



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:39 PM UTC

PDB ID : 1VRH / pdb_00001vrh
Title : HRV14/SDZ 880-061 COMPLEX
Authors : Oren, D.A.; Zhang, A.; Arnold, E.
Deposited on : 1996-02-26
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

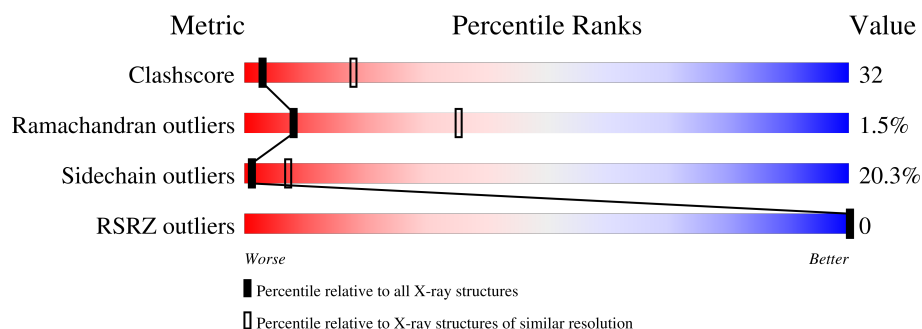
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	1	289	
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 6294 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
			2170	1373	375	414	8			

- 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	engineered mutation	UNP P03303

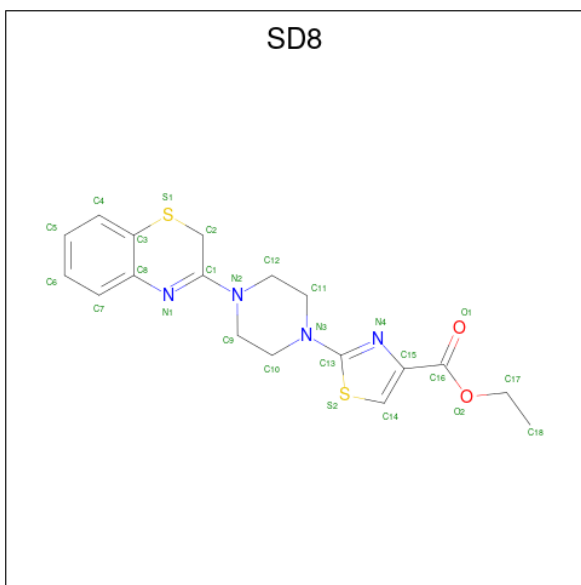
- Molecule 3 is a protein called RHINOVIRUS 14.

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 2-[4-(2H-1,4-BENZOTHAZINE-3-YL)-PIPERAZINE-1-LY]-1,3-THIAZOLE-4-CARBOXYLIC ACID ETHYLESTER (CCD ID: SD8) (formula: C₁₈H₂₀N₄O₂S₂).

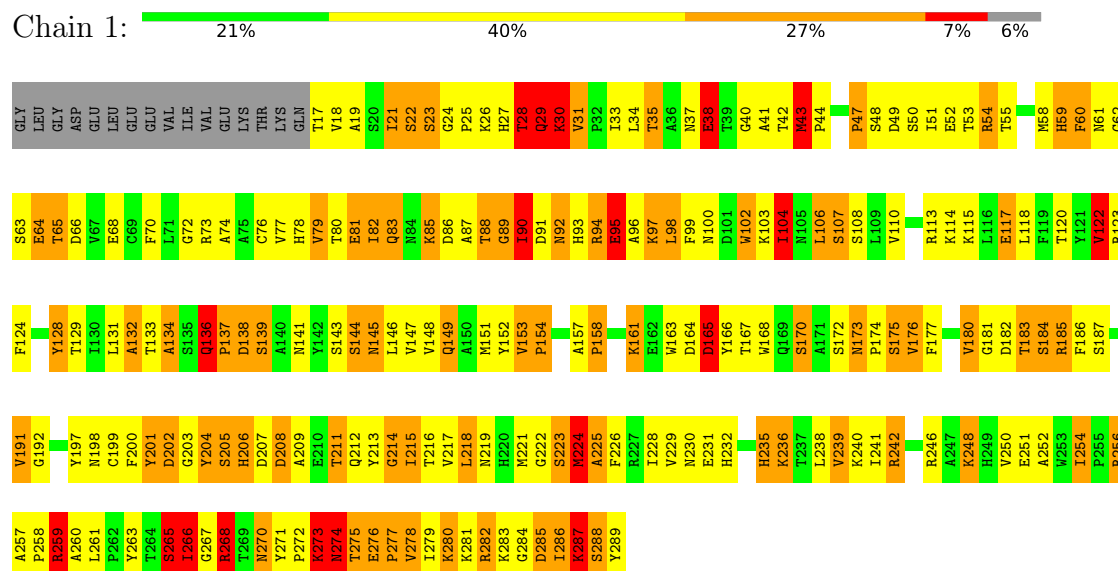


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	1	1	26	18	4	2	2	0	0

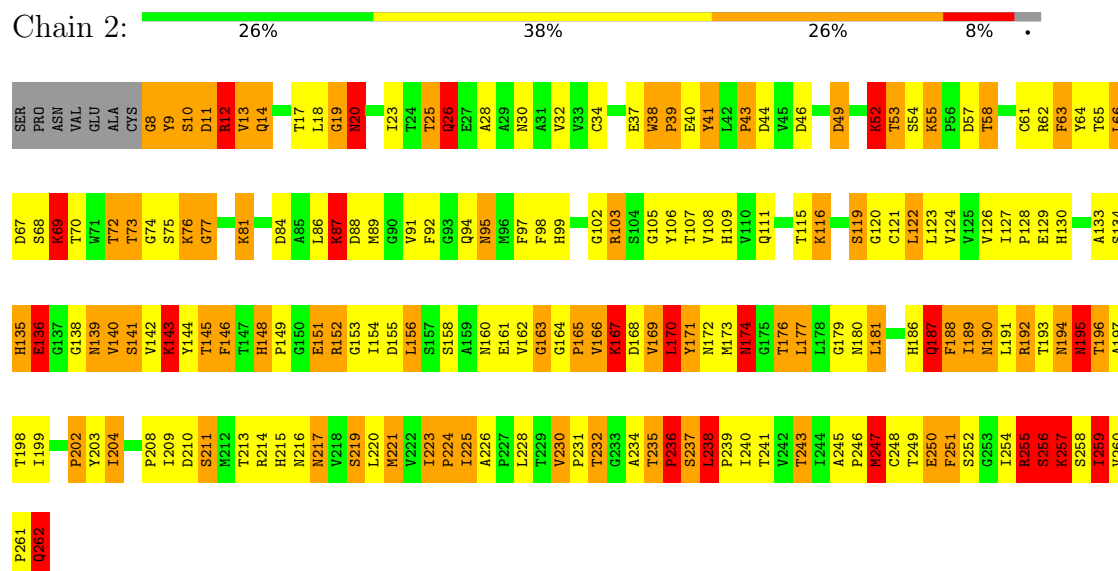
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

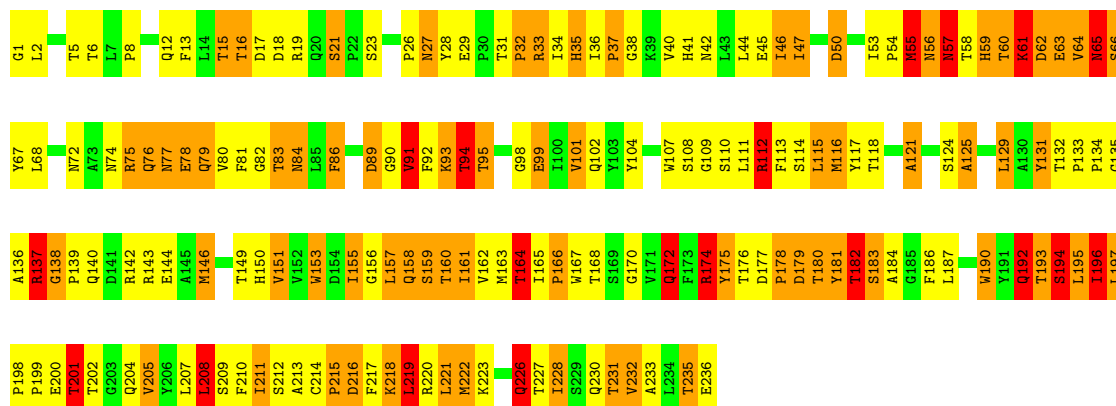
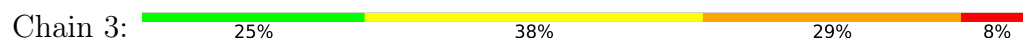
• Molecule 1: RHINOVIRUS 14



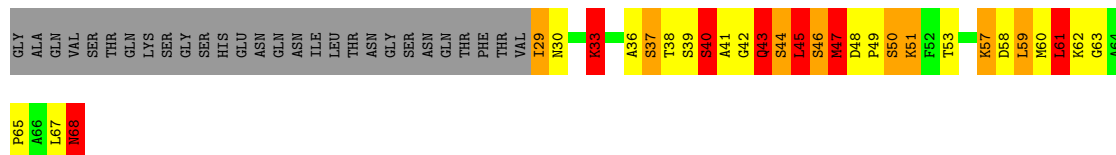
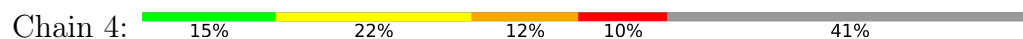
• Molecule 2: RHINOVIRUS 14



• Molecule 3: RHINOVIRUS 14



- Molecule 4: RHINOVIRUS 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00 200.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 25.4 (200.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.06 (at 3.01Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 18.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.116 for l,-k,h	Xtriage
F_o, F_c correlation	0.16	EDS
Total number of atoms	6294	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SD8

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	2.36	90/2228 (4.0%)	2.82	214/3031 (7.1%)
2	2	2.40	95/2001 (4.7%)	2.77	195/2735 (7.1%)
3	3	2.31	79/1898 (4.2%)	2.80	193/2597 (7.4%)
4	4	2.64	14/302 (4.6%)	3.14	34/406 (8.4%)
All	All	2.37	278/6429 (4.3%)	2.81	636/8769 (7.3%)

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	3
2	2	0	2
All	All	0	5

All (278) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	153	VAL	C-N	-18.81	1.11	1.33
1	1	285	ASP	CA-CB	17.77	1.79	1.53
1	1	198	ASN	C-N	15.96	1.57	1.33
1	1	128	TYR	C-N	15.09	1.55	1.33
4	4	41	ALA	C-O	13.30	1.41	1.24
3	3	57	ASN	CA-CB	12.72	1.75	1.53
4	4	42	GLY	N-CA	12.59	1.63	1.45
2	2	194	ASN	CA-CB	11.57	1.71	1.53
1	1	283	LYS	N-CA	10.88	1.61	1.46
1	1	144	SER	N-CA	10.33	1.58	1.45
3	3	164	THR	C-O	10.30	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	9.34	1.36	1.24
1	1	170	SER	CB-OG	-9.31	1.23	1.42
2	2	187	GLN	N-CA	9.27	1.57	1.45
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	8.98	1.58	1.46
2	2	102	GLY	N-CA	8.93	1.54	1.45
2	2	168	ASP	C-O	8.82	1.34	1.24
1	1	175	SER	N-CA	8.64	1.56	1.45
2	2	174	ASN	C-O	8.59	1.30	1.23
3	3	21	SER	CA-CB	8.58	1.66	1.54
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	7.93	1.55	1.44
2	2	77	GLY	N-CA	7.89	1.53	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	285	ASP	N-CA	-7.77	1.34	1.45
2	2	135	HIS	CE1-NE2	-7.66	1.24	1.32
3	3	1	GLY	N-CA	7.65	1.57	1.45
1	1	122	VAL	N-CA	7.60	1.55	1.46
1	1	72	GLY	C-O	7.56	1.34	1.23
2	2	12	ARG	NE-CZ	7.51	1.41	1.33
3	3	215	PRO	C-N	-7.43	1.23	1.33
2	2	52	LYS	N-CA	7.43	1.55	1.46
1	1	143	SER	C-O	7.43	1.33	1.24
2	2	11	ASP	CA-CB	7.36	1.66	1.53
1	1	94	ARG	CD-NE	7.33	1.56	1.46
1	1	288	SER	C-O	7.31	1.32	1.23
3	3	60	THR	CA-CB	7.23	1.65	1.54
2	2	260	VAL	N-CA	7.22	1.55	1.46
3	3	77	ASN	C-O	7.22	1.33	1.24
1	1	28	THR	CA-CB	7.21	1.64	1.53
2	2	120	GLY	N-CA	7.17	1.53	1.45
1	1	132	ALA	C-O	7.17	1.32	1.24
4	4	40	SER	CB-OG	7.07	1.56	1.42
1	1	276	GLU	C-O	7.04	1.31	1.24
2	2	58	THR	C-O	7.03	1.33	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	108	VAL	C-O	6.93	1.32	1.24
2	2	74	GLY	C-O	6.93	1.31	1.23
1	1	91	ASP	N-CA	6.91	1.55	1.46
4	4	49	PRO	C-N	-6.86	1.24	1.34
1	1	133	THR	N-CA	6.84	1.54	1.45
1	1	288	SER	CA-CB	6.84	1.65	1.53
3	3	86	PHE	CA-CB	-6.84	1.42	1.52
1	1	202	ASP	CA-CB	-6.80	1.42	1.53
2	2	152	ARG	CZ-NH2	6.80	1.42	1.33
2	2	223	ILE	CA-CB	6.80	1.59	1.54
3	3	216	ASP	CA-CB	6.77	1.64	1.53
1	1	23	SER	N-CA	6.76	1.54	1.45
2	2	243	THR	C-O	6.75	1.32	1.24
3	3	6	THR	N-CA	6.74	1.54	1.45
2	2	256	SER	CB-OG	6.74	1.55	1.42
2	2	194	ASN	N-CA	-6.72	1.37	1.45
2	2	197	ALA	C-O	6.71	1.31	1.23
1	1	280	LYS	C-O	6.70	1.31	1.24
1	1	148	VAL	C-N	-6.68	1.25	1.33
2	2	10	SER	C-N	-6.67	1.25	1.33
2	2	193	THR	C-N	-6.66	1.23	1.33
1	1	165	ASP	CA-CB	6.64	1.64	1.53
1	1	251	GLU	CA-CB	-6.62	1.42	1.53
1	1	73	ARG	N-CA	6.60	1.53	1.45
3	3	57	ASN	N-CA	-6.57	1.37	1.46
2	2	109	HIS	CE1-NE2	-6.54	1.26	1.32
4	4	44	SER	CB-OG	6.54	1.55	1.42
2	2	9	TYR	N-CA	6.54	1.53	1.46
1	1	85	LYS	C-O	6.54	1.31	1.23
3	3	15	THR	C-O	6.51	1.32	1.24
1	1	134	ALA	CA-CB	-6.50	1.42	1.53
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
3	3	156	GLY	C-O	-6.43	1.19	1.24
2	2	39	PRO	C-O	6.43	1.31	1.23
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
3	3	57	ASN	C-N	-6.40	1.25	1.33
1	1	231	GLU	CA-CB	-6.38	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	79	VAL	C-N	-6.37	1.24	1.33
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	-6.34	1.24	1.33
1	1	94	ARG	NE-CZ	6.34	1.40	1.33
2	2	8	GLY	N-CA	6.33	1.55	1.45
1	1	266	ILE	C-O	-6.32	1.16	1.24
1	1	95	GLU	CB-CG	6.31	1.71	1.52
3	3	5	THR	C-O	6.28	1.31	1.24
3	3	75	ARG	C-N	-6.28	1.24	1.33
4	4	63	GLY	N-CA	6.28	1.54	1.45
1	1	185	ARG	C-N	-6.27	1.25	1.33
1	1	203	GLY	N-CA	6.27	1.52	1.44
3	3	118	THR	CB-OG1	6.24	1.53	1.43
1	1	184	SER	N-CA	6.21	1.53	1.45
1	1	267	GLY	C-O	6.20	1.32	1.24
3	3	182	THR	CA-CB	6.20	1.62	1.53
1	1	251	GLU	N-CA	6.19	1.53	1.46
1	1	184	SER	C-O	6.19	1.31	1.23
2	2	257	LYS	N-CA	6.19	1.54	1.46
1	1	108	SER	C-O	6.18	1.31	1.24
3	3	16	THR	CA-CB	6.17	1.63	1.53
3	3	178	PRO	CA-CB	-6.17	1.45	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
2	2	259	ILE	C-O	6.12	1.30	1.24
3	3	164	THR	N-CA	6.12	1.53	1.46
3	3	155	ILE	N-CA	6.12	1.53	1.46
3	3	110	SER	N-CA	6.12	1.53	1.45
1	1	131	LEU	C-O	6.11	1.31	1.23
4	4	33	LYS	CE-NZ	6.11	1.67	1.49
4	4	45	LEU	N-CA	6.10	1.55	1.46
3	3	215	PRO	CA-CB	-6.09	1.44	1.53
1	1	274	ASN	N-CA	6.08	1.54	1.46
1	1	177	PHE	C-N	-6.07	1.25	1.33
1	1	28	THR	N-CA	-6.06	1.37	1.45
1	1	211	THR	N-CA	6.05	1.53	1.45
2	2	162	VAL	N-CA	6.05	1.53	1.46
2	2	19	GLY	C-N	-6.03	1.25	1.33
2	2	168	ASP	CA-CB	6.00	1.60	1.53
2	2	190	ASN	N-CA	6.00	1.54	1.46
3	3	36	ILE	N-CA	6.00	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	88	THR	CB-OG1	5.98	1.53	1.43
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	5.98	1.31	1.24
3	3	222	MET	CG-SD	5.94	1.95	1.80
1	1	107	SER	N-CA	5.93	1.53	1.46
2	2	180	ASN	C-N	-5.92	1.25	1.33
1	1	185	ARG	C-O	5.89	1.30	1.23
3	3	213	ALA	C-O	5.89	1.30	1.23
1	1	175	SER	CB-OG	-5.88	1.30	1.42
1	1	38	GLU	CB-CG	-5.88	1.34	1.52
2	2	17	THR	C-N	-5.86	1.25	1.33
2	2	103	ARG	C-O	5.85	1.31	1.23
3	3	27	ASN	C-N	-5.81	1.25	1.33
3	3	219	LEU	C-N	-5.81	1.26	1.33
3	3	158	GLN	C-O	5.80	1.30	1.24
1	1	287	LYS	C-O	5.75	1.31	1.24
1	1	180	VAL	C-O	5.74	1.29	1.24
1	1	276	GLU	N-CA	5.74	1.54	1.45
1	1	102	TRP	NE1-CE2	-5.74	1.31	1.37
3	3	33	ARG	NE-CZ	5.73	1.39	1.33
2	2	176	THR	N-CA	5.73	1.53	1.45
2	2	135	HIS	CG-CD2	-5.72	1.29	1.35
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	38	GLY	CA-C	-5.72	1.43	1.51
2	2	75	SER	C-O	5.71	1.30	1.23
2	2	88	ASP	C-O	5.71	1.32	1.24
2	2	55	LYS	N-CA	5.71	1.53	1.46
3	3	116	MET	N-CA	5.71	1.52	1.46
2	2	63	PHE	C-O	5.71	1.30	1.24
2	2	208	PRO	C-O	5.70	1.30	1.24
4	4	45	LEU	C-O	5.69	1.31	1.23
3	3	41	HIS	CE1-NE2	5.67	1.38	1.32
1	1	285	ASP	C-N	5.67	1.40	1.33
2	2	54	SER	CA-CB	-5.67	1.44	1.53
1	1	239	VAL	C-O	5.67	1.30	1.24
2	2	103	ARG	N-CA	5.67	1.52	1.46
2	2	195	ASN	CA-CB	-5.66	1.44	1.54
1	1	25	PRO	CA-CB	-5.64	1.45	1.53
2	2	87	LYS	CB-CG	-5.63	1.35	1.52
1	1	63	SER	CB-OG	-5.62	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	259	ILE	N-CA	5.62	1.53	1.46
1	1	268	ARG	N-CA	5.61	1.52	1.45
1	1	137	PRO	C-O	5.61	1.31	1.24
2	2	168	ASP	C-N	-5.61	1.26	1.33
3	3	35	HIS	C-N	-5.60	1.27	1.33
3	3	231	THR	CB-OG1	5.60	1.52	1.43
1	1	274	ASN	CA-C	5.59	1.60	1.52
1	1	117	GLU	CD-OE1	5.59	1.35	1.25
3	3	172	GLN	CG-CD	-5.58	1.38	1.52
2	2	194	ASN	C-O	5.58	1.30	1.23
4	4	51	LYS	CE-NZ	5.56	1.66	1.49
3	3	82	GLY	N-CA	5.54	1.50	1.45
3	3	108	SER	CA-CB	-5.54	1.44	1.53
2	2	151	GLU	CA-CB	-5.53	1.43	1.53
3	3	140	GLN	C-N	-5.53	1.26	1.33
2	2	223	ILE	CA-C	-5.52	1.48	1.52
3	3	75	ARG	N-CA	5.52	1.52	1.45
3	3	82	GLY	C-N	-5.52	1.26	1.33
2	2	109	HIS	C-O	5.51	1.30	1.24
3	3	66	SER	N-CA	5.51	1.53	1.46
3	3	174	ARG	NE-CZ	5.50	1.39	1.33
2	2	237	SER	C-O	5.49	1.30	1.23
3	3	40	VAL	C-O	5.49	1.30	1.24
3	3	61	LYS	CE-NZ	5.49	1.65	1.49
2	2	153	GLY	C-N	-5.47	1.25	1.33
1	1	153	VAL	CA-C	-5.46	1.47	1.52
2	2	237	SER	N-CA	5.45	1.52	1.46
3	3	77	ASN	CG-OD1	5.45	1.33	1.23
1	1	25	PRO	C-N	-5.45	1.25	1.33
1	1	254	ILE	CA-CB	5.44	1.61	1.54
1	1	277	PRO	N-CA	5.44	1.53	1.47
3	3	91	VAL	C-O	5.44	1.30	1.24
2	2	141	SER	N-CA	5.44	1.52	1.45
3	3	37	PRO	CA-CB	-5.42	1.45	1.53
3	3	209	SER	N-CA	5.41	1.52	1.46
2	2	256	SER	C-N	-5.38	1.26	1.33
1	1	279	ILE	C-O	5.38	1.29	1.24
2	2	148	HIS	ND1-CE1	5.36	1.38	1.32
3	3	228	ILE	C-O	5.35	1.30	1.24
3	3	74	ASN	CA-CB	5.34	1.61	1.53
2	2	68	SER	CA-C	-5.34	1.45	1.52
2	2	211	SER	C-O	5.34	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	176	VAL	CA-C	5.34	1.58	1.52
3	3	17	ASP	CG-OD1	5.32	1.35	1.25
4	4	61	LEU	C-O	5.32	1.30	1.24
3	3	64	VAL	C-N	-5.31	1.25	1.33
2	2	14	GLN	CD-NE2	5.30	1.44	1.33
2	2	61	CYS	CA-C	-5.30	1.47	1.53
1	1	30	LYS	CE-NZ	5.30	1.65	1.49
1	1	270	ASN	CA-C	5.29	1.59	1.52
2	2	103	ARG	CA-CB	-5.29	1.45	1.53
1	1	161	LYS	C-N	-5.29	1.26	1.33
2	2	72	THR	CB-OG1	5.29	1.52	1.43
2	2	171	TYR	C-O	5.29	1.31	1.24
1	1	122	VAL	C-O	5.28	1.29	1.24
1	1	33	ILE	C-O	5.27	1.30	1.24
2	2	202	PRO	C-O	5.27	1.30	1.23
2	2	246	PRO	C-O	5.27	1.30	1.23
3	3	209	SER	C-O	5.26	1.30	1.23
3	3	205	VAL	C-O	5.26	1.30	1.23
2	2	123	LEU	C-N	-5.25	1.26	1.33
1	1	54	ARG	C-O	5.23	1.30	1.23
3	3	133	PRO	CA-CB	-5.21	1.46	1.54
3	3	58	THR	CA-CB	5.21	1.62	1.53
2	2	219	SER	N-CA	5.21	1.52	1.46
3	3	146	MET	C-O	5.21	1.30	1.24
1	1	89	GLY	C-O	5.20	1.31	1.23
1	1	283	LYS	CE-NZ	5.20	1.65	1.49
3	3	2	LEU	CA-CB	5.20	1.63	1.53
2	2	38	TRP	CA-C	-5.18	1.45	1.52
2	2	202	PRO	C-N	-5.18	1.26	1.33
3	3	153	TRP	C-O	5.17	1.30	1.24
2	2	204	ILE	C-N	-5.16	1.26	1.33
2	2	99	HIS	C-N	-5.16	1.27	1.34
3	3	77	ASN	C-N	-5.14	1.26	1.33
1	1	252	ALA	C-O	5.14	1.30	1.23
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	225	ALA	N-CA	-5.11	1.39	1.46
1	1	166	TYR	N-CA	5.10	1.52	1.46
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	109	HIS	N-CA	5.09	1.53	1.46
1	1	209	ALA	C-N	-5.08	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	112	ARG	CA-CB	-5.08	1.45	1.53
3	3	216	ASP	N-CA	-5.08	1.40	1.46
2	2	128	PRO	CA-CB	-5.07	1.47	1.53
1	1	42	THR	C-O	5.07	1.29	1.23
2	2	220	LEU	C-N	-5.05	1.26	1.33
3	3	84	ASN	N-CA	5.05	1.52	1.45
1	1	117	GLU	N-CA	5.04	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
3	3	65	ASN	CA-CB	5.01	1.62	1.53
3	3	232	VAL	C-O	5.01	1.29	1.23
2	2	238	LEU	N-CA	5.00	1.51	1.45
3	3	163	MET	C-N	-5.00	1.26	1.33

All (636) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	50	ASP	CA-CB-CG	27.66	140.26	112.60
1	1	285	ASP	CA-CB-CG	-22.20	90.40	112.60
1	1	128	TYR	CA-C-N	-20.59	92.06	122.94
1	1	128	TYR	C-N-CA	-20.59	92.06	122.94
3	3	215	PRO	CA-C-N	20.36	149.21	120.29
3	3	215	PRO	C-N-CA	20.36	149.21	120.29
1	1	129	THR	O-C-N	-20.00	97.23	123.23
2	2	87	LYS	CA-CB-CG	19.04	152.18	114.10
2	2	11	ASP	CA-CB-CG	-18.96	93.64	112.60
1	1	145	ASN	OD1-CG-ND2	17.28	139.88	122.60
2	2	193	THR	CA-C-N	16.41	150.13	122.07
2	2	193	THR	C-N-CA	16.41	150.13	122.07
2	2	190	ASN	CA-CB-CG	16.38	128.98	112.60
1	1	153	VAL	CB-CA-C	-16.11	82.03	111.36
1	1	128	TYR	O-C-N	15.60	142.82	123.16
1	1	170	SER	CA-CB-OG	15.07	141.24	111.10
2	2	194	ASN	CA-CB-CG	-14.96	97.64	112.60
2	2	11	ASP	CA-C-N	14.79	140.56	120.44
2	2	11	ASP	C-N-CA	14.79	140.56	120.44
1	1	38	GLU	CB-CG-CD	13.69	135.87	112.60
3	3	57	ASN	CA-CB-CG	-13.66	98.94	112.60
3	3	74	ASN	CA-CB-CG	-13.47	99.13	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	202	ASP	CA-CB-CG	12.92	125.52	112.60
1	1	145	ASN	CA-CB-CG	-12.90	99.70	112.60
2	2	194	ASN	N-CA-CB	-12.65	89.78	110.41
2	2	44	ASP	CA-CB-CG	12.65	125.25	112.60
1	1	94	ARG	CD-NE-CZ	-12.57	106.80	124.40
1	1	256	ARG	NE-CZ-NH2	12.56	130.51	119.20
2	2	67	ASP	CA-CB-CG	-12.45	100.15	112.60
2	2	256	SER	CA-C-O	-12.27	105.31	119.79
4	4	30	ASN	CA-CB-CG	-12.08	100.52	112.60
3	3	172	GLN	CB-CG-CD	12.02	133.04	112.60
4	4	45	LEU	N-CA-CB	-11.87	94.16	111.84
3	3	74	ASN	OD1-CG-ND2	11.29	133.90	122.60
4	4	41	ALA	CA-C-O	-11.29	105.50	119.38
2	2	14	GLN	OE1-CD-NE2	11.16	133.76	122.60
3	3	29	GLU	CB-CG-CD	11.12	131.50	112.60
2	2	151	GLU	CA-CB-CG	11.11	136.32	114.10
1	1	285	ASP	N-CA-CB	-11.05	95.26	110.29
1	1	173	ASN	CA-CB-CG	10.96	123.56	112.60
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
4	4	48	ASP	CA-CB-CG	-10.65	101.95	112.60
2	2	219	SER	CA-CB-OG	10.64	132.38	111.10
1	1	282	ARG	CD-NE-CZ	-10.62	109.53	124.40
2	2	97	PHE	CA-CB-CG	-10.57	103.22	113.80
1	1	141	ASN	CA-CB-CG	-10.45	102.15	112.60
3	3	57	ASN	N-CA-CB	-10.38	92.95	110.49
1	1	153	VAL	O-C-N	10.21	132.74	121.10
4	4	48	ASP	O-C-N	10.15	128.34	121.23
3	3	72	ASN	CA-CB-CG	-10.14	102.46	112.60
1	1	246	ARG	NE-CZ-NH1	10.07	131.57	121.50
1	1	63	SER	CB-CA-C	-10.02	94.16	110.79
1	1	54	ARG	CD-NE-CZ	-9.93	110.50	124.40
4	4	44	SER	CA-C-N	-9.87	107.95	122.07
4	4	44	SER	C-N-CA	-9.87	107.95	122.07
1	1	91	ASP	CA-CB-CG	-9.81	102.79	112.60
1	1	285	ASP	N-CA-C	9.75	122.91	110.33
1	1	275	THR	CA-C-O	-9.73	109.23	121.88
1	1	22	SER	CA-C-O	-9.71	109.62	120.69
3	3	33	ARG	CA-C-O	-9.70	110.00	121.05
1	1	28	THR	CB-CA-C	-9.70	92.96	111.48
1	1	208	ASP	CA-CB-CG	-9.67	102.93	112.60
3	3	137	ARG	NE-CZ-NH1	-9.65	111.85	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	256	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	246	ARG	CD-NE-CZ	9.45	137.63	124.40
3	3	89	ASP	CA-CB-CG	-9.43	103.17	112.60
3	3	86	PHE	CA-CB-CG	9.42	123.22	113.80
1	1	38	GLU	CA-CB-CG	9.39	132.89	114.10
1	1	79	VAL	CA-C-O	-9.37	110.65	120.39
2	2	255	ARG	NE-CZ-NH2	-9.15	110.96	119.20
1	1	266	ILE	CB-CA-C	-9.11	96.35	111.29
3	3	57	ASN	CB-CA-C	-9.11	92.30	110.42
4	4	50	SER	CA-C-O	-9.04	109.88	120.10
1	1	268	ARG	CD-NE-CZ	-9.04	111.75	124.40
1	1	95	GLU	CB-CG-CD	-9.03	97.25	112.60
2	2	195	ASN	CA-CB-CG	8.97	121.58	112.60
3	3	196	ILE	CA-C-O	-8.97	111.21	120.27
2	2	136	GLU	CB-CG-CD	-8.81	97.63	112.60
1	1	266	ILE	O-C-N	-8.79	111.58	122.57
2	2	250	GLU	CA-CB-CG	8.78	131.65	114.10
4	4	68	ASN	CA-CB-CG	-8.76	103.84	112.60
1	1	270	ASN	CA-CB-CG	8.71	121.31	112.60
1	1	251	GLU	CA-CB-CG	8.66	131.42	114.10
2	2	139	ASN	CA-CB-CG	-8.47	104.13	112.60
2	2	255	ARG	CA-CB-CG	8.46	131.01	114.10
1	1	259	ARG	CA-CB-CG	-8.45	97.19	114.10
2	2	73	THR	CA-CB-OG1	-8.45	96.92	109.60
2	2	168	ASP	CA-C-O	-8.46	110.56	120.62
1	1	165	ASP	CB-CA-C	-8.42	93.66	110.42
3	3	174	ARG	CD-NE-CZ	-8.40	112.63	124.40
1	1	123	ARG	NE-CZ-NH1	8.40	129.90	121.50
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	-8.37	108.72	122.54
4	4	36	ALA	C-N-CA	-8.37	108.72	122.54
2	2	169	VAL	CB-CA-C	-8.37	101.25	111.97
3	3	74	ASN	CA-C-O	-8.36	109.85	120.55
4	4	41	ALA	N-CA-C	8.31	122.68	112.54
3	3	5	THR	CA-C-O	-8.29	111.12	120.32
3	3	172	GLN	CG-CD-NE2	8.25	128.77	116.40
1	1	122	VAL	N-CA-CB	-8.24	97.94	111.45
3	3	219	LEU	CA-C-O	-8.23	111.20	120.66
1	1	82	ILE	CA-C-O	-8.21	113.05	121.67
3	3	57	ASN	OD1-CG-ND2	8.18	130.78	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	182	THR	CA-CB-CG2	8.18	124.40	110.50
3	3	21	SER	CB-CA-C	-8.15	95.47	108.91
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
4	4	57	LYS	CA-C-O	-8.12	112.34	120.70
1	1	29	GLN	N-CA-C	-8.08	102.47	113.30
3	3	60	THR	CA-CB-OG1	-8.02	97.56	109.60
2	2	187	GLN	CA-CB-CG	8.02	130.14	114.10
3	3	233	ALA	CA-C-O	-8.01	112.38	121.19
1	1	288	SER	CA-C-O	-8.01	113.06	121.55
3	3	27	ASN	O-C-N	8.01	132.01	122.00
3	3	78	GLU	N-CA-C	8.00	120.85	110.53
1	1	198	ASN	O-C-N	-8.00	113.68	123.04
1	1	164	ASP	CA-C-N	7.99	136.80	121.54
1	1	164	ASP	C-N-CA	7.99	136.80	121.54
2	2	248	CYS	CA-C-O	-7.98	112.28	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	176	VAL	CA-C-O	-7.93	111.40	120.67
3	3	231	THR	CA-CB-OG1	-7.92	97.72	109.60
1	1	94	ARG	NE-CZ-NH2	-7.92	112.07	119.20
2	2	223	ILE	N-CA-CB	-7.92	101.50	112.27
1	1	37	ASN	CB-CG-ND2	7.87	128.20	116.40
2	2	216	ASN	CA-C-O	-7.86	112.07	120.80
1	1	123	ARG	CD-NE-CZ	7.81	135.33	124.40
3	3	216	ASP	N-CA-CB	-7.81	98.61	110.16
1	1	274	ASN	O-C-N	7.80	132.97	122.59
2	2	95	ASN	CA-CB-CG	-7.79	104.81	112.60
1	1	149	GLN	CB-CA-C	-7.77	99.96	111.77
4	4	45	LEU	CA-C-O	7.75	130.53	121.54
1	1	282	ARG	CA-C-N	-7.74	111.50	122.41
1	1	282	ARG	C-N-CA	-7.74	111.50	122.41
3	3	62	ASP	CA-CB-CG	7.71	120.31	112.60
2	2	109	HIS	CA-C-O	-7.71	110.85	120.57
4	4	37	SER	CB-CA-C	7.71	122.96	110.09
1	1	64	GLU	CB-CG-CD	7.70	125.70	112.60
2	2	190	ASN	OD1-CG-ND2	-7.70	114.91	122.60
1	1	176	VAL	CB-CA-C	-7.68	99.18	110.62
2	2	240	ILE	CA-C-O	-7.66	112.35	120.39
1	1	61	ASN	CA-CB-CG	-7.62	104.98	112.60
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	173	ASN	N-CA-CB	-7.61	97.00	109.94
1	1	17	THR	CA-C-N	-7.61	110.33	122.50
1	1	17	THR	C-N-CA	-7.61	110.33	122.50
3	3	59	HIS	CA-C-O	7.60	130.47	121.88
3	3	79	GLN	OE1-CD-NE2	-7.57	115.03	122.60
2	2	87	LYS	CB-CG-CD	7.55	128.68	111.30
3	3	142	ARG	CA-CB-CG	7.55	129.20	114.10
3	3	27	ASN	N-CA-C	7.54	124.05	113.56
1	1	277	PRO	N-CD-CG	-7.54	91.89	103.20
1	1	129	THR	CA-C-N	7.50	133.18	123.13
1	1	129	THR	C-N-CA	7.50	133.18	123.13
1	1	214	GLY	O-C-N	7.46	129.32	122.90
1	1	175	SER	CB-CA-C	7.44	126.07	109.56
4	4	30	ASN	CA-C-O	-7.42	112.23	120.69
1	1	288	SER	N-CA-C	7.41	120.42	110.35
2	2	140	VAL	CA-C-O	-7.39	113.32	121.23
2	2	98	PHE	CA-C-O	-7.35	111.00	119.60
2	2	107	THR	CA-C-O	-7.33	112.25	120.32
4	4	45	LEU	CB-CA-C	7.33	122.50	111.80
3	3	27	ASN	CB-CA-C	-7.32	97.22	111.06
3	3	129	LEU	CA-C-O	-7.31	112.96	120.71
2	2	77	GLY	CA-C-O	-7.28	114.77	122.05
2	2	180	ASN	CA-CB-CG	-7.27	105.33	112.60
3	3	118	THR	CA-CB-OG1	-7.26	98.71	109.60
2	2	39	PRO	CA-C-O	-7.25	113.07	121.34
3	3	46	ILE	CA-C-O	-7.25	112.42	120.25
2	2	68	SER	O-C-N	-7.25	114.77	122.96
2	2	187	GLN	CB-CA-C	7.24	125.37	109.94
3	3	124	SER	CA-C-O	-7.23	113.52	121.33
2	2	103	ARG	CD-NE-CZ	-7.23	114.28	124.40
3	3	61	LYS	CA-C-O	-7.23	112.67	121.06
1	1	275	THR	CA-CB-OG1	-7.22	98.77	109.60
1	1	26	LYS	CA-CB-CG	7.21	128.51	114.10
2	2	52	LYS	CA-C-O	-7.20	113.27	121.19
2	2	169	VAL	N-CA-C	7.18	117.31	110.42
4	4	30	ASN	OD1-CG-ND2	7.18	129.78	122.60
3	3	19	ARG	NE-CZ-NH2	7.17	125.66	119.20
1	1	158	PRO	O-C-N	7.14	130.76	122.98
2	2	146	PHE	CA-CB-CG	-7.14	106.66	113.80
1	1	59	HIS	CA-C-O	-7.13	111.97	120.81
1	1	284	GLY	CA-C-N	7.09	133.57	120.95
1	1	284	GLY	C-N-CA	7.09	133.57	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	47	MET	CA-CB-CG	-7.07	99.97	114.10
2	2	168	ASP	N-CA-CB	-7.06	98.02	109.60
1	1	285	ASP	CB-CA-C	-7.05	93.81	110.02
2	2	259	ILE	CB-CG1-CD1	-7.04	99.01	113.80
3	3	13	PHE	CA-CB-CG	7.04	120.84	113.80
2	2	134	SER	CA-C-O	-7.02	113.05	121.05
1	1	85	LYS	CA-C-O	-7.00	113.97	121.38
1	1	28	THR	OG1-CB-CG2	6.98	123.25	109.30
3	3	94	THR	O-C-N	6.97	131.56	122.42
1	1	43	MET	CA-C-O	6.97	126.30	119.75
3	3	35	HIS	CA-C-O	-6.97	112.90	120.92
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	77	ASN	OD1-CG-ND2	-6.94	115.66	122.60
3	3	109	GLY	CA-C-N	-6.94	110.85	122.64
3	3	109	GLY	C-N-CA	-6.94	110.85	122.64
3	3	121	ALA	CA-C-O	-6.92	112.28	120.10
3	3	66	SER	CB-CA-C	6.89	121.59	110.09
1	1	138	ASP	CA-CB-CG	6.88	119.47	112.60
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
2	2	186	HIS	CA-CB-CG	-6.86	106.94	113.80
1	1	89	GLY	CA-C-N	-6.86	114.29	122.93
1	1	89	GLY	C-N-CA	-6.86	114.29	122.93
2	2	9	TYR	CB-CA-C	6.85	121.37	109.65
1	1	154	PRO	N-CA-CB	-6.85	96.44	103.08
3	3	231	THR	CA-C-O	-6.85	110.50	119.06
2	2	57	ASP	CB-CA-C	-6.84	108.69	116.63
2	2	193	THR	O-C-N	-6.83	115.09	121.79
2	2	14	GLN	CB-CG-CD	-6.82	101.01	112.60
3	3	65	ASN	OD1-CG-ND2	6.81	129.41	122.60
3	3	146	MET	CG-SD-CE	6.81	115.89	100.90
1	1	183	THR	CA-CB-OG1	-6.81	99.38	109.60
1	1	42	THR	CA-CB-CG2	6.81	122.08	110.50
3	3	151	VAL	CA-C-O	-6.81	113.51	120.25
4	4	44	SER	O-C-N	6.80	131.64	122.59
2	2	219	SER	CB-CA-C	6.80	121.62	109.38
2	2	238	LEU	N-CA-CB	-6.80	98.75	110.72
1	1	35	THR	N-CA-CB	-6.76	99.06	110.49
1	1	49	ASP	N-CA-C	-6.76	105.32	113.97
3	3	202	THR	CA-C-O	6.76	128.46	121.23
1	1	206	HIS	CA-C-O	-6.75	114.06	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	143	ARG	N-CA-C	-6.75	104.01	111.36
3	3	178	PRO	O-C-N	6.74	130.76	123.01
4	4	58	ASP	O-C-N	6.73	130.89	123.22
1	1	62	GLY	CA-C-N	6.73	129.29	120.28
1	1	62	GLY	C-N-CA	6.73	129.29	120.28
2	2	224	PRO	CA-C-O	-6.72	114.03	121.23
2	2	249	THR	CA-CB-OG1	-6.71	99.53	109.60
2	2	170	LEU	CD1-CG-CD2	-6.71	96.05	110.80
2	2	124	VAL	CA-C-O	-6.70	112.82	120.66
1	1	198	ASN	CA-C-N	6.70	132.86	121.14
1	1	198	ASN	C-N-CA	6.70	132.86	121.14
3	3	42	ASN	CA-C-O	-6.69	112.97	120.66
2	2	255	ARG	CB-CG-CD	6.66	126.62	111.30
1	1	288	SER	CB-CA-C	-6.65	97.71	109.62
1	1	282	ARG	NE-CZ-NH2	-6.65	113.22	119.20
3	3	187	LEU	N-CA-CB	-6.65	100.33	110.77
3	3	187	LEU	CA-C-O	-6.65	113.19	120.24
3	3	227	THR	CA-CB-OG1	-6.65	99.63	109.60
1	1	95	GLU	CA-CB-CG	-6.64	100.82	114.10
1	1	90	ILE	CA-C-N	-6.62	109.75	122.06
1	1	90	ILE	C-N-CA	-6.62	109.75	122.06
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
1	1	118	LEU	CA-C-N	6.57	133.12	122.81
1	1	118	LEU	C-N-CA	6.57	133.12	122.81
3	3	134	PRO	CA-C-N	-6.57	116.34	123.30
3	3	134	PRO	C-N-CA	-6.57	116.34	123.30
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
1	1	60	PHE	CA-C-O	-6.56	113.68	120.89
3	3	202	THR	CA-CB-OG1	-6.55	99.77	109.60
4	4	48	ASP	OD1-CG-OD2	6.55	138.62	122.90
1	1	147	VAL	CA-C-O	-6.54	113.53	120.53
2	2	148	HIS	CA-CB-CG	6.54	120.34	113.80
2	2	12	ARG	N-CA-C	6.53	118.19	111.14
2	2	198	THR	CA-C-O	-6.53	113.07	120.32
2	2	145	THR	CA-CB-OG1	-6.52	99.81	109.60
2	2	226	ALA	N-CA-C	-6.52	99.12	109.04
2	2	11	ASP	OD1-CG-OD2	6.52	138.55	122.90
2	2	38	TRP	N-CA-CB	-6.52	99.36	110.11
2	2	163	GLY	O-C-N	6.52	130.19	122.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	122	VAL	CB-CA-C	6.51	121.98	110.71
2	2	193	THR	CA-C-O	6.50	126.55	119.40
3	3	19	ARG	CA-CB-CG	6.50	127.10	114.10
2	2	18	LEU	CB-CA-C	6.49	119.81	110.79
3	3	205	VAL	CB-CA-C	6.47	120.21	110.90
4	4	36	ALA	N-CA-C	-6.47	105.25	113.01
3	3	57	ASN	N-CA-C	6.46	124.56	110.80
3	3	74	ASN	N-CA-C	6.45	120.47	112.47
1	1	256	ARG	CD-NE-CZ	-6.45	115.38	124.40
3	3	182	THR	CA-CB-OG1	-6.44	99.94	109.60
3	3	99	GLU	CB-CG-CD	6.43	123.53	112.60
3	3	216	ASP	CA-C-N	6.43	129.84	120.71
3	3	216	ASP	C-N-CA	6.43	129.84	120.71
2	2	247	MET	CB-CA-C	6.43	122.40	109.68
2	2	142	VAL	CA-C-O	-6.42	113.14	120.66
2	2	194	ASN	N-CA-C	6.42	120.53	110.32
1	1	277	PRO	CB-CA-C	6.42	119.79	111.64
3	3	65	ASN	N-CA-CB	-6.41	100.98	110.53
2	2	111	GLN	OE1-CD-NE2	-6.41	116.19	122.60
2	2	241	THR	CA-C-O	-6.39	113.93	120.71
3	3	164	THR	CA-CB-OG1	-6.39	100.01	109.60
2	2	69	LYS	CA-CB-CG	6.38	126.87	114.10
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	98.35	111.10
4	4	39	SER	O-C-N	6.36	130.69	122.23
1	1	239	VAL	CB-CA-C	6.36	120.04	110.63
2	2	145	THR	CA-C-O	-6.36	113.77	120.63
3	3	181	TYR	O-C-N	6.36	128.86	122.12
2	2	223	ILE	CA-C-O	-6.35	116.64	119.94
1	1	144	SER	N-CA-CB	-6.35	100.76	110.42
3	3	226	GLN	CB-CG-CD	-6.35	101.80	112.60
2	2	203	TYR	CA-C-O	-6.35	113.22	120.58
1	1	137	PRO	CA-C-N	-6.34	113.01	122.39
1	1	137	PRO	C-N-CA	-6.34	113.01	122.39
3	3	204	GLN	O-C-N	6.34	130.16	123.06
2	2	235	THR	CB-CA-C	-6.33	99.52	109.52
3	3	202	THR	N-CA-C	6.32	118.46	108.79
3	3	83	THR	CA-CB-OG1	-6.32	100.12	109.60
1	1	219	ASN	O-C-N	6.31	130.98	122.59
1	1	250	VAL	N-CA-C	6.30	117.77	109.21
3	3	193	THR	CA-C-O	-6.29	111.52	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	80	VAL	CA-C-O	-6.29	113.98	120.71
1	1	288	SER	N-CA-CB	-6.28	100.80	110.04
1	1	117	GLU	CG-CD-OE2	6.28	132.84	118.40
1	1	70	PHE	CA-CB-CG	6.26	120.06	113.80
1	1	205	SER	O-C-N	6.26	131.04	122.46
3	3	41	HIS	CA-C-O	-6.26	112.47	119.67
3	3	216	ASP	CB-CG-OD2	6.26	132.79	118.40
1	1	282	ARG	NH1-CZ-NH2	6.25	127.42	119.30
2	2	143	LYS	O-C-N	6.24	130.48	122.81
3	3	63	GLU	CB-CG-CD	-6.24	102.00	112.60
3	3	196	ILE	N-CA-CB	-6.24	103.34	111.82
3	3	183	SER	N-CA-CB	-6.23	100.83	110.29
4	4	65	PRO	CB-CA-C	-6.22	103.43	111.46
1	1	31	VAL	N-CA-CB	-6.22	102.50	111.21
2	2	103	ARG	CA-CB-CG	6.22	126.54	114.10
3	3	161	ILE	CA-C-O	-6.20	113.88	120.39
1	1	48	SER	CA-C-O	-6.20	108.14	119.36
1	1	206	HIS	O-C-N	6.17	129.47	123.29
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
3	3	132	THR	CA-C-O	-6.17	113.92	119.59
1	1	153	VAL	CA-C-N	6.16	126.72	120.38
1	1	153	VAL	C-N-CA	6.16	126.72	120.38
2	2	11	ASP	O-C-N	6.16	130.39	122.39
1	1	260	ALA	CA-C-O	-6.15	111.52	120.13
1	1	265	SER	N-CA-CB	-6.14	100.51	110.71
1	1	236	LYS	CA-C-O	-6.13	114.23	121.16
1	1	252	ALA	CA-C-O	-6.12	113.62	120.66
2	2	28	ALA	CA-C-O	-6.12	114.90	121.94
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	163	MET	CA-CB-CG	-6.11	101.87	114.10
2	2	194	ASN	OD1-CG-ND2	6.11	128.71	122.60
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
2	2	12	ARG	CD-NE-CZ	-6.07	115.90	124.40
1	1	202	ASP	CB-CA-C	6.07	121.05	112.07
1	1	133	THR	CA-CB-OG1	-6.05	100.52	109.60
2	2	195	ASN	OD1-CG-ND2	-6.05	116.55	122.60
2	2	179	GLY	CA-C-O	-6.04	114.29	120.45
3	3	8	PRO	CA-C-O	-6.04	114.54	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	136	GLN	CG-CD-NE2	-6.03	107.35	116.40
3	3	41	HIS	N-CA-CB	6.03	119.15	110.40
2	2	241	THR	CA-CB-OG1	-6.03	100.55	109.60
3	3	193	THR	CA-CB-OG1	-6.03	100.56	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
4	4	43	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	1	41	ALA	CA-C-O	-6.01	114.62	121.72
1	1	141	ASN	O-C-N	6.01	129.67	122.27
3	3	194	SER	N-CA-CB	-6.01	100.33	110.49
1	1	68	GLU	CG-CD-OE2	6.00	132.21	118.40
3	3	47	ILE	CB-CG1-CD1	-6.00	101.19	113.80
2	2	86	LEU	CA-C-N	5.99	130.28	120.63
2	2	86	LEU	C-N-CA	5.99	130.28	120.63
3	3	137	ARG	CA-C-O	-5.99	115.05	121.94
2	2	169	VAL	N-CA-CB	5.99	117.55	110.55
3	3	121	ALA	CB-CA-C	-5.99	99.55	110.63
3	3	174	ARG	NH1-CZ-NH2	5.98	127.07	119.30
2	2	14	GLN	CA-CB-CG	-5.96	102.19	114.10
1	1	77	VAL	CA-C-O	-5.95	113.31	118.96
2	2	105	GLY	N-CA-C	-5.94	102.31	112.64
3	3	77	ASN	O-C-N	-5.94	114.69	122.59
2	2	136	GLU	CG-CD-OE1	-5.93	104.76	118.40
3	3	207	LEU	CA-C-O	-5.93	114.22	120.80
3	3	160	THR	CA-CB-OG1	-5.93	100.71	109.60
2	2	161	GLU	CA-CB-CG	5.92	125.93	114.10
2	2	41	TYR	N-CA-CB	5.91	118.48	110.38
1	1	259	ARG	CB-CA-C	-5.90	100.45	109.89
1	1	173	ASN	OD1-CG-ND2	-5.89	116.71	122.60
3	3	158	GLN	CA-C-O	5.89	127.62	120.62
1	1	185	ARG	NH1-CZ-NH2	-5.88	111.65	119.30
1	1	22	SER	N-CA-CB	-5.88	100.84	109.95
2	2	88	ASP	CA-C-O	-5.88	112.55	119.48
3	3	92	PHE	CA-CB-CG	-5.87	107.93	113.80
3	3	1	GLY	O-C-N	-5.86	113.62	123.00
1	1	55	THR	CA-CB-OG1	-5.85	100.82	109.60
1	1	280	LYS	CB-CA-C	-5.85	101.74	110.16
2	2	255	ARG	NE-CZ-NH1	5.85	127.35	121.50
3	3	55	MET	CA-CB-CG	-5.85	102.40	114.10
3	3	57	ASN	O-C-N	-5.84	114.82	122.59
1	1	242	ARG	CD-NE-CZ	-5.83	116.23	124.40
3	3	33	ARG	CB-CG-CD	-5.82	97.91	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	2	226	ALA	O-C-N	5.82	127.82	121.36
3	3	197	LEU	CB-CA-C	5.81	117.23	108.86
1	1	145	ASN	CB-CG-ND2	-5.81	107.69	116.40
4	4	65	PRO	CA-C-O	-5.81	114.72	121.34
1	1	270	ASN	CB-CA-C	-5.80	100.36	109.70
3	3	93	LYS	N-CA-C	5.80	118.38	111.71
1	1	267	GLY	CA-C-N	-5.79	113.08	122.81
1	1	267	GLY	C-N-CA	-5.79	113.08	122.81
2	2	198	THR	O-C-N	5.78	130.07	123.31
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
3	3	131	TYR	CA-C-O	-5.77	114.14	120.43
1	1	175	SER	CA-CB-OG	5.77	122.63	111.10
2	2	235	THR	OG1-CB-CG2	5.75	120.81	109.30
1	1	182	ASP	CA-C-N	5.74	131.57	122.62
1	1	182	ASP	C-N-CA	5.74	131.57	122.62
1	1	68	GLU	CG-CD-OE1	-5.72	105.24	118.40
2	2	189	ILE	CA-C-O	-5.72	113.26	120.69
3	3	45	GLU	CG-CD-OE2	5.71	131.54	118.40
1	1	83	GLN	CB-CG-CD	-5.71	102.90	112.60
2	2	86	LEU	CA-C-O	-5.71	112.89	119.56
2	2	210	ASP	N-CA-CB	-5.70	100.60	110.87
3	3	66	SER	N-CA-C	-5.70	105.99	113.17
1	1	129	THR	CA-C-O	-5.70	114.55	120.70
1	1	94	ARG	CG-CD-NE	-5.70	99.47	112.00
1	1	139	SER	CA-CB-OG	-5.69	99.73	111.10
3	3	38	GLY	N-CA-C	5.69	123.74	115.32
3	3	112	ARG	CA-CB-CG	5.69	125.47	114.10
3	3	137	ARG	O-C-N	5.68	129.63	122.65
3	3	161	ILE	CA-CB-CG1	-5.68	100.75	110.40
3	3	42	ASN	CB-CG-ND2	5.66	124.89	116.40
1	1	28	THR	N-CA-C	5.66	118.10	109.95
3	3	175	TYR	N-CA-CB	-5.65	101.52	110.06
1	1	94	ARG	NH1-CZ-NH2	5.65	126.64	119.30
2	2	190	ASN	CB-CA-C	5.65	120.00	110.79
1	1	27	HIS	CA-CB-CG	5.64	119.44	113.80
2	2	199	ILE	CA-C-O	-5.64	114.38	120.36
3	3	180	THR	CA-CB-OG1	-5.63	101.16	109.60
1	1	232	HIS	CA-CB-CG	-5.62	108.17	113.80
2	2	106	TYR	CA-C-O	-5.61	115.27	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	235	THR	CA-CB-OG1	-5.60	101.20	109.60
1	1	208	ASP	CA-C-O	-5.60	114.67	121.28
2	2	99	HIS	CA-CB-CG	-5.60	108.20	113.80
3	3	190	TRP	CA-C-O	-5.58	115.09	121.40
2	2	217	ASN	CB-CA-C	5.58	118.92	109.55
2	2	9	TYR	CA-CB-CG	-5.57	103.87	113.90
1	1	241	ILE	N-CA-CB	-5.57	104.31	110.99
2	2	262	GLN	OE1-CD-NE2	-5.56	117.04	122.60
2	2	188	PHE	CA-C-O	-5.55	114.89	121.66
4	4	58	ASP	CA-C-N	5.55	128.99	121.05
4	4	58	ASP	C-N-CA	5.55	128.99	121.05
3	3	166	PRO	CB-CA-C	5.55	118.62	111.46
1	1	273	LYS	CG-CD-CE	-5.54	98.56	111.30
2	2	251	PHE	CA-C-O	-5.54	114.85	121.11
3	3	107	TRP	CA-C-O	-5.54	115.14	121.40
1	1	64	GLU	CA-CB-CG	5.54	125.17	114.10
2	2	168	ASP	CA-C-N	5.53	127.53	120.56
2	2	168	ASP	C-N-CA	5.53	127.53	120.56
2	2	94	GLN	CG-CD-NE2	-5.52	108.12	116.40
3	3	140	GLN	CA-CB-CG	-5.52	103.07	114.10
2	2	215	HIS	CA-C-O	-5.51	112.56	120.11
3	3	76	GLN	CA-C-O	-5.50	115.19	121.68
2	2	68	SER	N-CA-CB	-5.50	101.93	110.29
3	3	90	GLY	CA-C-O	-5.50	114.75	121.68
2	2	99	HIS	CA-C-N	5.50	128.20	120.28
2	2	99	HIS	C-N-CA	5.50	128.20	120.28
1	1	63	SER	O-C-N	5.50	127.95	122.12
1	1	235	HIS	CA-CB-CG	-5.49	108.31	113.80
2	2	92	PHE	N-CA-C	-5.49	104.99	110.97
2	2	26	GLN	OE1-CD-NE2	-5.48	117.12	122.60
3	3	63	GLU	CG-CD-OE1	-5.47	105.82	118.40
3	3	57	ASN	CA-C-N	5.46	132.00	121.18
3	3	57	ASN	C-N-CA	5.46	132.00	121.18
2	2	167	LYS	CA-C-O	5.46	126.11	119.78
3	3	84	ASN	OD1-CG-ND2	5.46	128.06	122.60
2	2	43	PRO	N-CD-CG	-5.45	95.03	103.20
2	2	258	SER	O-C-N	5.45	129.51	122.81
2	2	38	TRP	CB-CA-C	5.45	116.25	108.68
2	2	123	LEU	CA-C-O	-5.45	114.50	120.43
2	2	187	GLN	CA-C-O	-5.44	114.89	120.99
3	3	168	THR	CA-CB-OG1	-5.44	101.43	109.60
2	2	232	THR	CA-CB-OG1	-5.44	101.44	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	164	THR	CB-CA-C	5.43	119.12	109.72
1	1	21	ILE	CA-CB-CG1	-5.43	101.17	110.40
4	4	50	SER	CA-CB-OG	-5.42	100.26	111.10
2	2	63	PHE	CA-CB-CG	5.42	119.22	113.80
2	2	219	SER	N-CA-C	-5.41	100.87	109.59
2	2	13	VAL	CA-C-O	-5.41	114.56	120.84
2	2	192	ARG	CA-C-O	-5.41	112.02	119.05
1	1	166	TYR	N-CA-C	-5.41	105.55	111.82
1	1	50	SER	CB-CA-C	5.40	117.45	109.29
3	3	195	LEU	CA-C-O	-5.40	114.89	121.05
1	1	144	SER	CA-C-N	-5.39	115.46	123.11
1	1	144	SER	C-N-CA	-5.39	115.46	123.11
2	2	53	THR	CA-C-O	-5.39	115.59	121.89
2	2	221	MET	CA-C-O	-5.38	114.34	120.32
2	2	129	GLU	CB-CA-C	-5.38	104.26	111.89
3	3	34	ILE	CA-C-O	-5.37	114.07	120.78
3	3	116	MET	CB-CG-SD	-5.37	96.59	112.70
2	2	81	LYS	CB-CG-CD	5.37	123.64	111.30
3	3	221	LEU	O-C-N	5.37	129.73	122.59
2	2	120	GLY	CA-C-O	-5.36	114.39	122.54
3	3	143	ARG	O-C-N	5.36	128.26	122.15
3	3	38	GLY	O-C-N	-5.36	116.00	122.38
3	3	78	GLU	CA-CB-CG	5.36	124.81	114.10
3	3	226	GLN	N-CA-C	-5.36	106.70	113.18
1	1	117	GLU	CG-CD-OE1	-5.35	106.09	118.40
1	1	288	SER	CA-CB-OG	-5.35	100.41	111.10
1	1	282	ARG	O-C-N	5.34	129.38	122.81
3	3	112	ARG	CB-CA-C	5.33	119.00	110.16
1	1	174	PRO	CA-C-O	-5.32	115.53	121.23
2	2	76	LYS	CA-C-O	-5.32	113.40	119.41
2	2	12	ARG	CB-CG-CD	-5.31	99.08	111.30
1	1	104	ILE	O-C-N	5.31	129.20	122.57
2	2	262	GLN	CG-CD-NE2	5.30	124.35	116.40
1	1	26	LYS	CG-CD-CE	-5.30	99.11	111.30
1	1	92	ASN	O-C-N	5.30	129.42	123.28
1	1	231	GLU	N-CA-C	-5.30	103.04	110.35
1	1	286	ILE	O-C-N	5.30	127.78	121.80
2	2	177	LEU	N-CA-CB	-5.29	101.65	110.23
3	3	192	GLN	N-CA-C	-5.29	105.10	112.45
3	3	77	ASN	CA-CB-CG	-5.29	107.31	112.60
3	3	16	THR	OG1-CB-CG2	5.29	119.87	109.30
3	3	222	MET	CB-CG-SD	-5.29	96.85	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	102	GLY	CA-C-O	-5.28	115.50	121.68
3	3	161	ILE	N-CA-CB	5.28	118.69	111.41
1	1	60	PHE	N-CA-CB	-5.27	102.17	111.39
3	3	204	GLN	CA-C-O	-5.26	115.04	121.36
2	2	168	ASP	OD1-CG-OD2	5.26	135.53	122.90
3	3	86	PHE	CB-CA-C	5.26	120.47	111.68
4	4	58	ASP	N-CA-CB	5.26	118.99	110.42
2	2	210	ASP	CA-CB-CG	-5.26	107.34	112.60
3	3	56	ASN	CA-C-N	5.25	131.57	121.54
3	3	56	ASN	C-N-CA	5.25	131.57	121.54
2	2	195	ASN	N-CA-C	-5.25	106.66	114.64
4	4	53	THR	CA-CB-OG1	-5.25	101.73	109.60
3	3	28	TYR	N-CA-CB	-5.25	102.26	109.97
1	1	201	TYR	CA-C-N	-5.25	114.77	122.06
1	1	201	TYR	C-N-CA	-5.25	114.77	122.06
1	1	136	GLN	OE1-CD-NE2	5.24	127.84	122.60
2	2	257	LYS	N-CA-CB	5.24	119.34	110.49
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
1	1	229	VAL	N-CA-C	-5.23	104.98	112.35
3	3	138	GLY	N-CA-C	-5.23	101.67	112.34
2	2	72	THR	CA-CB-OG1	-5.22	101.76	109.60
2	2	127	ILE	CA-C-O	-5.22	114.20	119.89
3	3	94	THR	CA-C-O	-5.21	113.21	119.15
3	3	144	GLU	CA-CB-CG	5.21	124.53	114.10
2	2	259	ILE	CA-C-O	-5.21	114.97	120.39
2	2	243	THR	CA-C-O	-5.21	114.70	120.38
1	1	282	ARG	CB-CA-C	-5.21	100.30	109.62
2	2	18	LEU	N-CA-CB	-5.21	102.74	110.71
1	1	268	ARG	CB-CA-C	5.20	119.75	109.66
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	20	ASN	CA-CB-CG	5.20	117.80	112.60
1	1	259	ARG	N-CA-CB	5.20	117.59	109.85
2	2	214	ARG	CD-NE-CZ	-5.20	117.12	124.40
3	3	158	GLN	CG-CD-OE1	5.20	131.19	120.80
1	1	63	SER	N-CA-C	5.19	116.94	111.28
1	1	257	ALA	N-CA-CB	-5.19	101.83	109.98
1	1	186	PHE	N-CA-C	-5.19	101.02	108.60
3	3	67	TYR	N-CA-C	-5.19	106.80	113.23
2	2	38	TRP	CA-CB-CG	-5.18	103.75	113.60
3	3	231	THR	CA-C-N	-5.18	115.34	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	231	THR	C-N-CA	-5.18	115.34	122.69
3	3	186	PHE	O-C-N	5.17	129.88	123.15
1	1	110	VAL	CA-C-O	-5.17	113.44	119.85
2	2	213	THR	CA-CB-OG1	-5.17	101.84	109.60
1	1	224	MET	O-C-N	5.17	129.47	122.59
3	3	45	GLU	CG-CD-OE1	-5.17	106.51	118.40
2	2	122	LEU	CA-C-O	-5.16	115.19	121.28
3	3	215	PRO	CB-CA-C	5.16	119.23	111.44
2	2	152	ARG	CD-NE-CZ	-5.16	117.18	124.40
2	2	75	SER	N-CA-CB	-5.14	102.06	109.83
2	2	143	LYS	CA-C-N	5.14	131.37	121.54
2	2	143	LYS	C-N-CA	5.14	131.37	121.54
3	3	233	ALA	O-C-N	5.14	129.19	122.87
2	2	181	LEU	N-CA-C	-5.14	106.27	112.54
3	3	82	GLY	N-CA-C	-5.14	102.96	110.87
1	1	23	SER	CA-C-O	-5.13	115.11	121.06
1	1	204	TYR	CA-C-O	-5.13	115.63	121.58
3	3	186	PHE	CA-CB-CG	-5.13	108.67	113.80
2	2	215	HIS	CA-CB-CG	5.13	118.93	113.80
3	3	208	LEU	CA-C-O	-5.12	115.11	120.80
3	3	109	GLY	N-CA-C	5.12	117.52	111.63
2	2	127	ILE	O-C-N	5.12	125.63	120.92
3	3	75	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	1	285	ASP	CA-C-N	-5.10	111.94	120.30
1	1	285	ASP	C-N-CA	-5.10	111.94	120.30
2	2	119	SER	O-C-N	5.10	129.34	123.17
1	1	66	ASP	CA-C-O	-5.09	115.59	121.19
3	3	177	ASP	N-CA-CB	-5.09	102.96	110.14
1	1	133	THR	CA-C-O	-5.09	115.36	121.11
1	1	170	SER	CA-C-O	-5.08	115.84	122.14
1	1	270	ASN	N-CA-CB	5.08	117.77	109.69
2	2	235	THR	CA-C-O	5.08	125.46	120.17
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	65	THR	CA-CB-OG1	-5.08	101.98	109.60
2	2	259	ILE	CA-C-N	-5.08	112.73	122.13
2	2	259	ILE	C-N-CA	-5.08	112.73	122.13
1	1	27	HIS	CA-C-O	-5.07	113.13	122.62
2	2	126	VAL	CA-C-O	-5.07	115.10	120.53
3	3	174	ARG	NE-CZ-NH2	-5.07	114.64	119.20
3	3	1	GLY	N-CA-C	5.07	128.01	113.30
2	2	168	ASP	CB-CG-OD1	-5.07	106.74	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	145	ASN	O-C-N	5.07	129.51	123.13
2	2	165	PRO	CA-C-O	-5.07	115.46	122.15
3	3	217	PHE	N-CA-C	5.07	117.57	110.23
1	1	165	ASP	CB-CG-OD2	5.06	130.04	118.40
2	2	119	SER	CA-C-O	-5.06	115.69	121.40
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
1	1	40	GLY	N-CA-C	-5.05	108.15	115.27
2	2	25	THR	CA-C-O	5.04	126.46	120.66
3	3	95	THR	CA-CB-OG1	-5.04	102.05	109.60
1	1	65	THR	N-CA-C	-5.04	106.06	113.61
1	1	282	ARG	CG-CD-NE	-5.03	100.93	112.00
2	2	32	VAL	O-C-N	5.03	128.27	123.14
3	3	60	THR	N-CA-CB	-5.02	103.27	110.65
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
3	3	146	MET	CB-CA-C	5.02	120.41	110.17
2	2	170	LEU	N-CA-C	-5.02	106.85	112.87
1	1	83	GLN	OE1-CD-NE2	5.01	127.61	122.60
2	2	196	THR	CA-CB-CG2	5.01	119.02	110.50
3	3	118	THR	CA-CB-CG2	5.00	119.01	110.50
2	2	115	THR	CA-C-O	-5.00	115.85	121.40
2	2	140	VAL	O-C-N	5.00	128.06	122.61
4	4	57	LYS	N-CA-CB	5.00	117.32	110.07

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	259	ARG	Sidechain
1	1	265	SER	Mainchain
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	180	0
2	2	1952	0	1926	118	0
3	3	1849	0	1832	147	0
4	4	297	0	294	29	0
5	1	26	0	20	3	0
All	All	6294	0	6179	399	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 32.

All (399) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.58
4:4:33:LYS:CE	4:4:33:LYS:NZ	1.67	1.55
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.54
1:1:285:ASP:CB	1:1:285:ASP:CA	1.79	1.54
1:1:266:ILE:HD12	3:3:235:THR:C	1.51	1.34
3:3:179:ASP:OD2	3:3:182:THR:HB	1.41	1.16
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.14
1:1:266:ILE:HD12	3:3:235:THR:CA	1.76	1.14
1:1:266:ILE:HG22	1:1:266:ILE:O	1.39	1.08
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.07
1:1:285:ASP:CA	1:1:285:ASP: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	1.42	1.02
1:1:266:ILE:CD1	3:3:235:THR:HA	1.93	0.99
1:1:83:GLN:HG2	1:1:97:LYS:HB2	1.44	0.99
3:3:57:ASN:CB	3:3:57:ASN:N	2.28	0.97
2:2:136:GLU:HB3	2:2:140:VAL:HG21	1.44	0.97
3:3:57:ASN:CB	3:3:57:ASN:C	2.36	0.97
1:1:136:GLN:HE21	1:1:235:HIS:CD2	1.84	0.95
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
1:1:266:ILE:O	1:1:266:ILE:CG2	2.14	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	1.28	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.90
1:1:58:MET:HE1	3:3:216:ASP:O	1.71	0.90
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.53	0.90
3:3:57:ASN:CA	3:3:57:ASN:CG	2.45	0.89
1:1:92:ASN:ND2	1:1:95:GLU:HB2	1.87	0.89
1:1:285:ASP:OD1	1:1:285:ASP:HA	1.73	0.89
1:1:266:ILE:CD1	3:3:235:THR:CA	2.50	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
1:1:158:PRO:HB2	1:1:167:THR:HG22	1.57	0.86
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.58	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
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
2:2:136: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
1:1:107:SER:HB2	1:1:113:ARG:HD2	1.63	0.81
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.80
2:2:9:TYR:HD1	2:2:9:TYR:N	1.77	0.80
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.79
1:1:266:ILE:HD11	3:3:235:THR:HA	1.64	0.79
2:2:9:TYR:N	2:2:9:TYR:CD1	2.43	0.78
1:1:58:MET:HE1	3:3:216:ASP:C	2.08	0.78
1:1:136:GLN:NE2	1:1:235:HIS:NE2	2.32	0.78
2:2:262:GLN:HE21	2:2:262:GLN:C	1.91	0.78
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.13	0.77
1:1:266:ILE:HD12	3:3:235:THR:HA	1.54	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
1:1:266:ILE:CD1	3:3:235:THR:C	2.47	0.76
1:1:153:VAL:HG12	1:1:153:VAL:O	1.85	0.76
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:224:MET:HG2	1:1:226:PHE:CZ	2.20	0.75
1:1:266:ILE:HD12	3:3:236:GLU:N	2.01	0.75
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.75
1:1:149:GLN:O	1:1:149:GLN:HG2	1.86	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
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.69	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	0.74
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.74
4:4:43:GLN:HG2	4:4:45:LEU:HB2	1.70	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
1:1:282: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
1:1:58:MET:HE1	3:3:216:ASP:HA	1.71	0.72
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.72
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
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.71
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.71
3:3:57:ASN:CA	3:3:57:ASN:OD1	2.38	0.70
1:1:191:VAL:HG23	1:1:191:VAL:O	1.90	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
2:2:195:ASN:OD1	2:2:196:THR:HG23	1.93	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
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
1:1:278: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
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.77	0.66
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
3:3:197:LEU:HB3	3:3:201:THR:HG22	1.77	0.66
1:1:285:ASP:CB	1:1:285:ASP:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:58:MET:HE1	3:3:216:ASP:CA	2.27	0.64
1:1:158:PRO:HB2	1:1:167:THR:CG2	2.26	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
2:2:23: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
1:1:104:ILE:HG13	1:1:222:GLY:O	1.99	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
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.61
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.30	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
1:1:87:ALA:HB2	1:1:98:LEU:HD11	1.82	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
1:1:149:GLN:O	1:1:149:GLN:CG	2.45	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
3:3:175:TYR:H	3:3:182:THR:HG21	1.66	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
1:1:51:ILE:HD13	3:3:166:PRO:HG3	1.82	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.84	0.59
1:1:96:ALA:C	1:1:97:LYS:HG2	2.27	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
1:1:83:GLN:NE2	1:1:97:LYS:HG3	2.18	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.02	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
2:2:64: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
1:1:205:SER:HB3	1:1:217:VAL:HG13	1.86	0.57
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:221:MET:HE2	2:2:223:ILE:HD11	1.87	0.57
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
3:3:179:ASP:OD2	3:3:182:THR:CG2	2.53	0.57
1:1:58:MET:HE3	3:3:216:ASP:HA	1.85	0.56
1:1:187:SER:O	3:3:23:SER:HA	2.05	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
3:3:175:TYR:H	3:3:182:THR:CG2	2.19	0.56
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.56
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
1:1:87:ALA:CB	1:1:98:LEU:HD11	2.36	0.56
1:1:136:GLN:NE2	1:1:235:HIS:CD2	2.64	0.56
1:1:117:GLU:HB3	1:1:200:PHE:HZ	1.70	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.56
1:1:97:LYS:C	1:1:99:PHE:N	2.59	0.56
1:1:107:SER:HB2	1:1:113:ARG:CD	2.34	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
1:1:153:VAL:O	1:1:153:VAL:CG1	2.32	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
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	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
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.55
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.87	0.54
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.54
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.54
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.54
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.54
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	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
3:3:117:TYR:CD1	3:3:155:ILE:HD13	2.43	0.54
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.53
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.53
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.53
1:1:152:TYR:O	1:1:154:PRO:HD3	2.09	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
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.53
3:3:86:PHE:CD1	3:3:178:PRO:HB3	2.44	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
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
1:1:152:TYR:C	1:1:154:PRO:HD3	2.33	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.52
2:2:66:LEU:HD12	2:2:89:MET:HE3	1.91	0.52
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.52
1:1:97:LYS:C	1:1:99:PHE:H	2.18	0.52
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.45	0.52
1:1:107:SER:CB	1:1:113:ARG:HD2	2.38	0.51
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.51
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.51
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.51
3:3:75:ARG:NH1	3:3:78:GLU:OE2	2.41	0.51
4:4:44:SER:C	4:4:46:SER:N	2.68	0.51
1:1:117:GLU:HB3	1:1:200:PHE:CZ	2.46	0.51
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.51
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
1:1:38:GLU:OE1	3:3:116:MET:HE2	2.10	0.51
2:2:158:SER:HG	2:2:167:LYS:HE2	1.71	0.51
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	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
1:1:81:GLU:HG2	1:1:97:LYS:NZ	2.25	0.50
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE2	2.44	0.50
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
2:2:255:ARG:CG	2:2:256:SER:H	2.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.50
1:1:151:MET:HA	1:1:175:SER:HB2	1.93	0.50
1:1:168:TRP:CH2	1:1:225:ALA:HB1	2.47	0.50
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
1:1:81:GLU:HG2	1:1:97:LYS:HZ2	1.78	0.49
1:1:157:ALA:HB1	1:1:158:PRO:HD2	1.94	0.49
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	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
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.49
1:1:96:ALA:O	1:1:97:LYS:HG2	2.12	0.49
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.49
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.48
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
1:1:204:TYR:HD1	1:1:212:GLN:O	1.97	0.48
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.48
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.95	0.48
1:1:280:LYS:HE3	3:3:89:ASP:OD1	2.13	0.48
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	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
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.47
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.96	0.47
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.44	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
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
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
1:1:206: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
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.47
2:2:63:PHE:CD1	2:2:245:ALA:HB2	2.50	0.47
2:2:158:SER:HG	2:2:167:LYS:CE	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:266:ILE:CD1	3:3:236:GLU:N	2.72	0.46
1:1:204:TYR:CZ	1:1:213:TYR:HD1	2.34	0.46
1:1:192:GLY:HA2	1:1:221:MET:HE1	1.97	0.46
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.46
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.46
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.63	0.46
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.46
1:1:82:ILE:HG22	1:1:100:ASN:HB2	1.97	0.46
1:1:78:HIS:CE1	1:1:102:TRP:CD1	3.03	0.46
1:1:236:LYS:HE2	1:1:236:LYS:HB3	1.83	0.46
1:1:87:ALA:CB	1:1:98:LEU:CD1	2.92	0.46
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.46
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.46
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	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
2:2:195:ASN:OD1	2:2:195:ASN:C	2.59	0.45
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.45
3:3:57:ASN:CB	3:3:57:ASN:H	2.26	0.45
1:1:218:LEU:HD23	1:1:218:LEU:HA	1.81	0.45
2:2:170:LEU:HD23	3:3:64:VAL:HG22	1.99	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.98	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.98	0.45
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.45
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	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
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.82	0.45
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.45
1:1:106:LEU:HG	5:1:290:SD8:H111	1.98	0.44
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	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
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
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.44
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.44
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.44
1:1:265:SER:OG	2:2:139:ASN:HB3	2.17	0.44
3:3:221:LEU:C	3:3:221:LEU:HD23	2.43	0.44
1:1:289:TYR:CD2	3:3:138:GLY:HA3	2.52	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
3:3:84:ASN:OD1	3:3:84:ASN:C	2.60	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.44
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.43
1:1:94:ARG:HD3	1:1:99:PHE:CE1	2.53	0.43
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.43
1:1:38:GLU:N	3:3:116:MET:HE1	2.33	0.43
1:1:120:THR:O	1:1:199:CYS:HB2	2.18	0.43
2:2:190:ASN:O	2:2:191:LEU:C	2.61	0.43
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.43
1:1:115:LYS:HZ3	3:3:222:MET:CE	2.31	0.43
1:1:132:ALA:O	1:1:181:GLY:N	2.41	0.43
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	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
1:1:215:ILE:C	1:1:217:VAL:H	2.26	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
1:1:285:ASP:C	1:1:285:ASP:HB3	2.38	0.43
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.53	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.42
4:4:43:GLN:C	4:4:45:LEU:N	2.74	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	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
3:3:174:ARG:HD2	3:3:182:THR:O	2.20	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
3:3:226:GLN:HE21	3:3:226:GLN:HB2	1.21	0.42
1:1:107:SER:HB3	5:1:290:SD8:H172	2.02	0.42
2:2:40:GLU:O	2:2:40:GLU:CG	2.61	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.42
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.38	0.42
1:1:128:TYR:CZ	5:1:290:SD8:H7	2.55	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD2	2.55	0.42
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	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
1:1:286: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
1:1:83:GLN:HE21	1:1:97:LYS:HG3	1.82	0.41
1:1:86:ASP:OD1	1:1:88:THR:HB	2.20	0.41
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.74	0.41
1:1:197:TYR:HE1	1:1:221:MET:CE	2.33	0.41
2:2:187:GLN:HE21	2:2:187:GLN:HB2	1.57	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	2.55	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
1:1:87:ALA:C	1:1:90:ILE:HG12	2.46	0.41
1:1:197:TYR:HE1	1:1:221:MET:HE3	1.86	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.02	0.41
3:3:137:ARG:HH11	3:3:137:ARG:HD3	1.22	0.41
1:1:83:GLN:HG2	1:1:97:LYS:CB	2.33	0.41
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.20	0.41
1:1:54:ARG:HH11	1:1:54:ARG:HD2	1.55	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
1:1:165:ASP:CB	1:1:167:THR:OG1	2.69	0.41
3:3:64:VAL:O	3:3:64:VAL:HG12	2.21	0.41
1:1:103:LYS:O	1:1:104:ILE:C	2.63	0.41
1:1:215:ILE:H	1:1:215:ILE:HG12	1.34	0.41
1:1:215:ILE:C	1:1:217:VAL:N	2.77	0.40
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
3:3:231:THR:C	3:3:232:VAL:HG13	2.45	0.40
1:1:201:TYR:HD2	1:1:214:GLY:O	2.04	0.40
1:1:208:ASP:HB3	1:1:211:THR:HB	2.04	0.40
3:3:101:VAL:HG13	3:3:176:THR:HB	2.04	0.40
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
1:1:228:ILE:HD11	1:1:239:VAL:CG2	2.52	0.40
2:2:172:ASN:CG	2:2:181:LEU:HD13	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:55:MET:HE1	3:3:83:THR:HG21	2.04	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%)	246 (91%)	18 (7%)	7 (3%)	4	23
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	16	50
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	14	48
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	4	23
All	All	796/855 (93%)	730 (92%)	54 (7%)	12 (2%)	8	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	SER
1	1	218	LEU
1	1	266	ILE
3	3	57	ASN
3	3	77	ASN
1	1	104	ILE
1	1	165	ASP
2	2	255	ARG
2	2	257	LYS
4	4	47	MET
1	1	223	SER
1	1	224	MET

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%)	191 (80%)	48 (20%)	1	7
2	2	223/229 (97%)	178 (80%)	45 (20%)	1	7
3	3	209/209 (100%)	172 (82%)	37 (18%)	2	10
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	1
All	All	704/748 (94%)	561 (80%)	143 (20%)	1	7

All (143) 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	98	LEU
1	1	104	ILE
1	1	106	LEU
1	1	122	VAL
1	1	136	GLN
1	1	137	PRO
1	1	138	ASP
1	1	144	SER
1	1	145	ASN
1	1	161	LYS

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Mol	Chain	Res	Type
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	191	VAL
1	1	202	ASP
1	1	215	ILE
1	1	216	THR
1	1	223	SER
1	1	224	MET
1	1	240	LYS
1	1	248	LYS
1	1	254	ILE
1	1	256	ARG
1	1	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	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

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

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

Mol	Chain	Res	Type
1	1	61	ASN
1	1	136	GLN
2	2	20	ASN

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Mol	Chain	Res	Type
2	2	94	GLN
2	2	111	GLN
2	2	135	HIS
2	2	174	ASN
2	2	187	GLN
2	2	262	GLN
3	3	27	ASN
3	3	65	ASN
3	3	74	ASN
3	3	140	GLN
3	3	192	GLN
3	3	226	GLN

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	SD8	1	290	-	28,29,29	3.63	11 (39%)	36,40,40	2.05	11 (30%)

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	SD8	1	290	-	-	2/15/34/34	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	290	SD8	C8-C3	10.11	1.55	1.41
5	1	290	SD8	C4-C3	8.95	1.54	1.39
5	1	290	SD8	C1-N2	8.37	1.48	1.35
5	1	290	SD8	C13-S2	-6.00	1.62	1.74
5	1	290	SD8	C8-N1	-4.06	1.32	1.39
5	1	290	SD8	C15-C16	3.73	1.53	1.48
5	1	290	SD8	O2-C16	3.42	1.40	1.33
5	1	290	SD8	C11-N3	2.33	1.51	1.47
5	1	290	SD8	C15-N4	2.26	1.43	1.38
5	1	290	SD8	C12-N2	2.22	1.51	1.47
5	1	290	SD8	C9-N2	2.04	1.50	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	290	SD8	C8-N1-C1	4.96	129.29	117.26
5	1	290	SD8	C8-C3-S1	4.92	122.74	119.58
5	1	290	SD8	C4-C3-C8	-4.10	114.16	119.30
5	1	290	SD8	S2-C13-N4	-3.57	111.86	116.28
5	1	290	SD8	C14-C15-N4	-3.39	110.77	115.43
5	1	290	SD8	S2-C13-N3	2.82	124.46	120.41
5	1	290	SD8	C4-C3-S1	2.65	123.06	117.48
5	1	290	SD8	C13-N4-C15	2.56	112.90	106.79
5	1	290	SD8	C5-C6-C7	2.35	123.14	120.24
5	1	290	SD8	C14-S2-C13	2.16	93.08	89.41
5	1	290	SD8	C3-C8-N1	-2.03	121.97	124.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

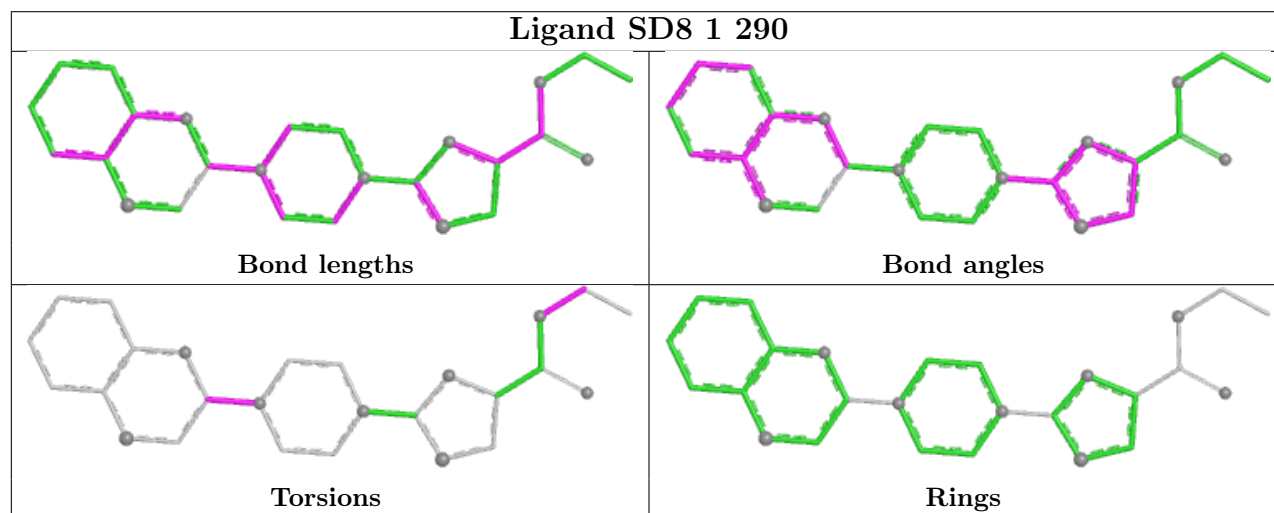
Mol	Chain	Res	Type	Atoms
5	1	290	SD8	N1-C1-N2-C12
5	1	290	SD8	C18-C17-O2-C16

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	290	SD8	3	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
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	153:VAL	C	154:PRO	N	1.11

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	273/289 (94%)	-1.35	0 100 100	8, 14, 30, 42	0
2	2	255/262 (97%)	-1.42	0 100 100	7, 12, 24, 42	0
3	3	236/236 (100%)	-1.37	0 100 100	8, 12, 23, 31	0
4	4	40/68 (58%)	-1.14	0 100 100	13, 24, 37, 38	0
All	All	804/855 (94%)	-1.37	0 100 100	7, 13, 28, 42	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

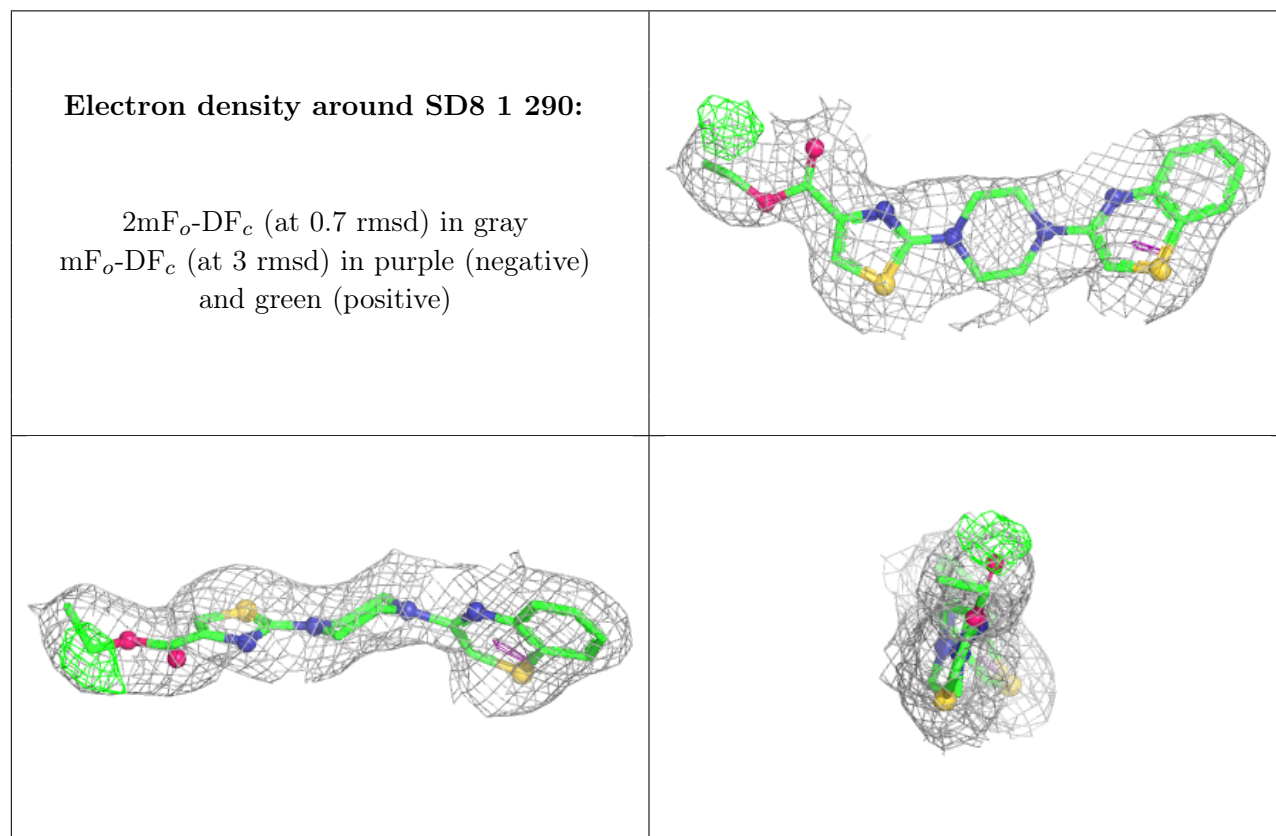
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SD8	1	290	26/26	0.99	0.05	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.