



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:59 AM EDT

PDB ID : 1CYC / pdb_00001cyc
Title : THE CRYSTAL STRUCTURE OF BONITO (KATSUO) FERROCYTOCHROME C AT 2.3 ANGSTROMS RESOLUTION. II. STRUCTURE AND FUNCTION
Authors : Tanaka, N.; Yamane, T.; Tsukihara, T.; Ashida, T.; Kakudo, M.
Deposited on : 1976-08-01
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

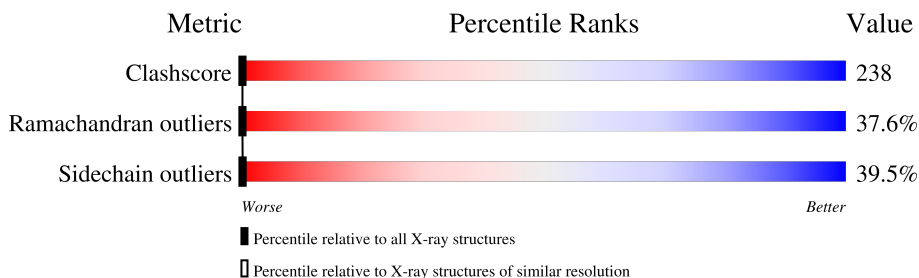
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	103	
1	B	103	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	104	X	X	X	-
2	HEC	B	104	X	X	X	-

2 Entry composition [i](#)

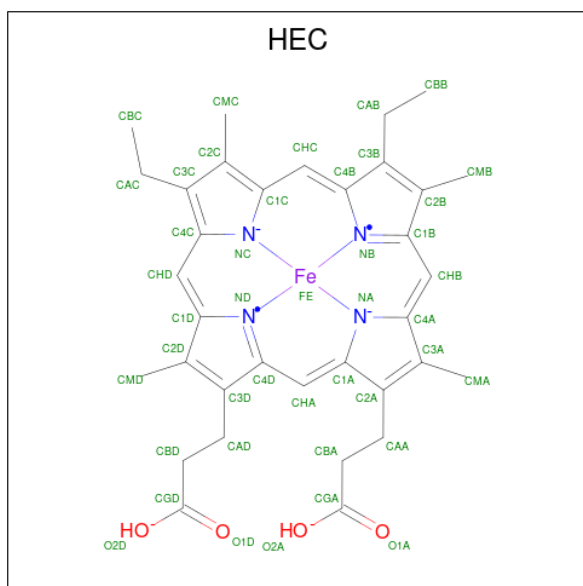
There are 3 unique types of molecules in this entry. The entry contains 1677 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 FERROCYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			795	505	139	147	4			
1	B	103	Total	C	N	O	S	0	0	0
			795	505	139	147	4			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

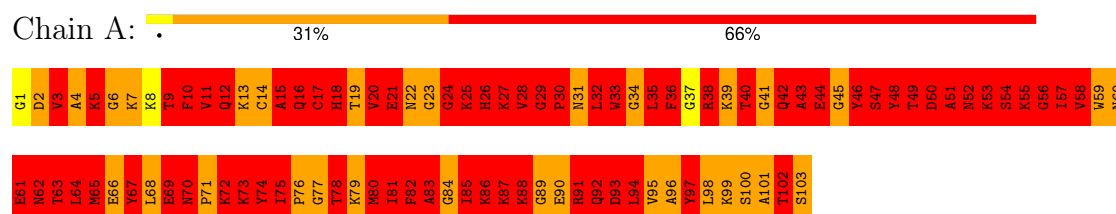
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		

3 Residue-property plots

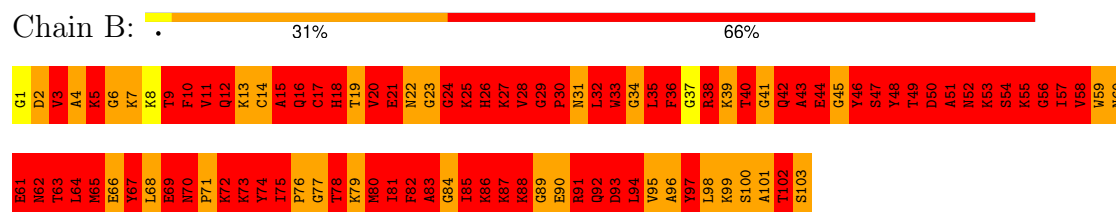
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: FERROCYTOCHROME C



• Molecule 1: FERROCYTOCHROME C



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.68Å 84.58Å 37.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1677	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC

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	A	9.78	457/811 (56.4%)	6.68	419/1084 (38.7%)
1	B	9.78	457/811 (56.4%)	6.68	419/1084 (38.7%)
All	All	9.78	914/1622 (56.4%)	6.68	838/2168 (38.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	35
1	B	2	35
All	All	4	70

All (914) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	VAL	CA-CB	108.38	2.81	1.54
1	B	3	VAL	CA-CB	108.38	2.81	1.54
1	A	49	THR	CA-C	-43.26	1.22	1.52
1	B	49	THR	CA-C	-43.26	1.22	1.52
1	A	81	ILE	C-O	30.47	1.60	1.24
1	B	81	ILE	C-O	30.47	1.60	1.24
1	A	30	PRO	N-CD	-27.27	1.09	1.47
1	B	30	PRO	N-CD	-27.27	1.09	1.47
1	A	24	GLY	N-CA	26.88	1.84	1.45
1	B	24	GLY	N-CA	26.88	1.84	1.45
1	A	43	ALA	N-CA	26.86	1.70	1.46
1	B	43	ALA	N-CA	26.86	1.70	1.46
1	A	28	VAL	CA-CB	-25.72	1.19	1.54
1	B	28	VAL	CA-CB	-25.72	1.19	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	LEU	C-O	-25.43	0.93	1.24
1	B	64	LEU	C-O	-25.43	0.93	1.24
1	A	19	THR	CB-OG1	-24.03	1.05	1.43
1	B	19	THR	CB-OG1	-24.03	1.05	1.43
1	A	64	LEU	CA-CB	23.58	1.91	1.53
1	B	64	LEU	CA-CB	23.58	1.91	1.53
1	A	63	THR	CB-OG1	-23.56	1.06	1.43
1	B	63	THR	CB-OG1	-23.56	1.06	1.43
1	A	92	GLN	N-CA	23.42	1.76	1.46
1	B	92	GLN	N-CA	23.42	1.76	1.46
1	A	46	TYR	CG-CD1	-23.29	0.90	1.39
1	B	46	TYR	CG-CD1	-23.29	0.90	1.39
1	A	98	LEU	N-CA	23.13	1.73	1.46
1	B	98	LEU	N-CA	23.13	1.73	1.46
1	A	91	ARG	NE-CZ	23.09	1.58	1.33
1	B	91	ARG	NE-CZ	23.09	1.58	1.33
1	A	44	GLU	CG-CD	22.65	2.08	1.52
1	B	44	GLU	CG-CD	22.65	2.08	1.52
1	A	83	ALA	CA-CB	22.53	1.91	1.53
1	B	83	ALA	CA-CB	22.53	1.91	1.53
1	A	92	GLN	CD-OE1	22.25	1.65	1.23
1	B	92	GLN	CD-OE1	22.25	1.65	1.23
1	A	71	PRO	N-CA	-22.01	1.19	1.47
1	B	71	PRO	N-CA	-22.01	1.19	1.47
1	A	101	ALA	N-CA	21.98	1.72	1.46
1	B	101	ALA	N-CA	21.98	1.72	1.46
1	A	10	PHE	CG-CD2	-21.81	0.93	1.38
1	B	10	PHE	CG-CD2	-21.81	0.93	1.38
1	A	91	ARG	N-CA	21.60	1.70	1.46
1	B	91	ARG	N-CA	21.60	1.70	1.46
1	A	57	ILE	CA-CB	-21.53	1.25	1.54
1	B	57	ILE	CA-CB	-21.53	1.25	1.54
1	A	3	VAL	CA-C	21.42	1.78	1.52
1	B	3	VAL	CA-C	21.42	1.78	1.52
1	A	45	GLY	C-O	21.32	1.52	1.23
1	B	45	GLY	C-O	21.32	1.52	1.23
1	A	52	ASN	CA-C	-20.82	1.24	1.52
1	B	52	ASN	CA-C	-20.82	1.24	1.52
1	A	12	GLN	CD-OE1	20.78	1.63	1.23
1	B	12	GLN	CD-OE1	20.78	1.63	1.23
1	A	38	ARG	CZ-NH1	-20.56	1.03	1.32
1	B	38	ARG	CZ-NH1	-20.56	1.03	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	HIS	CB-CG	20.43	1.78	1.50
1	B	26	HIS	CB-CG	20.43	1.78	1.50
1	A	32	LEU	C-N	-20.28	1.05	1.33
1	B	32	LEU	C-N	-20.28	1.05	1.33
1	A	16	GLN	N-CA	19.96	1.72	1.46
1	B	16	GLN	N-CA	19.96	1.72	1.46
1	A	91	ARG	CZ-NH1	19.79	1.60	1.32
1	B	91	ARG	CZ-NH1	19.79	1.60	1.32
1	A	2	ASP	CG-OD1	19.25	1.61	1.25
1	B	2	ASP	CG-OD1	19.25	1.61	1.25
1	A	82	PHE	N-CA	19.19	1.70	1.46
1	B	82	PHE	N-CA	19.19	1.70	1.46
1	A	44	GLU	CB-CG	19.09	2.09	1.52
1	B	44	GLU	CB-CG	19.09	2.09	1.52
1	A	13	LYS	C-O	-18.93	1.00	1.23
1	B	13	LYS	C-O	-18.93	1.00	1.23
1	A	62	ASN	N-CA	18.88	1.70	1.46
1	B	62	ASN	N-CA	18.88	1.70	1.46
1	A	33	TRP	CE2-CZ2	-18.85	1.00	1.39
1	B	33	TRP	CE2-CZ2	-18.85	1.00	1.39
1	A	30	PRO	CA-CB	-18.80	1.27	1.53
1	B	30	PRO	CA-CB	-18.80	1.27	1.53
1	A	98	LEU	CA-C	18.62	1.75	1.52
1	B	98	LEU	CA-C	18.62	1.75	1.52
1	A	33	TRP	N-CA	18.52	1.70	1.46
1	B	33	TRP	N-CA	18.52	1.70	1.46
1	A	2	ASP	CG-OD2	18.41	1.60	1.25
1	B	2	ASP	CG-OD2	18.41	1.60	1.25
1	A	30	PRO	C-N	18.31	1.58	1.33
1	B	30	PRO	C-N	18.31	1.58	1.33
1	A	54	SER	CA-CB	-18.26	1.22	1.53
1	B	54	SER	CA-CB	-18.26	1.22	1.53
1	A	59	TRP	C-N	-18.14	1.08	1.33
1	B	59	TRP	C-N	-18.14	1.08	1.33
1	A	32	LEU	N-CA	18.10	1.68	1.46
1	B	32	LEU	N-CA	18.10	1.68	1.46
1	A	50	ASP	C-O	17.82	1.44	1.23
1	B	50	ASP	C-O	17.82	1.44	1.23
1	A	86	LYS	C-N	-17.79	1.09	1.33
1	B	86	LYS	C-N	-17.79	1.09	1.33
1	A	93	ASP	C-N	-17.75	1.08	1.33
1	B	93	ASP	C-N	-17.75	1.08	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	TRP	N-CA	17.70	1.69	1.46
1	B	59	TRP	N-CA	17.70	1.69	1.46
1	A	59	TRP	CD2-CE2	-17.63	1.11	1.41
1	B	59	TRP	CD2-CE2	-17.63	1.11	1.41
1	A	73	LYS	CD-CE	17.48	2.04	1.52
1	B	73	LYS	CD-CE	17.48	2.04	1.52
1	A	78	THR	CA-C	-17.36	1.30	1.52
1	B	78	THR	CA-C	-17.36	1.30	1.52
1	A	17	CYS	CA-CB	17.17	1.75	1.53
1	B	17	CYS	CA-CB	17.17	1.75	1.53
1	A	8	LYS	C-O	-16.98	1.03	1.24
1	B	8	LYS	C-O	-16.98	1.03	1.24
1	A	18	HIS	N-CA	16.97	1.68	1.46
1	B	18	HIS	N-CA	16.97	1.68	1.46
1	A	100	SER	C-O	16.87	1.44	1.24
1	B	100	SER	C-O	16.87	1.44	1.24
1	A	12	GLN	CG-CD	16.70	1.93	1.52
1	B	12	GLN	CG-CD	16.70	1.93	1.52
1	A	57	ILE	C-N	16.66	1.56	1.33
1	B	57	ILE	C-N	16.66	1.56	1.33
1	A	7	LYS	N-CA	16.60	1.66	1.46
1	B	7	LYS	N-CA	16.60	1.66	1.46
1	A	49	THR	N-CA	16.42	1.63	1.46
1	B	49	THR	N-CA	16.42	1.63	1.46
1	A	22	ASN	C-N	-16.39	1.11	1.33
1	B	22	ASN	C-N	-16.39	1.11	1.33
1	A	91	ARG	CA-C	16.22	1.70	1.53
1	B	91	ARG	CA-C	16.22	1.70	1.53
1	A	65	MET	C-N	-16.12	1.14	1.33
1	B	65	MET	C-N	-16.12	1.14	1.33
1	A	55	LYS	CA-C	16.02	1.74	1.52
1	B	55	LYS	CA-C	16.02	1.74	1.52
1	A	93	ASP	CG-OD1	16.02	1.55	1.25
1	B	93	ASP	CG-OD1	16.02	1.55	1.25
1	A	56	GLY	N-CA	15.99	1.68	1.45
1	B	56	GLY	N-CA	15.99	1.68	1.45
1	A	26	HIS	CE1-NE2	-15.93	1.16	1.32
1	B	26	HIS	CE1-NE2	-15.93	1.16	1.32
1	A	46	TYR	N-CA	15.87	1.66	1.46
1	B	46	TYR	N-CA	15.87	1.66	1.46
1	A	40	THR	C-N	-15.65	1.08	1.32
1	B	40	THR	C-N	-15.65	1.08	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	THR	CA-C	15.60	1.73	1.52
1	B	102	THR	CA-C	15.60	1.73	1.52
1	A	53	LYS	N-CA	15.49	1.66	1.46
1	B	53	LYS	N-CA	15.49	1.66	1.46
1	A	61	GLU	CD-OE2	15.48	1.54	1.25
1	A	90	GLU	CD-OE2	15.48	1.54	1.25
1	B	61	GLU	CD-OE2	15.48	1.54	1.25
1	B	90	GLU	CD-OE2	15.48	1.54	1.25
1	A	62	ASN	CG-OD1	15.34	1.52	1.23
1	B	62	ASN	CG-OD1	15.34	1.52	1.23
1	A	17	CYS	CA-C	15.12	1.60	1.52
1	B	17	CYS	CA-C	15.12	1.60	1.52
1	A	18	HIS	CE1-NE2	15.11	1.47	1.32
1	B	18	HIS	CE1-NE2	15.11	1.47	1.32
1	A	46	TYR	CE2-CZ	-15.09	1.02	1.38
1	B	46	TYR	CE2-CZ	-15.09	1.02	1.38
1	A	70	ASN	CG-OD1	15.06	1.52	1.23
1	B	70	ASN	CG-OD1	15.06	1.52	1.23
1	A	65	MET	N-CA	15.02	1.64	1.46
1	B	65	MET	N-CA	15.02	1.64	1.46
1	A	51	ALA	C-O	-14.97	1.05	1.24
1	B	51	ALA	C-O	-14.97	1.05	1.24
1	A	90	GLU	C-N	-14.95	1.15	1.33
1	B	90	GLU	C-N	-14.95	1.15	1.33
1	A	12	GLN	N-CA	14.94	1.64	1.46
1	B	12	GLN	N-CA	14.94	1.64	1.46
1	A	89	GLY	C-N	-14.77	1.13	1.33
1	B	89	GLY	C-N	-14.77	1.13	1.33
1	A	61	GLU	N-CA	14.75	1.65	1.46
1	B	61	GLU	N-CA	14.75	1.65	1.46
1	A	82	PHE	C-N	-14.67	1.13	1.33
1	B	82	PHE	C-N	-14.67	1.13	1.33
1	A	49	THR	CA-CB	14.62	1.74	1.53
1	B	49	THR	CA-CB	14.62	1.74	1.53
1	A	101	ALA	CA-CB	-14.51	1.30	1.53
1	B	101	ALA	CA-CB	-14.51	1.30	1.53
1	A	91	ARG	C-O	-14.47	1.09	1.23
1	B	91	ARG	C-O	-14.47	1.09	1.23
1	A	66	GLU	C-N	-14.43	1.13	1.33
1	B	66	GLU	C-N	-14.43	1.13	1.33
1	A	77	GLY	C-N	14.41	1.52	1.33
1	B	77	GLY	C-N	14.41	1.52	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	GLU	CD-OE1	14.39	1.52	1.25
1	A	50	ASP	CG-OD1	14.39	1.52	1.25
1	A	69	GLU	CD-OE1	14.39	1.52	1.25
1	B	21	GLU	CD-OE1	14.39	1.52	1.25
1	B	50	ASP	CG-OD1	14.39	1.52	1.25
1	B	69	GLU	CD-OE1	14.39	1.52	1.25
1	A	102	THR	N-CA	14.38	1.64	1.46
1	B	102	THR	N-CA	14.38	1.64	1.46
1	A	81	ILE	N-CA	14.32	1.64	1.46
1	B	81	ILE	N-CA	14.32	1.64	1.46
1	A	46	TYR	C-N	-14.30	1.13	1.33
1	B	46	TYR	C-N	-14.30	1.13	1.33
1	A	21	GLU	CD-OE2	14.19	1.52	1.25
1	B	21	GLU	CD-OE2	14.19	1.52	1.25
1	A	80	MET	SD-CE	-14.12	1.44	1.79
1	B	80	MET	SD-CE	-14.12	1.44	1.79
1	A	82	PHE	CG-CD2	-13.94	1.09	1.38
1	B	82	PHE	CG-CD2	-13.94	1.09	1.38
1	A	46	TYR	CZ-OH	-13.91	1.08	1.38
1	B	46	TYR	CZ-OH	-13.91	1.08	1.38
1	A	11	VAL	CA-C	13.78	1.72	1.52
1	B	11	VAL	CA-C	13.78	1.72	1.52
1	A	71	PRO	CA-CB	-13.75	1.34	1.53
1	B	71	PRO	CA-CB	-13.75	1.34	1.53
1	A	62	ASN	CA-CB	-13.69	1.30	1.53
1	B	62	ASN	CA-CB	-13.69	1.30	1.53
1	A	26	HIS	CG-CD2	-13.67	1.20	1.35
1	B	26	HIS	CG-CD2	-13.67	1.20	1.35
1	A	37	GLY	CA-C	-13.57	1.32	1.51
1	B	37	GLY	CA-C	-13.57	1.32	1.51
1	A	3	VAL	C-O	-13.53	1.08	1.24
1	B	3	VAL	C-O	-13.53	1.08	1.24
1	A	42	GLN	CD-NE2	13.48	1.61	1.33
1	B	42	GLN	CD-NE2	13.48	1.61	1.33
1	A	47	SER	CB-OG	13.44	1.69	1.42
1	B	47	SER	CB-OG	13.44	1.69	1.42
1	A	89	GLY	N-CA	13.35	1.64	1.45
1	B	89	GLY	N-CA	13.35	1.64	1.45
1	A	47	SER	N-CA	13.34	1.63	1.46
1	B	47	SER	N-CA	13.34	1.63	1.46
1	A	100	SER	N-CA	13.28	1.62	1.46
1	B	100	SER	N-CA	13.28	1.62	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	ILE	C-N	13.23	1.48	1.33
1	B	75	ILE	C-N	13.23	1.48	1.33
1	A	21	GLU	N-CA	13.20	1.64	1.45
1	B	21	GLU	N-CA	13.20	1.64	1.45
1	A	98	LEU	CB-CG	-13.19	1.27	1.53
1	B	98	LEU	CB-CG	-13.19	1.27	1.53
1	A	60	ASN	C-N	-13.18	1.15	1.33
1	B	60	ASN	C-N	-13.18	1.15	1.33
1	A	7	LYS	C-O	13.15	1.39	1.24
1	B	7	LYS	C-O	13.15	1.39	1.24
1	A	14	CYS	N-CA	13.01	1.63	1.46
1	B	14	CYS	N-CA	13.01	1.63	1.46
1	A	18	HIS	ND1-CE1	12.94	1.45	1.32
1	B	18	HIS	ND1-CE1	12.94	1.45	1.32
1	A	31	ASN	CG-OD1	12.90	1.48	1.23
1	B	31	ASN	CG-OD1	12.90	1.48	1.23
1	A	61	GLU	CA-C	12.83	1.70	1.52
1	B	61	GLU	CA-C	12.83	1.70	1.52
1	A	99	LYS	CA-C	12.79	1.70	1.52
1	B	99	LYS	CA-C	12.79	1.70	1.52
1	A	16	GLN	CD-OE1	12.69	1.47	1.23
1	B	16	GLN	CD-OE1	12.69	1.47	1.23
1	A	60	ASN	CA-C	12.64	1.70	1.52
1	B	60	ASN	CA-C	12.64	1.70	1.52
1	A	60	ASN	CG-OD1	12.62	1.47	1.23
1	B	60	ASN	CG-OD1	12.62	1.47	1.23
1	A	58	VAL	CA-CB	-12.60	1.37	1.54
1	B	58	VAL	CA-CB	-12.60	1.37	1.54
1	A	33	TRP	CZ2-CH2	-12.59	1.13	1.37
1	B	33	TRP	CZ2-CH2	-12.59	1.13	1.37
1	A	20	VAL	CA-C	12.54	1.68	1.52
1	B	20	VAL	CA-C	12.54	1.68	1.52
1	A	81	ILE	CA-CB	-12.50	1.37	1.54
1	B	81	ILE	CA-CB	-12.50	1.37	1.54
1	A	19	THR	N-CA	12.49	1.62	1.46
1	B	19	THR	N-CA	12.49	1.62	1.46
1	A	12	GLN	CA-C	12.47	1.68	1.52
1	B	12	GLN	CA-C	12.47	1.68	1.52
1	A	103	SER	C-O	12.46	1.48	1.23
1	B	103	SER	C-O	12.46	1.48	1.23
1	A	90	GLU	CD-OE1	12.45	1.49	1.25
1	B	90	GLU	CD-OE1	12.45	1.49	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	GLN	C-N	-12.43	1.16	1.33
1	B	12	GLN	C-N	-12.43	1.16	1.33
1	A	52	ASN	C-O	12.41	1.39	1.24
1	B	52	ASN	C-O	12.41	1.39	1.24
1	A	42	GLN	CD-OE1	12.40	1.47	1.23
1	B	42	GLN	CD-OE1	12.40	1.47	1.23
1	A	9	THR	N-CA	12.36	1.61	1.46
1	B	9	THR	N-CA	12.36	1.61	1.46
1	A	19	THR	C-N	-12.27	1.17	1.33
1	B	19	THR	C-N	-12.27	1.17	1.33
1	A	77	GLY	C-O	-12.26	1.07	1.23
1	B	77	GLY	C-O	-12.26	1.07	1.23
1	A	88	LYS	CD-CE	-12.17	1.16	1.52
1	B	88	LYS	CD-CE	-12.17	1.16	1.52
1	A	60	ASN	N-CA	12.08	1.63	1.46
1	B	60	ASN	N-CA	12.08	1.63	1.46
1	A	48	TYR	C-O	-12.02	1.08	1.24
1	A	63	THR	C-O	-12.02	1.08	1.24
1	B	48	TYR	C-O	-12.02	1.08	1.24
1	B	63	THR	C-O	-12.02	1.08	1.24
1	A	33	TRP	CZ3-CH2	-11.99	1.10	1.40
1	B	33	TRP	CZ3-CH2	-11.99	1.10	1.40
1	A	44	GLU	CD-OE2	11.88	1.48	1.25
1	B	44	GLU	CD-OE2	11.88	1.48	1.25
1	A	97	TYR	C-N	-11.83	1.18	1.33
1	B	97	TYR	C-N	-11.83	1.18	1.33
1	A	90	GLU	N-CA	11.76	1.60	1.46
1	B	90	GLU	N-CA	11.76	1.60	1.46
1	A	50	ASP	CA-CB	-11.71	1.34	1.53
1	B	50	ASP	CA-CB	-11.71	1.34	1.53
1	A	54	SER	C-N	-11.71	1.17	1.33
1	B	54	SER	C-N	-11.71	1.17	1.33
1	A	40	THR	N-CA	11.67	1.60	1.46
1	A	68	LEU	CA-CB	-11.67	1.34	1.53
1	B	40	THR	N-CA	11.67	1.60	1.46
1	B	68	LEU	CA-CB	-11.67	1.34	1.53
1	A	31	ASN	C-N	-11.57	1.20	1.33
1	B	31	ASN	C-N	-11.57	1.20	1.33
1	A	7	LYS	CA-CB	11.52	1.71	1.53
1	B	7	LYS	CA-CB	11.52	1.71	1.53
1	A	80	MET	N-CA	11.50	1.60	1.46
1	B	80	MET	N-CA	11.50	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	TYR	CG-CD2	-11.48	1.15	1.39
1	B	48	TYR	CG-CD2	-11.48	1.15	1.39
1	A	55	LYS	C-N	-11.45	1.16	1.33
1	B	55	LYS	C-N	-11.45	1.16	1.33
1	A	83	ALA	C-O	-11.44	1.09	1.24
1	B	83	ALA	C-O	-11.44	1.09	1.24
1	A	23	GLY	N-CA	11.38	1.61	1.45
1	B	23	GLY	N-CA	11.38	1.61	1.45
1	A	10	PHE	C-N	11.21	1.47	1.33
1	B	10	PHE	C-N	11.21	1.47	1.33
1	A	42	GLN	CG-CD	-11.13	1.24	1.52
1	B	42	GLN	CG-CD	-11.13	1.24	1.52
1	A	14	CYS	CA-CB	11.11	1.71	1.53
1	B	14	CYS	CA-CB	11.11	1.71	1.53
1	A	8	LYS	C-N	-11.11	1.18	1.33
1	B	8	LYS	C-N	-11.11	1.18	1.33
1	A	41	GLY	C-O	-11.04	1.07	1.23
1	B	41	GLY	C-O	-11.04	1.07	1.23
1	A	93	ASP	CG-OD2	11.03	1.46	1.25
1	B	93	ASP	CG-OD2	11.03	1.46	1.25
1	A	3	VAL	N-CA	11.01	1.59	1.46
1	B	3	VAL	N-CA	11.01	1.59	1.46
1	A	48	TYR	CA-C	-10.99	1.38	1.52
1	B	48	TYR	CA-C	-10.99	1.38	1.52
1	A	67	TYR	CE1-CZ	-10.98	1.11	1.38
1	B	67	TYR	CE1-CZ	-10.98	1.11	1.38
1	A	74	TYR	CA-CB	10.86	1.71	1.53
1	B	74	TYR	CA-CB	10.86	1.71	1.53
1	A	16	GLN	CD-NE2	-10.85	1.10	1.33
1	B	16	GLN	CD-NE2	-10.85	1.10	1.33
1	A	38	ARG	C-O	-10.82	1.11	1.23
1	B	38	ARG	C-O	-10.82	1.11	1.23
1	A	79	LYS	CA-CB	-10.72	1.36	1.53
1	B	79	LYS	CA-CB	-10.72	1.36	1.53
1	A	93	ASP	C-O	10.71	1.36	1.24
1	B	93	ASP	C-O	10.71	1.36	1.24
1	A	18	HIS	C-O	10.70	1.37	1.24
1	B	18	HIS	C-O	10.70	1.37	1.24
1	A	98	LEU	CA-CB	-10.64	1.36	1.53
1	B	98	LEU	CA-CB	-10.64	1.36	1.53
1	A	35	LEU	C-N	-10.62	1.18	1.33
1	B	35	LEU	C-N	-10.62	1.18	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	VAL	CA-C	10.57	1.66	1.52
1	B	58	VAL	CA-C	10.57	1.66	1.52
1	A	32	LEU	CA-CB	-10.55	1.36	1.52
1	B	32	LEU	CA-CB	-10.55	1.36	1.52
1	A	32	LEU	C-O	10.41	1.41	1.23
1	B	32	LEU	C-O	10.41	1.41	1.23
1	A	95	VAL	C-O	10.28	1.36	1.24
1	B	95	VAL	C-O	10.28	1.36	1.24
1	A	67	TYR	CA-C	-10.27	1.39	1.52
1	B	67	TYR	CA-C	-10.27	1.39	1.52
1	A	61	GLU	C-N	-10.27	1.19	1.33
1	A	101	ALA	C-N	-10.27	1.19	1.33
1	B	61	GLU	C-N	-10.27	1.19	1.33
1	B	101	ALA	C-N	-10.27	1.19	1.33
1	A	11	VAL	C-N	-10.26	1.20	1.33
1	B	11	VAL	C-N	-10.26	1.20	1.33
1	A	24	GLY	C-O	10.25	1.37	1.23
1	B	24	GLY	C-O	10.25	1.37	1.23
1	A	44	GLU	C-O	10.24	1.36	1.24
1	B	44	GLU	C-O	10.24	1.36	1.24
1	A	26	HIS	CG-ND1	-10.16	1.27	1.38
1	B	26	HIS	CG-ND1	-10.16	1.27	1.38
1	A	77	GLY	CA-C	10.14	1.66	1.51
1	B	77	GLY	CA-C	10.14	1.66	1.51
1	A	96	ALA	N-CA	10.14	1.58	1.46
1	B	96	ALA	N-CA	10.14	1.58	1.46
1	A	16	GLN	C-O	10.13	1.36	1.24
1	A	40	THR	CB-OG1	10.13	1.59	1.43
1	A	42	GLN	C-O	10.13	1.36	1.24
1	B	16	GLN	C-O	10.13	1.36	1.24
1	B	40	THR	CB-OG1	10.13	1.59	1.43
1	B	42	GLN	C-O	10.13	1.36	1.24
1	A	64	LEU	CA-C	10.11	1.66	1.52
1	B	64	LEU	CA-C	10.11	1.66	1.52
1	A	62	ASN	CA-C	10.10	1.66	1.52
1	B	62	ASN	CA-C	10.10	1.66	1.52
1	A	24	GLY	C-N	10.07	1.47	1.33
1	B	24	GLY	C-N	10.07	1.47	1.33
1	A	36	PHE	CA-CB	10.04	1.70	1.53
1	B	36	PHE	CA-CB	10.04	1.70	1.53
1	A	102	THR	C-N	-10.02	1.19	1.33
1	B	102	THR	C-N	-10.02	1.19	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	THR	C-O	9.96	1.35	1.23
1	B	78	THR	C-O	9.96	1.35	1.23
1	A	80	MET	C-N	-9.92	1.20	1.33
1	B	80	MET	C-N	-9.92	1.20	1.33
1	A	59	TRP	CA-CB	-9.90	1.36	1.53
1	B	59	TRP	CA-CB	-9.90	1.36	1.53
1	A	64	LEU	CG-CD1	-9.87	1.20	1.52
1	B	64	LEU	CG-CD1	-9.87	1.20	1.52
1	A	100	SER	CA-CB	9.86	1.69	1.53
1	B	100	SER	CA-CB	9.86	1.69	1.53
1	A	26	HIS	CD2-NE2	-9.79	1.27	1.37
1	A	80	MET	C-O	-9.79	1.11	1.24
1	B	26	HIS	CD2-NE2	-9.79	1.27	1.37
1	B	80	MET	C-O	-9.79	1.11	1.24
1	A	26	HIS	C-N	-9.79	1.20	1.33
1	A	50	ASP	C-N	-9.79	1.20	1.33
1	B	26	HIS	C-N	-9.79	1.20	1.33
1	B	50	ASP	C-N	-9.79	1.20	1.33
1	A	54	SER	C-O	-9.72	1.11	1.24
1	B	54	SER	C-O	-9.72	1.11	1.24
1	A	79	LYS	CA-C	9.61	1.70	1.52
1	B	79	LYS	CA-C	9.61	1.70	1.52
1	A	69	GLU	CA-CB	-9.56	1.37	1.53
1	B	69	GLU	CA-CB	-9.56	1.37	1.53
1	A	38	ARG	CA-CB	-9.53	1.37	1.53
1	B	38	ARG	CA-CB	-9.53	1.37	1.53
1	A	65	MET	C-O	-9.52	1.13	1.24
1	B	65	MET	C-O	-9.52	1.13	1.24
1	A	75	ILE	N-CA	-9.42	1.34	1.46
1	B	75	ILE	N-CA	-9.42	1.34	1.46
1	A	85	ILE	CB-CG1	9.42	1.72	1.53
1	B	85	ILE	CB-CG1	9.42	1.72	1.53
1	A	69	GLU	N-CA	9.41	1.58	1.46
1	B	69	GLU	N-CA	9.41	1.58	1.46
1	A	67	TYR	C-N	-9.40	1.22	1.33
1	B	67	TYR	C-N	-9.40	1.22	1.33
1	A	19	THR	CA-C	9.38	1.65	1.52
1	A	67	TYR	N-CA	9.38	1.57	1.46
1	B	19	THR	CA-C	9.38	1.65	1.52
1	B	67	TYR	N-CA	9.38	1.57	1.46
1	A	86	LYS	CG-CD	9.32	1.80	1.52
1	B	86	LYS	CG-CD	9.32	1.80	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	ASP	CA-CB	9.30	1.69	1.53
1	B	2	ASP	CA-CB	9.30	1.69	1.53
1	A	30	PRO	C-O	-9.27	1.11	1.24
1	B	30	PRO	C-O	-9.27	1.11	1.24
1	A	21	GLU	CA-C	9.26	1.65	1.53
1	A	33	TRP	CG-CD2	-9.26	1.27	1.43
1	B	21	GLU	CA-C	9.26	1.65	1.53
1	B	33	TRP	CG-CD2	-9.26	1.27	1.43
1	A	11	VAL	CA-CB	-9.23	1.41	1.54
1	B	11	VAL	CA-CB	-9.23	1.41	1.54
1	A	10	PHE	CD2-CE2	-9.21	1.11	1.38
1	A	30	PRO	CB-CG	-9.21	1.03	1.49
1	B	10	PHE	CD2-CE2	-9.21	1.11	1.38
1	B	30	PRO	CB-CG	-9.21	1.03	1.49
1	A	13	LYS	C-N	-9.20	1.22	1.33
1	B	13	LYS	C-N	-9.20	1.22	1.33
1	A	69	GLU	C-N	-9.18	1.14	1.33
1	B	69	GLU	C-N	-9.18	1.14	1.33
1	A	16	GLN	CA-CB	-9.13	1.38	1.53
1	B	16	GLN	CA-CB	-9.13	1.38	1.53
1	A	4	ALA	N-CA	9.12	1.57	1.46
1	B	4	ALA	N-CA	9.12	1.57	1.46
1	A	78	THR	C-N	-9.11	1.18	1.33
1	B	78	THR	C-N	-9.11	1.18	1.33
1	A	3	VAL	C-N	-9.08	1.21	1.33
1	B	3	VAL	C-N	-9.08	1.21	1.33
1	A	66	GLU	CA-C	9.05	1.65	1.52
1	B	66	GLU	CA-C	9.05	1.65	1.52
1	A	50	ASP	CB-CG	-8.99	1.29	1.52
1	B	50	ASP	CB-CG	-8.99	1.29	1.52
1	A	10	PHE	C-O	-8.91	1.13	1.24
1	B	10	PHE	C-O	-8.91	1.13	1.24
1	A	95	VAL	N-CA	8.88	1.57	1.46
1	B	95	VAL	N-CA	8.88	1.57	1.46
1	A	29	GLY	N-CA	-8.84	1.32	1.44
1	B	29	GLY	N-CA	-8.84	1.32	1.44
1	A	88	LYS	C-N	8.77	1.46	1.33
1	B	88	LYS	C-N	8.77	1.46	1.33
1	A	2	ASP	C-N	-8.76	1.23	1.33
1	B	2	ASP	C-N	-8.76	1.23	1.33
1	A	34	GLY	C-O	8.74	1.35	1.23
1	B	34	GLY	C-O	8.74	1.35	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	VAL	CA-CB	-8.73	1.42	1.54
1	A	53	LYS	C-O	8.73	1.34	1.24
1	B	20	VAL	CA-CB	-8.73	1.42	1.54
1	B	53	LYS	C-O	8.73	1.34	1.24
1	A	66	GLU	CD-OE1	8.70	1.41	1.25
1	B	66	GLU	CD-OE1	8.70	1.41	1.25
1	A	63	THR	CA-C	8.66	1.64	1.52
1	B	63	THR	CA-C	8.66	1.64	1.52
1	A	53	LYS	CD-CE	8.62	1.78	1.52
1	B	53	LYS	CD-CE	8.62	1.78	1.52
1	A	27	LYS	CG-CD	-8.61	1.26	1.52
1	B	27	LYS	CG-CD	-8.61	1.26	1.52
1	A	66	GLU	N-CA	-8.57	1.36	1.46
1	B	66	GLU	N-CA	-8.57	1.36	1.46
1	A	13	LYS	CA-CB	-8.55	1.41	1.54
1	B	13	LYS	CA-CB	-8.55	1.41	1.54
1	A	23	GLY	CA-C	8.50	1.63	1.51
1	B	23	GLY	CA-C	8.50	1.63	1.51
1	A	20	VAL	CB-CG1	-8.44	1.24	1.52
1	A	32	LEU	CG-CD2	-8.44	1.24	1.52
1	B	20	VAL	CB-CG1	-8.44	1.24	1.52
1	B	32	LEU	CG-CD2	-8.44	1.24	1.52
1	A	61	GLU	CD-OE1	8.41	1.41	1.25
1	B	61	GLU	CD-OE1	8.41	1.41	1.25
1	A	80	MET	CG-SD	8.40	2.01	1.80
1	B	80	MET	CG-SD	8.40	2.01	1.80
1	A	28	VAL	CA-C	-8.34	1.42	1.52
1	B	28	VAL	CA-C	-8.34	1.42	1.52
1	A	40	THR	CA-CB	8.33	1.65	1.53
1	B	40	THR	CA-CB	8.33	1.65	1.53
1	A	81	ILE	C-N	-8.32	1.20	1.33
1	B	81	ILE	C-N	-8.32	1.20	1.33
1	A	39	LYS	CA-CB	8.29	1.65	1.53
1	B	39	LYS	CA-CB	8.29	1.65	1.53
1	A	86	LYS	CD-CE	8.28	1.77	1.52
1	B	86	LYS	CD-CE	8.28	1.77	1.52
1	A	29	GLY	C-O	8.27	1.35	1.24
1	B	29	GLY	C-O	8.27	1.35	1.24
1	A	73	LYS	CE-NZ	-8.27	1.24	1.49
1	B	73	LYS	CE-NZ	-8.27	1.24	1.49
1	A	39	LYS	C-N	-8.24	1.22	1.33
1	B	39	LYS	C-N	-8.24	1.22	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	PHE	CE2-CZ	-8.21	1.14	1.38
1	B	82	PHE	CE2-CZ	-8.21	1.14	1.38
1	A	11	VAL	N-CA	-8.20	1.35	1.46
1	B	11	VAL	N-CA	-8.20	1.35	1.46
1	A	19	THR	CA-CB	-8.19	1.39	1.53
1	B	19	THR	CA-CB	-8.19	1.39	1.53
1	A	15	ALA	C-N	-8.15	1.22	1.33
1	B	15	ALA	C-N	-8.15	1.22	1.33
1	A	59	TRP	CD2-CE3	-8.13	1.27	1.40
1	B	59	TRP	CD2-CE3	-8.13	1.27	1.40
1	A	52	ASN	N-CA	-8.12	1.35	1.46
1	B	52	ASN	N-CA	-8.12	1.35	1.46
1	A	43	ALA	C-O	-8.05	1.14	1.24
1	B	43	ALA	C-O	-8.05	1.14	1.24
1	A	44	GLU	N-CA	8.04	1.56	1.46
1	B	44	GLU	N-CA	8.04	1.56	1.46
1	A	71	PRO	N-CD	8.00	1.58	1.47
1	B	71	PRO	N-CD	8.00	1.58	1.47
1	A	67	TYR	C-O	-7.98	1.14	1.24
1	B	67	TYR	C-O	-7.98	1.14	1.24
1	A	86	LYS	CA-CB	7.92	1.63	1.53
1	B	86	LYS	CA-CB	7.92	1.63	1.53
1	A	78	THR	N-CA	7.92	1.55	1.46
1	B	78	THR	N-CA	7.92	1.55	1.46
1	A	33	TRP	C-O	-7.90	1.14	1.24
1	A	97	TYR	CA-C	7.90	1.63	1.52
1	B	33	TRP	C-O	-7.90	1.14	1.24
1	B	97	TYR	CA-C	7.90	1.63	1.52
1	A	91	ARG	CZ-NH2	7.88	1.43	1.33
1	B	91	ARG	CZ-NH2	7.88	1.43	1.33
1	A	36	PHE	N-CA	7.84	1.56	1.46
1	B	36	PHE	N-CA	7.84	1.56	1.46
1	A	25	LYS	C-N	7.84	1.44	1.33
1	B	25	LYS	C-N	7.84	1.44	1.33
1	A	27	LYS	CA-CB	7.80	1.66	1.53
1	B	27	LYS	CA-CB	7.80	1.66	1.53
1	A	28	VAL	N-CA	7.76	1.56	1.46
1	B	28	VAL	N-CA	7.76	1.56	1.46
1	A	89	GLY	CA-C	7.74	1.62	1.51
1	B	89	GLY	CA-C	7.74	1.62	1.51
1	A	16	GLN	CA-C	-7.60	1.42	1.52
1	B	16	GLN	CA-C	-7.60	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	TRP	CZ3-CH2	-7.59	1.21	1.40
1	B	59	TRP	CZ3-CH2	-7.59	1.21	1.40
1	A	5	LYS	CG-CD	7.57	1.75	1.52
1	B	5	LYS	CG-CD	7.57	1.75	1.52
1	A	48	TYR	CE1-CZ	-7.54	1.20	1.38
1	B	48	TYR	CE1-CZ	-7.54	1.20	1.38
1	A	37	GLY	C-O	7.54	1.34	1.23
1	B	37	GLY	C-O	7.54	1.34	1.23
1	A	64	LEU	N-CA	7.53	1.55	1.46
1	B	64	LEU	N-CA	7.53	1.55	1.46
1	A	95	VAL	CA-C	7.52	1.62	1.52
1	B	95	VAL	CA-C	7.52	1.62	1.52
1	A	29	GLY	C-N	7.50	1.51	1.33
1	B	29	GLY	C-N	7.50	1.51	1.33
1	A	37	GLY	C-N	7.50	1.42	1.33
1	B	37	GLY	C-N	7.50	1.42	1.33
1	A	71	PRO	C-N	-7.48	1.22	1.33
1	B	71	PRO	C-N	-7.48	1.22	1.33
1	A	103	SER	C-OXT	7.46	1.38	1.23
1	B	103	SER	C-OXT	7.46	1.38	1.23
1	A	89	GLY	C-O	-7.46	1.13	1.23
1	B	89	GLY	C-O	-7.46	1.13	1.23
1	A	26	HIS	C-O	7.43	1.33	1.24
1	B	26	HIS	C-O	7.43	1.33	1.24
1	A	58	VAL	C-O	-7.42	1.15	1.24
1	B	58	VAL	C-O	-7.42	1.15	1.24
1	A	6	GLY	N-CA	7.36	1.56	1.45
1	A	90	GLU	CA-C	7.36	1.62	1.52
1	B	6	GLY	N-CA	7.36	1.56	1.45
1	B	90	GLU	CA-C	7.36	1.62	1.52
1	A	64	LEU	C-N	-7.36	1.24	1.33
1	B	64	LEU	C-N	-7.36	1.24	1.33
1	A	36	PHE	CD2-CE2	-7.34	1.16	1.38
1	B	36	PHE	CD2-CE2	-7.34	1.16	1.38
1	A	2	ASP	N-CA	7.34	1.55	1.46
1	B	2	ASP	N-CA	7.34	1.55	1.46
1	A	49	THR	CB-CG2	-7.29	1.28	1.52
1	A	56	GLY	C-N	7.29	1.43	1.33
1	B	49	THR	CB-CG2	-7.29	1.28	1.52
1	B	56	GLY	C-N	7.29	1.43	1.33
1	A	76	PRO	CB-CG	-7.26	1.13	1.49
1	B	76	PRO	CB-CG	-7.26	1.13	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	CYS	N-CA	7.26	1.54	1.45
1	B	17	CYS	N-CA	7.26	1.54	1.45
1	A	74	TYR	C-N	-7.25	1.25	1.33
1	B	74	TYR	C-N	-7.25	1.25	1.33
1	A	82	PHE	CA-C	-7.24	1.43	1.52
1	B	82	PHE	CA-C	-7.24	1.43	1.52
1	A	26	HIS	CA-C	7.20	1.62	1.52
1	B	26	HIS	CA-C	7.20	1.62	1.52
1	A	51	ALA	CA-CB	-7.19	1.41	1.53
1	B	51	ALA	CA-CB	-7.19	1.41	1.53
1	A	93	ASP	CA-CB	7.19	1.64	1.53
1	B	93	ASP	CA-CB	7.19	1.64	1.53
1	A	97	TYR	C-O	7.17	1.32	1.24
1	B	97	TYR	C-O	7.17	1.32	1.24
1	A	96	ALA	C-N	-7.12	1.25	1.33
1	B	96	ALA	C-N	-7.12	1.25	1.33
1	A	59	TRP	CE2-CZ2	7.10	1.54	1.39
1	B	59	TRP	CE2-CZ2	7.10	1.54	1.39
1	A	99	LYS	C-N	-7.05	1.24	1.33
1	B	99	LYS	C-N	-7.05	1.24	1.33
1	A	33	TRP	CD2-CE2	-7.03	1.29	1.41
1	B	33	TRP	CD2-CE2	-7.03	1.29	1.41
1	A	48	TYR	CA-CB	7.02	1.65	1.53
1	B	48	TYR	CA-CB	7.02	1.65	1.53
1	A	30	PRO	CG-CD	-6.96	1.27	1.50
1	B	30	PRO	CG-CD	-6.96	1.27	1.50
1	A	82	PHE	CA-CB	-6.95	1.36	1.53
1	B	82	PHE	CA-CB	-6.95	1.36	1.53
1	A	75	ILE	CA-CB	-6.94	1.45	1.54
1	B	75	ILE	CA-CB	-6.94	1.45	1.54
1	A	86	LYS	CA-C	6.94	1.62	1.52
1	B	86	LYS	CA-C	6.94	1.62	1.52
1	A	17	CYS	C-N	-6.88	1.24	1.33
1	B	17	CYS	C-N	-6.88	1.24	1.33
1	A	47	SER	CA-CB	-6.86	1.41	1.53
1	A	92	GLN	CA-CB	-6.86	1.41	1.53
1	B	47	SER	CA-CB	-6.86	1.41	1.53
1	B	92	GLN	CA-CB	-6.86	1.41	1.53
1	A	22	ASN	CA-C	-6.85	1.43	1.52
1	B	22	ASN	CA-C	-6.85	1.43	1.52
1	A	73	LYS	C-O	6.84	1.32	1.24
1	B	73	LYS	C-O	6.84	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	GLN	CG-CD	6.84	1.69	1.52
1	B	16	GLN	CG-CD	6.84	1.69	1.52
1	A	82	PHE	CG-CD1	-6.81	1.24	1.38
1	B	82	PHE	CG-CD1	-6.81	1.24	1.38
1	A	93	ASP	CA-C	-6.81	1.43	1.52
1	B	93	ASP	CA-C	-6.81	1.43	1.52
1	A	55	LYS	CD-CE	6.81	1.72	1.52
1	B	55	LYS	CD-CE	6.81	1.72	1.52
1	A	73	LYS	N-CA	6.75	1.54	1.46
1	B	73	LYS	N-CA	6.75	1.54	1.46
1	A	18	HIS	CA-C	6.75	1.61	1.52
1	A	88	LYS	CA-C	6.75	1.61	1.52
1	B	18	HIS	CA-C	6.75	1.61	1.52
1	B	88	LYS	CA-C	6.75	1.61	1.52
1	A	52	ASN	CG-ND2	6.73	1.47	1.33
1	A	70	ASN	CG-ND2	6.73	1.47	1.33
1	B	52	ASN	CG-ND2	6.73	1.47	1.33
1	B	70	ASN	CG-ND2	6.73	1.47	1.33
1	A	23	GLY	C-N	6.70	1.43	1.33
1	B	23	GLY	C-N	6.70	1.43	1.33
1	A	38	ARG	CD-NE	-6.69	1.36	1.46
1	A	49	THR	C-O	6.69	1.32	1.23
1	B	38	ARG	CD-NE	-6.69	1.36	1.46
1	B	49	THR	C-O	6.69	1.32	1.23
1	A	16	GLN	C-N	-6.67	1.25	1.34
1	B	16	GLN	C-N	-6.67	1.25	1.34
1	A	25	LYS	CA-CB	6.67	1.64	1.53
1	B	25	LYS	CA-CB	6.67	1.64	1.53
1	A	12	GLN	CD-NE2	-6.63	1.19	1.33
1	B	12	GLN	CD-NE2	-6.63	1.19	1.33
1	A	96	ALA	CA-C	-6.63	1.44	1.52
1	A	96	ALA	C-O	6.63	1.31	1.24
1	B	96	ALA	CA-C	-6.63	1.44	1.52
1	B	96	ALA	C-O	6.63	1.31	1.24
1	A	42	GLN	CB-CG	-6.62	1.32	1.52
1	A	73	LYS	CG-CD	-6.62	1.32	1.52
1	B	42	GLN	CB-CG	-6.62	1.32	1.52
1	B	73	LYS	CG-CD	-6.62	1.32	1.52
1	A	31	ASN	C-O	6.60	1.31	1.23
1	B	31	ASN	C-O	6.60	1.31	1.23
1	A	64	LEU	CG-CD2	-6.59	1.30	1.52
1	B	64	LEU	CG-CD2	-6.59	1.30	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GLU	C-O	-6.58	1.16	1.24
1	B	66	GLU	C-O	-6.58	1.16	1.24
1	A	87	LYS	N-CA	6.57	1.54	1.46
1	B	87	LYS	N-CA	6.57	1.54	1.46
1	A	21	GLU	C-O	-6.56	1.15	1.24
1	B	21	GLU	C-O	-6.56	1.15	1.24
1	A	81	ILE	CB-CG1	-6.56	1.40	1.53
1	B	81	ILE	CB-CG1	-6.56	1.40	1.53
1	A	50	ASP	CA-C	-6.53	1.44	1.52
1	B	50	ASP	CA-C	-6.53	1.44	1.52
1	A	12	GLN	CA-CB	-6.48	1.43	1.53
1	B	12	GLN	CA-CB	-6.48	1.43	1.53
1	A	72	LYS	CE-NZ	6.40	1.68	1.49
1	B	72	LYS	CE-NZ	6.40	1.68	1.49
1	A	79	LYS	CE-NZ	-6.39	1.30	1.49
1	B	79	LYS	CE-NZ	-6.39	1.30	1.49
1	A	74	TYR	C-O	-6.39	1.16	1.24
1	B	74	TYR	C-O	-6.39	1.16	1.24
1	A	9	THR	C-O	6.38	1.31	1.24
1	B	9	THR	C-O	6.38	1.31	1.24
1	A	68	LEU	CB-CG	6.36	1.66	1.53
1	A	88	LYS	C-O	6.36	1.31	1.24
1	B	68	LEU	CB-CG	6.36	1.66	1.53
1	B	88	LYS	C-O	6.36	1.31	1.24
1	A	42	GLN	CA-C	-6.36	1.44	1.52
1	B	42	GLN	CA-C	-6.36	1.44	1.52
1	A	62	ASN	C-N	6.35	1.42	1.33
1	B	62	ASN	C-N	6.35	1.42	1.33
1	A	59	TRP	CZ2-CH2	-6.35	1.25	1.37
1	B	59	TRP	CZ2-CH2	-6.35	1.25	1.37
1	A	25	LYS	N-CA	6.35	1.54	1.46
1	B	25	LYS	N-CA	6.35	1.54	1.46
1	A	103	SER	CA-C	-6.35	1.39	1.52
1	B	103	SER	CA-C	-6.35	1.39	1.52
1	A	33	TRP	CD2-CE3	-6.30	1.30	1.40
1	B	33	TRP	CD2-CE3	-6.30	1.30	1.40
1	A	33	TRP	CB-CG	-6.28	1.30	1.50
1	B	33	TRP	CB-CG	-6.28	1.30	1.50
1	A	8	LYS	CA-C	6.24	1.61	1.52
1	B	8	LYS	CA-C	6.24	1.61	1.52
1	A	75	ILE	CB-CG1	6.18	1.65	1.53
1	A	94	LEU	CB-CG	6.18	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	ILE	CB-CG1	6.18	1.65	1.53
1	B	94	LEU	CB-CG	6.18	1.65	1.53
1	A	10	PHE	N-CA	-6.16	1.39	1.46
1	B	10	PHE	N-CA	-6.16	1.39	1.46
1	A	76	PRO	C-O	6.13	1.31	1.23
1	B	76	PRO	C-O	6.13	1.31	1.23
1	A	5	LYS	CE-NZ	6.13	1.67	1.49
1	B	5	LYS	CE-NZ	6.13	1.67	1.49
1	A	62	ASN	CB-CG	-6.12	1.36	1.52
1	B	62	ASN	CB-CG	-6.12	1.36	1.52
1	A	90	GLU	C-O	6.12	1.31	1.24
1	B	90	GLU	C-O	6.12	1.31	1.24
1	A	90	GLU	CA-CB	-6.11	1.43	1.53
1	B	90	GLU	CA-CB	-6.11	1.43	1.53
1	A	46	TYR	CA-CB	-6.11	1.43	1.53
1	A	76	PRO	N-CD	6.11	1.56	1.47
1	B	46	TYR	CA-CB	-6.11	1.43	1.53
1	B	76	PRO	N-CD	6.11	1.56	1.47
1	A	18	HIS	C-N	-6.08	1.25	1.33
1	A	41	GLY	C-N	-6.08	1.25	1.33
1	B	18	HIS	C-N	-6.08	1.25	1.33
1	B	41	GLY	C-N	-6.08	1.25	1.33
1	A	54	SER	CB-OG	6.05	1.54	1.42
1	A	67	TYR	CZ-OH	-6.05	1.25	1.38
1	A	100	SER	CB-OG	6.05	1.54	1.42
1	B	54	SER	CB-OG	6.05	1.54	1.42
1	B	67	TYR	CZ-OH	-6.05	1.25	1.38
1	B	100	SER	CB-OG	6.05	1.54	1.42
1	A	72	LYS	CA-CB	6.05	1.61	1.52
1	B	72	LYS	CA-CB	6.05	1.61	1.52
1	A	14	CYS	C-O	6.01	1.30	1.23
1	B	14	CYS	C-O	6.01	1.30	1.23
1	A	95	VAL	CA-CB	-6.00	1.46	1.54
1	B	95	VAL	CA-CB	-6.00	1.46	1.54
1	A	45	GLY	CA-C	5.99	1.60	1.51
1	B	45	GLY	CA-C	5.99	1.60	1.51
1	A	91	ARG	C-N	-5.96	1.25	1.33
1	A	97	TYR	CA-CB	-5.96	1.44	1.53
1	B	91	ARG	C-N	-5.96	1.25	1.33
1	B	97	TYR	CA-CB	-5.96	1.44	1.53
1	A	65	MET	CA-CB	-5.96	1.44	1.53
1	B	65	MET	CA-CB	-5.96	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	PHE	CE1-CZ	-5.95	1.20	1.38
1	B	82	PHE	CE1-CZ	-5.95	1.20	1.38
1	A	82	PHE	CB-CG	5.91	1.64	1.50
1	B	82	PHE	CB-CG	5.91	1.64	1.50
1	A	79	LYS	N-CA	5.90	1.54	1.46
1	B	79	LYS	N-CA	5.90	1.54	1.46
1	A	61	GLU	CG-CD	-5.89	1.37	1.52
1	B	61	GLU	CG-CD	-5.89	1.37	1.52
1	A	60	ASN	C-O	-5.88	1.16	1.23
1	B	60	ASN	C-O	-5.88	1.16	1.23
1	A	7	LYS	CD-CE	5.88	1.70	1.52
1	B	7	LYS	CD-CE	5.88	1.70	1.52
1	A	47	SER	C-N	5.85	1.41	1.33
1	B	47	SER	C-N	5.85	1.41	1.33
1	A	47	SER	C-O	-5.84	1.16	1.24
1	A	48	TYR	CG-CD1	-5.84	1.27	1.39
1	B	47	SER	C-O	-5.84	1.16	1.24
1	B	48	TYR	CG-CD1	-5.84	1.27	1.39
1	A	25	LYS	CD-CE	5.84	1.70	1.52
1	A	91	ARG	CG-CD	5.84	1.70	1.52
1	B	25	LYS	CD-CE	5.84	1.70	1.52
1	B	91	ARG	CG-CD	5.84	1.70	1.52
1	A	71	PRO	CA-C	-5.84	1.44	1.52
1	B	71	PRO	CA-C	-5.84	1.44	1.52
1	A	65	MET	CG-SD	-5.83	1.66	1.80
1	B	65	MET	CG-SD	-5.83	1.66	1.80
1	A	1	GLY	C-N	-5.81	1.25	1.33
1	B	1	GLY	C-N	-5.81	1.25	1.33
1	A	35	LEU	CA-C	5.73	1.60	1.52
1	B	35	LEU	CA-C	5.73	1.60	1.52
1	A	4	ALA	C-O	-5.71	1.16	1.24
1	B	4	ALA	C-O	-5.71	1.16	1.24
1	A	44	GLU	CD-OE1	5.69	1.36	1.25
1	B	44	GLU	CD-OE1	5.69	1.36	1.25
1	A	92	GLN	C-N	5.67	1.41	1.33
1	B	92	GLN	C-N	5.67	1.41	1.33
1	A	4	ALA	CA-CB	5.66	1.63	1.53
1	B	4	ALA	CA-CB	5.66	1.63	1.53
1	A	51	ALA	CA-C	5.64	1.60	1.52
1	A	59	TRP	CA-C	5.64	1.60	1.52
1	B	51	ALA	CA-C	5.64	1.60	1.52
1	B	59	TRP	CA-C	5.64	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	GLY	C-N	-5.62	1.25	1.33
1	A	68	LEU	C-N	-5.62	1.25	1.33
1	B	45	GLY	C-N	-5.62	1.25	1.33
1	B	68	LEU	C-N	-5.62	1.25	1.33
1	A	103	SER	N-CA	5.56	1.56	1.46
1	B	103	SER	N-CA	5.56	1.56	1.46
1	A	38	ARG	C-N	5.54	1.41	1.33
1	B	38	ARG	C-N	5.54	1.41	1.33
1	A	83	ALA	N-CA	-5.54	1.39	1.46
1	B	83	ALA	N-CA	-5.54	1.39	1.46
1	A	73	LYS	CA-CB	5.51	1.62	1.53
1	B	73	LYS	CA-CB	5.51	1.62	1.53
1	A	75	ILE	CG1-CD1	-5.49	1.30	1.51
1	B	75	ILE	CG1-CD1	-5.49	1.30	1.51
1	A	81	ILE	CB-CG2	5.46	1.70	1.52
1	B	81	ILE	CB-CG2	5.46	1.70	1.52
1	A	53	LYS	C-N	5.45	1.41	1.33
1	B	53	LYS	C-N	5.45	1.41	1.33
1	A	61	GLU	CB-CG	-5.43	1.36	1.52
1	B	61	GLU	CB-CG	-5.43	1.36	1.52
1	A	2	ASP	CA-C	5.42	1.59	1.52
1	B	2	ASP	CA-C	5.42	1.59	1.52
1	A	37	GLY	N-CA	5.41	1.53	1.45
1	B	37	GLY	N-CA	5.41	1.53	1.45
1	A	61	GLU	C-O	5.40	1.30	1.24
1	B	61	GLU	C-O	5.40	1.30	1.24
1	A	21	GLU	C-N	-5.39	1.25	1.33
1	B	21	GLU	C-N	-5.39	1.25	1.33
1	A	67	TYR	CE2-CZ	-5.38	1.25	1.38
1	B	67	TYR	CE2-CZ	-5.38	1.25	1.38
1	A	55	LYS	CB-CG	5.37	1.68	1.52
1	B	55	LYS	CB-CG	5.37	1.68	1.52
1	A	44	GLU	C-N	5.36	1.41	1.33
1	B	44	GLU	C-N	5.36	1.41	1.33
1	A	5	LYS	CA-C	5.34	1.60	1.52
1	B	5	LYS	CA-C	5.34	1.60	1.52
1	A	23	GLY	C-O	5.34	1.31	1.23
1	B	23	GLY	C-O	5.34	1.31	1.23
1	A	39	LYS	C-O	5.34	1.30	1.23
1	B	39	LYS	C-O	5.34	1.30	1.23
1	A	71	PRO	CG-CD	-5.34	1.32	1.50
1	A	103	SER	CB-OG	5.34	1.52	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	PRO	CG-CD	-5.34	1.32	1.50
1	B	103	SER	CB-OG	5.34	1.52	1.42
1	A	27	LYS	CE-NZ	-5.33	1.33	1.49
1	B	27	LYS	CE-NZ	-5.33	1.33	1.49
1	A	95	VAL	CB-CG2	-5.32	1.34	1.52
1	B	95	VAL	CB-CG2	-5.32	1.34	1.52
1	A	35	LEU	CA-CB	5.30	1.62	1.53
1	B	35	LEU	CA-CB	5.30	1.62	1.53
1	A	25	LYS	CB-CG	5.29	1.68	1.52
1	B	25	LYS	CB-CG	5.29	1.68	1.52
1	A	84	GLY	C-O	-5.28	1.16	1.23
1	B	84	GLY	C-O	-5.28	1.16	1.23
1	A	7	LYS	C-N	-5.25	1.27	1.33
1	B	7	LYS	C-N	-5.25	1.27	1.33
1	A	9	THR	C-N	-5.24	1.27	1.33
1	B	9	THR	C-N	-5.24	1.27	1.33
1	A	67	TYR	CD1-CE1	-5.24	1.23	1.38
1	B	67	TYR	CD1-CE1	-5.24	1.23	1.38
1	A	53	LYS	CA-C	-5.23	1.45	1.52
1	A	74	TYR	CA-C	-5.23	1.45	1.52
1	B	53	LYS	CA-C	-5.23	1.45	1.52
1	B	74	TYR	CA-C	-5.23	1.45	1.52
1	A	10	PHE	CA-C	5.22	1.59	1.52
1	A	74	TYR	CZ-OH	-5.22	1.27	1.38
1	A	97	TYR	CZ-OH	-5.22	1.27	1.38
1	B	10	PHE	CA-C	5.22	1.59	1.52
1	B	74	TYR	CZ-OH	-5.22	1.27	1.38
1	B	97	TYR	CZ-OH	-5.22	1.27	1.38
1	A	88	LYS	CA-CB	-5.21	1.44	1.53
1	B	88	LYS	CA-CB	-5.21	1.44	1.53
1	A	8	LYS	N-CA	5.20	1.52	1.46
1	B	8	LYS	N-CA	5.20	1.52	1.46
1	A	100	SER	C-N	-5.18	1.27	1.33
1	B	100	SER	C-N	-5.18	1.27	1.33
1	A	60	ASN	CG-ND2	5.17	1.44	1.33
1	B	60	ASN	CG-ND2	5.17	1.44	1.33
1	A	18	HIS	CA-CB	-5.13	1.44	1.53
1	A	42	GLN	CA-CB	-5.13	1.44	1.53
1	B	18	HIS	CA-CB	-5.13	1.44	1.53
1	B	42	GLN	CA-CB	-5.13	1.44	1.53
1	A	31	ASN	CB-CG	5.12	1.64	1.52
1	B	31	ASN	CB-CG	5.12	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	ASN	CG-OD1	-5.11	1.13	1.23
1	B	52	ASN	CG-OD1	-5.11	1.13	1.23
1	A	33	TRP	NE1-CE2	-5.09	1.31	1.37
1	B	33	TRP	NE1-CE2	-5.09	1.31	1.37
1	A	50	ASP	CG-OD2	5.07	1.34	1.25
1	B	50	ASP	CG-OD2	5.07	1.34	1.25
1	A	40	THR	CA-C	5.06	1.58	1.52
1	B	40	THR	CA-C	5.06	1.58	1.52
1	A	27	LYS	N-CA	5.04	1.52	1.46
1	B	27	LYS	N-CA	5.04	1.52	1.46
1	A	6	GLY	C-N	-5.04	1.27	1.33
1	A	94	LEU	C-O	5.04	1.30	1.24
1	B	6	GLY	C-N	-5.04	1.27	1.33
1	B	94	LEU	C-O	5.04	1.30	1.24
1	A	46	TYR	CA-C	-5.03	1.46	1.52
1	B	46	TYR	CA-C	-5.03	1.46	1.52
1	A	56	GLY	CA-C	5.02	1.58	1.51
1	B	56	GLY	CA-C	5.02	1.58	1.51

All (838) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	HIS	ND1-CG-CD2	-37.39	68.71	106.10
1	B	18	HIS	ND1-CG-CD2	-37.39	68.71	106.10
1	A	3	VAL	CA-CB-CG2	-33.73	53.07	110.40
1	B	3	VAL	CA-CB-CG2	-33.73	53.07	110.40
1	A	18	HIS	ND1-CE1-NE2	-31.95	76.45	108.40
1	B	18	HIS	ND1-CE1-NE2	-31.95	76.45	108.40
1	A	3	VAL	CA-CB-CG1	-29.61	60.05	110.40
1	B	3	VAL	CA-CB-CG1	-29.61	60.05	110.40
1	A	18	HIS	CG-ND1-CE1	27.14	155.43	109.30
1	B	18	HIS	CG-ND1-CE1	27.14	155.43	109.30
1	A	44	GLU	CB-CG-CD	-25.98	68.44	112.60
1	B	44	GLU	CB-CG-CD	-25.98	68.44	112.60
1	A	50	ASP	O-C-N	-24.19	95.28	123.10
1	B	50	ASP	O-C-N	-24.19	95.28	123.10
1	A	18	HIS	CG-CD2-NE2	23.05	130.25	107.20
1	B	18	HIS	CG-CD2-NE2	23.05	130.25	107.20
1	A	62	ASN	CA-CB-CG	22.52	135.12	112.60
1	B	62	ASN	CA-CB-CG	22.52	135.12	112.60
1	A	30	PRO	N-CD-CG	-20.85	71.93	103.20
1	B	30	PRO	N-CD-CG	-20.85	71.93	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	PRO	CA-N-CD	-20.39	83.46	112.00
1	B	76	PRO	CA-N-CD	-20.39	83.46	112.00
1	A	67	TYR	CA-C-O	20.21	142.17	120.55
1	B	67	TYR	CA-C-O	20.21	142.17	120.55
1	A	26	HIS	CA-CB-CG	-19.76	94.04	113.80
1	B	26	HIS	CA-CB-CG	-19.76	94.04	113.80
1	A	46	TYR	CB-CA-C	19.53	149.29	110.42
1	B	46	TYR	CB-CA-C	19.53	149.29	110.42
1	A	30	PRO	CA-CB-CG	-19.28	67.86	104.50
1	B	30	PRO	CA-CB-CG	-19.28	67.86	104.50
1	A	62	ASN	OD1-CG-ND2	-18.67	103.93	122.60
1	B	62	ASN	OD1-CG-ND2	-18.67	103.93	122.60
1	A	31	ASN	CA-CB-CG	-18.40	94.20	112.60
1	B	31	ASN	CA-CB-CG	-18.40	94.20	112.60
1	A	28	VAL	O-C-N	-18.01	100.05	122.57
1	B	28	VAL	O-C-N	-18.01	100.05	122.57
1	A	83	ALA	O-C-N	-17.71	99.03	122.59
1	B	83	ALA	O-C-N	-17.71	99.03	122.59
1	A	39	LYS	CA-CB-CG	17.65	149.40	114.10
1	B	39	LYS	CA-CB-CG	17.65	149.40	114.10
1	A	56	GLY	O-C-N	-17.40	100.08	122.70
1	B	56	GLY	O-C-N	-17.40	100.08	122.70
1	A	31	ASN	OD1-CG-ND2	-17.35	105.25	122.60
1	B	31	ASN	OD1-CG-ND2	-17.35	105.25	122.60
1	A	39	LYS	CA-C-O	-16.75	100.11	121.88
1	B	39	LYS	CA-C-O	-16.75	100.11	121.88
1	A	62	ASN	CA-C-O	-16.70	96.63	120.51
1	B	62	ASN	CA-C-O	-16.70	96.63	120.51
1	A	37	GLY	O-C-N	-16.54	101.20	122.70
1	B	37	GLY	O-C-N	-16.54	101.20	122.70
1	A	40	THR	O-C-N	16.47	141.88	123.27
1	B	40	THR	O-C-N	16.47	141.88	123.27
1	A	16	GLN	N-CA-CB	-16.41	82.75	110.49
1	B	16	GLN	N-CA-CB	-16.41	82.75	110.49
1	A	52	ASN	N-CA-CB	16.12	137.74	110.49
1	B	52	ASN	N-CA-CB	16.12	137.74	110.49
1	A	92	GLN	CG-CD-OE1	-16.03	88.74	120.80
1	B	92	GLN	CG-CD-OE1	-16.03	88.74	120.80
1	A	92	GLN	CG-CD-NE2	15.86	140.18	116.40
1	B	92	GLN	CG-CD-NE2	15.86	140.18	116.40
1	A	33	TRP	CG-CD2-CE3	-15.63	118.27	133.90
1	B	33	TRP	CG-CD2-CE3	-15.63	118.27	133.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	VAL	O-C-N	-15.63	106.59	121.91
1	B	3	VAL	O-C-N	-15.63	106.59	121.91
1	A	97	TYR	CZ-CE2-CD2	-15.54	91.63	119.60
1	B	97	TYR	CZ-CE2-CD2	-15.54	91.63	119.60
1	A	93	ASP	CA-CB-CG	15.46	128.06	112.60
1	B	93	ASP	CA-CB-CG	15.46	128.06	112.60
1	A	62	ASN	O-C-N	-15.43	102.07	122.59
1	B	62	ASN	O-C-N	-15.43	102.07	122.59
1	A	2	ASP	CA-CB-CG	15.05	127.65	112.60
1	B	2	ASP	CA-CB-CG	15.05	127.65	112.60
1	A	58	VAL	CA-C-O	-14.99	102.04	120.78
1	B	58	VAL	CA-C-O	-14.99	102.04	120.78
1	A	18	HIS	CA-CB-CG	-14.96	98.84	113.80
1	B	18	HIS	CA-CB-CG	-14.96	98.84	113.80
1	A	30	PRO	O-C-N	-14.91	102.50	122.64
1	B	30	PRO	O-C-N	-14.91	102.50	122.64
1	A	76	PRO	N-CA-CB	14.81	116.35	103.17
1	B	76	PRO	N-CA-CB	14.81	116.35	103.17
1	A	76	PRO	N-CD-CG	14.75	125.33	103.20
1	B	76	PRO	N-CD-CG	14.75	125.33	103.20
1	A	41	GLY	CA-C-N	14.72	149.66	121.54
1	A	41	GLY	C-N-CA	14.72	149.66	121.54
1	B	41	GLY	CA-C-N	14.72	149.66	121.54
1	B	41	GLY	C-N-CA	14.72	149.66	121.54
1	A	67	TYR	O-C-N	-14.53	104.59	122.17
1	B	67	TYR	O-C-N	-14.53	104.59	122.17
1	A	70	ASN	CA-C-N	14.51	137.97	119.84
1	A	70	ASN	C-N-CA	14.51	137.97	119.84
1	B	70	ASN	CA-C-N	14.51	137.97	119.84
1	B	70	ASN	C-N-CA	14.51	137.97	119.84
1	A	40	THR	CA-C-O	-14.26	104.89	120.43
1	B	40	THR	CA-C-O	-14.26	104.89	120.43
1	A	78	THR	O-C-N	-14.22	105.38	122.87
1	B	78	THR	O-C-N	-14.22	105.38	122.87
1	A	5	LYS	O-C-N	-14.09	106.14	122.20
1	B	5	LYS	O-C-N	-14.09	106.14	122.20
1	A	1	GLY	CA-C-N	-13.89	98.24	122.26
1	A	1	GLY	C-N-CA	-13.89	98.24	122.26
1	B	1	GLY	CA-C-N	-13.89	98.24	122.26
1	B	1	GLY	C-N-CA	-13.89	98.24	122.26
1	A	52	ASN	OD1-CG-ND2	-13.70	108.90	122.60
1	B	52	ASN	OD1-CG-ND2	-13.70	108.90	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	VAL	N-CA-CB	13.68	133.80	111.23
1	B	28	VAL	N-CA-CB	13.68	133.80	111.23
1	A	83	ALA	CA-C-O	13.64	140.02	120.51
1	B	83	ALA	CA-C-O	13.64	140.02	120.51
1	A	46	TYR	CZ-CE2-CD2	-13.58	95.15	119.60
1	B	46	TYR	CZ-CE2-CD2	-13.58	95.15	119.60
1	A	41	GLY	O-C-N	-13.56	102.37	123.93
1	B	41	GLY	O-C-N	-13.56	102.37	123.93
1	A	52	ASN	CB-CG-OD1	13.37	147.53	120.80
1	B	52	ASN	CB-CG-OD1	13.37	147.53	120.80
1	A	57	ILE	O-C-N	-13.28	105.97	122.57
1	B	57	ILE	O-C-N	-13.28	105.97	122.57
1	A	10	PHE	CA-C-O	-13.27	106.89	120.82
1	B	10	PHE	CA-C-O	-13.27	106.89	120.82
1	A	51	ALA	CA-C-O	13.19	139.38	120.51
1	B	51	ALA	CA-C-O	13.19	139.38	120.51
1	A	59	TRP	CD2-CE2-CZ2	-13.18	109.22	122.40
1	B	59	TRP	CD2-CE2-CZ2	-13.18	109.22	122.40
1	A	18	HIS	CB-CG-CD2	13.14	148.29	131.20
1	B	18	HIS	CB-CG-CD2	13.14	148.29	131.20
1	A	7	LYS	O-C-N	-13.07	107.25	122.15
1	B	7	LYS	O-C-N	-13.07	107.25	122.15
1	A	36	PHE	CD1-CG-CD2	-12.99	99.11	118.60
1	B	36	PHE	CD1-CG-CD2	-12.99	99.11	118.60
1	A	86	LYS	CA-C-O	12.90	136.57	121.34
1	B	86	LYS	CA-C-O	12.90	136.57	121.34
1	A	42	GLN	OE1-CD-NE2	-12.77	109.83	122.60
1	B	42	GLN	OE1-CD-NE2	-12.77	109.83	122.60
1	A	46	TYR	CA-CB-CG	12.69	136.73	113.90
1	B	46	TYR	CA-CB-CG	12.69	136.73	113.90
1	A	68	LEU	O-C-N	-12.66	107.55	122.11
1	B	68	LEU	O-C-N	-12.66	107.55	122.11
1	A	36	PHE	CG-CD2-CE2	12.65	142.20	120.70
1	B	36	PHE	CG-CD2-CE2	12.65	142.20	120.70
1	A	70	ASN	OD1-CG-ND2	-12.61	109.99	122.60
1	B	70	ASN	OD1-CG-ND2	-12.61	109.99	122.60
1	A	76	PRO	O-C-N	-12.60	109.25	122.98
1	B	76	PRO	O-C-N	-12.60	109.25	122.98
1	A	16	GLN	CA-C-N	-12.54	105.05	121.98
1	A	16	GLN	C-N-CA	-12.54	105.05	121.98
1	B	16	GLN	CA-C-N	-12.54	105.05	121.98
1	B	16	GLN	C-N-CA	-12.54	105.05	121.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	TYR	CB-CG-CD1	12.29	139.24	120.80
1	B	67	TYR	CB-CG-CD1	12.29	139.24	120.80
1	A	40	THR	CA-C-N	-12.21	101.82	121.97
1	A	40	THR	C-N-CA	-12.21	101.82	121.97
1	B	40	THR	CA-C-N	-12.21	101.82	121.97
1	B	40	THR	C-N-CA	-12.21	101.82	121.97
1	A	28	VAL	CA-CB-CG2	12.13	131.03	110.40
1	B	28	VAL	CA-CB-CG2	12.13	131.03	110.40
1	A	46	TYR	CG-CD2-CE2	11.97	139.16	121.20
1	B	46	TYR	CG-CD2-CE2	11.97	139.16	121.20
1	A	10	PHE	CZ-CE2-CD2	11.92	141.46	120.00
1	B	10	PHE	CZ-CE2-CD2	11.92	141.46	120.00
1	A	18	HIS	CB-CG-ND1	11.91	140.57	122.70
1	B	18	HIS	CB-CG-ND1	11.91	140.57	122.70
1	A	17	CYS	N-CA-C	-11.86	89.26	108.12
1	B	17	CYS	N-CA-C	-11.86	89.26	108.12
1	A	91	ARG	NE-CZ-NH1	-11.77	109.73	121.50
1	B	91	ARG	NE-CZ-NH1	-11.77	109.73	121.50
1	A	12	GLN	CG-CD-OE1	-11.59	97.62	120.80
1	B	12	GLN	CG-CD-OE1	-11.59	97.62	120.80
1	A	32	LEU	N-CA-CB	11.58	126.29	110.42
1	B	32	LEU	N-CA-CB	11.58	126.29	110.42
1	A	33	TRP	CB-CG-CD2	11.56	142.98	126.80
1	A	62	ASN	CB-CA-C	11.56	133.42	110.42
1	B	33	TRP	CB-CG-CD2	11.56	142.98	126.80
1	B	62	ASN	CB-CA-C	11.56	133.42	110.42
1	A	49	THR	O-C-N	-11.49	108.55	121.76
1	B	49	THR	O-C-N	-11.49	108.55	121.76
1	A	38	ARG	CA-C-O	11.46	133.71	121.10
1	A	59	TRP	CE2-CD2-CE3	11.46	130.26	118.80
1	B	38	ARG	CA-C-O	11.46	133.71	121.10
1	B	59	TRP	CE2-CD2-CE3	11.46	130.26	118.80
1	A	68	LEU	CB-CA-C	11.44	129.73	110.74
1	B	68	LEU	CB-CA-C	11.44	129.73	110.74
1	A	34	GLY	O-C-N	-11.42	107.86	122.70
1	B	34	GLY	O-C-N	-11.42	107.86	122.70
1	A	82	PHE	CD1-CG-CD2	-11.40	101.50	118.60
1	B	82	PHE	CD1-CG-CD2	-11.40	101.50	118.60
1	A	70	ASN	CA-CB-CG	11.39	123.99	112.60
1	B	70	ASN	CA-CB-CG	11.39	123.99	112.60
1	A	62	ASN	CB-CG-ND2	11.35	133.42	116.40
1	B	62	ASN	CB-CG-ND2	11.35	133.42	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	PHE	CA-C-N	11.33	143.62	121.41
1	A	36	PHE	C-N-CA	11.33	143.62	121.41
1	B	36	PHE	CA-C-N	11.33	143.62	121.41
1	B	36	PHE	C-N-CA	11.33	143.62	121.41
1	A	10	PHE	CE1-CZ-CE2	-11.23	99.78	120.00
1	B	10	PHE	CE1-CZ-CE2	-11.23	99.78	120.00
1	A	19	THR	O-C-N	-11.18	107.72	122.59
1	B	19	THR	O-C-N	-11.18	107.72	122.59
1	A	71	PRO	N-CA-CB	11.18	114.98	103.25
1	B	71	PRO	N-CA-CB	11.18	114.98	103.25
1	A	86	LYS	N-CA-C	-11.15	95.35	111.30
1	B	86	LYS	N-CA-C	-11.15	95.35	111.30
1	A	98	LEU	CB-CA-C	11.08	128.12	110.95
1	B	98	LEU	CB-CA-C	11.08	128.12	110.95
1	A	15	ALA	N-CA-C	11.07	134.37	110.80
1	B	15	ALA	N-CA-C	11.07	134.37	110.80
1	A	16	GLN	O-C-N	-11.01	107.95	122.59
1	B	16	GLN	O-C-N	-11.01	107.95	122.59
1	A	92	GLN	CB-CA-C	11.00	132.32	110.42
1	B	92	GLN	CB-CA-C	11.00	132.32	110.42
1	A	7	LYS	N-CA-C	-10.94	99.44	111.36
1	B	7	LYS	N-CA-C	-10.94	99.44	111.36
1	A	32	LEU	N-CA-C	-10.90	96.61	111.55
1	B	32	LEU	N-CA-C	-10.90	96.61	111.55
1	A	33	TRP	O-C-N	10.78	136.93	122.59
1	B	33	TRP	O-C-N	10.78	136.93	122.59
1	A	30	PRO	CA-C-O	10.73	140.13	120.60
1	B	30	PRO	CA-C-O	10.73	140.13	120.60
1	A	33	TRP	CE2-CD2-CG	10.71	120.05	107.20
1	B	33	TRP	CE2-CD2-CG	10.71	120.05	107.20
1	A	61	GLU	CG-CD-OE1	10.70	143.00	118.40
1	B	61	GLU	CG-CD-OE1	10.70	143.00	118.40
1	A	59	TRP	CG-CD2-CE3	-10.68	123.22	133.90
1	B	59	TRP	CG-CD2-CE3	-10.68	123.22	133.90
1	A	31	ASN	O-C-N	-10.66	109.97	122.97
1	B	31	ASN	O-C-N	-10.66	109.97	122.97
1	A	16	GLN	CB-CG-CD	-10.65	94.49	112.60
1	B	16	GLN	CB-CG-CD	-10.65	94.49	112.60
1	A	25	LYS	N-CA-CB	-10.63	92.52	110.49
1	B	25	LYS	N-CA-CB	-10.63	92.52	110.49
1	A	35	LEU	N-CA-CB	10.58	128.37	110.49
1	B	35	LEU	N-CA-CB	10.58	128.37	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	GLN	N-CA-CB	10.53	128.28	110.49
1	B	42	GLN	N-CA-CB	10.53	128.28	110.49
1	A	67	TYR	CB-CG-CD2	-10.53	105.01	120.80
1	B	67	TYR	CB-CG-CD2	-10.53	105.01	120.80
1	A	58	VAL	CB-CA-C	10.51	128.53	111.29
1	B	58	VAL	CB-CA-C	10.51	128.53	111.29
1	A	38	ARG	CD-NE-CZ	-10.38	109.87	124.40
1	B	38	ARG	CD-NE-CZ	-10.38	109.87	124.40
1	A	89	GLY	CA-C-N	10.36	135.00	120.29
1	A	89	GLY	C-N-CA	10.36	135.00	120.29
1	B	89	GLY	CA-C-N	10.36	135.00	120.29
1	B	89	GLY	C-N-CA	10.36	135.00	120.29
1	A	63	THR	CA-C-O	10.32	135.26	120.51
1	B	63	THR	CA-C-O	10.32	135.26	120.51
1	A	91	ARG	N-CA-C	-10.31	95.05	111.04
1	B	91	ARG	N-CA-C	-10.31	95.05	111.04
1	A	22	ASN	O-C-N	-10.27	108.24	122.41
1	B	22	ASN	O-C-N	-10.27	108.24	122.41
1	A	80	MET	CA-C-O	10.27	131.93	120.43
1	B	80	MET	CA-C-O	10.27	131.93	120.43
1	A	18	HIS	CB-CA-C	-10.26	90.00	110.42
1	B	18	HIS	CB-CA-C	-10.26	90.00	110.42
1	A	19	THR	N-CA-CB	10.26	127.82	110.49
1	B	19	THR	N-CA-CB	10.26	127.82	110.49
1	A	86	LYS	O-C-N	-10.25	108.12	121.95
1	B	86	LYS	O-C-N	-10.25	108.12	121.95
1	A	38	ARG	N-CA-C	-10.09	92.89	108.42
1	B	38	ARG	N-CA-C	-10.09	92.89	108.42
1	A	12	GLN	CB-CG-CD	10.04	129.66	112.60
1	B	12	GLN	CB-CG-CD	10.04	129.66	112.60
1	A	54	SER	O-C-N	-10.03	109.25	122.59
1	B	54	SER	O-C-N	-10.03	109.25	122.59
1	A	48	TYR	CB-CG-CD1	10.02	135.84	120.80
1	B	48	TYR	CB-CG-CD1	10.02	135.84	120.80
1	A	97	TYR	CE1-CZ-CE2	10.02	140.34	120.30
1	B	97	TYR	CE1-CZ-CE2	10.02	140.34	120.30
1	A	56	GLY	CA-C-O	9.99	137.95	120.57
1	B	56	GLY	CA-C-O	9.99	137.95	120.57
1	A	3	VAL	N-CA-C	-9.94	100.88	110.42
1	B	3	VAL	N-CA-C	-9.94	100.88	110.42
1	A	57	ILE	CA-C-O	9.89	133.14	120.78
1	B	57	ILE	CA-C-O	9.89	133.14	120.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ALA	O-C-N	-9.83	110.24	121.84
1	B	43	ALA	O-C-N	-9.83	110.24	121.84
1	A	97	TYR	O-C-N	-9.82	110.32	122.20
1	B	97	TYR	O-C-N	-9.82	110.32	122.20
1	A	90	GLU	O-C-N	-9.74	111.05	122.15
1	B	90	GLU	O-C-N	-9.74	111.05	122.15
1	A	75	ILE	CA-C-N	9.73	131.27	119.98
1	A	75	ILE	C-N-CA	9.73	131.27	119.98
1	B	75	ILE	CA-C-N	9.73	131.27	119.98
1	B	75	ILE	C-N-CA	9.73	131.27	119.98
1	A	23	GLY	N-CA-C	-9.72	100.11	115.08
1	B	23	GLY	N-CA-C	-9.72	100.11	115.08
1	A	63	THR	O-C-N	-9.64	109.77	122.59
1	B	63	THR	O-C-N	-9.64	109.77	122.59
1	A	88	LYS	O-C-N	-9.59	109.83	122.59
1	B	88	LYS	O-C-N	-9.59	109.83	122.59
1	A	13	LYS	N-CA-CB	-9.54	97.42	110.67
1	B	13	LYS	N-CA-CB	-9.54	97.42	110.67
1	A	79	LYS	CA-C-O	9.50	133.86	119.23
1	B	79	LYS	CA-C-O	9.50	133.86	119.23
1	A	29	GLY	CA-C-O	-9.48	107.97	121.52
1	B	29	GLY	CA-C-O	-9.48	107.97	121.52
1	A	93	ASP	O-C-N	-9.46	112.09	122.12
1	B	93	ASP	O-C-N	-9.46	112.09	122.12
1	A	44	GLU	O-C-N	-9.43	110.05	122.59
1	B	44	GLU	O-C-N	-9.43	110.05	122.59
1	A	71	PRO	CA-C-N	9.43	136.72	122.77
1	A	71	PRO	C-N-CA	9.43	136.72	122.77
1	B	71	PRO	CA-C-N	9.43	136.72	122.77
1	B	71	PRO	C-N-CA	9.43	136.72	122.77
1	A	39	LYS	CB-CG-CD	9.42	132.96	111.30
1	B	39	LYS	CB-CG-CD	9.42	132.96	111.30
1	A	93	ASP	N-CA-CB	-9.39	95.97	110.06
1	B	93	ASP	N-CA-CB	-9.39	95.97	110.06
1	A	9	THR	CA-CB-CG2	9.37	126.42	110.50
1	B	9	THR	CA-CB-CG2	9.37	126.42	110.50
1	A	46	TYR	CB-CG-CD2	9.32	134.78	120.80
1	B	46	TYR	CB-CG-CD2	9.32	134.78	120.80
1	A	48	TYR	N-CA-CB	-9.29	94.79	110.49
1	B	48	TYR	N-CA-CB	-9.29	94.79	110.49
1	A	55	LYS	O-C-N	9.27	134.91	122.59
1	B	55	LYS	O-C-N	9.27	134.91	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	VAL	N-CA-CB	9.12	126.28	111.23
1	B	58	VAL	N-CA-CB	9.12	126.28	111.23
1	A	52	ASN	CA-CB-CG	9.07	121.67	112.60
1	B	52	ASN	CA-CB-CG	9.07	121.67	112.60
1	A	48	TYR	CD1-CG-CD2	-9.03	104.55	118.10
1	B	48	TYR	CD1-CG-CD2	-9.03	104.55	118.10
1	A	35	LEU	CA-C-O	8.99	133.37	120.51
1	B	35	LEU	CA-C-O	8.99	133.37	120.51
1	A	52	ASN	CB-CG-ND2	-8.97	102.95	116.40
1	B	52	ASN	CB-CG-ND2	-8.97	102.95	116.40
1	A	16	GLN	CA-CB-CG	8.91	131.91	114.10
1	B	16	GLN	CA-CB-CG	8.91	131.91	114.10
1	A	67	TYR	CG-CD2-CE2	-8.89	107.87	121.20
1	B	67	TYR	CG-CD2-CE2	-8.89	107.87	121.20
1	A	26	HIS	N-CA-CB	-8.82	95.58	110.49
1	B	26	HIS	N-CA-CB	-8.82	95.58	110.49
1	A	42	GLN	CG-CD-OE1	8.80	138.39	120.80
1	B	42	GLN	CG-CD-OE1	8.80	138.39	120.80
1	A	58	VAL	O-C-N	-8.78	111.59	122.57
1	B	58	VAL	O-C-N	-8.78	111.59	122.57
1	A	95	VAL	CA-C-O	-8.75	109.84	120.78
1	B	95	VAL	CA-C-O	-8.75	109.84	120.78
1	A	58	VAL	N-CA-C	-8.74	91.15	109.34
1	B	58	VAL	N-CA-C	-8.74	91.15	109.34
1	A	38	ARG	CB-CA-C	-8.72	95.78	110.43
1	B	38	ARG	CB-CA-C	-8.72	95.78	110.43
1	A	42	GLN	CB-CG-CD	8.67	127.35	112.60
1	B	42	GLN	CB-CG-CD	8.67	127.35	112.60
1	A	97	TYR	N-CA-CB	8.67	124.46	109.72
1	B	97	TYR	N-CA-CB	8.67	124.46	109.72
1	A	90	GLU	N-CA-C	-8.59	102.00	111.36
1	B	90	GLU	N-CA-C	-8.59	102.00	111.36
1	A	5	LYS	CB-CA-C	-8.58	93.81	110.46
1	B	5	LYS	CB-CA-C	-8.58	93.81	110.46
1	A	97	TYR	CG-CD2-CE2	8.53	133.99	121.20
1	B	97	TYR	CG-CD2-CE2	8.53	133.99	121.20
1	A	70	ASN	CA-C-O	8.51	131.81	120.16
1	B	70	ASN	CA-C-O	8.51	131.81	120.16
1	A	17	CYS	CA-C-O	-8.50	114.36	119.55
1	B	17	CYS	CA-C-O	-8.50	114.36	119.55
1	A	63	THR	CA-CB-OG1	-8.50	96.85	109.60
1	B	63	THR	CA-CB-OG1	-8.50	96.85	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	GLY	N-CA-C	-8.46	93.12	113.18
1	B	6	GLY	N-CA-C	-8.46	93.12	113.18
1	A	36	PHE	N-CA-CB	-8.46	96.19	110.49
1	B	36	PHE	N-CA-CB	-8.46	96.19	110.49
1	A	6	GLY	O-C-N	-8.45	111.72	122.70
1	B	6	GLY	O-C-N	-8.45	111.72	122.70
1	A	33	TRP	N-CA-CB	8.44	124.76	110.49
1	B	33	TRP	N-CA-CB	8.44	124.76	110.49
1	A	77	GLY	O-C-N	-8.42	111.75	122.70
1	B	77	GLY	O-C-N	-8.42	111.75	122.70
1	A	97	TYR	CA-C-O	8.39	130.84	121.02
1	B	97	TYR	CA-C-O	8.39	130.84	121.02
1	A	98	LEU	N-CA-C	-8.36	101.75	111.03
1	B	98	LEU	N-CA-C	-8.36	101.75	111.03
1	A	81	ILE	CB-CA-C	8.31	124.92	111.29
1	B	81	ILE	CB-CA-C	8.31	124.92	111.29
1	A	59	TRP	CA-C-O	-8.29	108.66	120.51
1	B	59	TRP	CA-C-O	-8.29	108.66	120.51
1	A	92	GLN	CA-C-N	-8.28	109.04	120.38
1	A	92	GLN	C-N-CA	-8.28	109.04	120.38
1	B	92	GLN	CA-C-N	-8.28	109.04	120.38
1	B	92	GLN	C-N-CA	-8.28	109.04	120.38
1	A	66	GLU	N-CA-CB	8.28	123.79	109.72
1	B	66	GLU	N-CA-CB	8.28	123.79	109.72
1	A	10	PHE	O-C-N	-8.23	113.59	122.07
1	B	10	PHE	O-C-N	-8.23	113.59	122.07
1	A	65	MET	CA-C-N	8.19	134.21	121.19
1	A	65	MET	C-N-CA	8.19	134.21	121.19
1	B	65	MET	CA-C-N	8.19	134.21	121.19
1	B	65	MET	C-N-CA	8.19	134.21	121.19
1	A	97	TYR	CA-C-N	8.18	131.75	120.63
1	A	97	TYR	C-N-CA	8.18	131.75	120.63
1	B	97	TYR	CA-C-N	8.18	131.75	120.63
1	B	97	TYR	C-N-CA	8.18	131.75	120.63
1	A	14	CYS	N-CA-C	-8.16	100.45	111.96
1	B	14	CYS	N-CA-C	-8.16	100.45	111.96
1	A	12	GLN	CA-C-O	-8.13	112.52	120.90
1	B	12	GLN	CA-C-O	-8.13	112.52	120.90
1	A	65	MET	N-CA-C	-8.13	102.37	111.07
1	B	65	MET	N-CA-C	-8.13	102.37	111.07
1	A	44	GLU	CG-CD-OE1	-8.13	99.70	118.40
1	B	44	GLU	CG-CD-OE1	-8.13	99.70	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	TRP	CD2-CE3-CZ3	-8.10	108.08	118.60
1	B	33	TRP	CD2-CE3-CZ3	-8.10	108.08	118.60
1	A	46	TYR	N-CA-C	-8.09	93.57	110.80
1	B	46	TYR	N-CA-C	-8.09	93.57	110.80
1	A	91	ARG	NE-CZ-NH2	8.08	126.47	119.20
1	B	91	ARG	NE-CZ-NH2	8.08	126.47	119.20
1	A	61	GLU	OE1-CD-OE2	-8.08	103.52	122.90
1	B	61	GLU	OE1-CD-OE2	-8.08	103.52	122.90
1	A	92	GLN	CA-C-O	7.98	131.92	120.51
1	B	92	GLN	CA-C-O	7.98	131.92	120.51
1	A	21	GLU	N-CA-C	-7.97	97.75	109.63
1	A	40	THR	OG1-CB-CG2	-7.97	93.35	109.30
1	B	21	GLU	N-CA-C	-7.97	97.75	109.63
1	B	40	THR	OG1-CB-CG2	-7.97	93.35	109.30
1	A	48	TYR	CG-CD1-CE1	7.92	133.09	121.20
1	B	48	TYR	CG-CD1-CE1	7.92	133.09	121.20
1	A	77	GLY	CA-C-O	7.91	134.34	120.57
1	B	77	GLY	CA-C-O	7.91	134.34	120.57
1	A	66	GLU	O-C-N	7.83	131.67	122.20
1	B	66	GLU	O-C-N	7.83	131.67	122.20
1	A	10	PHE	CB-CG-CD1	-7.76	107.50	120.70
1	B	10	PHE	CB-CG-CD1	-7.76	107.50	120.70
1	A	97	TYR	OH-CZ-CE2	-7.71	96.76	119.90
1	B	97	TYR	OH-CZ-CE2	-7.71	96.76	119.90
1	A	67	TYR	CZ-CE2-CD2	7.70	133.46	119.60
1	B	67	TYR	CZ-CE2-CD2	7.70	133.46	119.60
1	A	82	PHE	CG-CD2-CE2	7.70	133.79	120.70
1	B	82	PHE	CG-CD2-CE2	7.70	133.79	120.70
1	A	5	LYS	CA-CB-CG	7.62	129.35	114.10
1	B	5	LYS	CA-CB-CG	7.62	129.35	114.10
1	A	19	THR	OG1-CB-CG2	7.61	124.52	109.30
1	B	19	THR	OG1-CB-CG2	7.61	124.52	109.30
1	A	36	PHE	O-C-N	-7.59	112.49	122.59
1	B	36	PHE	O-C-N	-7.59	112.49	122.59
1	A	79	LYS	N-CA-CB	7.58	122.14	110.46
1	B	79	LYS	N-CA-CB	7.58	122.14	110.46
1	A	33	TRP	CA-CB-CG	7.58	128.00	113.60
1	B	33	TRP	CA-CB-CG	7.58	128.00	113.60
1	A	81	ILE	CA-C-N	-7.53	110.53	122.73
1	A	81	ILE	C-N-CA	-7.53	110.53	122.73
1	B	81	ILE	CA-C-N	-7.53	110.53	122.73
1	B	81	ILE	C-N-CA	-7.53	110.53	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	TRP	O-C-N	7.52	132.59	122.59
1	B	59	TRP	O-C-N	7.52	132.59	122.59
1	A	5	LYS	N-CA-C	7.51	121.36	111.75
1	B	5	LYS	N-CA-C	7.51	121.36	111.75
1	A	68	LEU	CD1-CG-CD2	-7.48	94.34	110.80
1	B	68	LEU	CD1-CG-CD2	-7.48	94.34	110.80
1	A	40	THR	N-CA-C	7.47	121.41	109.24
1	A	79	LYS	O-C-N	-7.47	110.40	122.42
1	B	40	THR	N-CA-C	7.47	121.41	109.24
1	B	79	LYS	O-C-N	-7.47	110.40	122.42
1	A	31	ASN	CB-CG-ND2	7.27	127.31	116.40
1	B	31	ASN	CB-CG-ND2	7.27	127.31	116.40
1	A	48	TYR	CG-CD2-CE2	7.23	132.05	121.20
1	A	101	ALA	O-C-N	-7.23	113.72	122.11
1	B	48	TYR	CG-CD2-CE2	7.23	132.05	121.20
1	B	101	ALA	O-C-N	-7.23	113.72	122.11
1	A	84	GLY	N-CA-C	7.20	130.24	113.18
1	B	84	GLY	N-CA-C	7.20	130.24	113.18
1	A	93	ASP	N-CA-C	7.18	120.02	111.33
1	B	93	ASP	N-CA-C	7.18	120.02	111.33
1	A	82	PHE	O-C-N	-7.17	114.53	123.27
1	B	82	PHE	O-C-N	-7.17	114.53	123.27
1	A	59	TRP	NE1-CE2-CD2	7.16	116.71	107.40
1	B	59	TRP	NE1-CE2-CD2	7.16	116.71	107.40
1	A	47	SER	CA-CB-OG	-7.11	96.88	111.10
1	B	47	SER	CA-CB-OG	-7.11	96.88	111.10
1	A	13	LYS	N-CA-C	7.11	123.06	113.97
1	B	13	LYS	N-CA-C	7.11	123.06	113.97
1	A	44	GLU	CB-CA-C	7.09	124.54	110.42
1	B	44	GLU	CB-CA-C	7.09	124.54	110.42
1	A	90	GLU	CA-C-O	7.06	127.90	120.42
1	B	90	GLU	CA-C-O	7.06	127.90	120.42
1	A	73	LYS	CG-CD-CE	7.03	127.46	111.30
1	B	73	LYS	CG-CD-CE	7.03	127.46	111.30
1	A	55	LYS	CB-CG-CD	-7.02	95.16	111.30
1	B	55	LYS	CB-CG-CD	-7.02	95.16	111.30
1	A	51	ALA	O-C-N	-7.00	113.28	122.59
1	B	51	ALA	O-C-N	-7.00	113.28	122.59
1	A	52	ASN	O-C-N	-6.99	113.30	122.59
1	B	52	ASN	O-C-N	-6.99	113.30	122.59
1	A	69	GLU	CA-C-N	-6.96	104.81	121.80
1	A	69	GLU	C-N-CA	-6.96	104.81	121.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	GLU	CA-C-N	-6.96	104.81	121.80
1	B	69	GLU	C-N-CA	-6.96	104.81	121.80
1	A	10	PHE	CB-CG-CD2	6.95	132.51	120.70
1	B	10	PHE	CB-CG-CD2	6.95	132.51	120.70
1	A	57	ILE	CA-CB-CG2	6.93	122.29	110.50
1	B	57	ILE	CA-CB-CG2	6.93	122.29	110.50
1	A	92	GLN	O-C-N	-6.93	113.37	122.59
1	B	92	GLN	O-C-N	-6.93	113.37	122.59
1	A	48	TYR	CB-CA-C	6.91	124.16	110.42
1	B	48	TYR	CB-CA-C	6.91	124.16	110.42
1	A	90	GLU	CB-CG-CD	6.90	124.33	112.60
1	B	90	GLU	CB-CG-CD	6.90	124.33	112.60
1	A	67	TYR	N-CA-CB	-6.88	99.95	110.13
1	B	67	TYR	N-CA-CB	-6.88	99.95	110.13
1	A	79	LYS	CA-CB-CG	-6.87	100.36	114.10
1	B	79	LYS	CA-CB-CG	-6.87	100.36	114.10
1	A	45	GLY	CA-C-O	-6.86	108.64	120.57
1	A	71	PRO	O-C-N	-6.86	113.38	122.64
1	B	45	GLY	CA-C-O	-6.86	108.64	120.57
1	B	71	PRO	O-C-N	-6.86	113.38	122.64
1	A	61	GLU	N-CA-C	-6.85	96.20	110.80
1	B	61	GLU	N-CA-C	-6.85	96.20	110.80
1	A	49	THR	CB-CA-C	6.82	121.47	111.65
1	B	49	THR	CB-CA-C	6.82	121.47	111.65
1	A	59	TRP	NE1-CE2-CZ2	-6.81	119.88	130.10
1	B	59	TRP	NE1-CE2-CZ2	-6.81	119.88	130.10
1	A	29	GLY	CA-C-N	-6.78	111.37	119.84
1	A	29	GLY	C-N-CA	-6.78	111.37	119.84
1	B	29	GLY	CA-C-N	-6.78	111.37	119.84
1	B	29	GLY	C-N-CA	-6.78	111.37	119.84
1	A	8	LYS	O-C-N	6.77	129.89	122.11
1	B	8	LYS	O-C-N	6.77	129.89	122.11
1	A	50	ASP	OD1-CG-OD2	-6.76	106.67	122.90
1	A	79	LYS	CA-C-N	-6.76	113.17	122.30
1	A	79	LYS	C-N-CA	-6.76	113.17	122.30
1	B	50	ASP	OD1-CG-OD2	-6.76	106.67	122.90
1	B	79	LYS	CA-C-N	-6.76	113.17	122.30
1	B	79	LYS	C-N-CA	-6.76	113.17	122.30
1	A	37	GLY	CA-C-O	6.76	132.33	120.57
1	B	37	GLY	CA-C-O	6.76	132.33	120.57
1	A	69	GLU	CB-CG-CD	6.75	124.08	112.60
1	B	69	GLU	CB-CG-CD	6.75	124.08	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	PHE	CB-CA-C	-6.75	100.28	110.88
1	B	10	PHE	CB-CA-C	-6.75	100.28	110.88
1	A	73	LYS	CB-CG-CD	6.69	126.68	111.30
1	B	73	LYS	CB-CG-CD	6.69	126.68	111.30
1	A	84	GLY	O-C-N	-6.67	114.03	122.70
1	B	84	GLY	O-C-N	-6.67	114.03	122.70
1	A	60	ASN	N-CA-CB	6.66	121.75	111.22
1	B	60	ASN	N-CA-CB	6.66	121.75	111.22
1	A	10	PHE	N-CA-CB	6.57	119.54	110.01
1	B	10	PHE	N-CA-CB	6.57	119.54	110.01
1	A	101	ALA	N-CA-C	-6.56	102.77	111.24
1	B	101	ALA	N-CA-C	-6.56	102.77	111.24
1	A	51	ALA	N-CA-CB	6.56	121.57	110.49
1	B	51	ALA	N-CA-CB	6.56	121.57	110.49
1	A	12	GLN	O-C-N	-6.55	114.95	122.03
1	B	12	GLN	O-C-N	-6.55	114.95	122.03
1	A	48	TYR	CD1-CE1-CZ	-6.54	107.83	119.60
1	B	48	TYR	CD1-CE1-CZ	-6.54	107.83	119.60
1	A	75	ILE	N-CA-CB	6.54	120.36	111.21
1	B	75	ILE	N-CA-CB	6.54	120.36	111.21
1	A	64	LEU	CA-C-N	-6.48	112.02	120.44
1	A	64	LEU	C-N-CA	-6.48	112.02	120.44
1	B	64	LEU	CA-C-N	-6.48	112.02	120.44
1	B	64	LEU	C-N-CA	-6.48	112.02	120.44
1	A	9	THR	N-CA-CB	6.46	119.73	110.16
1	B	9	THR	N-CA-CB	6.46	119.73	110.16
1	A	26	HIS	CB-CG-CD2	-6.45	122.81	131.20
1	B	26	HIS	CB-CG-CD2	-6.45	122.81	131.20
1	A	79	LYS	CB-CG-CD	6.45	126.14	111.30
1	B	79	LYS	CB-CG-CD	6.45	126.14	111.30
1	A	36	PHE	CA-CB-CG	-6.44	107.36	113.80
1	B	36	PHE	CA-CB-CG	-6.44	107.36	113.80
1	A	34	GLY	CA-C-O	6.42	131.74	120.57
1	B	34	GLY	CA-C-O	6.42	131.74	120.57
1	A	46	TYR	CD1-CG-CD2	-6.42	108.47	118.10
1	B	46	TYR	CD1-CG-CD2	-6.42	108.47	118.10
1	A	55	LYS	N-CA-CB	6.35	121.22	110.49
1	B	55	LYS	N-CA-CB	6.35	121.22	110.49
1	A	79	LYS	CG-CD-CE	6.35	125.90	111.30
1	B	79	LYS	CG-CD-CE	6.35	125.90	111.30
1	A	70	ASN	O-C-N	-6.34	114.03	121.32
1	B	70	ASN	O-C-N	-6.34	114.03	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ASN	CA-C-N	-6.33	109.45	121.54
1	A	62	ASN	C-N-CA	-6.33	109.45	121.54
1	B	62	ASN	CA-C-N	-6.33	109.45	121.54
1	B	62	ASN	C-N-CA	-6.33	109.45	121.54
1	A	59	TRP	CD1-NE1-CE2	-6.32	97.52	108.90
1	B	59	TRP	CD1-NE1-CE2	-6.32	97.52	108.90
1	A	10	PHE	CG-CD1-CE1	-6.29	110.02	120.70
1	B	10	PHE	CG-CD1-CE1	-6.29	110.02	120.70
1	A	95	VAL	CA-C-N	-6.26	111.40	120.29
1	A	95	VAL	C-N-CA	-6.26	111.40	120.29
1	B	95	VAL	CA-C-N	-6.26	111.40	120.29
1	B	95	VAL	C-N-CA	-6.26	111.40	120.29
1	A	25	LYS	CA-C-N	-6.21	109.69	121.54
1	A	25	LYS	C-N-CA	-6.21	109.69	121.54
1	B	25	LYS	CA-C-N	-6.21	109.69	121.54
1	B	25	LYS	C-N-CA	-6.21	109.69	121.54
1	A	68	LEU	N-CA-C	-6.17	101.19	111.37
1	B	68	LEU	N-CA-C	-6.17	101.19	111.37
1	A	24	GLY	O-C-N	-6.15	114.70	122.70
1	B	24	GLY	O-C-N	-6.15	114.70	122.70
1	A	100	SER	CA-C-O	-6.15	113.97	120.55
1	B	100	SER	CA-C-O	-6.15	113.97	120.55
1	A	42	GLN	N-CA-C	-6.14	97.73	110.80
1	B	42	GLN	N-CA-C	-6.14	97.73	110.80
1	A	81	ILE	O-C-N	-6.12	114.92	122.57
1	B	81	ILE	O-C-N	-6.12	114.92	122.57
1	A	99	LYS	CA-C-O	-6.12	113.35	120.20
1	B	99	LYS	CA-C-O	-6.12	113.35	120.20
1	A	99	LYS	N-CA-C	6.09	119.55	111.75
1	B	99	LYS	N-CA-C	6.09	119.55	111.75
1	A	98	LEU	CA-C-N	-6.07	111.52	120.38
1	A	98	LEU	C-N-CA	-6.07	111.52	120.38
1	B	98	LEU	CA-C-N	-6.07	111.52	120.38
1	B	98	LEU	C-N-CA	-6.07	111.52	120.38
1	A	54	SER	CA-C-N	6.06	133.12	121.54
1	A	54	SER	C-N-CA	6.06	133.12	121.54
1	B	54	SER	CA-C-N	6.06	133.12	121.54
1	B	54	SER	C-N-CA	6.06	133.12	121.54
1	A	82	PHE	CB-CG-CD1	6.06	131.00	120.70
1	B	82	PHE	CB-CG-CD1	6.06	131.00	120.70
1	A	12	GLN	OE1-CD-NE2	6.03	128.63	122.60
1	B	12	GLN	OE1-CD-NE2	6.03	128.63	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	LEU	N-CA-C	-6.02	104.28	111.69
1	B	64	LEU	N-CA-C	-6.02	104.28	111.69
1	A	37	GLY	CA-C-N	-6.02	109.70	121.91
1	A	37	GLY	C-N-CA	-6.02	109.70	121.91
1	B	37	GLY	CA-C-N	-6.02	109.70	121.91
1	B	37	GLY	C-N-CA	-6.02	109.70	121.91
1	A	47	SER	CA-C-O	-6.01	111.91	120.51
1	B	47	SER	CA-C-O	-6.01	111.91	120.51
1	A	60	ASN	CA-C-N	-5.97	110.13	121.54
1	A	60	ASN	C-N-CA	-5.97	110.13	121.54
1	B	60	ASN	CA-C-N	-5.97	110.13	121.54
1	B	60	ASN	C-N-CA	-5.97	110.13	121.54
1	A	40	THR	CA-CB-OG1	-5.93	100.70	109.60
1	B	40	THR	CA-CB-OG1	-5.93	100.70	109.60
1	A	80	MET	O-C-N	-5.93	116.31	123.13
1	B	80	MET	O-C-N	-5.93	116.31	123.13
1	A	32	LEU	CB-CA-C	5.92	119.03	111.40
1	B	32	LEU	CB-CA-C	5.92	119.03	111.40
1	A	16	GLN	CG-CD-NE2	-5.90	107.55	116.40
1	B	16	GLN	CG-CD-NE2	-5.90	107.55	116.40
1	A	66	GLU	CG-CD-OE2	5.89	131.96	118.40
1	B	66	GLU	CG-CD-OE2	5.89	131.96	118.40
1	A	88	LYS	CA-C-O	5.88	128.92	120.51
1	B	88	LYS	CA-C-O	5.88	128.92	120.51
1	A	73	LYS	CB-CA-C	-5.87	98.74	110.42
1	B	73	LYS	CB-CA-C	-5.87	98.74	110.42
1	A	15	ALA	CA-C-N	-5.86	110.34	121.54
1	A	15	ALA	C-N-CA	-5.86	110.34	121.54
1	B	15	ALA	CA-C-N	-5.86	110.34	121.54
1	B	15	ALA	C-N-CA	-5.86	110.34	121.54
1	A	36	PHE	CB-CG-CD2	5.86	130.66	120.70
1	B	36	PHE	CB-CG-CD2	5.86	130.66	120.70
1	A	86	LYS	CB-CG-CD	5.84	124.74	111.30
1	B	86	LYS	CB-CG-CD	5.84	124.74	111.30
1	A	69	GLU	CB-CA-C	5.84	122.04	110.42
1	B	69	GLU	CB-CA-C	5.84	122.04	110.42
1	A	45	GLY	N-CA-C	5.82	126.97	113.18
1	B	45	GLY	N-CA-C	5.82	126.97	113.18
1	A	33	TRP	CH2-CZ2-CE2	5.80	125.05	117.50
1	B	33	TRP	CH2-CZ2-CE2	5.80	125.05	117.50
1	A	33	TRP	CB-CG-CD1	-5.80	118.20	126.90
1	B	33	TRP	CB-CG-CD1	-5.80	118.20	126.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ALA	N-CA-CB	-5.78	100.72	110.49
1	A	59	TRP	CA-C-N	-5.78	112.72	123.01
1	A	59	TRP	C-N-CA	-5.78	112.72	123.01
1	B	15	ALA	N-CA-CB	-5.78	100.72	110.49
1	B	59	TRP	CA-C-N	-5.78	112.72	123.01
1	B	59	TRP	C-N-CA	-5.78	112.72	123.01
1	A	25	LYS	N-CA-C	-5.78	98.50	110.80
1	B	25	LYS	N-CA-C	-5.78	98.50	110.80
1	A	33	TRP	CA-C-N	-5.77	110.09	121.41
1	A	33	TRP	C-N-CA	-5.77	110.09	121.41
1	A	48	TYR	CA-CB-CG	5.77	124.29	113.90
1	B	33	TRP	CA-C-N	-5.77	110.09	121.41
1	B	33	TRP	C-N-CA	-5.77	110.09	121.41
1	B	48	TYR	CA-CB-CG	5.77	124.29	113.90
1	A	92	GLN	CA-CB-CG	-5.76	102.57	114.10
1	B	92	GLN	CA-CB-CG	-5.76	102.57	114.10
1	A	32	LEU	CA-C-N	5.76	132.54	121.54
1	A	32	LEU	C-N-CA	5.76	132.54	121.54
1	B	32	LEU	CA-C-N	5.76	132.54	121.54
1	B	32	LEU	C-N-CA	5.76	132.54	121.54
1	A	19	THR	CA-CB-OG1	-5.75	100.98	109.60
1	B	19	THR	CA-CB-OG1	-5.75	100.98	109.60
1	A	5	LYS	CB-CG-CD	5.75	124.52	111.30
1	B	5	LYS	CB-CG-CD	5.75	124.52	111.30
1	A	97	TYR	CB-CA-C	-5.74	101.31	110.84
1	B	97	TYR	CB-CA-C	-5.74	101.31	110.84
1	A	82	PHE	CG-CD1-CE1	5.73	130.44	120.70
1	B	82	PHE	CG-CD1-CE1	5.73	130.44	120.70
1	A	41	GLY	CA-C-O	5.72	127.72	121.02
1	B	41	GLY	CA-C-O	5.72	127.72	121.02
1	A	66	GLU	CB-CG-CD	5.72	122.32	112.60
1	B	66	GLU	CB-CG-CD	5.72	122.32	112.60
1	A	14	CYS	CB-CA-C	-5.70	100.78	110.88
1	B	14	CYS	CB-CA-C	-5.70	100.78	110.88
1	A	82	PHE	N-CA-CB	-5.70	100.69	111.00
1	B	82	PHE	N-CA-CB	-5.70	100.69	111.00
1	A	99	LYS	CB-CG-CD	5.68	124.36	111.30
1	B	99	LYS	CB-CG-CD	5.68	124.36	111.30
1	A	8	LYS	CG-CD-CE	5.67	124.35	111.30
1	B	8	LYS	CG-CD-CE	5.67	124.35	111.30
1	A	67	TYR	N-CA-C	5.67	118.32	111.40
1	B	67	TYR	N-CA-C	5.67	118.32	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLU	N-CA-C	-5.67	98.73	110.80
1	B	44	GLU	N-CA-C	-5.67	98.73	110.80
1	A	10	PHE	N-CA-C	-5.64	105.03	111.07
1	B	10	PHE	N-CA-C	-5.64	105.03	111.07
1	A	87	LYS	CA-CB-CG	5.63	125.36	114.10
1	B	87	LYS	CA-CB-CG	5.63	125.36	114.10
1	A	85	ILE	CA-C-N	-5.62	113.75	123.25
1	A	85	ILE	C-N-CA	-5.62	113.75	123.25
1	B	85	ILE	CA-C-N	-5.62	113.75	123.25
1	B	85	ILE	C-N-CA	-5.62	113.75	123.25
1	A	49	THR	N-CA-C	5.62	119.56	111.02
1	B	49	THR	N-CA-C	5.62	119.56	111.02
1	A	68	LEU	CA-C-O	5.61	127.21	120.92
1	B	68	LEU	CA-C-O	5.61	127.21	120.92
1	A	46	TYR	CE1-CZ-CE2	5.59	131.47	120.30
1	B	46	TYR	CE1-CZ-CE2	5.59	131.47	120.30
1	A	102	THR	CA-CB-CG2	5.57	119.97	110.50
1	B	102	THR	CA-CB-CG2	5.57	119.97	110.50
1	A	2	ASP	CB-CG-OD1	-5.57	105.60	118.40
1	B	2	ASP	CB-CG-OD1	-5.57	105.60	118.40
1	A	68	LEU	N-CA-CB	-5.55	100.72	109.78
1	B	68	LEU	N-CA-CB	-5.55	100.72	109.78
1	A	8	LYS	CB-CA-C	-5.55	101.53	110.74
1	B	8	LYS	CB-CA-C	-5.55	101.53	110.74
1	A	102	THR	CA-CB-OG1	-5.52	101.32	109.60
1	B	102	THR	CA-CB-OG1	-5.52	101.32	109.60
1	A	65	MET	O-C-N	-5.51	116.39	122.07
1	B	65	MET	O-C-N	-5.51	116.39	122.07
1	A	5	LYS	N-CA-CB	5.51	118.84	110.14
1	A	27	LYS	CA-C-N	-5.51	112.06	121.97
1	A	27	LYS	C-N-CA	-5.51	112.06	121.97
1	B	5	LYS	N-CA-CB	5.51	118.84	110.14
1	B	27	LYS	CA-C-N	-5.51	112.06	121.97
1	B	27	LYS	C-N-CA	-5.51	112.06	121.97
1	A	36	PHE	N-CA-C	5.48	122.48	110.80
1	B	36	PHE	N-CA-C	5.48	122.48	110.80
1	A	32	LEU	O-C-N	-5.46	113.43	121.89
1	B	32	LEU	O-C-N	-5.46	113.43	121.89
1	A	60	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	66	GLU	OE1-CD-OE2	-5.45	109.82	122.90
1	B	60	ASN	CA-CB-CG	5.45	118.05	112.60
1	B	66	GLU	OE1-CD-OE2	-5.45	109.82	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	GLY	O-C-N	-5.44	115.63	122.70
1	B	45	GLY	O-C-N	-5.44	115.63	122.70
1	A	2	ASP	CA-C-N	5.42	127.39	120.56
1	A	2	ASP	C-N-CA	5.42	127.39	120.56
1	B	2	ASP	CA-C-N	5.42	127.39	120.56
1	B	2	ASP	C-N-CA	5.42	127.39	120.56
1	A	14	CYS	O-C-N	-5.42	115.79	122.19
1	B	14	CYS	O-C-N	-5.42	115.79	122.19
1	A	103	SER	CB-CA-C	5.40	120.37	110.10
1	B	103	SER	CB-CA-C	5.40	120.37	110.10
1	A	4	ALA	CA-C-N	-5.38	112.52	120.38
1	A	4	ALA	C-N-CA	-5.38	112.52	120.38
1	B	4	ALA	CA-C-N	-5.38	112.52	120.38
1	B	4	ALA	C-N-CA	-5.38	112.52	120.38
1	A	99	LYS	CD-CE-NZ	5.36	129.04	111.90
1	B	99	LYS	CD-CE-NZ	5.36	129.04	111.90
1	A	69	GLU	N-CA-CB	-5.35	101.44	110.49
1	B	69	GLU	N-CA-CB	-5.35	101.44	110.49
1	A	40	THR	CA-CB-CG2	-5.35	101.41	110.50
1	B	40	THR	CA-CB-CG2	-5.35	101.41	110.50
1	A	36	PHE	CG-CD1-CE1	5.34	129.78	120.70
1	B	36	PHE	CG-CD1-CE1	5.34	129.78	120.70
1	A	29	GLY	O-C-N	5.34	127.11	121.77
1	A	52	ASN	CB-CA-C	-5.34	99.80	110.42
1	B	29	GLY	O-C-N	5.34	127.11	121.77
1	B	52	ASN	CB-CA-C	-5.34	99.80	110.42
1	A	47	SER	N-CA-CB	5.34	119.51	110.49
1	B	47	SER	N-CA-CB	5.34	119.51	110.49
1	A	30	PRO	CB-CG-CD	5.33	123.16	106.10
1	B	30	PRO	CB-CG-CD	5.33	123.16	106.10
1	A	72	LYS	N-CA-CB	5.31	119.35	110.53
1	B	72	LYS	N-CA-CB	5.31	119.35	110.53
1	A	79	LYS	CD-CE-NZ	5.29	128.82	111.90
1	B	79	LYS	CD-CE-NZ	5.29	128.82	111.90
1	A	32	LEU	CA-C-O	-5.28	112.09	121.38
1	B	32	LEU	CA-C-O	-5.28	112.09	121.38
1	A	21	GLU	CA-C-N	-5.26	113.06	122.32
1	A	21	GLU	C-N-CA	-5.26	113.06	122.32
1	B	21	GLU	CA-C-N	-5.26	113.06	122.32
1	B	21	GLU	C-N-CA	-5.26	113.06	122.32
1	A	83	ALA	CB-CA-C	-5.26	99.95	110.42
1	B	83	ALA	CB-CA-C	-5.26	99.95	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ASN	CB-CG-OD1	5.25	131.29	120.80
1	B	70	ASN	CB-CG-OD1	5.25	131.29	120.80
1	A	36	PHE	CA-C-O	5.25	128.01	120.51
1	B	36	PHE	CA-C-O	5.25	128.01	120.51
1	A	43	ALA	N-CA-C	-5.24	104.85	113.50
1	B	43	ALA	N-CA-C	-5.24	104.85	113.50
1	A	50	ASP	CA-C-N	5.23	131.54	121.54
1	A	50	ASP	C-N-CA	5.23	131.54	121.54
1	B	50	ASP	CA-C-N	5.23	131.54	121.54
1	B	50	ASP	C-N-CA	5.23	131.54	121.54
1	A	25	LYS	O-C-N	-5.23	115.63	122.59
1	A	69	GLU	CA-CB-CG	5.23	124.57	114.10
1	B	25	LYS	O-C-N	-5.23	115.63	122.59
1	B	69	GLU	CA-CB-CG	5.23	124.57	114.10
1	A	63	THR	CA-C-N	-5.23	111.64	120.58
1	A	63	THR	C-N-CA	-5.23	111.64	120.58
1	B	63	THR	CA-C-N	-5.23	111.64	120.58
1	B	63	THR	C-N-CA	-5.23	111.64	120.58
1	A	7	LYS	CA-C-O	5.23	125.96	120.42
1	B	7	LYS	CA-C-O	5.23	125.96	120.42
1	A	57	ILE	CA-C-N	-5.20	112.61	121.97
1	A	57	ILE	C-N-CA	-5.20	112.61	121.97
1	B	57	ILE	CA-C-N	-5.20	112.61	121.97
1	B	57	ILE	C-N-CA	-5.20	112.61	121.97
1	A	22	ASN	CA-C-N	5.19	130.36	121.07
1	A	22	ASN	C-N-CA	5.19	130.36	121.07
1	B	22	ASN	CA-C-N	5.19	130.36	121.07
1	B	22	ASN	C-N-CA	5.19	130.36	121.07
1	A	7	LYS	CB-CA-C	-5.19	102.03	110.85
1	B	7	LYS	CB-CA-C	-5.19	102.03	110.85
1	A	21	GLU	CA-CB-CG	5.17	124.45	114.10
1	B	21	GLU	CA-CB-CG	5.17	124.45	114.10
1	A	93	ASP	OD1-CG-OD2	-5.16	110.51	122.90
1	B	93	ASP	OD1-CG-OD2	-5.16	110.51	122.90
1	A	39	LYS	CA-C-N	-5.13	115.64	122.72
1	A	39	LYS	C-N-CA	-5.13	115.64	122.72
1	B	39	LYS	CA-C-N	-5.13	115.64	122.72
1	B	39	LYS	C-N-CA	-5.13	115.64	122.72
1	A	74	TYR	CB-CA-C	-5.09	100.28	110.42
1	B	74	TYR	CB-CA-C	-5.09	100.28	110.42
1	A	99	LYS	O-C-N	-5.09	116.40	122.20
1	B	99	LYS	O-C-N	-5.09	116.40	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	LYS	N-CA-CB	-5.08	102.64	110.16
1	B	7	LYS	N-CA-CB	-5.08	102.64	110.16
1	A	69	GLU	CG-CD-OE1	5.07	130.07	118.40
1	B	69	GLU	CG-CD-OE1	5.07	130.07	118.40
1	A	74	TYR	CD1-CG-CD2	-5.06	110.50	118.10
1	B	74	TYR	CD1-CG-CD2	-5.06	110.50	118.10
1	A	36	PHE	CB-CA-C	5.06	120.48	110.42
1	B	36	PHE	CB-CA-C	5.06	120.48	110.42
1	A	44	GLU	CG-CD-OE2	5.05	130.01	118.40
1	B	44	GLU	CG-CD-OE2	5.05	130.01	118.40
1	A	33	TRP	CD2-CE2-CZ2	-5.05	117.35	122.40
1	B	33	TRP	CD2-CE2-CZ2	-5.05	117.35	122.40
1	A	57	ILE	N-CA-C	5.04	119.82	109.34
1	B	57	ILE	N-CA-C	5.04	119.82	109.34
1	A	9	THR	CB-CA-C	-5.04	102.29	110.85
1	B	9	THR	CB-CA-C	-5.04	102.29	110.85
1	A	72	LYS	CA-C-O	-5.03	115.76	121.39
1	B	72	LYS	CA-C-O	-5.03	115.76	121.39
1	A	21	GLU	CB-CA-C	-5.01	103.53	113.45
1	B	21	GLU	CB-CA-C	-5.01	103.53	113.45

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	40	THR	CB
1	A	78	THR	CB
1	B	40	THR	CB
1	B	78	THR	CB

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	PHE	Mainchain
1	A	12	GLN	Sidechain
1	A	16	GLN	Sidechain
1	A	17	CYS	Mainchain
1	A	18	HIS	Sidechain
1	A	2	ASP	Mainchain
1	A	21	GLU	Mainchain
1	A	26	HIS	Sidechain
1	A	29	GLY	Mainchain
1	A	32	LEU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	43	ALA	Mainchain
1	A	44	GLU	Mainchain,Sidechain
1	A	45	GLY	Mainchain
1	A	46	TYR	Sidechain
1	A	47	SER	Mainchain
1	A	49	THR	Mainchain
1	A	5	LYS	Mainchain
1	A	50	ASP	Sidechain
1	A	58	VAL	Mainchain
1	A	61	GLU	Mainchain
1	A	62	ASN	Mainchain,Sidechain
1	A	67	TYR	Sidechain
1	A	69	GLU	Mainchain
1	A	72	LYS	Mainchain
1	A	74	TYR	Mainchain
1	A	77	GLY	Mainchain
1	A	82	PHE	Mainchain
1	A	87	LYS	Mainchain
1	A	91	ARG	Sidechain
1	A	92	GLN	Sidechain
1	A	93	ASP	Sidechain
1	A	94	LEU	Mainchain
1	A	97	TYR	Sidechain
1	B	10	PHE	Mainchain
1	B	12	GLN	Sidechain
1	B	16	GLN	Sidechain
1	B	17	CYS	Mainchain
1	B	18	HIS	Sidechain
1	B	2	ASP	Mainchain
1	B	21	GLU	Mainchain
1	B	26	HIS	Sidechain
1	B	29	GLY	Mainchain
1	B	32	LEU	Mainchain
1	B	43	ALA	Mainchain
1	B	44	GLU	Mainchain,Sidechain
1	B	45	GLY	Mainchain
1	B	46	TYR	Sidechain
1	B	47	SER	Mainchain
1	B	49	THR	Mainchain
1	B	5	LYS	Mainchain
1	B	50	ASP	Sidechain
1	B	58	VAL	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	61	GLU	Mainchain
1	B	62	ASN	Mainchain,Sidechain
1	B	67	TYR	Sidechain
1	B	69	GLU	Mainchain
1	B	72	LYS	Mainchain
1	B	74	TYR	Mainchain
1	B	77	GLY	Mainchain
1	B	82	PHE	Mainchain
1	B	87	LYS	Mainchain
1	B	91	ARG	Sidechain
1	B	92	GLN	Sidechain
1	B	93	ASP	Sidechain
1	B	94	LEU	Mainchain
1	B	97	TYR	Sidechain

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	A	795	0	785	396	47
1	B	795	0	785	396	47
2	A	43	0	27	27	0
2	B	43	0	27	27	0
3	A	1	0	0	0	0
All	All	1677	0	1624	784	54

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 238.

All (784) 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:A:66:GLU:HB3	1:A:74:TYR:CE2	1.24	1.67
1:B:66:GLU:HB3	1:B:74:TYR:CE2	1.24	1.67
1:A:26:HIS:CB	1:A:26:HIS:CG	1.78	1.64
1:B:26:HIS:CG	1:B:26:HIS:CB	1.78	1.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:CA	1:A:49:THR:CB	1.74	1.63
1:B:49:THR:CB	1:B:49:THR:CA	1.74	1.63
1:A:5:LYS:CD	1:A:5:LYS:CG	1.75	1.63
1:B:5:LYS:CD	1:B:5:LYS:CG	1.75	1.63
1:A:53:LYS:CD	1:A:53:LYS:CE	1.78	1.62
1:A:86:LYS:CE	1:A:86:LYS:CD	1.77	1.62
1:B:53:LYS:CE	1:B:53:LYS:CD	1.78	1.62
1:B:86:LYS:CD	1:B:86:LYS:CE	1.77	1.62
1:A:17:CYS:CB	1:A:17:CYS:CA	1.75	1.60
1:B:17:CYS:CB	1:B:17:CYS:CA	1.75	1.60
1:A:98:LEU:C	1:A:98:LEU:CA	1.75	1.59
1:B:98:LEU:C	1:B:98:LEU:CA	1.75	1.59
1:A:56:GLY:N	1:A:56:GLY:CA	1.68	1.56
1:B:56:GLY:CA	1:B:56:GLY:N	1.68	1.56
1:A:91:ARG:N	1:A:91:ARG:CA	1.70	1.55
1:B:91:ARG:N	1:B:91:ARG:CA	1.70	1.55
1:A:32:LEU:N	1:A:32:LEU:CA	1.68	1.55
1:B:32:LEU:N	1:B:32:LEU:CA	1.68	1.55
1:A:86:LYS:CD	1:A:86:LYS:CG	1.80	1.54
1:B:86:LYS:CD	1:B:86:LYS:CG	1.80	1.54
1:A:5:LYS:CE	1:A:5:LYS:NZ	1.67	1.52
1:A:62:ASN:N	1:A:62:ASN:CA	1.70	1.52
1:B:5:LYS:CE	1:B:5:LYS:NZ	1.67	1.52
1:B:62:ASN:N	1:B:62:ASN:CA	1.70	1.52
1:A:72:LYS:NZ	1:A:72:LYS:CE	1.68	1.52
1:B:72:LYS:CE	1:B:72:LYS:NZ	1.68	1.52
1:A:3:VAL:CA	1:A:3:VAL:C	1.79	1.52
1:B:3:VAL:C	1:B:3:VAL:CA	1.79	1.52
1:A:43:ALA:N	1:A:43:ALA:CA	1.70	1.52
1:A:59:TRP:N	1:A:59:TRP:CA	1.69	1.52
1:B:43:ALA:N	1:B:43:ALA:CA	1.70	1.52
1:B:59:TRP:CA	1:B:59:TRP:N	1.69	1.52
1:A:82:PHE:CA	1:A:82:PHE:N	1.70	1.51
1:B:82:PHE:N	1:B:82:PHE:CA	1.70	1.51
1:A:98:LEU:CA	1:A:98:LEU:N	1.73	1.51
1:B:98:LEU:CA	1:B:98:LEU:N	1.73	1.51
1:A:33:TRP:N	1:A:33:TRP:CA	1.70	1.51
1:B:33:TRP:N	1:B:33:TRP:CA	1.70	1.51
1:A:18:HIS:N	1:A:18:HIS:CA	1.68	1.50
1:A:101:ALA:N	1:A:101:ALA:CA	1.72	1.50
1:B:18:HIS:N	1:B:18:HIS:CA	1.68	1.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ALA:CA	1:B:101:ALA:N	1.72	1.50
1:A:16:GLN:CA	1:A:16:GLN:N	1.71	1.49
1:B:16:GLN:N	1:B:16:GLN:CA	1.71	1.49
1:A:83:ALA:CB	1:A:83:ALA:CA	1.91	1.48
1:B:83:ALA:CA	1:B:83:ALA:CB	1.91	1.48
1:A:80:MET:CG	1:A:80:MET:SD	2.01	1.47
1:B:80:MET:CG	1:B:80:MET:SD	2.01	1.47
1:A:46:TYR:CD1	1:A:46:TYR:CB	1.97	1.46
1:B:46:TYR:CD1	1:B:46:TYR:CB	1.97	1.46
1:A:64:LEU:CB	1:A:64:LEU:CA	1.91	1.45
1:B:64:LEU:CB	1:B:64:LEU:CA	1.91	1.45
1:A:92:GLN:N	1:A:92:GLN:CA	1.76	1.45
1:B:92:GLN:CA	1:B:92:GLN:N	1.76	1.45
2:A:104:HEC:O1D	2:A:104:HEC:CGD	1.66	1.44
2:B:104:HEC:CGD	2:B:104:HEC:O1D	1.66	1.44
1:A:12:GLN:CG	1:A:12:GLN:CD	1.93	1.41
1:B:12:GLN:CD	1:B:12:GLN:CG	1.93	1.41
1:A:47:SER:CB	1:A:47:SER:OG	1.69	1.40
1:B:47:SER:CB	1:B:47:SER:OG	1.69	1.40
1:A:24:GLY:N	1:A:24:GLY:CA	1.84	1.40
1:B:24:GLY:N	1:B:24:GLY:CA	1.84	1.40
1:A:92:GLN:OE1	1:A:92:GLN:CD	1.65	1.39
1:B:92:GLN:OE1	1:B:92:GLN:CD	1.65	1.39
1:A:46:TYR:CD1	1:A:46:TYR:CD2	1.93	1.38
1:B:46:TYR:CD1	1:B:46:TYR:CD2	1.93	1.38
1:A:86:LYS:CE	1:B:103:SER:CA	2.01	1.38
1:A:66:GLU:HB3	1:A:74:TYR:CZ	1.57	1.38
1:B:66:GLU:HB3	1:B:74:TYR:CZ	1.57	1.38
1:A:73:LYS:CE	1:A:73:LYS:CD	2.04	1.35
1:B:73:LYS:CD	1:B:73:LYS:CE	2.04	1.35
1:A:86:LYS:NZ	1:B:103:SER:CB	1.91	1.32
1:A:48:TYR:HE2	2:A:104:HEC:O2D	1.09	1.30
1:B:48:TYR:HE2	2:B:104:HEC:O2D	1.09	1.30
1:A:86:LYS:CD	1:B:103:SER:HB3	1.61	1.30
1:A:44:GLU:CG	1:A:44:GLU:CB	2.09	1.29
1:B:44:GLU:CB	1:B:44:GLU:CG	2.09	1.29
1:A:46:TYR:CG	1:A:46:TYR:CE1	1.96	1.28
1:B:46:TYR:CG	1:B:46:TYR:CE1	1.96	1.28
1:A:66:GLU:CB	1:A:74:TYR:CE2	2.17	1.27
1:B:66:GLU:CB	1:B:74:TYR:CE2	2.17	1.27
1:A:10:PHE:CG	1:A:10:PHE:CE2	1.80	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:PHE:CG	1:B:10:PHE:CE2	1.80	1.26
1:A:44:GLU:CG	1:A:44:GLU:CD	2.08	1.26
1:B:44:GLU:CG	1:B:44:GLU:CD	2.08	1.26
1:A:16:GLN:N	1:A:16:GLN:CB	2.06	1.17
1:B:16:GLN:N	1:B:16:GLN:CB	2.06	1.17
1:A:24:GLY:O	1:A:25:LYS:HG2	1.45	1.17
1:B:24:GLY:O	1:B:25:LYS:HG2	1.45	1.17
1:A:86:LYS:HE3	1:B:103:SER:OG	1.45	1.15
1:A:86:LYS:HE2	1:B:103:SER:CA	1.67	1.14
1:A:16:GLN:N	1:A:16:GLN:HB3	1.62	1.14
1:A:57:ILE:HD12	1:A:58:VAL:H	1.04	1.14
1:B:16:GLN:N	1:B:16:GLN:HB3	1.62	1.14
1:B:57:ILE:HD12	1:B:58:VAL:H	1.04	1.14
1:A:67:TYR:O	1:A:68:LEU:C	1.80	1.14
1:B:67:TYR:O	1:B:68:LEU:C	1.80	1.14
1:A:10:PHE:CD2	1:A:10:PHE:CD1	2.06	1.13
1:B:10:PHE:CD2	1:B:10:PHE:CD1	2.06	1.13
1:A:3:VAL:CA	1:A:3:VAL:CG2	2.25	1.13
1:A:48:TYR:CE2	2:A:104:HEC:O2D	2.02	1.13
1:A:59:TRP:CE3	1:A:63:THR:HG21	1.81	1.13
1:B:3:VAL:CA	1:B:3:VAL:CG2	2.25	1.13
1:B:48:TYR:CE2	2:B:104:HEC:O2D	2.02	1.13
1:B:59:TRP:CE3	1:B:63:THR:HG21	1.81	1.13
1:A:86:LYS:CE	1:B:103:SER:OG	1.97	1.12
1:A:11:VAL:HA	1:A:15:ALA:HB2	1.16	1.12
1:B:11:VAL:HA	1:B:15:ALA:HB2	1.16	1.12
1:A:26:HIS:O	1:A:27:LYS:CG	1.98	1.11
1:B:26:HIS:O	1:B:27:LYS:CG	1.98	1.11
1:A:86:LYS:HZ3	1:B:102:THR:HG22	1.15	1.11
1:A:47:SER:O	1:A:48:TYR:CB	1.99	1.10
1:B:47:SER:O	1:B:48:TYR:CB	1.99	1.10
1:A:59:TRP:HZ3	1:A:63:THR:HG23	1.10	1.10
1:B:59:TRP:HZ3	1:B:63:THR:HG23	1.10	1.10
1:A:10:PHE:CD2	1:A:10:PHE:CB	2.33	1.10
1:B:10:PHE:CD2	1:B:10:PHE:CB	2.33	1.10
2:A:104:HEC:CMD	2:A:104:HEC:HBD1	1.81	1.08
2:B:104:HEC:CMD	2:B:104:HEC:HBD1	1.81	1.08
2:A:104:HEC:HBD1	2:A:104:HEC:HMD1	1.34	1.08
2:B:104:HEC:HBD1	2:B:104:HEC:HMD1	1.34	1.08
1:A:59:TRP:CZ3	1:A:63:THR:HG23	1.89	1.07
1:A:86:LYS:NZ	1:B:102:THR:HG22	1.67	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TRP:CZ3	1:B:63:THR:HG23	1.89	1.07
1:A:73:LYS:H	1:A:76:PRO:HB3	1.21	1.06
1:B:73:LYS:H	1:B:76:PRO:HB3	1.21	1.06
1:A:34:GLY:HA2	1:A:102:THR:HG23	1.32	1.06
1:B:34:GLY:HA2	1:B:102:THR:HG23	1.32	1.06
1:A:59:TRP:CZ3	1:A:63:THR:CG2	2.38	1.05
1:B:59:TRP:CZ3	1:B:63:THR:CG2	2.38	1.05
1:A:36:PHE:N	1:A:36:PHE:HD2	1.55	1.05
1:B:36:PHE:HD2	1:B:36:PHE:N	1.55	1.05
1:A:26:HIS:CG	1:A:26:HIS:CA	2.38	1.05
1:B:26:HIS:CG	1:B:26:HIS:CA	2.38	1.05
1:A:59:TRP:CE3	1:A:63:THR:CG2	2.40	1.04
1:B:59:TRP:CE3	1:B:63:THR:CG2	2.40	1.04
1:A:50:ASP:HB3	1:A:54:SER:OG	1.59	1.03
1:B:50:ASP:HB3	1:B:54:SER:OG	1.59	1.03
1:A:40:THR:CG2	1:A:57:ILE:HG12	1.88	1.03
1:A:57:ILE:CD1	1:A:58:VAL:H	1.70	1.03
1:A:80:MET:HB2	2:A:104:HEC:CHD	1.89	1.03
1:B:40:THR:CG2	1:B:57:ILE:HG12	1.88	1.03
1:B:57:ILE:CD1	1:B:58:VAL:H	1.70	1.03
1:B:80:MET:HB2	2:B:104:HEC:CHD	1.89	1.03
1:A:24:GLY:O	1:A:25:LYS:CG	2.08	1.02
1:B:24:GLY:O	1:B:25:LYS:CG	2.08	1.02
1:A:86:LYS:NZ	1:B:103:SER:HB3	1.58	1.01
1:A:70:ASN:HD21	1:A:72:LYS:HB2	1.26	1.00
1:B:70:ASN:HD21	1:B:72:LYS:HB2	1.26	1.00
1:A:47:SER:O	1:A:48:TYR:HB3	1.18	1.00
1:B:47:SER:O	1:B:48:TYR:HB3	1.18	1.00
1:A:74:TYR:H	1:A:76:PRO:HD3	1.26	0.98
1:B:74:TYR:H	1:B:76:PRO:HD3	1.26	0.98
1:A:44:GLU:CB	1:A:44:GLU:CD	2.35	0.98
1:A:66:GLU:CB	1:A:74:TYR:CZ	2.43	0.98
1:A:85:ILE:HG22	1:A:85:ILE:O	1.61	0.98
1:B:44:GLU:CB	1:B:44:GLU:CD	2.35	0.98
1:B:66:GLU:CB	1:B:74:TYR:CZ	2.43	0.98
1:B:85:ILE:HG22	1:B:85:ILE:O	1.61	0.98
1:A:16:GLN:HB3	1:A:16:GLN:H	1.28	0.98
1:B:16:GLN:HB3	1:B:16:GLN:H	1.28	0.98
1:A:72:LYS:O	1:A:73:LYS:HB2	1.61	0.98
1:B:72:LYS:O	1:B:73:LYS:HB2	1.61	0.98
1:A:86:LYS:HE2	1:B:103:SER:HA	1.46	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:MET:HB2	2:A:104:HEC:C1D	1.94	0.96
1:B:80:MET:HB2	2:B:104:HEC:C1D	1.94	0.96
1:A:3:VAL:CA	1:A:3:VAL:CG1	2.43	0.96
1:B:3:VAL:CA	1:B:3:VAL:CG1	2.43	0.96
1:A:24:GLY:C	1:A:25:LYS:HG2	1.90	0.96
1:B:24:GLY:C	1:B:25:LYS:HG2	1.90	0.96
1:A:48:TYR:CE1	1:A:51:ALA:HB3	2.01	0.96
1:B:48:TYR:CE1	1:B:51:ALA:HB3	2.01	0.96
1:A:68:LEU:HD21	1:A:94:LEU:HG	1.44	0.95
1:B:68:LEU:HD21	1:B:94:LEU:HG	1.44	0.95
1:A:11:VAL:CA	1:A:15:ALA:HB2	1.97	0.95
1:B:11:VAL:CA	1:B:15:ALA:HB2	1.97	0.95
1:A:56:GLY:O	1:A:57:ILE:HG22	1.67	0.94
1:B:56:GLY:O	1:B:57:ILE:HG22	1.67	0.94
1:A:81:ILE:C	1:A:82:PHE:CA	2.40	0.94
1:B:81:ILE:C	1:B:82:PHE:CA	2.40	0.94
1:A:3:VAL:CA	1:A:3:VAL:HG22	1.96	0.94
1:B:3:VAL:CA	1:B:3:VAL:HG22	1.96	0.94
1:A:3:VAL:CA	1:A:3:VAL:HG23	1.96	0.94
1:A:66:GLU:HB3	1:A:74:TYR:HE2	1.18	0.94
1:B:3:VAL:CA	1:B:3:VAL:HG23	1.96	0.94
1:B:66:GLU:HB3	1:B:74:TYR:HE2	1.18	0.94
1:A:46:TYR:CD1	1:A:46:TYR:HB2	2.02	0.93
1:B:46:TYR:CD1	1:B:46:TYR:HB2	2.02	0.93
1:A:35:LEU:HD12	1:A:64:LEU:HD21	1.49	0.93
1:B:35:LEU:HD12	1:B:64:LEU:HD21	1.49	0.93
1:A:10:PHE:CG	1:A:10:PHE:CD2	0.93	0.92
1:A:15:ALA:C	1:A:16:GLN:CA	2.42	0.92
1:B:10:PHE:CG	1:B:10:PHE:CD2	0.93	0.92
1:B:15:ALA:C	1:B:16:GLN:CA	2.42	0.92
1:A:11:VAL:HA	1:A:15:ALA:CB	1.99	0.92
1:B:11:VAL:HA	1:B:15:ALA:CB	1.99	0.92
1:A:50:ASP:O	1:A:51:ALA:CB	2.15	0.92
1:B:50:ASP:O	1:B:51:ALA:CB	2.15	0.92
1:A:26:HIS:O	1:A:27:LYS:HG2	1.68	0.92
1:B:26:HIS:O	1:B:27:LYS:HG2	1.68	0.92
1:A:28:VAL:CG1	1:A:29:GLY:N	2.34	0.91
1:B:28:VAL:CG1	1:B:29:GLY:N	2.34	0.91
1:A:46:TYR:CD1	1:A:46:TYR:CG	0.90	0.90
1:A:84:GLY:O	1:A:85:ILE:HB	1.71	0.90
1:B:46:TYR:CD1	1:B:46:TYR:CG	0.90	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLY:O	1:B:85:ILE:HB	1.71	0.90
1:A:57:ILE:HD12	1:A:58:VAL:N	1.85	0.90
1:B:57:ILE:HD12	1:B:58:VAL:N	1.85	0.90
1:A:73:LYS:O	1:A:74:TYR:HB2	1.72	0.89
1:B:73:LYS:O	1:B:74:TYR:HB2	1.72	0.89
1:A:70:ASN:ND2	1:A:72:LYS:HB2	1.87	0.89
1:B:70:ASN:ND2	1:B:72:LYS:HB2	1.87	0.89
1:A:40:THR:HG21	1:A:57:ILE:HG12	1.51	0.89
1:B:40:THR:HG21	1:B:57:ILE:HG12	1.51	0.89
1:A:28:VAL:HG12	1:A:29:GLY:H	1.36	0.88
1:A:63:THR:HA	1:A:66:GLU:HB2	1.56	0.88
1:B:28:VAL:HG12	1:B:29:GLY:H	1.36	0.88
1:B:63:THR:HA	1:B:66:GLU:HB2	1.56	0.88
1:A:24:GLY:O	1:A:25:LYS:CB	2.21	0.88
1:A:82:PHE:N	1:A:82:PHE:CB	2.36	0.88
1:B:24:GLY:O	1:B:25:LYS:CB	2.21	0.88
1:B:82:PHE:N	1:B:82:PHE:CB	2.36	0.88
1:A:17:CYS:C	1:A:18:HIS:CA	2.48	0.87
1:B:17:CYS:C	1:B:18:HIS:CA	2.48	0.87
1:A:26:HIS:O	1:A:27:LYS:CB	2.23	0.87
1:B:26:HIS:O	1:B:27:LYS:CB	2.23	0.87
1:A:60:ASN:O	1:A:61:GLU:C	2.17	0.87
1:B:60:ASN:O	1:B:61:GLU:C	2.17	0.87
1:A:32:LEU:HD11	2:A:104:HEC:C3A	2.05	0.87
1:B:32:LEU:HD11	2:B:104:HEC:C3A	2.05	0.87
1:A:48:TYR:OH	1:A:78:THR:HA	1.74	0.86
1:A:64:LEU:O	1:A:68:LEU:HB2	1.76	0.86
1:B:48:TYR:OH	1:B:78:THR:HA	1.74	0.86
1:B:64:LEU:O	1:B:68:LEU:HB2	1.76	0.86
1:A:86:LYS:NZ	1:B:103:SER:N	2.24	0.85
2:A:104:HEC:CMC	2:A:104:HEC:HBC3	2.07	0.85
2:B:104:HEC:CMC	2:B:104:HEC:HBC3	2.07	0.85
1:A:59:TRP:CZ3	1:A:63:THR:HG21	2.09	0.85
1:B:59:TRP:CZ3	1:B:63:THR:HG21	2.09	0.85
1:A:16:GLN:H	1:A:16:GLN:HE21	1.25	0.84
1:A:34:GLY:O	1:A:35:LEU:C	2.18	0.84
1:B:16:GLN:H	1:B:16:GLN:HE21	1.25	0.84
1:B:34:GLY:O	1:B:35:LEU:C	2.18	0.84
1:A:46:TYR:CG	1:A:46:TYR:HD1	1.58	0.84
1:B:46:TYR:CG	1:B:46:TYR:HD1	1.58	0.84
1:A:59:TRP:HE3	1:A:63:THR:HG21	1.39	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:NZ	1:B:103:SER:OG	2.04	0.84
1:B:59:TRP:HE3	1:B:63:THR:HG21	1.39	0.84
1:A:19:THR:HG23	1:A:27:LYS:HE3	1.59	0.83
1:B:19:THR:HG23	1:B:27:LYS:HE3	1.59	0.83
1:A:3:VAL:C	1:A:3:VAL:HG12	2.03	0.83
1:A:40:THR:CG2	1:A:57:ILE:CG1	2.55	0.83
1:B:3:VAL:C	1:B:3:VAL:HG12	2.03	0.83
1:B:40:THR:CG2	1:B:57:ILE:CG1	2.55	0.83
1:A:36:PHE:N	1:A:36:PHE:CD2	2.36	0.83
1:B:36:PHE:N	1:B:36:PHE:CD2	2.36	0.83
1:A:62:ASN:N	1:A:62:ASN:CB	2.41	0.83
1:B:62:ASN:N	1:B:62:ASN:CB	2.41	0.83
1:A:10:PHE:CG	1:A:10:PHE:HD2	1.59	0.83
1:B:10:PHE:CG	1:B:10:PHE:HD2	1.59	0.83
1:A:56:GLY:O	1:A:57:ILE:CG2	2.27	0.82
1:B:56:GLY:O	1:B:57:ILE:CG2	2.27	0.82
1:A:66:GLU:CG	1:A:74:TYR:HE2	1.93	0.81
1:B:66:GLU:CG	1:B:74:TYR:HE2	1.93	0.81
1:A:19:THR:O	1:A:20:VAL:HB	1.78	0.81
1:B:19:THR:O	1:B:20:VAL:HB	1.78	0.81
1:A:49:THR:CA	1:A:49:THR:CG2	2.55	0.81
1:A:74:TYR:N	1:A:76:PRO:HD3	1.96	0.81
1:B:49:THR:CA	1:B:49:THR:CG2	2.55	0.81
1:B:74:TYR:N	1:B:76:PRO:HD3	1.96	0.81
1:A:101:ALA:N	1:A:101:ALA:CB	2.44	0.81
1:B:101:ALA:N	1:B:101:ALA:CB	2.44	0.81
1:A:43:ALA:O	1:A:44:GLU:CB	2.29	0.80
1:B:43:ALA:O	1:B:44:GLU:CB	2.29	0.80
1:A:55:LYS:C	1:A:56:GLY:CA	2.54	0.80
1:B:55:LYS:C	1:B:56:GLY:CA	2.54	0.80
1:A:69:GLU:O	1:A:70:ASN:HB3	1.80	0.80
1:B:69:GLU:O	1:B:70:ASN:HB3	1.80	0.80
1:A:59:TRP:CE3	1:A:59:TRP:HA	2.17	0.80
1:B:59:TRP:CE3	1:B:59:TRP:HA	2.17	0.80
1:A:92:GLN:OE1	1:A:92:GLN:CG	2.30	0.80
1:B:92:GLN:OE1	1:B:92:GLN:CG	2.30	0.80
1:A:48:TYR:CE1	1:A:51:ALA:CB	2.65	0.80
2:A:104:HEC:HBC3	2:A:104:HEC:HMC1	1.64	0.80
1:B:48:TYR:CE1	1:B:51:ALA:CB	2.65	0.80
2:B:104:HEC:HBC3	2:B:104:HEC:HMC1	1.64	0.80
1:A:80:MET:CG	1:A:80:MET:CE	2.60	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:MET:CG	1:B:80:MET:CE	2.60	0.79
1:A:27:LYS:O	1:A:28:VAL:HB	1.75	0.79
1:B:27:LYS:O	1:B:28:VAL:HB	1.75	0.79
1:A:44:GLU:OE2	1:A:44:GLU:HB2	1.83	0.79
1:B:44:GLU:HB2	1:B:44:GLU:OE2	1.83	0.79
1:A:86:LYS:HE2	1:B:103:SER:CB	1.27	0.79
1:A:24:GLY:O	1:A:25:LYS:HB3	1.82	0.79
1:B:24:GLY:O	1:B:25:LYS:HB3	1.82	0.79
1:A:90:GLU:C	1:A:91:ARG:CA	2.53	0.77
1:B:90:GLU:C	1:B:91:ARG:CA	2.53	0.77
1:A:34:GLY:HA2	1:A:102:THR:CG2	2.15	0.77
1:B:34:GLY:HA2	1:B:102:THR:CG2	2.15	0.77
1:A:28:VAL:HG12	1:A:29:GLY:N	1.92	0.77
1:B:28:VAL:HG12	1:B:29:GLY:N	1.92	0.77
1:A:32:LEU:N	1:A:32:LEU:C	2.42	0.77
1:B:32:LEU:N	1:B:32:LEU:C	2.42	0.77
1:A:7:LYS:HB2	1:A:97:TYR:CE2	2.20	0.76
1:B:7:LYS:HB2	1:B:97:TYR:CE2	2.20	0.76
1:A:47:SER:OG	1:A:47:SER:CA	2.33	0.76
1:B:47:SER:OG	1:B:47:SER:CA	2.33	0.76
1:A:23:GLY:O	1:A:25:LYS:N	2.18	0.76
1:B:23:GLY:O	1:B:25:LYS:N	2.18	0.76
1:A:61:GLU:C	1:A:62:ASN:CA	2.57	0.75
1:B:61:GLU:C	1:B:62:ASN:CA	2.57	0.75
1:A:31:ASN:C	1:A:32:LEU:CA	2.57	0.75
1:A:50:ASP:CA	1:A:54:SER:HB2	2.15	0.75
1:B:31:ASN:C	1:B:32:LEU:CA	2.57	0.75
1:B:50:ASP:CA	1:B:54:SER:HB2	2.15	0.75
1:A:50:ASP:HB3	1:A:54:SER:CB	2.16	0.75
1:A:86:LYS:NZ	1:B:103:SER:CA	2.43	0.75
1:B:50:ASP:HB3	1:B:54:SER:CB	2.16	0.75
1:A:87:LYS:O	1:A:88:LYS:C	2.30	0.75
1:B:87:LYS:O	1:B:88:LYS:C	2.30	0.75
1:A:84:GLY:O	1:A:85:ILE:CB	2.32	0.74
1:B:84:GLY:O	1:B:85:ILE:CB	2.32	0.74
1:A:24:GLY:C	1:A:25:LYS:CG	2.58	0.74
1:A:91:ARG:C	1:A:92:GLN:CA	2.60	0.74
1:B:24:GLY:C	1:B:25:LYS:CG	2.58	0.74
1:B:91:ARG:C	1:B:92:GLN:CA	2.60	0.74
1:A:68:LEU:O	1:A:69:GLU:C	2.28	0.74
1:B:68:LEU:O	1:B:69:GLU:C	2.28	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLN:H	1:A:16:GLN:NE2	1.85	0.74
1:A:18:HIS:N	1:A:18:HIS:CB	2.50	0.74
1:B:16:GLN:H	1:B:16:GLN:NE2	1.85	0.74
1:B:18:HIS:N	1:B:18:HIS:CB	2.50	0.74
1:A:3:VAL:CA	1:A:3:VAL:HG12	2.17	0.73
1:B:3:VAL:CA	1:B:3:VAL:HG12	2.17	0.73
1:A:68:LEU:CD2	1:A:94:LEU:HG	2.18	0.73
1:B:68:LEU:CD2	1:B:94:LEU:HG	2.18	0.73
1:A:20:VAL:O	1:A:20:VAL:HG13	1.82	0.73
1:B:20:VAL:O	1:B:20:VAL:HG13	1.82	0.73
1:A:3:VAL:CA	1:A:3:VAL:HG13	2.17	0.73
1:B:3:VAL:CA	1:B:3:VAL:HG13	2.17	0.73
1:A:56:GLY:C	1:A:57:ILE:CG2	2.60	0.73
1:B:56:GLY:C	1:B:57:ILE:CG2	2.60	0.73
1:A:86:LYS:HZ3	1:B:103:SER:N	1.87	0.72
1:A:40:THR:HG23	1:A:57:ILE:CG1	2.19	0.72
1:B:40:THR:HG23	1:B:57:ILE:CG1	2.19	0.72
1:A:26:HIS:CE1	1:A:31:ASN:H	2.06	0.72
1:A:57:ILE:CG1	1:A:58:VAL:N	2.50	0.72
1:B:26:HIS:CE1	1:B:31:ASN:H	2.06	0.72
1:B:57:ILE:CG1	1:B:58:VAL:N	2.50	0.72
1:A:86:LYS:HE3	1:B:103:SER:HB2	0.72	0.72
1:A:66:GLU:CB	1:A:74:TYR:OH	2.37	0.72
1:B:66:GLU:CB	1:B:74:TYR:OH	2.37	0.72
1:A:79:LYS:HG3	1:A:79:LYS:O	1.87	0.71
1:B:79:LYS:O	1:B:79:LYS:HG3	1.87	0.71
1:A:59:TRP:HE3	1:A:63:THR:CG2	1.94	0.71
1:A:86:LYS:CD	1:B:103:SER:CB	2.39	0.71
1:B:59:TRP:HE3	1:B:63:THR:CG2	1.94	0.71
1:A:38:ARG:HH12	1:A:43:ALA:HB2	1.56	0.71
1:A:66:GLU:CD	1:A:74:TYR:HE2	1.99	0.71
1:B:38:ARG:HH12	1:B:43:ALA:HB2	1.56	0.71
1:B:66:GLU:CD	1:B:74:TYR:HE2	1.99	0.71
1:A:72:LYS:O	1:A:73:LYS:CB	2.35	0.71
1:B:72:LYS:O	1:B:73:LYS:CB	2.35	0.71
1:A:40:THR:HG23	1:A:57:ILE:HG12	1.72	0.71
1:A:60:ASN:CG	1:A:61:GLU:H	1.98	0.71
1:B:40:THR:HG23	1:B:57:ILE:HG12	1.72	0.71
1:B:60:ASN:CG	1:B:61:GLU:H	1.98	0.71
1:A:100:SER:C	1:A:101:ALA:CA	2.60	0.70
1:B:100:SER:C	1:B:101:ALA:CA	2.60	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:C	1:A:3:VAL:CG1	2.65	0.70
1:B:3:VAL:C	1:B:3:VAL:CG1	2.65	0.70
1:A:44:GLU:CD	1:A:44:GLU:HB2	2.17	0.70
1:A:57:ILE:O	1:A:58:VAL:HB	1.91	0.70
1:B:44:GLU:CD	1:B:44:GLU:HB2	2.17	0.70
1:B:57:ILE:O	1:B:58:VAL:HB	1.91	0.70
1:A:53:LYS:CD	1:A:53:LYS:NZ	2.50	0.70
1:B:53:LYS:CD	1:B:53:LYS:NZ	2.50	0.70
1:A:59:TRP:HZ3	1:A:63:THR:CG2	1.83	0.70
1:B:59:TRP:HZ3	1:B:63:THR:CG2	1.83	0.70
1:A:83:ALA:CB	1:A:83:ALA:C	2.65	0.69
1:B:83:ALA:CB	1:B:83:ALA:C	2.65	0.69
1:A:86:LYS:HE2	1:B:103:SER:HB3	1.04	0.69
1:A:57:ILE:CD1	1:A:58:VAL:N	2.48	0.69
1:B:57:ILE:CD1	1:B:58:VAL:N	2.48	0.69
1:A:32:LEU:C	1:A:33:TRP:CA	2.53	0.69
1:B:32:LEU:C	1:B:33:TRP:CA	2.53	0.69
1:A:3:VAL:HG22	1:A:3:VAL:HA	1.74	0.69
1:A:42:GLN:C	1:A:43:ALA:CA	2.65	0.69
1:B:3:VAL:HG22	1:B:3:VAL:HA	1.74	0.69
1:B:42:GLN:C	1:B:43:ALA:CA	2.65	0.69
1:A:26:HIS:O	1:A:27:LYS:HG3	1.90	0.69
1:A:35:LEU:HB2	1:A:36:PHE:CE2	2.28	0.69
1:A:48:TYR:OH	1:A:51:ALA:HB1	1.93	0.69
1:B:26:HIS:O	1:B:27:LYS:HG3	1.90	0.69
1:B:35:LEU:HB2	1:B:36:PHE:CE2	2.28	0.69
1:B:48:TYR:OH	1:B:51:ALA:HB1	1.93	0.69
1:A:50:ASP:HB3	1:A:54:SER:HG	1.55	0.69
1:B:50:ASP:HB3	1:B:54:SER:HG	1.55	0.69
1:A:91:ARG:N	1:A:91:ARG:C	2.50	0.68
1:B:91:ARG:N	1:B:91:ARG:C	2.50	0.68
1:A:26:HIS:C	1:A:27:LYS:HG3	2.18	0.68
1:B:26:HIS:C	1:B:27:LYS:HG3	2.18	0.68
1:A:98:LEU:N	1:A:98:LEU:CB	2.55	0.68
1:B:98:LEU:N	1:B:98:LEU:CB	2.55	0.68
1:A:85:ILE:O	1:A:85:ILE:CG2	2.39	0.68
1:B:85:ILE:O	1:B:85:ILE:CG2	2.39	0.68
1:A:32:LEU:HD13	1:A:35:LEU:HD21	1.75	0.68
1:A:66:GLU:HB3	1:A:74:TYR:OH	1.91	0.68
1:B:32:LEU:HD13	1:B:35:LEU:HD21	1.75	0.68
1:B:66:GLU:HB3	1:B:74:TYR:OH	1.91	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:N	1:A:33:TRP:HA	1.98	0.68
1:A:38:ARG:NH1	1:A:43:ALA:HB2	2.09	0.68
1:A:53:LYS:CE	1:A:53:LYS:CG	2.70	0.68
1:B:33:TRP:N	1:B:33:TRP:HA	1.98	0.68
1:B:38:ARG:NH1	1:B:43:ALA:HB2	2.09	0.68
1:B:53:LYS:CE	1:B:53:LYS:CG	2.70	0.68
1:A:44:GLU:CB	1:A:44:GLU:OE2	2.40	0.67
1:B:44:GLU:CB	1:B:44:GLU:OE2	2.40	0.67
1:A:64:LEU:CA	1:A:64:LEU:HD12	2.24	0.67
1:B:64:LEU:CA	1:B:64:LEU:HD12	2.24	0.67
1:A:86:LYS:HE3	1:B:103:SER:CB	0.43	0.67
1:A:36:PHE:HD2	1:A:36:PHE:H	1.34	0.67
1:A:57:ILE:HG13	1:A:58:VAL:N	2.10	0.67
1:B:36:PHE:HD2	1:B:36:PHE:H	1.34	0.67
1:B:57:ILE:HG13	1:B:58:VAL:N	2.10	0.67
1:A:34:GLY:O	1:A:36:PHE:N	2.28	0.67
1:B:34:GLY:O	1:B:36:PHE:N	2.28	0.67
1:A:7:LYS:O	1:A:11:VAL:N	2.27	0.66
1:A:41:GLY:O	1:A:42:GLN:C	2.38	0.66
1:B:7:LYS:O	1:B:11:VAL:N	2.27	0.66
1:B:41:GLY:O	1:B:42:GLN:C	2.38	0.66
1:A:7:LYS:HB2	1:A:97:TYR:HE2	1.58	0.66
1:A:86:LYS:CE	1:B:103:SER:HB2	1.39	0.66
1:B:7:LYS:HB2	1:B:97:TYR:HE2	1.58	0.66
1:A:5:LYS:O	1:A:6:GLY:C	2.38	0.66
1:B:5:LYS:O	1:B:6:GLY:C	2.38	0.66
1:A:86:LYS:CE	1:B:103:SER:CB	0.77	0.66
1:A:66:GLU:CB	1:A:74:TYR:HE2	1.81	0.66
1:B:66:GLU:CB	1:B:74:TYR:HE2	1.81	0.66
1:A:3:VAL:O	1:A:4:ALA:C	2.29	0.66
1:A:64:LEU:CA	1:A:64:LEU:CG	2.70	0.66
1:A:69:GLU:O	1:A:70:ASN:CB	2.37	0.66
1:B:3:VAL:O	1:B:4:ALA:C	2.29	0.66
1:B:64:LEU:CA	1:B:64:LEU:CG	2.70	0.66
1:B:69:GLU:O	1:B:70:ASN:CB	2.37	0.66
1:A:86:LYS:HZ3	1:B:102:THR:CG2	2.02	0.65
1:A:50:ASP:O	1:A:51:ALA:HB2	1.96	0.65
1:A:63:THR:HG22	1:A:64:LEU:N	2.11	0.65
1:B:50:ASP:O	1:B:51:ALA:HB2	1.96	0.65
1:B:63:THR:HG22	1:B:64:LEU:N	2.11	0.65
1:A:73:LYS:N	1:A:76:PRO:HB3	2.04	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:N	1:B:76:PRO:HB3	2.04	0.65
1:A:43:ALA:N	1:A:43:ALA:C	2.52	0.65
1:A:58:VAL:C	1:A:59:TRP:CA	2.65	0.65
1:B:43:ALA:N	1:B:43:ALA:C	2.52	0.65
1:B:58:VAL:C	1:B:59:TRP:CA	2.65	0.65
1:A:26:HIS:CB	1:A:26:HIS:CD2	2.64	0.65
1:B:26:HIS:CB	1:B:26:HIS:CD2	2.64	0.65
1:A:73:LYS:O	1:A:74:TYR:CB	2.43	0.65
1:B:73:LYS:O	1:B:74:TYR:CB	2.43	0.65
1:A:7:LYS:CA	1:A:97:TYR:CE2	2.80	0.64
1:B:7:LYS:CA	1:B:97:TYR:CE2	2.80	0.64
1:A:54:SER:O	1:A:56:GLY:N	2.30	0.64
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.80	0.64
1:B:54:SER:O	1:B:56:GLY:N	2.30	0.64
1:B:64:LEU:HD12	1:B:64:LEU:HA	1.80	0.64
1:A:65:MET:HE1	1:A:92:GLN:N	2.12	0.64
1:B:65:MET:HE1	1:B:92:GLN:N	2.12	0.64
1:A:50:ASP:HA	1:A:54:SER:HB2	1.77	0.64
1:A:62:ASN:C	1:A:64:LEU:N	2.55	0.64
1:B:50:ASP:HA	1:B:54:SER:HB2	1.77	0.64
1:B:62:ASN:C	1:B:64:LEU:N	2.55	0.64
1:A:60:ASN:CG	1:A:61:GLU:N	2.54	0.64
1:B:60:ASN:CG	1:B:61:GLU:N	2.54	0.64
1:A:67:TYR:O	1:A:68:LEU:O	2.15	0.63
1:B:67:TYR:O	1:B:68:LEU:O	2.15	0.63
1:A:17:CYS:CB	1:A:17:CYS:N	2.59	0.63
1:B:17:CYS:CB	1:B:17:CYS:N	2.59	0.63
1:A:26:HIS:CG	1:A:26:HIS:N	2.66	0.63
1:B:26:HIS:CG	1:B:26:HIS:N	2.66	0.63
1:A:46:TYR:O	1:A:47:SER:CB	2.46	0.63
1:A:48:TYR:CZ	1:A:51:ALA:CB	2.82	0.63
1:B:46:TYR:O	1:B:47:SER:CB	2.46	0.63
1:B:48:TYR:CZ	1:B:51:ALA:CB	2.82	0.63
1:A:50:ASP:O	1:A:51:ALA:HB3	1.99	0.62
1:A:102:THR:HG22	1:A:103:SER:N	2.13	0.62
1:B:50:ASP:O	1:B:51:ALA:HB3	1.99	0.62
1:B:102:THR:HG22	1:B:103:SER:N	2.13	0.62
2:A:104:HEC:HBD1	2:A:104:HEC:HMD2	1.81	0.62
2:B:104:HEC:HBD1	2:B:104:HEC:HMD2	1.81	0.62
1:A:17:CYS:CB	1:A:17:CYS:C	2.72	0.61
1:A:56:GLY:C	1:A:57:ILE:HG23	2.23	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLN:N	1:A:92:GLN:C	2.56	0.61
1:B:17:CYS:CB	1:B:17:CYS:C	2.72	0.61
1:B:56:GLY:C	1:B:57:ILE:HG23	2.23	0.61
1:B:92:GLN:N	1:B:92:GLN:C	2.56	0.61
1:A:18:HIS:CE1	1:A:29:GLY:HA3	2.36	0.61
1:B:18:HIS:CE1	1:B:29:GLY:HA3	2.36	0.61
1:A:59:TRP:N	1:A:59:TRP:CB	2.56	0.61
1:A:81:ILE:O	1:A:82:PHE:CA	2.48	0.61
1:B:59:TRP:N	1:B:59:TRP:CB	2.56	0.61
1:B:81:ILE:O	1:B:82:PHE:CA	2.48	0.61
1:A:26:HIS:C	1:A:27:LYS:CG	2.67	0.61
1:B:26:HIS:C	1:B:27:LYS:CG	2.67	0.61
1:A:67:TYR:O	1:A:69:GLU:N	2.30	0.60
1:B:67:TYR:O	1:B:69:GLU:N	2.30	0.60
1:A:93:ASP:O	1:A:94:LEU:C	2.40	0.60
1:B:93:ASP:O	1:B:94:LEU:C	2.40	0.60
1:A:49:THR:CB	1:A:49:THR:C	2.60	0.60
1:B:49:THR:CB	1:B:49:THR:C	2.60	0.60
1:A:3:VAL:HG12	1:A:4:ALA:N	2.16	0.59
1:A:65:MET:HE1	1:A:91:ARG:C	2.27	0.59
1:A:68:LEU:HD13	1:A:94:LEU:HB3	1.84	0.59
1:B:3:VAL:HG12	1:B:4:ALA:N	2.16	0.59
1:B:65:MET:HE1	1:B:91:ARG:C	2.27	0.59
1:B:68:LEU:HD13	1:B:94:LEU:HB3	1.84	0.59
1:A:48:TYR:CZ	1:A:51:ALA:HB3	2.33	0.59
1:B:48:TYR:CZ	1:B:51:ALA:HB3	2.33	0.59
1:A:64:LEU:CA	1:A:64:LEU:CD1	2.80	0.59
1:B:64:LEU:CA	1:B:64:LEU:CD1	2.80	0.59
1:A:26:HIS:ND1	1:A:31:ASN:N	2.50	0.59
1:B:26:HIS:ND1	1:B:31:ASN:N	2.50	0.59
1:A:3:VAL:CA	1:A:3:VAL:CB	2.81	0.59
1:A:5:LYS:CG	1:A:5:LYS:CE	2.74	0.59
1:B:3:VAL:CA	1:B:3:VAL:CB	2.81	0.59
1:B:5:LYS:CG	1:B:5:LYS:CE	2.74	0.59
1:A:3:VAL:C	1:A:3:VAL:N	2.61	0.58
1:A:7:LYS:CB	1:A:97:TYR:CE2	2.86	0.58
1:A:12:GLN:C	1:A:13:LYS:HG2	2.19	0.58
1:A:66:GLU:HB2	1:A:74:TYR:OH	2.02	0.58
1:B:3:VAL:C	1:B:3:VAL:N	2.61	0.58
1:B:7:LYS:CB	1:B:97:TYR:CE2	2.86	0.58
1:B:12:GLN:C	1:B:13:LYS:HG2	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:HB2	1:B:74:TYR:OH	2.02	0.58
1:A:57:ILE:CG1	1:A:58:VAL:H	2.13	0.58
1:B:57:ILE:CG1	1:B:58:VAL:H	2.13	0.58
1:A:101:ALA:N	1:A:101:ALA:C	2.59	0.58
1:B:101:ALA:N	1:B:101:ALA:C	2.59	0.58
1:A:81:ILE:O	1:A:82:PHE:HA	2.03	0.58
1:B:81:ILE:O	1:B:82:PHE:HA	2.03	0.58
1:A:43:ALA:O	1:A:44:GLU:HB2	2.03	0.58
1:B:43:ALA:O	1:B:44:GLU:HB2	2.03	0.58
1:A:51:ALA:H	1:A:54:SER:HB2	1.69	0.58
1:A:70:ASN:HD21	1:A:72:LYS:CB	2.10	0.58
1:B:51:ALA:H	1:B:54:SER:HB2	1.69	0.58
1:B:70:ASN:HD21	1:B:72:LYS:CB	2.10	0.58
1:A:11:VAL:O	1:A:15:ALA:HB3	2.04	0.58
1:A:48:TYR:OH	1:A:78:THR:CA	2.49	0.58
1:B:11:VAL:O	1:B:15:ALA:HB3	2.04	0.58
1:B:48:TYR:OH	1:B:78:THR:CA	2.49	0.58
1:A:28:VAL:HG13	1:A:29:GLY:N	2.13	0.57
1:A:63:THR:CA	1:A:66:GLU:HB2	2.31	0.57
1:B:28:VAL:HG13	1:B:29:GLY:N	2.13	0.57
1:B:63:THR:CA	1:B:66:GLU:HB2	2.31	0.57
1:A:50:ASP:C	1:A:54:SER:HB2	2.28	0.57
1:B:50:ASP:C	1:B:54:SER:HB2	2.28	0.57
1:A:38:ARG:O	1:A:59:TRP:N	2.37	0.57
1:B:38:ARG:O	1:B:59:TRP:N	2.37	0.57
1:A:19:THR:O	1:A:20:VAL:CB	2.33	0.57
1:B:19:THR:O	1:B:20:VAL:CB	2.33	0.57
1:A:40:THR:HG23	1:A:57:ILE:HG13	1.85	0.57
1:B:40:THR:HG23	1:B:57:ILE:HG13	1.85	0.57
1:A:86:LYS:CD	1:A:86:LYS:NZ	2.67	0.57
1:B:86:LYS:CD	1:B:86:LYS:NZ	2.67	0.57
1:A:6:GLY:O	1:A:7:LYS:C	2.45	0.57
1:B:6:GLY:O	1:B:7:LYS:C	2.45	0.57
1:A:66:GLU:CG	1:A:74:TYR:CE2	2.74	0.56
1:B:66:GLU:CG	1:B:74:TYR:CE2	2.74	0.56
1:A:91:ARG:O	1:A:92:GLN:C	2.49	0.56
1:B:91:ARG:O	1:B:92:GLN:C	2.49	0.56
1:A:30:PRO:O	1:A:31:ASN:C	2.48	0.55
1:B:30:PRO:O	1:B:31:ASN:C	2.48	0.55
1:A:54:SER:O	1:A:55:LYS:C	2.50	0.55
1:B:54:SER:O	1:B:55:LYS:C	2.50	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:CA	1:A:15:ALA:CB	2.72	0.55
1:B:11:VAL:CA	1:B:15:ALA:CB	2.72	0.55
1:A:47:SER:CB	1:A:47:SER:HG	2.12	0.55
1:B:47:SER:CB	1:B:47:SER:HG	2.12	0.55
1:A:26:HIS:CA	1:A:26:HIS:ND1	2.70	0.55
1:B:26:HIS:CA	1:B:26:HIS:ND1	2.70	0.55
1:A:51:ALA:N	1:A:54:SER:HB2	2.23	0.54
1:B:51:ALA:N	1:B:54:SER:HB2	2.23	0.54
1:A:96:ALA:O	1:A:97:TYR:C	2.50	0.54
1:B:96:ALA:O	1:B:97:TYR:C	2.50	0.54
1:A:51:ALA:O	1:A:53:LYS:N	2.41	0.54
1:B:51:ALA:O	1:B:53:LYS:N	2.41	0.54
1:A:26:HIS:O	1:A:27:LYS:HB3	2.04	0.54
1:B:26:HIS:O	1:B:27:LYS:HB3	2.04	0.54
1:A:32:LEU:CD1	2:A:104:HEC:HMA3	2.37	0.54
1:B:32:LEU:CD1	2:B:104:HEC:HMA3	2.37	0.54
1:A:59:TRP:HE3	1:A:59:TRP:HA	1.69	0.54
1:B:59:TRP:HE3	1:B:59:TRP:HA	1.69	0.54
1:A:24:GLY:N	1:A:24:GLY:C	2.63	0.53
1:B:24:GLY:N	1:B:24:GLY:C	2.63	0.53
1:A:80:MET:CB	2:A:104:HEC:C1D	2.79	0.53
1:B:80:MET:CB	2:B:104:HEC:C1D	2.79	0.53
1:A:56:GLY:N	1:A:56:GLY:C	2.63	0.53
1:B:56:GLY:N	1:B:56:GLY:C	2.63	0.53
1:A:98:LEU:N	1:A:98:LEU:CG	2.71	0.53
1:B:98:LEU:N	1:B:98:LEU:CG	2.71	0.53
1:A:63:THR:CG2	1:A:64:LEU:N	2.60	0.53
1:B:63:THR:CG2	1:B:64:LEU:N	2.60	0.53
1:A:63:THR:OG1	1:A:74:TYR:OH	2.20	0.53
1:B:63:THR:OG1	1:B:74:TYR:OH	2.20	0.53
1:A:86:LYS:HZ1	1:B:103:SER:H	1.57	0.53
1:A:26:HIS:CG	1:A:30:PRO:HA	2.45	0.52
1:B:26:HIS:CG	1:B:30:PRO:HA	2.45	0.52
1:A:94:LEU:O	1:A:97:TYR:N	2.41	0.52
1:B:94:LEU:O	1:B:97:TYR:N	2.41	0.52
1:A:70:ASN:ND2	1:A:70:ASN:C	2.68	0.52
1:B:70:ASN:ND2	1:B:70:ASN:C	2.68	0.52
1:A:46:TYR:HB2	1:A:46:TYR:HD1	1.59	0.52
1:B:46:TYR:HB2	1:B:46:TYR:HD1	1.59	0.52
1:A:32:LEU:HD13	1:A:35:LEU:CD2	2.39	0.52
1:A:86:LYS:HZ1	1:B:103:SER:N	2.06	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD13	1:B:35:LEU:CD2	2.39	0.52
1:A:91:ARG:N	1:A:91:ARG:CB	2.63	0.52
1:B:91:ARG:N	1:B:91:ARG:CB	2.63	0.52
1:A:46:TYR:O	1:A:47:SER:HB3	2.10	0.52
1:A:86:LYS:CE	1:A:86:LYS:CG	2.86	0.52
1:B:46:TYR:O	1:B:47:SER:HB3	2.10	0.52
1:B:86:LYS:CE	1:B:86:LYS:CG	2.86	0.52
1:A:94:LEU:O	1:A:95:VAL:C	2.53	0.51
1:B:94:LEU:O	1:B:95:VAL:C	2.53	0.51
1:A:48:TYR:OH	1:A:51:ALA:CB	2.59	0.51
1:A:50:ASP:HB3	1:A:54:SER:HB2	1.90	0.51
1:B:48:TYR:OH	1:B:51:ALA:CB	2.59	0.51
1:B:50:ASP:HB3	1:B:54:SER:HB2	1.90	0.51
1:A:32:LEU:CD1	1:A:35:LEU:HD21	2.40	0.50
1:A:44:GLU:CD	1:A:44:GLU:HA	2.35	0.50
1:B:32:LEU:CD1	1:B:35:LEU:HD21	2.40	0.50
1:B:44:GLU:CD	1:B:44:GLU:HA	2.35	0.50
1:A:3:VAL:HG23	1:A:3:VAL:N	2.26	0.50
1:B:3:VAL:HG23	1:B:3:VAL:N	2.26	0.50
1:A:70:ASN:ND2	1:A:72:LYS:CB	2.70	0.50
1:B:70:ASN:ND2	1:B:72:LYS:CB	2.70	0.50
1:A:92:GLN:O	1:A:93:ASP:C	2.50	0.50
1:B:92:GLN:O	1:B:93:ASP:C	2.50	0.50
1:A:32:LEU:HD11	2:A:104:HEC:CMA	2.41	0.50
1:B:32:LEU:HD11	2:B:104:HEC:CMA	2.41	0.50
1:A:91:ARG:C	1:A:92:GLN:C	2.80	0.50
1:B:91:ARG:C	1:B:92:GLN:C	2.80	0.50
1:A:10:PHE:CD2	1:A:14:CYS:HB2	2.47	0.49
1:B:10:PHE:CD2	1:B:14:CYS:HB2	2.47	0.49
1:A:55:LYS:HZ2	1:A:74:TYR:HA	1.78	0.49
1:B:55:LYS:HZ2	1:B:74:TYR:HA	1.78	0.49
1:A:19:THR:HG21	1:A:25:LYS:HE2	1.94	0.49
1:B:19:THR:HG21	1:B:25:LYS:HE2	1.94	0.49
1:A:50:ASP:CB	1:A:54:SER:HB2	2.42	0.49
1:B:50:ASP:CB	1:B:54:SER:HB2	2.42	0.49
1:A:14:CYS:SG	2:A:104:HEC:CMB	3.00	0.49
1:B:14:CYS:SG	2:B:104:HEC:CMB	3.00	0.49
1:A:17:CYS:O	1:A:18:HIS:CA	2.61	0.49
1:B:17:CYS:O	1:B:18:HIS:CA	2.61	0.49
1:A:32:LEU:HD11	2:A:104:HEC:C2A	2.43	0.48
1:A:83:ALA:CB	1:A:84:GLY:N	2.75	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD11	2:B:104:HEC:C2A	2.43	0.48
1:B:83:ALA:CB	1:B:84:GLY:N	2.75	0.48
1:A:57:ILE:O	1:A:58:VAL:CB	2.51	0.48
1:B:57:ILE:O	1:B:58:VAL:CB	2.51	0.48
1:A:66:GLU:CD	1:A:74:TYR:CE2	2.85	0.48
1:B:66:GLU:CD	1:B:74:TYR:CE2	2.85	0.48
1:A:44:GLU:CD	1:A:44:GLU:CA	2.87	0.47
1:B:44:GLU:CD	1:B:44:GLU:CA	2.87	0.47
1:A:79:LYS:HE2	2:A:104:HEC:CBD	2.45	0.47
1:B:79:LYS:HE2	2:B:104:HEC:CBD	2.45	0.47
1:A:49:THR:CA	1:A:49:THR:OG1	2.53	0.47
1:B:49:THR:CA	1:B:49:THR:OG1	2.53	0.47
1:A:65:MET:O	1:A:66:GLU:C	2.55	0.47
1:A:98:LEU:C	1:A:98:LEU:N	2.71	0.47
1:B:65:MET:O	1:B:66:GLU:C	2.55	0.47
1:B:98:LEU:C	1:B:98:LEU:N	2.71	0.47
1:A:9:THR:HG21	1:A:94:LEU:HD22	1.96	0.47
1:B:9:THR:HG21	1:B:94:LEU:HD22	1.96	0.47
1:A:74:TYR:O	1:A:75:ILE:C	2.56	0.46
1:B:74:TYR:O	1:B:75:ILE:C	2.56	0.46
1:A:39:LYS:HA	1:A:58:VAL:HA	1.97	0.46
1:B:39:LYS:HA	1:B:58:VAL:HA	1.97	0.46
1:A:48:TYR:OH	1:A:79:LYS:N	2.48	0.46
1:B:48:TYR:OH	1:B:79:LYS:N	2.48	0.46
1:A:10:PHE:CD2	1:A:14:CYS:CB	2.98	0.46
1:B:10:PHE:CD2	1:B:14:CYS:CB	2.98	0.46
1:A:86:LYS:CE	1:B:103:SER:HB3	0.21	0.45
1:A:53:LYS:O	1:A:54:SER:C	2.59	0.45
1:A:64:LEU:CB	1:A:64:LEU:C	2.86	0.45
1:B:53:LYS:O	1:B:54:SER:C	2.59	0.45
1:B:64:LEU:CB	1:B:64:LEU:C	2.86	0.45
1:A:85:ILE:HD12	1:A:94:LEU:HD23	1.97	0.45
1:B:85:ILE:HD12	1:B:94:LEU:HD23	1.97	0.45
1:A:79:LYS:HE2	2:A:104:HEC:HBD1	1.98	0.45
1:B:79:LYS:HE2	2:B:104:HEC:HBD1	1.98	0.45
1:A:25:LYS:O	1:A:26:HIS:O	2.35	0.45
1:A:31:ASN:O	1:A:32:LEU:CA	2.63	0.45
1:B:25:LYS:O	1:B:26:HIS:O	2.35	0.45
1:B:31:ASN:O	1:B:32:LEU:CA	2.63	0.45
1:A:10:PHE:CE2	1:A:14:CYS:HB3	2.52	0.45
1:A:31:ASN:HB3	1:A:33:TRP:CD1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:OE2	1:A:74:TYR:CE2	2.69	0.45
1:B:10:PHE:CE2	1:B:14:CYS:HB3	2.52	0.45
1:B:31:ASN:HB3	1:B:33:TRP:CD1	2.51	0.45
1:B:66:GLU:OE2	1:B:74:TYR:CE2	2.69	0.45
1:A:40:THR:HB	1:A:52:ASN:C	2.42	0.44
1:A:70:ASN:C	1:A:70:ASN:HD22	2.24	0.44
1:B:40:THR:HB	1:B:52:ASN:C	2.42	0.44
1:B:70:ASN:C	1:B:70:ASN:HD22	2.24	0.44
1:A:36:PHE:HE1	1:A:99:LYS:CA	2.31	0.44
1:A:70:ASN:O	1:A:72:LYS:N	2.50	0.44
1:B:36:PHE:HE1	1:B:99:LYS:CA	2.31	0.44
1:B:70:ASN:O	1:B:72:LYS:N	2.50	0.44
1:A:43:ALA:O	1:A:44:GLU:HB3	2.14	0.44
1:A:92:GLN:HG2	1:A:93:ASP:N	2.32	0.44
1:B:43:ALA:O	1:B:44:GLU:HB3	2.14	0.44
1:B:92:GLN:HG2	1:B:93:ASP:N	2.32	0.44
1:A:10:PHE:O	1:A:11:VAL:C	2.60	0.44
1:B:10:PHE:O	1:B:11:VAL:C	2.60	0.44
1:A:13:LYS:O	2:A:104:HEC:HMC3	2.17	0.44
1:A:80:MET:HB2	2:A:104:HEC:C2D	2.41	0.44
1:B:13:LYS:O	2:B:104:HEC:HMC3	2.17	0.44
1:B:80:MET:HB2	2:B:104:HEC:C2D	2.41	0.44
1:A:9:THR:CG2	1:A:94:LEU:HD22	2.48	0.43
1:A:70:ASN:HA	1:A:71:PRO:HD3	1.66	0.43
1:B:9:THR:CG2	1:B:94:LEU:HD22	2.48	0.43
1:B:70:ASN:HA	1:B:71:PRO:HD3	1.66	0.43
1:A:32:LEU:HD11	2:A:104:HEC:HMA3	2.01	0.43
1:A:32:LEU:CD1	2:A:104:HEC:CMA	2.96	0.43
1:B:32:LEU:HD11	2:B:104:HEC:HMA3	2.01	0.43
1:B:32:LEU:CD1	2:B:104:HEC:CMA	2.96	0.43
1:A:15:ALA:O	1:A:16:GLN:CA	2.63	0.43
1:A:44:GLU:OE2	1:A:44:GLU:CA	2.66	0.43
1:B:15:ALA:O	1:B:16:GLN:CA	2.63	0.43
1:B:44:GLU:OE2	1:B:44:GLU:CA	2.66	0.43
1:A:32:LEU:CD2	2:A:104:HEC:HBA1	2.49	0.43
1:A:94:LEU:HA	1:A:94:LEU:HD13	1.54	0.43
1:B:32:LEU:CD2	2:B:104:HEC:HBA1	2.49	0.43
1:B:94:LEU:HA	1:B:94:LEU:HD13	1.54	0.43
1:A:6:GLY:HA3	1:A:97:TYR:HB2	2.00	0.43
1:B:6:GLY:HA3	1:B:97:TYR:HB2	2.00	0.43
1:A:59:TRP:N	1:A:59:TRP:HA	2.07	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TRP:N	1:B:59:TRP:HA	2.07	0.43
1:A:68:LEU:CD1	1:A:94:LEU:HB3	2.48	0.43
1:B:68:LEU:CD1	1:B:94:LEU:HB3	2.48	0.43
1:A:18:HIS:N	1:A:18:HIS:CG	2.87	0.42
1:B:18:HIS:N	1:B:18:HIS:CG	2.87	0.42
1:A:90:GLU:O	1:A:91:ARG:CA	2.66	0.42
1:B:90:GLU:O	1:B:91:ARG:CA	2.66	0.42
1:A:17:CYS:HB3	1:A:18:HIS:H	1.84	0.42
1:A:86:LYS:NZ	1:B:102:THR:CG2	2.59	0.42
1:B:17:CYS:HB3	1:B:18:HIS:H	1.84	0.42
2:A:104:HEC:HBC3	2:A:104:HEC:HMC2	1.96	0.42
2:B:104:HEC:HBC3	2:B:104:HEC:HMC2	1.96	0.42
1:A:62:ASN:C	1:A:64:LEU:H	2.28	0.42
1:B:62:ASN:C	1:B:64:LEU:H	2.28	0.42
1:A:83:ALA:CB	1:A:83:ALA:N	2.71	0.42
1:B:83:ALA:CB	1:B:83:ALA:N	2.71	0.42
2:A:104:HEC:HMB1	2:A:104:HEC:HHB	1.79	0.41
2:B:104:HEC:HHB	2:B:104:HEC:HMB1	1.79	0.41
1:A:21:GLU:HB3	1:A:22:ASN:H	1.72	0.41
1:B:21:GLU:HB3	1:B:22:ASN:H	1.72	0.41
1:A:38:ARG:HH12	1:A:43:ALA:CB	2.30	0.41
1:A:72:LYS:NZ	1:A:72:LYS:CD	2.72	0.41
1:B:38:ARG:HH12	1:B:43:ALA:CB	2.30	0.41
1:B:72:LYS:NZ	1:B:72:LYS:CD	2.72	0.41
2:A:104:HEC:HMD1	2:A:104:HEC:CBD	2.15	0.41
2:B:104:HEC:HMD1	2:B:104:HEC:CBD	2.15	0.41
1:A:14:CYS:O	1:A:15:ALA:C	2.64	0.40
1:A:17:CYS:CB	1:A:18:HIS:N	2.84	0.40
1:A:32:LEU:HD21	2:A:104:HEC:HBA1	2.04	0.40
1:B:14:CYS:O	1:B:15:ALA:C	2.64	0.40
1:B:17:CYS:CB	1:B:18:HIS:N	2.84	0.40
1:B:32:LEU:HD21	2:B:104:HEC:HBA1	2.04	0.40
1:A:23:GLY:O	1:A:24:GLY:C	2.65	0.40
1:A:55:LYS:NZ	1:A:74:TYR:HA	2.37	0.40
1:A:64:LEU:O	1:A:68:LEU:CB	2.57	0.40
1:B:23:GLY:O	1:B:24:GLY:C	2.65	0.40
1:B:55:LYS:NZ	1:B:74:TYR:HA	2.37	0.40
1:B:64:LEU:O	1:B:68:LEU:CB	2.57	0.40
1:A:17:CYS:O	1:A:18:HIS:C	2.65	0.40
1:A:59:TRP:HA	1:A:63:THR:HG21	2.04	0.40
1:B:17:CYS:O	1:B:18:HIS:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TRP:HA	1:B:63:THR:HG21	2.04	0.40

All (54) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:CE	1:B:88:LYS:CD[4_455]	0.41	1.79
1:A:88:LYS:CD	1:B:88:LYS:CE[4_455]	0.41	1.79
1:A:16:GLN:OE1	1:A:47:SER:OG[2_454]	0.69	1.51
1:B:16:GLN:OE1	1:B:47:SER:OG[2_554]	0.69	1.51
1:A:103:SER:CB	1:B:86:LYS:CE[1_455]	0.77	1.43
1:A:55:LYS:O	1:B:62:ASN:CG[4_456]	0.79	1.41
1:A:62:ASN:CG	1:B:55:LYS:O[4_456]	0.79	1.41
1:A:88:LYS:CG	1:B:88:LYS:NZ[4_455]	0.90	1.30
1:A:88:LYS:NZ	1:B:88:LYS:CG[4_455]	0.90	1.30
1:A:55:LYS:O	1:B:62:ASN:ND2[4_456]	0.91	1.29
1:A:62:ASN:ND2	1:B:55:LYS:O[4_456]	0.91	1.29
1:A:55:LYS:C	1:B:62:ASN:ND2[4_456]	0.98	1.22
1:A:62:ASN:ND2	1:B:55:LYS:C[4_456]	0.98	1.22
1:A:88:LYS:CE	1:B:88:LYS:CE[4_455]	1.11	1.09
1:A:88:LYS:CD	1:B:88:LYS:NZ[4_455]	1.18	1.02
1:A:88:LYS:NZ	1:B:88:LYS:CD[4_455]	1.18	1.02
1:A:88:LYS:CD	1:B:88:LYS:CD[4_455]	1.24	0.96
1:A:92:GLN:CB	1:B:92:GLN:NE2[4_455]	1.27	0.93
1:A:92:GLN:NE2	1:B:92:GLN:CB[4_455]	1.27	0.93
1:A:73:LYS:CE	1:B:73:LYS:NZ[4_456]	1.38	0.82
1:A:73:LYS:NZ	1:B:73:LYS:CE[4_456]	1.38	0.82
1:A:16:GLN:OE1	1:A:47:SER:CB[2_454]	1.43	0.77
1:B:16:GLN:OE1	1:B:47:SER:CB[2_554]	1.43	0.77
1:A:73:LYS:CE	1:B:73:LYS:CE[4_456]	1.53	0.67
1:A:55:LYS:O	1:B:62:ASN:CB[4_456]	1.67	0.53
1:A:62:ASN:CB	1:B:55:LYS:O[4_456]	1.67	0.53
1:A:55:LYS:C	1:B:62:ASN:CG[4_456]	1.68	0.52
1:A:62:ASN:CG	1:B:55:LYS:C[4_456]	1.68	0.52
1:A:16:GLN:CD	1:A:47:SER:OG[2_454]	1.70	0.50
1:B:16:GLN:CD	1:B:47:SER:OG[2_554]	1.70	0.50
1:A:73:LYS:NZ	1:B:73:LYS:NZ[4_456]	1.72	0.48
1:A:88:LYS:CG	1:B:88:LYS:CE[4_455]	1.72	0.48
1:A:88:LYS:CE	1:B:88:LYS:CG[4_455]	1.72	0.48
1:A:58:VAL:CG1	1:B:58:VAL:CG1[4_456]	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:O	1:A:79:LYS:NZ[2_454]	1.86	0.34
1:B:11:VAL:O	1:B:79:LYS:NZ[2_554]	1.86	0.34
1:A:16:GLN:CG	1:A:47:SER:C[2_454]	1.89	0.31
1:B:16:GLN:CG	1:B:47:SER:C[2_554]	1.89	0.31
1:A:103:SER:CB	1:B:86:LYS:NZ[1_455]	1.91	0.29
1:A:56:GLY:N	1:B:62:ASN:ND2[4_456]	1.94	0.26
1:A:62:ASN:ND2	1:B:56:GLY:N[4_456]	1.94	0.26
1:A:103:SER:OG	1:B:86:LYS:CE[1_455]	1.97	0.23
1:A:103:SER:CA	1:B:86:LYS:CE[1_455]	2.01	0.19
1:A:55:LYS:CA	1:B:62:ASN:ND2[4_456]	2.03	0.17
1:A:62:ASN:ND2	1:B:55:LYS:CA[4_456]	2.03	0.17
1:A:92:GLN:CG	1:B:92:GLN:NE2[4_455]	2.04	0.16
1:A:92:GLN:NE2	1:B:92:GLN:CG[4_455]	2.04	0.16
1:A:103:SER:OG	1:B:86:LYS:NZ[1_455]	2.04	0.16
1:A:16:GLN:CG	1:A:48:TYR:CB[2_454]	2.06	0.14
1:B:16:GLN:CG	1:B:48:TYR:CB[2_554]	2.06	0.14
1:A:88:LYS:CE	1:B:88:LYS:NZ[4_455]	2.10	0.10
1:A:88:LYS:NZ	1:B:88:LYS:CE[4_455]	2.10	0.10
1:A:16:GLN:CB	1:A:48:TYR:CB[2_454]	2.15	0.05
1:B:16:GLN:CB	1:B:48:TYR:CB[2_554]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	101/103 (98%)	42 (42%)	21 (21%)	38 (38%)	0	0
1	B	101/103 (98%)	42 (42%)	21 (21%)	38 (38%)	0	0
All	All	202/206 (98%)	84 (42%)	42 (21%)	76 (38%)	0	0

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ALA
1	A	18	HIS
1	A	20	VAL
1	A	24	GLY
1	A	25	LYS
1	A	27	LYS
1	A	28	VAL
1	A	30	PRO
1	A	33	TRP
1	A	42	GLN
1	A	44	GLU
1	A	47	SER
1	A	48	TYR
1	A	53	LYS
1	A	55	LYS
1	A	56	GLY
1	A	57	ILE
1	A	62	ASN
1	A	63	THR
1	A	69	GLU
1	A	74	TYR
1	B	15	ALA
1	B	18	HIS
1	B	20	VAL
1	B	24	GLY
1	B	25	LYS
1	B	27	LYS
1	B	28	VAL
1	B	30	PRO
1	B	33	TRP
1	B	42	GLN
1	B	44	GLU
1	B	47	SER
1	B	48	TYR
1	B	53	LYS
1	B	55	LYS
1	B	56	GLY
1	B	57	ILE
1	B	62	ASN
1	B	63	THR
1	B	69	GLU
1	B	74	TYR
1	A	35	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	36	PHE
1	A	51	ALA
1	A	52	ASN
1	A	54	SER
1	A	73	LYS
1	A	85	ILE
1	B	35	LEU
1	B	36	PHE
1	B	51	ALA
1	B	52	ASN
1	B	54	SER
1	B	73	LYS
1	B	85	ILE
1	A	26	HIS
1	A	89	GLY
1	B	26	HIS
1	B	89	GLY
1	A	61	GLU
1	A	88	LYS
1	B	61	GLU
1	B	88	LYS
1	A	83	ALA
1	A	92	GLN
1	B	83	ALA
1	B	92	GLN
1	A	81	ILE
1	A	94	LEU
1	B	81	ILE
1	B	94	LEU
1	A	58	VAL
1	B	58	VAL
1	A	75	ILE
1	B	75	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	81/83 (98%)	49 (60%)	32 (40%)	0	0
1	B	81/83 (98%)	49 (60%)	32 (40%)	0	0
All	All	162/166 (98%)	98 (60%)	64 (40%)	0	0

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	9	THR
1	A	11	VAL
1	A	16	GLN
1	A	17	CYS
1	A	20	VAL
1	A	21	GLU
1	A	27	LYS
1	A	28	VAL
1	A	32	LEU
1	A	33	TRP
1	A	38	ARG
1	A	40	THR
1	A	42	GLN
1	A	46	TYR
1	A	50	ASP
1	A	57	ILE
1	A	61	GLU
1	A	63	THR
1	A	64	LEU
1	A	65	MET
1	A	70	ASN
1	A	75	ILE
1	A	78	THR
1	A	80	MET
1	A	81	ILE
1	A	85	ILE
1	A	86	LYS
1	A	88	LYS
1	A	92	GLN
1	A	94	LEU
1	A	102	THR
1	B	3	VAL
1	B	9	THR
1	B	11	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	16	GLN
1	B	17	CYS
1	B	20	VAL
1	B	21	GLU
1	B	27	LYS
1	B	28	VAL
1	B	32	LEU
1	B	33	TRP
1	B	38	ARG
1	B	40	THR
1	B	42	GLN
1	B	46	TYR
1	B	50	ASP
1	B	57	ILE
1	B	61	GLU
1	B	63	THR
1	B	64	LEU
1	B	65	MET
1	B	70	ASN
1	B	75	ILE
1	B	78	THR
1	B	80	MET
1	B	81	ILE
1	B	85	ILE
1	B	86	LYS
1	B	88	LYS
1	B	92	GLN
1	B	94	LEU
1	B	102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	16	GLN
1	A	42	GLN
1	A	62	ASN
1	A	70	ASN
1	A	92	GLN
1	B	12	GLN
1	B	16	GLN
1	B	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	62	ASN
1	B	70	ASN
1	B	92	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEC	B	104	1	50,50,50	6.72	34 (68%)	68,82,82	6.20	48 (70%)
2	HEC	A	104	1	50,50,50	6.72	34 (68%)	68,82,82	6.20	48 (70%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	104	1	1/1/3/7	10/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	104	1	1/1/3/7	10/14/54/54	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	104	HEC	C4B-C3B	-17.04	1.16	1.45
2	B	104	HEC	C4B-C3B	-17.04	1.16	1.45
2	A	104	HEC	C4D-C3D	-15.05	1.19	1.45
2	B	104	HEC	C4D-C3D	-15.05	1.19	1.45
2	A	104	HEC	O1D-CGD	13.53	1.66	1.22
2	B	104	HEC	O1D-CGD	13.53	1.66	1.22
2	A	104	HEC	CHA-C1A	-12.73	1.13	1.38
2	B	104	HEC	CHA-C1A	-12.73	1.13	1.38
2	A	104	HEC	C1B-NB	-11.24	1.16	1.38
2	B	104	HEC	C1B-NB	-11.24	1.16	1.38
2	A	104	HEC	C1D-C2D	-10.79	1.22	1.44
2	B	104	HEC	C1D-C2D	-10.79	1.22	1.44
2	A	104	HEC	C1A-C2A	-10.32	1.27	1.45
2	B	104	HEC	C1A-C2A	-10.32	1.27	1.45
2	A	104	HEC	C4A-C3A	-10.06	1.25	1.45
2	B	104	HEC	C4A-C3A	-10.06	1.25	1.45
2	A	104	HEC	CHC-C1C	-9.86	1.17	1.39
2	B	104	HEC	CHC-C1C	-9.86	1.17	1.39
2	A	104	HEC	CAA-C2A	-9.68	1.26	1.51
2	B	104	HEC	CAA-C2A	-9.68	1.26	1.51
2	A	104	HEC	FE-ND	-9.60	1.65	1.94
2	B	104	HEC	FE-ND	-9.60	1.65	1.94
2	A	104	HEC	CMD-C2D	-9.16	1.32	1.50
2	B	104	HEC	CMD-C2D	-9.16	1.32	1.50
2	A	104	HEC	C2A-C3A	7.63	1.53	1.36
2	B	104	HEC	C2A-C3A	7.63	1.53	1.36
2	A	104	HEC	CAB-C3B	7.62	1.70	1.51
2	B	104	HEC	CAB-C3B	7.62	1.70	1.51
2	A	104	HEC	C4A-NA	7.19	1.53	1.39
2	B	104	HEC	C4A-NA	7.19	1.53	1.39
2	A	104	HEC	FE-NB	-7.12	1.73	1.94
2	B	104	HEC	FE-NB	-7.12	1.73	1.94
2	A	104	HEC	C3C-C2C	-6.69	1.21	1.38
2	B	104	HEC	C3C-C2C	-6.69	1.21	1.38
2	A	104	HEC	CHC-C4B	-6.01	1.26	1.38
2	B	104	HEC	CHC-C4B	-6.01	1.26	1.38
2	A	104	HEC	CBD-CAD	-5.76	1.32	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	104	HEC	CBD-CAD	-5.76	1.32	1.51
2	A	104	HEC	C4C-NC	-5.67	1.28	1.39
2	B	104	HEC	C4C-NC	-5.67	1.28	1.39
2	A	104	HEC	CBC-CAC	-4.97	1.30	1.51
2	B	104	HEC	CBC-CAC	-4.97	1.30	1.51
2	A	104	HEC	C4B-NB	4.94	1.48	1.40
2	B	104	HEC	C4B-NB	4.94	1.48	1.40
2	A	104	HEC	C1C-NC	4.70	1.48	1.39
2	B	104	HEC	C1C-NC	4.70	1.48	1.39
2	A	104	HEC	C1B-C2B	-4.33	1.35	1.44
2	B	104	HEC	C1B-C2B	-4.33	1.35	1.44
2	A	104	HEC	CAC-C3C	4.20	1.61	1.51
2	B	104	HEC	CAC-C3C	4.20	1.61	1.51
2	A	104	HEC	CHB-C4A	-3.65	1.31	1.38
2	B	104	HEC	CHB-C4A	-3.65	1.31	1.38
2	A	104	HEC	CBB-CAB	-3.47	1.36	1.51
2	B	104	HEC	CBB-CAB	-3.47	1.36	1.51
2	A	104	HEC	C3B-C2B	3.47	1.44	1.36
2	B	104	HEC	C3B-C2B	3.47	1.44	1.36
2	A	104	HEC	CMB-C2B	-3.45	1.43	1.50
2	B	104	HEC	CMB-C2B	-3.45	1.43	1.50
2	A	104	HEC	CBA-CGA	3.35	1.58	1.50
2	B	104	HEC	CBA-CGA	3.35	1.58	1.50
2	A	104	HEC	O2A-CGA	-3.03	1.20	1.30
2	B	104	HEC	O2A-CGA	-3.03	1.20	1.30
2	A	104	HEC	CMC-C2C	2.51	1.55	1.50
2	B	104	HEC	CMC-C2C	2.51	1.55	1.50
2	A	104	HEC	CHB-C1B	2.22	1.44	1.39
2	B	104	HEC	CHB-C1B	2.22	1.44	1.39
2	A	104	HEC	O1A-CGA	-2.05	1.15	1.22
2	B	104	HEC	O1A-CGA	-2.05	1.15	1.22

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	104	HEC	CAB-C3B-C4B	16.31	146.02	124.79
2	B	104	HEC	CAB-C3B-C4B	16.31	146.02	124.79
2	A	104	HEC	C3D-C4D-ND	14.74	124.59	110.35
2	B	104	HEC	C3D-C4D-ND	14.74	124.59	110.35
2	A	104	HEC	C3C-C4C-NC	-12.94	95.79	110.15
2	B	104	HEC	C3C-C4C-NC	-12.94	95.79	110.15
2	A	104	HEC	C1D-ND-C4D	-12.84	90.00	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	104	HEC	C1D-ND-C4D	-12.84	90.00	105.21
2	A	104	HEC	C3B-C4B-NB	12.52	123.90	110.17
2	B	104	HEC	C3B-C4B-NB	12.52	123.90	110.17
2	A	104	HEC	CHB-C4A-NA	-12.00	111.39	124.45
2	B	104	HEC	CHB-C4A-NA	-12.00	111.39	124.45
2	A	104	HEC	C4C-C3C-C2C	11.22	124.23	106.87
2	B	104	HEC	C4C-C3C-C2C	11.22	124.23	106.87
2	A	104	HEC	C4B-NB-C1B	-10.28	93.03	105.21
2	B	104	HEC	C4B-NB-C1B	-10.28	93.03	105.21
2	A	104	HEC	CAD-C3D-C4D	9.42	141.11	124.70
2	B	104	HEC	CAD-C3D-C4D	9.42	141.11	124.70
2	A	104	HEC	C2B-C1B-NB	9.28	120.63	109.90
2	B	104	HEC	C2B-C1B-NB	9.28	120.63	109.90
2	A	104	HEC	CAC-C3C-C2C	-8.80	112.97	126.89
2	B	104	HEC	CAC-C3C-C2C	-8.80	112.97	126.89
2	A	104	HEC	CHB-C4A-C3A	8.79	143.76	125.49
2	B	104	HEC	CHB-C4A-C3A	8.79	143.76	125.49
2	A	104	HEC	C4A-C3A-C2A	7.60	118.26	106.97
2	B	104	HEC	C4A-C3A-C2A	7.60	118.26	106.97
2	A	104	HEC	CMA-C3A-C4A	-6.97	112.45	124.73
2	B	104	HEC	CMA-C3A-C4A	-6.97	112.45	124.73
2	A	104	HEC	CAA-C2A-C3A	6.92	140.83	127.87
2	B	104	HEC	CAA-C2A-C3A	6.92	140.83	127.87
2	A	104	HEC	CAB-C3B-C2B	-6.80	115.06	127.56
2	B	104	HEC	CAB-C3B-C2B	-6.80	115.06	127.56
2	A	104	HEC	CAD-C3D-C2D	-6.67	115.37	127.87
2	B	104	HEC	CAD-C3D-C2D	-6.67	115.37	127.87
2	A	104	HEC	CHC-C4B-C3B	-6.58	113.09	125.23
2	B	104	HEC	CHC-C4B-C3B	-6.58	113.09	125.23
2	A	104	HEC	C4C-CHD-C1D	-6.37	111.27	126.25
2	B	104	HEC	C4C-CHD-C1D	-6.37	111.27	126.25
2	A	104	HEC	O2D-CGD-CBD	6.30	133.92	114.00
2	B	104	HEC	O2D-CGD-CBD	6.30	133.92	114.00
2	A	104	HEC	C2D-C1D-ND	6.25	117.03	109.84
2	B	104	HEC	C2D-C1D-ND	6.25	117.03	109.84
2	A	104	HEC	C4B-C3B-C2B	-6.23	97.82	106.89
2	B	104	HEC	C4B-C3B-C2B	-6.23	97.82	106.89
2	A	104	HEC	CHB-C1B-C2B	-6.20	115.24	125.03
2	B	104	HEC	CHB-C1B-C2B	-6.20	115.24	125.03
2	A	104	HEC	C3A-C4A-NA	-5.83	98.85	109.64
2	B	104	HEC	C3A-C4A-NA	-5.83	98.85	109.64
2	A	104	HEC	CHA-C4D-ND	-5.59	118.41	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	104	HEC	CHA-C4D-ND	-5.59	118.41	124.42
2	A	104	HEC	C4C-NC-C1C	5.43	114.67	105.82
2	B	104	HEC	C4C-NC-C1C	5.43	114.67	105.82
2	A	104	HEC	CHA-C4D-C3D	-5.39	116.91	124.77
2	B	104	HEC	CHA-C4D-C3D	-5.39	116.91	124.77
2	A	104	HEC	CAD-CBD-CGD	5.20	127.47	113.67
2	B	104	HEC	CAD-CBD-CGD	5.20	127.47	113.67
2	A	104	HEC	C1A-C2A-C3A	-4.73	100.88	107.11
2	B	104	HEC	C1A-C2A-C3A	-4.73	100.88	107.11
2	A	104	HEC	C1C-C2C-C3C	-4.69	101.44	106.82
2	B	104	HEC	C1C-C2C-C3C	-4.69	101.44	106.82
2	A	104	HEC	CHD-C4C-NC	4.67	132.33	123.86
2	B	104	HEC	CHD-C4C-NC	4.67	132.33	123.86
2	A	104	HEC	O2D-CGD-O1D	-4.46	111.86	123.33
2	B	104	HEC	O2D-CGD-O1D	-4.46	111.86	123.33
2	A	104	HEC	O1D-CGD-CBD	-4.38	109.21	123.09
2	B	104	HEC	O1D-CGD-CBD	-4.38	109.21	123.09
2	A	104	HEC	CAA-C2A-C1A	-4.37	115.97	124.85
2	B	104	HEC	CAA-C2A-C1A	-4.37	115.97	124.85
2	A	104	HEC	CHD-C1D-C2D	-4.36	114.54	126.95
2	B	104	HEC	CHD-C1D-C2D	-4.36	114.54	126.95
2	A	104	HEC	C4D-C3D-C2D	-4.21	100.77	106.89
2	B	104	HEC	C4D-C3D-C2D	-4.21	100.77	106.89
2	A	104	HEC	CHA-C1A-C2A	-4.01	118.53	124.86
2	B	104	HEC	CHA-C1A-C2A	-4.01	118.53	124.86
2	A	104	HEC	C2C-C1C-NC	-3.95	103.81	110.14
2	B	104	HEC	C2C-C1C-NC	-3.95	103.81	110.14
2	A	104	HEC	CHA-C1A-NA	3.61	128.38	124.45
2	B	104	HEC	CHA-C1A-NA	3.61	128.38	124.45
2	A	104	HEC	O2A-CGA-O1A	-3.33	114.76	123.33
2	B	104	HEC	O2A-CGA-O1A	-3.33	114.76	123.33
2	A	104	HEC	CHD-C1D-ND	3.25	128.39	124.37
2	B	104	HEC	CHD-C1D-ND	3.25	128.39	124.37
2	A	104	HEC	CBB-CAB-C3B	-3.23	103.67	112.42
2	B	104	HEC	CBB-CAB-C3B	-3.23	103.67	112.42
2	A	104	HEC	CHD-C4C-C3C	2.90	131.63	125.30
2	B	104	HEC	CHD-C4C-C3C	2.90	131.63	125.30
2	A	104	HEC	C2A-C1A-NA	2.80	113.03	110.32
2	B	104	HEC	C2A-C1A-NA	2.80	113.03	110.32
2	A	104	HEC	C1B-C2B-C3B	-2.78	104.05	106.98
2	B	104	HEC	C1B-C2B-C3B	-2.78	104.05	106.98
2	A	104	HEC	CBA-CAA-C2A	2.52	119.50	112.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	104	HEC	CBA-CAA-C2A	2.52	119.50	112.53
2	A	104	HEC	O2A-CGA-CBA	2.28	121.20	114.00
2	B	104	HEC	O2A-CGA-CBA	2.28	121.20	114.00
2	A	104	HEC	CHC-C1C-NC	2.26	127.95	123.86
2	B	104	HEC	CHC-C1C-NC	2.26	127.95	123.86

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	104	HEC	NA
2	B	104	HEC	NA

All (20) torsion outliers are listed below:

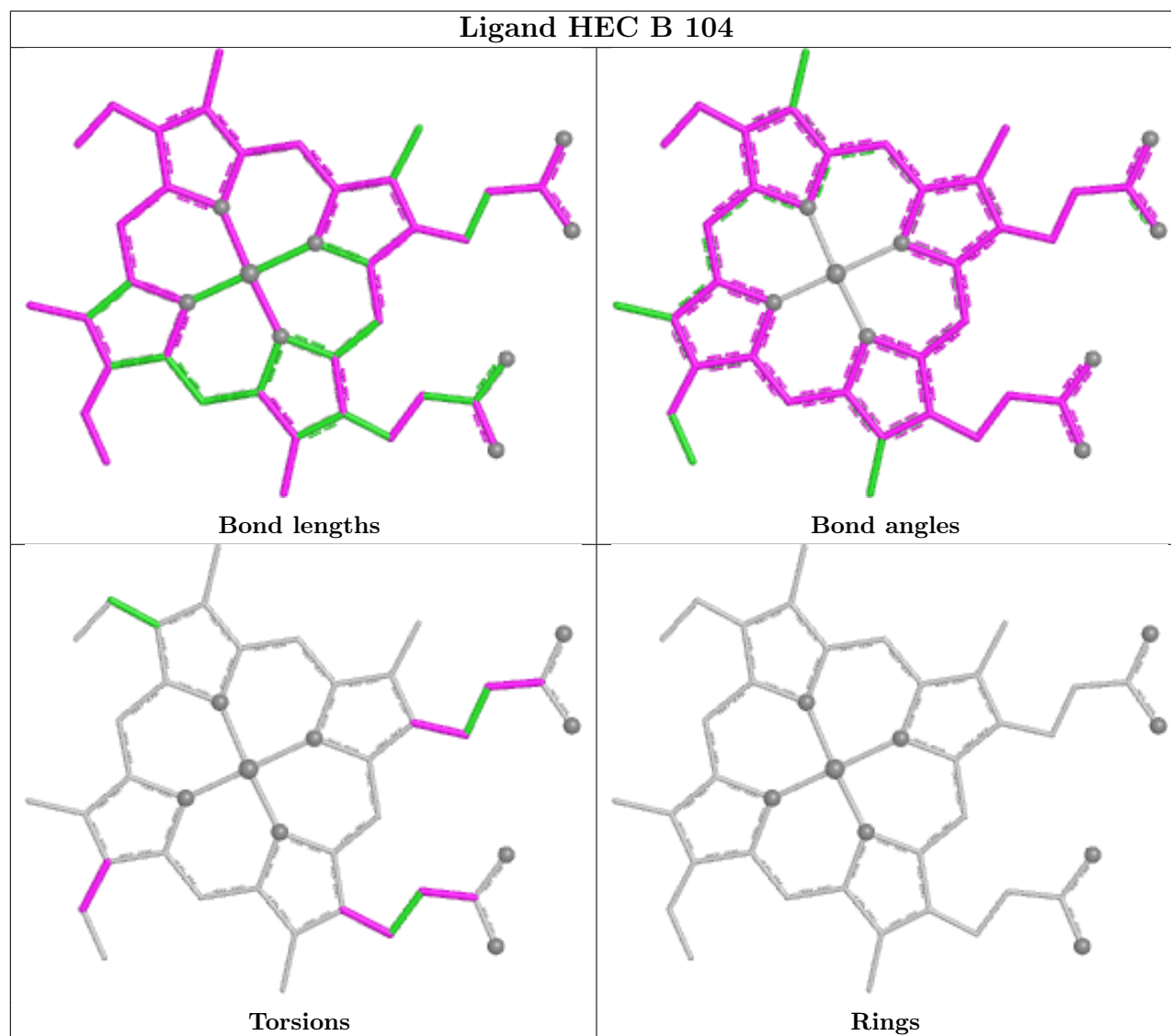
Mol	Chain	Res	Type	Atoms
2	A	104	HEC	C1A-C2A-CAA-CBA
2	B	104	HEC	C1A-C2A-CAA-CBA
2	A	104	HEC	C3A-C2A-CAA-CBA
2	B	104	HEC	C3A-C2A-CAA-CBA
2	A	104	HEC	C4D-C3D-CAD-CBD
2	B	104	HEC	C4D-C3D-CAD-CBD
2	A	104	HEC	C2D-C3D-CAD-CBD
2	B	104	HEC	C2D-C3D-CAD-CBD
2	A	104	HEC	C4C-C3C-CAC-CBC
2	B	104	HEC	C4C-C3C-CAC-CBC
2	A	104	HEC	C2C-C3C-CAC-CBC
2	B	104	HEC	C2C-C3C-CAC-CBC
2	A	104	HEC	CAA-CBA-CGA-O2A
2	B	104	HEC	CAA-CBA-CGA-O2A
2	A	104	HEC	CAA-CBA-CGA-O1A
2	B	104	HEC	CAA-CBA-CGA-O1A
2	A	104	HEC	CAD-CBD-CGD-O2D
2	B	104	HEC	CAD-CBD-CGD-O2D
2	A	104	HEC	CAD-CBD-CGD-O1D
2	B	104	HEC	CAD-CBD-CGD-O1D

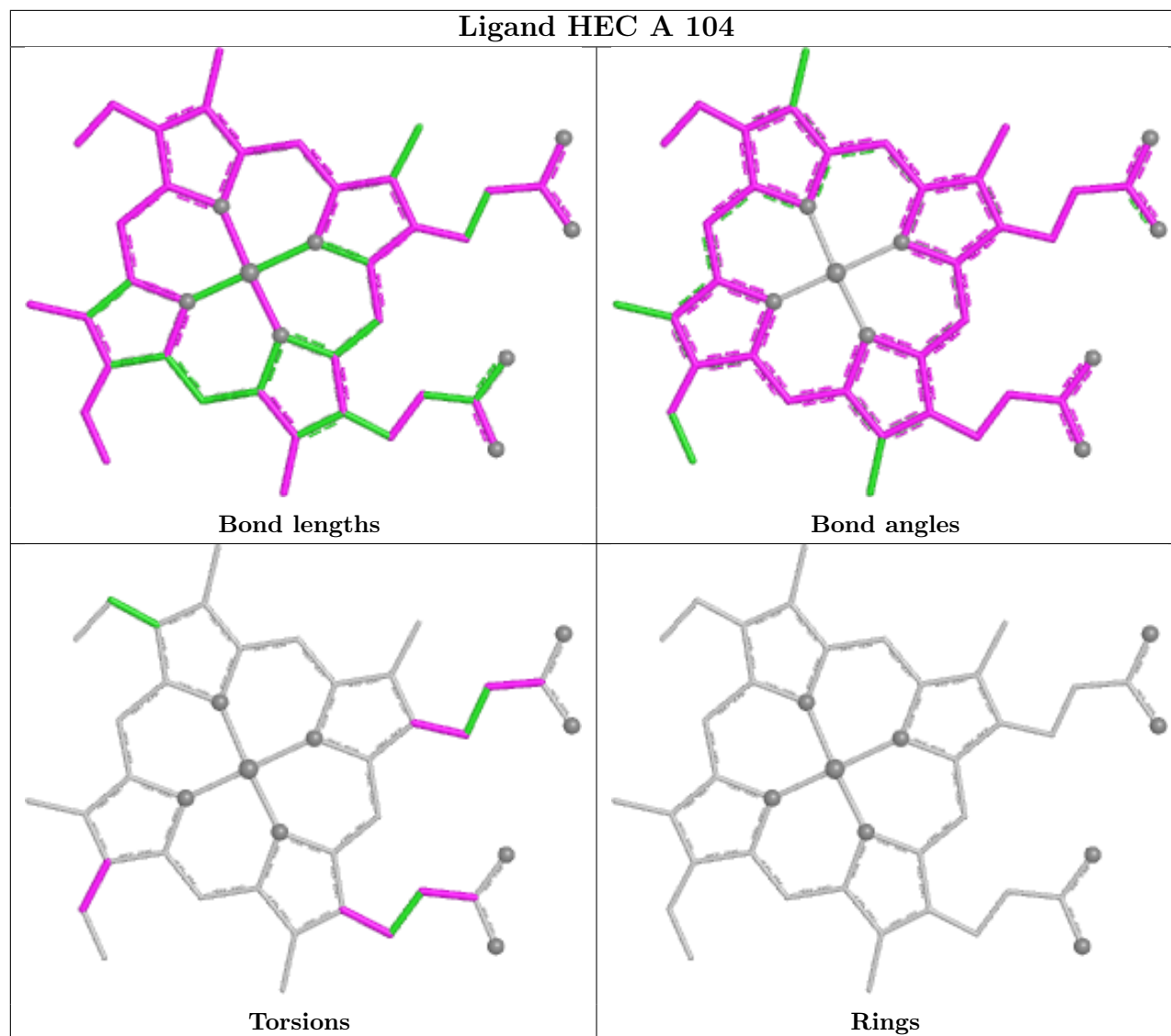
There are no ring outliers.

2 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	104	HEC	27	0
2	A	104	HEC	27	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	29
1	B	29

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	26:HIS	C	27:LYS	N	1.20
1	A	31:ASN	C	32:LEU	N	1.20
1	A	50:ASP	C	51:ALA	N	1.20
1	A	80:MET	C	81:ILE	N	1.20
1	B	26:HIS	C	27:LYS	N	1.20
1	B	31:ASN	C	32:LEU	N	1.20
1	B	50:ASP	C	51:ALA	N	1.20
1	B	80:MET	C	81:ILE	N	1.20
1	A	61:GLU	C	62:ASN	N	1.19
1	A	101:ALA	C	102:THR	N	1.19
1	A	102:THR	C	103:SER	N	1.19
1	B	61:GLU	C	62:ASN	N	1.19
1	B	101:ALA	C	102:THR	N	1.19
1	B	102:THR	C	103:SER	N	1.19
1	A	8:LYS	C	9:THR	N	1.18
1	A	35:LEU	C	36:PHE	N	1.18
1	A	78:THR	C	79:LYS	N	1.18
1	A	97:TYR	C	98:LEU	N	1.18
1	B	8:LYS	C	9:THR	N	1.18
1	B	35:LEU	C	36:PHE	N	1.18
1	B	78:THR	C	79:LYS	N	1.18
1	B	97:TYR	C	98:LEU	N	1.18
1	A	19:THR	C	20:VAL	N	1.17
1	A	54:SER	C	55:LYS	N	1.17
1	B	19:THR	C	20:VAL	N	1.17
1	B	54:SER	C	55:LYS	N	1.17
1	A	12:GLN	C	13:LYS	N	1.16
1	A	55:LYS	C	56:GLY	N	1.16
1	B	12:GLN	C	13:LYS	N	1.16
1	B	55:LYS	C	56:GLY	N	1.16
1	A	60:ASN	C	61:GLU	N	1.15
1	A	90:GLU	C	91:ARG	N	1.15
1	B	60:ASN	C	61:GLU	N	1.15
1	B	90:GLU	C	91:ARG	N	1.15
1	A	65:MET	C	66:GLU	N	1.14
1	A	69:GLU	C	70:ASN	N	1.14
1	B	65:MET	C	66:GLU	N	1.14
1	B	69:GLU	C	70:ASN	N	1.14
1	A	46:TYR	C	47:SER	N	1.13
1	A	66:GLU	C	67:TYR	N	1.13
1	A	82:PHE	C	83:ALA	N	1.13
1	A	89:GLY	C	90:GLU	N	1.13
1	B	46:TYR	C	47:SER	N	1.13

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	66:GLU	C	67:TYR	N	1.13
1	B	82:PHE	C	83:ALA	N	1.13
1	B	89:GLY	C	90:GLU	N	1.13
1	A	22:ASN	C	23:GLY	N	1.11
1	B	22:ASN	C	23:GLY	N	1.11
1	A	86:LYS	C	87:LYS	N	1.09
1	B	86:LYS	C	87:LYS	N	1.09
1	A	40:THR	C	41:GLY	N	1.08
1	A	59:TRP	C	60:ASN	N	1.08
1	A	93:ASP	C	94:LEU	N	1.08
1	B	40:THR	C	41:GLY	N	1.08
1	B	59:TRP	C	60:ASN	N	1.08
1	B	93:ASP	C	94:LEU	N	1.08
1	A	32:LEU	C	33:TRP	N	1.05
1	B	32:LEU	C	33:TRP	N	1.05

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.