



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:07 PM UTC

PDB ID : 1RUH / pdb_00001ruh
Title : RHINOVIRUS 14 MUTANT N1219S COMPLEXED WITH ANTIVIRAL COMPOUND WIN 52084
Authors : Hadfield, A.; Oliveira, M.A.; Kim, K.H.; Minor, I.; Kremer, M.J.; Heinz, B.A.; Shepard, D.; Pevear, D.C.; Rueckert, R.R.; Rossmann, M.G.
Deposited on : 1995-06-09
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

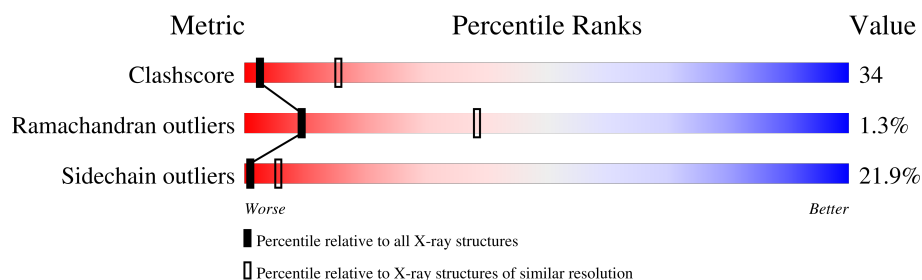
1 Overall quality at a glance

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

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 RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	273	Total	C	N	O	S	0	0	0
			2168	1372	374	414	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	219	SER	ASN	engineered mutation	UNP P03303

- Molecule 2 is a protein called RHINOVIRUS 14.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called RHINOVIRUS 14.

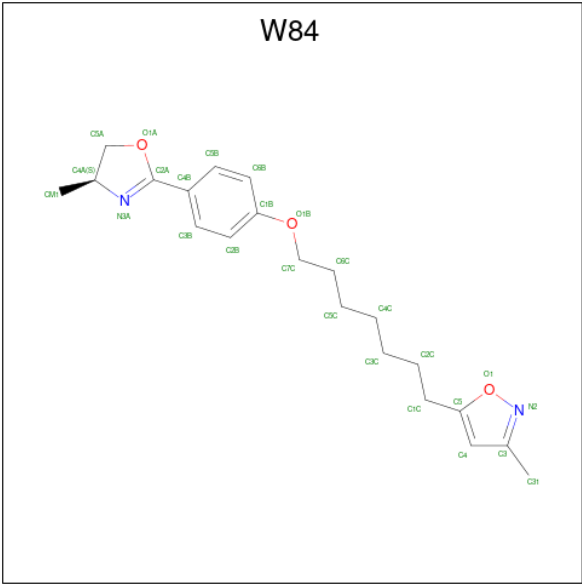
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	236	Total	C	N	O	S	0	0	0
			1849	1184	305	353	7			

- Molecule 4 is a protein called RHINOVIRUS 14.

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

- Molecule 5 is 5-(7-(5-HYDRO-4-METHYL-2-OXAZOLYL)PHENOXY)HEPTYL)-3-MET

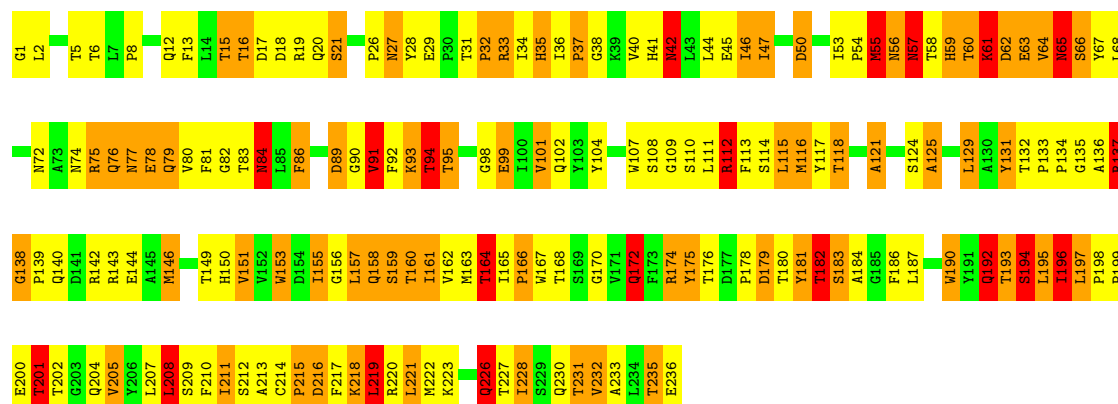
HYL ISOXAZOLE (CCD ID: W84) (formula: C₂₁H₂₈N₂O₃).



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

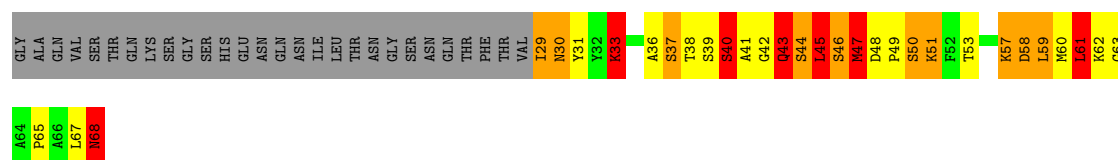
• Molecule 3: RHINOVIRUS 14

Chain 3: 25% 39% 28% 8%



• Molecule 4: RHINOVIRUS 14

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



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}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		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)	1.0	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: W84

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	2.50	85/2226 (3.8%)	2.71	201/3028 (6.6%)
2	2	2.40	94/2001 (4.7%)	2.77	194/2735 (7.1%)
3	3	2.29	79/1898 (4.2%)	2.78	187/2597 (7.2%)
4	4	2.64	14/302 (4.6%)	3.15	33/406 (8.1%)
All	All	2.42	272/6427 (4.2%)	2.77	615/8766 (7.0%)

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	4
2	2	0	2
All	All	0	6

All (272) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	220	HIS	C-N	-35.33	0.76	1.33
1	1	219	SER	C-N	-32.63	0.90	1.33
1	1	150	ALA	C-N	23.88	1.66	1.33
1	1	285	ASP	CA-CB	17.80	1.79	1.53
4	4	41	ALA	C-O	13.33	1.41	1.24
3	3	57	ASN	CA-CB	12.78	1.75	1.53
4	4	42	GLY	N-CA	12.59	1.63	1.45
1	1	187	SER	N-CA	11.77	1.60	1.46
2	2	194	ASN	CA-CB	11.51	1.71	1.53
1	1	283	LYS	N-CA	10.88	1.61	1.46
3	3	164	THR	C-O	10.31	1.36	1.24
4	4	45	LEU	C-N	9.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	256	SER	C-O	9.29	1.36	1.24
2	2	187	GLN	N-CA	9.27	1.57	1.45
1	1	170	SER	CB-OG	-9.25	1.23	1.42
1	1	52	GLU	C-O	9.14	1.35	1.24
1	1	282	ARG	CD-NE	9.09	1.58	1.46
2	2	152	ARG	CD-NE	8.92	1.58	1.46
2	2	102	GLY	N-CA	8.88	1.54	1.45
2	2	168	ASP	C-O	8.77	1.34	1.24
1	1	175	SER	N-CA	8.68	1.56	1.45
3	3	21	SER	CA-CB	8.61	1.66	1.54
2	2	174	ASN	C-O	8.59	1.30	1.23
3	3	50	ASP	CA-CB	-8.28	1.40	1.53
3	3	232	VAL	N-CA	8.26	1.55	1.46
1	1	73	ARG	C-O	8.02	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	-7.86	1.34	1.45
2	2	236	PRO	C-O	7.80	1.34	1.24
2	2	161	GLU	CA-CB	-7.78	1.42	1.53
1	1	158	PRO	CA-C	-7.67	1.41	1.52
2	2	135	HIS	CE1-NE2	-7.66	1.24	1.32
3	3	1	GLY	N-CA	7.65	1.57	1.45
1	1	122	VAL	N-CA	7.58	1.55	1.46
2	2	12	ARG	NE-CZ	7.57	1.41	1.33
1	1	72	GLY	C-O	7.53	1.34	1.23
2	2	52	LYS	N-CA	7.53	1.55	1.46
3	3	215	PRO	C-N	-7.47	1.23	1.33
2	2	108	VAL	C-O	7.43	1.32	1.24
1	1	94	ARG	CD-NE	7.42	1.56	1.46
2	2	11	ASP	CA-CB	7.36	1.66	1.53
1	1	288	SER	C-O	7.31	1.32	1.23
1	1	28	THR	CA-CB	7.27	1.64	1.53
2	2	120	GLY	N-CA	7.20	1.53	1.45
3	3	60	THR	CA-CB	7.20	1.65	1.54
3	3	77	ASN	C-O	7.17	1.33	1.24
2	2	260	VAL	N-CA	7.12	1.55	1.46
4	4	40	SER	CB-OG	7.05	1.56	1.42
1	1	276	GLU	C-O	7.04	1.31	1.24
2	2	219	SER	CA-CB	-7.01	1.41	1.53
2	2	74	GLY	C-O	7.00	1.31	1.23
1	1	30	LYS	C-O	7.00	1.32	1.23
2	2	9	TYR	C-O	6.99	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	58	THR	C-O	6.97	1.32	1.24
4	4	49	PRO	C-N	-6.91	1.24	1.34
1	1	91	ASP	N-CA	6.84	1.55	1.46
1	1	288	SER	CA-CB	6.84	1.65	1.53
3	3	86	PHE	CA-CB	-6.84	1.42	1.52
1	1	202	ASP	CA-CB	-6.80	1.42	1.53
2	2	223	ILE	CA-CB	6.80	1.59	1.54
3	3	6	THR	N-CA	6.76	1.54	1.45
2	2	194	ASN	N-CA	-6.74	1.37	1.45
1	1	23	SER	N-CA	6.74	1.54	1.45
2	2	243	THR	C-O	6.74	1.32	1.24
2	2	193	THR	C-N	-6.73	1.23	1.33
2	2	152	ARG	CZ-NH2	6.73	1.42	1.33
3	3	216	ASP	CA-CB	6.72	1.64	1.53
2	2	256	SER	CB-OG	6.71	1.55	1.42
2	2	197	ALA	C-O	6.71	1.31	1.23
2	2	10	SER	C-N	-6.67	1.25	1.33
1	1	280	LYS	C-O	6.66	1.31	1.24
1	1	165	ASP	CA-CB	6.63	1.64	1.53
1	1	251	GLU	CA-CB	-6.62	1.42	1.53
1	1	73	ARG	N-CA	6.59	1.53	1.45
2	2	109	HIS	CE1-NE2	-6.54	1.26	1.32
3	3	57	ASN	N-CA	-6.54	1.37	1.46
2	2	9	TYR	N-CA	6.54	1.53	1.46
1	1	85	LYS	C-O	6.54	1.31	1.23
1	1	79	VAL	C-N	-6.53	1.24	1.33
2	2	39	PRO	C-O	6.52	1.31	1.23
3	3	15	THR	C-O	6.51	1.32	1.24
4	4	44	SER	CB-OG	6.51	1.55	1.42
3	3	156	GLY	C-O	-6.51	1.18	1.24
2	2	190	ASN	CA-CB	-6.50	1.44	1.53
2	2	52	LYS	CE-NZ	6.50	1.68	1.49
4	4	62	LYS	C-O	6.50	1.31	1.24
2	2	262	GLN	CD-OE1	6.46	1.35	1.23
2	2	217	ASN	C-O	6.43	1.32	1.24
4	4	62	LYS	N-CA	6.42	1.54	1.46
1	1	231	GLU	CA-CB	-6.41	1.44	1.53
3	3	57	ASN	C-N	-6.40	1.25	1.33
2	2	30	ASN	N-CA	6.36	1.54	1.46
3	3	165	ILE	N-CA	6.35	1.54	1.46
3	3	205	VAL	N-CA	6.35	1.53	1.46
1	1	22	SER	C-N	-6.33	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	8	GLY	N-CA	6.33	1.55	1.45
1	1	95	GLU	CB-CG	6.31	1.71	1.52
1	1	94	ARG	NE-CZ	6.29	1.40	1.33
3	3	5	THR	C-O	6.28	1.31	1.24
3	3	118	THR	CB-OG1	6.28	1.53	1.43
4	4	63	GLY	N-CA	6.28	1.54	1.45
1	1	141	ASN	N-CA	6.27	1.50	1.46
1	1	185	ARG	C-N	-6.24	1.25	1.33
3	3	75	ARG	C-N	-6.23	1.24	1.33
1	1	184	SER	N-CA	6.21	1.53	1.45
2	2	259	ILE	C-O	6.20	1.31	1.24
1	1	184	SER	C-O	6.20	1.31	1.23
3	3	182	THR	CA-CB	6.20	1.62	1.53
3	3	16	THR	CA-CB	6.17	1.63	1.53
2	2	121	CYS	C-O	6.16	1.31	1.23
1	1	24	GLY	N-CA	6.14	1.53	1.44
4	4	45	LEU	N-CA	6.14	1.55	1.46
3	3	164	THR	N-CA	6.12	1.53	1.46
1	1	251	GLU	N-CA	6.12	1.53	1.46
2	2	257	LYS	N-CA	6.11	1.54	1.46
1	1	177	PHE	C-N	-6.10	1.25	1.33
4	4	33	LYS	CE-NZ	6.08	1.67	1.49
1	1	131	LEU	C-O	6.07	1.31	1.23
1	1	28	THR	N-CA	-6.06	1.37	1.45
2	2	19	GLY	C-N	-6.06	1.25	1.33
3	3	110	SER	N-CA	6.05	1.52	1.45
3	3	155	ILE	N-CA	6.05	1.53	1.46
2	2	162	VAL	N-CA	6.05	1.53	1.46
1	1	274	ASN	N-CA	6.04	1.53	1.46
2	2	168	ASP	CA-CB	6.03	1.60	1.53
1	1	211	THR	N-CA	6.03	1.53	1.45
3	3	215	PRO	CA-CB	-6.03	1.44	1.53
2	2	190	ASN	N-CA	6.02	1.54	1.46
3	3	36	ILE	N-CA	5.99	1.53	1.46
3	3	135	GLY	C-O	5.98	1.31	1.24
2	2	208	PRO	C-N	-5.98	1.28	1.33
3	3	57	ASN	C-O	5.96	1.31	1.24
1	1	88	THR	CB-OG1	5.93	1.53	1.43
3	3	222	MET	CG-SD	5.92	1.95	1.80
2	2	180	ASN	C-N	-5.92	1.25	1.33
3	3	213	ALA	C-O	5.89	1.30	1.23
1	1	175	SER	CB-OG	-5.88	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	185	ARG	C-O	5.87	1.30	1.23
2	2	17	THR	C-N	-5.86	1.25	1.33
2	2	103	ARG	C-O	5.85	1.31	1.23
1	1	38	GLU	CB-CG	-5.83	1.34	1.52
1	1	276	GLU	N-CA	5.81	1.54	1.45
3	3	27	ASN	C-N	-5.81	1.25	1.33
3	3	219	LEU	C-N	-5.81	1.26	1.33
2	2	55	LYS	N-CA	5.79	1.53	1.46
3	3	116	MET	N-CA	5.79	1.53	1.46
1	1	287	LYS	C-O	5.78	1.31	1.24
2	2	135	HIS	CG-CD2	-5.77	1.29	1.35
3	3	158	GLN	C-O	5.74	1.30	1.24
3	3	33	ARG	NE-CZ	5.73	1.39	1.33
2	2	88	ASP	C-O	5.72	1.32	1.24
2	2	152	ARG	NE-CZ	5.72	1.39	1.33
3	3	201	THR	C-O	5.72	1.31	1.23
3	3	41	HIS	CE1-NE2	5.72	1.38	1.32
3	3	38	GLY	CA-C	-5.72	1.43	1.51
1	1	187	SER	C-O	5.71	1.30	1.23
1	1	187	SER	CB-OG	-5.71	1.30	1.42
2	2	208	PRO	C-O	5.70	1.30	1.24
2	2	176	THR	N-CA	5.69	1.53	1.45
4	4	45	LEU	C-O	5.69	1.31	1.23
2	2	195	ASN	CA-CB	-5.68	1.44	1.54
1	1	285	ASP	C-N	5.67	1.40	1.33
2	2	54	SER	CA-CB	-5.67	1.44	1.53
1	1	180	VAL	C-O	5.66	1.29	1.24
1	1	268	ARG	N-CA	5.66	1.52	1.45
1	1	239	VAL	C-O	5.65	1.30	1.24
3	3	35	HIS	C-N	-5.65	1.26	1.33
1	1	25	PRO	CA-CB	-5.64	1.45	1.53
1	1	274	ASN	CA-C	5.64	1.60	1.52
1	1	63	SER	CB-OG	-5.63	1.30	1.42
3	3	82	GLY	N-CA	5.63	1.50	1.45
2	2	87	LYS	CB-CG	-5.63	1.35	1.52
2	2	259	ILE	N-CA	5.62	1.53	1.46
2	2	63	PHE	C-O	5.61	1.30	1.24
2	2	103	ARG	N-CA	5.61	1.52	1.46
2	2	75	SER	C-O	5.61	1.30	1.23
1	1	267	GLY	C-O	5.61	1.32	1.24
1	1	117	GLU	CD-OE1	5.59	1.35	1.25
3	3	172	GLN	CG-CD	-5.58	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	109	HIS	C-O	5.57	1.30	1.24
3	3	82	GLY	C-N	-5.57	1.26	1.33
2	2	237	SER	C-O	5.56	1.30	1.23
2	2	168	ASP	C-N	-5.56	1.26	1.33
3	3	231	THR	CB-OG1	5.56	1.52	1.43
4	4	51	LYS	CE-NZ	5.55	1.66	1.49
3	3	108	SER	CA-CB	-5.54	1.44	1.53
1	1	254	ILE	CA-CB	5.53	1.61	1.54
2	2	151	GLU	CA-CB	-5.53	1.43	1.53
2	2	223	ILE	CA-C	-5.52	1.48	1.52
3	3	75	ARG	N-CA	5.52	1.52	1.45
2	2	194	ASN	C-O	5.52	1.30	1.23
3	3	40	VAL	C-O	5.52	1.30	1.24
3	3	140	GLN	C-N	-5.52	1.26	1.33
3	3	66	SER	N-CA	5.51	1.53	1.46
3	3	61	LYS	CE-NZ	5.50	1.65	1.49
1	1	102	TRP	NE1-CE2	-5.49	1.31	1.37
2	2	153	GLY	C-N	-5.47	1.25	1.33
3	3	209	SER	N-CA	5.46	1.52	1.46
3	3	77	ASN	CG-OD1	5.45	1.33	1.23
2	2	141	SER	N-CA	5.45	1.52	1.45
1	1	25	PRO	C-N	-5.45	1.25	1.33
3	3	91	VAL	C-O	5.44	1.30	1.24
2	2	237	SER	N-CA	5.43	1.52	1.46
3	3	37	PRO	CA-CB	-5.42	1.45	1.53
2	2	211	SER	C-O	5.39	1.30	1.23
2	2	171	TYR	C-O	5.38	1.31	1.24
1	1	277	PRO	N-CA	5.38	1.53	1.47
2	2	61	CYS	CA-C	-5.37	1.47	1.53
4	4	61	LEU	C-O	5.36	1.30	1.24
2	2	148	HIS	ND1-CE1	5.36	1.38	1.32
1	1	279	ILE	C-O	5.35	1.29	1.24
3	3	17	ASP	CG-OD1	5.35	1.35	1.25
3	3	74	ASN	CA-CB	5.34	1.61	1.53
2	2	68	SER	CA-C	-5.34	1.45	1.52
1	1	176	VAL	CA-C	5.34	1.58	1.52
3	3	228	ILE	C-O	5.34	1.30	1.24
1	1	127	GLU	CA-CB	-5.33	1.46	1.53
2	2	103	ARG	CA-CB	-5.32	1.45	1.53
1	1	30	LYS	CE-NZ	5.32	1.65	1.49
2	2	256	SER	C-N	-5.32	1.26	1.33
3	3	209	SER	C-O	5.32	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	202	PRO	C-O	5.32	1.30	1.23
2	2	14	GLN	CD-NE2	5.30	1.44	1.33
2	2	72	THR	CB-OG1	5.29	1.52	1.43
1	1	122	VAL	C-O	5.28	1.29	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
3	3	64	VAL	C-N	-5.26	1.25	1.33
2	2	219	SER	N-CA	5.26	1.52	1.46
2	2	246	PRO	C-O	5.25	1.29	1.23
1	1	270	ASN	CA-C	5.25	1.59	1.52
3	3	2	LEU	CA-CB	5.25	1.63	1.53
1	1	161	LYS	C-N	-5.24	1.26	1.33
1	1	54	ARG	C-O	5.24	1.30	1.23
3	3	133	PRO	CA-CB	-5.21	1.46	1.54
3	3	174	ARG	CA-C	5.21	1.58	1.52
3	3	205	VAL	C-O	5.21	1.30	1.23
2	2	99	HIS	C-N	-5.21	1.26	1.34
1	1	283	LYS	CE-NZ	5.21	1.65	1.49
3	3	146	MET	C-O	5.21	1.30	1.24
1	1	89	GLY	C-O	5.20	1.31	1.23
3	3	58	THR	CA-CB	5.18	1.62	1.53
2	2	38	TRP	CA-C	-5.18	1.45	1.52
2	2	202	PRO	C-N	-5.17	1.26	1.33
3	3	153	TRP	C-O	5.17	1.30	1.24
1	1	166	TYR	N-CA	5.14	1.52	1.46
1	1	252	ALA	C-O	5.14	1.30	1.23
2	2	204	ILE	C-N	-5.13	1.26	1.33
3	3	77	ASN	C-N	-5.13	1.26	1.33
3	3	164	THR	CA-CB	5.13	1.61	1.53
1	1	85	LYS	N-CA	5.13	1.52	1.46
1	1	42	THR	C-O	5.10	1.29	1.23
3	3	136	ALA	C-O	5.10	1.30	1.23
2	2	248	CYS	C-N	-5.10	1.26	1.33
2	2	128	PRO	CA-CB	-5.08	1.46	1.53
1	1	209	ALA	C-N	-5.08	1.26	1.33
3	3	112	ARG	CA-CB	-5.08	1.45	1.53
3	3	34	ILE	C-O	5.07	1.30	1.24
2	2	220	LEU	C-N	-5.05	1.26	1.33
3	3	232	VAL	C-O	5.05	1.29	1.23
3	3	164	THR	CA-C	-5.05	1.46	1.52
1	1	117	GLU	N-CA	5.04	1.52	1.46
3	3	216	ASP	N-CA	-5.04	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	129	THR	N-CA	5.03	1.52	1.46
2	2	186	HIS	C-O	5.03	1.29	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
2	2	109	HIS	N-CA	5.00	1.53	1.46
3	3	65	ASN	CA-CB	5.00	1.62	1.53
1	1	246	ARG	CD-NE	-5.00	1.39	1.46
3	3	163	MET	C-N	-5.00	1.26	1.33

All (615) 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
1	1	285	ASP	CA-CB-CG	-22.20	90.39	112.60
3	3	215	PRO	CA-C-N	20.36	149.20	120.29
3	3	215	PRO	C-N-CA	20.36	149.20	120.29
2	2	87	LYS	CA-CB-CG	19.05	152.21	114.10
2	2	11	ASP	CA-CB-CG	-18.96	93.64	112.60
2	2	193	THR	CA-C-N	16.44	150.19	122.07
2	2	193	THR	C-N-CA	16.44	150.19	122.07
2	2	190	ASN	CA-CB-CG	16.38	128.98	112.60
1	1	159	ASN	CB-CA-C	15.62	130.16	108.76
1	1	170	SER	CA-CB-OG	15.05	141.20	111.10
2	2	194	ASN	CA-CB-CG	-14.93	97.67	112.60
2	2	11	ASP	CA-C-N	14.78	140.54	120.44
2	2	11	ASP	C-N-CA	14.78	140.54	120.44
1	1	197	TYR	N-CA-CB	-14.13	87.34	110.23
3	3	57	ASN	CA-CB-CG	-13.76	98.84	112.60
1	1	38	GLU	CB-CG-CD	13.64	135.79	112.60
3	3	74	ASN	CA-CB-CG	-13.45	99.15	112.60
3	3	65	ASN	CA-CB-CG	-13.08	99.52	112.60
3	3	27	ASN	CA-CB-CG	-12.94	99.66	112.60
1	1	202	ASP	CA-CB-CG	12.92	125.52	112.60
2	2	44	ASP	CA-CB-CG	12.65	125.25	112.60
2	2	194	ASN	N-CA-CB	-12.62	89.83	110.41
1	1	94	ARG	CD-NE-CZ	-12.61	106.75	124.40
1	1	256	ARG	NE-CZ-NH2	12.58	130.52	119.20
2	2	67	ASP	CA-CB-CG	-12.45	100.15	112.60
2	2	256	SER	CA-C-O	-12.20	105.39	119.79
4	4	30	ASN	CA-CB-CG	-12.05	100.55	112.60
3	3	172	GLN	CB-CG-CD	12.03	133.05	112.60
4	4	45	LEU	N-CA-CB	-11.89	94.13	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	219	SER	CA-C-N	-11.56	106.30	122.95
1	1	219	SER	C-N-CA	-11.56	106.30	122.95
4	4	41	ALA	CA-C-O	-11.31	105.46	119.38
3	3	74	ASN	OD1-CG-ND2	11.30	133.90	122.60
2	2	14	GLN	OE1-CD-NE2	11.13	133.73	122.60
3	3	29	GLU	CB-CG-CD	11.13	131.52	112.60
2	2	151	GLU	CA-CB-CG	11.09	136.28	114.10
1	1	285	ASP	N-CA-CB	-11.04	95.28	110.29
1	1	173	ASN	CA-CB-CG	10.98	123.58	112.60
1	1	197	TYR	CA-CB-CG	10.92	133.55	113.90
1	1	25	PRO	CA-C-O	-10.90	108.91	121.56
2	2	88	ASP	CA-CB-CG	-10.85	101.75	112.60
2	2	219	SER	CA-CB-OG	10.64	132.37	111.10
4	4	48	ASP	CA-CB-CG	-10.64	101.96	112.60
1	1	282	ARG	CD-NE-CZ	-10.61	109.55	124.40
2	2	97	PHE	CA-CB-CG	-10.57	103.22	113.80
3	3	57	ASN	N-CA-CB	-10.41	92.90	110.49
4	4	48	ASP	O-C-N	10.17	128.35	121.23
3	3	72	ASN	CA-CB-CG	-10.16	102.44	112.60
1	1	246	ARG	NE-CZ-NH1	10.05	131.55	121.50
1	1	63	SER	CB-CA-C	-9.99	94.20	110.79
1	1	54	ARG	CD-NE-CZ	-9.95	110.47	124.40
4	4	44	SER	CA-C-N	-9.87	107.96	122.07
4	4	44	SER	C-N-CA	-9.87	107.96	122.07
1	1	91	ASP	CA-CB-CG	-9.83	102.77	112.60
1	1	187	SER	CB-CA-C	9.78	129.24	109.38
1	1	285	ASP	N-CA-C	9.76	122.92	110.33
1	1	275	THR	CA-C-O	-9.75	109.21	121.88
3	3	179	ASP	CA-CB-CG	-9.71	102.89	112.60
1	1	22	SER	CA-C-O	-9.70	109.63	120.69
1	1	28	THR	CB-CA-C	-9.70	92.96	111.48
3	3	33	ARG	CA-C-O	-9.70	110.00	121.05
1	1	208	ASP	CA-CB-CG	-9.69	102.92	112.60
1	1	256	ARG	NE-CZ-NH1	-9.68	111.82	121.50
3	3	137	ARG	NE-CZ-NH1	-9.65	111.85	121.50
1	1	53	THR	CA-CB-OG1	-9.54	95.30	109.60
1	1	79	VAL	CA-C-O	-9.47	110.54	120.39
1	1	246	ARG	CD-NE-CZ	9.44	137.61	124.40
1	1	38	GLU	CA-CB-CG	9.42	132.95	114.10
3	3	86	PHE	CA-CB-CG	9.40	123.20	113.80
3	3	89	ASP	CA-CB-CG	-9.37	103.23	112.60
1	1	141	ASN	CB-CA-C	-9.34	103.62	117.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	157	ALA	O-C-N	9.32	129.69	121.39
2	2	255	ARG	NE-CZ-NH2	-9.16	110.96	119.20
3	3	57	ASN	CB-CA-C	-9.12	92.28	110.42
1	1	197	TYR	CB-CA-C	9.08	124.52	109.53
1	1	95	GLU	CB-CG-CD	-9.03	97.25	112.60
4	4	50	SER	CA-C-O	-9.02	109.90	120.10
1	1	268	ARG	CD-NE-CZ	-9.02	111.77	124.40
2	2	195	ASN	CA-CB-CG	9.01	121.61	112.60
3	3	196	ILE	CA-C-O	-8.96	111.23	120.27
2	2	136	GLU	CB-CG-CD	-8.83	97.58	112.60
2	2	250	GLU	CA-CB-CG	8.81	131.72	114.10
4	4	68	ASN	CA-CB-CG	-8.76	103.84	112.60
1	1	270	ASN	CA-CB-CG	8.73	121.33	112.60
1	1	150	ALA	CA-C-N	-8.70	108.87	122.87
1	1	150	ALA	C-N-CA	-8.70	108.87	122.87
1	1	251	GLU	CA-CB-CG	8.66	131.42	114.10
2	2	255	ARG	CA-CB-CG	8.49	131.08	114.10
2	2	139	ASN	CA-CB-CG	-8.48	104.12	112.60
1	1	259	ARG	CA-CB-CG	-8.44	97.22	114.10
2	2	73	THR	CA-CB-OG1	-8.44	96.94	109.60
2	2	169	VAL	CB-CA-C	-8.43	101.18	111.97
2	2	168	ASP	CA-C-O	-8.41	110.61	120.62
1	1	123	ARG	NE-CZ-NH1	8.40	129.90	121.50
1	1	165	ASP	CB-CA-C	-8.39	93.71	110.42
2	2	68	SER	N-CA-C	8.38	122.88	110.48
2	2	169	VAL	CA-C-O	-8.38	112.29	121.17
4	4	36	ALA	CA-C-N	-8.35	108.76	122.54
4	4	36	ALA	C-N-CA	-8.35	108.76	122.54
4	4	41	ALA	N-CA-C	8.34	122.72	112.54
3	3	74	ASN	CA-C-O	-8.33	109.89	120.55
3	3	5	THR	CA-C-O	-8.29	111.12	120.32
1	1	122	VAL	N-CA-CB	-8.26	97.90	111.45
3	3	172	GLN	CG-CD-NE2	8.25	128.77	116.40
1	1	186	PHE	CA-C-O	-8.24	112.49	121.31
1	1	82	ILE	CA-C-O	-8.20	113.06	121.67
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
3	3	21	SER	CB-CA-C	-8.13	95.50	108.91
4	4	57	LYS	CA-C-O	-8.13	112.33	120.70
3	3	16	THR	N-CA-CB	-8.12	98.35	110.61
2	2	49	ASP	CA-CB-CG	8.12	120.72	112.60
1	1	29	GLN	N-CA-C	-8.11	102.43	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	57	ASN	OD1-CG-ND2	8.11	130.71	122.60
3	3	78	GLU	N-CA-C	8.02	120.88	110.53
2	2	187	GLN	CA-CB-CG	8.02	130.14	114.10
3	3	60	THR	CA-CB-OG1	-8.02	97.57	109.60
3	3	233	ALA	CA-C-O	-8.00	112.39	121.19
1	1	164	ASP	CA-C-N	8.00	136.82	121.54
1	1	164	ASP	C-N-CA	8.00	136.82	121.54
3	3	27	ASN	O-C-N	7.99	131.98	122.00
1	1	288	SER	CA-C-O	-7.98	113.09	121.55
1	1	157	ALA	CA-C-N	7.98	129.82	119.84
1	1	157	ALA	C-N-CA	7.98	129.82	119.84
2	2	248	CYS	CA-C-O	-7.97	112.29	121.54
3	3	111	LEU	CA-C-N	-7.95	111.79	123.00
3	3	111	LEU	C-N-CA	-7.95	111.79	123.00
1	1	94	ARG	NE-CZ-NH2	-7.95	112.05	119.20
2	2	223	ILE	N-CA-CB	-7.92	101.50	112.27
1	1	176	VAL	CA-C-O	-7.92	111.41	120.67
3	3	231	THR	CA-CB-OG1	-7.91	97.74	109.60
1	1	37	ASN	CB-CG-ND2	7.87	128.20	116.40
2	2	216	ASN	CA-C-O	-7.86	112.08	120.80
1	1	274	ASN	O-C-N	7.83	133.01	122.59
2	2	95	ASN	CA-CB-CG	-7.83	104.77	112.60
1	1	123	ARG	CD-NE-CZ	7.81	135.33	124.40
3	3	216	ASP	N-CA-CB	-7.79	98.63	110.16
1	1	150	ALA	O-C-N	7.78	132.93	123.13
2	2	109	HIS	CA-C-O	-7.77	110.78	120.57
4	4	45	LEU	CA-C-O	7.76	130.54	121.54
1	1	282	ARG	CA-C-N	-7.75	111.48	122.41
1	1	282	ARG	C-N-CA	-7.75	111.48	122.41
3	3	62	ASP	CA-CB-CG	7.71	120.31	112.60
4	4	37	SER	CB-CA-C	7.71	122.96	110.09
1	1	64	GLU	CB-CG-CD	7.69	125.67	112.60
1	1	176	VAL	CB-CA-C	-7.68	99.18	110.62
2	2	190	ASN	OD1-CG-ND2	-7.66	114.94	122.60
2	2	240	ILE	CA-C-O	-7.64	112.37	120.39
3	3	137	ARG	CD-NE-CZ	-7.62	113.74	124.40
3	3	184	ALA	N-CA-C	7.61	122.76	113.17
3	3	59	HIS	CA-C-O	7.60	130.47	121.88
1	1	173	ASN	N-CA-CB	-7.59	97.04	109.94
1	1	61	ASN	CA-CB-CG	-7.58	105.03	112.60
3	3	142	ARG	CA-CB-CG	7.57	129.24	114.10
1	1	17	THR	CA-C-N	-7.57	110.39	122.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	17	THR	C-N-CA	-7.57	110.39	122.50
2	2	87	LYS	CB-CG-CD	7.56	128.70	111.30
3	3	79	GLN	OE1-CD-NE2	-7.54	115.06	122.60
3	3	27	ASN	N-CA-C	7.53	124.03	113.56
1	1	277	PRO	N-CD-CG	-7.53	91.91	103.20
1	1	197	TYR	CA-C-O	-7.44	112.37	120.92
1	1	175	SER	CB-CA-C	7.44	126.07	109.56
4	4	30	ASN	CA-C-O	-7.43	112.22	120.69
1	1	288	SER	N-CA-C	7.40	120.42	110.35
2	2	140	VAL	CA-C-O	-7.39	113.32	121.23
2	2	98	PHE	CA-C-O	-7.37	110.97	119.60
4	4	45	LEU	CB-CA-C	7.35	122.53	111.80
2	2	107	THR	CA-C-O	-7.32	112.27	120.32
3	3	27	ASN	CB-CA-C	-7.32	97.22	111.06
2	2	39	PRO	CA-C-O	-7.31	113.01	121.34
3	3	129	LEU	CA-C-O	-7.31	112.96	120.71
3	3	118	THR	CA-CB-OG1	-7.30	98.64	109.60
2	2	180	ASN	CA-CB-CG	-7.27	105.33	112.60
3	3	61	LYS	CA-C-O	-7.26	112.64	121.06
3	3	124	SER	CA-C-O	-7.26	113.49	121.33
2	2	77	GLY	CA-C-O	-7.25	114.81	122.05
2	2	103	ARG	CD-NE-CZ	-7.23	114.28	124.40
3	3	46	ILE	CA-C-O	-7.23	112.45	120.25
1	1	187	SER	N-CA-CB	-7.22	98.20	111.13
2	2	187	GLN	CB-CA-C	7.22	125.33	109.94
1	1	26	LYS	CA-CB-CG	7.21	128.51	114.10
1	1	275	THR	CA-CB-OG1	-7.20	98.80	109.60
2	2	52	LYS	CA-C-O	-7.20	113.27	121.19
2	2	68	SER	O-C-N	-7.18	114.84	122.96
2	2	169	VAL	N-CA-C	7.18	117.32	110.42
3	3	19	ARG	NE-CZ-NH2	7.17	125.66	119.20
4	4	30	ASN	OD1-CG-ND2	7.15	129.75	122.60
2	2	146	PHE	CA-CB-CG	-7.13	106.67	113.80
1	1	284	GLY	CA-C-N	7.12	133.63	120.95
1	1	284	GLY	C-N-CA	7.12	133.63	120.95
1	1	59	HIS	CA-C-O	-7.10	112.00	120.81
2	2	168	ASP	N-CA-CB	-7.09	97.97	109.60
1	1	285	ASP	CB-CA-C	-7.07	93.75	110.02
4	4	47	MET	CA-CB-CG	-7.06	99.98	114.10
2	2	134	SER	CA-C-O	-7.06	113.01	121.05
2	2	259	ILE	CB-CG1-CD1	-7.04	99.03	113.80
3	3	94	THR	O-C-N	7.01	131.60	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	13	PHE	CA-CB-CG	7.00	120.80	113.80
1	1	28	THR	OG1-CB-CG2	6.98	123.25	109.30
3	3	35	HIS	CA-C-O	-6.97	112.90	120.92
1	1	85	LYS	CA-C-O	-6.97	113.99	121.38
1	1	43	MET	CA-C-O	6.96	126.29	119.75
3	3	164	THR	N-CA-CB	-6.96	99.65	110.57
1	1	285	ASP	CB-CG-OD1	-6.95	102.43	118.40
3	3	121	ALA	CA-C-O	-6.93	112.27	120.10
3	3	77	ASN	OD1-CG-ND2	-6.91	115.69	122.60
3	3	109	GLY	CA-C-N	-6.91	110.89	122.64
3	3	109	GLY	C-N-CA	-6.91	110.89	122.64
3	3	66	SER	CB-CA-C	6.90	121.61	110.09
2	2	57	ASP	CB-CA-C	-6.89	108.64	116.63
3	3	65	ASN	OD1-CG-ND2	6.87	129.47	122.60
1	1	35	THR	CA-CB-OG1	-6.87	99.29	109.60
1	1	270	ASN	O-C-N	6.87	131.35	122.97
1	1	89	GLY	CA-C-N	-6.85	114.30	122.93
1	1	89	GLY	C-N-CA	-6.85	114.30	122.93
2	2	9	TYR	CB-CA-C	6.85	121.37	109.65
4	4	44	SER	O-C-N	6.84	131.69	122.59
2	2	186	HIS	CA-CB-CG	-6.84	106.96	113.80
1	1	183	THR	CA-CB-OG1	-6.82	99.36	109.60
2	2	14	GLN	CB-CG-CD	-6.82	101.01	112.60
3	3	231	THR	CA-C-O	-6.81	110.54	119.06
3	3	146	MET	CG-SD-CE	6.81	115.89	100.90
1	1	42	THR	CA-CB-CG2	6.81	122.08	110.50
2	2	193	THR	O-C-N	-6.81	115.12	121.79
2	2	219	SER	CB-CA-C	6.80	121.62	109.38
3	3	202	THR	CA-C-O	6.79	128.50	121.23
3	3	151	VAL	CA-C-O	-6.78	113.54	120.25
1	1	49	ASP	N-CA-C	-6.76	105.32	113.97
2	2	124	VAL	CA-C-O	-6.75	112.77	120.66
3	3	143	ARG	N-CA-C	-6.75	104.01	111.36
1	1	35	THR	N-CA-CB	-6.74	99.09	110.49
1	1	206	HIS	CA-C-O	-6.73	114.08	121.28
3	3	42	ASN	CA-C-O	-6.72	112.93	120.66
1	1	62	GLY	CA-C-N	6.72	129.28	120.28
1	1	62	GLY	C-N-CA	6.72	129.28	120.28
2	2	224	PRO	CA-C-O	-6.72	114.04	121.23
2	2	170	LEU	CD1-CG-CD2	-6.71	96.05	110.80
2	2	249	THR	CA-CB-OG1	-6.70	99.55	109.60
4	4	58	ASP	O-C-N	6.69	130.85	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	288	SER	CB-CA-C	-6.67	97.68	109.62
3	3	187	LEU	CA-C-O	-6.67	113.17	120.24
3	3	227	THR	CA-CB-OG1	-6.65	99.63	109.60
2	2	255	ARG	CB-CG-CD	6.64	126.58	111.30
1	1	95	GLU	CA-CB-CG	-6.64	100.82	114.10
1	1	90	ILE	CA-C-N	-6.62	109.74	122.06
1	1	90	ILE	C-N-CA	-6.62	109.74	122.06
3	3	187	LEU	N-CA-CB	-6.62	100.38	110.77
1	1	282	ARG	NE-CZ-NH2	-6.62	113.24	119.20
1	1	60	PHE	CA-C-O	-6.60	113.63	120.89
2	2	198	THR	CA-C-O	-6.59	113.01	120.32
1	1	25	PRO	CA-C-N	6.58	133.40	122.73
1	1	25	PRO	C-N-CA	6.58	133.40	122.73
1	1	259	ARG	CA-C-O	-6.58	113.24	120.81
3	3	134	PRO	CA-C-N	-6.57	116.33	123.30
3	3	134	PRO	C-N-CA	-6.57	116.33	123.30
3	3	202	THR	CA-CB-OG1	-6.57	99.75	109.60
1	1	118	LEU	CA-C-N	6.56	133.11	122.81
1	1	118	LEU	C-N-CA	6.56	133.11	122.81
2	2	161	GLU	CA-C-N	-6.56	114.50	122.90
2	2	161	GLU	C-N-CA	-6.56	114.50	122.90
2	2	145	THR	CA-CB-OG1	-6.55	99.78	109.60
2	2	12	ARG	N-CA-C	6.53	118.19	111.14
2	2	38	TRP	N-CA-CB	-6.53	99.34	110.11
2	2	148	HIS	CA-CB-CG	6.52	120.32	113.80
2	2	11	ASP	OD1-CG-OD2	6.52	138.55	122.90
4	4	48	ASP	OD1-CG-OD2	6.52	138.54	122.90
1	1	97	LYS	CB-CA-C	-6.51	102.48	111.73
2	2	226	ALA	N-CA-C	-6.51	99.14	109.04
2	2	163	GLY	O-C-N	6.50	130.17	122.50
3	3	19	ARG	CA-CB-CG	6.50	127.10	114.10
2	2	18	LEU	CB-CA-C	6.50	119.82	110.79
3	3	74	ASN	N-CA-C	6.48	120.51	112.47
1	1	122	VAL	CB-CA-C	6.47	121.90	110.71
4	4	36	ALA	N-CA-C	-6.47	105.25	113.01
3	3	205	VAL	CB-CA-C	6.46	120.21	110.90
1	1	256	ARG	CD-NE-CZ	-6.45	115.37	124.40
2	2	142	VAL	CA-C-O	-6.45	113.12	120.66
2	2	193	THR	CA-C-O	6.45	126.49	119.40
3	3	182	THR	CA-CB-OG1	-6.44	99.94	109.60
2	2	223	ILE	CA-C-O	-6.43	116.59	119.94
1	1	277	PRO	CB-CA-C	6.42	119.80	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	69	LYS	CA-CB-CG	6.42	126.94	114.10
3	3	57	ASN	N-CA-C	6.42	124.47	110.80
2	2	111	GLN	OE1-CD-NE2	-6.42	116.18	122.60
2	2	247	MET	CB-CA-C	6.42	122.39	109.68
2	2	194	ASN	N-CA-C	6.41	120.51	110.32
3	3	65	ASN	N-CA-CB	-6.41	100.98	110.53
3	3	216	ASP	CA-C-N	6.40	129.79	120.71
3	3	216	ASP	C-N-CA	6.40	129.79	120.71
4	4	39	SER	O-C-N	6.40	130.74	122.23
3	3	99	GLU	CB-CG-CD	6.39	123.47	112.60
3	3	164	THR	CA-CB-OG1	-6.39	100.01	109.60
3	3	204	GLN	O-C-N	6.39	130.22	123.06
3	3	172	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	1	50	SER	CA-C-O	-6.38	110.45	118.43
4	4	44	SER	CA-CB-OG	-6.38	98.34	111.10
2	2	203	TYR	CA-C-O	-6.38	113.18	120.58
3	3	226	GLN	CB-CG-CD	-6.37	101.78	112.60
1	1	159	ASN	CA-CB-CG	6.36	118.96	112.60
1	1	239	VAL	CB-CA-C	6.33	120.00	110.63
2	2	145	THR	CA-C-O	-6.32	113.80	120.63
2	2	235	THR	CB-CA-C	-6.32	99.53	109.52
3	3	181	TYR	O-C-N	6.32	128.82	122.12
2	2	241	THR	CA-C-O	-6.32	114.01	120.71
1	1	250	VAL	N-CA-C	6.31	117.80	109.21
1	1	265	SER	O-C-N	-6.31	115.95	123.27
3	3	202	THR	N-CA-C	6.31	118.45	108.79
3	3	193	THR	CA-C-O	-6.30	111.49	120.51
1	1	205	SER	O-C-N	6.29	131.08	122.46
1	1	288	SER	N-CA-CB	-6.28	100.80	110.04
3	3	41	HIS	CA-C-O	-6.28	112.45	119.67
3	3	83	THR	CA-CB-OG1	-6.28	100.18	109.60
3	3	216	ASP	CB-CG-OD2	6.28	132.84	118.40
3	3	80	VAL	CA-C-O	-6.27	114.00	120.71
1	1	154	PRO	O-C-N	6.27	128.85	121.46
1	1	117	GLU	CG-CD-OE2	6.26	132.81	118.40
3	3	63	GLU	CB-CG-CD	-6.26	101.95	112.60
2	2	103	ARG	CA-CB-CG	6.25	126.61	114.10
2	2	143	LYS	O-C-N	6.24	130.49	122.81
1	1	70	PHE	CA-CB-CG	6.23	120.03	113.80
3	3	183	SER	N-CA-CB	-6.23	100.82	110.29
1	1	282	ARG	NH1-CZ-NH2	6.23	127.40	119.30
4	4	65	PRO	CB-CA-C	-6.22	103.43	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	198	ASN	CA-CB-CG	6.22	118.82	112.60
3	3	196	ILE	N-CA-CB	-6.22	103.36	111.82
1	1	206	HIS	O-C-N	6.21	129.50	123.29
3	3	161	ILE	CA-C-O	-6.20	113.88	120.39
1	1	31	VAL	N-CA-CB	-6.20	102.53	111.21
1	1	48	SER	CA-C-O	-6.20	108.14	119.36
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	6	THR	CB-CA-C	6.17	120.05	109.51
2	2	11	ASP	O-C-N	6.16	130.40	122.39
2	2	28	ALA	CA-C-O	-6.15	114.87	121.94
2	2	238	LEU	N-CA-CB	-6.15	98.74	110.42
1	1	260	ALA	CA-C-O	-6.14	111.54	120.13
1	1	236	LYS	CA-C-O	-6.12	114.25	121.16
3	3	163	MET	CA-CB-CG	-6.12	101.86	114.10
1	1	252	ALA	CA-C-O	-6.12	113.63	120.66
3	3	137	ARG	NE-CZ-NH2	6.11	124.70	119.20
2	2	194	ASN	OD1-CG-ND2	6.11	128.71	122.60
2	2	111	GLN	CB-CG-CD	6.11	122.99	112.60
2	2	179	GLY	CA-C-O	-6.11	114.22	120.45
1	1	202	ASP	CB-CA-C	6.10	121.10	112.07
3	3	132	THR	CA-C-O	-6.09	113.98	119.59
3	3	170	GLY	CA-C-N	6.09	128.66	120.50
3	3	170	GLY	C-N-CA	6.09	128.66	120.50
4	4	43	GLN	OE1-CD-NE2	-6.07	116.53	122.60
2	2	195	ASN	OD1-CG-ND2	-6.06	116.54	122.60
2	2	12	ARG	CD-NE-CZ	-6.06	115.92	124.40
3	3	193	THR	CA-CB-OG1	-6.05	100.53	109.60
3	3	8	PRO	CA-C-O	-6.04	114.53	121.36
1	1	68	GLU	CG-CD-OE2	6.04	132.29	118.40
2	2	241	THR	CA-CB-OG1	-6.03	100.55	109.60
3	3	36	ILE	CA-C-O	-6.02	111.88	119.95
1	1	52	GLU	CA-C-O	-6.02	113.69	120.43
1	1	77	VAL	CA-C-O	-6.02	113.24	118.96
3	3	41	HIS	N-CA-CB	6.01	119.11	110.40
2	2	86	LEU	CA-C-N	6.00	130.30	120.63
2	2	86	LEU	C-N-CA	6.00	130.30	120.63
3	3	47	ILE	CB-CG1-CD1	-6.00	101.19	113.80
3	3	137	ARG	CA-C-O	-6.00	115.04	121.94
3	3	194	SER	N-CA-CB	-6.00	100.34	110.49
1	1	41	ALA	CA-C-O	-6.00	114.64	121.72
2	2	169	VAL	N-CA-CB	5.99	117.56	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	121	ALA	CB-CA-C	-5.99	99.55	110.63
2	2	14	GLN	CA-CB-CG	-5.96	102.19	114.10
2	2	105	GLY	N-CA-C	-5.94	102.31	112.64
3	3	160	THR	CA-CB-OG1	-5.93	100.70	109.60
3	3	158	GLN	CA-C-O	5.93	127.68	120.62
3	3	77	ASN	O-C-N	-5.92	114.71	122.59
2	2	136	GLU	CG-CD-OE1	-5.92	104.78	118.40
2	2	41	TYR	N-CA-CB	5.91	118.48	110.38
3	3	207	LEU	CA-C-O	-5.91	114.23	120.80
1	1	259	ARG	CB-CA-C	-5.90	100.45	109.89
1	1	265	SER	N-CA-CB	-5.90	100.55	111.53
1	1	22	SER	N-CA-CB	-5.90	100.81	109.95
1	1	55	THR	CA-CB-OG1	-5.90	100.75	109.60
2	2	161	GLU	CA-CB-CG	5.90	125.90	114.10
3	3	1	GLY	O-C-N	-5.89	113.58	123.00
3	3	57	ASN	O-C-N	-5.87	114.78	122.59
1	1	173	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	1	185	ARG	NH1-CZ-NH2	-5.86	111.69	119.30
3	3	55	MET	CA-CB-CG	-5.86	102.39	114.10
3	3	92	PHE	CA-CB-CG	-5.85	107.95	113.80
1	1	280	LYS	CB-CA-C	-5.85	101.74	110.16
2	2	88	ASP	CA-C-O	-5.84	112.58	119.48
1	1	242	ARG	CD-NE-CZ	-5.82	116.25	124.40
3	3	33	ARG	CB-CG-CD	-5.82	97.91	111.30
3	3	131	TYR	CA-C-O	-5.82	114.08	120.43
2	2	226	ALA	O-C-N	5.82	127.82	121.36
2	2	105	GLY	CA-C-O	-5.82	112.96	122.56
3	3	59	HIS	CA-CB-CG	-5.82	107.98	113.80
4	4	65	PRO	CA-C-O	-5.81	114.72	121.34
3	3	197	LEU	CB-CA-C	5.80	117.22	108.86
1	1	270	ASN	CB-CA-C	-5.80	100.36	109.70
2	2	54	SER	CA-C-N	-5.80	115.03	122.98
2	2	54	SER	C-N-CA	-5.80	115.03	122.98
3	3	93	LYS	N-CA-C	5.80	118.38	111.71
2	2	235	THR	OG1-CB-CG2	5.78	120.86	109.30
2	2	198	THR	O-C-N	5.78	130.07	123.31
1	1	267	GLY	CA-C-N	-5.78	113.11	122.81
1	1	267	GLY	C-N-CA	-5.78	113.11	122.81
2	2	255	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	1	175	SER	CA-CB-OG	5.77	122.63	111.10
1	1	182	ASP	CA-C-N	5.75	131.58	122.62
1	1	182	ASP	C-N-CA	5.75	131.58	122.62

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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
3	3	137	ARG	O-C-N	5.73	129.69	122.65
3	3	45	GLU	CG-CD-OE2	5.71	131.54	118.40
2	2	86	LEU	CA-C-O	-5.71	112.88	119.56
2	2	210	ASP	N-CA-CB	-5.70	100.61	110.87
3	3	66	SER	N-CA-C	-5.70	105.99	113.17
1	1	94	ARG	CG-CD-NE	-5.70	99.46	112.00
2	2	189	ILE	CA-C-O	-5.69	113.30	120.69
3	3	112	ARG	CA-CB-CG	5.69	125.47	114.10
1	1	83	GLN	CB-CG-CD	-5.68	102.94	112.60
3	3	161	ILE	CA-CB-CG1	-5.68	100.75	110.40
3	3	38	GLY	N-CA-C	5.67	123.71	115.32
1	1	129	THR	CA-C-O	-5.66	114.59	120.70
1	1	28	THR	N-CA-C	5.66	118.10	109.95
1	1	232	HIS	CA-CB-CG	-5.66	108.14	113.80
2	2	190	ASN	CB-CA-C	5.65	120.00	110.79
2	2	199	ILE	CA-C-O	-5.65	114.37	120.36
1	1	94	ARG	NH1-CZ-NH2	5.63	126.61	119.30
3	3	42	ASN	CB-CG-ND2	5.63	124.84	116.40
3	3	235	THR	CA-CB-OG1	-5.61	101.18	109.60
1	1	208	ASP	CA-C-O	-5.60	114.67	121.28
1	1	241	ILE	N-CA-CB	-5.60	104.27	110.99
2	2	99	HIS	CA-CB-CG	-5.58	108.22	113.80
2	2	188	PHE	CA-C-O	-5.58	114.86	121.66
4	4	58	ASP	CA-C-N	5.57	129.02	121.05
4	4	58	ASP	C-N-CA	5.57	129.02	121.05
1	1	27	HIS	CA-CB-CG	5.57	119.36	113.80
2	2	9	TYR	CA-CB-CG	-5.57	103.88	113.90
2	2	217	ASN	CB-CA-C	5.56	118.90	109.55
2	2	251	PHE	CA-C-O	-5.56	114.82	121.11
2	2	262	GLN	OE1-CD-NE2	-5.56	117.04	122.60
2	2	106	TYR	CA-C-O	-5.56	115.33	121.33
2	2	215	HIS	CA-C-O	-5.55	112.50	120.11
1	1	198	ASN	CA-C-O	-5.55	114.05	120.49
3	3	166	PRO	CB-CA-C	5.55	118.62	111.46
3	3	190	TRP	CA-C-O	-5.54	115.14	121.40
3	3	76	GLN	CA-C-O	-5.54	115.14	121.68
2	2	94	GLN	CG-CD-NE2	-5.54	108.09	116.40
3	3	107	TRP	CA-C-O	-5.54	115.14	121.40
2	2	68	SER	N-CA-CB	-5.53	101.88	110.29
1	1	141	ASN	CA-C-O	5.53	121.15	117.94
1	1	273	LYS	CG-CD-CE	-5.53	98.58	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	64	GLU	CA-CB-CG	5.53	125.15	114.10
1	1	235	HIS	CA-CB-CG	-5.53	108.28	113.80
2	2	168	ASP	CA-C-N	5.52	127.52	120.56
2	2	168	ASP	C-N-CA	5.52	127.52	120.56
3	3	140	GLN	CA-CB-CG	-5.52	103.07	114.10
2	2	99	HIS	CA-C-N	5.51	128.22	120.28
2	2	99	HIS	C-N-CA	5.51	128.22	120.28
3	3	175	TYR	CB-CA-C	-5.51	99.33	109.46
1	1	63	SER	O-C-N	5.48	127.93	122.12
1	1	186	PHE	O-C-N	5.48	128.86	122.99
3	3	57	ASN	CA-C-N	5.48	132.02	121.18
3	3	57	ASN	C-N-CA	5.48	132.02	121.18
2	2	26	GLN	OE1-CD-NE2	-5.48	117.12	122.60
2	2	258	SER	O-C-N	5.47	129.54	122.81
3	3	63	GLU	CG-CD-OE1	-5.47	105.83	118.40
2	2	123	LEU	CA-C-O	-5.46	114.47	120.43
2	2	192	ARG	CA-C-O	-5.46	111.95	119.05
2	2	43	PRO	N-CD-CG	-5.46	95.01	103.20
2	2	167	LYS	CA-C-O	5.46	126.11	119.78
2	2	38	TRP	CB-CA-C	5.45	116.25	108.68
2	2	92	PHE	N-CA-C	-5.45	105.03	110.97
3	3	84	ASN	OD1-CG-ND2	5.44	128.04	122.60
3	3	168	THR	CA-CB-OG1	-5.44	101.43	109.60
3	3	164	THR	CB-CA-C	5.44	119.12	109.72
1	1	166	TYR	N-CA-C	-5.43	105.52	111.82
1	1	21	ILE	CA-CB-CG1	-5.42	101.18	110.40
4	4	50	SER	CA-CB-OG	-5.42	100.26	111.10
2	2	232	THR	CA-CB-OG1	-5.42	101.48	109.60
3	3	90	GLY	CA-C-O	-5.42	114.86	121.68
2	2	13	VAL	CA-C-O	-5.41	114.56	120.84
2	2	221	MET	CA-C-O	-5.41	114.31	120.32
3	3	34	ILE	CA-C-O	-5.41	114.01	120.78
2	2	53	THR	CA-C-O	-5.41	115.56	121.89
1	1	50	SER	CB-CA-C	5.40	117.45	109.29
2	2	219	SER	N-CA-C	-5.40	100.90	109.59
2	2	63	PHE	CA-CB-CG	5.39	119.19	113.80
2	2	187	GLN	CA-C-O	-5.39	114.95	120.99
2	2	129	GLU	CB-CA-C	-5.39	104.24	111.89
3	3	38	GLY	O-C-N	-5.38	115.97	122.38
3	3	78	GLU	CA-CB-CG	5.38	124.87	114.10
1	1	282	ARG	O-C-N	5.38	129.43	122.81
3	3	195	LEU	CA-C-O	-5.38	114.92	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	116	MET	CB-CG-SD	-5.37	96.59	112.70
3	3	221	LEU	O-C-N	5.37	129.73	122.59
1	1	288	SER	CA-CB-OG	-5.36	100.37	111.10
3	3	143	ARG	O-C-N	5.36	128.26	122.15
2	2	81	LYS	CB-CG-CD	5.36	123.63	111.30
1	1	117	GLU	CG-CD-OE1	-5.35	106.09	118.40
2	2	102	GLY	CA-C-O	-5.34	115.43	121.68
1	1	286	ILE	O-C-N	5.33	127.82	121.80
1	1	174	PRO	CA-C-O	-5.33	115.53	121.23
3	3	112	ARG	CB-CA-C	5.33	119.00	110.16
1	1	92	ASN	O-C-N	5.32	129.46	123.28
1	1	231	GLU	N-CA-C	-5.32	103.00	110.35
2	2	177	LEU	N-CA-CB	-5.32	101.61	110.23
2	2	12	ARG	CB-CG-CD	-5.31	99.08	111.30
3	3	226	GLN	N-CA-C	-5.31	106.75	113.18
2	2	120	GLY	CA-C-O	-5.31	114.47	122.54
1	1	26	LYS	CG-CD-CE	-5.30	99.10	111.30
2	2	76	LYS	CA-C-O	-5.29	113.43	119.41
2	2	262	GLN	CG-CD-NE2	5.29	124.33	116.40
3	3	192	GLN	N-CA-C	-5.29	105.10	112.45
3	3	222	MET	CB-CG-SD	-5.29	96.83	112.70
3	3	16	THR	OG1-CB-CG2	5.29	119.87	109.30
2	2	210	ASP	CA-CB-CG	-5.28	107.32	112.60
1	1	140	ALA	N-CA-C	5.28	116.31	108.86
3	3	204	GLN	CA-C-O	-5.28	115.03	121.36
3	3	86	PHE	CB-CA-C	5.27	120.48	111.68
1	1	60	PHE	N-CA-CB	-5.27	102.17	111.39
3	3	56	ASN	CA-C-N	5.27	131.60	121.54
3	3	56	ASN	C-N-CA	5.27	131.60	121.54
3	3	77	ASN	CA-CB-CG	-5.27	107.33	112.60
1	1	229	VAL	N-CA-C	-5.26	104.93	112.35
3	3	28	TYR	N-CA-CB	-5.26	102.23	109.97
3	3	161	ILE	N-CA-CB	5.26	118.67	111.41
4	4	58	ASP	N-CA-CB	5.26	118.99	110.42
2	2	195	ASN	N-CA-C	-5.25	106.65	114.64
2	2	122	LEU	CA-C-O	-5.25	115.08	121.28
3	3	94	THR	CA-C-O	-5.25	113.16	119.15
2	2	72	THR	CA-CB-OG1	-5.25	101.73	109.60
4	4	53	THR	CA-CB-OG1	-5.25	101.73	109.60
2	2	168	ASP	OD1-CG-OD2	5.24	135.49	122.90
1	1	279	ILE	CA-C-N	5.23	128.77	121.02
1	1	279	ILE	C-N-CA	5.23	128.77	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	144	GLU	CA-CB-CG	5.23	124.56	114.10
1	1	268	ARG	CB-CA-C	5.22	119.78	109.66
2	2	257	LYS	N-CA-CB	5.22	119.31	110.49
3	3	67	TYR	N-CA-C	-5.22	106.76	113.23
2	2	20	ASN	CA-CB-CG	5.21	117.81	112.60
2	2	243	THR	CA-C-O	-5.21	114.70	120.38
2	2	181	LEU	N-CA-C	-5.21	106.19	112.54
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
1	1	259	ARG	N-CA-CB	5.20	117.59	109.85
3	3	138	GLY	N-CA-C	-5.20	101.74	112.34
1	1	23	SER	CA-C-O	-5.19	115.04	121.06
2	2	259	ILE	CA-C-O	-5.19	114.99	120.39
3	3	158	GLN	CG-CD-OE1	5.19	131.18	120.80
1	1	257	ALA	N-CA-CB	-5.19	101.83	109.98
1	1	127	GLU	CA-C-O	-5.19	114.61	120.32
1	1	201	TYR	CA-C-N	-5.18	114.85	122.06
1	1	201	TYR	C-N-CA	-5.18	114.85	122.06
2	2	38	TRP	CA-CB-CG	-5.18	103.75	113.60
3	3	208	LEU	CA-C-O	-5.18	115.05	120.80
1	1	63	SER	N-CA-C	5.18	116.92	111.28
1	1	282	ARG	CB-CA-C	-5.18	100.35	109.62
3	3	231	THR	CA-C-N	-5.18	115.34	122.69
3	3	231	THR	C-N-CA	-5.18	115.34	122.69
2	2	75	SER	N-CA-CB	-5.17	102.02	109.83
3	3	45	GLU	CG-CD-OE1	-5.17	106.50	118.40
1	1	187	SER	O-C-N	-5.17	117.07	123.33
3	3	186	PHE	CA-CB-CG	-5.17	108.63	113.80
2	2	127	ILE	CA-C-O	-5.17	114.25	119.89
3	3	215	PRO	CB-CA-C	5.17	119.25	111.44
3	3	233	ALA	O-C-N	5.17	129.23	122.87
1	1	204	TYR	CA-C-O	-5.17	115.58	121.58
3	3	186	PHE	O-C-N	5.17	129.87	123.15
2	2	213	THR	CA-CB-OG1	-5.16	101.86	109.60
2	2	18	LEU	N-CA-CB	-5.16	102.81	110.71
2	2	214	ARG	CD-NE-CZ	-5.15	117.19	124.40
2	2	143	LYS	CA-C-N	5.13	131.34	121.54
2	2	143	LYS	C-N-CA	5.13	131.34	121.54
3	3	82	GLY	N-CA-C	-5.13	102.97	110.87
3	3	109	GLY	N-CA-C	5.12	117.52	111.63
2	2	152	ARG	CD-NE-CZ	-5.12	117.24	124.40
2	2	119	SER	O-C-N	5.11	129.35	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	165	PRO	CA-C-O	-5.11	115.41	122.15
3	3	75	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	1	110	VAL	O-C-N	-5.10	117.23	122.23
2	2	65	THR	CA-CB-OG1	-5.10	101.95	109.60
1	1	285	ASP	CA-C-N	-5.09	111.95	120.30
1	1	285	ASP	C-N-CA	-5.09	111.95	120.30
2	2	32	VAL	O-C-N	5.09	128.33	123.14
1	1	40	GLY	N-CA-C	-5.08	108.10	115.27
1	1	170	SER	CA-C-O	-5.08	115.84	122.14
3	3	125	ALA	CA-C-O	-5.08	115.51	121.10
3	3	32	PRO	CA-C-O	-5.08	115.67	121.56
2	2	127	ILE	O-C-N	5.08	125.59	120.92
1	1	27	HIS	CA-C-O	-5.07	113.13	122.62
2	2	119	SER	CA-C-O	-5.07	115.67	121.40
3	3	1	GLY	N-CA-C	5.07	128.01	113.30
3	3	217	PHE	N-CA-C	5.07	117.58	110.23
2	2	126	VAL	CA-C-O	-5.07	115.11	120.53
1	1	165	ASP	CB-CG-OD2	5.06	130.04	118.40
2	2	168	ASP	CB-CG-OD1	-5.06	106.76	118.40
1	1	66	ASP	CA-C-O	-5.06	115.62	121.19
2	2	259	ILE	CA-C-N	-5.06	112.77	122.13
2	2	259	ILE	C-N-CA	-5.06	112.77	122.13
3	3	158	GLN	CB-CA-C	5.05	118.35	110.67
1	1	76	CYS	CA-C-O	-5.05	115.00	120.81
2	2	170	LEU	N-CA-C	-5.05	106.81	112.87
2	2	25	THR	CA-C-O	5.04	126.46	120.66
1	1	270	ASN	N-CA-CB	5.04	117.71	109.69
3	3	95	THR	CA-CB-OG1	-5.04	102.05	109.60
1	1	282	ARG	CG-CD-NE	-5.04	100.92	112.00
1	1	65	THR	N-CA-C	-5.03	106.06	113.61
2	2	235	THR	CA-C-O	5.03	125.40	120.17
3	3	146	MET	CB-CA-C	5.03	120.42	110.17
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
2	2	196	THR	CA-CB-CG2	5.02	119.03	110.50
1	1	189	PRO	CB-CA-C	-5.01	103.68	111.40
2	2	215	HIS	CA-CB-CG	5.01	118.81	113.80
2	2	115	THR	CA-C-O	-5.01	115.84	121.40
3	3	155	ILE	CB-CG1-CD1	5.00	124.31	113.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	219	SER	Mainchain
1	1	220	HIS	Mainchain
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	2168	0	2104	185	0
2	2	1952	0	1926	131	0
3	3	1849	0	1832	153	0
4	4	297	0	294	36	0
5	1	26	0	27	6	0
All	All	6292	0	6183	429	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 (429) 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	1.80	1.54
1:1:220:HIS:C	1:1:221:MET:CA	1.94	1.37
1:1:220:HIS:CA	1:1:221:MET:N	1.94	1.29
1:1:220:HIS:O	1:1:221:MET:N	1.74	1.21
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.14
1:1:136:GLN:NE2	1:1:140:ALA:CB	2.17	1.07
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.42	1.02
3:3:179:ASP:HB3	3:3:182:THR:HG22	1.44	1.00
1:1:99:PHE:CD1	1:1:99:PHE:O	2.15	1.00
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	0.97
1:1:136:GLN:NE2	1:1:140:ALA:HB1	1.80	0.96
1:1:285:ASP:CA	1:1:285:ASP:CG	2.37	0.95
1:1:83:GLN:HG3	1:1:85:LYS:HE2	1.47	0.94
1:1:285:ASP:CB	1:1:285:ASP:C	2.40	0.93
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.05	0.92
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.91
3:3:179:ASP:HB3	3:3:182:THR:CG2	2.01	0.91
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
2:2:12:ARG:HG3	2:2:12:ARG:HH11	1.28	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.90
1:1:58:MET:HE1	3:3:216:ASP:O	1.71	0.90
1:1:77:VAL:C	1:1:109:LEU:HD12	1.95	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
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
1:1:220:HIS:C	1:1:221:MET:N	0.76	0.86
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.90	0.86
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.57	0.85
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	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
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.82
1:1:220:HIS:O	1:1:221:MET:CA	2.18	0.82
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.82
2:2:30:ASN:HD22	2:2:31:ALA:H	1.27	0.82
2:2:52:LYS:NZ	2:2:52:LYS:CD	2.43	0.82
1:1:248:LYS:HE3	4:4:38:THR:O	1.80	0.82
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.82
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.61	0.81
1:1:38:GLU:CD	3:3:116:MET:HE2	2.05	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.47	0.79
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.79
2:2:9:TYR:N	2:2:9:TYR:CD1	2.43	0.79
1:1:142:TYR:O	1:1:142:TYR:CD1	2.36	0.78
1:1:58:MET:HE1	3:3:216:ASP:C	2.08	0.78
2:2:262:GLN:HE21	2:2:262:GLN:C	1.91	0.78
1:1:220:HIS:O	1:1:221:MET:HA	1.83	0.77
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.13	0.77
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
1:1:94:ARG:CZ	1:1:101:ASP:OD1	2.33	0.77
1:1:188:VAL:HG21	5:1:290:W84:H2C2	1.66	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	0.75
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.75
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.68	0.74
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.74
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	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
1:1:136:GLN:CD	1:1:140:ALA:CB	2.63	0.72
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.72
1:1:58:MET:HE1	3:3:216:ASP:HA	1.71	0.71
1:1:94:ARG:NH2	1:1:101:ASP:OD1	2.23	0.71
1:1:99:PHE:CD1	1:1:99:PHE:C	2.68	0.71
1:1:201:TYR:HD2	1:1:214:GLY:O	1.73	0.71
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.71
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.71
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.71
1:1:142:TYR:CD1	1:1:142:TYR:C	2.68	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	0.71
1:1:105:ASN:HD21	1:1:108:SER:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:57:ASN:CA	3:3:57:ASN:OD1	2.38	0.70
1:1:99:PHE:O	1:1:99:PHE:CG	2.43	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	0.69
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.69
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.69
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
1:1:82:ILE:HG22	1:1:100:ASN:H	1.57	0.69
1:1:136:GLN:HE21	1:1:235:HIS:CG	2.10	0.68
3:3:20:GLN:HE22	4:4:31:TYR:H	1.42	0.68
4:4:29:ILE:HG22	4:4:29:ILE:O	1.94	0.68
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.67
1:1:142:TYR:HE1	1:1:144:SER:HG	1.42	0.67
1:1:278:VAL:HG12	3:3:62:ASP:OD2	1.95	0.67
3:3:61:LYS:HD3	3:3:63:GLU:OE2	1.95	0.67
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.67
1:1:152:TYR:O	1:1:154:PRO:HD3	1.94	0.67
2:2:155:ASP:C	2:2:155:ASP:OD1	2.37	0.66
1:1:136:GLN:NE2	1:1:235:HIS:CD2	2.63	0.66
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.66
1:1:107:SER:HB3	1:1:113:ARG:HD2	1.77	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
1:1:285: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
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.64
1:1:58:MET:HE1	3:3:216:ASP:CA	2.27	0.64
1:1:77:VAL:C	1:1:109:LEU:CD1	2.69	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
3:3:179:ASP:OD1	3:3:180:THR:N	2.32	0.63
2:2:205:ASN:ND2	2:2:206:SER:H	1.97	0.63
2:2:187:GLN:HE21	2:2:197:ALA:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:136:GLN:NE2	1:1:235:HIS:CG	2.67	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62
3:3:84:ASN:ND2	3:3:86:PHE:H	1.98	0.62
1:1:136:GLN:HE22	1:1:140:ALA:HB1	1.65	0.61
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.61
1:1:188:VAL:HG11	5:1:290:W84:H3C1	1.82	0.61
2:2:38:TRP:CZ3	4:4:57:LYS:HD2	2.36	0.61
2:2:133:ALA:O	2:2:166:VAL:HG12	2.01	0.61
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.15	0.61
1:1:187:SER:HB3	3:3:21:SER:CB	2.31	0.61
1:1:136:GLN:CD	1:1:140:ALA:HB3	2.23	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
1:1:215:ILE:O	1:1:218:LEU:N	2.30	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	0.60
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
1:1:138:ASP:O	1:1:139:SER:C	2.44	0.60
3:3:179:ASP:CB	3:3:182:THR:HG22	2.26	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
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
1:1:188:VAL:HG21	5:1:290:W84:C2C	2.33	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
3:3:179:ASP:HB3	3:3:182:THR:HB	1.85	0.58
1:1:43:MET:HE3	1:1:43:MET:HA	1.85	0.58
1:1:136:GLN:NE2	1:1:140:ALA:HB2	2.15	0.58
1:1:151:MET:SD	1:1:170:SER:HB2	2.43	0.58
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.58
3:3:175:TYR:HD2	3:3:182:THR:HG21	1.68	0.57
2:2:64:TYR:CD1	2:2:89:MET:HB3	2.39	0.57
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	0.57
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.57
2:2:221:MET:HE2	2:2:223:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:57:ASN:HB3	3:3:57:ASN:C	2.27	0.57
2:2:52:LYS:NZ	2:2:52:LYS:HD3	2.20	0.57
1:1:188:VAL:HG21	5:1:290:W84:H3C1	1.86	0.57
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.56
1:1:102:TRP:O	1:1:223:SER:HB2	2.05	0.56
3:3:31:THR:CG2	3:3:32:PRO:HD2	2.34	0.56
1:1:58:MET:HE3	3:3:216:ASP:HA	1.86	0.56
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
1:1:103:LYS:O	1:1:104:ILE:C	2.49	0.56
2:2:174:ASN:C	2:2:174:ASN:ND2	2.63	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.56
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.56
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.55
2:2:189:ILE:HA	2:2:194:ASN:ND2	2.21	0.55
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.55
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.55
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.88	0.55
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.55
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.55
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	0.55
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
1:1:266:ILE:HD12	3:3:235:THR:HA	1.88	0.54
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.54
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.87	0.54
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.54
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.54
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.54
3:3:20:GLN:HE22	4:4:31:TYR:N	2.04	0.54
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.54
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.54
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.54
2:2:170:LEU:CD2	3:3:64:VAL:HA	2.38	0.54
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.54
3:3:117:TYR:CD1	3:3:155:ILE:HD13	2.43	0.54
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.53
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.53
3:3:175:TYR:CD2	3:3:182:THR:HG21	2.43	0.53
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.53
2:2:195:ASN:ND2	2:2:195:ASN:C	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.53
1:1:88:THR:O	1:1:90:ILE:HD13	2.09	0.52
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.52
1:1:188:VAL:HG21	5:1:290:W84:C3C	2.39	0.52
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
1:1:77:VAL:O	1:1:109:LEU:HD12	2.07	0.52
1:1:187:SER:HB3	3:3:21:SER:HB2	1.92	0.52
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.52
1:1:92:ASN:C	1:1:92:ASN:ND2	2.67	0.52
1:1:136:GLN:HE21	1:1:235:HIS:CD2	2.28	0.52
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	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
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.52
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.51
4:4:44:SER:C	4:4:46:SER:N	2.68	0.51
1:1:219:SER:O	1:1:219:SER:OG	2.19	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
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
3:3:84:ASN:ND2	3:3:84:ASN:C	2.69	0.51
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
1:1:38:GLU:OE1	3:3:116:MET:HE2	2.10	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
3:3:101:VAL:HG13	3:3:176:THR:CG2	2.41	0.51
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.51
3:3:84:ASN:HD22	3:3:86:PHE:N	2.08	0.51
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.50
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE2	2.44	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	2.00	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
2:2:171:TYR:HA	2:2:176:THR:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:142:TYR:C	1:1:142:TYR:HD1	2.18	0.50
3:3:84:ASN:HD22	3:3:84:ASN:C	2.20	0.49
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.49
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.49
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	0.49
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.49
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.94	0.49
3:3:20:GLN:NE2	4:4:31:TYR:H	2.11	0.49
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.49
2:2:30:ASN:ND2	2:2:31:ALA:H	2.05	0.48
1:1:82:ILE:CG2	1:1:100:ASN:H	2.23	0.48
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
3:3:54:PRO:O	3:3:91:VAL:HG12	2.13	0.48
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.48
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
1:1:280:LYS:HE3	3:3:89:ASP:OD1	2.13	0.48
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.95	0.48
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.48
1:1:122:VAL:O	1:1:197:TYR:HB2	2.13	0.48
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.78	0.48
1:1:158:PRO:HB2	1:1:167:THR:HG22	1.96	0.48
3:3:61:LYS:O	3:3:61:LYS:HG2	2.07	0.48
3:3:112:ARG:NH1	3:3:112:ARG:HG2	2.27	0.48
3:3:175:TYR:H	3:3:182:THR:HG21	1.78	0.48
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.47
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.95	0.47
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.44	0.47
1:1:104:ILE:HG13	1:1:223:SER:HA	1.96	0.47
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.95	0.47
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.47
1:1:268:ARG:CZ	2:2:139:ASN:HB2	2.44	0.47
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.47
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:165:ASP:HB3	1:1:167:THR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:206:HIS:ND1	1:1:206:HIS:N	2.62	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
1:1:102:TRP:CZ3	1:1:224:MET:HE2	2.50	0.47
1:1:188:VAL:CG2	5:1:290:W84:H2C2	2.40	0.47
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.47
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.43	0.46
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.46
1:1:110:VAL:O	1:1:111:GLN:C	2.53	0.46
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.46
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.46
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.63	0.46
1:1:236:LYS:HE2	1:1:236:LYS:HB3	1.83	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
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
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.46
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.46
1:1:102:TRP:HZ3	1:1:224:MET:HE2	1.81	0.45
3:3:57:ASN:CB	3:3:57:ASN:H	2.26	0.45
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.45
1:1:77:VAL:CA	1:1:109:LEU:HD12	2.46	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	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
1:1:132:ALA:O	1:1:181:GLY:N	2.39	0.45
2:2:170:LEU:HD23	3:3:64:VAL:HG22	1.99	0.45
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.98	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.98	0.45
1:1:152:TYR:O	1:1:173:ASN:ND2	2.50	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
3:3:192:GLN:HE21	3:3:192:GLN:HA	1.81	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.81	0.45
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
3:3:179:ASP:HB3	3:3:182:THR:CB	2.45	0.45
1:1:43:MET:HA	1:1:43:MET:CE	2.46	0.45
1:1:138:ASP:O	1:1:139:SER:O	2.33	0.45
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.45
1:1:198:ASN:HB3	1:1:200:PHE:O	2.17	0.44
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.44
1:1:92:ASN:C	1:1:92:ASN:HD22	2.26	0.44
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.44
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
1:1:289:TYR:CE2	3:3:138:GLY:HA3	2.53	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.17	0.44
1:1:207:ASP:HA	2:2:144:TYR:CE2	2.52	0.44
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.44
4:4:43:GLN:O	4:4:45:LEU:CB	2.66	0.44
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.44
1:1:289:TYR:CD2	3:3:138:GLY:HA3	2.52	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
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.44
3:3:101:VAL:HG13	3:3:176:THR:HG22	1.99	0.44
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.43
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	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
1:1:38:GLU:N	3:3:116:MET:HE1	2.34	0.43
1:1:215:ILE:C	1:1:217:VAL:N	2.74	0.43
1:1:82:ILE:HG22	1:1:100:ASN:HB2	2.00	0.43
1:1:159:ASN:HA	1:1:160:PRO:HD3	1.65	0.43
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	0.43
2:2:10:SER:CB	2:2:12:ARG:HB2	2.48	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
1:1:285:ASP:C	1:1:285:ASP:HB3	2.38	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
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
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.82	0.42
4:4:43:GLN:C	4:4:45:LEU:N	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	0.42
1:1:187:SER:HB3	3:3:21:SER:HB3	2.01	0.42
1:1:89:GLY:C	1:1:90:ILE:CD1	2.89	0.42
3:3:153:TRP:CD1	3:3:153:TRP:C	2.97	0.42
3:3:226:GLN:HE21	3:3:226:GLN:HB2	1.21	0.42
1:1:137:PRO:HG3	1:1:238:LEU:HD22	2.00	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
2:2:40: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
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.42
1:1:201:TYR:H	2:2:131:GLN:HE21	1.68	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42
3:3:44:LEU:HA	3:3:44:LEU:HD23	1.79	0.42
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.38	0.42
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.42
1:1:97:LYS:C	1:1:99:PHE:H	2.27	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	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.41
1:1:86:ASP:OD1	1:1:88:THR:HB	2.20	0.41
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.41
1:1:87:ALA:C	1:1:90:ILE:HG12	2.46	0.41
3:3:113:PHE:CE2	3:3:115:LEU:HD13	2.56	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.41
1:1:142:TYR:HE1	1:1:144:SER:OG	2.00	0.41
1:1:98:LEU:O	1:1:99:PHE:HB3	2.19	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.03	0.41
3:3:137:ARG:HH11	3:3:137:ARG:HD3	1.22	0.41
1:1:54:ARG:HH11	1:1:54:ARG:HD2	1.55	0.41
1:1:165:ASP:CB	1:1:167:THR:OG1	2.69	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
3:3:179:ASP:CB	3:3:182:THR:CG2	2.88	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
3:3:64:VAL:O	3:3:64:VAL:HG12	2.21	0.41
3:3:157:LEU:HD23	3:3:157:LEU:O	2.21	0.41
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40
3:3:20:GLN:NE2	4:4:30:ASN:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:231:THR:C	3:3:232:VAL:HG13	2.45	0.40
1:1:265:SER:OG	2:2:139:ASN:HB3	2.21	0.40
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
1:1:208:ASP:HB3	1:1:211:THR:HB	2.04	0.40
1:1:215:ILE:O	1:1:216:THR:C	2.64	0.40
1:1:228:ILE:HD11	1:1:239:VAL:CG2	2.52	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%)	251 (93%)	16 (6%)	4 (2%)	8	35
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	16	50
3	3	234/236 (99%)	216 (92%)	15 (6%)	3 (1%)	9	38
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	4	23
All	All	796/855 (93%)	734 (92%)	52 (6%)	10 (1%)	9	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	57	ASN
3	3	77	ASN
1	1	99	PHE
1	1	139	SER
1	1	165	ASP
2	2	255	ARG
2	2	257	LYS
4	4	47	MET
1	1	104	ILE

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Mol	Chain	Res	Type
3	3	178	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	239/253 (94%)	182 (76%)	57 (24%)	1	4
2	2	223/229 (97%)	177 (79%)	46 (21%)	1	7
3	3	209/209 (100%)	171 (82%)	38 (18%)	2	9
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	1
All	All	704/748 (94%)	550 (78%)	154 (22%)	1	5

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	VAL
1	1	21	ILE
1	1	22	SER
1	1	23	SER
1	1	28	THR
1	1	29	GLN
1	1	30	LYS
1	1	38	GLU
1	1	43	MET
1	1	47	PRO
1	1	81	GLU
1	1	90	ILE
1	1	95	GLU
1	1	97	LYS
1	1	99	PHE
1	1	100	ASN
1	1	101	ASP
1	1	103	LYS
1	1	105	ASN
1	1	106	LEU

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Mol	Chain	Res	Type
1	1	107	SER
1	1	122	VAL
1	1	138	ASP
1	1	142	TYR
1	1	143	SER
1	1	144	SER
1	1	145	ASN
1	1	151	MET
1	1	159	ASN
1	1	161	LYS
1	1	165	ASP
1	1	170	SER
1	1	172	SER
1	1	173	ASN
1	1	176	VAL
1	1	183	THR
1	1	184	SER
1	1	185	ARG
1	1	187	SER
1	1	202	ASP
1	1	215	ILE
1	1	216	THR
1	1	217	VAL
1	1	218	LEU
1	1	220	HIS
1	1	224	MET
1	1	240	LYS
1	1	248	LYS
1	1	254	ILE
1	1	256	ARG
1	1	266	ILE
1	1	268	ARG
1	1	273	LYS
1	1	274	ASN
1	1	275	THR
1	1	278	VAL
1	1	287	LYS
2	2	12	ARG
2	2	20	ASN
2	2	26	GLN
2	2	30	ASN
2	2	49	ASP

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Mol	Chain	Res	Type
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	170	LEU
2	2	174	ASN
2	2	187	GLN
2	2	192	ARG
2	2	195	ASN
2	2	209	ILE
2	2	211	SER
2	2	217	ASN
2	2	225	ILE
2	2	230	VAL
2	2	232	THR
2	2	236	PRO
2	2	238	LEU
2	2	247	MET
2	2	250	GLU
2	2	254	ILE
2	2	255	ARG
2	2	256	SER
2	2	259	ILE
2	2	262	GLN
3	3	12	GLN

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Mol	Chain	Res	Type
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	182	THR
3	3	192	GLN
3	3	194	SER
3	3	196	ILE
3	3	201	THR
3	3	208	LEU
3	3	211	ILE
3	3	218	LYS
3	3	219	LEU
3	3	220	ARG
3	3	223	LYS
3	3	226	GLN
3	3	228	ILE
3	3	230	GLN
4	4	29	ILE
4	4	33	LYS
4	4	40	SER
4	4	43	GLN
4	4	45	LEU

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Mol	Chain	Res	Type
4	4	46	SER
4	4	47	MET
4	4	50	SER
4	4	51	LYS
4	4	59	LEU
4	4	61	LEU
4	4	67	LEU
4	4	68	ASN

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

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

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Mol	Chain	Res	Type
4	4	30	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](#)

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	W84	1	290	-	28,28,28	2.81	5 (17%)	34,36,36	2.52	6 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	W84	1	290	-	-	6/15/24/24	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	290	W84	C2A-N3A	11.04	1.43	1.27
5	1	290	W84	C4A-N3A	-7.45	1.35	1.48
5	1	290	W84	O1A-C2A	-4.32	1.29	1.36
5	1	290	W84	O1A-C5A	-3.73	1.38	1.45
5	1	290	W84	O1B-C7C	2.62	1.52	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	290	W84	CM1-C4A-N3A	7.97	133.42	111.59
5	1	290	W84	O1A-C2A-N3A	-6.90	110.16	118.10
5	1	290	W84	O1A-C2A-C4B	6.52	124.09	115.85
5	1	290	W84	O1A-C5A-C4A	5.48	111.47	104.88
5	1	290	W84	C5A-C4A-N3A	-3.97	98.51	103.71
5	1	290	W84	CM1-C4A-C5A	-2.60	104.69	114.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	290	W84	C2C-C1C-C5-O1
5	1	290	W84	C3C-C4C-C5C-C6C
5	1	290	W84	C1C-C2C-C3C-C4C
5	1	290	W84	C2C-C1C-C5-C4
5	1	290	W84	C5-C1C-C2C-C3C
5	1	290	W84	C6C-C7C-O1B-C1B

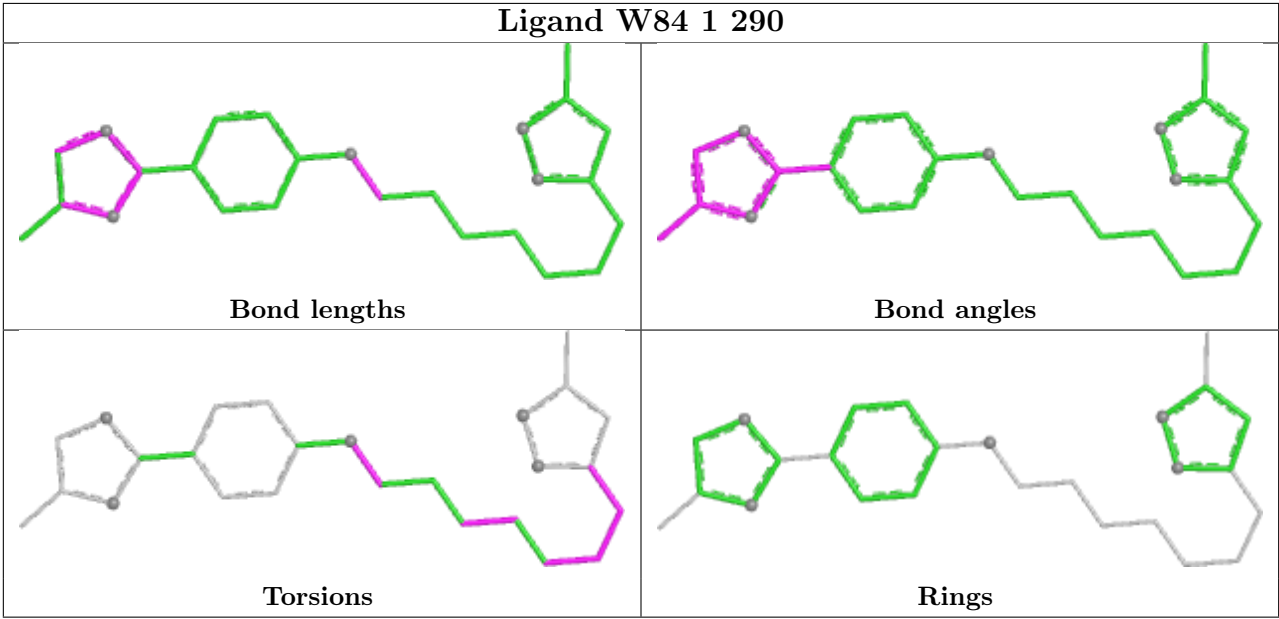
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	290	W84	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	150:ALA	C	151:MET	N	1.66
1	1	219:SER	C	220:HIS	N	0.90
1	1	220:HIS	C	221:MET	N	0.76

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.