



Full wwPDB EM Validation Report ⓘ

Jul 4, 2026 – 07:58 PM EDT

PDB ID : 9OP9 / pdb_00009op9
EMDB ID : EMD-70685
Title : Two Component Protein Nano-Particle (T=3). De Novo Design, Computationally Relaxed into Low Resolution Subtomogram Averaged CryoEM Map with Icosahedral Symmetry Applied
Authors : DiMaio, F.; Chmielewski, D.; Weidle, C.
Deposited on : 2025-05-17
Resolution : 31.60 Å (reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

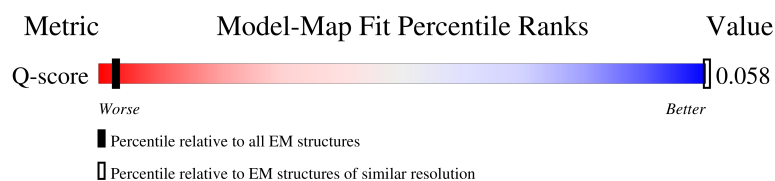
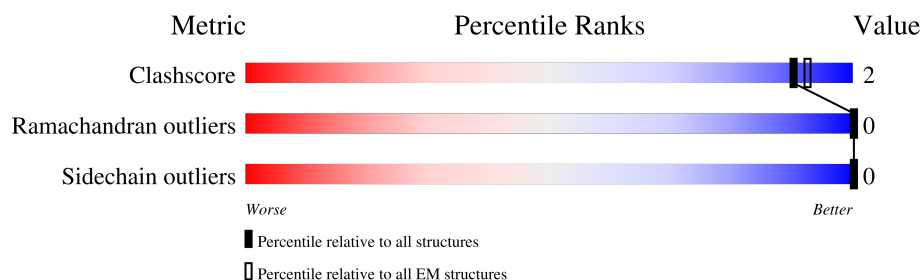
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 31.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



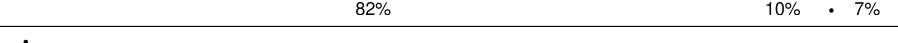
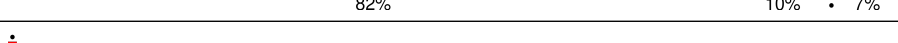
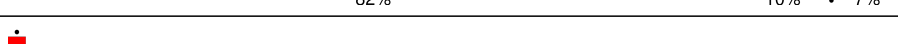
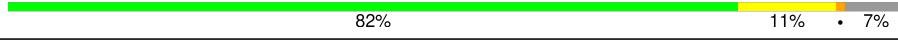
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1 (31.60 - 31.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	114	 82% 10% • 7%
1	AC	114	 83% 9% • 7%
1	AE	114	 79% 14% 7%
1	AG	114	 82% 10% • 7%

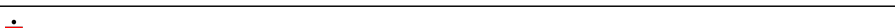
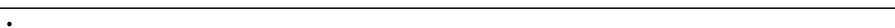
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AI	114	 83% 9% 7%
1	AK	114	 78% 15% 7%
1	AM	114	 82% 10% 7%
1	AP	114	 79% 14% 7%
1	AR	114	 82% 11% 7%
1	AS	114	 82% 10% 7%
1	AU	114	 84% 8% 7%
1	AW	114	 78% 15% 7%
1	AY	114	 82% 10% 7%
1	BA	114	 83% 9% 7%
1	BC	114	 78% 15% 7%
1	BE	114	 82% 10% 7%
1	BG	114	 82% 11% 7%
1	BI	114	 78% 15% 7%
1	BK	114	 82% 10% 7%
1	BM	114	 84% 8% 7%
1	BO	114	 79% 14% 7%
1	BQ	114	 82% 10% 7%
1	BS	114	 82% 11% 7%
1	BU	114	 79% 14% 7%
1	BW	114	 82% 10% 7%
1	BY	114	 82% 11% 7%
1	CA	114	 78% 15% 7%
1	CC	114	 82% 10% 7%
1	CE	114	82% 11% 7%

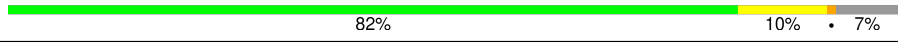
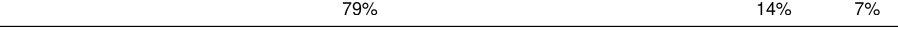
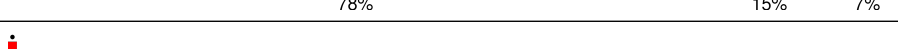
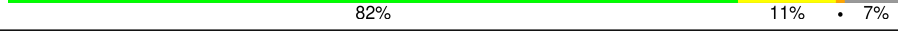
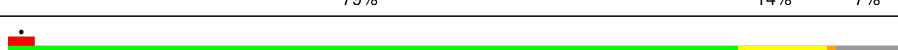
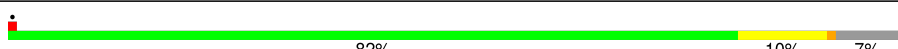
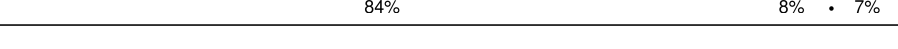
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CG	114	 79%14%7%
1	CI	114	 82%10%7%
1	CK	114	 82%11%7%
1	CM	114	 79%14%7%
1	CO	114	 82%10%7%
1	CQ	114	 84%8%7%
1	CS	114	 79%14%7%
1	CU	114	 82%10%7%
1	CW	114	 82%10%7%
1	CY	114	 79%14%7%
1	DA	114	 83%9%7%
1	DC	114	 82%11%7%
1	DE	114	 79%14%7%
1	DG	114	 82%10%7%
1	DI	114	 82%11%7%
1	DK	114	 79%14%7%
1	DM	114	 82%10%7%
1	DO	114	 84%8%7%
1	DQ	114	 79%14%7%
1	DS	114	 82%10%7%
1	DU	114	 82%11%7%
1	DX	114	 79%14%7%
1	DZ	114	 82%10%7%
1	EB	114	 83%9%7%
1	ED	114	 79%14%7%

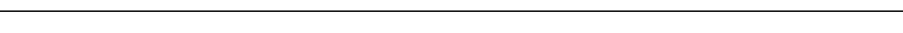
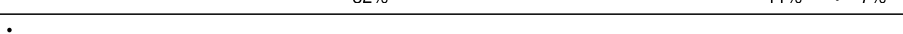
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	EF	114	
1	EH	114	
1	EJ	114	
1	EL	114	
1	EN	114	
1	EP	114	
1	ER	114	
1	ET	114	
1	EV	114	
1	EX	114	
1	EZ	114	
1	FB	114	
1	FD	114	
1	FF	114	
1	FH	114	
1	FJ	114	
1	FL	114	
1	FN	114	
1	FP	114	
1	FR	114	
1	FT	114	
1	FV	114	
1	FX	114	
1	FZ	114	
1	GB	114	

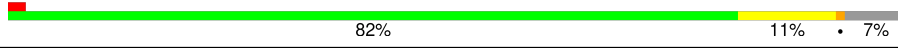
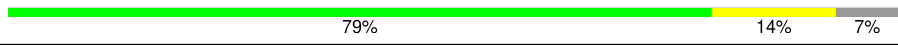
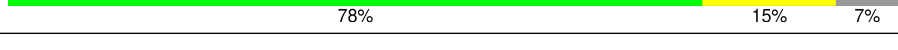
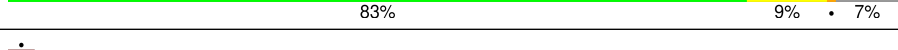
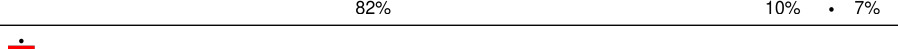
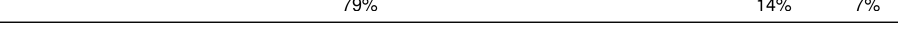
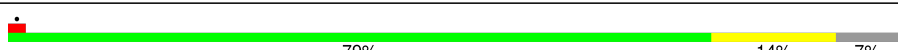
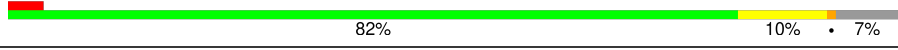
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	GD	114	 82% 11% • 7%
1	GF	114	 79% 14% 7%
1	GH	114	 82% 10% • 7%
1	GJ	114	 82% 11% • 7%
1	GL	114	 78% 15% 7%
1	GN	114	 82% 10% • 7%
1	GP	114	 82% 10% • 7%
1	GR	114	 79% 14% 7%
1	GT	114	 82% 10% • 7%
1	GV	114	 82% 11% • 7%
1	GX	114	 79% 14% 7%
1	GZ	114	 82% 10% • 7%
1	HB	114	 84% 8% • 7%
1	HD	114	 79% 14% 7%
1	HG	114	 82% 11% • 7%
1	HI	114	 79% 14% 7%
1	HL	114	 83% 9% • 7%
1	HN	114	 79% 14% 7%
1	HP	114	 82% 10% • 7%
1	HR	114	 82% 11% • 7%
1	HT	114	 79% 14% 7%
1	HV	114	 82% 10% • 7%
1	HX	114	 83% 9% • 7%
1	HZ	114	 79% 14% 7%
1	IC	114	 84% 8% • 7%

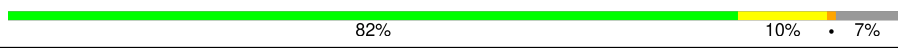
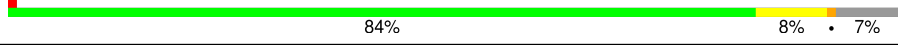
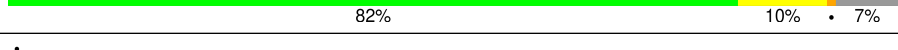
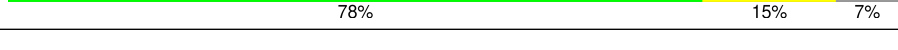
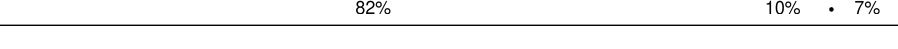
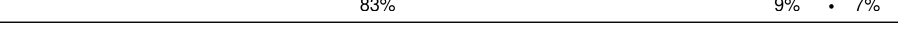
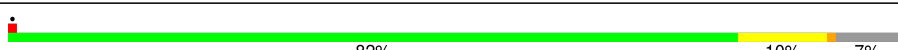
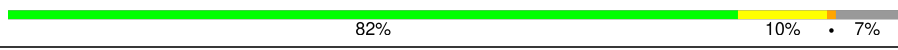
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	IE	114	
1	IH	114	
1	II	114	
1	IK	114	
1	IM	114	
1	IO	114	
1	IQ	114	
1	IS	114	
1	IU	114	
1	IW	114	
1	IY	114	
1	JA	114	
1	JC	114	
1	JE	114	
1	JG	114	
1	JI	114	
1	JK	114	
1	JM	114	
1	JO	114	
1	JQ	114	
1	JS	114	
1	JV	114	
1	JX	114	
1	JZ	114	
1	KB	114	

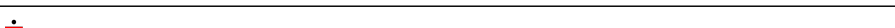
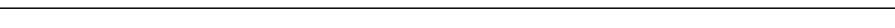
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	KD	114	 84%8%7%
1	KF	114	 79%14%7%
1	KH	114	 82%10%7%
1	KJ	114	 84%8%7%
1	KL	114	 78%15%7%
1	KN	114	 82%10%7%
1	KP	114	 82%10%7%
1	KR	114	 78%15%7%
1	KT	114	 82%10%7%
1	KV	114	 83%9%7%
1	KX	114	 79%14%7%
1	KZ	114	 82%10%7%
1	LB	114	 82%10%7%
1	LD	114	 78%15%7%
1	LF	114	 82%10%7%
1	LH	114	 82%10%7%
1	LJ	114	 79%14%7%
1	LL	114	 82%10%7%
1	LN	114	 82%11%7%
1	LP	114	 79%14%7%
1	LR	114	 82%10%7%
1	WA	114	 82%10%7%
1	WB	114	 82%10%7%
1	WC	114	 82%10%7%
1	WD	114	 79%14%7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	YA	114	 79%14%7%
1	YC	114	 82%10%7%
1	YE	114	 82%11%7%
1	YG	114	 79%14%7%
1	YI	114	 82%10%7%
1	YK	114	 82%10%7%
1	YM	114	 79%14%7%
1	YO	114	 82%10%7%
1	YQ	114	 82%11%7%
1	YS	114	 79%14%7%
1	YU	114	 82%10%7%
1	YW	114	 82%11%7%
1	YY	114	 79%14%7%
1	ZA	114	 82%11%7%
1	ZC	114	 79%14%7%
1	ZE	114	 82%10%7%
1	ZG	114	 82%10%7%
1	ZI	114	 78%15%7%
1	ZK	114	 82%10%7%
1	ZM	114	 82%10%7%
1	ZO	114	 79%14%7%
1	ZQ	114	 82%10%7%
1	ZS	114	 83%9%7%
1	ZU	114	 79%14%7%
1	ZW	114	 82%10%7%

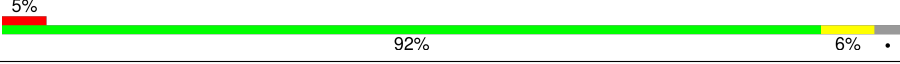
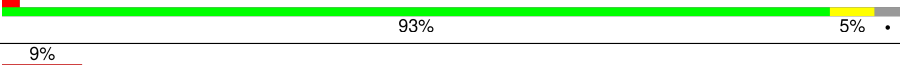
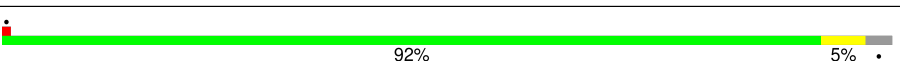
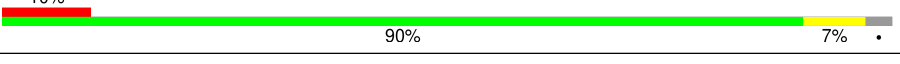
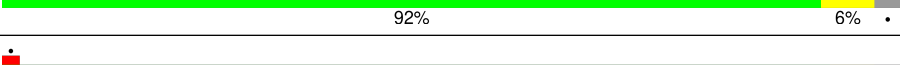
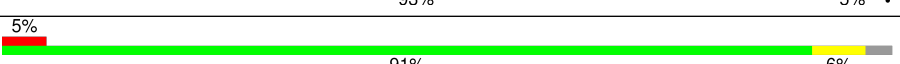
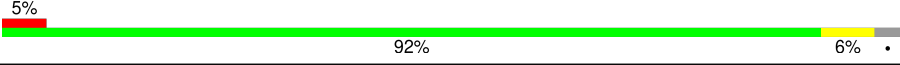
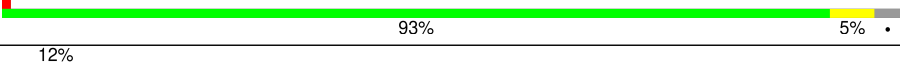
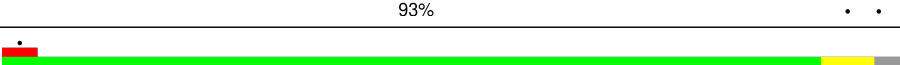
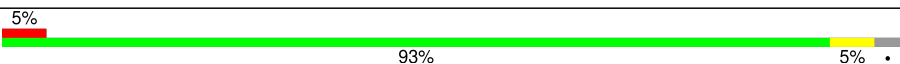
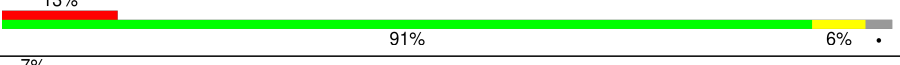
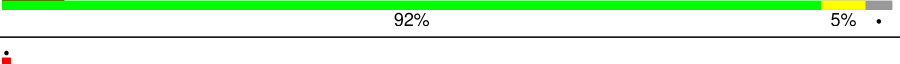
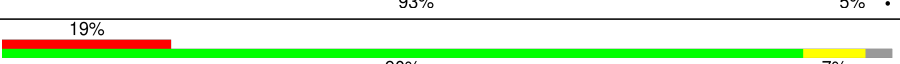
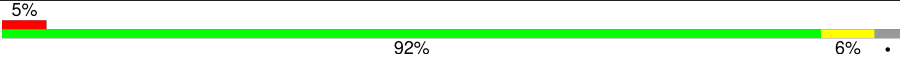
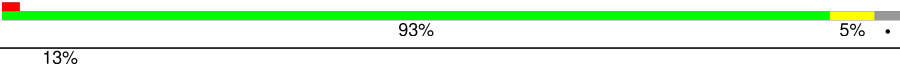
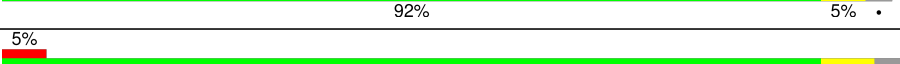
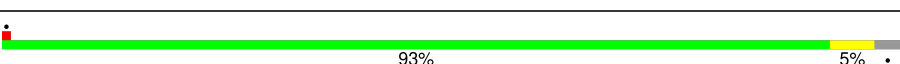
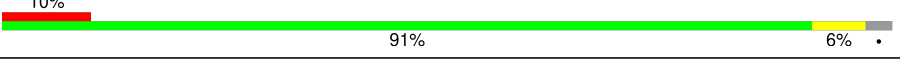
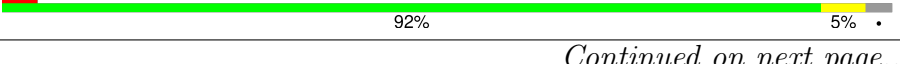
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	ZY	114	
2	AB	300	
2	AD	300	
2	AF	300	
2	AH	300	
2	AJ	300	
2	AL	300	
2	AN	300	
2	AO	300	
2	AQ	300	
2	AT	300	
2	AV	300	
2	AX	300	
2	AZ	300	
2	BB	300	
2	BD	300	
2	BF	300	
2	BH	300	
2	BJ	300	
2	BL	300	
2	BN	300	
2	BP	300	
2	BR	300	
2	BT	300	
2	BV	300	

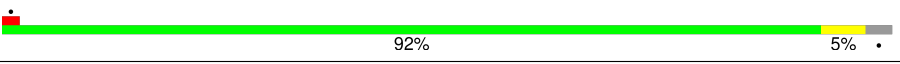
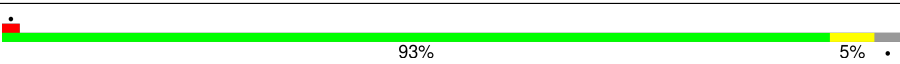
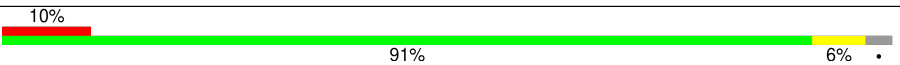
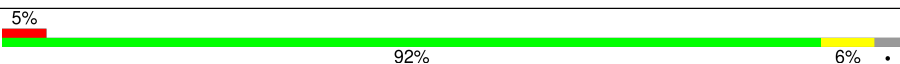
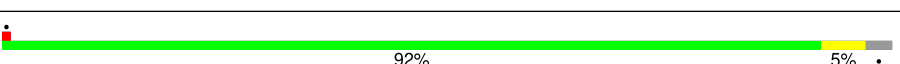
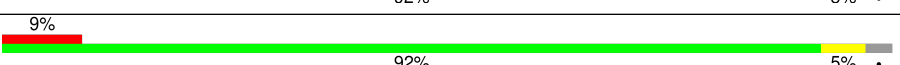
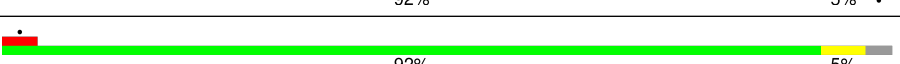
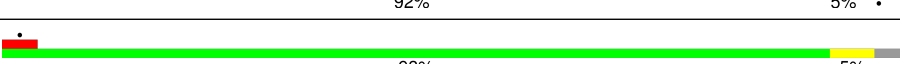
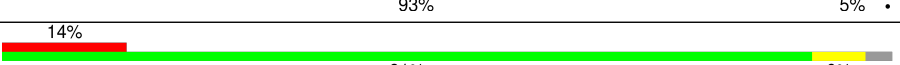
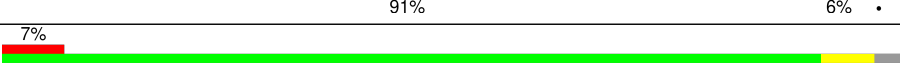
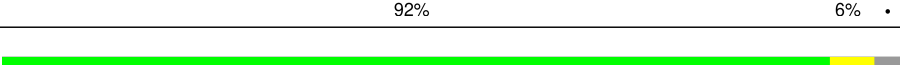
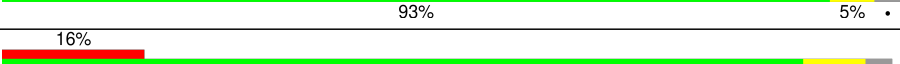
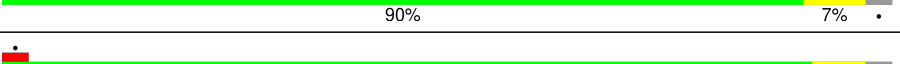
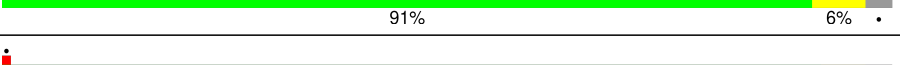
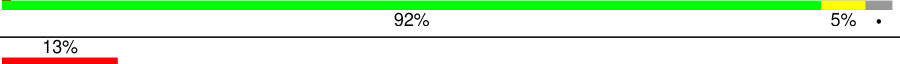
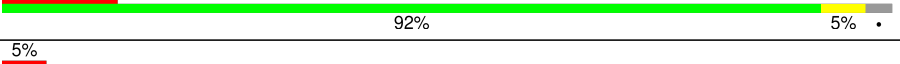
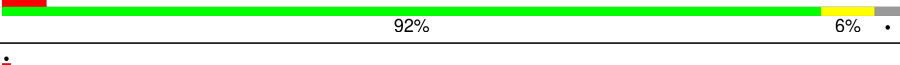
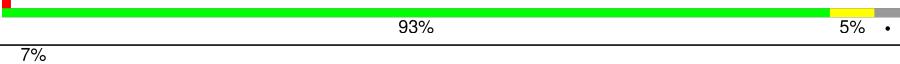
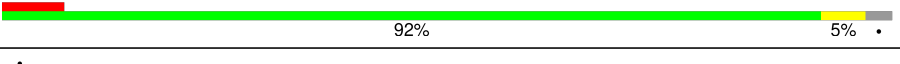
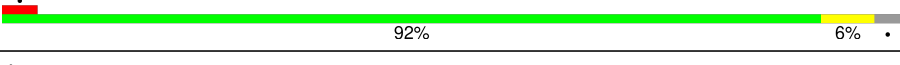
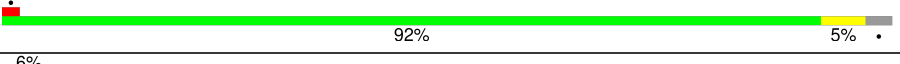
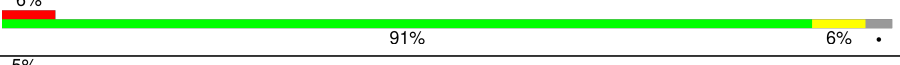
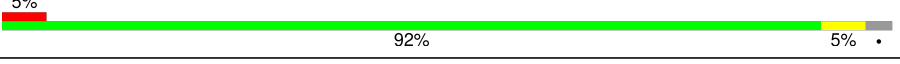
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	BX	300	
2	BZ	300	
2	CB	300	
2	CD	300	
2	CF	300	
2	CH	300	
2	CJ	300	
2	CL	300	
2	CN	300	
2	CP	300	
2	CR	300	
2	CT	300	
2	CV	300	
2	CX	300	
2	CZ	300	
2	DB	300	
2	DD	300	
2	DF	300	
2	DH	300	
2	DJ	300	
2	DL	300	
2	DN	300	
2	DP	300	
2	DR	300	
2	DT	300	

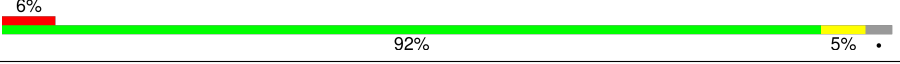
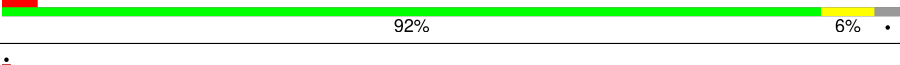
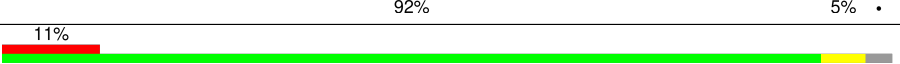
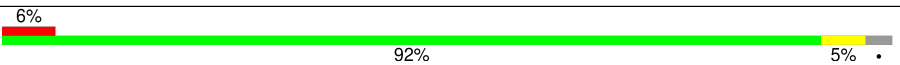
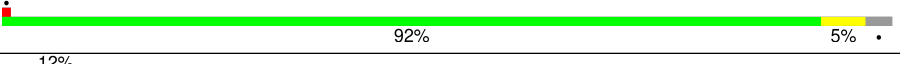
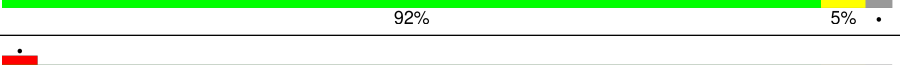
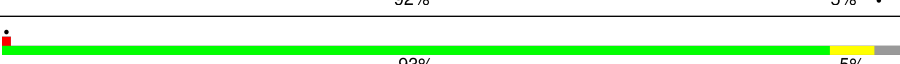
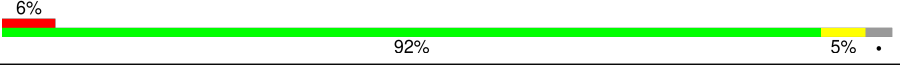
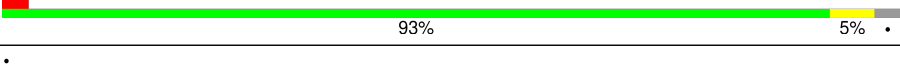
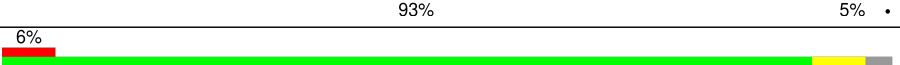
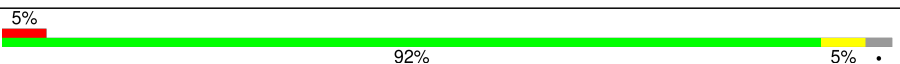
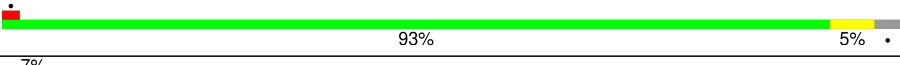
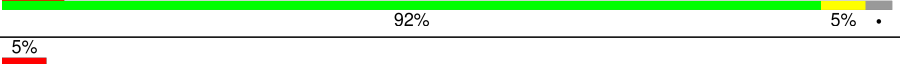
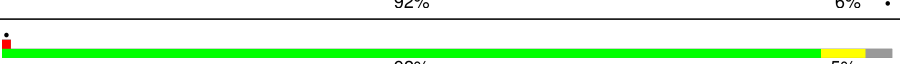
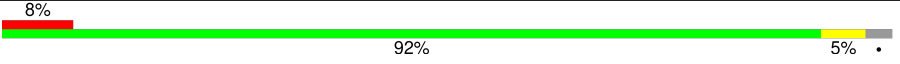
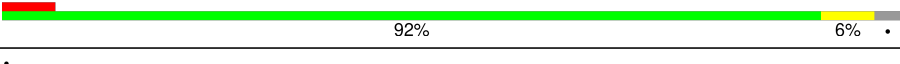
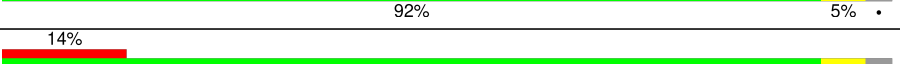
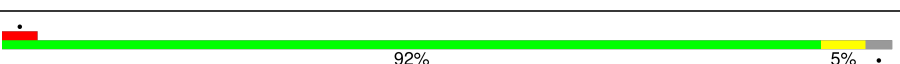
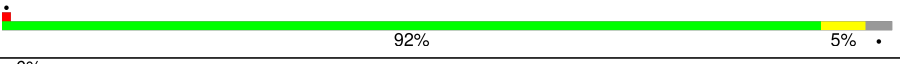
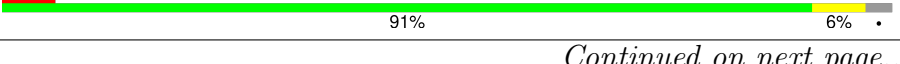
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	DW	300	
2	DY	300	
2	EA	300	
2	EC	300	
2	EE	300	
2	EG	300	
2	EI	300	
2	EK	300	
2	EM	300	
2	EO	300	
2	EQ	300	
2	ES	300	
2	EU	300	
2	EW	300	
2	EY	300	
2	FA	300	
2	FC	300	
2	FE	300	
2	FG	300	
2	FI	300	
2	FK	300	
2	FM	300	
2	FO	300	
2	FQ	300	
2	FS	300	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	FU	300	
2	FW	300	
2	FY	300	
2	GA	300	
2	GC	300	
2	GE	300	
2	GG	300	
2	GI	300	
2	GK	300	
2	GM	300	
2	GO	300	
2	GQ	300	
2	GS	300	
2	GU	300	
2	GW	300	
2	GY	300	
2	HA	300	
2	HC	300	
2	HE	300	
2	HF	300	
2	HH	300	
2	HJ	300	
2	HK	300	
2	HM	300	
2	HO	300	

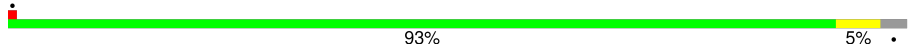
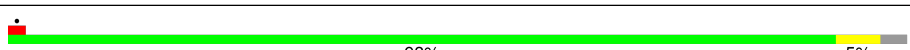
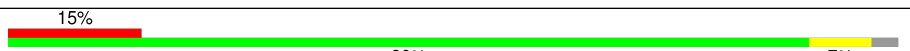
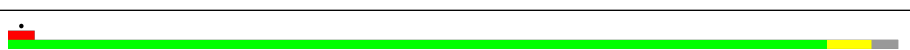
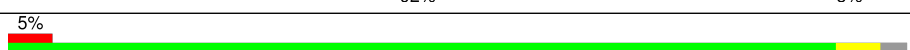
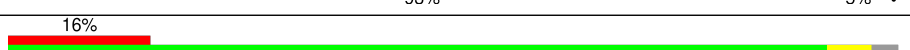
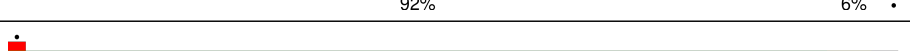
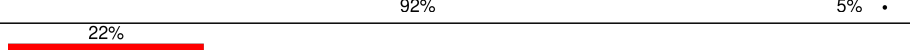
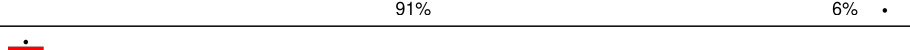
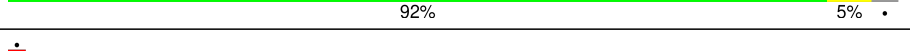
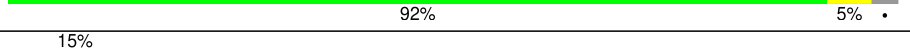
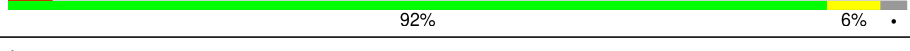
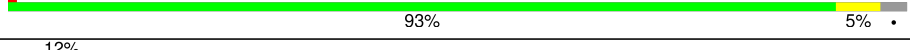
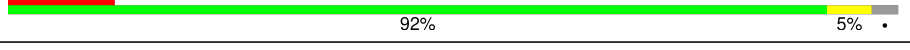
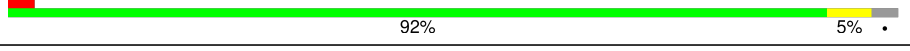
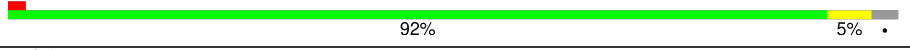
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	HQ	300	
2	HS	300	
2	HU	300	
2	HW	300	
2	HY	300	
2	IA	300	
2	IB	300	
2	ID	300	
2	IF	300	
2	IG	300	
2	IJ	300	
2	IL	300	
2	IN	300	
2	IP	300	
2	IR	300	
2	IT	300	
2	IV	300	
2	IX	300	
2	IZ	300	
2	JB	300	
2	JD	300	
2	JF	300	
2	JH	300	
2	JJ	300	
2	JL	300	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	JN	300	
2	JP	300	
2	JR	300	
2	JT	300	
2	JU	300	
2	JW	300	
2	JY	300	
2	KA	300	
2	KC	300	
2	KE	300	
2	KG	300	
2	KI	300	
2	KK	300	
2	KM	300	
2	KO	300	
2	KQ	300	
2	KS	300	
2	KU	300	
2	KW	300	
2	KY	300	
2	LA	300	
2	LC	300	
2	LE	300	
2	LG	300	
2	LI	300	

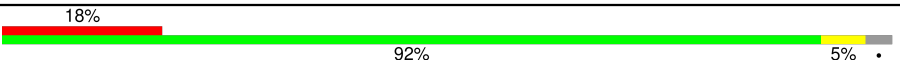
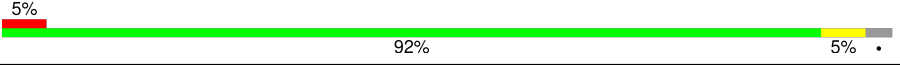
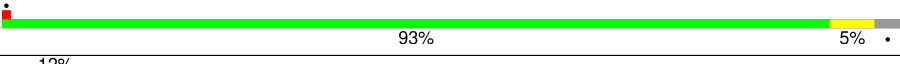
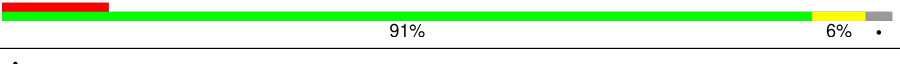
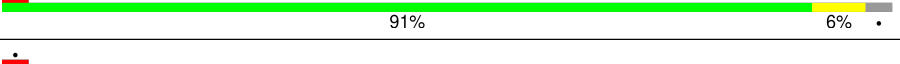
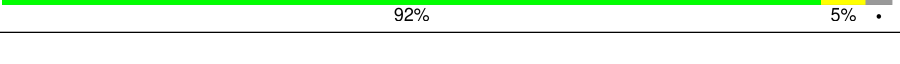
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	LK	300	
2	LM	300	
2	LO	300	
2	LQ	300	
2	LS	300	
2	YB	300	
2	YD	300	
2	YF	300	
2	YH	300	
2	YJ	300	
2	YL	300	
2	YN	300	
2	YP	300	
2	YR	300	
2	YT	300	
2	YV	300	
2	YX	300	
2	YZ	300	
2	ZB	300	
2	ZD	300	
2	ZF	300	
2	ZH	300	
2	ZJ	300	
2	ZL	300	
2	ZN	300	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	ZP	300	
2	ZR	300	
2	ZT	300	
2	ZV	300	
2	ZX	300	
2	ZZ	300	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 553500 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called C2-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	ZA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	YY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AE	106	Total 808	C 506	N 149	O 152	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AP	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AR	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	AY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BS	106	Total 808	C 506	N 149	O 152	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	BY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	CY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DG	106	Total 808	C 506	N 149	O 152	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DX	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	DZ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EB	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ED	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EF	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EH	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EJ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EL	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EN	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EP	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ER	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ET	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EV	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	EX	106	Total 808	C 506	N 149	O 152	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	EZ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FB	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FD	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FF	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FH	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FJ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FL	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FN	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FP	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FR	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FT	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FV	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FX	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	FZ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GB	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GD	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GF	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GH	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GJ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GL	106	Total 808	C 506	N 149	O 152	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	GN	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GP	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GR	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GT	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GV	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GX	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	GZ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HB	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HD	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	WB	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	WA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HL	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HN	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HP	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HR	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HT	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HV	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	HX	106	Total 808	C 506	N 149	O 152	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	HZ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	WC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IH	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	II	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IU	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IW	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	IY	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JA	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	ZK	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JC	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JE	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JG	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JI	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JK	106	Total 808	C 506	N 149	O 152	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	JM	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JO	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JQ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JS	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	WD	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JV	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JX	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	JZ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KB	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KD	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KF	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KH	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KJ	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KL	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KN	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KP	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KR	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KT	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KV	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KX	106	Total 808	C 506	N 149	O 152	S 1	0	0
1	KZ	106	Total 808	C 506	N 149	O 152	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	ZM	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	LB	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	LD	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	LF	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	LH	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	LJ	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	LL	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	LN	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	LP	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	LR	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	ZO	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	ZQ	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	ZS	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	ZU	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	ZW	106	Total	C	N	O	S	0	0
			808	506	149	152	1		
1	YA	106	Total	C	N	O	S	0	0
			808	506	149	152	1		

- Molecule 2 is a protein called C3-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	YD	292	Total	C	N	O	S	0	0
			2267	1421	413	430	3		
2	ZZ	292	Total	C	N	O	S	0	0
			2267	1421	413	430	3		
2	YF	292	Total	C	N	O	S	0	0
			2267	1421	413	430	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	YH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AO	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AQ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	AZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	BZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	CZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DW	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	DY	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	EA	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EC	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EE	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EG	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EI	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EK	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EM	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EO	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EQ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ES	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EU	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EW	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	EY	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FA	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FC	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FE	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FG	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FI	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FK	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FM	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FO	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FQ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FS	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FU	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FW	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	FY	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GA	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GC	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GE	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GG	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GI	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GK	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GM	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GO	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GQ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GS	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GU	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GW	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	GY	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HA	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	HC	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HE	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HK	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HM	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HO	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HQ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HS	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HU	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HW	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	HY	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IA	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ID	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IG	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	IN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	IZ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JD	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JF	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JH	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JJ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JU	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JW	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	JY	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KA	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	ZL	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KC	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KE	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KG	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KI	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KK	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KM	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KO	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KQ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KS	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KU	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KW	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	KY	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	LA	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	LC	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	LE	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	LG	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	LI	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	LK	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	LM	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	LO	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

Continued on next page...

Continued from previous page...

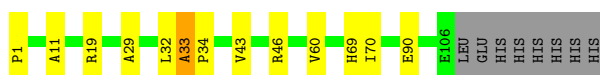
Mol	Chain	Residues	Atoms					AltConf	Trace
2	LQ	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	LS	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZN	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZP	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZR	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZT	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZV	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	ZX	292	Total 2267	C 1421	N 413	O 430	S 3	0	0
2	YB	292	Total 2267	C 1421	N 413	O 430	S 3	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: C2-B

Chain ZA:  82% 11% • 7%



- Molecule 1: C2-B

Chain YC:  82% 10% • 7%



- Molecule 1: C2-B

Chain ZY:  83% 9% • 7%



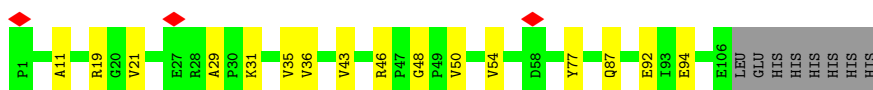
- Molecule 1: C2-B

Chain YE:  82% 11% • 7%



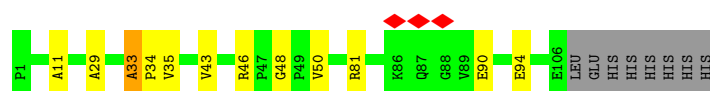
- Molecule 1: C2-B

Chain YG:  79% 14% • 7%



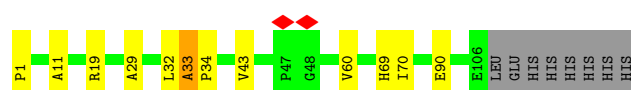
- Molecule 1: C2-B

Chain YI:  82% 10% 7%



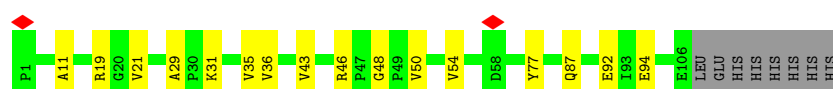
• Molecule 1: C2-B

Chain YK:  82% 10% 7%



• Molecule 1: C2-B

Chain YM:  79% 14% 7%



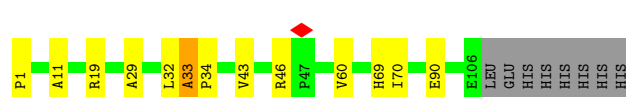
• Molecule 1: C2-B

Chain YO:  82% 10% 7%



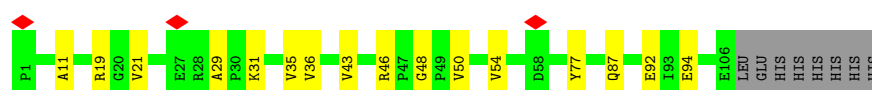
• Molecule 1: C2-B

Chain YQ:  82% 11% 7%



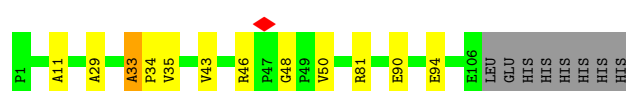
• Molecule 1: C2-B

Chain YS:  79% 14% 7%



• Molecule 1: C2-B

Chain YU:  82% 10% 7%



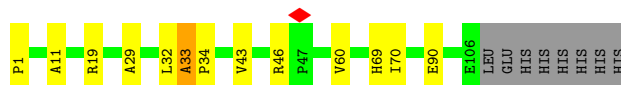
- Molecule 1: C2-B

Chain AA:  82% 10% • 7%



- Molecule 1: C2-B

Chain YW:  82% 11% • 7%



- Molecule 1: C2-B

Chain YY:  79% 14% 7%



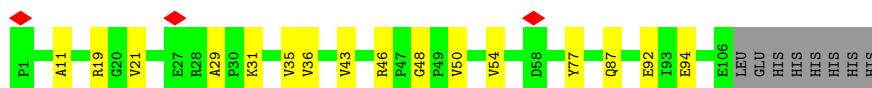
- Molecule 1: C2-B

Chain AC:  83% 9% • 7%



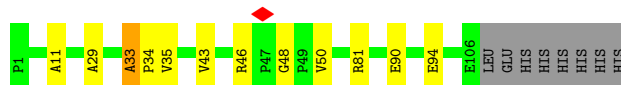
- Molecule 1: C2-B

Chain AE:  79% 14% 7%



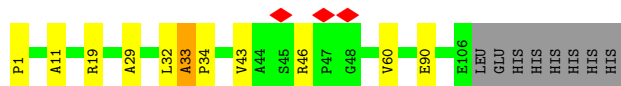
- Molecule 1: C2-B

Chain AG:  82% 10% • 7%

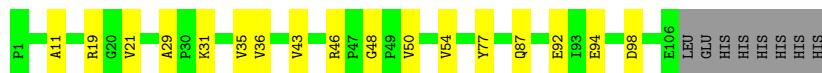


- Molecule 1: C2-B

Chain AI:  83% 9% • 7%



• Molecule 1: C2-B

Chain AK:  78% 15% 7%

• Molecule 1: C2-B

Chain AM:  82% 10% 7%

• Molecule 1: C2-B

Chain AP:  79% 14% 7%

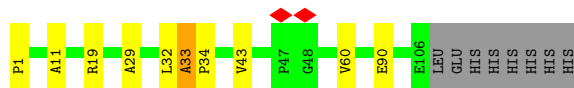
• Molecule 1: C2-B

Chain AR:  82% 11% 7%

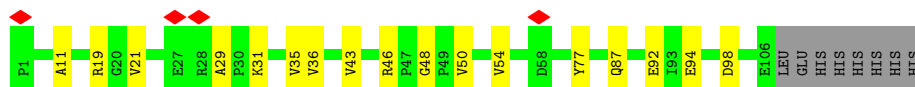
• Molecule 1: C2-B

Chain AS:  82% 10% 7%

• Molecule 1: C2-B

Chain AU:  84% 8% 7%

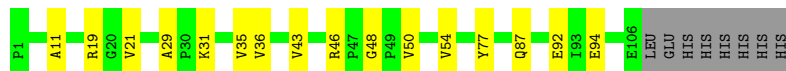
• Molecule 1: C2-B

Chain AW:  78% 15% 7%

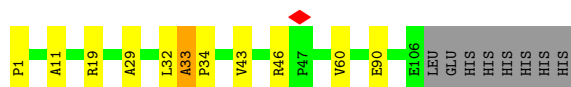
● Molecule 1: C2-B

Chain AY:  82% 10% • 7%

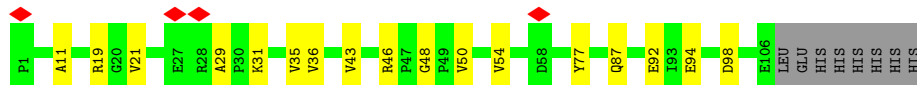
● Molecule 1: C2-B

Chain ZC:  79% 14% 7%

● Molecule 1: C2-B

Chain BA:  83% 9% • 7%

● Molecule 1: C2-B

Chain BC:  78% 15% 7%

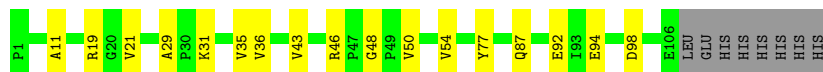
● Molecule 1: C2-B

Chain BE:  82% 10% • 7%

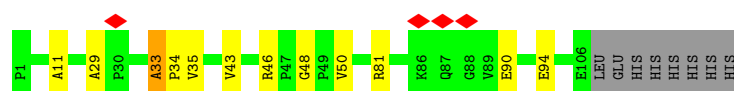
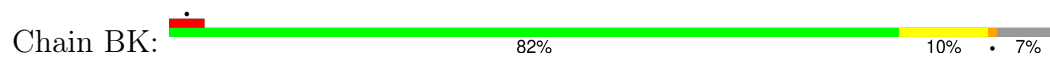
● Molecule 1: C2-B

Chain BG:  82% 11% • 7%

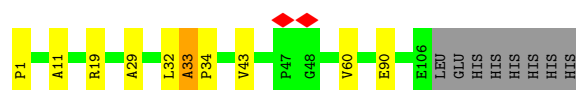
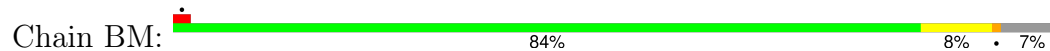
● Molecule 1: C2-B

Chain BI:  78% 15% 7%

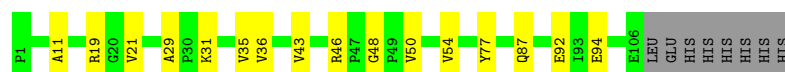
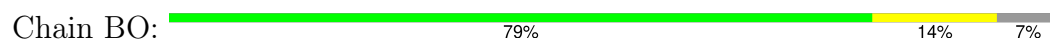
● Molecule 1: C2-B



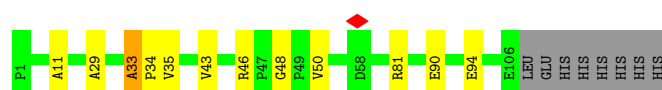
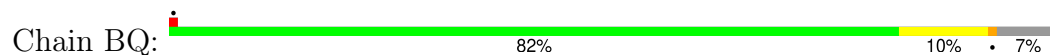
- Molecule 1: C2-B



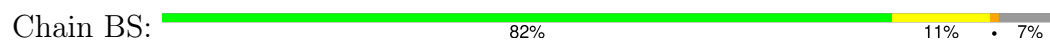
- Molecule 1: C2-B



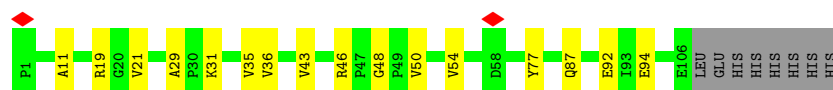
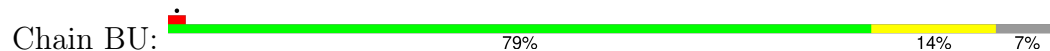
- Molecule 1: C2-B



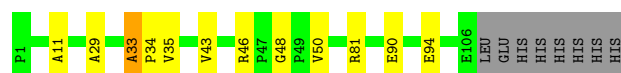
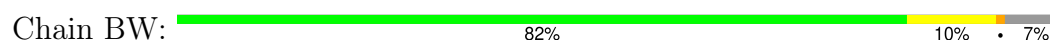
- Molecule 1: C2-B



- Molecule 1: C2-B



- Molecule 1: C2-B



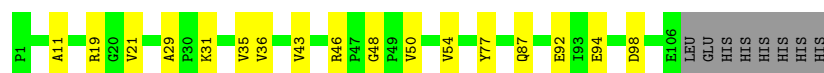
- Molecule 1: C2-B

Chain BY:  82% 11% • 7%



• Molecule 1: C2-B

Chain CA:  78% 15% 7%



• Molecule 1: C2-B

Chain CC:  82% 10% • 7%



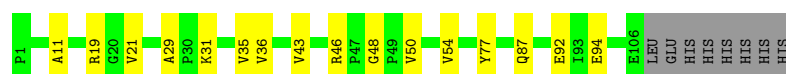
• Molecule 1: C2-B

Chain CE:  82% 11% • 7%



• Molecule 1: C2-B

Chain CG:  79% 14% 7%



• Molecule 1: C2-B

Chain CI:  82% 10% • 7%



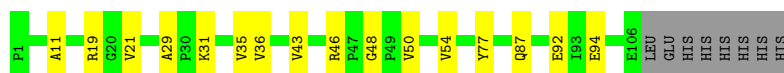
• Molecule 1: C2-B

Chain CK:  82% 11% • 7%

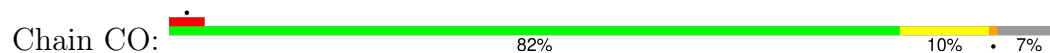


• Molecule 1: C2-B

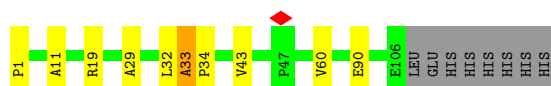
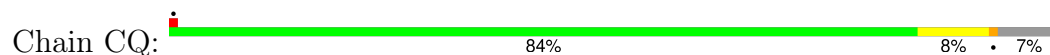
Chain CM:  79% 14% 7%



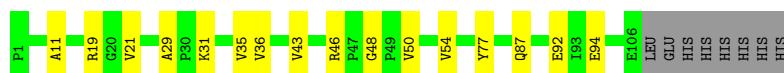
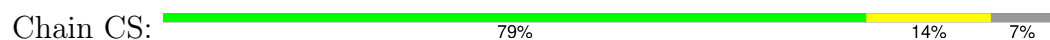
- Molecule 1: C2-B



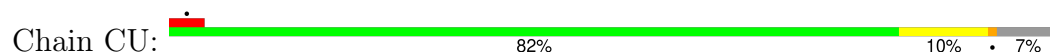
- Molecule 1: C2-B



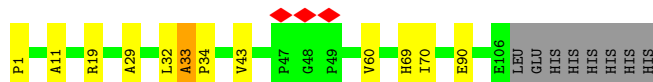
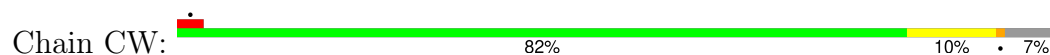
- Molecule 1: C2-B



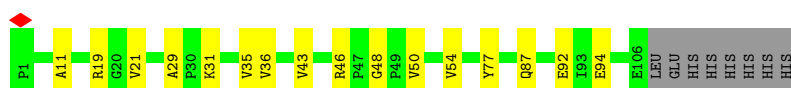
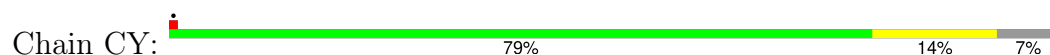
- Molecule 1: C2-B



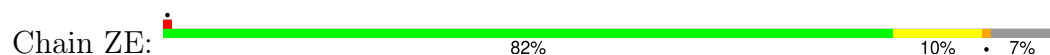
- Molecule 1: C2-B



- Molecule 1: C2-B

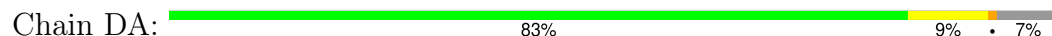


- Molecule 1: C2-B

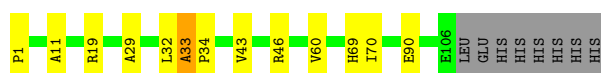
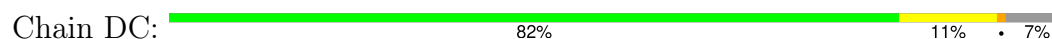




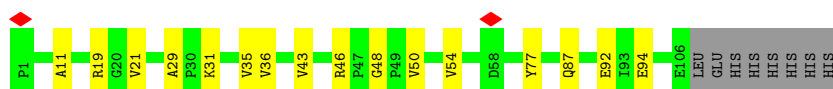
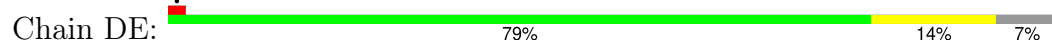
- Molecule 1: C2-B



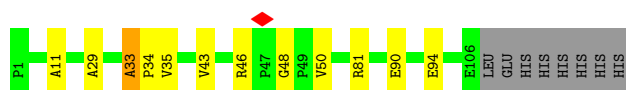
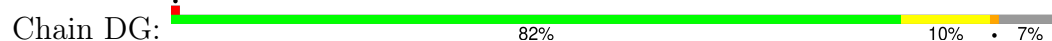
- Molecule 1: C2-B



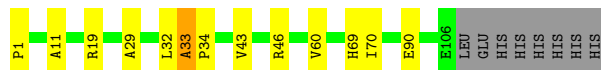
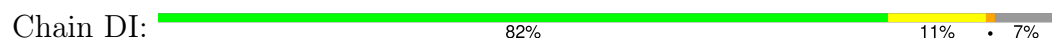
- Molecule 1: C2-B



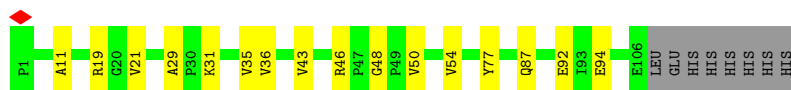
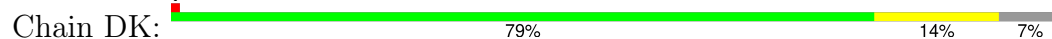
- Molecule 1: C2-B



- Molecule 1: C2-B



- Molecule 1: C2-B

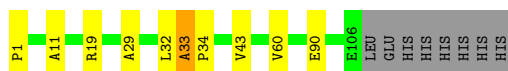
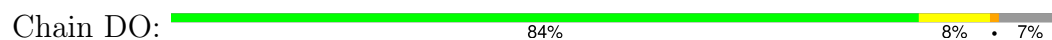


- Molecule 1: C2-B

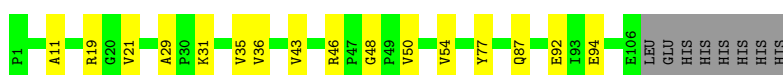
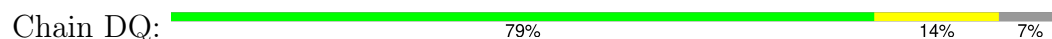




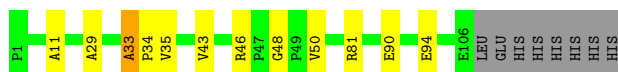
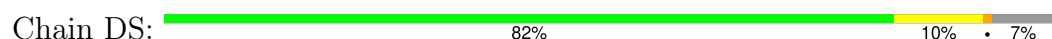
- Molecule 1: C2-B



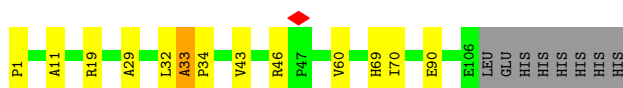
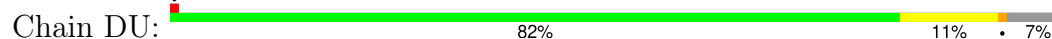
- Molecule 1: C2-B



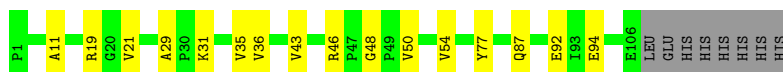
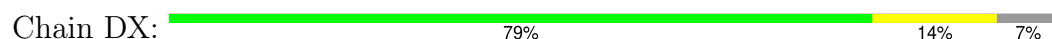
- Molecule 1: C2-B



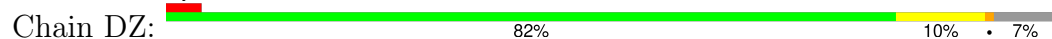
- Molecule 1: C2-B



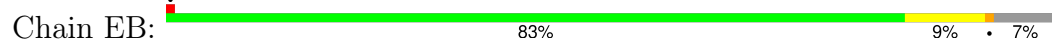
- Molecule 1: C2-B

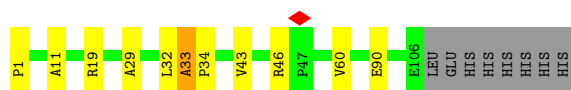


- Molecule 1: C2-B

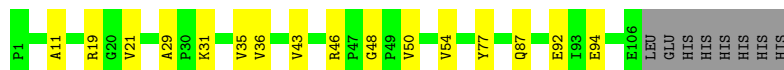
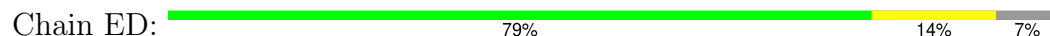


- Molecule 1: C2-B

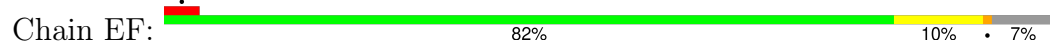




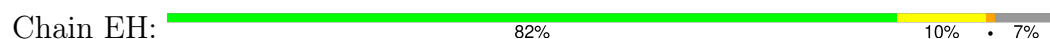
- Molecule 1: C2-B



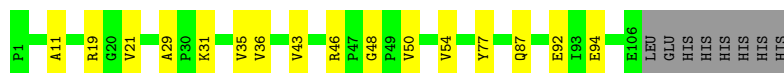
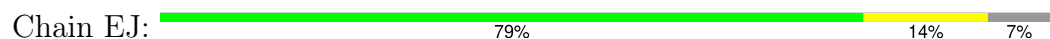
- Molecule 1: C2-B



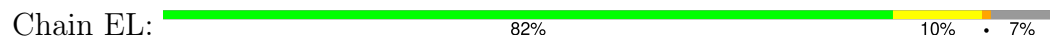
- Molecule 1: C2-B



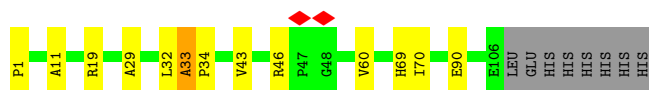
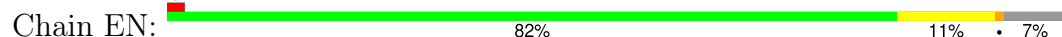
- Molecule 1: C2-B



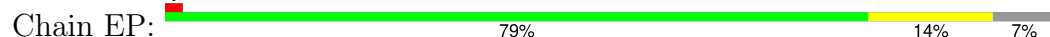
- Molecule 1: C2-B



- Molecule 1: C2-B

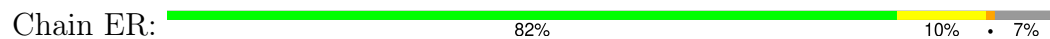


- Molecule 1: C2-B

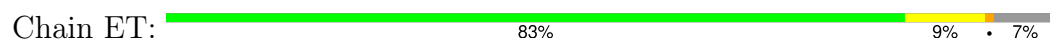




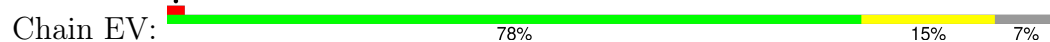
- Molecule 1: C2-B



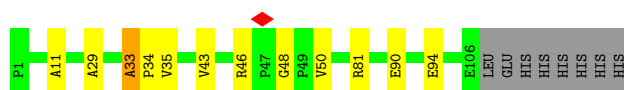
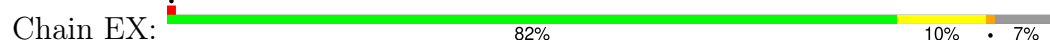
- Molecule 1: C2-B



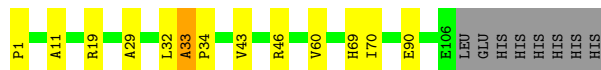
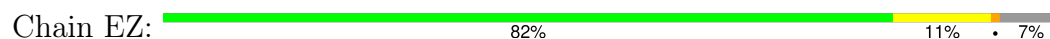
- Molecule 1: C2-B



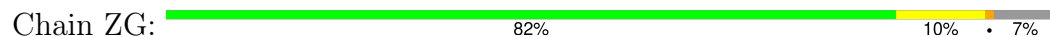
- Molecule 1: C2-B



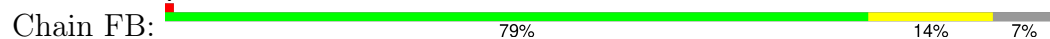
- Molecule 1: C2-B

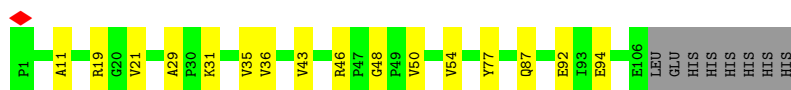


- Molecule 1: C2-B



- Molecule 1: C2-B





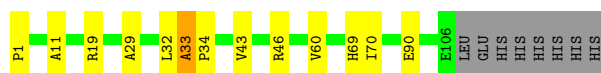
- Molecule 1: C2-B

Chain FD: 82% 10% • 7%



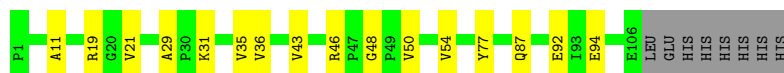
- Molecule 1: C2-B

Chain FF: 82% 11% • 7%



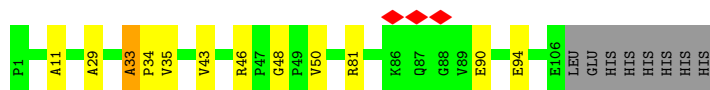
- Molecule 1: C2-B

Chain FH: 79% 14% 7%



- Molecule 1: C2-B

Chain FJ: 82% 10% • 7%



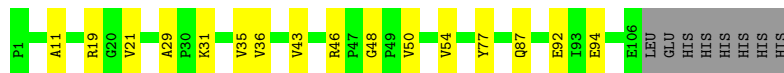
- Molecule 1: C2-B

Chain FL: 82% 10% • 7%



- Molecule 1: C2-B

Chain FN: 79% 14% 7%

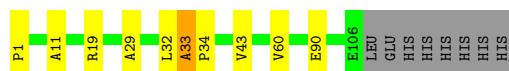
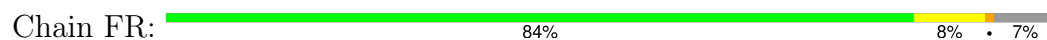


- Molecule 1: C2-B

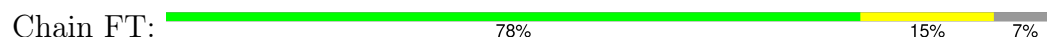
Chain FP: 82% 10% • 7%



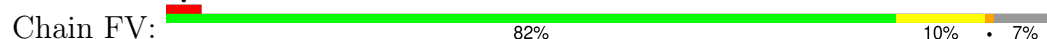
- Molecule 1: C2-B



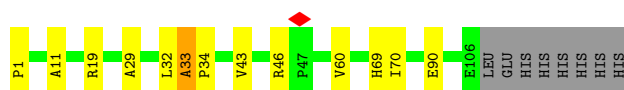
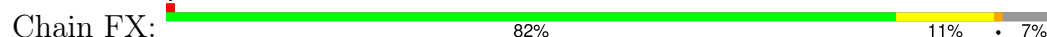
- Molecule 1: C2-B



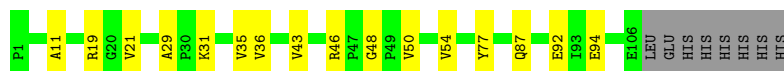
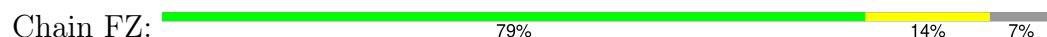
- Molecule 1: C2-B



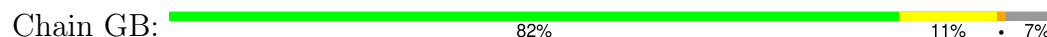
- Molecule 1: C2-B



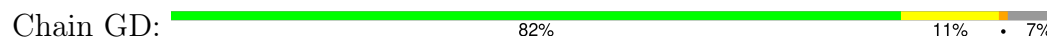
- Molecule 1: C2-B

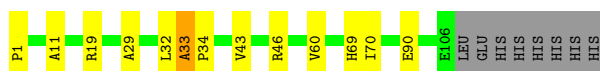


- Molecule 1: C2-B

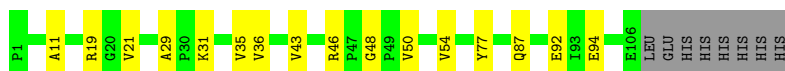
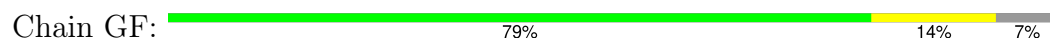


- Molecule 1: C2-B

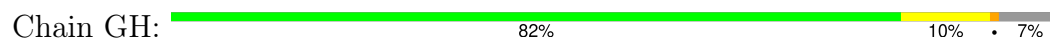




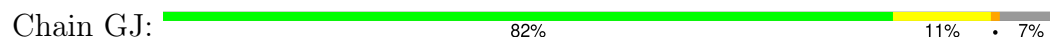
- Molecule 1: C2-B



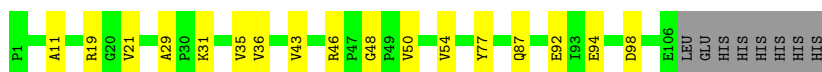
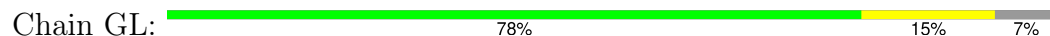
- Molecule 1: C2-B



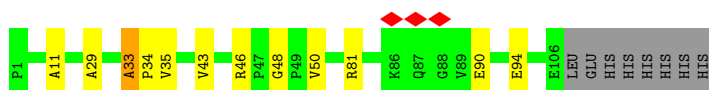
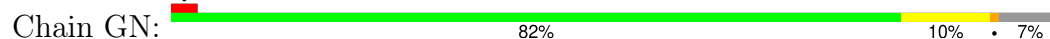
- Molecule 1: C2-B



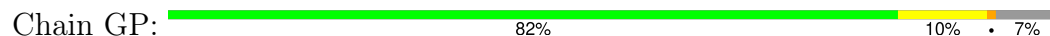
- Molecule 1: C2-B



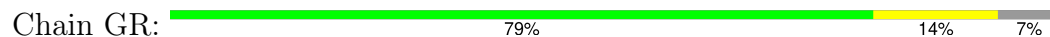
- Molecule 1: C2-B

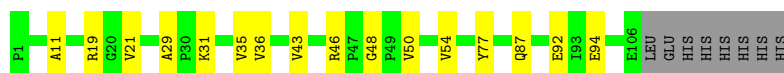


- Molecule 1: C2-B

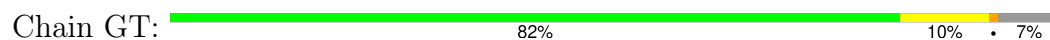


- Molecule 1: C2-B

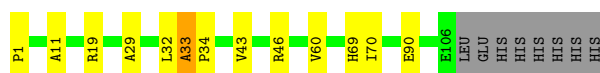
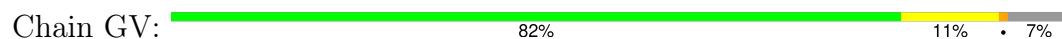




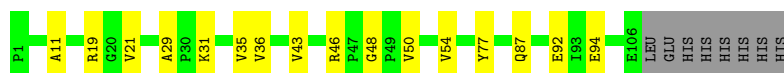
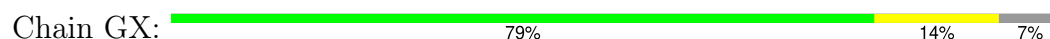
- Molecule 1: C2-B



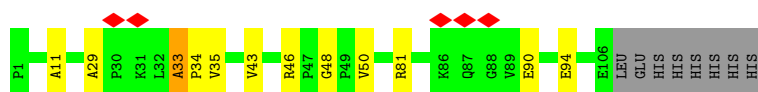
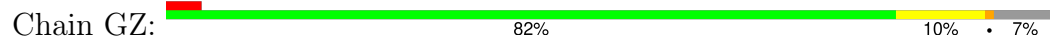
- Molecule 1: C2-B



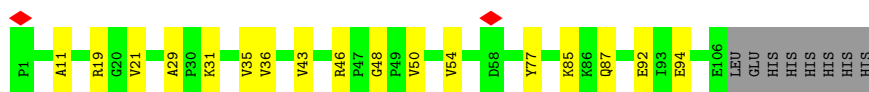
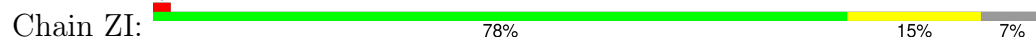
- Molecule 1: C2-B



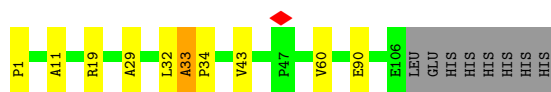
- Molecule 1: C2-B



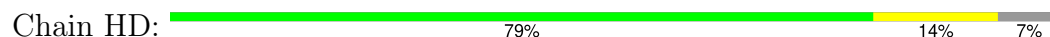
- Molecule 1: C2-B

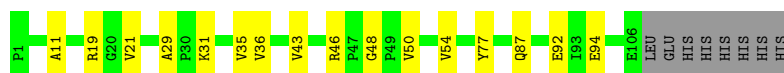


- Molecule 1: C2-B

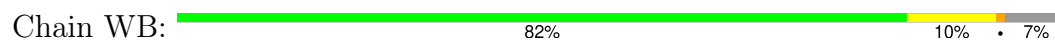


- Molecule 1: C2-B

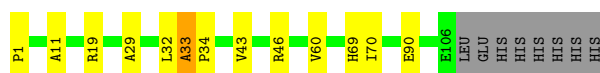
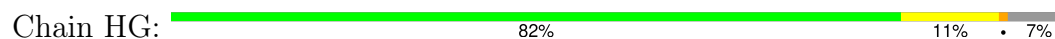




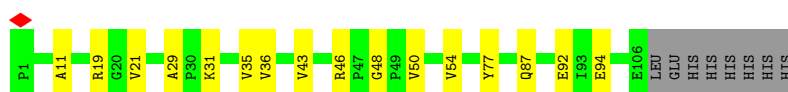
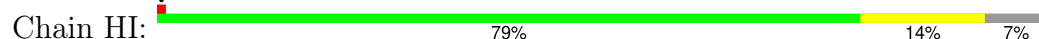
- Molecule 1: C2-B



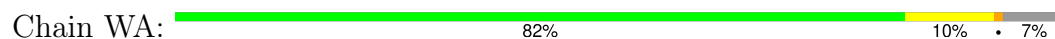
- Molecule 1: C2-B



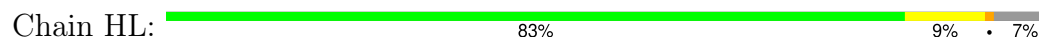
- Molecule 1: C2-B



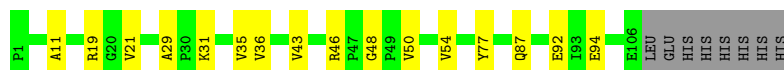
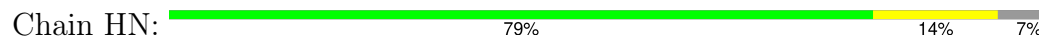
- Molecule 1: C2-B



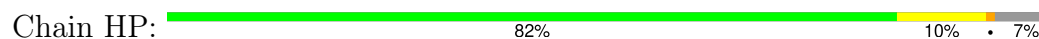
- Molecule 1: C2-B



- Molecule 1: C2-B

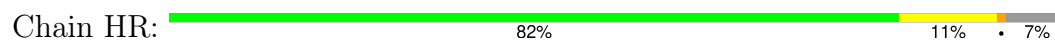


- Molecule 1: C2-B

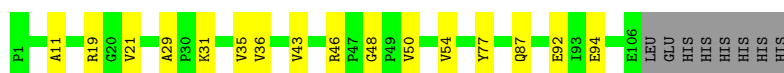
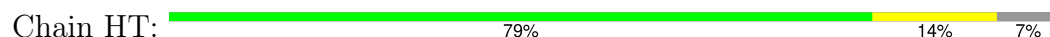




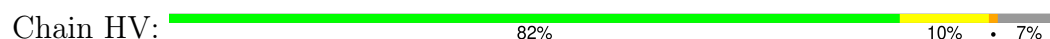
- Molecule 1: C2-B



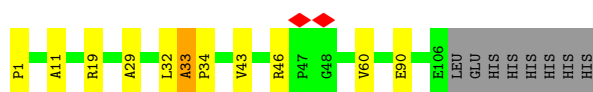
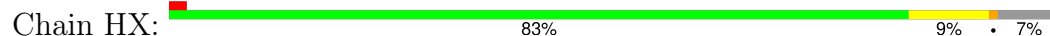
- Molecule 1: C2-B



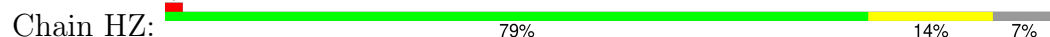
- Molecule 1: C2-B



- Molecule 1: C2-B



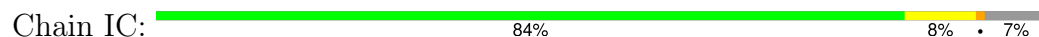
- Molecule 1: C2-B

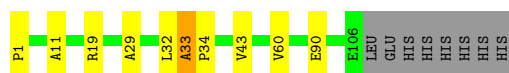


- Molecule 1: C2-B

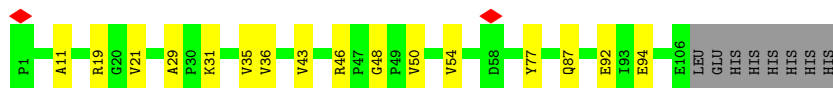
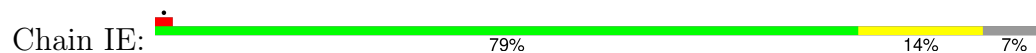


- Molecule 1: C2-B

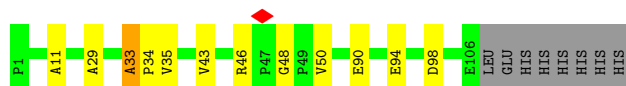
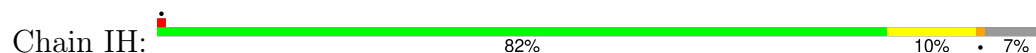




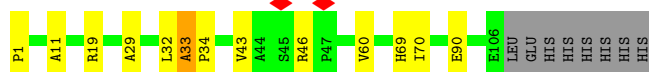
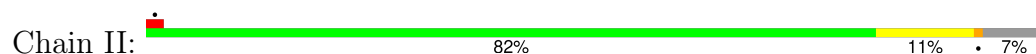
- Molecule 1: C2-B



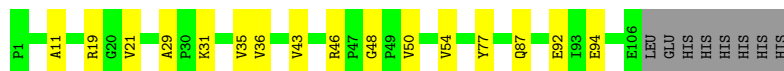
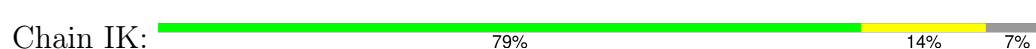
- Molecule 1: C2-B



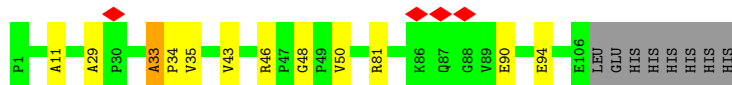
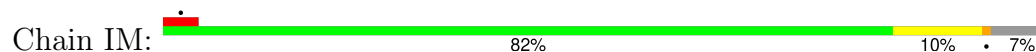
- Molecule 1: C2-B



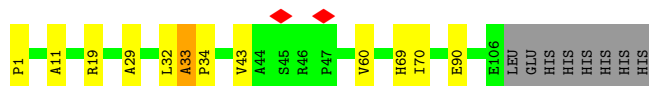
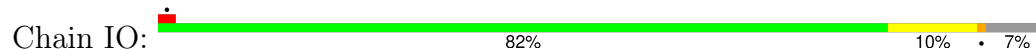
- Molecule 1: C2-B



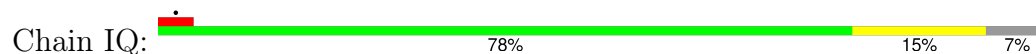
- Molecule 1: C2-B



- Molecule 1: C2-B



- Molecule 1: C2-B





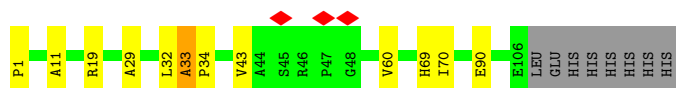
• Molecule 1: C2-B

Chain IS: 83% 9% 7%



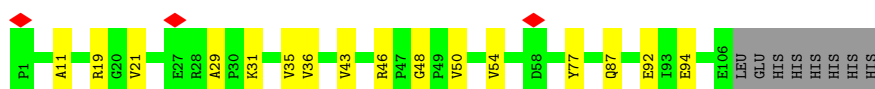
• Molecule 1: C2-B

Chain IU: 82% 10% 7%



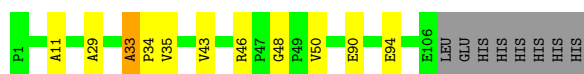
• Molecule 1: C2-B

Chain IW: 79% 14% 7%



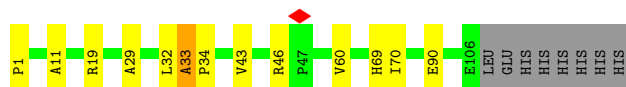
• Molecule 1: C2-B

Chain IY: 83% 9% 7%



• Molecule 1: C2-B

Chain JA: 82% 11% 7%



• Molecule 1: C2-B

Chain ZK: 82% 10% 7%



• Molecule 1: C2-B

Chain JC: 79% 14% 7%



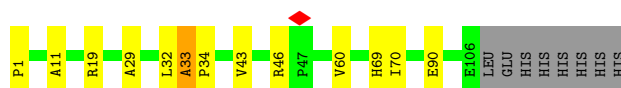
• Molecule 1: C2-B

Chain JE: 82% 10% 7%



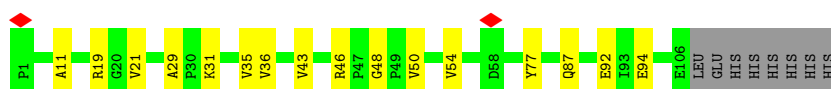
• Molecule 1: C2-B

Chain JG: 82% 11% 7%



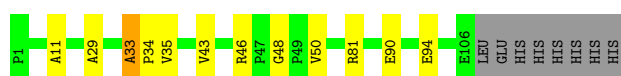
• Molecule 1: C2-B

Chain JI: 79% 14% 7%



• Molecule 1: C2-B

Chain JK: 82% 10% 7%



• Molecule 1: C2-B

Chain JM: 83% 9% 7%



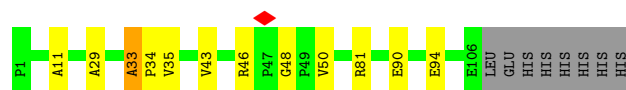
• Molecule 1: C2-B

Chain JO: 79% 14% 7%

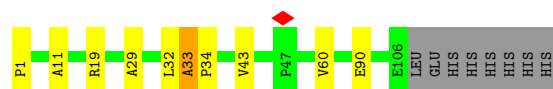
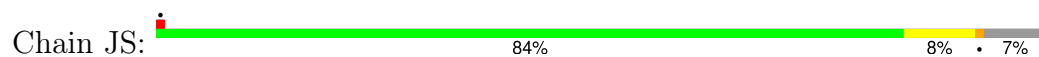


• Molecule 1: C2-B

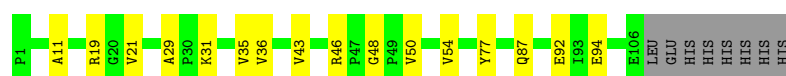
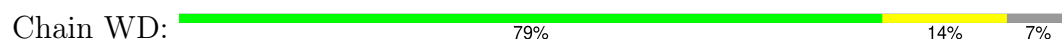
Chain JQ: 82% 10% 7%



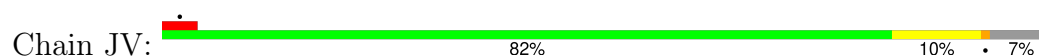
• Molecule 1: C2-B



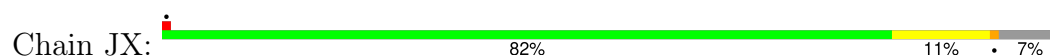
• Molecule 1: C2-B



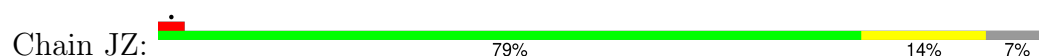
• Molecule 1: C2-B



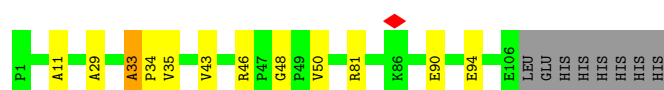
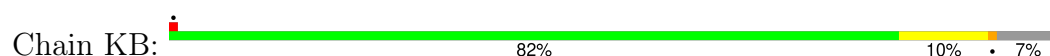
• Molecule 1: C2-B



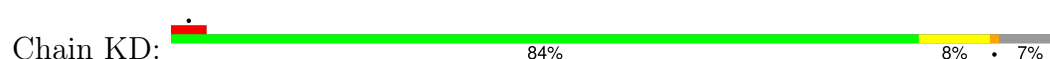
• Molecule 1: C2-B

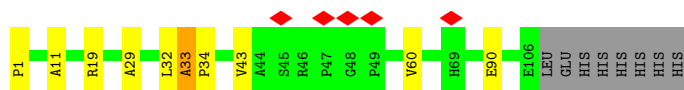


• Molecule 1: C2-B

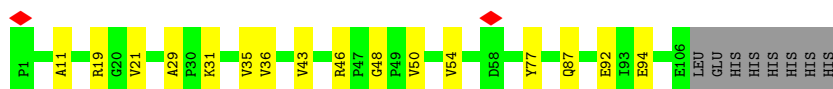
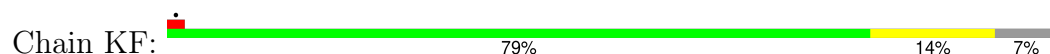


• Molecule 1: C2-B

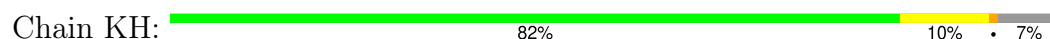




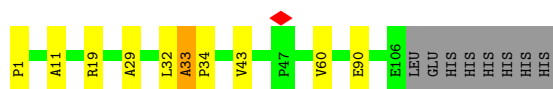
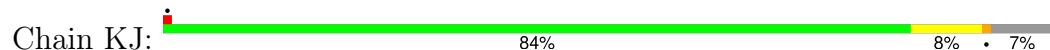
- Molecule 1: C2-B



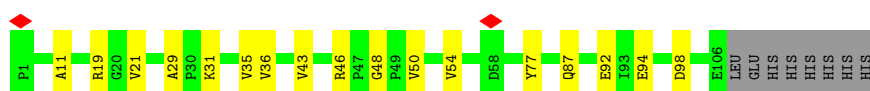
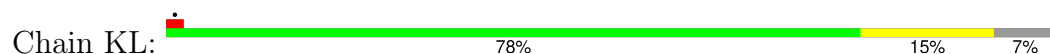
- Molecule 1: C2-B



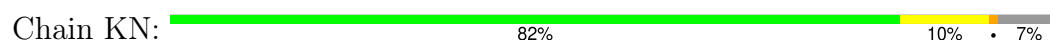
- Molecule 1: C2-B



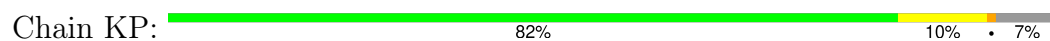
- Molecule 1: C2-B



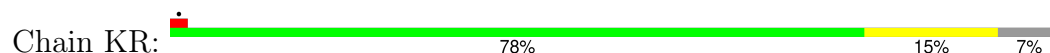
- Molecule 1: C2-B



- Molecule 1: C2-B



- Molecule 1: C2-B





- Molecule 1: C2-B

Chain KT: 82% 10% • 7%



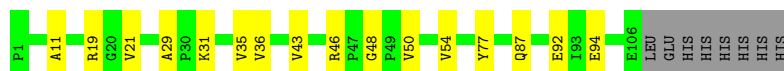
- Molecule 1: C2-B

Chain KV: 83% 9% • 7%



- Molecule 1: C2-B

Chain KX: 79% 14% 7%



- Molecule 1: C2-B

Chain KZ: 82% 10% • 7%



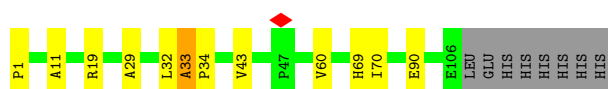
- Molecule 1: C2-B

Chain ZM: 82% 10% • 7%



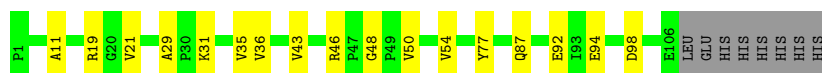
- Molecule 1: C2-B

Chain LB: 82% 10% • 7%

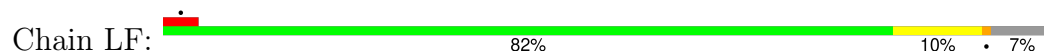


- Molecule 1: C2-B

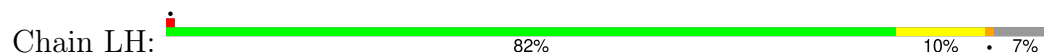
Chain LD: 78% 15% 7%



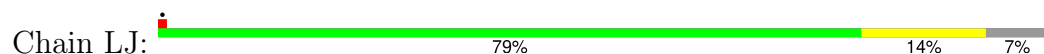
- Molecule 1: C2-B



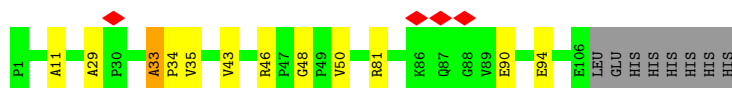
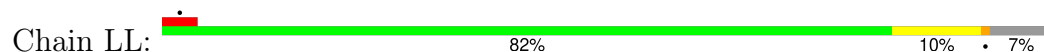
- Molecule 1: C2-B



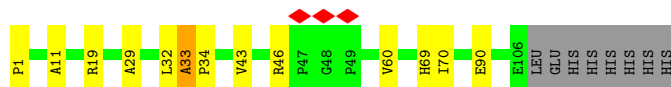
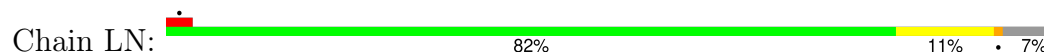
- Molecule 1: C2-B



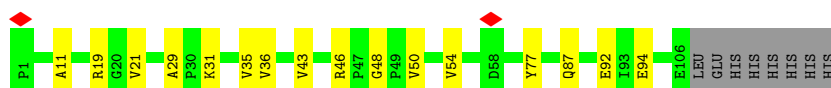
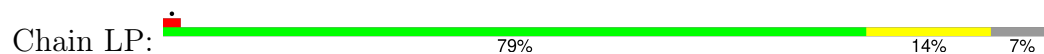
- Molecule 1: C2-B



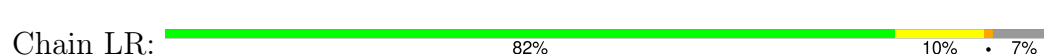
- Molecule 1: C2-B



- Molecule 1: C2-B

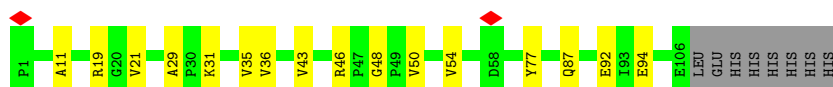
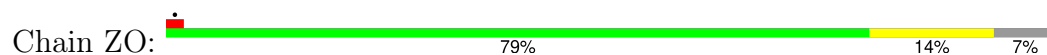


- Molecule 1: C2-B

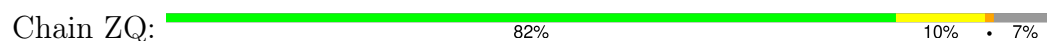




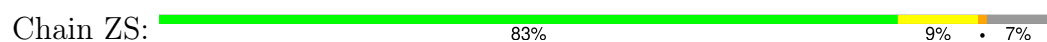
- Molecule 1: C2-B



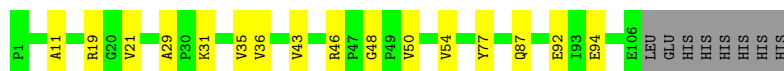
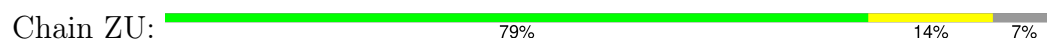
- Molecule 1: C2-B



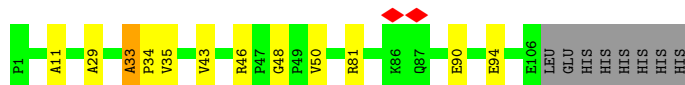
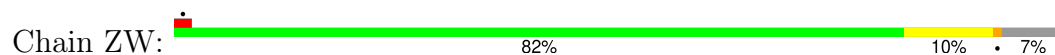
- Molecule 1: C2-B



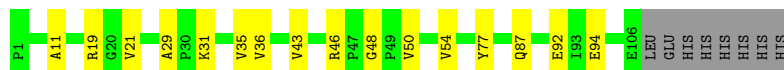
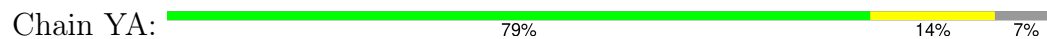
- Molecule 1: C2-B



- Molecule 1: C2-B

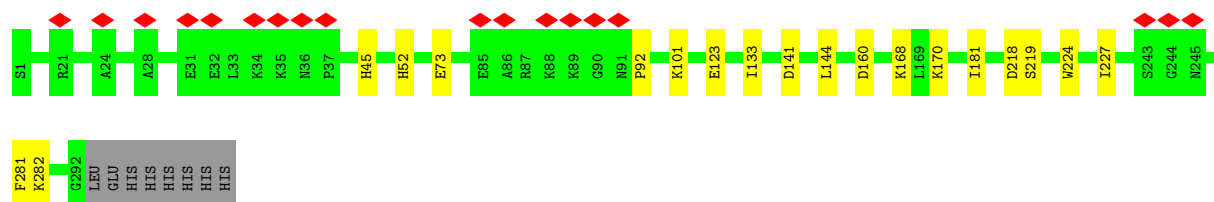


- Molecule 1: C2-B

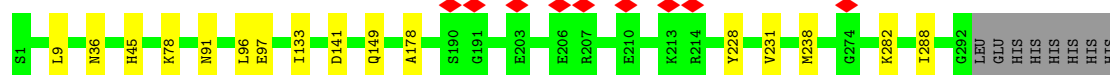


- Molecule 2: C3-A

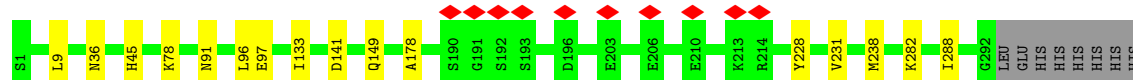




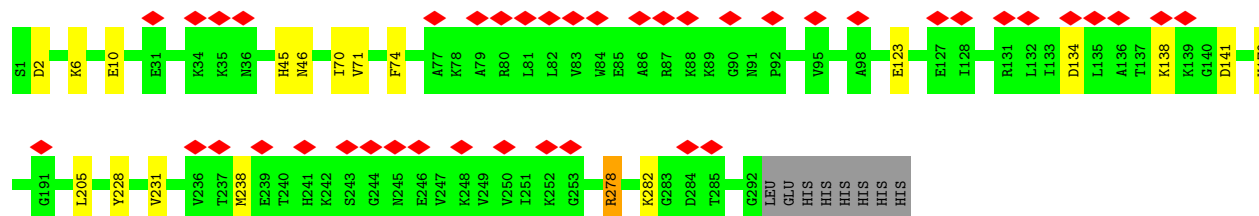
- Molecule 2: C3-A



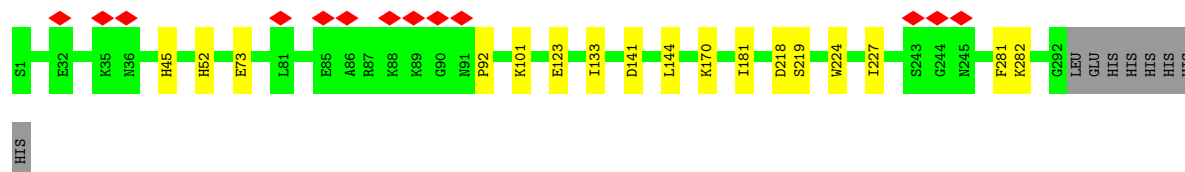
- Molecule 2: C3-A



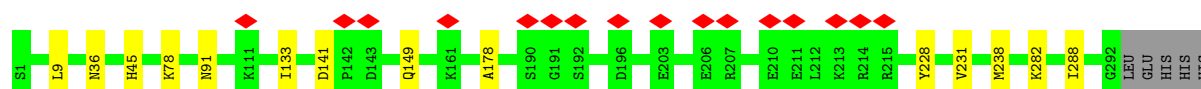
- Molecule 2: C3-A



- Molecule 2: C3-A



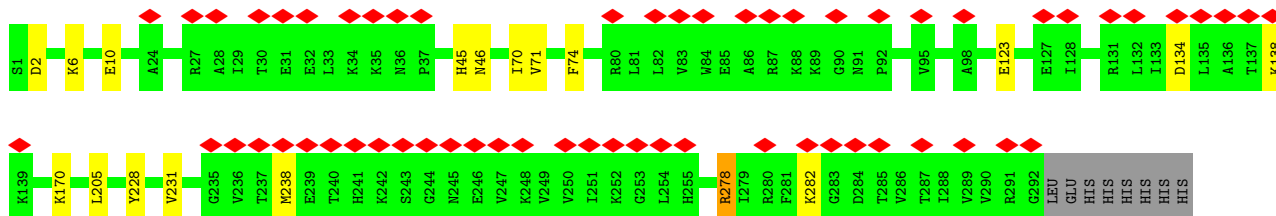
- Molecule 2: C3-A



HIS
HIS
HIS

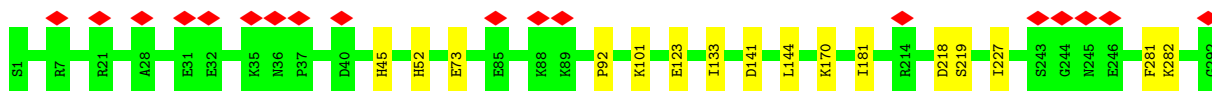
• Molecule 2: C3-A

Chain YN: 20% 91% 6% .



• Molecule 2: C3-A

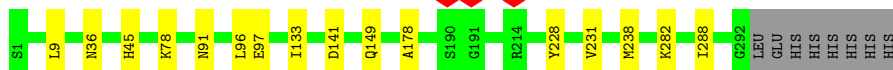
Chain YP: 6% 92% 5% .



LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

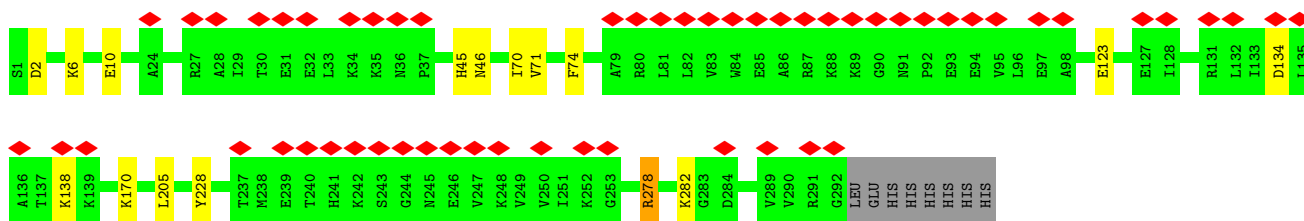
• Molecule 2: C3-A

Chain YR: 92% 5% .



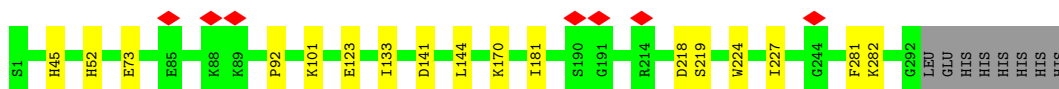
• Molecule 2: C3-A

Chain YT: 19% 92% 5% .

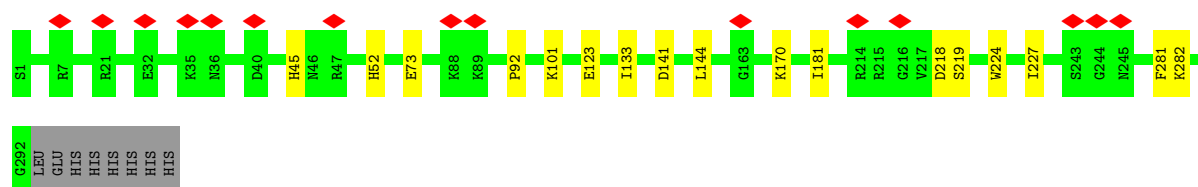


• Molecule 2: C3-A

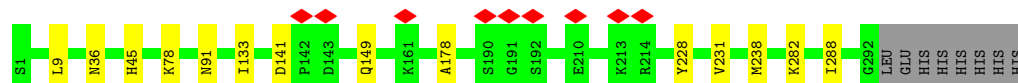
Chain YV: 92% 6% .



• Molecule 2: C3-A



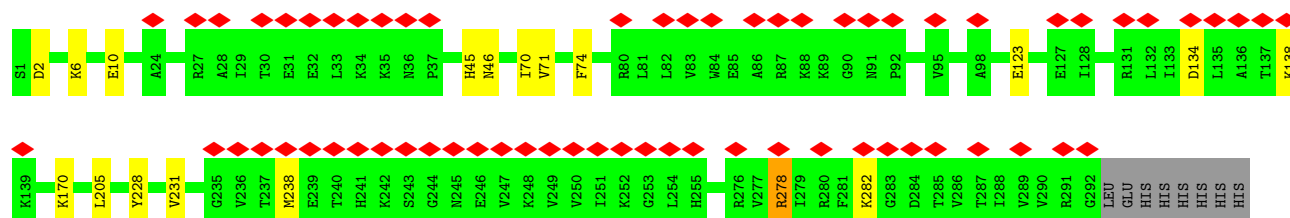
- Molecule 2: C3-A



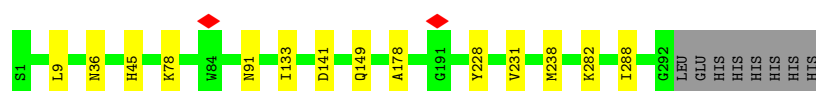
- Molecule 2: C3-A



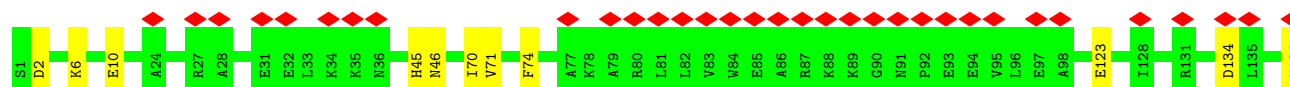
- Molecule 2: C3-A

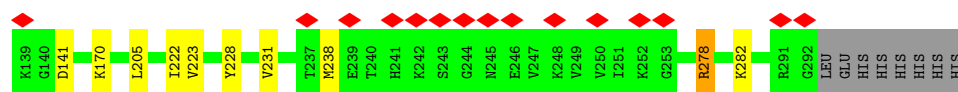


- Molecule 2: C3-A

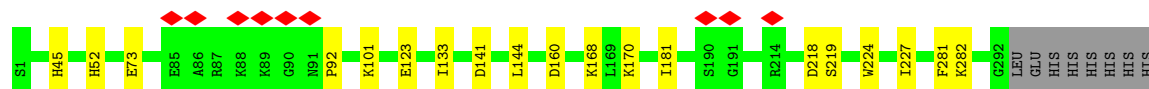


- Molecule 2: C3-A

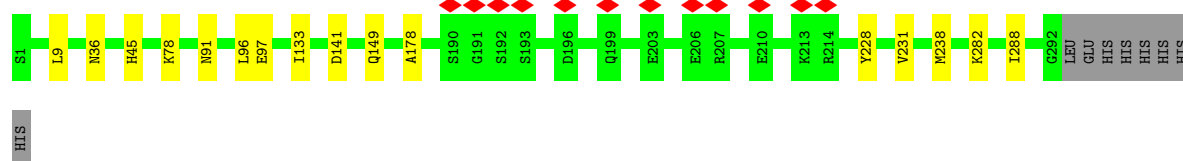




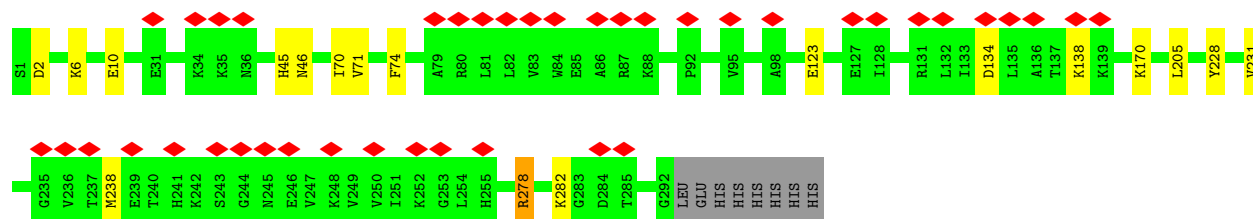
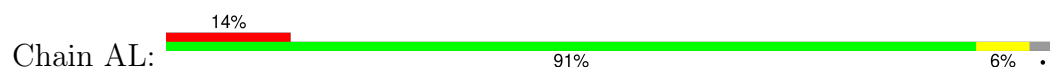
• Molecule 2: C3-A



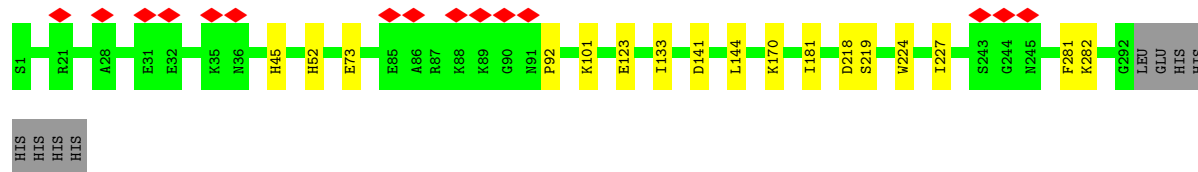
• Molecule 2: C3-A



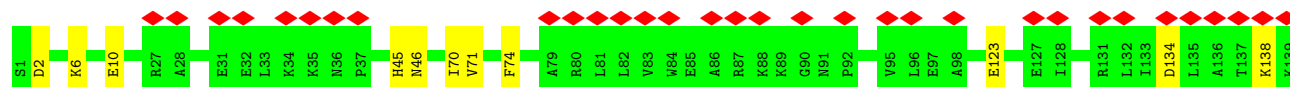
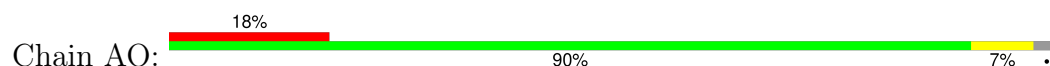
• Molecule 2: C3-A

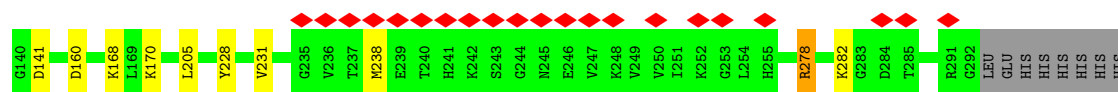


• Molecule 2: C3-A

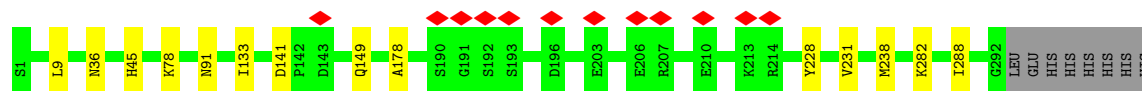


• Molecule 2: C3-A





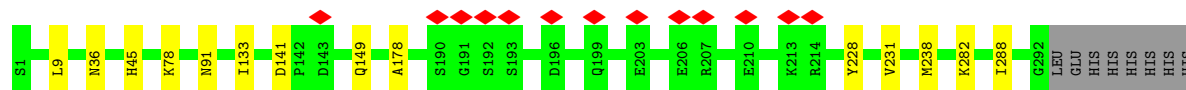
• Molecule 2: C3-A



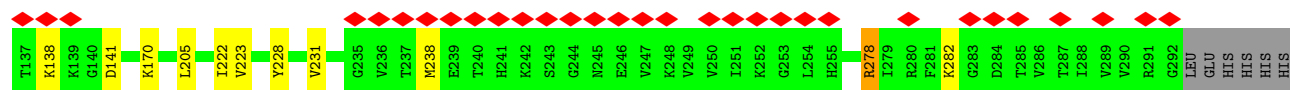
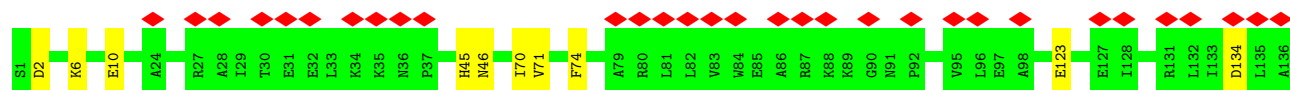
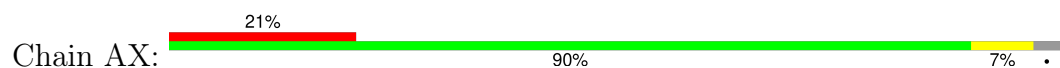
• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A



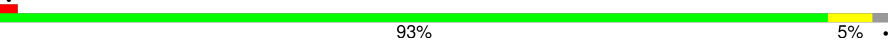
HIS
HIS

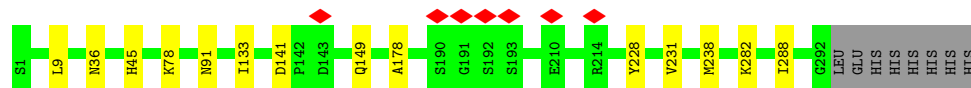
• Molecule 2: C3-A



G292
LEU
GLU
HIS
HIS
HIS
HIS
HIS

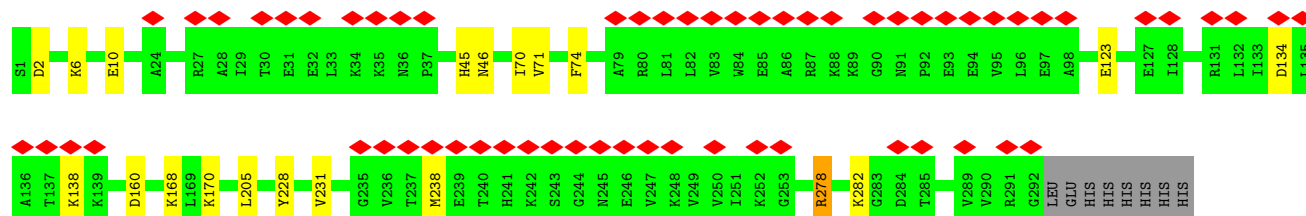
- Molecule 2: C3-A

Chain BB:  93% 5% .



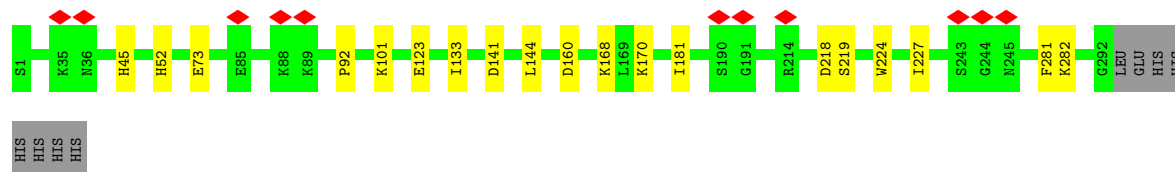
- Molecule 2: C3-A

Chain BD:  20% 91% 6% .



- Molecule 2: C3-A

Chain BF:  91% 6% .



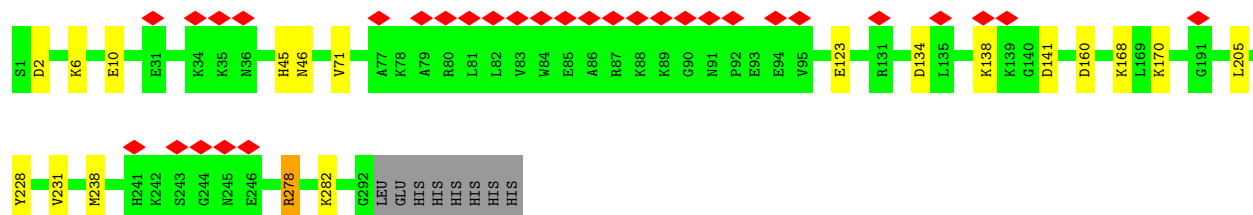
- Molecule 2: C3-A

Chain BH:  93% 5% .



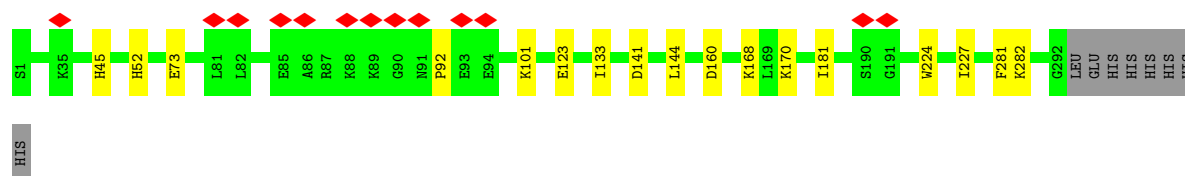
- Molecule 2: C3-A

Chain BJ:  10% 91% 6% .

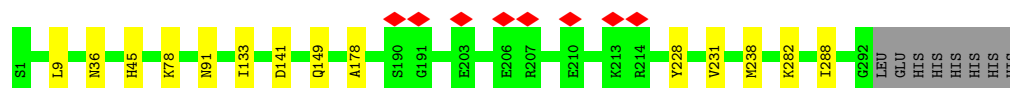


- Molecule 2: C3-A

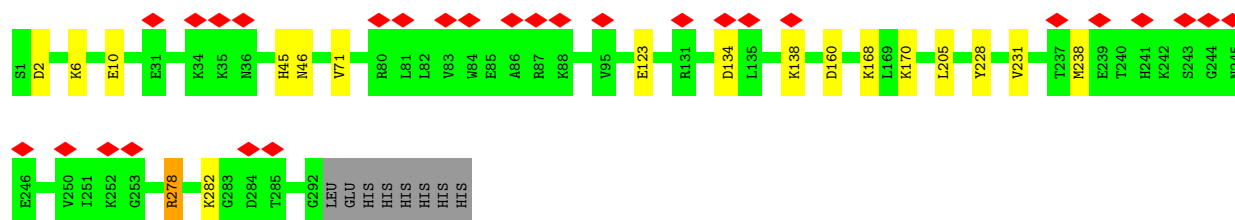
Chain BL:  92% 6% .



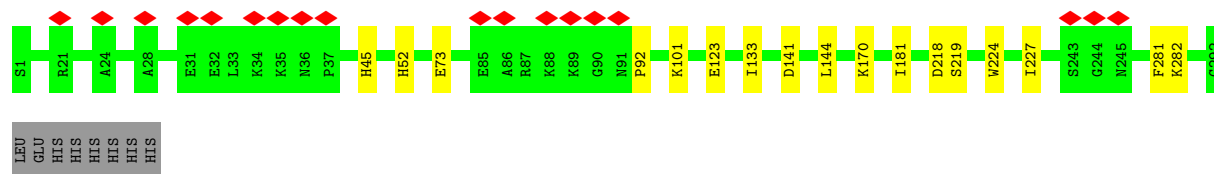
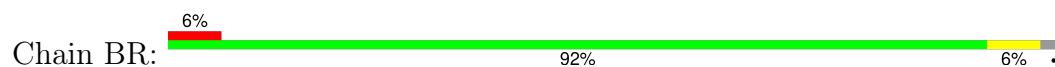
• Molecule 2: C3-A



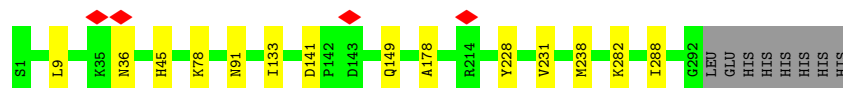
• Molecule 2: C3-A



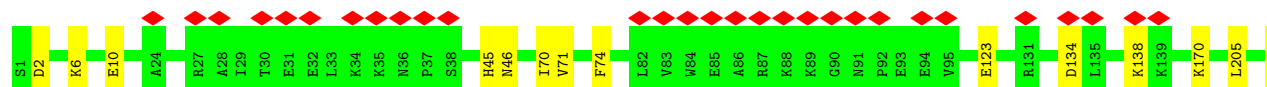
• Molecule 2: C3-A

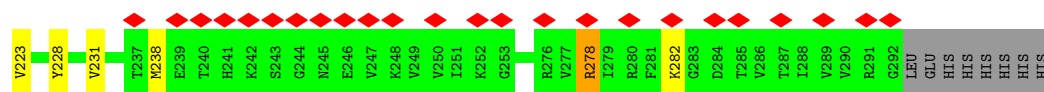


• Molecule 2: C3-A

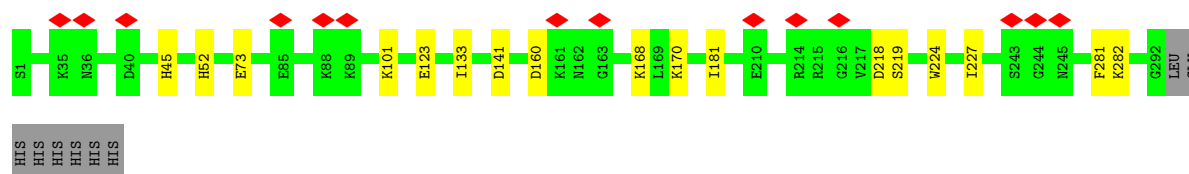


• Molecule 2: C3-A

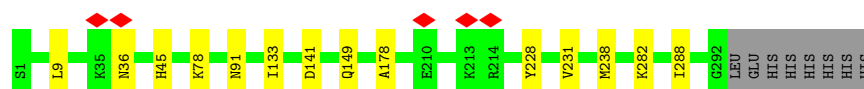




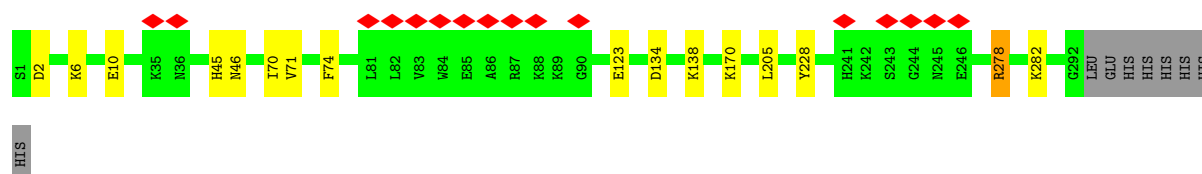
• Molecule 2: C3-A



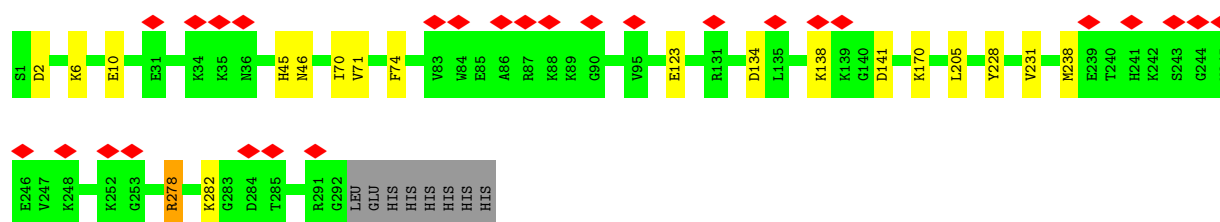
• Molecule 2: C3-A



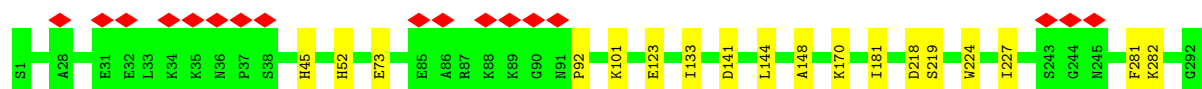
• Molecule 2: C3-A



• Molecule 2: C3-A

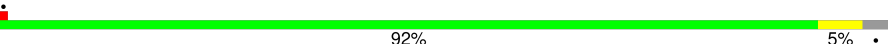


• Molecule 2: C3-A



GLU
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: C3-A

Chain CF:  92% 5%



• Molecule 2: C3-A

Chain CH:  10% 90% 7%



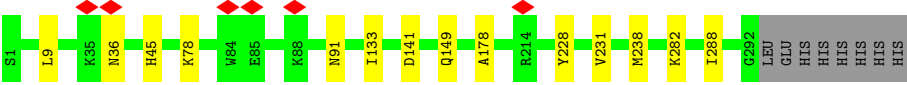
• Molecule 2: C3-A

Chain CJ:  92% 6%



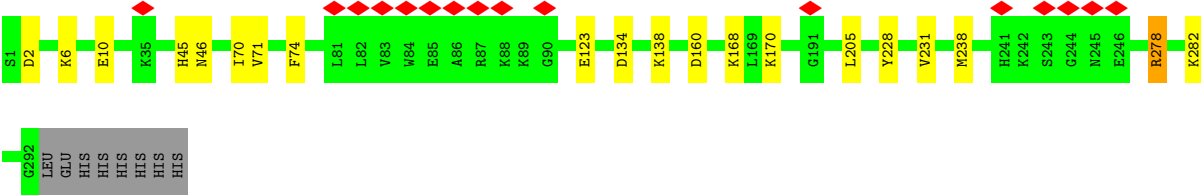
• Molecule 2: C3-A

Chain CL:  93% 5%



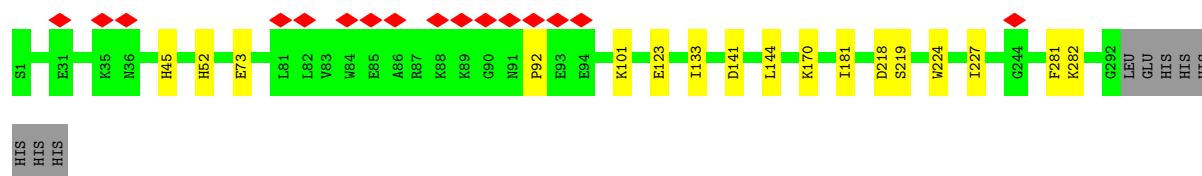
• Molecule 2: C3-A

Chain CN:  5% 91% 6%



• Molecule 2: C3-A

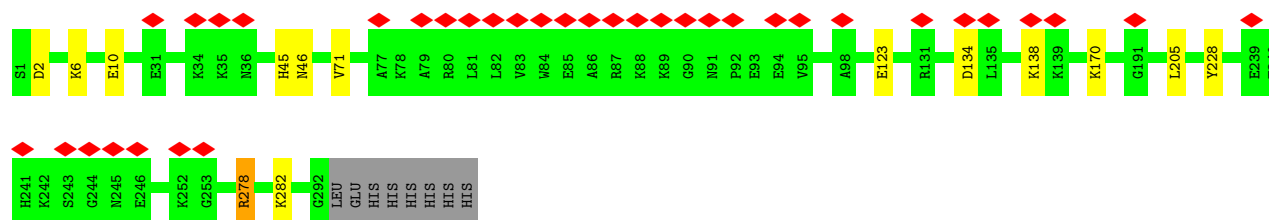
Chain CP:  5% 92% 6%



• Molecule 2: C3-A



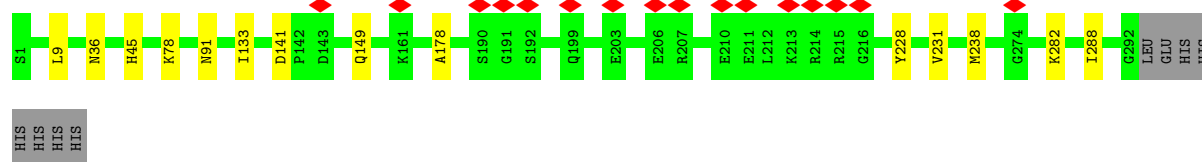
• Molecule 2: C3-A



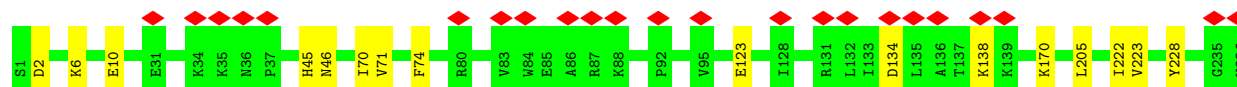
• Molecule 2: C3-A

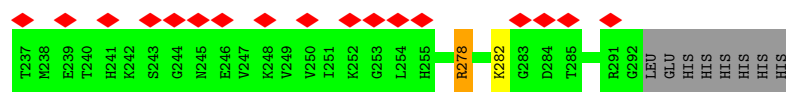


• Molecule 2: C3-A

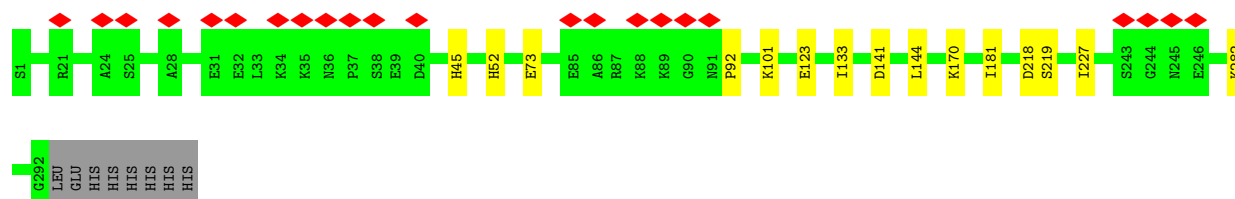


• Molecule 2: C3-A





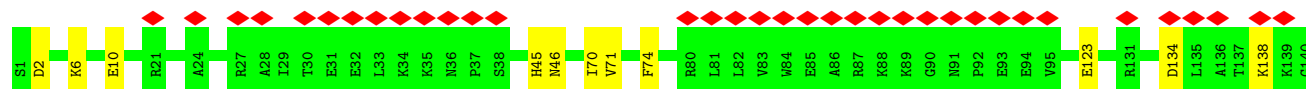
• Molecule 2: C3-A



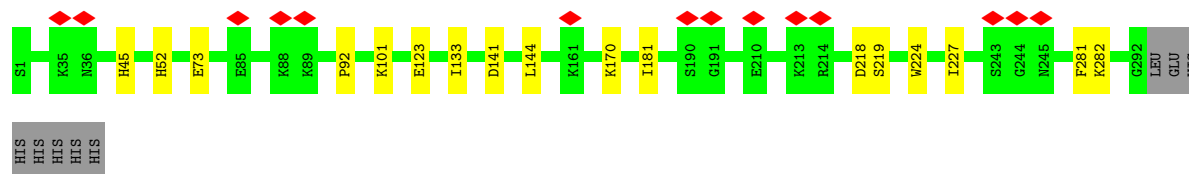
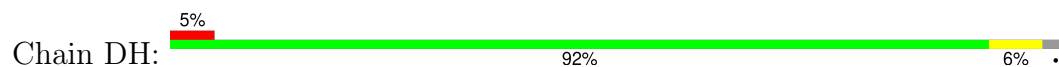
• Molecule 2: C3-A



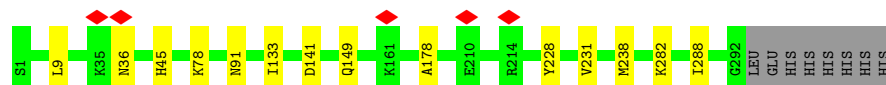
• Molecule 2: C3-A



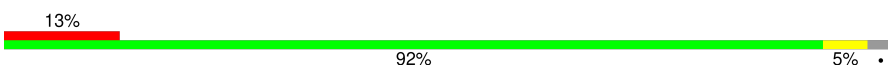
• Molecule 2: C3-A

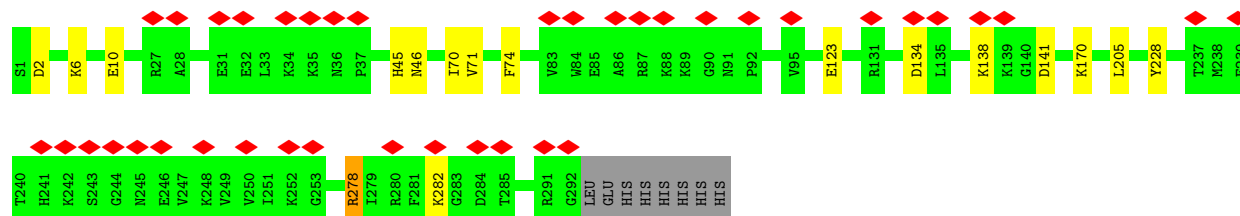


• Molecule 2: C3-A

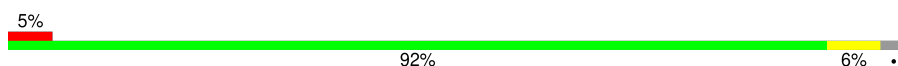


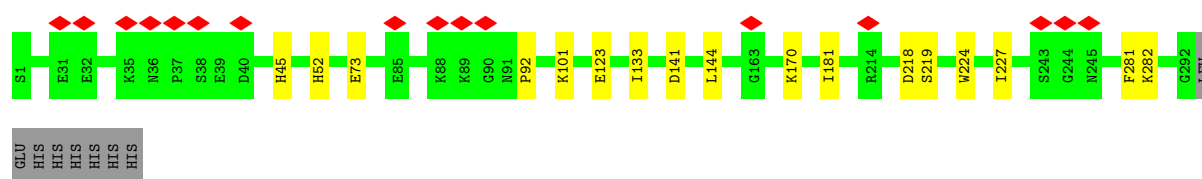
- Molecule 2: C3-A

Chain DL: 

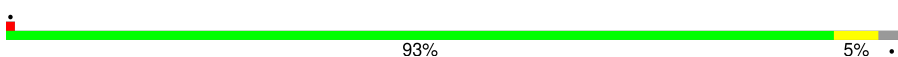


- Molecule 2: C3-A

Chain DN: 

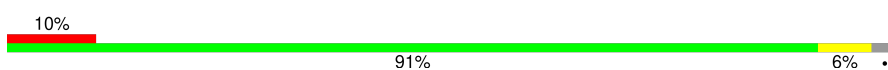


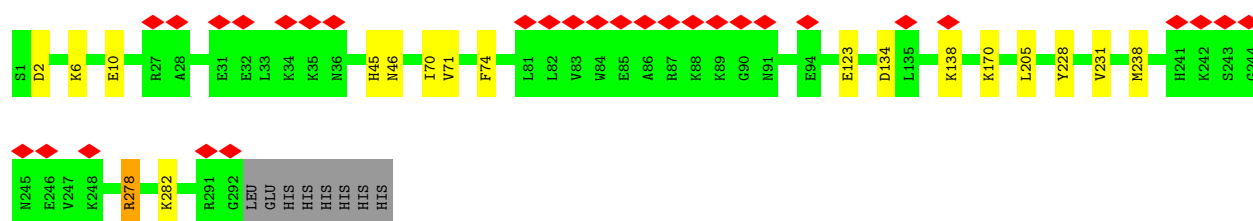
- Molecule 2: C3-A

Chain DP: 

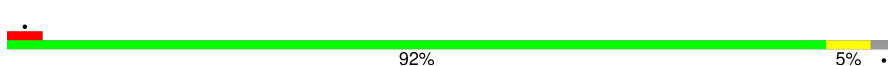


- Molecule 2: C3-A

Chain DR: 

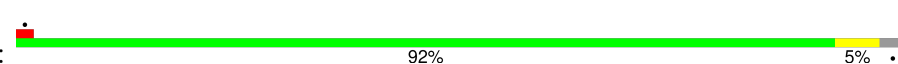


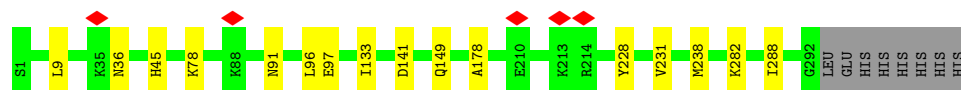
- Molecule 2: C3-A

Chain DT: 

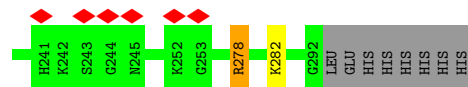
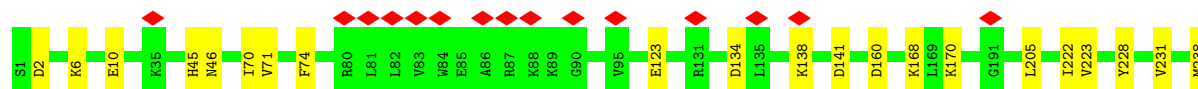
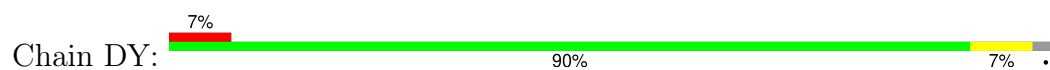


- Molecule 2: C3-A

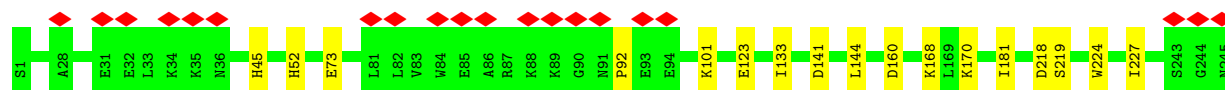
Chain DW: 



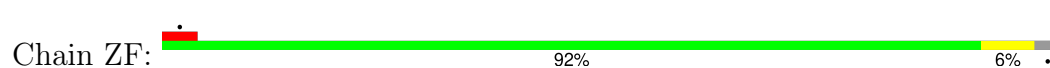
• Molecule 2: C3-A



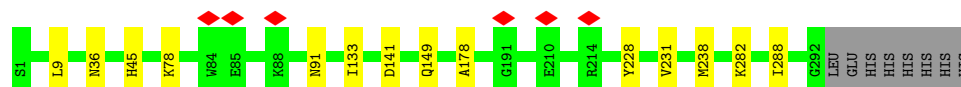
• Molecule 2: C3-A



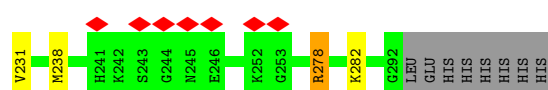
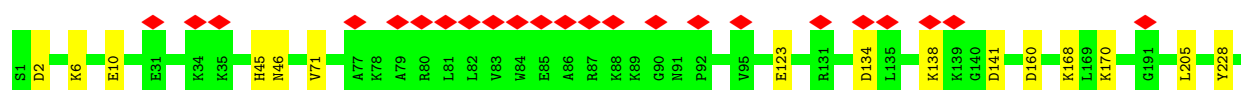
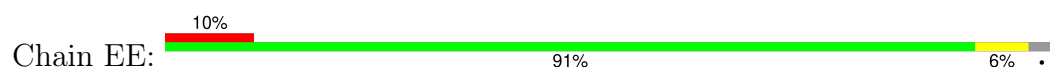
• Molecule 2: C3-A



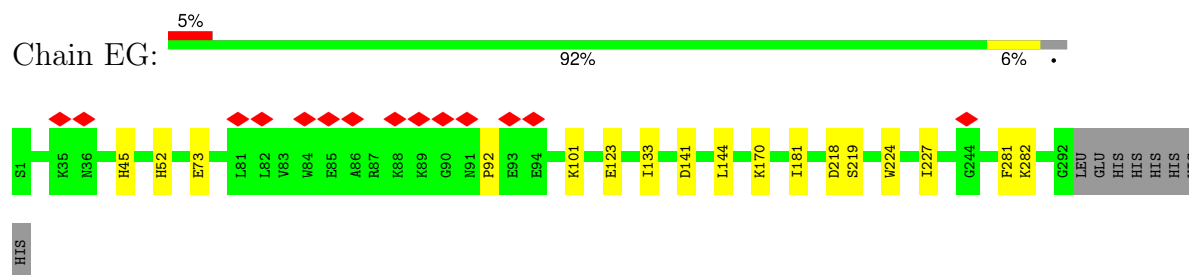
• Molecule 2: C3-A



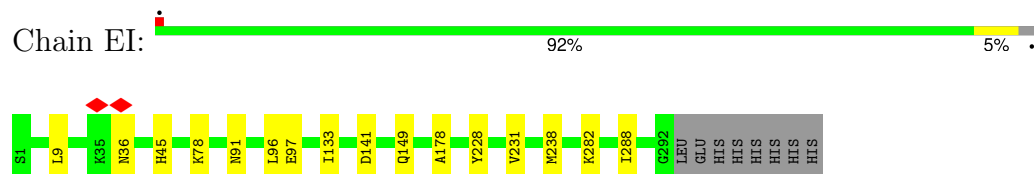
• Molecule 2: C3-A



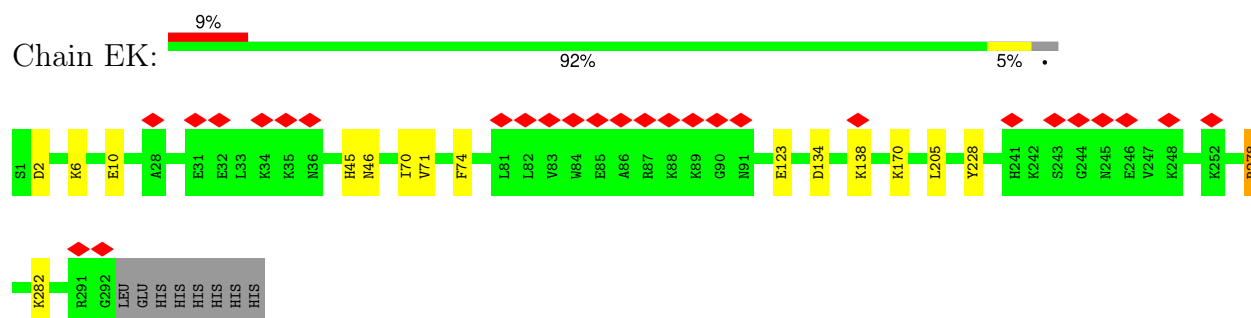
• Molecule 2: C3-A



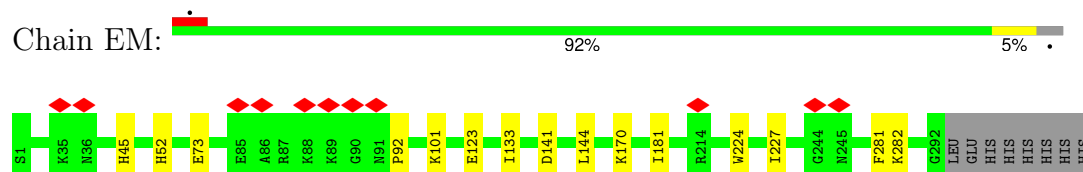
• Molecule 2: C3-A



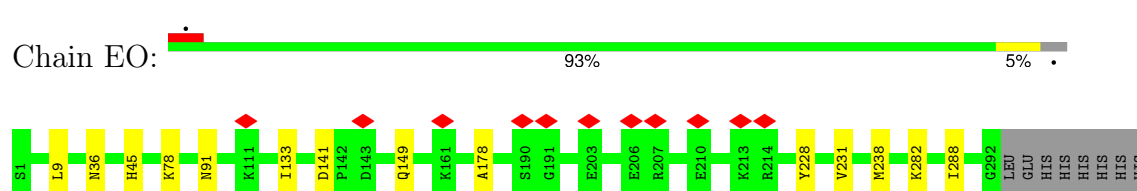
• Molecule 2: C3-A



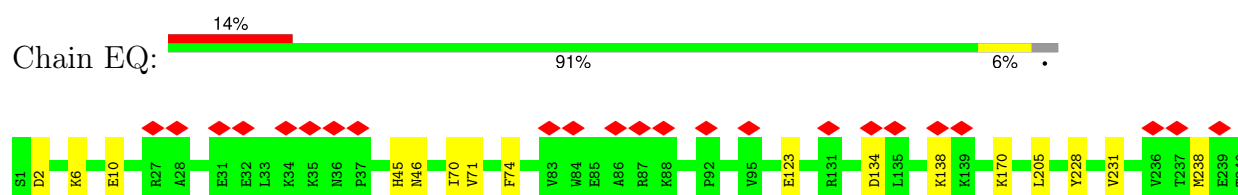
• Molecule 2: C3-A

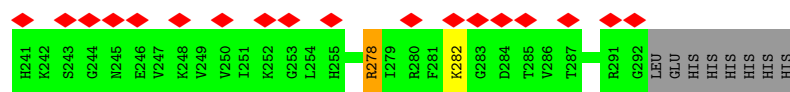


• Molecule 2: C3-A

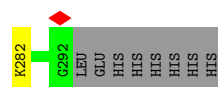
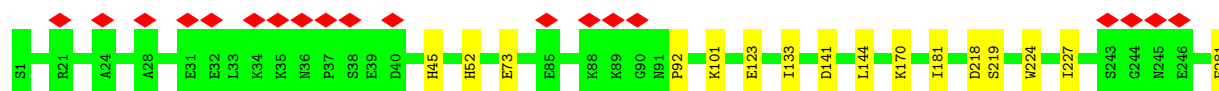
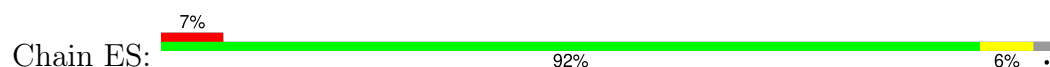


• Molecule 2: C3-A





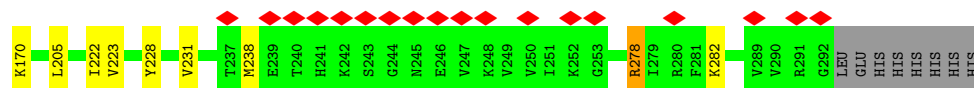
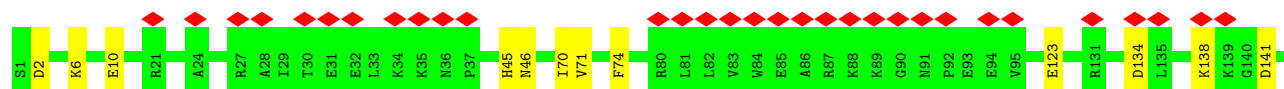
• Molecule 2: C3-A



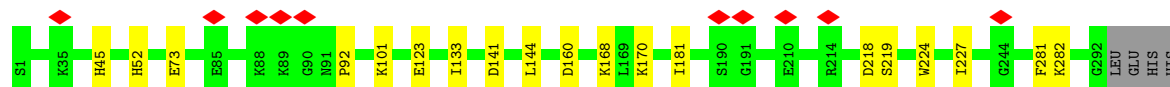
• Molecule 2: C3-A



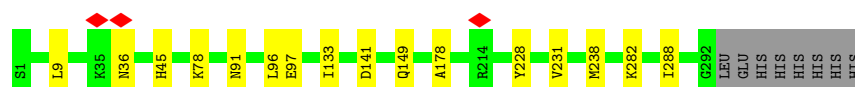
• Molecule 2: C3-A



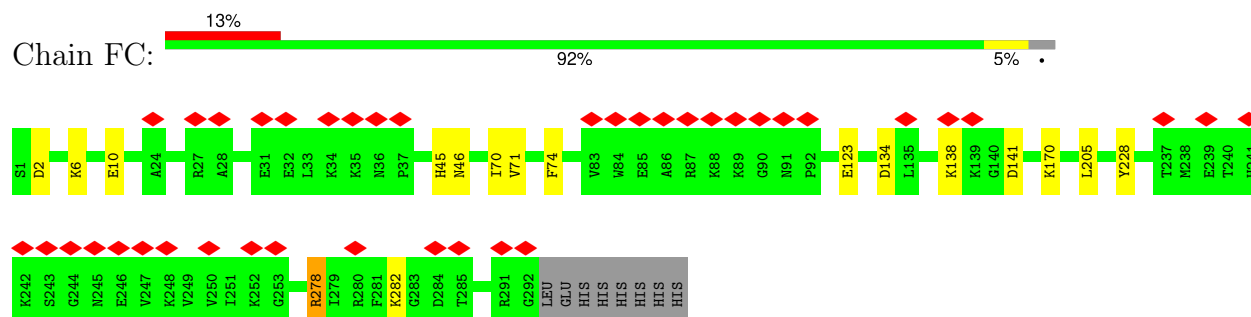
• Molecule 2: C3-A



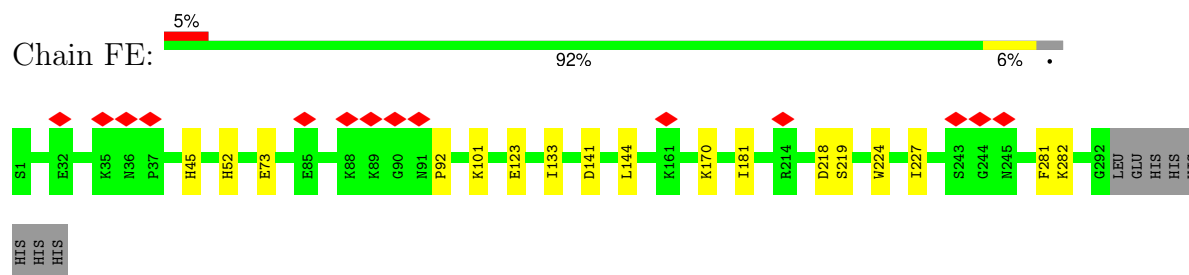
• Molecule 2: C3-A



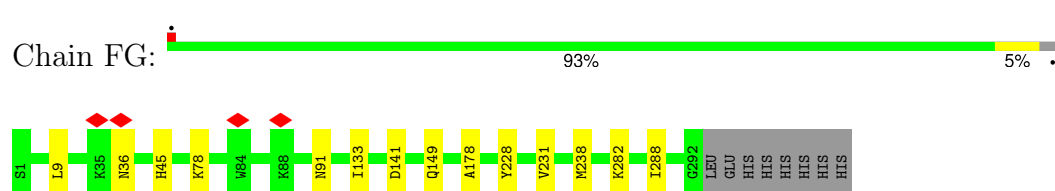
• Molecule 2: C3-A



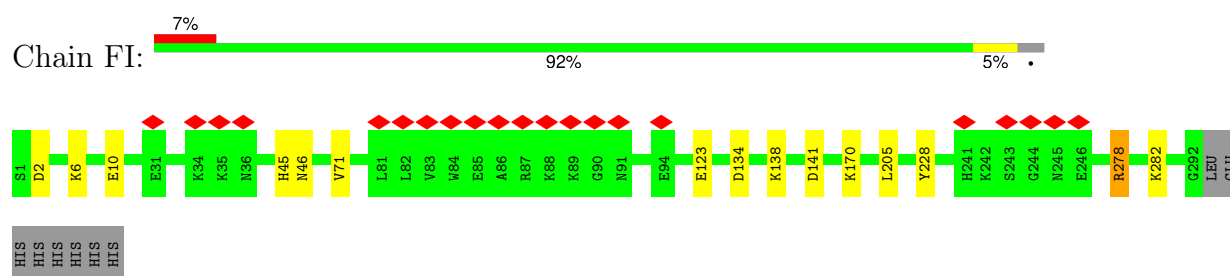
• Molecule 2: C3-A



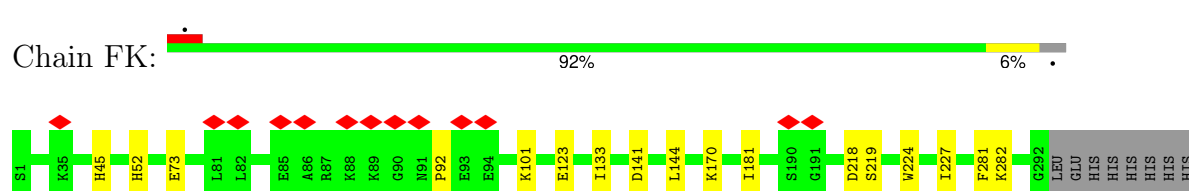
• Molecule 2: C3-A



• Molecule 2: C3-A

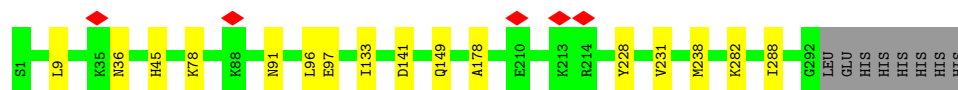


• Molecule 2: C3-A

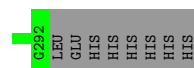
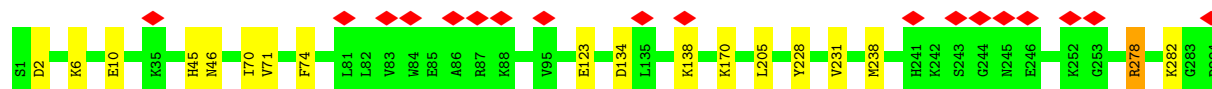


• Molecule 2: C3-A





- Molecule 2: C3-A



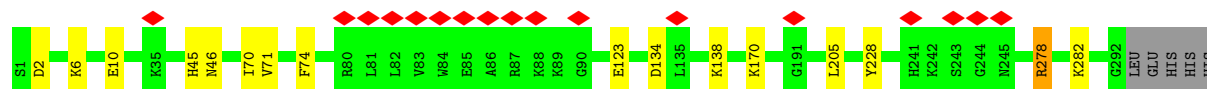
- Molecule 2: C3-A



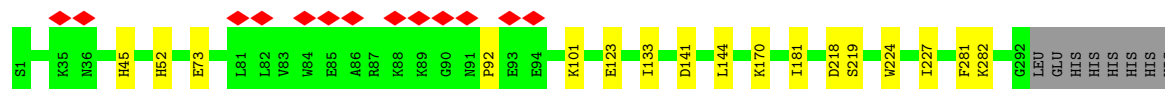
- Molecule 2: C3-A



- Molecule 2: C3-A

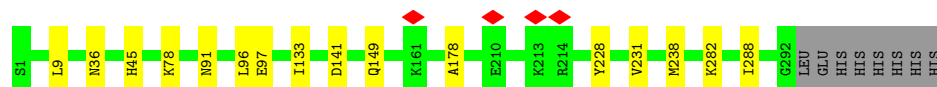


- Molecule 2: C3-A

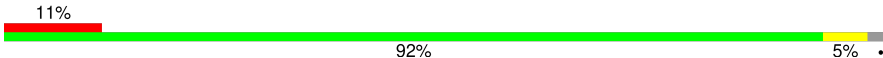


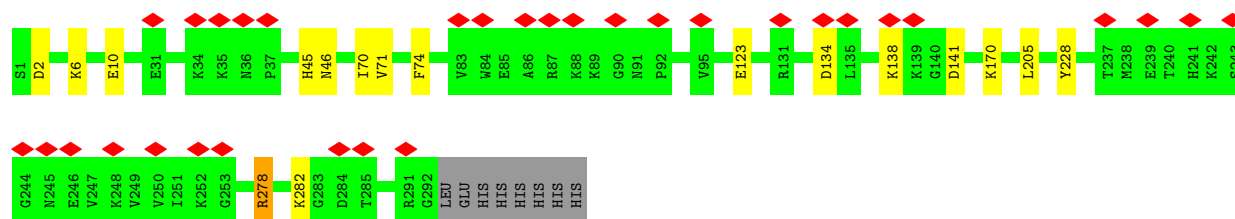
- Molecule 2: C3-A

Chain FY:  92% 5% .



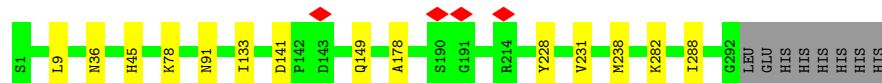
• Molecule 2: C3-A

Chain GA:  11% 92% 5% .



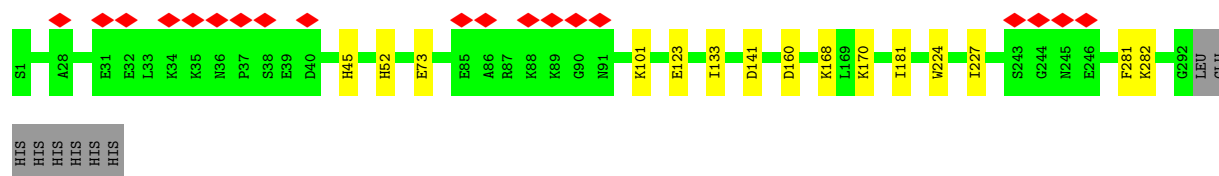
• Molecule 2: C3-A

Chain ZH:  93% 5% .



• Molecule 2: C3-A

Chain GC:  6% 92% 5% .



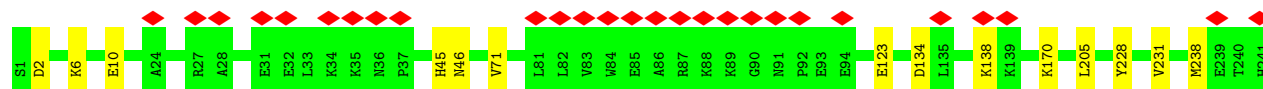
• Molecule 2: C3-A

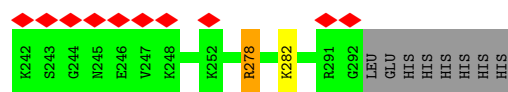
Chain GE:  92% 5% .



• Molecule 2: C3-A

Chain GG:  12% 92% 5% .





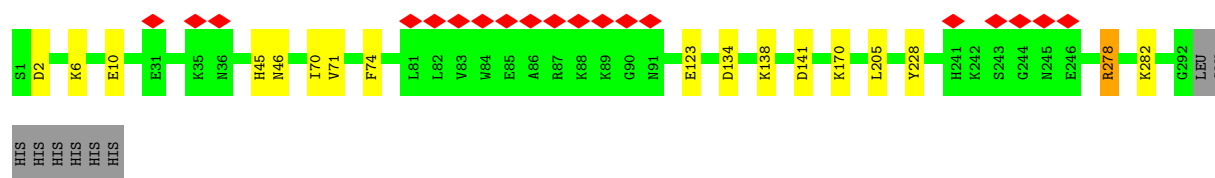
- Molecule 2: C3-A



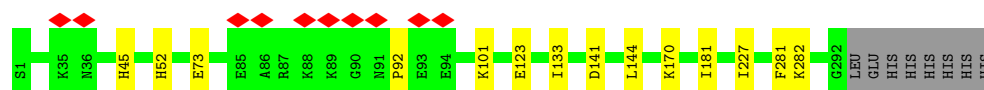
- Molecule 2: C3-A



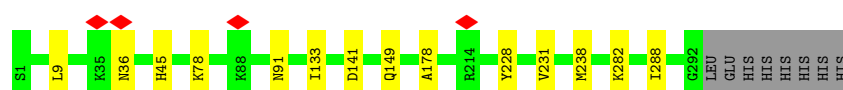
- Molecule 2: C3-A



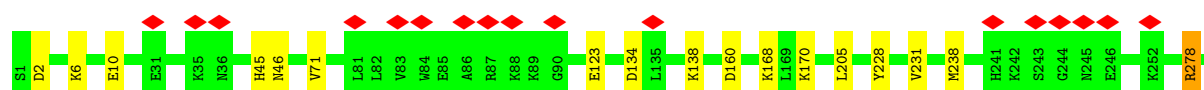
- Molecule 2: C3-A

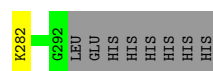


- Molecule 2: C3-A



- Molecule 2: C3-A





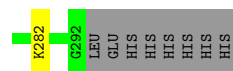
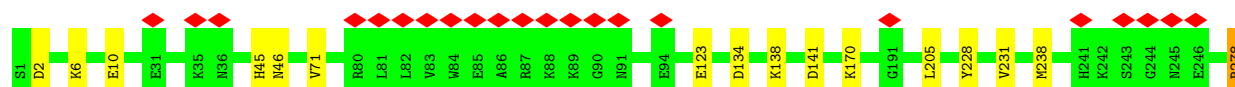
- Molecule 2: C3-A



- Molecule 2: C3-A



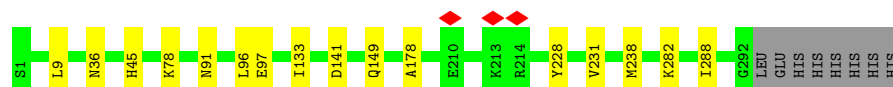
- Molecule 2: C3-A



- Molecule 2: C3-A

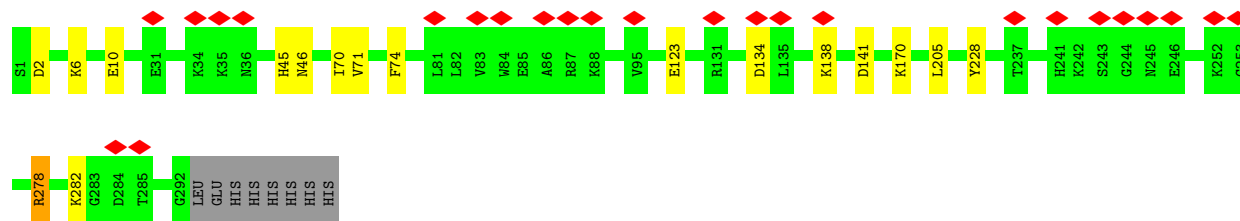


- Molecule 2: C3-A

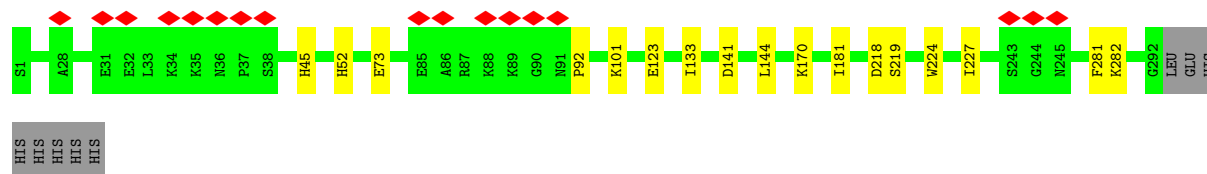


- Molecule 2: C3-A





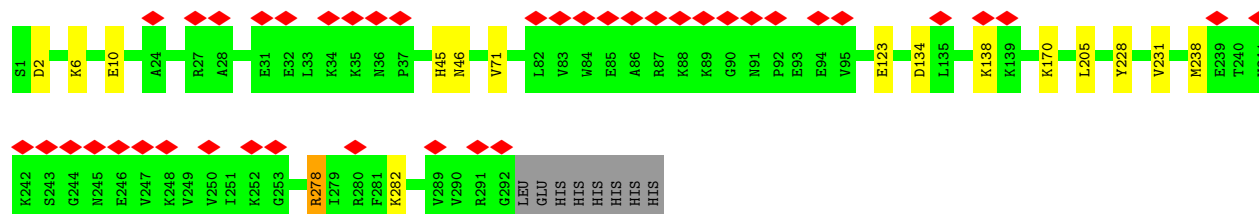
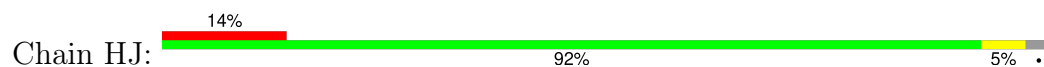
- Molecule 2: C3-A



- Molecule 2: C3-A



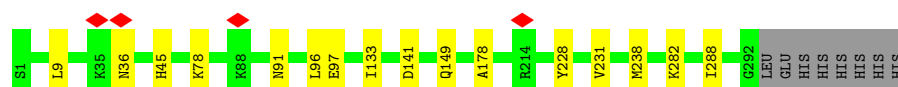
- Molecule 2: C3-A



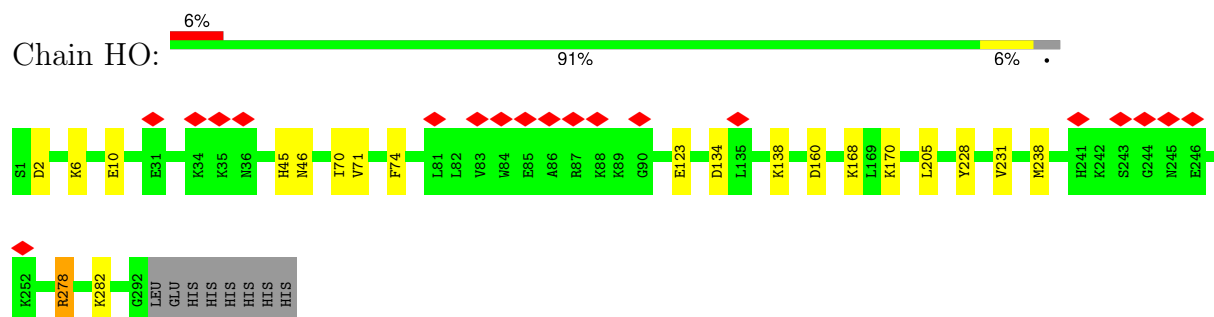
- Molecule 2: C3-A



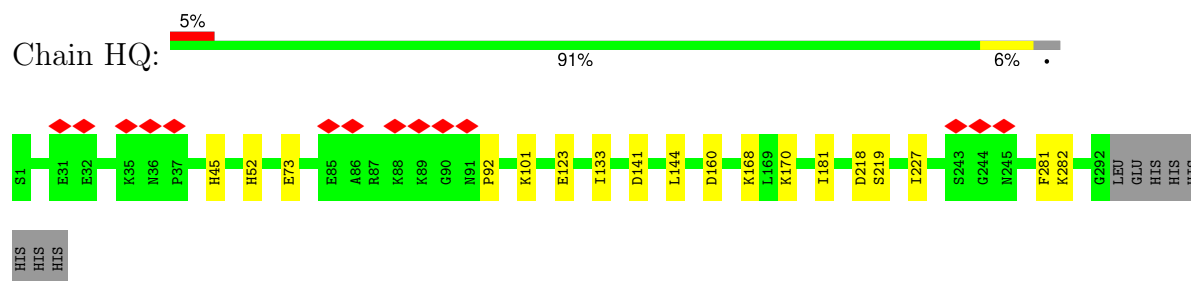
- Molecule 2: C3-A



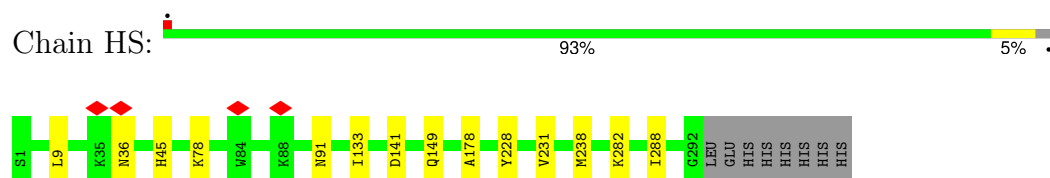
• Molecule 2: C3-A



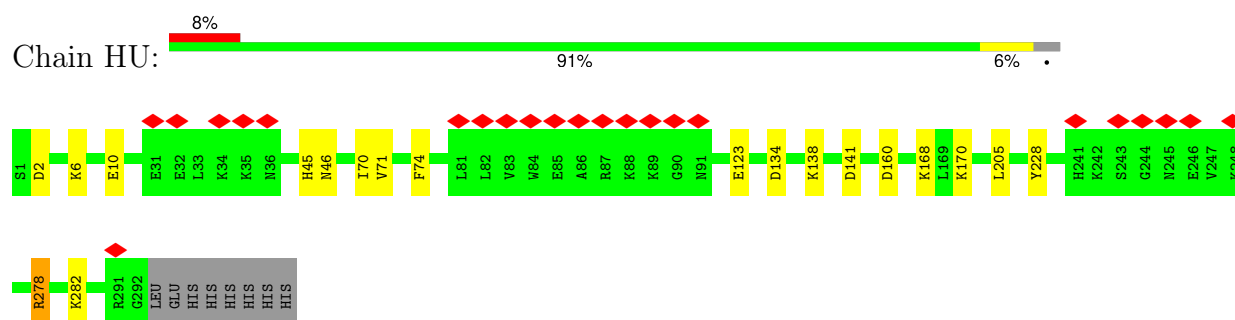
• Molecule 2: C3-A



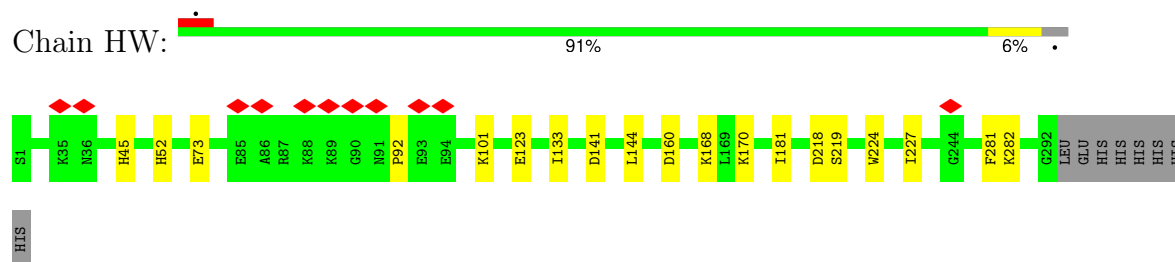
• Molecule 2: C3-A



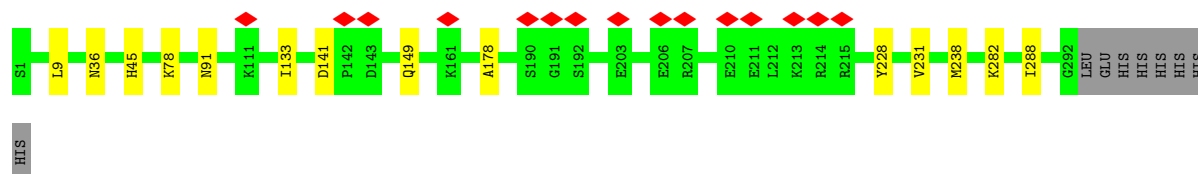
• Molecule 2: C3-A



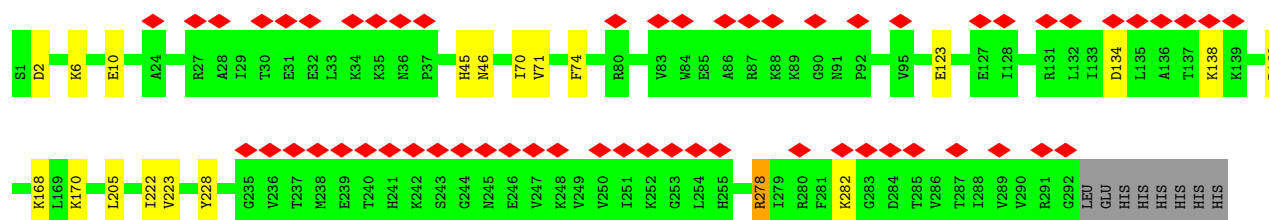
• Molecule 2: C3-A



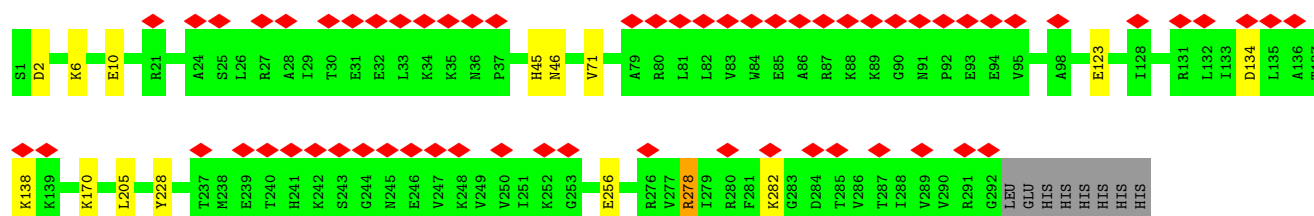
• Molecule 2: C3-A



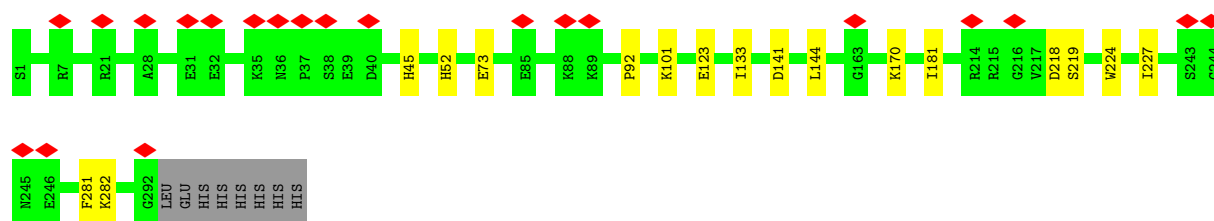
- Molecule 2: C3-A



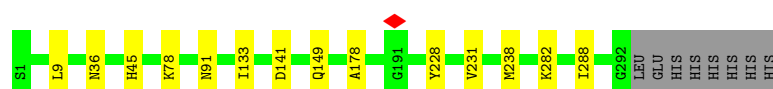
- Molecule 2: C3-A



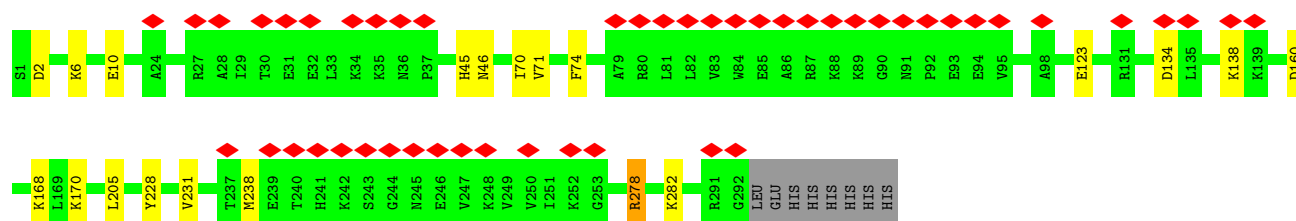
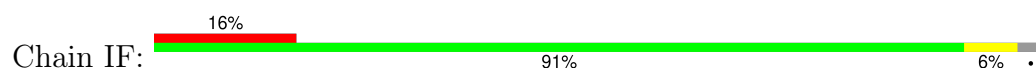
- Molecule 2: C3-A



- Molecule 2: C3-A



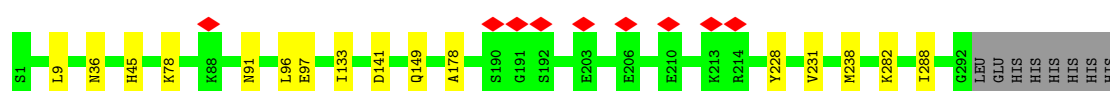
- Molecule 2: C3-A



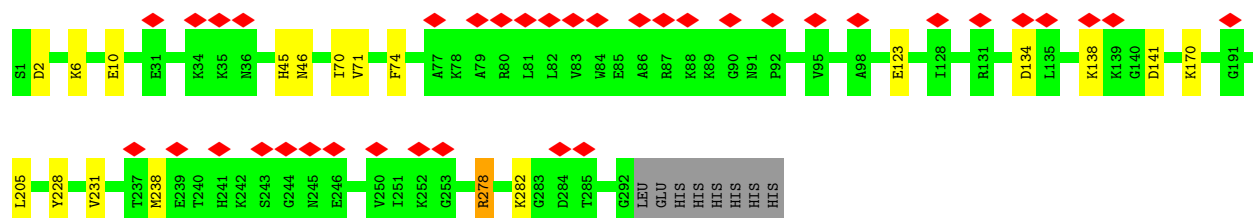
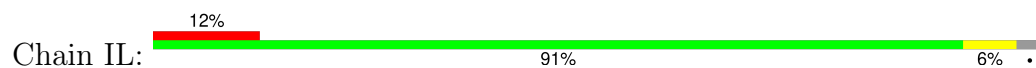
- Molecule 2: C3-A



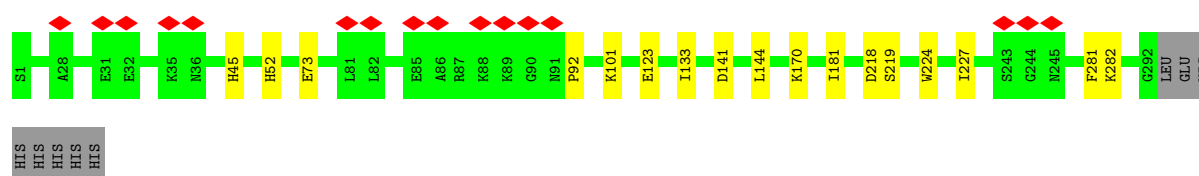
- Molecule 2: C3-A



- Molecule 2: C3-A

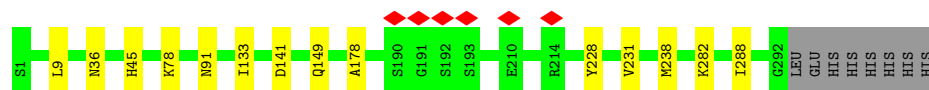


- Molecule 2: C3-A

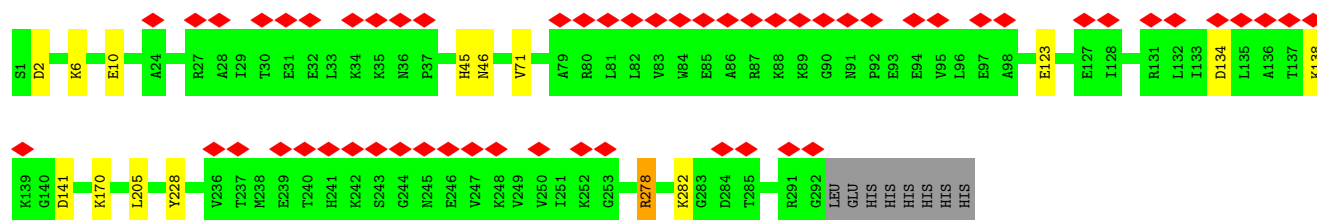


- Molecule 2: C3-A

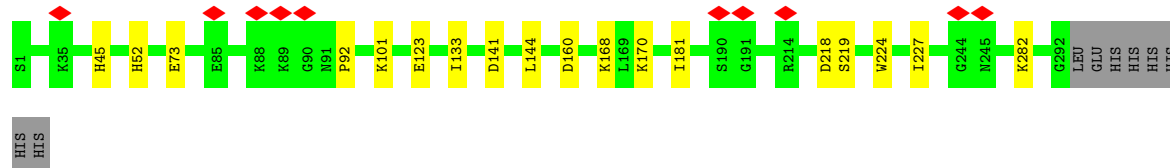




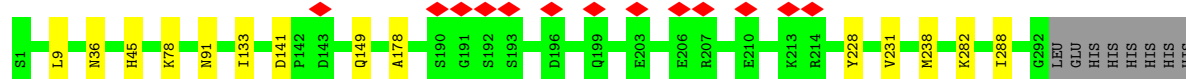
- Molecule 2: C3-A



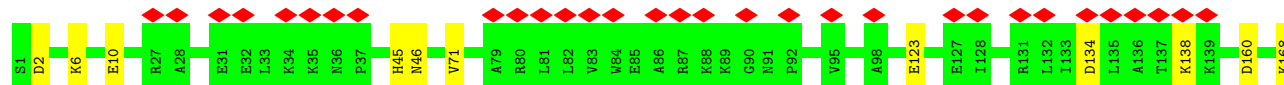
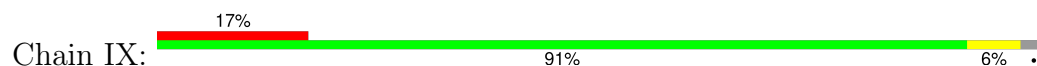
- Molecule 2: C3-A



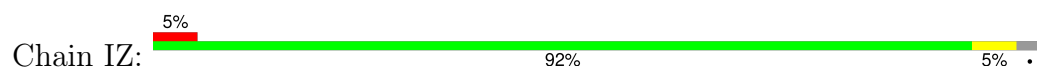
- Molecule 2: C3-A



- Molecule 2: C3-A

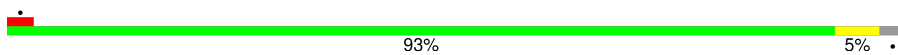


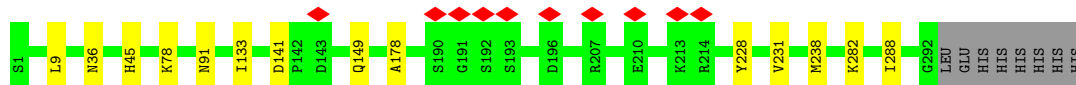
- Molecule 2: C3-A



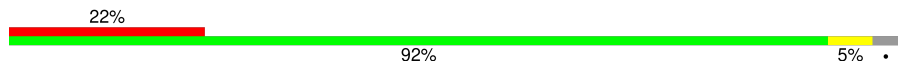
HIS
HIS
HIS

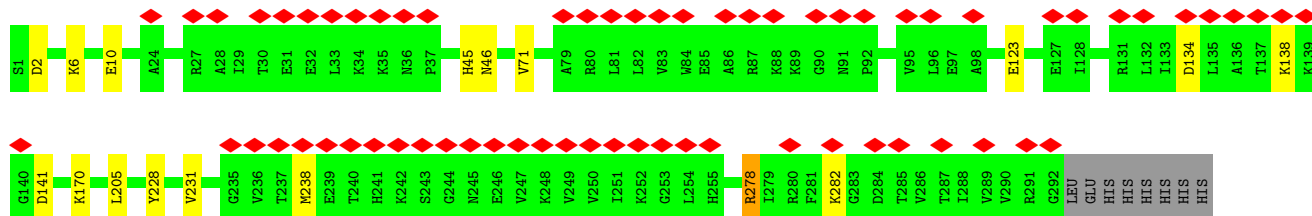
• Molecule 2: C3-A

Chain JB:  93% 5%



• Molecule 2: C3-A

Chain JD:  22% 92% 5%



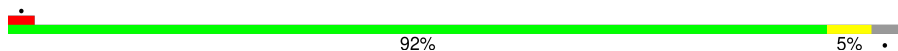
• Molecule 2: C3-A

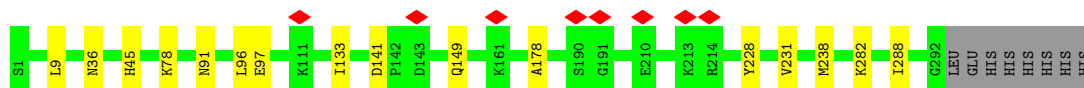
Chain JF:  92% 6%



HIS
HIS
HIS
HIS
HIS

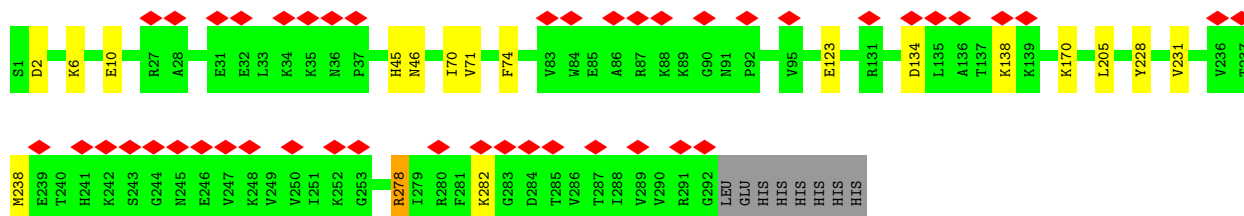
• Molecule 2: C3-A

Chain JH:  92% 5%

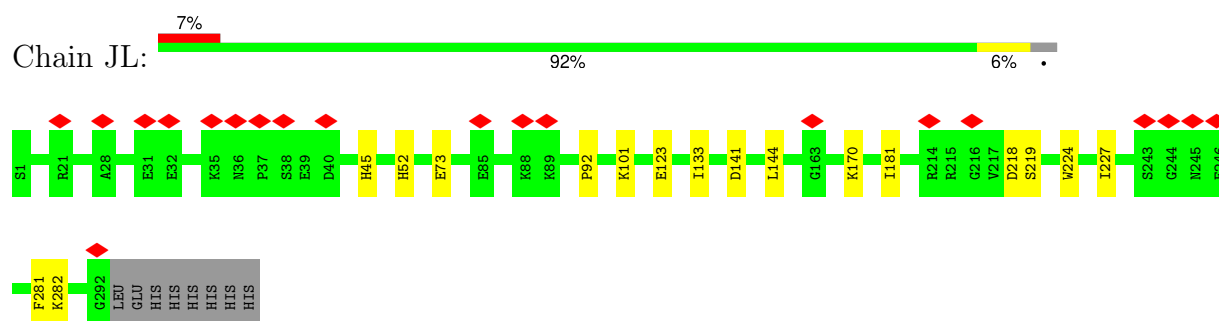


• Molecule 2: C3-A

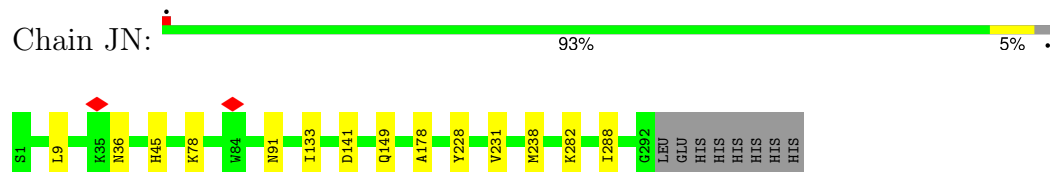
Chain JJ:  15% 91% 6%



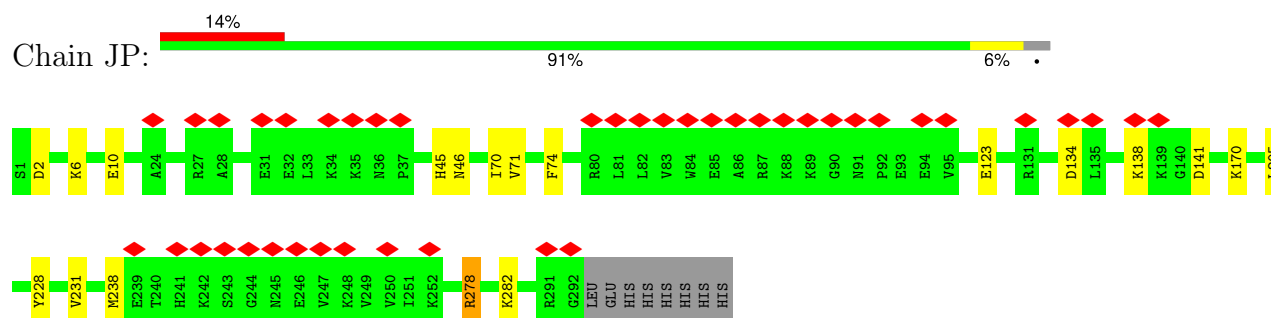
• Molecule 2: C3-A



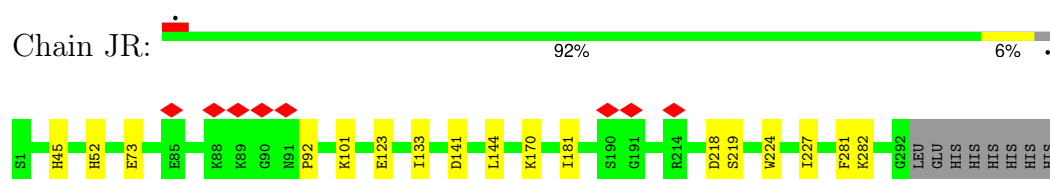
- Molecule 2: C3-A



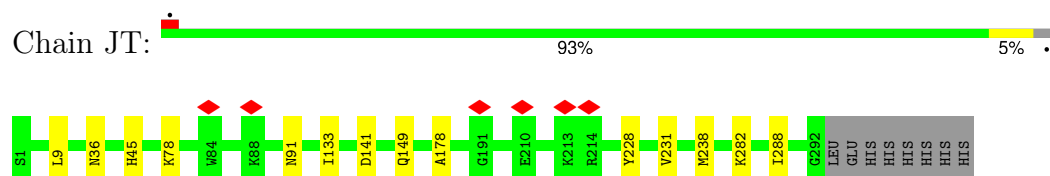
- Molecule 2: C3-A



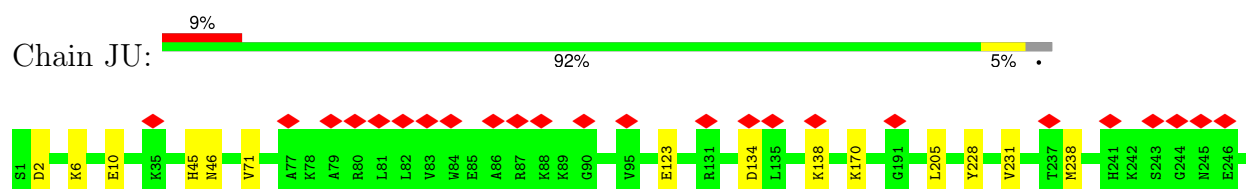
- Molecule 2: C3-A

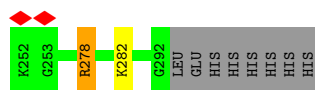


- Molecule 2: C3-A

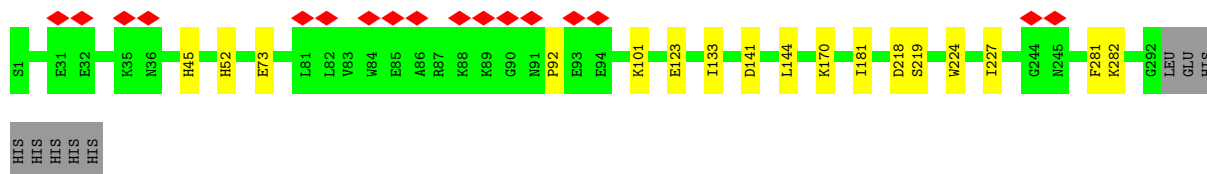


- Molecule 2: C3-A

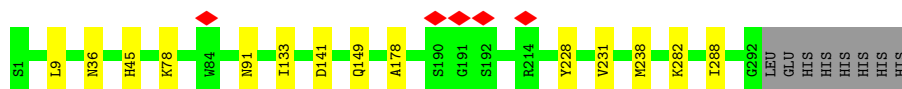




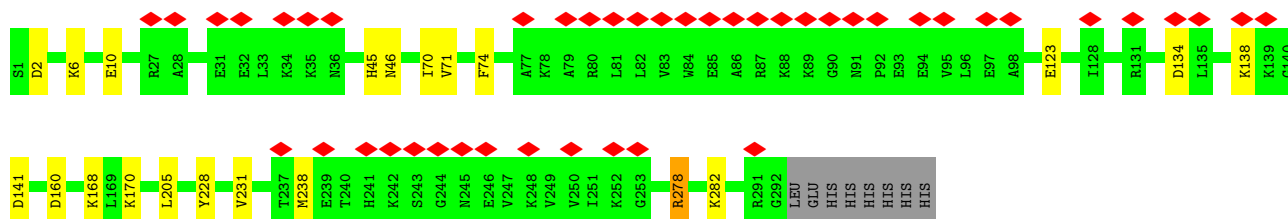
- Molecule 2: C3-A



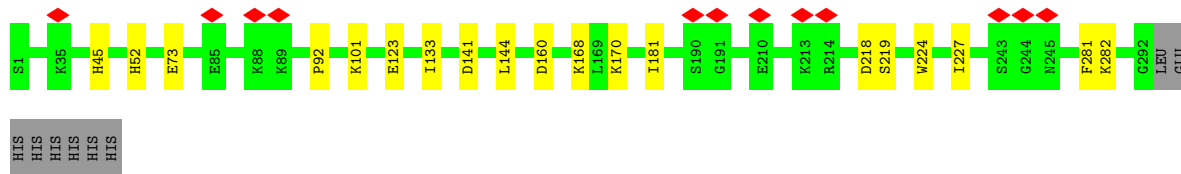
- Molecule 2: C3-A



- Molecule 2: C3-A



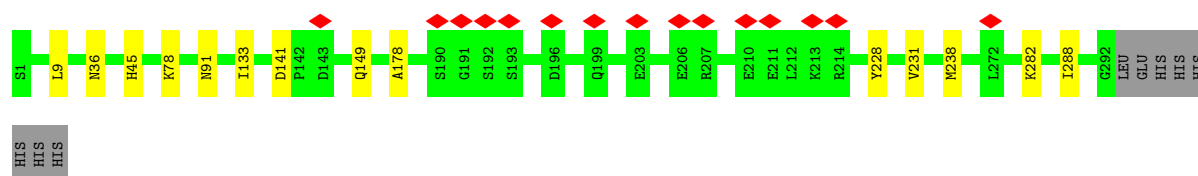
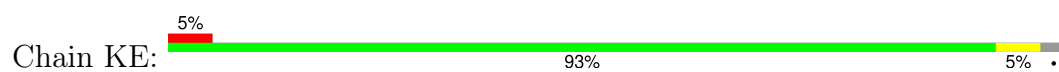
- Molecule 2: C3-A



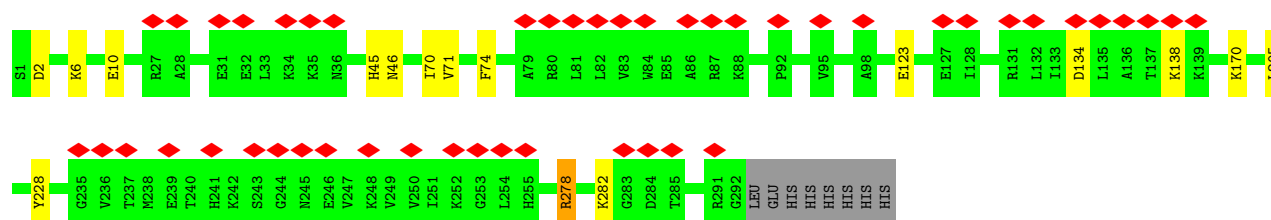
- Molecule 2: C3-A



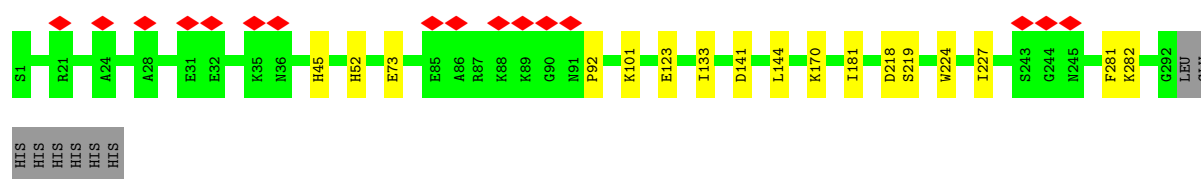
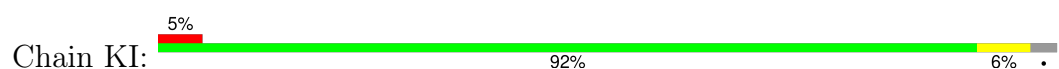
- Molecule 2: C3-A



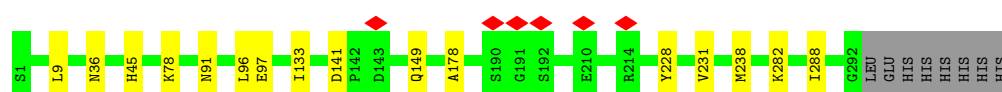
- Molecule 2: C3-A



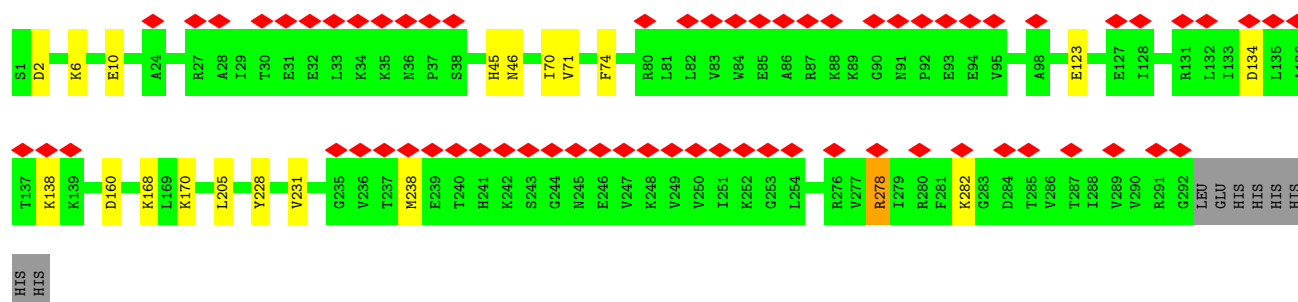
- Molecule 2: C3-A



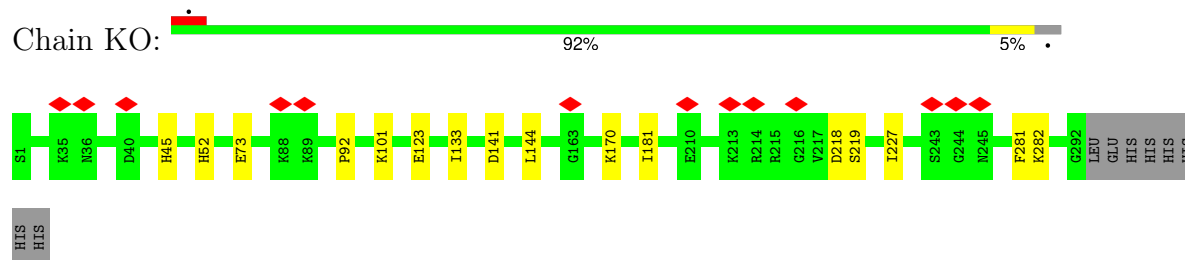
- Molecule 2: C3-A



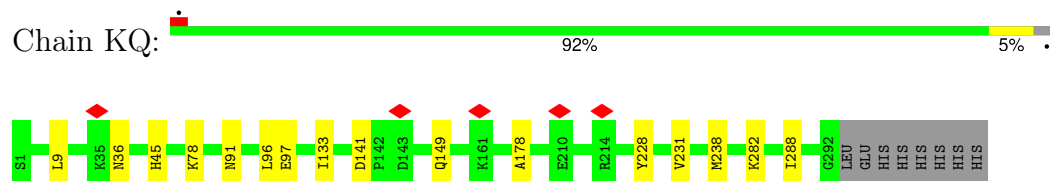
- Molecule 2: C3-A



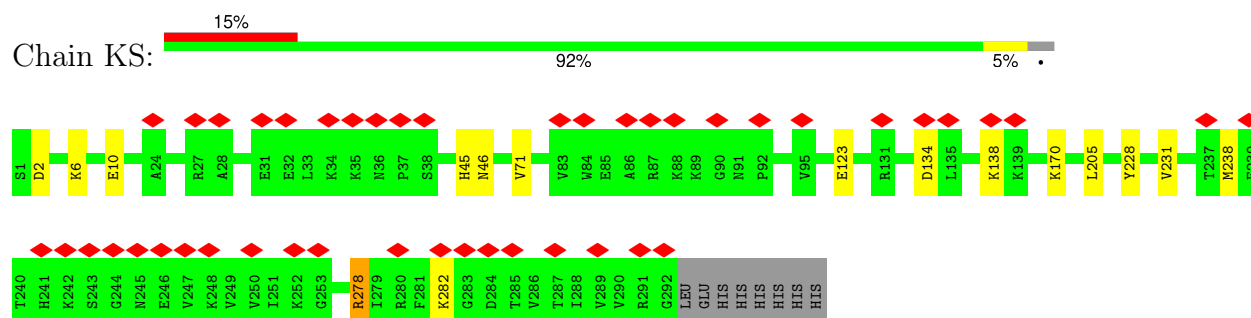
• Molecule 2: C3-A



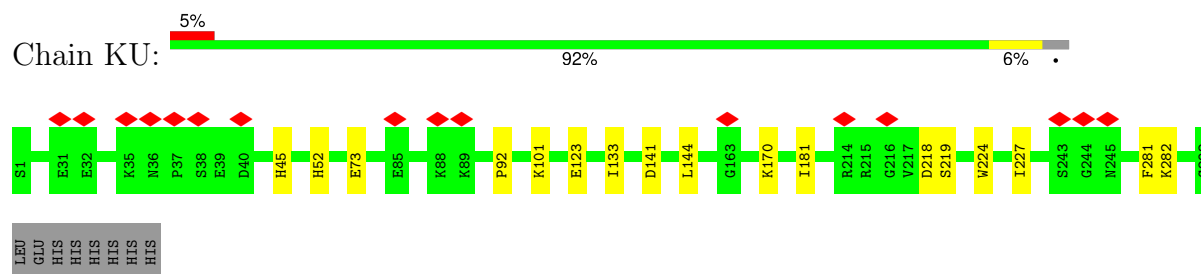
• Molecule 2: C3-A



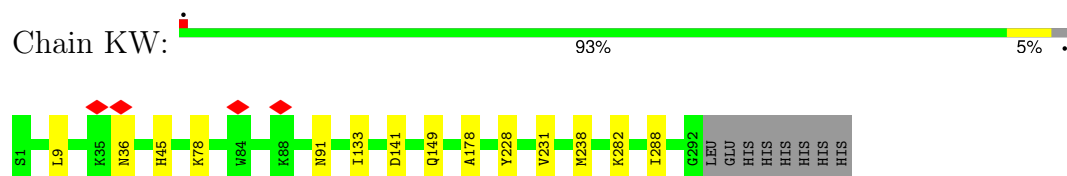
• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A





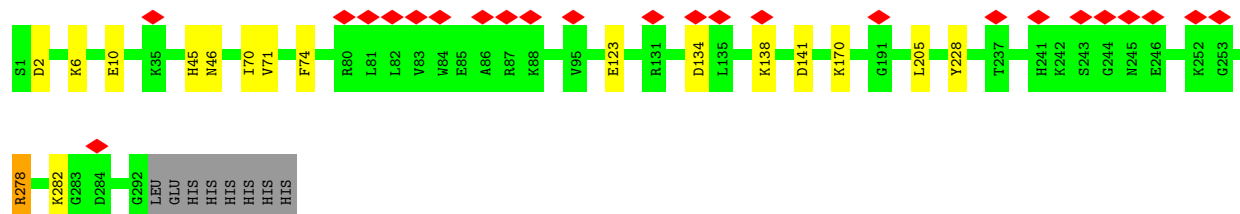
• Molecule 2: C3-A



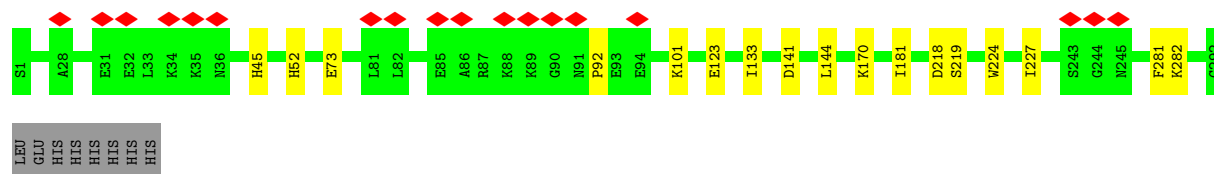
• Molecule 2: C3-A



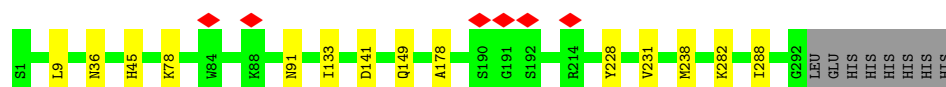
• Molecule 2: C3-A



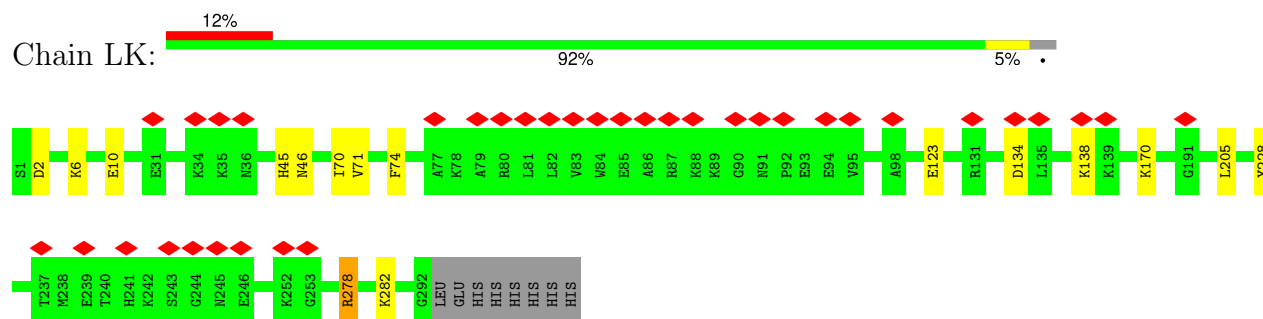
• Molecule 2: C3-A



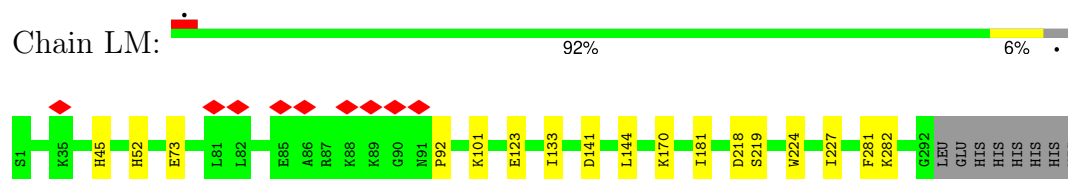
• Molecule 2: C3-A



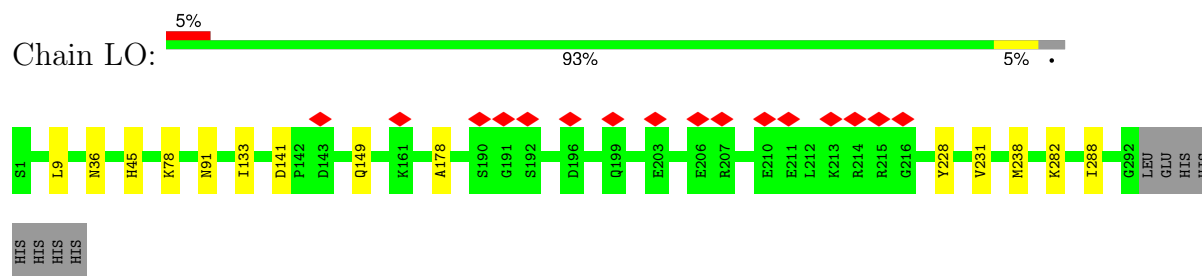
• Molecule 2: C3-A



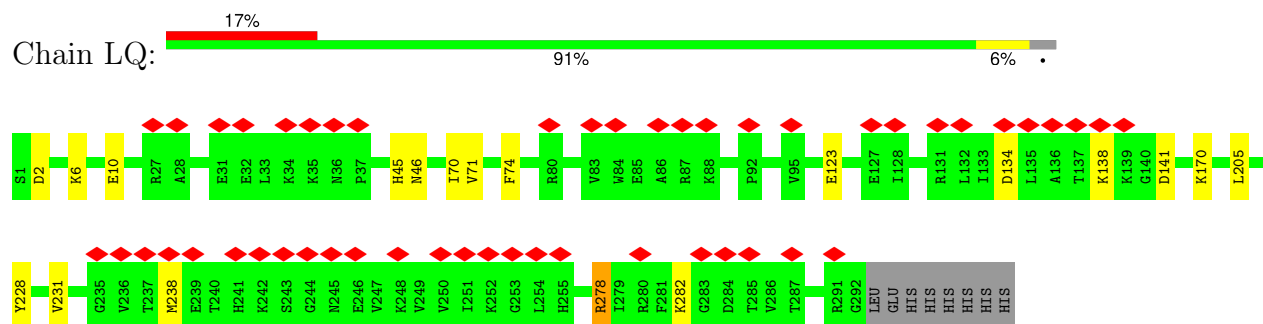
• Molecule 2: C3-A



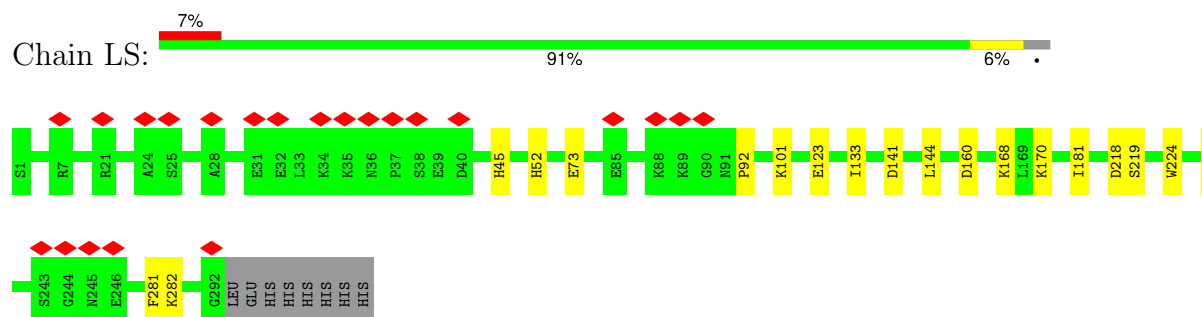
• Molecule 2: C3-A



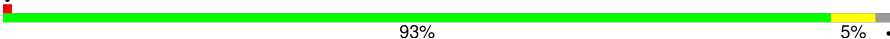
• Molecule 2: C3-A



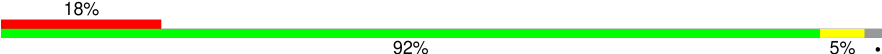
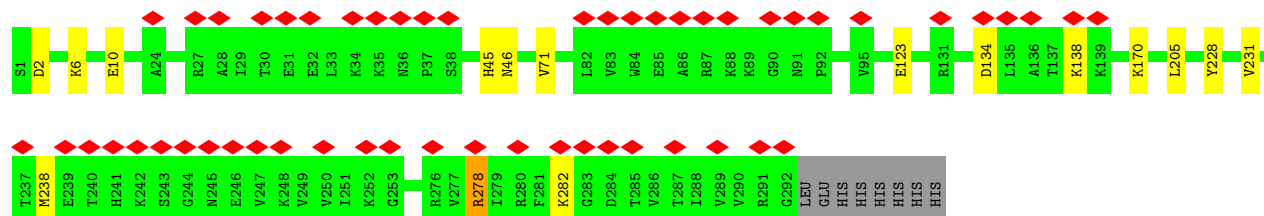
• Molecule 2: C3-A



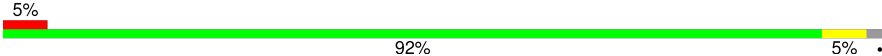
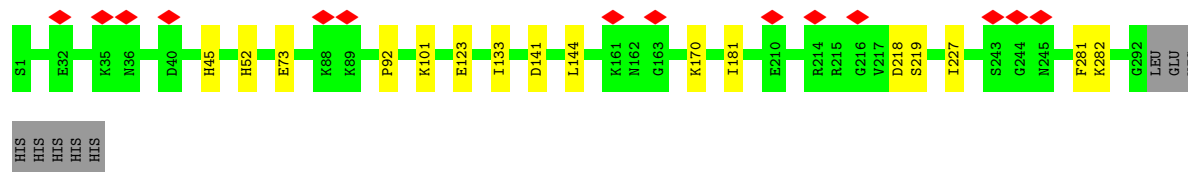
• Molecule 2: C3-A

Chain ZN:  93% 5% .

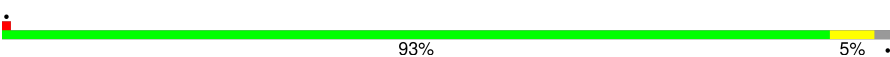
• Molecule 2: C3-A

Chain ZP:  18% 92% 5% .

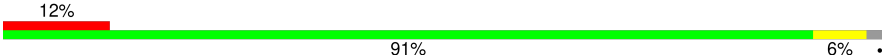
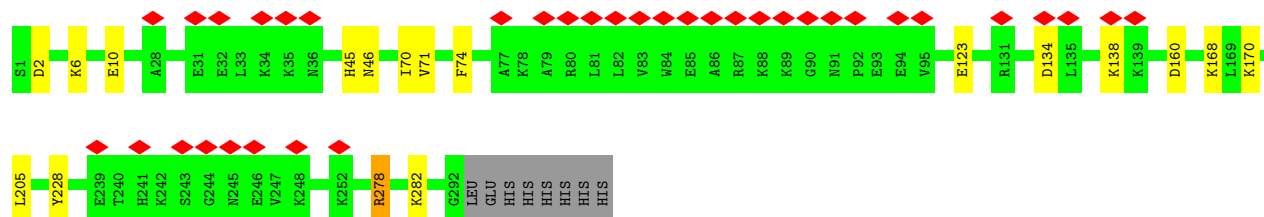
• Molecule 2: C3-A

Chain ZR:  5% 92% 5% .

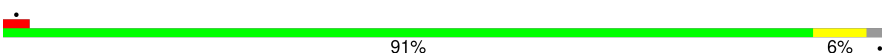
• Molecule 2: C3-A

Chain ZT:  93% 5% .

• Molecule 2: C3-A

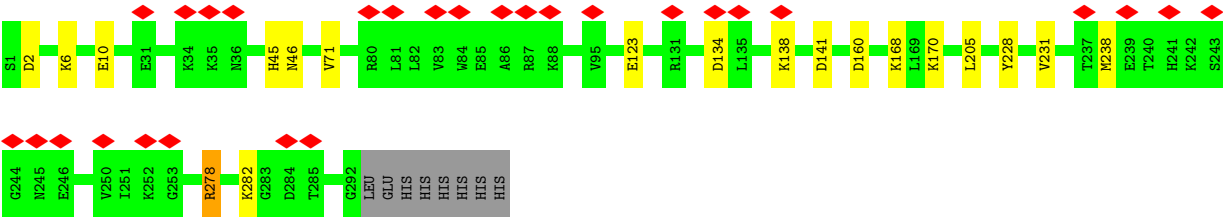
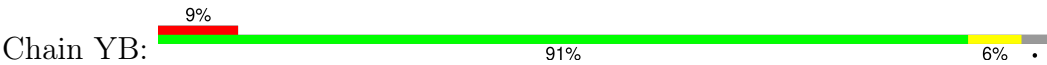
Chain ZV:  12% 91% 6% .

• Molecule 2: C3-A

Chain ZX:  91% 6% .



• Molecule 2: C3-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, I	Depositor
Number of subtomograms used	462	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	110	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	22000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4095.000	Depositor
Minimum map value	1.000	Depositor
Average map value	1211.762	Depositor
Map value standard deviation	264.152	Depositor
Recommended contour level	1854	Depositor
Map size (Å)	868.8, 868.8, 868.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.62, 3.62, 3.62	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	1.11	0/816	1.38	11/1106 (1.0%)
1	AC	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	AE	1.06	0/816	1.47	11/1106 (1.0%)
1	AG	1.11	0/816	1.38	11/1106 (1.0%)
1	AI	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	AK	1.06	0/816	1.47	11/1106 (1.0%)
1	AM	1.11	0/816	1.38	11/1106 (1.0%)
1	AP	1.06	0/816	1.47	11/1106 (1.0%)
1	AR	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	AS	1.11	0/816	1.38	11/1106 (1.0%)
1	AU	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	AW	1.06	0/816	1.47	11/1106 (1.0%)
1	AY	1.11	0/816	1.37	11/1106 (1.0%)
1	BA	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	BC	1.06	0/816	1.46	11/1106 (1.0%)
1	BE	1.11	0/816	1.38	11/1106 (1.0%)
1	BG	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	BI	1.06	0/816	1.47	11/1106 (1.0%)
1	BK	1.11	0/816	1.38	11/1106 (1.0%)
1	BM	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	BO	1.06	0/816	1.47	11/1106 (1.0%)
1	BQ	1.11	0/816	1.38	11/1106 (1.0%)
1	BS	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	BU	1.06	0/816	1.47	11/1106 (1.0%)
1	BW	1.11	0/816	1.38	11/1106 (1.0%)
1	BY	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	CA	1.06	0/816	1.47	11/1106 (1.0%)
1	CC	1.11	0/816	1.38	11/1106 (1.0%)
1	CE	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	CG	1.06	0/816	1.47	11/1106 (1.0%)
1	CI	1.11	0/816	1.37	11/1106 (1.0%)
1	CK	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	CM	1.06	0/816	1.46	11/1106 (1.0%)
1	CO	1.11	0/816	1.38	11/1106 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CQ	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	CS	1.06	0/816	1.47	11/1106 (1.0%)
1	CU	1.11	0/816	1.38	11/1106 (1.0%)
1	CW	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	CY	1.06	0/816	1.47	11/1106 (1.0%)
1	DA	1.11	0/816	1.37	11/1106 (1.0%)
1	DC	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	DE	1.06	0/816	1.47	11/1106 (1.0%)
1	DG	1.11	0/816	1.37	11/1106 (1.0%)
1	DI	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	DK	1.06	0/816	1.47	11/1106 (1.0%)
1	DM	1.11	0/816	1.38	11/1106 (1.0%)
1	DO	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	DQ	1.06	0/816	1.46	11/1106 (1.0%)
1	DS	1.11	0/816	1.37	11/1106 (1.0%)
1	DU	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	DX	1.06	0/816	1.47	11/1106 (1.0%)
1	DZ	1.11	0/816	1.37	11/1106 (1.0%)
1	EB	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	ED	1.06	0/816	1.47	11/1106 (1.0%)
1	EF	1.11	0/816	1.37	11/1106 (1.0%)
1	EH	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	EJ	1.06	0/816	1.47	11/1106 (1.0%)
1	EL	1.11	0/816	1.37	11/1106 (1.0%)
1	EN	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	EP	1.06	0/816	1.46	11/1106 (1.0%)
1	ER	1.11	0/816	1.38	11/1106 (1.0%)
1	ET	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	EV	1.06	0/816	1.47	11/1106 (1.0%)
1	EX	1.11	0/816	1.38	11/1106 (1.0%)
1	EZ	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	FB	1.06	0/816	1.47	11/1106 (1.0%)
1	FD	1.11	0/816	1.37	11/1106 (1.0%)
1	FF	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	FH	1.06	0/816	1.47	11/1106 (1.0%)
1	FJ	1.11	0/816	1.38	11/1106 (1.0%)
1	FL	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	FN	1.06	0/816	1.46	11/1106 (1.0%)
1	FP	1.11	0/816	1.37	11/1106 (1.0%)
1	FR	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	FT	1.06	0/816	1.47	11/1106 (1.0%)
1	FV	1.11	0/816	1.37	11/1106 (1.0%)
1	FX	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	FZ	1.06	0/816	1.47	11/1106 (1.0%)
1	GB	1.11	0/816	1.38	11/1106 (1.0%)
1	GD	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	GF	1.06	0/816	1.47	11/1106 (1.0%)
1	GH	1.11	0/816	1.37	11/1106 (1.0%)
1	GJ	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	GL	1.06	0/816	1.47	11/1106 (1.0%)
1	GN	1.11	0/816	1.37	11/1106 (1.0%)
1	GP	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	GR	1.06	0/816	1.47	11/1106 (1.0%)
1	GT	1.11	0/816	1.38	11/1106 (1.0%)
1	GV	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	GX	1.06	0/816	1.47	11/1106 (1.0%)
1	GZ	1.11	0/816	1.38	11/1106 (1.0%)
1	HB	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	HD	1.06	0/816	1.47	11/1106 (1.0%)
1	HG	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	HI	1.06	0/816	1.46	11/1106 (1.0%)
1	HL	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	HN	1.06	0/816	1.47	11/1106 (1.0%)
1	HP	1.11	0/816	1.38	11/1106 (1.0%)
1	HR	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	HT	1.06	0/816	1.47	11/1106 (1.0%)
1	HV	1.11	0/816	1.38	11/1106 (1.0%)
1	HX	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	HZ	1.06	0/816	1.47	11/1106 (1.0%)
1	IC	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	IE	1.06	0/816	1.47	11/1106 (1.0%)
1	IH	1.11	0/816	1.37	11/1106 (1.0%)
1	II	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	IK	1.06	0/816	1.47	11/1106 (1.0%)
1	IM	1.11	0/816	1.38	11/1106 (1.0%)
1	IO	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	IQ	1.06	0/816	1.47	11/1106 (1.0%)
1	IS	1.11	0/816	1.38	11/1106 (1.0%)
1	IU	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	IW	1.06	0/816	1.47	11/1106 (1.0%)
1	IY	1.11	0/816	1.38	11/1106 (1.0%)
1	JA	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	JC	1.06	0/816	1.47	11/1106 (1.0%)
1	JE	1.11	0/816	1.37	11/1106 (1.0%)
1	JG	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	JI	1.05	0/816	1.47	11/1106 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	JK	1.11	0/816	1.38	11/1106 (1.0%)
1	JM	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	JO	1.06	0/816	1.47	11/1106 (1.0%)
1	JQ	1.11	0/816	1.37	11/1106 (1.0%)
1	JS	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	JV	1.11	0/816	1.38	11/1106 (1.0%)
1	JX	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	JZ	1.06	0/816	1.47	11/1106 (1.0%)
1	KB	1.11	0/816	1.37	11/1106 (1.0%)
1	KD	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	KF	1.06	0/816	1.46	11/1106 (1.0%)
1	KH	1.11	0/816	1.38	11/1106 (1.0%)
1	KJ	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	KL	1.06	0/816	1.47	11/1106 (1.0%)
1	KN	1.11	0/816	1.37	11/1106 (1.0%)
1	KP	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	KR	1.06	0/816	1.47	11/1106 (1.0%)
1	KT	1.11	0/816	1.38	11/1106 (1.0%)
1	KV	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	KX	1.06	0/816	1.47	11/1106 (1.0%)
1	KZ	1.11	0/816	1.37	11/1106 (1.0%)
1	LB	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	LD	1.06	0/816	1.47	11/1106 (1.0%)
1	LF	1.11	0/816	1.38	11/1106 (1.0%)
1	LH	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	LJ	1.06	0/816	1.47	11/1106 (1.0%)
1	LL	1.11	0/816	1.37	11/1106 (1.0%)
1	LN	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	LP	1.06	0/816	1.47	11/1106 (1.0%)
1	LR	1.11	0/816	1.37	11/1106 (1.0%)
1	WA	1.11	0/816	1.38	11/1106 (1.0%)
1	WB	1.11	0/816	1.37	11/1106 (1.0%)
1	WC	1.11	0/816	1.37	11/1106 (1.0%)
1	WD	1.05	0/816	1.47	11/1106 (1.0%)
1	YA	1.06	0/816	1.47	11/1106 (1.0%)
1	YC	1.11	0/816	1.38	11/1106 (1.0%)
1	YE	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	YG	1.06	0/816	1.47	11/1106 (1.0%)
1	YI	1.11	0/816	1.37	11/1106 (1.0%)
1	YK	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	YM	1.05	0/816	1.47	11/1106 (1.0%)
1	YO	1.11	0/816	1.38	11/1106 (1.0%)
1	YQ	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	YS	1.05	0/816	1.47	11/1106 (1.0%)
1	YU	1.11	0/816	1.38	11/1106 (1.0%)
1	YW	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	YY	1.06	0/816	1.47	11/1106 (1.0%)
1	ZA	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	ZC	1.06	0/816	1.47	11/1106 (1.0%)
1	ZE	1.11	0/816	1.38	11/1106 (1.0%)
1	ZG	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	ZI	1.06	0/816	1.46	11/1106 (1.0%)
1	ZK	1.11	0/816	1.38	11/1106 (1.0%)
1	ZM	1.05	1/816 (0.1%)	1.39	9/1106 (0.8%)
1	ZO	1.06	0/816	1.47	11/1106 (1.0%)
1	ZQ	1.11	0/816	1.38	11/1106 (1.0%)
1	ZS	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
1	ZU	1.06	0/816	1.47	11/1106 (1.0%)
1	ZW	1.11	0/816	1.38	11/1106 (1.0%)
1	ZY	1.05	1/816 (0.1%)	1.39	11/1106 (1.0%)
2	AB	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	AD	0.94	0/2283	1.09	9/3073 (0.3%)
2	AF	0.98	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	AH	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	AJ	0.94	0/2283	1.09	9/3073 (0.3%)
2	AL	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	AN	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	AO	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	AQ	0.94	0/2283	1.09	9/3073 (0.3%)
2	AT	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	AV	0.95	0/2283	1.09	9/3073 (0.3%)
2	AX	0.98	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	AZ	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	BB	0.94	0/2283	1.09	9/3073 (0.3%)
2	BD	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	BF	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	BH	0.95	0/2283	1.09	9/3073 (0.3%)
2	BJ	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	BL	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	BN	0.94	0/2283	1.09	9/3073 (0.3%)
2	BP	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	BR	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	BT	0.94	0/2283	1.09	9/3073 (0.3%)
2	BV	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	BX	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	BZ	0.94	0/2283	1.09	9/3073 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	CB	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	CD	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	CF	0.94	0/2283	1.09	9/3073 (0.3%)
2	CH	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	CJ	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	CL	0.94	0/2283	1.09	9/3073 (0.3%)
2	CN	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	CP	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	CR	0.94	0/2283	1.09	9/3073 (0.3%)
2	CT	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	CV	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	CX	0.94	0/2283	1.09	9/3073 (0.3%)
2	CZ	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	DB	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	DD	0.94	0/2283	1.09	9/3073 (0.3%)
2	DF	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	DH	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	DJ	0.94	0/2283	1.09	9/3073 (0.3%)
2	DL	0.98	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	DN	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	DP	0.94	0/2283	1.09	9/3073 (0.3%)
2	DR	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	DT	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	DW	0.94	0/2283	1.09	9/3073 (0.3%)
2	DY	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	EA	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	EC	0.94	0/2283	1.09	9/3073 (0.3%)
2	EE	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	EG	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	EI	0.94	0/2283	1.09	9/3073 (0.3%)
2	EK	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	EM	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	EO	0.94	0/2283	1.09	9/3073 (0.3%)
2	EQ	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	ES	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	EU	0.94	0/2283	1.09	9/3073 (0.3%)
2	EW	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	EY	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	FA	0.94	0/2283	1.09	9/3073 (0.3%)
2	FC	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	FE	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	FG	0.94	0/2283	1.09	9/3073 (0.3%)
2	FI	0.98	2/2283 (0.1%)	1.07	4/3073 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	FK	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	FM	0.94	0/2283	1.09	9/3073 (0.3%)
2	FO	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	FQ	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	FS	0.95	0/2283	1.09	9/3073 (0.3%)
2	FU	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	FW	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	FY	0.95	0/2283	1.09	9/3073 (0.3%)
2	GA	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	GC	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	GE	0.94	0/2283	1.09	9/3073 (0.3%)
2	GG	0.98	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	GI	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	GK	0.94	0/2283	1.09	9/3073 (0.3%)
2	GM	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	GO	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	GQ	0.94	0/2283	1.09	9/3073 (0.3%)
2	GS	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	GU	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	GW	0.94	0/2283	1.09	9/3073 (0.3%)
2	GY	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	HA	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	HC	0.95	0/2283	1.09	9/3073 (0.3%)
2	HE	0.98	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	HF	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	HH	0.94	0/2283	1.09	9/3073 (0.3%)
2	HJ	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	HK	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	HM	0.94	0/2283	1.09	9/3073 (0.3%)
2	HO	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	HQ	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	HS	0.94	0/2283	1.09	9/3073 (0.3%)
2	HU	0.98	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	HW	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	HY	0.94	0/2283	1.09	9/3073 (0.3%)
2	IA	0.98	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	IB	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	ID	0.95	0/2283	1.09	9/3073 (0.3%)
2	IF	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	IG	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	IJ	0.95	0/2283	1.09	9/3073 (0.3%)
2	IL	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	IN	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	IP	0.94	0/2283	1.09	9/3073 (0.3%)
2	IR	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	IT	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	IV	0.94	0/2283	1.09	9/3073 (0.3%)
2	IX	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	IZ	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	JB	0.95	0/2283	1.09	9/3073 (0.3%)
2	JD	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	JF	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	JH	0.94	0/2283	1.09	9/3073 (0.3%)
2	JJ	0.98	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	JL	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	JN	0.94	0/2283	1.09	9/3073 (0.3%)
2	JP	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	JR	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	JT	0.94	0/2283	1.09	9/3073 (0.3%)
2	JU	0.98	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	JW	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	JY	0.94	0/2283	1.09	9/3073 (0.3%)
2	KA	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	KC	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	KE	0.94	0/2283	1.09	9/3073 (0.3%)
2	KG	0.98	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	KI	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	KK	0.94	0/2283	1.09	9/3073 (0.3%)
2	KM	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	KO	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	KQ	0.94	0/2283	1.09	9/3073 (0.3%)
2	KS	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	KU	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	KW	0.95	0/2283	1.09	9/3073 (0.3%)
2	KY	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	LA	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	LC	0.94	0/2283	1.09	9/3073 (0.3%)
2	LE	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	LG	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	LI	0.94	0/2283	1.09	9/3073 (0.3%)
2	LK	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	LM	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	LO	0.94	0/2283	1.09	9/3073 (0.3%)
2	LQ	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	LS	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	YB	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	YD	1.00	2/2283 (0.1%)	1.08	3/3073 (0.1%)
2	YF	0.94	0/2283	1.09	9/3073 (0.3%)
2	YH	0.99	2/2283 (0.1%)	1.07	4/3073 (0.1%)
2	YJ	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	YL	0.94	0/2283	1.09	9/3073 (0.3%)
2	YN	0.98	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	YP	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	YR	0.94	0/2283	1.09	9/3073 (0.3%)
2	YT	0.98	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	YV	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	YX	0.94	0/2283	1.09	9/3073 (0.3%)
2	YZ	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	ZB	0.94	0/2283	1.09	9/3073 (0.3%)
2	ZD	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	ZF	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	ZH	0.94	0/2283	1.09	9/3073 (0.3%)
2	ZJ	0.98	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	ZL	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	ZN	0.94	0/2283	1.09	9/3073 (0.3%)
2	ZP	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	ZR	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	ZT	0.94	0/2283	1.09	9/3073 (0.3%)
2	ZV	0.99	2/2283 (0.1%)	1.07	2/3073 (0.1%)
2	ZX	1.00	2/2283 (0.1%)	1.07	3/3073 (0.1%)
2	ZZ	0.95	0/2283	1.09	9/3073 (0.3%)
All	All	1.00	300/557820 (0.1%)	1.18	2832/752220 (0.4%)

All (300) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CW	1	PRO	N-CD	-8.01	1.36	1.47
1	EH	1	PRO	N-CD	-8.01	1.36	1.47
1	AC	1	PRO	N-CD	-7.98	1.36	1.47
1	HR	1	PRO	N-CD	-7.98	1.36	1.47
1	BA	1	PRO	N-CD	-7.98	1.36	1.47
1	HG	1	PRO	N-CD	-7.98	1.36	1.47
1	YK	1	PRO	N-CD	-7.97	1.36	1.47
1	JS	1	PRO	N-CD	-7.97	1.36	1.47
1	KJ	1	PRO	N-CD	-7.97	1.36	1.47
1	LH	1	PRO	N-CD	-7.97	1.36	1.47
1	ZG	1	PRO	N-CD	-7.97	1.36	1.47
1	KD	1	PRO	N-CD	-7.97	1.36	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	ZY	1	PRO	N-CD	-7.97	1.36	1.47
1	BG	1	PRO	N-CD	-7.97	1.36	1.47
1	DO	1	PRO	N-CD	-7.96	1.36	1.47
1	FL	1	PRO	N-CD	-7.96	1.36	1.47
1	CE	1	PRO	N-CD	-7.96	1.36	1.47
1	EB	1	PRO	N-CD	-7.96	1.36	1.47
1	IU	1	PRO	N-CD	-7.96	1.36	1.47
1	KP	1	PRO	N-CD	-7.96	1.36	1.47
1	ZA	1	PRO	N-CD	-7.95	1.36	1.47
1	AI	1	PRO	N-CD	-7.95	1.36	1.47
1	DC	1	PRO	N-CD	-7.95	1.36	1.47
1	GJ	1	PRO	N-CD	-7.95	1.36	1.47
1	JX	1	PRO	N-CD	-7.95	1.36	1.47
1	LN	1	PRO	N-CD	-7.95	1.36	1.47
1	BY	1	PRO	N-CD	-7.94	1.36	1.47
1	ET	1	PRO	N-CD	-7.94	1.36	1.47
1	JA	1	PRO	N-CD	-7.94	1.36	1.47
1	KV	1	PRO	N-CD	-7.94	1.36	1.47
1	BS	1	PRO	N-CD	-7.94	1.36	1.47
1	DU	1	PRO	N-CD	-7.94	1.36	1.47
1	EZ	1	PRO	N-CD	-7.94	1.36	1.47
1	ZS	1	PRO	N-CD	-7.94	1.36	1.47
1	CK	1	PRO	N-CD	-7.94	1.36	1.47
1	EN	1	PRO	N-CD	-7.94	1.36	1.47
1	FX	1	PRO	N-CD	-7.94	1.36	1.47
1	II	1	PRO	N-CD	-7.94	1.36	1.47
1	DI	1	PRO	N-CD	-7.93	1.36	1.47
1	FF	1	PRO	N-CD	-7.93	1.36	1.47
1	YE	1	PRO	N-CD	-7.93	1.36	1.47
1	YQ	1	PRO	N-CD	-7.93	1.36	1.47
1	GD	1	PRO	N-CD	-7.93	1.36	1.47
1	HX	1	PRO	N-CD	-7.93	1.36	1.47
1	JG	1	PRO	N-CD	-7.93	1.36	1.47
1	JM	1	PRO	N-CD	-7.93	1.36	1.47
1	YW	1	PRO	N-CD	-7.93	1.36	1.47
1	HL	1	PRO	N-CD	-7.93	1.36	1.47
1	AU	1	PRO	N-CD	-7.92	1.36	1.47
1	HB	1	PRO	N-CD	-7.92	1.36	1.47
1	AR	1	PRO	N-CD	-7.91	1.36	1.47
1	GV	1	PRO	N-CD	-7.91	1.36	1.47
1	FR	1	PRO	N-CD	-7.91	1.36	1.47
1	IC	1	PRO	N-CD	-7.91	1.36	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	IO	1	PRO	N-CD	-7.90	1.36	1.47
1	LB	1	PRO	N-CD	-7.90	1.36	1.47
1	BM	1	PRO	N-CD	-7.89	1.36	1.47
1	CQ	1	PRO	N-CD	-7.89	1.36	1.47
1	GP	1	PRO	N-CD	-7.89	1.36	1.47
1	ZM	1	PRO	N-CD	-7.89	1.36	1.47
2	AH	45	HIS	CB-CG	-6.75	1.40	1.50
2	HW	45	HIS	CB-CG	-6.75	1.40	1.50
2	YP	45	HIS	CB-CG	-6.75	1.40	1.50
2	JW	45	HIS	CB-CG	-6.75	1.40	1.50
2	GI	45	HIS	CB-CG	-6.74	1.40	1.50
2	IB	45	HIS	CB-CG	-6.74	1.40	1.50
2	ZL	45	HIS	CB-CG	-6.73	1.40	1.50
2	KI	45	HIS	CB-CG	-6.73	1.40	1.50
2	YD	45	HIS	CB-CG	-6.73	1.40	1.50
2	BL	45	HIS	CB-CG	-6.73	1.40	1.50
2	CJ	45	HIS	CB-CG	-6.72	1.40	1.50
2	EG	45	HIS	CB-CG	-6.72	1.40	1.50
2	IT	45	HIS	CB-CG	-6.72	1.40	1.50
2	LG	45	HIS	CB-CG	-6.72	1.40	1.50
2	CD	45	HIS	CB-CG	-6.71	1.40	1.50
2	CP	45	HIS	CB-CG	-6.71	1.40	1.50
2	ES	45	HIS	CB-CG	-6.71	1.40	1.50
2	EY	45	HIS	CB-CG	-6.71	1.40	1.50
2	AN	45	HIS	CB-CG	-6.71	1.40	1.50
2	AZ	45	HIS	CB-CG	-6.71	1.40	1.50
2	ZF	45	HIS	CB-CG	-6.71	1.40	1.50
2	HF	45	HIS	CB-CG	-6.71	1.40	1.50
2	BF	45	HIS	CB-CG	-6.71	1.40	1.50
2	DN	45	HIS	CB-CG	-6.71	1.40	1.50
2	EA	45	HIS	CB-CG	-6.71	1.40	1.50
2	FE	45	HIS	CB-CG	-6.71	1.40	1.50
2	FK	45	HIS	CB-CG	-6.71	1.40	1.50
2	FW	45	HIS	CB-CG	-6.71	1.40	1.50
2	HK	45	HIS	CB-CG	-6.71	1.40	1.50
2	IG	45	HIS	CB-CG	-6.71	1.40	1.50
2	DH	45	HIS	CB-CG	-6.71	1.40	1.50
2	DT	45	HIS	CB-CG	-6.71	1.40	1.50
2	FQ	45	HIS	CB-CG	-6.71	1.40	1.50
2	GO	45	HIS	CB-CG	-6.71	1.40	1.50
2	IZ	45	HIS	CB-CG	-6.71	1.40	1.50
2	KU	45	HIS	CB-CG	-6.71	1.40	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	KC	45	HIS	CB-CG	-6.71	1.40	1.50
2	LS	45	HIS	CB-CG	-6.71	1.40	1.50
2	BX	45	HIS	CB-CG	-6.70	1.40	1.50
2	ZX	45	HIS	CB-CG	-6.70	1.40	1.50
2	DB	45	HIS	CB-CG	-6.70	1.40	1.50
2	EM	45	HIS	CB-CG	-6.70	1.40	1.50
2	BR	45	HIS	CB-CG	-6.69	1.40	1.50
2	JF	45	HIS	CB-CG	-6.69	1.40	1.50
2	LA	45	HIS	CB-CG	-6.69	1.40	1.50
2	ZR	45	HIS	CB-CG	-6.69	1.40	1.50
2	CV	45	HIS	CB-CG	-6.69	1.40	1.50
2	GU	45	HIS	CB-CG	-6.69	1.40	1.50
2	GC	45	HIS	CB-CG	-6.69	1.40	1.50
2	IN	45	HIS	CB-CG	-6.69	1.40	1.50
2	KO	45	HIS	CB-CG	-6.69	1.40	1.50
2	LM	45	HIS	CB-CG	-6.69	1.40	1.50
2	YV	45	HIS	CB-CG	-6.68	1.40	1.50
2	JL	45	HIS	CB-CG	-6.68	1.40	1.50
2	AT	45	HIS	CB-CG	-6.68	1.40	1.50
2	HA	45	HIS	CB-CG	-6.68	1.40	1.50
2	YJ	45	HIS	CB-CG	-6.66	1.40	1.50
2	JR	45	HIS	CB-CG	-6.66	1.40	1.50
2	AB	45	HIS	CB-CG	-6.65	1.40	1.50
2	HQ	45	HIS	CB-CG	-6.65	1.40	1.50
2	DL	205	LEU	CB-CG	5.45	1.64	1.53
2	FI	205	LEU	CB-CG	5.45	1.64	1.53
2	KA	205	LEU	CB-CG	5.45	1.64	1.53
2	LQ	205	LEU	CB-CG	5.45	1.64	1.53
2	GA	205	LEU	CB-CG	5.44	1.64	1.53
2	IL	205	LEU	CB-CG	5.44	1.64	1.53
2	YT	205	LEU	CB-CG	5.44	1.64	1.53
2	JJ	205	LEU	CB-CG	5.44	1.64	1.53
2	IX	205	LEU	CB-CG	5.44	1.64	1.53
2	KS	205	LEU	CB-CG	5.44	1.64	1.53
2	AX	205	LEU	CB-CG	5.43	1.64	1.53
2	CH	205	LEU	CB-CG	5.43	1.64	1.53
2	EE	205	LEU	CB-CG	5.43	1.64	1.53
2	HE	205	LEU	CB-CG	5.43	1.64	1.53
2	JD	205	LEU	CB-CG	5.42	1.64	1.53
2	KY	205	LEU	CB-CG	5.42	1.64	1.53
2	AF	205	LEU	CB-CG	5.42	1.64	1.53
2	HU	205	LEU	CB-CG	5.42	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AL	205	LEU	CB-CG	5.42	1.64	1.53
2	ZD	205	LEU	CB-CG	5.42	1.64	1.53
2	AO	205	LEU	CB-CG	5.42	1.64	1.53
2	CB	205	LEU	CB-CG	5.42	1.64	1.53
2	EW	205	LEU	CB-CG	5.42	1.64	1.53
2	GY	205	LEU	CB-CG	5.42	1.64	1.53
2	CT	205	LEU	CB-CG	5.41	1.64	1.53
2	CZ	205	LEU	CB-CG	5.41	1.64	1.53
2	DY	205	LEU	CB-CG	5.41	1.64	1.53
2	EK	205	LEU	CB-CG	5.41	1.64	1.53
2	FC	205	LEU	CB-CG	5.41	1.64	1.53
2	GS	205	LEU	CB-CG	5.41	1.64	1.53
2	GG	205	LEU	CB-CG	5.41	1.64	1.53
2	IA	205	LEU	CB-CG	5.41	1.64	1.53
2	BV	205	LEU	CB-CG	5.41	1.64	1.53
2	DF	205	LEU	CB-CG	5.41	1.64	1.53
2	GM	205	LEU	CB-CG	5.41	1.64	1.53
2	ZV	205	LEU	CB-CG	5.41	1.64	1.53
2	BD	205	LEU	CB-CG	5.40	1.64	1.53
2	BJ	205	LEU	CB-CG	5.40	1.64	1.53
2	HJ	205	LEU	CB-CG	5.40	1.64	1.53
2	YB	205	LEU	CB-CG	5.40	1.64	1.53
2	YH	205	LEU	CB-CG	5.40	1.64	1.53
2	YZ	205	LEU	CB-CG	5.40	1.64	1.53
2	CN	205	LEU	CB-CG	5.40	1.64	1.53
2	EQ	205	LEU	CB-CG	5.40	1.64	1.53
2	HO	205	LEU	CB-CG	5.40	1.64	1.53
2	IR	205	LEU	CB-CG	5.40	1.64	1.53
2	JP	205	LEU	CB-CG	5.40	1.64	1.53
2	LE	205	LEU	CB-CG	5.40	1.64	1.53
2	FU	205	LEU	CB-CG	5.40	1.64	1.53
2	IF	205	LEU	CB-CG	5.40	1.64	1.53
2	DR	205	LEU	CB-CG	5.40	1.64	1.53
2	FO	205	LEU	CB-CG	5.40	1.64	1.53
2	KM	205	LEU	CB-CG	5.40	1.64	1.53
2	LK	205	LEU	CB-CG	5.40	1.64	1.53
2	YN	205	LEU	CB-CG	5.39	1.64	1.53
2	JU	205	LEU	CB-CG	5.39	1.64	1.53
2	ZJ	205	LEU	CB-CG	5.38	1.64	1.53
2	KG	205	LEU	CB-CG	5.38	1.64	1.53
2	BP	205	LEU	CB-CG	5.37	1.64	1.53
2	ZP	205	LEU	CB-CG	5.37	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DT	52	HIS	CB-CG	-5.23	1.42	1.50
2	FQ	52	HIS	CB-CG	-5.23	1.42	1.50
2	IZ	52	HIS	CB-CG	-5.21	1.42	1.50
2	KU	52	HIS	CB-CG	-5.21	1.42	1.50
2	FW	52	HIS	CB-CG	-5.21	1.42	1.50
2	IG	52	HIS	CB-CG	-5.21	1.42	1.50
2	GI	52	HIS	CB-CG	-5.21	1.42	1.50
2	IB	52	HIS	CB-CG	-5.21	1.42	1.50
2	YD	52	HIS	CB-CG	-5.21	1.42	1.50
2	BL	52	HIS	CB-CG	-5.21	1.42	1.50
2	CJ	52	HIS	CB-CG	-5.20	1.42	1.50
2	CT	45	HIS	CB-CG	-5.20	1.42	1.50
2	EG	52	HIS	CB-CG	-5.20	1.42	1.50
2	GS	45	HIS	CB-CG	-5.20	1.42	1.50
2	KO	52	HIS	CB-CG	-5.20	1.42	1.50
2	LM	52	HIS	CB-CG	-5.20	1.42	1.50
2	CZ	45	HIS	CB-CG	-5.19	1.42	1.50
2	EK	45	HIS	CB-CG	-5.19	1.42	1.50
2	CV	52	HIS	CB-CG	-5.19	1.42	1.50
2	GU	52	HIS	CB-CG	-5.19	1.42	1.50
2	GC	52	HIS	CB-CG	-5.18	1.42	1.50
2	IN	52	HIS	CB-CG	-5.18	1.42	1.50
2	BX	52	HIS	CB-CG	-5.18	1.43	1.50
2	IT	52	HIS	CB-CG	-5.18	1.43	1.50
2	IX	45	HIS	CB-CG	-5.18	1.43	1.50
2	KS	45	HIS	CB-CG	-5.18	1.43	1.50
2	LG	52	HIS	CB-CG	-5.18	1.43	1.50
2	ZX	52	HIS	CB-CG	-5.18	1.43	1.50
2	YT	45	HIS	CB-CG	-5.17	1.43	1.50
2	JJ	45	HIS	CB-CG	-5.17	1.43	1.50
2	DB	52	HIS	CB-CG	-5.17	1.43	1.50
2	EM	52	HIS	CB-CG	-5.17	1.43	1.50
2	BR	52	HIS	CB-CG	-5.17	1.43	1.50
2	ZR	52	HIS	CB-CG	-5.17	1.43	1.50
2	YH	45	HIS	CB-CG	-5.17	1.43	1.50
2	YJ	52	HIS	CB-CG	-5.17	1.43	1.50
2	JP	45	HIS	CB-CG	-5.17	1.43	1.50
2	JR	52	HIS	CB-CG	-5.17	1.43	1.50
2	ZL	52	HIS	CB-CG	-5.16	1.43	1.50
2	KI	52	HIS	CB-CG	-5.16	1.43	1.50
2	AZ	52	HIS	CB-CG	-5.16	1.43	1.50
2	DY	45	HIS	CB-CG	-5.16	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	FC	45	HIS	CB-CG	-5.16	1.43	1.50
2	GA	45	HIS	CB-CG	-5.16	1.43	1.50
2	HF	52	HIS	CB-CG	-5.16	1.43	1.50
2	IL	45	HIS	CB-CG	-5.16	1.43	1.50
2	FU	45	HIS	CB-CG	-5.16	1.43	1.50
2	IF	45	HIS	CB-CG	-5.16	1.43	1.50
2	KC	52	HIS	CB-CG	-5.16	1.43	1.50
2	LS	52	HIS	CB-CG	-5.16	1.43	1.50
2	AN	52	HIS	CB-CG	-5.15	1.43	1.50
2	ZF	52	HIS	CB-CG	-5.15	1.43	1.50
2	DR	45	HIS	CB-CG	-5.15	1.43	1.50
2	EA	52	HIS	CB-CG	-5.15	1.43	1.50
2	FE	52	HIS	CB-CG	-5.15	1.43	1.50
2	FO	45	HIS	CB-CG	-5.15	1.43	1.50
2	DH	52	HIS	CB-CG	-5.15	1.43	1.50
2	GO	52	HIS	CB-CG	-5.15	1.43	1.50
2	BV	45	HIS	CB-CG	-5.15	1.43	1.50
2	CH	45	HIS	CB-CG	-5.15	1.43	1.50
2	EE	45	HIS	CB-CG	-5.15	1.43	1.50
2	ZV	45	HIS	CB-CG	-5.15	1.43	1.50
2	AX	45	HIS	CB-CG	-5.15	1.43	1.50
2	HE	45	HIS	CB-CG	-5.15	1.43	1.50
2	KM	45	HIS	CB-CG	-5.15	1.43	1.50
2	LK	45	HIS	CB-CG	-5.15	1.43	1.50
2	AL	45	HIS	CB-CG	-5.14	1.43	1.50
2	ZD	45	HIS	CB-CG	-5.14	1.43	1.50
2	CD	52	HIS	CB-CG	-5.14	1.43	1.50
2	EY	52	HIS	CB-CG	-5.14	1.43	1.50
2	ZJ	45	HIS	CB-CG	-5.14	1.43	1.50
2	IR	45	HIS	CB-CG	-5.14	1.43	1.50
2	JD	45	HIS	CB-CG	-5.14	1.43	1.50
2	KG	45	HIS	CB-CG	-5.14	1.43	1.50
2	KY	45	HIS	CB-CG	-5.14	1.43	1.50
2	LE	45	HIS	CB-CG	-5.14	1.43	1.50
2	JF	52	HIS	CB-CG	-5.13	1.43	1.50
2	LA	52	HIS	CB-CG	-5.13	1.43	1.50
2	AH	52	HIS	CB-CG	-5.13	1.43	1.50
2	BF	52	HIS	CB-CG	-5.13	1.43	1.50
2	BJ	45	HIS	CB-CG	-5.13	1.43	1.50
2	HK	52	HIS	CB-CG	-5.13	1.43	1.50
2	HW	52	HIS	CB-CG	-5.13	1.43	1.50
2	YB	45	HIS	CB-CG	-5.13	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CN	45	HIS	CB-CG	-5.13	1.43	1.50
2	EQ	45	HIS	CB-CG	-5.13	1.43	1.50
2	BD	45	HIS	CB-CG	-5.13	1.43	1.50
2	HJ	45	HIS	CB-CG	-5.13	1.43	1.50
2	YZ	45	HIS	CB-CG	-5.12	1.43	1.50
2	CP	52	HIS	CB-CG	-5.12	1.43	1.50
2	ES	52	HIS	CB-CG	-5.12	1.43	1.50
2	HO	45	HIS	CB-CG	-5.12	1.43	1.50
2	DL	45	HIS	CB-CG	-5.11	1.43	1.50
2	FI	45	HIS	CB-CG	-5.11	1.43	1.50
2	BP	45	HIS	CB-CG	-5.11	1.43	1.50
2	KA	45	HIS	CB-CG	-5.11	1.43	1.50
2	LQ	45	HIS	CB-CG	-5.11	1.43	1.50
2	ZP	45	HIS	CB-CG	-5.11	1.43	1.50
2	YP	52	HIS	CB-CG	-5.11	1.43	1.50
2	JW	52	HIS	CB-CG	-5.11	1.43	1.50
2	AT	52	HIS	CB-CG	-5.10	1.43	1.50
2	GG	45	HIS	CB-CG	-5.10	1.43	1.50
2	HA	52	HIS	CB-CG	-5.10	1.43	1.50
2	IA	45	HIS	CB-CG	-5.10	1.43	1.50
2	DF	45	HIS	CB-CG	-5.10	1.43	1.50
2	GM	45	HIS	CB-CG	-5.10	1.43	1.50
2	AB	52	HIS	CB-CG	-5.10	1.43	1.50
2	HQ	52	HIS	CB-CG	-5.10	1.43	1.50
2	YV	52	HIS	CB-CG	-5.09	1.43	1.50
2	JL	52	HIS	CB-CG	-5.09	1.43	1.50
2	YN	45	HIS	CB-CG	-5.09	1.43	1.50
2	JU	45	HIS	CB-CG	-5.09	1.43	1.50
2	CB	45	HIS	CB-CG	-5.09	1.43	1.50
2	EW	45	HIS	CB-CG	-5.09	1.43	1.50
2	AF	45	HIS	CB-CG	-5.08	1.43	1.50
2	DN	52	HIS	CB-CG	-5.08	1.43	1.50
2	FK	52	HIS	CB-CG	-5.08	1.43	1.50
2	HU	45	HIS	CB-CG	-5.08	1.43	1.50
2	AO	45	HIS	CB-CG	-5.06	1.43	1.50
2	GY	45	HIS	CB-CG	-5.06	1.43	1.50

All (2832) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CY	48	GLY	CA-C-N	9.89	129.95	119.76
1	CY	48	GLY	C-N-CA	9.89	129.95	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EJ	48	GLY	CA-C-N	9.89	129.95	119.76
1	EJ	48	GLY	C-N-CA	9.89	129.95	119.76
1	BO	48	GLY	CA-C-N	9.87	129.92	119.76
1	BO	48	GLY	C-N-CA	9.87	129.92	119.76
1	ZO	48	GLY	CA-C-N	9.87	129.92	119.76
1	ZO	48	GLY	C-N-CA	9.87	129.92	119.76
1	IQ	48	GLY	CA-C-N	9.86	129.92	119.76
1	IQ	48	GLY	C-N-CA	9.86	129.92	119.76
1	LD	48	GLY	CA-C-N	9.86	129.92	119.76
1	LD	48	GLY	C-N-CA	9.86	129.92	119.76
1	CA	48	GLY	CA-C-N	9.86	129.91	119.76
1	CA	48	GLY	C-N-CA	9.86	129.91	119.76
1	EV	48	GLY	CA-C-N	9.86	129.91	119.76
1	EV	48	GLY	C-N-CA	9.86	129.91	119.76
1	AE	48	GLY	CA-C-N	9.86	129.91	119.76
1	AE	48	GLY	C-N-CA	9.86	129.91	119.76
1	HT	48	GLY	CA-C-N	9.86	129.91	119.76
1	HT	48	GLY	C-N-CA	9.86	129.91	119.76
1	AP	48	GLY	CA-C-N	9.85	129.91	119.76
1	AP	48	GLY	C-N-CA	9.85	129.91	119.76
1	GX	48	GLY	CA-C-N	9.85	129.91	119.76
1	GX	48	GLY	C-N-CA	9.85	129.91	119.76
1	JZ	48	GLY	CA-C-N	9.84	129.89	119.76
1	JZ	48	GLY	C-N-CA	9.84	129.89	119.76
1	LP	48	GLY	CA-C-N	9.84	129.89	119.76
1	LP	48	GLY	C-N-CA	9.84	129.89	119.76
1	YM	48	GLY	CA-C-N	9.83	129.88	119.76
1	YM	48	GLY	C-N-CA	9.83	129.88	119.76
1	YY	48	GLY	CA-C-N	9.83	129.88	119.76
1	YY	48	GLY	C-N-CA	9.83	129.88	119.76
1	HN	48	GLY	CA-C-N	9.83	129.88	119.76
1	HN	48	GLY	C-N-CA	9.83	129.88	119.76
1	WD	48	GLY	CA-C-N	9.83	129.88	119.76
1	WD	48	GLY	C-N-CA	9.83	129.88	119.76
1	KL	48	GLY	CA-C-N	9.83	129.88	119.76
1	KL	48	GLY	C-N-CA	9.83	129.88	119.76
1	LJ	48	GLY	CA-C-N	9.83	129.88	119.76
1	LJ	48	GLY	C-N-CA	9.83	129.88	119.76
1	BI	48	GLY	CA-C-N	9.83	129.88	119.76
1	BI	48	GLY	C-N-CA	9.83	129.88	119.76
1	YA	48	GLY	CA-C-N	9.83	129.88	119.76
1	YA	48	GLY	C-N-CA	9.83	129.88	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AK	48	GLY	CA-C-N	9.83	129.88	119.76
1	AK	48	GLY	C-N-CA	9.83	129.88	119.76
1	ZC	48	GLY	CA-C-N	9.83	129.88	119.76
1	ZC	48	GLY	C-N-CA	9.83	129.88	119.76
1	AW	48	GLY	CA-C-N	9.82	129.88	119.76
1	AW	48	GLY	C-N-CA	9.82	129.88	119.76
1	HD	48	GLY	CA-C-N	9.82	129.88	119.76
1	HD	48	GLY	C-N-CA	9.82	129.88	119.76
1	YG	48	GLY	CA-C-N	9.82	129.87	119.76
1	YG	48	GLY	C-N-CA	9.82	129.87	119.76
1	JO	48	GLY	CA-C-N	9.82	129.87	119.76
1	JO	48	GLY	C-N-CA	9.82	129.87	119.76
1	CM	48	GLY	CA-C-N	9.82	129.87	119.76
1	CM	48	GLY	C-N-CA	9.82	129.87	119.76
1	DK	48	GLY	CA-C-N	9.82	129.87	119.76
1	DK	48	GLY	C-N-CA	9.82	129.87	119.76
1	EP	48	GLY	CA-C-N	9.82	129.87	119.76
1	EP	48	GLY	C-N-CA	9.82	129.87	119.76
1	FH	48	GLY	CA-C-N	9.82	129.87	119.76
1	FH	48	GLY	C-N-CA	9.82	129.87	119.76
1	FT	48	GLY	CA-C-N	9.82	129.87	119.76
1	FT	48	GLY	C-N-CA	9.82	129.87	119.76
1	IE	48	GLY	CA-C-N	9.82	129.87	119.76
1	IE	48	GLY	C-N-CA	9.82	129.87	119.76
1	DE	48	GLY	CA-C-N	9.81	129.86	119.76
1	DE	48	GLY	C-N-CA	9.81	129.86	119.76
1	GL	48	GLY	CA-C-N	9.81	129.86	119.76
1	GL	48	GLY	C-N-CA	9.81	129.86	119.76
1	IW	48	GLY	CA-C-N	9.81	129.86	119.76
1	IW	48	GLY	C-N-CA	9.81	129.86	119.76
1	KR	48	GLY	CA-C-N	9.81	129.86	119.76
1	KR	48	GLY	C-N-CA	9.81	129.86	119.76
1	GF	48	GLY	CA-C-N	9.81	129.86	119.76
1	GF	48	GLY	C-N-CA	9.81	129.86	119.76
1	HZ	48	GLY	CA-C-N	9.81	129.86	119.76
1	HZ	48	GLY	C-N-CA	9.81	129.86	119.76
1	JC	48	GLY	CA-C-N	9.80	129.86	119.76
1	JC	48	GLY	C-N-CA	9.80	129.86	119.76
1	KX	48	GLY	CA-C-N	9.80	129.86	119.76
1	KX	48	GLY	C-N-CA	9.80	129.86	119.76
1	DX	48	GLY	CA-C-N	9.80	129.86	119.76
1	DX	48	GLY	C-N-CA	9.80	129.86	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FB	48	GLY	CA-C-N	9.80	129.86	119.76
1	FB	48	GLY	C-N-CA	9.80	129.86	119.76
1	BU	48	GLY	CA-C-N	9.80	129.85	119.76
1	BU	48	GLY	C-N-CA	9.80	129.85	119.76
1	ZU	48	GLY	CA-C-N	9.80	129.85	119.76
1	ZU	48	GLY	C-N-CA	9.80	129.85	119.76
1	CG	48	GLY	CA-C-N	9.80	129.85	119.76
1	CG	48	GLY	C-N-CA	9.80	129.85	119.76
1	ED	48	GLY	CA-C-N	9.80	129.85	119.76
1	ED	48	GLY	C-N-CA	9.80	129.85	119.76
1	BC	48	GLY	CA-C-N	9.79	129.85	119.76
1	BC	48	GLY	C-N-CA	9.79	129.85	119.76
1	HI	48	GLY	CA-C-N	9.79	129.85	119.76
1	HI	48	GLY	C-N-CA	9.79	129.85	119.76
1	DQ	48	GLY	CA-C-N	9.79	129.84	119.76
1	DQ	48	GLY	C-N-CA	9.79	129.84	119.76
1	FN	48	GLY	CA-C-N	9.79	129.84	119.76
1	FN	48	GLY	C-N-CA	9.79	129.84	119.76
1	FZ	48	GLY	CA-C-N	9.79	129.84	119.76
1	FZ	48	GLY	C-N-CA	9.79	129.84	119.76
1	IK	48	GLY	CA-C-N	9.79	129.84	119.76
1	IK	48	GLY	C-N-CA	9.79	129.84	119.76
1	YS	48	GLY	CA-C-N	9.79	129.84	119.76
1	YS	48	GLY	C-N-CA	9.79	129.84	119.76
1	JI	48	GLY	CA-C-N	9.79	129.84	119.76
1	JI	48	GLY	C-N-CA	9.79	129.84	119.76
1	CS	48	GLY	CA-C-N	9.77	129.82	119.76
1	CS	48	GLY	C-N-CA	9.77	129.82	119.76
1	GR	48	GLY	CA-C-N	9.77	129.82	119.76
1	GR	48	GLY	C-N-CA	9.77	129.82	119.76
1	ZI	48	GLY	CA-C-N	9.76	129.81	119.76
1	ZI	48	GLY	C-N-CA	9.76	129.81	119.76
1	KF	48	GLY	CA-C-N	9.76	129.81	119.76
1	KF	48	GLY	C-N-CA	9.76	129.81	119.76
1	YM	46	ARG	CA-C-N	9.28	129.52	119.87
1	YM	46	ARG	C-N-CA	9.28	129.52	119.87
1	WD	46	ARG	CA-C-N	9.28	129.52	119.87
1	WD	46	ARG	C-N-CA	9.28	129.52	119.87
1	BO	46	ARG	CA-C-N	9.27	129.50	119.87
1	BO	46	ARG	C-N-CA	9.27	129.50	119.87
1	BU	46	ARG	CA-C-N	9.27	129.51	119.87
1	BU	46	ARG	C-N-CA	9.27	129.51	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ZO	46	ARG	CA-C-N	9.27	129.50	119.87
1	ZO	46	ARG	C-N-CA	9.27	129.50	119.87
1	ZU	46	ARG	CA-C-N	9.27	129.51	119.87
1	ZU	46	ARG	C-N-CA	9.27	129.51	119.87
1	FZ	46	ARG	CA-C-N	9.26	129.50	119.87
1	FZ	46	ARG	C-N-CA	9.26	129.50	119.87
1	IK	46	ARG	CA-C-N	9.26	129.50	119.87
1	IK	46	ARG	C-N-CA	9.26	129.50	119.87
1	IW	46	ARG	CA-C-N	9.26	129.50	119.87
1	IW	46	ARG	C-N-CA	9.26	129.50	119.87
1	KR	46	ARG	CA-C-N	9.26	129.50	119.87
1	KR	46	ARG	C-N-CA	9.26	129.50	119.87
1	CG	46	ARG	CA-C-N	9.26	129.50	119.87
1	CG	46	ARG	C-N-CA	9.26	129.50	119.87
1	ED	46	ARG	CA-C-N	9.26	129.50	119.87
1	ED	46	ARG	C-N-CA	9.26	129.50	119.87
1	AW	46	ARG	CA-C-N	9.26	129.50	119.87
1	AW	46	ARG	C-N-CA	9.26	129.50	119.87
1	DE	46	ARG	CA-C-N	9.26	129.50	119.87
1	DE	46	ARG	C-N-CA	9.26	129.50	119.87
1	DX	46	ARG	CA-C-N	9.26	129.50	119.87
1	DX	46	ARG	C-N-CA	9.26	129.50	119.87
1	FB	46	ARG	CA-C-N	9.26	129.50	119.87
1	FB	46	ARG	C-N-CA	9.26	129.50	119.87
1	GL	46	ARG	CA-C-N	9.26	129.50	119.87
1	GL	46	ARG	C-N-CA	9.26	129.50	119.87
1	HD	46	ARG	CA-C-N	9.26	129.50	119.87
1	HD	46	ARG	C-N-CA	9.26	129.50	119.87
1	JC	46	ARG	CA-C-N	9.25	129.49	119.87
1	JC	46	ARG	C-N-CA	9.25	129.49	119.87
1	KX	46	ARG	CA-C-N	9.25	129.49	119.87
1	KX	46	ARG	C-N-CA	9.25	129.49	119.87
1	AE	46	ARG	CA-C-N	9.25	129.49	119.87
1	AE	46	ARG	C-N-CA	9.25	129.49	119.87
1	HT	46	ARG	CA-C-N	9.25	129.49	119.87
1	HT	46	ARG	C-N-CA	9.25	129.49	119.87
1	JZ	46	ARG	CA-C-N	9.24	129.48	119.87
1	JZ	46	ARG	C-N-CA	9.24	129.48	119.87
1	LP	46	ARG	CA-C-N	9.24	129.48	119.87
1	LP	46	ARG	C-N-CA	9.24	129.48	119.87
1	BC	46	ARG	CA-C-N	9.24	129.48	119.87
1	BC	46	ARG	C-N-CA	9.24	129.48	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HI	46	ARG	CA-C-N	9.24	129.48	119.87
1	HI	46	ARG	C-N-CA	9.24	129.48	119.87
1	FT	46	ARG	CA-C-N	9.24	129.48	119.87
1	FT	46	ARG	C-N-CA	9.24	129.48	119.87
1	IE	46	ARG	CA-C-N	9.24	129.48	119.87
1	IE	46	ARG	C-N-CA	9.24	129.48	119.87
1	YS	46	ARG	CA-C-N	9.24	129.47	119.87
1	YS	46	ARG	C-N-CA	9.24	129.47	119.87
1	AK	46	ARG	CA-C-N	9.24	129.47	119.87
1	AK	46	ARG	C-N-CA	9.24	129.47	119.87
1	ZC	46	ARG	CA-C-N	9.24	129.47	119.87
1	ZC	46	ARG	C-N-CA	9.24	129.47	119.87
1	BI	46	ARG	CA-C-N	9.24	129.48	119.87
1	BI	46	ARG	C-N-CA	9.24	129.48	119.87
1	JI	46	ARG	CA-C-N	9.24	129.47	119.87
1	JI	46	ARG	C-N-CA	9.24	129.47	119.87
1	YA	46	ARG	CA-C-N	9.24	129.48	119.87
1	YA	46	ARG	C-N-CA	9.24	129.48	119.87
1	CS	46	ARG	CA-C-N	9.23	129.47	119.87
1	CS	46	ARG	C-N-CA	9.23	129.47	119.87
1	GR	46	ARG	CA-C-N	9.23	129.47	119.87
1	GR	46	ARG	C-N-CA	9.23	129.47	119.87
1	YY	46	ARG	CA-C-N	9.23	129.47	119.87
1	YY	46	ARG	C-N-CA	9.23	129.47	119.87
1	AP	46	ARG	CA-C-N	9.23	129.47	119.87
1	AP	46	ARG	C-N-CA	9.23	129.47	119.87
1	CM	46	ARG	CA-C-N	9.23	129.47	119.87
1	CM	46	ARG	C-N-CA	9.23	129.47	119.87
1	EP	46	ARG	CA-C-N	9.23	129.47	119.87
1	EP	46	ARG	C-N-CA	9.23	129.47	119.87
1	GX	46	ARG	CA-C-N	9.23	129.47	119.87
1	GX	46	ARG	C-N-CA	9.23	129.47	119.87
1	HN	46	ARG	CA-C-N	9.23	129.47	119.87
1	HN	46	ARG	C-N-CA	9.23	129.47	119.87
1	DK	46	ARG	CA-C-N	9.22	129.46	119.87
1	DK	46	ARG	C-N-CA	9.22	129.46	119.87
1	FH	46	ARG	CA-C-N	9.22	129.46	119.87
1	FH	46	ARG	C-N-CA	9.22	129.46	119.87
1	IQ	46	ARG	CA-C-N	9.22	129.46	119.87
1	IQ	46	ARG	C-N-CA	9.22	129.46	119.87
1	LD	46	ARG	CA-C-N	9.22	129.46	119.87
1	LD	46	ARG	C-N-CA	9.22	129.46	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	46	ARG	CA-C-N	9.22	129.45	119.87
1	CA	46	ARG	C-N-CA	9.22	129.45	119.87
1	EV	46	ARG	CA-C-N	9.22	129.45	119.87
1	EV	46	ARG	C-N-CA	9.22	129.45	119.87
1	ZI	46	ARG	CA-C-N	9.22	129.46	119.87
1	ZI	46	ARG	C-N-CA	9.22	129.46	119.87
1	KF	46	ARG	CA-C-N	9.22	129.46	119.87
1	KF	46	ARG	C-N-CA	9.22	129.46	119.87
1	GF	46	ARG	CA-C-N	9.21	129.45	119.87
1	GF	46	ARG	C-N-CA	9.21	129.45	119.87
1	HZ	46	ARG	CA-C-N	9.21	129.45	119.87
1	HZ	46	ARG	C-N-CA	9.21	129.45	119.87
1	YG	46	ARG	CA-C-N	9.21	129.44	119.87
1	YG	46	ARG	C-N-CA	9.21	129.44	119.87
1	JO	46	ARG	CA-C-N	9.21	129.44	119.87
1	JO	46	ARG	C-N-CA	9.21	129.44	119.87
1	KL	46	ARG	CA-C-N	9.21	129.44	119.87
1	KL	46	ARG	C-N-CA	9.21	129.44	119.87
1	LJ	46	ARG	CA-C-N	9.21	129.44	119.87
1	LJ	46	ARG	C-N-CA	9.21	129.44	119.87
1	CY	46	ARG	CA-C-N	9.20	129.44	119.87
1	CY	46	ARG	C-N-CA	9.20	129.44	119.87
1	EJ	46	ARG	CA-C-N	9.20	129.44	119.87
1	EJ	46	ARG	C-N-CA	9.20	129.44	119.87
1	DQ	46	ARG	CA-C-N	9.20	129.43	119.87
1	DQ	46	ARG	C-N-CA	9.20	129.43	119.87
1	FN	46	ARG	CA-C-N	9.20	129.43	119.87
1	FN	46	ARG	C-N-CA	9.20	129.43	119.87
1	AE	29	ALA	CA-C-N	6.79	126.49	119.56
1	AE	29	ALA	C-N-CA	6.79	126.49	119.56
1	HT	29	ALA	CA-C-N	6.79	126.49	119.56
1	HT	29	ALA	C-N-CA	6.79	126.49	119.56
1	CA	29	ALA	CA-C-N	6.79	126.48	119.56
1	CA	29	ALA	C-N-CA	6.79	126.48	119.56
1	EV	29	ALA	CA-C-N	6.79	126.48	119.56
1	EV	29	ALA	C-N-CA	6.79	126.48	119.56
1	IW	29	ALA	CA-C-N	6.78	126.48	119.56
1	IW	29	ALA	C-N-CA	6.78	126.48	119.56
1	KR	29	ALA	CA-C-N	6.78	126.48	119.56
1	KR	29	ALA	C-N-CA	6.78	126.48	119.56
1	BI	29	ALA	CA-C-N	6.78	126.48	119.56
1	BI	29	ALA	C-N-CA	6.78	126.48	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YA	29	ALA	CA-C-N	6.78	126.48	119.56
1	YA	29	ALA	C-N-CA	6.78	126.48	119.56
1	AP	29	ALA	CA-C-N	6.78	126.47	119.56
1	AP	29	ALA	C-N-CA	6.78	126.47	119.56
1	BO	29	ALA	CA-C-N	6.78	126.47	119.56
1	BO	29	ALA	C-N-CA	6.78	126.47	119.56
1	CY	29	ALA	CA-C-N	6.78	126.47	119.56
1	CY	29	ALA	C-N-CA	6.78	126.47	119.56
1	EJ	29	ALA	CA-C-N	6.78	126.47	119.56
1	EJ	29	ALA	C-N-CA	6.78	126.47	119.56
1	GX	29	ALA	CA-C-N	6.78	126.47	119.56
1	GX	29	ALA	C-N-CA	6.78	126.47	119.56
1	ZO	29	ALA	CA-C-N	6.78	126.47	119.56
1	ZO	29	ALA	C-N-CA	6.78	126.47	119.56
1	DX	29	ALA	CA-C-N	6.77	126.47	119.56
1	DX	29	ALA	C-N-CA	6.77	126.47	119.56
1	FB	29	ALA	CA-C-N	6.77	126.47	119.56
1	FB	29	ALA	C-N-CA	6.77	126.47	119.56
1	YM	29	ALA	CA-C-N	6.77	126.47	119.56
1	YM	29	ALA	C-N-CA	6.77	126.47	119.56
1	WD	29	ALA	CA-C-N	6.77	126.47	119.56
1	WD	29	ALA	C-N-CA	6.77	126.47	119.56
1	FT	29	ALA	CA-C-N	6.77	126.47	119.56
1	FT	29	ALA	C-N-CA	6.77	126.47	119.56
1	IE	29	ALA	CA-C-N	6.77	126.47	119.56
1	IE	29	ALA	C-N-CA	6.77	126.47	119.56
1	IQ	29	ALA	CA-C-N	6.77	126.47	119.56
1	IQ	29	ALA	C-N-CA	6.77	126.47	119.56
1	LD	29	ALA	CA-C-N	6.77	126.47	119.56
1	LD	29	ALA	C-N-CA	6.77	126.47	119.56
1	FZ	29	ALA	CA-C-N	6.77	126.46	119.56
1	FZ	29	ALA	C-N-CA	6.77	126.46	119.56
1	IK	29	ALA	CA-C-N	6.77	126.46	119.56
1	IK	29	ALA	C-N-CA	6.77	126.46	119.56
1	KL	29	ALA	CA-C-N	6.76	126.46	119.56
1	KL	29	ALA	C-N-CA	6.76	126.46	119.56
1	LJ	29	ALA	CA-C-N	6.76	126.46	119.56
1	LJ	29	ALA	C-N-CA	6.76	126.46	119.56
1	AK	29	ALA	CA-C-N	6.76	126.45	119.56
1	AK	29	ALA	C-N-CA	6.76	126.45	119.56
1	ZC	29	ALA	CA-C-N	6.76	126.45	119.56
1	ZC	29	ALA	C-N-CA	6.76	126.45	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GF	29	ALA	CA-C-N	6.76	126.45	119.56
1	GF	29	ALA	C-N-CA	6.76	126.45	119.56
1	HZ	29	ALA	CA-C-N	6.76	126.45	119.56
1	HZ	29	ALA	C-N-CA	6.76	126.45	119.56
1	YS	29	ALA	CA-C-N	6.75	126.45	119.56
1	YS	29	ALA	C-N-CA	6.75	126.45	119.56
1	CK	29	ALA	CA-C-N	6.75	126.45	119.56
1	CK	29	ALA	C-N-CA	6.75	126.45	119.56
1	EN	29	ALA	CA-C-N	6.75	126.45	119.56
1	EN	29	ALA	C-N-CA	6.75	126.45	119.56
1	JI	29	ALA	CA-C-N	6.75	126.45	119.56
1	JI	29	ALA	C-N-CA	6.75	126.45	119.56
1	BU	29	ALA	CA-C-N	6.75	126.44	119.56
1	BU	29	ALA	C-N-CA	6.75	126.44	119.56
1	ZU	29	ALA	CA-C-N	6.75	126.44	119.56
1	ZU	29	ALA	C-N-CA	6.75	126.44	119.56
1	AW	29	ALA	CA-C-N	6.75	126.44	119.56
1	AW	29	ALA	C-N-CA	6.75	126.44	119.56
1	DQ	29	ALA	CA-C-N	6.75	126.44	119.56
1	DQ	29	ALA	C-N-CA	6.75	126.44	119.56
1	FN	29	ALA	CA-C-N	6.75	126.44	119.56
1	FN	29	ALA	C-N-CA	6.75	126.44	119.56
1	HD	29	ALA	CA-C-N	6.75	126.44	119.56
1	HD	29	ALA	C-N-CA	6.75	126.44	119.56
1	YY	29	ALA	CA-C-N	6.74	126.44	119.56
1	YY	29	ALA	C-N-CA	6.74	126.44	119.56
1	DE	29	ALA	CA-C-N	6.74	126.44	119.56
1	DE	29	ALA	C-N-CA	6.74	126.44	119.56
1	GL	29	ALA	CA-C-N	6.74	126.44	119.56
1	GL	29	ALA	C-N-CA	6.74	126.44	119.56
1	HN	29	ALA	CA-C-N	6.74	126.44	119.56
1	HN	29	ALA	C-N-CA	6.74	126.44	119.56
1	YE	29	ALA	CA-C-N	6.74	126.44	119.56
1	YE	29	ALA	C-N-CA	6.74	126.44	119.56
1	CG	29	ALA	CA-C-N	6.74	126.44	119.56
1	CG	29	ALA	C-N-CA	6.74	126.44	119.56
1	ED	29	ALA	CA-C-N	6.74	126.44	119.56
1	ED	29	ALA	C-N-CA	6.74	126.44	119.56
1	JM	29	ALA	CA-C-N	6.74	126.44	119.56
1	JM	29	ALA	C-N-CA	6.74	126.44	119.56
1	YG	29	ALA	CA-C-N	6.74	126.43	119.56
1	YG	29	ALA	C-N-CA	6.74	126.43	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	JO	29	ALA	CA-C-N	6.74	126.43	119.56
1	JO	29	ALA	C-N-CA	6.74	126.43	119.56
1	BC	29	ALA	CA-C-N	6.73	126.43	119.56
1	BC	29	ALA	C-N-CA	6.73	126.43	119.56
1	HI	29	ALA	CA-C-N	6.73	126.43	119.56
1	HI	29	ALA	C-N-CA	6.73	126.43	119.56
1	ZI	29	ALA	CA-C-N	6.73	126.42	119.56
1	ZI	29	ALA	C-N-CA	6.73	126.42	119.56
1	KF	29	ALA	CA-C-N	6.73	126.42	119.56
1	KF	29	ALA	C-N-CA	6.73	126.42	119.56
1	DK	29	ALA	CA-C-N	6.72	126.42	119.56
1	DK	29	ALA	C-N-CA	6.72	126.42	119.56
1	FH	29	ALA	CA-C-N	6.72	126.42	119.56
1	FH	29	ALA	C-N-CA	6.72	126.42	119.56
1	IS	29	ALA	CA-C-N	6.72	126.42	119.56
1	IS	29	ALA	C-N-CA	6.72	126.42	119.56
1	JC	29	ALA	CA-C-N	6.72	126.42	119.56
1	JC	29	ALA	C-N-CA	6.72	126.42	119.56
1	KX	29	ALA	CA-C-N	6.72	126.42	119.56
1	KX	29	ALA	C-N-CA	6.72	126.42	119.56
1	LF	29	ALA	CA-C-N	6.72	126.42	119.56
1	LF	29	ALA	C-N-CA	6.72	126.42	119.56
1	CQ	29	ALA	CA-C-N	6.72	126.42	119.56
1	CQ	29	ALA	C-N-CA	6.72	126.42	119.56
1	GD	29	ALA	CA-C-N	6.72	126.42	119.56
1	GD	29	ALA	C-N-CA	6.72	126.42	119.56
1	GP	29	ALA	CA-C-N	6.72	126.42	119.56
1	GP	29	ALA	C-N-CA	6.72	126.42	119.56
1	HX	29	ALA	CA-C-N	6.72	126.42	119.56
1	HX	29	ALA	C-N-CA	6.72	126.42	119.56
1	JZ	29	ALA	CA-C-N	6.72	126.42	119.56
1	JZ	29	ALA	C-N-CA	6.72	126.42	119.56
1	LP	29	ALA	CA-C-N	6.72	126.42	119.56
1	LP	29	ALA	C-N-CA	6.72	126.42	119.56
1	ZK	29	ALA	CA-C-N	6.72	126.42	119.56
1	ZK	29	ALA	C-N-CA	6.72	126.42	119.56
1	KH	29	ALA	CA-C-N	6.72	126.42	119.56
1	KH	29	ALA	C-N-CA	6.72	126.42	119.56
1	BA	29	ALA	CA-C-N	6.72	126.41	119.56
1	BA	29	ALA	C-N-CA	6.72	126.41	119.56
1	HG	29	ALA	CA-C-N	6.72	126.41	119.56
1	HG	29	ALA	C-N-CA	6.72	126.41	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ZY	29	ALA	CA-C-N	6.71	126.41	119.56
1	ZY	29	ALA	C-N-CA	6.71	126.41	119.56
1	BG	29	ALA	CA-C-N	6.71	126.41	119.56
1	BG	29	ALA	C-N-CA	6.71	126.41	119.56
1	YW	29	ALA	CA-C-N	6.71	126.41	119.56
1	YW	29	ALA	C-N-CA	6.71	126.41	119.56
1	HL	29	ALA	CA-C-N	6.71	126.41	119.56
1	HL	29	ALA	C-N-CA	6.71	126.41	119.56
1	CS	29	ALA	CA-C-N	6.71	126.40	119.56
1	CS	29	ALA	C-N-CA	6.71	126.40	119.56
1	GH	29	ALA	CA-C-N	6.71	126.40	119.56
1	GH	29	ALA	C-N-CA	6.71	126.40	119.56
1	GR	29	ALA	CA-C-N	6.71	126.40	119.56
1	GR	29	ALA	C-N-CA	6.71	126.40	119.56
1	WC	29	ALA	CA-C-N	6.71	126.40	119.56
1	WC	29	ALA	C-N-CA	6.71	126.40	119.56
1	AR	29	ALA	CA-C-N	6.71	126.40	119.56
1	AR	29	ALA	C-N-CA	6.71	126.40	119.56
1	GV	29	ALA	CA-C-N	6.71	126.40	119.56
1	GV	29	ALA	C-N-CA	6.71	126.40	119.56
1	IU	29	ALA	CA-C-N	6.70	126.40	119.56
1	IU	29	ALA	C-N-CA	6.70	126.40	119.56
1	KP	29	ALA	CA-C-N	6.70	126.40	119.56
1	KP	29	ALA	C-N-CA	6.70	126.40	119.56
1	YK	29	ALA	CA-C-N	6.70	126.39	119.56
1	YK	29	ALA	C-N-CA	6.70	126.39	119.56
1	DC	29	ALA	CA-C-N	6.70	126.39	119.56
1	DC	29	ALA	C-N-CA	6.70	126.39	119.56
1	GJ	29	ALA	CA-C-N	6.70	126.39	119.56
1	GJ	29	ALA	C-N-CA	6.70	126.39	119.56
1	JS	29	ALA	CA-C-N	6.70	126.39	119.56
1	JS	29	ALA	C-N-CA	6.70	126.39	119.56
1	KB	29	ALA	CA-C-N	6.70	126.39	119.56
1	KB	29	ALA	C-N-CA	6.70	126.39	119.56
1	LR	29	ALA	CA-C-N	6.70	126.39	119.56
1	LR	29	ALA	C-N-CA	6.70	126.39	119.56
1	DO	29	ALA	CA-C-N	6.70	126.39	119.56
1	DO	29	ALA	C-N-CA	6.70	126.39	119.56
1	FL	29	ALA	CA-C-N	6.70	126.39	119.56
1	FL	29	ALA	C-N-CA	6.70	126.39	119.56
1	CE	29	ALA	CA-C-N	6.70	126.39	119.56
1	CE	29	ALA	C-N-CA	6.70	126.39	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EB	29	ALA	CA-C-N	6.70	126.39	119.56
1	EB	29	ALA	C-N-CA	6.70	126.39	119.56
1	DM	29	ALA	CA-C-N	6.69	126.39	119.56
1	DM	29	ALA	C-N-CA	6.69	126.39	119.56
1	DZ	29	ALA	CA-C-N	6.69	126.39	119.56
1	DZ	29	ALA	C-N-CA	6.69	126.39	119.56
1	ZG	29	ALA	CA-C-N	6.69	126.39	119.56
1	ZG	29	ALA	C-N-CA	6.69	126.39	119.56
1	FD	29	ALA	CA-C-N	6.69	126.39	119.56
1	FD	29	ALA	C-N-CA	6.69	126.39	119.56
1	FJ	29	ALA	CA-C-N	6.69	126.39	119.56
1	FJ	29	ALA	C-N-CA	6.69	126.39	119.56
1	KD	29	ALA	CA-C-N	6.69	126.39	119.56
1	KD	29	ALA	C-N-CA	6.69	126.39	119.56
1	IO	29	ALA	CA-C-N	6.69	126.39	119.56
1	IO	29	ALA	C-N-CA	6.69	126.39	119.56
1	LB	29	ALA	CA-C-N	6.69	126.39	119.56
1	LB	29	ALA	C-N-CA	6.69	126.39	119.56
1	ZA	29	ALA	CA-C-N	6.69	126.38	119.56
1	ZA	29	ALA	C-N-CA	6.69	126.38	119.56
1	AI	29	ALA	CA-C-N	6.69	126.38	119.56
1	AI	29	ALA	C-N-CA	6.69	126.38	119.56
1	CM	29	ALA	CA-C-N	6.69	126.38	119.56
1	CM	29	ALA	C-N-CA	6.69	126.38	119.56
1	DI	29	ALA	CA-C-N	6.69	126.38	119.56
1	DI	29	ALA	C-N-CA	6.69	126.38	119.56
1	EP	29	ALA	CA-C-N	6.69	126.38	119.56
1	EP	29	ALA	C-N-CA	6.69	126.38	119.56
1	FF	29	ALA	CA-C-N	6.69	126.38	119.56
1	FF	29	ALA	C-N-CA	6.69	126.38	119.56
1	CO	29	ALA	CA-C-N	6.69	126.38	119.56
1	CO	29	ALA	C-N-CA	6.69	126.38	119.56
1	DG	29	ALA	CA-C-N	6.69	126.38	119.56
1	DG	29	ALA	C-N-CA	6.69	126.38	119.56
1	ER	29	ALA	CA-C-N	6.69	126.38	119.56
1	ER	29	ALA	C-N-CA	6.69	126.38	119.56
1	GN	29	ALA	CA-C-N	6.69	126.38	119.56
1	GN	29	ALA	C-N-CA	6.69	126.38	119.56
1	JA	29	ALA	CA-C-N	6.69	126.38	119.56
1	JA	29	ALA	C-N-CA	6.69	126.38	119.56
1	KV	29	ALA	CA-C-N	6.69	126.38	119.56
1	KV	29	ALA	C-N-CA	6.69	126.38	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DU	29	ALA	CA-C-N	6.69	126.38	119.56
1	DU	29	ALA	C-N-CA	6.69	126.38	119.56
1	EZ	29	ALA	CA-C-N	6.69	126.38	119.56
1	EZ	29	ALA	C-N-CA	6.69	126.38	119.56
1	CU	29	ALA	CA-C-N	6.68	126.38	119.56
1	CU	29	ALA	C-N-CA	6.68	126.38	119.56
1	GT	29	ALA	CA-C-N	6.68	126.38	119.56
1	GT	29	ALA	C-N-CA	6.68	126.38	119.56
1	CI	29	ALA	CA-C-N	6.68	126.38	119.56
1	CI	29	ALA	C-N-CA	6.68	126.38	119.56
1	EF	29	ALA	CA-C-N	6.68	126.38	119.56
1	EF	29	ALA	C-N-CA	6.68	126.38	119.56
1	JE	29	ALA	CA-C-N	6.68	126.37	119.56
1	JE	29	ALA	C-N-CA	6.68	126.37	119.56
1	KZ	29	ALA	CA-C-N	6.68	126.37	119.56
1	KZ	29	ALA	C-N-CA	6.68	126.37	119.56
1	YC	29	ALA	CA-C-N	6.68	126.37	119.56
1	YC	29	ALA	C-N-CA	6.68	126.37	119.56
1	AY	29	ALA	CA-C-N	6.68	126.37	119.56
1	AY	29	ALA	C-N-CA	6.68	126.37	119.56
1	BK	29	ALA	CA-C-N	6.68	126.37	119.56
1	BK	29	ALA	C-N-CA	6.68	126.37	119.56
1	WB	29	ALA	CA-C-N	6.68	126.37	119.56
1	WB	29	ALA	C-N-CA	6.68	126.37	119.56
1	DS	29	ALA	CA-C-N	6.67	126.37	119.56
1	DS	29	ALA	C-N-CA	6.67	126.37	119.56
1	FP	29	ALA	CA-C-N	6.67	126.37	119.56
1	FP	29	ALA	C-N-CA	6.67	126.37	119.56
1	AM	29	ALA	CA-C-N	6.67	126.37	119.56
1	AM	29	ALA	C-N-CA	6.67	126.37	119.56
1	ZE	29	ALA	CA-C-N	6.67	126.37	119.56
1	ZE	29	ALA	C-N-CA	6.67	126.37	119.56
1	AC	29	ALA	CA-C-N	6.67	126.36	119.56
1	AC	29	ALA	C-N-CA	6.67	126.36	119.56
1	AU	29	ALA	CA-C-N	6.67	126.36	119.56
1	AU	29	ALA	C-N-CA	6.67	126.36	119.56
1	FV	29	ALA	CA-C-N	6.67	126.36	119.56
1	FV	29	ALA	C-N-CA	6.67	126.36	119.56
1	HB	29	ALA	CA-C-N	6.67	126.36	119.56
1	HB	29	ALA	C-N-CA	6.67	126.36	119.56
1	HR	29	ALA	CA-C-N	6.67	126.36	119.56
1	HR	29	ALA	C-N-CA	6.67	126.36	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	IH	29	ALA	CA-C-N	6.67	126.36	119.56
1	IH	29	ALA	C-N-CA	6.67	126.36	119.56
1	KJ	29	ALA	CA-C-N	6.67	126.36	119.56
1	KJ	29	ALA	C-N-CA	6.67	126.36	119.56
1	LH	29	ALA	CA-C-N	6.67	126.36	119.56
1	LH	29	ALA	C-N-CA	6.67	126.36	119.56
1	AG	29	ALA	CA-C-N	6.67	126.36	119.56
1	AG	29	ALA	C-N-CA	6.67	126.36	119.56
1	CC	29	ALA	CA-C-N	6.67	126.36	119.56
1	CC	29	ALA	C-N-CA	6.67	126.36	119.56
1	EX	29	ALA	CA-C-N	6.67	126.36	119.56
1	EX	29	ALA	C-N-CA	6.67	126.36	119.56
1	HV	29	ALA	CA-C-N	6.67	126.36	119.56
1	HV	29	ALA	C-N-CA	6.67	126.36	119.56
1	IY	29	ALA	CA-C-N	6.67	126.36	119.56
1	IY	29	ALA	C-N-CA	6.67	126.36	119.56
1	KN	29	ALA	CA-C-N	6.67	126.36	119.56
1	KN	29	ALA	C-N-CA	6.67	126.36	119.56
1	KT	29	ALA	CA-C-N	6.67	126.36	119.56
1	KT	29	ALA	C-N-CA	6.67	126.36	119.56
1	LL	29	ALA	CA-C-N	6.67	126.36	119.56
1	LL	29	ALA	C-N-CA	6.67	126.36	119.56
1	BY	29	ALA	CA-C-N	6.67	126.36	119.56
1	BY	29	ALA	C-N-CA	6.67	126.36	119.56
1	ET	29	ALA	CA-C-N	6.67	126.36	119.56
1	ET	29	ALA	C-N-CA	6.67	126.36	119.56
1	BE	29	ALA	CA-C-N	6.66	126.36	119.56
1	BE	29	ALA	C-N-CA	6.66	126.36	119.56
1	WA	29	ALA	CA-C-N	6.66	126.36	119.56
1	WA	29	ALA	C-N-CA	6.66	126.36	119.56
1	JX	29	ALA	CA-C-N	6.66	126.35	119.56
1	JX	29	ALA	C-N-CA	6.66	126.35	119.56
1	LN	29	ALA	CA-C-N	6.66	126.35	119.56
1	LN	29	ALA	C-N-CA	6.66	126.35	119.56
1	YQ	29	ALA	CA-C-N	6.66	126.35	119.56
1	YQ	29	ALA	C-N-CA	6.66	126.35	119.56
1	JG	29	ALA	CA-C-N	6.66	126.35	119.56
1	JG	29	ALA	C-N-CA	6.66	126.35	119.56
1	YU	29	ALA	CA-C-N	6.66	126.35	119.56
1	YU	29	ALA	C-N-CA	6.66	126.35	119.56
1	CW	29	ALA	CA-C-N	6.66	126.35	119.56
1	CW	29	ALA	C-N-CA	6.66	126.35	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EH	29	ALA	CA-C-N	6.66	126.35	119.56
1	EH	29	ALA	C-N-CA	6.66	126.35	119.56
1	FX	29	ALA	CA-C-N	6.66	126.35	119.56
1	FX	29	ALA	C-N-CA	6.66	126.35	119.56
1	II	29	ALA	CA-C-N	6.66	126.35	119.56
1	II	29	ALA	C-N-CA	6.66	126.35	119.56
1	JK	29	ALA	CA-C-N	6.66	126.35	119.56
1	JK	29	ALA	C-N-CA	6.66	126.35	119.56
1	DA	29	ALA	CA-C-N	6.65	126.35	119.56
1	DA	29	ALA	C-N-CA	6.65	126.35	119.56
1	EL	29	ALA	CA-C-N	6.65	126.35	119.56
1	EL	29	ALA	C-N-CA	6.65	126.35	119.56
1	YO	29	ALA	CA-C-N	6.65	126.34	119.56
1	YO	29	ALA	C-N-CA	6.65	126.34	119.56
1	GB	29	ALA	CA-C-N	6.65	126.34	119.56
1	GB	29	ALA	C-N-CA	6.65	126.34	119.56
1	IM	29	ALA	CA-C-N	6.65	126.34	119.56
1	IM	29	ALA	C-N-CA	6.65	126.34	119.56
1	JV	29	ALA	CA-C-N	6.65	126.34	119.56
1	JV	29	ALA	C-N-CA	6.65	126.34	119.56
1	BW	29	ALA	CA-C-N	6.65	126.34	119.56
1	BW	29	ALA	C-N-CA	6.65	126.34	119.56
1	ZW	29	ALA	CA-C-N	6.65	126.34	119.56
1	ZW	29	ALA	C-N-CA	6.65	126.34	119.56
1	AA	29	ALA	CA-C-N	6.65	126.34	119.56
1	AA	29	ALA	C-N-CA	6.65	126.34	119.56
1	BM	29	ALA	CA-C-N	6.65	126.34	119.56
1	BM	29	ALA	C-N-CA	6.65	126.34	119.56
1	HP	29	ALA	CA-C-N	6.65	126.34	119.56
1	HP	29	ALA	C-N-CA	6.65	126.34	119.56
1	ZM	29	ALA	CA-C-N	6.65	126.34	119.56
1	ZM	29	ALA	C-N-CA	6.65	126.34	119.56
1	BS	29	ALA	CA-C-N	6.64	126.33	119.56
1	BS	29	ALA	C-N-CA	6.64	126.33	119.56
1	ZS	29	ALA	CA-C-N	6.64	126.33	119.56
1	ZS	29	ALA	C-N-CA	6.64	126.33	119.56
1	YI	29	ALA	CA-C-N	6.64	126.33	119.56
1	YI	29	ALA	C-N-CA	6.64	126.33	119.56
1	JQ	29	ALA	CA-C-N	6.64	126.33	119.56
1	JQ	29	ALA	C-N-CA	6.64	126.33	119.56
1	AS	29	ALA	CA-C-N	6.63	126.33	119.56
1	AS	29	ALA	C-N-CA	6.63	126.33	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BQ	29	ALA	CA-C-N	6.63	126.33	119.56
1	BQ	29	ALA	C-N-CA	6.63	126.33	119.56
1	GZ	29	ALA	CA-C-N	6.63	126.33	119.56
1	GZ	29	ALA	C-N-CA	6.63	126.33	119.56
1	ZQ	29	ALA	CA-C-N	6.63	126.33	119.56
1	ZQ	29	ALA	C-N-CA	6.63	126.33	119.56
1	FR	29	ALA	CA-C-N	6.61	126.31	119.56
1	FR	29	ALA	C-N-CA	6.61	126.31	119.56
1	IC	29	ALA	CA-C-N	6.61	126.31	119.56
1	IC	29	ALA	C-N-CA	6.61	126.31	119.56
1	ZK	48	GLY	CA-C-N	6.27	126.03	119.76
1	ZK	48	GLY	C-N-CA	6.27	126.03	119.76
1	KH	48	GLY	CA-C-N	6.27	126.03	119.76
1	KH	48	GLY	C-N-CA	6.27	126.03	119.76
1	BQ	48	GLY	CA-C-N	6.27	126.03	119.76
1	BQ	48	GLY	C-N-CA	6.27	126.03	119.76
1	ZQ	48	GLY	CA-C-N	6.27	126.03	119.76
1	ZQ	48	GLY	C-N-CA	6.27	126.03	119.76
1	AY	48	GLY	CA-C-N	6.25	126.02	119.76
1	AY	48	GLY	C-N-CA	6.25	126.02	119.76
1	WB	48	GLY	CA-C-N	6.25	126.02	119.76
1	WB	48	GLY	C-N-CA	6.25	126.02	119.76
1	CU	48	GLY	CA-C-N	6.25	126.01	119.76
1	CU	48	GLY	C-N-CA	6.25	126.01	119.76
1	GT	48	GLY	CA-C-N	6.25	126.01	119.76
1	GT	48	GLY	C-N-CA	6.25	126.01	119.76
1	AS	48	GLY	CA-C-N	6.25	126.01	119.76
1	AS	48	GLY	C-N-CA	6.25	126.01	119.76
1	GH	48	GLY	CA-C-N	6.25	126.01	119.76
1	GH	48	GLY	C-N-CA	6.25	126.01	119.76
1	GZ	48	GLY	CA-C-N	6.25	126.01	119.76
1	GZ	48	GLY	C-N-CA	6.25	126.01	119.76
1	WC	48	GLY	CA-C-N	6.25	126.01	119.76
1	WC	48	GLY	C-N-CA	6.25	126.01	119.76
1	YU	48	GLY	CA-C-N	6.24	126.00	119.76
1	YU	48	GLY	C-N-CA	6.24	126.00	119.76
1	CO	48	GLY	CA-C-N	6.24	126.00	119.76
1	CO	48	GLY	C-N-CA	6.24	126.00	119.76
1	ER	48	GLY	CA-C-N	6.24	126.00	119.76
1	ER	48	GLY	C-N-CA	6.24	126.00	119.76
1	JK	48	GLY	CA-C-N	6.24	126.00	119.76
1	JK	48	GLY	C-N-CA	6.24	126.00	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CI	48	GLY	CA-C-N	6.24	126.00	119.76
1	CI	48	GLY	C-N-CA	6.24	126.00	119.76
1	EF	48	GLY	CA-C-N	6.24	126.00	119.76
1	EF	48	GLY	C-N-CA	6.24	126.00	119.76
1	IS	48	GLY	CA-C-N	6.24	126.00	119.76
1	IS	48	GLY	C-N-CA	6.24	126.00	119.76
1	LF	48	GLY	CA-C-N	6.24	126.00	119.76
1	LF	48	GLY	C-N-CA	6.24	126.00	119.76
1	YI	48	GLY	CA-C-N	6.24	126.00	119.76
1	YI	48	GLY	C-N-CA	6.24	126.00	119.76
1	JQ	48	GLY	CA-C-N	6.24	126.00	119.76
1	JQ	48	GLY	C-N-CA	6.24	126.00	119.76
1	AM	48	GLY	CA-C-N	6.23	125.99	119.76
1	AM	48	GLY	C-N-CA	6.23	125.99	119.76
1	ZE	48	GLY	CA-C-N	6.23	125.99	119.76
1	ZE	48	GLY	C-N-CA	6.23	125.99	119.76
1	FV	48	GLY	CA-C-N	6.23	125.99	119.76
1	FV	48	GLY	C-N-CA	6.23	125.99	119.76
1	IH	48	GLY	CA-C-N	6.23	125.99	119.76
1	IH	48	GLY	C-N-CA	6.23	125.99	119.76
1	DM	48	GLY	CA-C-N	6.23	125.99	119.76
1	DM	48	GLY	C-N-CA	6.23	125.99	119.76
1	FJ	48	GLY	CA-C-N	6.23	125.99	119.76
1	FJ	48	GLY	C-N-CA	6.23	125.99	119.76
1	BE	48	GLY	CA-C-N	6.23	125.99	119.76
1	BE	48	GLY	C-N-CA	6.23	125.99	119.76
1	DA	48	GLY	CA-C-N	6.23	125.99	119.76
1	DA	48	GLY	C-N-CA	6.23	125.99	119.76
1	EL	48	GLY	CA-C-N	6.23	125.99	119.76
1	EL	48	GLY	C-N-CA	6.23	125.99	119.76
1	WA	48	GLY	CA-C-N	6.23	125.99	119.76
1	WA	48	GLY	C-N-CA	6.23	125.99	119.76
1	IY	48	GLY	CA-C-N	6.22	125.98	119.76
1	IY	48	GLY	C-N-CA	6.22	125.98	119.76
1	KT	48	GLY	CA-C-N	6.22	125.98	119.76
1	KT	48	GLY	C-N-CA	6.22	125.98	119.76
1	CC	48	GLY	CA-C-N	6.22	125.98	119.76
1	CC	48	GLY	C-N-CA	6.22	125.98	119.76
1	EX	48	GLY	CA-C-N	6.22	125.98	119.76
1	EX	48	GLY	C-N-CA	6.22	125.98	119.76
1	YC	46	ARG	CA-C-N	6.22	125.84	119.56
1	YC	46	ARG	C-N-CA	6.22	125.84	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YC	48	GLY	CA-C-N	6.22	125.98	119.76
1	YC	48	GLY	C-N-CA	6.22	125.98	119.76
1	YO	48	GLY	CA-C-N	6.22	125.98	119.76
1	YO	48	GLY	C-N-CA	6.22	125.98	119.76
1	BK	46	ARG	CA-C-N	6.22	125.84	119.56
1	BK	46	ARG	C-N-CA	6.22	125.84	119.56
1	BK	48	GLY	CA-C-N	6.22	125.98	119.76
1	BK	48	GLY	C-N-CA	6.22	125.98	119.76
1	DZ	48	GLY	CA-C-N	6.22	125.98	119.76
1	DZ	48	GLY	C-N-CA	6.22	125.98	119.76
1	FD	48	GLY	CA-C-N	6.22	125.98	119.76
1	FD	48	GLY	C-N-CA	6.22	125.98	119.76
1	JV	48	GLY	CA-C-N	6.22	125.98	119.76
1	JV	48	GLY	C-N-CA	6.22	125.98	119.76
1	KN	48	GLY	CA-C-N	6.22	125.98	119.76
1	KN	48	GLY	C-N-CA	6.22	125.98	119.76
1	LL	48	GLY	CA-C-N	6.22	125.98	119.76
1	LL	48	GLY	C-N-CA	6.22	125.98	119.76
1	DG	48	GLY	CA-C-N	6.21	125.97	119.76
1	DG	48	GLY	C-N-CA	6.21	125.97	119.76
1	DS	48	GLY	CA-C-N	6.21	125.97	119.76
1	DS	48	GLY	C-N-CA	6.21	125.97	119.76
1	FP	48	GLY	CA-C-N	6.21	125.97	119.76
1	FP	48	GLY	C-N-CA	6.21	125.97	119.76
1	GN	48	GLY	CA-C-N	6.21	125.97	119.76
1	GN	48	GLY	C-N-CA	6.21	125.97	119.76
1	KB	48	GLY	CA-C-N	6.21	125.97	119.76
1	KB	48	GLY	C-N-CA	6.21	125.97	119.76
1	LR	48	GLY	CA-C-N	6.21	125.97	119.76
1	LR	48	GLY	C-N-CA	6.21	125.97	119.76
1	AA	48	GLY	CA-C-N	6.20	125.96	119.76
1	AA	48	GLY	C-N-CA	6.20	125.96	119.76
1	CC	46	ARG	CA-C-N	6.20	125.82	119.56
1	CC	46	ARG	C-N-CA	6.20	125.82	119.56
1	EX	46	ARG	CA-C-N	6.20	125.82	119.56
1	EX	46	ARG	C-N-CA	6.20	125.82	119.56
1	HP	48	GLY	CA-C-N	6.20	125.96	119.76
1	HP	48	GLY	C-N-CA	6.20	125.96	119.76
1	JE	48	GLY	CA-C-N	6.20	125.96	119.76
1	JE	48	GLY	C-N-CA	6.20	125.96	119.76
1	KZ	48	GLY	CA-C-N	6.20	125.96	119.76
1	KZ	48	GLY	C-N-CA	6.20	125.96	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BW	48	GLY	CA-C-N	6.20	125.96	119.76
1	BW	48	GLY	C-N-CA	6.20	125.96	119.76
1	ZW	48	GLY	CA-C-N	6.20	125.96	119.76
1	ZW	48	GLY	C-N-CA	6.20	125.96	119.76
1	YO	46	ARG	CA-C-N	6.20	125.82	119.56
1	YO	46	ARG	C-N-CA	6.20	125.82	119.56
1	AG	48	GLY	CA-C-N	6.20	125.95	119.76
1	AG	48	GLY	C-N-CA	6.20	125.95	119.76
1	HV	48	GLY	CA-C-N	6.20	125.95	119.76
1	HV	48	GLY	C-N-CA	6.20	125.95	119.76
1	ZK	46	ARG	CA-C-N	6.20	125.82	119.56
1	ZK	46	ARG	C-N-CA	6.20	125.82	119.56
1	JV	46	ARG	CA-C-N	6.20	125.82	119.56
1	JV	46	ARG	C-N-CA	6.20	125.82	119.56
1	KH	46	ARG	CA-C-N	6.20	125.82	119.56
1	KH	46	ARG	C-N-CA	6.20	125.82	119.56
1	AG	46	ARG	CA-C-N	6.19	125.82	119.56
1	AG	46	ARG	C-N-CA	6.19	125.82	119.56
1	HV	46	ARG	CA-C-N	6.19	125.82	119.56
1	HV	46	ARG	C-N-CA	6.19	125.82	119.56
1	YU	46	ARG	CA-C-N	6.18	125.81	119.56
1	YU	46	ARG	C-N-CA	6.18	125.81	119.56
1	JK	46	ARG	CA-C-N	6.18	125.81	119.56
1	JK	46	ARG	C-N-CA	6.18	125.81	119.56
1	IS	46	ARG	CA-C-N	6.18	125.80	119.56
1	IS	46	ARG	C-N-CA	6.18	125.80	119.56
1	LF	46	ARG	CA-C-N	6.18	125.80	119.56
1	LF	46	ARG	C-N-CA	6.18	125.80	119.56
1	BW	46	ARG	CA-C-N	6.17	125.79	119.56
1	BW	46	ARG	C-N-CA	6.17	125.79	119.56
1	ZW	46	ARG	CA-C-N	6.17	125.79	119.56
1	ZW	46	ARG	C-N-CA	6.17	125.79	119.56
1	CO	46	ARG	CA-C-N	6.17	125.79	119.56
1	CO	46	ARG	C-N-CA	6.17	125.79	119.56
1	CU	46	ARG	CA-C-N	6.17	125.79	119.56
1	CU	46	ARG	C-N-CA	6.17	125.79	119.56
1	ER	46	ARG	CA-C-N	6.17	125.79	119.56
1	ER	46	ARG	C-N-CA	6.17	125.79	119.56
1	GT	46	ARG	CA-C-N	6.17	125.79	119.56
1	GT	46	ARG	C-N-CA	6.17	125.79	119.56
1	AM	46	ARG	CA-C-N	6.17	125.79	119.56
1	AM	46	ARG	C-N-CA	6.17	125.79	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BQ	46	ARG	CA-C-N	6.17	125.79	119.56
1	BQ	46	ARG	C-N-CA	6.17	125.79	119.56
1	ZE	46	ARG	CA-C-N	6.17	125.79	119.56
1	ZE	46	ARG	C-N-CA	6.17	125.79	119.56
1	ZQ	46	ARG	CA-C-N	6.17	125.79	119.56
1	ZQ	46	ARG	C-N-CA	6.17	125.79	119.56
1	AS	46	ARG	CA-C-N	6.16	125.79	119.56
1	AS	46	ARG	C-N-CA	6.16	125.79	119.56
1	GZ	46	ARG	CA-C-N	6.16	125.79	119.56
1	GZ	46	ARG	C-N-CA	6.16	125.79	119.56
1	IY	46	ARG	CA-C-N	6.16	125.78	119.56
1	IY	46	ARG	C-N-CA	6.16	125.78	119.56
1	KT	46	ARG	CA-C-N	6.16	125.78	119.56
1	KT	46	ARG	C-N-CA	6.16	125.78	119.56
1	GB	48	GLY	CA-C-N	6.16	125.92	119.76
1	GB	48	GLY	C-N-CA	6.16	125.92	119.76
1	IM	48	GLY	CA-C-N	6.16	125.92	119.76
1	IM	48	GLY	C-N-CA	6.16	125.92	119.76
1	AA	46	ARG	CA-C-N	6.16	125.78	119.56
1	AA	46	ARG	C-N-CA	6.16	125.78	119.56
1	HP	46	ARG	CA-C-N	6.16	125.78	119.56
1	HP	46	ARG	C-N-CA	6.16	125.78	119.56
1	BE	46	ARG	CA-C-N	6.16	125.78	119.56
1	BE	46	ARG	C-N-CA	6.16	125.78	119.56
1	DM	46	ARG	CA-C-N	6.16	125.78	119.56
1	DM	46	ARG	C-N-CA	6.16	125.78	119.56
1	FJ	46	ARG	CA-C-N	6.16	125.78	119.56
1	FJ	46	ARG	C-N-CA	6.16	125.78	119.56
1	WA	46	ARG	CA-C-N	6.16	125.78	119.56
1	WA	46	ARG	C-N-CA	6.16	125.78	119.56
1	GB	46	ARG	CA-C-N	6.15	125.78	119.56
1	GB	46	ARG	C-N-CA	6.15	125.78	119.56
1	IM	46	ARG	CA-C-N	6.15	125.78	119.56
1	IM	46	ARG	C-N-CA	6.15	125.78	119.56
1	CC	33	ALA	CA-C-N	6.00	125.68	119.56
1	CC	33	ALA	C-N-CA	6.00	125.68	119.56
1	EX	33	ALA	CA-C-N	6.00	125.68	119.56
1	EX	33	ALA	C-N-CA	6.00	125.68	119.56
1	YO	33	ALA	CA-C-N	6.00	125.68	119.56
1	YO	33	ALA	C-N-CA	6.00	125.68	119.56
1	JV	33	ALA	CA-C-N	6.00	125.68	119.56
1	JV	33	ALA	C-N-CA	6.00	125.68	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BW	33	ALA	CA-C-N	6.00	125.68	119.56
1	BW	33	ALA	C-N-CA	6.00	125.68	119.56
1	ZW	33	ALA	CA-C-N	6.00	125.68	119.56
1	ZW	33	ALA	C-N-CA	6.00	125.68	119.56
1	AG	33	ALA	CA-C-N	6.00	125.67	119.56
1	AG	33	ALA	C-N-CA	6.00	125.67	119.56
1	HV	33	ALA	CA-C-N	6.00	125.67	119.56
1	HV	33	ALA	C-N-CA	6.00	125.67	119.56
1	DA	33	ALA	CA-C-N	5.99	125.67	119.56
1	DA	33	ALA	C-N-CA	5.99	125.67	119.56
1	EL	33	ALA	CA-C-N	5.99	125.67	119.56
1	EL	33	ALA	C-N-CA	5.99	125.67	119.56
1	DM	33	ALA	CA-C-N	5.99	125.67	119.56
1	DM	33	ALA	C-N-CA	5.99	125.67	119.56
1	FJ	33	ALA	CA-C-N	5.99	125.67	119.56
1	FJ	33	ALA	C-N-CA	5.99	125.67	119.56
1	AA	33	ALA	CA-C-N	5.98	125.66	119.56
1	AA	33	ALA	C-N-CA	5.98	125.66	119.56
1	HP	33	ALA	CA-C-N	5.98	125.66	119.56
1	HP	33	ALA	C-N-CA	5.98	125.66	119.56
1	AS	33	ALA	CA-C-N	5.98	125.66	119.56
1	AS	33	ALA	C-N-CA	5.98	125.66	119.56
1	GZ	33	ALA	CA-C-N	5.98	125.66	119.56
1	GZ	33	ALA	C-N-CA	5.98	125.66	119.56
1	BQ	33	ALA	CA-C-N	5.98	125.66	119.56
1	BQ	33	ALA	C-N-CA	5.98	125.66	119.56
1	ZQ	33	ALA	CA-C-N	5.98	125.66	119.56
1	ZQ	33	ALA	C-N-CA	5.98	125.66	119.56
1	YC	33	ALA	CA-C-N	5.98	125.66	119.56
1	YC	33	ALA	C-N-CA	5.98	125.66	119.56
1	BK	33	ALA	CA-C-N	5.98	125.66	119.56
1	BK	33	ALA	C-N-CA	5.98	125.66	119.56
1	CO	33	ALA	CA-C-N	5.97	125.65	119.56
1	CO	33	ALA	C-N-CA	5.97	125.65	119.56
1	ER	33	ALA	CA-C-N	5.97	125.65	119.56
1	ER	33	ALA	C-N-CA	5.97	125.65	119.56
1	IS	33	ALA	CA-C-N	5.97	125.65	119.56
1	IS	33	ALA	C-N-CA	5.97	125.65	119.56
1	LF	33	ALA	CA-C-N	5.97	125.65	119.56
1	LF	33	ALA	C-N-CA	5.97	125.65	119.56
1	GH	33	ALA	CA-C-N	5.97	125.65	119.56
1	GH	33	ALA	C-N-CA	5.97	125.65	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	WC	33	ALA	CA-C-N	5.97	125.65	119.56
1	WC	33	ALA	C-N-CA	5.97	125.65	119.56
1	ZK	33	ALA	CA-C-N	5.96	125.64	119.56
1	ZK	33	ALA	C-N-CA	5.96	125.64	119.56
1	KH	33	ALA	CA-C-N	5.96	125.64	119.56
1	KH	33	ALA	C-N-CA	5.96	125.64	119.56
1	JE	33	ALA	CA-C-N	5.96	125.64	119.56
1	JE	33	ALA	C-N-CA	5.96	125.64	119.56
1	KZ	33	ALA	CA-C-N	5.96	125.64	119.56
1	KZ	33	ALA	C-N-CA	5.96	125.64	119.56
1	BE	33	ALA	CA-C-N	5.96	125.64	119.56
1	BE	33	ALA	C-N-CA	5.96	125.64	119.56
1	WA	33	ALA	CA-C-N	5.96	125.64	119.56
1	WA	33	ALA	C-N-CA	5.96	125.64	119.56
1	DS	33	ALA	CA-C-N	5.96	125.64	119.56
1	DS	33	ALA	C-N-CA	5.96	125.64	119.56
1	FP	33	ALA	CA-C-N	5.96	125.64	119.56
1	FP	33	ALA	C-N-CA	5.96	125.64	119.56
1	AY	33	ALA	CA-C-N	5.96	125.63	119.56
1	AY	33	ALA	C-N-CA	5.96	125.63	119.56
1	WB	33	ALA	CA-C-N	5.96	125.63	119.56
1	WB	33	ALA	C-N-CA	5.96	125.63	119.56
1	AM	33	ALA	CA-C-N	5.95	125.63	119.56
1	AM	33	ALA	C-N-CA	5.95	125.63	119.56
1	ZE	33	ALA	CA-C-N	5.95	125.63	119.56
1	ZE	33	ALA	C-N-CA	5.95	125.63	119.56
1	CI	33	ALA	CA-C-N	5.95	125.62	119.56
1	CI	33	ALA	C-N-CA	5.95	125.62	119.56
1	EF	33	ALA	CA-C-N	5.95	125.62	119.56
1	EF	33	ALA	C-N-CA	5.95	125.62	119.56
1	KN	33	ALA	CA-C-N	5.94	125.62	119.56
1	KN	33	ALA	C-N-CA	5.94	125.62	119.56
1	LL	33	ALA	CA-C-N	5.94	125.62	119.56
1	LL	33	ALA	C-N-CA	5.94	125.62	119.56
1	KB	33	ALA	CA-C-N	5.94	125.62	119.56
1	KB	33	ALA	C-N-CA	5.94	125.62	119.56
1	LR	33	ALA	CA-C-N	5.94	125.62	119.56
1	LR	33	ALA	C-N-CA	5.94	125.62	119.56
1	DG	33	ALA	CA-C-N	5.94	125.62	119.56
1	DG	33	ALA	C-N-CA	5.94	125.62	119.56
1	GN	33	ALA	CA-C-N	5.94	125.62	119.56
1	GN	33	ALA	C-N-CA	5.94	125.62	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	IY	33	ALA	CA-C-N	5.94	125.62	119.56
1	IY	33	ALA	C-N-CA	5.94	125.62	119.56
1	KT	33	ALA	CA-C-N	5.94	125.62	119.56
1	KT	33	ALA	C-N-CA	5.94	125.62	119.56
1	DZ	33	ALA	CA-C-N	5.93	125.61	119.56
1	DZ	33	ALA	C-N-CA	5.93	125.61	119.56
1	FD	33	ALA	CA-C-N	5.93	125.61	119.56
1	FD	33	ALA	C-N-CA	5.93	125.61	119.56
1	FV	33	ALA	CA-C-N	5.93	125.61	119.56
1	FV	33	ALA	C-N-CA	5.93	125.61	119.56
1	IH	33	ALA	CA-C-N	5.93	125.61	119.56
1	IH	33	ALA	C-N-CA	5.93	125.61	119.56
1	CU	33	ALA	CA-C-N	5.93	125.61	119.56
1	CU	33	ALA	C-N-CA	5.93	125.61	119.56
1	GT	33	ALA	CA-C-N	5.93	125.61	119.56
1	GT	33	ALA	C-N-CA	5.93	125.61	119.56
1	GB	33	ALA	CA-C-N	5.92	125.60	119.56
1	GB	33	ALA	C-N-CA	5.92	125.60	119.56
1	IM	33	ALA	CA-C-N	5.92	125.60	119.56
1	IM	33	ALA	C-N-CA	5.92	125.60	119.56
1	YI	33	ALA	CA-C-N	5.91	125.59	119.56
1	YI	33	ALA	C-N-CA	5.91	125.59	119.56
1	JQ	33	ALA	CA-C-N	5.91	125.59	119.56
1	JQ	33	ALA	C-N-CA	5.91	125.59	119.56
1	YU	33	ALA	CA-C-N	5.91	125.58	119.56
1	YU	33	ALA	C-N-CA	5.91	125.58	119.56
1	JK	33	ALA	CA-C-N	5.91	125.58	119.56
1	JK	33	ALA	C-N-CA	5.91	125.58	119.56
1	YS	19	ARG	N-CA-C	-5.83	105.01	111.36
1	JI	19	ARG	N-CA-C	-5.83	105.01	111.36
1	YY	19	ARG	N-CA-C	-5.83	105.01	111.36
1	HN	19	ARG	N-CA-C	-5.83	105.01	111.36
1	BI	19	ARG	N-CA-C	-5.82	105.01	111.36
1	YA	19	ARG	N-CA-C	-5.82	105.01	111.36
1	JZ	19	ARG	N-CA-C	-5.82	105.02	111.36
1	LP	19	ARG	N-CA-C	-5.82	105.02	111.36
1	FT	19	ARG	N-CA-C	-5.82	105.02	111.36
1	IE	19	ARG	N-CA-C	-5.82	105.02	111.36
1	JC	19	ARG	N-CA-C	-5.82	105.02	111.36
1	KX	19	ARG	N-CA-C	-5.82	105.02	111.36
1	GF	19	ARG	N-CA-C	-5.81	105.03	111.36
1	HZ	19	ARG	N-CA-C	-5.81	105.03	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CY	19	ARG	N-CA-C	-5.81	105.03	111.36
1	EJ	19	ARG	N-CA-C	-5.81	105.03	111.36
1	CM	19	ARG	N-CA-C	-5.80	105.03	111.36
1	EP	19	ARG	N-CA-C	-5.80	105.03	111.36
1	ZI	19	ARG	N-CA-C	-5.80	105.03	111.36
1	KF	19	ARG	N-CA-C	-5.80	105.03	111.36
1	AK	19	ARG	N-CA-C	-5.80	105.04	111.36
1	ZC	19	ARG	N-CA-C	-5.80	105.04	111.36
1	KL	19	ARG	N-CA-C	-5.80	105.04	111.36
1	LJ	19	ARG	N-CA-C	-5.80	105.04	111.36
1	YG	19	ARG	N-CA-C	-5.79	105.05	111.36
1	CA	19	ARG	N-CA-C	-5.79	105.05	111.36
1	CG	19	ARG	N-CA-C	-5.79	105.05	111.36
1	DK	19	ARG	N-CA-C	-5.79	105.05	111.36
1	ED	19	ARG	N-CA-C	-5.79	105.05	111.36
1	EV	19	ARG	N-CA-C	-5.79	105.05	111.36
1	FH	19	ARG	N-CA-C	-5.79	105.05	111.36
1	IQ	19	ARG	N-CA-C	-5.79	105.05	111.36
1	JO	19	ARG	N-CA-C	-5.79	105.05	111.36
1	LD	19	ARG	N-CA-C	-5.79	105.05	111.36
1	BC	19	ARG	N-CA-C	-5.79	105.05	111.36
1	DQ	19	ARG	N-CA-C	-5.79	105.05	111.36
1	FN	19	ARG	N-CA-C	-5.79	105.05	111.36
1	HI	19	ARG	N-CA-C	-5.79	105.05	111.36
1	AP	19	ARG	N-CA-C	-5.79	105.05	111.36
1	GX	19	ARG	N-CA-C	-5.79	105.05	111.36
1	BO	19	ARG	N-CA-C	-5.78	105.06	111.36
1	ZO	19	ARG	N-CA-C	-5.78	105.06	111.36
1	AE	19	ARG	N-CA-C	-5.78	105.06	111.36
1	HT	19	ARG	N-CA-C	-5.78	105.06	111.36
1	DX	19	ARG	N-CA-C	-5.78	105.06	111.36
1	FB	19	ARG	N-CA-C	-5.78	105.06	111.36
1	AW	19	ARG	N-CA-C	-5.78	105.06	111.36
1	FZ	19	ARG	N-CA-C	-5.78	105.06	111.36
1	HD	19	ARG	N-CA-C	-5.78	105.06	111.36
1	IK	19	ARG	N-CA-C	-5.78	105.06	111.36
1	BU	19	ARG	N-CA-C	-5.78	105.06	111.36
1	ZU	19	ARG	N-CA-C	-5.78	105.06	111.36
1	DE	19	ARG	N-CA-C	-5.77	105.07	111.36
1	GL	19	ARG	N-CA-C	-5.77	105.07	111.36
1	YM	19	ARG	N-CA-C	-5.77	105.07	111.36
1	WD	19	ARG	N-CA-C	-5.77	105.07	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CS	19	ARG	N-CA-C	-5.77	105.07	111.36
1	GR	19	ARG	N-CA-C	-5.77	105.07	111.36
1	IW	19	ARG	N-CA-C	-5.77	105.07	111.36
1	KR	19	ARG	N-CA-C	-5.77	105.07	111.36
1	GH	46	ARG	CA-C-N	5.70	125.80	119.87
1	GH	46	ARG	C-N-CA	5.70	125.80	119.87
1	WC	46	ARG	CA-C-N	5.70	125.80	119.87
1	WC	46	ARG	C-N-CA	5.70	125.80	119.87
1	AY	46	ARG	CA-C-N	5.70	125.80	119.87
1	AY	46	ARG	C-N-CA	5.70	125.80	119.87
1	WB	46	ARG	CA-C-N	5.70	125.80	119.87
1	WB	46	ARG	C-N-CA	5.70	125.80	119.87
1	YI	46	ARG	CA-C-N	5.70	125.80	119.87
1	YI	46	ARG	C-N-CA	5.70	125.80	119.87
1	JQ	46	ARG	CA-C-N	5.70	125.80	119.87
1	JQ	46	ARG	C-N-CA	5.70	125.80	119.87
1	CI	46	ARG	CA-C-N	5.69	125.79	119.87
1	CI	46	ARG	C-N-CA	5.69	125.79	119.87
1	DZ	46	ARG	CA-C-N	5.69	125.78	119.87
1	DZ	46	ARG	C-N-CA	5.69	125.78	119.87
1	EF	46	ARG	CA-C-N	5.69	125.79	119.87
1	EF	46	ARG	C-N-CA	5.69	125.79	119.87
1	FD	46	ARG	CA-C-N	5.69	125.78	119.87
1	FD	46	ARG	C-N-CA	5.69	125.78	119.87
1	DG	46	ARG	CA-C-N	5.68	125.77	119.87
1	DG	46	ARG	C-N-CA	5.68	125.77	119.87
1	GN	46	ARG	CA-C-N	5.68	125.77	119.87
1	GN	46	ARG	C-N-CA	5.68	125.77	119.87
1	KB	46	ARG	CA-C-N	5.67	125.76	119.87
1	KB	46	ARG	C-N-CA	5.67	125.76	119.87
1	LR	46	ARG	CA-C-N	5.67	125.76	119.87
1	LR	46	ARG	C-N-CA	5.67	125.76	119.87
1	KN	46	ARG	CA-C-N	5.66	125.75	119.87
1	KN	46	ARG	C-N-CA	5.66	125.75	119.87
1	LL	46	ARG	CA-C-N	5.66	125.75	119.87
1	LL	46	ARG	C-N-CA	5.66	125.75	119.87
1	DS	46	ARG	CA-C-N	5.65	125.75	119.87
1	DS	46	ARG	C-N-CA	5.65	125.75	119.87
1	FP	46	ARG	CA-C-N	5.65	125.75	119.87
1	FP	46	ARG	C-N-CA	5.65	125.75	119.87
1	DA	46	ARG	CA-C-N	5.65	125.75	119.87
1	DA	46	ARG	C-N-CA	5.65	125.75	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EL	46	ARG	CA-C-N	5.65	125.75	119.87
1	EL	46	ARG	C-N-CA	5.65	125.75	119.87
1	FV	46	ARG	CA-C-N	5.65	125.75	119.87
1	FV	46	ARG	C-N-CA	5.65	125.75	119.87
1	IH	46	ARG	CA-C-N	5.65	125.75	119.87
1	IH	46	ARG	C-N-CA	5.65	125.75	119.87
1	JE	46	ARG	CA-C-N	5.65	125.74	119.87
1	JE	46	ARG	C-N-CA	5.65	125.74	119.87
1	KZ	46	ARG	CA-C-N	5.65	125.74	119.87
1	KZ	46	ARG	C-N-CA	5.65	125.74	119.87
1	CQ	33	ALA	CA-C-N	5.61	125.29	119.56
1	CQ	33	ALA	C-N-CA	5.61	125.29	119.56
1	GP	33	ALA	CA-C-N	5.61	125.29	119.56
1	GP	33	ALA	C-N-CA	5.61	125.29	119.56
1	ZG	33	ALA	CA-C-N	5.61	125.28	119.56
1	ZG	33	ALA	C-N-CA	5.61	125.28	119.56
1	KD	33	ALA	CA-C-N	5.61	125.28	119.56
1	KD	33	ALA	C-N-CA	5.61	125.28	119.56
1	GD	33	ALA	CA-C-N	5.58	125.26	119.56
1	GD	33	ALA	C-N-CA	5.58	125.26	119.56
1	HX	33	ALA	CA-C-N	5.58	125.26	119.56
1	HX	33	ALA	C-N-CA	5.58	125.26	119.56
1	YW	33	ALA	CA-C-N	5.57	125.24	119.56
1	YW	33	ALA	C-N-CA	5.57	125.24	119.56
1	HL	33	ALA	CA-C-N	5.57	125.24	119.56
1	HL	33	ALA	C-N-CA	5.57	125.24	119.56
1	IO	33	ALA	CA-C-N	5.57	125.24	119.56
1	IO	33	ALA	C-N-CA	5.57	125.24	119.56
1	LB	33	ALA	CA-C-N	5.57	125.24	119.56
1	LB	33	ALA	C-N-CA	5.57	125.24	119.56
1	YK	33	ALA	CA-C-N	5.57	125.24	119.56
1	YK	33	ALA	C-N-CA	5.57	125.24	119.56
1	JS	33	ALA	CA-C-N	5.57	125.24	119.56
1	JS	33	ALA	C-N-CA	5.57	125.24	119.56
1	AU	33	ALA	CA-C-N	5.57	125.24	119.56
1	AU	33	ALA	C-N-CA	5.57	125.24	119.56
1	HB	33	ALA	CA-C-N	5.57	125.24	119.56
1	HB	33	ALA	C-N-CA	5.57	125.24	119.56
1	JA	33	ALA	CA-C-N	5.56	125.23	119.56
1	JA	33	ALA	C-N-CA	5.56	125.23	119.56
1	KV	33	ALA	CA-C-N	5.56	125.23	119.56
1	KV	33	ALA	C-N-CA	5.56	125.23	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CK	33	ALA	CA-C-N	5.56	125.23	119.56
1	CK	33	ALA	C-N-CA	5.56	125.23	119.56
1	EN	33	ALA	CA-C-N	5.56	125.23	119.56
1	EN	33	ALA	C-N-CA	5.56	125.23	119.56
1	DO	33	ALA	CA-C-N	5.56	125.23	119.56
1	DO	33	ALA	C-N-CA	5.56	125.23	119.56
1	DU	33	ALA	CA-C-N	5.56	125.23	119.56
1	DU	33	ALA	C-N-CA	5.56	125.23	119.56
1	EZ	33	ALA	CA-C-N	5.56	125.23	119.56
1	EZ	33	ALA	C-N-CA	5.56	125.23	119.56
1	FL	33	ALA	CA-C-N	5.56	125.23	119.56
1	FL	33	ALA	C-N-CA	5.56	125.23	119.56
1	CW	33	ALA	CA-C-N	5.56	125.23	119.56
1	CW	33	ALA	C-N-CA	5.56	125.23	119.56
1	EH	33	ALA	CA-C-N	5.56	125.23	119.56
1	EH	33	ALA	C-N-CA	5.56	125.23	119.56
1	AR	33	ALA	CA-C-N	5.55	125.22	119.56
1	AR	33	ALA	C-N-CA	5.55	125.22	119.56
1	GV	33	ALA	CA-C-N	5.55	125.22	119.56
1	GV	33	ALA	C-N-CA	5.55	125.22	119.56
1	AC	60	VAL	N-CA-C	5.55	116.11	108.12
1	BS	33	ALA	CA-C-N	5.55	125.22	119.56
1	BS	33	ALA	C-N-CA	5.55	125.22	119.56
2	DD	91	ASN	CA-C-N	5.55	125.64	119.87
2	DD	91	ASN	C-N-CA	5.55	125.64	119.87
1	DI	33	ALA	CA-C-N	5.55	125.22	119.56
1	DI	33	ALA	C-N-CA	5.55	125.22	119.56
1	FF	33	ALA	CA-C-N	5.55	125.22	119.56
1	FF	33	ALA	C-N-CA	5.55	125.22	119.56
2	GK	91	ASN	CA-C-N	5.55	125.64	119.87
2	GK	91	ASN	C-N-CA	5.55	125.64	119.87
1	HR	60	VAL	N-CA-C	5.55	116.11	108.12
1	ZS	33	ALA	CA-C-N	5.55	125.22	119.56
1	ZS	33	ALA	C-N-CA	5.55	125.22	119.56
1	BA	60	VAL	N-CA-C	5.54	116.11	108.12
1	HG	60	VAL	N-CA-C	5.54	116.11	108.12
1	YE	33	ALA	CA-C-N	5.54	125.21	119.56
1	YE	33	ALA	C-N-CA	5.54	125.21	119.56
1	YE	60	VAL	N-CA-C	5.54	116.10	108.12
1	DC	33	ALA	CA-C-N	5.54	125.21	119.56
1	DC	33	ALA	C-N-CA	5.54	125.21	119.56
1	FX	33	ALA	CA-C-N	5.54	125.21	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FX	33	ALA	C-N-CA	5.54	125.21	119.56
1	GJ	33	ALA	CA-C-N	5.54	125.21	119.56
1	GJ	33	ALA	C-N-CA	5.54	125.21	119.56
1	II	33	ALA	CA-C-N	5.54	125.21	119.56
1	II	33	ALA	C-N-CA	5.54	125.21	119.56
1	JM	33	ALA	CA-C-N	5.54	125.21	119.56
1	JM	33	ALA	C-N-CA	5.54	125.21	119.56
1	JM	60	VAL	N-CA-C	5.54	116.10	108.12
1	BA	33	ALA	CA-C-N	5.54	125.21	119.56
1	BA	33	ALA	C-N-CA	5.54	125.21	119.56
1	HG	33	ALA	CA-C-N	5.54	125.21	119.56
1	HG	33	ALA	C-N-CA	5.54	125.21	119.56
1	JX	60	VAL	N-CA-C	5.54	116.10	108.12
1	LN	60	VAL	N-CA-C	5.54	116.10	108.12
1	AC	33	ALA	CA-C-N	5.54	125.21	119.56
1	AC	33	ALA	C-N-CA	5.54	125.21	119.56
1	HR	33	ALA	CA-C-N	5.54	125.21	119.56
1	HR	33	ALA	C-N-CA	5.54	125.21	119.56
1	JA	60	VAL	N-CA-C	5.54	116.10	108.12
1	KV	60	VAL	N-CA-C	5.54	116.10	108.12
1	ZA	33	ALA	CA-C-N	5.54	125.21	119.56
1	ZA	33	ALA	C-N-CA	5.54	125.21	119.56
1	AI	33	ALA	CA-C-N	5.54	125.21	119.56
1	AI	33	ALA	C-N-CA	5.54	125.21	119.56
1	DU	60	VAL	N-CA-C	5.54	116.09	108.12
1	EZ	60	VAL	N-CA-C	5.54	116.09	108.12
1	CE	60	VAL	N-CA-C	5.53	116.09	108.12
1	DC	60	VAL	N-CA-C	5.53	116.09	108.12
1	EB	60	VAL	N-CA-C	5.53	116.09	108.12
1	GJ	60	VAL	N-CA-C	5.53	116.09	108.12
1	CK	60	VAL	N-CA-C	5.53	116.09	108.12
1	EN	60	VAL	N-CA-C	5.53	116.09	108.12
2	YL	91	ASN	CA-C-N	5.53	125.62	119.87
2	YL	91	ASN	C-N-CA	5.53	125.62	119.87
1	DO	60	VAL	N-CA-C	5.53	116.08	108.12
1	FL	60	VAL	N-CA-C	5.53	116.08	108.12
2	JT	91	ASN	CA-C-N	5.53	125.62	119.87
2	JT	91	ASN	C-N-CA	5.53	125.62	119.87
1	ZA	60	VAL	N-CA-C	5.53	116.08	108.12
1	YQ	60	VAL	N-CA-C	5.53	116.08	108.12
1	AI	60	VAL	N-CA-C	5.53	116.08	108.12
2	DF	278	ARG	CA-C-N	-5.53	115.90	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DF	278	ARG	C-N-CA	-5.53	115.90	123.14
1	ZG	60	VAL	N-CA-C	5.53	116.08	108.12
2	GM	278	ARG	CA-C-N	-5.53	115.90	123.14
2	GM	278	ARG	C-N-CA	-5.53	115.90	123.14
1	JG	60	VAL	N-CA-C	5.53	116.08	108.12
1	KD	60	VAL	N-CA-C	5.53	116.08	108.12
1	ZY	33	ALA	CA-C-N	5.53	125.20	119.56
1	ZY	33	ALA	C-N-CA	5.53	125.20	119.56
1	BG	33	ALA	CA-C-N	5.53	125.20	119.56
1	BG	33	ALA	C-N-CA	5.53	125.20	119.56
1	YW	60	VAL	N-CA-C	5.53	116.08	108.12
2	AX	278	ARG	CA-C-N	-5.53	115.90	123.14
2	AX	278	ARG	C-N-CA	-5.53	115.90	123.14
1	BS	60	VAL	N-CA-C	5.53	116.08	108.12
1	CQ	60	VAL	N-CA-C	5.53	116.08	108.12
1	FR	60	VAL	N-CA-C	5.53	116.08	108.12
1	GP	60	VAL	N-CA-C	5.53	116.08	108.12
2	HE	278	ARG	CA-C-N	-5.53	115.90	123.14
2	HE	278	ARG	C-N-CA	-5.53	115.90	123.14
1	HL	60	VAL	N-CA-C	5.53	116.08	108.12
1	IC	60	VAL	N-CA-C	5.53	116.08	108.12
1	IU	60	VAL	N-CA-C	5.53	116.08	108.12
1	KP	60	VAL	N-CA-C	5.53	116.08	108.12
1	ZS	60	VAL	N-CA-C	5.53	116.08	108.12
1	YQ	33	ALA	CA-C-N	5.52	125.19	119.56
1	YQ	33	ALA	C-N-CA	5.52	125.19	119.56
2	DY	278	ARG	CA-C-N	-5.52	115.90	123.14
2	DY	278	ARG	C-N-CA	-5.52	115.90	123.14
2	FC	278	ARG	CA-C-N	-5.52	115.90	123.14
2	FC	278	ARG	C-N-CA	-5.52	115.90	123.14
2	JB	91	ASN	CA-C-N	5.52	125.61	119.87
2	JB	91	ASN	C-N-CA	5.52	125.61	119.87
1	JG	33	ALA	CA-C-N	5.52	125.19	119.56
1	JG	33	ALA	C-N-CA	5.52	125.19	119.56
2	KW	91	ASN	CA-C-N	5.52	125.61	119.87
2	KW	91	ASN	C-N-CA	5.52	125.61	119.87
1	CW	60	VAL	N-CA-C	5.52	116.07	108.12
1	EH	60	VAL	N-CA-C	5.52	116.07	108.12
1	FR	33	ALA	CA-C-N	5.52	125.19	119.56
1	FR	33	ALA	C-N-CA	5.52	125.19	119.56
2	FY	91	ASN	CA-C-N	5.52	125.61	119.87
2	FY	91	ASN	C-N-CA	5.52	125.61	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	IC	33	ALA	CA-C-N	5.52	125.19	119.56
1	IC	33	ALA	C-N-CA	5.52	125.19	119.56
2	IJ	91	ASN	CA-C-N	5.52	125.61	119.87
2	IJ	91	ASN	C-N-CA	5.52	125.61	119.87
1	IO	60	VAL	N-CA-C	5.52	116.07	108.12
1	KJ	33	ALA	CA-C-N	5.52	125.19	119.56
1	KJ	33	ALA	C-N-CA	5.52	125.19	119.56
1	LB	60	VAL	N-CA-C	5.52	116.07	108.12
1	LH	33	ALA	CA-C-N	5.52	125.19	119.56
1	LH	33	ALA	C-N-CA	5.52	125.19	119.56
1	BY	33	ALA	CA-C-N	5.52	125.19	119.56
1	BY	33	ALA	C-N-CA	5.52	125.19	119.56
2	DP	36	ASN	CA-C-N	5.52	125.42	119.85
2	DP	36	ASN	C-N-CA	5.52	125.42	119.85
1	ET	33	ALA	CA-C-N	5.52	125.19	119.56
1	ET	33	ALA	C-N-CA	5.52	125.19	119.56
2	FM	36	ASN	CA-C-N	5.52	125.42	119.85
2	FM	36	ASN	C-N-CA	5.52	125.42	119.85
2	GE	91	ASN	CA-C-N	5.52	125.61	119.87
2	GE	91	ASN	C-N-CA	5.52	125.61	119.87
2	HY	91	ASN	CA-C-N	5.52	125.61	119.87
2	HY	91	ASN	C-N-CA	5.52	125.61	119.87
1	KJ	60	VAL	N-CA-C	5.52	116.07	108.12
1	LH	60	VAL	N-CA-C	5.52	116.07	108.12
2	AF	278	ARG	CA-C-N	-5.52	115.91	123.14
2	AF	278	ARG	C-N-CA	-5.52	115.91	123.14
2	CF	91	ASN	CA-C-N	5.52	125.61	119.87
2	CF	91	ASN	C-N-CA	5.52	125.61	119.87
2	CX	36	ASN	CA-C-N	5.52	125.42	119.85
2	CX	36	ASN	C-N-CA	5.52	125.42	119.85
2	EC	91	ASN	CA-C-N	5.52	125.61	119.87
2	EC	91	ASN	C-N-CA	5.52	125.61	119.87
2	EI	36	ASN	CA-C-N	5.52	125.42	119.85
2	EI	36	ASN	C-N-CA	5.52	125.42	119.85
1	FX	60	VAL	N-CA-C	5.52	116.07	108.12
2	HU	278	ARG	CA-C-N	-5.52	115.91	123.14
2	HU	278	ARG	C-N-CA	-5.52	115.91	123.14
1	II	60	VAL	N-CA-C	5.52	116.07	108.12
2	BD	278	ARG	CA-C-N	-5.52	115.91	123.14
2	BD	278	ARG	C-N-CA	-5.52	115.91	123.14
2	BN	91	ASN	CA-C-N	5.52	125.61	119.87
2	BN	91	ASN	C-N-CA	5.52	125.61	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BY	60	VAL	N-CA-C	5.52	116.06	108.12
2	BZ	36	ASN	CA-C-N	5.52	125.42	119.85
2	BZ	36	ASN	C-N-CA	5.52	125.42	119.85
1	ET	60	VAL	N-CA-C	5.52	116.06	108.12
2	EU	36	ASN	CA-C-N	5.52	125.42	119.85
2	EU	36	ASN	C-N-CA	5.52	125.42	119.85
2	HJ	278	ARG	CA-C-N	-5.52	115.91	123.14
2	HJ	278	ARG	C-N-CA	-5.52	115.91	123.14
1	IU	33	ALA	CA-C-N	5.52	125.19	119.56
1	IU	33	ALA	C-N-CA	5.52	125.19	119.56
1	JX	33	ALA	CA-C-N	5.52	125.19	119.56
1	JX	33	ALA	C-N-CA	5.52	125.19	119.56
1	KP	33	ALA	CA-C-N	5.52	125.19	119.56
1	KP	33	ALA	C-N-CA	5.52	125.19	119.56
1	LN	33	ALA	CA-C-N	5.52	125.19	119.56
1	LN	33	ALA	C-N-CA	5.52	125.19	119.56
2	ZN	91	ASN	CA-C-N	5.52	125.61	119.87
2	ZN	91	ASN	C-N-CA	5.52	125.61	119.87
2	AO	278	ARG	CA-C-N	-5.51	115.92	123.14
2	AO	278	ARG	C-N-CA	-5.51	115.92	123.14
2	DW	141	ASP	CA-C-N	5.51	125.61	119.87
2	DW	141	ASP	C-N-CA	5.51	125.61	119.87
2	FA	141	ASP	CA-C-N	5.51	125.61	119.87
2	FA	141	ASP	C-N-CA	5.51	125.61	119.87
2	GY	278	ARG	CA-C-N	-5.51	115.92	123.14
2	GY	278	ARG	C-N-CA	-5.51	115.92	123.14
1	YK	60	VAL	N-CA-C	5.51	116.06	108.12
2	JD	278	ARG	CA-C-N	-5.51	115.92	123.14
2	JD	278	ARG	C-N-CA	-5.51	115.92	123.14
1	JS	60	VAL	N-CA-C	5.51	116.06	108.12
2	KY	278	ARG	CA-C-N	-5.51	115.92	123.14
2	KY	278	ARG	C-N-CA	-5.51	115.92	123.14
2	AV	91	ASN	CA-C-N	5.51	125.60	119.87
2	AV	91	ASN	C-N-CA	5.51	125.60	119.87
1	GD	60	VAL	N-CA-C	5.51	116.06	108.12
2	HC	91	ASN	CA-C-N	5.51	125.60	119.87
2	HC	91	ASN	C-N-CA	5.51	125.60	119.87
1	HX	60	VAL	N-CA-C	5.51	116.06	108.12
1	ZY	60	VAL	N-CA-C	5.51	116.05	108.12
1	BG	60	VAL	N-CA-C	5.51	116.05	108.12
1	AR	60	VAL	N-CA-C	5.51	116.05	108.12
1	BM	60	VAL	N-CA-C	5.51	116.05	108.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DI	60	VAL	N-CA-C	5.51	116.05	108.12
2	DP	91	ASN	CA-C-N	5.51	125.60	119.87
2	DP	91	ASN	C-N-CA	5.51	125.60	119.87
1	FF	60	VAL	N-CA-C	5.51	116.05	108.12
2	FM	91	ASN	CA-C-N	5.51	125.60	119.87
2	FM	91	ASN	C-N-CA	5.51	125.60	119.87
1	GV	60	VAL	N-CA-C	5.51	116.05	108.12
2	IP	141	ASP	CA-C-N	5.51	125.60	119.87
2	IP	141	ASP	C-N-CA	5.51	125.60	119.87
1	ZM	60	VAL	N-CA-C	5.51	116.05	108.12
2	LC	141	ASP	CA-C-N	5.51	125.60	119.87
2	LC	141	ASP	C-N-CA	5.51	125.60	119.87
2	AD	91	ASN	CA-C-N	5.51	125.60	119.87
2	AD	91	ASN	C-N-CA	5.51	125.60	119.87
2	AQ	91	ASN	CA-C-N	5.51	125.60	119.87
2	AQ	91	ASN	C-N-CA	5.51	125.60	119.87
2	BT	91	ASN	CA-C-N	5.51	125.60	119.87
2	BT	91	ASN	C-N-CA	5.51	125.60	119.87
2	FS	36	ASN	CA-C-N	5.51	125.41	119.85
2	FS	36	ASN	C-N-CA	5.51	125.41	119.85
2	GW	91	ASN	CA-C-N	5.51	125.60	119.87
2	GW	91	ASN	C-N-CA	5.51	125.60	119.87
2	HS	91	ASN	CA-C-N	5.51	125.60	119.87
2	HS	91	ASN	C-N-CA	5.51	125.60	119.87
2	ID	36	ASN	CA-C-N	5.51	125.41	119.85
2	ID	36	ASN	C-N-CA	5.51	125.41	119.85
2	ZT	91	ASN	CA-C-N	5.51	125.60	119.87
2	ZT	91	ASN	C-N-CA	5.51	125.60	119.87
2	CF	36	ASN	CA-C-N	5.50	125.41	119.85
2	CF	36	ASN	C-N-CA	5.50	125.41	119.85
2	EC	36	ASN	CA-C-N	5.50	125.41	119.85
2	EC	36	ASN	C-N-CA	5.50	125.41	119.85
2	YR	91	ASN	CA-C-N	5.50	125.59	119.87
2	YR	91	ASN	C-N-CA	5.50	125.59	119.87
2	ZB	91	ASN	CA-C-N	5.50	125.59	119.87
2	ZB	91	ASN	C-N-CA	5.50	125.59	119.87
2	AJ	91	ASN	CA-C-N	5.50	125.59	119.87
2	AJ	91	ASN	C-N-CA	5.50	125.59	119.87
2	AQ	36	ASN	CA-C-N	5.50	125.41	119.85
2	AQ	36	ASN	C-N-CA	5.50	125.41	119.85
2	GW	36	ASN	CA-C-N	5.50	125.41	119.85
2	GW	36	ASN	C-N-CA	5.50	125.41	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	JH	91	ASN	CA-C-N	5.50	125.59	119.87
2	JH	91	ASN	C-N-CA	5.50	125.59	119.87
1	AU	60	VAL	N-CA-C	5.50	116.04	108.12
1	CE	33	ALA	CA-C-N	5.50	125.17	119.56
1	CE	33	ALA	C-N-CA	5.50	125.17	119.56
1	EB	33	ALA	CA-C-N	5.50	125.17	119.56
1	EB	33	ALA	C-N-CA	5.50	125.17	119.56
1	HB	60	VAL	N-CA-C	5.50	116.04	108.12
2	DR	278	ARG	CA-C-N	-5.50	115.94	123.14
2	DR	278	ARG	C-N-CA	-5.50	115.94	123.14
2	FO	278	ARG	CA-C-N	-5.50	115.94	123.14
2	FO	278	ARG	C-N-CA	-5.50	115.94	123.14
2	KK	141	ASP	CA-C-N	5.50	125.59	119.87
2	KK	141	ASP	C-N-CA	5.50	125.59	119.87
2	LI	141	ASP	CA-C-N	5.50	125.59	119.87
2	LI	141	ASP	C-N-CA	5.50	125.59	119.87
2	ZZ	36	ASN	CA-C-N	5.50	125.40	119.85
2	ZZ	36	ASN	C-N-CA	5.50	125.40	119.85
2	BH	36	ASN	CA-C-N	5.50	125.40	119.85
2	BH	36	ASN	C-N-CA	5.50	125.40	119.85
2	DL	278	ARG	CA-C-N	-5.50	115.94	123.14
2	DL	278	ARG	C-N-CA	-5.50	115.94	123.14
2	FI	278	ARG	CA-C-N	-5.50	115.94	123.14
2	FI	278	ARG	C-N-CA	-5.50	115.94	123.14
2	YZ	278	ARG	CA-C-N	-5.50	115.94	123.14
2	YZ	278	ARG	C-N-CA	-5.50	115.94	123.14
2	ZH	91	ASN	CA-C-N	5.50	125.59	119.87
2	ZH	91	ASN	C-N-CA	5.50	125.59	119.87
2	HO	278	ARG	CA-C-N	-5.50	115.94	123.14
2	HO	278	ARG	C-N-CA	-5.50	115.94	123.14
2	KE	91	ASN	CA-C-N	5.50	125.59	119.87
2	KE	91	ASN	C-N-CA	5.50	125.59	119.87
2	KK	91	ASN	CA-C-N	5.50	125.59	119.87
2	KK	91	ASN	C-N-CA	5.50	125.59	119.87
2	LI	91	ASN	CA-C-N	5.50	125.59	119.87
2	LI	91	ASN	C-N-CA	5.50	125.59	119.87
2	FS	91	ASN	CA-C-N	5.50	125.58	119.87
2	FS	91	ASN	C-N-CA	5.50	125.58	119.87
2	ID	91	ASN	CA-C-N	5.50	125.58	119.87
2	ID	91	ASN	C-N-CA	5.50	125.58	119.87
2	YT	278	ARG	CA-C-N	-5.49	115.94	123.14
2	YT	278	ARG	C-N-CA	-5.49	115.94	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BZ	91	ASN	CA-C-N	5.49	125.58	119.87
2	BZ	91	ASN	C-N-CA	5.49	125.58	119.87
2	EU	91	ASN	CA-C-N	5.49	125.58	119.87
2	EU	91	ASN	C-N-CA	5.49	125.58	119.87
2	GA	278	ARG	CA-C-N	-5.49	115.94	123.14
2	GA	278	ARG	C-N-CA	-5.49	115.94	123.14
2	IL	278	ARG	CA-C-N	-5.49	115.94	123.14
2	IL	278	ARG	C-N-CA	-5.49	115.94	123.14
2	IV	91	ASN	CA-C-N	5.49	125.58	119.87
2	IV	91	ASN	C-N-CA	5.49	125.58	119.87
2	JJ	278	ARG	CA-C-N	-5.49	115.94	123.14
2	JJ	278	ARG	C-N-CA	-5.49	115.94	123.14
2	KQ	91	ASN	CA-C-N	5.49	125.58	119.87
2	KQ	91	ASN	C-N-CA	5.49	125.58	119.87
2	BN	36	ASN	CA-C-N	5.49	125.39	119.85
2	BN	36	ASN	C-N-CA	5.49	125.39	119.85
2	CL	36	ASN	CA-C-N	5.49	125.39	119.85
2	CL	36	ASN	C-N-CA	5.49	125.39	119.85
2	CL	91	ASN	CA-C-N	5.49	125.58	119.87
2	CL	91	ASN	C-N-CA	5.49	125.58	119.87
2	EO	36	ASN	CA-C-N	5.49	125.39	119.85
2	EO	36	ASN	C-N-CA	5.49	125.39	119.85
2	EO	91	ASN	CA-C-N	5.49	125.58	119.87
2	EO	91	ASN	C-N-CA	5.49	125.58	119.87
2	IR	278	ARG	CA-C-N	-5.49	115.95	123.14
2	IR	278	ARG	C-N-CA	-5.49	115.95	123.14
2	KA	278	ARG	CA-C-N	-5.49	115.95	123.14
2	KA	278	ARG	C-N-CA	-5.49	115.95	123.14
2	LE	278	ARG	CA-C-N	-5.49	115.95	123.14
2	LE	278	ARG	C-N-CA	-5.49	115.95	123.14
2	LQ	278	ARG	CA-C-N	-5.49	115.95	123.14
2	LQ	278	ARG	C-N-CA	-5.49	115.95	123.14
2	ZN	36	ASN	CA-C-N	5.49	125.39	119.85
2	ZN	36	ASN	C-N-CA	5.49	125.39	119.85
2	YR	36	ASN	CA-C-N	5.49	125.39	119.85
2	YR	36	ASN	C-N-CA	5.49	125.39	119.85
2	DW	91	ASN	CA-C-N	5.49	125.58	119.87
2	DW	91	ASN	C-N-CA	5.49	125.58	119.87
2	FA	91	ASN	CA-C-N	5.49	125.58	119.87
2	FA	91	ASN	C-N-CA	5.49	125.58	119.87
2	JH	36	ASN	CA-C-N	5.49	125.39	119.85
2	JH	36	ASN	C-N-CA	5.49	125.39	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	KK	36	ASN	CA-C-N	5.49	125.39	119.85
2	KK	36	ASN	C-N-CA	5.49	125.39	119.85
2	KM	278	ARG	CA-C-N	-5.49	115.95	123.14
2	KM	278	ARG	C-N-CA	-5.49	115.95	123.14
2	LI	36	ASN	CA-C-N	5.49	125.39	119.85
2	LI	36	ASN	C-N-CA	5.49	125.39	119.85
2	LK	278	ARG	CA-C-N	-5.49	115.95	123.14
2	LK	278	ARG	C-N-CA	-5.49	115.95	123.14
2	BP	278	ARG	CA-C-N	-5.49	115.95	123.14
2	BP	278	ARG	C-N-CA	-5.49	115.95	123.14
2	ZP	278	ARG	CA-C-N	-5.49	115.95	123.14
2	ZP	278	ARG	C-N-CA	-5.49	115.95	123.14
2	GE	36	ASN	CA-C-N	5.49	125.39	119.85
2	GE	36	ASN	C-N-CA	5.49	125.39	119.85
2	HY	36	ASN	CA-C-N	5.49	125.39	119.85
2	HY	36	ASN	C-N-CA	5.49	125.39	119.85
2	ZJ	278	ARG	CA-C-N	-5.49	115.95	123.14
2	ZJ	278	ARG	C-N-CA	-5.49	115.95	123.14
2	KG	278	ARG	CA-C-N	-5.49	115.95	123.14
2	KG	278	ARG	C-N-CA	-5.49	115.95	123.14
2	AL	278	ARG	CA-C-N	-5.48	115.96	123.14
2	AL	278	ARG	C-N-CA	-5.48	115.96	123.14
2	ZD	278	ARG	CA-C-N	-5.48	115.96	123.14
2	ZD	278	ARG	C-N-CA	-5.48	115.96	123.14
2	CN	278	ARG	CA-C-N	-5.48	115.96	123.14
2	CN	278	ARG	C-N-CA	-5.48	115.96	123.14
2	CX	91	ASN	CA-C-N	5.48	125.57	119.87
2	CX	91	ASN	C-N-CA	5.48	125.57	119.87
2	EI	91	ASN	CA-C-N	5.48	125.57	119.87
2	EI	91	ASN	C-N-CA	5.48	125.57	119.87
2	EQ	278	ARG	CA-C-N	-5.48	115.96	123.14
2	EQ	278	ARG	C-N-CA	-5.48	115.96	123.14
2	FU	278	ARG	CA-C-N	-5.48	115.96	123.14
2	FU	278	ARG	C-N-CA	-5.48	115.96	123.14
2	IF	278	ARG	CA-C-N	-5.48	115.96	123.14
2	IF	278	ARG	C-N-CA	-5.48	115.96	123.14
2	IV	36	ASN	CA-C-N	5.48	125.39	119.85
2	IV	36	ASN	C-N-CA	5.48	125.39	119.85
2	KQ	36	ASN	CA-C-N	5.48	125.39	119.85
2	KQ	36	ASN	C-N-CA	5.48	125.39	119.85
2	CT	278	ARG	CA-C-N	-5.48	115.96	123.14
2	CT	278	ARG	C-N-CA	-5.48	115.96	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GS	278	ARG	CA-C-N	-5.48	115.96	123.14
2	GS	278	ARG	C-N-CA	-5.48	115.96	123.14
2	IP	36	ASN	CA-C-N	5.48	125.39	119.85
2	IP	36	ASN	C-N-CA	5.48	125.39	119.85
2	JY	91	ASN	CA-C-N	5.48	125.57	119.87
2	JY	91	ASN	C-N-CA	5.48	125.57	119.87
2	LC	36	ASN	CA-C-N	5.48	125.39	119.85
2	LC	36	ASN	C-N-CA	5.48	125.39	119.85
2	LO	91	ASN	CA-C-N	5.48	125.57	119.87
2	LO	91	ASN	C-N-CA	5.48	125.57	119.87
2	CL	141	ASP	CA-C-N	5.48	125.57	119.87
2	CL	141	ASP	C-N-CA	5.48	125.57	119.87
2	DJ	36	ASN	CA-C-N	5.48	125.38	119.85
2	DJ	36	ASN	C-N-CA	5.48	125.38	119.85
2	EO	141	ASP	CA-C-N	5.48	125.57	119.87
2	EO	141	ASP	C-N-CA	5.48	125.57	119.87
2	FG	36	ASN	CA-C-N	5.48	125.38	119.85
2	FG	36	ASN	C-N-CA	5.48	125.38	119.85
2	BZ	141	ASP	CA-C-N	5.48	125.57	119.87
2	BZ	141	ASP	C-N-CA	5.48	125.57	119.87
2	CZ	278	ARG	CA-C-N	-5.48	115.97	123.14
2	CZ	278	ARG	C-N-CA	-5.48	115.97	123.14
2	EK	278	ARG	CA-C-N	-5.48	115.97	123.14
2	EK	278	ARG	C-N-CA	-5.48	115.97	123.14
2	EU	141	ASP	CA-C-N	5.48	125.57	119.87
2	EU	141	ASP	C-N-CA	5.48	125.57	119.87
2	GG	278	ARG	CA-C-N	-5.48	115.97	123.14
2	GG	278	ARG	C-N-CA	-5.48	115.97	123.14
2	IA	278	ARG	CA-C-N	-5.48	115.97	123.14
2	IA	278	ARG	C-N-CA	-5.48	115.97	123.14
2	YN	278	ARG	CA-C-N	-5.48	115.97	123.14
2	YN	278	ARG	C-N-CA	-5.48	115.97	123.14
2	ZH	36	ASN	CA-C-N	5.48	125.38	119.85
2	ZH	36	ASN	C-N-CA	5.48	125.38	119.85
2	JU	278	ARG	CA-C-N	-5.48	115.97	123.14
2	JU	278	ARG	C-N-CA	-5.48	115.97	123.14
2	KE	36	ASN	CA-C-N	5.48	125.38	119.85
2	KE	36	ASN	C-N-CA	5.48	125.38	119.85
2	BJ	278	ARG	CA-C-N	-5.47	115.97	123.14
2	BJ	278	ARG	C-N-CA	-5.47	115.97	123.14
1	BM	33	ALA	CA-C-N	5.47	125.14	119.56
1	BM	33	ALA	C-N-CA	5.47	125.14	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DJ	141	ASP	CA-C-N	5.47	125.56	119.87
2	DJ	141	ASP	C-N-CA	5.47	125.56	119.87
2	FG	141	ASP	CA-C-N	5.47	125.56	119.87
2	FG	141	ASP	C-N-CA	5.47	125.56	119.87
2	JB	36	ASN	CA-C-N	5.47	125.38	119.85
2	JB	36	ASN	C-N-CA	5.47	125.38	119.85
2	KW	36	ASN	CA-C-N	5.47	125.38	119.85
2	KW	36	ASN	C-N-CA	5.47	125.38	119.85
1	ZM	33	ALA	CA-C-N	5.47	125.14	119.56
1	ZM	33	ALA	C-N-CA	5.47	125.14	119.56
2	YB	278	ARG	CA-C-N	-5.47	115.97	123.14
2	YB	278	ARG	C-N-CA	-5.47	115.97	123.14
2	AV	36	ASN	CA-C-N	5.47	125.38	119.85
2	AV	36	ASN	C-N-CA	5.47	125.38	119.85
2	BB	141	ASP	CA-C-N	5.47	125.56	119.87
2	BB	141	ASP	C-N-CA	5.47	125.56	119.87
2	HC	36	ASN	CA-C-N	5.47	125.38	119.85
2	HC	36	ASN	C-N-CA	5.47	125.38	119.85
2	HH	141	ASP	CA-C-N	5.47	125.56	119.87
2	HH	141	ASP	C-N-CA	5.47	125.56	119.87
2	YX	91	ASN	CA-C-N	5.47	125.56	119.87
2	YX	91	ASN	C-N-CA	5.47	125.56	119.87
2	DD	141	ASP	CA-C-N	5.47	125.56	119.87
2	DD	141	ASP	C-N-CA	5.47	125.56	119.87
2	GK	141	ASP	CA-C-N	5.47	125.56	119.87
2	GK	141	ASP	C-N-CA	5.47	125.56	119.87
2	HM	91	ASN	CA-C-N	5.47	125.56	119.87
2	HM	91	ASN	C-N-CA	5.47	125.56	119.87
2	ZZ	91	ASN	CA-C-N	5.47	125.56	119.87
2	ZZ	91	ASN	C-N-CA	5.47	125.56	119.87
2	YL	36	ASN	CA-C-N	5.47	125.37	119.85
2	YL	36	ASN	C-N-CA	5.47	125.37	119.85
2	ZB	36	ASN	CA-C-N	5.47	125.37	119.85
2	ZB	36	ASN	C-N-CA	5.47	125.37	119.85
2	AJ	36	ASN	CA-C-N	5.47	125.37	119.85
2	AJ	36	ASN	C-N-CA	5.47	125.37	119.85
2	BH	91	ASN	CA-C-N	5.47	125.56	119.87
2	BH	91	ASN	C-N-CA	5.47	125.56	119.87
2	CH	278	ARG	CA-C-N	-5.47	115.97	123.14
2	CH	278	ARG	C-N-CA	-5.47	115.97	123.14
2	EE	278	ARG	CA-C-N	-5.47	115.97	123.14
2	EE	278	ARG	C-N-CA	-5.47	115.97	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	JT	36	ASN	CA-C-N	5.47	125.37	119.85
2	JT	36	ASN	C-N-CA	5.47	125.37	119.85
2	CR	36	ASN	CA-C-N	5.47	125.37	119.85
2	CR	36	ASN	C-N-CA	5.47	125.37	119.85
2	DJ	91	ASN	CA-C-N	5.47	125.56	119.87
2	DJ	91	ASN	C-N-CA	5.47	125.56	119.87
2	FG	91	ASN	CA-C-N	5.47	125.56	119.87
2	FG	91	ASN	C-N-CA	5.47	125.56	119.87
2	GQ	36	ASN	CA-C-N	5.47	125.37	119.85
2	GQ	36	ASN	C-N-CA	5.47	125.37	119.85
2	YH	278	ARG	CA-C-N	-5.47	115.98	123.14
2	YH	278	ARG	C-N-CA	-5.47	115.98	123.14
2	IX	278	ARG	CA-C-N	-5.47	115.98	123.14
2	IX	278	ARG	C-N-CA	-5.47	115.98	123.14
2	JP	278	ARG	CA-C-N	-5.47	115.98	123.14
2	JP	278	ARG	C-N-CA	-5.47	115.98	123.14
2	KS	278	ARG	CA-C-N	-5.47	115.98	123.14
2	KS	278	ARG	C-N-CA	-5.47	115.98	123.14
2	ZZ	141	ASP	CA-C-N	5.46	125.55	119.87
2	ZZ	141	ASP	C-N-CA	5.46	125.55	119.87
2	BH	141	ASP	CA-C-N	5.46	125.55	119.87
2	BH	141	ASP	C-N-CA	5.46	125.55	119.87
2	DW	36	ASN	CA-C-N	5.46	125.37	119.85
2	DW	36	ASN	C-N-CA	5.46	125.37	119.85
2	FA	36	ASN	CA-C-N	5.46	125.37	119.85
2	FA	36	ASN	C-N-CA	5.46	125.37	119.85
2	ZB	141	ASP	CA-C-N	5.46	125.55	119.87
2	ZB	141	ASP	C-N-CA	5.46	125.55	119.87
2	AD	36	ASN	CA-C-N	5.46	125.37	119.85
2	AD	36	ASN	C-N-CA	5.46	125.37	119.85
2	AJ	141	ASP	CA-C-N	5.46	125.55	119.87
2	AJ	141	ASP	C-N-CA	5.46	125.55	119.87
2	CR	141	ASP	CA-C-N	5.46	125.55	119.87
2	CR	141	ASP	C-N-CA	5.46	125.55	119.87
2	CX	141	ASP	CA-C-N	5.46	125.55	119.87
2	CX	141	ASP	C-N-CA	5.46	125.55	119.87
2	EI	141	ASP	CA-C-N	5.46	125.55	119.87
2	EI	141	ASP	C-N-CA	5.46	125.55	119.87
2	GQ	141	ASP	CA-C-N	5.46	125.55	119.87
2	GQ	141	ASP	C-N-CA	5.46	125.55	119.87
2	HS	36	ASN	CA-C-N	5.46	125.37	119.85
2	HS	36	ASN	C-N-CA	5.46	125.37	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YX	141	ASP	CA-C-N	5.46	125.55	119.87
2	YX	141	ASP	C-N-CA	5.46	125.55	119.87
2	BV	278	ARG	CA-C-N	-5.46	115.98	123.14
2	BV	278	ARG	C-N-CA	-5.46	115.98	123.14
2	HM	141	ASP	CA-C-N	5.46	125.55	119.87
2	HM	141	ASP	C-N-CA	5.46	125.55	119.87
2	IP	91	ASN	CA-C-N	5.46	125.55	119.87
2	IP	91	ASN	C-N-CA	5.46	125.55	119.87
2	LC	91	ASN	CA-C-N	5.46	125.55	119.87
2	LC	91	ASN	C-N-CA	5.46	125.55	119.87
2	ZV	278	ARG	CA-C-N	-5.46	115.98	123.14
2	ZV	278	ARG	C-N-CA	-5.46	115.98	123.14
2	YR	141	ASP	CA-C-N	5.46	125.55	119.87
2	YR	141	ASP	C-N-CA	5.46	125.55	119.87
2	YX	36	ASN	CA-C-N	5.46	125.36	119.85
2	YX	36	ASN	C-N-CA	5.46	125.36	119.85
2	CR	91	ASN	CA-C-N	5.46	125.55	119.87
2	CR	91	ASN	C-N-CA	5.46	125.55	119.87
2	GQ	91	ASN	CA-C-N	5.46	125.55	119.87
2	GQ	91	ASN	C-N-CA	5.46	125.55	119.87
2	HM	36	ASN	CA-C-N	5.46	125.36	119.85
2	HM	36	ASN	C-N-CA	5.46	125.36	119.85
2	JH	141	ASP	CA-C-N	5.46	125.55	119.87
2	JH	141	ASP	C-N-CA	5.46	125.55	119.87
2	IV	141	ASP	CA-C-N	5.46	125.54	119.87
2	IV	141	ASP	C-N-CA	5.46	125.54	119.87
2	KQ	141	ASP	CA-C-N	5.46	125.54	119.87
2	KQ	141	ASP	C-N-CA	5.46	125.54	119.87
2	YF	141	ASP	CA-C-N	5.45	125.54	119.87
2	YF	141	ASP	C-N-CA	5.45	125.54	119.87
2	JN	141	ASP	CA-C-N	5.45	125.54	119.87
2	JN	141	ASP	C-N-CA	5.45	125.54	119.87
2	CB	278	ARG	CA-C-N	-5.45	116.00	123.14
2	CB	278	ARG	C-N-CA	-5.45	116.00	123.14
2	EW	278	ARG	CA-C-N	-5.45	116.00	123.14
2	EW	278	ARG	C-N-CA	-5.45	116.00	123.14
2	GE	141	ASP	CA-C-N	5.45	125.54	119.87
2	GE	141	ASP	C-N-CA	5.45	125.54	119.87
2	HY	141	ASP	CA-C-N	5.45	125.54	119.87
2	HY	141	ASP	C-N-CA	5.45	125.54	119.87
2	JB	141	ASP	CA-C-N	5.45	125.54	119.87
2	JB	141	ASP	C-N-CA	5.45	125.54	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	KW	141	ASP	CA-C-N	5.45	125.54	119.87
2	KW	141	ASP	C-N-CA	5.45	125.54	119.87
2	CF	141	ASP	CA-C-N	5.45	125.54	119.87
2	CF	141	ASP	C-N-CA	5.45	125.54	119.87
2	EC	141	ASP	CA-C-N	5.45	125.54	119.87
2	EC	141	ASP	C-N-CA	5.45	125.54	119.87
2	YF	36	ASN	CA-C-N	5.45	125.35	119.85
2	YF	36	ASN	C-N-CA	5.45	125.35	119.85
2	JN	36	ASN	CA-C-N	5.45	125.35	119.85
2	JN	36	ASN	C-N-CA	5.45	125.35	119.85
2	AQ	141	ASP	CA-C-N	5.45	125.53	119.87
2	AQ	141	ASP	C-N-CA	5.45	125.53	119.87
2	BN	141	ASP	CA-C-N	5.45	125.53	119.87
2	BN	141	ASP	C-N-CA	5.45	125.53	119.87
2	BT	141	ASP	CA-C-N	5.45	125.53	119.87
2	BT	141	ASP	C-N-CA	5.45	125.53	119.87
2	GW	141	ASP	CA-C-N	5.45	125.53	119.87
2	GW	141	ASP	C-N-CA	5.45	125.53	119.87
2	JY	141	ASP	CA-C-N	5.45	125.53	119.87
2	JY	141	ASP	C-N-CA	5.45	125.53	119.87
2	LO	141	ASP	CA-C-N	5.45	125.53	119.87
2	LO	141	ASP	C-N-CA	5.45	125.53	119.87
2	ZN	141	ASP	CA-C-N	5.45	125.53	119.87
2	ZN	141	ASP	C-N-CA	5.45	125.53	119.87
2	ZT	141	ASP	CA-C-N	5.45	125.53	119.87
2	ZT	141	ASP	C-N-CA	5.45	125.53	119.87
2	BB	36	ASN	CA-C-N	5.44	125.35	119.85
2	BB	36	ASN	C-N-CA	5.44	125.35	119.85
2	HH	36	ASN	CA-C-N	5.44	125.35	119.85
2	HH	36	ASN	C-N-CA	5.44	125.35	119.85
2	YF	91	ASN	CA-C-N	5.44	125.53	119.87
2	YF	91	ASN	C-N-CA	5.44	125.53	119.87
2	DP	141	ASP	CA-C-N	5.44	125.53	119.87
2	DP	141	ASP	C-N-CA	5.44	125.53	119.87
2	FM	141	ASP	CA-C-N	5.44	125.53	119.87
2	FM	141	ASP	C-N-CA	5.44	125.53	119.87
2	JN	91	ASN	CA-C-N	5.44	125.53	119.87
2	JN	91	ASN	C-N-CA	5.44	125.53	119.87
2	BT	36	ASN	CA-C-N	5.44	125.34	119.85
2	BT	36	ASN	C-N-CA	5.44	125.34	119.85
2	ZT	36	ASN	CA-C-N	5.44	125.34	119.85
2	ZT	36	ASN	C-N-CA	5.44	125.34	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	FY	141	ASP	CA-C-N	5.44	125.52	119.87
2	FY	141	ASP	C-N-CA	5.44	125.52	119.87
2	IJ	141	ASP	CA-C-N	5.44	125.52	119.87
2	IJ	141	ASP	C-N-CA	5.44	125.52	119.87
2	YL	141	ASP	CA-C-N	5.43	125.52	119.87
2	YL	141	ASP	C-N-CA	5.43	125.52	119.87
2	ZH	141	ASP	CA-C-N	5.43	125.52	119.87
2	ZH	141	ASP	C-N-CA	5.43	125.52	119.87
2	JT	141	ASP	CA-C-N	5.43	125.52	119.87
2	JT	141	ASP	C-N-CA	5.43	125.52	119.87
2	KE	141	ASP	CA-C-N	5.43	125.52	119.87
2	KE	141	ASP	C-N-CA	5.43	125.52	119.87
2	DD	36	ASN	CA-C-N	5.43	125.34	119.85
2	DD	36	ASN	C-N-CA	5.43	125.34	119.85
2	GK	36	ASN	CA-C-N	5.43	125.34	119.85
2	GK	36	ASN	C-N-CA	5.43	125.34	119.85
2	FS	141	ASP	CA-C-N	5.43	125.52	119.87
2	FS	141	ASP	C-N-CA	5.43	125.52	119.87
2	ID	141	ASP	CA-C-N	5.43	125.52	119.87
2	ID	141	ASP	C-N-CA	5.43	125.52	119.87
2	JY	36	ASN	CA-C-N	5.43	125.33	119.85
2	JY	36	ASN	C-N-CA	5.43	125.33	119.85
2	LO	36	ASN	CA-C-N	5.43	125.33	119.85
2	LO	36	ASN	C-N-CA	5.43	125.33	119.85
2	BB	91	ASN	CA-C-N	5.43	125.52	119.87
2	BB	91	ASN	C-N-CA	5.43	125.52	119.87
2	FY	36	ASN	CA-C-N	5.43	125.33	119.85
2	FY	36	ASN	C-N-CA	5.43	125.33	119.85
2	HH	91	ASN	CA-C-N	5.43	125.52	119.87
2	HH	91	ASN	C-N-CA	5.43	125.52	119.87
2	IJ	36	ASN	CA-C-N	5.43	125.33	119.85
2	IJ	36	ASN	C-N-CA	5.43	125.33	119.85
2	AV	141	ASP	CA-C-N	5.42	125.51	119.87
2	AV	141	ASP	C-N-CA	5.42	125.51	119.87
2	HC	141	ASP	CA-C-N	5.42	125.51	119.87
2	HC	141	ASP	C-N-CA	5.42	125.51	119.87
2	DN	227	ILE	CB-CA-C	-5.42	105.04	111.97
2	FK	227	ILE	CB-CA-C	-5.42	105.04	111.97
2	AD	141	ASP	CA-C-N	5.41	125.50	119.87
2	AD	141	ASP	C-N-CA	5.41	125.50	119.87
2	HS	141	ASP	CA-C-N	5.41	125.50	119.87
2	HS	141	ASP	C-N-CA	5.41	125.50	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	ZL	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	KI	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	BX	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	IT	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	LG	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	ZX	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	GC	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	IN	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	GI	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	IB	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	IZ	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	KU	227	ILE	CB-CA-C	-5.39	105.07	111.97
2	YV	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	BR	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	DH	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	GO	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	JL	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	ZR	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	CV	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	GU	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	AN	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	ZF	227	ILE	CB-CA-C	-5.38	105.08	111.97
2	YJ	227	ILE	CB-CA-C	-5.38	105.09	111.97
2	AZ	227	ILE	CB-CA-C	-5.38	105.09	111.97
2	HF	227	ILE	CB-CA-C	-5.38	105.09	111.97
2	JR	227	ILE	CB-CA-C	-5.38	105.09	111.97
2	FW	227	ILE	CB-CA-C	-5.38	105.09	111.97
2	IG	227	ILE	CB-CA-C	-5.38	105.09	111.97
2	YP	227	ILE	CB-CA-C	-5.38	105.09	111.97
2	JW	227	ILE	CB-CA-C	-5.38	105.09	111.97
2	CJ	227	ILE	CB-CA-C	-5.37	105.09	111.97
2	EG	227	ILE	CB-CA-C	-5.37	105.09	111.97
2	AT	227	ILE	CB-CA-C	-5.37	105.09	111.97
2	DB	227	ILE	CB-CA-C	-5.37	105.09	111.97
2	EM	227	ILE	CB-CA-C	-5.37	105.09	111.97
2	HA	227	ILE	CB-CA-C	-5.37	105.09	111.97
2	KC	227	ILE	CB-CA-C	-5.37	105.09	111.97
2	LS	227	ILE	CB-CA-C	-5.37	105.09	111.97
2	AB	227	ILE	CB-CA-C	-5.37	105.10	111.97
2	HQ	227	ILE	CB-CA-C	-5.37	105.10	111.97
2	KO	227	ILE	CB-CA-C	-5.37	105.10	111.97
2	LM	227	ILE	CB-CA-C	-5.37	105.10	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YD	227	ILE	CB-CA-C	-5.37	105.10	111.97
2	BL	227	ILE	CB-CA-C	-5.37	105.10	111.97
2	CP	227	ILE	CB-CA-C	-5.37	105.10	111.97
2	ES	227	ILE	CB-CA-C	-5.37	105.10	111.97
2	BF	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	CD	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	EY	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	HK	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	EA	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	FE	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	DT	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	FQ	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	JF	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	LA	227	ILE	CB-CA-C	-5.36	105.11	111.97
2	AH	227	ILE	CB-CA-C	-5.34	105.13	111.97
2	HW	227	ILE	CB-CA-C	-5.34	105.13	111.97
1	CS	36	VAL	N-CA-C	-5.33	105.18	110.62
1	GR	36	VAL	N-CA-C	-5.33	105.18	110.62
1	IQ	36	VAL	N-CA-C	-5.33	105.19	110.62
1	LD	36	VAL	N-CA-C	-5.33	105.19	110.62
1	JZ	36	VAL	N-CA-C	-5.31	105.20	110.62
1	LP	36	VAL	N-CA-C	-5.31	105.20	110.62
1	CM	36	VAL	N-CA-C	-5.31	105.20	110.62
1	EP	36	VAL	N-CA-C	-5.31	105.20	110.62
1	AW	36	VAL	N-CA-C	-5.30	105.21	110.62
1	CY	35	VAL	N-CA-C	-5.30	105.22	111.00
1	DX	36	VAL	N-CA-C	-5.30	105.21	110.62
1	EJ	35	VAL	N-CA-C	-5.30	105.22	111.00
1	FB	36	VAL	N-CA-C	-5.30	105.21	110.62
1	HD	36	VAL	N-CA-C	-5.30	105.21	110.62
1	FT	36	VAL	N-CA-C	-5.30	105.22	110.62
1	IE	36	VAL	N-CA-C	-5.30	105.22	110.62
1	YS	36	VAL	N-CA-C	-5.30	105.22	110.62
1	CA	36	VAL	N-CA-C	-5.30	105.22	110.62
1	EV	36	VAL	N-CA-C	-5.30	105.22	110.62
1	JI	36	VAL	N-CA-C	-5.30	105.22	110.62
1	ZI	36	VAL	N-CA-C	-5.29	105.22	110.62
1	KF	36	VAL	N-CA-C	-5.29	105.22	110.62
1	BA	1	PRO	CA-C-N	5.29	128.99	121.42
1	BA	1	PRO	C-N-CA	5.29	128.99	121.42
1	HG	1	PRO	CA-C-N	5.29	128.99	121.42
1	HG	1	PRO	C-N-CA	5.29	128.99	121.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DO	1	PRO	CA-C-N	5.29	128.99	121.42
1	DO	1	PRO	C-N-CA	5.29	128.99	121.42
1	FL	1	PRO	CA-C-N	5.29	128.99	121.42
1	FL	1	PRO	C-N-CA	5.29	128.99	121.42
1	IW	36	VAL	N-CA-C	-5.29	105.22	110.62
1	JC	35	VAL	N-CA-C	-5.29	105.23	111.00
1	KR	36	VAL	N-CA-C	-5.29	105.22	110.62
1	KX	35	VAL	N-CA-C	-5.29	105.23	111.00
1	CG	36	VAL	N-CA-C	-5.29	105.22	110.62
1	DE	36	VAL	N-CA-C	-5.29	105.22	110.62
1	ED	36	VAL	N-CA-C	-5.29	105.22	110.62
1	GL	36	VAL	N-CA-C	-5.29	105.22	110.62
1	DQ	36	VAL	N-CA-C	-5.29	105.22	110.62
1	FN	36	VAL	N-CA-C	-5.29	105.22	110.62
1	YW	1	PRO	CA-C-N	5.29	128.98	121.42
1	YW	1	PRO	C-N-CA	5.29	128.98	121.42
1	AK	36	VAL	N-CA-C	-5.29	105.23	110.62
1	ZC	36	VAL	N-CA-C	-5.29	105.23	110.62
1	CM	35	VAL	N-CA-C	-5.29	105.24	111.00
1	DE	35	VAL	N-CA-C	-5.29	105.24	111.00
1	EP	35	VAL	N-CA-C	-5.29	105.24	111.00
1	GL	35	VAL	N-CA-C	-5.29	105.24	111.00
1	HL	1	PRO	CA-C-N	5.29	128.98	121.42
1	HL	1	PRO	C-N-CA	5.29	128.98	121.42
1	CY	36	VAL	N-CA-C	-5.29	105.23	110.62
1	EJ	36	VAL	N-CA-C	-5.29	105.23	110.62
1	FZ	36	VAL	N-CA-C	-5.29	105.23	110.62
1	IK	36	VAL	N-CA-C	-5.29	105.23	110.62
1	KL	35	VAL	N-CA-C	-5.29	105.24	111.00
1	LJ	35	VAL	N-CA-C	-5.29	105.24	111.00
1	ZY	1	PRO	CA-C-N	5.28	128.98	121.42
1	ZY	1	PRO	C-N-CA	5.28	128.98	121.42
1	YY	35	VAL	N-CA-C	-5.28	105.24	111.00
1	AP	35	VAL	N-CA-C	-5.28	105.24	111.00
1	BG	1	PRO	CA-C-N	5.28	128.98	121.42
1	BG	1	PRO	C-N-CA	5.28	128.98	121.42
1	GX	35	VAL	N-CA-C	-5.28	105.24	111.00
1	HN	35	VAL	N-CA-C	-5.28	105.24	111.00
1	YS	35	VAL	N-CA-C	-5.28	105.24	111.00
1	JI	35	VAL	N-CA-C	-5.28	105.24	111.00
1	YG	35	VAL	N-CA-C	-5.28	105.25	111.00
1	BC	36	VAL	N-CA-C	-5.28	105.24	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DK	36	VAL	N-CA-C	-5.28	105.24	110.62
1	FH	36	VAL	N-CA-C	-5.28	105.24	110.62
1	HI	36	VAL	N-CA-C	-5.28	105.24	110.62
1	JO	35	VAL	N-CA-C	-5.28	105.25	111.00
1	JZ	35	VAL	N-CA-C	-5.28	105.25	111.00
1	LP	35	VAL	N-CA-C	-5.28	105.25	111.00
1	BI	35	VAL	N-CA-C	-5.28	105.25	111.00
1	JC	36	VAL	N-CA-C	-5.28	105.24	110.62
1	KX	36	VAL	N-CA-C	-5.28	105.24	110.62
1	YA	35	VAL	N-CA-C	-5.28	105.25	111.00
1	ZG	1	PRO	CA-C-N	5.27	128.96	121.42
1	ZG	1	PRO	C-N-CA	5.27	128.96	121.42
1	IO	1	PRO	CA-C-N	5.27	128.96	121.42
1	IO	1	PRO	C-N-CA	5.27	128.96	121.42
1	KD	1	PRO	CA-C-N	5.27	128.96	121.42
1	KD	1	PRO	C-N-CA	5.27	128.96	121.42
1	LB	1	PRO	CA-C-N	5.27	128.96	121.42
1	LB	1	PRO	C-N-CA	5.27	128.96	121.42
1	AR	1	PRO	CA-C-N	5.27	128.96	121.42
1	AR	1	PRO	C-N-CA	5.27	128.96	121.42
1	DQ	35	VAL	N-CA-C	-5.27	105.25	111.00
1	FN	35	VAL	N-CA-C	-5.27	105.25	111.00
1	GD	1	PRO	CA-C-N	5.27	128.96	121.42
1	GD	1	PRO	C-N-CA	5.27	128.96	121.42
1	GV	1	PRO	CA-C-N	5.27	128.96	121.42
1	GV	1	PRO	C-N-CA	5.27	128.96	121.42
1	HX	1	PRO	CA-C-N	5.27	128.96	121.42
1	HX	1	PRO	C-N-CA	5.27	128.96	121.42
1	YM	35	VAL	N-CA-C	-5.27	105.26	111.00
1	AP	36	VAL	N-CA-C	-5.27	105.25	110.62
1	BU	36	VAL	N-CA-C	-5.27	105.25	110.62
1	DU	32	LEU	N-CA-C	-5.27	106.98	113.41
1	EZ	32	LEU	N-CA-C	-5.27	106.98	113.41
1	FT	35	VAL	N-CA-C	-5.27	105.25	111.00
1	FZ	35	VAL	N-CA-C	-5.27	105.25	111.00
1	GX	36	VAL	N-CA-C	-5.27	105.25	110.62
1	IE	35	VAL	N-CA-C	-5.27	105.25	111.00
1	IK	35	VAL	N-CA-C	-5.27	105.25	111.00
1	WD	35	VAL	N-CA-C	-5.27	105.26	111.00
1	ZU	36	VAL	N-CA-C	-5.27	105.25	110.62
1	YE	1	PRO	CA-C-N	5.27	128.95	121.42
1	YE	1	PRO	C-N-CA	5.27	128.95	121.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YG	36	VAL	N-CA-C	-5.27	105.25	110.62
1	BC	35	VAL	N-CA-C	-5.27	105.26	111.00
1	CK	1	PRO	CA-C-N	5.27	128.95	121.42
1	CK	1	PRO	C-N-CA	5.27	128.95	121.42
1	DC	1	PRO	CA-C-N	5.27	128.95	121.42
1	DC	1	PRO	C-N-CA	5.27	128.95	121.42
1	EN	1	PRO	CA-C-N	5.27	128.95	121.42
1	EN	1	PRO	C-N-CA	5.27	128.95	121.42
1	GJ	1	PRO	CA-C-N	5.27	128.95	121.42
1	GJ	1	PRO	C-N-CA	5.27	128.95	121.42
1	HI	35	VAL	N-CA-C	-5.27	105.26	111.00
1	JM	1	PRO	CA-C-N	5.27	128.95	121.42
1	JM	1	PRO	C-N-CA	5.27	128.95	121.42
1	JO	36	VAL	N-CA-C	-5.27	105.25	110.62
1	CE	1	PRO	CA-C-N	5.27	128.95	121.42
1	CE	1	PRO	C-N-CA	5.27	128.95	121.42
1	EB	1	PRO	CA-C-N	5.27	128.95	121.42
1	EB	1	PRO	C-N-CA	5.27	128.95	121.42
1	ZI	35	VAL	N-CA-C	-5.27	105.26	111.00
1	KF	35	VAL	N-CA-C	-5.27	105.26	111.00
1	KL	36	VAL	N-CA-C	-5.27	105.25	110.62
1	LJ	36	VAL	N-CA-C	-5.27	105.25	110.62
1	ZA	1	PRO	CA-C-N	5.26	128.95	121.42
1	ZA	1	PRO	C-N-CA	5.26	128.95	121.42
1	AI	1	PRO	CA-C-N	5.26	128.95	121.42
1	AI	1	PRO	C-N-CA	5.26	128.95	121.42
1	CW	1	PRO	CA-C-N	5.26	128.95	121.42
1	CW	1	PRO	C-N-CA	5.26	128.95	121.42
1	DM	35	VAL	N-CA-C	-5.26	105.26	111.00
1	EH	1	PRO	CA-C-N	5.26	128.95	121.42
1	EH	1	PRO	C-N-CA	5.26	128.95	121.42
1	FJ	35	VAL	N-CA-C	-5.26	105.26	111.00
1	YQ	1	PRO	CA-C-N	5.26	128.95	121.42
1	YQ	1	PRO	C-N-CA	5.26	128.95	121.42
1	BS	1	PRO	CA-C-N	5.26	128.95	121.42
1	BS	1	PRO	C-N-CA	5.26	128.95	121.42
1	BY	1	PRO	CA-C-N	5.26	128.95	121.42
1	BY	1	PRO	C-N-CA	5.26	128.95	121.42
1	CS	35	VAL	N-CA-C	-5.26	105.26	111.00
1	ET	1	PRO	CA-C-N	5.26	128.95	121.42
1	ET	1	PRO	C-N-CA	5.26	128.95	121.42
1	GR	35	VAL	N-CA-C	-5.26	105.26	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	JG	1	PRO	CA-C-N	5.26	128.95	121.42
1	JG	1	PRO	C-N-CA	5.26	128.95	121.42
1	KB	35	VAL	N-CA-C	-5.26	105.26	111.00
1	LR	35	VAL	N-CA-C	-5.26	105.26	111.00
1	ZS	1	PRO	CA-C-N	5.26	128.95	121.42
1	ZS	1	PRO	C-N-CA	5.26	128.95	121.42
1	ZY	32	LEU	N-CA-C	-5.26	106.99	113.41
1	YY	36	VAL	N-CA-C	-5.26	105.25	110.62
1	BG	32	LEU	N-CA-C	-5.26	106.99	113.41
1	HN	36	VAL	N-CA-C	-5.26	105.25	110.62
1	IU	1	PRO	CA-C-N	5.26	128.94	121.42
1	IU	1	PRO	C-N-CA	5.26	128.94	121.42
1	KJ	1	PRO	CA-C-N	5.26	128.94	121.42
1	KJ	1	PRO	C-N-CA	5.26	128.94	121.42
1	KP	1	PRO	CA-C-N	5.26	128.94	121.42
1	KP	1	PRO	C-N-CA	5.26	128.94	121.42
1	LH	1	PRO	CA-C-N	5.26	128.94	121.42
1	LH	1	PRO	C-N-CA	5.26	128.94	121.42
1	KJ	32	LEU	N-CA-C	-5.26	106.99	113.41
1	LH	32	LEU	N-CA-C	-5.26	106.99	113.41
1	AC	1	PRO	CA-C-N	5.26	128.94	121.42
1	AC	1	PRO	C-N-CA	5.26	128.94	121.42
1	AU	1	PRO	CA-C-N	5.26	128.94	121.42
1	AU	1	PRO	C-N-CA	5.26	128.94	121.42
1	BO	36	VAL	N-CA-C	-5.26	105.26	110.62
1	CQ	1	PRO	CA-C-N	5.26	128.94	121.42
1	CQ	1	PRO	C-N-CA	5.26	128.94	121.42
1	ZG	32	LEU	N-CA-C	-5.26	107.00	113.41
1	GP	1	PRO	CA-C-N	5.26	128.94	121.42
1	GP	1	PRO	C-N-CA	5.26	128.94	121.42
1	HB	1	PRO	CA-C-N	5.26	128.94	121.42
1	HB	1	PRO	C-N-CA	5.26	128.94	121.42
1	HR	1	PRO	CA-C-N	5.26	128.94	121.42
1	HR	1	PRO	C-N-CA	5.26	128.94	121.42
1	KD	32	LEU	N-CA-C	-5.26	107.00	113.41
1	ZO	36	VAL	N-CA-C	-5.26	105.26	110.62
1	YK	1	PRO	CA-C-N	5.26	128.94	121.42
1	YK	1	PRO	C-N-CA	5.26	128.94	121.42
1	AK	35	VAL	N-CA-C	-5.26	105.27	111.00
1	ZC	35	VAL	N-CA-C	-5.26	105.27	111.00
1	IW	35	VAL	N-CA-C	-5.26	105.27	111.00
1	JS	1	PRO	CA-C-N	5.26	128.94	121.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	JS	1	PRO	C-N-CA	5.26	128.94	121.42
1	KR	35	VAL	N-CA-C	-5.26	105.27	111.00
1	BO	35	VAL	N-CA-C	-5.25	105.27	111.00
1	DK	35	VAL	N-CA-C	-5.25	105.27	111.00
1	DU	1	PRO	CA-C-N	5.25	128.94	121.42
1	DU	1	PRO	C-N-CA	5.25	128.94	121.42
1	EZ	1	PRO	CA-C-N	5.25	128.94	121.42
1	EZ	1	PRO	C-N-CA	5.25	128.94	121.42
1	FH	35	VAL	N-CA-C	-5.25	105.27	111.00
1	ZO	35	VAL	N-CA-C	-5.25	105.27	111.00
1	YW	32	LEU	N-CA-C	-5.25	107.00	113.41
1	DG	35	VAL	N-CA-C	-5.25	105.27	111.00
1	GF	36	VAL	N-CA-C	-5.25	105.26	110.62
1	GN	35	VAL	N-CA-C	-5.25	105.27	111.00
1	HL	32	LEU	N-CA-C	-5.25	107.00	113.41
1	HZ	36	VAL	N-CA-C	-5.25	105.26	110.62
1	DX	35	VAL	N-CA-C	-5.25	105.28	111.00
1	FB	35	VAL	N-CA-C	-5.25	105.28	111.00
1	DS	35	VAL	N-CA-C	-5.25	105.28	111.00
1	FP	35	VAL	N-CA-C	-5.25	105.28	111.00
1	FX	32	LEU	N-CA-C	-5.25	107.00	113.41
1	II	32	LEU	N-CA-C	-5.25	107.00	113.41
1	IY	35	VAL	N-CA-C	-5.25	105.28	111.00
1	KT	35	VAL	N-CA-C	-5.25	105.28	111.00
1	AE	36	VAL	N-CA-C	-5.25	105.27	110.62
1	AR	32	LEU	N-CA-C	-5.25	107.01	113.41
1	BU	35	VAL	N-CA-C	-5.25	105.28	111.00
1	GV	32	LEU	N-CA-C	-5.25	107.01	113.41
1	HT	36	VAL	N-CA-C	-5.25	105.27	110.62
1	JA	1	PRO	CA-C-N	5.25	128.92	121.42
1	JA	1	PRO	C-N-CA	5.25	128.92	121.42
1	JX	1	PRO	CA-C-N	5.25	128.92	121.42
1	JX	1	PRO	C-N-CA	5.25	128.92	121.42
1	KV	1	PRO	CA-C-N	5.25	128.92	121.42
1	KV	1	PRO	C-N-CA	5.25	128.92	121.42
1	LN	1	PRO	CA-C-N	5.25	128.92	121.42
1	LN	1	PRO	C-N-CA	5.25	128.92	121.42
1	ZU	35	VAL	N-CA-C	-5.25	105.28	111.00
1	FV	35	VAL	N-CA-C	-5.25	105.28	111.00
1	IH	35	VAL	N-CA-C	-5.25	105.28	111.00
1	JX	32	LEU	N-CA-C	-5.25	107.01	113.41
1	LN	32	LEU	N-CA-C	-5.25	107.01	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BY	32	LEU	N-CA-C	-5.24	107.01	113.41
1	ET	32	LEU	N-CA-C	-5.24	107.01	113.41
1	FX	1	PRO	CA-C-N	5.24	128.92	121.42
1	FX	1	PRO	C-N-CA	5.24	128.92	121.42
1	GB	35	VAL	N-CA-C	-5.24	105.28	111.00
1	II	1	PRO	CA-C-N	5.24	128.92	121.42
1	II	1	PRO	C-N-CA	5.24	128.92	121.42
1	IM	35	VAL	N-CA-C	-5.24	105.28	111.00
1	DI	1	PRO	CA-C-N	5.24	128.92	121.42
1	DI	1	PRO	C-N-CA	5.24	128.92	121.42
1	FF	1	PRO	CA-C-N	5.24	128.92	121.42
1	FF	1	PRO	C-N-CA	5.24	128.92	121.42
1	GH	35	VAL	N-CA-C	-5.24	105.29	111.00
1	WC	35	VAL	N-CA-C	-5.24	105.29	111.00
1	CG	35	VAL	N-CA-C	-5.24	105.29	111.00
1	ED	35	VAL	N-CA-C	-5.24	105.29	111.00
1	IU	32	LEU	N-CA-C	-5.24	107.02	113.41
1	KP	32	LEU	N-CA-C	-5.24	107.02	113.41
1	ZA	32	LEU	N-CA-C	-5.24	107.02	113.41
1	YM	36	VAL	N-CA-C	-5.24	105.28	110.62
1	AI	32	LEU	N-CA-C	-5.24	107.02	113.41
1	BI	36	VAL	N-CA-C	-5.24	105.28	110.62
1	DO	32	LEU	N-CA-C	-5.24	107.02	113.41
1	FL	32	LEU	N-CA-C	-5.24	107.02	113.41
1	GD	32	LEU	N-CA-C	-5.24	107.02	113.41
1	HX	32	LEU	N-CA-C	-5.24	107.02	113.41
1	WD	36	VAL	N-CA-C	-5.24	105.28	110.62
1	YA	36	VAL	N-CA-C	-5.24	105.28	110.62
1	AE	35	VAL	N-CA-C	-5.24	105.29	111.00
1	CK	32	LEU	N-CA-C	-5.24	107.02	113.41
1	DA	35	VAL	N-CA-C	-5.24	105.29	111.00
1	EL	35	VAL	N-CA-C	-5.24	105.29	111.00
1	EN	32	LEU	N-CA-C	-5.24	107.02	113.41
1	HT	35	VAL	N-CA-C	-5.24	105.29	111.00
1	YK	32	LEU	N-CA-C	-5.24	107.02	113.41
1	AU	32	LEU	N-CA-C	-5.24	107.02	113.41
1	GF	35	VAL	N-CA-C	-5.24	105.29	111.00
1	HB	32	LEU	N-CA-C	-5.24	107.02	113.41
1	HZ	35	VAL	N-CA-C	-5.24	105.29	111.00
1	IO	32	LEU	N-CA-C	-5.24	107.02	113.41
1	JS	32	LEU	N-CA-C	-5.24	107.02	113.41
1	LB	32	LEU	N-CA-C	-5.24	107.02	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CE	32	LEU	N-CA-C	-5.23	107.02	113.41
1	EB	32	LEU	N-CA-C	-5.23	107.02	113.41
1	YC	35	VAL	N-CA-C	-5.23	105.30	111.00
1	AC	32	LEU	N-CA-C	-5.23	107.03	113.41
1	BK	35	VAL	N-CA-C	-5.23	105.30	111.00
1	BM	1	PRO	CA-C-N	5.23	128.90	121.42
1	BM	1	PRO	C-N-CA	5.23	128.90	121.42
1	HR	32	LEU	N-CA-C	-5.23	107.03	113.41
1	JA	32	LEU	N-CA-C	-5.23	107.03	113.41
1	KV	32	LEU	N-CA-C	-5.23	107.03	113.41
1	ZM	1	PRO	CA-C-N	5.23	128.90	121.42
1	ZM	1	PRO	C-N-CA	5.23	128.90	121.42
1	DC	32	LEU	N-CA-C	-5.23	107.03	113.41
1	GJ	32	LEU	N-CA-C	-5.23	107.03	113.41
1	ZK	35	VAL	N-CA-C	-5.23	105.30	111.00
1	KH	35	VAL	N-CA-C	-5.23	105.30	111.00
1	YI	35	VAL	N-CA-C	-5.23	105.30	111.00
1	AW	35	VAL	N-CA-C	-5.23	105.30	111.00
1	HD	35	VAL	N-CA-C	-5.23	105.30	111.00
1	JQ	35	VAL	N-CA-C	-5.23	105.30	111.00
1	BA	32	LEU	N-CA-C	-5.23	107.03	113.41
1	BE	35	VAL	N-CA-C	-5.23	105.30	111.00
1	BM	32	LEU	N-CA-C	-5.23	107.03	113.41
1	BQ	35	VAL	N-CA-C	-5.23	105.30	111.00
1	CO	35	VAL	N-CA-C	-5.23	105.30	111.00
1	CU	35	VAL	N-CA-C	-5.23	105.30	111.00
1	DI	32	LEU	N-CA-C	-5.23	107.03	113.41
1	ER	35	VAL	N-CA-C	-5.23	105.30	111.00
1	FF	32	LEU	N-CA-C	-5.23	107.03	113.41
1	GT	35	VAL	N-CA-C	-5.23	105.30	111.00
1	HG	32	LEU	N-CA-C	-5.23	107.03	113.41
1	WA	35	VAL	N-CA-C	-5.23	105.30	111.00
1	ZM	32	LEU	N-CA-C	-5.23	107.03	113.41
1	ZQ	35	VAL	N-CA-C	-5.23	105.30	111.00
1	KN	35	VAL	N-CA-C	-5.23	105.30	111.00
1	LL	35	VAL	N-CA-C	-5.23	105.30	111.00
1	YU	35	VAL	N-CA-C	-5.22	105.31	111.00
1	AY	35	VAL	N-CA-C	-5.22	105.31	111.00
1	WB	35	VAL	N-CA-C	-5.22	105.31	111.00
1	JE	35	VAL	N-CA-C	-5.22	105.30	111.00
1	JK	35	VAL	N-CA-C	-5.22	105.31	111.00
1	JZ	50	VAL	CA-C-N	-5.22	115.74	123.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	JZ	50	VAL	C-N-CA	-5.22	115.74	123.05
1	KZ	35	VAL	N-CA-C	-5.22	105.30	111.00
1	LP	50	VAL	CA-C-N	-5.22	115.74	123.05
1	LP	50	VAL	C-N-CA	-5.22	115.74	123.05
1	CA	35	VAL	N-CA-C	-5.22	105.31	111.00
1	EV	35	VAL	N-CA-C	-5.22	105.31	111.00
1	YE	32	LEU	N-CA-C	-5.22	107.04	113.41
1	CI	35	VAL	N-CA-C	-5.22	105.31	111.00
1	EF	35	VAL	N-CA-C	-5.22	105.31	111.00
1	FR	1	PRO	CA-C-N	5.22	128.89	121.42
1	FR	1	PRO	C-N-CA	5.22	128.89	121.42
1	IC	1	PRO	CA-C-N	5.22	128.89	121.42
1	IC	1	PRO	C-N-CA	5.22	128.89	121.42
1	JM	32	LEU	N-CA-C	-5.22	107.04	113.41
1	YO	35	VAL	N-CA-C	-5.22	105.31	111.00
1	AM	35	VAL	N-CA-C	-5.22	105.31	111.00
1	ZE	35	VAL	N-CA-C	-5.22	105.31	111.00
1	DZ	35	VAL	N-CA-C	-5.22	105.31	111.00
1	FD	35	VAL	N-CA-C	-5.22	105.31	111.00
1	JV	35	VAL	N-CA-C	-5.22	105.31	111.00
1	YQ	32	LEU	N-CA-C	-5.22	107.05	113.41
1	JG	32	LEU	N-CA-C	-5.22	107.05	113.41
1	AA	35	VAL	N-CA-C	-5.22	105.31	111.00
1	BW	35	VAL	N-CA-C	-5.22	105.31	111.00
1	HP	35	VAL	N-CA-C	-5.22	105.31	111.00
1	ZW	35	VAL	N-CA-C	-5.22	105.31	111.00
1	BS	32	LEU	N-CA-C	-5.21	107.05	113.41
1	ZS	32	LEU	N-CA-C	-5.21	107.05	113.41
1	IQ	35	VAL	N-CA-C	-5.21	105.32	111.00
1	LD	35	VAL	N-CA-C	-5.21	105.32	111.00
1	CC	35	VAL	N-CA-C	-5.21	105.32	111.00
1	EX	35	VAL	N-CA-C	-5.21	105.32	111.00
1	AS	35	VAL	N-CA-C	-5.21	105.32	111.00
1	GZ	35	VAL	N-CA-C	-5.21	105.32	111.00
1	FR	32	LEU	N-CA-C	-5.21	107.06	113.41
1	IC	32	LEU	N-CA-C	-5.21	107.06	113.41
1	IS	35	VAL	N-CA-C	-5.21	105.32	111.00
1	LF	35	VAL	N-CA-C	-5.21	105.32	111.00
1	BU	50	VAL	CA-C-N	-5.20	115.77	123.05
1	BU	50	VAL	C-N-CA	-5.20	115.77	123.05
1	CY	50	VAL	CA-C-N	-5.20	115.76	123.05
1	CY	50	VAL	C-N-CA	-5.20	115.76	123.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EJ	50	VAL	CA-C-N	-5.20	115.76	123.05
1	EJ	50	VAL	C-N-CA	-5.20	115.76	123.05
1	FZ	50	VAL	CA-C-N	-5.20	115.77	123.05
1	FZ	50	VAL	C-N-CA	-5.20	115.77	123.05
1	IK	50	VAL	CA-C-N	-5.20	115.77	123.05
1	IK	50	VAL	C-N-CA	-5.20	115.77	123.05
1	ZU	50	VAL	CA-C-N	-5.20	115.77	123.05
1	ZU	50	VAL	C-N-CA	-5.20	115.77	123.05
1	CQ	32	LEU	N-CA-C	-5.20	107.07	113.41
1	GP	32	LEU	N-CA-C	-5.20	107.07	113.41
1	JC	50	VAL	CA-C-N	-5.20	115.77	123.05
1	JC	50	VAL	C-N-CA	-5.20	115.77	123.05
1	KX	50	VAL	CA-C-N	-5.20	115.77	123.05
1	KX	50	VAL	C-N-CA	-5.20	115.77	123.05
1	KL	50	VAL	CA-C-N	-5.19	115.78	123.05
1	KL	50	VAL	C-N-CA	-5.19	115.78	123.05
1	LJ	50	VAL	CA-C-N	-5.19	115.78	123.05
1	LJ	50	VAL	C-N-CA	-5.19	115.78	123.05
1	CG	50	VAL	CA-C-N	-5.19	115.79	123.05
1	CG	50	VAL	C-N-CA	-5.19	115.79	123.05
1	ED	50	VAL	CA-C-N	-5.19	115.79	123.05
1	ED	50	VAL	C-N-CA	-5.19	115.79	123.05
1	FT	50	VAL	CA-C-N	-5.19	115.79	123.05
1	FT	50	VAL	C-N-CA	-5.19	115.79	123.05
1	IE	50	VAL	CA-C-N	-5.19	115.79	123.05
1	IE	50	VAL	C-N-CA	-5.19	115.79	123.05
1	IQ	50	VAL	CA-C-N	-5.19	115.79	123.05
1	IQ	50	VAL	C-N-CA	-5.19	115.79	123.05
1	LD	50	VAL	CA-C-N	-5.19	115.79	123.05
1	LD	50	VAL	C-N-CA	-5.19	115.79	123.05
1	CW	32	LEU	N-CA-C	-5.19	107.08	113.41
1	EH	32	LEU	N-CA-C	-5.19	107.08	113.41
1	CS	50	VAL	CA-C-N	-5.18	115.79	123.05
1	CS	50	VAL	C-N-CA	-5.18	115.79	123.05
1	DS	94	GLU	CA-C-N	-5.18	116.20	123.10
1	DS	94	GLU	C-N-CA	-5.18	116.20	123.10
1	FP	94	GLU	CA-C-N	-5.18	116.20	123.10
1	FP	94	GLU	C-N-CA	-5.18	116.20	123.10
1	GR	50	VAL	CA-C-N	-5.18	115.79	123.05
1	GR	50	VAL	C-N-CA	-5.18	115.79	123.05
1	YG	50	VAL	CA-C-N	-5.18	115.80	123.05
1	YG	50	VAL	C-N-CA	-5.18	115.80	123.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DK	50	VAL	CA-C-N	-5.18	115.79	123.05
1	DK	50	VAL	C-N-CA	-5.18	115.79	123.05
1	FH	50	VAL	CA-C-N	-5.18	115.79	123.05
1	FH	50	VAL	C-N-CA	-5.18	115.79	123.05
1	JO	50	VAL	CA-C-N	-5.18	115.80	123.05
1	JO	50	VAL	C-N-CA	-5.18	115.80	123.05
1	AW	50	VAL	CA-C-N	-5.18	115.80	123.05
1	AW	50	VAL	C-N-CA	-5.18	115.80	123.05
1	ZI	50	VAL	CA-C-N	-5.18	115.80	123.05
1	ZI	50	VAL	C-N-CA	-5.18	115.80	123.05
1	HD	50	VAL	CA-C-N	-5.18	115.80	123.05
1	HD	50	VAL	C-N-CA	-5.18	115.80	123.05
1	KF	50	VAL	CA-C-N	-5.18	115.80	123.05
1	KF	50	VAL	C-N-CA	-5.18	115.80	123.05
1	CM	50	VAL	CA-C-N	-5.18	115.80	123.05
1	CM	50	VAL	C-N-CA	-5.18	115.80	123.05
1	DG	94	GLU	CA-C-N	-5.18	116.21	123.10
1	DG	94	GLU	C-N-CA	-5.18	116.21	123.10
1	EP	50	VAL	CA-C-N	-5.18	115.80	123.05
1	EP	50	VAL	C-N-CA	-5.18	115.80	123.05
1	GN	94	GLU	CA-C-N	-5.18	116.21	123.10
1	GN	94	GLU	C-N-CA	-5.18	116.21	123.10
1	AK	50	VAL	CA-C-N	-5.18	115.80	123.05
1	AK	50	VAL	C-N-CA	-5.18	115.80	123.05
1	ZC	50	VAL	CA-C-N	-5.18	115.80	123.05
1	ZC	50	VAL	C-N-CA	-5.18	115.80	123.05
1	BI	50	VAL	CA-C-N	-5.18	115.80	123.05
1	BI	50	VAL	C-N-CA	-5.18	115.80	123.05
1	DX	50	VAL	CA-C-N	-5.18	115.80	123.05
1	DX	50	VAL	C-N-CA	-5.18	115.80	123.05
1	FB	50	VAL	CA-C-N	-5.18	115.80	123.05
1	FB	50	VAL	C-N-CA	-5.18	115.80	123.05
1	GF	50	VAL	CA-C-N	-5.18	115.80	123.05
1	GF	50	VAL	C-N-CA	-5.18	115.80	123.05
1	HZ	50	VAL	CA-C-N	-5.18	115.80	123.05
1	HZ	50	VAL	C-N-CA	-5.18	115.80	123.05
1	YA	50	VAL	CA-C-N	-5.18	115.80	123.05
1	YA	50	VAL	C-N-CA	-5.18	115.80	123.05
1	BO	50	VAL	CA-C-N	-5.17	115.81	123.05
1	BO	50	VAL	C-N-CA	-5.17	115.81	123.05
1	CU	94	GLU	CA-C-N	-5.17	116.22	123.10
1	CU	94	GLU	C-N-CA	-5.17	116.22	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GT	94	GLU	CA-C-N	-5.17	116.22	123.10
1	GT	94	GLU	C-N-CA	-5.17	116.22	123.10
1	ZO	50	VAL	CA-C-N	-5.17	115.81	123.05
1	ZO	50	VAL	C-N-CA	-5.17	115.81	123.05
2	BT	133	ILE	CB-CA-C	-5.17	105.16	112.14
1	CA	50	VAL	CA-C-N	-5.17	115.81	123.05
1	CA	50	VAL	C-N-CA	-5.17	115.81	123.05
1	EV	50	VAL	CA-C-N	-5.17	115.81	123.05
1	EV	50	VAL	C-N-CA	-5.17	115.81	123.05
2	ZT	133	ILE	CB-CA-C	-5.17	105.16	112.14
2	YF	133	ILE	CB-CA-C	-5.17	105.16	112.14
1	YI	94	GLU	CA-C-N	-5.17	116.22	123.10
1	YI	94	GLU	C-N-CA	-5.17	116.22	123.10
1	CO	94	GLU	CA-C-N	-5.17	116.22	123.10
1	CO	94	GLU	C-N-CA	-5.17	116.22	123.10
1	ER	94	GLU	CA-C-N	-5.17	116.22	123.10
1	ER	94	GLU	C-N-CA	-5.17	116.22	123.10
2	JN	133	ILE	CB-CA-C	-5.17	105.16	112.14
1	JQ	94	GLU	CA-C-N	-5.17	116.22	123.10
1	JQ	94	GLU	C-N-CA	-5.17	116.22	123.10
1	YY	50	VAL	CA-C-N	-5.17	115.81	123.05
1	YY	50	VAL	C-N-CA	-5.17	115.81	123.05
1	HN	50	VAL	CA-C-N	-5.17	115.81	123.05
1	HN	50	VAL	C-N-CA	-5.17	115.81	123.05
1	AA	94	GLU	CA-C-N	-5.17	116.23	123.10
1	AA	94	GLU	C-N-CA	-5.17	116.23	123.10
1	AP	50	VAL	CA-C-N	-5.17	115.81	123.05
1	AP	50	VAL	C-N-CA	-5.17	115.81	123.05
1	DE	50	VAL	CA-C-N	-5.17	115.81	123.05
1	DE	50	VAL	C-N-CA	-5.17	115.81	123.05
2	FY	133	ILE	CB-CA-C	-5.17	105.16	112.14
1	GL	50	VAL	CA-C-N	-5.17	115.81	123.05
1	GL	50	VAL	C-N-CA	-5.17	115.81	123.05
1	GX	50	VAL	CA-C-N	-5.17	115.81	123.05
1	GX	50	VAL	C-N-CA	-5.17	115.81	123.05
1	HP	94	GLU	CA-C-N	-5.17	116.23	123.10
1	HP	94	GLU	C-N-CA	-5.17	116.23	123.10
2	IJ	133	ILE	CB-CA-C	-5.17	105.16	112.14
1	ZK	94	GLU	CA-C-N	-5.17	116.22	123.10
1	ZK	94	GLU	C-N-CA	-5.17	116.22	123.10
1	KH	94	GLU	CA-C-N	-5.17	116.22	123.10
1	KH	94	GLU	C-N-CA	-5.17	116.22	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AE	50	VAL	CA-C-N	-5.17	115.82	123.05
1	AE	50	VAL	C-N-CA	-5.17	115.82	123.05
1	AG	35	VAL	N-CA-C	-5.17	105.37	111.00
2	BN	133	ILE	CB-CA-C	-5.17	105.17	112.14
1	DM	94	GLU	CA-C-N	-5.17	116.23	123.10
1	DM	94	GLU	C-N-CA	-5.17	116.23	123.10
1	DQ	50	VAL	CA-C-N	-5.17	115.82	123.05
1	DQ	50	VAL	C-N-CA	-5.17	115.82	123.05
1	FJ	94	GLU	CA-C-N	-5.17	116.23	123.10
1	FJ	94	GLU	C-N-CA	-5.17	116.23	123.10
1	FN	50	VAL	CA-C-N	-5.17	115.82	123.05
1	FN	50	VAL	C-N-CA	-5.17	115.82	123.05
1	HT	50	VAL	CA-C-N	-5.17	115.82	123.05
1	HT	50	VAL	C-N-CA	-5.17	115.82	123.05
1	HV	35	VAL	N-CA-C	-5.17	105.37	111.00
2	ZN	133	ILE	CB-CA-C	-5.17	105.17	112.14
1	YU	94	GLU	CA-C-N	-5.17	116.23	123.10
1	YU	94	GLU	C-N-CA	-5.17	116.23	123.10
1	BE	94	GLU	CA-C-N	-5.17	116.23	123.10
1	BE	94	GLU	C-N-CA	-5.17	116.23	123.10
1	WA	94	GLU	CA-C-N	-5.17	116.23	123.10
1	WA	94	GLU	C-N-CA	-5.17	116.23	123.10
1	JK	94	GLU	CA-C-N	-5.17	116.23	123.10
1	JK	94	GLU	C-N-CA	-5.17	116.23	123.10
1	YS	50	VAL	CA-C-N	-5.16	115.82	123.05
1	YS	50	VAL	C-N-CA	-5.16	115.82	123.05
1	AG	94	GLU	CA-C-N	-5.16	116.23	123.10
1	AG	94	GLU	C-N-CA	-5.16	116.23	123.10
2	CX	133	ILE	CB-CA-C	-5.16	105.17	112.14
2	EI	133	ILE	CB-CA-C	-5.16	105.17	112.14
1	HV	94	GLU	CA-C-N	-5.16	116.23	123.10
1	HV	94	GLU	C-N-CA	-5.16	116.23	123.10
1	JI	50	VAL	CA-C-N	-5.16	115.82	123.05
1	JI	50	VAL	C-N-CA	-5.16	115.82	123.05
2	YR	133	ILE	CB-CA-C	-5.16	105.17	112.14
1	AM	94	GLU	CA-C-N	-5.16	116.24	123.10
1	AM	94	GLU	C-N-CA	-5.16	116.24	123.10
1	BW	94	GLU	CA-C-N	-5.16	116.24	123.10
1	BW	94	GLU	C-N-CA	-5.16	116.24	123.10
2	CR	133	ILE	CB-CA-C	-5.16	105.17	112.14
1	ZE	94	GLU	CA-C-N	-5.16	116.24	123.10
1	ZE	94	GLU	C-N-CA	-5.16	116.24	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GQ	133	ILE	CB-CA-C	-5.16	105.17	112.14
2	JH	133	ILE	CB-CA-C	-5.16	105.17	112.14
1	KB	94	GLU	CA-C-N	-5.16	116.24	123.10
1	KB	94	GLU	C-N-CA	-5.16	116.24	123.10
1	LR	94	GLU	CA-C-N	-5.16	116.24	123.10
1	LR	94	GLU	C-N-CA	-5.16	116.24	123.10
1	ZW	94	GLU	CA-C-N	-5.16	116.24	123.10
1	ZW	94	GLU	C-N-CA	-5.16	116.24	123.10
1	JE	94	GLU	CA-C-N	-5.16	116.24	123.10
1	JE	94	GLU	C-N-CA	-5.16	116.24	123.10
1	KZ	94	GLU	CA-C-N	-5.16	116.24	123.10
1	KZ	94	GLU	C-N-CA	-5.16	116.24	123.10
2	AQ	133	ILE	CB-CA-C	-5.16	105.18	112.14
2	GW	133	ILE	CB-CA-C	-5.16	105.18	112.14
2	JB	133	ILE	CB-CA-C	-5.16	105.18	112.14
2	KW	133	ILE	CB-CA-C	-5.16	105.18	112.14
1	BQ	94	GLU	CA-C-N	-5.16	116.24	123.10
1	BQ	94	GLU	C-N-CA	-5.16	116.24	123.10
2	DW	133	ILE	CB-CA-C	-5.16	105.18	112.14
2	FA	133	ILE	CB-CA-C	-5.16	105.18	112.14
1	ZQ	94	GLU	CA-C-N	-5.16	116.24	123.10
1	ZQ	94	GLU	C-N-CA	-5.16	116.24	123.10
1	YO	94	GLU	CA-C-N	-5.15	116.25	123.10
1	YO	94	GLU	C-N-CA	-5.15	116.25	123.10
1	AS	94	GLU	CA-C-N	-5.15	116.25	123.10
1	AS	94	GLU	C-N-CA	-5.15	116.25	123.10
1	CI	94	GLU	CA-C-N	-5.15	116.25	123.10
1	CI	94	GLU	C-N-CA	-5.15	116.25	123.10
1	EF	94	GLU	CA-C-N	-5.15	116.25	123.10
1	EF	94	GLU	C-N-CA	-5.15	116.25	123.10
1	GZ	94	GLU	CA-C-N	-5.15	116.25	123.10
1	GZ	94	GLU	C-N-CA	-5.15	116.25	123.10
1	JV	94	GLU	CA-C-N	-5.15	116.25	123.10
1	JV	94	GLU	C-N-CA	-5.15	116.25	123.10
1	CC	94	GLU	CA-C-N	-5.15	116.25	123.10
1	CC	94	GLU	C-N-CA	-5.15	116.25	123.10
1	DA	94	GLU	CA-C-N	-5.15	116.25	123.10
1	DA	94	GLU	C-N-CA	-5.15	116.25	123.10
1	EL	94	GLU	CA-C-N	-5.15	116.25	123.10
1	EL	94	GLU	C-N-CA	-5.15	116.25	123.10
1	EX	94	GLU	CA-C-N	-5.15	116.25	123.10
1	EX	94	GLU	C-N-CA	-5.15	116.25	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	IY	94	GLU	CA-C-N	-5.15	116.25	123.10
1	IY	94	GLU	C-N-CA	-5.15	116.25	123.10
2	JY	133	ILE	CB-CA-C	-5.15	105.19	112.14
1	KT	94	GLU	CA-C-N	-5.15	116.25	123.10
1	KT	94	GLU	C-N-CA	-5.15	116.25	123.10
2	LO	133	ILE	CB-CA-C	-5.15	105.19	112.14
1	BC	50	VAL	CA-C-N	-5.15	115.84	123.05
1	BC	50	VAL	C-N-CA	-5.15	115.84	123.05
1	HI	50	VAL	CA-C-N	-5.15	115.84	123.05
1	HI	50	VAL	C-N-CA	-5.15	115.84	123.05
2	DD	133	ILE	CB-CA-C	-5.15	105.19	112.14
1	DZ	94	GLU	CA-C-N	-5.15	116.25	123.10
1	DZ	94	GLU	C-N-CA	-5.15	116.25	123.10
1	FD	94	GLU	CA-C-N	-5.15	116.25	123.10
1	FD	94	GLU	C-N-CA	-5.15	116.25	123.10
2	GK	133	ILE	CB-CA-C	-5.15	105.19	112.14
1	YM	50	VAL	CA-C-N	-5.15	115.84	123.05
1	YM	50	VAL	C-N-CA	-5.15	115.84	123.05
2	DP	133	ILE	CB-CA-C	-5.15	105.19	112.14
2	FM	133	ILE	CB-CA-C	-5.15	105.19	112.14
2	ZH	133	ILE	CB-CA-C	-5.15	105.19	112.14
1	WD	50	VAL	CA-C-N	-5.15	115.84	123.05
1	WD	50	VAL	C-N-CA	-5.15	115.84	123.05
2	KE	133	ILE	CB-CA-C	-5.15	105.19	112.14
2	YL	133	ILE	CB-CA-C	-5.15	105.19	112.14
2	JT	133	ILE	CB-CA-C	-5.15	105.19	112.14
1	YC	94	GLU	CA-C-N	-5.14	116.26	123.10
1	YC	94	GLU	C-N-CA	-5.14	116.26	123.10
2	YX	133	ILE	CB-CA-C	-5.14	105.19	112.14
1	BK	94	GLU	CA-C-N	-5.14	116.26	123.10
1	BK	94	GLU	C-N-CA	-5.14	116.26	123.10
2	BZ	133	ILE	CB-CA-C	-5.14	105.19	112.14
2	CL	133	ILE	CB-CA-C	-5.14	105.19	112.14
2	EO	133	ILE	CB-CA-C	-5.14	105.19	112.14
2	EU	133	ILE	CB-CA-C	-5.14	105.19	112.14
1	GB	94	GLU	CA-C-N	-5.14	116.26	123.10
1	GB	94	GLU	C-N-CA	-5.14	116.26	123.10
2	HM	133	ILE	CB-CA-C	-5.14	105.19	112.14
1	IM	94	GLU	CA-C-N	-5.14	116.26	123.10
1	IM	94	GLU	C-N-CA	-5.14	116.26	123.10
1	IW	50	VAL	CA-C-N	-5.14	115.85	123.05
1	IW	50	VAL	C-N-CA	-5.14	115.85	123.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	KN	94	GLU	CA-C-N	-5.14	116.26	123.10
1	KN	94	GLU	C-N-CA	-5.14	116.26	123.10
1	KR	50	VAL	CA-C-N	-5.14	115.85	123.05
1	KR	50	VAL	C-N-CA	-5.14	115.85	123.05
1	LL	94	GLU	CA-C-N	-5.14	116.26	123.10
1	LL	94	GLU	C-N-CA	-5.14	116.26	123.10
1	AY	94	GLU	CA-C-N	-5.14	116.26	123.10
1	AY	94	GLU	C-N-CA	-5.14	116.26	123.10
2	CF	133	ILE	CB-CA-C	-5.14	105.20	112.14
2	EC	133	ILE	CB-CA-C	-5.14	105.20	112.14
1	WB	94	GLU	CA-C-N	-5.14	116.26	123.10
1	WB	94	GLU	C-N-CA	-5.14	116.26	123.10
2	KK	133	ILE	CB-CA-C	-5.14	105.20	112.14
2	LI	133	ILE	CB-CA-C	-5.14	105.20	112.14
2	ZB	133	ILE	CB-CA-C	-5.14	105.20	112.14
2	AJ	133	ILE	CB-CA-C	-5.14	105.20	112.14
2	BR	141	ASP	CA-C-N	5.14	125.22	119.87
2	BR	141	ASP	C-N-CA	5.14	125.22	119.87
2	FS	133	ILE	CB-CA-C	-5.14	105.20	112.14
2	ID	133	ILE	CB-CA-C	-5.14	105.20	112.14
2	IP	133	ILE	CB-CA-C	-5.14	105.20	112.14
2	LC	133	ILE	CB-CA-C	-5.14	105.20	112.14
2	ZR	141	ASP	CA-C-N	5.14	125.22	119.87
2	ZR	141	ASP	C-N-CA	5.14	125.22	119.87
2	AD	133	ILE	CB-CA-C	-5.14	105.20	112.14
1	GH	94	GLU	CA-C-N	-5.14	116.26	123.10
1	GH	94	GLU	C-N-CA	-5.14	116.26	123.10
2	HS	133	ILE	CB-CA-C	-5.14	105.20	112.14
1	WC	94	GLU	CA-C-N	-5.14	116.26	123.10
1	WC	94	GLU	C-N-CA	-5.14	116.26	123.10
2	DD	288	ILE	CA-C-N	-5.14	116.44	123.12
2	DD	288	ILE	C-N-CA	-5.14	116.44	123.12
2	GK	288	ILE	CA-C-N	-5.14	116.44	123.12
2	GK	288	ILE	C-N-CA	-5.14	116.44	123.12
2	AV	133	ILE	CB-CA-C	-5.14	105.21	112.14
2	BB	133	ILE	CB-CA-C	-5.14	105.21	112.14
2	HC	133	ILE	CB-CA-C	-5.14	105.21	112.14
2	HH	133	ILE	CB-CA-C	-5.14	105.21	112.14
1	IS	94	GLU	CA-C-N	-5.14	116.27	123.10
1	IS	94	GLU	C-N-CA	-5.14	116.27	123.10
1	LF	94	GLU	CA-C-N	-5.14	116.27	123.10
1	LF	94	GLU	C-N-CA	-5.14	116.27	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BT	288	ILE	CA-C-N	-5.13	116.44	123.12
2	BT	288	ILE	C-N-CA	-5.13	116.44	123.12
1	FV	94	GLU	CA-C-N	-5.13	116.27	123.10
1	FV	94	GLU	C-N-CA	-5.13	116.27	123.10
1	IH	94	GLU	CA-C-N	-5.13	116.27	123.10
1	IH	94	GLU	C-N-CA	-5.13	116.27	123.10
2	ZT	288	ILE	CA-C-N	-5.13	116.44	123.12
2	ZT	288	ILE	C-N-CA	-5.13	116.44	123.12
2	GE	288	ILE	CA-C-N	-5.13	116.45	123.12
2	GE	288	ILE	C-N-CA	-5.13	116.45	123.12
2	HY	288	ILE	CA-C-N	-5.13	116.45	123.12
2	HY	288	ILE	C-N-CA	-5.13	116.45	123.12
2	FY	288	ILE	CA-C-N	-5.13	116.45	123.12
2	FY	288	ILE	C-N-CA	-5.13	116.45	123.12
2	IJ	288	ILE	CA-C-N	-5.13	116.45	123.12
2	IJ	288	ILE	C-N-CA	-5.13	116.45	123.12
2	ZZ	288	ILE	CA-C-N	-5.13	116.45	123.12
2	ZZ	288	ILE	C-N-CA	-5.13	116.45	123.12
2	YL	288	ILE	CA-C-N	-5.13	116.45	123.12
2	YL	288	ILE	C-N-CA	-5.13	116.45	123.12
2	BH	288	ILE	CA-C-N	-5.13	116.45	123.12
2	BH	288	ILE	C-N-CA	-5.13	116.45	123.12
2	DJ	133	ILE	CB-CA-C	-5.13	105.22	112.14
2	FG	133	ILE	CB-CA-C	-5.13	105.22	112.14
2	JT	288	ILE	CA-C-N	-5.13	116.45	123.12
2	JT	288	ILE	C-N-CA	-5.13	116.45	123.12
2	IV	133	ILE	CB-CA-C	-5.13	105.22	112.14
2	KQ	133	ILE	CB-CA-C	-5.13	105.22	112.14
2	YV	141	ASP	CA-C-N	5.12	125.20	119.87
2	YV	141	ASP	C-N-CA	5.12	125.20	119.87
2	DP	288	ILE	CA-C-N	-5.12	116.46	123.12
2	DP	288	ILE	C-N-CA	-5.12	116.46	123.12
2	DW	288	ILE	CA-C-N	-5.12	116.46	123.12
2	DW	288	ILE	C-N-CA	-5.12	116.46	123.12
2	FA	288	ILE	CA-C-N	-5.12	116.46	123.12
2	FA	288	ILE	C-N-CA	-5.12	116.46	123.12
2	FM	288	ILE	CA-C-N	-5.12	116.46	123.12
2	FM	288	ILE	C-N-CA	-5.12	116.46	123.12
2	JL	141	ASP	CA-C-N	5.12	125.20	119.87
2	JL	141	ASP	C-N-CA	5.12	125.20	119.87
2	AD	288	ILE	CA-C-N	-5.12	116.46	123.12
2	AD	288	ILE	C-N-CA	-5.12	116.46	123.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	HS	288	ILE	CA-C-N	-5.12	116.46	123.12
2	HS	288	ILE	C-N-CA	-5.12	116.46	123.12
2	JB	288	ILE	CA-C-N	-5.12	116.46	123.12
2	JB	288	ILE	C-N-CA	-5.12	116.46	123.12
2	KW	288	ILE	CA-C-N	-5.12	116.46	123.12
2	KW	288	ILE	C-N-CA	-5.12	116.46	123.12
2	YF	288	ILE	CA-C-N	-5.12	116.47	123.12
2	YF	288	ILE	C-N-CA	-5.12	116.47	123.12
2	YR	288	ILE	CA-C-N	-5.12	116.47	123.12
2	YR	288	ILE	C-N-CA	-5.12	116.47	123.12
2	DJ	288	ILE	CA-C-N	-5.12	116.47	123.12
2	DJ	288	ILE	C-N-CA	-5.12	116.47	123.12
2	FG	288	ILE	CA-C-N	-5.12	116.47	123.12
2	FG	288	ILE	C-N-CA	-5.12	116.47	123.12
2	JH	288	ILE	CA-C-N	-5.12	116.47	123.12
2	JH	288	ILE	C-N-CA	-5.12	116.47	123.12
2	JN	288	ILE	CA-C-N	-5.12	116.47	123.12
2	JN	288	ILE	C-N-CA	-5.12	116.47	123.12
2	CV	141	ASP	CA-C-N	5.12	125.19	119.87
2	CV	141	ASP	C-N-CA	5.12	125.19	119.87
2	GU	141	ASP	CA-C-N	5.12	125.19	119.87
2	GU	141	ASP	C-N-CA	5.12	125.19	119.87
2	ZB	288	ILE	CA-C-N	-5.11	116.47	123.12
2	ZB	288	ILE	C-N-CA	-5.11	116.47	123.12
2	AJ	288	ILE	CA-C-N	-5.11	116.47	123.12
2	AJ	288	ILE	C-N-CA	-5.11	116.47	123.12
2	IV	288	ILE	CA-C-N	-5.11	116.47	123.12
2	IV	288	ILE	C-N-CA	-5.11	116.47	123.12
2	KQ	288	ILE	CA-C-N	-5.11	116.47	123.12
2	KQ	288	ILE	C-N-CA	-5.11	116.47	123.12
2	BF	141	ASP	CA-C-N	5.11	125.18	119.87
2	BF	141	ASP	C-N-CA	5.11	125.18	119.87
2	DN	141	ASP	CA-C-N	5.11	125.19	119.87
2	DN	141	ASP	C-N-CA	5.11	125.19	119.87
2	FK	141	ASP	CA-C-N	5.11	125.19	119.87
2	FK	141	ASP	C-N-CA	5.11	125.19	119.87
2	HK	141	ASP	CA-C-N	5.11	125.18	119.87
2	HK	141	ASP	C-N-CA	5.11	125.18	119.87
2	ZZ	133	ILE	CB-CA-C	-5.11	105.24	112.14
2	AV	288	ILE	CA-C-N	-5.11	116.48	123.12
2	AV	288	ILE	C-N-CA	-5.11	116.48	123.12
2	BH	133	ILE	CB-CA-C	-5.11	105.24	112.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	HC	288	ILE	CA-C-N	-5.11	116.48	123.12
2	HC	288	ILE	C-N-CA	-5.11	116.48	123.12
2	GE	133	ILE	CB-CA-C	-5.11	105.24	112.14
2	HY	133	ILE	CB-CA-C	-5.11	105.24	112.14
2	IP	288	ILE	CA-C-N	-5.11	116.48	123.12
2	IP	288	ILE	C-N-CA	-5.11	116.48	123.12
2	LC	288	ILE	CA-C-N	-5.11	116.48	123.12
2	LC	288	ILE	C-N-CA	-5.11	116.48	123.12
2	BB	288	ILE	CA-C-N	-5.11	116.48	123.12
2	BB	288	ILE	C-N-CA	-5.11	116.48	123.12
2	FS	288	ILE	CA-C-N	-5.11	116.48	123.12
2	FS	288	ILE	C-N-CA	-5.11	116.48	123.12
2	ZH	288	ILE	CA-C-N	-5.11	116.48	123.12
2	ZH	288	ILE	C-N-CA	-5.11	116.48	123.12
2	HH	288	ILE	CA-C-N	-5.11	116.48	123.12
2	HH	288	ILE	C-N-CA	-5.11	116.48	123.12
2	ID	288	ILE	CA-C-N	-5.11	116.48	123.12
2	ID	288	ILE	C-N-CA	-5.11	116.48	123.12
2	KE	288	ILE	CA-C-N	-5.11	116.48	123.12
2	KE	288	ILE	C-N-CA	-5.11	116.48	123.12
2	YD	141	ASP	CA-C-N	5.10	125.18	119.87
2	YD	141	ASP	C-N-CA	5.10	125.18	119.87
2	BL	141	ASP	CA-C-N	5.10	125.18	119.87
2	BL	141	ASP	C-N-CA	5.10	125.18	119.87
2	BN	288	ILE	CA-C-N	-5.10	116.48	123.12
2	BN	288	ILE	C-N-CA	-5.10	116.48	123.12
2	CX	288	ILE	CA-C-N	-5.10	116.48	123.12
2	CX	288	ILE	C-N-CA	-5.10	116.48	123.12
2	EI	288	ILE	CA-C-N	-5.10	116.48	123.12
2	EI	288	ILE	C-N-CA	-5.10	116.48	123.12
2	GI	141	ASP	CA-C-N	5.10	125.18	119.87
2	GI	141	ASP	C-N-CA	5.10	125.18	119.87
2	IB	141	ASP	CA-C-N	5.10	125.18	119.87
2	IB	141	ASP	C-N-CA	5.10	125.18	119.87
2	ZN	288	ILE	CA-C-N	-5.10	116.48	123.12
2	ZN	288	ILE	C-N-CA	-5.10	116.48	123.12
2	AZ	141	ASP	CA-C-N	5.10	125.18	119.87
2	AZ	141	ASP	C-N-CA	5.10	125.18	119.87
2	BZ	288	ILE	CA-C-N	-5.10	116.49	123.12
2	BZ	288	ILE	C-N-CA	-5.10	116.49	123.12
2	CL	288	ILE	CA-C-N	-5.10	116.49	123.12
2	CL	288	ILE	C-N-CA	-5.10	116.49	123.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EO	288	ILE	CA-C-N	-5.10	116.49	123.12
2	EO	288	ILE	C-N-CA	-5.10	116.49	123.12
2	EU	288	ILE	CA-C-N	-5.10	116.49	123.12
2	EU	288	ILE	C-N-CA	-5.10	116.49	123.12
2	HF	141	ASP	CA-C-N	5.10	125.18	119.87
2	HF	141	ASP	C-N-CA	5.10	125.18	119.87
2	DB	141	ASP	CA-C-N	5.10	125.17	119.87
2	DB	141	ASP	C-N-CA	5.10	125.17	119.87
2	EM	141	ASP	CA-C-N	5.10	125.17	119.87
2	EM	141	ASP	C-N-CA	5.10	125.17	119.87
2	AH	141	ASP	CA-C-N	5.10	125.17	119.87
2	AH	141	ASP	C-N-CA	5.10	125.17	119.87
2	BX	141	ASP	CA-C-N	5.10	125.17	119.87
2	BX	141	ASP	C-N-CA	5.10	125.17	119.87
2	HW	141	ASP	CA-C-N	5.10	125.17	119.87
2	HW	141	ASP	C-N-CA	5.10	125.17	119.87
2	ZX	141	ASP	CA-C-N	5.10	125.17	119.87
2	ZX	141	ASP	C-N-CA	5.10	125.17	119.87
2	JY	288	ILE	CA-C-N	-5.10	116.49	123.12
2	JY	288	ILE	C-N-CA	-5.10	116.49	123.12
2	ZL	141	ASP	CA-C-N	5.10	125.17	119.87
2	ZL	141	ASP	C-N-CA	5.10	125.17	119.87
2	KI	141	ASP	CA-C-N	5.10	125.17	119.87
2	KI	141	ASP	C-N-CA	5.10	125.17	119.87
2	LO	288	ILE	CA-C-N	-5.10	116.49	123.12
2	LO	288	ILE	C-N-CA	-5.10	116.49	123.12
2	CR	288	ILE	CA-C-N	-5.10	116.50	123.12
2	CR	288	ILE	C-N-CA	-5.10	116.50	123.12
2	GQ	288	ILE	CA-C-N	-5.10	116.50	123.12
2	GQ	288	ILE	C-N-CA	-5.10	116.50	123.12
2	FW	141	ASP	CA-C-N	5.09	125.17	119.87
2	FW	141	ASP	C-N-CA	5.09	125.17	119.87
2	IG	141	ASP	CA-C-N	5.09	125.17	119.87
2	IG	141	ASP	C-N-CA	5.09	125.17	119.87
1	FR	19	ARG	N-CA-C	-5.09	105.81	111.36
1	IC	19	ARG	N-CA-C	-5.09	105.81	111.36
1	ZY	19	ARG	N-CA-C	-5.09	105.81	111.36
1	BG	19	ARG	N-CA-C	-5.09	105.81	111.36
2	CF	288	ILE	CA-C-N	-5.09	116.50	123.12
2	CF	288	ILE	C-N-CA	-5.09	116.50	123.12
2	EC	288	ILE	CA-C-N	-5.09	116.50	123.12
2	EC	288	ILE	C-N-CA	-5.09	116.50	123.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	IT	141	ASP	CA-C-N	5.09	125.17	119.87
2	IT	141	ASP	C-N-CA	5.09	125.17	119.87
2	LG	141	ASP	CA-C-N	5.09	125.17	119.87
2	LG	141	ASP	C-N-CA	5.09	125.17	119.87
2	KK	288	ILE	CA-C-N	-5.09	116.50	123.12
2	KK	288	ILE	C-N-CA	-5.09	116.50	123.12
2	LI	288	ILE	CA-C-N	-5.09	116.50	123.12
2	LI	288	ILE	C-N-CA	-5.09	116.50	123.12
1	KJ	19	ARG	N-CA-C	-5.08	105.82	111.36
1	LH	19	ARG	N-CA-C	-5.08	105.82	111.36
2	GC	141	ASP	CA-C-N	5.08	125.16	119.87
2	GC	141	ASP	C-N-CA	5.08	125.16	119.87
2	IN	141	ASP	CA-C-N	5.08	125.16	119.87
2	IN	141	ASP	C-N-CA	5.08	125.16	119.87
2	AN	141	ASP	CA-C-N	5.08	125.16	119.87
2	AN	141	ASP	C-N-CA	5.08	125.16	119.87
2	AQ	288	ILE	CA-C-N	-5.08	116.52	123.12
2	AQ	288	ILE	C-N-CA	-5.08	116.52	123.12
1	AU	19	ARG	N-CA-C	-5.08	105.82	111.36
1	BS	19	ARG	N-CA-C	-5.08	105.82	111.36
2	ZF	141	ASP	CA-C-N	5.08	125.16	119.87
2	ZF	141	ASP	C-N-CA	5.08	125.16	119.87
2	GW	288	ILE	CA-C-N	-5.08	116.52	123.12
2	GW	288	ILE	C-N-CA	-5.08	116.52	123.12
1	HB	19	ARG	N-CA-C	-5.08	105.82	111.36
1	ZS	19	ARG	N-CA-C	-5.08	105.82	111.36
2	AB	141	ASP	CA-C-N	5.08	125.15	119.87
2	AB	141	ASP	C-N-CA	5.08	125.15	119.87
1	DU	19	ARG	N-CA-C	-5.08	105.83	111.36
1	EZ	19	ARG	N-CA-C	-5.08	105.83	111.36
2	HQ	141	ASP	CA-C-N	5.08	125.15	119.87
2	HQ	141	ASP	C-N-CA	5.08	125.15	119.87
2	CP	141	ASP	CA-C-N	5.08	125.15	119.87
2	CP	141	ASP	C-N-CA	5.08	125.15	119.87
2	ES	141	ASP	CA-C-N	5.08	125.15	119.87
2	ES	141	ASP	C-N-CA	5.08	125.15	119.87
2	YX	288	ILE	CA-C-N	-5.07	116.52	123.12
2	YX	288	ILE	C-N-CA	-5.07	116.52	123.12
2	HM	288	ILE	CA-C-N	-5.07	116.52	123.12
2	HM	288	ILE	C-N-CA	-5.07	116.52	123.12
1	IU	19	ARG	N-CA-C	-5.07	105.83	111.36
1	KP	19	ARG	N-CA-C	-5.07	105.83	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DC	19	ARG	N-CA-C	-5.07	105.83	111.36
1	GJ	19	ARG	N-CA-C	-5.07	105.83	111.36
1	JX	19	ARG	N-CA-C	-5.07	105.84	111.36
1	LN	19	ARG	N-CA-C	-5.07	105.84	111.36
1	CK	19	ARG	N-CA-C	-5.07	105.84	111.36
1	EN	19	ARG	N-CA-C	-5.07	105.84	111.36
2	KC	141	ASP	CA-C-N	5.07	125.14	119.87
2	KC	141	ASP	C-N-CA	5.07	125.14	119.87
2	KO	141	ASP	CA-C-N	5.07	125.14	119.87
2	KO	141	ASP	C-N-CA	5.07	125.14	119.87
2	LM	141	ASP	CA-C-N	5.07	125.14	119.87
2	LM	141	ASP	C-N-CA	5.07	125.14	119.87
2	LS	141	ASP	CA-C-N	5.07	125.14	119.87
2	LS	141	ASP	C-N-CA	5.07	125.14	119.87
1	AR	19	ARG	N-CA-C	-5.06	105.84	111.36
1	GV	19	ARG	N-CA-C	-5.06	105.84	111.36
1	YE	19	ARG	N-CA-C	-5.06	105.84	111.36
2	EA	141	ASP	CA-C-N	5.06	125.14	119.87
2	EA	141	ASP	C-N-CA	5.06	125.14	119.87
2	FE	141	ASP	CA-C-N	5.06	125.14	119.87
2	FE	141	ASP	C-N-CA	5.06	125.14	119.87
1	JM	19	ARG	N-CA-C	-5.06	105.84	111.36
1	CW	19	ARG	N-CA-C	-5.06	105.84	111.36
2	DT	141	ASP	CA-C-N	5.06	125.13	119.87
2	DT	141	ASP	C-N-CA	5.06	125.13	119.87
1	EH	19	ARG	N-CA-C	-5.06	105.84	111.36
2	FQ	141	ASP	CA-C-N	5.06	125.13	119.87
2	FQ	141	ASP	C-N-CA	5.06	125.13	119.87
1	ZA	19	ARG	N-CA-C	-5.06	105.84	111.36
1	AI	19	ARG	N-CA-C	-5.06	105.84	111.36
1	BA	19	ARG	N-CA-C	-5.06	105.84	111.36
1	HG	19	ARG	N-CA-C	-5.06	105.84	111.36
2	YJ	141	ASP	CA-C-N	5.06	125.13	119.87
2	YJ	141	ASP	C-N-CA	5.06	125.13	119.87
1	BM	19	ARG	N-CA-C	-5.06	105.85	111.36
1	IO	19	ARG	N-CA-C	-5.06	105.85	111.36
2	JR	141	ASP	CA-C-N	5.06	125.13	119.87
2	JR	141	ASP	C-N-CA	5.06	125.13	119.87
1	ZM	19	ARG	N-CA-C	-5.06	105.85	111.36
1	LB	19	ARG	N-CA-C	-5.06	105.85	111.36
1	FX	19	ARG	N-CA-C	-5.06	105.85	111.36
1	II	19	ARG	N-CA-C	-5.06	105.85	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	YK	19	ARG	N-CA-C	-5.05	105.85	111.36
1	DO	19	ARG	N-CA-C	-5.05	105.85	111.36
1	FL	19	ARG	N-CA-C	-5.05	105.85	111.36
1	JS	19	ARG	N-CA-C	-5.05	105.85	111.36
2	CJ	141	ASP	CA-C-N	5.05	125.12	119.87
2	CJ	141	ASP	C-N-CA	5.05	125.12	119.87
2	EG	141	ASP	CA-C-N	5.05	125.12	119.87
2	EG	141	ASP	C-N-CA	5.05	125.12	119.87
1	ZG	19	ARG	N-CA-C	-5.05	105.85	111.36
2	JF	141	ASP	CA-C-N	5.05	125.12	119.87
2	JF	141	ASP	C-N-CA	5.05	125.12	119.87
1	KD	19	ARG	N-CA-C	-5.05	105.85	111.36
2	LA	141	ASP	CA-C-N	5.05	125.12	119.87
2	LA	141	ASP	C-N-CA	5.05	125.12	119.87
1	DI	19	ARG	N-CA-C	-5.05	105.86	111.36
1	FF	19	ARG	N-CA-C	-5.05	105.86	111.36
2	IR	141	ASP	CA-C-N	5.05	125.12	119.87
2	IR	141	ASP	C-N-CA	5.05	125.12	119.87
1	JA	19	ARG	N-CA-C	-5.05	105.86	111.36
1	KV	19	ARG	N-CA-C	-5.05	105.86	111.36
2	LE	141	ASP	CA-C-N	5.05	125.12	119.87
2	LE	141	ASP	C-N-CA	5.05	125.12	119.87
1	YW	46	ARG	CA-C-N	5.05	126.86	121.00
1	YW	46	ARG	C-N-CA	5.05	126.86	121.00
1	HL	46	ARG	CA-C-N	5.05	126.86	121.00
1	HL	46	ARG	C-N-CA	5.05	126.86	121.00
1	AC	19	ARG	N-CA-C	-5.04	105.86	111.36
1	HR	19	ARG	N-CA-C	-5.04	105.86	111.36
2	AT	141	ASP	CA-C-N	5.04	125.11	119.87
2	AT	141	ASP	C-N-CA	5.04	125.11	119.87
1	CE	19	ARG	N-CA-C	-5.04	105.86	111.36
1	EB	19	ARG	N-CA-C	-5.04	105.86	111.36
2	HA	141	ASP	CA-C-N	5.04	125.11	119.87
2	HA	141	ASP	C-N-CA	5.04	125.11	119.87
1	YQ	19	ARG	N-CA-C	-5.04	105.87	111.36
1	BS	46	ARG	CA-C-N	5.04	126.84	121.00
1	BS	46	ARG	C-N-CA	5.04	126.84	121.00
2	CB	141	ASP	CA-C-N	5.04	125.11	119.87
2	CB	141	ASP	C-N-CA	5.04	125.11	119.87
2	EW	141	ASP	CA-C-N	5.04	125.11	119.87
2	EW	141	ASP	C-N-CA	5.04	125.11	119.87
1	JG	19	ARG	N-CA-C	-5.04	105.87	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ZS	46	ARG	CA-C-N	5.04	126.84	121.00
1	ZS	46	ARG	C-N-CA	5.04	126.84	121.00
1	BY	19	ARG	N-CA-C	-5.04	105.87	111.36
1	ET	19	ARG	N-CA-C	-5.04	105.87	111.36
1	YW	19	ARG	N-CA-C	-5.03	105.87	111.36
2	CD	141	ASP	CA-C-N	5.03	125.11	119.87
2	CD	141	ASP	C-N-CA	5.03	125.11	119.87
2	EY	141	ASP	CA-C-N	5.03	125.11	119.87
2	EY	141	ASP	C-N-CA	5.03	125.11	119.87
1	FX	46	ARG	CA-C-N	5.03	126.84	121.00
1	FX	46	ARG	C-N-CA	5.03	126.84	121.00
1	GD	19	ARG	N-CA-C	-5.03	105.87	111.36
1	HL	19	ARG	N-CA-C	-5.03	105.87	111.36
1	HX	19	ARG	N-CA-C	-5.03	105.87	111.36
1	II	46	ARG	CA-C-N	5.03	126.84	121.00
1	II	46	ARG	C-N-CA	5.03	126.84	121.00
2	AF	141	ASP	CA-C-N	5.03	125.10	119.87
2	AF	141	ASP	C-N-CA	5.03	125.10	119.87
2	HU	141	ASP	CA-C-N	5.03	125.10	119.87
2	HU	141	ASP	C-N-CA	5.03	125.10	119.87
2	IZ	141	ASP	CA-C-N	5.03	125.10	119.87
2	IZ	141	ASP	C-N-CA	5.03	125.10	119.87
2	KU	141	ASP	CA-C-N	5.03	125.10	119.87
2	KU	141	ASP	C-N-CA	5.03	125.10	119.87
1	DI	46	ARG	CA-C-N	5.03	126.83	121.00
1	DI	46	ARG	C-N-CA	5.03	126.83	121.00
1	DU	46	ARG	CA-C-N	5.03	126.83	121.00
1	DU	46	ARG	C-N-CA	5.03	126.83	121.00
1	EZ	46	ARG	CA-C-N	5.03	126.83	121.00
1	EZ	46	ARG	C-N-CA	5.03	126.83	121.00
1	FF	46	ARG	CA-C-N	5.03	126.83	121.00
1	FF	46	ARG	C-N-CA	5.03	126.83	121.00
1	CK	46	ARG	CA-C-N	5.02	126.83	121.00
1	CK	46	ARG	C-N-CA	5.02	126.83	121.00
1	EN	46	ARG	CA-C-N	5.02	126.83	121.00
1	EN	46	ARG	C-N-CA	5.02	126.83	121.00
1	YE	46	ARG	CA-C-N	5.02	126.83	121.00
1	YE	46	ARG	C-N-CA	5.02	126.83	121.00
2	GA	141	ASP	CA-C-N	5.02	125.09	119.87
2	GA	141	ASP	C-N-CA	5.02	125.09	119.87
2	IL	141	ASP	CA-C-N	5.02	125.09	119.87
2	IL	141	ASP	C-N-CA	5.02	125.09	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	JM	46	ARG	CA-C-N	5.02	126.83	121.00
1	JM	46	ARG	C-N-CA	5.02	126.83	121.00
2	AO	141	ASP	CA-C-N	5.02	125.09	119.87
2	AO	141	ASP	C-N-CA	5.02	125.09	119.87
2	GY	141	ASP	CA-C-N	5.02	125.09	119.87
2	GY	141	ASP	C-N-CA	5.02	125.09	119.87
2	YP	141	ASP	CA-C-N	5.02	125.09	119.87
2	YP	141	ASP	C-N-CA	5.02	125.09	119.87
1	AR	46	ARG	CA-C-N	5.02	126.82	121.00
1	AR	46	ARG	C-N-CA	5.02	126.82	121.00
2	AX	141	ASP	CA-C-N	5.02	125.09	119.87
2	AX	141	ASP	C-N-CA	5.02	125.09	119.87
1	GV	46	ARG	CA-C-N	5.02	126.82	121.00
1	GV	46	ARG	C-N-CA	5.02	126.82	121.00
2	HE	141	ASP	CA-C-N	5.02	125.09	119.87
2	HE	141	ASP	C-N-CA	5.02	125.09	119.87
2	JW	141	ASP	CA-C-N	5.02	125.09	119.87
2	JW	141	ASP	C-N-CA	5.02	125.09	119.87
2	KA	141	ASP	CA-C-N	5.02	125.09	119.87
2	KA	141	ASP	C-N-CA	5.02	125.09	119.87
2	LQ	141	ASP	CA-C-N	5.02	125.09	119.87
2	LQ	141	ASP	C-N-CA	5.02	125.09	119.87
2	DF	141	ASP	CA-C-N	5.02	125.09	119.87
2	DF	141	ASP	C-N-CA	5.02	125.09	119.87
2	GM	141	ASP	CA-C-N	5.02	125.09	119.87
2	GM	141	ASP	C-N-CA	5.02	125.09	119.87
1	JX	46	ARG	CA-C-N	5.02	126.82	121.00
1	JX	46	ARG	C-N-CA	5.02	126.82	121.00
1	LN	46	ARG	CA-C-N	5.02	126.82	121.00
1	LN	46	ARG	C-N-CA	5.02	126.82	121.00
1	ZY	46	ARG	CA-C-N	5.01	126.82	121.00
1	ZY	46	ARG	C-N-CA	5.01	126.82	121.00
1	BG	46	ARG	CA-C-N	5.01	126.82	121.00
1	BG	46	ARG	C-N-CA	5.01	126.82	121.00
1	CQ	19	ARG	N-CA-C	-5.01	105.89	111.36
1	GP	19	ARG	N-CA-C	-5.01	105.89	111.36
1	BA	46	ARG	CA-C-N	5.01	126.82	121.00
1	BA	46	ARG	C-N-CA	5.01	126.82	121.00
1	HG	46	ARG	CA-C-N	5.01	126.82	121.00
1	HG	46	ARG	C-N-CA	5.01	126.82	121.00
2	DH	141	ASP	CA-C-N	5.01	125.08	119.87
2	DH	141	ASP	C-N-CA	5.01	125.08	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DY	141	ASP	CA-C-N	5.01	125.08	119.87
2	DY	141	ASP	C-N-CA	5.01	125.08	119.87
2	FC	141	ASP	CA-C-N	5.01	125.08	119.87
2	FC	141	ASP	C-N-CA	5.01	125.08	119.87
2	GO	141	ASP	CA-C-N	5.01	125.08	119.87
2	GO	141	ASP	C-N-CA	5.01	125.08	119.87
1	BY	46	ARG	CA-C-N	5.01	126.81	121.00
1	BY	46	ARG	C-N-CA	5.01	126.81	121.00
1	DC	46	ARG	CA-C-N	5.01	126.81	121.00
1	DC	46	ARG	C-N-CA	5.01	126.81	121.00
2	DL	141	ASP	CA-C-N	5.01	125.08	119.87
2	DL	141	ASP	C-N-CA	5.01	125.08	119.87
1	ET	46	ARG	CA-C-N	5.01	126.81	121.00
1	ET	46	ARG	C-N-CA	5.01	126.81	121.00
2	FI	141	ASP	CA-C-N	5.01	125.08	119.87
2	FI	141	ASP	C-N-CA	5.01	125.08	119.87
1	GJ	46	ARG	CA-C-N	5.01	126.81	121.00
1	GJ	46	ARG	C-N-CA	5.01	126.81	121.00
1	ZA	46	ARG	CA-C-N	5.01	126.81	121.00
1	ZA	46	ARG	C-N-CA	5.01	126.81	121.00
1	AI	46	ARG	CA-C-N	5.01	126.81	121.00
1	AI	46	ARG	C-N-CA	5.01	126.81	121.00
1	AC	46	ARG	CA-C-N	5.01	126.81	121.00
1	AC	46	ARG	C-N-CA	5.01	126.81	121.00
2	BJ	141	ASP	CA-C-N	5.01	125.08	119.87
2	BJ	141	ASP	C-N-CA	5.01	125.08	119.87
1	HR	46	ARG	CA-C-N	5.01	126.81	121.00
1	HR	46	ARG	C-N-CA	5.01	126.81	121.00
1	JA	46	ARG	CA-C-N	5.01	126.81	121.00
1	JA	46	ARG	C-N-CA	5.01	126.81	121.00
1	KV	46	ARG	CA-C-N	5.01	126.81	121.00
1	KV	46	ARG	C-N-CA	5.01	126.81	121.00
2	YB	141	ASP	CA-C-N	5.01	125.08	119.87
2	YB	141	ASP	C-N-CA	5.01	125.08	119.87
2	YH	141	ASP	CA-C-N	5.00	125.07	119.87
2	YH	141	ASP	C-N-CA	5.00	125.07	119.87
1	YQ	46	ARG	CA-C-N	5.00	126.81	121.00
1	YQ	46	ARG	C-N-CA	5.00	126.81	121.00
2	CH	141	ASP	CA-C-N	5.00	125.07	119.87
2	CH	141	ASP	C-N-CA	5.00	125.07	119.87
2	EE	141	ASP	CA-C-N	5.00	125.07	119.87
2	EE	141	ASP	C-N-CA	5.00	125.07	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GD	46	ARG	CA-C-N	5.00	126.81	121.00
1	GD	46	ARG	C-N-CA	5.00	126.81	121.00
1	HX	46	ARG	CA-C-N	5.00	126.81	121.00
1	HX	46	ARG	C-N-CA	5.00	126.81	121.00
1	JG	46	ARG	CA-C-N	5.00	126.81	121.00
1	JG	46	ARG	C-N-CA	5.00	126.81	121.00
2	JP	141	ASP	CA-C-N	5.00	125.07	119.87
2	JP	141	ASP	C-N-CA	5.00	125.07	119.87
1	CE	46	ARG	CA-C-N	5.00	126.80	121.00
1	CE	46	ARG	C-N-CA	5.00	126.80	121.00
1	EB	46	ARG	CA-C-N	5.00	126.80	121.00
1	EB	46	ARG	C-N-CA	5.00	126.80	121.00
2	JD	141	ASP	CA-C-N	5.00	125.07	119.87
2	JD	141	ASP	C-N-CA	5.00	125.07	119.87
2	KY	141	ASP	CA-C-N	5.00	125.07	119.87
2	KY	141	ASP	C-N-CA	5.00	125.07	119.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	808	0	851	5	0
1	AC	808	0	851	3	0
1	AE	808	0	851	6	0
1	AG	808	0	851	5	0
1	AI	808	0	851	3	0
1	AK	808	0	851	7	0
1	AM	808	0	851	5	0
1	AP	808	0	851	6	0
1	AR	808	0	851	4	0
1	AS	808	0	851	5	0
1	AU	808	0	851	3	0
1	AW	808	0	851	7	0
1	AY	808	0	851	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	808	0	851	3	0
1	BC	808	0	851	7	0
1	BE	808	0	851	5	0
1	BG	808	0	851	4	0
1	BI	808	0	851	7	0
1	BK	808	0	851	5	0
1	BM	808	0	851	3	0
1	BO	808	0	851	6	0
1	BQ	808	0	851	5	0
1	BS	808	0	851	4	0
1	BU	808	0	851	6	0
1	BW	808	0	851	5	0
1	BY	808	0	851	4	0
1	CA	808	0	851	7	0
1	CC	808	0	851	5	0
1	CE	808	0	851	4	0
1	CG	808	0	851	6	0
1	CI	808	0	851	5	0
1	CK	808	0	851	4	0
1	CM	808	0	851	6	0
1	CO	808	0	851	5	0
1	CQ	808	0	851	3	0
1	CS	808	0	851	6	0
1	CU	808	0	851	5	0
1	CW	808	0	851	4	0
1	CY	808	0	851	6	0
1	DA	808	0	851	4	0
1	DC	808	0	851	4	0
1	DE	808	0	851	6	0
1	DG	808	0	851	5	0
1	DI	808	0	851	4	0
1	DK	808	0	851	6	0
1	DM	808	0	851	5	0
1	DO	808	0	851	3	0
1	DQ	808	0	851	6	0
1	DS	808	0	851	5	0
1	DU	808	0	851	4	0
1	DX	808	0	851	6	0
1	DZ	808	0	851	5	0
1	EB	808	0	851	3	0
1	ED	808	0	851	6	0
1	EF	808	0	851	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EH	808	0	851	4	0
1	EJ	808	0	851	6	0
1	EL	808	0	851	5	0
1	EN	808	0	851	4	0
1	EP	808	0	851	6	0
1	ER	808	0	851	5	0
1	ET	808	0	851	3	0
1	EV	808	0	851	7	0
1	EX	808	0	851	5	0
1	EZ	808	0	851	4	0
1	FB	808	0	851	6	0
1	FD	808	0	851	5	0
1	FF	808	0	851	4	0
1	FH	808	0	851	6	0
1	FJ	808	0	851	5	0
1	FL	808	0	851	4	0
1	FN	808	0	851	6	0
1	FP	808	0	851	5	0
1	FR	808	0	851	3	0
1	FT	808	0	851	7	0
1	FV	808	0	851	5	0
1	FX	808	0	851	4	0
1	FZ	808	0	851	6	0
1	GB	808	0	851	6	0
1	GD	808	0	851	4	0
1	GF	808	0	851	6	0
1	GH	808	0	851	5	0
1	GJ	808	0	851	4	0
1	GL	808	0	851	7	0
1	GN	808	0	851	5	0
1	GP	808	0	851	4	0
1	GR	808	0	851	6	0
1	GT	808	0	851	5	0
1	GV	808	0	851	4	0
1	GX	808	0	851	6	0
1	GZ	808	0	851	5	0
1	HB	808	0	851	3	0
1	HD	808	0	851	6	0
1	HG	808	0	851	4	0
1	HI	808	0	851	6	0
1	HL	808	0	851	3	0
1	HN	808	0	851	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HP	808	0	851	5	0
1	HR	808	0	851	4	0
1	HT	808	0	851	6	0
1	HV	808	0	851	5	0
1	HX	808	0	851	3	0
1	HZ	808	0	851	6	0
1	IC	808	0	851	3	0
1	IE	808	0	851	6	0
1	IH	808	0	851	5	0
1	II	808	0	851	4	0
1	IK	808	0	851	6	0
1	IM	808	0	851	5	0
1	IO	808	0	851	4	0
1	IQ	808	0	851	7	0
1	IS	808	0	851	4	0
1	IU	808	0	851	4	0
1	IW	808	0	851	6	0
1	IY	808	0	851	4	0
1	JA	808	0	851	4	0
1	JC	808	0	851	6	0
1	JE	808	0	851	5	0
1	JG	808	0	851	4	0
1	JI	808	0	851	6	0
1	JK	808	0	851	5	0
1	JM	808	0	851	3	0
1	JO	808	0	851	6	0
1	JQ	808	0	851	5	0
1	JS	808	0	851	3	0
1	JV	808	0	851	5	0
1	JX	808	0	851	4	0
1	JZ	808	0	851	6	0
1	KB	808	0	851	5	0
1	KD	808	0	851	3	0
1	KF	808	0	851	6	0
1	KH	808	0	851	5	0
1	KJ	808	0	851	3	0
1	KL	808	0	851	7	0
1	KN	808	0	851	5	0
1	KP	808	0	851	4	0
1	KR	808	0	851	7	0
1	KT	808	0	851	5	0
1	KV	808	0	851	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	KX	808	0	851	6	0
1	KZ	808	0	851	5	0
1	LB	808	0	851	4	0
1	LD	808	0	851	7	0
1	LF	808	0	851	5	0
1	LH	808	0	851	4	0
1	LJ	808	0	851	6	0
1	LL	808	0	851	5	0
1	LN	808	0	851	4	0
1	LP	808	0	851	6	0
1	LR	808	0	851	5	0
1	WA	808	0	851	5	0
1	WB	808	0	851	5	0
1	WC	808	0	851	5	0
1	WD	808	0	851	6	0
1	YA	808	0	851	6	0
1	YC	808	0	851	5	0
1	YE	808	0	851	4	0
1	YG	808	0	851	6	0
1	YI	808	0	851	5	0
1	YK	808	0	851	4	0
1	YM	808	0	851	6	0
1	YO	808	0	851	5	0
1	YQ	808	0	851	4	0
1	YS	808	0	851	6	0
1	YU	808	0	851	5	0
1	YW	808	0	851	4	0
1	YY	808	0	851	6	0
1	ZA	808	0	851	4	0
1	ZC	808	0	851	6	0
1	ZE	808	0	851	5	0
1	ZG	808	0	851	4	0
1	ZI	808	0	851	7	0
1	ZK	808	0	851	5	0
1	ZM	808	0	851	4	0
1	ZO	808	0	851	6	0
1	ZQ	808	0	851	5	0
1	ZS	808	0	851	3	0
1	ZU	808	0	851	6	0
1	ZW	808	0	851	5	0
1	ZY	808	0	851	3	0
2	AB	2267	0	2393	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AD	2267	0	2393	7	0
2	AF	2267	0	2393	12	0
2	AH	2267	0	2393	10	0
2	AJ	2267	0	2393	8	0
2	AL	2267	0	2393	11	0
2	AN	2267	0	2393	9	0
2	AO	2267	0	2393	12	0
2	AQ	2267	0	2393	7	0
2	AT	2267	0	2393	9	0
2	AV	2267	0	2393	7	0
2	AX	2267	0	2393	12	0
2	AZ	2267	0	2393	10	0
2	BB	2267	0	2393	7	0
2	BD	2267	0	2393	12	0
2	BF	2267	0	2393	10	0
2	BH	2267	0	2393	7	0
2	BJ	2267	0	2393	11	0
2	BL	2267	0	2393	9	0
2	BN	2267	0	2393	7	0
2	BP	2267	0	2393	11	0
2	BR	2267	0	2393	9	0
2	BT	2267	0	2393	7	0
2	BV	2267	0	2393	12	0
2	BX	2267	0	2393	9	0
2	BZ	2267	0	2393	7	0
2	CB	2267	0	2393	11	0
2	CD	2267	0	2393	10	0
2	CF	2267	0	2393	8	0
2	CH	2267	0	2393	12	0
2	CJ	2267	0	2393	9	0
2	CL	2267	0	2393	7	0
2	CN	2267	0	2393	12	0
2	CP	2267	0	2393	9	0
2	CR	2267	0	2393	7	0
2	CT	2267	0	2393	9	0
2	CV	2267	0	2393	9	0
2	CX	2267	0	2393	7	0
2	CZ	2267	0	2393	11	0
2	DB	2267	0	2393	7	0
2	DD	2267	0	2393	7	0
2	DF	2267	0	2393	12	0
2	DH	2267	0	2393	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DJ	2267	0	2393	7	0
2	DL	2267	0	2393	10	0
2	DN	2267	0	2393	9	0
2	DP	2267	0	2393	7	0
2	DR	2267	0	2393	11	0
2	DT	2267	0	2393	8	0
2	DW	2267	0	2393	8	0
2	DY	2267	0	2393	13	0
2	EA	2267	0	2393	10	0
2	EC	2267	0	2393	7	0
2	EE	2267	0	2393	11	0
2	EG	2267	0	2393	9	0
2	EI	2267	0	2393	8	0
2	EK	2267	0	2393	10	0
2	EM	2267	0	2393	8	0
2	EO	2267	0	2393	7	0
2	EQ	2267	0	2393	11	0
2	ES	2267	0	2393	9	0
2	EU	2267	0	2393	7	0
2	EW	2267	0	2393	12	0
2	EY	2267	0	2393	10	0
2	FA	2267	0	2393	8	0
2	FC	2267	0	2393	10	0
2	FE	2267	0	2393	9	0
2	FG	2267	0	2393	7	0
2	FI	2267	0	2393	9	0
2	FK	2267	0	2393	9	0
2	FM	2267	0	2393	8	0
2	FO	2267	0	2393	11	0
2	FQ	2267	0	2393	8	0
2	FS	2267	0	2393	8	0
2	FU	2267	0	2393	10	0
2	FW	2267	0	2393	9	0
2	FY	2267	0	2393	8	0
2	GA	2267	0	2393	10	0
2	GC	2267	0	2393	8	0
2	GE	2267	0	2393	8	0
2	GG	2267	0	2393	10	0
2	GI	2267	0	2393	8	0
2	GK	2267	0	2393	7	0
2	GM	2267	0	2393	10	0
2	GO	2267	0	2393	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	GQ	2267	0	2393	7	0
2	GS	2267	0	2393	11	0
2	GU	2267	0	2393	8	0
2	GW	2267	0	2393	7	0
2	GY	2267	0	2393	10	0
2	HA	2267	0	2393	9	0
2	HC	2267	0	2393	8	0
2	HE	2267	0	2393	10	0
2	HF	2267	0	2393	9	0
2	HH	2267	0	2393	8	0
2	HJ	2267	0	2393	10	0
2	HK	2267	0	2393	8	0
2	HM	2267	0	2393	8	0
2	HO	2267	0	2393	12	0
2	HQ	2267	0	2393	9	0
2	HS	2267	0	2393	7	0
2	HU	2267	0	2393	11	0
2	HW	2267	0	2393	10	0
2	HY	2267	0	2393	7	0
2	IA	2267	0	2393	12	0
2	IB	2267	0	2393	9	0
2	ID	2267	0	2393	7	0
2	IF	2267	0	2393	12	0
2	IG	2267	0	2393	7	0
2	IJ	2267	0	2393	8	0
2	IL	2267	0	2393	11	0
2	IN	2267	0	2393	9	0
2	IP	2267	0	2393	7	0
2	IR	2267	0	2393	9	0
2	IT	2267	0	2393	9	0
2	IV	2267	0	2393	7	0
2	IX	2267	0	2393	12	0
2	IZ	2267	0	2393	8	0
2	JB	2267	0	2393	7	0
2	JD	2267	0	2393	10	0
2	JF	2267	0	2393	9	0
2	JH	2267	0	2393	8	0
2	JJ	2267	0	2393	11	0
2	JL	2267	0	2393	9	0
2	JN	2267	0	2393	7	0
2	JP	2267	0	2393	11	0
2	JR	2267	0	2393	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	JT	2267	0	2393	7	0
2	JU	2267	0	2393	10	0
2	JW	2267	0	2393	9	0
2	JY	2267	0	2393	7	0
2	KA	2267	0	2393	12	0
2	KC	2267	0	2393	8	0
2	KE	2267	0	2393	7	0
2	KG	2267	0	2393	10	0
2	KI	2267	0	2393	9	0
2	KK	2267	0	2393	8	0
2	KM	2267	0	2393	12	0
2	KO	2267	0	2393	8	0
2	KQ	2267	0	2393	8	0
2	KS	2267	0	2393	10	0
2	KU	2267	0	2393	9	0
2	KW	2267	0	2393	7	0
2	KY	2267	0	2393	10	0
2	LA	2267	0	2393	8	0
2	LC	2267	0	2393	8	0
2	LE	2267	0	2393	10	0
2	LG	2267	0	2393	9	0
2	LI	2267	0	2393	7	0
2	LK	2267	0	2393	10	0
2	LM	2267	0	2393	9	0
2	LO	2267	0	2393	7	0
2	LQ	2267	0	2393	11	0
2	LS	2267	0	2393	10	0
2	YB	2267	0	2393	11	0
2	YD	2267	0	2393	10	0
2	YF	2267	0	2393	8	0
2	YH	2267	0	2393	11	0
2	YJ	2267	0	2393	9	0
2	YL	2267	0	2393	7	0
2	YN	2267	0	2393	11	0
2	YP	2267	0	2393	8	0
2	YR	2267	0	2393	8	0
2	YT	2267	0	2393	10	0
2	YV	2267	0	2393	9	0
2	YX	2267	0	2393	7	0
2	YZ	2267	0	2393	11	0
2	ZB	2267	0	2393	8	0
2	ZD	2267	0	2393	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	ZF	2267	0	2393	9	0
2	ZH	2267	0	2393	7	0
2	ZJ	2267	0	2393	10	0
2	ZL	2267	0	2393	10	0
2	ZN	2267	0	2393	7	0
2	ZP	2267	0	2393	10	0
2	ZR	2267	0	2393	8	0
2	ZT	2267	0	2393	7	0
2	ZV	2267	0	2393	11	0
2	ZX	2267	0	2393	10	0
2	ZZ	2267	0	2393	8	0
All	All	553500	0	583920	1976	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (1976) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:90:GLU:OE2	2:LC:282:LYS:NZ	2.34	0.61
1:YE:90:GLU:OE2	2:YF:282:LYS:NZ	2.34	0.61
1:BS:90:GLU:OE2	2:BT:282:LYS:NZ	2.34	0.61
1:DC:90:GLU:OE2	2:DD:282:LYS:NZ	2.34	0.61
1:ZG:90:GLU:OE2	2:ZH:282:LYS:NZ	2.34	0.61
1:HL:90:GLU:OE2	2:HM:282:LYS:NZ	2.34	0.61
1:II:90:GLU:OE2	2:IJ:282:LYS:NZ	2.34	0.61
2:AQ:282:LYS:NZ	1:AR:90:GLU:OE2	2.34	0.61
1:EN:90:GLU:OE2	2:EO:282:LYS:NZ	2.34	0.61
1:FR:90:GLU:OE2	2:FS:282:LYS:NZ	2.34	0.61
1:HB:90:GLU:OE2	2:HC:282:LYS:NZ	2.34	0.61
1:JA:90:GLU:OE2	2:JB:282:LYS:NZ	2.34	0.61
1:KP:90:GLU:OE2	2:KQ:282:LYS:NZ	2.34	0.61
1:ZS:90:GLU:OE2	2:ZT:282:LYS:NZ	2.34	0.61
1:AC:90:GLU:OE2	2:AD:282:LYS:NZ	2.34	0.61
1:HG:90:GLU:OE2	2:HH:282:LYS:NZ	2.34	0.61
1:KJ:90:GLU:OE2	2:KK:282:LYS:NZ	2.34	0.61
1:BY:90:GLU:OE2	2:BZ:282:LYS:NZ	2.34	0.61
1:DU:90:GLU:OE2	2:DW:282:LYS:NZ	2.34	0.61
1:EH:90:GLU:OE2	2:EI:282:LYS:NZ	2.34	0.61
1:LH:90:GLU:OE2	2:LI:282:LYS:NZ	2.34	0.61
1:AI:90:GLU:OE2	2:AJ:282:LYS:NZ	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GP:90:GLU:OE2	2:GQ:282:LYS:NZ	2.34	0.61
1:BG:90:GLU:OE2	2:BH:282:LYS:NZ	2.34	0.61
1:CK:90:GLU:OE2	2:CL:282:LYS:NZ	2.34	0.61
1:CQ:90:GLU:OE2	2:CR:282:LYS:NZ	2.34	0.61
1:GD:90:GLU:OE2	2:GE:282:LYS:NZ	2.34	0.61
1:IO:90:GLU:OE2	2:IP:282:LYS:NZ	2.34	0.61
1:IU:90:GLU:OE2	2:IV:282:LYS:NZ	2.34	0.61
1:KV:90:GLU:OE2	2:KW:282:LYS:NZ	2.34	0.61
1:LN:90:GLU:OE2	2:LO:282:LYS:NZ	2.34	0.61
1:YQ:90:GLU:OE2	2:YR:282:LYS:NZ	2.34	0.61
1:AU:90:GLU:OE2	2:AV:282:LYS:NZ	2.34	0.61
1:FL:90:GLU:OE2	2:FM:282:LYS:NZ	2.34	0.61
1:BA:90:GLU:OE2	2:BB:282:LYS:NZ	2.34	0.60
1:EB:90:GLU:OE2	2:EC:282:LYS:NZ	2.34	0.60
1:HX:90:GLU:OE2	2:HY:282:LYS:NZ	2.34	0.60
1:KD:90:GLU:OE2	2:KE:282:LYS:NZ	2.34	0.60
1:ZM:90:GLU:OE2	2:ZN:282:LYS:NZ	2.34	0.60
1:ZY:90:GLU:OE2	2:ZZ:282:LYS:NZ	2.34	0.60
1:CE:90:GLU:OE2	2:CF:282:LYS:NZ	2.34	0.60
1:ZA:90:GLU:OE2	2:ZB:282:LYS:NZ	2.34	0.60
1:DI:90:GLU:OE2	2:DJ:282:LYS:NZ	2.34	0.60
2:FE:123:GLU:OE2	2:FE:170:LYS:NZ	2.34	0.60
1:FX:90:GLU:OE2	2:FY:282:LYS:NZ	2.34	0.60
1:IC:90:GLU:OE2	2:ID:282:LYS:NZ	2.34	0.60
2:IG:123:GLU:OE2	2:IG:170:LYS:NZ	2.34	0.60
1:JS:90:GLU:OE2	2:JT:282:LYS:NZ	2.34	0.60
1:JX:90:GLU:OE2	2:JY:282:LYS:NZ	2.34	0.60
1:FF:90:GLU:OE2	2:FG:282:LYS:NZ	2.34	0.60
1:BM:90:GLU:OE2	2:BN:282:LYS:NZ	2.34	0.60
1:DO:90:GLU:OE2	2:DP:282:LYS:NZ	2.34	0.60
2:EQ:2:ASP:OD2	2:ES:101:LYS:NZ	2.33	0.60
1:ET:90:GLU:OE2	2:EU:282:LYS:NZ	2.34	0.60
2:FW:123:GLU:OE2	2:FW:170:LYS:NZ	2.34	0.60
1:HR:90:GLU:OE2	2:HS:282:LYS:NZ	2.34	0.60
1:JG:90:GLU:OE2	2:JH:282:LYS:NZ	2.34	0.60
1:JM:90:GLU:OE2	2:JN:282:LYS:NZ	2.34	0.60
1:YK:90:GLU:OE2	2:YL:282:LYS:NZ	2.34	0.60
1:CW:90:GLU:OE2	2:CX:282:LYS:NZ	2.34	0.60
1:EZ:90:GLU:OE2	2:FA:282:LYS:NZ	2.34	0.60
2:HW:123:GLU:OE2	2:HW:170:LYS:NZ	2.34	0.60
2:AT:123:GLU:OE2	2:AT:170:LYS:NZ	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GJ:90:GLU:OE2	2:GK:282:LYS:NZ	2.34	0.60
1:GV:90:GLU:OE2	2:GW:282:LYS:NZ	2.34	0.60
2:KO:123:GLU:OE2	2:KO:170:LYS:NZ	2.34	0.60
1:YW:90:GLU:OE2	2:YX:282:LYS:NZ	2.34	0.60
2:DT:123:GLU:OE2	2:DT:170:LYS:NZ	2.34	0.60
2:IL:123:GLU:OE2	2:IL:170:LYS:NZ	2.34	0.60
2:CV:123:GLU:OE2	2:CV:170:LYS:NZ	2.34	0.60
2:FK:123:GLU:OE2	2:FK:170:LYS:NZ	2.34	0.60
2:BD:123:GLU:OE2	2:BD:170:LYS:NZ	2.34	0.59
1:BQ:90:GLU:OE2	2:BR:282:LYS:NZ	2.35	0.59
2:GO:123:GLU:OE2	2:GO:170:LYS:NZ	2.34	0.59
1:GT:90:GLU:OE2	2:GU:282:LYS:NZ	2.35	0.59
1:JE:90:GLU:OE2	2:JF:282:LYS:NZ	2.35	0.59
1:KH:90:GLU:OE2	2:KI:282:LYS:NZ	2.35	0.59
2:LG:123:GLU:OE2	2:LG:170:LYS:NZ	2.34	0.59
2:ZR:123:GLU:OE2	2:ZR:170:LYS:NZ	2.34	0.59
1:YI:90:GLU:OE2	2:YJ:282:LYS:NZ	2.35	0.59
1:AA:90:GLU:OE2	2:AB:282:LYS:NZ	2.35	0.59
1:BE:90:GLU:OE2	2:BF:282:LYS:NZ	2.35	0.59
1:CU:90:GLU:OE2	2:CV:282:LYS:NZ	2.35	0.59
1:FV:90:GLU:OE2	2:FW:282:LYS:NZ	2.36	0.59
1:IM:90:GLU:OE2	2:IN:282:LYS:NZ	2.35	0.59
2:JF:123:GLU:OE2	2:JF:170:LYS:NZ	2.34	0.59
1:JK:90:GLU:OE2	2:JL:282:LYS:NZ	2.35	0.59
1:KT:90:GLU:OE2	2:KU:282:LYS:NZ	2.36	0.59
1:KZ:90:GLU:OE2	2:LA:282:LYS:NZ	2.35	0.59
1:YO:90:GLU:OE2	2:YP:282:LYS:NZ	2.35	0.59
1:AG:90:GLU:OE2	2:AH:282:LYS:NZ	2.35	0.59
1:CC:90:GLU:OE2	2:CD:282:LYS:NZ	2.35	0.59
1:EF:90:GLU:OE2	2:EG:282:LYS:NZ	2.35	0.59
1:HP:90:GLU:OE2	2:HQ:282:LYS:NZ	2.35	0.59
2:IB:123:GLU:OE2	2:IB:170:LYS:NZ	2.34	0.59
1:ZQ:90:GLU:OE2	2:ZR:282:LYS:NZ	2.35	0.59
1:DG:90:GLU:OE2	2:DH:282:LYS:NZ	2.35	0.59
1:LF:90:GLU:OE2	2:LG:282:LYS:NZ	2.35	0.59
2:ZX:123:GLU:OE2	2:ZX:170:LYS:NZ	2.34	0.59
2:BX:123:GLU:OE2	2:BX:170:LYS:NZ	2.34	0.59
1:DA:90:GLU:OE2	2:DB:282:LYS:NZ	2.35	0.59
1:FJ:90:GLU:OE2	2:FK:282:LYS:NZ	2.35	0.59
1:GH:90:GLU:OE2	2:GI:282:LYS:NZ	2.35	0.59
2:IG:282:LYS:NZ	1:IH:90:GLU:OE2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KC:123:GLU:OE2	2:KC:170:LYS:NZ	2.34	0.59
2:LK:2:ASP:OD2	2:LM:101:LYS:NZ	2.34	0.59
1:ZW:90:GLU:OE2	2:ZX:282:LYS:NZ	2.35	0.59
1:YU:90:GLU:OE2	2:YV:282:LYS:NZ	2.35	0.59
1:AM:90:GLU:OE2	2:AN:282:LYS:NZ	2.35	0.59
1:CO:90:GLU:OE2	2:CP:282:LYS:NZ	2.35	0.59
1:FD:90:GLU:OE2	2:FE:282:LYS:NZ	2.35	0.59
1:GN:90:GLU:OE2	2:GO:282:LYS:NZ	2.35	0.59
1:GZ:90:GLU:OE2	2:HA:282:LYS:NZ	2.35	0.59
1:HV:90:GLU:OE2	2:HW:282:LYS:NZ	2.35	0.59
1:IS:90:GLU:OE2	2:IT:282:LYS:NZ	2.35	0.59
1:JQ:90:GLU:OE2	2:JR:282:LYS:NZ	2.35	0.59
1:AS:90:GLU:OE2	2:AT:282:LYS:NZ	2.35	0.59
2:CJ:123:GLU:OE2	2:CJ:170:LYS:NZ	2.34	0.59
1:ZE:90:GLU:OE2	2:ZF:282:LYS:NZ	2.35	0.59
1:EL:90:GLU:OE2	2:EM:282:LYS:NZ	2.35	0.59
1:ER:90:GLU:OE2	2:ES:282:LYS:NZ	2.35	0.59
2:HF:282:LYS:NZ	1:WB:90:GLU:OE2	2.35	0.59
2:KI:123:GLU:OE2	2:KI:170:LYS:NZ	2.34	0.59
1:BW:90:GLU:OE2	2:BX:282:LYS:NZ	2.35	0.59
1:DM:90:GLU:OE2	2:DN:282:LYS:NZ	2.35	0.59
2:BF:123:GLU:OE2	2:BF:170:LYS:NZ	2.34	0.59
2:CP:123:GLU:OE2	2:CP:170:LYS:NZ	2.34	0.59
1:KB:90:GLU:OE2	2:KC:282:LYS:NZ	2.35	0.59
1:LL:90:GLU:OE2	2:LM:282:LYS:NZ	2.36	0.59
1:LR:90:GLU:OE2	2:LS:282:LYS:NZ	2.35	0.59
1:EX:90:GLU:OE2	2:EY:282:LYS:NZ	2.35	0.59
2:FQ:123:GLU:OE2	2:FQ:170:LYS:NZ	2.34	0.59
2:IX:2:ASP:OD2	2:IZ:101:LYS:NZ	2.33	0.59
1:ZK:90:GLU:OE2	2:ZL:282:LYS:NZ	2.35	0.59
1:JV:90:GLU:OE2	2:JW:282:LYS:NZ	2.35	0.59
1:YC:90:GLU:OE2	2:YD:282:LYS:NZ	2.36	0.58
2:CZ:2:ASP:OD2	2:DB:101:LYS:NZ	2.34	0.58
1:FP:90:GLU:OE2	2:FQ:282:LYS:NZ	2.35	0.58
2:HA:123:GLU:OE2	2:HA:170:LYS:NZ	2.34	0.58
2:HK:282:LYS:NZ	1:WA:90:GLU:OE2	2.35	0.58
1:CI:90:GLU:OE2	2:CJ:282:LYS:NZ	2.35	0.58
1:DS:90:GLU:OE2	2:DT:282:LYS:NZ	2.35	0.58
1:DZ:90:GLU:OE2	2:EA:282:LYS:NZ	2.35	0.58
2:EM:123:GLU:OE2	2:EM:170:LYS:NZ	2.34	0.58
1:AY:90:GLU:OE2	2:AZ:282:LYS:NZ	2.35	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GS:2:ASP:OD2	2:GU:101:LYS:NZ	2.33	0.58
2:IB:282:LYS:NZ	1:WC:90:GLU:OE2	2.35	0.58
1:IY:90:GLU:OE2	2:IZ:282:LYS:NZ	2.36	0.58
2:IX:123:GLU:OE2	2:IX:170:LYS:NZ	2.34	0.58
2:YJ:123:GLU:OE2	2:YJ:170:LYS:NZ	2.34	0.58
1:BK:90:GLU:OE2	2:BL:282:LYS:NZ	2.36	0.58
2:CD:123:GLU:OE2	2:CD:170:LYS:NZ	2.34	0.58
1:GB:90:GLU:OE2	2:GC:282:LYS:NZ	2.35	0.58
2:GC:123:GLU:OE2	2:GC:170:LYS:NZ	2.34	0.58
2:GI:123:GLU:OE2	2:GI:170:LYS:NZ	2.34	0.58
1:KN:90:GLU:OE2	2:KO:282:LYS:NZ	2.36	0.58
2:DB:123:GLU:OE2	2:DB:170:LYS:NZ	2.34	0.58
2:EY:123:GLU:OE2	2:EY:170:LYS:NZ	2.34	0.58
2:HQ:123:GLU:OE2	2:HQ:170:LYS:NZ	2.34	0.58
2:EA:123:GLU:OE2	2:EA:170:LYS:NZ	2.34	0.58
2:GA:2:ASP:OD2	2:GC:101:LYS:NZ	2.34	0.58
2:IT:123:GLU:OE2	2:IT:170:LYS:NZ	2.34	0.58
2:JL:123:GLU:OE2	2:JL:170:LYS:NZ	2.34	0.58
2:ZP:123:GLU:OE2	2:ZP:170:LYS:NZ	2.34	0.58
2:GG:123:GLU:OE2	2:GG:170:LYS:NZ	2.34	0.58
2:YH:123:GLU:OE2	2:YH:170:LYS:NZ	2.34	0.58
2:AN:123:GLU:OE2	2:AN:170:LYS:NZ	2.34	0.57
2:DH:123:GLU:OE2	2:DH:170:LYS:NZ	2.34	0.57
2:FU:2:ASP:OD2	2:FW:101:LYS:NZ	2.34	0.57
2:ZF:123:GLU:OE2	2:ZF:170:LYS:NZ	2.34	0.57
2:BJ:123:GLU:OE2	2:BJ:170:LYS:NZ	2.34	0.57
2:GM:123:GLU:OE2	2:GM:170:LYS:NZ	2.34	0.57
2:ZL:123:GLU:OE2	2:ZL:170:LYS:NZ	2.34	0.57
2:YZ:123:GLU:OE2	2:YZ:170:LYS:NZ	2.34	0.57
2:AL:123:GLU:OE2	2:AL:170:LYS:NZ	2.34	0.57
2:GA:123:GLU:OE2	2:GA:170:LYS:NZ	2.34	0.57
2:JW:123:GLU:OE2	2:JW:170:LYS:NZ	2.34	0.57
2:KS:2:ASP:OD2	2:KU:101:LYS:NZ	2.33	0.57
2:LS:123:GLU:OE2	2:LS:170:LYS:NZ	2.34	0.57
2:YZ:134:ASP:OD1	2:YZ:138:LYS:NZ	2.38	0.57
2:DN:123:GLU:OE2	2:DN:170:LYS:NZ	2.34	0.57
1:YG:92:GLU:OE2	2:YH:282:LYS:NZ	2.38	0.57
2:AF:134:ASP:OD1	2:AF:138:LYS:NZ	2.38	0.57
1:CS:92:GLU:OE2	2:CT:282:LYS:NZ	2.38	0.57
2:CZ:134:ASP:OD1	2:CZ:138:LYS:NZ	2.38	0.57
1:DK:92:GLU:OE2	2:DL:282:LYS:NZ	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DL:134:ASP:OD1	2:DL:138:LYS:NZ	2.38	0.57
2:DR:134:ASP:OD1	2:DR:138:LYS:NZ	2.38	0.57
1:FN:92:GLU:OE2	2:FO:282:LYS:NZ	2.38	0.57
2:FO:134:ASP:OD1	2:FO:138:LYS:NZ	2.38	0.57
2:GM:134:ASP:OD1	2:GM:138:LYS:NZ	2.38	0.57
2:HJ:134:ASP:OD1	2:HJ:138:LYS:NZ	2.38	0.57
2:HO:134:ASP:OD1	2:HO:138:LYS:NZ	2.38	0.57
2:JU:134:ASP:OD1	2:JU:138:LYS:NZ	2.38	0.57
2:KY:134:ASP:OD1	2:KY:138:LYS:NZ	2.38	0.57
2:ZP:134:ASP:OD1	2:ZP:138:LYS:NZ	2.38	0.57
1:YS:92:GLU:OE2	2:YT:282:LYS:NZ	2.38	0.57
2:BL:123:GLU:OE2	2:BL:170:LYS:NZ	2.34	0.57
1:DE:92:GLU:OE2	2:DF:282:LYS:NZ	2.38	0.57
1:DQ:92:GLU:OE2	2:DR:282:LYS:NZ	2.38	0.57
2:DY:134:ASP:OD1	2:DY:138:LYS:NZ	2.38	0.57
2:EK:134:ASP:OD1	2:EK:138:LYS:NZ	2.38	0.57
1:FZ:92:GLU:OE2	2:GA:282:LYS:NZ	2.38	0.57
2:GU:123:GLU:OE2	2:GU:170:LYS:NZ	2.34	0.57
1:ZI:92:GLU:OE2	2:ZJ:282:LYS:NZ	2.38	0.57
2:IZ:123:GLU:OE2	2:IZ:170:LYS:NZ	2.34	0.57
1:JI:92:GLU:OE2	2:JJ:282:LYS:NZ	2.38	0.57
1:ZC:92:GLU:OE2	2:ZD:282:LYS:NZ	2.38	0.57
2:ZD:134:ASP:OD1	2:ZD:138:LYS:NZ	2.38	0.57
2:DF:134:ASP:OD1	2:DF:138:LYS:NZ	2.38	0.57
2:EE:134:ASP:OD1	2:EE:138:LYS:NZ	2.38	0.57
1:EJ:92:GLU:OE2	2:EK:282:LYS:NZ	2.38	0.57
1:HD:92:GLU:OE2	2:HE:282:LYS:NZ	2.38	0.57
2:YV:123:GLU:OE2	2:YV:170:LYS:NZ	2.34	0.57
2:AH:123:GLU:OE2	2:AH:170:LYS:NZ	2.34	0.57
2:AL:134:ASP:OD1	2:AL:138:LYS:NZ	2.38	0.57
2:AO:2:ASP:OD2	2:AT:101:LYS:NZ	2.34	0.57
1:AW:92:GLU:OE2	2:AX:282:LYS:NZ	2.38	0.57
2:BD:134:ASP:OD1	2:BD:138:LYS:NZ	2.38	0.57
2:CH:134:ASP:OD1	2:CH:138:LYS:NZ	2.38	0.57
1:CM:92:GLU:OE2	2:CN:282:LYS:NZ	2.38	0.57
2:EQ:134:ASP:OD1	2:EQ:138:LYS:NZ	2.38	0.57
2:EW:2:ASP:OD2	2:EY:101:LYS:NZ	2.34	0.57
1:GL:92:GLU:OE2	2:GM:282:LYS:NZ	2.38	0.57
2:GY:134:ASP:OD1	2:GY:138:LYS:NZ	2.38	0.57
2:HE:134:ASP:OD1	2:HE:138:LYS:NZ	2.38	0.57
1:HT:92:GLU:OE2	2:HU:282:LYS:NZ	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HZ:92:GLU:OE2	2:IA:282:LYS:NZ	2.38	0.57
2:JD:134:ASP:OD1	2:JD:138:LYS:NZ	2.38	0.57
2:LK:123:GLU:OE2	2:LK:170:LYS:NZ	2.34	0.57
2:LQ:134:ASP:OD1	2:LQ:138:LYS:NZ	2.38	0.57
2:AB:123:GLU:OE2	2:AB:170:LYS:NZ	2.34	0.56
1:EV:92:GLU:OE2	2:EW:282:LYS:NZ	2.38	0.56
2:FU:134:ASP:OD1	2:FU:138:LYS:NZ	2.38	0.56
2:HU:123:GLU:OE2	2:HU:170:LYS:NZ	2.34	0.56
1:IW:92:GLU:OE2	2:IX:282:LYS:NZ	2.38	0.56
1:KF:92:GLU:OE2	2:KG:282:LYS:NZ	2.38	0.56
2:YH:134:ASP:OD1	2:YH:138:LYS:NZ	2.38	0.56
1:YM:92:GLU:OE2	2:YN:282:LYS:NZ	2.38	0.56
1:BO:92:GLU:OE2	2:BP:282:LYS:NZ	2.38	0.56
2:BV:134:ASP:OD1	2:BV:138:LYS:NZ	2.38	0.56
2:CT:123:GLU:OE2	2:CT:170:LYS:NZ	2.34	0.56
1:CY:92:GLU:OE2	2:CZ:282:LYS:NZ	2.38	0.56
1:DX:92:GLU:OE2	2:DY:282:LYS:NZ	2.38	0.56
2:EW:134:ASP:OD1	2:EW:138:LYS:NZ	2.38	0.56
2:FC:134:ASP:OD1	2:FC:138:LYS:NZ	2.38	0.56
1:HI:92:GLU:OE2	2:HJ:282:LYS:NZ	2.38	0.56
1:HN:92:GLU:OE2	2:HO:282:LYS:NZ	2.38	0.56
2:HU:134:ASP:OD1	2:HU:138:LYS:NZ	2.38	0.56
2:IF:134:ASP:OD1	2:IF:138:LYS:NZ	2.38	0.56
2:IR:134:ASP:OD1	2:IR:138:LYS:NZ	2.38	0.56
1:JC:92:GLU:OE2	2:JD:282:LYS:NZ	2.38	0.56
2:KS:134:ASP:OD1	2:KS:138:LYS:NZ	2.38	0.56
1:KX:92:GLU:OE2	2:KY:282:LYS:NZ	2.38	0.56
1:LJ:92:GLU:OE2	2:LK:282:LYS:NZ	2.38	0.56
2:ZP:2:ASP:OD2	2:ZR:101:LYS:NZ	2.34	0.56
2:YD:123:GLU:OE2	2:YD:170:LYS:NZ	2.34	0.56
1:AK:92:GLU:OE2	2:AL:282:LYS:NZ	2.38	0.56
2:BD:2:ASP:OD2	2:BF:101:LYS:NZ	2.33	0.56
1:BI:92:GLU:OE2	2:BJ:282:LYS:NZ	2.38	0.56
2:BJ:134:ASP:OD1	2:BJ:138:LYS:NZ	2.38	0.56
2:CN:134:ASP:OD1	2:CN:138:LYS:NZ	2.38	0.56
2:CT:134:ASP:OD1	2:CT:138:LYS:NZ	2.38	0.56
1:ED:92:GLU:OE2	2:EE:282:LYS:NZ	2.38	0.56
1:FT:92:GLU:OE2	2:FU:282:LYS:NZ	2.38	0.56
2:GA:134:ASP:OD1	2:GA:138:LYS:NZ	2.38	0.56
1:GR:92:GLU:OE2	2:GS:282:LYS:NZ	2.38	0.56
2:GS:134:ASP:OD1	2:GS:138:LYS:NZ	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GX:92:GLU:OE2	2:GY:282:LYS:NZ	2.38	0.56
2:ZJ:134:ASP:OD1	2:ZJ:138:LYS:NZ	2.38	0.56
2:IF:2:ASP:OD2	2:IG:101:LYS:NZ	2.34	0.56
1:IK:92:GLU:OE2	2:IL:282:LYS:NZ	2.38	0.56
2:IL:134:ASP:OD1	2:IL:138:LYS:NZ	2.38	0.56
2:IX:134:ASP:OD1	2:IX:138:LYS:NZ	2.38	0.56
2:KA:2:ASP:OD2	2:KC:101:LYS:NZ	2.33	0.56
1:KL:92:GLU:OE2	2:KM:282:LYS:NZ	2.38	0.56
1:KR:92:GLU:OE2	2:KS:282:LYS:NZ	2.38	0.56
2:KU:123:GLU:OE2	2:KU:170:LYS:NZ	2.34	0.56
1:YA:92:GLU:OE2	2:YB:282:LYS:NZ	2.38	0.56
2:YT:134:ASP:OD1	2:YT:138:LYS:NZ	2.38	0.56
2:AO:134:ASP:OD1	2:AO:138:LYS:NZ	2.38	0.56
2:BP:134:ASP:OD1	2:BP:138:LYS:NZ	2.38	0.56
2:CB:134:ASP:OD1	2:CB:138:LYS:NZ	2.38	0.56
2:GY:2:ASP:OD2	2:HA:101:LYS:NZ	2.34	0.56
2:IA:134:ASP:OD1	2:IA:138:LYS:NZ	2.38	0.56
1:IE:92:GLU:OE2	2:IF:282:LYS:NZ	2.38	0.56
1:JZ:92:GLU:OE2	2:KA:282:LYS:NZ	2.38	0.56
1:LP:92:GLU:OE2	2:LQ:282:LYS:NZ	2.38	0.56
1:YY:92:GLU:OE2	2:YZ:282:LYS:NZ	2.38	0.56
1:AE:92:GLU:OE2	2:AF:282:LYS:NZ	2.38	0.56
1:BU:92:GLU:OE2	2:BV:282:LYS:NZ	2.38	0.56
2:ZD:2:ASP:OD2	2:ZF:101:LYS:NZ	2.33	0.56
1:CA:92:GLU:OE2	2:CB:282:LYS:NZ	2.38	0.56
1:CG:92:GLU:OE2	2:CH:282:LYS:NZ	2.38	0.56
1:EP:92:GLU:OE2	2:EQ:282:LYS:NZ	2.38	0.56
2:IA:123:GLU:OE2	2:IA:170:LYS:NZ	2.34	0.56
2:LE:123:GLU:OE2	2:LE:170:LYS:NZ	2.34	0.56
2:IR:123:GLU:OE2	2:IR:170:LYS:NZ	2.34	0.56
2:LE:134:ASP:OD1	2:LE:138:LYS:NZ	2.38	0.56
2:LK:134:ASP:OD1	2:LK:138:LYS:NZ	2.38	0.56
1:ZO:92:GLU:OE2	2:ZP:282:LYS:NZ	2.38	0.56
2:FI:134:ASP:OD1	2:FI:138:LYS:NZ	2.38	0.56
2:JJ:134:ASP:OD1	2:JJ:138:LYS:NZ	2.38	0.56
1:JO:92:GLU:OE2	2:JP:282:LYS:NZ	2.38	0.56
2:KA:134:ASP:OD1	2:KA:138:LYS:NZ	2.38	0.56
2:ZV:134:ASP:OD1	2:ZV:138:LYS:NZ	2.38	0.56
2:YB:134:ASP:OD1	2:YB:138:LYS:NZ	2.38	0.56
2:YP:123:GLU:OE2	2:YP:170:LYS:NZ	2.34	0.56
2:YT:2:ASP:OD2	2:YV:101:LYS:NZ	2.33	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AO:282:LYS:NZ	1:AP:92:GLU:OE2	2.38	0.56
2:AX:134:ASP:OD1	2:AX:138:LYS:NZ	2.38	0.56
1:FB:92:GLU:OE2	2:FC:282:LYS:NZ	2.38	0.56
2:FO:2:ASP:OD2	2:FQ:101:LYS:NZ	2.33	0.56
1:GF:92:GLU:OE2	2:GG:282:LYS:NZ	2.38	0.56
1:IQ:92:GLU:OE2	2:IR:282:LYS:NZ	2.38	0.56
2:JR:123:GLU:OE2	2:JR:170:LYS:NZ	2.34	0.56
2:JU:282:LYS:NZ	1:WD:92:GLU:OE2	2.38	0.56
2:AZ:123:GLU:OE2	2:AZ:170:LYS:NZ	2.34	0.56
1:BC:92:GLU:OE2	2:BD:282:LYS:NZ	2.38	0.56
1:FH:92:GLU:OE2	2:FI:282:LYS:NZ	2.38	0.56
2:LM:123:GLU:OE2	2:LM:170:LYS:NZ	2.34	0.56
2:YN:134:ASP:OD1	2:YN:138:LYS:NZ	2.38	0.56
2:GG:134:ASP:OD1	2:GG:138:LYS:NZ	2.38	0.56
2:HJ:123:GLU:OE2	2:HJ:170:LYS:NZ	2.34	0.56
2:HW:160:ASP:OD1	2:HW:168:LYS:NZ	2.36	0.56
2:KM:134:ASP:OD1	2:KM:138:LYS:NZ	2.38	0.56
1:ZU:92:GLU:OE2	2:ZV:282:LYS:NZ	2.38	0.56
2:LQ:2:ASP:OD2	2:LS:101:LYS:NZ	2.33	0.55
2:CH:123:GLU:OE2	2:CH:170:LYS:NZ	2.34	0.55
2:GG:2:ASP:OD2	2:GI:101:LYS:NZ	2.33	0.55
2:HF:123:GLU:OE2	2:HF:170:LYS:NZ	2.34	0.55
2:JP:134:ASP:OD1	2:JP:138:LYS:NZ	2.38	0.55
2:LA:123:GLU:OE2	2:LA:170:LYS:NZ	2.34	0.55
2:HU:2:ASP:OD2	2:HW:101:LYS:NZ	2.34	0.55
2:IR:2:ASP:OD2	2:IT:101:LYS:NZ	2.33	0.55
2:JU:2:ASP:OD2	2:JW:101:LYS:NZ	2.34	0.55
2:KG:134:ASP:OD1	2:KG:138:LYS:NZ	2.38	0.55
2:KS:123:GLU:OE2	2:KS:170:LYS:NZ	2.34	0.55
2:ZJ:2:ASP:OD2	2:ZL:101:LYS:NZ	2.33	0.55
1:LD:92:GLU:OE2	2:LE:282:LYS:NZ	2.38	0.55
2:ZV:2:ASP:OD2	2:ZX:101:LYS:NZ	2.34	0.55
2:ZV:123:GLU:OE2	2:ZV:170:LYS:NZ	2.34	0.55
2:FU:123:GLU:OE2	2:FU:170:LYS:NZ	2.34	0.55
2:JJ:123:GLU:OE2	2:JJ:170:LYS:NZ	2.34	0.55
2:KM:2:ASP:OD2	2:KO:101:LYS:NZ	2.34	0.55
2:BR:123:GLU:OE2	2:BR:170:LYS:NZ	2.34	0.55
2:DR:123:GLU:OE2	2:DR:170:LYS:NZ	2.34	0.55
2:ES:123:GLU:OE2	2:ES:170:LYS:NZ	2.34	0.55
2:YN:123:GLU:OE2	2:YN:170:LYS:NZ	2.34	0.55
2:FO:123:GLU:OE2	2:FO:170:LYS:NZ	2.34	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KG:2:ASP:OD2	2:KI:101:LYS:NZ	2.33	0.55
2:EG:123:GLU:OE2	2:EG:170:LYS:NZ	2.34	0.54
2:AX:123:GLU:OE2	2:AX:170:LYS:NZ	2.34	0.54
2:HK:123:GLU:OE2	2:HK:170:LYS:NZ	2.34	0.54
2:HO:2:ASP:OD2	2:HQ:101:LYS:NZ	2.33	0.54
2:IN:123:GLU:OE2	2:IN:170:LYS:NZ	2.34	0.54
2:FC:2:ASP:OD2	2:FE:101:LYS:NZ	2.34	0.54
2:HO:123:GLU:OE2	2:HO:170:LYS:NZ	2.34	0.54
2:CH:2:ASP:OD2	2:CJ:101:LYS:NZ	2.33	0.54
2:EK:123:GLU:OE2	2:EK:170:LYS:NZ	2.34	0.54
2:YH:2:ASP:OD2	2:YJ:101:LYS:NZ	2.34	0.54
2:AF:123:GLU:OE2	2:AF:170:LYS:NZ	2.34	0.54
2:BJ:2:ASP:OD2	2:BL:101:LYS:NZ	2.33	0.54
2:KY:2:ASP:OD2	2:LA:101:LYS:NZ	2.33	0.54
2:GY:123:GLU:OE2	2:GY:170:LYS:NZ	2.34	0.54
2:DF:2:ASP:OD2	2:DH:101:LYS:NZ	2.33	0.53
2:JD:2:ASP:OD2	2:JF:101:LYS:NZ	2.33	0.53
2:KM:123:GLU:OE2	2:KM:170:LYS:NZ	2.34	0.53
2:HE:2:ASP:OD2	2:HF:101:LYS:NZ	2.33	0.53
2:YN:2:ASP:OD2	2:YP:101:LYS:NZ	2.34	0.53
2:EK:2:ASP:OD2	2:EM:101:LYS:NZ	2.34	0.53
2:AF:2:ASP:OD2	2:AH:101:LYS:NZ	2.34	0.53
2:EQ:123:GLU:OE2	2:EQ:170:LYS:NZ	2.34	0.53
2:JP:123:GLU:OE2	2:JP:170:LYS:NZ	2.34	0.53
2:AX:2:ASP:OD2	2:AZ:101:LYS:NZ	2.33	0.53
2:YD:101:LYS:NZ	2:YB:2:ASP:OD2	2.33	0.53
2:CT:2:ASP:OD2	2:CV:101:LYS:NZ	2.33	0.53
2:CB:123:GLU:OE2	2:CB:170:LYS:NZ	2.34	0.53
2:FI:2:ASP:OD2	2:FK:101:LYS:NZ	2.33	0.53
2:EA:160:ASP:OD1	2:EA:168:LYS:NZ	2.36	0.52
2:FI:123:GLU:OE2	2:FI:170:LYS:NZ	2.34	0.52
2:JJ:2:ASP:OD2	2:JL:101:LYS:NZ	2.33	0.52
2:IA:2:ASP:OD2	2:IB:101:LYS:NZ	2.33	0.52
2:KY:123:GLU:OE2	2:KY:170:LYS:NZ	2.34	0.52
2:ZD:123:GLU:OE2	2:ZD:170:LYS:NZ	2.34	0.52
2:FC:123:GLU:OE2	2:FC:170:LYS:NZ	2.34	0.52
2:HJ:2:ASP:OD2	2:HK:101:LYS:NZ	2.33	0.52
2:CN:123:GLU:OE2	2:CN:170:LYS:NZ	2.34	0.52
2:DL:2:ASP:OD2	2:DN:101:LYS:NZ	2.33	0.52
2:AZ:160:ASP:OD1	2:AZ:168:LYS:NZ	2.36	0.52
2:GM:2:ASP:OD2	2:GO:101:LYS:NZ	2.33	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JP:2:ASP:OD2	2:JR:101:LYS:NZ	2.34	0.52
2:CN:2:ASP:OD2	2:CP:101:LYS:NZ	2.33	0.52
2:LE:2:ASP:OD2	2:LG:101:LYS:NZ	2.33	0.52
2:BP:2:ASP:OD2	2:BR:101:LYS:NZ	2.34	0.51
2:DF:123:GLU:OE2	2:DF:170:LYS:NZ	2.34	0.51
2:BP:123:GLU:OE2	2:BP:170:LYS:NZ	2.34	0.51
2:JU:123:GLU:OE2	2:JU:170:LYS:NZ	2.34	0.51
2:GS:123:GLU:OE2	2:GS:170:LYS:NZ	2.34	0.51
2:IL:2:ASP:OD2	2:IN:101:LYS:NZ	2.34	0.51
2:KA:123:GLU:OE2	2:KA:170:LYS:NZ	2.34	0.51
2:CB:2:ASP:OD2	2:CD:101:LYS:NZ	2.34	0.51
1:DS:43:VAL:HG13	1:DS:50:VAL:HG11	1.93	0.51
2:HE:123:GLU:OE2	2:HE:170:LYS:NZ	2.34	0.51
1:JE:43:VAL:HG13	1:JE:50:VAL:HG11	1.93	0.51
1:LR:43:VAL:HG13	1:LR:50:VAL:HG11	1.93	0.51
1:DZ:43:VAL:HG13	1:DZ:50:VAL:HG11	1.93	0.51
2:FU:228:TYR:CD1	2:FU:228:TYR:C	2.89	0.51
1:HP:43:VAL:HG13	1:HP:50:VAL:HG11	1.93	0.51
1:IY:43:VAL:HG13	1:IY:50:VAL:HG11	1.93	0.51
2:JD:228:TYR:CD1	2:JD:228:TYR:C	2.89	0.51
2:LE:228:TYR:CD1	2:LE:228:TYR:C	2.89	0.51
1:YC:43:VAL:HG13	1:YC:50:VAL:HG11	1.93	0.51
2:YN:228:TYR:CD1	2:YN:228:TYR:C	2.89	0.51
2:AF:228:TYR:C	2:AF:228:TYR:CD1	2.89	0.51
2:AL:228:TYR:C	2:AL:228:TYR:CD1	2.89	0.51
1:BE:43:VAL:HG13	1:BE:50:VAL:HG11	1.93	0.51
1:BK:43:VAL:HG13	1:BK:50:VAL:HG11	1.93	0.51
2:BP:228:TYR:C	2:BP:228:TYR:CD1	2.89	0.51
2:CZ:123:GLU:OE2	2:CZ:170:LYS:NZ	2.34	0.51
2:EE:123:GLU:OE2	2:EE:170:LYS:NZ	2.34	0.51
2:EK:228:TYR:CD1	2:EK:228:TYR:C	2.89	0.51
1:GN:43:VAL:HG13	1:GN:50:VAL:HG11	1.93	0.51
1:HV:43:VAL:HG13	1:HV:50:VAL:HG11	1.93	0.51
2:JD:123:GLU:OE2	2:JD:170:LYS:NZ	2.34	0.51
1:ZQ:43:VAL:HG13	1:ZQ:50:VAL:HG11	1.93	0.51
1:AM:43:VAL:HG13	1:AM:50:VAL:HG11	1.93	0.51
2:CH:228:TYR:CD1	2:CH:228:TYR:C	2.89	0.51
1:WA:43:VAL:HG13	1:WA:50:VAL:HG11	1.93	0.51
2:ZJ:123:GLU:OE2	2:ZJ:170:LYS:NZ	2.34	0.51
2:KS:228:TYR:CD1	2:KS:228:TYR:C	2.89	0.51
2:YH:228:TYR:CD1	2:YH:228:TYR:C	2.89	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:YT:228:TYR:CD1	2:YT:228:TYR:C	2.89	0.51
1:CU:43:VAL:HG13	1:CU:50:VAL:HG11	1.93	0.51
1:DG:43:VAL:HG13	1:DG:50:VAL:HG11	1.93	0.51
1:EF:43:VAL:HG13	1:EF:50:VAL:HG11	1.93	0.51
1:GB:43:VAL:HG13	1:GB:50:VAL:HG11	1.93	0.51
2:GG:228:TYR:CD1	2:GG:228:TYR:C	2.89	0.51
1:WB:43:VAL:HG13	1:WB:50:VAL:HG11	1.93	0.51
1:IM:43:VAL:HG13	1:IM:50:VAL:HG11	1.93	0.51
2:KG:228:TYR:C	2:KG:228:TYR:CD1	2.89	0.51
2:BL:160:ASP:OD1	2:BL:168:LYS:NZ	2.36	0.50
2:BV:2:ASP:OD2	2:BX:101:LYS:NZ	2.34	0.50
1:BW:43:VAL:HG13	1:BW:50:VAL:HG11	1.93	0.50
2:CT:228:TYR:CD1	2:CT:228:TYR:C	2.89	0.50
1:ER:43:VAL:HG13	1:ER:50:VAL:HG11	1.93	0.50
2:HO:228:TYR:CD1	2:HO:228:TYR:C	2.89	0.50
1:WC:43:VAL:HG13	1:WC:50:VAL:HG11	1.93	0.50
2:IF:123:GLU:OE2	2:IF:170:LYS:NZ	2.34	0.50
2:JJ:228:TYR:CD1	2:JJ:228:TYR:C	2.89	0.50
1:JK:43:VAL:HG13	1:JK:50:VAL:HG11	1.93	0.50
2:LQ:228:TYR:CD1	2:LQ:228:TYR:C	2.89	0.50
1:YI:43:VAL:HG13	1:YI:50:VAL:HG11	1.93	0.50
2:YT:123:GLU:OE2	2:YT:170:LYS:NZ	2.34	0.50
2:AO:123:GLU:OE2	2:AO:170:LYS:NZ	2.34	0.50
2:BV:228:TYR:CD1	2:BV:228:TYR:C	2.89	0.50
2:GY:228:TYR:C	2:GY:228:TYR:CD1	2.89	0.50
2:HU:228:TYR:C	2:HU:228:TYR:CD1	2.89	0.50
1:KH:43:VAL:HG13	1:KH:50:VAL:HG11	1.93	0.50
2:AO:228:TYR:C	2:AO:228:TYR:CD1	2.89	0.50
2:EW:228:TYR:CD1	2:EW:228:TYR:C	2.89	0.50
2:FC:228:TYR:CD1	2:FC:228:TYR:C	2.89	0.50
1:LL:43:VAL:HG13	1:LL:50:VAL:HG11	1.93	0.50
2:AX:228:TYR:CD1	2:AX:228:TYR:C	2.89	0.50
2:BV:123:GLU:OE2	2:BV:170:LYS:NZ	2.34	0.50
2:CN:228:TYR:CD1	2:CN:228:TYR:C	2.89	0.50
1:FJ:43:VAL:HG13	1:FJ:50:VAL:HG11	1.93	0.50
2:IL:228:TYR:C	2:IL:228:TYR:CD1	2.89	0.50
2:JU:228:TYR:CD1	2:JU:228:TYR:C	2.89	0.50
2:LK:228:TYR:CD1	2:LK:228:TYR:C	2.89	0.50
2:AL:2:ASP:OD2	2:AN:101:LYS:NZ	2.33	0.50
2:DY:228:TYR:CD1	2:DY:228:TYR:C	2.89	0.50
2:EE:2:ASP:OD2	2:EG:101:LYS:NZ	2.33	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GT:43:VAL:HG13	1:GT:50:VAL:HG11	1.93	0.50
2:HE:228:TYR:CD1	2:HE:228:TYR:C	2.89	0.50
2:IX:228:TYR:CD1	2:IX:228:TYR:C	2.89	0.50
1:KB:43:VAL:HG13	1:KB:50:VAL:HG11	1.93	0.50
1:AA:43:VAL:HG13	1:AA:50:VAL:HG11	1.93	0.50
2:ZD:228:TYR:CD1	2:ZD:228:TYR:C	2.89	0.50
2:DF:228:TYR:CD1	2:DF:228:TYR:C	2.89	0.50
2:FO:228:TYR:C	2:FO:228:TYR:CD1	2.89	0.50
2:GA:228:TYR:CD1	2:GA:228:TYR:C	2.89	0.50
2:GM:228:TYR:CD1	2:GM:228:TYR:C	2.89	0.50
2:KG:123:GLU:OE2	2:KG:170:LYS:NZ	2.34	0.50
1:ZW:43:VAL:HG13	1:ZW:50:VAL:HG11	1.93	0.50
2:YB:123:GLU:OE2	2:YB:170:LYS:NZ	2.34	0.50
2:AB:101:LYS:NZ	2:YZ:2:ASP:OD2	2.33	0.50
2:YZ:228:TYR:C	2:YZ:228:TYR:CD1	2.89	0.50
2:CB:228:TYR:CD1	2:CB:228:TYR:C	2.89	0.50
2:DL:228:TYR:CD1	2:DL:228:TYR:C	2.89	0.50
2:DR:228:TYR:CD1	2:DR:228:TYR:C	2.89	0.50
2:EE:228:TYR:C	2:EE:228:TYR:CD1	2.89	0.50
2:FI:228:TYR:CD1	2:FI:228:TYR:C	2.89	0.50
1:GH:43:VAL:HG13	1:GH:50:VAL:HG11	1.93	0.50
2:IF:228:TYR:C	2:IF:228:TYR:CD1	2.89	0.50
1:JV:43:VAL:HG13	1:JV:50:VAL:HG11	1.93	0.50
2:YB:228:TYR:CD1	2:YB:228:TYR:C	2.89	0.50
2:DL:123:GLU:OE2	2:DL:170:LYS:NZ	2.34	0.50
2:EW:123:GLU:OE2	2:EW:170:LYS:NZ	2.34	0.50
1:EX:43:VAL:HG13	1:EX:50:VAL:HG11	1.93	0.50
1:GF:11:ALA:HB1	1:GF:43:VAL:O	2.12	0.50
2:GS:228:TYR:CD1	2:GS:228:TYR:C	2.89	0.50
1:IS:43:VAL:HG13	1:IS:50:VAL:HG11	1.93	0.50
1:ZK:43:VAL:HG13	1:ZK:50:VAL:HG11	1.93	0.50
1:JQ:43:VAL:HG13	1:JQ:50:VAL:HG11	1.93	0.50
1:LP:11:ALA:HB1	1:LP:43:VAL:O	2.12	0.50
1:YG:11:ALA:HB1	1:YG:43:VAL:O	2.12	0.50
1:AP:11:ALA:HB1	1:AP:43:VAL:O	2.12	0.50
1:BC:11:ALA:HB1	1:BC:43:VAL:O	2.12	0.50
2:BJ:228:TYR:CD1	2:BJ:228:TYR:C	2.89	0.50
1:BU:11:ALA:HB1	1:BU:43:VAL:O	2.12	0.50
1:CA:11:ALA:HB1	1:CA:43:VAL:O	2.12	0.50
1:CM:11:ALA:HB1	1:CM:43:VAL:O	2.12	0.50
1:FT:11:ALA:HB1	1:FT:43:VAL:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IA:228:TYR:C	2:IA:228:TYR:CD1	2.89	0.50
2:ZJ:228:TYR:CD1	2:ZJ:228:TYR:C	2.89	0.50
1:IH:43:VAL:HG13	1:IH:50:VAL:HG11	1.93	0.50
2:JP:228:TYR:CD1	2:JP:228:TYR:C	2.89	0.50
2:KA:228:TYR:CD1	2:KA:228:TYR:C	2.89	0.50
2:ZL:160:ASP:OD1	2:ZL:168:LYS:NZ	2.36	0.50
1:KL:11:ALA:HB1	1:KL:43:VAL:O	2.12	0.50
1:KN:43:VAL:HG13	1:KN:50:VAL:HG11	1.93	0.50
1:KZ:43:VAL:HG13	1:KZ:50:VAL:HG11	1.93	0.50
1:AY:43:VAL:HG13	1:AY:50:VAL:HG11	1.93	0.49
1:BO:11:ALA:HB1	1:BO:43:VAL:O	2.12	0.49
1:DM:43:VAL:HG13	1:DM:50:VAL:HG11	1.93	0.49
1:EP:11:ALA:HB1	1:EP:43:VAL:O	2.12	0.49
2:EQ:228:TYR:CD1	2:EQ:228:TYR:C	2.89	0.49
1:FV:43:VAL:HG13	1:FV:50:VAL:HG11	1.93	0.49
1:ZO:11:ALA:HB1	1:ZO:43:VAL:O	2.12	0.49
1:BI:11:ALA:HB1	1:BI:43:VAL:O	2.12	0.49
1:BQ:43:VAL:HG13	1:BQ:50:VAL:HG11	1.93	0.49
1:CO:43:VAL:HG13	1:CO:50:VAL:HG11	1.93	0.49
1:DQ:11:ALA:HB1	1:DQ:43:VAL:O	2.12	0.49
1:DX:11:ALA:HB1	1:DX:43:VAL:O	2.12	0.49
1:FD:43:VAL:HG13	1:FD:50:VAL:HG11	1.93	0.49
1:FN:11:ALA:HB1	1:FN:43:VAL:O	2.12	0.49
1:FP:43:VAL:HG13	1:FP:50:VAL:HG11	1.93	0.49
1:GL:11:ALA:HB1	1:GL:43:VAL:O	2.12	0.49
2:HJ:228:TYR:C	2:HJ:228:TYR:CD1	2.89	0.49
1:HZ:11:ALA:HB1	1:HZ:43:VAL:O	2.12	0.49
1:IQ:11:ALA:HB1	1:IQ:43:VAL:O	2.12	0.49
1:KT:43:VAL:HG13	1:KT:50:VAL:HG11	1.93	0.49
1:LF:43:VAL:HG13	1:LF:50:VAL:HG11	1.93	0.49
1:YO:43:VAL:HG13	1:YO:50:VAL:HG11	1.93	0.49
1:YS:11:ALA:HB1	1:YS:43:VAL:O	2.12	0.49
2:CZ:228:TYR:CD1	2:CZ:228:TYR:C	2.89	0.49
1:DA:43:VAL:HG13	1:DA:50:VAL:HG11	1.93	0.49
1:DK:11:ALA:HB1	1:DK:43:VAL:O	2.12	0.49
2:DY:123:GLU:OE2	2:DY:170:LYS:NZ	2.34	0.49
1:EV:11:ALA:HB1	1:EV:43:VAL:O	2.12	0.49
1:HN:11:ALA:HB1	1:HN:43:VAL:O	2.12	0.49
1:KF:11:ALA:HB1	1:KF:43:VAL:O	2.12	0.49
2:KY:228:TYR:CD1	2:KY:228:TYR:C	2.89	0.49
2:ZP:228:TYR:CD1	2:ZP:228:TYR:C	2.89	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ZV:228:TYR:C	2:ZV:228:TYR:CD1	2.89	0.49
1:YM:11:ALA:HB1	1:YM:43:VAL:O	2.12	0.49
1:AS:43:VAL:HG13	1:AS:50:VAL:HG11	1.93	0.49
1:AW:11:ALA:HB1	1:AW:43:VAL:O	2.12	0.49
1:IW:11:ALA:HB1	1:IW:43:VAL:O	2.12	0.49
1:AG:43:VAL:HG13	1:AG:50:VAL:HG11	1.93	0.49
2:BD:228:TYR:CD1	2:BD:228:TYR:C	2.89	0.49
1:GZ:43:VAL:HG13	1:GZ:50:VAL:HG11	1.93	0.49
1:ZI:11:ALA:HB1	1:ZI:43:VAL:O	2.12	0.49
1:HI:11:ALA:HB1	1:HI:43:VAL:O	2.12	0.49
2:KM:228:TYR:C	2:KM:228:TYR:CD1	2.89	0.49
1:CG:11:ALA:HB1	1:CG:43:VAL:O	2.12	0.49
2:DY:2:ASP:OD2	2:EA:101:LYS:NZ	2.34	0.49
1:FZ:11:ALA:HB1	1:FZ:43:VAL:O	2.12	0.49
2:IF:6:LYS:NZ	2:IF:10:GLU:OE2	2.45	0.49
2:IR:228:TYR:CD1	2:IR:228:TYR:C	2.89	0.49
1:WD:11:ALA:HB1	1:WD:43:VAL:O	2.12	0.49
1:AE:11:ALA:HB1	1:AE:43:VAL:O	2.12	0.49
1:CY:11:ALA:HB1	1:CY:43:VAL:O	2.12	0.49
1:EJ:11:ALA:HB1	1:EJ:43:VAL:O	2.12	0.49
1:EL:43:VAL:HG13	1:EL:50:VAL:HG11	1.93	0.49
1:GR:11:ALA:HB1	1:GR:43:VAL:O	2.12	0.49
1:HT:11:ALA:HB1	1:HT:43:VAL:O	2.12	0.49
1:ZE:43:VAL:HG13	1:ZE:50:VAL:HG11	1.93	0.49
1:FH:11:ALA:HB1	1:FH:43:VAL:O	2.12	0.49
1:JC:11:ALA:HB1	1:JC:43:VAL:O	2.12	0.49
1:LD:11:ALA:HB1	1:LD:43:VAL:O	2.12	0.49
1:CI:43:VAL:HG13	1:CI:50:VAL:HG11	1.93	0.49
2:ZJ:6:LYS:NZ	2:ZJ:10:GLU:OE2	2.45	0.49
2:KY:6:LYS:NZ	2:KY:10:GLU:OE2	2.45	0.49
1:LJ:11:ALA:HB1	1:LJ:43:VAL:O	2.12	0.49
1:YY:11:ALA:HB1	1:YY:43:VAL:O	2.12	0.49
1:CC:43:VAL:HG13	1:CC:50:VAL:HG11	1.93	0.49
1:ED:11:ALA:HB1	1:ED:43:VAL:O	2.12	0.49
1:IK:11:ALA:HB1	1:IK:43:VAL:O	2.12	0.49
1:JO:11:ALA:HB1	1:JO:43:VAL:O	2.12	0.49
1:YA:11:ALA:HB1	1:YA:43:VAL:O	2.12	0.49
2:CH:6:LYS:NZ	2:CH:10:GLU:OE2	2.45	0.48
2:KS:6:LYS:NZ	2:KS:10:GLU:OE2	2.45	0.48
1:YU:43:VAL:HG13	1:YU:50:VAL:HG11	1.93	0.48
2:BT:228:TYR:CD1	2:BT:228:TYR:C	2.92	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DJ:228:TYR:CD1	2:DJ:228:TYR:C	2.92	0.48
2:DL:6:LYS:NZ	2:DL:10:GLU:OE2	2.45	0.48
2:FM:228:TYR:CD1	2:FM:228:TYR:C	2.92	0.48
1:GX:11:ALA:HB1	1:GX:43:VAL:O	2.12	0.48
2:HH:228:TYR:CD1	2:HH:228:TYR:C	2.92	0.48
1:JZ:11:ALA:HB1	1:JZ:43:VAL:O	2.12	0.48
2:KK:228:TYR:CD1	2:KK:228:TYR:C	2.92	0.48
1:KR:11:ALA:HB1	1:KR:43:VAL:O	2.12	0.48
2:LI:228:TYR:CD1	2:LI:228:TYR:C	2.92	0.48
1:AK:11:ALA:HB1	1:AK:43:VAL:O	2.12	0.48
1:ZC:11:ALA:HB1	1:ZC:43:VAL:O	2.12	0.48
2:EC:228:TYR:CD1	2:EC:228:TYR:C	2.92	0.48
2:FO:6:LYS:NZ	2:FO:10:GLU:OE2	2.45	0.48
2:FY:228:TYR:CD1	2:FY:228:TYR:C	2.92	0.48
2:ZH:228:TYR:C	2:ZH:228:TYR:CD1	2.92	0.48
2:IA:6:LYS:NZ	2:IA:10:GLU:OE2	2.45	0.48
1:IE:11:ALA:HB1	1:IE:43:VAL:O	2.12	0.48
1:JI:11:ALA:HB1	1:JI:43:VAL:O	2.12	0.48
2:YN:6:LYS:NZ	2:YN:10:GLU:OE2	2.45	0.48
2:DD:228:TYR:CD1	2:DD:228:TYR:C	2.91	0.48
2:DP:228:TYR:CD1	2:DP:228:TYR:C	2.92	0.48
2:EE:6:LYS:NZ	2:EE:10:GLU:OE2	2.45	0.48
2:EI:228:TYR:CD1	2:EI:228:TYR:C	2.92	0.48
2:EO:228:TYR:CD1	2:EO:228:TYR:C	2.92	0.48
1:FB:11:ALA:HB1	1:FB:43:VAL:O	2.12	0.48
2:GY:6:LYS:NZ	2:GY:10:GLU:OE2	2.45	0.48
1:HD:11:ALA:HB1	1:HD:43:VAL:O	2.12	0.48
2:IP:228:TYR:CD1	2:IP:228:TYR:C	2.92	0.48
2:ZZ:228:TYR:CD1	2:ZZ:228:TYR:C	2.92	0.48
2:EW:6:LYS:NZ	2:EW:10:GLU:OE2	2.45	0.48
2:KQ:228:TYR:CD1	2:KQ:228:TYR:C	2.92	0.48
2:LO:228:TYR:CD1	2:LO:228:TYR:C	2.91	0.48
2:AQ:228:TYR:C	2:AQ:228:TYR:CD1	2.92	0.48
1:CS:11:ALA:HB1	1:CS:43:VAL:O	2.12	0.48
2:CX:228:TYR:C	2:CX:228:TYR:CD1	2.92	0.48
2:FS:228:TYR:CD1	2:FS:228:TYR:C	2.92	0.48
1:KX:11:ALA:HB1	1:KX:43:VAL:O	2.12	0.48
2:AJ:228:TYR:CD1	2:AJ:228:TYR:C	2.92	0.48
2:BZ:228:TYR:CD1	2:BZ:228:TYR:C	2.92	0.48
2:CL:228:TYR:CD1	2:CL:228:TYR:C	2.92	0.48
2:HM:78:LYS:NZ	2:HQ:73:GLU:OE1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HY:228:TYR:CD1	2:HY:228:TYR:C	2.92	0.48
1:ZU:11:ALA:HB1	1:ZU:43:VAL:O	2.12	0.48
2:YL:228:TYR:CD1	2:YL:228:TYR:C	2.92	0.48
2:YT:6:LYS:NZ	2:YT:10:GLU:OE2	2.45	0.48
2:AB:73:GLU:OE1	2:YX:78:LYS:NZ	2.47	0.48
2:AV:78:LYS:NZ	2:AZ:73:GLU:OE1	2.47	0.48
2:BB:228:TYR:C	2:BB:228:TYR:CD1	2.92	0.48
2:CT:6:LYS:NZ	2:CT:10:GLU:OE2	2.45	0.48
2:DW:228:TYR:C	2:DW:228:TYR:CD1	2.91	0.48
2:GC:160:ASP:OD1	2:GC:168:LYS:NZ	2.36	0.48
2:GQ:228:TYR:C	2:GQ:228:TYR:CD1	2.92	0.48
2:GS:6:LYS:NZ	2:GS:10:GLU:OE2	2.45	0.48
2:HM:228:TYR:CD1	2:HM:228:TYR:C	2.92	0.48
2:JH:228:TYR:CD1	2:JH:228:TYR:C	2.92	0.48
2:ZT:78:LYS:NZ	2:ZX:73:GLU:OE1	2.47	0.48
2:ZT:228:TYR:CD1	2:ZT:228:TYR:C	2.92	0.48
2:YD:73:GLU:OE1	2:ZZ:78:LYS:NZ	2.47	0.48
2:YF:78:LYS:NZ	2:YJ:73:GLU:OE1	2.47	0.48
2:ZB:228:TYR:CD1	2:ZB:228:TYR:C	2.92	0.48
2:CF:78:LYS:NZ	2:CJ:73:GLU:OE1	2.47	0.48
2:DD:78:LYS:NZ	2:DH:73:GLU:OE1	2.47	0.48
1:DE:11:ALA:HB1	1:DE:43:VAL:O	2.12	0.48
2:EI:78:LYS:NZ	2:EM:73:GLU:OE1	2.47	0.48
2:FG:78:LYS:NZ	2:FK:73:GLU:OE1	2.47	0.48
2:FU:6:LYS:NZ	2:FU:10:GLU:OE2	2.45	0.48
2:GA:6:LYS:NZ	2:GA:10:GLU:OE2	2.45	0.48
2:GK:78:LYS:NZ	2:GO:73:GLU:OE1	2.47	0.48
2:GQ:78:LYS:NZ	2:GU:73:GLU:OE1	2.47	0.48
2:HO:6:LYS:NZ	2:HO:10:GLU:OE2	2.45	0.48
2:ID:78:LYS:NZ	2:IG:73:GLU:OE1	2.47	0.48
2:JB:78:LYS:NZ	2:JF:73:GLU:OE1	2.47	0.48
2:JN:78:LYS:NZ	2:JR:73:GLU:OE1	2.47	0.48
2:KW:228:TYR:CD1	2:KW:228:TYR:C	2.91	0.48
2:LI:78:LYS:NZ	2:LM:73:GLU:OE1	2.47	0.48
2:ZP:6:LYS:NZ	2:ZP:10:GLU:OE2	2.45	0.48
2:YF:228:TYR:CD1	2:YF:228:TYR:C	2.92	0.48
2:AF:6:LYS:NZ	2:AF:10:GLU:OE2	2.45	0.48
2:BB:78:LYS:NZ	2:BF:73:GLU:OE1	2.47	0.48
2:CR:78:LYS:NZ	2:CV:73:GLU:OE1	2.47	0.48
2:CR:228:TYR:C	2:CR:228:TYR:CD1	2.92	0.48
2:DR:6:LYS:NZ	2:DR:10:GLU:OE2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ZH:78:LYS:NZ	2:ZL:73:GLU:OE1	2.47	0.48
2:GW:78:LYS:NZ	2:HA:73:GLU:OE1	2.47	0.48
2:IR:6:LYS:NZ	2:IR:10:GLU:OE2	2.45	0.48
2:IV:78:LYS:NZ	2:IZ:73:GLU:OE1	2.47	0.48
2:KW:78:LYS:NZ	2:LA:73:GLU:OE1	2.47	0.48
2:LC:78:LYS:NZ	2:LG:73:GLU:OE1	2.47	0.48
2:LO:78:LYS:NZ	2:LS:73:GLU:OE1	2.47	0.48
2:LQ:123:GLU:OE2	2:LQ:170:LYS:NZ	2.34	0.48
2:AV:228:TYR:CD1	2:AV:228:TYR:C	2.92	0.47
2:BN:228:TYR:C	2:BN:228:TYR:CD1	2.92	0.47
2:BT:78:LYS:NZ	2:BX:73:GLU:OE1	2.47	0.47
2:CL:78:LYS:NZ	2:CP:73:GLU:OE1	2.47	0.47
2:DP:78:LYS:NZ	2:DT:73:GLU:OE1	2.47	0.47
2:FG:228:TYR:C	2:FG:228:TYR:CD1	2.92	0.47
2:HC:228:TYR:CD1	2:HC:228:TYR:C	2.92	0.47
2:IV:228:TYR:CD1	2:IV:228:TYR:C	2.92	0.47
2:IX:6:LYS:NZ	2:IX:10:GLU:OE2	2.45	0.47
2:ZN:228:TYR:C	2:ZN:228:TYR:CD1	2.92	0.47
2:AJ:78:LYS:NZ	2:AN:73:GLU:OE1	2.47	0.47
2:EU:78:LYS:NZ	2:EY:73:GLU:OE1	2.47	0.47
2:FM:78:LYS:NZ	2:FQ:73:GLU:OE1	2.47	0.47
2:GE:228:TYR:CD1	2:GE:228:TYR:C	2.92	0.47
2:GK:228:TYR:CD1	2:GK:228:TYR:C	2.91	0.47
2:HC:78:LYS:NZ	2:HF:73:GLU:OE1	2.47	0.47
2:HH:78:LYS:NZ	2:HK:73:GLU:OE1	2.47	0.47
2:JU:6:LYS:NZ	2:JU:10:GLU:OE2	2.45	0.47
2:JY:78:LYS:NZ	2:KC:73:GLU:OE1	2.47	0.47
2:JY:228:TYR:C	2:JY:228:TYR:CD1	2.91	0.47
2:KE:228:TYR:CD1	2:KE:228:TYR:C	2.92	0.47
2:LA:160:ASP:OD1	2:LA:168:LYS:NZ	2.36	0.47
2:ZV:6:LYS:NZ	2:ZV:10:GLU:OE2	2.45	0.47
2:YR:228:TYR:C	2:YR:228:TYR:CD1	2.92	0.47
1:AW:94:GLU:OE1	2:AX:278:ARG:NH2	2.48	0.47
2:FS:78:LYS:NZ	2:FW:73:GLU:OE1	2.47	0.47
1:GR:94:GLU:OE1	2:GS:278:ARG:NH2	2.48	0.47
2:HS:228:TYR:CD1	2:HS:228:TYR:C	2.92	0.47
1:HT:94:GLU:OE1	2:HU:278:ARG:NH2	2.48	0.47
2:ID:228:TYR:CD1	2:ID:228:TYR:C	2.92	0.47
2:IJ:78:LYS:NZ	2:IN:73:GLU:OE1	2.47	0.47
2:IJ:228:TYR:CD1	2:IJ:228:TYR:C	2.92	0.47
1:IW:94:GLU:OE1	2:IX:278:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JT:78:LYS:NZ	2:JW:73:GLU:OE1	2.47	0.47
2:KE:78:LYS:NZ	2:KI:73:GLU:OE1	2.47	0.47
2:KQ:78:LYS:NZ	2:KU:73:GLU:OE1	2.47	0.47
2:LC:228:TYR:C	2:LC:228:TYR:CD1	2.92	0.47
2:ZN:78:LYS:NZ	2:ZR:73:GLU:OE1	2.47	0.47
2:ZB:78:LYS:NZ	2:ZF:73:GLU:OE1	2.47	0.47
2:BH:228:TYR:C	2:BH:228:TYR:CD1	2.92	0.47
1:BU:94:GLU:OE1	2:BV:278:ARG:NH2	2.48	0.47
2:BZ:78:LYS:NZ	2:CD:73:GLU:OE1	2.47	0.47
2:ZD:6:LYS:NZ	2:ZD:10:GLU:OE2	2.45	0.47
1:CG:94:GLU:OE1	2:CH:278:ARG:NH2	2.48	0.47
1:CS:94:GLU:OE1	2:CT:278:ARG:NH2	2.48	0.47
2:DR:2:ASP:OD2	2:DT:101:LYS:NZ	2.33	0.47
2:EU:228:TYR:CD1	2:EU:228:TYR:C	2.92	0.47
2:FA:78:LYS:NZ	2:FE:73:GLU:OE1	2.47	0.47
2:GW:228:TYR:CD1	2:GW:228:TYR:C	2.92	0.47
2:HQ:160:ASP:OD1	2:HQ:168:LYS:NZ	2.36	0.47
2:IP:78:LYS:NZ	2:IT:73:GLU:OE1	2.47	0.47
1:JC:94:GLU:OE1	2:JD:278:ARG:NH2	2.48	0.47
2:JN:228:TYR:C	2:JN:228:TYR:CD1	2.92	0.47
2:JU:278:ARG:NH2	1:WD:94:GLU:OE1	2.48	0.47
1:KL:94:GLU:OE1	2:KM:278:ARG:NH2	2.48	0.47
2:YR:78:LYS:NZ	2:YV:73:GLU:OE1	2.47	0.47
1:YS:94:GLU:OE1	2:YT:278:ARG:NH2	2.48	0.47
2:AD:78:LYS:NZ	2:AH:73:GLU:OE1	2.47	0.47
2:AD:228:TYR:CD1	2:AD:228:TYR:C	2.92	0.47
2:AO:278:ARG:NH2	1:AP:94:GLU:OE1	2.48	0.47
1:BI:94:GLU:OE1	2:BJ:278:ARG:NH2	2.48	0.47
2:CF:228:TYR:CD1	2:CF:228:TYR:C	2.92	0.47
2:CX:78:LYS:NZ	2:DB:73:GLU:OE1	2.47	0.47
1:HZ:94:GLU:OE1	2:IA:278:ARG:NH2	2.48	0.47
2:JH:78:LYS:NZ	2:JL:73:GLU:OE1	2.47	0.47
2:JT:228:TYR:CD1	2:JT:228:TYR:C	2.92	0.47
1:JZ:94:GLU:OE1	2:KA:278:ARG:NH2	2.48	0.47
1:KR:94:GLU:OE1	2:KS:278:ARG:NH2	2.48	0.47
2:LK:6:LYS:NZ	2:LK:10:GLU:OE2	2.45	0.47
1:ZO:94:GLU:OE1	2:ZP:278:ARG:NH2	2.48	0.47
2:EO:78:LYS:NZ	2:ES:73:GLU:OE1	2.47	0.47
1:EP:94:GLU:OE1	2:EQ:278:ARG:NH2	2.48	0.47
2:EQ:6:LYS:NZ	2:EQ:10:GLU:OE2	2.45	0.47
1:GL:94:GLU:OE1	2:GM:278:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GX:94:GLU:OE1	2:GY:278:ARG:NH2	2.48	0.47
2:HU:6:LYS:NZ	2:HU:10:GLU:OE2	2.45	0.47
2:HY:78:LYS:NZ	2:IB:73:GLU:OE1	2.47	0.47
1:JO:94:GLU:OE1	2:JP:278:ARG:NH2	2.48	0.47
1:LP:94:GLU:OE1	2:LQ:278:ARG:NH2	2.48	0.47
1:YC:33:ALA:N	1:YC:34:PRO:CD	2.78	0.47
1:YM:94:GLU:OE1	2:YN:278:ARG:NH2	2.48	0.47
1:YY:94:GLU:OE1	2:YZ:278:ARG:NH2	2.48	0.47
2:AQ:78:LYS:NZ	2:AT:73:GLU:OE1	2.47	0.47
1:ZC:94:GLU:OE1	2:ZD:278:ARG:NH2	2.48	0.47
2:BN:231:VAL:HG11	2:BN:238:MET:HB2	1.97	0.47
2:BP:6:LYS:NZ	2:BP:10:GLU:OE2	2.45	0.47
2:DJ:78:LYS:NZ	2:DN:73:GLU:OE1	2.47	0.47
2:DW:78:LYS:NZ	2:EA:73:GLU:OE1	2.47	0.47
1:EL:33:ALA:N	1:EL:34:PRO:CD	2.78	0.47
1:EV:94:GLU:OE1	2:EW:278:ARG:NH2	2.48	0.47
1:EX:33:ALA:N	1:EX:34:PRO:CD	2.78	0.47
1:FH:94:GLU:OE1	2:FI:278:ARG:NH2	2.48	0.47
1:FN:94:GLU:OE1	2:FO:278:ARG:NH2	2.48	0.47
1:FP:33:ALA:N	1:FP:34:PRO:CD	2.78	0.47
1:FT:94:GLU:OE1	2:FU:278:ARG:NH2	2.48	0.47
2:FY:78:LYS:NZ	2:GC:73:GLU:OE1	2.47	0.47
2:GM:6:LYS:NZ	2:GM:10:GLU:OE2	2.45	0.47
1:ZI:94:GLU:OE1	2:ZJ:278:ARG:NH2	2.48	0.47
1:KH:33:ALA:N	1:KH:34:PRO:CD	2.78	0.47
2:KM:6:LYS:NZ	2:KM:10:GLU:OE2	2.45	0.47
1:LD:94:GLU:OE1	2:LE:278:ARG:NH2	2.48	0.47
2:YX:228:TYR:CD1	2:YX:228:TYR:C	2.92	0.47
1:AE:94:GLU:OE1	2:AF:278:ARG:NH2	2.48	0.47
1:AK:94:GLU:OE1	2:AL:278:ARG:NH2	2.48	0.47
1:BO:94:GLU:OE1	2:BP:278:ARG:NH2	2.48	0.47
1:DQ:94:GLU:OE1	2:DR:278:ARG:NH2	2.48	0.47
2:EC:78:LYS:NZ	2:EG:73:GLU:OE1	2.47	0.47
1:ED:94:GLU:OE1	2:EE:278:ARG:NH2	2.48	0.47
1:FB:94:GLU:OE1	2:FC:278:ARG:NH2	2.48	0.47
1:GT:33:ALA:N	1:GT:34:PRO:CD	2.78	0.47
1:HP:33:ALA:N	1:HP:34:PRO:CD	2.78	0.47
2:HS:78:LYS:NZ	2:HW:73:GLU:OE1	2.47	0.47
2:JB:228:TYR:CD1	2:JB:228:TYR:C	2.91	0.47
1:JK:33:ALA:N	1:JK:34:PRO:CD	2.78	0.47
2:KK:78:LYS:NZ	2:KO:73:GLU:OE1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LJ:94:GLU:OE1	2:LK:278:ARG:NH2	2.48	0.47
2:ZN:231:VAL:HG11	2:ZN:238:MET:HB2	1.97	0.47
1:AG:33:ALA:N	1:AG:34:PRO:CD	2.78	0.47
1:AS:33:ALA:N	1:AS:34:PRO:CD	2.78	0.47
1:BK:33:ALA:N	1:BK:34:PRO:CD	2.78	0.47
1:CC:33:ALA:N	1:CC:34:PRO:CD	2.78	0.47
2:CX:231:VAL:HG11	2:CX:238:MET:HB2	1.97	0.47
1:IK:94:GLU:OE1	2:IL:278:ARG:NH2	2.48	0.47
1:IQ:94:GLU:OE1	2:IR:278:ARG:NH2	2.48	0.47
1:KX:94:GLU:OE1	2:KY:278:ARG:NH2	2.48	0.47
1:KZ:33:ALA:N	1:KZ:34:PRO:CD	2.78	0.47
1:CU:33:ALA:N	1:CU:34:PRO:CD	2.78	0.47
1:CY:94:GLU:OE1	2:CZ:278:ARG:NH2	2.48	0.47
1:DX:94:GLU:OE1	2:DY:278:ARG:NH2	2.48	0.47
2:FA:228:TYR:CD1	2:FA:228:TYR:C	2.91	0.47
2:FY:231:VAL:HG11	2:FY:238:MET:HB2	1.97	0.47
2:GE:78:LYS:NZ	2:GI:73:GLU:OE1	2.47	0.47
1:GF:94:GLU:OE1	2:GG:278:ARG:NH2	2.48	0.47
2:GW:231:VAL:HG11	2:GW:238:MET:HB2	1.97	0.47
1:HD:94:GLU:OE1	2:HE:278:ARG:NH2	2.48	0.47
1:WB:33:ALA:N	1:WB:34:PRO:CD	2.78	0.47
2:HH:231:VAL:HG11	2:HH:238:MET:HB2	1.97	0.47
2:ID:231:VAL:HG11	2:ID:238:MET:HB2	1.97	0.47
1:IE:94:GLU:OE1	2:IF:278:ARG:NH2	2.48	0.47
1:JE:33:ALA:N	1:JE:34:PRO:CD	2.78	0.47
1:KF:94:GLU:OE1	2:KG:278:ARG:NH2	2.48	0.47
1:YA:94:GLU:OE1	2:YB:278:ARG:NH2	2.48	0.47
1:YI:33:ALA:N	1:YI:34:PRO:CD	2.78	0.46
2:YZ:6:LYS:NZ	2:YZ:10:GLU:OE2	2.45	0.46
2:AJ:231:VAL:HG11	2:AJ:238:MET:HB2	1.97	0.46
1:BE:33:ALA:N	1:BE:34:PRO:CD	2.78	0.46
2:BZ:231:VAL:HG11	2:BZ:238:MET:HB2	1.97	0.46
1:CA:94:GLU:OE1	2:CB:278:ARG:NH2	2.48	0.46
1:DK:94:GLU:OE1	2:DL:278:ARG:NH2	2.48	0.46
1:EJ:94:GLU:OE1	2:EK:278:ARG:NH2	2.48	0.46
2:EO:231:VAL:HG11	2:EO:238:MET:HB2	1.97	0.46
2:FS:231:VAL:HG11	2:FS:238:MET:HB2	1.97	0.46
1:FZ:94:GLU:OE1	2:GA:278:ARG:NH2	2.48	0.46
1:HV:33:ALA:N	1:HV:34:PRO:CD	2.78	0.46
2:JH:231:VAL:HG11	2:JH:238:MET:HB2	1.97	0.46
2:KQ:231:VAL:HG11	2:KQ:238:MET:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KW:231:VAL:HG11	2:KW:238:MET:HB2	1.97	0.46
1:ZW:33:ALA:N	1:ZW:34:PRO:CD	2.78	0.46
2:YH:6:LYS:NZ	2:YH:10:GLU:OE2	2.45	0.46
2:YL:78:LYS:NZ	2:YP:73:GLU:OE1	2.47	0.46
2:YL:231:VAL:HG11	2:YL:238:MET:HB2	1.97	0.46
1:AY:33:ALA:N	1:AY:34:PRO:CD	2.78	0.46
1:BC:94:GLU:OE1	2:BD:278:ARG:NH2	2.48	0.46
2:BH:78:LYS:NZ	2:BL:73:GLU:OE1	2.47	0.46
2:BJ:6:LYS:NZ	2:BJ:10:GLU:OE2	2.45	0.46
2:EU:231:VAL:HG11	2:EU:238:MET:HB2	1.97	0.46
1:FD:33:ALA:N	1:FD:34:PRO:CD	2.78	0.46
1:IS:33:ALA:N	1:IS:34:PRO:CD	2.78	0.46
1:JQ:33:ALA:N	1:JQ:34:PRO:CD	2.78	0.46
2:JT:231:VAL:HG11	2:JT:238:MET:HB2	1.97	0.46
1:KB:33:ALA:N	1:KB:34:PRO:CD	2.78	0.46
1:ZU:94:GLU:OE1	2:ZV:278:ARG:NH2	2.48	0.46
2:ZZ:231:VAL:HG11	2:ZZ:238:MET:HB2	1.97	0.46
2:AD:231:VAL:HG11	2:AD:238:MET:HB2	1.97	0.46
1:CM:94:GLU:OE1	2:CN:278:ARG:NH2	2.48	0.46
2:DD:231:VAL:HG11	2:DD:238:MET:HB2	1.97	0.46
1:ER:33:ALA:N	1:ER:34:PRO:CD	2.78	0.46
1:FV:33:ALA:N	1:FV:34:PRO:CD	2.78	0.46
1:GZ:33:ALA:N	1:GZ:34:PRO:CD	2.78	0.46
2:HY:231:VAL:HG11	2:HY:238:MET:HB2	1.97	0.46
1:WC:33:ALA:N	1:WC:34:PRO:CD	2.78	0.46
1:KT:33:ALA:N	1:KT:34:PRO:CD	2.78	0.46
2:LE:6:LYS:NZ	2:LE:10:GLU:OE2	2.45	0.46
1:YG:94:GLU:OE1	2:YH:278:ARG:NH2	2.48	0.46
1:YO:33:ALA:N	1:YO:34:PRO:CD	2.78	0.46
2:YR:231:VAL:HG11	2:YR:238:MET:HB2	1.97	0.46
1:BA:11:ALA:HB1	1:BA:43:VAL:O	2.16	0.46
2:CR:231:VAL:HG11	2:CR:238:MET:HB2	1.97	0.46
1:DZ:33:ALA:N	1:DZ:34:PRO:CD	2.78	0.46
2:EC:231:VAL:HG11	2:EC:238:MET:HB2	1.97	0.46
2:FG:231:VAL:HG11	2:FG:238:MET:HB2	1.97	0.46
1:HN:94:GLU:OE1	2:HO:278:ARG:NH2	2.48	0.46
2:JN:231:VAL:HG11	2:JN:238:MET:HB2	1.97	0.46
1:KN:33:ALA:N	1:KN:34:PRO:CD	2.78	0.46
1:LF:33:ALA:N	1:LF:34:PRO:CD	2.78	0.46
1:LL:33:ALA:N	1:LL:34:PRO:CD	2.78	0.46
2:ZB:231:VAL:HG11	2:ZB:238:MET:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BQ:33:ALA:N	1:BQ:34:PRO:CD	2.78	0.46
1:CO:33:ALA:N	1:CO:34:PRO:CD	2.78	0.46
1:DE:94:GLU:OE1	2:DF:278:ARG:NH2	2.48	0.46
1:DG:33:ALA:N	1:DG:34:PRO:CD	2.78	0.46
1:EF:33:ALA:N	1:EF:34:PRO:CD	2.78	0.46
2:EK:6:LYS:NZ	2:EK:10:GLU:OE2	2.45	0.46
1:GN:33:ALA:N	1:GN:34:PRO:CD	2.78	0.46
2:HE:6:LYS:NZ	2:HE:10:GLU:OE2	2.45	0.46
1:WA:33:ALA:N	1:WA:34:PRO:CD	2.78	0.46
1:IM:33:ALA:N	1:IM:34:PRO:CD	2.78	0.46
2:JY:231:VAL:HG11	2:JY:238:MET:HB2	1.97	0.46
1:KP:11:ALA:HB1	1:KP:43:VAL:O	2.16	0.46
1:ZA:11:ALA:HB1	1:ZA:43:VAL:O	2.16	0.46
2:BT:231:VAL:HG11	2:BT:238:MET:HB2	1.97	0.46
2:CL:231:VAL:HG11	2:CL:238:MET:HB2	1.97	0.46
2:EI:231:VAL:HG11	2:EI:238:MET:HB2	1.97	0.46
1:EZ:11:ALA:HB1	1:EZ:43:VAL:O	2.16	0.46
1:GD:11:ALA:HB1	1:GD:43:VAL:O	2.16	0.46
1:HX:11:ALA:HB1	1:HX:43:VAL:O	2.16	0.46
1:IH:33:ALA:N	1:IH:34:PRO:CD	2.78	0.46
1:IU:11:ALA:HB1	1:IU:43:VAL:O	2.16	0.46
1:IY:33:ALA:N	1:IY:34:PRO:CD	2.78	0.46
1:ZK:33:ALA:N	1:ZK:34:PRO:CD	2.78	0.46
2:KG:6:LYS:NZ	2:KG:10:GLU:OE2	2.45	0.46
1:KJ:11:ALA:HB1	1:KJ:43:VAL:O	2.16	0.46
2:LC:231:VAL:HG11	2:LC:238:MET:HB2	1.97	0.46
2:LQ:6:LYS:NZ	2:LQ:10:GLU:OE2	2.45	0.46
1:ZQ:33:ALA:N	1:ZQ:34:PRO:CD	2.78	0.46
1:ZS:11:ALA:HB1	1:ZS:43:VAL:O	2.16	0.46
1:AC:11:ALA:HB1	1:AC:43:VAL:O	2.16	0.46
1:BM:11:ALA:HB1	1:BM:43:VAL:O	2.16	0.46
1:CI:33:ALA:N	1:CI:34:PRO:CD	2.78	0.46
2:FI:6:LYS:NZ	2:FI:10:GLU:OE2	2.45	0.46
2:GG:6:LYS:NZ	2:GG:10:GLU:OE2	2.45	0.46
1:GV:11:ALA:HB1	1:GV:43:VAL:O	2.16	0.46
1:HB:11:ALA:HB1	1:HB:43:VAL:O	2.16	0.46
1:HI:94:GLU:OE1	2:HJ:278:ARG:NH2	2.48	0.46
2:HS:231:VAL:HG11	2:HS:238:MET:HB2	1.97	0.46
1:IC:11:ALA:HB1	1:IC:43:VAL:O	2.16	0.46
2:IV:231:VAL:HG11	2:IV:238:MET:HB2	1.97	0.46
1:JI:94:GLU:OE1	2:JJ:278:ARG:NH2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JJ:6:LYS:NZ	2:JJ:10:GLU:OE2	2.45	0.46
1:LH:11:ALA:HB1	1:LH:43:VAL:O	2.16	0.46
1:LR:33:ALA:N	1:LR:34:PRO:CD	2.78	0.46
2:AQ:231:VAL:HG11	2:AQ:238:MET:HB2	1.97	0.46
2:BB:231:VAL:HG11	2:BB:238:MET:HB2	1.97	0.46
2:BN:78:LYS:NZ	2:BR:73:GLU:OE1	2.47	0.46
1:CQ:11:ALA:HB1	1:CQ:43:VAL:O	2.16	0.46
1:DS:33:ALA:N	1:DS:34:PRO:CD	2.78	0.46
2:DY:6:LYS:NZ	2:DY:10:GLU:OE2	2.45	0.46
1:GP:11:ALA:HB1	1:GP:43:VAL:O	2.16	0.46
2:KK:231:VAL:HG11	2:KK:238:MET:HB2	1.97	0.46
1:YE:11:ALA:HB1	1:YE:43:VAL:O	2.16	0.46
1:CW:11:ALA:HB1	1:CW:43:VAL:O	2.16	0.46
1:ET:11:ALA:HB1	1:ET:43:VAL:O	2.16	0.46
1:FJ:33:ALA:N	1:FJ:34:PRO:CD	2.78	0.46
1:GB:33:ALA:N	1:GB:34:PRO:CD	2.78	0.46
1:GH:33:ALA:N	1:GH:34:PRO:CD	2.78	0.46
2:GQ:231:VAL:HG11	2:GQ:238:MET:HB2	1.97	0.46
1:HL:11:ALA:HB1	1:HL:43:VAL:O	2.16	0.46
2:JD:6:LYS:NZ	2:JD:10:GLU:OE2	2.45	0.46
1:JV:33:ALA:N	1:JV:34:PRO:CD	2.78	0.46
1:ZM:11:ALA:HB1	1:ZM:43:VAL:O	2.16	0.46
2:ZV:160:ASP:OD1	2:ZV:168:LYS:NZ	2.45	0.46
1:YQ:11:ALA:HB1	1:YQ:43:VAL:O	2.16	0.46
1:YU:33:ALA:N	1:YU:34:PRO:CD	2.78	0.46
1:YW:11:ALA:HB1	1:YW:43:VAL:O	2.16	0.46
2:YX:231:VAL:HG11	2:YX:238:MET:HB2	1.97	0.46
1:AM:33:ALA:N	1:AM:34:PRO:CD	2.78	0.46
1:DA:33:ALA:N	1:DA:34:PRO:CD	2.78	0.46
1:EH:11:ALA:HB1	1:EH:43:VAL:O	2.16	0.46
1:FL:11:ALA:HB1	1:FL:43:VAL:O	2.16	0.46
2:GK:231:VAL:HG11	2:GK:238:MET:HB2	1.97	0.46
2:HJ:6:LYS:NZ	2:HJ:10:GLU:OE2	2.45	0.46
2:IJ:231:VAL:HG11	2:IJ:238:MET:HB2	1.97	0.46
2:IL:6:LYS:NZ	2:IL:10:GLU:OE2	2.45	0.46
1:JX:11:ALA:HB1	1:JX:43:VAL:O	2.16	0.46
2:BD:6:LYS:NZ	2:BD:10:GLU:OE2	2.45	0.45
1:EB:11:ALA:HB1	1:EB:43:VAL:O	2.16	0.45
2:FM:231:VAL:HG11	2:FM:238:MET:HB2	1.97	0.45
1:FX:11:ALA:HB1	1:FX:43:VAL:O	2.16	0.45
1:GJ:11:ALA:HB1	1:GJ:43:VAL:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HM:231:VAL:HG11	2:HM:238:MET:HB2	1.97	0.45
1:HR:11:ALA:HB1	1:HR:43:VAL:O	2.16	0.45
2:JB:231:VAL:HG11	2:JB:238:MET:HB2	1.97	0.45
1:AA:33:ALA:N	1:AA:34:PRO:CD	2.78	0.45
1:BG:11:ALA:HB1	1:BG:43:VAL:O	2.16	0.45
1:BW:33:ALA:N	1:BW:34:PRO:CD	2.78	0.45
1:CE:11:ALA:HB1	1:CE:43:VAL:O	2.16	0.45
1:ZE:33:ALA:N	1:ZE:34:PRO:CD	2.78	0.45
1:DC:11:ALA:HB1	1:DC:43:VAL:O	2.16	0.45
1:DM:33:ALA:N	1:DM:34:PRO:CD	2.78	0.45
2:DW:231:VAL:HG11	2:DW:238:MET:HB2	1.97	0.45
2:FA:231:VAL:HG11	2:FA:238:MET:HB2	1.97	0.45
2:ZH:231:VAL:HG11	2:ZH:238:MET:HB2	1.97	0.45
2:HC:231:VAL:HG11	2:HC:238:MET:HB2	1.97	0.45
1:IO:11:ALA:HB1	1:IO:43:VAL:O	2.16	0.45
2:IP:231:VAL:HG11	2:IP:238:MET:HB2	1.97	0.45
1:ZY:11:ALA:HB1	1:ZY:43:VAL:O	2.16	0.45
1:YK:11:ALA:HB1	1:YK:43:VAL:O	2.16	0.45
2:CN:6:LYS:NZ	2:CN:10:GLU:OE2	2.45	0.45
2:DJ:231:VAL:HG11	2:DJ:238:MET:HB2	1.97	0.45
1:FR:11:ALA:HB1	1:FR:43:VAL:O	2.16	0.45
2:HM:9:LEU:HD11	2:HO:71:VAL:HG21	1.99	0.45
1:KV:11:ALA:HB1	1:KV:43:VAL:O	2.16	0.45
1:LB:11:ALA:HB1	1:LB:43:VAL:O	2.16	0.45
1:LP:77:TYR:N	1:LP:77:TYR:CD1	2.84	0.45
2:AO:6:LYS:NZ	2:AO:10:GLU:OE2	2.45	0.45
2:AV:231:VAL:HG11	2:AV:238:MET:HB2	1.97	0.45
1:BY:11:ALA:HB1	1:BY:43:VAL:O	2.16	0.45
1:CK:11:ALA:HB1	1:CK:43:VAL:O	2.16	0.45
2:DJ:9:LEU:HD11	2:DL:71:VAL:HG21	1.99	0.45
2:GE:231:VAL:HG11	2:GE:238:MET:HB2	1.97	0.45
1:AR:11:ALA:HB1	1:AR:43:VAL:O	2.16	0.45
2:BH:9:LEU:HD11	2:BJ:71:VAL:HG21	1.99	0.45
2:CZ:6:LYS:NZ	2:CZ:10:GLU:OE2	2.45	0.45
1:DI:11:ALA:HB1	1:DI:43:VAL:O	2.16	0.45
1:ZG:11:ALA:HB1	1:ZG:43:VAL:O	2.16	0.45
1:FF:11:ALA:HB1	1:FF:43:VAL:O	2.16	0.45
1:GL:77:TYR:N	1:GL:77:TYR:CD1	2.84	0.45
1:JM:11:ALA:HB1	1:JM:43:VAL:O	2.16	0.45
1:KD:11:ALA:HB1	1:KD:43:VAL:O	2.16	0.45
2:KE:231:VAL:HG11	2:KE:238:MET:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YM:77:TYR:N	1:YM:77:TYR:CD1	2.84	0.45
2:AO:160:ASP:OD1	2:AO:168:LYS:NZ	2.45	0.45
1:BI:77:TYR:N	1:BI:77:TYR:CD1	2.84	0.45
1:BS:11:ALA:HB1	1:BS:43:VAL:O	2.16	0.45
2:FA:9:LEU:HD11	2:FC:71:VAL:HG21	1.99	0.45
1:HG:11:ALA:HB1	1:HG:43:VAL:O	2.16	0.45
1:HI:77:TYR:N	1:HI:77:TYR:CD1	2.84	0.45
2:LC:9:LEU:HD11	2:LE:71:VAL:HG21	1.99	0.45
1:LJ:77:TYR:N	1:LJ:77:TYR:CD1	2.84	0.45
2:YF:9:LEU:HD11	2:YH:71:VAL:HG21	1.99	0.45
2:YF:231:VAL:HG11	2:YF:238:MET:HB2	1.97	0.45
1:AI:11:ALA:HB1	1:AI:43:VAL:O	2.16	0.45
2:BN:9:LEU:HD11	2:BP:71:VAL:HG21	1.99	0.45
1:BO:77:TYR:CD1	1:BO:77:TYR:N	2.84	0.45
2:CF:231:VAL:HG11	2:CF:238:MET:HB2	1.97	0.45
1:DU:11:ALA:HB1	1:DU:43:VAL:O	2.16	0.45
1:DX:77:TYR:CD1	1:DX:77:TYR:N	2.84	0.45
1:EN:11:ALA:HB1	1:EN:43:VAL:O	2.16	0.45
2:GE:9:LEU:HD11	2:GG:71:VAL:HG21	1.99	0.45
2:HY:9:LEU:HD11	2:IA:71:VAL:HG21	1.99	0.45
1:II:11:ALA:HB1	1:II:43:VAL:O	2.16	0.45
1:JS:11:ALA:HB1	1:JS:43:VAL:O	2.16	0.45
2:KE:9:LEU:HD11	2:KG:71:VAL:HG21	1.99	0.45
1:KL:77:TYR:N	1:KL:77:TYR:CD1	2.84	0.45
2:KW:9:LEU:HD11	2:KY:71:VAL:HG21	1.99	0.45
2:LI:231:VAL:HG11	2:LI:238:MET:HB2	1.97	0.45
2:LO:231:VAL:HG11	2:LO:238:MET:HB2	1.97	0.45
2:YX:9:LEU:HD11	2:YZ:71:VAL:HG21	1.99	0.45
2:BH:231:VAL:HG11	2:BH:238:MET:HB2	1.97	0.45
2:HC:9:LEU:HD11	2:HE:71:VAL:HG21	1.99	0.45
1:LN:11:ALA:HB1	1:LN:43:VAL:O	2.16	0.45
2:ZT:231:VAL:HG11	2:ZT:238:MET:HB2	1.97	0.45
2:ZZ:9:LEU:HD11	2:YB:71:VAL:HG21	1.99	0.45
2:BX:160:ASP:OD1	2:BX:168:LYS:NZ	2.36	0.45
2:EI:9:LEU:HD11	2:EK:71:VAL:HG21	1.99	0.45
2:FS:9:LEU:HD11	2:FU:71:VAL:HG21	1.99	0.45
1:JG:11:ALA:HB1	1:JG:43:VAL:O	2.16	0.45
2:JP:6:LYS:NZ	2:JP:10:GLU:OE2	2.45	0.45
2:LI:9:LEU:HD11	2:LK:71:VAL:HG21	1.99	0.45
2:ZT:9:LEU:HD11	2:ZV:71:VAL:HG21	1.99	0.45
2:ZB:9:LEU:HD11	2:ZD:71:VAL:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:9:LEU:HD11	2:BD:71:VAL:HG21	1.99	0.45
2:DP:231:VAL:HG11	2:DP:238:MET:HB2	1.97	0.45
1:FZ:77:TYR:N	1:FZ:77:TYR:CD1	2.84	0.45
1:JA:11:ALA:HB1	1:JA:43:VAL:O	2.16	0.45
2:KQ:9:LEU:HD11	2:KS:71:VAL:HG21	1.99	0.45
1:LD:77:TYR:N	1:LD:77:TYR:CD1	2.84	0.45
2:DF:6:LYS:NZ	2:DF:10:GLU:OE2	2.45	0.44
2:DP:9:LEU:HD11	2:DR:71:VAL:HG21	1.99	0.44
1:GF:77:TYR:N	1:GF:77:TYR:CD1	2.84	0.44
2:JY:9:LEU:HD11	2:KA:71:VAL:HG21	1.99	0.44
2:AD:9:LEU:HD11	2:AF:71:VAL:HG21	1.99	0.44
2:AH:160:ASP:OD1	2:AH:168:LYS:NZ	2.36	0.44
1:DO:11:ALA:HB1	1:DO:43:VAL:O	2.16	0.44
1:AU:11:ALA:HB1	1:AU:43:VAL:O	2.16	0.44
2:EC:9:LEU:HD11	2:EE:71:VAL:HG21	1.99	0.44
1:FB:77:TYR:N	1:FB:77:TYR:CD1	2.84	0.44
2:FC:6:LYS:NZ	2:FC:10:GLU:OE2	2.45	0.44
2:FY:9:LEU:HD11	2:GA:71:VAL:HG21	1.99	0.44
2:ZH:9:LEU:HD11	2:ZJ:71:VAL:HG21	1.99	0.44
2:IF:160:ASP:OD1	2:IF:168:LYS:NZ	2.45	0.44
1:IW:77:TYR:N	1:IW:77:TYR:CD1	2.84	0.44
2:AO:71:VAL:HG21	2:AQ:9:LEU:HD11	1.99	0.44
1:CO:81:ARG:NH2	2:CP:281:PHE:O	2.51	0.44
1:JK:81:ARG:NH2	2:JL:281:PHE:O	2.51	0.44
1:KN:81:ARG:NH2	2:KO:281:PHE:O	2.51	0.44
1:CU:81:ARG:NH2	2:CV:281:PHE:O	2.51	0.44
1:DM:81:ARG:NH2	2:DN:281:PHE:O	2.51	0.44
1:DQ:77:TYR:N	1:DQ:77:TYR:CD1	2.84	0.44
2:FG:9:LEU:HD11	2:FI:71:VAL:HG21	1.99	0.44
2:FM:9:LEU:HD11	2:FO:71:VAL:HG21	1.99	0.44
1:JZ:31:LYS:O	1:JZ:87:GLN:NE2	2.51	0.44
2:LO:9:LEU:HD11	2:LQ:71:VAL:HG21	1.99	0.44
2:YR:9:LEU:HD11	2:YT:71:VAL:HG21	1.99	0.44
1:YY:77:TYR:N	1:YY:77:TYR:CD1	2.84	0.44
1:BI:31:LYS:O	1:BI:87:GLN:NE2	2.51	0.44
2:DW:9:LEU:HD11	2:DY:71:VAL:HG21	1.99	0.44
2:EU:9:LEU:HD11	2:EW:71:VAL:HG21	1.99	0.44
2:GQ:9:LEU:HD11	2:GS:71:VAL:HG21	1.99	0.44
1:GR:31:LYS:O	1:GR:87:GLN:NE2	2.51	0.44
1:IE:77:TYR:N	1:IE:77:TYR:CD1	2.84	0.44
1:ZO:31:LYS:O	1:ZO:87:GLN:NE2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YG:31:LYS:O	1:YG:87:GLN:NE2	2.51	0.44
2:AJ:9:LEU:HD11	2:AL:71:VAL:HG21	1.99	0.44
1:ZC:31:LYS:O	1:ZC:87:GLN:NE2	2.51	0.44
2:BF:160:ASP:OD1	2:BF:168:LYS:NZ	2.36	0.44
1:CM:31:LYS:O	1:CM:87:GLN:NE2	2.51	0.44
1:CM:77:TYR:N	1:CM:77:TYR:CD1	2.84	0.44
1:CS:31:LYS:O	1:CS:87:GLN:NE2	2.51	0.44
1:DE:31:LYS:O	1:DE:87:GLN:NE2	2.51	0.44
1:GZ:81:ARG:NH2	2:HA:281:PHE:O	2.51	0.44
1:IK:31:LYS:O	1:IK:87:GLN:NE2	2.51	0.44
1:ZW:81:ARG:NH2	2:ZX:281:PHE:O	2.51	0.44
2:YB:6:LYS:NZ	2:YB:10:GLU:OE2	2.45	0.44
1:YC:81:ARG:NH2	2:YD:281:PHE:O	2.51	0.44
1:AP:31:LYS:O	1:AP:87:GLN:NE2	2.51	0.44
1:CA:31:LYS:O	1:CA:87:GLN:NE2	2.51	0.44
2:CB:6:LYS:NZ	2:CB:10:GLU:OE2	2.45	0.44
1:CG:31:LYS:O	1:CG:87:GLN:NE2	2.51	0.44
1:FB:31:LYS:O	1:FB:87:GLN:NE2	2.51	0.44
1:GX:21:VAL:HG11	1:GX:54:VAL:HG11	2.00	0.44
2:HS:9:LEU:HD11	2:HU:71:VAL:HG21	1.99	0.44
1:HZ:31:LYS:O	1:HZ:87:GLN:NE2	2.51	0.44
2:ID:149:GLN:HG2	2:ID:178:ALA:HB3	2.00	0.44
2:IV:9:LEU:HD11	2:IX:71:VAL:HG21	1.99	0.44
1:IW:31:LYS:O	1:IW:87:GLN:NE2	2.51	0.44
2:JN:9:LEU:HD11	2:JP:71:VAL:HG21	1.99	0.44
1:KT:81:ARG:NH2	2:KU:281:PHE:O	2.51	0.44
1:LL:81:ARG:NH2	2:LM:281:PHE:O	2.51	0.44
1:ZU:31:LYS:O	1:ZU:87:GLN:NE2	2.51	0.44
2:YF:149:GLN:HG2	2:YF:178:ALA:HB3	2.00	0.44
1:ZC:21:VAL:HG11	1:ZC:54:VAL:HG11	2.00	0.44
2:CL:149:GLN:HG2	2:CL:178:ALA:HB3	2.00	0.44
2:CX:9:LEU:HD11	2:CZ:71:VAL:HG21	1.99	0.44
2:CX:149:GLN:HG2	2:CX:178:ALA:HB3	2.00	0.44
2:DP:149:GLN:HG2	2:DP:178:ALA:HB3	2.00	0.44
2:EO:149:GLN:HG2	2:EO:178:ALA:HB3	2.00	0.44
1:EV:21:VAL:HG11	1:EV:54:VAL:HG11	2.00	0.44
1:FB:21:VAL:HG11	1:FB:54:VAL:HG11	2.00	0.44
2:FG:45:HIS:CE1	2:FI:46:ASN:HD21	2.36	0.44
1:FT:31:LYS:O	1:FT:87:GLN:NE2	2.51	0.44
1:GF:31:LYS:O	1:GF:87:GLN:NE2	2.51	0.44
1:GL:31:LYS:O	1:GL:87:GLN:NE2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZI:31:LYS:O	1:ZI:87:GLN:NE2	2.51	0.44
2:HH:9:LEU:HD11	2:HJ:71:VAL:HG21	1.99	0.44
1:HN:31:LYS:O	1:HN:87:GLN:NE2	2.51	0.44
1:HT:31:LYS:O	1:HT:87:GLN:NE2	2.51	0.44
1:IE:31:LYS:O	1:IE:87:GLN:NE2	2.51	0.44
2:IP:9:LEU:HD11	2:IR:71:VAL:HG21	1.99	0.44
2:IV:149:GLN:HG2	2:IV:178:ALA:HB3	2.00	0.44
2:JH:9:LEU:HD11	2:JJ:71:VAL:HG21	1.99	0.44
1:JI:77:TYR:N	1:JI:77:TYR:CD1	2.84	0.44
1:KF:31:LYS:O	1:KF:87:GLN:NE2	2.51	0.44
1:KR:21:VAL:HG11	1:KR:54:VAL:HG11	2.00	0.44
2:LI:149:GLN:HG2	2:LI:178:ALA:HB3	2.00	0.44
2:ZN:9:LEU:HD11	2:ZP:71:VAL:HG21	1.99	0.44
2:ZZ:149:GLN:HG2	2:ZZ:178:ALA:HB3	2.00	0.43
1:YS:21:VAL:HG11	1:YS:54:VAL:HG11	2.00	0.43
2:CL:9:LEU:HD11	2:CN:71:VAL:HG21	1.99	0.43
2:EI:149:GLN:HG2	2:EI:178:ALA:HB3	2.00	0.43
1:EJ:31:LYS:O	1:EJ:87:GLN:NE2	2.51	0.43
1:FH:21:VAL:HG11	1:FH:54:VAL:HG11	2.00	0.43
1:FT:77:TYR:CD1	1:FT:77:TYR:N	2.84	0.43
2:GE:149:GLN:HG2	2:GE:178:ALA:HB3	2.00	0.43
2:GK:9:LEU:HD11	2:GM:71:VAL:HG21	1.99	0.43
2:GQ:45:HIS:CE1	2:GS:46:ASN:HD21	2.36	0.43
1:GX:31:LYS:O	1:GX:87:GLN:NE2	2.51	0.43
1:ZI:21:VAL:HG11	1:ZI:54:VAL:HG11	2.00	0.43
2:HH:149:GLN:HG2	2:HH:178:ALA:HB3	2.00	0.43
2:HM:149:GLN:HG2	2:HM:178:ALA:HB3	2.00	0.43
1:IQ:31:LYS:O	1:IQ:87:GLN:NE2	2.51	0.43
2:JB:9:LEU:HD11	2:JD:71:VAL:HG21	1.99	0.43
1:JC:31:LYS:O	1:JC:87:GLN:NE2	2.51	0.43
2:JN:149:GLN:HG2	2:JN:178:ALA:HB3	2.00	0.43
1:KF:21:VAL:HG11	1:KF:54:VAL:HG11	2.00	0.43
1:KH:81:ARG:NH2	2:KI:281:PHE:O	2.51	0.43
1:KX:31:LYS:O	1:KX:87:GLN:NE2	2.51	0.43
1:ZO:21:VAL:HG11	1:ZO:54:VAL:HG11	2.00	0.43
1:YA:31:LYS:O	1:YA:87:GLN:NE2	2.51	0.43
2:YL:9:LEU:HD11	2:YN:71:VAL:HG21	1.99	0.43
2:YX:149:GLN:HG2	2:YX:178:ALA:HB3	2.00	0.43
1:YY:21:VAL:HG11	1:YY:54:VAL:HG11	2.00	0.43
1:YY:31:LYS:O	1:YY:87:GLN:NE2	2.51	0.43
1:AW:31:LYS:O	1:AW:87:GLN:NE2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:149:GLN:HG2	2:BB:178:ALA:HB3	2.00	0.43
1:BC:77:TYR:N	1:BC:77:TYR:CD1	2.84	0.43
1:BE:81:ARG:NH2	2:BF:281:PHE:O	2.51	0.43
1:BI:21:VAL:HG11	1:BI:54:VAL:HG11	2.01	0.43
2:BT:9:LEU:HD11	2:BV:71:VAL:HG21	1.99	0.43
1:CG:21:VAL:HG11	1:CG:54:VAL:HG11	2.00	0.43
1:EP:31:LYS:O	1:EP:87:GLN:NE2	2.51	0.43
1:FN:21:VAL:HG11	1:FN:54:VAL:HG11	2.00	0.43
1:FZ:31:LYS:O	1:FZ:87:GLN:NE2	2.51	0.43
1:GR:77:TYR:N	1:GR:77:TYR:CD1	2.84	0.43
2:GW:9:LEU:HD11	2:GY:71:VAL:HG21	1.99	0.43
2:HS:45:HIS:CE1	2:HU:46:ASN:HD21	2.37	0.43
1:IK:21:VAL:HG11	1:IK:54:VAL:HG11	2.00	0.43
1:JO:31:LYS:O	1:JO:87:GLN:NE2	2.51	0.43
2:KA:6:LYS:NZ	2:KA:10:GLU:OE2	2.45	0.43
1:KR:31:LYS:O	1:KR:87:GLN:NE2	2.51	0.43
2:LC:149:GLN:HG2	2:LC:178:ALA:HB3	2.00	0.43
1:LP:31:LYS:O	1:LP:87:GLN:NE2	2.51	0.43
2:ZN:45:HIS:CE1	2:ZP:46:ASN:HD21	2.37	0.43
1:ZU:21:VAL:HG11	1:ZU:54:VAL:HG11	2.00	0.43
1:YA:77:TYR:N	1:YA:77:TYR:CD1	2.84	0.43
2:YR:45:HIS:CE1	2:YT:46:ASN:HD21	2.37	0.43
1:YS:77:TYR:CD1	1:YS:77:TYR:N	2.84	0.43
2:ZB:149:GLN:HG2	2:ZB:178:ALA:HB3	2.00	0.43
1:AE:77:TYR:N	1:AE:77:TYR:CD1	2.84	0.43
2:AV:45:HIS:CE1	2:AX:46:ASN:HD21	2.37	0.43
1:BC:21:VAL:HG11	1:BC:54:VAL:HG11	2.00	0.43
2:BH:149:GLN:HG2	2:BH:178:ALA:HB3	2.00	0.43
2:CF:9:LEU:HD11	2:CH:71:VAL:HG21	1.99	0.43
2:CF:149:GLN:HG2	2:CF:178:ALA:HB3	2.00	0.43
2:CR:9:LEU:HD11	2:CT:71:VAL:HG21	1.99	0.43
2:CR:45:HIS:CE1	2:CT:46:ASN:HD21	2.36	0.43
1:CY:77:TYR:CD1	1:CY:77:TYR:N	2.84	0.43
2:DJ:45:HIS:CE1	2:DL:46:ASN:HD21	2.36	0.43
1:FH:31:LYS:O	1:FH:87:GLN:NE2	2.51	0.43
1:GH:81:ARG:NH2	2:GI:281:PHE:O	2.51	0.43
2:GQ:149:GLN:HG2	2:GQ:178:ALA:HB3	2.00	0.43
1:HT:21:VAL:HG11	1:HT:54:VAL:HG11	2.00	0.43
2:IP:45:HIS:CE1	2:IR:46:ASN:HD21	2.36	0.43
1:WD:21:VAL:HG11	1:WD:54:VAL:HG11	2.00	0.43
2:KK:9:LEU:HD11	2:KM:71:VAL:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KK:149:GLN:HG2	2:KK:178:ALA:HB3	2.00	0.43
1:LF:81:ARG:NH2	2:LG:281:PHE:O	2.51	0.43
2:YR:149:GLN:HG2	2:YR:178:ALA:HB3	2.00	0.43
1:AW:21:VAL:HG11	1:AW:54:VAL:HG11	2.00	0.43
1:DZ:81:ARG:NH2	2:EA:281:PHE:O	2.51	0.43
1:ED:31:LYS:O	1:ED:87:GLN:NE2	2.51	0.43
1:EL:81:ARG:NH2	2:EM:281:PHE:O	2.51	0.43
1:FN:31:LYS:O	1:FN:87:GLN:NE2	2.51	0.43
2:FS:149:GLN:HG2	2:FS:178:ALA:HB3	2.00	0.43
1:ZI:77:TYR:N	1:ZI:77:TYR:CD1	2.84	0.43
1:IQ:98:ASP:OD1	1:IQ:98:ASP:N	2.52	0.43
1:ZK:81:ARG:NH2	2:ZL:281:PHE:O	2.51	0.43
2:JB:45:HIS:CE1	2:JD:46:ASN:HD21	2.37	0.43
1:JC:21:VAL:HG11	1:JC:54:VAL:HG11	2.00	0.43
2:LC:45:HIS:CE1	2:LE:46:ASN:HD21	2.36	0.43
2:AD:149:GLN:HG2	2:AD:178:ALA:HB3	2.00	0.43
1:AK:77:TYR:N	1:AK:77:TYR:CD1	2.84	0.43
2:AV:9:LEU:HD11	2:AX:71:VAL:HG21	1.99	0.43
2:AV:149:GLN:HG2	2:AV:178:ALA:HB3	2.00	0.43
1:AW:77:TYR:N	1:AW:77:TYR:CD1	2.84	0.43
2:DJ:149:GLN:HG2	2:DJ:178:ALA:HB3	2.00	0.43
1:DK:21:VAL:HG11	1:DK:54:VAL:HG11	2.00	0.43
2:DW:45:HIS:CE1	2:DY:46:ASN:HD21	2.37	0.43
2:DY:160:ASP:OD1	2:DY:168:LYS:NZ	2.45	0.43
2:FM:149:GLN:HG2	2:FM:178:ALA:HB3	2.00	0.43
1:FV:81:ARG:NH2	2:FW:281:PHE:O	2.51	0.43
2:ZH:149:GLN:HG2	2:ZH:178:ALA:HB3	2.00	0.43
1:GR:21:VAL:HG11	1:GR:54:VAL:HG11	2.00	0.43
1:HD:31:LYS:O	1:HD:87:GLN:NE2	2.51	0.43
1:HI:31:LYS:O	1:HI:87:GLN:NE2	2.51	0.43
1:JE:81:ARG:NH2	2:JF:281:PHE:O	2.51	0.43
2:JT:9:LEU:HD11	2:JU:71:VAL:HG21	1.99	0.43
1:WD:77:TYR:N	1:WD:77:TYR:CD1	2.84	0.43
1:LJ:21:VAL:HG11	1:LJ:54:VAL:HG11	2.00	0.43
1:LP:21:VAL:HG11	1:LP:54:VAL:HG11	2.00	0.43
1:ZO:77:TYR:N	1:ZO:77:TYR:CD1	2.84	0.43
2:YL:45:HIS:CE1	2:YN:46:ASN:HD21	2.37	0.43
1:YO:81:ARG:NH2	2:YP:281:PHE:O	2.51	0.43
1:YS:31:LYS:O	1:YS:87:GLN:NE2	2.51	0.43
2:ZB:45:HIS:CE1	2:ZD:46:ASN:HD21	2.37	0.43
1:ZC:77:TYR:N	1:ZC:77:TYR:CD1	2.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:31:LYS:O	1:BC:87:GLN:NE2	2.51	0.43
2:BT:45:HIS:CE1	2:BV:46:ASN:HD21	2.37	0.43
1:CG:77:TYR:N	1:CG:77:TYR:CD1	2.84	0.43
1:CS:21:VAL:HG11	1:CS:54:VAL:HG11	2.00	0.43
2:DD:9:LEU:HD11	2:DF:71:VAL:HG21	1.99	0.43
1:DK:31:LYS:O	1:DK:87:GLN:NE2	2.51	0.43
1:DQ:31:LYS:O	1:DQ:87:GLN:NE2	2.51	0.43
1:EF:81:ARG:NH2	2:EG:281:PHE:O	2.51	0.43
1:EV:31:LYS:O	1:EV:87:GLN:NE2	2.51	0.43
1:FH:77:TYR:CD1	1:FH:77:TYR:N	2.84	0.43
1:FZ:21:VAL:HG11	1:FZ:54:VAL:HG11	2.00	0.43
2:GE:45:HIS:CE1	2:GG:46:ASN:HD21	2.36	0.43
2:GW:45:HIS:CE1	2:GY:46:ASN:HD21	2.37	0.43
2:HC:45:HIS:CE1	2:HE:46:ASN:HD21	2.37	0.43
2:ID:9:LEU:HD11	2:IF:71:VAL:HG21	1.99	0.43
2:IJ:9:LEU:HD11	2:IL:71:VAL:HG21	1.99	0.43
2:IJ:45:HIS:CE1	2:IL:46:ASN:HD21	2.37	0.43
1:WD:31:LYS:O	1:WD:87:GLN:NE2	2.51	0.43
1:KL:31:LYS:O	1:KL:87:GLN:NE2	2.51	0.43
2:KQ:149:GLN:HG2	2:KQ:178:ALA:HB3	2.00	0.43
1:KX:77:TYR:N	1:KX:77:TYR:CD1	2.84	0.43
1:LJ:31:LYS:O	1:LJ:87:GLN:NE2	2.51	0.43
2:ZZ:45:HIS:CE1	2:YB:46:ASN:HD21	2.36	0.43
2:YF:45:HIS:CE1	2:YH:46:ASN:HD21	2.37	0.43
1:YM:21:VAL:HG11	1:YM:54:VAL:HG11	2.00	0.43
1:AW:98:ASP:OD1	1:AW:98:ASP:N	2.52	0.43
1:AY:81:ARG:NH2	2:AZ:281:PHE:O	2.51	0.43
1:BO:31:LYS:O	1:BO:87:GLN:NE2	2.51	0.43
2:EO:9:LEU:HD11	2:EQ:71:VAL:HG21	1.99	0.43
1:HD:21:VAL:HG11	1:HD:54:VAL:HG11	2.00	0.43
1:JZ:21:VAL:HG11	1:JZ:54:VAL:HG11	2.00	0.43
2:LI:45:HIS:CE1	2:LK:46:ASN:HD21	2.36	0.43
2:ZT:149:GLN:HG2	2:ZT:178:ALA:HB3	2.00	0.43
1:ZU:77:TYR:N	1:ZU:77:TYR:CD1	2.84	0.43
1:AE:21:VAL:HG11	1:AE:54:VAL:HG11	2.00	0.43
1:AE:31:LYS:O	1:AE:87:GLN:NE2	2.51	0.43
1:AP:77:TYR:CD1	1:AP:77:TYR:N	2.84	0.43
1:AS:81:ARG:NH2	2:AT:281:PHE:O	2.51	0.43
1:BU:21:VAL:HG11	1:BU:54:VAL:HG11	2.00	0.43
1:BU:77:TYR:N	1:BU:77:TYR:CD1	2.84	0.43
1:CA:98:ASP:OD1	1:CA:98:ASP:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DS:81:ARG:NH2	2:DT:281:PHE:O	2.51	0.43
1:DX:31:LYS:O	1:DX:87:GLN:NE2	2.51	0.43
2:EI:45:HIS:CE1	2:EK:46:ASN:HD21	2.36	0.43
2:HH:45:HIS:CE1	2:HJ:46:ASN:HD21	2.37	0.43
1:JI:31:LYS:O	1:JI:87:GLN:NE2	2.51	0.43
1:JO:77:TYR:CD1	1:JO:77:TYR:N	2.84	0.43
1:JQ:81:ARG:NH2	2:JR:281:PHE:O	2.51	0.43
2:JT:149:GLN:HG2	2:JT:178:ALA:HB3	2.00	0.43
1:JZ:77:TYR:N	1:JZ:77:TYR:CD1	2.84	0.43
1:LD:31:LYS:O	1:LD:87:GLN:NE2	2.51	0.43
2:YL:149:GLN:HG2	2:YL:178:ALA:HB3	2.00	0.43
1:YM:31:LYS:O	1:YM:87:GLN:NE2	2.51	0.43
2:BH:45:HIS:CE1	2:BJ:46:ASN:HD21	2.36	0.43
1:DE:21:VAL:HG11	1:DE:54:VAL:HG11	2.00	0.43
1:DQ:21:VAL:HG11	1:DQ:54:VAL:HG11	2.00	0.43
1:FP:81:ARG:NH2	2:FQ:281:PHE:O	2.51	0.43
1:HP:81:ARG:NH2	2:HQ:281:PHE:O	2.51	0.43
1:IK:77:TYR:N	1:IK:77:TYR:CD1	2.84	0.43
2:JH:45:HIS:CE1	2:JJ:46:ASN:HD21	2.37	0.43
2:JY:149:GLN:HG2	2:JY:178:ALA:HB3	2.00	0.43
2:LO:45:HIS:CE1	2:LQ:46:ASN:HD21	2.37	0.43
2:BZ:9:LEU:HD11	2:CB:71:VAL:HG21	1.99	0.43
2:BZ:149:GLN:HG2	2:BZ:178:ALA:HB3	2.00	0.43
2:DD:45:HIS:CE1	2:DF:46:ASN:HD21	2.37	0.43
1:DG:81:ARG:NH2	2:DH:281:PHE:O	2.51	0.43
1:EJ:21:VAL:HG11	1:EJ:54:VAL:HG11	2.01	0.43
2:FS:45:HIS:CE1	2:FU:46:ASN:HD21	2.37	0.43
2:ZH:45:HIS:CE1	2:ZJ:46:ASN:HD21	2.36	0.43
2:HY:45:HIS:CE1	2:IA:46:ASN:HD21	2.36	0.43
1:IM:81:ARG:NH2	2:IN:281:PHE:O	2.51	0.43
1:JV:81:ARG:NH2	2:JW:281:PHE:O	2.51	0.43
2:KK:45:HIS:CE1	2:KM:46:ASN:HD21	2.36	0.43
1:AK:21:VAL:HG11	1:AK:54:VAL:HG11	2.00	0.42
1:BQ:81:ARG:NH2	2:BR:281:PHE:O	2.51	0.42
2:BZ:45:HIS:CE1	2:CB:46:ASN:HD21	2.37	0.42
2:DD:149:GLN:HG2	2:DD:178:ALA:HB3	2.00	0.42
1:DE:77:TYR:N	1:DE:77:TYR:CD1	2.84	0.42
1:ED:21:VAL:HG11	1:ED:54:VAL:HG11	2.00	0.42
2:EU:45:HIS:CE1	2:EW:46:ASN:HD21	2.37	0.42
2:FG:149:GLN:HG2	2:FG:178:ALA:HB3	2.00	0.42
1:GT:81:ARG:NH2	2:GU:281:PHE:O	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GX:77:TYR:N	1:GX:77:TYR:CD1	2.84	0.42
2:HS:149:GLN:HG2	2:HS:178:ALA:HB3	2.00	0.42
1:HT:77:TYR:N	1:HT:77:TYR:CD1	2.84	0.42
1:HZ:21:VAL:HG11	1:HZ:54:VAL:HG11	2.00	0.42
2:IP:149:GLN:HG2	2:IP:178:ALA:HB3	2.00	0.42
2:JB:149:GLN:HG2	2:JB:178:ALA:HB3	2.00	0.42
1:JO:21:VAL:HG11	1:JO:54:VAL:HG11	2.00	0.42
1:LD:21:VAL:HG11	1:LD:54:VAL:HG11	2.00	0.42
2:ZT:45:HIS:CE1	2:ZV:46:ASN:HD21	2.37	0.42
2:AJ:45:HIS:CE1	2:AL:46:ASN:HD21	2.37	0.42
1:AK:31:LYS:O	1:AK:87:GLN:NE2	2.51	0.42
2:BN:149:GLN:HG2	2:BN:178:ALA:HB3	2.00	0.42
1:BU:31:LYS:O	1:BU:87:GLN:NE2	2.51	0.42
1:BW:81:ARG:NH2	2:BX:281:PHE:O	2.51	0.42
1:CA:21:VAL:HG11	1:CA:54:VAL:HG11	2.00	0.42
2:CF:45:HIS:CE1	2:CH:46:ASN:HD21	2.36	0.42
1:CM:21:VAL:HG11	1:CM:54:VAL:HG11	2.00	0.42
2:DW:149:GLN:HG2	2:DW:178:ALA:HB3	2.00	0.42
2:EE:160:ASP:OD1	2:EE:168:LYS:NZ	2.45	0.42
1:FJ:81:ARG:NH2	2:FK:281:PHE:O	2.51	0.42
1:FT:21:VAL:HG11	1:FT:54:VAL:HG11	2.00	0.42
2:FY:149:GLN:HG2	2:FY:178:ALA:HB3	2.00	0.42
2:IT:133:ILE:HG21	2:IT:181:ILE:HD13	2.02	0.42
1:KR:98:ASP:OD1	1:KR:98:ASP:N	2.52	0.42
1:LR:81:ARG:NH2	2:LS:281:PHE:O	2.51	0.42
2:ZR:133:ILE:HG21	2:ZR:181:ILE:HD13	2.02	0.42
2:YP:133:ILE:HG21	2:YP:181:ILE:HD13	2.02	0.42
2:YX:45:HIS:CE1	2:YZ:46:ASN:HD21	2.37	0.42
2:AT:133:ILE:HG21	2:AT:181:ILE:HD13	2.02	0.42
1:BO:21:VAL:HG11	1:BO:54:VAL:HG11	2.00	0.42
2:BT:149:GLN:HG2	2:BT:178:ALA:HB3	2.00	0.42
1:ZE:81:ARG:NH2	2:ZF:281:PHE:O	2.51	0.42
2:FA:45:HIS:CE1	2:FC:46:ASN:HD21	2.37	0.42
2:FA:149:GLN:HG2	2:FA:178:ALA:HB3	2.00	0.42
2:FM:45:HIS:CE1	2:FO:46:ASN:HD21	2.36	0.42
2:FQ:133:ILE:HG21	2:FQ:181:ILE:HD13	2.01	0.42
2:FY:45:HIS:CE1	2:GA:46:ASN:HD21	2.37	0.42
2:GI:133:ILE:HG21	2:GI:181:ILE:HD13	2.02	0.42
2:GK:149:GLN:HG2	2:GK:178:ALA:HB3	2.00	0.42
2:GO:133:ILE:HG21	2:GO:181:ILE:HD13	2.02	0.42
2:HW:133:ILE:HG21	2:HW:181:ILE:HD13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IQ:21:VAL:HG11	1:IQ:54:VAL:HG11	2.00	0.42
2:IV:45:HIS:CE1	2:IX:46:ASN:HD21	2.36	0.42
1:JC:77:TYR:N	1:JC:77:TYR:CD1	2.84	0.42
2:KW:149:GLN:HG2	2:KW:178:ALA:HB3	2.00	0.42
1:LD:98:ASP:OD1	1:LD:98:ASP:N	2.52	0.42
1:AP:21:VAL:HG11	1:AP:54:VAL:HG11	2.00	0.42
2:BB:45:HIS:CE1	2:BD:46:ASN:HD21	2.37	0.42
2:BD:160:ASP:OD1	2:BD:168:LYS:NZ	2.45	0.42
2:CX:45:HIS:CE1	2:CZ:46:ASN:HD21	2.36	0.42
1:CY:31:LYS:O	1:CY:87:GLN:NE2	2.51	0.42
2:DN:133:ILE:HG21	2:DN:181:ILE:HD13	2.02	0.42
2:DP:45:HIS:CE1	2:DR:46:ASN:HD21	2.36	0.42
1:DX:21:VAL:HG11	1:DX:54:VAL:HG11	2.00	0.42
2:ES:133:ILE:HG21	2:ES:181:ILE:HD13	2.02	0.42
2:EU:149:GLN:HG2	2:EU:178:ALA:HB3	2.00	0.42
2:EY:160:ASP:OD1	2:EY:168:LYS:NZ	2.35	0.42
2:GC:133:ILE:HG21	2:GC:181:ILE:HD13	2.02	0.42
2:GK:45:HIS:CE1	2:GM:46:ASN:HD21	2.37	0.42
2:IB:133:ILE:HG21	2:IB:181:ILE:HD13	2.02	0.42
1:JI:21:VAL:HG11	1:JI:54:VAL:HG11	2.00	0.42
2:JR:133:ILE:HG21	2:JR:181:ILE:HD13	2.02	0.42
2:JY:45:HIS:CE1	2:KA:46:ASN:HD21	2.37	0.42
2:LG:133:ILE:HG21	2:LG:181:ILE:HD13	2.02	0.42
2:BF:92:PRO:HB2	2:BF:144:LEU:HD13	2.02	0.42
2:BR:133:ILE:HG21	2:BR:181:ILE:HD13	2.02	0.42
1:BW:11:ALA:HB1	1:BW:43:VAL:O	2.20	0.42
1:CA:77:TYR:N	1:CA:77:TYR:CD1	2.84	0.42
2:CP:92:PRO:HB2	2:CP:144:LEU:HD13	2.02	0.42
2:DB:133:ILE:HG21	2:DB:181:ILE:HD13	2.02	0.42
2:DH:133:ILE:HG21	2:DH:181:ILE:HD13	2.02	0.42
1:FV:11:ALA:HB1	1:FV:43:VAL:O	2.20	0.42
1:GF:21:VAL:HG11	1:GF:54:VAL:HG11	2.00	0.42
2:HC:149:GLN:HG2	2:HC:178:ALA:HB3	2.00	0.42
1:HI:21:VAL:HG11	1:HI:54:VAL:HG11	2.00	0.42
2:IJ:149:GLN:HG2	2:IJ:178:ALA:HB3	2.00	0.42
2:ZL:133:ILE:HG21	2:ZL:181:ILE:HD13	2.02	0.42
2:KE:45:HIS:CE1	2:KG:46:ASN:HD21	2.36	0.42
1:KL:21:VAL:HG11	1:KL:54:VAL:HG11	2.00	0.42
2:KU:133:ILE:HG21	2:KU:181:ILE:HD13	2.02	0.42
1:ZQ:81:ARG:NH2	2:ZR:281:PHE:O	2.51	0.42
2:AB:133:ILE:HG21	2:AB:181:ILE:HD13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AO:46:ASN:HD21	2:AQ:45:HIS:CE1	2.37	0.42
2:AQ:149:GLN:HG2	2:AQ:178:ALA:HB3	2.00	0.42
2:BL:92:PRO:HB2	2:BL:144:LEU:HD13	2.02	0.42
2:BN:45:HIS:CE1	2:BP:46:ASN:HD21	2.37	0.42
1:ZE:11:ALA:HB1	1:ZE:43:VAL:O	2.20	0.42
1:DK:77:TYR:N	1:DK:77:TYR:CD1	2.84	0.42
2:FW:133:ILE:HG21	2:FW:181:ILE:HD13	2.01	0.42
2:GU:133:ILE:HG21	2:GU:181:ILE:HD13	2.02	0.42
2:GW:149:GLN:HG2	2:GW:178:ALA:HB3	2.00	0.42
2:HM:45:HIS:CE1	2:HO:46:ASN:HD21	2.37	0.42
1:HN:77:TYR:N	1:HN:77:TYR:CD1	2.84	0.42
2:HO:160:ASP:OD1	2:HO:168:LYS:NZ	2.45	0.42
1:IH:11:ALA:HB1	1:IH:43:VAL:O	2.20	0.42
1:IS:11:ALA:HB1	1:IS:43:VAL:O	2.20	0.42
2:IT:160:ASP:OD1	2:IT:168:LYS:NZ	2.36	0.42
1:IW:21:VAL:HG11	1:IW:54:VAL:HG11	2.00	0.42
1:ZK:11:ALA:HB1	1:ZK:43:VAL:O	2.20	0.42
2:JL:133:ILE:HG21	2:JL:181:ILE:HD13	2.02	0.42
2:JN:45:HIS:CE1	2:JP:46:ASN:HD21	2.37	0.42
2:KC:92:PRO:HB2	2:KC:144:LEU:HD13	2.02	0.42
1:KF:77:TYR:N	1:KF:77:TYR:CD1	2.84	0.42
2:KQ:45:HIS:CE1	2:KS:46:ASN:HD21	2.36	0.42
2:LO:149:GLN:HG2	2:LO:178:ALA:HB3	2.00	0.42
1:YC:11:ALA:HB1	1:YC:43:VAL:O	2.20	0.42
2:YD:133:ILE:HG21	2:YD:181:ILE:HD13	2.02	0.42
2:AD:45:HIS:CE1	2:AF:46:ASN:HD21	2.37	0.42
1:AG:81:ARG:NH2	2:AH:281:PHE:O	2.51	0.42
2:AH:133:ILE:HG21	2:AH:181:ILE:HD13	2.02	0.42
2:AJ:149:GLN:HG2	2:AJ:178:ALA:HB3	2.00	0.42
2:AN:133:ILE:HG21	2:AN:181:ILE:HD13	2.02	0.42
2:AT:92:PRO:HB2	2:AT:144:LEU:HD13	2.02	0.42
1:BQ:11:ALA:HB1	1:BQ:43:VAL:O	2.20	0.42
2:CD:92:PRO:HB2	2:CD:144:LEU:HD13	2.02	0.42
2:CD:133:ILE:HG21	2:CD:181:ILE:HD13	2.02	0.42
1:CI:81:ARG:NH2	2:CJ:281:PHE:O	2.51	0.42
2:CL:45:HIS:CE1	2:CN:46:ASN:HD21	2.36	0.42
1:DM:11:ALA:HB1	1:DM:43:VAL:O	2.20	0.42
1:EX:11:ALA:HB1	1:EX:43:VAL:O	2.20	0.42
2:EY:133:ILE:HG21	2:EY:181:ILE:HD13	2.02	0.42
2:FK:133:ILE:HG21	2:FK:181:ILE:HD13	2.02	0.42
1:GH:11:ALA:HB1	1:GH:43:VAL:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GT:11:ALA:HB1	1:GT:43:VAL:O	2.20	0.42
2:HK:133:ILE:HG21	2:HK:181:ILE:HD13	2.02	0.42
1:HL:33:ALA:N	1:HL:34:PRO:CD	2.83	0.42
2:HW:92:PRO:HB2	2:HW:144:LEU:HD13	2.02	0.42
2:ID:45:HIS:CE1	2:IF:46:ASN:HD21	2.37	0.42
2:IN:133:ILE:HG21	2:IN:181:ILE:HD13	2.02	0.42
2:JT:45:HIS:CE1	2:JU:46:ASN:HD21	2.37	0.42
2:JW:133:ILE:HG21	2:JW:181:ILE:HD13	2.02	0.42
2:KO:133:ILE:HG21	2:KO:181:ILE:HD13	2.02	0.42
2:LS:133:ILE:HG21	2:LS:181:ILE:HD13	2.02	0.42
2:ZN:149:GLN:HG2	2:ZN:178:ALA:HB3	2.00	0.42
1:YA:21:VAL:HG11	1:YA:54:VAL:HG11	2.01	0.42
2:YD:218:ASP:OD1	2:YD:219:SER:N	2.53	0.42
1:AA:11:ALA:HB1	1:AA:43:VAL:O	2.20	0.42
1:AI:33:ALA:N	1:AI:34:PRO:CD	2.83	0.42
1:BS:33:ALA:N	1:BS:34:PRO:CD	2.83	0.42
1:DA:11:ALA:HB1	1:DA:43:VAL:O	2.20	0.42
1:EV:77:TYR:N	1:EV:77:TYR:CD1	2.84	0.42
2:FE:92:PRO:HB2	2:FE:144:LEU:HD13	2.02	0.42
2:GI:92:PRO:HB2	2:GI:144:LEU:HD13	2.02	0.42
1:GP:33:ALA:N	1:GP:34:PRO:CD	2.83	0.42
2:HA:133:ILE:HG21	2:HA:181:ILE:HD13	2.02	0.42
1:WA:11:ALA:HB1	1:WA:43:VAL:O	2.20	0.42
1:WC:11:ALA:HB1	1:WC:43:VAL:O	2.20	0.42
2:IG:133:ILE:HG21	2:IG:181:ILE:HD13	2.01	0.42
1:IQ:77:TYR:N	1:IQ:77:TYR:CD1	2.84	0.42
1:JX:33:ALA:N	1:JX:34:PRO:CD	2.83	0.42
2:KC:218:ASP:OD1	2:KC:219:SER:N	2.53	0.42
2:KI:133:ILE:HG21	2:KI:181:ILE:HD13	2.02	0.42
2:LG:92:PRO:HB2	2:LG:144:LEU:HD13	2.02	0.42
1:LH:33:ALA:N	1:LH:34:PRO:CD	2.83	0.42
1:ZW:11:ALA:HB1	1:ZW:43:VAL:O	2.20	0.42
2:YP:92:PRO:HB2	2:YP:144:LEU:HD13	2.02	0.42
2:AB:92:PRO:HB2	2:AB:144:LEU:HD13	2.02	0.42
1:AR:69:HIS:O	1:AR:70:ILE:C	2.63	0.42
1:AY:11:ALA:HB1	1:AY:43:VAL:O	2.20	0.42
1:BK:81:ARG:NH2	2:BL:281:PHE:O	2.51	0.42
1:CE:33:ALA:N	1:CE:34:PRO:CD	2.83	0.42
2:CV:133:ILE:HG21	2:CV:181:ILE:HD13	2.02	0.42
1:DG:11:ALA:HB1	1:DG:43:VAL:O	2.20	0.42
1:EH:33:ALA:N	1:EH:34:PRO:CD	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EV:98:ASP:OD1	1:EV:98:ASP:N	2.52	0.42
2:EY:218:ASP:OD1	2:EY:219:SER:N	2.53	0.42
1:EZ:33:ALA:N	1:EZ:34:PRO:CD	2.83	0.42
1:FP:11:ALA:HB1	1:FP:43:VAL:O	2.20	0.42
1:HD:77:TYR:N	1:HD:77:TYR:CD1	2.84	0.42
1:HN:21:VAL:HG11	1:HN:54:VAL:HG11	2.00	0.42
2:HY:149:GLN:HG2	2:HY:178:ALA:HB3	2.00	0.42
2:IG:218:ASP:OD1	2:IG:219:SER:N	2.53	0.42
2:IT:218:ASP:OD1	2:IT:219:SER:N	2.53	0.42
2:JF:218:ASP:OD1	2:JF:219:SER:N	2.53	0.42
2:JL:218:ASP:OD1	2:JL:219:SER:N	2.53	0.42
1:JS:33:ALA:N	1:JS:34:PRO:CD	2.83	0.42
1:JV:11:ALA:HB1	1:JV:43:VAL:O	2.20	0.42
1:KN:11:ALA:HB1	1:KN:43:VAL:O	2.20	0.42
2:KW:45:HIS:CE1	2:KY:46:ASN:HD21	2.37	0.42
1:KZ:11:ALA:HB1	1:KZ:43:VAL:O	2.20	0.42
2:ZR:92:PRO:HB2	2:ZR:144:LEU:HD13	2.02	0.42
2:YJ:218:ASP:OD1	2:YJ:219:SER:N	2.53	0.42
2:YP:218:ASP:OD1	2:YP:219:SER:N	2.53	0.42
1:YW:33:ALA:N	1:YW:34:PRO:CD	2.83	0.42
1:YW:69:HIS:O	1:YW:70:ILE:C	2.63	0.42
2:AL:6:LYS:NZ	2:AL:10:GLU:OE2	2.45	0.42
2:AN:218:ASP:OD1	2:AN:219:SER:N	2.53	0.42
1:BI:98:ASP:OD1	1:BI:98:ASP:N	2.52	0.42
2:CD:218:ASP:OD1	2:CD:219:SER:N	2.53	0.42
1:CK:33:ALA:N	1:CK:34:PRO:CD	2.83	0.42
1:DC:33:ALA:N	1:DC:34:PRO:CD	2.83	0.42
2:DH:92:PRO:HB2	2:DH:144:LEU:HD13	2.02	0.42
2:EC:149:GLN:HG2	2:EC:178:ALA:HB3	2.00	0.42
2:FE:218:ASP:OD1	2:FE:219:SER:N	2.53	0.42
2:FK:92:PRO:HB2	2:FK:144:LEU:HD13	2.02	0.42
2:FQ:92:PRO:HB2	2:FQ:144:LEU:HD13	2.02	0.42
1:GD:33:ALA:N	1:GD:34:PRO:CD	2.83	0.42
1:GP:69:HIS:O	1:GP:70:ILE:C	2.63	0.42
1:HR:33:ALA:N	1:HR:34:PRO:CD	2.83	0.42
1:HX:33:ALA:N	1:HX:34:PRO:CD	2.83	0.42
2:IB:218:ASP:OD1	2:IB:219:SER:N	2.53	0.42
1:JK:11:ALA:HB1	1:JK:43:VAL:O	2.20	0.42
1:JX:69:HIS:O	1:JX:70:ILE:C	2.63	0.42
2:KC:133:ILE:HG21	2:KC:181:ILE:HD13	2.02	0.42
1:KT:11:ALA:HB1	1:KT:43:VAL:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ZR:218:ASP:OD1	2:ZR:219:SER:N	2.53	0.42
2:ZX:160:ASP:OD1	2:ZX:168:LYS:NZ	2.36	0.42
2:YJ:92:PRO:HB2	2:YJ:144:LEU:HD13	2.02	0.41
2:AJ:96:LEU:O	2:AJ:97:GLU:C	2.63	0.41
1:AM:11:ALA:HB1	1:AM:43:VAL:O	2.20	0.41
1:BG:33:ALA:N	1:BG:34:PRO:CD	2.83	0.41
1:BK:11:ALA:HB1	1:BK:43:VAL:O	2.20	0.41
2:BR:92:PRO:HB2	2:BR:144:LEU:HD13	2.02	0.41
2:BX:133:ILE:HG21	2:BX:181:ILE:HD13	2.02	0.41
1:BY:69:HIS:O	1:BY:70:ILE:C	2.63	0.41
2:CN:160:ASP:OD1	2:CN:168:LYS:NZ	2.45	0.41
2:CP:218:ASP:OD1	2:CP:219:SER:N	2.53	0.41
2:CV:218:ASP:OD1	2:CV:219:SER:N	2.53	0.41
2:EG:133:ILE:HG21	2:EG:181:ILE:HD13	2.02	0.41
1:EP:21:VAL:HG11	1:EP:54:VAL:HG11	2.00	0.41
1:ZG:33:ALA:N	1:ZG:34:PRO:CD	2.83	0.41
1:ZG:69:HIS:O	1:ZG:70:ILE:C	2.63	0.41
1:FN:77:TYR:N	1:FN:77:TYR:CD1	2.84	0.41
1:FX:69:HIS:O	1:FX:70:ILE:C	2.63	0.41
1:HB:33:ALA:N	1:HB:34:PRO:CD	2.83	0.41
1:HP:11:ALA:HB1	1:HP:43:VAL:O	2.20	0.41
1:IE:21:VAL:HG11	1:IE:54:VAL:HG11	2.00	0.41
1:JG:33:ALA:N	1:JG:34:PRO:CD	2.83	0.41
2:KE:149:GLN:HG2	2:KE:178:ALA:HB3	2.00	0.41
2:KO:218:ASP:OD1	2:KO:219:SER:N	2.53	0.41
1:KX:21:VAL:HG11	1:KX:54:VAL:HG11	2.00	0.41
2:LA:133:ILE:HG21	2:LA:181:ILE:HD13	2.02	0.41
1:YK:33:ALA:N	1:YK:34:PRO:CD	2.83	0.41
1:YK:69:HIS:O	1:YK:70:ILE:C	2.63	0.41
1:YU:11:ALA:HB1	1:YU:43:VAL:O	2.20	0.41
1:AC:33:ALA:N	1:AC:34:PRO:CD	2.83	0.41
1:AG:11:ALA:HB1	1:AG:43:VAL:O	2.20	0.41
1:AU:33:ALA:N	1:AU:34:PRO:CD	2.83	0.41
2:BL:133:ILE:HG21	2:BL:181:ILE:HD13	2.02	0.41
2:BR:218:ASP:OD1	2:BR:219:SER:N	2.53	0.41
1:BS:69:HIS:O	1:BS:70:ILE:C	2.63	0.41
1:CK:69:HIS:O	1:CK:70:ILE:C	2.63	0.41
2:CR:149:GLN:HG2	2:CR:178:ALA:HB3	2.00	0.41
1:CS:77:TYR:N	1:CS:77:TYR:CD1	2.84	0.41
2:DN:218:ASP:OD1	2:DN:219:SER:N	2.53	0.41
2:ZF:92:PRO:HB2	2:ZF:144:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:33:ALA:N	1:EB:34:PRO:CD	2.83	0.41
2:EC:45:HIS:CE1	2:EE:46:ASN:HD21	2.36	0.41
1:FJ:11:ALA:HB1	1:FJ:43:VAL:O	2.20	0.41
1:GD:69:HIS:O	1:GD:70:ILE:C	2.63	0.41
1:GL:21:VAL:HG11	1:GL:54:VAL:HG11	2.00	0.41
1:GN:81:ARG:NH2	2:GO:281:PHE:O	2.51	0.41
2:GU:92:PRO:HB2	2:GU:144:LEU:HD13	2.02	0.41
1:GZ:11:ALA:HB1	1:GZ:43:VAL:O	2.20	0.41
1:WB:11:ALA:HB1	1:WB:43:VAL:O	2.20	0.41
1:HG:33:ALA:N	1:HG:34:PRO:CD	2.83	0.41
2:HK:92:PRO:HB2	2:HK:144:LEU:HD13	2.02	0.41
2:HU:160:ASP:OD1	2:HU:168:LYS:NZ	2.45	0.41
1:IO:33:ALA:N	1:IO:34:PRO:CD	2.83	0.41
2:IZ:218:ASP:OD1	2:IZ:219:SER:N	2.53	0.41
2:KA:160:ASP:OD1	2:KA:168:LYS:NZ	2.45	0.41
2:KU:92:PRO:HB2	2:KU:144:LEU:HD13	2.02	0.41
1:ZM:33:ALA:N	1:ZM:34:PRO:CD	2.83	0.41
1:LL:11:ALA:HB1	1:LL:43:VAL:O	2.20	0.41
1:ZQ:11:ALA:HB1	1:ZQ:43:VAL:O	2.20	0.41
1:YG:21:VAL:HG11	1:YG:54:VAL:HG11	2.00	0.41
1:YU:81:ARG:NH2	2:YV:281:PHE:O	2.51	0.41
1:AS:11:ALA:HB1	1:AS:43:VAL:O	2.20	0.41
1:BA:33:ALA:N	1:BA:34:PRO:CD	2.83	0.41
2:BV:6:LYS:NZ	2:BV:10:GLU:OE2	2.45	0.41
2:EA:133:ILE:HG21	2:EA:181:ILE:HD13	2.02	0.41
2:EA:218:ASP:OD1	2:EA:219:SER:N	2.53	0.41
1:ER:11:ALA:HB1	1:ER:43:VAL:O	2.20	0.41
1:ER:81:ARG:NH2	2:ES:281:PHE:O	2.51	0.41
2:FM:96:LEU:O	2:FM:97:GLU:C	2.63	0.41
1:FR:33:ALA:N	1:FR:34:PRO:CD	2.83	0.41
1:FX:33:ALA:N	1:FX:34:PRO:CD	2.83	0.41
1:GB:11:ALA:HB1	1:GB:43:VAL:O	2.20	0.41
1:GN:11:ALA:HB1	1:GN:43:VAL:O	2.20	0.41
2:HF:92:PRO:HB2	2:HF:144:LEU:HD13	2.02	0.41
1:HG:69:HIS:O	1:HG:70:ILE:C	2.63	0.41
1:HV:11:ALA:HB1	1:HV:43:VAL:O	2.20	0.41
1:IM:11:ALA:HB1	1:IM:43:VAL:O	2.20	0.41
1:IU:33:ALA:N	1:IU:34:PRO:CD	2.83	0.41
1:JQ:11:ALA:HB1	1:JQ:43:VAL:O	2.20	0.41
2:JW:218:ASP:OD1	2:JW:219:SER:N	2.53	0.41
2:KO:92:PRO:HB2	2:KO:144:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LM:218:ASP:OD1	2:LM:219:SER:N	2.53	0.41
1:LR:11:ALA:HB1	1:LR:43:VAL:O	2.20	0.41
2:ZX:92:PRO:HB2	2:ZX:144:LEU:HD13	2.02	0.41
1:AK:98:ASP:OD1	1:AK:98:ASP:N	2.52	0.41
1:CW:69:HIS:O	1:CW:70:ILE:C	2.63	0.41
2:EA:92:PRO:HB2	2:EA:144:LEU:HD13	2.02	0.41
2:EG:218:ASP:OD1	2:EG:219:SER:N	2.53	0.41
1:EN:33:ALA:N	1:EN:34:PRO:CD	2.83	0.41
2:EO:45:HIS:CE1	2:EQ:46:ASN:HD21	2.36	0.41
1:ET:33:ALA:N	1:ET:34:PRO:CD	2.83	0.41
1:FL:69:HIS:O	1:FL:70:ILE:C	2.63	0.41
2:FY:96:LEU:O	2:FY:97:GLU:C	2.63	0.41
1:GJ:33:ALA:N	1:GJ:34:PRO:CD	2.83	0.41
1:GV:33:ALA:N	1:GV:34:PRO:CD	2.83	0.41
2:IJ:96:LEU:O	2:IJ:97:GLU:C	2.63	0.41
1:IY:11:ALA:HB1	1:IY:43:VAL:O	2.20	0.41
1:KB:11:ALA:HB1	1:KB:43:VAL:O	2.20	0.41
1:KB:81:ARG:NH2	2:KC:281:PHE:O	2.51	0.41
2:KI:92:PRO:HB2	2:KI:144:LEU:HD13	2.02	0.41
2:YD:92:PRO:HB2	2:YD:144:LEU:HD13	2.02	0.41
2:YD:160:ASP:OD1	2:YD:168:LYS:NZ	2.36	0.41
1:YE:69:HIS:O	1:YE:70:ILE:C	2.63	0.41
2:AN:92:PRO:HB2	2:AN:144:LEU:HD13	2.02	0.41
2:BF:133:ILE:HG21	2:BF:181:ILE:HD13	2.02	0.41
1:BM:33:ALA:N	1:BM:34:PRO:CD	2.83	0.41
2:BX:218:ASP:OD1	2:BX:219:SER:N	2.53	0.41
1:CC:81:ARG:NH2	2:CD:281:PHE:O	2.51	0.41
1:CI:11:ALA:HB1	1:CI:43:VAL:O	2.20	0.41
2:CJ:133:ILE:HG21	2:CJ:181:ILE:HD13	2.02	0.41
2:CN:231:VAL:HG11	2:CN:238:MET:HB2	2.03	0.41
1:DS:11:ALA:HB1	1:DS:43:VAL:O	2.20	0.41
1:DU:69:HIS:O	1:DU:70:ILE:C	2.63	0.41
2:ZF:170:LYS:HG2	2:ZF:224:TRP:CH2	2.56	0.41
2:ZF:218:ASP:OD1	2:ZF:219:SER:N	2.53	0.41
2:EM:133:ILE:HG21	2:EM:181:ILE:HD13	2.02	0.41
2:GU:170:LYS:HG2	2:GU:224:TRP:CH2	2.56	0.41
2:HA:92:PRO:HB2	2:HA:144:LEU:HD13	2.02	0.41
2:HK:170:LYS:HG2	2:HK:224:TRP:CH2	2.56	0.41
2:HQ:133:ILE:HG21	2:HQ:181:ILE:HD13	2.02	0.41
1:IC:33:ALA:N	1:IC:34:PRO:CD	2.83	0.41
2:IN:92:PRO:HB2	2:IN:144:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IZ:92:PRO:HB2	2:IZ:144:LEU:HD13	2.02	0.41
2:KI:218:ASP:OD1	2:KI:219:SER:N	2.53	0.41
1:KP:33:ALA:N	1:KP:34:PRO:CD	2.83	0.41
1:LF:11:ALA:HB1	1:LF:43:VAL:O	2.20	0.41
2:LM:92:PRO:HB2	2:LM:144:LEU:HD13	2.02	0.41
1:LN:69:HIS:O	1:LN:70:ILE:C	2.63	0.41
1:ZS:33:ALA:N	1:ZS:34:PRO:CD	2.83	0.41
1:YQ:33:ALA:N	1:YQ:34:PRO:CD	2.83	0.41
2:YR:96:LEU:O	2:YR:97:GLU:C	2.63	0.41
2:YV:218:ASP:OD1	2:YV:219:SER:N	2.53	0.41
2:AB:218:ASP:OD1	2:AB:219:SER:N	2.53	0.41
2:AF:231:VAL:HG11	2:AF:238:MET:HB2	2.03	0.41
2:AZ:218:ASP:OD1	2:AZ:219:SER:N	2.53	0.41
2:BD:231:VAL:HG11	2:BD:238:MET:HB2	2.03	0.41
2:BV:231:VAL:HG11	2:BV:238:MET:HB2	2.03	0.41
1:CC:11:ALA:HB1	1:CC:43:VAL:O	2.20	0.41
2:CD:170:LYS:HG2	2:CD:224:TRP:CH2	2.56	0.41
1:CU:11:ALA:HB1	1:CU:43:VAL:O	2.20	0.41
2:CV:170:LYS:HG2	2:CV:224:TRP:CH2	2.56	0.41
1:DC:69:HIS:O	1:DC:70:ILE:C	2.63	0.41
1:DI:69:HIS:O	1:DI:70:ILE:C	2.63	0.41
2:DN:170:LYS:HG2	2:DN:224:TRP:CH2	2.56	0.41
2:EG:170:LYS:HG2	2:EG:224:TRP:CH2	2.56	0.41
2:ES:92:PRO:HB2	2:ES:144:LEU:HD13	2.02	0.41
1:EZ:69:HIS:O	1:EZ:70:ILE:C	2.63	0.41
2:FO:231:VAL:HG11	2:FO:238:MET:HB2	2.03	0.41
1:ZI:85:LYS:NZ	2:ZJ:256:GLU:OE1	2.50	0.41
2:HW:218:ASP:OD1	2:HW:219:SER:N	2.53	0.41
2:IL:231:VAL:HG11	2:IL:238:MET:HB2	2.03	0.41
2:IN:218:ASP:OD1	2:IN:219:SER:N	2.53	0.41
2:IZ:133:ILE:HG21	2:IZ:181:ILE:HD13	2.02	0.41
1:JA:33:ALA:N	1:JA:34:PRO:CD	2.83	0.41
2:JF:92:PRO:HB2	2:JF:144:LEU:HD13	2.02	0.41
2:JF:133:ILE:HG21	2:JF:181:ILE:HD13	2.02	0.41
2:JH:149:GLN:HG2	2:JH:178:ALA:HB3	2.00	0.41
2:JR:92:PRO:HB2	2:JR:144:LEU:HD13	2.02	0.41
2:LS:92:PRO:HB2	2:LS:144:LEU:HD13	2.02	0.41
2:ZX:218:ASP:OD1	2:ZX:219:SER:N	2.53	0.41
1:ZY:33:ALA:N	1:ZY:34:PRO:CD	2.83	0.41
1:YE:33:ALA:N	1:YE:34:PRO:CD	2.83	0.41
1:YI:11:ALA:HB1	1:YI:43:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YO:11:ALA:HB1	1:YO:43:VAL:O	2.20	0.41
1:AA:81:ARG:NH2	2:AB:281:PHE:O	2.51	0.41
2:AH:92:PRO:HB2	2:AH:144:LEU:HD13	2.02	0.41
2:AL:231:VAL:HG11	2:AL:238:MET:HB2	2.03	0.41
1:AM:81:ARG:NH2	2:AN:281:PHE:O	2.51	0.41
2:BF:170:LYS:HG2	2:BF:224:TRP:CH2	2.56	0.41
2:BL:170:LYS:HG2	2:BL:224:TRP:CH2	2.56	0.41
1:CY:21:VAL:HG11	1:CY:54:VAL:HG11	2.01	0.41
2:DW:96:LEU:O	2:DW:97:GLU:C	2.63	0.41
2:EG:92:PRO:HB2	2:EG:144:LEU:HD13	2.02	0.41
1:EJ:77:TYR:CD1	1:EJ:77:TYR:N	2.84	0.41
2:ES:170:LYS:HG2	2:ES:224:TRP:CH2	2.56	0.41
2:EW:231:VAL:HG11	2:EW:238:MET:HB2	2.03	0.41
2:FE:133:ILE:HG21	2:FE:181:ILE:HD13	2.02	0.41
2:GY:231:VAL:HG11	2:GY:238:MET:HB2	2.03	0.41
2:HM:96:LEU:O	2:HM:97:GLU:C	2.63	0.41
2:IA:160:ASP:OD1	2:IA:168:LYS:NZ	2.45	0.41
1:II:33:ALA:N	1:II:34:PRO:CD	2.83	0.41
2:IT:170:LYS:HG2	2:IT:224:TRP:CH2	2.56	0.41
2:IX:160:ASP:OD1	2:IX:168:LYS:NZ	2.45	0.41
1:JA:69:HIS:O	1:JA:70:ILE:C	2.63	0.41
2:JD:231:VAL:HG11	2:JD:238:MET:HB2	2.03	0.41
2:KK:96:LEU:O	2:KK:97:GLU:C	2.63	0.41
2:KM:231:VAL:HG11	2:KM:238:MET:HB2	2.03	0.41
2:LG:218:ASP:OD1	2:LG:219:SER:N	2.53	0.41
2:LS:160:ASP:OD1	2:LS:168:LYS:NZ	2.36	0.41
2:ZX:133:ILE:HG21	2:ZX:181:ILE:HD13	2.02	0.41
2:ZZ:96:LEU:O	2:ZZ:97:GLU:C	2.63	0.41
2:YH:231:VAL:HG11	2:YH:238:MET:HB2	2.03	0.41
1:YI:81:ARG:NH2	2:YJ:281:PHE:O	2.51	0.41
2:YJ:133:ILE:HG21	2:YJ:181:ILE:HD13	2.02	0.41
2:YV:92:PRO:HB2	2:YV:144:LEU:HD13	2.02	0.41
2:AH:218:ASP:OD1	2:AH:219:SER:N	2.53	0.41
2:AZ:92:PRO:HB2	2:AZ:144:LEU:HD13	2.02	0.41
1:BC:98:ASP:OD1	1:BC:98:ASP:N	2.52	0.41
1:BG:69:HIS:O	1:BG:70:ILE:C	2.63	0.41
1:BY:33:ALA:N	1:BY:34:PRO:CD	2.83	0.41
2:DB:92:PRO:HB2	2:DB:144:LEU:HD13	2.02	0.41
2:DH:218:ASP:OD1	2:DH:219:SER:N	2.53	0.41
1:DI:33:ALA:N	1:DI:34:PRO:CD	2.83	0.41
2:DT:133:ILE:HG21	2:DT:181:ILE:HD13	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ZF:133:ILE:HG21	2:ZF:181:ILE:HD13	2.02	0.41
1:EL:11:ALA:HB1	1:EL:43:VAL:O	2.20	0.41
1:FL:33:ALA:N	1:FL:34:PRO:CD	2.83	0.41
2:FW:92:PRO:HB2	2:FW:144:LEU:HD13	2.02	0.41
2:FW:170:LYS:HG2	2:FW:224:TRP:CH2	2.56	0.41
1:GL:98:ASP:OD1	1:GL:98:ASP:N	2.52	0.41
2:HF:133:ILE:HG21	2:HF:181:ILE:HD13	2.02	0.41
2:HQ:218:ASP:OD1	2:HQ:219:SER:N	2.53	0.41
1:HR:69:HIS:O	1:HR:70:ILE:C	2.63	0.41
2:IB:281:PHE:O	1:WC:81:ARG:NH2	2.51	0.41
1:IH:98:ASP:OD1	1:IH:98:ASP:N	2.50	0.41
2:IT:92:PRO:HB2	2:IT:144:LEU:HD13	2.02	0.41
1:IU:69:HIS:O	1:IU:70:ILE:C	2.63	0.41
2:ZL:92:PRO:HB2	2:ZL:144:LEU:HD13	2.02	0.41
2:KI:170:LYS:HG2	2:KI:224:TRP:CH2	2.56	0.41
2:LA:92:PRO:HB2	2:LA:144:LEU:HD13	2.02	0.41
1:LB:69:HIS:O	1:LB:70:ILE:C	2.63	0.41
1:ZA:69:HIS:O	1:ZA:70:ILE:C	2.63	0.41
1:YG:77:TYR:N	1:YG:77:TYR:CD1	2.84	0.41
2:YV:133:ILE:HG21	2:YV:181:ILE:HD13	2.02	0.41
2:YV:170:LYS:HG2	2:YV:224:TRP:CH2	2.56	0.41
2:AF:70:ILE:HG23	2:AF:74:PHE:CE1	2.56	0.41
2:AN:170:LYS:HG2	2:AN:224:TRP:CH2	2.56	0.41
1:AR:33:ALA:N	1:AR:34:PRO:CD	2.83	0.41
2:AT:170:LYS:HG2	2:AT:224:TRP:CH2	2.56	0.41
2:AT:218:ASP:OD1	2:AT:219:SER:N	2.53	0.41
2:AX:6:LYS:NZ	2:AX:10:GLU:OE2	2.45	0.41
2:AX:231:VAL:HG11	2:AX:238:MET:HB2	2.03	0.41
1:BE:11:ALA:HB1	1:BE:43:VAL:O	2.20	0.41
2:BJ:160:ASP:OD1	2:BJ:168:LYS:NZ	2.45	0.41
2:BP:160:ASP:OD1	2:BP:168:LYS:NZ	2.45	0.41
2:BP:231:VAL:HG11	2:BP:238:MET:HB2	2.03	0.41
2:BX:170:LYS:HG2	2:BX:224:TRP:CH2	2.56	0.41
1:CE:69:HIS:O	1:CE:70:ILE:C	2.63	0.41
2:CJ:92:PRO:HB2	2:CJ:144:LEU:HD13	2.02	0.41
2:CJ:218:ASP:OD1	2:CJ:219:SER:N	2.53	0.41
1:CO:11:ALA:HB1	1:CO:43:VAL:O	2.20	0.41
1:CW:33:ALA:N	1:CW:34:PRO:CD	2.83	0.41
2:CZ:70:ILE:HG23	2:CZ:74:PHE:CE1	2.56	0.41
2:DB:218:ASP:OD1	2:DB:219:SER:N	2.53	0.41
2:DF:231:VAL:HG11	2:DF:238:MET:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DL:70:ILE:HG23	2:DL:74:PHE:CE1	2.56	0.41
1:DO:33:ALA:N	1:DO:34:PRO:CD	2.83	0.41
2:DT:170:LYS:HG2	2:DT:224:TRP:CH2	2.56	0.41
1:DU:33:ALA:N	1:DU:34:PRO:CD	2.83	0.41
2:DY:231:VAL:HG11	2:DY:238:MET:HB2	2.03	0.41
1:DZ:11:ALA:HB1	1:DZ:43:VAL:O	2.20	0.41
1:EH:69:HIS:O	1:EH:70:ILE:C	2.63	0.41
2:EM:92:PRO:HB2	2:EM:144:LEU:HD13	2.02	0.41
2:EM:170:LYS:HG2	2:EM:224:TRP:CH2	2.56	0.41
1:EN:69:HIS:O	1:EN:70:ILE:C	2.63	0.41
1:FD:11:ALA:HB1	1:FD:43:VAL:O	2.20	0.41
2:FE:170:LYS:HG2	2:FE:224:TRP:CH2	2.56	0.41
1:FF:33:ALA:N	1:FF:34:PRO:CD	2.83	0.41
2:FS:96:LEU:O	2:FS:97:GLU:C	2.63	0.41
1:FT:98:ASP:OD1	1:FT:98:ASP:N	2.52	0.41
1:GB:81:ARG:NH2	2:GC:281:PHE:O	2.51	0.41
2:GE:96:LEU:O	2:GE:97:GLU:C	2.63	0.41
2:GG:231:VAL:HG11	2:GG:238:MET:HB2	2.03	0.41
2:GI:170:LYS:HG2	2:GI:224:TRP:CH2	2.56	0.41
2:GM:70:ILE:HG23	2:GM:74:PHE:CE1	2.56	0.41
2:GS:160:ASP:OD1	2:GS:168:LYS:NZ	2.45	0.41
2:GS:231:VAL:HG11	2:GS:238:MET:HB2	2.03	0.41
2:HA:170:LYS:HG2	2:HA:224:TRP:CH2	2.56	0.41
2:IB:92:PRO:HB2	2:IB:144:LEU:HD13	2.02	0.41
2:JF:170:LYS:HG2	2:JF:224:TRP:CH2	2.56	0.41
1:JG:69:HIS:O	1:JG:70:ILE:C	2.63	0.41
2:JL:92:PRO:HB2	2:JL:144:LEU:HD13	2.02	0.41
2:JP:70:ILE:HG23	2:JP:74:PHE:CE1	2.56	0.41
2:JP:231:VAL:HG11	2:JP:238:MET:HB2	2.03	0.41
2:JR:218:ASP:OD1	2:JR:219:SER:N	2.53	0.41
2:JU:231:VAL:HG11	2:JU:238:MET:HB2	2.03	0.41
1:KD:33:ALA:N	1:KD:34:PRO:CD	2.83	0.41
1:KH:11:ALA:HB1	1:KH:43:VAL:O	2.20	0.41
1:KL:98:ASP:OD1	1:KL:98:ASP:N	2.52	0.41
1:KV:33:ALA:N	1:KV:34:PRO:CD	2.83	0.41
1:ZM:69:HIS:O	1:ZM:70:ILE:C	2.63	0.41
1:LH:69:HIS:O	1:LH:70:ILE:C	2.63	0.41
2:LM:133:ILE:HG21	2:LM:181:ILE:HD13	2.02	0.41
2:ZP:231:VAL:HG11	2:ZP:238:MET:HB2	2.03	0.41
2:YD:170:LYS:HG2	2:YD:224:TRP:CH2	2.56	0.41
2:YN:70:ILE:HG23	2:YN:74:PHE:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YQ:69:HIS:O	1:YQ:70:ILE:C	2.63	0.41
2:AB:170:LYS:HG2	2:AB:224:TRP:CH2	2.56	0.41
2:YZ:231:VAL:HG11	2:YZ:238:MET:HB2	2.03	0.41
2:AH:170:LYS:HG2	2:AH:224:TRP:CH2	2.56	0.41
2:AZ:170:LYS:HG2	2:AZ:224:TRP:CH2	2.56	0.41
2:BJ:231:VAL:HG11	2:BJ:238:MET:HB2	2.03	0.41
2:CF:96:LEU:O	2:CF:97:GLU:C	2.63	0.41
1:CQ:33:ALA:N	1:CQ:34:PRO:CD	2.83	0.41
2:CV:92:PRO:HB2	2:CV:144:LEU:HD13	2.02	0.41
2:EA:170:LYS:HG2	2:EA:224:TRP:CH2	2.56	0.41
2:FA:96:LEU:O	2:FA:97:GLU:C	2.63	0.41
1:GB:98:ASP:OD1	1:GB:98:ASP:N	2.50	0.41
1:GJ:69:HIS:O	1:GJ:70:ILE:C	2.63	0.41
2:HA:218:ASP:OD1	2:HA:219:SER:N	2.53	0.41
2:HF:281:PHE:O	1:WB:81:ARG:NH2	2.51	0.41
2:HH:96:LEU:O	2:HH:97:GLU:C	2.63	0.41
2:IF:231:VAL:HG11	2:IF:238:MET:HB2	2.03	0.41
2:IL:70:ILE:HG23	2:IL:74:PHE:CE1	2.56	0.41
2:IN:170:LYS:HG2	2:IN:224:TRP:CH2	2.56	0.41
2:IX:231:VAL:HG11	2:IX:238:MET:HB2	2.03	0.41
2:JH:96:LEU:O	2:JH:97:GLU:C	2.63	0.41
2:JJ:231:VAL:HG11	2:JJ:238:MET:HB2	2.03	0.41
2:JL:170:LYS:HG2	2:JL:224:TRP:CH2	2.56	0.41
2:KM:70:ILE:HG23	2:KM:74:PHE:CE1	2.56	0.41
2:KU:170:LYS:HG2	2:KU:224:TRP:CH2	2.56	0.41
2:KY:70:ILE:HG23	2:KY:74:PHE:CE1	2.56	0.41
2:LM:170:LYS:HG2	2:LM:224:TRP:CH2	2.56	0.41
2:ZX:170:LYS:HG2	2:ZX:224:TRP:CH2	2.56	0.41
2:YB:160:ASP:OD1	2:YB:168:LYS:NZ	2.45	0.41
2:YF:96:LEU:O	2:YF:97:GLU:C	2.63	0.40
2:AO:70:ILE:HG23	2:AO:74:PHE:CE1	2.56	0.40
2:AZ:133:ILE:HG21	2:AZ:181:ILE:HD13	2.02	0.40
2:BF:218:ASP:OD1	2:BF:219:SER:N	2.53	0.40
2:BR:170:LYS:HG2	2:BR:224:TRP:CH2	2.56	0.40
2:CB:70:ILE:HG23	2:CB:74:PHE:CE1	2.56	0.40
2:CH:70:ILE:HG23	2:CH:74:PHE:CE1	2.56	0.40
2:CH:222:ILE:O	2:CH:223:VAL:C	2.63	0.40
2:DY:222:ILE:O	2:DY:223:VAL:C	2.63	0.40
1:EF:11:ALA:HB1	1:EF:43:VAL:O	2.20	0.40
1:EP:77:TYR:N	1:EP:77:TYR:CD1	2.84	0.40
2:EQ:70:ILE:HG23	2:EQ:74:PHE:CE1	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ES:218:ASP:OD1	2:ES:219:SER:N	2.53	0.40
2:GO:92:PRO:HB2	2:GO:144:LEU:HD13	2.02	0.40
2:HK:281:PHE:O	1:WA:81:ARG:NH2	2.51	0.40
2:HQ:92:PRO:HB2	2:HQ:144:LEU:HD13	2.02	0.40
2:HU:70:ILE:HG23	2:HU:74:PHE:CE1	2.56	0.40
1:HZ:77:TYR:N	1:HZ:77:TYR:CD1	2.84	0.40
2:IG:92:PRO:HB2	2:IG:144:LEU:HD13	2.02	0.40
1:JE:11:ALA:HB1	1:JE:43:VAL:O	2.20	0.40
2:JW:92:PRO:HB2	2:JW:144:LEU:HD13	2.02	0.40
2:KM:160:ASP:OD1	2:KM:168:LYS:NZ	2.45	0.40
2:ZV:70:ILE:HG23	2:ZV:74:PHE:CE1	2.56	0.40
2:YH:70:ILE:HG23	2:YH:74:PHE:CE1	2.56	0.40
2:YZ:70:ILE:HG23	2:YZ:74:PHE:CE1	2.56	0.40
2:AF:222:ILE:O	2:AF:223:VAL:C	2.63	0.40
2:AL:70:ILE:HG23	2:AL:74:PHE:CE1	2.56	0.40
2:AO:231:VAL:HG11	2:AO:238:MET:HB2	2.03	0.40
2:BV:70:ILE:HG23	2:BV:74:PHE:CE1	2.56	0.40
2:CJ:170:LYS:HG2	2:CJ:224:TRP:CH2	2.56	0.40
2:CN:70:ILE:HG23	2:CN:74:PHE:CE1	2.56	0.40
2:CP:133:ILE:HG21	2:CP:181:ILE:HD13	2.02	0.40
2:CP:170:LYS:HG2	2:CP:224:TRP:CH2	2.56	0.40
2:DF:70:ILE:HG23	2:DF:74:PHE:CE1	2.56	0.40
2:DF:160:ASP:OD1	2:DF:168:LYS:NZ	2.45	0.40
1:ED:77:TYR:N	1:ED:77:TYR:CD1	2.84	0.40
2:EI:96:LEU:O	2:EI:97:GLU:C	2.63	0.40
2:EQ:231:VAL:HG11	2:EQ:238:MET:HB2	2.03	0.40
1:EX:81:ARG:NH2	2:EY:281:PHE:O	2.51	0.40
2:EY:92:PRO:HB2	2:EY:144:LEU:HD13	2.02	0.40
2:EY:170:LYS:HG2	2:EY:224:TRP:CH2	2.56	0.40
2:HF:218:ASP:OD1	2:HF:219:SER:N	2.53	0.40
1:HV:81:ARG:NH2	2:HW:281:PHE:O	2.51	0.40
2:JJ:70:ILE:HG23	2:JJ:74:PHE:CE1	2.56	0.40
1:JM:33:ALA:N	1:JM:34:PRO:CD	2.83	0.40
2:KA:70:ILE:HG23	2:KA:74:PHE:CE1	2.56	0.40
2:KQ:96:LEU:O	2:KQ:97:GLU:C	2.63	0.40
2:KU:218:ASP:OD1	2:KU:219:SER:N	2.53	0.40
2:LS:218:ASP:OD1	2:LS:219:SER:N	2.53	0.40
2:ZB:96:LEU:O	2:ZB:97:GLU:C	2.63	0.40
2:AX:70:ILE:HG23	2:AX:74:PHE:CE1	2.56	0.40
2:BD:70:ILE:HG23	2:BD:74:PHE:CE1	2.56	0.40
2:BV:222:ILE:O	2:BV:223:VAL:C	2.63	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:231:VAL:HG11	2:CB:238:MET:HB2	2.03	0.40
2:DR:70:ILE:HG23	2:DR:74:PHE:CE1	2.56	0.40
2:DT:218:ASP:OD1	2:DT:219:SER:N	2.53	0.40
2:DY:70:ILE:HG23	2:DY:74:PHE:CE1	2.56	0.40
2:EW:222:ILE:O	2:EW:223:VAL:C	2.63	0.40
2:FC:70:ILE:HG23	2:FC:74:PHE:CE1	2.56	0.40
1:FD:81:ARG:NH2	2:FE:281:PHE:O	2.51	0.40
2:FK:218:ASP:OD1	2:FK:219:SER:N	2.53	0.40
2:FQ:170:LYS:HG2	2:FQ:224:TRP:CH2	2.56	0.40
2:FW:218:ASP:OD1	2:FW:219:SER:N	2.53	0.40
2:HC:96:LEU:O	2:HC:97:GLU:C	2.63	0.40
2:HE:70:ILE:HG23	2:HE:74:PHE:CE1	2.56	0.40
2:HF:170:LYS:HG2	2:HF:224:TRP:CH2	2.56	0.40
2:HO:70:ILE:HG23	2:HO:74:PHE:CE1	2.56	0.40
2:HO:231:VAL:HG11	2:HO:238:MET:HB2	2.03	0.40
2:IF:70:ILE:HG23	2:IF:74:PHE:CE1	2.56	0.40
1:II:69:HIS:O	1:II:70:ILE:C	2.63	0.40
1:IO:69:HIS:O	1:IO:70:ILE:C	2.63	0.40
2:IZ:170:LYS:HG2	2:IZ:224:TRP:CH2	2.56	0.40
2:JR:170:LYS:HG2	2:JR:224:TRP:CH2	2.56	0.40
2:ZL:170:LYS:HG2	2:ZL:224:TRP:CH2	2.56	0.40
1:KP:69:HIS:O	1:KP:70:ILE:C	2.63	0.40
2:LE:70:ILE:HG23	2:LE:74:PHE:CE1	2.56	0.40
2:AX:222:ILE:O	2:AX:223:VAL:C	2.63	0.40
2:ZD:70:ILE:HG23	2:ZD:74:PHE:CE1	2.56	0.40
2:CZ:222:ILE:O	2:CZ:223:VAL:C	2.63	0.40
2:DH:170:LYS:HG2	2:DH:224:TRP:CH2	2.56	0.40
2:DR:231:VAL:HG11	2:DR:238:MET:HB2	2.03	0.40
2:EE:231:VAL:HG11	2:EE:238:MET:HB2	2.03	0.40
2:EK:70:ILE:HG23	2:EK:74:PHE:CE1	2.56	0.40
1:GV:69:HIS:O	1:GV:70:ILE:C	2.63	0.40
2:HW:170:LYS:HG2	2:HW:224:TRP:CH2	2.56	0.40
2:IB:170:LYS:HG2	2:IB:224:TRP:CH2	2.56	0.40
2:JW:170:LYS:HG2	2:JW:224:TRP:CH2	2.56	0.40
2:KA:231:VAL:HG11	2:KA:238:MET:HB2	2.03	0.40
2:KG:70:ILE:HG23	2:KG:74:PHE:CE1	2.56	0.40
1:LB:33:ALA:N	1:LB:34:PRO:CD	2.83	0.40
2:LK:70:ILE:HG23	2:LK:74:PHE:CE1	2.56	0.40
1:LN:33:ALA:N	1:LN:34:PRO:CD	2.83	0.40
2:LS:170:LYS:HG2	2:LS:224:TRP:CH2	2.56	0.40
1:ZA:33:ALA:N	1:ZA:34:PRO:CD	2.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:YJ:170:LYS:HG2	2:YJ:224:TRP:CH2	2.56	0.40
2:YN:231:VAL:HG11	2:YN:238:MET:HB2	2.03	0.40
2:YT:70:ILE:HG23	2:YT:74:PHE:CE1	2.56	0.40
2:CD:133:ILE:HG13	2:CD:148:ALA:CB	2.52	0.40
2:CH:231:VAL:HG11	2:CH:238:MET:HB2	2.03	0.40
2:DN:92:PRO:HB2	2:DN:144:LEU:HD13	2.02	0.40
2:EW:70:ILE:HG23	2:EW:74:PHE:CE1	2.56	0.40
1:FF:69:HIS:O	1:FF:70:ILE:C	2.63	0.40
2:FK:170:LYS:HG2	2:FK:224:TRP:CH2	2.56	0.40
2:FO:70:ILE:HG23	2:FO:74:PHE:CE1	2.56	0.40
2:FU:70:ILE:HG23	2:FU:74:PHE:CE1	2.56	0.40
2:GA:70:ILE:HG23	2:GA:74:PHE:CE1	2.56	0.40
2:GC:170:LYS:HG2	2:GC:224:TRP:CH2	2.56	0.40
2:HJ:231:VAL:HG11	2:HJ:238:MET:HB2	2.03	0.40
2:IA:70:ILE:HG23	2:IA:74:PHE:CE1	2.56	0.40
2:IA:222:ILE:O	2:IA:223:VAL:C	2.63	0.40
2:IX:222:ILE:O	2:IX:223:VAL:C	2.63	0.40
2:ZL:218:ASP:OD1	2:ZL:219:SER:N	2.53	0.40
1:KJ:33:ALA:N	1:KJ:34:PRO:CD	2.83	0.40
1:KR:77:TYR:N	1:KR:77:TYR:CD1	2.84	0.40
2:KS:231:VAL:HG11	2:KS:238:MET:HB2	2.03	0.40
1:KZ:81:ARG:NH2	2:LA:281:PHE:O	2.51	0.40
2:LC:96:LEU:O	2:LC:97:GLU:C	2.63	0.40
2:LG:170:LYS:HG2	2:LG:224:TRP:CH2	2.56	0.40
2:LQ:70:ILE:HG23	2:LQ:74:PHE:CE1	2.56	0.40
2:LQ:231:VAL:HG11	2:LQ:238:MET:HB2	2.03	0.40
2:YB:231:VAL:HG11	2:YB:238:MET:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	104/114 (91%)	104 (100%)	0	0	100	100
1	AC	104/114 (91%)	104 (100%)	0	0	100	100
1	AE	104/114 (91%)	104 (100%)	0	0	100	100
1	AG	104/114 (91%)	104 (100%)	0	0	100	100
1	AI	104/114 (91%)	104 (100%)	0	0	100	100
1	AK	104/114 (91%)	104 (100%)	0	0	100	100
1	AM	104/114 (91%)	104 (100%)	0	0	100	100
1	AP	104/114 (91%)	104 (100%)	0	0	100	100
1	AR	104/114 (91%)	104 (100%)	0	0	100	100
1	AS	104/114 (91%)	104 (100%)	0	0	100	100
1	AU	104/114 (91%)	104 (100%)	0	0	100	100
1	AW	104/114 (91%)	104 (100%)	0	0	100	100
1	AY	104/114 (91%)	104 (100%)	0	0	100	100
1	BA	104/114 (91%)	104 (100%)	0	0	100	100
1	BC	104/114 (91%)	104 (100%)	0	0	100	100
1	BE	104/114 (91%)	104 (100%)	0	0	100	100
1	BG	104/114 (91%)	104 (100%)	0	0	100	100
1	BI	104/114 (91%)	104 (100%)	0	0	100	100
1	BK	104/114 (91%)	104 (100%)	0	0	100	100
1	BM	104/114 (91%)	104 (100%)	0	0	100	100
1	BO	104/114 (91%)	104 (100%)	0	0	100	100
1	BQ	104/114 (91%)	104 (100%)	0	0	100	100
1	BS	104/114 (91%)	104 (100%)	0	0	100	100
1	BU	104/114 (91%)	104 (100%)	0	0	100	100
1	BW	104/114 (91%)	104 (100%)	0	0	100	100
1	BY	104/114 (91%)	104 (100%)	0	0	100	100
1	CA	104/114 (91%)	104 (100%)	0	0	100	100
1	CC	104/114 (91%)	104 (100%)	0	0	100	100
1	CE	104/114 (91%)	104 (100%)	0	0	100	100
1	CG	104/114 (91%)	104 (100%)	0	0	100	100
1	CI	104/114 (91%)	104 (100%)	0	0	100	100
1	CK	104/114 (91%)	104 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CM	104/114 (91%)	104 (100%)	0	0	100	100
1	CO	104/114 (91%)	104 (100%)	0	0	100	100
1	CQ	104/114 (91%)	104 (100%)	0	0	100	100
1	CS	104/114 (91%)	104 (100%)	0	0	100	100
1	CU	104/114 (91%)	104 (100%)	0	0	100	100
1	CW	104/114 (91%)	104 (100%)	0	0	100	100
1	CY	104/114 (91%)	104 (100%)	0	0	100	100
1	DA	104/114 (91%)	104 (100%)	0	0	100	100
1	DC	104/114 (91%)	104 (100%)	0	0	100	100
1	DE	104/114 (91%)	104 (100%)	0	0	100	100
1	DG	104/114 (91%)	104 (100%)	0	0	100	100
1	DI	104/114 (91%)	104 (100%)	0	0	100	100
1	DK	104/114 (91%)	104 (100%)	0	0	100	100
1	DM	104/114 (91%)	104 (100%)	0	0	100	100
1	DO	104/114 (91%)	104 (100%)	0	0	100	100
1	DQ	104/114 (91%)	104 (100%)	0	0	100	100
1	DS	104/114 (91%)	104 (100%)	0	0	100	100
1	DU	104/114 (91%)	104 (100%)	0	0	100	100
1	DX	104/114 (91%)	104 (100%)	0	0	100	100
1	DZ	104/114 (91%)	104 (100%)	0	0	100	100
1	EB	104/114 (91%)	104 (100%)	0	0	100	100
1	ED	104/114 (91%)	104 (100%)	0	0	100	100
1	EF	104/114 (91%)	104 (100%)	0	0	100	100
1	EH	104/114 (91%)	104 (100%)	0	0	100	100
1	EJ	104/114 (91%)	104 (100%)	0	0	100	100
1	EL	104/114 (91%)	104 (100%)	0	0	100	100
1	EN	104/114 (91%)	104 (100%)	0	0	100	100
1	EP	104/114 (91%)	104 (100%)	0	0	100	100
1	ER	104/114 (91%)	104 (100%)	0	0	100	100
1	ET	104/114 (91%)	104 (100%)	0	0	100	100
1	EV	104/114 (91%)	104 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EX	104/114 (91%)	104 (100%)	0	0	100	100
1	EZ	104/114 (91%)	104 (100%)	0	0	100	100
1	FB	104/114 (91%)	104 (100%)	0	0	100	100
1	FD	104/114 (91%)	104 (100%)	0	0	100	100
1	FF	104/114 (91%)	104 (100%)	0	0	100	100
1	FH	104/114 (91%)	104 (100%)	0	0	100	100
1	FJ	104/114 (91%)	104 (100%)	0	0	100	100
1	FL	104/114 (91%)	104 (100%)	0	0	100	100
1	FN	104/114 (91%)	104 (100%)	0	0	100	100
1	FP	104/114 (91%)	104 (100%)	0	0	100	100
1	FR	104/114 (91%)	104 (100%)	0	0	100	100
1	FT	104/114 (91%)	104 (100%)	0	0	100	100
1	FV	104/114 (91%)	104 (100%)	0	0	100	100
1	FX	104/114 (91%)	104 (100%)	0	0	100	100
1	FZ	104/114 (91%)	104 (100%)	0	0	100	100
1	GB	104/114 (91%)	104 (100%)	0	0	100	100
1	GD	104/114 (91%)	104 (100%)	0	0	100	100
1	GF	104/114 (91%)	104 (100%)	0	0	100	100
1	GH	104/114 (91%)	104 (100%)	0	0	100	100
1	GJ	104/114 (91%)	104 (100%)	0	0	100	100
1	GL	104/114 (91%)	104 (100%)	0	0	100	100
1	GN	104/114 (91%)	104 (100%)	0	0	100	100
1	GP	104/114 (91%)	104 (100%)	0	0	100	100
1	GR	104/114 (91%)	104 (100%)	0	0	100	100
1	GT	104/114 (91%)	104 (100%)	0	0	100	100
1	GV	104/114 (91%)	104 (100%)	0	0	100	100
1	GX	104/114 (91%)	104 (100%)	0	0	100	100
1	GZ	104/114 (91%)	104 (100%)	0	0	100	100
1	HB	104/114 (91%)	104 (100%)	0	0	100	100
1	HD	104/114 (91%)	104 (100%)	0	0	100	100
1	HG	104/114 (91%)	104 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HI	104/114 (91%)	104 (100%)	0	0	100	100
1	HL	104/114 (91%)	104 (100%)	0	0	100	100
1	HN	104/114 (91%)	104 (100%)	0	0	100	100
1	HP	104/114 (91%)	104 (100%)	0	0	100	100
1	HR	104/114 (91%)	104 (100%)	0	0	100	100
1	HT	104/114 (91%)	104 (100%)	0	0	100	100
1	HV	104/114 (91%)	104 (100%)	0	0	100	100
1	HX	104/114 (91%)	104 (100%)	0	0	100	100
1	HZ	104/114 (91%)	104 (100%)	0	0	100	100
1	IC	104/114 (91%)	104 (100%)	0	0	100	100
1	IE	104/114 (91%)	104 (100%)	0	0	100	100
1	IH	104/114 (91%)	104 (100%)	0	0	100	100
1	II	104/114 (91%)	104 (100%)	0	0	100	100
1	IK	104/114 (91%)	104 (100%)	0	0	100	100
1	IM	104/114 (91%)	104 (100%)	0	0	100	100
1	IO	104/114 (91%)	104 (100%)	0	0	100	100
1	IQ	104/114 (91%)	104 (100%)	0	0	100	100
1	IS	104/114 (91%)	104 (100%)	0	0	100	100
1	IU	104/114 (91%)	104 (100%)	0	0	100	100
1	IW	104/114 (91%)	104 (100%)	0	0	100	100
1	IY	104/114 (91%)	104 (100%)	0	0	100	100
1	JA	104/114 (91%)	104 (100%)	0	0	100	100
1	JC	104/114 (91%)	104 (100%)	0	0	100	100
1	JE	104/114 (91%)	104 (100%)	0	0	100	100
1	JG	104/114 (91%)	104 (100%)	0	0	100	100
1	JI	104/114 (91%)	104 (100%)	0	0	100	100
1	JK	104/114 (91%)	104 (100%)	0	0	100	100
1	JM	104/114 (91%)	104 (100%)	0	0	100	100
1	JO	104/114 (91%)	104 (100%)	0	0	100	100
1	JQ	104/114 (91%)	104 (100%)	0	0	100	100
1	JS	104/114 (91%)	104 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JV	104/114 (91%)	104 (100%)	0	0	100	100
1	JX	104/114 (91%)	104 (100%)	0	0	100	100
1	JZ	104/114 (91%)	104 (100%)	0	0	100	100
1	KB	104/114 (91%)	104 (100%)	0	0	100	100
1	KD	104/114 (91%)	104 (100%)	0	0	100	100
1	KF	104/114 (91%)	104 (100%)	0	0	100	100
1	KH	104/114 (91%)	104 (100%)	0	0	100	100
1	KJ	104/114 (91%)	104 (100%)	0	0	100	100
1	KL	104/114 (91%)	104 (100%)	0	0	100	100
1	KN	104/114 (91%)	104 (100%)	0	0	100	100
1	KP	104/114 (91%)	104 (100%)	0	0	100	100
1	KR	104/114 (91%)	104 (100%)	0	0	100	100
1	KT	104/114 (91%)	104 (100%)	0	0	100	100
1	KV	104/114 (91%)	104 (100%)	0	0	100	100
1	KX	104/114 (91%)	104 (100%)	0	0	100	100
1	KZ	104/114 (91%)	104 (100%)	0	0	100	100
1	LB	104/114 (91%)	104 (100%)	0	0	100	100
1	LD	104/114 (91%)	104 (100%)	0	0	100	100
1	LF	104/114 (91%)	104 (100%)	0	0	100	100
1	LH	104/114 (91%)	104 (100%)	0	0	100	100
1	LJ	104/114 (91%)	104 (100%)	0	0	100	100
1	LL	104/114 (91%)	104 (100%)	0	0	100	100
1	LN	104/114 (91%)	104 (100%)	0	0	100	100
1	LP	104/114 (91%)	104 (100%)	0	0	100	100
1	LR	104/114 (91%)	104 (100%)	0	0	100	100
1	WA	104/114 (91%)	104 (100%)	0	0	100	100
1	WB	104/114 (91%)	104 (100%)	0	0	100	100
1	WC	104/114 (91%)	104 (100%)	0	0	100	100
1	WD	104/114 (91%)	104 (100%)	0	0	100	100
1	YA	104/114 (91%)	104 (100%)	0	0	100	100
1	YC	104/114 (91%)	104 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	YE	104/114 (91%)	104 (100%)	0	0	100	100
1	YG	104/114 (91%)	104 (100%)	0	0	100	100
1	YI	104/114 (91%)	104 (100%)	0	0	100	100
1	YK	104/114 (91%)	104 (100%)	0	0	100	100
1	YM	104/114 (91%)	104 (100%)	0	0	100	100
1	YO	104/114 (91%)	104 (100%)	0	0	100	100
1	YQ	104/114 (91%)	104 (100%)	0	0	100	100
1	YS	104/114 (91%)	104 (100%)	0	0	100	100
1	YU	104/114 (91%)	104 (100%)	0	0	100	100
1	YW	104/114 (91%)	104 (100%)	0	0	100	100
1	YY	104/114 (91%)	104 (100%)	0	0	100	100
1	ZA	104/114 (91%)	104 (100%)	0	0	100	100
1	ZC	104/114 (91%)	104 (100%)	0	0	100	100
1	ZE	104/114 (91%)	104 (100%)	0	0	100	100
1	ZG	104/114 (91%)	104 (100%)	0	0	100	100
1	ZI	104/114 (91%)	104 (100%)	0	0	100	100
1	ZK	104/114 (91%)	104 (100%)	0	0	100	100
1	ZM	104/114 (91%)	104 (100%)	0	0	100	100
1	ZO	104/114 (91%)	104 (100%)	0	0	100	100
1	ZQ	104/114 (91%)	104 (100%)	0	0	100	100
1	ZS	104/114 (91%)	104 (100%)	0	0	100	100
1	ZU	104/114 (91%)	104 (100%)	0	0	100	100
1	ZW	104/114 (91%)	104 (100%)	0	0	100	100
1	ZY	104/114 (91%)	104 (100%)	0	0	100	100
2	AB	290/300 (97%)	290 (100%)	0	0	100	100
2	AD	290/300 (97%)	290 (100%)	0	0	100	100
2	AF	290/300 (97%)	290 (100%)	0	0	100	100
2	AH	290/300 (97%)	290 (100%)	0	0	100	100
2	AJ	290/300 (97%)	290 (100%)	0	0	100	100
2	AL	290/300 (97%)	290 (100%)	0	0	100	100
2	AN	290/300 (97%)	290 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AO	290/300 (97%)	290 (100%)	0	0	100	100
2	AQ	290/300 (97%)	290 (100%)	0	0	100	100
2	AT	290/300 (97%)	290 (100%)	0	0	100	100
2	AV	290/300 (97%)	290 (100%)	0	0	100	100
2	AX	290/300 (97%)	290 (100%)	0	0	100	100
2	AZ	290/300 (97%)	290 (100%)	0	0	100	100
2	BB	290/300 (97%)	290 (100%)	0	0	100	100
2	BD	290/300 (97%)	290 (100%)	0	0	100	100
2	BF	290/300 (97%)	290 (100%)	0	0	100	100
2	BH	290/300 (97%)	290 (100%)	0	0	100	100
2	BJ	290/300 (97%)	290 (100%)	0	0	100	100
2	BL	290/300 (97%)	290 (100%)	0	0	100	100
2	BN	290/300 (97%)	290 (100%)	0	0	100	100
2	BP	290/300 (97%)	290 (100%)	0	0	100	100
2	BR	290/300 (97%)	290 (100%)	0	0	100	100
2	BT	290/300 (97%)	290 (100%)	0	0	100	100
2	BV	290/300 (97%)	290 (100%)	0	0	100	100
2	BX	290/300 (97%)	290 (100%)	0	0	100	100
2	BZ	290/300 (97%)	290 (100%)	0	0	100	100
2	CB	290/300 (97%)	290 (100%)	0	0	100	100
2	CD	290/300 (97%)	290 (100%)	0	0	100	100
2	CF	290/300 (97%)	290 (100%)	0	0	100	100
2	CH	290/300 (97%)	290 (100%)	0	0	100	100
2	CJ	290/300 (97%)	290 (100%)	0	0	100	100
2	CL	290/300 (97%)	290 (100%)	0	0	100	100
2	CN	290/300 (97%)	290 (100%)	0	0	100	100
2	CP	290/300 (97%)	290 (100%)	0	0	100	100
2	CR	290/300 (97%)	290 (100%)	0	0	100	100
2	CT	290/300 (97%)	290 (100%)	0	0	100	100
2	CV	290/300 (97%)	290 (100%)	0	0	100	100
2	CX	290/300 (97%)	290 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CZ	290/300 (97%)	290 (100%)	0	0	100	100
2	DB	290/300 (97%)	290 (100%)	0	0	100	100
2	DD	290/300 (97%)	290 (100%)	0	0	100	100
2	DF	290/300 (97%)	290 (100%)	0	0	100	100
2	DH	290/300 (97%)	290 (100%)	0	0	100	100
2	DJ	290/300 (97%)	290 (100%)	0	0	100	100
2	DL	290/300 (97%)	290 (100%)	0	0	100	100
2	DN	290/300 (97%)	290 (100%)	0	0	100	100
2	DP	290/300 (97%)	290 (100%)	0	0	100	100
2	DR	290/300 (97%)	290 (100%)	0	0	100	100
2	DT	290/300 (97%)	290 (100%)	0	0	100	100
2	DW	290/300 (97%)	290 (100%)	0	0	100	100
2	DY	290/300 (97%)	290 (100%)	0	0	100	100
2	EA	290/300 (97%)	290 (100%)	0	0	100	100
2	EC	290/300 (97%)	290 (100%)	0	0	100	100
2	EE	290/300 (97%)	290 (100%)	0	0	100	100
2	EG	290/300 (97%)	290 (100%)	0	0	100	100
2	EI	290/300 (97%)	290 (100%)	0	0	100	100
2	EK	290/300 (97%)	290 (100%)	0	0	100	100
2	EM	290/300 (97%)	290 (100%)	0	0	100	100
2	EO	290/300 (97%)	290 (100%)	0	0	100	100
2	EQ	290/300 (97%)	290 (100%)	0	0	100	100
2	ES	290/300 (97%)	290 (100%)	0	0	100	100
2	EU	290/300 (97%)	290 (100%)	0	0	100	100
2	EW	290/300 (97%)	290 (100%)	0	0	100	100
2	EY	290/300 (97%)	290 (100%)	0	0	100	100
2	FA	290/300 (97%)	290 (100%)	0	0	100	100
2	FC	290/300 (97%)	290 (100%)	0	0	100	100
2	FE	290/300 (97%)	290 (100%)	0	0	100	100
2	FG	290/300 (97%)	290 (100%)	0	0	100	100
2	FI	290/300 (97%)	290 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	FK	290/300 (97%)	290 (100%)	0	0	100	100
2	FM	290/300 (97%)	290 (100%)	0	0	100	100
2	FO	290/300 (97%)	290 (100%)	0	0	100	100
2	FQ	290/300 (97%)	290 (100%)	0	0	100	100
2	FS	290/300 (97%)	290 (100%)	0	0	100	100
2	FU	290/300 (97%)	290 (100%)	0	0	100	100
2	FW	290/300 (97%)	290 (100%)	0	0	100	100
2	FY	290/300 (97%)	290 (100%)	0	0	100	100
2	GA	290/300 (97%)	290 (100%)	0	0	100	100
2	GC	290/300 (97%)	290 (100%)	0	0	100	100
2	GE	290/300 (97%)	290 (100%)	0	0	100	100
2	GG	290/300 (97%)	290 (100%)	0	0	100	100
2	GI	290/300 (97%)	290 (100%)	0	0	100	100
2	GK	290/300 (97%)	290 (100%)	0	0	100	100
2	GM	290/300 (97%)	290 (100%)	0	0	100	100
2	GO	290/300 (97%)	290 (100%)	0	0	100	100
2	GQ	290/300 (97%)	290 (100%)	0	0	100	100
2	GS	290/300 (97%)	290 (100%)	0	0	100	100
2	GU	290/300 (97%)	290 (100%)	0	0	100	100
2	GW	290/300 (97%)	290 (100%)	0	0	100	100
2	GY	290/300 (97%)	290 (100%)	0	0	100	100
2	HA	290/300 (97%)	290 (100%)	0	0	100	100
2	HC	290/300 (97%)	290 (100%)	0	0	100	100
2	HE	290/300 (97%)	290 (100%)	0	0	100	100
2	HF	290/300 (97%)	290 (100%)	0	0	100	100
2	HH	290/300 (97%)	290 (100%)	0	0	100	100
2	HJ	290/300 (97%)	290 (100%)	0	0	100	100
2	HK	290/300 (97%)	290 (100%)	0	0	100	100
2	HM	290/300 (97%)	290 (100%)	0	0	100	100
2	HO	290/300 (97%)	290 (100%)	0	0	100	100
2	HQ	290/300 (97%)	290 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	HS	290/300 (97%)	290 (100%)	0	0	100	100
2	HU	290/300 (97%)	290 (100%)	0	0	100	100
2	HW	290/300 (97%)	290 (100%)	0	0	100	100
2	HY	290/300 (97%)	290 (100%)	0	0	100	100
2	IA	290/300 (97%)	290 (100%)	0	0	100	100
2	IB	290/300 (97%)	290 (100%)	0	0	100	100
2	ID	290/300 (97%)	290 (100%)	0	0	100	100
2	IF	290/300 (97%)	290 (100%)	0	0	100	100
2	IG	290/300 (97%)	290 (100%)	0	0	100	100
2	IJ	290/300 (97%)	290 (100%)	0	0	100	100
2	IL	290/300 (97%)	290 (100%)	0	0	100	100
2	IN	290/300 (97%)	290 (100%)	0	0	100	100
2	IP	290/300 (97%)	290 (100%)	0	0	100	100
2	IR	290/300 (97%)	290 (100%)	0	0	100	100
2	IT	290/300 (97%)	290 (100%)	0	0	100	100
2	IV	290/300 (97%)	290 (100%)	0	0	100	100
2	IX	290/300 (97%)	290 (100%)	0	0	100	100
2	IZ	290/300 (97%)	290 (100%)	0	0	100	100
2	JB	290/300 (97%)	290 (100%)	0	0	100	100
2	JD	290/300 (97%)	290 (100%)	0	0	100	100
2	JF	290/300 (97%)	290 (100%)	0	0	100	100
2	JH	290/300 (97%)	290 (100%)	0	0	100	100
2	JJ	290/300 (97%)	290 (100%)	0	0	100	100
2	JL	290/300 (97%)	290 (100%)	0	0	100	100
2	JN	290/300 (97%)	290 (100%)	0	0	100	100
2	JP	290/300 (97%)	290 (100%)	0	0	100	100
2	JR	290/300 (97%)	290 (100%)	0	0	100	100
2	JT	290/300 (97%)	290 (100%)	0	0	100	100
2	JU	290/300 (97%)	290 (100%)	0	0	100	100
2	JW	290/300 (97%)	290 (100%)	0	0	100	100
2	JY	290/300 (97%)	290 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	KA	290/300 (97%)	290 (100%)	0	0	100	100
2	KC	290/300 (97%)	290 (100%)	0	0	100	100
2	KE	290/300 (97%)	290 (100%)	0	0	100	100
2	KG	290/300 (97%)	290 (100%)	0	0	100	100
2	KI	290/300 (97%)	290 (100%)	0	0	100	100
2	KK	290/300 (97%)	290 (100%)	0	0	100	100
2	KM	290/300 (97%)	290 (100%)	0	0	100	100
2	KO	290/300 (97%)	290 (100%)	0	0	100	100
2	KQ	290/300 (97%)	290 (100%)	0	0	100	100
2	KS	290/300 (97%)	290 (100%)	0	0	100	100
2	KU	290/300 (97%)	290 (100%)	0	0	100	100
2	KW	290/300 (97%)	290 (100%)	0	0	100	100
2	KY	290/300 (97%)	290 (100%)	0	0	100	100
2	LA	290/300 (97%)	290 (100%)	0	0	100	100
2	LC	290/300 (97%)	290 (100%)	0	0	100	100
2	LE	290/300 (97%)	290 (100%)	0	0	100	100
2	LG	290/300 (97%)	290 (100%)	0	0	100	100
2	LI	290/300 (97%)	290 (100%)	0	0	100	100
2	LK	290/300 (97%)	290 (100%)	0	0	100	100
2	LM	290/300 (97%)	290 (100%)	0	0	100	100
2	LO	290/300 (97%)	290 (100%)	0	0	100	100
2	LQ	290/300 (97%)	290 (100%)	0	0	100	100
2	LS	290/300 (97%)	290 (100%)	0	0	100	100
2	YB	290/300 (97%)	290 (100%)	0	0	100	100
2	YD	290/300 (97%)	290 (100%)	0	0	100	100
2	YF	290/300 (97%)	290 (100%)	0	0	100	100
2	YH	290/300 (97%)	290 (100%)	0	0	100	100
2	YJ	290/300 (97%)	290 (100%)	0	0	100	100
2	YL	290/300 (97%)	290 (100%)	0	0	100	100
2	YN	290/300 (97%)	290 (100%)	0	0	100	100
2	YP	290/300 (97%)	290 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	YR	290/300 (97%)	290 (100%)	0	0	100	100
2	YT	290/300 (97%)	290 (100%)	0	0	100	100
2	YV	290/300 (97%)	290 (100%)	0	0	100	100
2	YX	290/300 (97%)	290 (100%)	0	0	100	100
2	YZ	290/300 (97%)	290 (100%)	0	0	100	100
2	ZB	290/300 (97%)	290 (100%)	0	0	100	100
2	ZD	290/300 (97%)	290 (100%)	0	0	100	100
2	ZF	290/300 (97%)	290 (100%)	0	0	100	100
2	ZH	290/300 (97%)	290 (100%)	0	0	100	100
2	ZJ	290/300 (97%)	290 (100%)	0	0	100	100
2	ZL	290/300 (97%)	290 (100%)	0	0	100	100
2	ZN	290/300 (97%)	290 (100%)	0	0	100	100
2	ZP	290/300 (97%)	290 (100%)	0	0	100	100
2	ZR	290/300 (97%)	290 (100%)	0	0	100	100
2	ZT	290/300 (97%)	290 (100%)	0	0	100	100
2	ZV	290/300 (97%)	290 (100%)	0	0	100	100
2	ZX	290/300 (97%)	290 (100%)	0	0	100	100
2	ZZ	290/300 (97%)	290 (100%)	0	0	100	100
All	All	70920/74520 (95%)	70920 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	86/94 (92%)	86 (100%)	0	100	100
1	AC	86/94 (92%)	86 (100%)	0	100	100
1	AE	86/94 (92%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AG	86/94 (92%)	86 (100%)	0	100	100
1	AI	86/94 (92%)	86 (100%)	0	100	100
1	AK	86/94 (92%)	86 (100%)	0	100	100
1	AM	86/94 (92%)	86 (100%)	0	100	100
1	AP	86/94 (92%)	86 (100%)	0	100	100
1	AR	86/94 (92%)	86 (100%)	0	100	100
1	AS	86/94 (92%)	86 (100%)	0	100	100
1	AU	86/94 (92%)	86 (100%)	0	100	100
1	AW	86/94 (92%)	86 (100%)	0	100	100
1	AY	86/94 (92%)	86 (100%)	0	100	100
1	BA	86/94 (92%)	86 (100%)	0	100	100
1	BC	86/94 (92%)	86 (100%)	0	100	100
1	BE	86/94 (92%)	86 (100%)	0	100	100
1	BG	86/94 (92%)	86 (100%)	0	100	100
1	BI	86/94 (92%)	86 (100%)	0	100	100
1	BK	86/94 (92%)	86 (100%)	0	100	100
1	BM	86/94 (92%)	86 (100%)	0	100	100
1	BO	86/94 (92%)	86 (100%)	0	100	100
1	BQ	86/94 (92%)	86 (100%)	0	100	100
1	BS	86/94 (92%)	86 (100%)	0	100	100
1	BU	86/94 (92%)	86 (100%)	0	100	100
1	BW	86/94 (92%)	86 (100%)	0	100	100
1	BY	86/94 (92%)	86 (100%)	0	100	100
1	CA	86/94 (92%)	86 (100%)	0	100	100
1	CC	86/94 (92%)	86 (100%)	0	100	100
1	CE	86/94 (92%)	86 (100%)	0	100	100
1	CG	86/94 (92%)	86 (100%)	0	100	100
1	CI	86/94 (92%)	86 (100%)	0	100	100
1	CK	86/94 (92%)	86 (100%)	0	100	100
1	CM	86/94 (92%)	86 (100%)	0	100	100
1	CO	86/94 (92%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CQ	86/94 (92%)	86 (100%)	0	100	100
1	CS	86/94 (92%)	86 (100%)	0	100	100
1	CU	86/94 (92%)	86 (100%)	0	100	100
1	CW	86/94 (92%)	86 (100%)	0	100	100
1	CY	86/94 (92%)	86 (100%)	0	100	100
1	DA	86/94 (92%)	86 (100%)	0	100	100
1	DC	86/94 (92%)	86 (100%)	0	100	100
1	DE	86/94 (92%)	86 (100%)	0	100	100
1	DG	86/94 (92%)	86 (100%)	0	100	100
1	DI	86/94 (92%)	86 (100%)	0	100	100
1	DK	86/94 (92%)	86 (100%)	0	100	100
1	DM	86/94 (92%)	86 (100%)	0	100	100
1	DO	86/94 (92%)	86 (100%)	0	100	100
1	DQ	86/94 (92%)	86 (100%)	0	100	100
1	DS	86/94 (92%)	86 (100%)	0	100	100
1	DU	86/94 (92%)	86 (100%)	0	100	100
1	DX	86/94 (92%)	86 (100%)	0	100	100
1	DZ	86/94 (92%)	86 (100%)	0	100	100
1	EB	86/94 (92%)	86 (100%)	0	100	100
1	ED	86/94 (92%)	86 (100%)	0	100	100
1	EF	86/94 (92%)	86 (100%)	0	100	100
1	EH	86/94 (92%)	86 (100%)	0	100	100
1	EJ	86/94 (92%)	86 (100%)	0	100	100
1	EL	86/94 (92%)	86 (100%)	0	100	100
1	EN	86/94 (92%)	86 (100%)	0	100	100
1	EP	86/94 (92%)	86 (100%)	0	100	100
1	ER	86/94 (92%)	86 (100%)	0	100	100
1	ET	86/94 (92%)	86 (100%)	0	100	100
1	EV	86/94 (92%)	86 (100%)	0	100	100
1	EX	86/94 (92%)	86 (100%)	0	100	100
1	EZ	86/94 (92%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FB	86/94 (92%)	86 (100%)	0	100	100
1	FD	86/94 (92%)	86 (100%)	0	100	100
1	FF	86/94 (92%)	86 (100%)	0	100	100
1	FH	86/94 (92%)	86 (100%)	0	100	100
1	FJ	86/94 (92%)	86 (100%)	0	100	100
1	FL	86/94 (92%)	86 (100%)	0	100	100
1	FN	86/94 (92%)	86 (100%)	0	100	100
1	FP	86/94 (92%)	86 (100%)	0	100	100
1	FR	86/94 (92%)	86 (100%)	0	100	100
1	FT	86/94 (92%)	86 (100%)	0	100	100
1	FV	86/94 (92%)	86 (100%)	0	100	100
1	FX	86/94 (92%)	86 (100%)	0	100	100
1	FZ	86/94 (92%)	86 (100%)	0	100	100
1	GB	86/94 (92%)	86 (100%)	0	100	100
1	GD	86/94 (92%)	86 (100%)	0	100	100
1	GF	86/94 (92%)	86 (100%)	0	100	100
1	GH	86/94 (92%)	86 (100%)	0	100	100
1	GJ	86/94 (92%)	86 (100%)	0	100	100
1	GL	86/94 (92%)	86 (100%)	0	100	100
1	GN	86/94 (92%)	86 (100%)	0	100	100
1	GP	86/94 (92%)	86 (100%)	0	100	100
1	GR	86/94 (92%)	86 (100%)	0	100	100
1	GT	86/94 (92%)	86 (100%)	0	100	100
1	GV	86/94 (92%)	86 (100%)	0	100	100
1	GX	86/94 (92%)	86 (100%)	0	100	100
1	GZ	86/94 (92%)	86 (100%)	0	100	100
1	HB	86/94 (92%)	86 (100%)	0	100	100
1	HD	86/94 (92%)	86 (100%)	0	100	100
1	HG	86/94 (92%)	86 (100%)	0	100	100
1	HI	86/94 (92%)	86 (100%)	0	100	100
1	HL	86/94 (92%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HN	86/94 (92%)	86 (100%)	0	100	100
1	HP	86/94 (92%)	86 (100%)	0	100	100
1	HR	86/94 (92%)	86 (100%)	0	100	100
1	HT	86/94 (92%)	86 (100%)	0	100	100
1	HV	86/94 (92%)	86 (100%)	0	100	100
1	HX	86/94 (92%)	86 (100%)	0	100	100
1	HZ	86/94 (92%)	86 (100%)	0	100	100
1	IC	86/94 (92%)	86 (100%)	0	100	100
1	IE	86/94 (92%)	86 (100%)	0	100	100
1	IH	86/94 (92%)	86 (100%)	0	100	100
1	II	86/94 (92%)	86 (100%)	0	100	100
1	IK	86/94 (92%)	86 (100%)	0	100	100
1	IM	86/94 (92%)	86 (100%)	0	100	100
1	IO	86/94 (92%)	86 (100%)	0	100	100
1	IQ	86/94 (92%)	86 (100%)	0	100	100
1	IS	86/94 (92%)	86 (100%)	0	100	100
1	IU	86/94 (92%)	86 (100%)	0	100	100
1	IW	86/94 (92%)	86 (100%)	0	100	100
1	IY	86/94 (92%)	86 (100%)	0	100	100
1	JA	86/94 (92%)	86 (100%)	0	100	100
1	JC	86/94 (92%)	86 (100%)	0	100	100
1	JE	86/94 (92%)	86 (100%)	0	100	100
1	JG	86/94 (92%)	86 (100%)	0	100	100
1	JI	86/94 (92%)	86 (100%)	0	100	100
1	JK	86/94 (92%)	86 (100%)	0	100	100
1	JM	86/94 (92%)	86 (100%)	0	100	100
1	JO	86/94 (92%)	86 (100%)	0	100	100
1	JQ	86/94 (92%)	86 (100%)	0	100	100
1	JS	86/94 (92%)	86 (100%)	0	100	100
1	JV	86/94 (92%)	86 (100%)	0	100	100
1	JX	86/94 (92%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JZ	86/94 (92%)	86 (100%)	0	100	100
1	KB	86/94 (92%)	86 (100%)	0	100	100
1	KD	86/94 (92%)	86 (100%)	0	100	100
1	KF	86/94 (92%)	86 (100%)	0	100	100
1	KH	86/94 (92%)	86 (100%)	0	100	100
1	KJ	86/94 (92%)	86 (100%)	0	100	100
1	KL	86/94 (92%)	86 (100%)	0	100	100
1	KN	86/94 (92%)	86 (100%)	0	100	100
1	KP	86/94 (92%)	86 (100%)	0	100	100
1	KR	86/94 (92%)	86 (100%)	0	100	100
1	KT	86/94 (92%)	86 (100%)	0	100	100
1	KV	86/94 (92%)	86 (100%)	0	100	100
1	KX	86/94 (92%)	86 (100%)	0	100	100
1	KZ	86/94 (92%)	86 (100%)	0	100	100
1	LB	86/94 (92%)	86 (100%)	0	100	100
1	LD	86/94 (92%)	86 (100%)	0	100	100
1	LF	86/94 (92%)	86 (100%)	0	100	100
1	LH	86/94 (92%)	86 (100%)	0	100	100
1	LJ	86/94 (92%)	86 (100%)	0	100	100
1	LL	86/94 (92%)	86 (100%)	0	100	100
1	LN	86/94 (92%)	86 (100%)	0	100	100
1	LP	86/94 (92%)	86 (100%)	0	100	100
1	LR	86/94 (92%)	86 (100%)	0	100	100
1	WA	86/94 (92%)	86 (100%)	0	100	100
1	WB	86/94 (92%)	86 (100%)	0	100	100
1	WC	86/94 (92%)	86 (100%)	0	100	100
1	WD	86/94 (92%)	86 (100%)	0	100	100
1	YA	86/94 (92%)	86 (100%)	0	100	100
1	YC	86/94 (92%)	86 (100%)	0	100	100
1	YE	86/94 (92%)	86 (100%)	0	100	100
1	YG	86/94 (92%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	YI	86/94 (92%)	86 (100%)	0	100	100
1	YK	86/94 (92%)	86 (100%)	0	100	100
1	YM	86/94 (92%)	86 (100%)	0	100	100
1	YO	86/94 (92%)	86 (100%)	0	100	100
1	YQ	86/94 (92%)	86 (100%)	0	100	100
1	YS	86/94 (92%)	86 (100%)	0	100	100
1	YU	86/94 (92%)	86 (100%)	0	100	100
1	YW	86/94 (92%)	86 (100%)	0	100	100
1	YY	86/94 (92%)	86 (100%)	0	100	100
1	ZA	86/94 (92%)	86 (100%)	0	100	100
1	ZC	86/94 (92%)	86 (100%)	0	100	100
1	ZE	86/94 (92%)	86 (100%)	0	100	100
1	ZG	86/94 (92%)	86 (100%)	0	100	100
1	ZI	86/94 (92%)	86 (100%)	0	100	100
1	ZK	86/94 (92%)	86 (100%)	0	100	100
1	ZM	86/94 (92%)	86 (100%)	0	100	100
1	ZO	86/94 (92%)	86 (100%)	0	100	100
1	ZQ	86/94 (92%)	86 (100%)	0	100	100
1	ZS	86/94 (92%)	86 (100%)	0	100	100
1	ZU	86/94 (92%)	86 (100%)	0	100	100
1	ZW	86/94 (92%)	86 (100%)	0	100	100
1	ZY	86/94 (92%)	86 (100%)	0	100	100
2	AB	233/241 (97%)	233 (100%)	0	100	100
2	AD	233/241 (97%)	233 (100%)	0	100	100
2	AF	233/241 (97%)	233 (100%)	0	100	100
2	AH	233/241 (97%)	233 (100%)	0	100	100
2	AJ	233/241 (97%)	233 (100%)	0	100	100
2	AL	233/241 (97%)	233 (100%)	0	100	100
2	AN	233/241 (97%)	233 (100%)	0	100	100
2	AO	233/241 (97%)	233 (100%)	0	100	100
2	AQ	233/241 (97%)	233 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AT	233/241 (97%)	233 (100%)	0	100	100
2	AV	233/241 (97%)	233 (100%)	0	100	100
2	AX	233/241 (97%)	233 (100%)	0	100	100
2	AZ	233/241 (97%)	233 (100%)	0	100	100
2	BB	233/241 (97%)	233 (100%)	0	100	100
2	BD	233/241 (97%)	233 (100%)	0	100	100
2	BF	233/241 (97%)	233 (100%)	0	100	100
2	BH	233/241 (97%)	233 (100%)	0	100	100
2	BJ	233/241 (97%)	233 (100%)	0	100	100
2	BL	233/241 (97%)	233 (100%)	0	100	100
2	BN	233/241 (97%)	233 (100%)	0	100	100
2	BP	233/241 (97%)	233 (100%)	0	100	100
2	BR	233/241 (97%)	233 (100%)	0	100	100
2	BT	233/241 (97%)	233 (100%)	0	100	100
2	BV	233/241 (97%)	233 (100%)	0	100	100
2	BX	233/241 (97%)	233 (100%)	0	100	100
2	BZ	233/241 (97%)	233 (100%)	0	100	100
2	CB	233/241 (97%)	233 (100%)	0	100	100
2	CD	233/241 (97%)	233 (100%)	0	100	100
2	CF	233/241 (97%)	233 (100%)	0	100	100
2	CH	233/241 (97%)	233 (100%)	0	100	100
2	CJ	233/241 (97%)	233 (100%)	0	100	100
2	CL	233/241 (97%)	233 (100%)	0	100	100
2	CN	233/241 (97%)	233 (100%)	0	100	100
2	CP	233/241 (97%)	233 (100%)	0	100	100
2	CR	233/241 (97%)	233 (100%)	0	100	100
2	CT	233/241 (97%)	233 (100%)	0	100	100
2	CV	233/241 (97%)	233 (100%)	0	100	100
2	CX	233/241 (97%)	233 (100%)	0	100	100
2	CZ	233/241 (97%)	233 (100%)	0	100	100
2	DB	233/241 (97%)	233 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DD	233/241 (97%)	233 (100%)	0	100	100
2	DF	233/241 (97%)	233 (100%)	0	100	100
2	DH	233/241 (97%)	233 (100%)	0	100	100
2	DJ	233/241 (97%)	233 (100%)	0	100	100
2	DL	233/241 (97%)	233 (100%)	0	100	100
2	DN	233/241 (97%)	233 (100%)	0	100	100
2	DP	233/241 (97%)	233 (100%)	0	100	100
2	DR	233/241 (97%)	233 (100%)	0	100	100
2	DT	233/241 (97%)	233 (100%)	0	100	100
2	DW	233/241 (97%)	233 (100%)	0	100	100
2	DY	233/241 (97%)	233 (100%)	0	100	100
2	EA	233/241 (97%)	233 (100%)	0	100	100
2	EC	233/241 (97%)	233 (100%)	0	100	100
2	EE	233/241 (97%)	233 (100%)	0	100	100
2	EG	233/241 (97%)	233 (100%)	0	100	100
2	EI	233/241 (97%)	233 (100%)	0	100	100
2	EK	233/241 (97%)	233 (100%)	0	100	100
2	EM	233/241 (97%)	233 (100%)	0	100	100
2	EO	233/241 (97%)	233 (100%)	0	100	100
2	EQ	233/241 (97%)	233 (100%)	0	100	100
2	ES	233/241 (97%)	233 (100%)	0	100	100
2	EU	233/241 (97%)	233 (100%)	0	100	100
2	EW	233/241 (97%)	233 (100%)	0	100	100
2	EY	233/241 (97%)	233 (100%)	0	100	100
2	FA	233/241 (97%)	233 (100%)	0	100	100
2	FC	233/241 (97%)	233 (100%)	0	100	100
2	FE	233/241 (97%)	233 (100%)	0	100	100
2	FG	233/241 (97%)	233 (100%)	0	100	100
2	FI	233/241 (97%)	233 (100%)	0	100	100
2	FK	233/241 (97%)	233 (100%)	0	100	100
2	FM	233/241 (97%)	233 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	FO	233/241 (97%)	233 (100%)	0	100	100
2	FQ	233/241 (97%)	233 (100%)	0	100	100
2	FS	233/241 (97%)	233 (100%)	0	100	100
2	FU	233/241 (97%)	233 (100%)	0	100	100
2	FW	233/241 (97%)	233 (100%)	0	100	100
2	FY	233/241 (97%)	233 (100%)	0	100	100
2	GA	233/241 (97%)	233 (100%)	0	100	100
2	GC	233/241 (97%)	233 (100%)	0	100	100
2	GE	233/241 (97%)	233 (100%)	0	100	100
2	GG	233/241 (97%)	233 (100%)	0	100	100
2	GI	233/241 (97%)	233 (100%)	0	100	100
2	GK	233/241 (97%)	233 (100%)	0	100	100
2	GM	233/241 (97%)	233 (100%)	0	100	100
2	GO	233/241 (97%)	233 (100%)	0	100	100
2	GQ	233/241 (97%)	233 (100%)	0	100	100
2	GS	233/241 (97%)	233 (100%)	0	100	100
2	GU	233/241 (97%)	233 (100%)	0	100	100
2	GW	233/241 (97%)	233 (100%)	0	100	100
2	GY	233/241 (97%)	233 (100%)	0	100	100
2	HA	233/241 (97%)	233 (100%)	0	100	100
2	HC	233/241 (97%)	233 (100%)	0	100	100
2	HE	233/241 (97%)	233 (100%)	0	100	100
2	HF	233/241 (97%)	233 (100%)	0	100	100
2	HH	233/241 (97%)	233 (100%)	0	100	100
2	HJ	233/241 (97%)	233 (100%)	0	100	100
2	HK	233/241 (97%)	233 (100%)	0	100	100
2	HM	233/241 (97%)	233 (100%)	0	100	100
2	HO	233/241 (97%)	233 (100%)	0	100	100
2	HQ	233/241 (97%)	233 (100%)	0	100	100
2	HS	233/241 (97%)	233 (100%)	0	100	100
2	HU	233/241 (97%)	233 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	HW	233/241 (97%)	233 (100%)	0	100	100
2	HY	233/241 (97%)	233 (100%)	0	100	100
2	IA	233/241 (97%)	233 (100%)	0	100	100
2	IB	233/241 (97%)	233 (100%)	0	100	100
2	ID	233/241 (97%)	233 (100%)	0	100	100
2	IF	233/241 (97%)	233 (100%)	0	100	100
2	IG	233/241 (97%)	233 (100%)	0	100	100
2	IJ	233/241 (97%)	233 (100%)	0	100	100
2	IL	233/241 (97%)	233 (100%)	0	100	100
2	IN	233/241 (97%)	233 (100%)	0	100	100
2	IP	233/241 (97%)	233 (100%)	0	100	100
2	IR	233/241 (97%)	233 (100%)	0	100	100
2	IT	233/241 (97%)	233 (100%)	0	100	100
2	IV	233/241 (97%)	233 (100%)	0	100	100
2	IX	233/241 (97%)	233 (100%)	0	100	100
2	IZ	233/241 (97%)	233 (100%)	0	100	100
2	JB	233/241 (97%)	233 (100%)	0	100	100
2	JD	233/241 (97%)	233 (100%)	0	100	100
2	JF	233/241 (97%)	233 (100%)	0	100	100
2	JH	233/241 (97%)	233 (100%)	0	100	100
2	JJ	233/241 (97%)	233 (100%)	0	100	100
2	JL	233/241 (97%)	233 (100%)	0	100	100
2	JN	233/241 (97%)	233 (100%)	0	100	100
2	JP	233/241 (97%)	233 (100%)	0	100	100
2	JR	233/241 (97%)	233 (100%)	0	100	100
2	JT	233/241 (97%)	233 (100%)	0	100	100
2	JU	233/241 (97%)	233 (100%)	0	100	100
2	JW	233/241 (97%)	233 (100%)	0	100	100
2	JY	233/241 (97%)	233 (100%)	0	100	100
2	KA	233/241 (97%)	233 (100%)	0	100	100
2	KC	233/241 (97%)	233 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	KE	233/241 (97%)	233 (100%)	0	100	100
2	KG	233/241 (97%)	233 (100%)	0	100	100
2	KI	233/241 (97%)	233 (100%)	0	100	100
2	KK	233/241 (97%)	233 (100%)	0	100	100
2	KM	233/241 (97%)	233 (100%)	0	100	100
2	KO	233/241 (97%)	233 (100%)	0	100	100
2	KQ	233/241 (97%)	233 (100%)	0	100	100
2	KS	233/241 (97%)	233 (100%)	0	100	100
2	KU	233/241 (97%)	233 (100%)	0	100	100
2	KW	233/241 (97%)	233 (100%)	0	100	100
2	KY	233/241 (97%)	233 (100%)	0	100	100
2	LA	233/241 (97%)	233 (100%)	0	100	100
2	LC	233/241 (97%)	233 (100%)	0	100	100
2	LE	233/241 (97%)	233 (100%)	0	100	100
2	LG	233/241 (97%)	233 (100%)	0	100	100
2	LI	233/241 (97%)	233 (100%)	0	100	100
2	LK	233/241 (97%)	233 (100%)	0	100	100
2	LM	233/241 (97%)	233 (100%)	0	100	100
2	LO	233/241 (97%)	233 (100%)	0	100	100
2	LQ	233/241 (97%)	233 (100%)	0	100	100
2	LS	233/241 (97%)	233 (100%)	0	100	100
2	YB	233/241 (97%)	233 (100%)	0	100	100
2	YD	233/241 (97%)	233 (100%)	0	100	100
2	YF	233/241 (97%)	233 (100%)	0	100	100
2	YH	233/241 (97%)	233 (100%)	0	100	100
2	YJ	233/241 (97%)	233 (100%)	0	100	100
2	YL	233/241 (97%)	233 (100%)	0	100	100
2	YN	233/241 (97%)	233 (100%)	0	100	100
2	YP	233/241 (97%)	233 (100%)	0	100	100
2	YR	233/241 (97%)	233 (100%)	0	100	100
2	YT	233/241 (97%)	233 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	YV	233/241 (97%)	233 (100%)	0	100	100
2	YX	233/241 (97%)	233 (100%)	0	100	100
2	YZ	233/241 (97%)	233 (100%)	0	100	100
2	ZB	233/241 (97%)	233 (100%)	0	100	100
2	ZD	233/241 (97%)	233 (100%)	0	100	100
2	ZF	233/241 (97%)	233 (100%)	0	100	100
2	ZH	233/241 (97%)	233 (100%)	0	100	100
2	ZJ	233/241 (97%)	233 (100%)	0	100	100
2	ZL	233/241 (97%)	233 (100%)	0	100	100
2	ZN	233/241 (97%)	233 (100%)	0	100	100
2	ZP	233/241 (97%)	233 (100%)	0	100	100
2	ZR	233/241 (97%)	233 (100%)	0	100	100
2	ZT	233/241 (97%)	233 (100%)	0	100	100
2	ZV	233/241 (97%)	233 (100%)	0	100	100
2	ZX	233/241 (97%)	233 (100%)	0	100	100
2	ZZ	233/241 (97%)	233 (100%)	0	100	100
All	All	57420/60300 (95%)	57420 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
2	YD	59	ASN
2	ZZ	259	GLN
2	YH	46	ASN
1	YI	87	GLN
2	YJ	59	ASN
2	YN	46	ASN
2	YP	59	ASN
2	YR	259	GLN
1	YU	87	GLN
2	YV	59	ASN
2	YZ	46	ASN
2	AF	46	ASN
2	AL	46	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AM	87	GLN
2	AN	59	ASN
2	AO	46	ASN
2	AX	46	ASN
2	AZ	59	ASN
2	BN	259	GLN
2	BR	59	ASN
2	BX	59	ASN
2	BZ	259	GLN
2	ZD	46	ASN
2	CB	46	ASN
1	CC	87	GLN
2	CD	59	ASN
2	CH	46	ASN
2	CJ	59	ASN
2	CP	59	ASN
2	CT	46	ASN
2	CV	59	ASN
2	CX	259	GLN
2	DB	59	ASN
2	DF	46	ASN
2	DH	59	ASN
2	DL	46	ASN
1	DM	87	GLN
2	DN	59	ASN
2	DT	59	ASN
2	DY	46	ASN
2	EA	59	ASN
2	ZF	59	ASN
2	EG	59	ASN
2	EI	259	GLN
2	EO	259	GLN
2	EQ	46	ASN
2	ES	59	ASN
2	EW	46	ASN
1	EX	87	GLN
2	FC	46	ASN
2	FE	59	ASN
2	FK	59	ASN
2	FQ	59	ASN
2	FU	46	ASN
2	FW	59	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	FY	259	GLN
2	GA	46	ASN
2	GG	46	ASN
2	GI	59	ASN
1	GN	87	GLN
2	GO	59	ASN
2	GS	46	ASN
2	GU	59	ASN
2	GY	46	ASN
2	HA	59	ASN
2	HE	46	ASN
2	HF	59	ASN
1	WB	87	GLN
2	HJ	46	ASN
2	HK	59	ASN
2	HS	259	GLN
2	HU	46	ASN
2	HW	59	ASN
2	ZJ	46	ASN
2	IB	59	ASN
2	ID	259	GLN
2	IG	59	ASN
2	IL	46	ASN
2	IN	59	ASN
2	IT	59	ASN
2	IZ	59	ASN
2	JJ	46	ASN
2	JL	59	ASN
2	JW	59	ASN
2	KA	46	ASN
2	ZL	59	ASN
2	KC	59	ASN
2	KG	46	ASN
2	KI	59	ASN
2	KM	46	ASN
2	KO	59	ASN
2	KS	46	ASN
2	KU	59	ASN
2	KY	46	ASN
1	KZ	87	GLN
2	LA	59	ASN
2	LC	259	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	LE	46	ASN
1	LF	87	GLN
2	LM	59	ASN
2	LQ	46	ASN
2	LS	59	ASN
2	ZN	259	GLN
2	ZP	46	ASN
2	ZR	59	ASN
2	ZV	46	ASN
1	ZW	87	GLN
2	ZX	59	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70685. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

6.1.2 Raw map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

6.2.2 Raw map



X Index: 120



Y Index: 120



Z Index: 120

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 120



Y Index: 99



Z Index: 75

6.3.2 Raw map



X Index: 120



Y Index: 99



Z Index: 163

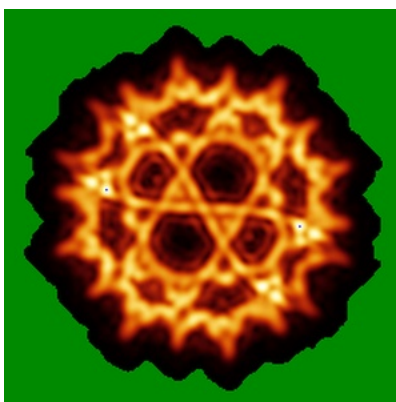
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y

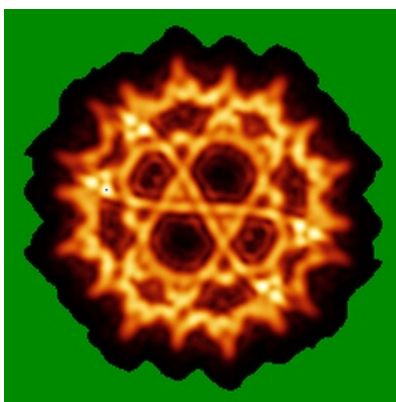


Z

6.4.2 Raw map



X



Y

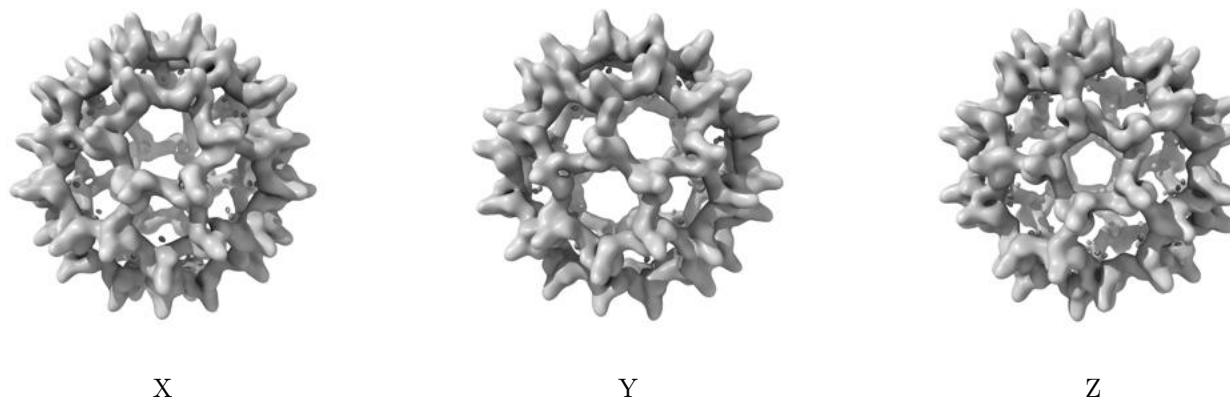


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

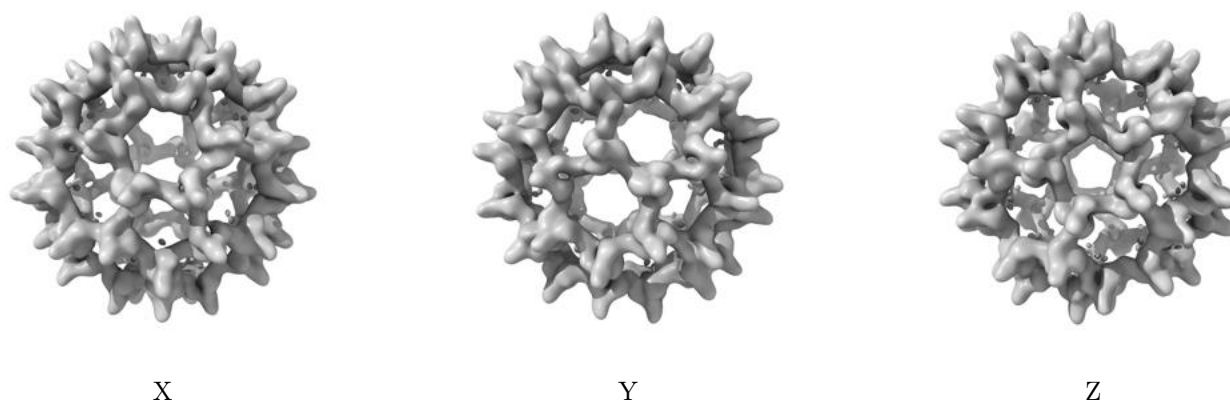
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1854.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

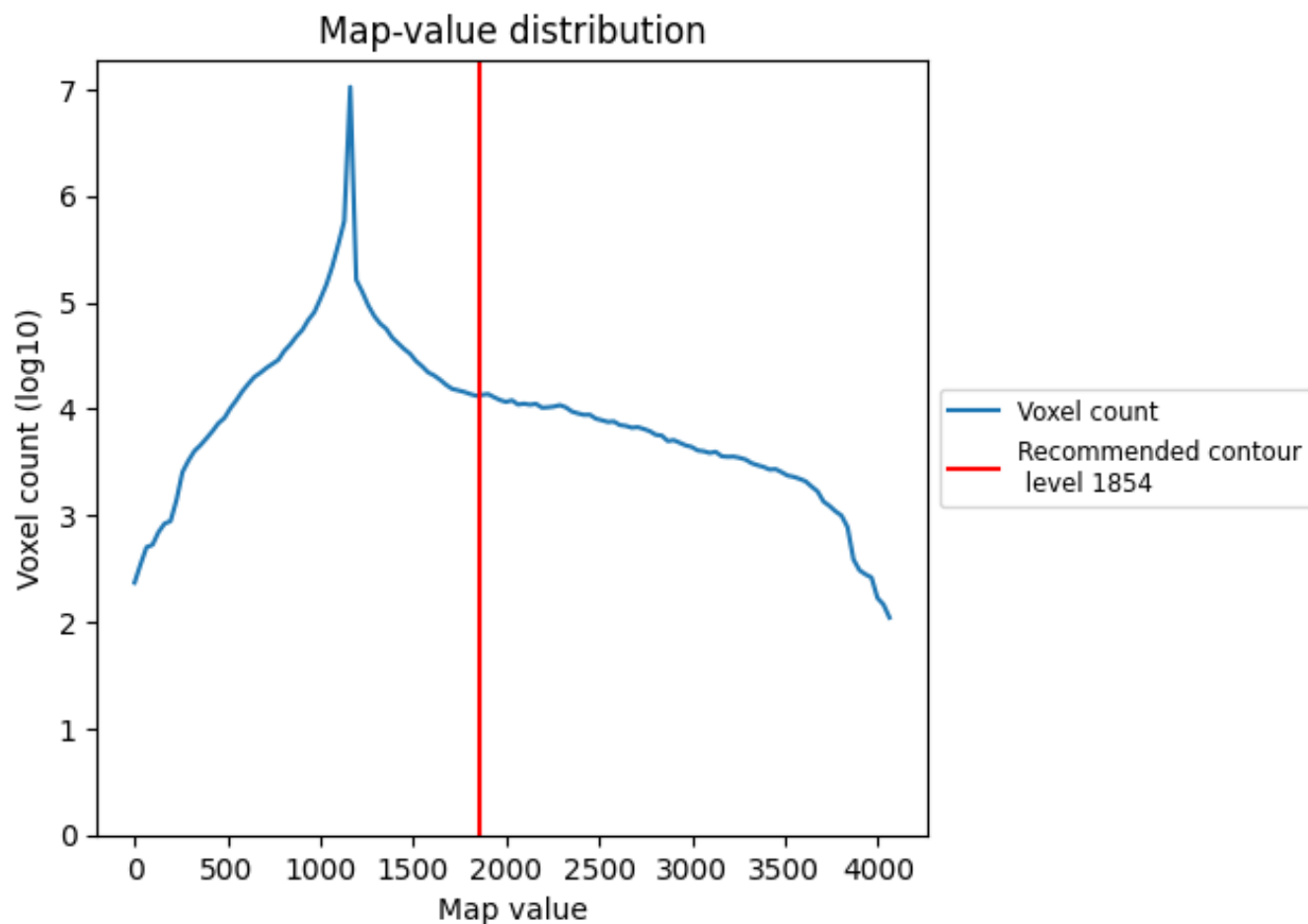
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

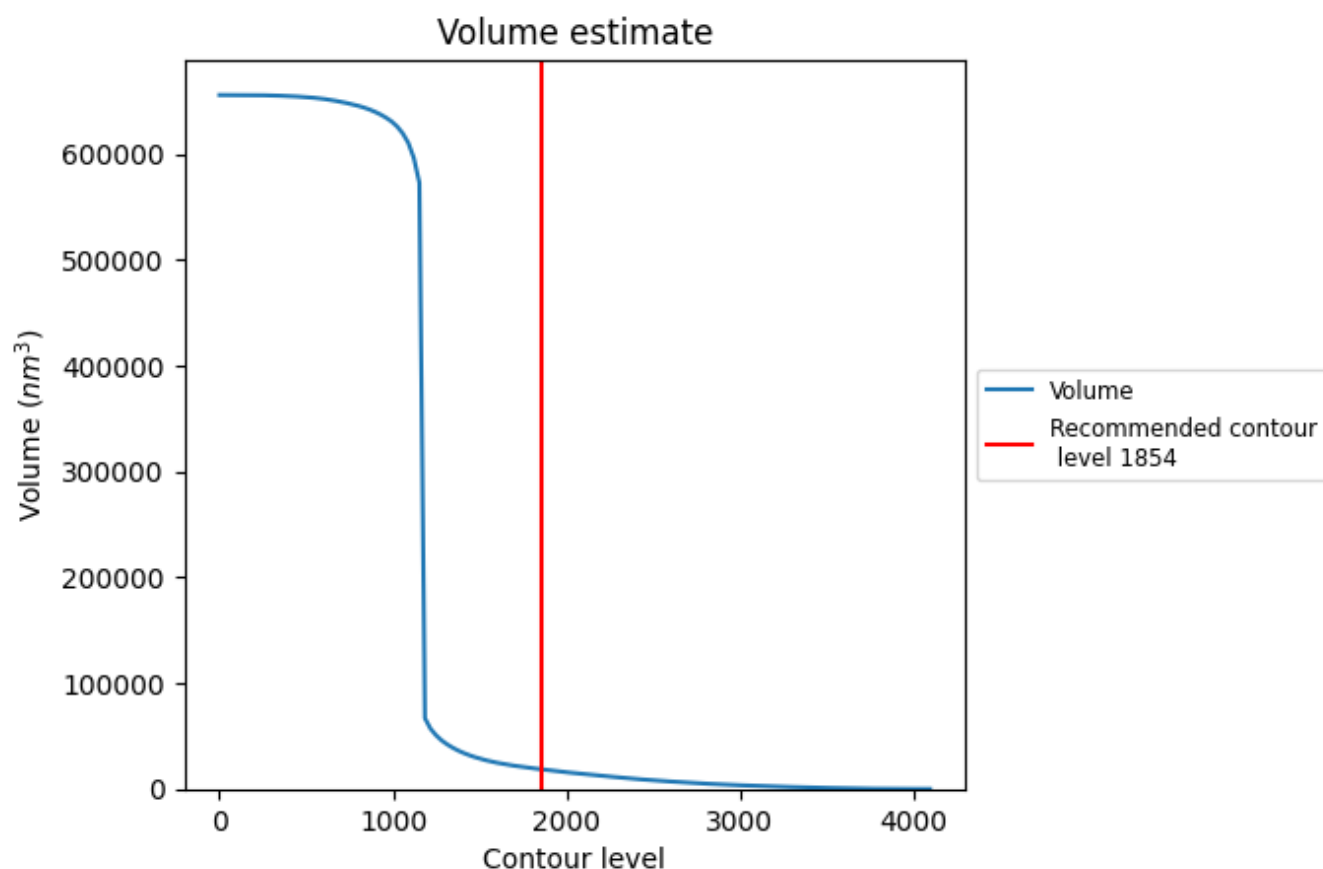
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

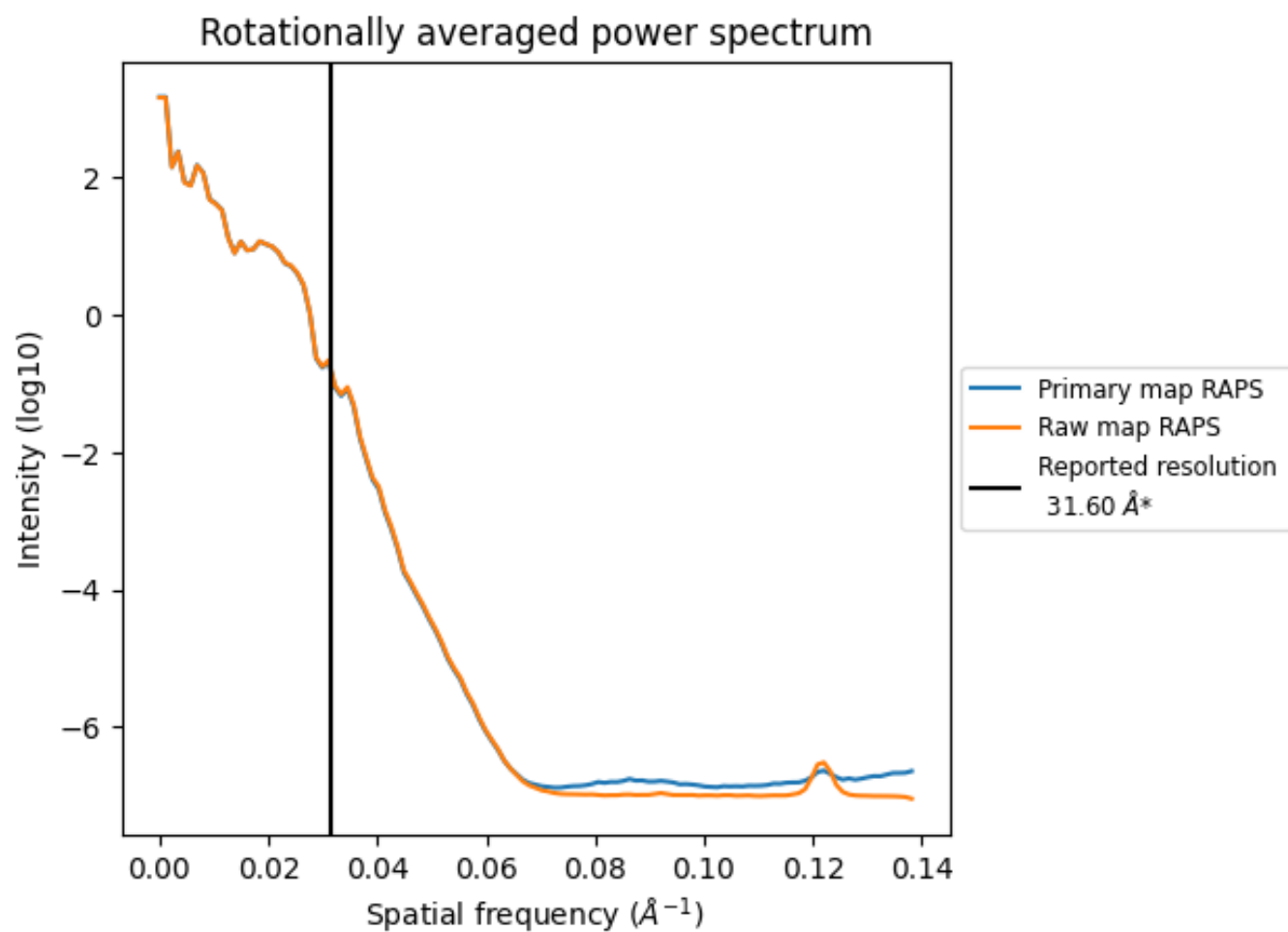
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 18602 nm^3 ; this corresponds to an approximate mass of 16804 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

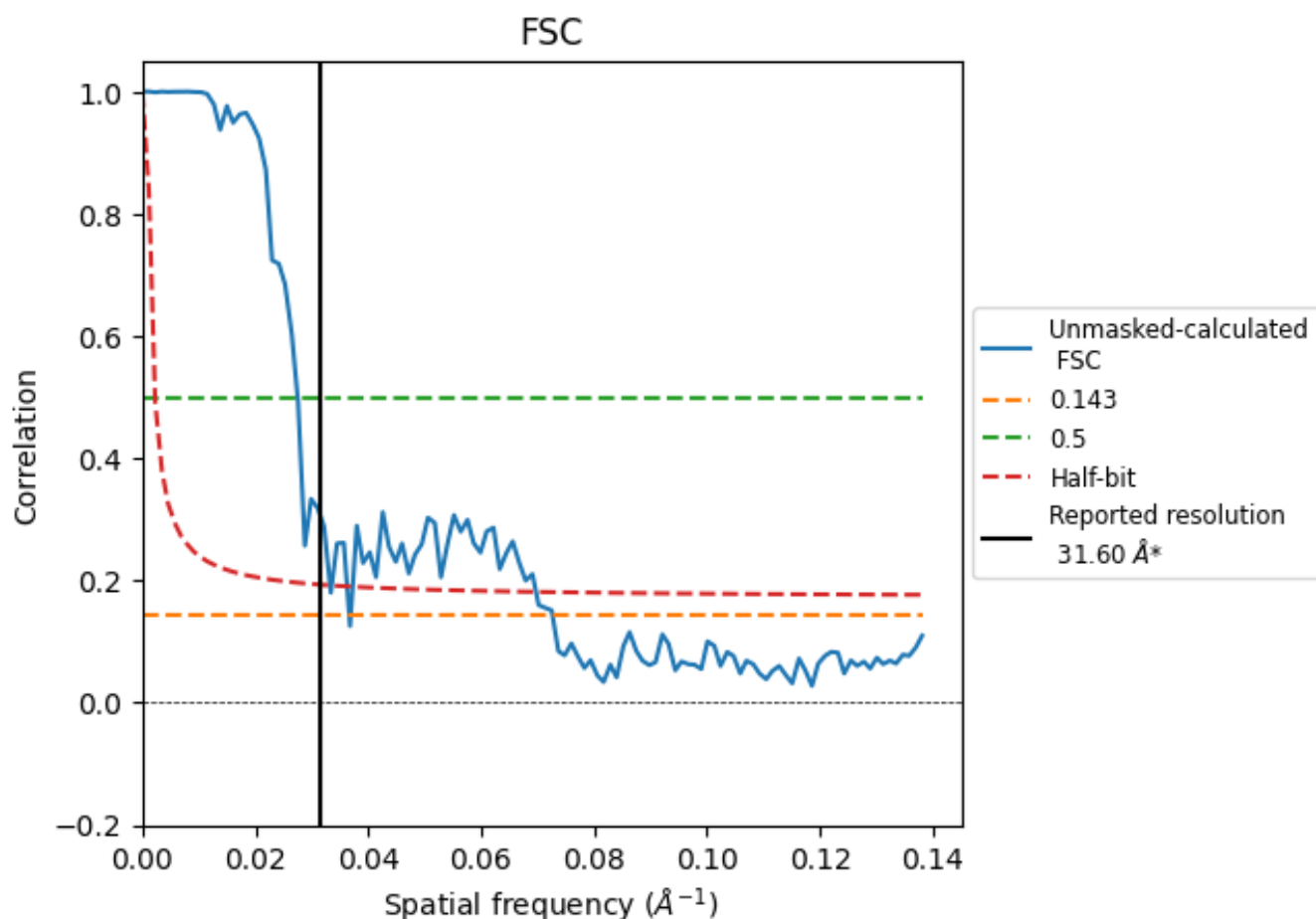


*Reported resolution corresponds to spatial frequency of 0.032 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.032 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

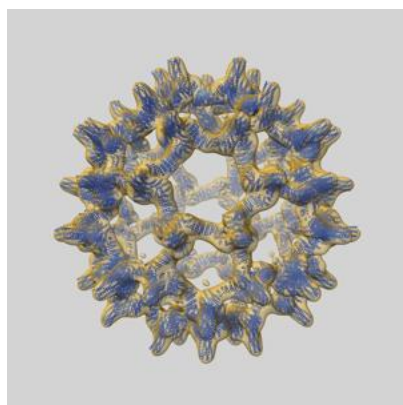
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	31.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	27.25	36.36	30.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 27.25 differs from the reported value 31.6 by more than 10 %

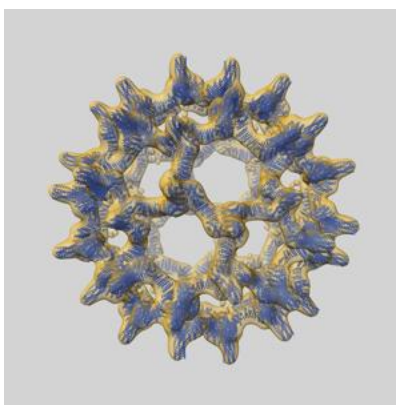
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70685 and PDB model 9OP9. Per-residue inclusion information can be found in section [3](#) on page [36](#).

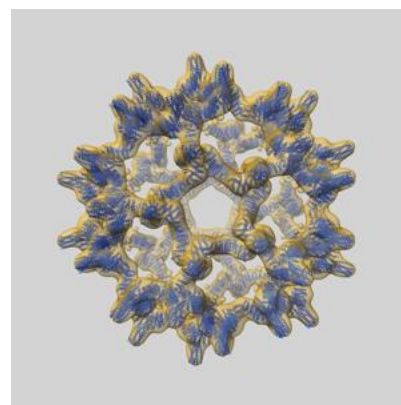
9.1 Map-model overlay [i](#)



X



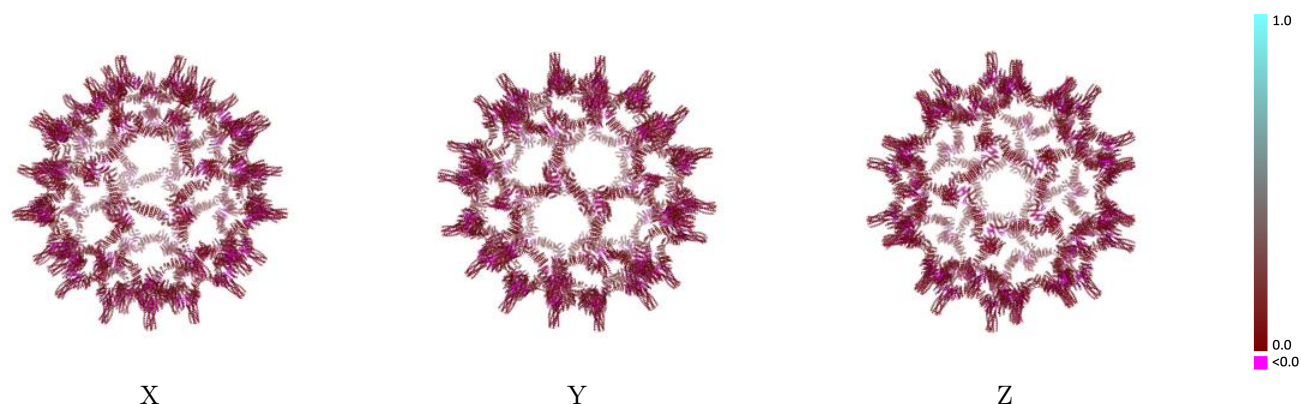
Y



Z

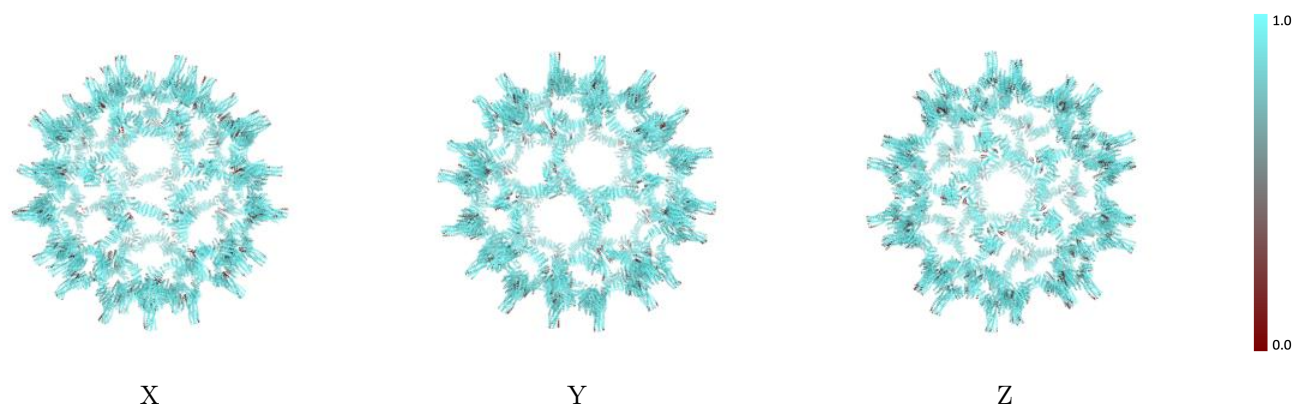
The images above show the 3D surface view of the map at the recommended contour level 1854.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



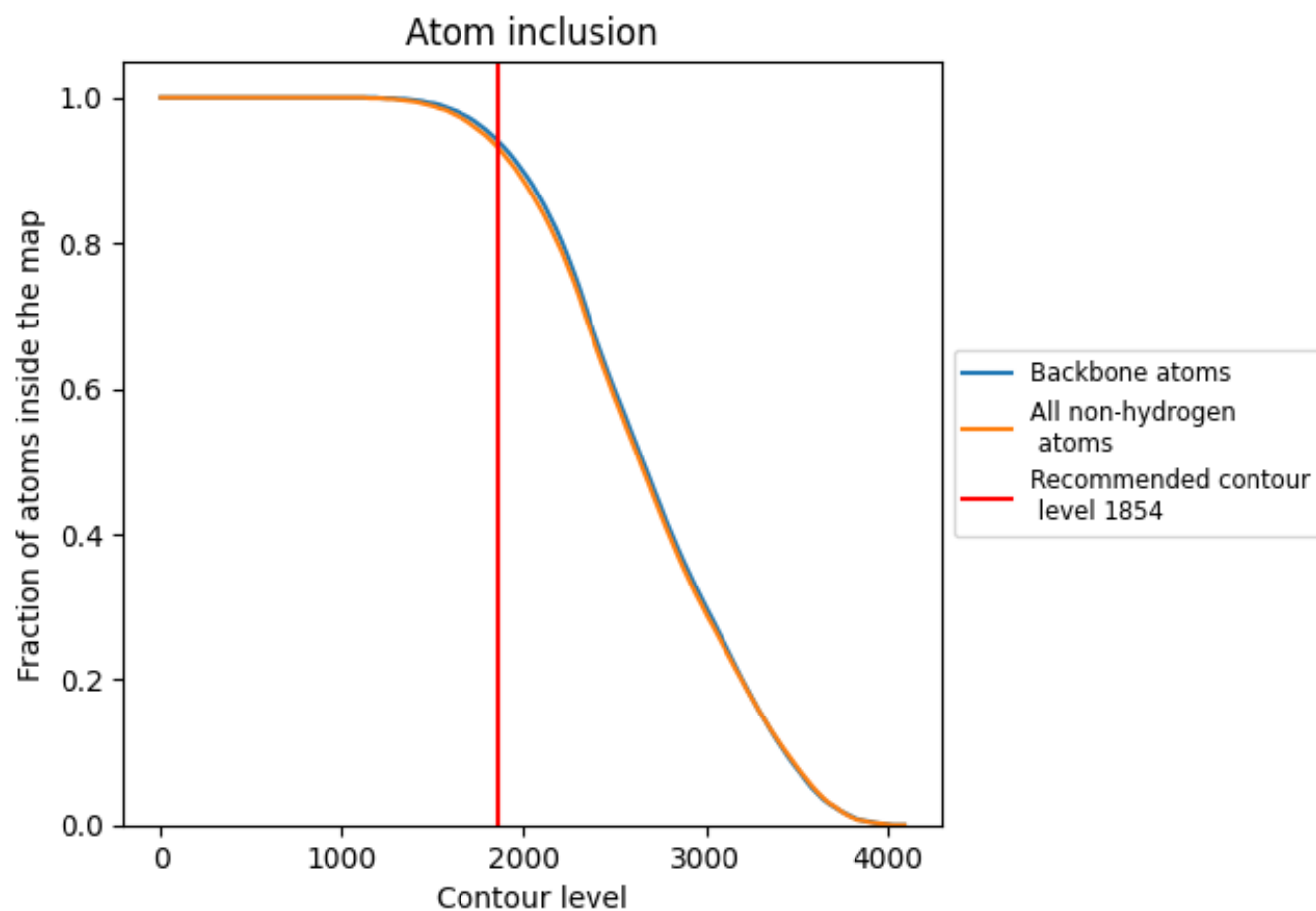
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1854).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1854) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9330	0.0580
AA	0.9990	0.0590
AB	0.9170	0.0550
AC	0.9860	0.0680
AD	0.9790	0.0590
AE	0.9620	0.0870
AF	0.8180	0.0440
AG	0.9820	0.0690
AH	0.9540	0.0560
AI	0.9630	0.0680
AJ	0.9430	0.0570
AK	0.9890	0.0860
AL	0.8370	0.0480
AM	0.9720	0.0680
AN	0.9330	0.0490
AO	0.7970	0.0430
AP	0.9470	0.0860
AQ	0.9500	0.0580
AR	0.9620	0.0690
AS	0.9950	0.0670
AT	0.9480	0.0560
AU	0.9710	0.0670
AV	0.9370	0.0550
AW	0.9410	0.0920
AX	0.7720	0.0380
AY	0.9980	0.0640
AZ	0.9350	0.0520
BA	0.9780	0.0690
BB	0.9610	0.0590
BC	0.9380	0.0840
BD	0.7820	0.0370
BE	0.9950	0.0680
BF	0.9490	0.0530
BG	0.9920	0.0690
BH	0.9770	0.0570



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BI	 0.9950	 0.0780
BJ	 0.8770	 0.0450
BK	 0.9570	 0.0630
BL	 0.9470	 0.0580
BM	 0.9730	 0.0610
BN	 0.9510	 0.0550
BO	 0.9980	 0.0770
BP	 0.8820	 0.0480
BQ	 0.9760	 0.0680
BR	 0.9200	 0.0510
BS	 0.9990	 0.0610
BT	 0.9750	 0.0600
BU	 0.9720	 0.0840
BV	 0.8040	 0.0410
BW	 0.9980	 0.0630
BX	 0.9330	 0.0570
BY	 0.9920	 0.0600
BZ	 0.9660	 0.0580
CA	 0.9950	 0.0810
CB	 0.8840	 0.0470
CC	 0.9950	 0.0670
CD	 0.9320	 0.0550
CE	 0.9990	 0.0690
CF	 0.9800	 0.0610
CG	 0.9950	 0.0840
CH	 0.8700	 0.0460
CI	 0.9940	 0.0580
CJ	 0.9520	 0.0600
CK	 0.9980	 0.0650
CL	 0.9700	 0.0570
CM	 1.0000	 0.0750
CN	 0.9180	 0.0470
CO	 0.9430	 0.0680
CP	 0.9360	 0.0530
CQ	 0.9890	 0.0720
CR	 0.9720	 0.0580
CS	 0.9890	 0.0850
CT	 0.8650	 0.0410
CU	 0.9520	 0.0730
CV	 0.9490	 0.0540
CW	 0.9640	 0.0630
CX	 0.9330	 0.0580

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
CY	 0.9890	 0.0910
CZ	 0.8400	 0.0450
DA	 0.9870	 0.0740
DB	 0.9150	 0.0590
DC	 0.9980	 0.0640
DD	 0.9780	 0.0600
DE	 0.9640	 0.0900
DF	 0.7840	 0.0390
DG	 0.9940	 0.0640
DH	 0.9350	 0.0610
DI	 0.9950	 0.0630
DJ	 0.9670	 0.0590
DK	 0.9890	 0.0870
DL	 0.8460	 0.0490
DM	 0.9990	 0.0700
DN	 0.9280	 0.0590
DO	 0.9990	 0.0690
DP	 0.9800	 0.0560
DQ	 0.9960	 0.0870
DR	 0.8710	 0.0440
DS	 0.9890	 0.0620
DT	 0.9490	 0.0590
DU	 0.9890	 0.0640
DW	 0.9650	 0.0550
DX	 0.9990	 0.0810
DY	 0.9120	 0.0450
DZ	 0.9390	 0.0710
EA	 0.9260	 0.0560
EB	 0.9910	 0.0700
EC	 0.9670	 0.0560
ED	 0.9950	 0.0830
EE	 0.8850	 0.0490
EF	 0.9390	 0.0680
EG	 0.9440	 0.0530
EH	 0.9990	 0.0640
EI	 0.9780	 0.0570
EJ	 0.9990	 0.0910
EK	 0.8860	 0.0470
EL	 0.9960	 0.0580
EM	 0.9480	 0.0590
EN	 0.9770	 0.0690
EO	 0.9450	 0.0590

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
EP	 0.9870	 0.0880
EQ	 0.8340	 0.0490
ER	 0.9920	 0.0670
ES	 0.9150	 0.0560
ET	 1.0000	 0.0670
EU	 0.9820	 0.0560
EV	 0.9810	 0.0870
EW	 0.8130	 0.0440
EX	 0.9910	 0.0620
EY	 0.9490	 0.0570
EZ	 0.9990	 0.0620
FA	 0.9780	 0.0600
FB	 0.9890	 0.0870
FC	 0.8430	 0.0450
FD	 0.9990	 0.0630
FE	 0.9440	 0.0580
FF	 0.9990	 0.0660
FG	 0.9760	 0.0570
FH	 0.9990	 0.0780
FI	 0.8980	 0.0460
FJ	 0.9670	 0.0710
FK	 0.9440	 0.0540
FL	 0.9870	 0.0590
FM	 0.9660	 0.0570
FN	 0.9990	 0.0820
FO	 0.9090	 0.0470
FP	 0.9660	 0.0700
FQ	 0.9270	 0.0560
FR	 0.9960	 0.0590
FS	 0.9700	 0.0560
FT	 0.9990	 0.0800
FU	 0.9100	 0.0460
FV	 0.9400	 0.0640
FW	 0.9390	 0.0570
FX	 0.9850	 0.0580
FY	 0.9590	 0.0620
FZ	 0.9920	 0.0880
GA	 0.8730	 0.0460
GB	 0.9920	 0.0670
GC	 0.9240	 0.0550
GD	 0.9990	 0.0690
GE	 0.9820	 0.0570

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
GF	 0.9900	 0.0820
GG	 0.8450	 0.0420
GH	 0.9920	 0.0660
GI	 0.9500	 0.0570
GJ	 0.9990	 0.0680
GK	 0.9740	 0.0570
GL	 1.0000	 0.0780
GM	 0.9110	 0.0420
GN	 0.9690	 0.0700
GO	 0.9450	 0.0580
GP	 0.9980	 0.0620
GQ	 0.9740	 0.0590
GR	 0.9990	 0.0780
GS	 0.9120	 0.0480
GT	 0.9850	 0.0640
GU	 0.9360	 0.0570
GV	 1.0000	 0.0600
GW	 0.9730	 0.0550
GX	 0.9990	 0.0790
GY	 0.9030	 0.0450
GZ	 0.9500	 0.0690
HA	 0.9440	 0.0580
HB	 0.9850	 0.0620
HC	 0.9620	 0.0570
HD	 0.9990	 0.0850
HE	 0.8960	 0.0470
HF	 0.9240	 0.0560
HG	 0.9990	 0.0660
HH	 0.9810	 0.0570
HI	 0.9890	 0.0810
HJ	 0.8390	 0.0430
HK	 0.9410	 0.0580
HL	 0.9990	 0.0670
HM	 0.9750	 0.0580
HN	 0.9990	 0.0780
HO	 0.9050	 0.0460
HP	 0.9910	 0.0630
HQ	 0.9400	 0.0540
HR	 0.9990	 0.0600
HS	 0.9770	 0.0590
HT	 0.9990	 0.0880
HU	 0.8950	 0.0470

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
HV	 0.9940	 0.0660
HW	 0.9470	 0.0630
HX	 0.9780	 0.0640
HY	 0.9330	 0.0610
HZ	 0.9710	 0.0870
IA	 0.7880	 0.0400
IB	 0.9130	 0.0580
IC	 0.9960	 0.0650
ID	 0.9810	 0.0570
IE	 0.9690	 0.0870
IF	 0.8060	 0.0420
IG	 0.9560	 0.0580
IH	 0.9910	 0.0650
II	 0.9670	 0.0670
IJ	 0.9580	 0.0560
IK	 0.9870	 0.0900
IL	 0.8550	 0.0400
IM	 0.9540	 0.0740
IN	 0.9400	 0.0530
IO	 0.9730	 0.0730
IP	 0.9630	 0.0570
IQ	 0.9400	 0.0820
IR	 0.7910	 0.0400
IS	 0.9940	 0.0680
IT	 0.9530	 0.0550
IU	 0.9610	 0.0660
IV	 0.9420	 0.0550
IW	 0.9540	 0.0880
IX	 0.7990	 0.0390
IY	 0.9950	 0.0680
IZ	 0.9410	 0.0540
JA	 0.9770	 0.0610
JB	 0.9460	 0.0620
JC	 0.9380	 0.0900
JD	 0.7650	 0.0370
JE	 0.9980	 0.0660
JF	 0.9330	 0.0590
JG	 0.9800	 0.0620
JH	 0.9480	 0.0580
JI	 0.9820	 0.0830
JJ	 0.8200	 0.0410
JK	 0.9980	 0.0670

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
JL	 0.9140	 0.0570
JM	 1.0000	 0.0730
JN	 0.9820	 0.0590
JO	 0.9850	 0.0820
JP	 0.8320	 0.0390
JQ	 0.9900	 0.0620
JR	 0.9550	 0.0590
JS	 0.9800	 0.0610
JT	 0.9630	 0.0550
JU	 0.8910	 0.0460
JV	 0.9380	 0.0710
JW	 0.9360	 0.0520
JX	 0.9820	 0.0670
JY	 0.9720	 0.0560
JZ	 0.9620	 0.0880
KA	 0.8220	 0.0350
KB	 0.9720	 0.0730
KC	 0.9560	 0.0530
KD	 0.9580	 0.0640
KE	 0.9350	 0.0600
KF	 0.9820	 0.0840
KG	 0.8220	 0.0370
KH	 0.9860	 0.0720
KI	 0.9270	 0.0560
KJ	 0.9910	 0.0570
KK	 0.9570	 0.0570
KL	 0.9470	 0.0830
KM	 0.7630	 0.0390
KN	 0.9980	 0.0650
KO	 0.9270	 0.0590
KP	 0.9920	 0.0570
KQ	 0.9620	 0.0600
KR	 0.9800	 0.0870
KS	 0.8200	 0.0440
KT	 1.0000	 0.0620
KU	 0.9240	 0.0580
KV	 0.9960	 0.0680
KW	 0.9800	 0.0580
KX	 0.9920	 0.0830
KY	 0.8620	 0.0360
KZ	 0.9810	 0.0710
LA	 0.9520	 0.0550

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LB	 0.9810	 0.0610
LC	 0.9620	 0.0570
LD	 0.9990	 0.0720
LE	 0.9020	 0.0450
LF	 0.9400	 0.0650
LG	 0.9280	 0.0580
LH	 0.9800	 0.0660
LI	 0.9670	 0.0540
LJ	 0.9750	 0.0810
LK	 0.8530	 0.0410
LL	 0.9580	 0.0690
LM	 0.9530	 0.0510
LN	 0.9660	 0.0580
LO	 0.9310	 0.0590
LP	 0.9830	 0.0870
LQ	 0.8130	 0.0420
LR	 0.9920	 0.0670
LS	 0.9160	 0.0560
WA	 0.9960	 0.0600
WB	 0.9820	 0.0680
WC	 0.9990	 0.0720
WD	 0.9980	 0.0770
YA	 0.9950	 0.0860
YB	 0.8720	 0.0520
YC	 0.9680	 0.0610
YD	 0.9210	 0.0550
YE	 0.9660	 0.0690
YF	 0.9550	 0.0610
YG	 0.9660	 0.0840
YH	 0.8280	 0.0430
YI	 0.9660	 0.0670
YJ	 0.9490	 0.0540
YK	 0.9720	 0.0630
YL	 0.9300	 0.0610
YM	 0.9660	 0.0880
YN	 0.7820	 0.0410
YO	 0.9990	 0.0650
YP	 0.9170	 0.0570
YQ	 0.9920	 0.0720
YR	 0.9740	 0.0570
YS	 0.9480	 0.0850
YT	 0.7870	 0.0360

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
YU	 0.9910	 0.0700
YV	 0.9480	 0.0530
YW	 0.9860	 0.0640
YX	 0.9490	 0.0600
YY	 0.9530	 0.0870
YZ	 0.7670	 0.0400
ZA	 0.9990	 0.0630
ZB	 0.9740	 0.0580
ZC	 1.0000	 0.0790
ZD	 0.9170	 0.0490
ZE	 0.9710	 0.0650
ZF	 0.9390	 0.0560
ZG	 0.9980	 0.0680
ZH	 0.9730	 0.0580
ZI	 0.9610	 0.0880
ZJ	 0.7760	 0.0360
ZK	 0.9940	 0.0660
ZL	 0.9370	 0.0600
ZM	 0.9980	 0.0630
ZN	 0.9660	 0.0570
ZO	 0.9620	 0.0900
ZP	 0.7920	 0.0460
ZQ	 0.9980	 0.0610
ZR	 0.9260	 0.0590
ZS	 0.9910	 0.0720
ZT	 0.9810	 0.0560
ZU	 0.9900	 0.0850
ZV	 0.8570	 0.0400
ZW	 0.9670	 0.0720
ZX	 0.9510	 0.0530
ZY	 0.9680	 0.0690
ZZ	 0.9470	 0.0590