



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:37 AM UTC

PDB ID : 1G6Q / pdb_00001g6q
Title : CRYSTAL STRUCTURE OF YEAST ARGININE METHYLTRANSFERASE, HMT1
Authors : Weiss, V.H.; McBride, A.E.; Soriano, M.A.; Filman, D.J.; Silver, P.A.; Hogle, J.M.
Deposited on : 2000-11-07
Resolution : 2.90 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

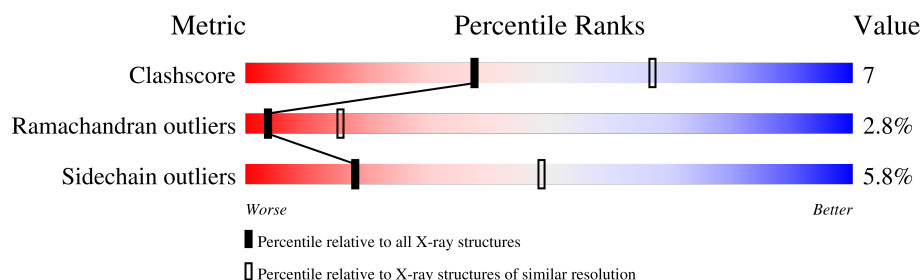
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	328	
1	2	328	
1	3	328	
1	4	328	
1	5	328	
1	6	328	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 15520 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 HNRNP ARGININE N-METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	328	Total	C	N	O	S	0	0	0
			2656	1705	431	508	12			
1	2	320	Total	C	N	O	S	0	0	0
			2579	1654	423	490	12			
1	3	319	Total	C	N	O	S	0	0	0
			2562	1642	420	488	12			
1	4	318	Total	C	N	O	S	0	0	0
			2557	1639	419	487	12			
1	5	321	Total	C	N	O	S	0	0	0
			2587	1658	424	493	12			
1	6	320	Total	C	N	O	S	0	0	0
			2579	1654	423	490	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	21	ASP	GLN	engineered mutation	UNP P38074
1	22	TYR	HIS	engineered mutation	UNP P38074
1	25	ASP	ASN	engineered mutation	UNP P38074
2	21	ASP	GLN	engineered mutation	UNP P38074
2	22	TYR	HIS	engineered mutation	UNP P38074
2	25	ASP	ASN	engineered mutation	UNP P38074
3	21	ASP	GLN	engineered mutation	UNP P38074
3	22	TYR	HIS	engineered mutation	UNP P38074
3	25	ASP	ASN	engineered mutation	UNP P38074
4	21	ASP	GLN	engineered mutation	UNP P38074
4	22	TYR	HIS	engineered mutation	UNP P38074
4	25	ASP	ASN	engineered mutation	UNP P38074
5	21	ASP	GLN	engineered mutation	UNP P38074
5	22	TYR	HIS	engineered mutation	UNP P38074
5	25	ASP	ASN	engineered mutation	UNP P38074
6	21	ASP	GLN	engineered mutation	UNP P38074
6	22	TYR	HIS	engineered mutation	UNP P38074

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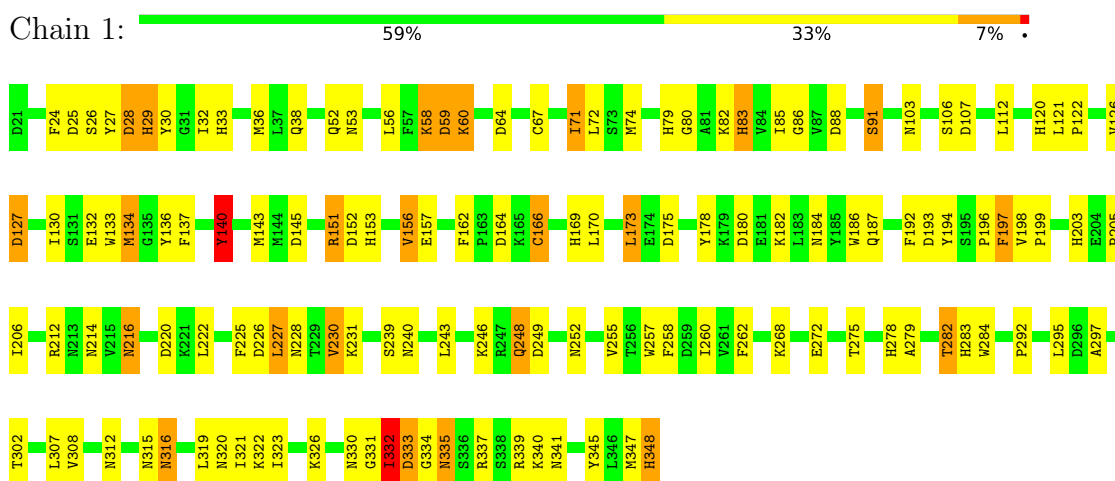
Chain	Residue	Modelled	Actual	Comment	Reference
6	25	ASP	ASN	engineered mutation	UNP P38074

3 Residue-property plots

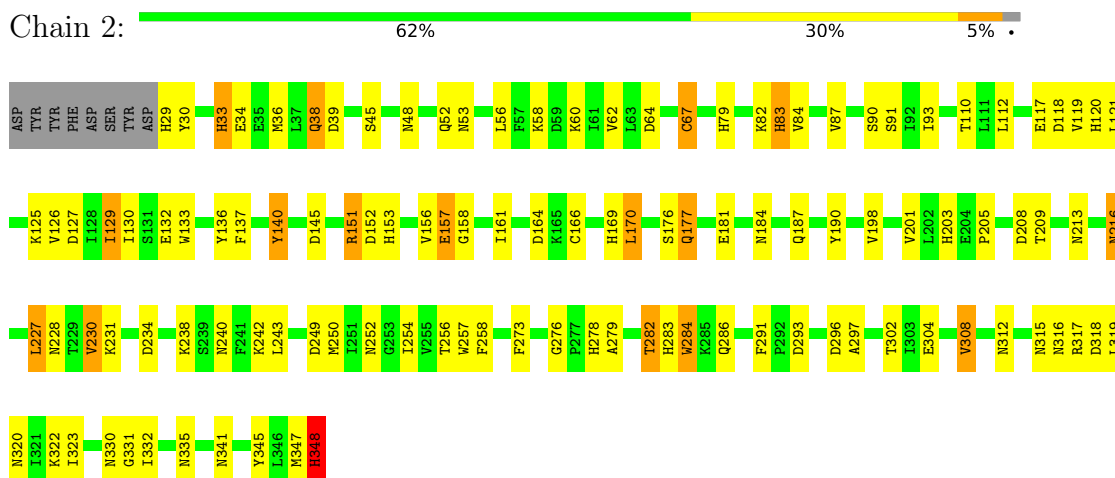
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE

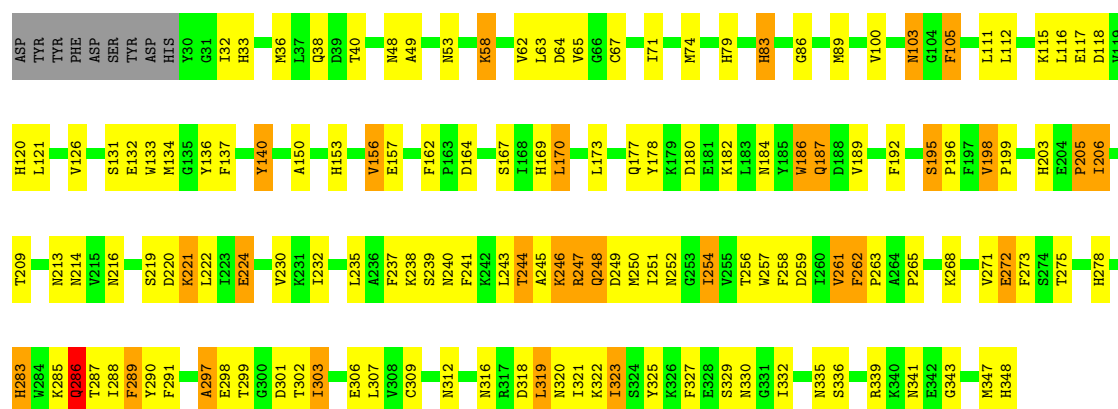


• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE



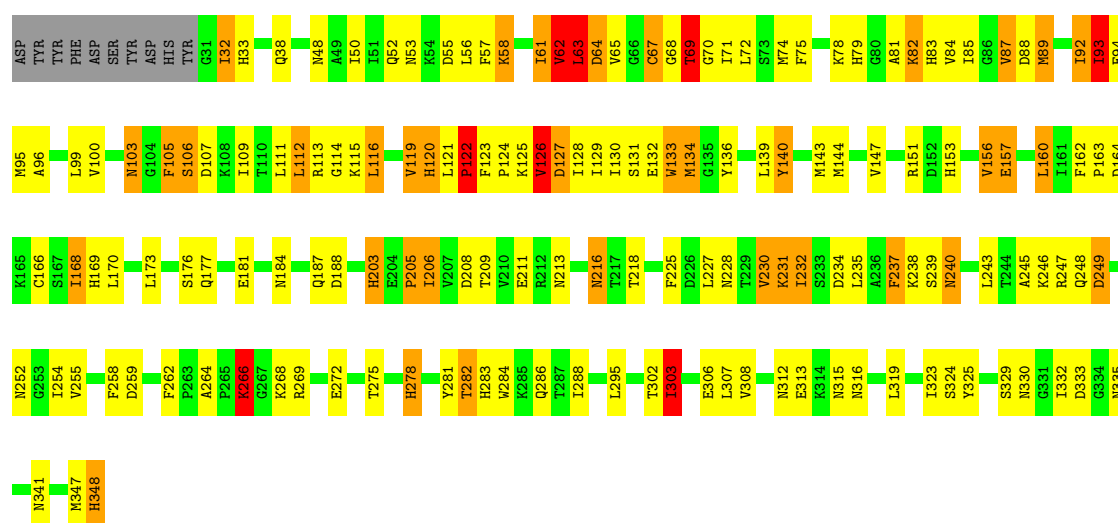
• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE





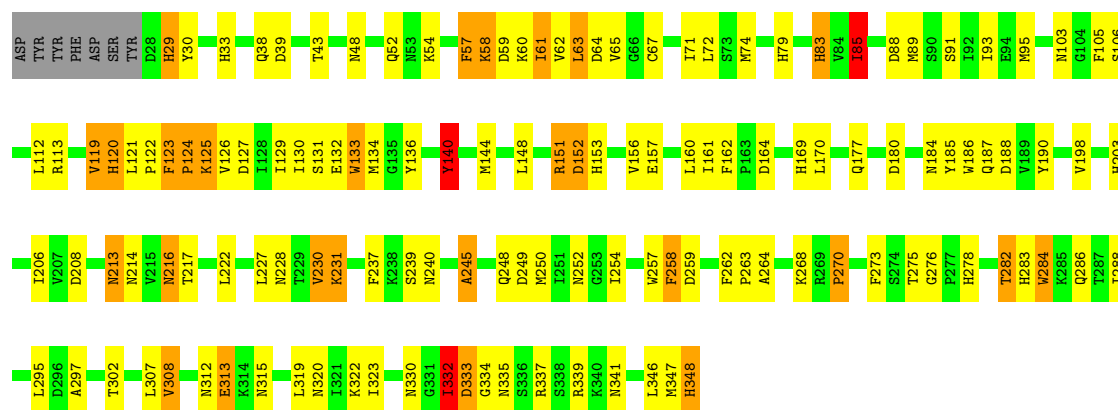
• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE

Chain 4: 48% 35% 11% . .



• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE

Chain 5: 57% 32% 8% . .



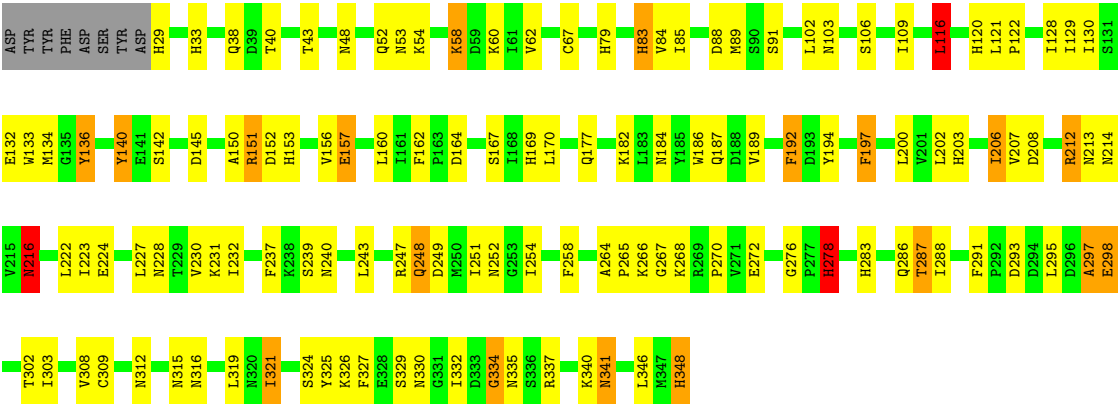
• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE

Chain 6:

58%

33%

5% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.10Å 129.43Å 101.43Å 90.00° 102.74° 90.00°	Depositor
Resolution (Å)	28.00 – 2.90	Depositor
% Data completeness (in resolution range)	99.1 (28.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.253 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15520	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	1.08	15/2722 (0.6%)	2.00	103/3684 (2.8%)
1	2	1.12	11/2641 (0.4%)	1.99	97/3573 (2.7%)
1	3	1.04	14/2622 (0.5%)	2.09	118/3547 (3.3%)
1	4	1.05	10/2617 (0.4%)	2.15	120/3540 (3.4%)
1	5	1.06	14/2649 (0.5%)	2.00	100/3584 (2.8%)
1	6	1.06	13/2641 (0.5%)	1.99	94/3573 (2.6%)
All	All	1.07	77/15892 (0.5%)	2.04	632/21501 (2.9%)

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	1
1	2	0	1
All	All	0	2

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	278	HIS	CD2-NE2	-8.03	1.29	1.37
1	6	153	HIS	CD2-NE2	-7.68	1.29	1.37
1	2	83	HIS	CD2-NE2	-7.54	1.29	1.37
1	2	29	HIS	CD2-NE2	-7.45	1.29	1.37
1	2	283	HIS	CD2-NE2	-7.34	1.29	1.37
1	2	348	HIS	CD2-NE2	-7.30	1.29	1.37
1	1	29	HIS	CD2-NE2	-7.22	1.29	1.37
1	5	169	HIS	CD2-NE2	-7.20	1.29	1.37
1	1	153	HIS	CD2-NE2	-7.13	1.30	1.37
1	3	153	HIS	CG-ND1	-7.10	1.30	1.38
1	6	33	HIS	CD2-NE2	-7.04	1.30	1.37
1	5	348	HIS	CD2-NE2	-6.99	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	348	HIS	CD2-NE2	-6.94	1.30	1.37
1	4	153	HIS	CD2-NE2	-6.86	1.30	1.37
1	6	83	HIS	CD2-NE2	-6.75	1.30	1.37
1	4	33	HIS	CD2-NE2	-6.65	1.30	1.37
1	1	83	HIS	CD2-NE2	-6.62	1.30	1.37
1	3	83	HIS	CD2-NE2	-6.61	1.30	1.37
1	1	33	HIS	CD2-NE2	-6.61	1.30	1.37
1	3	153	HIS	CD2-NE2	-6.59	1.30	1.37
1	5	120	HIS	CD2-NE2	-6.58	1.30	1.37
1	3	203	HIS	CD2-NE2	-6.57	1.30	1.37
1	3	283	HIS	CD2-NE2	-6.54	1.30	1.37
1	5	29	HIS	CD2-NE2	-6.52	1.30	1.37
1	4	283	HIS	CD2-NE2	-6.48	1.30	1.37
1	3	120	HIS	CD2-NE2	-6.43	1.30	1.37
1	5	79	HIS	CD2-NE2	-6.43	1.30	1.37
1	2	153	HIS	CD2-NE2	-6.41	1.30	1.37
1	5	283	HIS	CD2-NE2	-6.40	1.30	1.37
1	3	169	HIS	CD2-NE2	-6.38	1.30	1.37
1	3	33	HIS	CD2-NE2	-6.38	1.30	1.37
1	5	83	HIS	CD2-NE2	-6.36	1.30	1.37
1	4	120	HIS	CD2-NE2	-6.32	1.30	1.37
1	6	120	HIS	CD2-NE2	-6.31	1.30	1.37
1	5	278	HIS	CD2-NE2	-6.31	1.30	1.37
1	1	203	HIS	CD2-NE2	-6.30	1.30	1.37
1	6	348	HIS	CD2-NE2	-6.29	1.30	1.37
1	4	169	HIS	CD2-NE2	-6.25	1.30	1.37
1	1	348	HIS	CD2-NE2	-6.24	1.30	1.37
1	4	348	HIS	CD2-NE2	-6.23	1.30	1.37
1	5	153	HIS	CD2-NE2	-6.21	1.31	1.37
1	4	83	HIS	CD2-NE2	-6.20	1.31	1.37
1	4	278	HIS	CD2-NE2	-6.20	1.31	1.37
1	1	169	HIS	CD2-NE2	-6.20	1.31	1.37
1	2	169	HIS	CD2-NE2	-6.19	1.31	1.37
1	2	33	HIS	CD2-NE2	-6.12	1.31	1.37
1	1	283	HIS	CD2-NE2	-6.11	1.31	1.37
1	4	79	HIS	CD2-NE2	-6.08	1.31	1.37
1	6	29	HIS	CD2-NE2	-6.08	1.31	1.37
1	1	120	HIS	CD2-NE2	-6.06	1.31	1.37
1	2	79	HIS	CD2-NE2	-6.04	1.31	1.37
1	2	203	HIS	CD2-NE2	-6.00	1.31	1.37
1	4	203	HIS	CD2-NE2	-5.97	1.31	1.37
1	6	283	HIS	CD2-NE2	-5.92	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	278	HIS	CD2-NE2	-5.91	1.31	1.37
1	1	278	HIS	CD2-NE2	-5.88	1.31	1.37
1	6	278	HIS	CG-ND1	-5.86	1.31	1.38
1	3	278	HIS	CD2-NE2	-5.78	1.31	1.37
1	5	169	HIS	CG-ND1	-5.76	1.31	1.38
1	6	79	HIS	CD2-NE2	-5.74	1.31	1.37
1	6	203	HIS	CD2-NE2	-5.69	1.31	1.37
1	3	198	VAL	CA-CB	5.68	1.61	1.54
1	1	29	HIS	CG-ND1	-5.67	1.32	1.38
1	5	283	HIS	CG-ND1	-5.61	1.32	1.38
1	5	33	HIS	CD2-NE2	-5.58	1.31	1.37
1	5	348	HIS	CG-ND1	-5.55	1.32	1.38
1	1	169	HIS	CG-ND1	-5.55	1.32	1.38
1	5	203	HIS	CD2-NE2	-5.54	1.31	1.37
1	1	203	HIS	CG-ND1	-5.49	1.32	1.38
1	6	153	HIS	CG-ND1	-5.46	1.32	1.38
1	3	79	HIS	CD2-NE2	-5.45	1.31	1.37
1	2	120	HIS	CD2-NE2	-5.26	1.32	1.37
1	6	169	HIS	CD2-NE2	-5.19	1.32	1.37
1	1	79	HIS	CD2-NE2	-5.16	1.32	1.37
1	1	83	HIS	CG-ND1	-5.08	1.32	1.38
1	3	203	HIS	CG-ND1	-5.02	1.32	1.38
1	3	209	THR	CA-CB	5.01	1.59	1.52

All (632) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	203	HIS	CA-CB-CG	-13.56	100.24	113.80
1	4	133	TRP	N-CA-C	12.66	125.08	111.28
1	6	164	ASP	CA-CB-CG	12.04	124.64	112.60
1	5	60	LYS	N-CA-C	11.56	125.79	110.53
1	4	264	ALA	N-CA-C	11.41	118.49	108.22
1	6	38	GLN	OE1-CD-NE2	-11.26	111.34	122.60
1	5	240	ASN	OD1-CG-ND2	-11.11	111.49	122.60
1	2	136	TYR	N-CA-C	11.08	124.40	111.11
1	5	48	ASN	OD1-CG-ND2	-10.76	111.84	122.60
1	2	228	ASN	OD1-CG-ND2	-10.56	112.03	122.60
1	1	136	TYR	N-CA-C	10.42	123.61	111.11
1	2	184	ASN	OD1-CG-ND2	-10.26	112.34	122.60
1	1	248	GLN	OE1-CD-NE2	-10.17	112.43	122.60
1	3	33	HIS	CA-CB-CG	-10.15	103.65	113.80
1	4	109	ILE	N-CA-C	10.14	122.38	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	136	TYR	N-CA-C	10.07	121.85	111.07
1	4	112	LEU	N-CA-C	10.05	124.34	109.07
1	5	136	TYR	N-CA-C	10.01	123.44	111.33
1	1	312	ASN	CA-CB-CG	9.97	122.57	112.60
1	5	230	VAL	N-CA-C	9.93	121.71	109.30
1	4	240	ASN	OD1-CG-ND2	-9.83	112.77	122.60
1	6	228	ASN	OD1-CG-ND2	-9.82	112.78	122.60
1	1	240	ASN	OD1-CG-ND2	-9.77	112.83	122.60
1	3	341	ASN	OD1-CG-ND2	-9.75	112.85	122.60
1	4	134	MET	N-CA-C	9.75	123.40	110.53
1	4	286	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	1	184	ASN	OD1-CG-ND2	-9.55	113.05	122.60
1	2	341	ASN	OD1-CG-ND2	-9.51	113.09	122.60
1	4	216	ASN	OD1-CG-ND2	-9.42	113.18	122.60
1	3	134	MET	N-CA-C	9.34	124.02	110.10
1	2	302	THR	N-CA-C	9.31	124.07	108.90
1	2	52	GLN	OE1-CD-NE2	-9.30	113.30	122.60
1	1	192	PHE	CA-CB-CG	-9.22	104.58	113.80
1	5	341	ASN	OD1-CG-ND2	-9.20	113.41	122.60
1	4	184	ASN	OD1-CG-ND2	-9.19	113.41	122.60
1	2	330	ASN	CA-CB-CG	9.19	121.79	112.60
1	3	120	HIS	CA-C-O	9.16	130.26	120.36
1	6	214	ASN	OD1-CG-ND2	-9.11	113.49	122.60
1	2	332	ILE	N-CA-C	9.11	119.70	110.23
1	6	252	ASN	OD1-CG-ND2	-9.08	113.52	122.60
1	5	312	ASN	OD1-CG-ND2	-9.07	113.53	122.60
1	3	283	HIS	CA-CB-CG	9.04	122.84	113.80
1	4	248	GLN	OE1-CD-NE2	-9.03	113.57	122.60
1	1	312	ASN	OD1-CG-ND2	-9.00	113.60	122.60
1	1	230	VAL	N-CA-C	8.96	120.49	109.30
1	2	316	ASN	OD1-CG-ND2	-8.93	113.67	122.60
1	6	83	HIS	CB-CG-CD2	-8.90	119.63	131.20
1	1	228	ASN	OD1-CG-ND2	-8.89	113.71	122.60
1	5	152	ASP	CA-CB-CG	8.89	121.49	112.60
1	3	316	ASN	OD1-CG-ND2	-8.88	113.72	122.60
1	3	252	ASN	N-CA-C	8.86	121.90	111.71
1	3	286	GLN	OE1-CD-NE2	-8.84	113.76	122.60
1	4	62	VAL	N-CA-C	8.81	122.86	109.20
1	5	38	GLN	OE1-CD-NE2	-8.78	113.82	122.60
1	6	302	THR	N-CA-C	8.77	123.96	109.06
1	1	121	LEU	N-CA-C	8.75	119.66	109.60
1	3	336	SER	N-CA-C	8.75	120.74	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	83	HIS	CB-CG-CD2	-8.72	119.87	131.20
1	5	134	MET	N-CA-C	8.63	122.95	110.10
1	1	187	GLN	OE1-CD-NE2	-8.61	113.99	122.60
1	6	203	HIS	CA-CB-CG	-8.61	105.19	113.80
1	3	241	PHE	N-CA-C	8.55	123.00	109.50
1	3	335	ASN	OD1-CG-ND2	-8.55	114.05	122.60
1	6	249	ASP	CA-CB-CG	8.51	121.11	112.60
1	1	103	ASN	OD1-CG-ND2	-8.49	114.11	122.60
1	2	330	ASN	CA-C-N	8.48	132.60	120.56
1	2	330	ASN	C-N-CA	8.48	132.60	120.56
1	4	38	GLN	OE1-CD-NE2	-8.47	114.13	122.60
1	6	83	HIS	CB-CG-ND1	8.46	135.40	122.70
1	4	61	ILE	N-CA-CB	-8.44	99.77	111.25
1	5	312	ASN	N-CA-C	8.42	122.98	110.52
1	4	213	ASN	OD1-CG-ND2	-8.41	114.19	122.60
1	5	103	ASN	CA-CB-CG	-8.41	104.19	112.60
1	6	103	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	1	28	ASP	N-CA-C	8.38	128.66	110.80
1	3	302	THR	N-CA-C	8.36	122.52	108.90
1	4	341	ASN	OD1-CG-ND2	-8.31	114.29	122.60
1	4	237	PHE	N-CA-C	8.31	122.77	110.48
1	5	85	ILE	CB-CG1-CD1	8.24	131.10	113.80
1	6	283	HIS	CA-CB-CG	8.23	122.03	113.80
1	3	214	ASN	OD1-CG-ND2	-8.21	114.39	122.60
1	5	248	GLN	OE1-CD-NE2	-8.20	114.40	122.60
1	1	28	ASP	CA-C-O	8.20	132.23	120.51
1	5	214	ASN	OD1-CG-ND2	-8.18	114.42	122.60
1	3	240	ASN	OD1-CG-ND2	-8.18	114.42	122.60
1	1	335	ASN	OD1-CG-ND2	-8.17	114.43	122.60
1	3	48	ASN	OD1-CG-ND2	-8.16	114.44	122.60
1	6	230	VAL	N-CA-C	8.14	119.92	108.93
1	3	169	HIS	CB-CG-CD2	-8.13	120.63	131.20
1	4	48	ASN	OD1-CG-ND2	-8.13	114.47	122.60
1	3	239	SER	N-CA-C	8.11	121.80	109.23
1	3	323	ILE	N-CA-C	8.09	119.53	107.80
1	6	330	ASN	OD1-CG-ND2	-8.06	114.53	122.60
1	2	286	GLN	OE1-CD-NE2	-8.06	114.54	122.60
1	5	57	PHE	N-CA-C	8.06	121.23	111.40
1	6	316	ASN	OD1-CG-ND2	-8.06	114.54	122.60
1	2	48	ASN	OD1-CG-ND2	-8.04	114.56	122.60
1	6	48	ASN	OD1-CG-ND2	-8.01	114.59	122.60
1	4	139	LEU	N-CA-C	7.99	122.61	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	330	ASN	OD1-CG-ND2	-7.99	114.61	122.60
1	5	286	GLN	OE1-CD-NE2	-7.98	114.62	122.60
1	4	295	LEU	N-CA-C	7.98	121.32	109.59
1	6	315	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	3	140	TYR	O-C-N	-7.95	112.02	122.59
1	6	248	GLN	OE1-CD-NE2	-7.94	114.66	122.60
1	1	58	LYS	N-CA-C	7.93	127.69	110.80
1	2	312	ASN	OD1-CG-ND2	-7.87	114.73	122.60
1	3	301	ASP	N-CA-C	7.86	120.90	110.53
1	2	216	ASN	N-CA-C	7.84	122.60	112.41
1	4	312	ASN	N-CA-C	7.82	122.75	110.32
1	5	273	PHE	CA-CB-CG	7.80	121.60	113.80
1	1	140	TYR	O-C-N	-7.77	112.25	122.59
1	6	335	ASN	OD1-CG-ND2	-7.76	114.84	122.60
1	5	67	CYS	N-CA-C	7.75	120.63	111.71
1	5	319	LEU	N-CA-C	7.74	121.53	109.07
1	4	83	HIS	CB-CG-CD2	-7.73	121.15	131.20
1	6	297	ALA	N-CA-C	7.73	121.82	108.76
1	4	125	LYS	CA-CB-CG	7.70	129.50	114.10
1	6	177	GLN	OE1-CD-NE2	-7.68	114.92	122.60
1	4	105	PHE	N-CA-C	7.68	127.15	110.80
1	1	33	HIS	CB-CG-CD2	-7.68	121.22	131.20
1	3	216	ASN	OD1-CG-ND2	-7.67	114.93	122.60
1	4	120	HIS	N-CA-C	7.67	121.67	108.02
1	4	252	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	5	59	ASP	CA-CB-CG	7.62	120.22	112.60
1	1	302	THR	N-CA-C	7.61	121.03	109.23
1	3	320	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	3	237	PHE	N-CA-C	7.59	121.64	110.17
1	2	216	ASN	OD1-CG-ND2	-7.59	115.01	122.60
1	5	160	LEU	N-CA-C	7.58	121.81	109.76
1	6	237	PHE	N-CA-C	7.58	120.31	110.53
1	2	316	ASN	CA-CB-CG	7.58	120.18	112.60
1	5	62	VAL	N-CA-C	7.55	119.71	108.46
1	4	111	LEU	N-CA-C	7.54	121.21	109.52
1	6	208	ASP	CA-CB-CG	7.54	120.14	112.60
1	4	335	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	6	216	ASN	OD1-CG-ND2	-7.53	115.07	122.60
1	2	29	HIS	CB-CG-CD2	-7.52	121.43	131.20
1	3	33	HIS	CB-CG-CD2	-7.51	121.44	131.20
1	6	312	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	3	121	LEU	N-CA-C	7.49	119.15	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	286	GLN	OE1-CD-NE2	-7.48	115.12	122.60
1	6	216	ASN	N-CA-C	7.44	121.20	112.72
1	3	83	HIS	CB-CG-ND1	7.43	133.85	122.70
1	2	331	GLY	O-C-N	-7.40	115.11	123.62
1	2	330	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	3	259	ASP	CA-CB-CG	7.39	119.99	112.60
1	6	184	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	5	216	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	3	83	HIS	CB-CG-CD2	-7.36	121.64	131.20
1	3	33	HIS	CB-CG-ND1	7.35	133.72	122.70
1	2	296	ASP	CA-CB-CG	7.33	119.93	112.60
1	3	195	SER	N-CA-C	7.30	125.94	109.81
1	1	239	SER	N-CA-C	7.30	120.55	109.23
1	2	297	ALA	N-CA-C	7.28	121.30	109.59
1	5	264	ALA	N-CA-C	7.28	116.69	108.25
1	1	316	ASN	OD1-CG-ND2	-7.27	115.33	122.60
1	6	316	ASN	CA-CB-CG	7.27	119.87	112.60
1	4	61	ILE	N-CA-C	7.27	118.35	108.17
1	4	87	VAL	N-CA-C	7.27	118.36	107.75
1	3	301	ASP	CA-CB-CG	7.26	119.86	112.60
1	2	60	LYS	N-CA-C	7.26	120.81	110.14
1	1	214	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	2	67	CYS	N-CA-C	7.26	121.23	112.38
1	6	341	ASN	N-CA-C	7.24	119.17	108.60
1	5	320	ASN	CA-CB-CG	7.24	119.84	112.60
1	3	120	HIS	N-CA-C	7.23	120.69	108.90
1	4	329	SER	N-CA-C	7.23	120.26	108.26
1	5	177	GLN	OE1-CD-NE2	-7.22	115.38	122.60
1	5	330	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	2	176	SER	CB-CA-C	-7.20	98.89	110.84
1	5	270	PRO	N-CA-C	7.20	122.52	111.15
1	4	231	LYS	N-CA-C	7.20	119.51	109.15
1	3	103	ASN	OD1-CG-ND2	-7.19	115.41	122.60
1	2	177	GLN	OE1-CD-NE2	-7.17	115.43	122.60
1	5	79	HIS	CA-CB-CG	-7.16	106.64	113.80
1	2	315	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	6	136	TYR	N-CA-C	7.14	126.02	110.80
1	6	52	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	4	131	SER	N-CA-C	7.13	121.32	108.69
1	4	52	GLN	OE1-CD-NE2	-7.13	115.47	122.60
1	4	107	ASP	CA-CB-CG	7.12	119.72	112.60
1	2	133	TRP	N-CA-C	7.10	121.17	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	208	ASP	CA-CB-CG	7.07	119.67	112.60
1	3	240	ASN	N-CA-C	7.07	120.38	108.23
1	3	173	LEU	N-CA-C	7.05	120.89	109.40
1	1	53	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	2	273	PHE	CA-CB-CG	7.03	120.83	113.80
1	4	313	GLU	N-CA-C	7.03	122.97	111.37
1	5	71	ILE	N-CA-C	7.02	117.73	110.36
1	1	248	GLN	CG-CD-NE2	7.00	126.91	116.40
1	5	315	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	1	137	PHE	CA-CB-CG	6.96	120.76	113.80
1	2	213	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	6	38	GLN	CG-CD-NE2	6.96	126.84	116.40
1	2	320	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	5	332	ILE	N-CA-C	6.95	123.79	109.34
1	6	319	LEU	N-CA-C	6.94	119.72	108.41
1	2	230	VAL	N-CA-C	6.92	118.71	109.37
1	4	53	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	4	234	ASP	CA-CB-CG	6.91	119.51	112.60
1	3	306	GLU	N-CA-C	6.90	120.91	108.69
1	1	319	LEU	N-CA-C	6.89	119.96	108.73
1	2	317	ARG	CA-CB-CG	-6.88	100.33	114.10
1	6	216	ASN	CA-CB-CG	6.88	119.47	112.60
1	1	26	SER	N-CA-C	6.87	120.60	109.40
1	4	125	LYS	N-CA-C	6.86	118.92	109.18
1	1	107	ASP	CA-CB-CG	6.85	119.45	112.60
1	1	52	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	2	187	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	6	134	MET	N-CA-C	6.85	120.42	110.28
1	5	237	PHE	N-CA-C	6.82	120.17	110.14
1	1	312	ASN	N-CA-C	6.81	120.92	110.36
1	1	216	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	1	282	THR	O-C-N	-6.80	115.39	123.27
1	5	33	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	4	63	LEU	N-CA-C	6.76	120.06	108.02
1	1	258	PHE	N-CA-C	6.76	119.45	109.24
1	1	339	ARG	N-CA-C	6.76	119.44	108.76
1	6	53	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	4	164	ASP	CA-CB-CG	6.74	119.34	112.60
1	4	103	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	3	319	LEU	N-CA-C	6.72	119.47	108.52
1	1	315	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	4	69	THR	CB-CA-C	-6.70	97.09	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	228	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	1	60	LYS	N-CA-C	6.69	120.42	110.52
1	1	279	ALA	O-C-N	-6.68	116.33	121.14
1	2	38	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	6	103	ASN	CB-CG-ND2	6.68	126.42	116.40
1	1	134	MET	N-CA-C	6.68	120.16	110.28
1	5	184	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	4	319	LEU	N-CA-C	6.66	120.09	109.24
1	3	330	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	1	326	LYS	CA-CB-CG	6.66	127.41	114.10
1	3	262	PHE	N-CA-C	6.66	119.04	110.39
1	6	79	HIS	CA-CB-CG	-6.65	107.15	113.80
1	1	38	GLN	OE1-CD-NE2	-6.64	115.95	122.60
1	6	140	TYR	O-C-N	-6.64	113.75	122.59
1	1	193	ASP	CA-CB-CG	6.64	119.24	112.60
1	1	120	HIS	CB-CG-CD2	-6.64	122.57	131.20
1	3	83	HIS	CA-CB-CG	-6.64	107.16	113.80
1	6	295	LEU	N-CA-C	6.63	119.85	109.96
1	1	252	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	3	67	CYS	N-CA-C	6.61	119.31	111.71
1	5	186	TRP	CG-CD2-CE3	6.60	140.50	133.90
1	6	54	LYS	N-CA-C	6.60	120.20	111.75
1	4	114	GLY	N-CA-C	6.59	120.76	111.00
1	3	58	LYS	N-CA-C	6.59	124.84	110.80
1	6	341	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	3	169	HIS	CB-CG-ND1	6.56	132.55	122.70
1	3	286	GLN	CG-CD-NE2	6.55	126.22	116.40
1	5	335	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	2	145	ASP	CA-CB-CG	6.53	119.13	112.60
1	1	216	ASN	CB-CG-ND2	6.52	126.18	116.40
1	3	167	SER	N-CA-C	6.50	120.20	108.69
1	2	52	GLN	CG-CD-NE2	6.49	126.14	116.40
1	4	330	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	3	312	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	6	240	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	3	250	MET	N-CA-C	6.47	118.70	108.67
1	3	248	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	6	330	ASN	CB-CG-ND2	6.44	126.06	116.40
1	1	240	ASN	CB-CG-ND2	6.43	126.05	116.40
1	4	169	HIS	CB-CG-CD2	-6.43	122.83	131.20
1	1	126	VAL	N-CA-CB	-6.43	103.71	110.72
1	5	320	ASN	OD1-CG-ND2	-6.42	116.18	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	240	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	5	58	LYS	N-CA-C	6.41	124.44	110.80
1	4	160	LEU	N-CA-C	6.40	119.14	108.96
1	3	187	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	3	186	TRP	CB-CG-CD1	-6.37	117.34	126.90
1	2	137	PHE	CA-CB-CG	6.37	120.17	113.80
1	3	38	GLN	OE1-CD-NE2	-6.37	116.23	122.60
1	6	186	TRP	N-CA-C	6.36	120.76	113.19
1	5	295	LEU	N-CA-C	6.35	118.30	109.15
1	4	247	ARG	O-C-N	-6.35	116.94	123.29
1	1	203	HIS	CA-CB-CG	-6.34	107.46	113.80
1	6	327	PHE	CA-CB-CG	6.32	120.12	113.80
1	4	239	SER	N-CA-C	6.31	119.69	109.40
1	5	103	ASN	N-CA-C	6.30	120.65	113.15
1	5	39	ASP	CA-CB-CG	6.30	118.90	112.60
1	2	330	ASN	O-C-N	6.28	130.58	123.42
1	3	252	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	2	330	ASN	CB-CG-ND2	6.28	125.82	116.40
1	2	83	HIS	CB-CG-ND1	6.26	132.09	122.70
1	2	152	ASP	CA-CB-CG	6.25	118.85	112.60
1	5	52	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	6	186	TRP	CB-CG-CD1	-6.24	117.54	126.90
1	5	38	GLN	CG-CD-NE2	6.23	125.74	116.40
1	2	312	ASN	CB-CG-ND2	6.21	125.72	116.40
1	3	205	PRO	CA-C-N	-6.20	115.51	123.19
1	3	205	PRO	C-N-CA	-6.20	115.51	123.19
1	6	186	TRP	CG-CD2-CE3	6.19	140.09	133.90
1	3	312	ASN	N-CA-C	6.19	119.79	109.95
1	5	164	ASP	CA-CB-CG	6.19	118.79	112.60
1	1	151	ARG	CB-CG-CD	6.18	125.53	111.30
1	2	151	ARG	CA-CB-CG	6.18	126.47	114.10
1	2	319	LEU	N-CA-C	6.18	118.48	108.41
1	5	268	LYS	N-CA-C	6.18	118.78	108.96
1	1	268	LYS	O-C-N	-6.17	116.15	123.06
1	2	283	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	2	318	ASP	CA-CB-CG	6.17	118.77	112.60
1	5	124	PRO	N-CA-C	6.16	125.16	112.47
1	6	272	GLU	CA-CB-CG	6.16	126.42	114.10
1	5	252	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	1	184	ASN	CB-CG-ND2	6.15	125.63	116.40
1	4	228	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	6	278	HIS	CA-CB-CG	6.15	119.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	33	HIS	CA-CB-CG	-6.14	107.66	113.80
1	1	295	LEU	N-CA-C	6.14	118.65	109.25
1	3	273	PHE	N-CA-C	6.14	118.40	109.07
1	4	107	ASP	N-CA-C	6.13	118.77	111.71
1	5	213	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	1	29	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	2	234	ASP	CA-CB-CG	6.11	118.71	112.60
1	3	316	ASN	CB-CG-ND2	6.09	125.54	116.40
1	3	137	PHE	N-CA-C	-6.09	103.20	111.55
1	4	75	PHE	CA-CB-CG	6.08	119.88	113.80
1	5	187	GLN	OE1-CD-NE2	-6.08	116.52	122.60
1	4	303	ILE	CA-C-O	6.07	126.70	120.39
1	3	285	LYS	CB-CA-C	-6.05	109.58	116.54
1	4	168	ILE	N-CA-C	6.04	117.00	108.36
1	3	177	GLN	OE1-CD-NE2	-6.04	116.56	122.60
1	6	213	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	5	297	ALA	N-CA-C	6.02	119.35	109.72
1	4	126	VAL	N-CA-C	6.02	117.36	108.45
1	3	332	ILE	N-CA-C	6.01	118.56	111.05
1	1	272	GLU	CA-CB-CG	6.00	126.10	114.10
1	3	318	ASP	CA-CB-CG	6.00	118.60	112.60
1	3	156	VAL	N-CA-C	5.99	121.79	109.34
1	5	89	MET	N-CA-C	5.97	120.08	113.21
1	4	83	HIS	CB-CG-ND1	5.97	131.66	122.70
1	3	263	PRO	N-CA-CB	5.97	108.62	103.31
1	3	105	PHE	N-CA-C	5.96	122.56	113.61
1	5	188	ASP	CA-C-O	5.96	126.77	120.33
1	6	264	ALA	N-CA-C	5.96	115.17	108.25
1	6	335	ASN	N-CA-C	5.96	118.57	111.71
1	5	248	GLN	CA-CB-CG	5.96	126.01	114.10
1	5	282	THR	O-C-N	-5.96	116.00	123.27
1	6	186	TRP	CE2-CD2-CG	-5.95	100.06	107.20
1	4	32	ILE	N-CA-C	5.95	121.71	109.34
1	5	313	GLU	CB-CA-C	-5.95	101.47	110.92
1	1	228	ASN	CB-CG-ND2	5.94	125.31	116.40
1	2	140	TYR	O-C-N	-5.93	114.70	122.59
1	2	164	ASP	CA-CB-CG	5.93	118.53	112.60
1	4	58	LYS	N-CA-C	5.92	123.41	110.80
1	1	332	ILE	CB-CG1-CD1	-5.92	101.37	113.80
1	5	59	ASP	CA-C-O	5.91	125.30	118.97
1	1	59	ASP	CA-CB-CG	5.91	118.51	112.60
1	3	62	VAL	N-CA-C	5.91	116.44	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	187	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	4	249	ASP	N-CA-C	5.90	116.20	107.88
1	3	297	ALA	N-CA-C	5.89	119.55	110.42
1	1	120	HIS	CB-CG-ND1	5.89	131.53	122.70
1	1	341	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	4	316	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	3	71	ILE	O-C-N	-5.88	116.16	121.87
1	2	250	MET	O-C-N	-5.87	116.33	123.19
1	3	335	ASN	CB-CG-ND2	5.87	125.20	116.40
1	4	119	VAL	O-C-N	-5.86	116.73	123.00
1	4	315	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	1	33	HIS	CB-CG-ND1	5.85	131.47	122.70
1	1	206	ILE	CB-CA-C	-5.85	102.89	110.84
1	5	120	HIS	N-CA-C	5.85	123.25	110.80
1	4	92	ILE	O-C-N	-5.84	116.20	121.87
1	2	293	ASP	O-C-N	-5.84	116.36	123.19
1	1	169	HIS	CB-CG-CD2	-5.83	123.61	131.20
1	4	177	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	4	123	PHE	N-CA-C	5.83	119.02	110.10
1	6	239	SER	N-CA-C	5.82	117.82	109.14
1	2	169	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	1	140	TYR	CA-C-O	-5.82	112.19	120.51
1	1	24	PHE	N-CA-C	5.82	118.93	108.17
1	1	25	ASP	CA-CB-CG	5.82	118.42	112.60
1	1	133	TRP	CG-CD2-CE3	5.82	139.72	133.90
1	6	160	LEU	N-CA-C	5.81	119.10	109.46
1	3	246	LYS	N-CA-C	5.81	118.56	111.82
1	5	258	PHE	N-CA-C	5.80	118.22	109.23
1	1	297	ALA	N-CA-C	5.80	119.50	110.17
1	3	224	GLU	CA-CB-CG	5.80	125.69	114.10
1	3	289	PHE	CA-CB-CG	-5.80	108.00	113.80
1	4	205	PRO	N-CA-CB	5.80	107.11	103.23
1	1	348	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	2	284	TRP	CG-CD2-CE3	5.79	139.69	133.90
1	3	112	LEU	CA-C-O	5.79	126.69	120.32
1	4	246	LYS	N-CA-C	5.78	120.17	113.18
1	3	186	TRP	CG-CD2-CE3	5.78	139.68	133.90
1	5	140	TYR	O-C-N	-5.78	114.91	122.59
1	5	346	LEU	N-CA-C	5.77	118.29	108.02
1	5	48	ASN	CB-CG-ND2	5.76	125.04	116.40
1	5	312	ASN	CB-CG-ND2	5.76	125.04	116.40
1	4	232	ILE	N-CA-C	5.76	121.32	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	239	SER	N-CA-C	5.74	117.79	109.07
1	1	88	ASP	CA-CB-CG	5.73	118.33	112.60
1	6	169	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	3	133	TRP	N-CA-C	5.71	120.32	113.23
1	5	245	ALA	N-CA-C	5.70	118.60	110.10
1	6	88	ASP	O-C-N	-5.70	116.98	123.48
1	1	257	TRP	CG-CD2-CE3	5.70	139.60	133.90
1	5	203	HIS	CA-CB-CG	-5.70	108.10	113.80
1	4	348	HIS	CB-CG-CD2	-5.70	123.80	131.20
1	6	121	LEU	N-CA-C	5.70	117.68	109.48
1	2	238	LYS	O-C-N	-5.69	116.41	123.36
1	2	33	HIS	CA-CB-CG	-5.69	108.11	113.80
1	2	203	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	5	208	ASP	CA-CB-CG	5.68	118.28	112.60
1	1	67	CYS	N-CA-C	5.67	119.30	112.38
1	5	33	HIS	CA-CB-CG	-5.67	108.13	113.80
1	4	122	PRO	N-CA-C	5.67	124.16	112.47
1	2	252	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	5	119	VAL	CA-C-O	5.66	127.66	121.04
1	4	103	ASN	CA-CB-CG	-5.66	106.94	112.60
1	3	164	ASP	CA-CB-CG	5.65	118.25	112.60
1	6	293	ASP	O-C-N	-5.65	116.88	123.27
1	1	164	ASP	CA-CB-CG	5.64	118.24	112.60
1	1	272	GLU	N-CA-C	5.64	117.64	109.07
1	5	88	ASP	O-C-N	-5.64	116.99	123.42
1	6	325	TYR	N-CA-C	5.63	117.64	109.07
1	1	321	ILE	O-C-N	-5.63	117.27	123.18
1	4	258	PHE	N-CA-C	5.63	117.74	109.24
1	5	335	ASN	N-CA-C	5.63	119.66	112.34
1	2	119	VAL	N-CA-C	5.63	115.96	107.80
1	3	206	ILE	N-CA-C	5.61	116.03	108.17
1	3	335	ASN	CA-CB-CG	5.61	118.21	112.60
1	5	85	ILE	N-CA-CB	-5.61	104.65	111.21
1	5	125	LYS	CA-CB-CG	5.61	125.31	114.10
1	5	33	HIS	CB-CG-ND1	5.61	131.11	122.70
1	1	184	ASN	CA-CB-CG	-5.60	107.00	112.60
1	2	284	TRP	CE2-CD2-CG	-5.60	100.48	107.20
1	3	327	PHE	CA-CB-CG	5.60	119.40	113.80
1	4	33	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	4	262	PHE	N-CA-C	5.59	116.56	110.13
1	3	184	ASN	N-CA-C	5.59	118.90	111.75
1	1	24	PHE	CA-CB-CG	-5.57	108.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	216	ASN	N-CA-C	5.57	119.88	112.30
1	5	302	THR	N-CA-C	5.54	117.82	109.23
1	4	302	THR	N-CA-C	5.54	118.42	109.40
1	2	126	VAL	N-CA-CB	-5.53	102.92	110.56
1	2	166	CYS	N-CA-C	5.53	117.48	109.07
1	3	245	ALA	N-CA-C	5.53	118.26	109.96
1	3	53	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	4	187	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	1	262	PHE	N-CA-C	5.52	117.57	110.39
1	2	127	ASP	N-CA-C	5.52	120.13	112.90
1	4	248	GLN	CG-CD-NE2	5.52	124.68	116.40
1	2	276	GLY	N-CA-C	5.51	118.88	112.10
1	1	173	LEU	CD1-CG-CD2	-5.51	98.68	110.80
1	2	257	TRP	CE2-CD2-CG	-5.51	100.59	107.20
1	3	339	ARG	N-CA-C	5.50	118.67	110.52
1	2	29	HIS	CB-CG-ND1	5.50	130.95	122.70
1	3	248	GLN	CA-C-O	5.50	126.78	120.84
1	4	173	LEU	N-CA-C	5.50	118.42	109.24
1	4	33	HIS	CB-CG-ND1	5.49	130.94	122.70
1	1	283	HIS	CA-CB-CG	5.49	119.29	113.80
1	1	143	MET	CA-CB-CG	-5.48	103.13	114.10
1	6	83	HIS	N-CA-C	5.48	122.48	110.80
1	6	67	CYS	N-CA-C	5.48	119.07	112.38
1	4	240	ASN	CB-CG-ND2	5.48	124.61	116.40
1	4	82	LYS	N-CA-C	5.47	122.46	110.80
1	5	339	ARG	N-CA-C	5.47	118.38	109.24
1	6	145	ASP	CA-CB-CG	5.47	118.07	112.60
1	6	252	ASN	CB-CG-ND2	5.47	124.61	116.40
1	4	153	HIS	N-CA-C	5.45	120.42	113.55
1	2	198	VAL	O-C-N	-5.45	116.94	120.42
1	6	276	GLY	O-C-N	-5.44	115.83	122.03
1	4	55	ASP	CA-CB-CG	5.43	118.03	112.60
1	3	170	LEU	N-CA-C	5.42	117.22	109.14
1	3	325	TYR	N-CA-C	5.42	118.32	109.59
1	3	327	PHE	N-CA-C	5.42	117.83	107.75
1	4	85	ILE	O-C-N	-5.42	117.41	123.26
1	5	213	ASN	CA-CB-CG	5.42	118.02	112.60
1	1	127	ASP	CA-CB-CG	5.42	118.02	112.60
1	4	69	THR	N-CA-CB	5.41	119.63	110.49
1	2	335	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	4	93	ILE	CB-CA-C	-5.41	101.46	111.79
1	1	166	CYS	CA-CB-SG	-5.40	101.97	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	284	TRP	CE2-CD2-CG	-5.40	100.72	107.20
1	4	127	ASP	CA-CB-CG	5.40	118.00	112.60
1	6	267	GLY	CA-C-O	5.40	124.73	119.27
1	4	312	ASN	CA-CB-CG	5.40	118.00	112.60
1	4	79	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	4	264	ALA	O-C-N	-5.39	116.80	121.71
1	5	63	LEU	N-CA-C	5.39	117.31	108.52
1	1	320	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	2	184	ASN	CA-CB-CG	5.39	117.99	112.60
1	3	247	ARG	N-CA-C	5.39	116.17	108.74
1	2	341	ASN	CB-CG-ND2	5.38	124.47	116.40
1	4	269	ARG	N-CA-C	5.38	120.41	109.60
1	6	283	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	3	118	ASP	CA-CB-CG	5.37	117.97	112.60
1	4	246	LYS	CA-CB-CG	5.37	124.85	114.10
1	4	245	ALA	N-CA-C	5.37	117.48	109.59
1	6	58	LYS	N-CA-C	5.37	122.23	110.80
1	2	228	ASN	CB-CG-ND2	5.37	124.45	116.40
1	3	341	ASN	CB-CG-ND2	5.36	124.43	116.40
1	1	79	HIS	N-CA-C	5.35	118.64	112.97
1	2	151	ARG	NE-CZ-NH1	5.35	126.85	121.50
1	6	202	LEU	CD1-CG-CD2	-5.35	99.03	110.80
1	6	298	GLU	CA-CB-CG	5.35	124.79	114.10
1	5	186	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	5	257	TRP	N-CA-C	5.34	115.60	108.38
1	1	292	PRO	N-CA-C	-5.34	106.24	113.40
1	3	257	TRP	CB-CG-CD1	-5.34	118.89	126.90
1	4	284	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	3	220	ASP	N-CA-C	5.34	118.76	110.17
1	5	259	ASP	CA-CB-CG	5.33	117.93	112.60
1	2	302	THR	N-CA-CB	-5.33	101.73	110.68
1	5	198	VAL	CA-C-O	-5.33	115.12	118.69
1	5	284	TRP	CG-CD2-CE3	5.33	139.23	133.90
1	5	313	GLU	N-CA-C	5.33	117.52	111.02
1	2	39	ASP	CA-CB-CG	5.32	117.92	112.60
1	2	91	SER	N-CA-C	5.32	118.56	111.75
1	2	249	ASP	CA-CB-CG	5.31	117.91	112.60
1	3	290	TYR	CB-CA-C	-5.31	101.39	109.89
1	5	186	TRP	CB-CG-CD1	-5.31	118.94	126.90
1	1	186	TRP	CE2-CD2-CG	-5.30	100.84	107.20
1	3	285	LYS	CB-CG-CD	-5.30	99.12	111.30
1	2	136	TYR	O-C-N	-5.29	116.58	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	186	TRP	CD1-CG-CD2	5.29	114.77	106.30
1	3	89	MET	N-CA-C	5.29	119.37	113.02
1	1	283	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	4	325	TYR	N-CA-C	5.28	117.41	109.23
1	4	188	ASP	CA-CB-CG	5.28	117.88	112.60
1	2	121	LEU	N-CA-C	5.27	117.07	109.48
1	4	316	ASN	N-CA-C	5.27	120.64	113.37
1	1	186	TRP	CG-CD2-CE3	5.27	139.17	133.90
1	3	235	LEU	N-CA-C	5.27	119.42	112.89
1	4	259	ASP	CA-CB-CG	5.27	117.87	112.60
1	6	33	HIS	CA-CB-CG	-5.26	108.54	113.80
1	5	333	ASP	CA-CB-CG	5.26	117.86	112.60
1	6	116	LEU	N-CA-C	5.26	122.00	110.80
1	4	208	ASP	CA-CB-CG	5.25	117.85	112.60
1	2	184	ASN	CB-CG-ND2	5.25	124.27	116.40
1	3	112	LEU	N-CA-C	5.25	117.07	108.52
1	5	284	TRP	CG-CD1-NE1	-5.25	103.38	110.20
1	3	230	VAL	N-CA-C	5.24	116.34	109.58
1	4	266	LYS	N-CA-C	5.24	121.96	110.80
1	1	284	TRP	CG-CD2-CE3	5.24	139.13	133.90
1	5	276	GLY	CA-C-N	5.24	124.90	119.56
1	5	276	GLY	C-N-CA	5.24	124.90	119.56
1	6	346	LEU	N-CA-C	5.23	117.60	108.76
1	6	89	MET	N-CA-C	5.23	118.79	112.93
1	4	169	HIS	CB-CG-ND1	5.23	130.54	122.70
1	2	118	ASP	CA-CB-CG	5.23	117.83	112.60
1	4	272	GLU	N-CA-C	5.23	117.02	108.76
1	3	272	GLU	N-CA-C	5.22	116.92	109.14
1	6	129	ILE	N-CA-C	5.22	115.37	107.75
1	6	270	PRO	N-CA-C	5.22	119.29	111.14
1	5	284	TRP	CD1-CG-CD2	5.21	114.64	106.30
1	2	140	TYR	CA-C-O	-5.21	113.06	120.51
1	2	331	GLY	CA-C-O	-5.21	115.91	121.38
1	5	106	SER	N-CA-C	5.21	121.89	110.80
1	3	195	SER	O-C-N	-5.20	115.34	121.32
1	4	216	ASN	N-CA-C	5.20	119.38	112.30
1	4	230	VAL	N-CA-C	5.20	120.16	109.34
1	4	283	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	2	279	ALA	O-C-N	-5.20	116.93	121.35
1	3	283	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	4	140	TYR	O-C-N	-5.19	115.69	122.59
1	6	153	HIS	N-CA-C	5.19	119.70	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	295	LEU	O-C-N	-5.18	116.64	123.02
1	3	258	PHE	N-CA-C	5.18	117.69	109.50
1	5	120	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	4	206	ILE	N-CA-C	5.18	116.43	108.71
1	2	157	GLU	N-CA-C	5.18	121.83	110.80
1	3	257	TRP	N-CA-C	5.18	116.16	108.60
1	2	125	LYS	CA-C-O	5.17	127.71	120.52
1	3	257	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	4	89	MET	N-CA-C	5.16	118.70	110.70
1	4	132	GLU	N-CA-CB	-5.16	103.15	110.79
1	1	74	MET	CG-SD-CE	-5.16	89.55	100.90
1	3	291	PHE	CA-CB-CG	5.16	118.96	113.80
1	1	198	VAL	N-CA-CB	-5.15	107.07	110.52
1	1	330	ASN	CB-CG-ND2	5.15	124.13	116.40
1	4	216	ASN	CB-CG-ND2	5.15	124.13	116.40
1	6	258	PHE	N-CA-C	5.15	117.22	109.23
1	3	257	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	1	71	ILE	N-CA-C	5.14	115.76	110.36
1	1	220	ASP	CA-CB-CG	5.14	117.74	112.60
1	3	244	THR	O-C-N	-5.14	116.48	122.96
1	5	257	TRP	CE2-CD2-CG	-5.14	101.04	107.20
1	1	180	ASP	CA-CB-CG	5.13	117.73	112.60
1	4	252	ASN	N-CA-C	5.13	119.54	113.28
1	6	120	HIS	N-CA-C	5.13	117.62	107.98
1	3	243	LEU	N-CA-C	5.13	118.56	107.49
1	5	186	TRP	N-CA-C	5.12	119.15	113.01
1	1	91	SER	N-CA-C	5.11	118.98	112.34
1	2	151	ARG	N-CA-CB	-5.11	102.61	110.12
1	2	117	GLU	CB-CG-CD	5.11	121.28	112.60
1	2	153	HIS	N-CA-C	5.11	120.36	113.72
1	2	348	HIS	CE1-NE2-CD2	5.11	114.11	109.00
1	4	282	THR	O-C-N	-5.11	117.15	123.33
1	6	276	GLY	CA-C-N	5.11	124.77	119.56
1	6	276	GLY	C-N-CA	5.11	124.77	119.56
1	5	185	TYR	O-C-N	-5.10	116.71	122.12
1	6	321	ILE	O-C-N	-5.10	117.82	123.18
1	6	348	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	6	335	ASN	CB-CG-ND2	5.09	124.04	116.40
1	5	133	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	4	281	TYR	N-CA-C	5.09	117.42	110.24
1	3	79	HIS	N-CA-C	5.09	118.98	112.26
1	1	249	ASP	N-CA-C	5.09	116.57	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	192	PHE	N-CA-C	5.08	118.49	109.96
1	3	40	THR	N-CA-C	5.07	116.81	111.28
1	6	167	SER	O-C-N	-5.06	117.21	123.44
1	2	320	ASN	CB-CG-ND2	5.06	123.99	116.40
1	3	120	HIS	O-C-N	5.06	129.32	123.30
1	5	263	PRO	N-CA-CB	5.06	107.75	103.35
1	6	237	PHE	CA-CB-CG	5.06	118.86	113.80
1	2	258	PHE	N-CA-C	5.05	116.87	109.24
1	3	329	SER	N-CA-C	5.05	118.53	110.70
1	1	216	ASN	N-CA-C	5.04	118.96	112.41
1	3	186	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	6	120	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	4	61	ILE	CB-CA-C	5.03	118.33	110.83
1	4	264	ALA	CA-C-N	5.03	124.93	119.85
1	4	264	ALA	C-N-CA	5.03	124.93	119.85
1	3	137	PHE	N-CA-CB	-5.03	103.53	110.42
1	6	142	SER	N-CA-C	5.03	117.93	110.48
1	1	226	ASP	CA-CB-CG	5.03	117.63	112.60
1	4	64	ASP	N-CA-C	5.03	117.30	108.56
1	2	121	LEU	CA-C-N	5.02	124.81	119.28
1	2	121	LEU	C-N-CA	5.02	124.81	119.28
1	2	64	ASP	CA-C-O	5.02	125.76	120.54
1	3	303	ILE	N-CA-CB	5.02	117.02	110.99
1	4	176	SER	N-CA-C	5.02	119.66	111.37
1	3	240	ASN	CB-CG-ND2	5.02	123.93	116.40
1	1	257	TRP	N-CA-C	5.01	114.95	107.88
1	6	133	TRP	CE2-CD2-CG	-5.01	101.18	107.20
1	4	332	ILE	N-CA-C	5.01	119.76	109.34
1	1	112	LEU	CA-C-O	5.00	125.76	120.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	140	TYR	Sidechain
1	2	190	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2656	0	2579	36	0
1	2	2579	0	2526	25	0
1	3	2562	0	2512	47	0
1	4	2557	0	2510	54	0
1	5	2587	0	2530	38	0
1	6	2579	0	2526	33	0
All	All	15520	0	15183	216	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 7.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:87:VAL:HG11	1:4:116:LEU:HB2	1.53	0.88
1:4:170:LEU:HD12	1:4:254:ILE:HG21	1.53	0.87
1:2:242:LYS:HG3	1:2:304:GLU:HG2	1.60	0.82
1:4:89:MET:SD	1:4:115:LYS:HG2	2.20	0.81
1:4:112:LEU:HD23	1:4:121:LEU:HG	1.62	0.79
1:4:96:ALA:HA	1:4:99:LEU:HD12	1.69	0.75
1:1:308:VAL:HG22	1:1:322:LYS:HB3	1.70	0.72
1:5:170:LEU:HD22	1:5:222:LEU:HG	1.73	0.70
1:1:332:ILE:HD13	1:3:246:LYS:HA	1.74	0.69
1:6:130:ILE:HG22	1:6:162:PHE:HB2	1.74	0.69
1:5:93:ILE:HG21	1:5:113:ARG:HB2	1.73	0.69
1:1:205:PRO:HG2	1:1:347:MET:HG3	1.76	0.67
1:2:205:PRO:HG2	1:2:347:MET:HG3	1.76	0.67
1:3:74:MET:HE3	1:3:100:VAL:HA	1.75	0.67
1:2:170:LEU:HD13	1:2:243:LEU:HD21	1.77	0.67
1:3:192:PHE:CE2	1:4:74:MET:HB3	2.30	0.67
1:3:195:SER:O	1:3:198:VAL:HG22	1.97	0.65
1:5:130:ILE:HG22	1:5:162:PHE:HB2	1.80	0.64
1:5:222:LEU:HD11	1:5:307:LEU:HD13	1.80	0.64
1:1:248:GLN:HE21	1:3:247:ARG:NH2	1.96	0.63
1:4:62:VAL:HG12	1:4:128:ILE:HB	1.79	0.63
1:3:261:VAL:HG13	1:3:272:GLU:HB3	1.80	0.62
1:3:186:TRP:HA	1:3:189:VAL:HG23	1.82	0.61
1:5:74:MET:HB3	1:6:192:PHE:CE2	2.34	0.61
1:3:49:ALA:HA	1:3:271:VAL:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:87:VAL:HG22	1:2:112:LEU:HB2	1.83	0.60
1:4:128:ILE:HG12	1:4:160:LEU:HB2	1.83	0.59
1:4:67:CYS:SG	1:4:70:GLY:N	2.75	0.59
1:4:127:ASP:HA	1:4:156:VAL:HG22	1.85	0.59
1:6:116:LEU:HD21	1:6:150:ALA:HB2	1.84	0.58
1:2:33:HIS:HD2	1:2:36:MET:HE2	1.68	0.58
1:4:87:VAL:HG21	1:4:116:LEU:HD13	1.85	0.58
1:3:65:VAL:HB	1:3:131:SER:HB2	1.86	0.58
1:6:298:GLU:HG2	1:6:337:ARG:NH2	2.20	0.57
1:5:65:VAL:HB	1:5:131:SER:HB2	1.87	0.57
1:4:168:ILE:HD11	1:4:237:PHE:CZ	2.40	0.56
1:3:256:THR:HG22	1:3:287:THR:O	2.05	0.56
1:6:206:ILE:HG13	1:6:288:ILE:HB	1.87	0.56
1:2:83:HIS:HE1	1:2:110:THR:OG1	1.90	0.55
1:3:198:VAL:HG23	1:3:199:PRO:HD3	1.88	0.55
1:3:116:LEU:HD21	1:3:150:ALA:HB2	1.89	0.55
1:4:72:LEU:HD13	1:4:130:ILE:HG12	1.87	0.55
1:5:254:ILE:HD11	1:5:323:ILE:HD13	1.89	0.54
1:1:27:TYR:HB3	1:1:91:SER:OG	2.08	0.54
1:2:34:GLU:HG2	1:2:38:GLN:NE2	2.23	0.54
1:1:151:ARG:HG3	1:1:152:ASP:N	2.24	0.53
1:3:251:ILE:HG21	1:3:303:ILE:HD11	1.91	0.53
1:5:217:THR:HG22	1:5:245:ALA:HA	1.90	0.53
1:2:177:GLN:O	1:2:181:GLU:HG2	2.08	0.53
1:4:62:VAL:CG1	1:4:128:ILE:HB	2.39	0.53
1:4:307:LEU:HD12	1:4:323:ILE:HG12	1.89	0.52
1:6:85:ILE:HD12	1:6:122:PRO:HG2	1.91	0.52
1:1:173:LEU:HD22	1:1:175:ASP:HB2	1.92	0.52
1:3:222:LEU:HD21	1:3:307:LEU:HD23	1.91	0.52
1:1:56:LEU:O	1:1:60:LYS:HD2	2.10	0.52
1:3:170:LEU:HD12	1:3:254:ILE:HD13	1.91	0.52
1:3:206:ILE:HG23	1:3:288:ILE:HB	1.91	0.52
1:4:112:LEU:CD2	1:4:121:LEU:HG	2.38	0.52
1:3:205:PRO:HG2	1:3:347:MET:HG3	1.91	0.52
1:1:166:CYS:SG	1:1:225:PHE:HB2	2.50	0.52
1:4:206:ILE:HG13	1:4:288:ILE:HB	1.91	0.52
1:4:227:LEU:HA	1:4:230:VAL:HG12	1.92	0.52
1:1:173:LEU:HD12	1:1:255:VAL:HB	1.93	0.51
1:4:116:LEU:HA	1:4:119:VAL:HG12	1.92	0.51
1:3:63:LEU:HB2	1:3:126:VAL:HG21	1.91	0.51
1:4:93:ILE:HG12	1:4:112:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:128:ILE:HG23	1:4:160:LEU:HB2	1.92	0.51
1:1:130:ILE:HG22	1:1:162:PHE:HB2	1.93	0.51
1:4:61:ILE:HG23	1:4:126:VAL:HA	1.92	0.51
1:4:64:ASP:HA	1:4:130:ILE:O	2.11	0.51
1:4:166:CYS:SG	1:4:225:PHE:HB2	2.50	0.50
1:2:67:CYS:SG	1:2:93:ILE:HD11	2.52	0.50
1:3:32:ILE:O	1:3:36:MET:HG2	2.11	0.50
1:3:115:LYS:HG3	1:3:117:GLU:HG2	1.93	0.50
1:3:196:PRO:O	1:3:199:PRO:HD2	2.11	0.50
1:5:61:ILE:HD13	1:5:126:VAL:HA	1.93	0.50
1:2:308:VAL:HG22	1:2:322:LYS:HB3	1.94	0.50
1:1:127:ASP:HA	1:1:156:VAL:HG22	1.93	0.50
1:1:323:ILE:HD12	1:1:345:TYR:CE1	2.47	0.50
1:4:254:ILE:HG22	1:4:255:VAL:N	2.27	0.50
1:5:112:LEU:HD13	1:5:119:VAL:HG12	1.94	0.50
1:4:133:TRP:HB3	1:4:147:VAL:HG21	1.95	0.49
1:1:197:PHE:HE2	1:2:30:TYR:HB2	1.77	0.49
1:4:133:TRP:CZ3	1:4:144:MET:SD	3.05	0.49
1:2:254:ILE:HG23	1:2:291:PHE:CZ	2.47	0.49
1:2:62:VAL:HB	1:2:84:VAL:HG13	1.95	0.49
1:4:144:MET:HE2	1:4:235:LEU:HD21	1.93	0.49
1:6:212:ARG:HD3	1:6:278:HIS:HB3	1.94	0.49
1:3:74:MET:HE2	1:3:105:PHE:HD2	1.78	0.49
1:4:50:ILE:HG23	1:4:57:PHE:CZ	2.48	0.49
1:4:306:GLU:HB3	1:4:324:SER:OG	2.13	0.49
1:4:56:LEU:HG	1:4:160:LEU:HD11	1.95	0.49
1:6:254:ILE:HG23	1:6:291:PHE:CZ	2.48	0.48
1:3:63:LEU:HD21	1:3:116:LEU:HD11	1.95	0.48
1:3:162:PHE:HD1	1:3:262:PHE:HD1	1.61	0.48
1:6:265:PRO:HG2	1:6:268:LYS:HD2	1.94	0.48
1:3:192:PHE:HE1	1:4:78:LYS:HD2	1.77	0.48
1:5:95:MET:HE3	1:6:200:LEU:HD22	1.94	0.48
1:5:127:ASP:HA	1:5:156:VAL:HG22	1.96	0.48
1:6:340:LYS:HD3	1:6:341:ASN:N	2.28	0.48
1:5:151:ARG:HG3	1:5:152:ASP:N	2.29	0.48
1:6:248:GLN:HA	1:6:297:ALA:O	2.14	0.47
1:3:74:MET:HE2	1:3:105:PHE:CD2	2.49	0.47
1:5:112:LEU:HD11	1:5:122:PRO:HD3	1.96	0.47
1:4:275:THR:CA	1:4:282:THR:HG21	2.44	0.47
1:6:223:ILE:HG13	1:6:224:GLU:N	2.30	0.47
1:4:88:ASP:HB3	1:4:93:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:178:TYR:O	1:3:182:LYS:HG2	2.14	0.47
1:4:203:HIS:O	1:4:205:PRO:HD3	2.14	0.47
1:6:298:GLU:HG2	1:6:337:ARG:HH22	1.79	0.47
1:1:27:TYR:O	1:2:348:HIS:NE2	2.48	0.47
1:2:282:THR:OG1	1:2:284:TRP:HE3	1.98	0.47
1:3:307:LEU:HD11	1:3:321:ILE:HG23	1.97	0.47
1:1:196:PRO:O	1:1:199:PRO:HD2	2.15	0.47
1:4:275:THR:HA	1:4:282:THR:HG21	1.96	0.47
1:5:72:LEU:HB3	1:5:130:ILE:HD12	1.97	0.46
1:4:68:GLY:O	1:4:69:THR:HG23	2.15	0.46
1:2:170:LEU:HB3	1:2:256:THR:HG22	1.96	0.46
1:4:100:VAL:HG12	1:4:106:SER:HA	1.96	0.46
1:5:227:LEU:HA	1:5:230:VAL:HG12	1.96	0.46
1:1:178:TYR:CE1	1:1:182:LYS:HD2	2.51	0.46
1:2:323:ILE:HD12	1:2:345:TYR:CE1	2.51	0.46
1:3:162:PHE:HD1	1:3:262:PHE:CD1	2.34	0.46
1:4:205:PRO:HG2	1:4:347:MET:HG2	1.97	0.46
1:3:198:VAL:CG2	1:3:199:PRO:HD3	2.46	0.45
1:6:170:LEU:HD23	1:6:222:LEU:HD11	1.96	0.45
1:5:333:ASP:HB3	1:5:337:ARG:HD3	1.99	0.45
1:1:64:ASP:HB3	1:1:86:GLY:HA2	1.99	0.45
1:2:53:ASN:OD1	1:2:56:LEU:HD12	2.17	0.45
1:4:63:LEU:HD22	1:4:65:VAL:HG22	1.97	0.45
1:6:243:LEU:HB2	1:6:303:ILE:HB	1.99	0.45
1:3:256:THR:HG21	1:3:289:PHE:HE2	1.81	0.45
1:5:105:PHE:HE2	1:6:192:PHE:HE2	1.64	0.45
1:1:246:LYS:HA	1:5:332:ILE:HG13	1.99	0.45
1:2:129:ILE:HG23	1:2:161:ILE:HG12	1.99	0.44
1:2:156:VAL:O	1:2:158:GLY:N	2.51	0.44
1:3:265:PRO:HG2	1:3:268:LYS:HG3	1.98	0.44
1:4:143:MET:O	1:4:147:VAL:HG23	2.17	0.44
1:6:329:SER:HB3	1:6:334:GLY:HA2	1.99	0.44
1:1:222:LEU:HD11	1:1:307:LEU:HD13	1.99	0.44
1:4:93:ILE:HD11	1:4:113:ARG:HE	1.83	0.44
1:1:85:ILE:HD13	1:1:122:PRO:HD2	2.00	0.44
1:3:309:CYS:SG	1:3:319:LEU:HD22	2.57	0.44
1:4:92:ILE:O	1:4:95:MET:HB3	2.18	0.44
1:3:275:THR:O	1:3:286:GLN:NE2	2.50	0.44
1:4:121:LEU:HB3	1:4:122:PRO:HD2	1.98	0.44
1:6:216:ASN:ND2	1:6:251:ILE:HG12	2.33	0.44
1:1:59:ASP:O	1:1:82:LYS:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:140:TYR:CE2	1:5:347:MET:HB3	2.53	0.44
1:6:189:VAL:HG21	1:6:194:TYR:CD1	2.53	0.44
1:2:62:VAL:HB	1:2:84:VAL:HG22	1.99	0.43
1:6:329:SER:OG	1:6:337:ARG:NH2	2.52	0.43
1:1:248:GLN:OE1	1:3:213:ASN:HB3	2.19	0.43
1:3:170:LEU:HD22	1:3:222:LEU:HD13	2.00	0.43
1:4:93:ILE:HD12	1:4:94:GLU:N	2.32	0.43
1:6:309:CYS:SG	1:6:321:ILE:CD1	3.07	0.43
1:5:144:MET:SD	1:5:227:LEU:HD11	2.58	0.43
1:2:82:LYS:HB2	1:2:82:LYS:HE2	1.87	0.43
1:3:64:ASP:HB3	1:3:86:GLY:HA2	2.00	0.43
1:4:62:VAL:HG23	1:4:84:VAL:HB	2.00	0.43
1:4:162:PHE:HA	1:4:163:PRO:HA	1.84	0.43
1:1:134:MET:HG2	1:1:260:ILE:HD11	2.00	0.43
1:4:93:ILE:HG12	1:4:113:ARG:HA	2.01	0.43
1:1:333:ASP:HB2	1:1:337:ARG:HE	1.83	0.43
1:4:63:LEU:HB3	1:4:129:ILE:HG22	2.00	0.43
1:5:151:ARG:HG3	1:5:152:ASP:H	1.84	0.43
1:6:197:PHE:O	1:6:200:LEU:HB3	2.18	0.43
1:6:207:VAL:HG22	1:6:287:THR:HG23	2.01	0.43
1:1:194:TYR:C	1:1:196:PRO:HD2	2.44	0.43
1:3:254:ILE:HG13	1:3:289:PHE:HB2	2.01	0.43
1:1:58:LYS:HA	1:1:58:LYS:HD3	1.85	0.42
1:1:30:TYR:CD2	1:2:201:VAL:HG22	2.54	0.42
1:4:63:LEU:HB2	1:4:126:VAL:HG21	2.02	0.42
1:6:326:LYS:HB3	1:6:326:LYS:HE2	1.78	0.42
1:4:218:THR:O	1:4:243:LEU:HD22	2.19	0.42
1:5:64:ASP:HA	1:5:130:ILE:O	2.19	0.42
1:1:32:ILE:O	1:1:36:MET:HG2	2.20	0.42
1:5:206:ILE:HG13	1:5:288:ILE:HB	2.02	0.42
1:5:133:TRP:H	1:5:133:TRP:CD1	2.38	0.42
1:3:248:GLN:HA	1:3:297:ALA:O	2.20	0.42
1:5:151:ARG:HH21	1:5:231:LYS:NZ	2.18	0.42
1:2:130:ILE:HD13	1:2:130:ILE:HG21	1.90	0.42
1:5:262:PHE:O	1:5:270:PRO:HB3	2.18	0.42
1:1:71:ILE:HG23	1:1:72:LEU:N	2.34	0.42
1:5:105:PHE:HE2	1:6:192:PHE:CE2	2.38	0.42
1:6:84:VAL:HB	1:6:109:ILE:HG23	2.02	0.41
1:1:231:LYS:HD3	1:1:231:LYS:HA	1.84	0.41
1:5:54:LYS:HA	1:5:57:PHE:HB2	2.01	0.41
1:5:129:ILE:HG23	1:5:161:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:182:LYS:HD3	1:6:182:LYS:HA	1.74	0.41
1:3:36:MET:SD	1:3:283:HIS:CE1	3.14	0.41
1:3:100:VAL:HG21	1:3:111:LEU:HD11	2.01	0.41
1:1:212:ARG:CZ	1:5:250:MET:SD	3.08	0.41
1:2:227:LEU:HA	1:2:230:VAL:HG12	2.02	0.41
1:5:30:TYR:HB2	1:6:197:PHE:HE2	1.85	0.41
1:5:308:VAL:HG22	1:5:322:LYS:HB3	2.02	0.41
1:3:221:LYS:NZ	1:3:221:LYS:HB3	2.36	0.41
1:1:170:LEU:CD1	1:1:243:LEU:HD21	2.51	0.41
1:1:227:LEU:HA	1:1:230:VAL:HG12	2.03	0.41
1:1:248:GLN:NE2	1:3:247:ARG:NH2	2.67	0.41
1:3:307:LEU:HD13	1:3:323:ILE:HG12	2.02	0.41
1:4:63:LEU:HD22	1:4:65:VAL:CG2	2.50	0.41
1:4:238:LYS:HG3	1:4:308:VAL:HB	2.02	0.41
1:5:63:LEU:HD12	1:5:85:ILE:O	2.21	0.41
1:5:258:PHE:CE1	1:5:275:THR:HG21	2.56	0.41
1:6:151:ARG:HH21	1:6:231:LYS:NZ	2.19	0.41
1:1:275:THR:HG22	1:1:282:THR:HG21	2.02	0.41
1:3:74:MET:HE1	1:3:103:ASN:HB2	2.02	0.40
1:5:148:LEU:O	1:5:151:ARG:HG3	2.21	0.40
1:6:62:VAL:HA	1:6:128:ILE:O	2.20	0.40
1:4:243:LEU:HB2	1:4:303:ILE:CG2	2.51	0.40
1:3:205:PRO:HB3	1:3:289:PHE:CE1	2.55	0.40
1:3:322:LYS:HA	1:3:343:GLY:O	2.21	0.40
1:5:190:TYR:OH	1:6:40:THR:HA	2.21	0.40
1:5:282:THR:OG1	1:5:284:TRP:HE3	2.04	0.40
1:6:151:ARG:HG3	1:6:152:ASP:N	2.37	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	1	326/328 (99%)	304 (93%)	14 (4%)	8 (2%)	4	17
1	2	318/328 (97%)	295 (93%)	20 (6%)	3 (1%)	14	41
1	3	317/328 (97%)	275 (87%)	35 (11%)	7 (2%)	5	20
1	4	316/328 (96%)	273 (86%)	26 (8%)	17 (5%)	1	5
1	5	319/328 (97%)	284 (89%)	25 (8%)	10 (3%)	3	14
1	6	318/328 (97%)	290 (91%)	19 (6%)	9 (3%)	4	15
All	All	1914/1968 (97%)	1721 (90%)	139 (7%)	54 (3%)	4	15

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	140	TYR
1	1	157	GLU
1	1	334	GLY
1	2	140	TYR
1	2	157	GLU
1	3	58	LYS
1	3	140	TYR
1	4	32	ILE
1	4	58	LYS
1	4	105	PHE
1	4	136	TYR
1	4	232	ILE
1	5	58	LYS
1	5	120	HIS
1	5	123	PHE
1	5	140	TYR
1	5	157	GLU
1	5	332	ILE
1	5	334	GLY
1	6	58	LYS
1	6	116	LEU
1	6	140	TYR
1	1	28	ASP
1	2	58	LYS
1	3	157	GLU
1	3	219	SER
1	3	232	ILE
1	4	67	CYS
1	4	69	THR
1	4	81	ALA

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Mol	Chain	Res	Type
1	4	124	PRO
1	4	157	GLU
1	6	157	GLU
1	1	332	ILE
1	4	106	SER
1	4	116	LEU
1	4	122	PRO
1	4	140	TYR
1	4	156	VAL
1	4	266	LYS
1	5	91	SER
1	5	124	PRO
1	6	136	TYR
1	6	332	ILE
1	3	156	VAL
1	3	299	THR
1	4	82	LYS
1	6	91	SER
1	1	156	VAL
1	5	29	HIS
1	6	156	VAL
1	6	334	GLY
1	1	80	GLY
1	1	331	GLY

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	1	295/295 (100%)	282 (96%)	13 (4%)	25	59
1	2	287/295 (97%)	274 (96%)	13 (4%)	24	58
1	3	285/295 (97%)	272 (95%)	13 (5%)	24	57
1	4	285/295 (97%)	262 (92%)	23 (8%)	11	33
1	5	288/295 (98%)	271 (94%)	17 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6	287/295 (97%)	266 (93%)	21 (7%)	13	38
All	All	1727/1770 (98%)	1627 (94%)	100 (6%)	18	49

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	29	HIS
1	1	83	HIS
1	1	106	SER
1	1	132	GLU
1	1	145	ASP
1	1	197	PHE
1	1	216	ASN
1	1	227	LEU
1	1	316	ASN
1	1	333	ASP
1	1	335	ASN
1	1	340	LYS
1	1	348	HIS
1	2	45	SER
1	2	90	SER
1	2	129	ILE
1	2	132	GLU
1	2	151	ARG
1	2	170	LEU
1	2	209	THR
1	2	216	ASN
1	2	227	LEU
1	2	231	LYS
1	2	282	THR
1	2	308	VAL
1	2	348	HIS
1	3	83	HIS
1	3	132	GLU
1	3	180	ASP
1	3	187	GLN
1	3	221	LYS
1	3	224	GLU
1	3	238	LYS
1	3	244	THR
1	3	249	ASP
1	3	254	ILE

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Mol	Chain	Res	Type
1	3	261	VAL
1	3	286	GLN
1	3	298	GLU
1	4	62	VAL
1	4	63	LEU
1	4	71	ILE
1	4	93	ILE
1	4	103	ASN
1	4	120	HIS
1	4	126	VAL
1	4	134	MET
1	4	151	ARG
1	4	157	GLU
1	4	181	GLU
1	4	209	THR
1	4	211	GLU
1	4	216	ASN
1	4	231	LYS
1	4	240	ASN
1	4	249	ASP
1	4	266	LYS
1	4	268	LYS
1	4	278	HIS
1	4	303	ILE
1	4	333	ASP
1	4	348	HIS
1	5	43	THR
1	5	61	ILE
1	5	83	HIS
1	5	85	ILE
1	5	121	LEU
1	5	123	PHE
1	5	125	LYS
1	5	132	GLU
1	5	151	ARG
1	5	180	ASP
1	5	213	ASN
1	5	216	ASN
1	5	231	LYS
1	5	249	ASP
1	5	308	VAL
1	5	313	GLU

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Mol	Chain	Res	Type
1	5	348	HIS
1	6	43	THR
1	6	60	LYS
1	6	83	HIS
1	6	102	LEU
1	6	106	SER
1	6	132	GLU
1	6	151	ARG
1	6	157	GLU
1	6	197	PHE
1	6	206	ILE
1	6	212	ARG
1	6	216	ASN
1	6	227	LEU
1	6	232	ILE
1	6	247	ARG
1	6	266	LYS
1	6	278	HIS
1	6	287	THR
1	6	308	VAL
1	6	324	SER
1	6	348	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	38	GLN
1	1	52	GLN
1	2	33	HIS
1	2	52	GLN
1	2	83	HIS
1	2	169	HIS
1	2	187	GLN
1	2	203	HIS
1	2	216	ASN
1	3	83	HIS
1	3	169	HIS
1	3	216	ASN
1	3	283	HIS
1	4	169	HIS
1	4	187	GLN
1	4	240	ASN

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Mol	Chain	Res	Type
1	4	335	ASN
1	5	38	GLN
1	5	228	ASN
1	5	240	ASN
1	5	312	ASN
1	6	52	GLN
1	6	83	HIS
1	6	169	HIS
1	6	240	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.