



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:34 PM UTC

PDB ID : 3LQA / pdb_00003lqa
Title : Crystal structure of clade C gp120 in complex with sCD4 and 21c Fab
Authors : Diskin, R.; Marcovecchio, P.M.; Bjorkman, P.J.
Deposited on : 2010-02-08
Resolution : 3.40 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

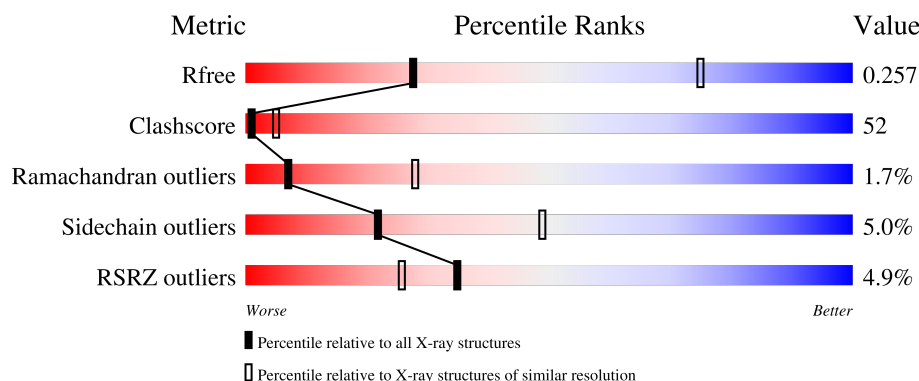
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	192	4% 20% 49% 21% 9%
2	G	332	5% 21% 37% 27% 13%
3	H	231	4% 24% 46% 24% . .
4	L	217	5% 33% 42% 20% . .

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
5	NAG	G	2500	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6945 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 T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	175	Total	C	N	O	S	0	0	0
			1361	850	238	269	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	183	ILE	-	expression tag	UNP P01730
C	184	ASP	-	expression tag	UNP P01730
C	185	GLY	-	expression tag	UNP P01730
C	186	ARG	-	expression tag	UNP P01730
C	187	HIS	-	expression tag	UNP P01730
C	188	HIS	-	expression tag	UNP P01730
C	189	HIS	-	expression tag	UNP P01730
C	190	HIS	-	expression tag	UNP P01730
C	191	HIS	-	expression tag	UNP P01730
C	192	HIS	-	expression tag	UNP P01730

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	290	Total	C	N	O	S	0	0	0
			2271	1434	386	433	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	294	GLY	-	linker	UNP Q1PHM6
G	323	ALA	-	linker	UNP Q1PHM6
G	324	GLY	-	linker	UNP Q1PHM6
G	89	ILE	THR	engineered mutation	UNP Q1PHM6
G	226	ASP	ASN	engineered mutation	UNP Q1PHM6
G	232	ILE	THR	engineered mutation	UNP Q1PHM6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	285	THR	ASN	engineered mutation	UNP Q1PHM6
G	329	ASN	SER	engineered mutation	UNP Q1PHM6
G	388	ILE	THR	engineered mutation	UNP Q1PHM6
G	447	ASP	ASN	engineered mutation	UNP Q1PHM6
G	495	SER	-	expression tag	UNP Q1PHM6
G	496	GLY	-	expression tag	UNP Q1PHM6
G	497	HIS	-	expression tag	UNP Q1PHM6
G	498	HIS	-	expression tag	UNP Q1PHM6
G	499	HIS	-	expression tag	UNP Q1PHM6
G	500	HIS	-	expression tag	UNP Q1PHM6
G	501	HIS	-	expression tag	UNP Q1PHM6
G	502	HIS	-	expression tag	UNP Q1PHM6

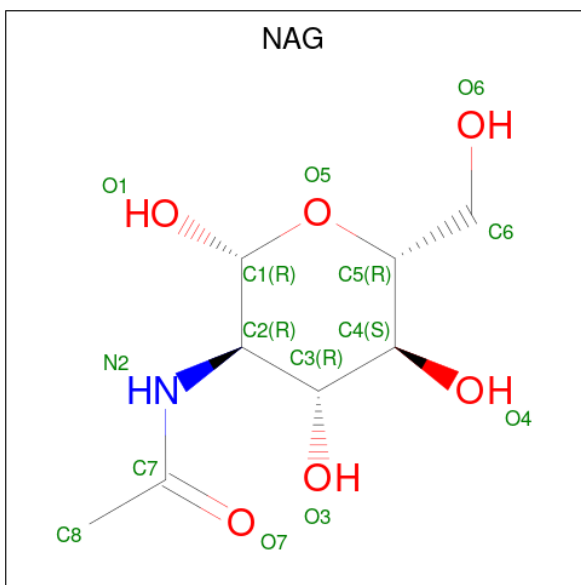
- Molecule 3 is a protein called Heavy chain of anti HIV Fab from human 21c antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	225	Total	C	N	O	S	0	0	0
			1685	1068	277	333	7			

- Molecule 4 is a protein called Light chain of anti HIV Fab from human 21c antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1572	984	262	321	5			

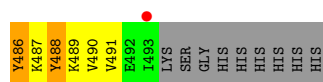
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



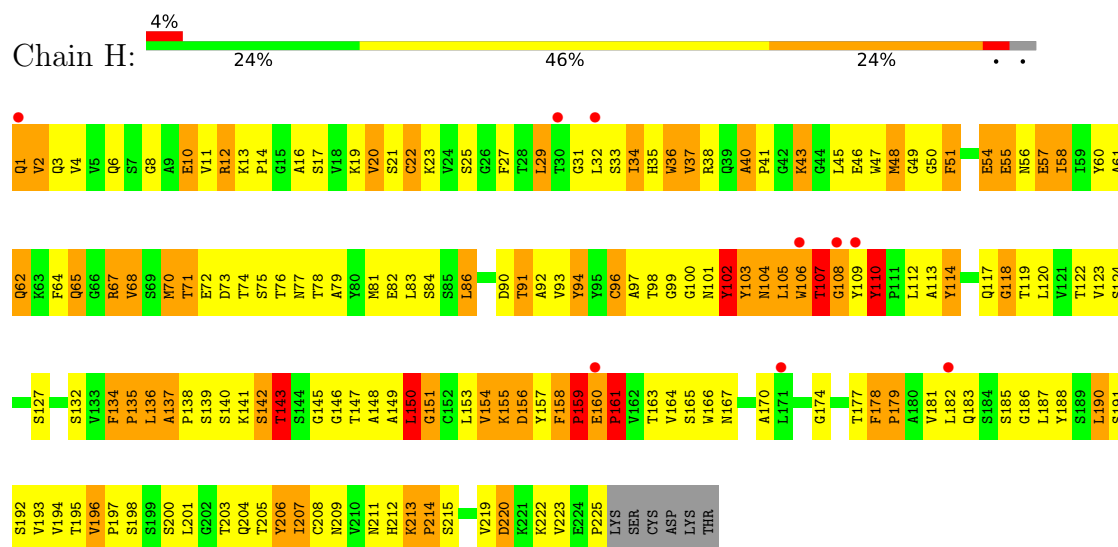
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 1: T-cell surface glycoprotein CD4

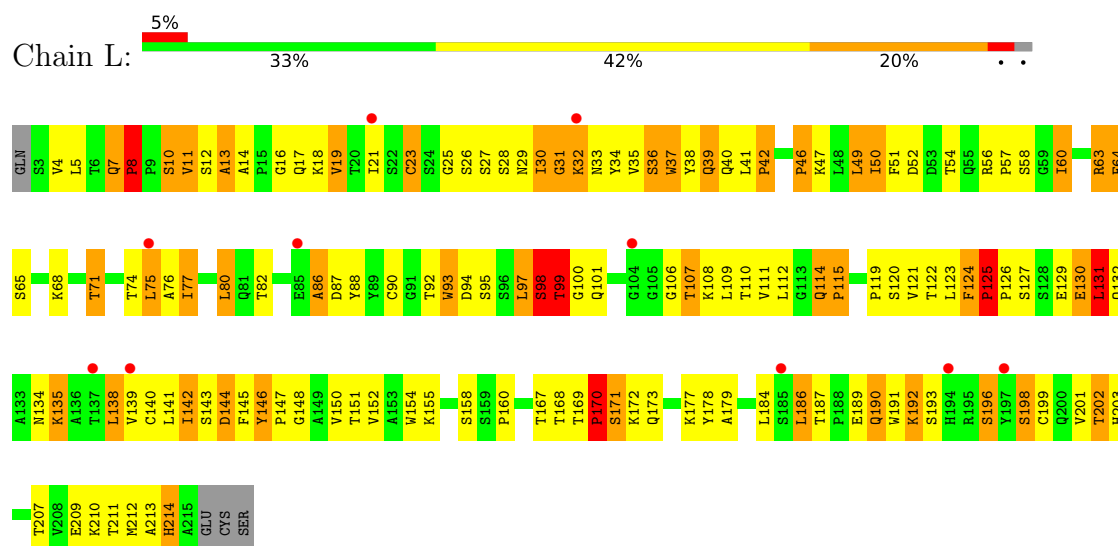




• Molecule 3: Heavy chain of anti HIV Fab from human 21c antibody



• Molecule 4: Light chain of anti HIV Fab from human 21c antibody



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	93.73Å 187.93Å 151.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.00 – 3.40 84.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	79.6 (84.00-3.40) 79.5 (84.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 3.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.322 0.241 , 0.257	Depositor DCC
R_{free} test set	71 reflections (0.47%)	wwPDB-VP
Wilson B-factor (Å ²)	90.5	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6945	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	C	1.18	3/1380 (0.2%)	2.23	78/1862 (4.2%)
2	G	1.38	21/2316 (0.9%)	2.45	166/3142 (5.3%)
3	H	1.46	8/1728 (0.5%)	2.58	127/2358 (5.4%)
4	L	1.44	11/1610 (0.7%)	2.26	79/2197 (3.6%)
All	All	1.38	43/7034 (0.6%)	2.40	450/9559 (4.7%)

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
3	H	0	4
4	L	0	3
All	All	0	7

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	258	ASN	CB-CG	10.83	1.79	1.52
2	G	258	ASN	CA-CB	10.60	1.70	1.53
2	G	258	ASN	CA-C	8.78	1.64	1.53
2	G	380	ASN	CA-CB	8.76	1.63	1.52
2	G	441	ASN	CA-C	8.03	1.62	1.52
2	G	272	ASN	CA-CB	7.93	1.66	1.53
4	L	109	LEU	CA-C	-7.78	1.43	1.52
2	G	442	ILE	CA-CB	7.67	1.64	1.54
4	L	57	PRO	C-O	-7.17	1.14	1.23
4	L	146	TYR	C-O	-7.03	1.16	1.24
3	H	48	MET	SD-CE	-7.00	1.62	1.79
2	G	272	ASN	CB-CG	6.95	1.69	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	272	ASN	CA-C	6.82	1.60	1.52
2	G	254	GLN	CA-C	6.50	1.61	1.52
3	H	113	ALA	C-O	-6.45	1.16	1.24
3	H	108	GLY	C-O	-6.45	1.16	1.23
4	L	80	LEU	C-O	-6.31	1.16	1.23
4	L	37	TRP	CA-C	6.24	1.60	1.52
4	L	110	THR	CA-CB	6.15	1.66	1.54
2	G	441	ASN	CA-CB	6.09	1.65	1.53
2	G	441	ASN	CB-CG	5.99	1.67	1.52
4	L	52	ASP	C-O	-5.97	1.16	1.23
2	G	247	ILE	CA-CB	5.95	1.61	1.54
3	H	4	VAL	CA-CB	-5.90	1.47	1.54
2	G	442	ILE	N-CA	5.84	1.53	1.46
4	L	75	LEU	CA-C	5.79	1.59	1.52
2	G	276	ASN	N-CA	-5.77	1.39	1.46
4	L	37	TRP	N-CA	5.73	1.53	1.46
3	H	219	VAL	CA-C	-5.65	1.45	1.52
4	L	49	LEU	CA-C	-5.62	1.45	1.52
3	H	211	ASN	C-O	-5.58	1.17	1.24
1	C	86	VAL	CA-CB	5.53	1.62	1.54
3	H	102	TYR	CA-C	-5.47	1.45	1.52
2	G	441	ASN	CG-ND2	5.46	1.44	1.33
2	G	103	MET	CG-SD	5.38	1.94	1.80
2	G	469	ILE	CA-CB	5.32	1.61	1.54
2	G	341	VAL	CA-CB	5.26	1.61	1.54
3	H	70	MET	SD-CE	-5.16	1.66	1.79
1	C	100	LEU	C-O	-5.15	1.17	1.24
2	G	422	ILE	CA-C	-5.14	1.45	1.52
4	L	57	PRO	CA-C	-5.03	1.47	1.52
1	C	150	GLU	CA-C	5.03	1.58	1.52
2	G	365	ILE	CA-CB	-5.01	1.48	1.54

All (450) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	160	GLU	CA-C-N	28.76	155.79	119.84
3	H	160	GLU	C-N-CA	28.76	155.79	119.84
3	H	58	ILE	N-CA-C	-26.10	70.53	108.12
4	L	124	PHE	CA-C-N	19.11	140.06	120.38
4	L	124	PHE	C-N-CA	19.11	140.06	120.38
2	G	277	VAL	N-CA-C	17.64	128.53	110.72
2	G	114	SER	N-CA-C	16.84	129.72	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	467	THR	N-CA-C	16.61	133.92	110.50
3	H	75	SER	N-CA-C	15.84	128.55	111.28
2	G	343	LYS	N-CA-C	15.75	128.53	111.36
1	C	174	ILE	N-CA-C	15.64	130.01	108.11
4	L	7	GLN	CA-C-N	-15.19	104.73	120.38
4	L	7	GLN	C-N-CA	-15.19	104.73	120.38
2	G	389	HIS	N-CA-C	15.16	134.38	108.76
4	L	193	SER	N-CA-C	14.97	127.68	111.36
2	G	390	ASN	N-CA-C	14.75	131.60	111.54
2	G	263	GLU	N-CA-C	14.65	127.25	111.28
3	H	106	TRP	N-CA-C	-14.64	95.32	111.28
3	H	67	ARG	N-CA-C	14.06	130.59	113.16
3	H	105	LEU	N-CA-C	-13.53	96.54	111.28
3	H	34	ILE	N-CA-C	13.46	127.01	108.17
2	G	207	ASP	CA-C-N	13.45	136.65	119.84
2	G	207	ASP	C-N-CA	13.45	136.65	119.84
2	G	463	GLU	N-CA-C	-13.22	96.87	111.28
2	G	456	ASP	N-CA-C	12.96	125.40	111.28
1	C	98	PHE	CA-C-N	-12.92	112.86	121.65
1	C	98	PHE	C-N-CA	-12.92	112.86	121.65
1	C	105	ASP	N-CA-C	12.89	125.33	111.28
2	G	382	THR	N-CA-C	-12.81	97.31	111.28
2	G	251	VAL	N-CA-C	-12.75	89.31	107.80
4	L	17	GLN	N-CA-C	12.50	128.35	110.23
3	H	164	VAL	N-CA-C	12.45	125.53	108.11
3	H	109	TYR	N-CA-C	12.44	128.58	113.16
1	C	110	GLN	N-CA-C	12.41	128.22	110.23
4	L	30	ILE	N-CA-C	12.31	123.18	110.62
2	G	276	ASN	N-CA-CB	-12.14	92.27	110.12
2	G	278	LYS	N-CA-C	12.06	128.12	110.28
2	G	442	ILE	N-CA-C	11.91	124.79	108.11
4	L	60	ILE	CA-C-N	-11.74	108.18	120.85
4	L	60	ILE	C-N-CA	-11.74	108.18	120.85
3	H	160	GLU	C-N-CD	-11.57	77.58	125.00
3	H	33	SER	N-CA-C	11.33	123.63	111.28
4	L	32	LYS	N-CA-C	10.91	123.17	111.28
3	H	40	ALA	CA-C-N	-10.75	107.98	120.13
3	H	40	ALA	C-N-CA	-10.75	107.98	120.13
2	G	284	LEU	N-CA-C	10.69	127.30	109.76
2	G	271	GLU	N-CA-C	-10.67	99.65	111.28
3	H	105	LEU	CB-CA-C	-10.61	93.17	110.79
3	H	143	THR	N-CA-C	10.57	126.27	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	450	GLY	N-CA-C	10.55	127.85	110.55
2	G	380	ASN	N-CA-C	-10.54	89.44	107.99
3	H	190	LEU	N-CA-C	10.51	126.52	108.76
2	G	238	VAL	N-CA-C	10.30	122.95	108.12
1	C	3	VAL	N-CA-C	10.10	122.25	108.11
3	H	178	PHE	N-CA-C	9.98	123.85	110.08
2	G	225	ASN	N-CA-C	9.91	122.08	111.28
3	H	55	GLU	N-CA-C	9.85	122.02	111.28
3	H	213	LYS	CA-C-N	9.83	129.19	118.97
3	H	213	LYS	C-N-CA	9.83	129.19	118.97
1	C	128	VAL	N-CA-C	9.74	121.74	108.11
2	G	436	PRO	CA-C-N	9.73	132.00	119.84
2	G	436	PRO	C-N-CA	9.73	132.00	119.84
4	L	209	GLU	N-CA-C	9.64	125.34	109.24
3	H	113	ALA	N-CA-C	9.64	121.86	111.36
2	G	281	ILE	N-CA-C	9.59	120.40	110.72
2	G	341	VAL	N-CA-C	-9.55	101.07	110.72
2	G	287	SER	N-CA-C	9.51	123.39	110.55
2	G	257	LEU	N-CA-C	9.51	124.90	109.40
4	L	11	VAL	N-CA-C	9.38	122.34	108.45
2	G	244	THR	N-CA-C	-9.38	98.15	110.53
1	C	151	LEU	CA-C-N	9.32	132.78	120.28
1	C	151	LEU	C-N-CA	9.32	132.78	120.28
2	G	213	TYR	N-CA-C	-9.28	93.60	108.73
4	L	77	ILE	N-CA-C	9.23	121.03	108.11
4	L	142	ILE	N-CA-C	-9.21	94.30	107.75
1	C	146	VAL	N-CA-C	-9.21	94.45	107.80
2	G	221	ILE	N-CA-C	-9.21	95.28	108.17
4	L	50	ILE	N-CA-C	9.19	122.06	108.45
3	H	158	PHE	CA-C-N	9.11	131.23	119.84
3	H	158	PHE	C-N-CA	9.11	131.23	119.84
2	G	427	GLN	N-CA-C	9.08	121.17	111.28
2	G	476	ASP	N-CA-C	-9.06	92.70	108.20
4	L	82	THR	N-CA-C	-8.96	101.51	111.28
1	C	83	ILE	N-CA-C	8.95	120.82	107.75
3	H	86	LEU	N-CA-C	8.95	123.21	110.23
1	C	60	SER	CA-C-N	8.89	132.20	120.28
1	C	60	SER	C-N-CA	8.89	132.20	120.28
3	H	158	PHE	C-N-CD	-8.87	88.63	125.00
2	G	436	PRO	N-CA-C	8.87	121.52	110.70
2	G	353	ILE	N-CA-C	8.86	120.57	108.17
2	G	333	TRP	N-CA-C	8.81	120.88	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	12	ARG	N-CA-C	8.78	123.90	109.24
3	H	201	LEU	N-CA-C	8.78	120.84	111.28
1	C	136	LYS	N-CA-C	-8.77	97.03	110.10
3	H	137	ALA	CA-C-N	-8.72	110.60	119.93
3	H	137	ALA	C-N-CA	-8.72	110.60	119.93
4	L	93	TRP	N-CA-C	-8.65	95.57	109.76
1	C	149	LEU	N-CA-C	8.63	122.20	110.55
4	L	98	SER	CB-CA-C	-8.62	96.48	110.79
4	L	95	SER	N-CA-C	8.62	120.75	111.36
3	H	142	SER	N-CA-C	8.61	120.67	111.28
1	C	42	SER	N-CA-C	8.58	120.63	111.28
1	C	59	ARG	N-CA-C	8.50	120.54	111.28
2	G	464	ASN	N-CA-C	-8.49	100.28	111.74
1	C	158	THR	N-CA-C	8.47	122.71	108.90
3	H	214	PRO	CA-C-N	8.47	131.62	120.28
3	H	214	PRO	C-N-CA	8.47	131.62	120.28
1	C	106	THR	N-CA-C	8.46	120.95	108.60
3	H	1	GLN	CA-C-N	8.46	135.53	122.25
3	H	1	GLN	C-N-CA	8.46	135.53	122.25
2	G	384	LEU	CA-C-N	-8.45	111.85	122.84
2	G	384	LEU	C-N-CA	-8.45	111.85	122.84
4	L	19	VAL	N-CA-C	8.44	120.94	108.45
2	G	376	PHE	N-CA-C	-8.39	95.73	109.40
4	L	138	LEU	CA-C-N	-8.35	112.20	123.14
4	L	138	LEU	C-N-CA	-8.35	112.20	123.14
3	H	27	PHE	N-CA-C	8.33	121.53	108.79
4	L	99	THR	N-CA-C	8.26	128.39	110.80
4	L	192	LYS	N-CA-C	8.24	120.26	111.28
3	H	156	ASP	N-CA-C	8.23	123.05	111.52
2	G	285	THR	N-CA-C	8.18	120.28	111.36
2	G	118	CYS	N-CA-C	-8.15	102.47	111.36
2	G	234	PRO	N-CA-C	-8.15	97.26	110.55
3	H	37	VAL	N-CA-C	8.11	119.47	108.11
1	C	112	GLN	N-CA-C	-8.09	99.63	110.55
2	G	236	ASN	N-CA-C	8.05	120.06	111.28
2	G	471	ARG	CA-C-N	-8.05	109.78	119.84
2	G	471	ARG	C-N-CA	-8.05	109.78	119.84
1	C	150	GLU	N-CA-C	8.03	121.36	109.24
3	H	10	GLU	N-CA-C	8.01	121.65	109.23
2	G	348	PHE	CA-C-N	7.94	127.87	119.85
2	G	348	PHE	C-N-CA	7.94	127.87	119.85
2	G	424	ASN	CA-C-N	-7.89	112.12	123.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	424	ASN	C-N-CA	-7.89	112.12	123.00
2	G	338	LYS	N-CA-C	7.88	119.86	111.28
4	L	10	SER	N-CA-C	7.86	121.32	108.99
3	H	83	LEU	N-CA-C	-7.85	96.11	108.90
1	C	133	PRO	N-CA-C	-7.85	102.06	113.75
2	G	478	LYS	N-CA-C	-7.82	102.76	111.28
3	H	186	GLY	N-CA-C	-7.82	103.75	115.00
2	G	119	VAL	N-CA-C	7.81	119.37	108.12
4	L	13	ALA	N-CA-C	7.80	120.72	108.79
4	L	8	PRO	N-CA-C	7.78	120.19	110.70
3	H	65	GLN	CB-CA-C	-7.75	97.92	110.79
2	G	116	LYS	CA-C-N	-7.74	112.03	119.85
2	G	116	LYS	C-N-CA	-7.74	112.03	119.85
3	H	155	LYS	N-CA-C	7.73	122.01	109.40
4	L	143	SER	N-CA-C	7.73	120.92	109.24
3	H	132	SER	N-CA-C	-7.68	96.42	109.24
4	L	33	ASN	N-CA-C	7.67	121.96	109.85
2	G	113	GLN	N-CA-C	7.66	119.27	111.07
4	L	144	ASP	N-CA-C	7.64	122.06	111.74
2	G	437	PRO	N-CA-C	7.62	128.17	112.47
1	C	17	THR	N-CA-C	7.62	121.31	108.90
2	G	359	VAL	N-CA-C	7.60	118.37	110.62
3	H	118	GLY	N-CA-C	-7.60	101.77	111.72
1	C	58	ARG	CA-C-N	7.57	130.42	120.28
1	C	58	ARG	C-N-CA	7.57	130.42	120.28
3	H	20	VAL	N-CA-C	7.57	118.79	107.75
2	G	453	LEU	N-CA-C	7.55	120.94	109.23
1	C	81	THR	N-CA-C	-7.50	96.51	108.73
4	L	171	SER	N-CA-C	7.49	121.33	109.50
2	G	482	ARG	N-CA-C	7.44	119.39	111.28
3	H	104	ASN	N-CA-C	7.43	122.07	112.26
1	C	124	SER	N-CA-C	7.41	121.21	109.50
3	H	68	VAL	N-CA-C	7.39	118.76	108.12
3	H	91	THR	N-CA-C	-7.36	99.56	110.23
3	H	48	MET	N-CA-C	7.34	119.36	111.36
3	H	127	SER	N-CA-C	-7.33	98.26	109.41
3	H	140	SER	CA-C-N	7.33	130.11	120.28
3	H	140	SER	C-N-CA	7.33	130.11	120.28
1	C	142	LYS	N-CA-C	7.33	119.27	111.28
3	H	8	GLY	N-CA-C	7.31	120.34	111.93
1	C	170	PHE	N-CA-C	-7.29	97.52	109.40
3	H	65	GLN	N-CA-C	7.27	119.20	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	32	ASN	N-CA-C	-7.25	100.76	110.55
3	H	139	SER	N-CA-C	7.24	119.87	110.53
2	G	275	ASN	CA-C-N	7.22	129.96	120.28
2	G	275	ASN	C-N-CA	7.22	129.96	120.28
1	C	162	LEU	N-CA-C	7.20	120.25	108.52
2	G	438	SER	N-CA-C	7.18	121.30	112.54
2	G	441	ASN	CB-CA-C	7.17	122.67	109.70
1	C	89	GLN	CA-C-N	-7.15	113.14	123.00
1	C	89	GLN	C-N-CA	-7.15	113.14	123.00
2	G	272	ASN	CB-CG-ND2	7.14	127.11	116.40
3	H	102	TYR	CA-C-N	-7.13	113.57	122.84
3	H	102	TYR	C-N-CA	-7.13	113.57	122.84
1	C	51	LEU	N-CA-C	7.13	119.05	111.28
4	L	115	PRO	N-CA-C	-7.12	100.75	111.57
4	L	167	THR	N-CA-C	7.12	121.12	109.24
4	L	74	THR	N-CA-C	7.08	120.44	108.90
2	G	443	THR	N-CA-C	7.08	120.27	108.73
3	H	213	LYS	N-CA-C	7.07	122.44	113.25
2	G	461	LYS	N-CA-C	7.07	121.28	111.74
1	C	105	ASP	CB-CA-C	-7.06	99.08	110.79
2	G	435	ALA	CA-C-N	7.06	127.65	120.38
2	G	435	ALA	C-N-CA	7.06	127.65	120.38
1	C	59	ARG	CA-CB-CG	-7.04	100.03	114.10
4	L	207	THR	N-CA-C	7.03	120.36	108.90
3	H	140	SER	N-CA-C	-7.02	103.63	111.28
2	G	381	THR	N-CA-C	-7.00	104.31	112.92
2	G	459	GLU	N-CA-C	7.00	121.06	111.54
1	C	119	GLU	N-CA-C	-6.99	97.81	109.07
2	G	201	CYS	N-CA-C	6.98	119.71	110.08
3	H	203	THR	N-CA-C	6.94	118.93	111.36
4	L	12	SER	N-CA-C	6.93	119.71	109.24
2	G	110	LEU	N-CA-C	-6.90	103.76	111.28
2	G	89	ILE	N-CA-C	6.90	117.82	107.75
4	L	111	VAL	N-CA-C	-6.89	98.24	108.85
3	H	159	PRO	CA-N-CD	-6.87	102.38	112.00
4	L	39	GLN	CA-C-N	-6.87	113.04	123.07
4	L	39	GLN	C-N-CA	-6.87	113.04	123.07
1	C	123	GLY	N-CA-C	6.85	125.84	114.48
2	G	440	GLY	N-CA-C	6.84	120.93	112.73
2	G	266	VAL	CA-C-N	6.82	131.65	123.19
2	G	266	VAL	C-N-CA	6.82	131.65	123.19
4	L	122	THR	N-CA-C	-6.81	97.86	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	121	LEU	N-CA-C	-6.80	97.81	108.90
3	H	159	PRO	N-CA-C	-6.80	98.46	112.47
1	C	24	ILE	N-CA-C	6.79	117.61	108.11
2	G	466	ASP	N-CA-C	-6.78	103.89	111.28
3	H	57	GLU	CA-C-N	6.78	132.42	122.99
3	H	57	GLU	C-N-CA	6.78	132.42	122.99
2	G	206	PHE	N-CA-C	-6.77	98.17	109.07
3	H	196	VAL	N-CA-C	6.76	116.65	109.01
2	G	230	ASN	N-CA-C	-6.76	101.81	110.53
1	C	59	ARG	CA-C-N	6.72	129.29	120.28
1	C	59	ARG	C-N-CA	6.72	129.29	120.28
2	G	343	LYS	CB-CA-C	-6.72	99.43	110.85
2	G	105	GLN	N-CA-C	6.72	118.60	111.28
4	L	63	ARG	N-CA-C	-6.71	103.96	111.28
2	G	196	THR	N-CA-C	6.71	120.46	109.06
3	H	204	GLN	N-CA-C	6.71	120.17	109.24
4	L	58	SER	N-CA-C	6.70	119.94	110.23
2	G	420	ARG	CB-CG-CD	6.69	126.69	111.30
2	G	274	SER	N-CA-C	-6.68	104.39	112.54
4	L	36	SER	N-CA-C	-6.63	99.24	109.52
3	H	65	GLN	CA-CB-CG	6.60	127.29	114.10
3	H	179	PRO	N-CA-C	-6.59	100.73	111.21
1	C	139	GLN	N-CA-CB	-6.58	100.82	110.49
2	G	355	PHE	N-CA-C	-6.57	97.81	108.52
1	C	35	LYS	N-CA-CB	-6.55	99.17	110.17
2	G	445	ILE	N-CA-C	-6.54	98.95	108.11
2	G	354	GLU	N-CA-C	6.54	119.90	109.24
3	H	43	LYS	N-CA-C	6.54	119.65	109.52
2	G	215	ALA	CA-C-N	6.53	128.00	119.84
2	G	215	ALA	C-N-CA	6.53	128.00	119.84
2	G	419	ILE	CA-C-N	-6.52	112.17	122.73
2	G	419	ILE	C-N-CA	-6.52	112.17	122.73
2	G	256	LEU	N-CA-C	-6.51	98.58	109.07
4	L	131	LEU	CA-C-N	6.51	129.00	120.28
4	L	131	LEU	C-N-CA	6.51	129.00	120.28
4	L	16	GLY	CA-C-N	6.49	129.92	120.71
4	L	16	GLY	C-N-CA	6.49	129.92	120.71
3	H	107	THR	CA-C-N	6.47	127.17	119.98
3	H	107	THR	C-N-CA	6.47	127.17	119.98
2	G	431	ARG	N-CA-C	6.47	120.37	109.76
1	C	12	VAL	CB-CA-C	-6.45	100.57	110.50
3	H	103	TYR	CA-C-N	6.45	132.72	122.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	103	TYR	C-N-CA	6.45	132.72	122.86
1	C	23	SER	CA-C-N	6.44	131.57	123.14
1	C	23	SER	C-N-CA	6.44	131.57	123.14
2	G	97	ASN	CA-C-N	6.43	128.90	120.28
2	G	97	ASN	C-N-CA	6.43	128.90	120.28
2	G	347	TYR	N-CA-CB	6.42	119.67	110.16
4	L	198	SER	N-CA-C	6.42	119.96	109.24
3	H	67	ARG	CA-C-N	-6.40	114.10	122.99
3	H	67	ARG	C-N-CA	-6.40	114.10	122.99
4	L	210	LYS	N-CA-C	6.36	119.77	109.40
1	C	139	GLN	CA-C-N	6.33	127.00	119.98
1	C	139	GLN	C-N-CA	6.33	127.00	119.98
2	G	273	ILE	CB-CA-C	-6.33	103.49	112.22
3	H	220	ASP	N-CA-C	-6.30	99.14	109.40
4	L	98	SER	N-CA-C	6.29	118.14	111.28
4	L	196	SER	N-CA-C	6.29	118.41	108.79
2	G	481	TRP	N-CA-C	-6.28	104.52	111.36
2	G	275	ASN	CA-C-O	6.22	127.79	120.58
1	C	111	GLY	N-CA-C	-6.21	107.14	115.21
2	G	285	THR	CB-CA-C	-6.20	100.31	110.85
2	G	258	ASN	CA-CB-CG	6.16	118.76	112.60
2	G	463	GLU	CA-C-N	6.16	130.87	122.19
2	G	463	GLU	C-N-CA	6.16	130.87	122.19
3	H	62	GLN	N-CA-C	6.13	117.97	111.28
3	H	151	GLY	N-CA-C	6.13	119.45	110.80
2	G	384	LEU	N-CA-C	6.13	118.04	111.36
1	C	116	LEU	N-CA-C	-6.11	99.76	109.59
3	H	219	VAL	N-CA-C	6.09	116.63	108.11
3	H	36	TRP	CA-C-N	6.09	131.11	123.14
3	H	36	TRP	C-N-CA	6.09	131.11	123.14
1	C	133	PRO	CA-C-N	6.08	128.43	120.28
1	C	133	PRO	C-N-CA	6.08	128.43	120.28
3	H	76	THR	N-CA-C	-6.08	105.87	113.28
1	C	169	GLU	N-CA-C	6.07	118.63	108.73
4	L	14	ALA	CA-C-N	6.04	126.15	119.87
4	L	14	ALA	C-N-CA	6.04	126.15	119.87
3	H	51	PHE	N-CA-C	6.02	119.19	110.28
2	G	414	THR	N-CA-C	6.02	118.70	108.90
2	G	89	ILE	CA-C-N	6.01	132.03	122.59
2	G	89	ILE	C-N-CA	6.01	132.03	122.59
4	L	138	LEU	N-CA-C	-6.01	99.91	109.76
1	C	28	TRP	N-CA-C	6.00	119.17	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	163	THR	N-CA-C	5.99	118.97	109.50
2	G	389	HIS	CA-C-N	5.99	130.63	122.07
2	G	389	HIS	C-N-CA	5.99	130.63	122.07
4	L	54	THR	CA-C-N	-5.97	114.83	122.77
4	L	54	THR	C-N-CA	-5.97	114.83	122.77
4	L	31	GLY	N-CA-C	-5.96	105.59	112.50
2	G	420	ARG	CA-CB-CG	-5.92	102.25	114.10
2	G	280	ILE	N-CA-C	5.91	116.37	107.75
4	L	30	ILE	CB-CA-C	-5.88	104.20	112.14
4	L	46	PRO	CA-C-N	5.88	132.05	122.81
4	L	46	PRO	C-N-CA	5.88	132.05	122.81
3	H	21	SER	N-CA-C	5.86	118.46	110.55
1	C	171	LYS	N-CA-C	-5.84	99.49	109.24
3	H	161	PRO	CA-N-CD	-5.84	103.83	112.00
2	G	448	ILE	CB-CA-C	-5.83	102.14	110.83
1	C	76	ILE	CB-CA-C	-5.83	104.26	112.14
2	G	380	ASN	CB-CG-ND2	5.83	125.15	116.40
3	H	160	GLU	N-CA-C	5.83	119.19	108.69
2	G	122	THR	N-CA-C	5.83	117.64	108.55
4	L	4	VAL	N-CA-C	5.83	117.07	108.45
3	H	105	LEU	CA-CB-CG	5.81	136.64	116.30
2	G	477	MET	CA-C-N	5.81	128.06	120.28
2	G	477	MET	C-N-CA	5.81	128.06	120.28
3	H	136	LEU	N-CA-C	-5.80	99.28	108.73
2	G	351	LYS	N-CA-C	5.78	118.48	109.52
2	G	259	GLY	N-CA-C	5.77	126.86	113.18
1	C	59	ARG	N-CA-CB	-5.77	101.64	110.12
2	G	243	CYS	N-CA-C	5.76	118.61	109.50
2	G	486	TYR	N-CA-C	5.76	117.56	111.28
2	G	194	THR	CA-C-N	-5.75	115.13	122.77
2	G	194	THR	C-N-CA	-5.75	115.13	122.77
2	G	375	GLU	N-CA-C	-5.74	100.53	109.72
1	C	15	THR	N-CA-C	5.74	118.60	109.24
4	L	63	ARG	NE-CZ-NH1	-5.72	115.78	121.50
2	G	346	LYS	CB-CA-C	5.72	120.28	110.79
3	H	29	LEU	N-CA-CB	-5.71	100.95	109.69
2	G	365	ILE	CA-C-N	5.71	127.94	120.28
2	G	365	ILE	C-N-CA	5.71	127.94	120.28
2	G	105	GLN	CB-CG-CD	-5.71	102.90	112.60
3	H	71	THR	N-CA-C	5.71	118.07	109.23
1	C	34	ILE	N-CA-CB	5.70	119.01	111.25
2	G	470	PHE	N-CA-C	-5.68	100.14	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	LEU	N-CA-C	5.67	117.96	108.73
1	C	61	LEU	CA-C-N	5.65	127.85	120.28
1	C	61	LEU	C-N-CA	5.65	127.85	120.28
4	L	64	PHE	N-CA-C	5.65	118.74	109.76
1	C	53	ASP	N-CA-C	-5.63	103.26	110.53
3	H	73	ASP	N-CA-CB	5.62	119.58	110.42
4	L	114	GLN	N-CA-C	5.62	118.86	109.09
4	L	160	PRO	N-CA-C	5.60	120.39	111.26
4	L	130	GLU	N-CA-C	5.59	117.37	111.28
2	G	429	VAL	CB-CA-C	-5.59	104.20	110.96
4	L	152	VAL	N-CA-C	5.57	118.15	108.95
3	H	29	LEU	CB-CA-C	5.57	118.59	109.90
4	L	125	PRO	CA-N-CD	-5.55	104.23	112.00
3	H	22	CYS	CA-C-N	-5.54	114.63	122.94
3	H	22	CYS	C-N-CA	-5.54	114.63	122.94
3	H	98	THR	N-CA-C	5.54	117.81	109.23
3	H	206	TYR	N-CA-C	5.53	117.91	108.90
3	H	207	ILE	N-CA-C	5.52	115.83	108.11
4	L	97	LEU	CA-CB-CG	5.51	135.59	116.30
4	L	134	ASN	N-CA-C	5.50	119.17	111.74
3	H	1	GLN	CB-CA-C	-5.50	99.65	110.10
2	G	276	ASN	CB-CA-C	5.48	119.89	110.79
3	H	27	PHE	CA-C-N	-5.48	115.48	122.77
3	H	27	PHE	C-N-CA	-5.48	115.48	122.77
2	G	378	TYR	N-CA-CB	-5.47	101.31	110.83
3	H	11	VAL	N-CA-C	5.47	115.83	108.17
3	H	185	SER	N-CA-C	-5.46	105.32	111.28
2	G	368	HIS	N-CA-C	5.46	117.62	108.23
2	G	488	TYR	N-CA-C	5.46	118.36	110.28
3	H	1	GLN	CB-CG-CD	5.45	121.87	112.60
2	G	276	ASN	CA-C-N	5.44	128.15	120.42
2	G	276	ASN	C-N-CA	5.44	128.15	120.42
3	H	11	VAL	CB-CA-C	-5.43	102.74	110.83
3	H	86	LEU	CA-C-N	5.43	132.47	122.92
3	H	86	LEU	C-N-CA	5.43	132.47	122.92
2	G	111	TRP	N-CA-C	5.43	117.19	111.28
1	C	33	GLN	CA-C-N	5.42	129.92	123.19
1	C	33	GLN	C-N-CA	5.42	129.92	123.19
2	G	354	GLU	CA-CB-CG	5.42	124.94	114.10
1	C	62	TRP	CA-C-O	-5.42	114.81	120.55
3	H	104	ASN	CA-CB-CG	5.39	117.99	112.60
2	G	462	THR	CA-C-N	5.39	127.50	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	462	THR	C-N-CA	5.39	127.50	120.28
2	G	252	SER	N-CA-C	5.38	117.25	109.07
1	C	50	LYS	CA-C-N	5.37	127.48	120.28
1	C	50	LYS	C-N-CA	5.37	127.48	120.28
2	G	420	ARG	N-CA-CB	-5.36	101.30	111.00
2	G	441	ASN	CA-CB-CG	5.36	117.96	112.60
3	H	124	SER	CA-C-N	5.36	127.46	120.28
3	H	124	SER	C-N-CA	5.36	127.46	120.28
3	H	73	ASP	N-CA-C	-5.36	100.00	108.73
3	H	208	CYS	N-CA-C	-5.34	101.45	109.95
2	G	263	GLU	N-CA-CB	-5.34	102.27	110.12
2	G	447	ASP	CA-C-N	-5.33	116.58	123.19
2	G	447	ASP	C-N-CA	-5.33	116.58	123.19
3	H	54	GLU	N-CA-C	-5.33	100.04	108.73
2	G	258	ASN	N-CA-CB	5.31	119.76	111.84
1	C	85	GLU	N-CA-C	5.30	117.17	108.52
4	L	202	THR	CA-C-N	-5.30	115.30	122.77
4	L	202	THR	C-N-CA	-5.30	115.30	122.77
4	L	147	PRO	N-CA-C	-5.29	98.33	112.10
2	G	92	PHE	N-CA-C	-5.29	100.78	109.40
2	G	266	VAL	N-CA-C	-5.28	100.14	107.80
4	L	120	SER	N-CA-C	-5.27	100.31	108.90
1	C	29	LYS	N-CA-C	5.27	117.82	109.50
3	H	211	ASN	CA-C-N	-5.27	114.80	122.44
3	H	211	ASN	C-N-CA	-5.27	114.80	122.44
3	H	145	GLY	N-CA-C	-5.26	107.99	115.30
2	G	364	GLU	CA-C-N	5.26	127.89	120.42
2	G	364	GLU	C-N-CA	5.26	127.89	120.42
1	C	61	LEU	N-CA-C	5.25	117.00	111.28
3	H	134	PHE	N-CA-C	-5.25	101.00	109.82
2	G	490	VAL	N-CA-C	5.23	115.39	107.80
2	G	290	ILE	N-CA-CB	5.23	118.44	111.64
3	H	3	GLN	N-CA-C	5.21	117.30	109.23
2	G	482	ARG	CA-CB-CG	-5.20	103.70	114.10
4	L	190	GLN	N-CA-C	5.20	117.03	111.36
2	G	484	GLU	N-CA-C	5.19	117.02	111.36
1	C	13	GLU	N-CA-C	5.17	117.33	108.90
1	C	22	LYS	N-CA-C	5.16	117.84	109.06
2	G	419	ILE	N-CA-C	-5.16	100.94	108.17
1	C	120	SER	N-CA-C	-5.16	102.21	110.10
1	C	29	LYS	CA-C-N	5.14	131.74	122.02
1	C	29	LYS	C-N-CA	5.14	131.74	122.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	GLN	CB-CA-C	5.13	119.31	110.79
2	G	205	SER	CA-C-N	-5.13	115.91	123.00
2	G	205	SER	C-N-CA	-5.13	115.91	123.00
2	G	228	THR	N-CA-C	-5.12	100.69	109.24
3	H	150	LEU	N-CA-C	-5.11	101.30	109.07
3	H	29	LEU	CA-CB-CG	5.10	134.14	116.30
4	L	172	LYS	N-CA-C	-5.09	103.67	110.55
2	G	345	VAL	N-CA-C	-5.08	105.44	110.62
3	H	76	THR	CA-C-N	5.07	129.56	122.36
3	H	76	THR	C-N-CA	5.07	129.56	122.36
4	L	148	GLY	N-CA-C	5.07	118.81	112.73
2	G	250	VAL	N-CA-C	-5.07	101.18	108.48
2	G	248	LYS	N-CA-C	-5.07	101.34	109.04
2	G	100	VAL	N-CA-C	-5.04	105.48	110.62
4	L	121	VAL	N-CA-C	5.03	115.16	108.11
3	H	154	VAL	N-CA-C	-5.03	100.51	107.80
3	H	61	ALA	N-CA-C	-5.02	103.90	110.53
3	H	113	ALA	CA-C-N	-5.02	115.41	122.94
3	H	113	ALA	C-N-CA	-5.02	115.41	122.94
1	C	55	ALA	N-CA-C	-5.01	99.25	108.02
2	G	226	ASP	N-CA-C	-5.01	102.96	110.23
4	L	98	SER	O-C-N	5.01	127.44	122.12
2	G	451	LEU	N-CA-C	5.00	117.40	109.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	102	TYR	Sidechain
3	H	110	TYR	Sidechain
3	H	114	TYR	Sidechain
3	H	94	TYR	Sidechain
4	L	34	TYR	Sidechain
4	L	98	SER	Peptide,Mainchain

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	C	1361	0	1382	162	0
2	G	2271	0	2232	287	0
3	H	1685	0	1645	202	0
4	L	1572	0	1530	129	0
5	G	56	0	51	11	0
All	All	6945	0	6840	717	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (717) 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)
2:G:258:ASN:CG	2:G:258:ASN:CB	1.79	1.56
5:G:2500:NAG:C2	5:G:2500:NAG:C1	1.75	1.56
3:H:158:PHE:HB3	3:H:159:PRO:HD2	1.22	1.20
2:G:420:ARG:HH12	3:H:55:GLU:HB2	1.06	1.13
2:G:355:PHE:HB3	2:G:385:PHE:HB3	1.23	1.12
4:L:7:GLN:HE21	4:L:107:THR:HG22	1.06	1.10
1:C:37:LEU:HD11	1:C:44:LEU:HD11	1.30	1.09
1:C:3:VAL:HG22	1:C:94:GLN:HB3	1.32	1.08
3:H:91:THR:HG22	3:H:123:VAL:H	1.05	1.08
2:G:354:GLU:HG3	2:G:469:ILE:HG12	1.29	1.08
2:G:420:ARG:HG2	3:H:56:ASN:HB3	1.34	1.08
2:G:420:ARG:HH22	3:H:55:GLU:N	1.54	1.05
2:G:420:ARG:NE	3:H:56:ASN:HD22	1.55	1.04
4:L:29:ASN:ND2	4:L:30:ILE:HG12	1.73	1.03
1:C:157:TRP:HE1	1:C:174:ILE:HD12	1.19	1.02
3:H:16:ALA:O	3:H:86:LEU:HD13	1.60	1.02
2:G:123:PRO:HD3	3:H:105:LEU:HD13	1.40	1.02
3:H:158:PHE:CB	3:H:159:PRO:HD2	1.86	1.01
2:G:223:LYS:HE3	2:G:241:VAL:HG11	1.44	0.99
2:G:329:ASN:HD21	2:G:331:LYS:HB2	1.26	0.98
4:L:7:GLN:NE2	4:L:107:THR:HG22	1.79	0.98
4:L:5:LEU:HD21	4:L:29:ASN:ND2	1.79	0.97
3:H:29:LEU:H	3:H:77:ASN:ND2	1.62	0.96
2:G:337:LEU:O	2:G:341:VAL:HG13	1.66	0.96
3:H:86:LEU:HD23	3:H:123:VAL:HG22	1.48	0.95
3:H:56:ASN:OD1	3:H:57:GLU:HG3	1.66	0.95
2:G:100:VAL:HG11	2:G:482:ARG:HG2	1.48	0.95
1:C:21:LYS:HA	1:C:64:GLN:O	1.66	0.94
3:H:149:ALA:HB2	3:H:195:THR:HG22	1.49	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:VAL:HG11	1:C:164:ASN:HD22	1.33	0.94
2:G:420:ARG:HH12	3:H:55:GLU:CB	1.81	0.93
4:L:155:LYS:HG2	4:L:158:SER:HA	1.50	0.93
2:G:275:ASN:HD21	2:G:277:VAL:HB	1.32	0.93
2:G:247:ILE:HG23	2:G:484:GLU:OE1	1.68	0.92
3:H:29:LEU:H	3:H:77:ASN:HD21	1.12	0.92
3:H:48:MET:HG2	3:H:64:PHE:CZ	2.04	0.92
3:H:91:THR:HG22	3:H:123:VAL:N	1.83	0.91
1:C:103:ASN:HD22	1:C:104:SER:H	1.12	0.91
2:G:420:ARG:NH1	3:H:55:GLU:HB2	1.85	0.91
2:G:420:ARG:HE	3:H:56:ASN:HD22	1.15	0.91
2:G:420:ARG:CG	3:H:56:ASN:HB3	2.00	0.90
1:C:103:ASN:HD22	1:C:104:SER:N	1.70	0.90
2:G:354:GLU:HB2	2:G:469:ILE:HA	1.51	0.90
1:C:132:SER:HA	1:C:157:TRP:CE3	2.08	0.88
3:H:36:TRP:HB2	3:H:70:MET:HE3	1.53	0.88
4:L:97:LEU:HD22	4:L:99:THR:HG23	1.53	0.88
3:H:35:HIS:CD2	3:H:50:GLY:HA3	2.09	0.88
3:H:158:PHE:HB3	3:H:159:PRO:CD	2.05	0.87
2:G:337:LEU:O	2:G:340:VAL:HG22	1.73	0.87
1:C:53:ASP:O	1:C:54:ARG:HG2	1.74	0.86
1:C:37:LEU:HD11	1:C:44:LEU:CD1	2.05	0.86
1:C:154:SER:HA	1:C:174:ILE:HG22	1.58	0.85
2:G:329:ASN:ND2	2:G:331:LYS:HB2	1.90	0.85
2:G:253:THR:CG2	2:G:369:SER:H	1.90	0.84
2:G:383:LYS:NZ	2:G:416:PRO:HG3	1.93	0.84
2:G:383:LYS:HZ3	2:G:416:PRO:HG3	1.41	0.84
3:H:91:THR:CG2	3:H:123:VAL:H	1.89	0.84
2:G:85:LEU:HD22	2:G:240:THR:H	1.43	0.84
2:G:262:ALA:HB2	2:G:283:HIS:CD2	2.12	0.84
2:G:223:LYS:HE2	2:G:488:TYR:HE2	1.43	0.84
2:G:420:ARG:CZ	3:H:56:ASN:H	1.91	0.84
2:G:420:ARG:NH2	3:H:56:ASN:H	1.76	0.83
2:G:272:ASN:HB3	2:G:275:ASN:HB2	1.61	0.83
2:G:333:TRP:CZ2	2:G:384:LEU:HD21	2.13	0.83
4:L:186:LEU:N	4:L:186:LEU:HD23	1.92	0.83
1:C:37:LEU:CD1	1:C:44:LEU:HD11	2.10	0.82
2:G:266:VAL:HB	2:G:343:LYS:HE2	1.62	0.81
3:H:32:LEU:HD13	3:H:107:THR:HG21	1.62	0.81
2:G:348:PHE:HB3	2:G:351:LYS:HD2	1.61	0.81
2:G:92:PHE:CE2	2:G:224:CYS:HB2	2.16	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:SER:OG	1:C:134:ARG:HB2	1.81	0.81
3:H:158:PHE:CB	3:H:159:PRO:CD	2.57	0.81
1:C:54:ARG:HA	1:C:72:LYS:HE2	1.63	0.80
2:G:95:TRP:HA	2:G:482:ARG:NH1	1.96	0.80
1:C:53:ASP:HB2	4:L:32:LYS:NZ	1.96	0.80
2:G:435:ALA:HB1	2:G:436:PRO:HD2	1.63	0.80
4:L:7:GLN:HE21	4:L:107:THR:CG2	1.92	0.79
2:G:270:SER:CB	2:G:273:ILE:HD13	2.13	0.79
2:G:223:LYS:CE	2:G:241:VAL:HG11	2.13	0.78
1:C:157:TRP:NE1	1:C:174:ILE:HD12	1.97	0.78
3:H:36:TRP:CD1	3:H:81:MET:HG3	2.19	0.78
2:G:422:ILE:HG12	2:G:433:MET:HG3	1.65	0.78
1:C:46:LYS:HB2	2:G:360:GLY:HA3	1.65	0.77
3:H:29:LEU:HD11	3:H:34:ILE:HD11	1.66	0.77
1:C:45:THR:HG22	2:G:365:ILE:HG21	1.66	0.77
3:H:86:LEU:HD23	3:H:123:VAL:CG2	2.15	0.77
2:G:420:ARG:HG2	3:H:56:ASN:CB	2.13	0.77
1:C:150:GLU:O	1:C:176:VAL:HG11	1.84	0.77
1:C:53:ASP:HB2	4:L:32:LYS:HZ3	1.48	0.77
4:L:71:THR:HG23	4:L:71:THR:O	1.84	0.77
4:L:150:VAL:HG12	4:L:170:PRO:HG3	1.67	0.77
3:H:22:CYS:HB2	3:H:36:TRP:HH2	1.48	0.76
4:L:126:PRO:HB2	4:L:131:LEU:HD11	1.68	0.76
1:C:43:PHE:CB	2:G:365:ILE:HD11	2.16	0.75
3:H:29:LEU:N	3:H:77:ASN:HD21	1.85	0.75
2:G:382:THR:HG21	5:G:2000:NAG:H62	1.69	0.74
1:C:51:LEU:O	1:C:53:ASP:O	2.05	0.74
2:G:97:ASN:HD21	2:G:99:MET:HE3	1.53	0.74
4:L:29:ASN:HD21	4:L:30:ILE:HG12	1.49	0.74
2:G:349:PRO:O	2:G:351:LYS:HG3	1.88	0.74
4:L:29:ASN:CG	4:L:30:ILE:H	1.95	0.74
2:G:272:ASN:ND2	5:G:1500:NAG:H62	2.01	0.74
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.69	0.74
4:L:19:VAL:CG1	4:L:80:LEU:HD22	2.18	0.74
2:G:333:TRP:CH2	2:G:384:LEU:HD21	2.22	0.73
2:G:388:ILE:HD13	2:G:388:ILE:H	1.52	0.73
2:G:294:GLY:HA2	2:G:324:GLY:N	2.03	0.73
2:G:381:THR:HG22	2:G:415:LEU:HD13	1.69	0.73
4:L:123:LEU:HD22	4:L:212:MET:HB2	1.70	0.73
2:G:270:SER:HB2	2:G:273:ILE:HD13	1.71	0.73
4:L:97:LEU:HD23	4:L:98:SER:H	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:124:PHE:HB3	4:L:125:PRO:HD2	1.71	0.73
3:H:32:LEU:HD13	3:H:107:THR:CG2	2.18	0.73
2:G:100:VAL:HG11	2:G:482:ARG:CG	2.17	0.73
2:G:275:ASN:ND2	2:G:277:VAL:HB	2.04	0.73
3:H:182:LEU:HD12	3:H:188:TYR:CE1	2.24	0.73
1:C:109:LEU:O	1:C:112:GLN:HB2	1.90	0.72
2:G:459:GLU:O	2:G:460:ASN:HB2	1.88	0.72
2:G:123:PRO:CD	3:H:105:LEU:HD13	2.20	0.72
2:G:253:THR:O	2:G:255:LEU:N	2.21	0.72
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.72	0.72
2:G:418:ARG:HB3	2:G:420:ARG:HD2	1.71	0.72
4:L:7:GLN:NE2	4:L:107:THR:CG2	2.51	0.72
2:G:215:ALA:HB2	2:G:221:ILE:HG12	1.72	0.72
2:G:119:VAL:HB	2:G:433:MET:HB3	1.72	0.71
2:G:461:LYS:HE2	2:G:463:GLU:OE2	1.91	0.71
1:C:129:GLN:CD	1:C:137:ASN:HD21	1.98	0.71
2:G:275:ASN:HD22	2:G:278:LYS:HG2	1.53	0.71
1:C:43:PHE:HB3	2:G:365:ILE:HD11	1.71	0.71
1:C:27:HIS:CE1	1:C:35:LYS:HE3	2.24	0.71
1:C:45:THR:CG2	2:G:365:ILE:HG21	2.21	0.71
2:G:111:TRP:CZ2	2:G:251:VAL:HG21	2.26	0.71
3:H:142:SER:HB3	3:H:148:ALA:HB1	1.73	0.71
4:L:186:LEU:HD12	4:L:190:GLN:CB	2.21	0.71
1:C:35:LYS:O	1:C:47:GLY:HA3	1.92	0.70
1:C:40:GLN:HG3	2:G:474:GLY:O	1.91	0.70
3:H:190:LEU:HD12	3:H:191:SER:N	2.06	0.70
2:G:422:ILE:O	3:H:55:GLU:HB3	1.92	0.70
1:C:31:SER:HB2	1:C:80:ASP:OD1	1.92	0.70
2:G:206:PHE:CE2	2:G:208:PRO:HA	2.26	0.70
1:C:129:GLN:CG	1:C:137:ASN:HD21	2.03	0.70
2:G:91:ASN:ND2	2:G:234:PRO:HA	2.06	0.70
2:G:459:GLU:O	2:G:460:ASN:CB	2.40	0.70
3:H:19:LYS:HB2	3:H:82:GLU:HG2	1.74	0.69
3:H:193:VAL:HG11	4:L:141:LEU:HD13	1.74	0.69
3:H:159:PRO:HB2	3:H:214:PRO:CB	2.22	0.69
4:L:87:ASP:OD1	4:L:108:LYS:HG3	1.92	0.69
2:G:290:ILE:HG12	2:G:328:ILE:HG12	1.74	0.69
2:G:419:ILE:C	2:G:420:ARG:HG3	2.15	0.69
2:G:111:TRP:CZ3	2:G:115:LEU:HD12	2.28	0.69
2:G:455:ARG:HB3	2:G:470:PHE:CD1	2.27	0.69
3:H:158:PHE:HD1	3:H:159:PRO:HD3	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ILE:CG2	1:C:144:LEU:HD21	2.23	0.68
2:G:270:SER:OG	2:G:273:ILE:HD13	1.93	0.68
2:G:337:LEU:HD22	2:G:389:HIS:CE1	2.28	0.68
3:H:17:SER:HA	3:H:84:SER:HA	1.74	0.68
2:G:97:ASN:HD21	2:G:99:MET:CE	2.06	0.68
4:L:186:LEU:HD12	4:L:190:GLN:HB2	1.73	0.68
2:G:385:PHE:CE1	2:G:472:PRO:HG3	2.29	0.68
1:C:7:LYS:HE3	1:C:169:GLU:O	1.94	0.68
4:L:49:LEU:HD11	4:L:64:PHE:CD1	2.29	0.67
4:L:127:SER:O	4:L:131:LEU:HD13	1.94	0.67
1:C:108:LEU:O	1:C:176:VAL:HA	1.93	0.67
3:H:48:MET:HE3	3:H:64:PHE:CE2	2.30	0.67
1:C:71:ILE:HG22	1:C:74:LEU:HD23	1.76	0.67
3:H:174:GLY:O	3:H:194:VAL:HG23	1.94	0.67
4:L:30:ILE:HD13	4:L:92:THR:OG1	1.94	0.67
2:G:206:PHE:HE2	2:G:208:PRO:HA	1.60	0.67
3:H:97:ALA:HB1	3:H:112:LEU:HD22	1.76	0.67
3:H:167:ASN:HB3	3:H:170:ALA:HB3	1.77	0.67
4:L:41:LEU:HD23	4:L:86:ALA:HB2	1.76	0.67
2:G:253:THR:C	2:G:255:LEU:H	2.02	0.67
3:H:62:GLN:HA	3:H:65:GLN:HG2	1.75	0.67
2:G:91:ASN:HD22	2:G:234:PRO:HA	1.61	0.66
3:H:141:LYS:HZ3	4:L:212:MET:HG3	1.60	0.66
4:L:155:LYS:CG	4:L:158:SER:HA	2.24	0.66
1:C:33:GLN:HB2	2:G:459:GLU:CG	2.25	0.66
2:G:455:ARG:HB3	2:G:470:PHE:CE1	2.30	0.66
4:L:112:LEU:HA	4:L:146:TYR:OH	1.95	0.66
2:G:418:ARG:CB	2:G:420:ARG:HD2	2.24	0.66
2:G:253:THR:HG22	2:G:369:SER:N	2.12	0.65
2:G:354:GLU:CG	2:G:469:ILE:HG12	2.17	0.65
3:H:29:LEU:HD11	3:H:34:ILE:CD1	2.26	0.65
3:H:104:ASN:O	3:H:107:THR:OG1	2.07	0.65
4:L:36:SER:CB	4:L:51:PHE:HA	2.27	0.65
2:G:338:LYS:HA	2:G:341:VAL:HG22	1.78	0.65
2:G:363:LEU:HD21	2:G:420:ARG:CZ	2.27	0.65
4:L:18:LYS:HG3	4:L:77:ILE:O	1.96	0.65
2:G:336:THR:O	2:G:340:VAL:HG13	1.97	0.65
2:G:123:PRO:HD3	3:H:105:LEU:CD1	2.22	0.64
2:G:254:GLN:NE2	2:G:368:HIS:HB2	2.12	0.64
2:G:481:TRP:CE3	2:G:481:TRP:HA	2.31	0.64
4:L:138:LEU:HD22	4:L:184:LEU:HD23	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ILE:HG22	1:C:144:LEU:HD21	1.79	0.64
2:G:424:ASN:OD1	2:G:431:ARG:HG2	1.97	0.64
3:H:158:PHE:CD1	3:H:159:PRO:CD	2.80	0.64
1:C:20:GLN:HE21	1:C:22:LYS:HD2	1.62	0.64
2:G:223:LYS:HE2	2:G:488:TYR:CE2	2.30	0.64
2:G:261:LEU:HD21	2:G:287:SER:HB3	1.78	0.64
2:G:119:VAL:CG2	2:G:433:MET:HE2	2.28	0.64
3:H:158:PHE:CD1	3:H:159:PRO:HD3	2.32	0.64
2:G:100:VAL:HG21	2:G:482:ARG:HD3	1.80	0.64
2:G:420:ARG:HH21	3:H:54:GLU:HG2	1.61	0.64
2:G:384:LEU:HD23	2:G:384:LEU:C	2.23	0.63
4:L:192:LYS:O	4:L:214:HIS:NE2	2.32	0.63
3:H:64:PHE:O	3:H:68:VAL:HG12	1.99	0.63
3:H:212:HIS:ND1	3:H:214:PRO:HD2	2.14	0.63
4:L:130:GLU:HG2	4:L:135:LYS:O	1.98	0.63
2:G:103:MET:HE1	2:G:213:TYR:HB2	1.79	0.63
3:H:36:TRP:HB2	3:H:70:MET:CE	2.28	0.63
3:H:117:GLN:HG3	3:H:118:GLY:O	1.98	0.63
3:H:158:PHE:O	3:H:159:PRO:HG2	1.97	0.63
4:L:36:SER:HB2	4:L:51:PHE:HA	1.80	0.63
2:G:338:LYS:O	2:G:341:VAL:HG22	1.99	0.63
4:L:129:GLU:O	4:L:132:GLN:HB3	1.99	0.63
3:H:99:GLY:HA3	3:H:110:TYR:HD1	1.63	0.62
4:L:114:GLN:NE2	4:L:177:LYS:HG2	2.14	0.62
2:G:261:LEU:HD21	2:G:287:SER:CB	2.29	0.62
4:L:119:PRO:HA	4:L:145:PHE:HB3	1.81	0.62
2:G:420:ARG:HE	3:H:56:ASN:ND2	1.93	0.62
2:G:253:THR:HG22	2:G:369:SER:H	1.64	0.62
2:G:107:ILE:HG22	2:G:426:TRP:HH2	1.64	0.62
1:C:113:SER:HB3	1:C:147:SER:O	2.00	0.62
3:H:177:THR:HG22	3:H:190:LEU:HD11	1.82	0.62
4:L:154:TRP:CZ3	4:L:199:CYS:HB2	2.34	0.62
2:G:227:LYS:HD2	2:G:263:GLU:OE1	2.00	0.61
2:G:381:THR:HG22	2:G:415:LEU:CD1	2.30	0.61
1:C:103:ASN:ND2	1:C:104:SER:N	2.45	0.61
2:G:253:THR:CG2	2:G:369:SER:N	2.61	0.61
2:G:256:LEU:HD23	2:G:480:ASN:ND2	2.14	0.61
4:L:123:LEU:HD12	4:L:199:CYS:HB3	1.83	0.61
2:G:426:TRP:H	2:G:426:TRP:CD1	2.19	0.61
2:G:254:GLN:HE21	2:G:368:HIS:HB2	1.63	0.61
3:H:37:VAL:HG13	3:H:46:GLU:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:146:GLY:O	3:H:198:SER:N	2.25	0.61
4:L:19:VAL:HG11	4:L:80:LEU:HD22	1.82	0.61
2:G:103:MET:HG2	2:G:485:LEU:HD11	1.82	0.61
2:G:332:ALA:O	2:G:336:THR:HG23	2.01	0.61
1:C:28:TRP:CE2	1:C:69:LEU:HB2	2.36	0.61
1:C:36:ILE:HD11	1:C:51:LEU:HD12	1.82	0.60
3:H:94:TYR:O	3:H:119:THR:HG22	2.00	0.60
4:L:5:LEU:HD21	4:L:29:ASN:HD21	1.65	0.60
3:H:141:LYS:NZ	4:L:212:MET:HG3	2.16	0.60
4:L:173:GLN:HB3	4:L:177:LYS:O	2.01	0.60
1:C:20:GLN:HE21	1:C:22:LYS:CD	2.15	0.60
1:C:103:ASN:ND2	1:C:104:SER:H	1.92	0.60
2:G:461:LYS:NZ	2:G:461:LYS:HB3	2.17	0.60
3:H:159:PRO:HB2	3:H:214:PRO:HB3	1.84	0.60
3:H:177:THR:HG23	3:H:192:SER:HB2	1.82	0.60
3:H:142:SER:O	3:H:148:ALA:HA	2.01	0.60
2:G:95:TRP:HA	2:G:482:ARG:HH11	1.65	0.60
2:G:254:GLN:NE2	2:G:381:THR:OG1	2.33	0.60
2:G:104:HIS:HE1	2:G:477:MET:HB2	1.67	0.60
2:G:253:THR:HG21	2:G:369:SER:H	1.67	0.60
3:H:47:TRP:CD2	4:L:101:GLN:HB3	2.37	0.60
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.37	0.59
2:G:119:VAL:HG21	2:G:433:MET:HE2	1.84	0.59
3:H:206:TYR:O	3:H:222:LYS:HG3	2.02	0.59
2:G:266:VAL:HB	2:G:343:LYS:CE	2.31	0.59
4:L:19:VAL:HG12	4:L:80:LEU:HD22	1.83	0.59
1:C:40:GLN:O	1:C:41:GLY:C	2.44	0.59
1:C:43:PHE:HB2	2:G:365:ILE:HD11	1.82	0.59
3:H:23:LYS:HA	3:H:78:THR:HG22	1.84	0.59
3:H:207:ILE:HG12	3:H:222:LYS:HB2	1.85	0.59
2:G:290:ILE:HD11	2:G:448:ILE:HD11	1.83	0.59
5:G:2500:NAG:C2	5:G:2500:NAG:O5	2.42	0.59
3:H:138:PRO:HG2	3:H:225:PRO:HB3	1.84	0.59
4:L:71:THR:O	4:L:71:THR:CG2	2.51	0.59
2:G:280:ILE:HG22	2:G:282:VAL:HG23	1.83	0.59
1:C:43:PHE:HB3	2:G:365:ILE:CD1	2.33	0.58
2:G:420:ARG:HH22	3:H:55:GLU:H	1.44	0.58
2:G:420:ARG:NE	3:H:56:ASN:ND2	2.39	0.58
2:G:420:ARG:CZ	3:H:56:ASN:N	2.66	0.58
4:L:29:ASN:CG	4:L:30:ILE:N	2.61	0.58
3:H:23:LYS:HG3	3:H:78:THR:HG22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:30:ILE:CG2	4:L:68:LYS:HE2	2.34	0.58
2:G:111:TRP:CE3	2:G:115:LEU:HD12	2.38	0.58
3:H:193:VAL:HG11	4:L:141:LEU:CD1	2.33	0.58
4:L:186:LEU:HD23	4:L:186:LEU:H	1.67	0.58
4:L:41:LEU:HB3	4:L:42:PRO:HD2	1.85	0.58
1:C:58:ARG:HB3	1:C:61:LEU:HD23	1.84	0.58
2:G:356:ALA:HB1	2:G:357:PRO:HD2	1.86	0.58
2:G:383:LYS:HE2	5:G:2000:NAG:O7	2.03	0.58
3:H:178:PHE:HB3	3:H:179:PRO:HD2	1.86	0.58
2:G:253:THR:HG23	2:G:368:HIS:HA	1.84	0.57
3:H:110:TYR:HD2	3:H:110:TYR:N	2.02	0.57
2:G:333:TRP:O	2:G:337:LEU:HG	2.03	0.57
3:H:48:MET:HG2	3:H:64:PHE:CE2	2.38	0.57
2:G:388:ILE:HD13	2:G:388:ILE:N	2.19	0.57
3:H:20:VAL:HG11	3:H:119:THR:HG21	1.87	0.57
4:L:186:LEU:N	4:L:186:LEU:CD2	2.65	0.57
1:C:144:LEU:HD13	1:C:144:LEU:C	2.29	0.57
3:H:143:THR:HA	3:H:147:THR:O	2.04	0.57
3:H:154:VAL:HB	3:H:190:LEU:O	2.04	0.57
1:C:61:LEU:N	1:C:61:LEU:HD22	2.20	0.57
2:G:225:ASN:HB2	2:G:237:ASN:O	2.05	0.57
3:H:150:LEU:H	3:H:150:LEU:HD23	1.69	0.57
1:C:37:LEU:HD11	1:C:44:LEU:CG	2.34	0.57
3:H:182:LEU:HD23	3:H:182:LEU:C	2.30	0.56
4:L:142:ILE:HD12	4:L:201:VAL:CG2	2.35	0.56
2:G:266:VAL:HG22	2:G:285:THR:H	1.70	0.56
3:H:165:SER:OG	3:H:209:ASN:HB2	2.04	0.56
1:C:33:GLN:HB2	2:G:459:GLU:HG3	1.85	0.56
2:G:253:THR:HG21	2:G:364:GLU:O	2.04	0.56
2:G:290:ILE:CD1	2:G:448:ILE:HD11	2.35	0.56
3:H:137:ALA:O	3:H:138:PRO:C	2.46	0.56
4:L:7:GLN:NE2	4:L:106:GLY:HA2	2.20	0.56
1:C:14:LEU:HD22	1:C:93:VAL:HG11	1.87	0.56
1:C:44:LEU:HD13	1:C:62:TRP:HH2	1.69	0.56
2:G:268:ILE:HG23	2:G:280:ILE:HG23	1.87	0.56
2:G:436:PRO:HB2	2:G:437:PRO:HD2	1.87	0.56
3:H:104:ASN:C	3:H:107:THR:H	2.13	0.56
4:L:87:ASP:CG	4:L:108:LYS:HG3	2.31	0.56
2:G:461:LYS:O	2:G:461:LYS:HG2	2.04	0.56
3:H:110:TYR:N	3:H:110:TYR:CD2	2.74	0.56
1:C:3:VAL:HG22	1:C:94:GLN:CB	2.22	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LEU:O	1:C:52:ASN:C	2.48	0.56
2:G:261:LEU:HD21	2:G:287:SER:OG	2.06	0.56
3:H:212:HIS:CE1	3:H:215:SER:OG	2.59	0.56
2:G:455:ARG:HA	2:G:469:ILE:O	2.05	0.56
1:C:107:HIS:HD2	1:C:175:VAL:HG11	1.70	0.56
3:H:60:TYR:HE1	3:H:70:MET:HG3	1.70	0.56
3:H:160:GLU:N	3:H:161:PRO:HD3	2.16	0.55
4:L:8:PRO:O	4:L:107:THR:HB	2.06	0.55
4:L:21:ILE:HG21	4:L:107:THR:HG21	1.88	0.55
3:H:103:TYR:CD1	3:H:103:TYR:O	2.58	0.55
2:G:85:LEU:HD23	2:G:240:THR:HG22	1.87	0.55
1:C:52:ASN:N	1:C:52:ASN:HD22	2.02	0.55
4:L:140:CYS:HB2	4:L:154:TRP:CZ2	2.41	0.55
3:H:135:PRO:HB2	3:H:223:VAL:HG13	1.89	0.55
1:C:5:LEU:CD2	1:C:96:LEU:HB2	2.36	0.55
3:H:150:LEU:HD23	3:H:150:LEU:O	2.06	0.55
4:L:5:LEU:HD11	4:L:92:THR:CG2	2.37	0.55
4:L:93:TRP:CZ3	4:L:100:GLY:HA2	2.42	0.55
2:G:425:MET:SD	2:G:432:ALA:HB2	2.47	0.54
4:L:138:LEU:N	4:L:138:LEU:HD12	2.22	0.54
2:G:462:THR:HG22	2:G:462:THR:O	2.07	0.54
2:G:117:PRO:HD3	2:G:434:TYR:OH	2.07	0.54
2:G:245:HIS:N	2:G:488:TYR:OH	2.40	0.54
2:G:268:ILE:HG22	2:G:273:ILE:HD12	1.89	0.54
2:G:335:GLU:O	2:G:338:LYS:HB2	2.08	0.54
2:G:419:ILE:C	2:G:420:ARG:CG	2.81	0.54
2:G:97:ASN:O	2:G:100:VAL:HG22	2.08	0.54
3:H:99:GLY:HA3	3:H:110:TYR:CD1	2.43	0.54
4:L:30:ILE:HD12	4:L:35:VAL:HG22	1.89	0.54
4:L:171:SER:O	4:L:178:TYR:HA	2.08	0.54
1:C:12:VAL:HG22	1:C:13:GLU:N	2.23	0.54
2:G:228:THR:HG21	2:G:265:GLU:HB2	1.90	0.54
2:G:461:LYS:HB3	2:G:461:LYS:HZ3	1.73	0.54
3:H:167:ASN:CB	3:H:170:ALA:HB3	2.38	0.54
4:L:125:PRO:HA	4:L:212:MET:HE1	1.90	0.54
2:G:214:CYS:SG	2:G:242:GLN:O	2.66	0.53
2:G:89:ILE:HG12	2:G:236:ASN:HA	1.89	0.53
2:G:481:TRP:HA	2:G:481:TRP:HE3	1.71	0.53
4:L:191:TRP:CH2	4:L:214:HIS:HB2	2.42	0.53
2:G:383:LYS:HZ1	5:G:2000:NAG:H81	1.72	0.53
3:H:2:VAL:HG11	3:H:114:TYR:CE1	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:193:VAL:HG21	4:L:141:LEU:HD11	1.90	0.53
1:C:20:GLN:NE2	1:C:22:LYS:HD2	2.23	0.53
2:G:272:ASN:ND2	5:G:1500:NAG:C6	2.65	0.53
4:L:125:PRO:HB3	4:L:212:MET:SD	2.48	0.53
3:H:103:TYR:CD2	3:H:103:TYR:N	2.76	0.53
3:H:142:SER:HB3	3:H:149:ALA:H	1.73	0.53
4:L:37:TRP:CD2	4:L:75:LEU:HD13	2.44	0.53
2:G:471:ARG:HH11	2:G:471:ARG:HG2	1.73	0.53
3:H:100:GLY:O	3:H:101:ASN:C	2.51	0.53
4:L:186:LEU:HD12	4:L:190:GLN:HB3	1.91	0.53
1:C:36:ILE:O	1:C:47:GLY:N	2.31	0.53
1:C:37:LEU:HD12	1:C:45:THR:O	2.08	0.53
2:G:275:ASN:ND2	2:G:278:LYS:HG2	2.23	0.53
2:G:282:VAL:HB	2:G:451:LEU:HB2	1.91	0.53
4:L:29:ASN:ND2	4:L:30:ILE:H	2.07	0.53
2:G:215:ALA:HB2	2:G:221:ILE:CD1	2.40	0.52
3:H:102:TYR:CE2	3:H:110:TYR:HA	2.43	0.52
2:G:367:THR:HB	2:G:379:CYS:O	2.09	0.52
1:C:21:LYS:O	1:C:21:LYS:HG3	2.09	0.52
2:G:426:TRP:CE3	2:G:477:MET:HG3	2.43	0.52
3:H:197:PRO:HG2	3:H:200:SER:HB2	1.89	0.52
4:L:40:GLN:O	4:L:86:ALA:HB1	2.09	0.52
4:L:155:LYS:HG2	4:L:158:SER:CA	2.31	0.52
1:C:46:LYS:HE3	2:G:360:GLY:HA3	1.92	0.52
1:C:53:ASP:O	1:C:54:ARG:CG	2.54	0.52
1:C:138:ILE:HG21	1:C:144:LEU:HD21	1.91	0.52
1:C:144:LEU:HD22	1:C:145:SER:N	2.25	0.52
3:H:209:ASN:OD1	3:H:220:ASP:HB3	2.10	0.52
2:G:348:PHE:HB3	2:G:351:LYS:CD	2.34	0.52
3:H:31:GLY:HA2	3:H:72:GLU:OE1	2.08	0.52
2:G:253:THR:C	2:G:255:LEU:N	2.66	0.52
1:C:133:PRO:HG3	1:C:157:TRP:HB3	1.92	0.52
1:C:33:GLN:HG3	2:G:459:GLU:HG3	1.92	0.52
3:H:35:HIS:CD2	3:H:47:TRP:HE1	2.28	0.52
2:G:281:ILE:O	2:G:451:LEU:O	2.28	0.52
1:C:45:THR:CG2	2:G:365:ILE:HD13	2.40	0.51
4:L:29:ASN:HD22	4:L:92:THR:HG21	1.75	0.51
2:G:103:MET:CE	2:G:213:TYR:HB2	2.39	0.51
2:G:328:ILE:HG21	2:G:333:TRP:HE1	1.74	0.51
2:G:339:LYS:O	2:G:343:LYS:HG2	2.10	0.51
3:H:34:ILE:HD12	3:H:72:GLU:HG2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ILE:HD11	1:C:82:TYR:HE2	1.75	0.51
2:G:338:LYS:NZ	2:G:338:LYS:HB3	2.26	0.51
4:L:151:THR:HG23	4:L:202:THR:HB	1.92	0.51
2:G:253:THR:OG1	2:G:254:GLN:N	2.44	0.51
2:G:256:LEU:HD23	2:G:480:ASN:HD22	1.74	0.51
2:G:270:SER:OG	2:G:280:ILE:HG12	2.10	0.51
1:C:109:LEU:HD23	1:C:176:VAL:C	2.35	0.51
2:G:85:LEU:HD22	2:G:239:SER:OG	2.10	0.51
2:G:229:PHE:CE2	2:G:235:CYS:HB2	2.45	0.51
2:G:483:SER:O	2:G:486:TYR:HD2	1.92	0.51
4:L:41:LEU:HB3	4:L:42:PRO:CD	2.40	0.51
1:C:53:ASP:HB2	4:L:32:LYS:HZ1	1.75	0.51
1:C:58:ARG:CB	1:C:61:LEU:HD23	2.41	0.51
1:C:154:SER:HB3	1:C:176:VAL:HB	1.92	0.51
2:G:340:VAL:CG2	2:G:341:VAL:N	2.73	0.51
3:H:60:TYR:HE1	3:H:70:MET:CG	2.23	0.51
3:H:97:ALA:CB	3:H:112:LEU:HD22	2.41	0.51
3:H:106:TRP:C	3:H:108:GLY:H	2.17	0.51
1:C:24:ILE:HD13	1:C:87:GLU:HB3	1.92	0.51
3:H:38:ARG:O	3:H:38:ARG:HG3	2.11	0.51
4:L:5:LEU:HD11	4:L:92:THR:HG22	1.91	0.51
2:G:254:GLN:O	2:G:255:LEU:HD23	2.11	0.50
2:G:282:VAL:HG11	2:G:451:LEU:HD12	1.92	0.50
3:H:110:TYR:HD2	3:H:110:TYR:H	1.58	0.50
2:G:272:ASN:ND2	5:G:1500:NAG:H4	2.26	0.50
2:G:435:ALA:HB1	2:G:436:PRO:CD	2.37	0.50
3:H:60:TYR:OH	3:H:70:MET:N	2.42	0.50
1:C:36:ILE:HG23	1:C:55:ALA:HB1	1.94	0.50
1:C:120:SER:OG	1:C:121:PRO:HD2	2.12	0.50
3:H:36:TRP:CH2	3:H:96:CYS:HB2	2.46	0.50
3:H:71:THR:O	3:H:79:ALA:HB1	2.11	0.50
2:G:453:LEU:HD23	2:G:472:PRO:HA	1.94	0.50
1:C:138:ILE:HG22	1:C:144:LEU:CD2	2.41	0.50
2:G:272:ASN:CB	2:G:275:ASN:HB2	2.36	0.50
1:C:83:ILE:HG12	1:C:92:GLU:CB	2.42	0.50
2:G:376:PHE:CD2	2:G:423:ILE:HD13	2.47	0.50
2:G:378:TYR:CD1	2:G:420:ARG:HD3	2.46	0.50
3:H:38:ARG:HA	3:H:93:VAL:O	2.12	0.50
4:L:65:SER:OG	4:L:76:ALA:HB3	2.12	0.50
4:L:198:SER:OG	4:L:211:THR:HA	2.12	0.50
2:G:268:ILE:HG23	2:G:280:ILE:CG2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:326:CYS:O	2:G:414:THR:HG23	2.12	0.50
1:C:71:ILE:CG2	1:C:74:LEU:HD23	2.41	0.49
2:G:267:VAL:HG11	2:G:269:ARG:NH2	2.26	0.49
2:G:334:ASN:HA	2:G:337:LEU:HG	1.94	0.49
2:G:420:ARG:CB	3:H:56:ASN:HB3	2.41	0.49
2:G:420:ARG:CB	2:G:420:ARG:HH11	2.24	0.49
3:H:150:LEU:HD23	3:H:194:VAL:O	2.11	0.49
4:L:151:THR:CG2	4:L:202:THR:HB	2.42	0.49
3:H:138:PRO:HD3	3:H:150:LEU:CB	2.43	0.49
3:H:158:PHE:O	3:H:159:PRO:O	2.30	0.49
1:C:33:GLN:CG	2:G:459:GLU:HG3	2.43	0.49
2:G:215:ALA:HB2	2:G:221:ILE:CG1	2.40	0.49
4:L:142:ILE:HD12	4:L:201:VAL:HG21	1.94	0.49
2:G:269:ARG:HH12	2:G:283:HIS:CD2	2.30	0.49
1:C:132:SER:O	1:C:133:PRO:C	2.54	0.49
1:C:79:SER:OG	1:C:97:VAL:N	2.44	0.49
2:G:463:GLU:CB	2:G:465:ASN:HD22	2.26	0.49
1:C:28:TRP:CD2	1:C:84:CYS:HB2	2.48	0.48
1:C:144:LEU:HD22	1:C:145:SER:H	1.79	0.48
3:H:22:CYS:HB2	3:H:36:TRP:CH2	2.39	0.48
3:H:158:PHE:CG	3:H:159:PRO:CD	2.97	0.48
4:L:28:SER:O	4:L:94:ASP:OD2	2.30	0.48
1:C:27:HIS:NE2	1:C:35:LYS:HE3	2.28	0.48
2:G:420:ARG:NH1	2:G:420:ARG:HB3	2.28	0.48
1:C:121:PRO:O	1:C:122:PRO:C	2.57	0.48
3:H:23:LYS:HG3	3:H:78:THR:CG2	2.43	0.48
2:G:103:MET:O	2:G:107:ILE:HG12	2.14	0.48
2:G:208:PRO:HG3	5:G:1000:NAG:O7	2.13	0.48
3:H:31:GLY:CA	3:H:72:GLU:OE1	2.61	0.48
3:H:151:GLY:HA2	3:H:166:TRP:HH2	1.77	0.48
3:H:182:LEU:HD12	3:H:188:TYR:CZ	2.49	0.48
3:H:142:SER:CB	3:H:148:ALA:HB1	2.44	0.48
3:H:150:LEU:HD23	3:H:150:LEU:N	2.28	0.48
1:C:44:LEU:HD13	1:C:62:TRP:CH2	2.49	0.48
1:C:85:GLU:HG2	1:C:90:LYS:HD3	1.96	0.48
3:H:13:LYS:O	3:H:14:PRO:C	2.54	0.48
4:L:19:VAL:HG11	4:L:80:LEU:CD2	2.43	0.48
1:C:37:LEU:HD23	1:C:57:SER:HB3	1.96	0.48
2:G:461:LYS:O	2:G:463:GLU:N	2.46	0.48
4:L:37:TRP:CG	4:L:75:LEU:HD13	2.49	0.48
4:L:173:GLN:OE1	4:L:179:ALA:HB2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:420:ARG:HH11	2:G:420:ARG:HB3	1.78	0.48
1:C:86:VAL:O	1:C:87:GLU:C	2.57	0.47
2:G:272:ASN:HB3	2:G:275:ASN:CB	2.40	0.47
3:H:179:PRO:HG2	4:L:168:THR:CG2	2.44	0.47
4:L:7:GLN:HB3	4:L:23:CYS:HB2	1.95	0.47
1:C:61:LEU:HD22	1:C:61:LEU:H	1.79	0.47
1:C:132:SER:C	1:C:135:GLY:H	2.22	0.47
2:G:252:SER:OG	2:G:255:LEU:O	2.22	0.47
1:C:129:GLN:HG2	1:C:137:ASN:HD21	1.76	0.47
3:H:19:LYS:CB	3:H:82:GLU:HG2	2.44	0.47
2:G:223:LYS:O	2:G:238:VAL:HG13	2.13	0.47
3:H:150:LEU:N	3:H:150:LEU:CD2	2.77	0.47
2:G:250:VAL:HG23	2:G:250:VAL:O	2.14	0.47
4:L:25:GLY:O	4:L:71:THR:HG23	2.15	0.47
1:C:11:THR:HG23	1:C:72:LYS:HB3	1.95	0.47
1:C:12:VAL:CG2	1:C:13:GLU:N	2.78	0.47
1:C:33:GLN:HB2	2:G:459:GLU:HG2	1.96	0.47
2:G:225:ASN:O	2:G:226:ASP:C	2.56	0.47
2:G:420:ARG:NH2	3:H:55:GLU:N	2.40	0.47
3:H:1:GLN:NE2	3:H:25:SER:HB3	2.30	0.47
3:H:47:TRP:CG	4:L:101:GLN:HB3	2.50	0.47
3:H:90:ASP:O	3:H:91:THR:C	2.58	0.47
3:H:159:PRO:CB	3:H:214:PRO:HB3	2.44	0.47
3:H:205:THR:HB	3:H:222:LYS:HD2	1.95	0.47
2:G:104:HIS:HD1	2:G:481:TRP:CD1	2.33	0.47
2:G:338:LYS:C	2:G:341:VAL:HG22	2.39	0.47
4:L:13:ALA:HB3	4:L:80:LEU:HD23	1.97	0.47
4:L:29:ASN:HD22	4:L:30:ILE:HG12	1.74	0.47
2:G:97:ASN:OD1	2:G:97:ASN:C	2.57	0.47
2:G:333:TRP:HA	2:G:336:THR:OG1	2.15	0.46
1:C:128:VAL:HG23	1:C:141:GLY:O	2.15	0.46
3:H:64:PHE:HB3	3:H:68:VAL:CG1	2.45	0.46
3:H:183:GLN:HB3	3:H:187:LEU:O	2.16	0.46
3:H:6:GLN:OE1	3:H:118:GLY:N	2.47	0.46
3:H:212:HIS:HE1	3:H:214:PRO:HB2	1.79	0.46
3:H:190:LEU:HD12	3:H:191:SER:H	1.78	0.46
1:C:61:LEU:H	1:C:61:LEU:CD2	2.29	0.46
1:C:132:SER:O	1:C:135:GLY:N	2.49	0.46
2:G:436:PRO:CB	2:G:437:PRO:HD2	2.45	0.46
3:H:91:THR:HG22	3:H:122:THR:HA	1.97	0.46
1:C:100:LEU:HD12	1:C:170:PHE:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:10:GLU:OE2	3:H:12:ARG:CZ	2.64	0.46
1:C:131:ARG:HG2	1:C:137:ASN:HD22	1.80	0.46
2:G:121:LEU:HD23	2:G:196:THR:OG1	2.15	0.46
2:G:420:ARG:HH22	3:H:55:GLU:CA	2.28	0.46
3:H:64:PHE:HB3	3:H:68:VAL:HG11	1.97	0.46
1:C:57:SER:HB2	1:C:68:PRO:O	2.14	0.46
3:H:31:GLY:C	3:H:72:GLU:OE1	2.59	0.46
1:C:36:ILE:CG2	1:C:55:ALA:HB1	2.45	0.46
1:C:43:PHE:CE1	2:G:426:TRP:HA	2.51	0.46
1:C:56:ASP:O	1:C:70:ILE:HB	2.15	0.46
2:G:340:VAL:HG23	2:G:341:VAL:N	2.31	0.46
2:G:370:PHE:CE2	2:G:377:PHE:HB2	2.51	0.46
3:H:134:PHE:CD2	4:L:130:GLU:HB2	2.50	0.46
4:L:10:SER:C	4:L:11:VAL:HG23	2.39	0.46
4:L:191:TRP:CZ3	4:L:214:HIS:HB2	2.51	0.46
3:H:138:PRO:HD3	3:H:150:LEU:HB3	1.98	0.45
4:L:114:GLN:HB3	4:L:115:PRO:HD2	1.98	0.45
1:C:158:THR:HG23	1:C:169:GLU:HG3	1.97	0.45
2:G:261:LEU:N	2:G:261:LEU:HD12	2.30	0.45
3:H:51:PHE:HA	3:H:58:ILE:HA	1.98	0.45
4:L:38:TYR:HA	4:L:47:LYS:O	2.17	0.45
1:C:28:TRP:CE2	1:C:84:CYS:HB2	2.51	0.45
4:L:63:ARG:HH11	4:L:63:ARG:HD2	1.49	0.45
1:C:20:GLN:O	1:C:22:LYS:N	2.49	0.45
1:C:174:ILE:HG23	1:C:175:VAL:N	2.31	0.45
4:L:39:GLN:HG3	4:L:88:TYR:CE1	2.52	0.45
1:C:12:VAL:O	1:C:12:VAL:HG13	2.17	0.45
1:C:133:PRO:HD3	1:C:157:TRP:CD2	2.51	0.45
2:G:331:LYS:O	2:G:335:GLU:OE2	2.35	0.45
2:G:378:TYR:O	2:G:417:CYS:SG	2.74	0.45
3:H:35:HIS:HD2	3:H:47:TRP:HE1	1.64	0.45
2:G:378:TYR:OH	2:G:423:ILE:HG13	2.16	0.45
4:L:97:LEU:CD2	4:L:99:THR:HG23	2.36	0.45
4:L:126:PRO:HG2	4:L:191:TRP:CD1	2.52	0.45
2:G:262:ALA:O	2:G:285:THR:HA	2.17	0.45
3:H:32:LEU:HD22	3:H:51:PHE:CE2	2.51	0.45
4:L:30:ILE:HG22	4:L:68:LYS:HE2	1.99	0.45
1:C:58:ARG:HA	3:H:106:TRP:HH2	1.80	0.45
1:C:100:LEU:HD11	1:C:159:CYS:HB2	1.98	0.45
2:G:112:ASP:O	2:G:116:LYS:HG2	2.17	0.45
3:H:45:LEU:HD21	4:L:46:PRO:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:136:LEU:HB3	4:L:124:PHE:CD2	2.52	0.45
1:C:132:SER:C	1:C:134:ARG:N	2.69	0.44
2:G:210:PRO:HA	2:G:247:ILE:O	2.17	0.44
2:G:266:VAL:O	2:G:343:LYS:HE2	2.17	0.44
2:G:420:ARG:HH21	3:H:54:GLU:CG	2.29	0.44
4:L:37:TRP:CE3	4:L:75:LEU:HD22	2.52	0.44
1:C:61:LEU:HB3	1:C:66:ASN:HB3	1.98	0.44
2:G:99:MET:HE1	2:G:488:TYR:HB3	1.99	0.44
4:L:114:GLN:HE22	4:L:177:LYS:HG2	1.81	0.44
2:G:111:TRP:CE2	2:G:251:VAL:HG21	2.52	0.44
2:G:354:GLU:OE2	2:G:388:ILE:HG22	2.18	0.44
4:L:37:TRP:CD1	4:L:50:ILE:HB	2.52	0.44
1:C:36:ILE:CD1	1:C:51:LEU:HD12	2.47	0.44
2:G:337:LEU:HD22	2:G:389:HIS:NE2	2.33	0.44
3:H:47:TRP:CH2	3:H:49:GLY:HA2	2.53	0.44
3:H:68:VAL:HG23	3:H:82:GLU:O	2.17	0.44
4:L:56:ARG:HD2	4:L:60:ILE:CG2	2.47	0.44
1:C:46:LYS:HD2	1:C:52:ASN:O	2.17	0.44
4:L:144:ASP:OD2	4:L:173:GLN:NE2	2.51	0.44
1:C:134:ARG:HD3	1:C:152:GLN:HB3	2.00	0.44
2:G:420:ARG:NH1	3:H:56:ASN:N	2.65	0.44
2:G:461:LYS:NZ	2:G:461:LYS:CB	2.80	0.44
3:H:148:ALA:O	3:H:196:VAL:N	2.42	0.44
4:L:154:TRP:CH2	4:L:199:CYS:HB2	2.52	0.44
3:H:158:PHE:CD1	3:H:159:PRO:N	2.86	0.44
4:L:169:THR:O	4:L:170:PRO:O	2.36	0.44
2:G:118:CYS:N	2:G:201:CYS:SG	2.91	0.44
2:G:276:ASN:OD1	2:G:277:VAL:HG23	2.18	0.44
1:C:125:SER:O	1:C:163:GLN:CD	2.61	0.43
2:G:97:ASN:ND2	2:G:99:MET:HE3	2.28	0.43
2:G:207:ASP:HA	2:G:208:PRO:HD2	1.47	0.43
2:G:463:GLU:HB3	2:G:465:ASN:HD22	1.83	0.43
1:C:30:ASN:OD1	1:C:34:ILE:O	2.36	0.43
1:C:46:LYS:HE3	2:G:360:GLY:CA	2.48	0.43
1:C:51:LEU:O	1:C:53:ASP:N	2.51	0.43
2:G:452:LEU:O	2:G:453:LEU:HD23	2.17	0.43
4:L:26:SER:O	4:L:27:SER:C	2.60	0.43
1:C:12:VAL:CG1	1:C:74:LEU:HD21	2.48	0.43
1:C:39:ASN:HD22	1:C:39:ASN:H	1.65	0.43
3:H:38:ARG:O	3:H:38:ARG:CG	2.64	0.43
4:L:30:ILE:O	4:L:31:GLY:C	2.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:187:THR:OG1	4:L:189:GLU:HB3	2.18	0.43
2:G:267:VAL:HG11	2:G:269:ARG:HH21	1.82	0.43
2:G:272:ASN:ND2	5:G:1500:NAG:C4	2.76	0.43
3:H:36:TRP:CG	3:H:81:MET:HG3	2.53	0.43
1:C:130:CYS:HA	1:C:158:THR:O	2.18	0.43
2:G:426:TRP:HE3	2:G:477:MET:HG3	1.82	0.43
1:C:132:SER:HA	1:C:157:TRP:HE3	1.71	0.43
3:H:6:GLN:OE1	3:H:118:GLY:CA	2.67	0.43
2:G:215:ALA:HB1	2:G:219:TYR:O	2.18	0.43
2:G:338:LYS:CA	2:G:341:VAL:HG22	2.48	0.43
2:G:357:PRO:HB2	2:G:382:THR:HB	2.01	0.43
2:G:471:ARG:HG2	2:G:471:ARG:NH1	2.34	0.43
2:G:483:SER:O	2:G:486:TYR:CD2	2.70	0.43
3:H:67:ARG:HD2	3:H:84:SER:O	2.19	0.43
1:C:160:THR:HG21	1:C:167:LYS:HD2	2.00	0.43
2:G:213:TYR:O	2:G:244:THR:HG23	2.19	0.43
1:C:85:GLU:OE2	1:C:90:LYS:HE2	2.19	0.43
1:C:114:LEU:HB2	1:C:149:LEU:HD11	2.00	0.43
2:G:108:ILE:HD12	2:G:427:GLN:HG2	2.01	0.43
2:G:267:VAL:HG11	2:G:269:ARG:NE	2.34	0.43
3:H:149:ALA:CB	3:H:195:THR:HG22	2.34	0.43
3:H:213:LYS:N	3:H:214:PRO:CD	2.82	0.43
4:L:37:TRP:CZ2	4:L:75:LEU:HB2	2.54	0.43
2:G:227:LYS:CD	2:G:263:GLU:OE1	2.66	0.42
1:C:3:VAL:HG21	1:C:164:ASN:ND2	2.35	0.42
2:G:418:ARG:HB2	2:G:420:ARG:HD2	1.98	0.42
4:L:124:PHE:CB	4:L:125:PRO:HD2	2.41	0.42
1:C:96:LEU:HD22	1:C:121:PRO:HG3	2.00	0.42
2:G:116:LYS:HG3	2:G:202:PRO:HG3	2.02	0.42
1:C:129:GLN:CD	1:C:137:ASN:ND2	2.74	0.42
1:C:24:ILE:HG22	1:C:25:GLN:O	2.20	0.42
2:G:99:MET:HE1	2:G:488:TYR:CB	2.50	0.42
3:H:136:LEU:HD21	4:L:139:VAL:HG21	2.00	0.42
1:C:58:ARG:HA	3:H:106:TRP:CH2	2.55	0.42
3:H:153:LEU:HD12	3:H:191:SER:HB3	2.01	0.42
2:G:223:LYS:HE3	2:G:241:VAL:HG21	2.02	0.42
3:H:47:TRP:CZ2	3:H:49:GLY:CA	3.03	0.42
1:C:133:PRO:N	1:C:157:TRP:HB3	2.34	0.42
3:H:58:ILE:O	3:H:58:ILE:CG2	2.68	0.42
4:L:187:THR:C	4:L:189:GLU:N	2.78	0.42
2:G:93:ASN:CG	2:G:232:ILE:HD12	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:146:GLY:O	3:H:197:PRO:HA	2.20	0.42
3:H:193:VAL:HG21	4:L:141:LEU:HD21	2.02	0.42
4:L:150:VAL:HG22	4:L:151:THR:N	2.35	0.42
4:L:196:SER:HB3	4:L:213:ALA:HB2	2.01	0.42
2:G:103:MET:HE1	2:G:213:TYR:CB	2.47	0.41
2:G:338:LYS:HB3	2:G:338:LYS:HZ3	1.84	0.41
2:G:368:HIS:O	2:G:368:HIS:CG	2.73	0.41
2:G:489:LYS:HE2	2:G:491:VAL:HG13	2.02	0.41
1:C:12:VAL:HG12	1:C:74:LEU:HD21	2.02	0.41
1:C:114:LEU:O	1:C:145:SER:HA	2.20	0.41
2:G:420:ARG:NH2	3:H:54:GLU:HG2	2.30	0.41
1:C:85:GLU:HG2	1:C:90:LYS:CD	2.51	0.41
1:C:133:PRO:HD3	1:C:157:TRP:CG	2.54	0.41
2:G:270:SER:O	2:G:271:GLU:C	2.62	0.41
2:G:280:ILE:O	2:G:453:LEU:N	2.48	0.41
2:G:348:PHE:CB	2:G:351:LYS:HD2	2.42	0.41
3:H:41:PRO:HD3	3:H:92:ALA:HA	2.02	0.41
3:H:153:LEU:HD12	3:H:153:LEU:HA	1.70	0.41
1:C:58:ARG:HG2	3:H:106:TRP:CH2	2.55	0.41
1:C:133:PRO:CD	1:C:157:TRP:HB3	2.50	0.41
2:G:420:ARG:NH2	3:H:56:ASN:N	2.58	0.41
3:H:1:GLN:HE22	3:H:25:SER:HB3	1.85	0.41
4:L:169:THR:O	4:L:170:PRO:C	2.64	0.41
3:H:32:LEU:HD13	3:H:107:THR:HG23	2.01	0.41
1:C:33:GLN:CB	2:G:459:GLU:HG3	2.49	0.41
1:C:133:PRO:CG	1:C:157:TRP:HB3	2.50	0.41
2:G:92:PHE:CD1	2:G:489:LYS:HB2	2.56	0.41
1:C:36:ILE:HG22	1:C:37:LEU:N	2.34	0.41
1:C:52:ASN:ND2	1:C:53:ASP:H	2.18	0.41
1:C:57:SER:CB	1:C:68:PRO:O	2.69	0.41
1:C:118:LEU:HD23	1:C:126:PRO:HB2	2.03	0.41
1:C:174:ILE:CG2	1:C:176:VAL:HG23	2.50	0.41
2:G:253:THR:HG23	2:G:254:GLN:HG2	2.02	0.41
5:G:1000:NAG:H83	5:G:1000:NAG:O3	2.21	0.41
1:C:124:SER:HB3	1:C:163:GLN:HE21	1.86	0.41
2:G:244:THR:HA	2:G:488:TYR:CZ	2.55	0.41
2:G:436:PRO:HA	2:G:437:PRO:HD3	1.90	0.41
3:H:48:MET:HE3	3:H:64:PHE:CD2	2.54	0.41
3:H:93:VAL:HG22	3:H:120:LEU:HD13	2.02	0.41
3:H:149:ALA:HA	3:H:195:THR:HA	2.02	0.41
3:H:157:TYR:CE2	3:H:188:TYR:O	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LYS:HD2	1:C:10:ASP:OD2	2.20	0.41
1:C:45:THR:HG21	2:G:365:ILE:HG21	2.00	0.41
2:G:223:LYS:HE3	2:G:241:VAL:CG1	2.31	0.41
3:H:158:PHE:CG	3:H:159:PRO:N	2.89	0.41
3:H:197:PRO:HG2	3:H:200:SER:CB	2.51	0.41
4:L:37:TRP:N	4:L:50:ILE:O	2.43	0.41
4:L:37:TRP:CZ3	4:L:90:CYS:HB3	2.56	0.41
1:C:36:ILE:HG21	1:C:69:LEU:HD11	2.03	0.41
1:C:58:ARG:HG2	3:H:106:TRP:HH2	1.85	0.41
1:C:61:LEU:N	1:C:61:LEU:CD2	2.84	0.41
2:G:104:HIS:O	2:G:108:ILE:HG12	2.21	0.41
1:C:110:GLN:C	1:C:112:GLN:H	2.26	0.40
2:G:233:GLY:HA2	2:G:234:PRO:HD3	1.85	0.40
2:G:341:VAL:HG23	2:G:342:GLU:N	2.36	0.40
4:L:119:PRO:HD3	4:L:203:HIS:CD2	2.56	0.40
1:C:85:GLU:CD	1:C:90:LYS:HE2	2.47	0.40
2:G:114:SER:OG	2:G:206:PHE:HB2	2.21	0.40
2:G:245:HIS:CE1	2:G:487:LYS:NZ	2.89	0.40
4:L:123:LEU:HD22	4:L:212:MET:CB	2.45	0.40
1:C:92:GLU:N	1:C:92:GLU:CD	2.79	0.40
2:G:100:VAL:HG12	2:G:485:LEU:HD12	2.03	0.40
2:G:111:TRP:CZ2	2:G:251:VAL:CG2	2.98	0.40
2:G:276:ASN:OD1	2:G:277:VAL:N	2.52	0.40
2:G:455:ARG:CA	2:G:469:ILE:O	2.70	0.40
2:G:388:ILE:N	2:G:388:ILE:CD1	2.85	0.40
3:H:158:PHE:O	3:H:159:PRO:CG	2.60	0.40
4:L:56:ARG:HD2	4:L:60:ILE:HG22	2.03	0.40
1:C:37:LEU:HD21	1:C:57:SER:OG	2.21	0.40
1:C:98:PHE:HE1	1:C:120:SER:OG	2.05	0.40
3:H:36:TRP:O	3:H:48:MET:HB2	2.21	0.40
3:H:138:PRO:HD3	3:H:150:LEU:HB2	2.04	0.40
3:H:155:LYS:HG3	3:H:156:ASP:CG	2.46	0.40

There are no symmetry-related clashes.

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	C	173/192 (90%)	168 (97%)	3 (2%)	2 (1%)	10	35
2	G	282/332 (85%)	273 (97%)	3 (1%)	6 (2%)	5	24
3	H	223/231 (96%)	216 (97%)	4 (2%)	3 (1%)	9	33
4	L	211/217 (97%)	204 (97%)	3 (1%)	4 (2%)	6	26
All	All	889/972 (92%)	861 (97%)	13 (2%)	15 (2%)	7	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	ASN
1	C	126	PRO
2	G	208	PRO
2	G	216	PRO
2	G	254	GLN
2	G	460	ASN
2	G	462	THR
3	H	159	PRO
3	H	161	PRO
4	L	99	THR
3	H	107	THR
4	L	42	PRO
4	L	86	ALA
4	L	170	PRO
2	G	249	PRO

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	C	159/173 (92%)	151 (95%)	8 (5%)	22	49
2	G	261/296 (88%)	248 (95%)	13 (5%)	22	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	188/194 (97%)	180 (96%)	8 (4%)	26	51
4	L	176/180 (98%)	166 (94%)	10 (6%)	18	45
All	All	784/843 (93%)	745 (95%)	39 (5%)	22	49

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	16	CYS
1	C	39	ASN
1	C	52	ASN
1	C	103	ASN
1	C	106	THR
1	C	121	PRO
1	C	130	CYS
1	C	167	LYS
2	G	116	LYS
2	G	293	ILE
2	G	357	PRO
2	G	372	CYS
2	G	388	ILE
2	G	391	SER
2	G	415	LEU
2	G	417	CYS
2	G	420	ARG
2	G	436	PRO
2	G	443	THR
2	G	445	ILE
2	G	461	LYS
3	H	2	VAL
3	H	74	THR
3	H	96	CYS
3	H	110	TYR
3	H	135	PRO
3	H	143	THR
3	H	150	LEU
3	H	181	VAL
4	L	8	PRO
4	L	23	CYS
4	L	71	THR
4	L	107	THR
4	L	125	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	131	LEU
4	L	135	LYS
4	L	170	PRO
4	L	186	LEU
4	L	214	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	GLN
1	C	33	GLN
1	C	39	ASN
1	C	52	ASN
1	C	73	ASN
1	C	103	ASN
1	C	107	HIS
1	C	110	GLN
1	C	129	GLN
1	C	137	ASN
1	C	139	GLN
1	C	164	ASN
2	G	91	ASN
2	G	102	GLN
2	G	104	HIS
2	G	105	GLN
2	G	193	ASN
2	G	236	ASN
2	G	254	GLN
2	G	275	ASN
2	G	283	HIS
2	G	329	ASN
2	G	390	ASN
2	G	464	ASN
2	G	465	ASN
2	G	480	ASN
3	H	1	GLN
3	H	35	HIS
3	H	56	ASN
3	H	77	ASN
3	H	204	GLN
4	L	7	GLN
4	L	40	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	81	GLN
4	L	194	HIS

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 ⓘ

4 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$
5	NAG	G	1000	2	14,14,15	2.49	3 (21%)	17,19,21	2.06	6 (35%)
5	NAG	G	1500	2	14,14,15	2.97	3 (21%)	17,19,21	1.93	4 (23%)
5	NAG	G	2000	2	14,14,15	2.55	4 (28%)	17,19,21	1.41	3 (17%)
5	NAG	G	2500	2	14,14,15	4.73	4 (28%)	17,19,21	3.00	3 (17%)

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
5	NAG	G	2500	2	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	G	1500	2	-	5/6/23/26	0/1/1/1
5	NAG	G	2000	2	-	4/6/23/26	0/1/1/1
5	NAG	G	1000	2	-	3/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	2500	NAG	C1-C2	16.68	1.75	1.52
5	G	1500	NAG	C1-C2	10.26	1.66	1.52
5	G	2000	NAG	C1-C2	8.38	1.63	1.52
5	G	1000	NAG	O5-C1	6.31	1.54	1.43
5	G	1000	NAG	O5-C5	5.65	1.54	1.43
5	G	2500	NAG	C3-C2	4.17	1.61	1.52
5	G	2000	NAG	O5-C5	2.51	1.48	1.43
5	G	1500	NAG	C8-C7	2.48	1.55	1.50
5	G	2000	NAG	C4-C5	2.40	1.58	1.53
5	G	1500	NAG	C2-N2	2.32	1.50	1.46
5	G	1000	NAG	C3-C2	2.31	1.57	1.52
5	G	2000	NAG	C3-C2	2.26	1.57	1.52
5	G	2500	NAG	C2-N2	2.10	1.49	1.46
5	G	2500	NAG	C8-C7	2.01	1.54	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2500	NAG	C1-C2-N2	8.78	124.27	110.43
5	G	2500	NAG	O5-C1-C2	-7.56	99.60	111.29
5	G	1500	NAG	O5-C1-C2	-5.01	103.54	111.29
5	G	1000	NAG	O5-C1-C2	-4.11	104.93	111.29
5	G	1500	NAG	C8-C7-N2	3.85	122.50	116.12
5	G	1000	NAG	C2-N2-C7	-3.74	117.89	122.90
5	G	1000	NAG	C1-O5-C5	3.45	116.82	112.19
5	G	2000	NAG	C1-O5-C5	3.34	116.66	112.19
5	G	1500	NAG	O7-C7-C8	-2.98	116.74	122.05
5	G	1500	NAG	C1-C2-N2	2.91	115.01	110.43
5	G	1000	NAG	C1-C2-N2	-2.70	106.17	110.43
5	G	2500	NAG	O7-C7-C8	-2.51	117.59	122.05
5	G	1000	NAG	C4-C3-C2	2.18	114.21	111.02
5	G	2000	NAG	O5-C1-C2	-2.05	108.12	111.29
5	G	1000	NAG	O5-C5-C6	2.05	111.64	107.66
5	G	2000	NAG	C1-C2-N2	2.04	113.65	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	2500	NAG	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1000	NAG	C8-C7-N2-C2
5	G	1000	NAG	O7-C7-N2-C2
5	G	1500	NAG	C8-C7-N2-C2
5	G	1500	NAG	O7-C7-N2-C2
5	G	2000	NAG	C8-C7-N2-C2
5	G	2000	NAG	O7-C7-N2-C2
5	G	2500	NAG	C8-C7-N2-C2
5	G	2500	NAG	O7-C7-N2-C2
5	G	2000	NAG	O5-C5-C6-O6
5	G	1500	NAG	O5-C5-C6-O6
5	G	2000	NAG	C4-C5-C6-O6
5	G	1000	NAG	O5-C5-C6-O6
5	G	1500	NAG	C4-C5-C6-O6
5	G	1500	NAG	C3-C2-N2-C7
5	G	2500	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1000	NAG	2	0
5	G	1500	NAG	4	0
5	G	2000	NAG	3	0
5	G	2500	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	175/192 (91%)	0.38	7 (4%) 42 30	51, 103, 139, 185	0
2	G	290/332 (87%)	0.56	18 (6%) 26 21	52, 118, 174, 225	0
3	H	225/231 (97%)	0.38	9 (4%) 42 30	36, 84, 136, 185	0
4	L	213/217 (98%)	0.32	10 (4%) 36 27	39, 83, 133, 162	0
All	All	903/972 (92%)	0.42	44 (4%) 35 26	36, 97, 162, 225	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	106	TRP	6.2
2	G	451	LEU	5.6
2	G	443	THR	4.7
2	G	282	VAL	3.9
3	H	109	TYR	3.8
1	C	41	GLY	3.6
2	G	257	LEU	3.5
4	L	139	VAL	3.3
2	G	484	GLU	3.3
4	L	197	TYR	3.2
2	G	355	PHE	3.2
3	H	182	LEU	3.0
4	L	185	SER	2.9
4	L	137	THR	2.9
2	G	493	ILE	2.7
2	G	371	ASN	2.7
4	L	194	HIS	2.6
1	C	36	ILE	2.6
3	H	171	LEU	2.6
4	L	21	ILE	2.5
4	L	85	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	376	PHE	2.4
3	H	1	GLN	2.4
2	G	427	GLN	2.3
1	C	61	LEU	2.3
2	G	453	LEU	2.3
3	H	108	GLY	2.3
2	G	220	ALA	2.3
1	C	45	THR	2.3
2	G	110	LEU	2.3
1	C	151	LEU	2.2
2	G	346	LYS	2.2
2	G	353	ILE	2.2
3	H	30	THR	2.2
2	G	358	PRO	2.2
3	H	160	GLU	2.2
2	G	260	SER	2.1
4	L	32	LYS	2.1
3	H	32	LEU	2.1
1	C	114	LEU	2.1
2	G	276	ASN	2.1
1	C	82	TYR	2.1
4	L	104	GLY	2.1
4	L	75	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	G	1500	14/15	0.64	0.11	122,122,122,122	0
5	NAG	G	2000	14/15	0.66	0.14	125,125,125,125	0
5	NAG	G	2500	14/15	0.74	0.10	136,136,136,136	0
5	NAG	G	1000	14/15	0.85	0.11	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.