



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:50 PM UTC

PDB ID : 2HWC / pdb_00002hwc
Title : A COMPARISON OF THE ANTI-RHINOVIRAL DRUG BINDING
POCKET IN HRV14 AND HRV1A
Authors : Kim, K.H.; Rossmann, M.G.
Deposited on : 1994-01-25
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

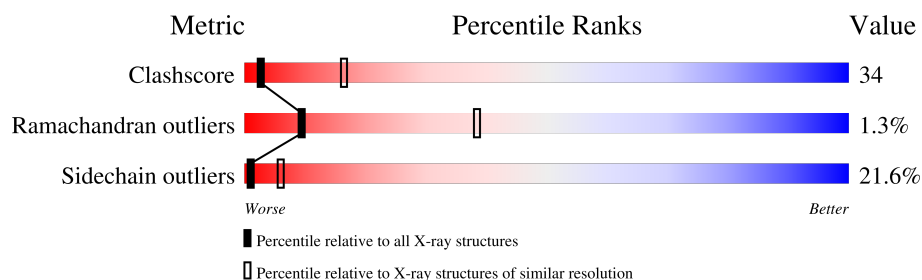
1 Overall quality at a glance

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)

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	289	
2	2	262	
3	3	236	
4	4	68	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6292 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
			1951	1237	330	372	12			

There is a discrepancy between the modelled and reference sequences:

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

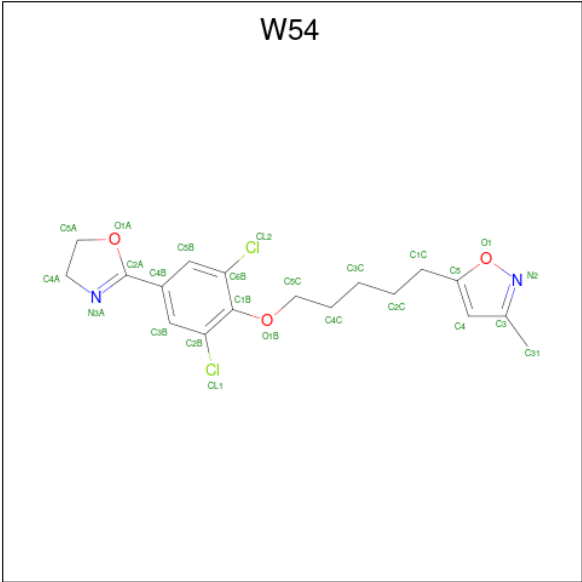
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

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-(5-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLY)PHENOXY)PENTYL)-3-METHYL ISOXAZOLE (CCD ID: W54) (formula: C₁₈H₂₀Cl₂N₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	1	1	25	18	2	2	3	0	0

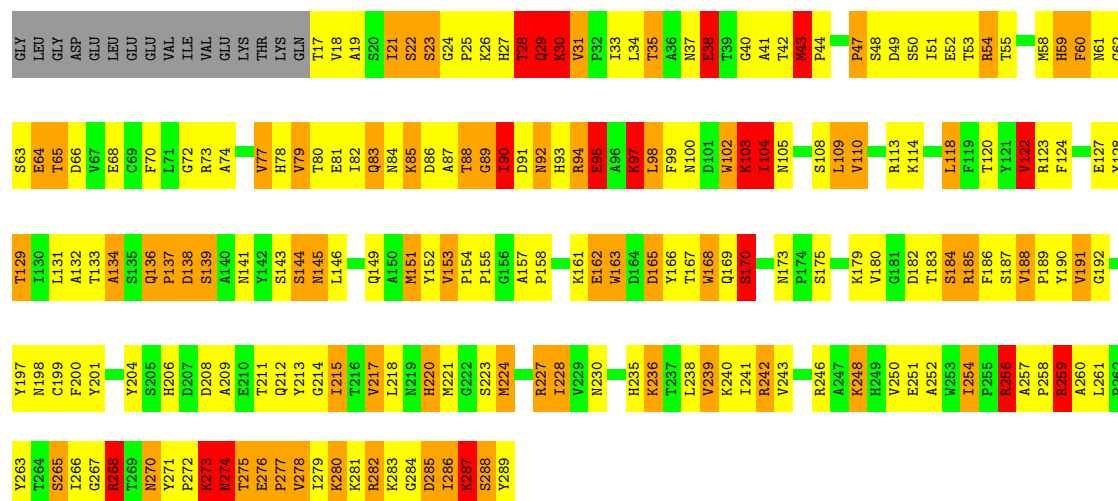
3 Residue-property plots

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.

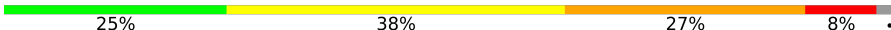
Note EDS was not executed.

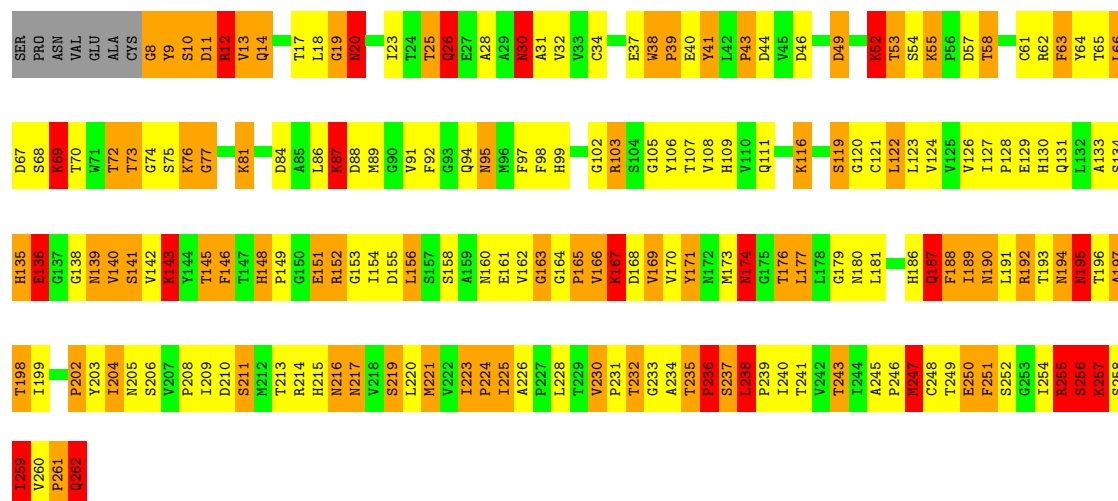
• Molecule 1: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

Chain 1: 



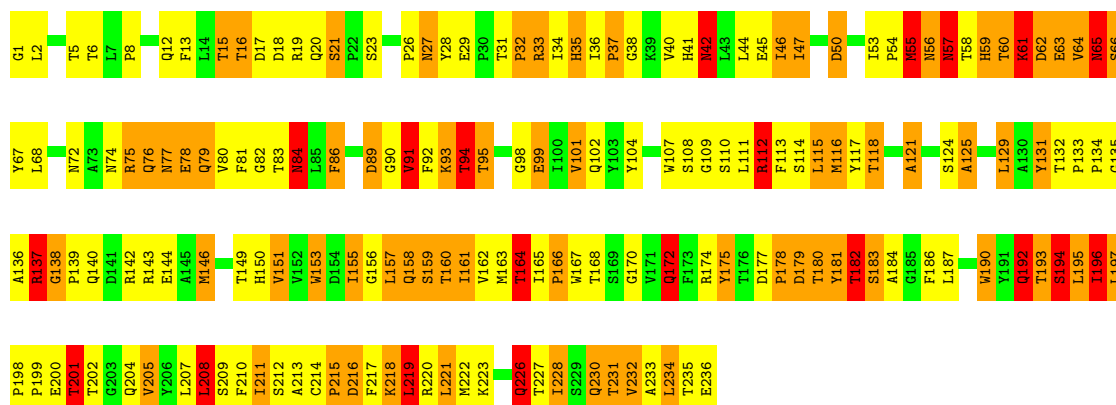
• Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)

Chain 2: 



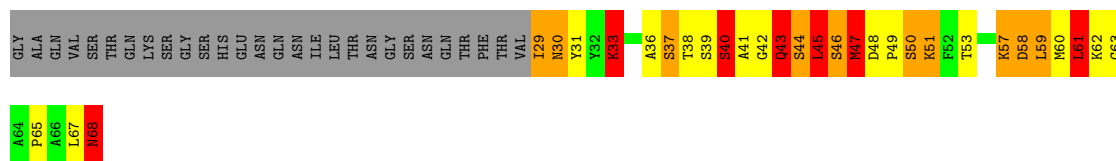
• Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)

Chain 3: 



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

Chain 4: 



4 Data and refinement statistics

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

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	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6292	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W54

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	2.02	69/2228 (3.1%)	2.41	162/3031 (5.3%)
2	2	2.43	96/2000 (4.8%)	2.76	190/2734 (6.9%)
3	3	2.45	80/1898 (4.2%)	2.80	188/2597 (7.2%)
4	4	2.64	14/302 (4.6%)	3.14	33/406 (8.1%)
All	All	2.31	259/6428 (4.0%)	2.68	573/8768 (6.5%)

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 (259) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	234	LEU	C-N	36.09	1.82	1.33
1	1	285	ASP	CA-CB	17.77	1.79	1.53
2	2	169	VAL	C-N	-16.99	1.10	1.33
4	4	41	ALA	C-O	13.29	1.41	1.24
3	3	57	ASN	CA-CB	12.81	1.75	1.53
4	4	42	GLY	N-CA	12.62	1.63	1.45
2	2	194	ASN	CA-CB	11.52	1.71	1.53
1	1	283	LYS	N-CA	10.92	1.61	1.46
1	1	144	SER	N-CA	10.40	1.58	1.45
3	3	164	THR	C-O	10.22	1.36	1.24
4	4	45	LEU	C-N	9.39	1.46	1.33
2	2	256	SER	C-O	9.29	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	187	GLN	N-CA	9.25	1.57	1.45
1	1	52	GLU	C-O	9.12	1.35	1.24
1	1	282	ARG	CD-NE	9.06	1.58	1.46
2	2	102	GLY	N-CA	8.93	1.54	1.45
2	2	152	ARG	CD-NE	8.87	1.58	1.46
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	8.51	1.30	1.23
3	3	50	ASP	CA-CB	-8.30	1.40	1.53
3	3	232	VAL	N-CA	8.25	1.55	1.46
1	1	73	ARG	C-O	7.95	1.33	1.23
3	3	138	GLY	N-CA	7.91	1.55	1.44
2	2	77	GLY	N-CA	7.88	1.53	1.45
1	1	285	ASP	N-CA	-7.83	1.34	1.45
2	2	236	PRO	C-O	7.83	1.34	1.24
2	2	161	GLU	CA-CB	-7.80	1.42	1.53
3	3	1	GLY	N-CA	7.66	1.57	1.45
2	2	135	HIS	CE1-NE2	-7.66	1.24	1.32
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	7.58	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	94	ARG	CD-NE	7.47	1.56	1.46
1	1	143	SER	C-O	7.44	1.33	1.24
1	1	28	THR	CA-CB	7.36	1.64	1.53
2	2	11	ASP	CA-CB	7.36	1.66	1.53
1	1	288	SER	C-O	7.29	1.32	1.23
3	3	60	THR	CA-CB	7.25	1.65	1.54
3	3	77	ASN	C-O	7.22	1.33	1.24
1	1	132	ALA	C-O	7.20	1.32	1.24
2	2	120	GLY	N-CA	7.16	1.53	1.45
2	2	260	VAL	N-CA	7.15	1.55	1.46
1	1	276	GLU	C-O	7.03	1.31	1.24
4	4	40	SER	CB-OG	7.03	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
2	2	58	THR	C-O	6.99	1.32	1.24
1	1	288	SER	CA-CB	6.89	1.65	1.53
2	2	74	GLY	C-O	6.88	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	49	PRO	C-N	-6.86	1.24	1.34
3	3	86	PHE	CA-CB	-6.84	1.42	1.52
1	1	23	SER	N-CA	6.84	1.54	1.45
1	1	133	THR	N-CA	6.83	1.54	1.45
2	2	194	ASN	N-CA	-6.79	1.37	1.45
3	3	216	ASP	CA-CB	6.79	1.64	1.53
1	1	91	ASP	N-CA	6.78	1.55	1.46
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	10	SER	C-N	-6.73	1.24	1.33
3	3	6	THR	N-CA	6.72	1.54	1.45
2	2	152	ARG	CZ-NH2	6.70	1.42	1.33
2	2	223	ILE	CA-CB	6.67	1.59	1.54
1	1	251	GLU	CA-CB	-6.67	1.42	1.53
2	2	256	SER	CB-OG	6.67	1.55	1.42
1	1	280	LYS	C-O	6.62	1.31	1.24
2	2	39	PRO	C-O	6.61	1.31	1.23
2	2	197	ALA	C-O	6.61	1.31	1.23
1	1	73	ARG	N-CA	6.59	1.53	1.45
3	3	156	GLY	C-O	-6.58	1.18	1.24
1	1	85	LYS	C-O	6.57	1.31	1.23
3	3	57	ASN	N-CA	-6.57	1.37	1.46
2	2	109	HIS	CE1-NE2	-6.54	1.26	1.32
3	3	15	THR	C-O	6.54	1.32	1.24
1	1	134	ALA	CA-CB	-6.53	1.42	1.53
3	3	57	ASN	C-N	-6.52	1.24	1.33
2	2	262	GLN	CD-OE1	6.51	1.35	1.23
4	4	62	LYS	C-O	6.50	1.31	1.24
2	2	52	LYS	CE-NZ	6.50	1.68	1.49
4	4	44	SER	CB-OG	6.49	1.55	1.42
2	2	9	TYR	N-CA	6.48	1.53	1.46
2	2	190	ASN	CA-CB	-6.48	1.44	1.53
1	1	79	VAL	C-N	-6.47	1.24	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	22	SER	C-N	-6.34	1.24	1.33
3	3	205	VAL	N-CA	6.32	1.53	1.46
1	1	95	GLU	CB-CG	6.31	1.71	1.52
2	2	8	GLY	N-CA	6.30	1.55	1.45
3	3	5	THR	C-O	6.28	1.31	1.24
3	3	165	ILE	N-CA	6.28	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	94	ARG	NE-CZ	6.25	1.40	1.33
2	2	259	ILE	C-O	6.24	1.31	1.24
4	4	63	GLY	N-CA	6.24	1.54	1.45
3	3	118	THR	CB-OG1	6.22	1.53	1.43
2	2	162	VAL	N-CA	6.16	1.53	1.46
3	3	16	THR	CA-CB	6.14	1.63	1.53
4	4	45	LEU	N-CA	6.14	1.55	1.46
1	1	184	SER	C-O	6.14	1.31	1.23
1	1	24	GLY	N-CA	6.14	1.53	1.44
3	3	182	THR	CA-CB	6.13	1.62	1.53
3	3	75	ARG	C-N	-6.13	1.25	1.33
1	1	251	GLU	N-CA	6.12	1.53	1.46
2	2	168	ASP	CA-CB	6.11	1.60	1.53
2	2	257	LYS	N-CA	6.11	1.54	1.46
4	4	33	LYS	CE-NZ	6.11	1.67	1.49
3	3	164	THR	N-CA	6.10	1.53	1.46
2	2	121	CYS	C-O	6.10	1.31	1.23
3	3	178	PRO	CA-CB	-6.10	1.45	1.53
3	3	215	PRO	CA-CB	-6.09	1.44	1.53
3	3	155	ILE	N-CA	6.05	1.53	1.46
1	1	28	THR	N-CA	-6.04	1.37	1.45
1	1	274	ASN	N-CA	6.04	1.53	1.46
3	3	57	ASN	C-O	6.03	1.31	1.24
2	2	19	GLY	C-N	-6.02	1.25	1.33
2	2	190	ASN	N-CA	6.02	1.54	1.46
1	1	131	LEU	C-O	6.02	1.31	1.23
3	3	110	SER	N-CA	5.99	1.52	1.45
2	2	208	PRO	C-N	-5.98	1.28	1.33
3	3	222	MET	CG-SD	5.94	1.95	1.80
3	3	36	ILE	N-CA	5.94	1.53	1.46
3	3	135	GLY	C-O	5.93	1.30	1.24
2	2	180	ASN	C-N	-5.92	1.25	1.33
2	2	17	THR	C-N	-5.90	1.25	1.33
1	1	88	THR	CB-OG1	5.89	1.53	1.43
3	3	175	TYR	CA-C	5.88	1.60	1.52
3	3	116	MET	N-CA	5.87	1.53	1.46
1	1	38	GLU	CB-CG	-5.85	1.34	1.52
2	2	103	ARG	C-O	5.85	1.31	1.23
3	3	213	ALA	C-O	5.83	1.30	1.23
3	3	2	LEU	CA-CB	5.81	1.63	1.52
3	3	41	HIS	CE1-NE2	5.81	1.38	1.32
3	3	27	ASN	C-N	-5.81	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	219	LEU	C-N	-5.80	1.26	1.33
2	2	88	ASP	C-O	5.80	1.32	1.24
2	2	135	HIS	CG-CD2	-5.79	1.29	1.35
1	1	239	VAL	C-O	5.76	1.30	1.24
2	2	171	TYR	C-O	5.74	1.31	1.24
2	2	176	THR	N-CA	5.74	1.53	1.45
1	1	276	GLU	N-CA	5.73	1.54	1.45
3	3	33	ARG	NE-CZ	5.73	1.39	1.33
3	3	38	GLY	CA-C	-5.73	1.43	1.51
2	2	152	ARG	NE-CZ	5.72	1.39	1.33
3	3	158	GLN	C-O	5.72	1.30	1.24
1	1	287	LYS	C-O	5.72	1.31	1.24
2	2	55	LYS	N-CA	5.71	1.53	1.46
2	2	54	SER	CA-CB	-5.71	1.44	1.53
1	1	274	ASN	CA-C	5.70	1.60	1.52
4	4	45	LEU	C-O	5.69	1.31	1.23
3	3	82	GLY	C-N	-5.68	1.26	1.33
3	3	201	THR	C-O	5.66	1.30	1.23
2	2	259	ILE	N-CA	5.66	1.53	1.46
2	2	63	PHE	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	87	LYS	CB-CG	-5.64	1.35	1.52
1	1	63	SER	CB-OG	-5.63	1.30	1.42
3	3	35	HIS	C-N	-5.63	1.27	1.33
3	3	82	GLY	N-CA	5.63	1.50	1.45
2	2	208	PRO	C-O	5.63	1.30	1.24
1	1	267	GLY	C-O	5.62	1.32	1.24
1	1	268	ARG	N-CA	5.61	1.52	1.45
2	2	103	ARG	N-CA	5.61	1.52	1.46
2	2	195	ASN	CA-CB	-5.60	1.44	1.54
1	1	285	ASP	C-N	5.60	1.40	1.33
3	3	140	GLN	C-N	-5.60	1.26	1.33
3	3	172	GLN	CG-CD	-5.59	1.38	1.52
4	4	51	LYS	CE-NZ	5.58	1.66	1.49
1	1	137	PRO	C-O	5.58	1.31	1.24
1	1	254	ILE	CA-CB	5.57	1.61	1.54
3	3	108	SER	CA-CB	-5.54	1.44	1.53
2	2	75	SER	C-O	5.53	1.30	1.23
2	2	168	ASP	C-N	-5.52	1.26	1.33
2	2	194	ASN	C-O	5.51	1.30	1.23
2	2	109	HIS	C-O	5.51	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	40	VAL	C-O	5.50	1.30	1.24
3	3	61	LYS	CE-NZ	5.50	1.65	1.49
2	2	237	SER	C-O	5.49	1.30	1.23
3	3	231	THR	CB-OG1	5.49	1.52	1.43
3	3	75	ARG	N-CA	5.48	1.52	1.45
2	2	151	GLU	CA-CB	-5.47	1.43	1.53
3	3	66	SER	N-CA	5.47	1.53	1.46
3	3	77	ASN	CG-OD1	5.47	1.33	1.23
2	2	153	GLY	C-N	-5.47	1.25	1.33
1	1	279	ILE	C-O	5.46	1.29	1.24
3	3	209	SER	N-CA	5.45	1.52	1.46
2	2	141	SER	N-CA	5.45	1.52	1.45
2	2	237	SER	N-CA	5.43	1.52	1.46
1	1	163	TRP	NE1-CE2	-5.43	1.31	1.37
1	1	25	PRO	C-N	-5.41	1.25	1.33
1	1	277	PRO	N-CA	5.40	1.53	1.47
3	3	37	PRO	CA-CB	-5.39	1.45	1.53
1	1	122	VAL	C-O	5.38	1.29	1.24
3	3	91	VAL	C-O	5.38	1.30	1.24
1	1	168	TRP	NE1-CE2	-5.37	1.31	1.37
2	2	61	CYS	CA-C	-5.37	1.47	1.53
1	1	270	ASN	CA-C	5.36	1.59	1.52
3	3	17	ASP	CG-OD1	5.36	1.35	1.25
3	3	74	ASN	CA-CB	5.34	1.61	1.53
2	2	103	ARG	CA-CB	-5.32	1.45	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
2	2	68	SER	CA-C	-5.31	1.45	1.52
1	1	127	GLU	CA-CB	-5.30	1.46	1.53
1	1	30	LYS	CE-NZ	5.29	1.65	1.49
2	2	211	SER	C-O	5.29	1.30	1.23
3	3	209	SER	C-O	5.29	1.30	1.23
2	2	14	GLN	CD-NE2	5.29	1.44	1.33
3	3	228	ILE	C-O	5.29	1.30	1.24
2	2	123	LEU	C-N	-5.28	1.26	1.33
1	1	33	ILE	C-O	5.27	1.30	1.24
2	2	72	THR	CB-OG1	5.27	1.52	1.43
2	2	99	HIS	C-N	-5.27	1.26	1.34
2	2	219	SER	N-CA	5.26	1.52	1.46
3	3	64	VAL	C-N	-5.25	1.25	1.33
4	4	61	LEU	C-O	5.25	1.30	1.24
2	2	246	PRO	C-O	5.23	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	164	THR	CA-CB	5.22	1.61	1.53
2	2	202	PRO	C-O	5.19	1.29	1.23
1	1	54	ARG	C-O	5.19	1.30	1.23
1	1	252	ALA	C-O	5.19	1.30	1.23
1	1	283	LYS	CE-NZ	5.18	1.64	1.49
3	3	146	MET	C-O	5.17	1.30	1.24
2	2	38	TRP	CA-C	-5.17	1.45	1.52
3	3	153	TRP	C-O	5.17	1.30	1.24
3	3	77	ASN	C-N	-5.15	1.26	1.33
3	3	133	PRO	CA-CB	-5.13	1.47	1.54
3	3	232	VAL	C-O	5.13	1.29	1.23
2	2	204	ILE	C-N	-5.13	1.26	1.33
3	3	112	ARG	CA-CB	-5.11	1.45	1.53
2	2	202	PRO	C-N	-5.10	1.26	1.33
1	1	42	THR	C-O	5.10	1.29	1.23
3	3	58	THR	CA-CB	5.10	1.62	1.53
3	3	205	VAL	C-O	5.10	1.29	1.23
2	2	109	HIS	N-CA	5.09	1.53	1.46
2	2	128	PRO	CA-CB	-5.08	1.46	1.53
1	1	85	LYS	N-CA	5.07	1.51	1.46
1	1	89	GLY	C-O	5.07	1.31	1.24
2	2	220	LEU	C-N	-5.07	1.26	1.33
2	2	248	CYS	C-N	-5.07	1.26	1.33
1	1	48	SER	C-N	-5.06	1.26	1.33
3	3	65	ASN	CA-CB	5.05	1.62	1.53
2	2	233	GLY	C-O	5.05	1.30	1.24
1	1	246	ARG	CD-NE	-5.05	1.39	1.46
3	3	164	THR	CA-C	-5.05	1.46	1.52
2	2	186	HIS	C-O	5.05	1.29	1.23
3	3	84	ASN	N-CA	5.04	1.52	1.45
3	3	216	ASP	N-CA	-5.04	1.40	1.46
1	1	129	THR	N-CA	5.03	1.52	1.46
3	3	136	ALA	C-O	5.03	1.30	1.23
3	3	109	GLY	C-N	5.02	1.40	1.33
2	2	12	ARG	N-CA	-5.01	1.40	1.46
1	1	102	TRP	NE1-CE2	-5.01	1.31	1.37
1	1	275	THR	C-O	5.00	1.30	1.23

All (573) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	50	ASP	CA-CB-CG	27.70	140.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	285	ASP	CA-CB-CG	-22.18	90.42	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	19.04	152.17	114.10
2	2	11	ASP	CA-CB-CG	-18.96	93.64	112.60
1	1	145	ASN	OD1-CG-ND2	17.21	139.81	122.60
2	2	190	ASN	CA-CB-CG	16.45	129.05	112.60
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	194	ASN	CA-CB-CG	-14.87	97.73	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
3	3	57	ASN	CA-CB-CG	-13.81	98.78	112.60
1	1	38	GLU	CB-CG-CD	13.59	135.69	112.60
3	3	74	ASN	CA-CB-CG	-13.45	99.15	112.60
3	3	65	ASN	CA-CB-CG	-13.05	99.55	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
2	2	194	ASN	N-CA-CB	-12.63	89.82	110.41
1	1	94	ARG	CD-NE-CZ	-12.63	106.72	124.40
2	2	44	ASP	CA-CB-CG	12.62	125.22	112.60
1	1	256	ARG	NE-CZ-NH2	12.53	130.47	119.20
2	2	67	ASP	CA-CB-CG	-12.49	100.11	112.60
2	2	256	SER	CA-C-O	-12.21	105.38	119.79
4	4	30	ASN	CA-CB-CG	-12.13	100.47	112.60
3	3	172	GLN	CB-CG-CD	12.02	133.03	112.60
4	4	45	LEU	N-CA-CB	-11.95	94.04	111.84
4	4	41	ALA	CA-C-O	-11.31	105.47	119.38
3	3	74	ASN	OD1-CG-ND2	11.23	133.83	122.60
2	2	14	GLN	OE1-CD-NE2	11.18	133.78	122.60
3	3	29	GLU	CB-CG-CD	11.12	131.50	112.60
2	2	151	GLU	CA-CB-CG	11.08	136.27	114.10
1	1	285	ASP	N-CA-CB	-11.04	95.27	110.29
1	1	25	PRO	CA-C-O	-10.88	108.94	121.56
2	2	88	ASP	CA-CB-CG	-10.86	101.74	112.60
2	2	219	SER	CA-CB-OG	10.64	132.39	111.10
4	4	48	ASP	CA-CB-CG	-10.60	102.00	112.60
1	1	282	ARG	CD-NE-CZ	-10.59	109.57	124.40
2	2	97	PHE	CA-CB-CG	-10.57	103.23	113.80
1	1	141	ASN	CA-CB-CG	-10.41	102.19	112.60
3	3	57	ASN	N-CA-CB	-10.40	92.91	110.49
3	3	72	ASN	CA-CB-CG	-10.13	102.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	48	ASP	O-C-N	10.11	128.31	121.23
1	1	63	SER	CB-CA-C	-10.00	94.20	110.79
1	1	246	ARG	NE-CZ-NH1	9.97	131.47	121.50
1	1	54	ARG	CD-NE-CZ	-9.96	110.45	124.40
1	1	91	ASP	CA-CB-CG	-9.86	102.74	112.60
4	4	44	SER	CA-C-N	-9.83	108.02	122.07
4	4	44	SER	C-N-CA	-9.83	108.02	122.07
1	1	285	ASP	N-CA-C	9.79	122.95	110.33
1	1	275	THR	CA-C-O	-9.77	109.17	121.88
1	1	22	SER	CA-C-O	-9.73	109.60	120.69
1	1	28	THR	CB-CA-C	-9.71	92.94	111.48
3	3	137	ARG	NE-CZ-NH1	-9.70	111.81	121.50
3	3	33	ARG	CA-C-O	-9.66	110.03	121.05
3	3	234	LEU	O-C-N	9.65	134.25	122.86
1	1	256	ARG	NE-CZ-NH1	-9.64	111.86	121.50
1	1	53	THR	CA-CB-OG1	-9.54	95.30	109.60
1	1	246	ARG	CD-NE-CZ	9.49	137.69	124.40
1	1	79	VAL	CA-C-O	-9.47	110.54	120.39
1	1	38	GLU	CA-CB-CG	9.45	133.00	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
2	2	255	ARG	NE-CZ-NH2	-9.14	110.97	119.20
3	3	57	ASN	CB-CA-C	-9.09	92.33	110.42
1	1	95	GLU	CB-CG-CD	-9.03	97.25	112.60
1	1	268	ARG	CD-NE-CZ	-8.99	111.81	124.40
3	3	196	ILE	CA-C-O	-8.99	111.19	120.27
4	4	50	SER	CA-C-O	-8.99	109.94	120.10
2	2	195	ASN	CA-CB-CG	8.97	121.57	112.60
2	2	136	GLU	CB-CG-CD	-8.82	97.61	112.60
2	2	250	GLU	CA-CB-CG	8.81	131.72	114.10
4	4	68	ASN	CA-CB-CG	-8.78	103.82	112.60
1	1	251	GLU	CA-CB-CG	8.68	131.45	114.10
1	1	270	ASN	CA-CB-CG	8.67	121.27	112.60
2	2	139	ASN	CA-CB-CG	-8.53	104.07	112.60
2	2	255	ARG	CA-CB-CG	8.48	131.07	114.10
3	3	234	LEU	CA-C-N	-8.47	107.86	123.03
3	3	234	LEU	C-N-CA	-8.47	107.86	123.03
2	2	73	THR	CA-CB-OG1	-8.45	96.92	109.60
1	1	259	ARG	CA-CB-CG	-8.44	97.22	114.10
2	2	169	VAL	CB-CA-C	-8.42	101.19	111.97
2	2	168	ASP	CA-C-O	-8.41	110.61	120.62
2	2	68	SER	N-CA-C	8.38	122.89	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	41	ALA	N-CA-C	8.37	122.75	112.54
2	2	169	VAL	CA-C-O	-8.36	112.30	121.17
4	4	36	ALA	CA-C-N	-8.35	108.77	122.54
4	4	36	ALA	C-N-CA	-8.35	108.77	122.54
1	1	123	ARG	NE-CZ-NH1	8.33	129.83	121.50
3	3	74	ASN	CA-C-O	-8.29	109.94	120.55
3	3	5	THR	CA-C-O	-8.28	111.13	120.32
1	1	122	VAL	N-CA-CB	-8.28	97.87	111.45
3	3	57	ASN	OD1-CG-ND2	8.26	130.86	122.60
3	3	172	GLN	CG-CD-NE2	8.26	128.78	116.40
4	4	57	LYS	CA-C-O	-8.21	112.24	120.70
3	3	219	LEU	CA-C-O	-8.20	111.23	120.66
3	3	182	THR	CA-CB-CG2	8.18	124.40	110.50
1	1	82	ILE	CA-C-O	-8.14	113.12	121.67
3	3	16	THR	N-CA-CB	-8.14	98.32	110.61
3	3	21	SER	CB-CA-C	-8.13	95.50	108.91
2	2	49	ASP	CA-CB-CG	8.12	120.72	112.60
1	1	29	GLN	N-CA-C	-8.10	102.45	113.30
3	3	27	ASN	O-C-N	8.02	132.03	122.00
1	1	94	ARG	NE-CZ-NH2	-8.01	111.99	119.20
3	3	60	THR	CA-CB-OG1	-8.01	97.59	109.60
3	3	78	GLU	N-CA-C	8.00	120.85	110.53
2	2	187	GLN	CA-CB-CG	7.99	130.09	114.10
1	1	288	SER	CA-C-O	-7.99	113.08	121.55
2	2	248	CYS	CA-C-O	-7.97	112.29	121.54
3	3	233	ALA	CA-C-O	-7.95	112.44	121.19
2	2	223	ILE	N-CA-CB	-7.91	101.52	112.27
3	3	111	LEU	CA-C-N	-7.89	111.87	123.00
3	3	111	LEU	C-N-CA	-7.89	111.87	123.00
3	3	231	THR	CA-CB-OG1	-7.88	97.79	109.60
1	1	37	ASN	CB-CG-ND2	7.86	128.18	116.40
2	2	216	ASN	CA-C-O	-7.85	112.09	120.80
1	1	123	ARG	CD-NE-CZ	7.83	135.36	124.40
3	3	216	ASP	N-CA-CB	-7.80	98.61	110.16
1	1	274	ASN	O-C-N	7.79	132.95	122.59
4	4	45	LEU	CA-C-O	7.76	130.54	121.54
2	2	95	ASN	CA-CB-CG	-7.75	104.85	112.60
1	1	282	ARG	CA-C-N	-7.73	111.51	122.41
1	1	282	ARG	C-N-CA	-7.73	111.51	122.41
3	3	62	ASP	CA-CB-CG	7.73	120.33	112.60
2	2	109	HIS	CA-C-O	-7.71	110.85	120.57
2	2	240	ILE	CA-C-O	-7.70	112.31	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	64	GLU	CB-CG-CD	7.68	125.66	112.60
2	2	190	ASN	OD1-CG-ND2	-7.68	114.92	122.60
4	4	37	SER	CB-CA-C	7.67	122.89	110.09
1	1	61	ASN	CA-CB-CG	-7.63	104.97	112.60
1	1	17	THR	CA-C-N	-7.60	110.34	122.50
1	1	17	THR	C-N-CA	-7.60	110.34	122.50
3	3	137	ARG	CD-NE-CZ	-7.60	113.76	124.40
2	2	87	LYS	CB-CG-CD	7.59	128.75	111.30
3	3	59	HIS	CA-C-O	7.59	130.46	121.88
3	3	142	ARG	CA-CB-CG	7.59	129.27	114.10
3	3	184	ALA	N-CA-C	7.57	122.70	113.17
1	1	277	PRO	N-CD-CG	-7.53	91.90	103.20
3	3	27	ASN	N-CA-C	7.53	124.03	113.56
3	3	79	GLN	OE1-CD-NE2	-7.50	115.09	122.60
4	4	30	ASN	CA-C-O	-7.43	112.22	120.69
2	2	140	VAL	CA-C-O	-7.40	113.31	121.23
1	1	288	SER	N-CA-C	7.38	120.38	110.35
2	2	98	PHE	CA-C-O	-7.37	110.97	119.60
2	2	107	THR	CA-C-O	-7.37	112.21	120.32
2	2	39	PRO	CA-C-O	-7.34	112.97	121.34
3	3	129	LEU	CA-C-O	-7.33	112.94	120.71
4	4	45	LEU	CB-CA-C	7.32	122.49	111.80
3	3	118	THR	CA-CB-OG1	-7.31	98.64	109.60
3	3	27	ASN	CB-CA-C	-7.30	97.25	111.06
2	2	187	GLN	CB-CA-C	7.26	125.39	109.94
3	3	61	LYS	CA-C-O	-7.25	112.64	121.06
3	3	19	ARG	NE-CZ-NH2	7.25	125.73	119.20
2	2	169	VAL	N-CA-C	7.25	117.38	110.42
3	3	124	SER	CA-C-O	-7.23	113.52	121.33
2	2	77	GLY	CA-C-O	-7.22	114.83	122.05
2	2	180	ASN	CA-CB-CG	-7.22	105.38	112.60
1	1	26	LYS	CA-CB-CG	7.21	128.53	114.10
2	2	68	SER	O-C-N	-7.21	114.81	122.96
2	2	103	ARG	CD-NE-CZ	-7.20	114.31	124.40
2	2	52	LYS	CA-C-O	-7.17	113.30	121.19
1	1	275	THR	CA-CB-OG1	-7.17	98.84	109.60
3	3	46	ILE	CA-C-O	-7.14	112.54	120.25
1	1	284	GLY	CA-C-N	7.13	133.64	120.95
1	1	284	GLY	C-N-CA	7.13	133.64	120.95
1	1	59	HIS	CA-C-O	-7.12	111.98	120.81
4	4	30	ASN	OD1-CG-ND2	7.12	129.72	122.60
2	2	146	PHE	CA-CB-CG	-7.09	106.70	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	168	ASP	N-CA-CB	-7.09	97.96	109.60
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	-7.04	93.82	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
3	3	35	HIS	CA-C-O	-7.00	112.87	120.92
1	1	28	THR	OG1-CB-CG2	6.99	123.28	109.30
3	3	164	THR	N-CA-CB	-6.99	99.60	110.57
1	1	43	MET	CA-C-O	6.98	126.31	119.75
1	1	85	LYS	CA-C-O	-6.96	114.00	121.38
3	3	121	ALA	CA-C-O	-6.96	112.23	120.10
1	1	285	ASP	CB-CG-OD1	-6.96	102.40	118.40
2	2	57	ASP	CB-CA-C	-6.91	108.61	116.63
1	1	270	ASN	O-C-N	6.90	131.39	122.97
3	3	109	GLY	CA-C-N	-6.90	110.91	122.64
3	3	109	GLY	C-N-CA	-6.90	110.91	122.64
3	3	66	SER	CB-CA-C	6.90	121.61	110.09
2	2	186	HIS	CA-CB-CG	-6.89	106.91	113.80
1	1	138	ASP	CA-CB-CG	6.88	119.48	112.60
3	3	77	ASN	OD1-CG-ND2	-6.86	115.74	122.60
2	2	9	TYR	CB-CA-C	6.86	121.38	109.65
3	3	65	ASN	OD1-CG-ND2	6.84	129.44	122.60
3	3	231	THR	CA-C-O	-6.84	110.50	119.06
1	1	35	THR	CA-CB-OG1	-6.84	99.34	109.60
2	2	219	SER	CB-CA-C	6.84	121.69	109.38
2	2	14	GLN	CB-CG-CD	-6.82	101.00	112.60
4	4	44	SER	O-C-N	6.82	131.66	122.59
3	3	202	THR	CA-C-O	6.81	128.52	121.23
2	2	193	THR	O-C-N	-6.81	115.12	121.79
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
3	3	146	MET	CG-SD-CE	6.80	115.86	100.90
1	1	42	THR	CA-CB-CG2	6.79	122.04	110.50
1	1	35	THR	N-CA-CB	-6.76	99.06	110.49
3	3	187	LEU	CA-C-O	-6.75	113.08	120.24
1	1	49	ASP	N-CA-C	-6.75	105.33	113.97
3	3	151	VAL	CA-C-O	-6.73	113.58	120.25
4	4	58	ASP	O-C-N	6.73	130.90	123.22
1	1	62	GLY	CA-C-N	6.72	129.29	120.28
1	1	62	GLY	C-N-CA	6.72	129.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	249	THR	CA-CB-OG1	-6.71	99.53	109.60
3	3	143	ARG	N-CA-C	-6.71	104.05	111.36
3	3	178	PRO	O-C-N	6.70	130.72	123.01
2	2	124	VAL	CA-C-O	-6.70	112.83	120.66
2	2	224	PRO	CA-C-O	-6.69	114.07	121.23
1	1	288	SER	CB-CA-C	-6.69	97.65	109.62
1	1	282	ARG	NE-CZ-NH2	-6.68	113.19	119.20
3	3	227	THR	CA-CB-OG1	-6.67	99.59	109.60
3	3	42	ASN	CA-C-O	-6.67	112.99	120.66
2	2	255	ARG	CB-CG-CD	6.66	126.61	111.30
1	1	95	GLU	CA-CB-CG	-6.64	100.82	114.10
1	1	259	ARG	CA-C-O	-6.62	113.20	120.81
1	1	90	ILE	CA-C-N	-6.61	109.76	122.06
1	1	90	ILE	C-N-CA	-6.61	109.76	122.06
1	1	25	PRO	CA-C-N	6.60	133.42	122.73
1	1	25	PRO	C-N-CA	6.60	133.42	122.73
3	3	202	THR	CA-CB-OG1	-6.60	99.70	109.60
3	3	134	PRO	CA-C-N	-6.60	116.31	123.30
3	3	134	PRO	C-N-CA	-6.60	116.31	123.30
2	2	198	THR	CA-C-O	-6.59	113.00	120.32
2	2	161	GLU	CA-C-N	-6.59	114.46	122.90
2	2	161	GLU	C-N-CA	-6.59	114.46	122.90
3	3	187	LEU	N-CA-CB	-6.59	100.42	110.77
1	1	60	PHE	CA-C-O	-6.59	113.64	120.89
1	1	98	LEU	N-CA-C	-6.58	105.11	113.01
2	2	145	THR	CA-CB-OG1	-6.55	99.78	109.60
2	2	11	ASP	OD1-CG-OD2	6.53	138.58	122.90
2	2	38	TRP	N-CA-CB	-6.53	99.34	110.11
3	3	74	ASN	N-CA-C	6.53	120.56	112.47
4	4	48	ASP	OD1-CG-OD2	6.52	138.54	122.90
2	2	142	VAL	CA-C-O	-6.51	113.04	120.66
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
3	3	19	ARG	CA-CB-CG	6.50	127.10	114.10
2	2	111	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	1	97	LYS	CB-CA-C	-6.50	102.50	111.73
2	2	163	GLY	O-C-N	6.48	130.15	122.50
1	1	256	ARG	CD-NE-CZ	-6.48	115.33	124.40
1	1	122	VAL	CB-CA-C	6.48	121.92	110.71
2	2	226	ALA	N-CA-C	-6.47	99.20	109.04
2	2	148	HIS	CA-CB-CG	6.47	120.27	113.80
4	4	36	ALA	N-CA-C	-6.47	105.25	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	205	VAL	CB-CA-C	6.46	120.20	110.90
2	2	194	ASN	N-CA-C	6.46	120.59	110.32
4	4	39	SER	O-C-N	6.45	130.80	122.23
1	1	277	PRO	CB-CA-C	6.44	119.82	111.64
3	3	65	ASN	N-CA-CB	-6.43	100.94	110.53
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
3	3	182	THR	CA-CB-OG1	-6.42	99.96	109.60
3	3	57	ASN	N-CA-C	6.42	124.48	110.80
2	2	69	LYS	CA-CB-CG	6.41	126.91	114.10
3	3	164	THR	CA-CB-OG1	-6.40	99.99	109.60
3	3	204	GLN	O-C-N	6.40	130.23	123.06
3	3	216	ASP	CA-C-N	6.39	129.78	120.71
3	3	216	ASP	C-N-CA	6.39	129.78	120.71
3	3	172	GLN	OE1-CD-NE2	-6.38	116.22	122.60
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
2	2	241	THR	CA-C-O	-6.38	113.95	120.71
3	3	226	GLN	CB-CG-CD	-6.37	101.76	112.60
1	1	239	VAL	CB-CA-C	6.36	120.04	110.63
4	4	44	SER	CA-CB-OG	-6.36	98.38	111.10
3	3	41	HIS	CA-C-O	-6.36	112.36	119.67
2	2	223	ILE	CA-C-O	-6.35	116.64	119.94
3	3	181	TYR	O-C-N	6.35	128.85	122.12
2	2	145	THR	CA-C-O	-6.35	113.78	120.63
1	1	265	SER	O-C-N	-6.34	115.92	123.27
2	2	235	THR	CB-CA-C	-6.34	99.50	109.52
1	1	50	SER	CA-C-O	-6.34	110.51	118.43
1	1	144	SER	N-CA-CB	-6.33	100.80	110.42
1	1	250	VAL	N-CA-C	6.31	117.79	109.21
1	1	288	SER	N-CA-CB	-6.30	100.77	110.04
3	3	202	THR	N-CA-C	6.30	118.43	108.79
3	3	63	GLU	CB-CG-CD	-6.28	101.92	112.60
1	1	137	PRO	CA-C-N	-6.28	113.10	122.39
1	1	137	PRO	C-N-CA	-6.28	113.10	122.39
3	3	80	VAL	CA-C-O	-6.27	114.00	120.71
3	3	216	ASP	CB-CG-OD2	6.26	132.79	118.40
2	2	103	ARG	CA-CB-CG	6.25	126.61	114.10
3	3	193	THR	CA-C-O	-6.25	111.57	120.51
3	3	83	THR	CA-CB-OG1	-6.25	100.23	109.60
1	1	282	ARG	NH1-CZ-NH2	6.25	127.42	119.30
3	3	183	SER	N-CA-CB	-6.23	100.82	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	70	PHE	CA-CB-CG	6.23	120.03	113.80
4	4	65	PRO	CB-CA-C	-6.23	103.42	111.46
2	2	143	LYS	O-C-N	6.21	130.45	122.81
1	1	31	VAL	N-CA-CB	-6.20	102.53	111.21
2	2	179	GLY	CA-C-O	-6.18	114.14	120.45
2	2	28	ALA	CA-C-O	-6.18	114.83	121.94
1	1	48	SER	CA-C-O	-6.17	108.19	119.36
1	1	260	ALA	CA-C-O	-6.17	111.49	120.13
1	1	274	ASN	N-CA-CB	6.17	120.92	110.49
3	3	27	ASN	N-CA-CB	-6.17	103.09	113.15
3	3	196	ILE	N-CA-CB	-6.17	103.44	111.82
2	2	11	ASP	O-C-N	6.16	130.40	122.39
3	3	6	THR	CB-CA-C	6.15	120.03	109.51
3	3	161	ILE	CA-C-O	-6.15	113.93	120.39
3	3	132	THR	CA-C-O	-6.15	113.93	119.59
4	4	43	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	1	236	LYS	CA-C-O	-6.13	114.23	121.16
2	2	238	LEU	N-CA-CB	-6.13	98.77	110.42
3	3	163	MET	CA-CB-CG	-6.13	101.85	114.10
2	2	111	GLN	CB-CG-CD	6.12	123.01	112.60
3	3	137	ARG	NE-CZ-NH2	6.11	124.70	119.20
3	3	170	GLY	CA-C-N	6.11	128.69	120.50
3	3	170	GLY	C-N-CA	6.11	128.69	120.50
1	1	141	ASN	O-C-N	6.09	129.76	122.27
2	2	12	ARG	CD-NE-CZ	-6.08	115.88	124.40
1	1	252	ALA	CA-C-O	-6.07	113.68	120.66
1	1	77	VAL	CA-C-O	-6.06	113.20	118.96
3	3	193	THR	CA-CB-OG1	-6.06	100.52	109.60
3	3	36	ILE	CA-C-O	-6.05	111.84	119.95
2	2	86	LEU	CA-C-N	6.05	130.37	120.63
2	2	86	LEU	C-N-CA	6.05	130.37	120.63
2	2	194	ASN	OD1-CG-ND2	6.05	128.65	122.60
1	1	68	GLU	CG-CD-OE2	6.04	132.29	118.40
2	2	241	THR	CA-CB-OG1	-6.03	100.55	109.60
1	1	52	GLU	CA-C-O	-6.03	113.68	120.43
3	3	8	PRO	CA-C-O	-6.03	114.55	121.36
1	1	136	GLN	CG-CD-NE2	-6.03	107.36	116.40
3	3	47	ILE	CB-CG1-CD1	-6.01	101.18	113.80
1	1	41	ALA	CA-C-O	-6.00	114.64	121.72
3	3	137	ARG	CA-C-O	-5.99	115.05	121.94
1	1	133	THR	CA-CB-OG1	-5.99	100.62	109.60
3	3	121	ALA	CB-CA-C	-5.98	99.56	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	194	SER	N-CA-CB	-5.98	100.39	110.49
2	2	14	GLN	CA-CB-CG	-5.98	102.15	114.10
3	3	41	HIS	N-CA-CB	5.97	119.06	110.40
2	2	195	ASN	OD1-CG-ND2	-5.97	116.63	122.60
2	2	169	VAL	N-CA-CB	5.96	117.53	110.55
2	2	105	GLY	N-CA-C	-5.95	102.29	112.64
2	2	136	GLU	CG-CD-OE1	-5.95	104.72	118.40
3	3	77	ASN	O-C-N	-5.94	114.69	122.59
1	1	55	THR	CA-CB-OG1	-5.93	100.70	109.60
2	2	161	GLU	CA-CB-CG	5.93	125.95	114.10
3	3	160	THR	CA-CB-OG1	-5.92	100.72	109.60
1	1	259	ARG	CB-CA-C	-5.91	100.44	109.89
3	3	1	GLY	O-C-N	-5.90	113.56	123.00
2	2	41	TYR	N-CA-CB	5.90	118.46	110.38
3	3	158	GLN	CA-C-O	5.90	127.64	120.62
1	1	22	SER	N-CA-CB	-5.90	100.81	109.95
1	1	265	SER	N-CA-CB	-5.90	100.56	111.53
3	3	92	PHE	CA-CB-CG	-5.88	107.92	113.80
3	3	55	MET	CA-CB-CG	-5.87	102.35	114.10
3	3	57	ASN	O-C-N	-5.87	114.79	122.59
1	1	270	ASN	CB-CA-C	-5.84	100.29	109.70
3	3	131	TYR	CA-C-O	-5.84	114.06	120.43
2	2	255	ARG	NE-CZ-NH1	5.84	127.34	121.50
2	2	226	ALA	O-C-N	5.83	127.83	121.36
1	1	280	LYS	CB-CA-C	-5.83	101.77	110.16
3	3	207	LEU	CA-C-O	-5.83	114.33	120.80
1	1	242	ARG	CD-NE-CZ	-5.82	116.25	124.40
3	3	59	HIS	CA-CB-CG	-5.82	107.98	113.80
2	2	88	ASP	CA-C-O	-5.82	112.62	119.48
3	3	197	LEU	CB-CA-C	5.81	117.23	108.86
4	4	65	PRO	CA-C-O	-5.81	114.71	121.34
3	3	93	LYS	N-CA-C	5.81	118.39	111.71
3	3	33	ARG	CB-CG-CD	-5.80	97.96	111.30
1	1	145	ASN	CB-CG-ND2	-5.80	107.70	116.40
2	2	235	THR	OG1-CB-CG2	5.78	120.86	109.30
2	2	54	SER	CA-C-N	-5.77	115.08	122.98
2	2	54	SER	C-N-CA	-5.77	115.08	122.98
2	2	105	GLY	CA-C-O	-5.77	113.04	122.56
1	1	267	GLY	CA-C-N	-5.77	113.12	122.81
1	1	267	GLY	C-N-CA	-5.77	113.12	122.81
2	2	198	THR	O-C-N	5.76	130.05	123.31
3	3	66	SER	N-CA-C	-5.75	105.92	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	68	GLU	CG-CD-OE1	-5.74	105.20	118.40
2	2	210	ASP	N-CA-CB	-5.73	100.56	110.87
2	2	189	ILE	CA-C-O	-5.72	113.25	120.69
1	1	94	ARG	CG-CD-NE	-5.71	99.44	112.00
3	3	45	GLU	CG-CD-OE2	5.71	131.52	118.40
1	1	129	THR	CA-C-O	-5.70	114.55	120.70
3	3	38	GLY	N-CA-C	5.69	123.74	115.32
1	1	83	GLN	CB-CG-CD	-5.68	102.94	112.60
3	3	112	ARG	CA-CB-CG	5.67	125.44	114.10
1	1	104	ILE	O-C-N	5.67	129.66	122.57
3	3	137	ARG	O-C-N	5.67	129.62	122.65
1	1	139	SER	CA-CB-OG	-5.67	99.77	111.10
3	3	161	ILE	CA-CB-CG1	-5.66	100.78	110.40
2	2	199	ILE	CA-C-O	-5.66	114.36	120.36
2	2	86	LEU	CA-C-O	-5.65	112.95	119.56
1	1	28	THR	N-CA-C	5.62	118.05	109.95
1	1	94	ARG	NH1-CZ-NH2	5.62	126.61	119.30
2	2	190	ASN	CB-CA-C	5.62	119.94	110.79
2	2	262	GLN	OE1-CD-NE2	-5.62	116.98	122.60
2	2	217	ASN	CB-CA-C	5.61	118.98	109.55
1	1	241	ILE	N-CA-CB	-5.61	104.26	110.99
3	3	180	THR	CA-CB-OG1	-5.61	101.18	109.60
2	2	99	HIS	CA-CB-CG	-5.60	108.20	113.80
2	2	106	TYR	CA-C-O	-5.59	115.29	121.33
2	2	94	GLN	CG-CD-NE2	-5.58	108.03	116.40
1	1	27	HIS	CA-CB-CG	5.57	119.36	113.80
1	1	273	LYS	CG-CD-CE	-5.56	98.52	111.30
3	3	42	ASN	CB-CG-ND2	5.56	124.73	116.40
2	2	99	HIS	CA-C-N	5.55	128.28	120.28
2	2	99	HIS	C-N-CA	5.55	128.28	120.28
2	2	215	HIS	CA-C-O	-5.55	112.50	120.11
3	3	166	PRO	CB-CA-C	5.55	118.62	111.46
3	3	107	TRP	CA-C-O	-5.54	115.14	121.40
3	3	190	TRP	CA-C-O	-5.54	115.14	121.40
2	2	9	TYR	CA-CB-CG	-5.54	103.94	113.90
2	2	251	PHE	CA-C-O	-5.54	114.86	121.11
4	4	58	ASP	CA-C-N	5.53	128.96	121.05
4	4	58	ASP	C-N-CA	5.53	128.96	121.05
3	3	140	GLN	CA-CB-CG	-5.52	103.07	114.10
2	2	188	PHE	CA-C-O	-5.51	114.93	121.66
2	2	68	SER	N-CA-CB	-5.51	101.91	110.29
1	1	64	GLU	CA-CB-CG	5.51	125.11	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	76	GLN	CA-C-O	-5.51	115.18	121.68
1	1	63	SER	O-C-N	5.50	127.95	122.12
2	2	192	ARG	CA-C-O	-5.50	111.90	119.05
3	3	57	ASN	CA-C-N	5.50	132.06	121.18
3	3	57	ASN	C-N-CA	5.50	132.06	121.18
2	2	168	ASP	CA-C-N	5.49	127.48	120.56
2	2	168	ASP	C-N-CA	5.49	127.48	120.56
2	2	167	LYS	CA-C-O	5.49	126.15	119.78
1	1	235	HIS	CA-CB-CG	-5.47	108.33	113.80
1	1	144	SER	CA-C-N	-5.47	115.35	123.11
1	1	144	SER	C-N-CA	-5.47	115.35	123.11
2	2	43	PRO	N-CD-CG	-5.47	95.00	103.20
2	2	13	VAL	CA-C-O	-5.46	114.51	120.84
3	3	164	THR	CB-CA-C	5.46	119.16	109.72
2	2	38	TRP	CB-CA-C	5.45	116.26	108.68
3	3	63	GLU	CG-CD-OE1	-5.45	105.86	118.40
2	2	26	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	2	258	SER	O-C-N	5.45	129.51	122.81
2	2	187	GLN	CA-C-O	-5.44	114.89	120.99
1	1	21	ILE	CA-CB-CG1	-5.44	101.15	110.40
2	2	92	PHE	N-CA-C	-5.44	105.05	110.97
4	4	50	SER	CA-CB-OG	-5.43	100.23	111.10
2	2	219	SER	N-CA-C	-5.42	100.87	109.59
1	1	50	SER	CB-CA-C	5.42	117.47	109.29
2	2	63	PHE	CA-CB-CG	5.41	119.21	113.80
2	2	123	LEU	CA-C-O	-5.41	114.53	120.43
2	2	129	GLU	CB-CA-C	-5.40	104.22	111.89
2	2	53	THR	CA-C-O	-5.40	115.57	121.89
3	3	34	ILE	CA-C-O	-5.40	114.03	120.78
3	3	90	GLY	CA-C-O	-5.40	114.87	121.68
3	3	168	THR	CA-CB-OG1	-5.40	101.50	109.60
2	2	232	THR	CA-CB-OG1	-5.39	101.51	109.60
2	2	221	MET	CA-C-O	-5.38	114.34	120.32
3	3	84	ASN	OD1-CG-ND2	5.37	127.97	122.60
3	3	116	MET	CB-CG-SD	-5.37	96.60	112.70
3	3	78	GLU	CA-CB-CG	5.36	124.83	114.10
1	1	288	SER	CA-CB-OG	-5.36	100.38	111.10
2	2	81	LYS	CB-CG-CD	5.36	123.62	111.30
3	3	112	ARG	CB-CA-C	5.36	119.05	110.16
1	1	92	ASN	O-C-N	5.36	129.49	123.28
3	3	195	LEU	CA-C-O	-5.35	114.95	121.05
1	1	282	ARG	O-C-N	5.35	129.39	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	102	GLY	CA-C-O	-5.34	115.43	121.68
3	3	38	GLY	O-C-N	-5.34	116.02	122.38
2	2	177	LEU	N-CA-CB	-5.34	101.58	110.23
2	2	262	GLN	CG-CD-NE2	5.32	124.39	116.40
3	3	143	ARG	O-C-N	5.32	128.22	122.15
1	1	26	LYS	CG-CD-CE	-5.32	99.07	111.30
2	2	120	GLY	CA-C-O	-5.31	114.46	122.54
3	3	221	LEU	O-C-N	5.31	129.66	122.59
3	3	226	GLN	N-CA-C	-5.31	106.76	113.18
1	1	113	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	2	12	ARG	CB-CG-CD	-5.30	99.12	111.30
2	2	210	ASP	CA-CB-CG	-5.30	107.30	112.60
4	4	58	ASP	N-CA-CB	5.29	119.05	110.42
3	3	161	ILE	N-CA-CB	5.29	118.71	111.41
3	3	222	MET	CB-CG-SD	-5.29	96.84	112.70
3	3	192	GLN	N-CA-C	-5.28	105.11	112.45
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
2	2	72	THR	CA-CB-OG1	-5.27	101.69	109.60
3	3	28	TYR	N-CA-CB	-5.27	102.22	109.97
1	1	286	ILE	O-C-N	5.27	127.75	121.80
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
3	3	144	GLU	CA-CB-CG	5.26	124.63	114.10
3	3	204	GLN	CA-C-O	-5.26	115.05	121.36
2	2	76	LYS	CA-C-O	-5.26	113.47	119.41
1	1	136	GLN	OE1-CD-NE2	5.25	127.85	122.60
1	1	60	PHE	N-CA-CB	-5.25	102.21	111.39
1	1	103	LYS	O-C-N	5.24	129.56	122.59
3	3	94	THR	CA-C-O	-5.24	113.18	119.15
2	2	168	ASP	OD1-CG-OD2	5.23	135.46	122.90
2	2	195	ASN	N-CA-C	-5.23	106.69	114.64
1	1	127	GLU	CA-C-O	-5.23	114.57	120.32
1	1	227	ARG	NE-CZ-NH2	5.22	123.90	119.20
3	3	77	ASN	CA-CB-CG	-5.22	107.38	112.60
2	2	257	LYS	N-CA-CB	5.22	119.31	110.49
4	4	53	THR	CA-CB-OG1	-5.22	101.77	109.60
1	1	282	ARG	CB-CA-C	-5.22	100.28	109.62
2	2	122	LEU	CA-C-O	-5.22	115.12	121.28
3	3	186	PHE	CA-CB-CG	-5.22	108.58	113.80
1	1	279	ILE	CA-C-N	5.21	128.74	121.02
1	1	279	ILE	C-N-CA	5.21	128.74	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	158	GLN	CG-CD-OE1	5.21	131.22	120.80
3	3	208	LEU	CA-C-O	-5.21	115.02	120.80
3	3	138	GLY	N-CA-C	-5.21	101.71	112.34
2	2	259	ILE	CA-C-O	-5.21	114.97	120.39
2	2	127	ILE	CA-C-O	-5.21	114.21	119.89
2	2	8	GLY	CA-C-N	-5.20	113.48	120.87
2	2	8	GLY	C-N-CA	-5.20	113.48	120.87
2	2	213	THR	CA-CB-OG1	-5.20	101.80	109.60
1	1	259	ARG	N-CA-CB	5.20	117.60	109.85
3	3	67	TYR	N-CA-C	-5.20	106.78	113.23
1	1	268	ARG	CB-CA-C	5.19	119.73	109.66
2	2	75	SER	N-CA-CB	-5.19	101.99	109.83
2	2	214	ARG	CD-NE-CZ	-5.19	117.13	124.40
1	1	63	SER	N-CA-C	5.18	116.93	111.28
2	2	32	VAL	O-C-N	5.18	128.43	123.14
2	2	18	LEU	N-CA-CB	-5.18	102.78	110.71
2	2	243	THR	CA-C-O	-5.18	114.73	120.38
2	2	20	ASN	CA-CB-CG	5.18	117.78	112.60
2	2	38	TRP	CA-CB-CG	-5.18	103.77	113.60
1	1	145	ASN	O-C-N	5.17	129.65	123.13
1	1	257	ALA	N-CA-CB	-5.17	101.86	109.98
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	231	THR	CA-C-N	-5.16	115.36	122.69
3	3	231	THR	C-N-CA	-5.16	115.36	122.69
3	3	45	GLU	CG-CD-OE1	-5.16	106.54	118.40
2	2	143	LYS	CA-C-N	5.15	131.38	121.54
2	2	143	LYS	C-N-CA	5.15	131.38	121.54
1	1	23	SER	CA-C-O	-5.15	115.09	121.06
3	3	186	PHE	O-C-N	5.14	129.83	123.15
2	2	165	PRO	CA-C-O	-5.14	115.37	122.15
1	1	128	TYR	CA-CB-CG	-5.13	104.67	113.90
1	1	285	ASP	CA-C-N	-5.12	111.91	120.30
1	1	285	ASP	C-N-CA	-5.12	111.91	120.30
2	2	181	LEU	N-CA-C	-5.12	106.30	112.54
3	3	233	ALA	O-C-N	5.12	129.16	122.87
1	1	27	HIS	CA-C-O	-5.11	113.06	122.62
2	2	259	ILE	CA-C-N	-5.11	112.67	122.13
2	2	259	ILE	C-N-CA	-5.11	112.67	122.13
3	3	109	GLY	N-CA-C	5.11	117.50	111.63
3	3	82	GLY	N-CA-C	-5.11	103.01	110.87
3	3	75	ARG	CD-NE-CZ	-5.10	117.26	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	215	HIS	CA-CB-CG	5.09	118.89	113.80
2	2	119	SER	O-C-N	5.08	129.32	123.17
3	3	32	PRO	CA-C-O	-5.08	115.67	121.56
3	3	125	ALA	CA-C-O	-5.08	115.51	121.10
2	2	152	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	1	40	GLY	N-CA-C	-5.08	108.11	115.27
3	3	1	GLY	N-CA-C	5.07	128.01	113.30
3	3	177	ASP	N-CA-CB	-5.07	102.99	110.14
1	1	66	ASP	CA-C-O	-5.07	115.62	121.19
1	1	270	ASN	N-CA-CB	5.07	117.75	109.69
2	2	119	SER	CA-C-O	-5.06	115.68	121.40
2	2	65	THR	CA-CB-OG1	-5.06	102.01	109.60
2	2	25	THR	CA-C-O	5.06	126.48	120.66
2	2	168	ASP	CB-CG-OD1	-5.06	106.77	118.40
1	1	83	GLN	OE1-CD-NE2	5.05	127.65	122.60
3	3	158	GLN	CB-CA-C	5.05	118.35	110.67
2	2	126	VAL	CA-C-O	-5.04	115.14	120.53
1	1	65	THR	N-CA-C	-5.04	106.06	113.61
3	3	217	PHE	N-CA-C	5.04	117.53	110.23
1	1	68	GLU	N-CA-C	-5.03	105.98	111.82
3	3	95	THR	CA-CB-OG1	-5.03	102.05	109.60
2	2	235	THR	CA-C-O	5.03	125.40	120.17
1	1	133	THR	CA-C-O	-5.02	115.43	121.11
2	2	261	PRO	CA-C-N	5.02	130.74	121.70
2	2	261	PRO	C-N-CA	5.02	130.74	121.70
1	1	282	ARG	CG-CD-NE	-5.01	100.99	112.00

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	179	0
2	2	1951	0	1923	132	0
3	3	1849	0	1831	145	0
4	4	297	0	294	36	0
5	1	25	0	20	1	0
All	All	6292	0	6175	419	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 34.

All (419) 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
3:3:234:LEU:C	3:3:235:THR:N	1.82	1.35
3:3:179:ASP:OD2	3:3:182:THR:HB	1.40	1.17
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.14
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.07
1:1:285:ASP:CA	1:1:285:ASP:OD1	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
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
1:1:151:MET:HE1	1:1:167:THR:O	1.64	0.98
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
1:1:152:TYR:O	1:1:154:PRO:HD3	1.69	0.93
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.04	0.92
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.91
2:2:12:ARG:HG3	2:2:12:ARG:HH11	1.27	0.91
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
1:1:103:LYS:HG3	1:1:103:LYS:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:58:MET:HE1	3:3:216:ASP:O	1.71	0.90
1:1:28:THR:HB	1:1:30:LYS:H	1.36	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:OD1	1:1:285:ASP:HA	1.73	0.88
1:1:102:TRP:CZ3	1:1:243:VAL:HG11	2.08	0.88
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.88
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
1:1:162:GLU:HB2	1:1:165:ASP:OD1	1.75	0.86
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.91	0.86
1:1:191:VAL:HG23	1:1:191:VAL:O	1.75	0.85
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.85
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.58	0.85
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
1:1:103:LYS:O	1:1:103:LYS:CG	2.27	0.83
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
2:2:52: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
2:2:30:ASN:HD22	2:2:31:ALA:H	1.27	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
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.48	0.79
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.79
1:1:102:TRP:CZ3	1:1:224:MET:HE3	2.18	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	0.77
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
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
1:1:220:HIS:CG	1:1:220:HIS:O	2.39	0.75
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.69	0.74
3:3:179:ASP:OD2	3:3:182:THR:CB	2.31	0.74
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:92:ASN:OD1	1:1:95:GLU:HB2	1.87	0.73
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.73
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.72
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.72
1:1:58:MET:HE1	3:3:216:ASP:HA	1.71	0.71
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.71
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.71
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.71
2:2:195:ASN:HD22	2:2:195:ASN:C	1.99	0.71
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.71
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	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
1:1:170:SER:O	1:1:170:SER:OG	2.09	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
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:OD2	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:OE2	1.95	0.67
2:2:155:ASP:C	2:2:155:ASP:OD1	2.37	0.66
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	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
1:1:151:MET:SD	1:1:170:SER:HB2	2.35	0.65
1:1:201:TYR:HD2	1:1:214:GLY:O	1.79	0.65
1:1:102:TRP:CE3	1:1:224:MET:HE3	2.32	0.65
1:1:285:ASP:CB	1:1:285:ASP:H	2.08	0.65
2:2:190:ASN:HD21	3:3:118:THR:HA	1.62	0.65
3:3:234:LEU:C	3:3:235:THR:CA	2.69	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	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.64
1:1:163:TRP:O	1:1:227:ARG:NH1	2.30	0.64
3:3:234:LEU:CA	3:3:235:THR:N	2.61	0.64
1:1:58:MET:HE1	3:3:216:ASP:CA	2.27	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.64
2:2:30:ASN:HD22	2:2:31:ALA:N	1.94	0.64
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
2:2:187:GLN:HE21	2:2:197:ALA:HA	1.63	0.63
2:2:205:ASN:ND2	2:2:206:SER:H	1.97	0.63
1:1:151:MET:HE1	1:1:167:THR:C	2.24	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
1:1:166:TYR:O	1:1:169:GLN:HB2	1.99	0.62
3:3:84:ASN:ND2	3:3:86:PHE:H	1.98	0.62
1:1:120:THR:O	1:1:199:CYS:HB2	1.99	0.62
2:2:170:VAL:CG1	2:2:170:VAL:O	2.47	0.61
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
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
1:1:204:TYR:CE2	1:1:213:TYR:HB2	2.36	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
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.60
1:1:204:TYR:HD2	1:1:212:GLN:O	1.85	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
1:1:259:ARG:HD2	1:1:263:TYR:CE1	2.38	0.59
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.59
3:3:175:TYR:H	3:3:182:THR:HG21	1.68	0.59
1:1:94:ARG:NH1	1:1:94:ARG:CG	2.60	0.59
3:3:84:ASN:HD22	3:3:86:PHE:H	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:206:HIS:CE1	1:1:208:ASP:HB2	2.38	0.58
2:2:30:ASN:HD21	4:4:58:ASP:H	1.51	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
1:1:209:ALA:HB2	2:2:261:PRO:HB3	1.85	0.58
1:1:43:MET:HE3	1:1:43:MET:HA	1.85	0.58
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.57
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.86	0.57
1:1:151:MET:HB2	1:1:175:SER:OG	2.04	0.57
2:2:64:TYR:CD1	2:2:89:MET:HB3	2.39	0.57
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.57
1:1:78:HIS:NE2	1:1:102:TRP:HB2	2.19	0.57
1:1:104:ILE:HG12	1:1:223:SER:HA	1.86	0.57
1:1:155:PRO:HB3	1:1:220:HIS:HE1	1.70	0.57
2:2:221:MET:HE2	2:2:223:ILE:HD11	1.87	0.57
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.22	0.57
3:3:179:ASP:OD2	3:3:182:THR:CG2	2.52	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
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
1:1:93:HIS:CE1	1:1:162:GLU:HG2	2.41	0.56
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	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
2:2:170:VAL:O	2:2:170:VAL:HG12	2.05	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
1:1:102:TRP:CH2	1:1:243:VAL:HG11	2.40	0.55
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.55
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.55
1:1:155:PRO:HB3	1:1:220:HIS:CE1	2.42	0.55
1:1:208:ASP:O	2:2:261:PRO:HG2	2.07	0.55
1:1:204:TYR:HE2	1:1:213:TYR:HB2	1.72	0.55
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	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
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.54
1:1:158:PRO:HB2	1:1:167:THR:HG22	1.90	0.54
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.87	0.54
1:1:208:ASP:HB3	1:1:211:THR:HB	1.90	0.54
3:3:175:TYR:H	3:3:182:THR:CG2	2.21	0.54
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.54
3:3:20:GLN:HE22	4:4:31:TYR:N	2.04	0.54
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.54
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.54
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.54
1:1:208:ASP:C	2:2:261:PRO:HG2	2.32	0.54
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	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	0.53
3:3:117:TYR:CD1	3:3:155:ILE:HD13	2.44	0.53
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
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.41	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:OD2	4:4:40:SER:HB2	2.09	0.53
1:1:185:ARG:HG3	1:1:186:PHE:N	2.21	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	0.53
1:1:190:TYR:HD1	1:1:197:TYR:CZ	2.28	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
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.92	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
1:1:92:ASN:C	1:1:92:ASN:ND2	2.67	0.52
1:1:104:ILE:HG21	5:1:500:W54:H3C1	1.90	0.52
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.52
1:1:114:LYS:NZ	3:3:99:GLU:OE2	2.43	0.52
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.52
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.45	0.52
2:2:66:LEU:HD12	2:2:89:MET:HE3	1.91	0.52
4:4:44:SER:C	4:4:46:SER:N	2.68	0.51
1:1:273:LYS:O	1:1:274:ASN:O	2.27	0.51
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.51
3:3:75:ARG:NH1	3:3:78:GLU:OE2	2.41	0.51
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
1:1:84:ASN:HB2	1:1:228:ILE:HD12	1.91	0.51
3:3:84:ASN:ND2	3:3:84:ASN:C	2.69	0.51
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
1:1:38:GLU:OE1	3:3:116:MET:HE2	2.10	0.51
1:1:153:VAL:HG12	1:1:157:ALA:HB3	1.91	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	2.78	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
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
2:2:255:ARG:CG	2:2:256:SER:H	1.99	0.50
1:1:102:TRP:CZ3	1:1:224:MET:CE	2.94	0.50
1:1:215:ILE:C	1:1:217:VAL:H	2.20	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
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
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.49
3:3:84:ASN:HD22	3:3:84:ASN:C	2.20	0.49
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.49
1:1:103:LYS:HA	1:1:223:SER:CB	2.43	0.49
1:1:58:MET:O	1:1:59:HIS:HB2	2.12	0.49
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.49
1:1:77:VAL:C	1:1:109:LEU:CD2	2.86	0.49
1:1:179:LYS:O	1:1:182:ASP:HB2	2.12	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	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
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.49
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.49
1:1:102:TRP:HZ3	1:1:243:VAL:HG11	1.69	0.48
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.95	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
1:1:103:LYS:HD3	3:3:236:GLU:OE2	2.14	0.48
1:1:191:VAL:O	1:1:191:VAL:CG2	2.46	0.48
1:1:280:LYS:HE3	3:3:89:ASP:OD1	2.13	0.48
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.48
1:1:102:TRP:HZ3	1:1:224:MET:HE3	1.77	0.48
3:3:61:LYS:O	3:3:61:LYS:HG2	2.07	0.48
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.96	0.48
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.48
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.79	0.48
3:3:112:ARG:NH1	3:3:112:ARG:HG2	2.28	0.48
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.47
1:1:110:VAL:HG13	3:3:230:GLN:CD	2.39	0.47
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.43	0.47
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.47
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.47
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
1:1:268:ARG:CZ	2:2:139:ASN:HB2	2.44	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.97	0.47
2:2:13:VAL:HA	2:2:25:THR:O	2.15	0.47
2:2:63:PHE:CD1	2:2:245:ALA:HB2	2.50	0.47
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.47
1:1:268:ARG:HH11	1:1:268:ARG:HD3	1.50	0.46
1:1:200:PHE:CE2	1:1:256:ARG:HD2	2.50	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
1:1:103:LYS:O	1:1:104:ILE:C	2.58	0.46
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.46
1:1:215:ILE:C	1:1:217:VAL:N	2.71	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.63	0.46
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.46
2:2:158:SER:HG	2:2:167:LYS:CE	2.26	0.46
1:1:236:LYS:HE2	1:1:236:LYS:HB3	1.83	0.46
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.46
1:1:169:GLN:O	1:1:170:SER:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.45
1:1:198:ASN:ND2	2:2:206:SER:OG	2.40	0.45
3:3:57:ASN:CB	3:3:57:ASN:H	2.26	0.45
1:1:97:LYS:C	1:1:99:PHE:N	2.71	0.45
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
1:1:188:VAL:HG23	1:1:189:PRO:O	2.16	0.45
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.98	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
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.98	0.45
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
3:3:192:GLN:HE21	3:3:192:GLN:HA	1.81	0.45
1:1:43:MET:HA	1:1:43:MET:CE	2.46	0.45
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.82	0.44
1:1:215:ILE:O	1:1:218:LEU:N	2.43	0.44
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
1:1:92:ASN:C	1:1:92:ASN:HD22	2.26	0.44
1:1:201:TYR:H	2:2:131:GLN:HE21	1.66	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
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
1:1:289:TYR:CE2	3:3:138:GLY:HA3	2.53	0.44
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.44
1:1:124:PHE:O	1:1:190:TYR:HB2	2.18	0.44
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.44
1:1:187:SER:O	3:3:23:SER:HA	2.17	0.44
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.44
3:3:221:LEU:C	3:3:221:LEU:HD23	2.43	0.44
1:1:98:LEU:O	1:1:99:PHE:HB3	2.18	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.44
1:1:154:PRO:HD2	1:1:173:ASN:HD21	1.83	0.44
1:1:190:TYR:CD1	1:1:197:TYR:CZ	3.05	0.44
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:289:TYR:CD2	3:3:138:GLY:HA3	2.53	0.44
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.99	0.43
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.43
1:1:38:GLU:N	3:3:116:MET:HE1	2.33	0.43
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.48	0.43
2:2:190:ASN:O	2:2:191:LEU:C	2.61	0.43
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.43
1:1:103:LYS:HA	1:1:223:SER:HB3	2.00	0.43
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.18	0.43
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	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
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	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
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	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
1:1:146:LEU:HD13	1:1:228:ILE:CD1	2.50	0.42
1:1:190:TYR:CE1	1:1:192:GLY:HA3	2.54	0.42
1:1:214:GLY:O	1:1:217:VAL:CG1	2.67	0.42
1:1:77:VAL:C	1:1:109:LEU:HD22	2.44	0.42
1:1:104:ILE:HG12	1:1:104:ILE:H	1.62	0.42
4:4:43:GLN:C	4:4:45:LEU:N	2.74	0.42
1:1:89:GLY:C	1:1:90:ILE:CD1	2.89	0.42
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.42
3:3:153:TRP:CD1	3:3:153:TRP:C	2.97	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.19	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
3:3:226:GLN:HE21	3:3:226:GLN:HB2	1.21	0.42
1:1:165:ASP:N	1:1:168:TRP:HD1	2.18	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42
2:2:40:GLU:O	2:2:40:GLU:CG	2.61	0.42
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.42
3:3:44:LEU:HA	3:3:44:LEU:HD23	1.79	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD2	2.55	0.42
1:1:286:ILE:HD13	1:1:286:ILE:HG21	1.77	0.42
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.42
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.42
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.80	0.41
1:1:86:ASP:OD1	1:1:88:THR:HB	2.21	0.41
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.41
1:1:87:ALA:C	1:1:90:ILE:HG12	2.46	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.41
3:3:113:PHE:CE2	3:3:115:LEU:HD13	2.56	0.41
3:3:137:ARG:HH11	3:3:137:ARG:HD3	1.22	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.03	0.41
3:3:64:VAL:O	3:3:64:VAL:HG12	2.21	0.41
1:1:97:LYS:C	1:1:99:PHE:H	2.23	0.41
1:1:54:ARG:HH11	1:1:54:ARG:HD2	1.55	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40
3:3:157:LEU:HD23	3:3:157:LEU:O	2.21	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
1:1:265:SER:OG	2:2:139:ASN:HB3	2.21	0.40
1:1:118:LEU:HD12	1:1:118:LEU:HA	1.91	0.40
1:1:285:ASP:HB3	1:1:287:LYS:H	1.87	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%)	243 (90%)	23 (8%)	5 (2%)	6	31
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	727 (91%)	59 (7%)	10 (1%)	9	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	104	ILE
1	1	139	SER
3	3	57	ASN
3	3	77	ASN
2	2	255	ARG
2	2	257	LYS
1	1	165	ASP
1	1	108	SER
1	1	170	SER
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%)	178 (80%)	45 (20%)	1	7
3	3	209/209 (100%)	170 (81%)	39 (19%)	1	9
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	1
All	All	704/748 (94%)	552 (78%)	152 (22%)	1	6

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	VAL
1	1	21	ILE

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Mol	Chain	Res	Type
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	100	ASN
1	1	103	LYS
1	1	104	ILE
1	1	105	ASN
1	1	109	LEU
1	1	110	VAL
1	1	118	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	149	GLN
1	1	151	MET
1	1	153	VAL
1	1	161	LYS
1	1	162	GLU
1	1	170	SER
1	1	183	THR
1	1	184	SER
1	1	185	ARG
1	1	188	VAL
1	1	191	VAL
1	1	215	ILE
1	1	217	VAL
1	1	220	HIS
1	1	221	MET
1	1	224	MET
1	1	228	ILE

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Mol	Chain	Res	Type
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	103	ARG
2	2	116	LYS
2	2	119	SER
2	2	136	GLU
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	174	ASN
2	2	187	GLN
2	2	192	ARG
2	2	195	ASN
2	2	209	ILE

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Mol	Chain	Res	Type
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
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	179	ASP
3	3	182	THR
3	3	192	GLN
3	3	194	SER

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Mol	Chain	Res	Type
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 (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	92	ASN
1	1	93	HIS
1	1	100	ASN
1	1	136	GLN
1	1	173	ASN
1	1	198	ASN
1	1	220	HIS
2	2	15	GLN
2	2	20	ASN
2	2	30	ASN
2	2	94	GLN
2	2	111	GLN
2	2	131	GLN

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Mol	Chain	Res	Type
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	W54	1	500	-	27,27,27	3.05	4 (14%)	35,36,36	2.69	8 (22%)

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	W54	1	500	-	-	1/13/20/20	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	500	W54	C2A-N3A	13.09	1.43	1.27
5	1	500	W54	C4A-N3A	-6.88	1.36	1.47
5	1	500	W54	O1A-C2A	-4.26	1.29	1.36
5	1	500	W54	O1A-C5A	-3.14	1.38	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	500	W54	O1A-C2A-N3A	-9.42	110.11	118.25
5	1	500	W54	C4A-N3A-C2A	6.68	112.68	106.75
5	1	500	W54	O1A-C2A-C4B	6.26	123.76	115.85
5	1	500	W54	O1B-C1B-C6B	-5.07	114.96	121.14
5	1	500	W54	O1A-C5A-C4A	4.02	111.72	104.24
5	1	500	W54	O1B-C1B-C2B	3.41	125.30	121.14
5	1	500	W54	C5A-C4A-N3A	-2.66	98.62	104.42
5	1	500	W54	C5C-O1B-C1B	2.09	120.50	114.22

There are no chirality outliers.

All (1) torsion outliers are listed below:

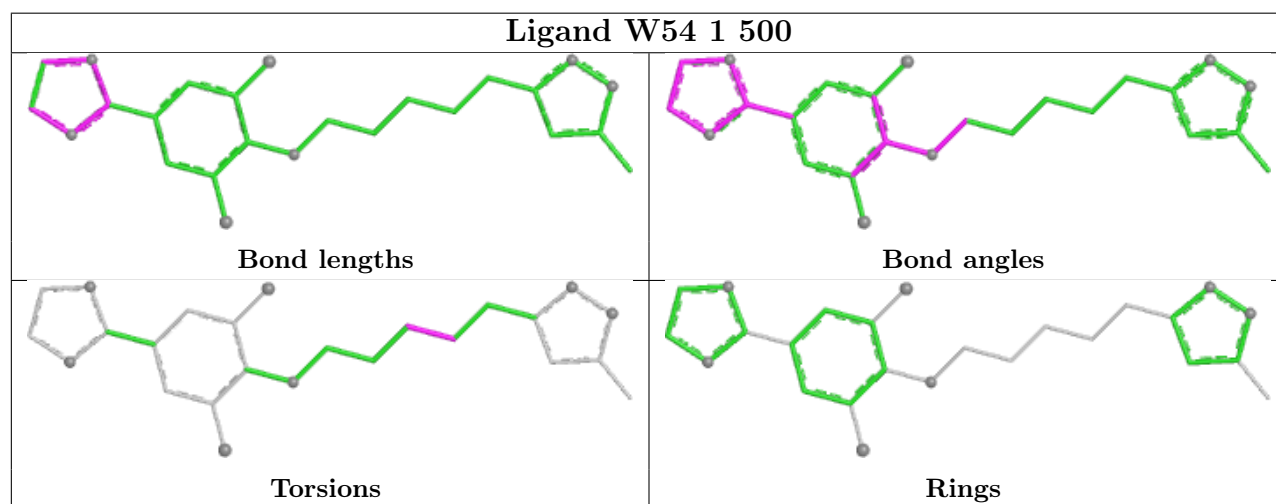
Mol	Chain	Res	Type	Atoms
5	1	500	W54	C1C-C2C-C3C-C4C

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	500	W54	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	3	1
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	234:LEU	C	235:THR	N	1.82
1	2	169:VAL	C	170:VAL	N	1.10

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.