



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:08 AM UTC

PDB ID : 2RR1 / pdb_00002rr1
Title : STRUCTURAL ANALYSIS OF ANTIVIRAL AGENTS THAT INTERACT
WITH THE CAPSID OF HUMAN RHINOVIRUSES
Authors : Badger, J.; Smith, T.J.; Rossmann, M.G.
Deposited on : 1988-10-03
Resolution : 3.00 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

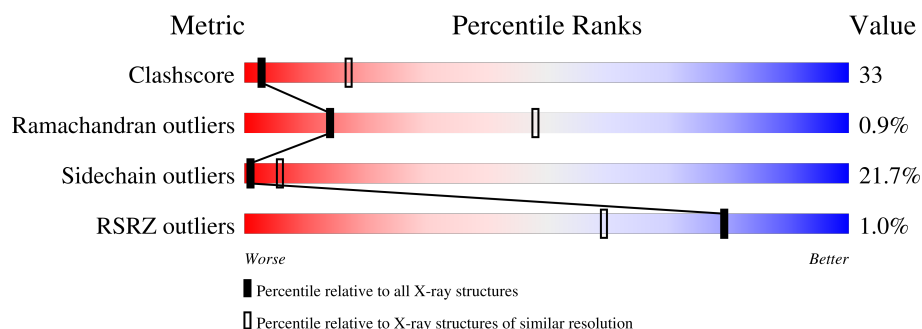
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1	289	 24% 39% 25% 7% 6%
2	2	262	 24% 38% 27% 8% 3%
3	3	236	 25% 39% 28% 8%
4	4	68	 13% 21% 15% 10% 41%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6301 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 HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	273	Total	C	N	O	S	0	0	0
			2170	1373	375	414	8			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total	C	N	O	S	0	0	0
			1952	1238	330	372	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	conflict	UNP P03303

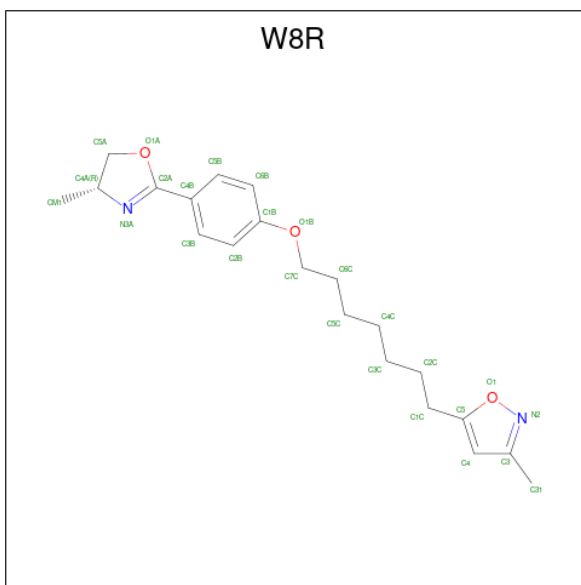
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	236	Total	C	N	O	S	0	0	0
			1849	1184	305	353	7			

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	40	Total	C	N	O	S	0	0	0
			297	186	47	62	2			

- Molecule 5 is 5-(7-(5-HYDRO-4-METHYL-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYL ISOXAZOLE (CCD ID: W8R) (formula: C₂₁H₂₈N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1	1	Total	C	N	O	0	0
			26	21	2	3		

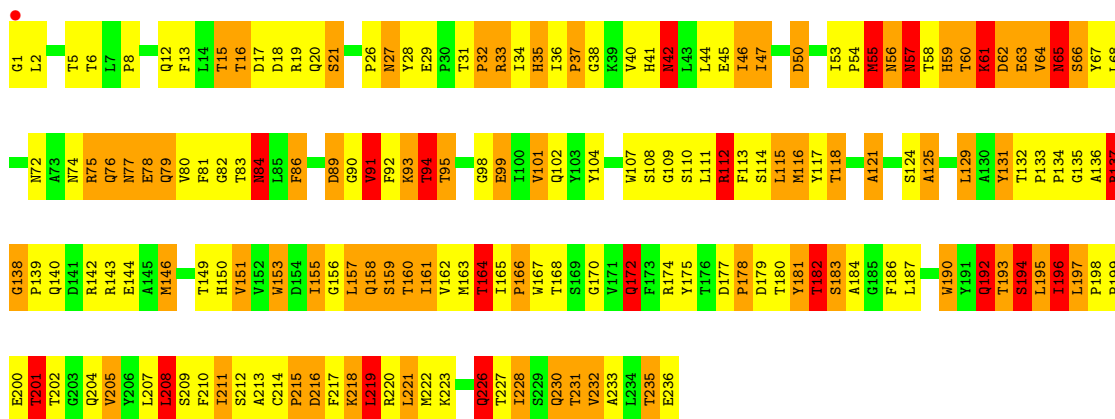
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	6	Total O 6 6	0	0
6	2	1	Total O 1 1	0	0

S258
L259
V260
P261
Q262

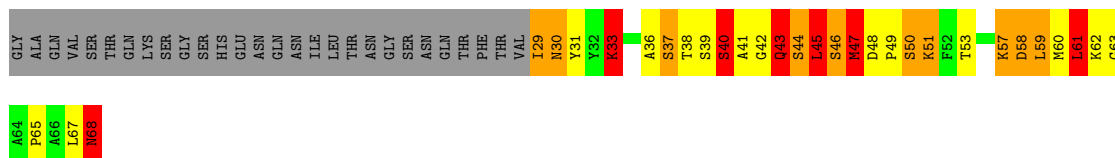
• Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)

Chain 3: 25% 39% 28% 8%



• Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4)

Chain 4: 13% 21% 15% 10% 41%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00 0.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 2.0 (0.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 3.01Å)	Xtriage
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 108.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.079 for l,-k,h	Xtriage
F_o, F_c correlation	0.37	EDS
Total number of atoms	6301	wwPDB-VP
Average B, all atoms (Å ²)	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W8R

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	1	2.31	90/2228 (4.0%)	2.73	211/3031 (7.0%)
2	2	2.40	96/2001 (4.8%)	2.77	193/2735 (7.1%)
3	3	2.30	80/1898 (4.2%)	2.78	186/2597 (7.2%)
4	4	2.64	14/302 (4.6%)	3.14	33/406 (8.1%)
All	All	2.35	280/6429 (4.4%)	2.78	623/8769 (7.1%)

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	1	0	2
2	2	0	2
All	All	0	4

All (280) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	285	ASP	CA-CB	17.77	1.79	1.53
4	4	41	ALA	C-O	13.33	1.41	1.24
3	3	57	ASN	CA-CB	12.78	1.75	1.53
4	4	42	GLY	N-CA	12.59	1.63	1.45
1	1	187	SER	N-CA	11.77	1.60	1.46
2	2	194	ASN	CA-CB	11.51	1.71	1.53
1	1	283	LYS	N-CA	10.88	1.61	1.46
1	1	144	SER	N-CA	10.33	1.58	1.45
3	3	164	THR	C-O	10.22	1.36	1.24
1	1	154	PRO	CA-C	-10.14	1.42	1.52
4	4	45	LEU	C-N	9.39	1.46	1.33
2	2	187	GLN	N-CA	9.31	1.57	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	256	SER	C-O	9.29	1.36	1.24
1	1	170	SER	CB-OG	-9.23	1.23	1.42
1	1	52	GLU	C-O	9.14	1.35	1.24
1	1	282	ARG	CD-NE	9.12	1.59	1.46
2	2	152	ARG	CD-NE	8.88	1.58	1.46
2	2	102	GLY	N-CA	8.88	1.54	1.45
2	2	168	ASP	C-O	8.82	1.34	1.24
3	3	21	SER	CA-CB	8.61	1.66	1.54
2	2	174	ASN	C-O	8.43	1.30	1.23
3	3	50	ASP	CA-CB	-8.28	1.40	1.53
3	3	232	VAL	N-CA	8.17	1.55	1.46
1	1	73	ARG	C-O	8.02	1.33	1.23
2	2	77	GLY	N-CA	7.83	1.53	1.45
3	3	138	GLY	N-CA	7.83	1.55	1.44
2	2	236	PRO	C-O	7.80	1.34	1.24
2	2	161	GLU	CA-CB	-7.78	1.42	1.53
1	1	285	ASP	N-CA	-7.77	1.34	1.45
2	2	135	HIS	CE1-NE2	-7.66	1.24	1.32
3	3	1	GLY	N-CA	7.65	1.57	1.45
2	2	12	ARG	NE-CZ	7.59	1.41	1.33
1	1	122	VAL	N-CA	7.58	1.55	1.46
1	1	72	GLY	C-O	7.53	1.34	1.23
2	2	52	LYS	N-CA	7.53	1.55	1.46
3	3	215	PRO	C-N	-7.47	1.23	1.33
1	1	143	SER	C-O	7.47	1.33	1.24
1	1	94	ARG	CD-NE	7.42	1.56	1.46
2	2	11	ASP	CA-CB	7.36	1.66	1.53
1	1	28	THR	CA-CB	7.34	1.64	1.53
1	1	288	SER	C-O	7.31	1.32	1.23
2	2	120	GLY	N-CA	7.22	1.53	1.45
1	1	132	ALA	C-O	7.20	1.32	1.24
3	3	77	ASN	C-O	7.17	1.33	1.24
3	3	60	THR	CA-CB	7.16	1.65	1.54
2	2	260	VAL	N-CA	7.15	1.55	1.46
4	4	40	SER	CB-OG	7.05	1.56	1.42
2	2	108	VAL	C-O	7.01	1.32	1.24
2	2	219	SER	CA-CB	-7.01	1.41	1.53
1	1	30	LYS	C-O	7.00	1.32	1.23
2	2	9	TYR	C-O	6.99	1.32	1.23
1	1	276	GLU	C-O	6.97	1.30	1.24
2	2	58	THR	C-O	6.97	1.32	1.24
2	2	74	GLY	C-O	6.94	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	202	ASP	CA-CB	-6.86	1.42	1.53
4	4	49	PRO	C-N	-6.85	1.24	1.34
1	1	91	ASP	N-CA	6.84	1.55	1.46
1	1	133	THR	N-CA	6.84	1.54	1.45
1	1	288	SER	CA-CB	6.84	1.65	1.53
3	3	86	PHE	CA-CB	-6.84	1.42	1.52
1	1	23	SER	N-CA	6.81	1.54	1.45
2	2	223	ILE	CA-CB	6.80	1.59	1.54
3	3	6	THR	N-CA	6.76	1.54	1.45
2	2	243	THR	C-O	6.74	1.32	1.24
2	2	193	THR	C-N	-6.73	1.23	1.33
2	2	152	ARG	CZ-NH2	6.73	1.42	1.33
2	2	194	ASN	N-CA	-6.72	1.37	1.45
3	3	216	ASP	CA-CB	6.72	1.64	1.53
2	2	197	ALA	C-O	6.71	1.31	1.23
1	1	73	ARG	N-CA	6.67	1.53	1.45
1	1	165	ASP	CA-CB	6.67	1.64	1.53
2	2	256	SER	CB-OG	6.67	1.55	1.42
2	2	10	SER	C-N	-6.66	1.25	1.33
1	1	161	LYS	N-CA	-6.62	1.38	1.46
1	1	251	GLU	CA-CB	-6.62	1.42	1.53
1	1	280	LYS	C-O	6.62	1.31	1.24
2	2	39	PRO	C-O	6.58	1.31	1.23
3	3	57	ASN	N-CA	-6.57	1.37	1.46
1	1	134	ALA	CA-CB	-6.56	1.42	1.53
2	2	109	HIS	CE1-NE2	-6.54	1.26	1.32
2	2	9	TYR	N-CA	6.54	1.53	1.46
3	3	15	THR	C-O	6.54	1.32	1.24
1	1	85	LYS	C-O	6.54	1.31	1.23
3	3	156	GLY	C-O	-6.51	1.18	1.24
2	2	190	ASN	CA-CB	-6.50	1.44	1.53
2	2	52	LYS	CE-NZ	6.50	1.68	1.49
4	4	62	LYS	C-O	6.50	1.31	1.24
4	4	44	SER	CB-OG	6.49	1.55	1.42
2	2	262	GLN	CD-OE1	6.46	1.35	1.23
1	1	79	VAL	C-N	-6.44	1.24	1.33
3	3	57	ASN	C-N	-6.43	1.25	1.33
2	2	30	ASN	N-CA	6.43	1.54	1.46
2	2	217	ASN	C-O	6.43	1.32	1.24
4	4	62	LYS	N-CA	6.42	1.54	1.46
1	1	231	GLU	CA-CB	-6.41	1.44	1.53
3	3	205	VAL	N-CA	6.35	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	22	SER	C-N	-6.33	1.25	1.33
1	1	95	GLU	CB-CG	6.33	1.71	1.52
1	1	148	VAL	C-N	-6.33	1.25	1.33
2	2	8	GLY	N-CA	6.30	1.55	1.45
1	1	94	ARG	NE-CZ	6.29	1.40	1.33
4	4	63	GLY	N-CA	6.29	1.54	1.45
3	3	165	ILE	N-CA	6.28	1.54	1.46
1	1	160	PRO	CA-C	-6.27	1.44	1.52
3	3	5	THR	C-O	6.24	1.31	1.24
3	3	118	THR	CB-OG1	6.24	1.53	1.43
1	1	185	ARG	C-N	-6.24	1.25	1.33
1	1	184	SER	N-CA	6.21	1.53	1.45
2	2	259	ILE	C-O	6.20	1.31	1.24
3	3	182	THR	CA-CB	6.20	1.62	1.53
3	3	75	ARG	C-N	-6.18	1.24	1.33
3	3	164	THR	N-CA	6.18	1.53	1.46
2	2	121	CYS	C-O	6.16	1.31	1.23
1	1	177	PHE	C-N	-6.16	1.25	1.33
3	3	16	THR	CA-CB	6.14	1.63	1.53
1	1	184	SER	C-O	6.14	1.31	1.23
4	4	45	LEU	N-CA	6.14	1.55	1.46
2	2	168	ASP	CA-CB	6.14	1.60	1.53
1	1	172	SER	C-N	-6.13	1.25	1.33
1	1	251	GLU	N-CA	6.12	1.53	1.46
1	1	28	THR	N-CA	-6.10	1.37	1.45
2	2	162	VAL	N-CA	6.10	1.53	1.46
1	1	274	ASN	N-CA	6.10	1.54	1.46
3	3	178	PRO	CA-CB	-6.09	1.45	1.53
3	3	215	PRO	CA-CB	-6.09	1.44	1.53
4	4	33	LYS	CE-NZ	6.08	1.67	1.49
1	1	24	GLY	N-CA	6.07	1.53	1.44
3	3	110	SER	N-CA	6.05	1.52	1.45
2	2	19	GLY	C-N	-6.05	1.25	1.33
2	2	190	ASN	N-CA	6.04	1.54	1.46
2	2	257	LYS	N-CA	6.04	1.53	1.46
1	1	211	THR	N-CA	6.03	1.53	1.45
3	3	57	ASN	C-O	6.03	1.31	1.24
1	1	131	LEU	C-O	6.02	1.31	1.23
3	3	155	ILE	N-CA	5.99	1.53	1.46
3	3	36	ILE	N-CA	5.99	1.53	1.46
3	3	135	GLY	C-O	5.99	1.31	1.24
2	2	208	PRO	C-N	-5.98	1.28	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	222	MET	CG-SD	5.96	1.95	1.80
1	1	88	THR	CB-OG1	5.93	1.53	1.43
2	2	180	ASN	C-N	-5.92	1.25	1.33
2	2	17	THR	C-N	-5.90	1.25	1.33
3	3	27	ASN	C-N	-5.87	1.25	1.33
1	1	185	ARG	C-O	5.84	1.30	1.23
1	1	38	GLU	CB-CG	-5.83	1.34	1.52
3	3	213	ALA	C-O	5.83	1.30	1.23
3	3	219	LEU	C-N	-5.81	1.26	1.33
1	1	276	GLU	N-CA	5.80	1.54	1.45
2	2	55	LYS	N-CA	5.79	1.53	1.46
3	3	116	MET	N-CA	5.79	1.53	1.46
2	2	103	ARG	C-O	5.77	1.30	1.23
2	2	135	HIS	CG-CD2	-5.77	1.29	1.35
1	1	287	LYS	C-O	5.75	1.31	1.24
2	2	88	ASP	C-O	5.74	1.32	1.24
3	3	33	ARG	NE-CZ	5.73	1.39	1.33
2	2	176	THR	N-CA	5.73	1.53	1.45
3	3	38	GLY	CA-C	-5.73	1.43	1.51
2	2	152	ARG	NE-CZ	5.72	1.39	1.33
1	1	274	ASN	CA-C	5.71	1.60	1.52
1	1	187	SER	CB-OG	-5.71	1.30	1.42
1	1	187	SER	C-O	5.71	1.30	1.23
2	2	54	SER	CA-CB	-5.71	1.44	1.53
4	4	45	LEU	C-O	5.69	1.31	1.23
3	3	41	HIS	CE1-NE2	5.67	1.38	1.32
1	1	285	ASP	C-N	5.67	1.40	1.33
1	1	239	VAL	C-O	5.67	1.30	1.24
3	3	201	THR	C-O	5.66	1.30	1.23
2	2	103	ARG	N-CA	5.66	1.52	1.46
2	2	195	ASN	CA-CB	-5.66	1.44	1.54
3	3	35	HIS	C-N	-5.65	1.26	1.33
1	1	268	ARG	N-CA	5.65	1.52	1.45
3	3	158	GLN	C-O	5.65	1.30	1.24
1	1	25	PRO	CA-CB	-5.64	1.45	1.53
2	2	223	ILE	CA-C	-5.64	1.48	1.52
2	2	63	PHE	C-O	5.64	1.30	1.24
2	2	208	PRO	C-O	5.63	1.30	1.24
2	2	87	LYS	CB-CG	-5.63	1.35	1.52
1	1	63	SER	CB-OG	-5.62	1.30	1.42
1	1	267	GLY	C-O	5.62	1.32	1.24
3	3	82	GLY	N-CA	5.62	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	259	ILE	N-CA	5.62	1.53	1.46
1	1	180	VAL	C-O	5.62	1.29	1.24
2	2	75	SER	C-O	5.61	1.30	1.23
1	1	117	GLU	CD-OE2	5.59	1.35	1.25
3	3	172	GLN	CG-CD	-5.58	1.38	1.52
2	2	168	ASP	C-N	-5.58	1.26	1.33
1	1	137	PRO	C-O	5.58	1.31	1.24
2	2	194	ASN	C-O	5.58	1.30	1.23
1	1	254	ILE	CA-CB	5.57	1.61	1.54
3	3	82	GLY	C-N	-5.57	1.26	1.33
3	3	231	THR	CB-OG1	5.56	1.52	1.43
4	4	51	LYS	CE-NZ	5.55	1.66	1.49
3	3	75	ARG	N-CA	5.54	1.52	1.45
3	3	108	SER	CA-CB	-5.54	1.44	1.53
1	1	102	TRP	NE1-CE2	-5.54	1.31	1.37
3	3	140	GLN	C-N	-5.52	1.26	1.33
2	2	109	HIS	C-O	5.51	1.30	1.24
3	3	66	SER	N-CA	5.51	1.53	1.46
3	3	61	LYS	CE-NZ	5.50	1.65	1.49
2	2	153	GLY	C-N	-5.50	1.25	1.33
2	2	237	SER	C-O	5.49	1.30	1.23
2	2	237	SER	N-CA	5.49	1.52	1.46
2	2	151	GLU	CA-CB	-5.46	1.43	1.53
3	3	77	ASN	CG-OD1	5.45	1.33	1.23
1	1	25	PRO	C-N	-5.45	1.25	1.33
3	3	209	SER	N-CA	5.45	1.52	1.46
2	2	141	SER	N-CA	5.45	1.52	1.45
1	1	277	PRO	N-CA	5.44	1.53	1.47
3	3	40	VAL	C-O	5.44	1.30	1.24
3	3	37	PRO	CA-CB	-5.42	1.45	1.53
2	2	171	TYR	C-O	5.41	1.31	1.24
3	3	74	ASN	CA-CB	5.38	1.61	1.53
3	3	91	VAL	C-O	5.38	1.30	1.24
1	1	279	ILE	C-O	5.38	1.29	1.24
2	2	61	CYS	CA-C	-5.37	1.47	1.53
1	1	270	ASN	CA-C	5.36	1.59	1.52
1	1	122	VAL	C-O	5.35	1.29	1.24
2	2	103	ARG	CA-CB	-5.35	1.44	1.53
3	3	17	ASP	CG-OD2	5.35	1.35	1.25
2	2	72	THR	CB-OG1	5.34	1.52	1.43
3	3	209	SER	C-O	5.34	1.30	1.23
1	1	108	SER	N-CA	5.34	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	68	SER	CA-C	-5.34	1.45	1.52
2	2	211	SER	C-O	5.34	1.30	1.23
1	1	176	VAL	CA-C	5.33	1.58	1.52
1	1	127	GLU	CA-CB	-5.33	1.46	1.53
2	2	148	HIS	ND1-CE1	5.32	1.37	1.32
2	2	256	SER	C-N	-5.32	1.26	1.33
4	4	61	LEU	C-O	5.32	1.30	1.24
2	2	219	SER	N-CA	5.30	1.52	1.46
1	1	30	LYS	CE-NZ	5.30	1.65	1.49
2	2	14	GLN	CD-NE2	5.29	1.44	1.33
2	2	123	LEU	C-N	-5.28	1.26	1.33
3	3	228	ILE	C-O	5.28	1.30	1.24
1	1	33	ILE	C-O	5.27	1.30	1.24
3	3	64	VAL	C-N	-5.26	1.25	1.33
3	3	2	LEU	CA-CB	5.25	1.63	1.53
1	1	89	GLY	C-O	5.25	1.31	1.23
2	2	246	PRO	C-O	5.23	1.29	1.23
2	2	99	HIS	C-N	-5.21	1.26	1.34
3	3	164	THR	CA-CB	5.21	1.61	1.53
1	1	283	LYS	CE-NZ	5.21	1.65	1.49
2	2	202	PRO	C-O	5.20	1.29	1.23
1	1	54	ARG	C-O	5.20	1.30	1.23
1	1	161	LYS	C-N	-5.20	1.26	1.33
3	3	146	MET	C-O	5.19	1.30	1.24
3	3	77	ASN	C-N	-5.19	1.26	1.33
2	2	38	TRP	CA-C	-5.18	1.45	1.52
3	3	153	TRP	C-O	5.17	1.30	1.24
1	1	252	ALA	C-O	5.15	1.30	1.23
3	3	58	THR	CA-CB	5.15	1.62	1.53
3	3	133	PRO	CA-CB	-5.13	1.47	1.54
2	2	204	ILE	C-N	-5.13	1.26	1.33
3	3	112	ARG	CA-CB	-5.12	1.45	1.53
1	1	129	THR	N-CA	5.12	1.52	1.46
2	2	202	PRO	C-N	-5.10	1.26	1.33
3	3	136	ALA	C-O	5.10	1.30	1.23
3	3	205	VAL	C-O	5.10	1.29	1.23
1	1	166	TYR	N-CA	5.10	1.52	1.46
1	1	85	LYS	N-CA	5.08	1.51	1.46
2	2	128	PRO	CA-CB	-5.08	1.46	1.53
1	1	209	ALA	C-N	-5.08	1.26	1.33
2	2	186	HIS	C-O	5.06	1.29	1.23
3	3	65	ASN	CA-CB	5.06	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	248	CYS	C-N	-5.06	1.26	1.33
3	3	232	VAL	C-O	5.05	1.29	1.23
2	2	233	GLY	C-O	5.05	1.30	1.24
1	1	42	THR	C-O	5.05	1.29	1.23
3	3	34	ILE	C-O	5.04	1.30	1.24
3	3	216	ASP	N-CA	-5.04	1.40	1.46
3	3	109	GLY	C-N	5.02	1.40	1.33
2	2	109	HIS	N-CA	5.02	1.53	1.46
2	2	12	ARG	N-CA	-5.01	1.40	1.46
3	3	164	THR	CA-C	-5.01	1.46	1.52
1	1	117	GLU	N-CA	5.01	1.52	1.46
2	2	220	LEU	C-N	-5.01	1.26	1.33
1	1	246	ARG	CD-NE	-5.00	1.39	1.46
2	2	223	ILE	N-CA	5.00	1.49	1.45
3	3	163	MET	C-N	-5.00	1.26	1.33
3	3	84	ASN	N-CA	5.00	1.51	1.45

All (623) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	50	ASP	CA-CB-CG	27.73	140.33	112.60
1	1	285	ASP	CA-CB-CG	-22.21	90.39	112.60
3	3	215	PRO	CA-C-N	20.36	149.20	120.29
3	3	215	PRO	C-N-CA	20.36	149.20	120.29
2	2	87	LYS	CA-CB-CG	19.05	152.21	114.10
2	2	11	ASP	CA-CB-CG	-18.96	93.64	112.60
1	1	145	ASN	OD1-CG-ND2	17.24	139.84	122.60
2	2	193	THR	CA-C-N	16.42	150.15	122.07
2	2	193	THR	C-N-CA	16.42	150.15	122.07
2	2	190	ASN	CA-CB-CG	16.38	128.98	112.60
1	1	170	SER	CA-CB-OG	15.05	141.21	111.10
2	2	194	ASN	CA-CB-CG	-14.89	97.71	112.60
2	2	11	ASP	CA-C-N	14.78	140.54	120.44
2	2	11	ASP	C-N-CA	14.78	140.54	120.44
1	1	197	TYR	N-CA-CB	-14.13	87.34	110.23
3	3	57	ASN	CA-CB-CG	-13.74	98.86	112.60
1	1	38	GLU	CB-CG-CD	13.64	135.78	112.60
3	3	74	ASN	CA-CB-CG	-13.47	99.13	112.60
3	3	65	ASN	CA-CB-CG	-13.09	99.51	112.60
1	1	202	ASP	CA-CB-CG	12.96	125.56	112.60
3	3	27	ASN	CA-CB-CG	-12.94	99.66	112.60
1	1	145	ASN	CA-CB-CG	-12.89	99.71	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	194	ASN	N-CA-CB	-12.65	89.79	110.41
2	2	44	ASP	CA-CB-CG	12.64	125.24	112.60
1	1	94	ARG	CD-NE-CZ	-12.61	106.75	124.40
1	1	256	ARG	NE-CZ-NH2	12.57	130.51	119.20
2	2	67	ASP	CA-CB-CG	-12.45	100.15	112.60
1	1	197	TYR	CA-CB-CG	12.21	135.89	113.90
2	2	256	SER	CA-C-O	-12.21	105.38	119.79
4	4	30	ASN	CA-CB-CG	-12.10	100.50	112.60
3	3	172	GLN	CB-CG-CD	12.03	133.05	112.60
4	4	45	LEU	N-CA-CB	-11.89	94.13	111.84
4	4	41	ALA	CA-C-O	-11.31	105.46	119.38
3	3	74	ASN	OD1-CG-ND2	11.30	133.90	122.60
2	2	14	GLN	OE1-CD-NE2	11.18	133.78	122.60
3	3	29	GLU	CB-CG-CD	11.13	131.52	112.60
1	1	285	ASP	N-CA-CB	-11.05	95.26	110.29
2	2	151	GLU	CA-CB-CG	11.04	136.19	114.10
1	1	25	PRO	CA-C-O	-10.88	108.94	121.56
2	2	88	ASP	CA-CB-CG	-10.83	101.77	112.60
2	2	219	SER	CA-CB-OG	10.64	132.39	111.10
1	1	282	ARG	CD-NE-CZ	-10.62	109.53	124.40
2	2	97	PHE	CA-CB-CG	-10.60	103.20	113.80
4	4	48	ASP	CA-CB-CG	-10.60	102.00	112.60
1	1	141	ASN	CA-CB-CG	-10.45	102.15	112.60
3	3	57	ASN	N-CA-CB	-10.40	92.92	110.49
3	3	72	ASN	CA-CB-CG	-10.16	102.44	112.60
4	4	48	ASP	O-C-N	10.14	128.33	121.23
1	1	246	ARG	NE-CZ-NH1	10.01	131.51	121.50
1	1	63	SER	CB-CA-C	-10.00	94.20	110.79
1	1	54	ARG	CD-NE-CZ	-9.96	110.45	124.40
4	4	44	SER	CA-C-N	-9.87	107.96	122.07
4	4	44	SER	C-N-CA	-9.87	107.96	122.07
1	1	91	ASP	CA-CB-CG	-9.79	102.81	112.60
1	1	187	SER	CB-CA-C	9.78	129.24	109.38
1	1	275	THR	CA-C-O	-9.78	109.17	121.88
1	1	285	ASP	N-CA-C	9.75	122.91	110.33
1	1	28	THR	CB-CA-C	-9.73	92.89	111.48
1	1	22	SER	CA-C-O	-9.71	109.62	120.69
1	1	208	ASP	CA-CB-CG	-9.69	102.92	112.60
1	1	256	ARG	NE-CZ-NH1	-9.66	111.83	121.50
3	3	33	ARG	CA-C-O	-9.66	110.04	121.05
3	3	137	ARG	NE-CZ-NH1	-9.63	111.87	121.50
1	1	53	THR	CA-CB-OG1	-9.54	95.30	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	246	ARG	CD-NE-CZ	9.44	137.62	124.40
1	1	79	VAL	CA-C-O	-9.42	110.59	120.39
1	1	38	GLU	CA-CB-CG	9.41	132.93	114.10
3	3	86	PHE	CA-CB-CG	9.40	123.20	113.80
3	3	89	ASP	CA-CB-CG	-9.37	103.23	112.60
1	1	197	TYR	CB-CA-C	9.08	124.52	109.53
3	3	57	ASN	CB-CA-C	-9.07	92.36	110.42
2	2	255	ARG	NE-CZ-NH2	-9.06	111.04	119.20
1	1	95	GLU	CB-CG-CD	-9.03	97.25	112.60
1	1	268	ARG	CD-NE-CZ	-9.03	111.76	124.40
4	4	50	SER	CA-C-O	-9.02	109.90	120.10
3	3	196	ILE	CA-C-O	-8.98	111.20	120.27
2	2	195	ASN	CA-CB-CG	8.94	121.54	112.60
2	2	136	GLU	CB-CG-CD	-8.84	97.57	112.60
2	2	250	GLU	CA-CB-CG	8.81	131.72	114.10
4	4	68	ASN	CA-CB-CG	-8.76	103.84	112.60
1	1	270	ASN	CA-CB-CG	8.67	121.27	112.60
1	1	251	GLU	CA-CB-CG	8.64	131.38	114.10
1	1	154	PRO	O-C-N	8.58	131.59	121.46
2	2	139	ASN	CA-CB-CG	-8.48	104.12	112.60
2	2	255	ARG	CA-CB-CG	8.48	131.07	114.10
2	2	73	THR	CA-CB-OG1	-8.47	96.89	109.60
1	1	259	ARG	CA-CB-CG	-8.44	97.22	114.10
2	2	168	ASP	CA-C-O	-8.41	110.61	120.62
1	1	123	ARG	NE-CZ-NH1	8.40	129.90	121.50
1	1	165	ASP	CB-CA-C	-8.40	93.70	110.42
2	2	68	SER	N-CA-C	8.38	122.88	110.48
2	2	169	VAL	CA-C-O	-8.38	112.29	121.17
2	2	169	VAL	CB-CA-C	-8.37	101.25	111.97
4	4	41	ALA	N-CA-C	8.35	122.73	112.54
4	4	36	ALA	CA-C-N	-8.33	108.80	122.54
4	4	36	ALA	C-N-CA	-8.33	108.80	122.54
3	3	74	ASN	CA-C-O	-8.33	109.89	120.55
3	3	5	THR	CA-C-O	-8.29	111.11	120.32
1	1	122	VAL	N-CA-CB	-8.26	97.90	111.45
3	3	172	GLN	CG-CD-NE2	8.25	128.77	116.40
1	1	186	PHE	CA-C-O	-8.24	112.49	121.31
3	3	219	LEU	CA-C-O	-8.22	111.21	120.66
1	1	82	ILE	CA-C-O	-8.20	113.06	121.67
3	3	182	THR	CA-CB-CG2	8.16	124.37	110.50
3	3	57	ASN	OD1-CG-ND2	8.15	130.75	122.60
3	3	16	THR	N-CA-CB	-8.15	98.30	110.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	21	SER	CB-CA-C	-8.13	95.50	108.91
4	4	57	LYS	CA-C-O	-8.12	112.33	120.70
1	1	29	GLN	N-CA-C	-8.11	102.43	113.30
2	2	49	ASP	CA-CB-CG	8.09	120.69	112.60
3	3	78	GLU	N-CA-C	8.00	120.85	110.53
3	3	233	ALA	CA-C-O	-8.00	112.39	121.19
1	1	164	ASP	CA-C-N	8.00	136.82	121.54
1	1	164	ASP	C-N-CA	8.00	136.82	121.54
3	3	60	THR	CA-CB-OG1	-8.00	97.61	109.60
2	2	187	GLN	CA-CB-CG	7.99	130.09	114.10
1	1	288	SER	CA-C-O	-7.98	113.09	121.55
2	2	248	CYS	CA-C-O	-7.97	112.29	121.54
3	3	27	ASN	O-C-N	7.96	131.95	122.00
1	1	94	ARG	NE-CZ-NH2	-7.95	112.05	119.20
3	3	111	LEU	CA-C-N	-7.94	111.80	123.00
3	3	111	LEU	C-N-CA	-7.94	111.80	123.00
3	3	231	THR	CA-CB-OG1	-7.91	97.74	109.60
2	2	223	ILE	N-CA-CB	-7.91	101.52	112.27
1	1	176	VAL	CA-C-O	-7.90	111.42	120.67
1	1	37	ASN	CB-CG-ND2	7.87	128.20	116.40
2	2	216	ASN	CA-C-O	-7.85	112.09	120.80
1	1	274	ASN	O-C-N	7.83	133.01	122.59
2	2	95	ASN	CA-CB-CG	-7.83	104.77	112.60
1	1	123	ARG	CD-NE-CZ	7.81	135.33	124.40
3	3	216	ASP	N-CA-CB	-7.79	98.63	110.16
4	4	45	LEU	CA-C-O	7.76	130.54	121.54
1	1	282	ARG	CA-C-N	-7.74	111.50	122.41
1	1	282	ARG	C-N-CA	-7.74	111.50	122.41
2	2	109	HIS	CA-C-O	-7.73	110.83	120.57
4	4	37	SER	CB-CA-C	7.71	122.96	110.09
1	1	176	VAL	CB-CA-C	-7.70	99.14	110.62
3	3	62	ASP	CA-CB-CG	7.68	120.28	112.60
1	1	64	GLU	CB-CG-CD	7.67	125.64	112.60
2	2	190	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	1	17	THR	CA-C-N	-7.65	110.26	122.50
1	1	17	THR	C-N-CA	-7.65	110.26	122.50
2	2	240	ILE	CA-C-O	-7.63	112.37	120.39
3	3	137	ARG	CD-NE-CZ	-7.62	113.74	124.40
1	1	61	ASN	CA-CB-CG	-7.61	104.99	112.60
3	3	59	HIS	CA-C-O	7.60	130.47	121.88
3	3	184	ALA	N-CA-C	7.58	122.72	113.17
3	3	142	ARG	CA-CB-CG	7.58	129.25	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	87	LYS	CB-CG-CD	7.56	128.70	111.30
1	1	277	PRO	N-CD-CG	-7.54	91.88	103.20
3	3	27	ASN	N-CA-C	7.52	124.01	113.56
3	3	79	GLN	OE1-CD-NE2	-7.50	115.10	122.60
1	1	197	TYR	CA-C-O	-7.44	112.37	120.92
1	1	173	ASN	N-CA-CB	-7.43	97.08	110.23
4	4	30	ASN	CA-C-O	-7.43	112.22	120.69
1	1	288	SER	N-CA-C	7.40	120.42	110.35
2	2	98	PHE	CA-C-O	-7.37	110.97	119.60
2	2	140	VAL	CA-C-O	-7.36	113.36	121.23
4	4	45	LEU	CB-CA-C	7.35	122.53	111.80
2	2	107	THR	CA-C-O	-7.34	112.24	120.32
3	3	129	LEU	CA-C-O	-7.34	112.93	120.71
2	2	39	PRO	CA-C-O	-7.31	113.01	121.34
3	3	27	ASN	CB-CA-C	-7.30	97.26	111.06
3	3	118	THR	CA-CB-OG1	-7.30	98.65	109.60
2	2	187	GLN	CB-CA-C	7.26	125.39	109.94
2	2	77	GLY	CA-C-O	-7.23	114.82	122.05
4	4	30	ASN	OD1-CG-ND2	7.23	129.83	122.60
3	3	46	ILE	CA-C-O	-7.23	112.45	120.25
3	3	61	LYS	CA-C-O	-7.23	112.68	121.06
1	1	187	SER	N-CA-CB	-7.22	98.20	111.13
2	2	169	VAL	N-CA-C	7.22	117.36	110.42
3	3	124	SER	CA-C-O	-7.22	113.53	121.33
1	1	26	LYS	CA-CB-CG	7.21	128.53	114.10
3	3	19	ARG	NE-CZ-NH2	7.21	125.69	119.20
2	2	180	ASN	CA-CB-CG	-7.21	105.39	112.60
2	2	103	ARG	CD-NE-CZ	-7.20	114.31	124.40
1	1	275	THR	CA-CB-OG1	-7.18	98.83	109.60
2	2	68	SER	O-C-N	-7.18	114.84	122.96
2	2	52	LYS	CA-C-O	-7.17	113.30	121.19
2	2	146	PHE	CA-CB-CG	-7.14	106.66	113.80
2	2	168	ASP	N-CA-CB	-7.14	97.90	109.60
1	1	59	HIS	CA-C-O	-7.12	111.98	120.81
1	1	284	GLY	CA-C-N	7.11	133.60	120.95
1	1	284	GLY	C-N-CA	7.11	133.60	120.95
4	4	47	MET	CA-CB-CG	-7.08	99.95	114.10
2	2	134	SER	CA-C-O	-7.06	113.01	121.05
1	1	285	ASP	CB-CA-C	-7.05	93.81	110.02
3	3	94	THR	O-C-N	7.04	131.65	122.42
2	2	259	ILE	CB-CG1-CD1	-7.04	99.03	113.80
3	3	13	PHE	CA-CB-CG	7.03	120.83	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	85	LYS	CA-C-O	-7.00	113.97	121.38
3	3	164	THR	N-CA-CB	-6.98	99.61	110.57
1	1	28	THR	OG1-CB-CG2	6.98	123.25	109.30
3	3	35	HIS	CA-C-O	-6.97	112.90	120.92
1	1	43	MET	CA-C-O	6.94	126.28	119.75
1	1	285	ASP	CB-CG-OD2	-6.93	102.46	118.40
3	3	109	GLY	CA-C-N	-6.93	110.86	122.64
3	3	109	GLY	C-N-CA	-6.93	110.86	122.64
3	3	121	ALA	CA-C-O	-6.93	112.27	120.10
3	3	66	SER	CB-CA-C	6.91	121.63	110.09
3	3	77	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	1	270	ASN	O-C-N	6.90	131.39	122.97
2	2	57	ASP	CB-CA-C	-6.88	108.65	116.63
1	1	138	ASP	CA-CB-CG	6.88	119.48	112.60
2	2	9	TYR	CB-CA-C	6.88	121.41	109.65
1	1	35	THR	CA-CB-OG1	-6.87	99.29	109.60
3	3	231	THR	CA-C-O	-6.85	110.49	119.06
4	4	44	SER	O-C-N	6.85	131.70	122.59
2	2	186	HIS	CA-CB-CG	-6.84	106.96	113.80
3	3	65	ASN	OD1-CG-ND2	6.84	129.44	122.60
2	2	219	SER	CB-CA-C	6.84	121.69	109.38
1	1	183	THR	CA-CB-OG1	-6.82	99.36	109.60
3	3	146	MET	CG-SD-CE	6.82	115.90	100.90
2	2	193	THR	O-C-N	-6.81	115.12	121.79
2	2	14	GLN	CB-CG-CD	-6.81	101.03	112.60
1	1	89	GLY	CA-C-N	-6.81	114.35	122.93
1	1	89	GLY	C-N-CA	-6.81	114.35	122.93
1	1	42	THR	CA-CB-CG2	6.78	122.03	110.50
3	3	202	THR	CA-C-O	6.78	128.49	121.23
1	1	49	ASP	N-CA-C	-6.76	105.32	113.97
3	3	151	VAL	CA-C-O	-6.74	113.57	120.25
1	1	110	VAL	N-CA-C	6.74	119.51	111.09
3	3	187	LEU	CA-C-O	-6.74	113.10	120.24
1	1	35	THR	N-CA-CB	-6.73	99.11	110.49
3	3	143	ARG	N-CA-C	-6.73	104.02	111.36
2	2	124	VAL	CA-C-O	-6.73	112.78	120.66
1	1	62	GLY	CA-C-N	6.73	129.29	120.28
1	1	62	GLY	C-N-CA	6.73	129.29	120.28
2	2	170	LEU	CD1-CG-CD2	-6.73	96.00	110.80
3	3	42	ASN	CA-C-O	-6.72	112.93	120.66
4	4	58	ASP	O-C-N	6.72	130.88	123.22
2	2	249	THR	CA-CB-OG1	-6.71	99.53	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	206	HIS	CA-C-O	-6.71	114.10	121.28
2	2	224	PRO	CA-C-O	-6.71	114.05	121.23
1	1	288	SER	CB-CA-C	-6.67	97.68	109.62
2	2	255	ARG	CB-CG-CD	6.66	126.61	111.30
1	1	282	ARG	NE-CZ-NH2	-6.65	113.22	119.20
3	3	227	THR	CA-CB-OG1	-6.65	99.63	109.60
1	1	95	GLU	CA-CB-CG	-6.64	100.82	114.10
1	1	90	ILE	CA-C-N	-6.62	109.74	122.06
1	1	90	ILE	C-N-CA	-6.62	109.74	122.06
1	1	259	ARG	CA-C-O	-6.62	113.20	120.81
2	2	198	THR	CA-C-O	-6.62	112.97	120.32
1	1	60	PHE	CA-C-O	-6.60	113.63	120.89
3	3	187	LEU	N-CA-CB	-6.59	100.42	110.77
1	1	147	VAL	CA-C-O	-6.59	113.48	120.53
3	3	134	PRO	CA-C-N	-6.59	116.32	123.30
3	3	134	PRO	C-N-CA	-6.59	116.32	123.30
1	1	25	PRO	CA-C-N	6.58	133.40	122.73
1	1	25	PRO	C-N-CA	6.58	133.40	122.73
3	3	202	THR	CA-CB-OG1	-6.58	99.73	109.60
2	2	145	THR	CA-CB-OG1	-6.57	99.75	109.60
1	1	118	LEU	CA-C-N	6.56	133.11	122.81
1	1	118	LEU	C-N-CA	6.56	133.11	122.81
2	2	161	GLU	CA-C-N	-6.54	114.52	122.90
2	2	161	GLU	C-N-CA	-6.54	114.52	122.90
2	2	38	TRP	N-CA-CB	-6.53	99.34	110.11
2	2	11	ASP	OD1-CG-OD2	6.52	138.55	122.90
2	2	226	ALA	N-CA-C	-6.52	99.14	109.04
4	4	48	ASP	OD1-CG-OD2	6.52	138.54	122.90
3	3	19	ARG	CA-CB-CG	6.51	127.13	114.10
2	2	18	LEU	CB-CA-C	6.51	119.84	110.79
2	2	12	ARG	N-CA-C	6.51	118.17	111.14
2	2	148	HIS	CA-CB-CG	6.50	120.30	113.80
2	2	163	GLY	O-C-N	6.50	130.17	122.50
1	1	97	LYS	CB-CA-C	-6.50	102.50	111.73
1	1	277	PRO	CB-CA-C	6.48	119.87	111.64
3	3	74	ASN	N-CA-C	6.48	120.51	112.47
1	1	122	VAL	CB-CA-C	6.47	121.90	110.71
4	4	36	ALA	N-CA-C	-6.47	105.25	113.01
3	3	205	VAL	CB-CA-C	6.46	120.20	110.90
1	1	256	ARG	CD-NE-CZ	-6.45	115.37	124.40
4	4	39	SER	O-C-N	6.45	130.80	122.23
2	2	142	VAL	CA-C-O	-6.44	113.12	120.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	182	THR	CA-CB-OG1	-6.44	99.94	109.60
3	3	65	ASN	N-CA-CB	-6.44	100.94	110.53
3	3	57	ASN	N-CA-C	6.43	124.50	110.80
2	2	247	MET	CB-CA-C	6.43	122.41	109.68
2	2	193	THR	CA-C-O	6.43	126.47	119.40
2	2	194	ASN	N-CA-C	6.43	120.54	110.32
3	3	164	THR	CA-CB-OG1	-6.43	99.96	109.60
2	2	111	GLN	OE1-CD-NE2	-6.42	116.18	122.60
2	2	69	LYS	CA-CB-CG	6.41	126.91	114.10
3	3	216	ASP	CA-C-N	6.40	129.80	120.71
3	3	216	ASP	C-N-CA	6.40	129.80	120.71
1	1	205	SER	O-C-N	6.39	131.22	122.46
3	3	204	GLN	O-C-N	6.39	130.22	123.06
3	3	172	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	1	50	SER	CA-C-O	-6.38	110.45	118.43
2	2	203	TYR	CA-C-O	-6.38	113.18	120.58
3	3	99	GLU	CB-CG-CD	6.38	123.44	112.60
3	3	226	GLN	CB-CG-CD	-6.38	101.76	112.60
4	4	44	SER	CA-CB-OG	-6.37	98.36	111.10
1	1	239	VAL	CB-CA-C	6.36	120.04	110.63
2	2	223	ILE	CA-C-O	-6.35	116.64	119.94
3	3	41	HIS	CA-C-O	-6.34	112.38	119.67
1	1	144	SER	N-CA-CB	-6.33	100.79	110.42
2	2	235	THR	CB-CA-C	-6.33	99.52	109.52
1	1	250	VAL	N-CA-C	6.33	117.82	109.21
2	2	241	THR	CA-C-O	-6.32	114.01	120.71
3	3	181	TYR	O-C-N	6.32	128.82	122.12
1	1	137	PRO	CA-C-N	-6.31	113.05	122.39
1	1	137	PRO	C-N-CA	-6.31	113.05	122.39
3	3	80	VAL	CA-C-O	-6.31	113.96	120.71
1	1	265	SER	O-C-N	-6.31	115.95	123.27
3	3	202	THR	N-CA-C	6.29	118.42	108.79
2	2	145	THR	CA-C-O	-6.29	113.84	120.63
1	1	288	SER	N-CA-CB	-6.28	100.80	110.04
3	3	216	ASP	CB-CG-OD1	6.28	132.84	118.40
3	3	63	GLU	CB-CG-CD	-6.28	101.93	112.60
3	3	193	THR	CA-C-O	-6.27	111.54	120.51
3	3	83	THR	CA-CB-OG1	-6.27	100.19	109.60
1	1	117	GLU	CG-CD-OE1	6.26	132.81	118.40
2	2	103	ARG	CA-CB-CG	6.26	126.62	114.10
2	2	143	LYS	O-C-N	6.26	130.51	122.81
1	1	70	PHE	CA-CB-CG	6.23	120.03	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	183	SER	N-CA-CB	-6.23	100.82	110.29
4	4	65	PRO	CB-CA-C	-6.23	103.42	111.46
1	1	206	HIS	O-C-N	6.23	129.52	123.29
1	1	282	ARG	NH1-CZ-NH2	6.22	127.38	119.30
1	1	198	ASN	CA-CB-CG	6.21	118.81	112.60
3	3	161	ILE	CA-C-O	-6.20	113.88	120.39
1	1	31	VAL	N-CA-CB	-6.20	102.53	111.21
3	3	196	ILE	N-CA-CB	-6.19	103.41	111.82
1	1	274	ASN	N-CA-CB	6.17	120.92	110.49
1	1	48	SER	CA-C-O	-6.17	108.19	119.36
2	2	28	ALA	CA-C-O	-6.17	114.85	121.94
3	3	27	ASN	N-CA-CB	-6.17	103.09	113.15
3	3	6	THR	CB-CA-C	6.17	120.05	109.51
3	3	132	THR	CA-C-O	-6.16	113.92	119.59
1	1	260	ALA	CA-C-O	-6.16	111.51	120.13
2	2	11	ASP	O-C-N	6.16	130.39	122.39
2	2	194	ASN	OD1-CG-ND2	6.15	128.75	122.60
2	2	111	GLN	CB-CG-CD	6.13	123.01	112.60
2	2	238	LEU	N-CA-CB	-6.13	98.78	110.42
1	1	236	LYS	CA-C-O	-6.12	114.25	121.16
2	2	179	GLY	CA-C-O	-6.12	114.21	120.45
3	3	163	MET	CA-CB-CG	-6.11	101.87	114.10
1	1	202	ASP	CB-CA-C	6.11	121.11	112.07
1	1	52	GLU	CA-C-O	-6.10	113.60	120.43
3	3	137	ARG	NE-CZ-NH2	6.09	124.68	119.20
3	3	170	GLY	CA-C-N	6.09	128.66	120.50
3	3	170	GLY	C-N-CA	6.09	128.66	120.50
1	1	252	ALA	CA-C-O	-6.08	113.67	120.66
3	3	193	THR	CA-CB-OG1	-6.08	100.48	109.60
2	2	12	ARG	CD-NE-CZ	-6.08	115.89	124.40
1	1	141	ASN	O-C-N	6.07	129.74	122.27
4	4	43	GLN	OE1-CD-NE2	-6.07	116.53	122.60
2	2	241	THR	CA-CB-OG1	-6.05	100.53	109.60
3	3	8	PRO	CA-C-O	-6.04	114.53	121.36
1	1	68	GLU	CG-CD-OE1	6.04	132.29	118.40
2	2	195	ASN	OD1-CG-ND2	-6.03	116.57	122.60
3	3	36	ILE	CA-C-O	-6.02	111.88	119.95
1	1	77	VAL	CA-C-O	-6.01	113.25	118.96
1	1	133	THR	CA-CB-OG1	-6.00	100.59	109.60
1	1	136	GLN	CG-CD-NE2	-6.00	107.39	116.40
2	2	86	LEU	CA-C-N	6.00	130.30	120.63
2	2	86	LEU	C-N-CA	6.00	130.30	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	47	ILE	CB-CG1-CD1	-6.00	101.19	113.80
1	1	41	ALA	CA-C-O	-6.00	114.64	121.72
2	2	169	VAL	N-CA-CB	5.99	117.56	110.55
3	3	121	ALA	CB-CA-C	-5.99	99.55	110.63
1	1	101	ASP	CB-CA-C	-5.98	97.55	109.33
3	3	41	HIS	N-CA-CB	5.98	119.08	110.40
2	2	14	GLN	CA-CB-CG	-5.98	102.15	114.10
3	3	137	ARG	CA-C-O	-5.97	115.07	121.94
3	3	194	SER	N-CA-CB	-5.97	100.40	110.49
3	3	158	GLN	CA-C-O	5.95	127.70	120.62
2	2	105	GLY	N-CA-C	-5.94	102.31	112.64
2	2	136	GLU	CG-CD-OE2	-5.94	104.75	118.40
3	3	77	ASN	O-C-N	-5.93	114.71	122.59
3	3	207	LEU	CA-C-O	-5.91	114.23	120.80
3	3	160	THR	CA-CB-OG1	-5.91	100.74	109.60
1	1	22	SER	N-CA-CB	-5.90	100.80	109.95
1	1	265	SER	N-CA-CB	-5.90	100.55	111.53
1	1	55	THR	CA-CB-OG1	-5.90	100.75	109.60
2	2	161	GLU	CA-CB-CG	5.90	125.90	114.10
3	3	1	GLY	O-C-N	-5.90	113.57	123.00
3	3	57	ASN	O-C-N	-5.89	114.75	122.59
1	1	259	ARG	CB-CA-C	-5.89	100.47	109.89
2	2	41	TYR	N-CA-CB	5.89	118.45	110.38
1	1	185	ARG	NH1-CZ-NH2	-5.88	111.66	119.30
3	3	55	MET	CA-CB-CG	-5.86	102.39	114.10
2	2	226	ALA	O-C-N	5.85	127.86	121.36
3	3	92	PHE	CA-CB-CG	-5.85	107.95	113.80
1	1	270	ASN	CB-CA-C	-5.84	100.29	109.70
1	1	280	LYS	CB-CA-C	-5.84	101.75	110.16
3	3	131	TYR	CA-C-O	-5.84	114.06	120.43
2	2	88	ASP	CA-C-O	-5.83	112.60	119.48
1	1	159	ASN	CA-C-N	5.82	125.73	119.85
1	1	159	ASN	C-N-CA	5.82	125.73	119.85
1	1	242	ARG	CD-NE-CZ	-5.82	116.25	124.40
1	1	267	GLY	CA-C-N	-5.82	113.04	122.81
1	1	267	GLY	C-N-CA	-5.82	113.04	122.81
2	2	198	THR	O-C-N	5.82	130.11	123.31
3	3	197	LEU	CB-CA-C	5.81	117.23	108.86
2	2	105	GLY	CA-C-O	-5.80	112.99	122.56
3	3	33	ARG	CB-CG-CD	-5.80	97.96	111.30
3	3	93	LYS	N-CA-C	5.80	118.38	111.71
2	2	54	SER	CA-C-N	-5.80	115.03	122.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	54	SER	C-N-CA	-5.80	115.03	122.98
3	3	59	HIS	CA-CB-CG	-5.80	108.00	113.80
1	1	175	SER	CB-CA-C	5.80	120.30	109.86
2	2	255	ARG	NE-CZ-NH1	5.79	127.29	121.50
4	4	65	PRO	CA-C-O	-5.79	114.74	121.34
1	1	145	ASN	CB-CG-ND2	-5.78	107.73	116.40
2	2	235	THR	OG1-CB-CG2	5.76	120.83	109.30
1	1	68	GLU	CG-CD-OE2	-5.74	105.20	118.40
2	2	189	ILE	CA-C-O	-5.73	113.24	120.69
2	2	210	ASP	N-CA-CB	-5.73	100.56	110.87
1	1	182	ASP	CA-C-N	5.72	131.55	122.62
1	1	182	ASP	C-N-CA	5.72	131.55	122.62
1	1	94	ARG	CG-CD-NE	-5.71	99.43	112.00
2	2	86	LEU	CA-C-O	-5.71	112.88	119.56
3	3	38	GLY	N-CA-C	5.69	123.74	115.32
3	3	66	SER	N-CA-C	-5.69	106.00	113.17
1	1	83	GLN	CB-CG-CD	-5.68	102.94	112.60
3	3	45	GLU	CG-CD-OE1	5.68	131.47	118.40
3	3	137	ARG	O-C-N	5.68	129.64	122.65
1	1	129	THR	CA-C-O	-5.68	114.57	120.70
3	3	112	ARG	CA-CB-CG	5.68	125.45	114.10
1	1	139	SER	CA-CB-OG	-5.67	99.77	111.10
2	2	190	ASN	CB-CA-C	5.66	120.01	110.79
3	3	161	ILE	CA-CB-CG1	-5.66	100.79	110.40
2	2	199	ILE	CA-C-O	-5.65	114.37	120.36
1	1	28	THR	N-CA-C	5.64	118.08	109.95
1	1	232	HIS	CA-CB-CG	-5.64	108.16	113.80
1	1	94	ARG	NH1-CZ-NH2	5.63	126.62	119.30
3	3	235	THR	CA-CB-OG1	-5.61	101.18	109.60
1	1	208	ASP	CA-C-O	-5.61	114.66	121.28
3	3	42	ASN	CB-CG-ND2	5.60	124.80	116.40
2	2	99	HIS	CA-CB-CG	-5.58	108.22	113.80
1	1	241	ILE	N-CA-CB	-5.58	104.29	110.99
1	1	27	HIS	CA-CB-CG	5.58	119.38	113.80
2	2	217	ASN	CB-CA-C	5.58	118.92	109.55
2	2	251	PHE	CA-C-O	-5.58	114.81	121.11
4	4	58	ASP	CA-C-N	5.57	129.02	121.05
4	4	58	ASP	C-N-CA	5.57	129.02	121.05
2	2	262	GLN	OE1-CD-NE2	-5.57	117.03	122.60
2	2	106	TYR	CA-C-O	-5.56	115.33	121.33
2	2	215	HIS	CA-C-O	-5.55	112.50	120.11
1	1	273	LYS	CG-CD-CE	-5.55	98.54	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	166	PRO	CB-CA-C	5.55	118.62	111.46
1	1	173	ASN	CA-CB-CG	5.54	118.14	112.60
2	2	9	TYR	CA-CB-CG	-5.54	103.93	113.90
3	3	190	TRP	CA-C-O	-5.54	115.14	121.40
2	2	94	GLN	CG-CD-NE2	-5.54	108.10	116.40
2	2	68	SER	N-CA-CB	-5.53	101.88	110.29
2	2	168	ASP	CA-C-N	5.53	127.52	120.56
2	2	168	ASP	C-N-CA	5.53	127.52	120.56
3	3	107	TRP	CA-C-O	-5.53	115.16	121.40
1	1	198	ASN	CA-C-O	-5.52	114.09	120.49
2	2	99	HIS	CA-C-N	5.51	128.22	120.28
2	2	99	HIS	C-N-CA	5.51	128.22	120.28
2	2	188	PHE	CA-C-O	-5.51	114.93	121.66
1	1	64	GLU	CA-CB-CG	5.51	125.12	114.10
1	1	235	HIS	CA-CB-CG	-5.51	108.29	113.80
3	3	57	ASN	CA-C-N	5.51	132.08	121.18
3	3	57	ASN	C-N-CA	5.51	132.08	121.18
3	3	76	GLN	CA-C-O	-5.50	115.18	121.68
2	2	192	ARG	CA-C-O	-5.49	111.92	119.05
3	3	140	GLN	CA-CB-CG	-5.49	103.12	114.10
1	1	186	PHE	O-C-N	5.48	128.86	122.99
1	1	63	SER	O-C-N	5.48	127.92	122.12
3	3	63	GLU	CG-CD-OE2	-5.47	105.83	118.40
2	2	123	LEU	CA-C-O	-5.46	114.47	120.43
2	2	43	PRO	N-CD-CG	-5.46	95.01	103.20
2	2	167	LYS	CA-C-O	5.46	126.11	119.78
1	1	144	SER	CA-C-N	-5.45	115.37	123.11
1	1	144	SER	C-N-CA	-5.45	115.37	123.11
2	2	26	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	2	92	PHE	N-CA-C	-5.45	105.03	110.97
2	2	258	SER	O-C-N	5.45	129.51	122.81
2	2	38	TRP	CB-CA-C	5.45	116.25	108.68
3	3	164	THR	CB-CA-C	5.45	119.14	109.72
2	2	187	GLN	CA-C-O	-5.44	114.89	120.99
3	3	34	ILE	CA-C-O	-5.44	113.97	120.78
3	3	168	THR	CA-CB-OG1	-5.44	101.43	109.60
1	1	21	ILE	CA-CB-CG1	-5.44	101.15	110.40
3	3	84	ASN	OD1-CG-ND2	5.44	128.04	122.60
2	2	53	THR	CA-C-O	-5.43	115.54	121.89
1	1	50	SER	CB-CA-C	5.42	117.48	109.29
4	4	50	SER	CA-CB-OG	-5.42	100.26	111.10
2	2	13	VAL	CA-C-O	-5.42	114.56	120.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	232	THR	CA-CB-OG1	-5.42	101.48	109.60
2	2	63	PHE	CA-CB-CG	5.41	119.21	113.80
3	3	78	GLU	CA-CB-CG	5.40	124.91	114.10
1	1	166	TYR	N-CA-C	-5.40	105.55	111.82
2	2	219	SER	N-CA-C	-5.40	100.89	109.59
3	3	90	GLY	CA-C-O	-5.40	114.87	121.68
2	2	129	GLU	CB-CA-C	-5.40	104.22	111.89
2	2	221	MET	CA-C-O	-5.38	114.34	120.32
2	2	81	LYS	CB-CG-CD	5.37	123.66	111.30
3	3	112	ARG	CB-CA-C	5.37	119.08	110.16
1	1	231	GLU	N-CA-C	-5.37	102.94	110.35
3	3	38	GLY	O-C-N	-5.36	116.00	122.38
3	3	116	MET	CB-CG-SD	-5.36	96.63	112.70
1	1	92	ASN	O-C-N	5.36	129.49	123.28
1	1	117	GLU	CG-CD-OE2	-5.35	106.09	118.40
1	1	288	SER	CA-CB-OG	-5.35	100.41	111.10
2	2	120	GLY	CA-C-O	-5.35	114.41	122.54
3	3	195	LEU	CA-C-O	-5.34	114.97	121.05
2	2	210	ASP	CA-CB-CG	-5.33	107.27	112.60
1	1	286	ILE	O-C-N	5.33	127.82	121.80
2	2	177	LEU	N-CA-CB	-5.33	101.60	110.23
1	1	282	ARG	O-C-N	5.32	129.35	122.81
3	3	226	GLN	N-CA-C	-5.32	106.74	113.18
2	2	102	GLY	CA-C-O	-5.31	115.46	121.68
3	3	221	LEU	O-C-N	5.31	129.66	122.59
4	4	58	ASP	N-CA-CB	5.31	119.08	110.42
1	1	26	LYS	CG-CD-CE	-5.30	99.10	111.30
2	2	12	ARG	CB-CG-CD	-5.30	99.11	111.30
3	3	161	ILE	N-CA-CB	5.30	118.72	111.41
3	3	222	MET	CB-CG-SD	-5.30	96.80	112.70
2	2	72	THR	CA-CB-OG1	-5.28	101.68	109.60
3	3	143	ARG	O-C-N	5.28	128.17	122.15
2	2	262	GLN	CG-CD-NE2	5.28	124.32	116.40
3	3	16	THR	OG1-CB-CG2	5.28	119.85	109.30
3	3	86	PHE	CB-CA-C	5.28	120.49	111.68
3	3	204	GLN	CA-C-O	-5.28	115.03	121.36
3	3	192	GLN	N-CA-C	-5.27	105.13	112.45
1	1	60	PHE	N-CA-CB	-5.27	102.17	111.39
3	3	56	ASN	CA-C-N	5.27	131.60	121.54
3	3	56	ASN	C-N-CA	5.27	131.60	121.54
2	2	76	LYS	CA-C-O	-5.27	113.46	119.41
2	2	195	ASN	N-CA-C	-5.26	106.64	114.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	229	VAL	N-CA-C	-5.26	104.94	112.35
2	2	122	LEU	CA-C-O	-5.26	115.08	121.28
2	2	257	LYS	N-CA-CB	5.25	119.36	110.49
4	4	53	THR	CA-CB-OG1	-5.25	101.73	109.60
3	3	77	ASN	CA-CB-CG	-5.25	107.35	112.60
2	2	168	ASP	OD1-CG-OD2	5.24	135.49	122.90
3	3	94	THR	CA-C-O	-5.24	113.18	119.15
1	1	201	TYR	CA-C-N	-5.23	114.79	122.06
1	1	201	TYR	C-N-CA	-5.23	114.79	122.06
3	3	208	LEU	CA-C-O	-5.23	114.99	120.80
1	1	279	ILE	CA-C-N	5.23	128.76	121.02
1	1	279	ILE	C-N-CA	5.23	128.76	121.02
2	2	20	ASN	CA-CB-CG	5.23	117.83	112.60
3	3	28	TYR	N-CA-CB	-5.23	102.29	109.97
1	1	127	GLU	CA-C-O	-5.22	114.58	120.32
3	3	144	GLU	CA-CB-CG	5.22	124.54	114.10
1	1	136	GLN	OE1-CD-NE2	5.22	127.82	122.60
2	2	75	SER	N-CA-CB	-5.22	101.95	109.83
1	1	155	PRO	O-C-N	5.21	128.66	122.98
1	1	63	SER	N-CA-C	5.21	116.96	111.28
3	3	158	GLN	CG-CD-OE1	5.21	131.22	120.80
2	2	243	THR	CA-C-O	-5.21	114.70	120.38
2	2	127	ILE	CA-C-O	-5.21	114.21	119.89
1	1	187	SER	O-C-N	-5.20	117.03	123.33
2	2	214	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	1	282	ARG	CB-CA-C	-5.20	100.31	109.62
3	3	67	TYR	N-CA-C	-5.20	106.78	113.23
1	1	259	ARG	N-CA-CB	5.20	117.59	109.85
1	1	268	ARG	CB-CA-C	5.20	119.74	109.66
2	2	8	GLY	CA-C-N	-5.19	113.50	120.87
2	2	8	GLY	C-N-CA	-5.19	113.50	120.87
3	3	138	GLY	N-CA-C	-5.19	101.75	112.34
2	2	18	LEU	N-CA-CB	-5.18	102.78	110.71
2	2	38	TRP	CA-CB-CG	-5.18	103.77	113.60
2	2	213	THR	CA-CB-OG1	-5.17	101.84	109.60
1	1	257	ALA	N-CA-CB	-5.17	101.86	109.98
2	2	259	ILE	CA-C-O	-5.17	115.01	120.39
3	3	233	ALA	O-C-N	5.17	129.23	122.87
3	3	215	PRO	CB-CA-C	5.17	119.24	111.44
2	2	127	ILE	O-C-N	5.16	125.67	120.92
3	3	186	PHE	O-C-N	5.16	129.85	123.15
1	1	149	GLN	CB-CA-C	-5.15	102.84	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	45	GLU	CG-CD-OE2	-5.15	106.55	118.40
1	1	23	SER	CA-C-O	-5.15	115.09	121.06
1	1	145	ASN	O-C-N	5.14	129.61	123.13
2	2	181	LEU	N-CA-C	-5.14	106.27	112.54
2	2	165	PRO	CA-C-O	-5.14	115.37	122.15
3	3	186	PHE	CA-CB-CG	-5.14	108.66	113.80
3	3	231	THR	CA-C-N	-5.14	115.39	122.69
3	3	231	THR	C-N-CA	-5.14	115.39	122.69
2	2	152	ARG	CD-NE-CZ	-5.13	117.22	124.40
2	2	143	LYS	CA-C-N	5.12	131.32	121.54
2	2	143	LYS	C-N-CA	5.12	131.32	121.54
1	1	204	TYR	CA-C-O	-5.12	115.64	121.58
3	3	125	ALA	CA-C-O	-5.11	115.48	121.10
1	1	170	SER	CA-C-O	-5.11	115.80	122.14
2	2	259	ILE	CA-C-N	-5.11	112.68	122.13
2	2	259	ILE	C-N-CA	-5.11	112.68	122.13
3	3	109	GLY	N-CA-C	5.11	117.50	111.63
2	2	119	SER	O-C-N	5.10	129.34	123.17
1	1	27	HIS	CA-C-O	-5.10	113.09	122.62
1	1	285	ASP	CA-C-N	-5.09	111.95	120.30
1	1	285	ASP	C-N-CA	-5.09	111.95	120.30
2	2	32	VAL	O-C-N	5.09	128.33	123.14
3	3	82	GLY	N-CA-C	-5.09	103.03	110.87
3	3	32	PRO	CA-C-O	-5.08	115.67	121.56
2	2	126	VAL	CA-C-O	-5.08	115.09	120.53
2	2	65	THR	CA-CB-OG1	-5.08	101.98	109.60
3	3	1	GLY	N-CA-C	5.07	128.01	113.30
1	1	40	GLY	N-CA-C	-5.07	108.12	115.27
2	2	119	SER	CA-C-O	-5.07	115.67	121.40
2	2	215	HIS	CA-CB-CG	5.07	118.87	113.80
2	2	235	THR	CA-C-O	5.07	125.44	120.17
2	2	25	THR	CA-C-O	5.07	126.49	120.66
3	3	75	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	1	165	ASP	CB-CG-OD1	5.06	130.04	118.40
3	3	217	PHE	N-CA-C	5.06	117.57	110.23
2	2	168	ASP	CB-CG-OD2	-5.06	106.76	118.40
1	1	133	THR	CA-C-O	-5.06	115.39	121.11
1	1	83	GLN	OE1-CD-NE2	5.06	127.66	122.60
3	3	95	THR	CA-CB-OG1	-5.05	102.02	109.60
3	3	177	ASP	N-CA-CB	-5.05	103.02	110.14
2	2	170	LEU	N-CA-C	-5.05	106.81	112.87
3	3	158	GLN	CB-CA-C	5.05	118.34	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	270	ASN	N-CA-CB	5.04	117.71	109.69
1	1	66	ASP	CA-C-O	-5.04	115.64	121.19
1	1	213	TYR	O-C-N	-5.04	117.30	123.10
3	3	146	MET	CB-CA-C	5.03	120.43	110.17
2	2	261	PRO	CA-C-N	5.03	130.75	121.70
2	2	261	PRO	C-N-CA	5.03	130.75	121.70
1	1	65	THR	N-CA-C	-5.03	106.07	113.61
1	1	76	CYS	CA-C-O	-5.03	115.03	120.81
1	1	282	ARG	CG-CD-NE	-5.02	100.95	112.00
2	2	121	CYS	N-CA-CB	-5.02	102.31	110.59
3	3	217	PHE	CA-C-O	-5.02	115.67	121.19
1	1	189	PRO	CB-CA-C	-5.01	103.68	111.40
1	1	68	GLU	N-CA-C	-5.01	106.01	111.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	259	ARG	Sidechain
1	1	268	ARG	Sidechain
2	2	12	ARG	Sidechain
2	2	255	ARG	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	1	2170	0	2107	167	0
2	2	1952	0	1926	132	0
3	3	1849	0	1832	154	0
4	4	297	0	294	36	0
5	1	26	0	27	6	0
6	1	6	0	0	1	0
6	2	1	0	0	0	0
All	All	6301	0	6186	408	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 33.

All (408) 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)
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.58
4:4:33:LYS:CE	4:4:33:LYS:NZ	1.67	1.55
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.54
1:1:285:ASP:CB	1:1:285:ASP:CA	1.79	1.54
1:1:94:ARG:CZ	1:1:101:ASP:OD2	1.95	1.15
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.14
1:1:151:MET:HE3	1:1:170:SER:HB2	1.22	1.12
1:1:151:MET:CE	1:1:170:SER:HB2	1.84	1.08
1:1:188:VAL:HG21	5:1:900:W8R:H2C2	1.33	1.08
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.07
1:1:285:ASP:CA	1:1:285:ASP:OD2	2.00	1.07
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.36	1.06
1:1:47:PRO:HA	3:3:164:THR:HG21	1.34	1.05
1:1:151:MET:HE3	1:1:170:SER:CB	1.86	1.05
2:2:12:ARG:NH1	2:2:12:ARG:HG3	1.69	1.05
2:2:255:ARG:HG2	2:2:256:SER:H	1.24	1.03
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.41	1.02
2:2:136:GLU:HB3	2:2:140:VAL:HG21	1.44	0.97
3:3:57:ASN:CB	3:3:57:ASN:N	2.28	0.97
3:3:57:ASN:CB	3:3:57:ASN:C	2.37	0.96
1:1:285:ASP:CA	1:1:285:ASP:CG	2.37	0.95
1:1:83:GLN:HG3	1:1:85:LYS:HE2	1.47	0.94
1:1:285:ASP:CB	1:1:285:ASP:C	2.40	0.93
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.05	0.92
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.91
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
2:2:12:ARG:HG3	2:2:12:ARG:HH11	1.27	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.90
1:1:58:MET:HE1	3:3:216:ASP:O	1.71	0.90
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
3:3:57:ASN:CA	3:3:57:ASN:CG	2.45	0.89
1:1:285:ASP:OD2	1:1:285:ASP:HA	1.73	0.88
3:3:179:ASP:HB3	3:3:182:THR:HG22	1.55	0.88
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.88
1:1:151:MET:HE1	1:1:167:THR:O	1.74	0.87
2:2:20:ASN:ND2	2:2:62:ARG:HE	1.72	0.87
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	0.87
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.91	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.85
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.57	0.85
1:1:198:ASN:O	1:1:215:ILE:HD11	1.75	0.84
1:1:90:ILE:HD13	1:1:90:ILE:N	1.92	0.84
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.84
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.82
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.82
2:2:30:ASN:HD22	2:2:31:ALA:H	1.27	0.82
2:2:52:LYS:NZ	2:2:52:LYS:CD	2.43	0.82
1:1:248:LYS:HE3	4:4:38:THR:O	1.80	0.82
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.82
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.61	0.81
1:1:38:GLU:CD	3:3:116:MET:HE2	2.05	0.81
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.80
2:2:9:TYR:HD1	2:2:9:TYR:N	1.77	0.80
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.79
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.48	0.79
1:1:188:VAL:HG21	5:1:900:W8R:C2C	2.11	0.79
2:2:9:TYR:N	2:2:9:TYR:CD1	2.43	0.79
1:1:58:MET:HE1	3:3:216:ASP:C	2.08	0.78
2:2:262:GLN:HE21	2:2:262:GLN:C	1.91	0.78
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.13	0.77
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
2:2:255:ARG:HG2	2:2:256:SER:N	2.00	0.77
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.20	0.76
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.19	0.76
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.75
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.68	0.74
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	0.74
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.74
4:4:43:GLN:HG2	4:4:45:LEU:HB2	1.70	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
1:1:122:VAL:HG13	1:1:124:PHE:HE2	1.53	0.73
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.73
1:1:92:ASN:OD1	1:1:95:GLU:HB2	1.87	0.73
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.72
1:1:58:MET:HE1	3:3:216:ASP:HA	1.71	0.71
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.71
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.71
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.71
2:2:195:ASN:HD22	2:2:195:ASN:C	1.99	0.71
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.71
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.71
1:1:188:VAL:CG2	5:1:900:W8R:H2C2	2.17	0.70
3:3:57:ASN:CA	3:3:57:ASN:OD1	2.38	0.70
2:2:39:PRO:HG2	2:2:247:MET:HE2	1.74	0.70
2:2:235:THR:CG2	2:2:236:PRO:HD2	2.21	0.70
1:1:152:TYR:O	1:1:173:ASN:ND2	2.26	0.69
1:1:104:ILE:HD11	1:1:224:MET:HG3	1.74	0.69
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.69
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.69
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.76	0.68
1:1:201:TYR:HD2	1:1:214:GLY:O	1.76	0.68
4:4:29:ILE:HG22	4:4:29:ILE:O	1.94	0.68
3:3:20:GLN:HE22	4:4:31:TYR:H	1.42	0.68
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.67
1:1:278:VAL:HG12	3:3:62:ASP:OD1	1.95	0.67
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.67
3:3:61:LYS:HD3	3:3:63:GLU:OE1	1.95	0.67
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.77	0.66
2:2:155:ASP:OD2	2:2:155:ASP:C	2.37	0.66
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.66
1:1:94:ARG:NH1	1:1:101:ASP:OD2	2.28	0.66
1:1:151:MET:CE	1:1:167:THR:O	2.44	0.66
3:3:42:ASN:HD22	3:3:44:LEU:H	1.43	0.66
3:3:197:LEU:HB3	3:3:201:THR:HG22	1.77	0.66
3:3:179:ASP:HB3	3:3:182:THR:CG2	2.23	0.65
1:1:176:VAL:HG22	5:1:900:W8R:H312	1.79	0.65
1:1:285:ASP:CB	1:1:285:ASP:H	2.09	0.65
2:2:190:ASN:HD21	3:3:118:THR:HA	1.62	0.65
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.64
1:1:58:MET:HE1	3:3:216:ASP:CA	2.27	0.64
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64
2:2:30:ASN:HD22	2:2:31:ALA:N	1.94	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.64
2:2:12:ARG:NH1	4:4:68:ASN:O	2.31	0.64
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.33	0.64
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.63
2:2:39:PRO:CG	2:2:247:MET:HE2	2.29	0.63
2:2:205:ASN:ND2	2:2:206:SER:H	1.96	0.63
2:2:187:GLN:HE21	2:2:197:ALA:HA	1.63	0.63
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.80	0.63
3:3:75:ARG:O	3:3:194:SER:HB2	1.99	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62
3:3:84:ASN:ND2	3:3:86:PHE:H	1.98	0.62
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.61
2:2:38:TRP:CZ3	4:4:57:LYS:HD2	2.36	0.61
2:2:133:ALA:O	2:2:166:VAL:HG12	2.01	0.61
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.15	0.61
1:1:187:SER:HB3	3:3:21:SER:CB	2.31	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
3:3:55:MET:HG3	3:3:55:MET:O	1.99	0.61
1:1:90:ILE:N	1:1:90:ILE:CD1	2.62	0.61
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
1:1:94:ARG:NH2	1:1:101:ASP:OD2	2.34	0.60
1:1:51:ILE:HD13	3:3:166:PRO:HG3	1.82	0.59
3:3:131:TYR:HB3	3:3:149:THR:HB	1.82	0.59
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.59
1:1:94:ARG:NH1	1:1:94:ARG:CG	2.60	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE2	2.38	0.59
3:3:84:ASN:HD22	3:3:86:PHE:H	1.49	0.59
2:2:30:ASN:HD21	4:4:58:ASP:H	1.51	0.59
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
1:1:100:ASN:HD22	1:1:101:ASP:H	1.49	0.58
1:1:43:MET:HE3	1:1:43:MET:HA	1.85	0.57
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.57
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	0.57
1:1:82:ILE:HG22	1:1:100:ASN:HB2	1.86	0.57
2:2:64:TYR:CD2	2:2:89:MET:HB3	2.39	0.57
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.57
2:2:221:MET:HE2	2:2:223:ILE:HD11	1.87	0.57
2:2:52:LYS:NZ	2:2:52:LYS:HD3	2.20	0.57
3:3:57:ASN:HB3	3:3:57:ASN:C	2.28	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.56
1:1:58:MET:HE3	3:3:216:ASP:HA	1.85	0.56
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
2:2:174:ASN:C	2:2:174:ASN:ND2	2.63	0.56
3:3:31:THR:CG2	3:3:32:PRO:HD2	2.34	0.56
1:1:117:GLU:HB3	1:1:200:PHE:HZ	1.70	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.56
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.56
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.56
1:1:102:TRP:CZ3	1:1:224:MET:HE3	2.41	0.55
2:2:189:ILE:HA	2:2:194:ASN:ND2	2.21	0.55
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.55
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.55
3:3:175:TYR:H	3:3:182:THR:HG21	1.70	0.55
1:1:176:VAL:CG2	5:1:900:W8R:H312	2.35	0.55
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.55
3:3:175:TYR:H	3:3:182:THR:CG2	2.20	0.55
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.88	0.55
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	0.55
1:1:110:VAL:HG22	3:3:230:GLN:OE1	2.06	0.55
1:1:151:MET:HE3	1:1:170:SER:CA	2.37	0.55
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.55
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
1:1:266:ILE:HD12	3:3:235:THR:HA	1.88	0.54
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.54
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.87	0.54
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.54
1:1:103:LYS:HA	1:1:223:SER:HB2	1.89	0.54
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.54
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.54
3:3:20:GLN:HE22	4:4:31:TYR:N	2.04	0.54
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.54
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.54
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.54
2:2:170:LEU:CD2	3:3:64:VAL:HA	2.38	0.54
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.54
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.54
1:1:216:THR:HG21	3:3:236:GLU:HG2	1.88	0.53
3:3:117:TYR:CD2	3:3:155:ILE:HD13	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.53
2:2:195:ASN:ND2	2:2:195:ASN:C	2.66	0.53
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.53
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
3:3:18:ASP:OD1	4:4:40:SER:HB2	2.09	0.53
3:3:86:PHE:CD1	3:3:178:PRO:HB3	2.44	0.53
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.52
1:1:214:GLY:O	1:1:217:VAL:CG1	2.57	0.52
1:1:88:THR:O	1:1:90:ILE:HD13	2.10	0.52
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.52
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
1:1:187:SER:HB3	3:3:21:SER:HB2	1.92	0.52
1:1:92:ASN:C	1:1:92:ASN:ND2	2.67	0.52
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.52
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.52
1:1:194:ALA:HB3	6:1:504:HOH:O	2.10	0.52
2:2:66:LEU:HD12	2:2:89:MET:HE3	1.91	0.52
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.51
4:4:44:SER:C	4:4:46:SER:N	2.68	0.51
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.51
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.51
3:3:75:ARG:NH1	3:3:78:GLU:OE1	2.41	0.51
1:1:117:GLU:HB3	1:1:200:PHE:CZ	2.46	0.51
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.51
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
3:3:84:ASN:ND2	3:3:84:ASN:C	2.69	0.51
1:1:38:GLU:OE1	3:3:116:MET:HE2	2.10	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.51
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.51
3:3:84:ASN:HD22	3:3:86:PHE:N	2.08	0.51
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE1	2.44	0.50
1:1:151:MET:HE3	1:1:170:SER:HB3	1.87	0.50
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.50
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
2:2:255:ARG:CG	2:2:256:SER:H	2.00	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.50
2:2:158:SER:HG	2:2:167:LYS:HE2	1.71	0.50
3:3:84:ASN:HD22	3:3:84:ASN:C	2.20	0.49
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.49
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.49
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	0.49
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.49
1:1:122:VAL:CG1	1:1:124:PHE:HE2	2.25	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.49
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.94	0.49
3:3:20:GLN:NE2	4:4:31:TYR:H	2.11	0.49
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.49
2:2:30:ASN:ND2	2:2:31:ALA:H	2.05	0.48
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.48
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
1:1:216:THR:HG21	3:3:236:GLU:CG	2.43	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.48
1:1:280:LYS:HE3	3:3:89:ASP:OD2	2.13	0.48
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.48
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.96	0.48
1:1:152:TYR:O	1:1:154:PRO:HD3	2.13	0.48
3:3:61:LYS:O	3:3:61:LYS:HG2	2.07	0.48
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.48
1:1:216:THR:CG2	3:3:236:GLU:CG	2.91	0.48
3:3:112:ARG:NH1	3:3:112:ARG:HG2	2.28	0.48
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.96	0.48
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.79	0.48
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.47
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.43	0.47
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.47
1:1:165:ASP:HB3	1:1:167:THR:H	1.79	0.47
1:1:201:TYR:CG	1:1:218:LEU:HD22	2.49	0.47
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:268:ARG:CZ	2:2:139:ASN:HB2	2.44	0.47
2:2:13:VAL:HA	2:2:25:THR:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
1:1:206:HIS:ND1	1:1:206:HIS:N	2.62	0.47
2:2:63:PHE:CD2	2:2:245:ALA:HB2	2.50	0.47
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.47
3:3:175:TYR:CD1	3:3:182:THR:HG21	2.49	0.47
1:1:268:ARG:HH11	1:1:268:ARG:HD3	1.50	0.47
1:1:122:VAL:O	1:1:197:TYR:HB2	2.14	0.46
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.43	0.46
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.46
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.46
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.46
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.62	0.46
1:1:102:TRP:CE3	1:1:224:MET:HE3	2.50	0.46
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.46
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.46
1:1:236:LYS:HE2	1:1:236:LYS:HB3	1.83	0.46
2:2:158:SER:HG	2:2:167:LYS:CE	2.26	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
1:1:110:VAL:O	1:1:111:GLN:C	2.58	0.46
1:1:151:MET:HE2	1:1:170:SER:HB2	1.83	0.46
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.46
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.45
3:3:57:ASN:CB	3:3:57:ASN:H	2.26	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.45
4:4:30:ASN:HA	4:4:30:ASN:HD22	1.40	0.45
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.45
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.97	0.45
2:2:170:LEU:HD23	3:3:64:VAL:HG22	1.99	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.98	0.45
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.81	0.45
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.45
3:3:192:GLN:HE21	3:3:192:GLN:HA	1.81	0.45
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.44
1:1:43:MET:HA	1:1:43:MET:CE	2.46	0.44
1:1:92:ASN:C	1:1:92:ASN:HD22	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:198:ASN:HB3	1:1:200:PHE:O	2.17	0.44
1:1:207:ASP:HA	2:2:144:TYR:CE1	2.52	0.44
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.44
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.17	0.44
1:1:289:TYR:CE1	3:3:138:GLY:HA3	2.53	0.44
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.44
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.44
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
3:3:221:LEU:C	3:3:221:LEU:HD23	2.43	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.44
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.44
1:1:289:TYR:CD1	3:3:138:GLY:HA3	2.53	0.44
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.43
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.48	0.43
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.43
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.43
2:2:190:ASN:O	2:2:191:LEU:C	2.61	0.43
1:1:38:GLU:N	3:3:116:MET:HE1	2.34	0.43
1:1:132:ALA:O	1:1:181:GLY:N	2.41	0.43
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	0.43
3:3:175:TYR:CB	3:3:182:THR:HG21	2.47	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
2:2:10:SER:CB	2:2:12:ARG:HB2	2.48	0.43
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.43
1:1:285:ASP:C	1:1:285:ASP:HB3	2.38	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.80	0.43
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.53	0.43
2:2:205:ASN:ND2	2:2:206:SER:N	2.66	0.43
4:4:43:GLN:C	4:4:45:LEU:N	2.74	0.42
1:1:216:THR:HG22	3:3:236:GLU:CD	2.44	0.42
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.42
1:1:89:GLY:C	1:1:90:ILE:CD1	2.89	0.42
1:1:187:SER:HB3	3:3:21:SER:HB3	2.01	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:153:TRP:CD1	3:3:153:TRP:C	2.97	0.42
1:1:191:VAL:CG2	5:1:900:W8R:H6C1	2.50	0.42
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.19	0.42
3:3:226:GLN:HE21	3:3:226:GLN:HB2	1.21	0.42
2:2:40:GLU:O	2:2:40:GLU:CG	2.61	0.42
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.42
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.38	0.42
1:1:201:TYR:H	2:2:131:GLN:HE21	1.68	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42
3:3:44:LEU:HA	3:3:44:LEU:HD23	1.79	0.42
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.42
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD1	2.55	0.41
1:1:286:ILE:HD13	1:1:286:ILE:HG21	1.77	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
1:1:102:TRP:HZ3	1:1:224:MET:HE3	1.84	0.41
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.41
3:3:113:PHE:CE1	3:3:115:LEU:HD13	2.55	0.41
1:1:86:ASP:OD2	1:1:88:THR:HB	2.21	0.41
1:1:87:ALA:C	1:1:90:ILE:HG12	2.45	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.02	0.41
3:3:137:ARG:HH11	3:3:137:ARG:HD3	1.22	0.41
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.20	0.41
1:1:165:ASP:CB	1:1:167:THR:OG1	2.69	0.41
1:1:54:ARG:HH11	1:1:54:ARG:HD2	1.55	0.41
1:1:97:LYS:C	1:1:99:PHE:H	2.25	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
3:3:64:VAL:O	3:3:64:VAL:HG12	2.21	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
3:3:157:LEU:HD23	3:3:157:LEU:O	2.21	0.41
1:1:100:ASN:ND2	1:1:101:ASP:H	2.17	0.40
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
3:3:231:THR:C	3:3:232:VAL:HG13	2.45	0.40
3:3:20:GLN:NE2	4:4:30:ASN:HA	2.36	0.40
1:1:208:ASP:HB3	1:1:211:THR:HB	2.04	0.40
1:1:265:SER:OG	2:2:139:ASN:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:172:ASN:CG	2:2:181:LEU:HD13	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1	271/289 (94%)	249 (92%)	20 (7%)	2 (1%)	18	53
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	16	50
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	14	48
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	4	23
All	All	796/855 (93%)	733 (92%)	56 (7%)	7 (1%)	14	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	SER
3	3	57	ASN
3	3	77	ASN
1	1	165	ASP
2	2	255	ARG
2	2	257	LYS
4	4	47	MET

5.3.2 Protein sidechains [i](#)

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	1	239/253 (94%)	184 (77%)	55 (23%)	1	5
2	2	223/229 (97%)	176 (79%)	47 (21%)	1	6
3	3	209/209 (100%)	171 (82%)	38 (18%)	2	9
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	1
All	All	704/748 (94%)	551 (78%)	153 (22%)	1	6

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	VAL
1	1	21	ILE
1	1	22	SER
1	1	23	SER
1	1	28	THR
1	1	29	GLN
1	1	30	LYS
1	1	38	GLU
1	1	43	MET
1	1	47	PRO
1	1	81	GLU
1	1	90	ILE
1	1	95	GLU
1	1	97	LYS
1	1	103	LYS
1	1	105	ASN
1	1	106	LEU
1	1	107	SER
1	1	109	LEU
1	1	122	VAL
1	1	136	GLN
1	1	137	PRO
1	1	138	ASP
1	1	144	SER
1	1	145	ASN
1	1	161	LYS
1	1	165	ASP
1	1	170	SER
1	1	172	SER
1	1	173	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	175	SER
1	1	176	VAL
1	1	183	THR
1	1	184	SER
1	1	185	ARG
1	1	187	SER
1	1	202	ASP
1	1	215	ILE
1	1	216	THR
1	1	217	VAL
1	1	218	LEU
1	1	221	MET
1	1	223	SER
1	1	224	MET
1	1	240	LYS
1	1	248	LYS
1	1	254	ILE
1	1	256	ARG
1	1	266	ILE
1	1	268	ARG
1	1	273	LYS
1	1	274	ASN
1	1	275	THR
1	1	278	VAL
1	1	287	LYS
2	2	12	ARG
2	2	20	ASN
2	2	26	GLN
2	2	30	ASN
2	2	49	ASP
2	2	52	LYS
2	2	66	LEU
2	2	69	LYS
2	2	73	THR
2	2	76	LYS
2	2	81	LYS
2	2	87	LYS
2	2	88	ASP
2	2	103	ARG
2	2	116	LYS
2	2	119	SER
2	2	136	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	141	SER
2	2	143	LYS
2	2	145	THR
2	2	151	GLU
2	2	152	ARG
2	2	156	LEU
2	2	165	PRO
2	2	166	VAL
2	2	167	LYS
2	2	169	VAL
2	2	170	LEU
2	2	174	ASN
2	2	187	GLN
2	2	192	ARG
2	2	195	ASN
2	2	209	ILE
2	2	211	SER
2	2	217	ASN
2	2	225	ILE
2	2	230	VAL
2	2	232	THR
2	2	236	PRO
2	2	238	LEU
2	2	247	MET
2	2	250	GLU
2	2	254	ILE
2	2	255	ARG
2	2	256	SER
2	2	259	ILE
2	2	262	GLN
3	3	12	GLN
3	3	16	THR
3	3	33	ARG
3	3	42	ASN
3	3	46	ILE
3	3	55	MET
3	3	60	THR
3	3	61	LYS
3	3	65	ASN
3	3	84	ASN
3	3	91	VAL
3	3	94	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	101	VAL
3	3	112	ARG
3	3	114	SER
3	3	115	LEU
3	3	137	ARG
3	3	146	MET
3	3	157	LEU
3	3	158	GLN
3	3	159	SER
3	3	164	THR
3	3	172	GLN
3	3	174	ARG
3	3	182	THR
3	3	192	GLN
3	3	194	SER
3	3	196	ILE
3	3	201	THR
3	3	208	LEU
3	3	211	ILE
3	3	218	LYS
3	3	219	LEU
3	3	220	ARG
3	3	223	LYS
3	3	226	GLN
3	3	228	ILE
3	3	230	GLN
4	4	29	ILE
4	4	33	LYS
4	4	40	SER
4	4	43	GLN
4	4	45	LEU
4	4	46	SER
4	4	47	MET
4	4	50	SER
4	4	51	LYS
4	4	59	LEU
4	4	61	LEU
4	4	67	LEU
4	4	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	92	ASN
1	1	100	ASN
1	1	136	GLN
1	1	173	ASN
1	1	198	ASN
2	2	15	GLN
2	2	20	ASN
2	2	30	ASN
2	2	94	GLN
2	2	111	GLN
2	2	131	GLN
2	2	135	HIS
2	2	174	ASN
2	2	187	GLN
2	2	190	ASN
2	2	195	ASN
2	2	205	ASN
2	2	216	ASN
2	2	262	GLN
3	3	20	GLN
3	3	27	ASN
3	3	42	ASN
3	3	56	ASN
3	3	65	ASN
3	3	74	ASN
3	3	84	ASN
3	3	140	GLN
3	3	192	GLN
3	3	226	GLN
4	4	30	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	W8R	1	900	-	28,28,28	2.77	4 (14%)	34,36,36	2.63	6 (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	W8R	1	900	-	-	7/15/24/24	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	900	W8R	C2A-N3A	11.46	1.43	1.27
5	1	900	W8R	C4A-N3A	-7.03	1.36	1.48
5	1	900	W8R	O1A-C2A	-4.18	1.29	1.36
5	1	900	W8R	O1A-C5A	-3.70	1.38	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	900	W8R	CM1-C4A-N3A	8.71	135.45	111.59
5	1	900	W8R	O1A-C2A-N3A	-7.15	109.87	118.10
5	1	900	W8R	O1A-C2A-C4B	6.69	124.30	115.85
5	1	900	W8R	O1A-C5A-C4A	5.68	111.71	104.88
5	1	900	W8R	C5A-C4A-N3A	-3.93	98.57	103.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	900	W8R	CM1-C4A-C5A	-2.73	104.25	114.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

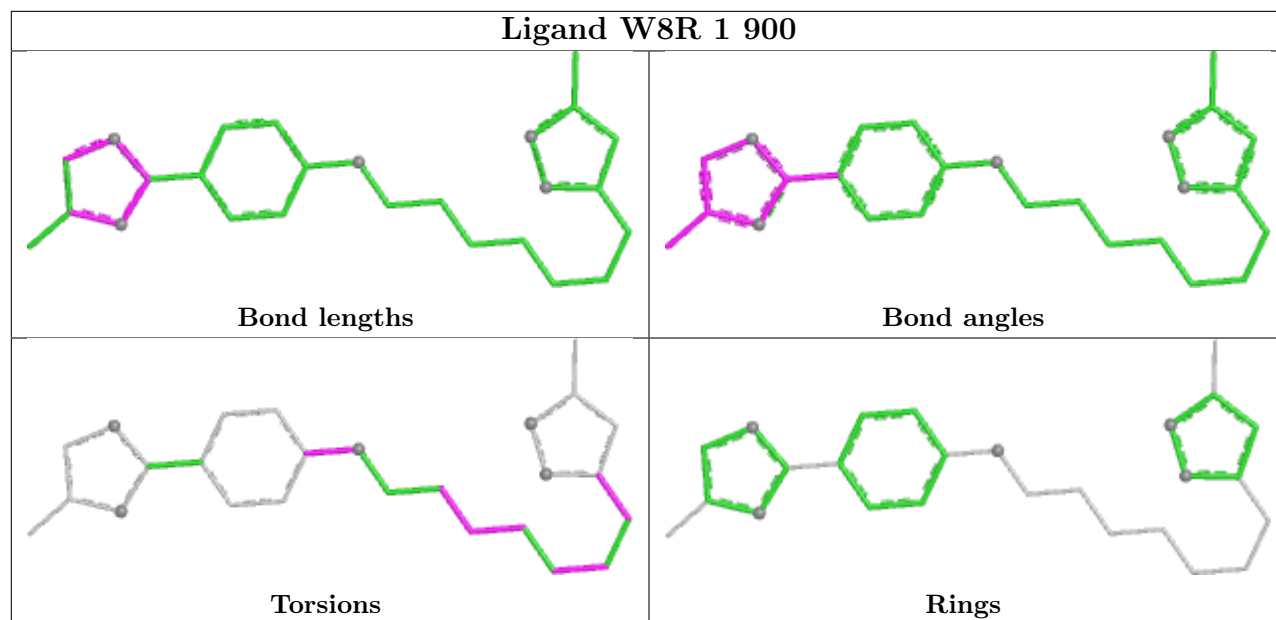
Mol	Chain	Res	Type	Atoms
5	1	900	W8R	C2C-C1C-C5-O1
5	1	900	W8R	C2B-C1B-O1B-C7C
5	1	900	W8R	C6B-C1B-O1B-C7C
5	1	900	W8R	C1C-C2C-C3C-C4C
5	1	900	W8R	C2C-C1C-C5-C4
5	1	900	W8R	C3C-C4C-C5C-C6C
5	1	900	W8R	C4C-C5C-C6C-C7C

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	900	W8R	6	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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1	273/289 (94%)	-0.21	2 (0%) 84 66	1, 1, 1, 1	0
2	2	255/262 (97%)	-0.23	5 (1%) 65 41	1, 1, 1, 1	0
3	3	236/236 (100%)	-0.27	1 (0%) 88 76	1, 1, 1, 1	0
4	4	40/68 (58%)	-0.35	0 100 100	1, 1, 1, 1	0
All	All	804/855 (94%)	-0.24	8 (0%) 79 59	1, 1, 1, 1	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	61	ASN	3.1
2	2	119	SER	3.0
2	2	68	SER	2.9
2	2	211	SER	2.8
1	1	40	GLY	2.4
2	2	151	GLU	2.1
2	2	112	CYS	2.1
3	3	1	GLY	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](#)

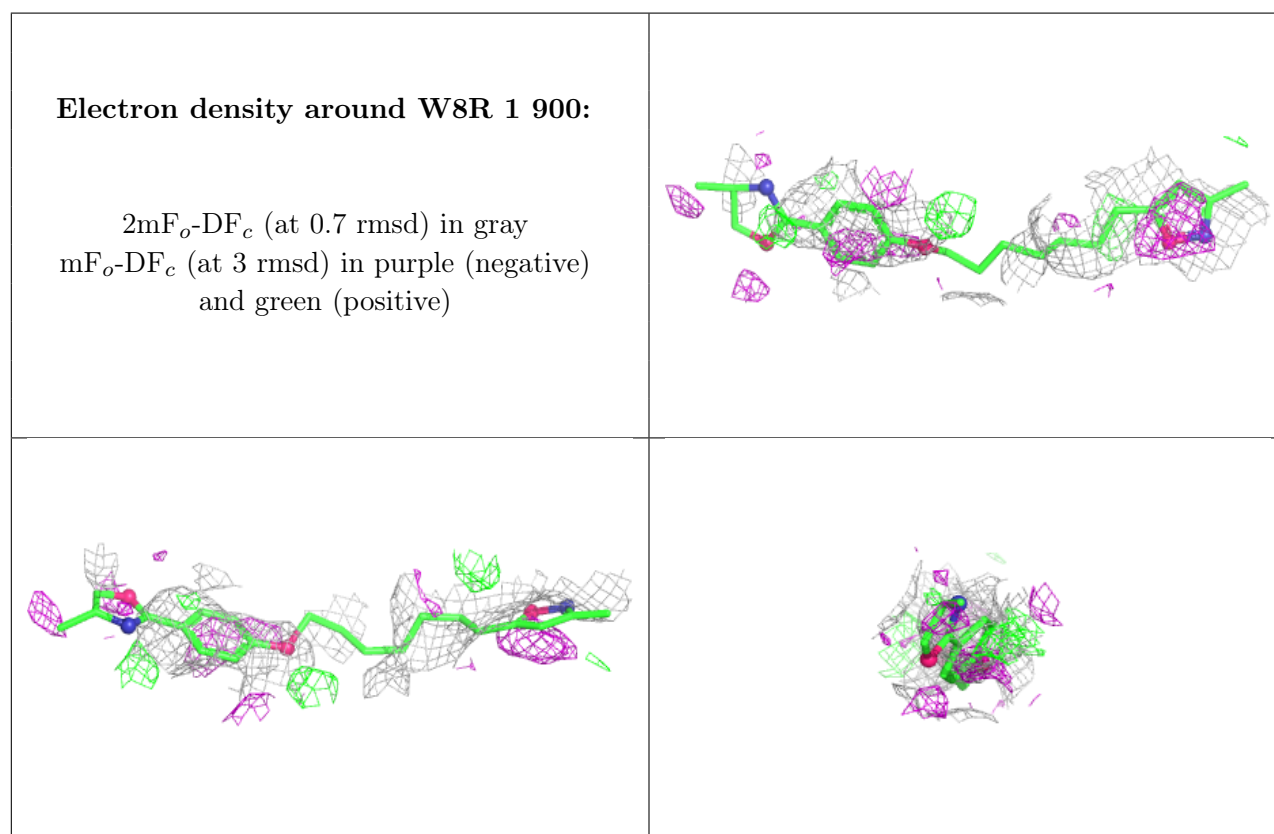
There are no oligosaccharides in this entry.

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	W8R	1	900	26/26	0.98	0.11	1,1,1,1	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.