



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:41 AM UTC

PDB ID : 2RS1 / pdb_00002rs1
Title : STRUCTURAL ANALYSIS OF ANTIVIRAL AGENTS THAT INTERACT
WITH THE CAPSID OF HUMAN RHINOVIRUSES
Authors : Badger, J.; Smith, T.J.; Rossmann, M.G.
Deposited on : 1988-10-03
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

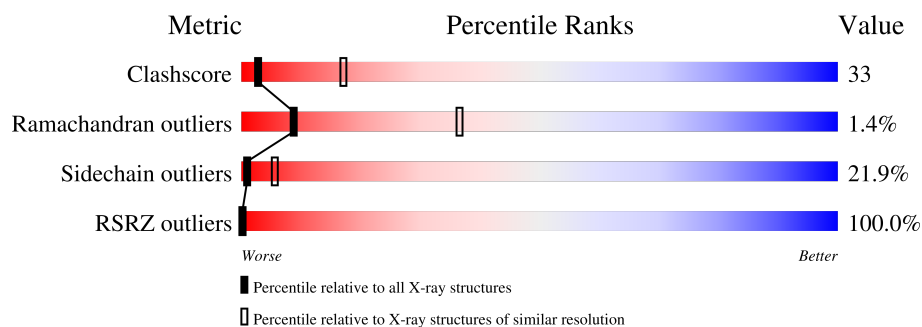
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	289	
2	2	262	
3	3	236	
4	4	68	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	W84	1	900	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6302 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1).

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

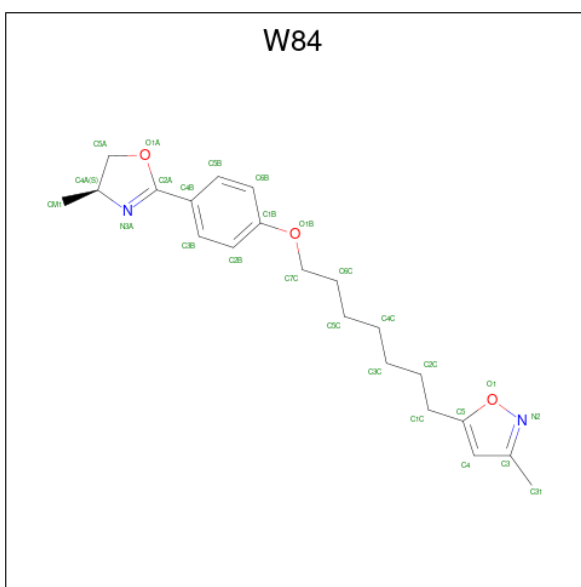
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

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

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

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

- Molecule 5 is 5-(7-(5-HYDRO-4-METHYL-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYL ISOXAZOLE (CCD ID: W84) (formula: C₂₁H₂₈N₂O₃).



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

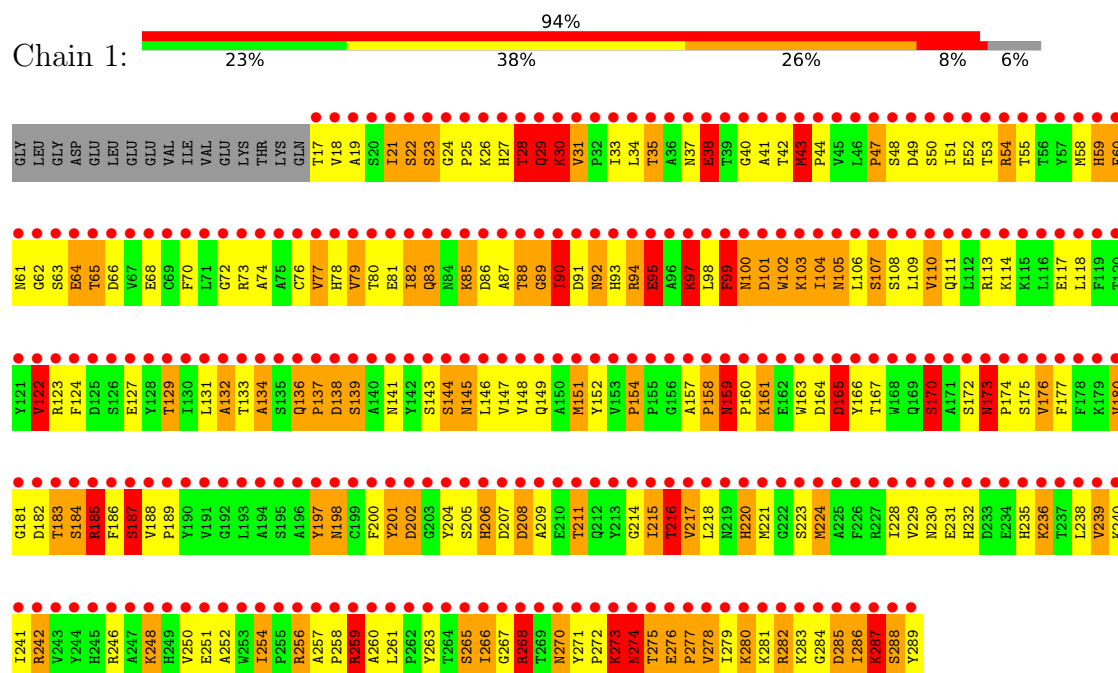
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	7	Total O 7 7	0	0
6	2	1	Total O 1 1	0	0

3 Residue-property plots

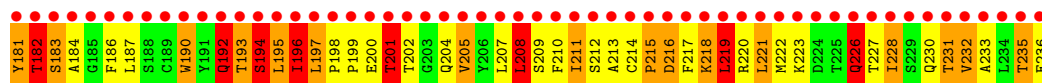
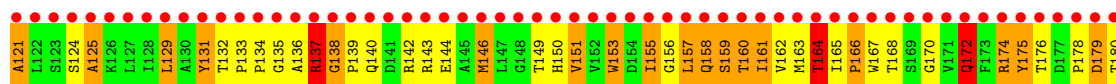
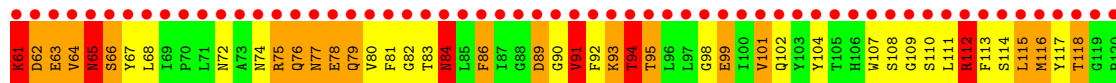
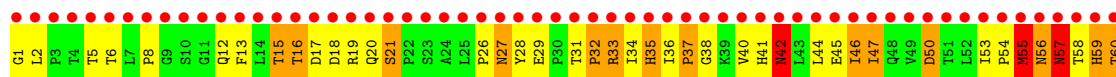
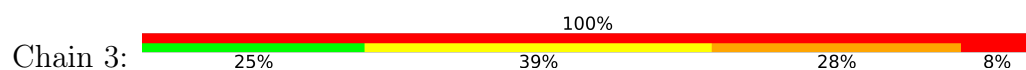
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

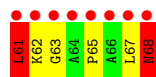
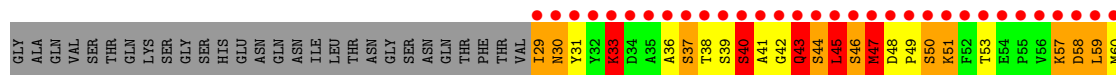
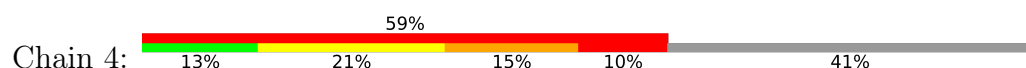




• Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00 0.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 8.6 (0.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.81Å)	Xtriage
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 330.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for l,-k,h	Xtriage
F_o, F_c correlation	-0.01	EDS
Total number of atoms	6302	wwPDB-VP
Average B, all atoms (Å ²)	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.26% 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 i

5.1 Standard geometry i

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	2.31	90/2228 (4.0%)	2.76	214/3031 (7.1%)
2	2	2.40	96/2001 (4.8%)	2.77	193/2735 (7.1%)
3	3	2.29	80/1898 (4.2%)	2.78	187/2597 (7.2%)
4	4	2.64	14/302 (4.6%)	3.14	33/406 (8.1%)
All	All	2.35	280/6429 (4.4%)	2.79	627/8769 (7.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2
2	2	0	2
All	All	0	4

All (280) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	285	ASP	CA-CB	17.77	1.79	1.53
4	4	41	ALA	C-O	13.33	1.41	1.24
3	3	57	ASN	CA-CB	12.78	1.75	1.53
4	4	42	GLY	N-CA	12.59	1.63	1.45
1	1	187	SER	N-CA	11.77	1.60	1.46
2	2	194	ASN	CA-CB	11.51	1.71	1.53
1	1	283	LYS	N-CA	10.88	1.61	1.46
1	1	144	SER	N-CA	10.33	1.58	1.45
3	3	164	THR	C-O	10.22	1.36	1.24
4	4	45	LEU	C-N	9.39	1.46	1.33
2	2	187	GLN	N-CA	9.31	1.57	1.45
2	2	256	SER	C-O	9.29	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	170	SER	CB-OG	-9.23	1.23	1.42
1	1	52	GLU	C-O	9.14	1.35	1.24
1	1	282	ARG	CD-NE	9.12	1.59	1.46
2	2	152	ARG	CD-NE	8.88	1.58	1.46
2	2	102	GLY	N-CA	8.88	1.54	1.45
2	2	168	ASP	C-O	8.82	1.34	1.24
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	8.43	1.30	1.23
3	3	50	ASP	CA-CB	-8.28	1.40	1.53
3	3	232	VAL	N-CA	8.17	1.55	1.46
1	1	73	ARG	C-O	8.02	1.33	1.23
2	2	77	GLY	N-CA	7.83	1.53	1.45
3	3	138	GLY	N-CA	7.83	1.55	1.44
2	2	236	PRO	C-O	7.80	1.34	1.24
2	2	161	GLU	CA-CB	-7.78	1.42	1.53
1	1	285	ASP	N-CA	-7.77	1.34	1.45
1	1	158	PRO	CA-C	-7.72	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
2	2	12	ARG	NE-CZ	7.59	1.41	1.33
1	1	122	VAL	N-CA	7.58	1.55	1.46
1	1	72	GLY	C-O	7.53	1.34	1.23
2	2	52	LYS	N-CA	7.53	1.55	1.46
3	3	215	PRO	C-N	-7.47	1.23	1.33
1	1	143	SER	C-O	7.47	1.33	1.24
1	1	94	ARG	CD-NE	7.42	1.56	1.46
2	2	11	ASP	CA-CB	7.36	1.66	1.53
1	1	28	THR	CA-CB	7.34	1.64	1.53
1	1	288	SER	C-O	7.31	1.32	1.23
2	2	120	GLY	N-CA	7.22	1.53	1.45
1	1	132	ALA	C-O	7.20	1.32	1.24
3	3	77	ASN	C-O	7.17	1.33	1.24
3	3	60	THR	CA-CB	7.16	1.65	1.54
2	2	260	VAL	N-CA	7.15	1.55	1.46
4	4	40	SER	CB-OG	7.05	1.56	1.42
2	2	108	VAL	C-O	7.01	1.32	1.24
2	2	219	SER	CA-CB	-7.01	1.41	1.53
1	1	30	LYS	C-O	7.00	1.32	1.23
2	2	9	TYR	C-O	6.99	1.32	1.23
1	1	276	GLU	C-O	6.97	1.30	1.24
2	2	58	THR	C-O	6.97	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	74	GLY	C-O	6.94	1.31	1.23
1	1	202	ASP	CA-CB	-6.86	1.42	1.53
4	4	49	PRO	C-N	-6.85	1.24	1.34
1	1	91	ASP	N-CA	6.84	1.55	1.46
1	1	133	THR	N-CA	6.84	1.54	1.45
1	1	288	SER	CA-CB	6.84	1.65	1.53
3	3	86	PHE	CA-CB	-6.84	1.42	1.52
1	1	23	SER	N-CA	6.81	1.54	1.45
2	2	223	ILE	CA-CB	6.80	1.59	1.54
3	3	6	THR	N-CA	6.76	1.54	1.45
2	2	243	THR	C-O	6.74	1.32	1.24
2	2	193	THR	C-N	-6.73	1.23	1.33
2	2	152	ARG	CZ-NH2	6.73	1.42	1.33
2	2	194	ASN	N-CA	-6.72	1.37	1.45
3	3	216	ASP	CA-CB	6.72	1.64	1.53
2	2	197	ALA	C-O	6.71	1.31	1.23
1	1	73	ARG	N-CA	6.67	1.53	1.45
1	1	165	ASP	CA-CB	6.67	1.64	1.53
2	2	256	SER	CB-OG	6.67	1.55	1.42
2	2	10	SER	C-N	-6.66	1.25	1.33
1	1	251	GLU	CA-CB	-6.62	1.42	1.53
1	1	280	LYS	C-O	6.62	1.31	1.24
2	2	39	PRO	C-O	6.58	1.31	1.23
3	3	57	ASN	N-CA	-6.57	1.37	1.46
1	1	134	ALA	CA-CB	-6.56	1.42	1.53
2	2	109	HIS	CE1-NE2	-6.54	1.26	1.32
2	2	9	TYR	N-CA	6.54	1.53	1.46
3	3	15	THR	C-O	6.54	1.32	1.24
1	1	85	LYS	C-O	6.54	1.31	1.23
3	3	156	GLY	C-O	-6.51	1.18	1.24
2	2	190	ASN	CA-CB	-6.50	1.44	1.53
2	2	52	LYS	CE-NZ	6.50	1.68	1.49
4	4	62	LYS	C-O	6.50	1.31	1.24
4	4	44	SER	CB-OG	6.49	1.55	1.42
2	2	262	GLN	CD-OE1	6.46	1.35	1.23
1	1	79	VAL	C-N	-6.44	1.24	1.33
3	3	57	ASN	C-N	-6.43	1.25	1.33
2	2	30	ASN	N-CA	6.43	1.54	1.46
2	2	217	ASN	C-O	6.43	1.32	1.24
4	4	62	LYS	N-CA	6.42	1.54	1.46
1	1	231	GLU	CA-CB	-6.41	1.44	1.53
3	3	205	VAL	N-CA	6.35	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	22	SER	C-N	-6.33	1.25	1.33
1	1	95	GLU	CB-CG	6.33	1.71	1.52
1	1	148	VAL	C-N	-6.33	1.25	1.33
2	2	8	GLY	N-CA	6.30	1.55	1.45
1	1	94	ARG	NE-CZ	6.29	1.40	1.33
4	4	63	GLY	N-CA	6.29	1.54	1.45
3	3	165	ILE	N-CA	6.28	1.54	1.46
3	3	5	THR	C-O	6.24	1.31	1.24
3	3	118	THR	CB-OG1	6.24	1.53	1.43
1	1	185	ARG	C-N	-6.24	1.25	1.33
1	1	184	SER	N-CA	6.21	1.53	1.45
2	2	259	ILE	C-O	6.20	1.31	1.24
3	3	182	THR	CA-CB	6.20	1.62	1.53
3	3	75	ARG	C-N	-6.18	1.24	1.33
3	3	164	THR	N-CA	6.18	1.53	1.46
2	2	121	CYS	C-O	6.16	1.31	1.23
1	1	177	PHE	C-N	-6.16	1.25	1.33
3	3	16	THR	CA-CB	6.14	1.63	1.53
1	1	184	SER	C-O	6.14	1.31	1.23
4	4	45	LEU	N-CA	6.14	1.55	1.46
2	2	168	ASP	CA-CB	6.14	1.60	1.53
1	1	251	GLU	N-CA	6.12	1.53	1.46
1	1	28	THR	N-CA	-6.10	1.37	1.45
2	2	162	VAL	N-CA	6.10	1.53	1.46
1	1	274	ASN	N-CA	6.10	1.54	1.46
3	3	215	PRO	CA-CB	-6.09	1.44	1.53
4	4	33	LYS	CE-NZ	6.08	1.67	1.49
1	1	24	GLY	N-CA	6.07	1.53	1.44
3	3	110	SER	N-CA	6.05	1.52	1.45
2	2	19	GLY	C-N	-6.05	1.25	1.33
2	2	190	ASN	N-CA	6.04	1.54	1.46
2	2	257	LYS	N-CA	6.04	1.53	1.46
1	1	211	THR	N-CA	6.03	1.53	1.45
3	3	57	ASN	C-O	6.03	1.31	1.24
1	1	131	LEU	C-O	6.02	1.31	1.23
3	3	155	ILE	N-CA	5.99	1.53	1.46
3	3	36	ILE	N-CA	5.99	1.53	1.46
3	3	135	GLY	C-O	5.99	1.31	1.24
2	2	208	PRO	C-N	-5.98	1.28	1.33
3	3	222	MET	CG-SD	5.96	1.95	1.80
1	1	220	HIS	CA-C	-5.94	1.46	1.53
1	1	88	THR	CB-OG1	5.93	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	180	ASN	C-N	-5.92	1.25	1.33
1	1	220	HIS	C-N	-5.91	1.25	1.33
2	2	17	THR	C-N	-5.90	1.25	1.33
1	1	175	SER	CB-OG	-5.88	1.30	1.42
3	3	27	ASN	C-N	-5.87	1.25	1.33
1	1	185	ARG	C-O	5.84	1.30	1.23
1	1	38	GLU	CB-CG	-5.83	1.34	1.52
3	3	213	ALA	C-O	5.83	1.30	1.23
3	3	219	LEU	C-N	-5.81	1.26	1.33
1	1	276	GLU	N-CA	5.80	1.54	1.45
2	2	55	LYS	N-CA	5.79	1.53	1.46
3	3	116	MET	N-CA	5.79	1.53	1.46
2	2	103	ARG	C-O	5.77	1.30	1.23
2	2	135	HIS	CG-CD2	-5.77	1.29	1.35
1	1	287	LYS	C-O	5.75	1.31	1.24
2	2	88	ASP	C-O	5.74	1.32	1.24
3	3	33	ARG	NE-CZ	5.73	1.39	1.33
2	2	176	THR	N-CA	5.73	1.53	1.45
3	3	38	GLY	CA-C	-5.73	1.43	1.51
2	2	152	ARG	NE-CZ	5.72	1.39	1.33
1	1	274	ASN	CA-C	5.71	1.60	1.52
1	1	187	SER	CB-OG	-5.71	1.30	1.42
1	1	187	SER	C-O	5.71	1.30	1.23
2	2	54	SER	CA-CB	-5.71	1.44	1.53
4	4	45	LEU	C-O	5.69	1.31	1.23
3	3	41	HIS	CE1-NE2	5.67	1.38	1.32
1	1	285	ASP	C-N	5.67	1.40	1.33
1	1	239	VAL	C-O	5.67	1.30	1.24
3	3	201	THR	C-O	5.66	1.30	1.23
2	2	103	ARG	N-CA	5.66	1.52	1.46
2	2	195	ASN	CA-CB	-5.66	1.44	1.54
3	3	35	HIS	C-N	-5.65	1.26	1.33
1	1	268	ARG	N-CA	5.65	1.52	1.45
3	3	158	GLN	C-O	5.65	1.30	1.24
1	1	25	PRO	CA-CB	-5.64	1.45	1.53
2	2	223	ILE	CA-C	-5.64	1.48	1.52
2	2	63	PHE	C-O	5.64	1.30	1.24
2	2	208	PRO	C-O	5.63	1.30	1.24
2	2	87	LYS	CB-CG	-5.63	1.35	1.52
1	1	63	SER	CB-OG	-5.62	1.30	1.42
1	1	267	GLY	C-O	5.62	1.32	1.24
3	3	82	GLY	N-CA	5.62	1.50	1.45

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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	180	VAL	C-O	5.62	1.29	1.24
2	2	75	SER	C-O	5.61	1.30	1.23
1	1	117	GLU	CD-OE2	5.59	1.35	1.25
3	3	172	GLN	CG-CD	-5.58	1.38	1.52
2	2	168	ASP	C-N	-5.58	1.26	1.33
1	1	137	PRO	C-O	5.58	1.31	1.24
2	2	194	ASN	C-O	5.58	1.30	1.23
1	1	254	ILE	CA-CB	5.57	1.61	1.54
3	3	82	GLY	C-N	-5.57	1.26	1.33
3	3	231	THR	CB-OG1	5.56	1.52	1.43
4	4	51	LYS	CE-NZ	5.55	1.66	1.49
3	3	75	ARG	N-CA	5.54	1.52	1.45
3	3	108	SER	CA-CB	-5.54	1.44	1.53
3	3	140	GLN	C-N	-5.52	1.26	1.33
2	2	109	HIS	C-O	5.51	1.30	1.24
3	3	66	SER	N-CA	5.51	1.53	1.46
3	3	61	LYS	CE-NZ	5.50	1.65	1.49
2	2	153	GLY	C-N	-5.50	1.25	1.33
1	1	102	TRP	NE1-CE2	-5.49	1.31	1.37
2	2	237	SER	C-O	5.49	1.30	1.23
2	2	237	SER	N-CA	5.49	1.52	1.46
2	2	151	GLU	CA-CB	-5.46	1.43	1.53
3	3	77	ASN	CG-OD1	5.45	1.33	1.23
1	1	25	PRO	C-N	-5.45	1.25	1.33
3	3	209	SER	N-CA	5.45	1.52	1.46
2	2	141	SER	N-CA	5.45	1.52	1.45
1	1	277	PRO	N-CA	5.44	1.53	1.47
3	3	40	VAL	C-O	5.44	1.30	1.24
3	3	37	PRO	CA-CB	-5.42	1.45	1.53
2	2	171	TYR	C-O	5.41	1.31	1.24
3	3	74	ASN	CA-CB	5.38	1.61	1.53
3	3	91	VAL	C-O	5.38	1.30	1.24
1	1	279	ILE	C-O	5.38	1.29	1.24
2	2	61	CYS	CA-C	-5.37	1.47	1.53
1	1	270	ASN	CA-C	5.36	1.59	1.52
1	1	122	VAL	C-O	5.35	1.29	1.24
2	2	103	ARG	CA-CB	-5.35	1.44	1.53
3	3	17	ASP	CG-OD2	5.35	1.35	1.25
2	2	72	THR	CB-OG1	5.34	1.52	1.43
3	3	209	SER	C-O	5.34	1.30	1.23
2	2	68	SER	CA-C	-5.34	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	211	SER	C-O	5.34	1.30	1.23
1	1	176	VAL	CA-C	5.33	1.58	1.52
1	1	127	GLU	CA-CB	-5.33	1.46	1.53
2	2	148	HIS	ND1-CE1	5.32	1.37	1.32
2	2	256	SER	C-N	-5.32	1.26	1.33
4	4	61	LEU	C-O	5.32	1.30	1.24
2	2	219	SER	N-CA	5.30	1.52	1.46
1	1	30	LYS	CE-NZ	5.30	1.65	1.49
2	2	14	GLN	CD-NE2	5.29	1.44	1.33
2	2	123	LEU	C-N	-5.28	1.26	1.33
3	3	228	ILE	C-O	5.28	1.30	1.24
1	1	33	ILE	C-O	5.27	1.30	1.24
3	3	64	VAL	C-N	-5.26	1.25	1.33
3	3	2	LEU	CA-CB	5.25	1.63	1.53
1	1	89	GLY	C-O	5.25	1.31	1.23
2	2	246	PRO	C-O	5.23	1.29	1.23
2	2	99	HIS	C-N	-5.21	1.26	1.34
3	3	164	THR	CA-CB	5.21	1.61	1.53
1	1	283	LYS	CE-NZ	5.21	1.65	1.49
2	2	202	PRO	C-O	5.20	1.29	1.23
1	1	54	ARG	C-O	5.20	1.30	1.23
1	1	161	LYS	C-N	-5.20	1.26	1.33
3	3	146	MET	C-O	5.19	1.30	1.24
3	3	77	ASN	C-N	-5.19	1.26	1.33
2	2	38	TRP	CA-C	-5.18	1.45	1.52
3	3	153	TRP	C-O	5.17	1.30	1.24
3	3	174	ARG	CA-C	5.16	1.58	1.52
1	1	252	ALA	C-O	5.15	1.30	1.23
3	3	58	THR	CA-CB	5.15	1.62	1.53
3	3	133	PRO	CA-CB	-5.13	1.47	1.54
2	2	204	ILE	C-N	-5.13	1.26	1.33
3	3	112	ARG	CA-CB	-5.12	1.45	1.53
1	1	129	THR	N-CA	5.12	1.52	1.46
2	2	202	PRO	C-N	-5.10	1.26	1.33
3	3	136	ALA	C-O	5.10	1.30	1.23
3	3	205	VAL	C-O	5.10	1.29	1.23
1	1	166	TYR	N-CA	5.10	1.52	1.46
1	1	85	LYS	N-CA	5.08	1.51	1.46
2	2	128	PRO	CA-CB	-5.08	1.46	1.53
1	1	209	ALA	C-N	-5.08	1.26	1.33
2	2	186	HIS	C-O	5.06	1.29	1.23
3	3	65	ASN	CA-CB	5.06	1.62	1.53

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

All (627) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	50	ASP	CA-CB-CG	27.73	140.33	112.60
1	1	285	ASP	CA-CB-CG	-22.21	90.39	112.60
3	3	215	PRO	CA-C-N	20.36	149.20	120.29
3	3	215	PRO	C-N-CA	20.36	149.20	120.29
2	2	87	LYS	CA-CB-CG	19.05	152.21	114.10
2	2	11	ASP	CA-CB-CG	-18.96	93.64	112.60
1	1	145	ASN	OD1-CG-ND2	17.24	139.84	122.60
2	2	193	THR	CA-C-N	16.42	150.15	122.07
2	2	193	THR	C-N-CA	16.42	150.15	122.07
2	2	190	ASN	CA-CB-CG	16.38	128.98	112.60
1	1	159	ASN	CB-CA-C	15.59	130.12	108.76
1	1	170	SER	CA-CB-OG	15.05	141.21	111.10
2	2	194	ASN	CA-CB-CG	-14.89	97.71	112.60
2	2	11	ASP	CA-C-N	14.78	140.54	120.44
2	2	11	ASP	C-N-CA	14.78	140.54	120.44
1	1	197	TYR	N-CA-CB	-14.13	87.34	110.23
3	3	57	ASN	CA-CB-CG	-13.74	98.86	112.60
1	1	38	GLU	CB-CG-CD	13.64	135.78	112.60
3	3	74	ASN	CA-CB-CG	-13.47	99.13	112.60
3	3	65	ASN	CA-CB-CG	-13.09	99.51	112.60
1	1	202	ASP	CA-CB-CG	12.96	125.56	112.60
3	3	27	ASN	CA-CB-CG	-12.94	99.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	145	ASN	CA-CB-CG	-12.89	99.71	112.60
2	2	194	ASN	N-CA-CB	-12.65	89.79	110.41
2	2	44	ASP	CA-CB-CG	12.64	125.24	112.60
1	1	94	ARG	CD-NE-CZ	-12.61	106.75	124.40
1	1	256	ARG	NE-CZ-NH2	12.57	130.51	119.20
2	2	67	ASP	CA-CB-CG	-12.45	100.15	112.60
2	2	256	SER	CA-C-O	-12.21	105.38	119.79
4	4	30	ASN	CA-CB-CG	-12.10	100.50	112.60
3	3	172	GLN	CB-CG-CD	12.03	133.05	112.60
4	4	45	LEU	N-CA-CB	-11.89	94.13	111.84
4	4	41	ALA	CA-C-O	-11.31	105.46	119.38
3	3	74	ASN	OD1-CG-ND2	11.30	133.90	122.60
2	2	14	GLN	OE1-CD-NE2	11.18	133.78	122.60
3	3	29	GLU	CB-CG-CD	11.13	131.52	112.60
1	1	285	ASP	N-CA-CB	-11.05	95.26	110.29
2	2	151	GLU	CA-CB-CG	11.04	136.19	114.10
1	1	173	ASN	CA-CB-CG	11.01	123.61	112.60
1	1	197	TYR	CA-CB-CG	10.92	133.55	113.90
1	1	25	PRO	CA-C-O	-10.88	108.94	121.56
2	2	88	ASP	CA-CB-CG	-10.83	101.77	112.60
2	2	219	SER	CA-CB-OG	10.64	132.39	111.10
1	1	282	ARG	CD-NE-CZ	-10.62	109.53	124.40
2	2	97	PHE	CA-CB-CG	-10.60	103.20	113.80
4	4	48	ASP	CA-CB-CG	-10.60	102.00	112.60
1	1	141	ASN	CA-CB-CG	-10.45	102.15	112.60
3	3	57	ASN	N-CA-CB	-10.40	92.92	110.49
3	3	72	ASN	CA-CB-CG	-10.16	102.44	112.60
4	4	48	ASP	O-C-N	10.14	128.33	121.23
1	1	246	ARG	NE-CZ-NH1	10.01	131.51	121.50
1	1	63	SER	CB-CA-C	-10.00	94.20	110.79
1	1	54	ARG	CD-NE-CZ	-9.96	110.45	124.40
4	4	44	SER	CA-C-N	-9.87	107.96	122.07
4	4	44	SER	C-N-CA	-9.87	107.96	122.07
1	1	91	ASP	CA-CB-CG	-9.79	102.81	112.60
1	1	187	SER	CB-CA-C	9.78	129.24	109.38
1	1	275	THR	CA-C-O	-9.78	109.17	121.88
1	1	285	ASP	N-CA-C	9.75	122.91	110.33
3	3	179	ASP	CA-CB-CG	-9.74	102.86	112.60
1	1	28	THR	CB-CA-C	-9.73	92.89	111.48
1	1	22	SER	CA-C-O	-9.71	109.62	120.69
1	1	208	ASP	CA-CB-CG	-9.69	102.92	112.60
1	1	256	ARG	NE-CZ-NH1	-9.66	111.83	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	33	ARG	CA-C-O	-9.66	110.04	121.05
3	3	137	ARG	NE-CZ-NH1	-9.63	111.87	121.50
1	1	53	THR	CA-CB-OG1	-9.54	95.30	109.60
1	1	246	ARG	CD-NE-CZ	9.44	137.62	124.40
1	1	79	VAL	CA-C-O	-9.42	110.59	120.39
1	1	38	GLU	CA-CB-CG	9.41	132.93	114.10
3	3	86	PHE	CA-CB-CG	9.40	123.20	113.80
3	3	89	ASP	CA-CB-CG	-9.37	103.23	112.60
1	1	157	ALA	O-C-N	9.30	129.67	121.39
1	1	197	TYR	CB-CA-C	9.08	124.52	109.53
3	3	57	ASN	CB-CA-C	-9.07	92.36	110.42
2	2	255	ARG	NE-CZ-NH2	-9.06	111.04	119.20
1	1	95	GLU	CB-CG-CD	-9.03	97.25	112.60
1	1	268	ARG	CD-NE-CZ	-9.03	111.76	124.40
4	4	50	SER	CA-C-O	-9.02	109.90	120.10
3	3	196	ILE	CA-C-O	-8.98	111.20	120.27
2	2	195	ASN	CA-CB-CG	8.94	121.54	112.60
2	2	136	GLU	CB-CG-CD	-8.84	97.57	112.60
2	2	250	GLU	CA-CB-CG	8.81	131.72	114.10
4	4	68	ASN	CA-CB-CG	-8.76	103.84	112.60
1	1	270	ASN	CA-CB-CG	8.67	121.27	112.60
1	1	251	GLU	CA-CB-CG	8.64	131.38	114.10
2	2	139	ASN	CA-CB-CG	-8.48	104.12	112.60
2	2	255	ARG	CA-CB-CG	8.48	131.07	114.10
2	2	73	THR	CA-CB-OG1	-8.47	96.89	109.60
1	1	259	ARG	CA-CB-CG	-8.44	97.22	114.10
2	2	168	ASP	CA-C-O	-8.41	110.61	120.62
1	1	123	ARG	NE-CZ-NH1	8.40	129.90	121.50
1	1	165	ASP	CB-CA-C	-8.40	93.70	110.42
2	2	68	SER	N-CA-C	8.38	122.88	110.48
2	2	169	VAL	CA-C-O	-8.38	112.29	121.17
2	2	169	VAL	CB-CA-C	-8.37	101.25	111.97
4	4	41	ALA	N-CA-C	8.35	122.73	112.54
4	4	36	ALA	CA-C-N	-8.33	108.80	122.54
4	4	36	ALA	C-N-CA	-8.33	108.80	122.54
3	3	74	ASN	CA-C-O	-8.33	109.89	120.55
3	3	5	THR	CA-C-O	-8.29	111.11	120.32
1	1	122	VAL	N-CA-CB	-8.26	97.90	111.45
3	3	172	GLN	CG-CD-NE2	8.25	128.77	116.40
1	1	186	PHE	CA-C-O	-8.24	112.49	121.31
3	3	219	LEU	CA-C-O	-8.22	111.21	120.66
1	1	82	ILE	CA-C-O	-8.20	113.06	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	182	THR	CA-CB-CG2	8.16	124.37	110.50
3	3	57	ASN	OD1-CG-ND2	8.15	130.75	122.60
3	3	16	THR	N-CA-CB	-8.15	98.30	110.61
3	3	21	SER	CB-CA-C	-8.13	95.50	108.91
4	4	57	LYS	CA-C-O	-8.12	112.33	120.70
1	1	29	GLN	N-CA-C	-8.11	102.43	113.30
2	2	49	ASP	CA-CB-CG	8.09	120.69	112.60
3	3	78	GLU	N-CA-C	8.00	120.85	110.53
3	3	233	ALA	CA-C-O	-8.00	112.39	121.19
1	1	164	ASP	CA-C-N	8.00	136.82	121.54
1	1	164	ASP	C-N-CA	8.00	136.82	121.54
3	3	60	THR	CA-CB-OG1	-8.00	97.61	109.60
2	2	187	GLN	CA-CB-CG	7.99	130.09	114.10
1	1	288	SER	CA-C-O	-7.98	113.09	121.55
2	2	248	CYS	CA-C-O	-7.97	112.29	121.54
3	3	27	ASN	O-C-N	7.96	131.95	122.00
1	1	94	ARG	NE-CZ-NH2	-7.95	112.05	119.20
3	3	111	LEU	CA-C-N	-7.94	111.80	123.00
3	3	111	LEU	C-N-CA	-7.94	111.80	123.00
1	1	157	ALA	CA-C-N	7.93	129.75	119.84
1	1	157	ALA	C-N-CA	7.93	129.75	119.84
3	3	231	THR	CA-CB-OG1	-7.91	97.74	109.60
2	2	223	ILE	N-CA-CB	-7.91	101.52	112.27
1	1	176	VAL	CA-C-O	-7.90	111.42	120.67
1	1	37	ASN	CB-CG-ND2	7.87	128.20	116.40
2	2	216	ASN	CA-C-O	-7.85	112.09	120.80
1	1	274	ASN	O-C-N	7.83	133.01	122.59
2	2	95	ASN	CA-CB-CG	-7.83	104.77	112.60
1	1	123	ARG	CD-NE-CZ	7.81	135.33	124.40
3	3	216	ASP	N-CA-CB	-7.79	98.63	110.16
4	4	45	LEU	CA-C-O	7.76	130.54	121.54
1	1	282	ARG	CA-C-N	-7.74	111.50	122.41
1	1	282	ARG	C-N-CA	-7.74	111.50	122.41
2	2	109	HIS	CA-C-O	-7.73	110.83	120.57
4	4	37	SER	CB-CA-C	7.71	122.96	110.09
1	1	176	VAL	CB-CA-C	-7.70	99.14	110.62
3	3	62	ASP	CA-CB-CG	7.68	120.28	112.60
1	1	64	GLU	CB-CG-CD	7.67	125.64	112.60
2	2	190	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	1	17	THR	CA-C-N	-7.65	110.26	122.50
1	1	17	THR	C-N-CA	-7.65	110.26	122.50
2	2	240	ILE	CA-C-O	-7.63	112.37	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	137	ARG	CD-NE-CZ	-7.62	113.74	124.40
1	1	61	ASN	CA-CB-CG	-7.61	104.99	112.60
3	3	59	HIS	CA-C-O	7.60	130.47	121.88
3	3	184	ALA	N-CA-C	7.58	122.72	113.17
3	3	142	ARG	CA-CB-CG	7.58	129.25	114.10
1	1	173	ASN	N-CA-CB	-7.57	97.08	109.94
2	2	87	LYS	CB-CG-CD	7.56	128.70	111.30
1	1	277	PRO	N-CD-CG	-7.54	91.88	103.20
3	3	27	ASN	N-CA-C	7.52	124.01	113.56
3	3	79	GLN	OE1-CD-NE2	-7.50	115.10	122.60
1	1	197	TYR	CA-C-O	-7.44	112.37	120.92
1	1	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	98	PHE	CA-C-O	-7.37	110.97	119.60
2	2	140	VAL	CA-C-O	-7.36	113.36	121.23
4	4	45	LEU	CB-CA-C	7.35	122.53	111.80
2	2	107	THR	CA-C-O	-7.34	112.24	120.32
3	3	129	LEU	CA-C-O	-7.34	112.93	120.71
2	2	39	PRO	CA-C-O	-7.31	113.01	121.34
3	3	27	ASN	CB-CA-C	-7.30	97.26	111.06
3	3	118	THR	CA-CB-OG1	-7.30	98.65	109.60
2	2	187	GLN	CB-CA-C	7.26	125.39	109.94
2	2	77	GLY	CA-C-O	-7.23	114.82	122.05
4	4	30	ASN	OD1-CG-ND2	7.23	129.83	122.60
3	3	46	ILE	CA-C-O	-7.23	112.45	120.25
3	3	61	LYS	CA-C-O	-7.23	112.68	121.06
1	1	187	SER	N-CA-CB	-7.22	98.20	111.13
2	2	169	VAL	N-CA-C	7.22	117.36	110.42
3	3	124	SER	CA-C-O	-7.22	113.53	121.33
1	1	26	LYS	CA-CB-CG	7.21	128.53	114.10
3	3	19	ARG	NE-CZ-NH2	7.21	125.69	119.20
2	2	180	ASN	CA-CB-CG	-7.21	105.39	112.60
2	2	103	ARG	CD-NE-CZ	-7.20	114.31	124.40
1	1	275	THR	CA-CB-OG1	-7.18	98.83	109.60
2	2	68	SER	O-C-N	-7.18	114.84	122.96
2	2	52	LYS	CA-C-O	-7.17	113.30	121.19
2	2	146	PHE	CA-CB-CG	-7.14	106.66	113.80
2	2	168	ASP	N-CA-CB	-7.14	97.90	109.60
1	1	59	HIS	CA-C-O	-7.12	111.98	120.81
1	1	284	GLY	CA-C-N	7.11	133.60	120.95
1	1	284	GLY	C-N-CA	7.11	133.60	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	47	MET	CA-CB-CG	-7.08	99.95	114.10
2	2	134	SER	CA-C-O	-7.06	113.01	121.05
1	1	285	ASP	CB-CA-C	-7.05	93.81	110.02
3	3	94	THR	O-C-N	7.04	131.65	122.42
2	2	259	ILE	CB-CG1-CD1	-7.04	99.03	113.80
3	3	13	PHE	CA-CB-CG	7.03	120.83	113.80
1	1	85	LYS	CA-C-O	-7.00	113.97	121.38
3	3	164	THR	N-CA-CB	-6.98	99.61	110.57
1	1	28	THR	OG1-CB-CG2	6.98	123.25	109.30
3	3	35	HIS	CA-C-O	-6.97	112.90	120.92
1	1	43	MET	CA-C-O	6.94	126.28	119.75
1	1	285	ASP	CB-CG-OD2	-6.93	102.46	118.40
3	3	109	GLY	CA-C-N	-6.93	110.86	122.64
3	3	109	GLY	C-N-CA	-6.93	110.86	122.64
3	3	121	ALA	CA-C-O	-6.93	112.27	120.10
3	3	66	SER	CB-CA-C	6.91	121.63	110.09
3	3	77	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	1	270	ASN	O-C-N	6.90	131.39	122.97
2	2	57	ASP	CB-CA-C	-6.88	108.65	116.63
1	1	138	ASP	CA-CB-CG	6.88	119.48	112.60
2	2	9	TYR	CB-CA-C	6.88	121.41	109.65
1	1	35	THR	CA-CB-OG1	-6.87	99.29	109.60
3	3	231	THR	CA-C-O	-6.85	110.49	119.06
4	4	44	SER	O-C-N	6.85	131.70	122.59
2	2	186	HIS	CA-CB-CG	-6.84	106.96	113.80
3	3	65	ASN	OD1-CG-ND2	6.84	129.44	122.60
2	2	219	SER	CB-CA-C	6.84	121.69	109.38
1	1	183	THR	CA-CB-OG1	-6.82	99.36	109.60
3	3	146	MET	CG-SD-CE	6.82	115.90	100.90
2	2	193	THR	O-C-N	-6.81	115.12	121.79
2	2	14	GLN	CB-CG-CD	-6.81	101.03	112.60
1	1	89	GLY	CA-C-N	-6.81	114.35	122.93
1	1	89	GLY	C-N-CA	-6.81	114.35	122.93
1	1	42	THR	CA-CB-CG2	6.78	122.03	110.50
3	3	202	THR	CA-C-O	6.78	128.49	121.23
1	1	49	ASP	N-CA-C	-6.76	105.32	113.97
3	3	151	VAL	CA-C-O	-6.74	113.57	120.25
3	3	187	LEU	CA-C-O	-6.74	113.10	120.24
1	1	35	THR	N-CA-CB	-6.73	99.11	110.49
3	3	143	ARG	N-CA-C	-6.73	104.02	111.36
2	2	124	VAL	CA-C-O	-6.73	112.78	120.66
1	1	62	GLY	CA-C-N	6.73	129.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	62	GLY	C-N-CA	6.73	129.29	120.28
2	2	170	LEU	CD1-CG-CD2	-6.73	96.00	110.80
3	3	42	ASN	CA-C-O	-6.72	112.93	120.66
4	4	58	ASP	O-C-N	6.72	130.88	123.22
2	2	249	THR	CA-CB-OG1	-6.71	99.53	109.60
1	1	206	HIS	CA-C-O	-6.71	114.10	121.28
2	2	224	PRO	CA-C-O	-6.71	114.05	121.23
1	1	288	SER	CB-CA-C	-6.67	97.68	109.62
2	2	255	ARG	CB-CG-CD	6.66	126.61	111.30
1	1	282	ARG	NE-CZ-NH2	-6.65	113.22	119.20
3	3	227	THR	CA-CB-OG1	-6.65	99.63	109.60
1	1	95	GLU	CA-CB-CG	-6.64	100.82	114.10
1	1	90	ILE	CA-C-N	-6.62	109.74	122.06
1	1	90	ILE	C-N-CA	-6.62	109.74	122.06
1	1	259	ARG	CA-C-O	-6.62	113.20	120.81
2	2	198	THR	CA-C-O	-6.62	112.97	120.32
1	1	60	PHE	CA-C-O	-6.60	113.63	120.89
3	3	187	LEU	N-CA-CB	-6.59	100.42	110.77
1	1	147	VAL	CA-C-O	-6.59	113.48	120.53
3	3	134	PRO	CA-C-N	-6.59	116.32	123.30
3	3	134	PRO	C-N-CA	-6.59	116.32	123.30
1	1	25	PRO	CA-C-N	6.58	133.40	122.73
1	1	25	PRO	C-N-CA	6.58	133.40	122.73
3	3	202	THR	CA-CB-OG1	-6.58	99.73	109.60
2	2	145	THR	CA-CB-OG1	-6.57	99.75	109.60
1	1	118	LEU	CA-C-N	6.56	133.11	122.81
1	1	118	LEU	C-N-CA	6.56	133.11	122.81
2	2	161	GLU	CA-C-N	-6.54	114.52	122.90
2	2	161	GLU	C-N-CA	-6.54	114.52	122.90
2	2	38	TRP	N-CA-CB	-6.53	99.34	110.11
2	2	11	ASP	OD1-CG-OD2	6.52	138.55	122.90
2	2	226	ALA	N-CA-C	-6.52	99.14	109.04
4	4	48	ASP	OD1-CG-OD2	6.52	138.54	122.90
3	3	19	ARG	CA-CB-CG	6.51	127.13	114.10
2	2	18	LEU	CB-CA-C	6.51	119.84	110.79
2	2	12	ARG	N-CA-C	6.51	118.17	111.14
2	2	148	HIS	CA-CB-CG	6.50	120.30	113.80
2	2	163	GLY	O-C-N	6.50	130.17	122.50
1	1	97	LYS	CB-CA-C	-6.50	102.50	111.73
1	1	277	PRO	CB-CA-C	6.48	119.87	111.64
3	3	74	ASN	N-CA-C	6.48	120.51	112.47
1	1	122	VAL	CB-CA-C	6.47	121.90	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	36	ALA	N-CA-C	-6.47	105.25	113.01
3	3	205	VAL	CB-CA-C	6.46	120.20	110.90
1	1	256	ARG	CD-NE-CZ	-6.45	115.37	124.40
4	4	39	SER	O-C-N	6.45	130.80	122.23
2	2	142	VAL	CA-C-O	-6.44	113.12	120.66
3	3	182	THR	CA-CB-OG1	-6.44	99.94	109.60
3	3	65	ASN	N-CA-CB	-6.44	100.94	110.53
3	3	57	ASN	N-CA-C	6.43	124.50	110.80
2	2	247	MET	CB-CA-C	6.43	122.41	109.68
2	2	193	THR	CA-C-O	6.43	126.47	119.40
2	2	194	ASN	N-CA-C	6.43	120.54	110.32
3	3	164	THR	CA-CB-OG1	-6.43	99.96	109.60
2	2	111	GLN	OE1-CD-NE2	-6.42	116.18	122.60
2	2	69	LYS	CA-CB-CG	6.41	126.91	114.10
3	3	216	ASP	CA-C-N	6.40	129.80	120.71
3	3	216	ASP	C-N-CA	6.40	129.80	120.71
1	1	205	SER	O-C-N	6.39	131.22	122.46
3	3	204	GLN	O-C-N	6.39	130.22	123.06
3	3	172	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	1	50	SER	CA-C-O	-6.38	110.45	118.43
2	2	203	TYR	CA-C-O	-6.38	113.18	120.58
3	3	99	GLU	CB-CG-CD	6.38	123.44	112.60
1	1	159	ASN	CA-CB-CG	6.38	118.98	112.60
3	3	226	GLN	CB-CG-CD	-6.38	101.76	112.60
4	4	44	SER	CA-CB-OG	-6.37	98.36	111.10
1	1	239	VAL	CB-CA-C	6.36	120.04	110.63
2	2	223	ILE	CA-C-O	-6.35	116.64	119.94
3	3	41	HIS	CA-C-O	-6.34	112.38	119.67
1	1	144	SER	N-CA-CB	-6.33	100.79	110.42
2	2	235	THR	CB-CA-C	-6.33	99.52	109.52
1	1	250	VAL	N-CA-C	6.33	117.82	109.21
2	2	241	THR	CA-C-O	-6.32	114.01	120.71
3	3	181	TYR	O-C-N	6.32	128.82	122.12
1	1	137	PRO	CA-C-N	-6.31	113.05	122.39
1	1	137	PRO	C-N-CA	-6.31	113.05	122.39
3	3	80	VAL	CA-C-O	-6.31	113.96	120.71
1	1	265	SER	O-C-N	-6.31	115.95	123.27
3	3	202	THR	N-CA-C	6.29	118.42	108.79
2	2	145	THR	CA-C-O	-6.29	113.84	120.63
1	1	288	SER	N-CA-CB	-6.28	100.80	110.04
3	3	216	ASP	CB-CG-OD1	6.28	132.84	118.40
3	3	63	GLU	CB-CG-CD	-6.28	101.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	193	THR	CA-C-O	-6.27	111.54	120.51
3	3	83	THR	CA-CB-OG1	-6.27	100.19	109.60
1	1	117	GLU	CG-CD-OE1	6.26	132.81	118.40
2	2	103	ARG	CA-CB-CG	6.26	126.62	114.10
2	2	143	LYS	O-C-N	6.26	130.51	122.81
1	1	154	PRO	O-C-N	6.23	128.81	121.46
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
4	4	65	PRO	CB-CA-C	-6.23	103.42	111.46
1	1	206	HIS	O-C-N	6.23	129.52	123.29
1	1	282	ARG	NH1-CZ-NH2	6.22	127.38	119.30
1	1	198	ASN	CA-CB-CG	6.21	118.81	112.60
3	3	161	ILE	CA-C-O	-6.20	113.88	120.39
1	1	31	VAL	N-CA-CB	-6.20	102.53	111.21
3	3	196	ILE	N-CA-CB	-6.19	103.41	111.82
1	1	274	ASN	N-CA-CB	6.17	120.92	110.49
1	1	48	SER	CA-C-O	-6.17	108.19	119.36
2	2	28	ALA	CA-C-O	-6.17	114.85	121.94
3	3	27	ASN	N-CA-CB	-6.17	103.09	113.15
3	3	6	THR	CB-CA-C	6.17	120.05	109.51
3	3	132	THR	CA-C-O	-6.16	113.92	119.59
1	1	260	ALA	CA-C-O	-6.16	111.51	120.13
2	2	11	ASP	O-C-N	6.16	130.39	122.39
2	2	194	ASN	OD1-CG-ND2	6.15	128.75	122.60
2	2	111	GLN	CB-CG-CD	6.13	123.01	112.60
2	2	238	LEU	N-CA-CB	-6.13	98.78	110.42
1	1	236	LYS	CA-C-O	-6.12	114.25	121.16
2	2	179	GLY	CA-C-O	-6.12	114.21	120.45
3	3	163	MET	CA-CB-CG	-6.11	101.87	114.10
1	1	202	ASP	CB-CA-C	6.11	121.11	112.07
1	1	52	GLU	CA-C-O	-6.10	113.60	120.43
3	3	137	ARG	NE-CZ-NH2	6.09	124.68	119.20
3	3	170	GLY	CA-C-N	6.09	128.66	120.50
3	3	170	GLY	C-N-CA	6.09	128.66	120.50
1	1	252	ALA	CA-C-O	-6.08	113.67	120.66
3	3	193	THR	CA-CB-OG1	-6.08	100.48	109.60
2	2	12	ARG	CD-NE-CZ	-6.08	115.89	124.40
1	1	141	ASN	O-C-N	6.07	129.74	122.27
4	4	43	GLN	OE1-CD-NE2	-6.07	116.53	122.60
2	2	241	THR	CA-CB-OG1	-6.05	100.53	109.60
3	3	8	PRO	CA-C-O	-6.04	114.53	121.36
1	1	68	GLU	CG-CD-OE1	6.04	132.29	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	195	ASN	OD1-CG-ND2	-6.03	116.57	122.60
3	3	36	ILE	CA-C-O	-6.02	111.88	119.95
1	1	77	VAL	CA-C-O	-6.01	113.25	118.96
1	1	133	THR	CA-CB-OG1	-6.00	100.59	109.60
1	1	136	GLN	CG-CD-NE2	-6.00	107.39	116.40
2	2	86	LEU	CA-C-N	6.00	130.30	120.63
2	2	86	LEU	C-N-CA	6.00	130.30	120.63
3	3	47	ILE	CB-CG1-CD1	-6.00	101.19	113.80
1	1	41	ALA	CA-C-O	-6.00	114.64	121.72
2	2	169	VAL	N-CA-CB	5.99	117.56	110.55
3	3	121	ALA	CB-CA-C	-5.99	99.55	110.63
3	3	41	HIS	N-CA-CB	5.98	119.08	110.40
2	2	14	GLN	CA-CB-CG	-5.98	102.15	114.10
3	3	137	ARG	CA-C-O	-5.97	115.07	121.94
3	3	194	SER	N-CA-CB	-5.97	100.40	110.49
3	3	158	GLN	CA-C-O	5.95	127.70	120.62
2	2	105	GLY	N-CA-C	-5.94	102.31	112.64
2	2	136	GLU	CG-CD-OE2	-5.94	104.75	118.40
1	1	173	ASN	OD1-CG-ND2	-5.93	116.67	122.60
3	3	77	ASN	O-C-N	-5.93	114.71	122.59
3	3	207	LEU	CA-C-O	-5.91	114.23	120.80
3	3	160	THR	CA-CB-OG1	-5.91	100.74	109.60
1	1	22	SER	N-CA-CB	-5.90	100.80	109.95
1	1	265	SER	N-CA-CB	-5.90	100.55	111.53
1	1	55	THR	CA-CB-OG1	-5.90	100.75	109.60
2	2	161	GLU	CA-CB-CG	5.90	125.90	114.10
3	3	1	GLY	O-C-N	-5.90	113.57	123.00
3	3	57	ASN	O-C-N	-5.89	114.75	122.59
1	1	259	ARG	CB-CA-C	-5.89	100.47	109.89
2	2	41	TYR	N-CA-CB	5.89	118.45	110.38
1	1	185	ARG	NH1-CZ-NH2	-5.88	111.66	119.30
3	3	55	MET	CA-CB-CG	-5.86	102.39	114.10
2	2	226	ALA	O-C-N	5.85	127.86	121.36
3	3	92	PHE	CA-CB-CG	-5.85	107.95	113.80
1	1	270	ASN	CB-CA-C	-5.84	100.29	109.70
1	1	280	LYS	CB-CA-C	-5.84	101.75	110.16
3	3	131	TYR	CA-C-O	-5.84	114.06	120.43
2	2	88	ASP	CA-C-O	-5.83	112.60	119.48
1	1	242	ARG	CD-NE-CZ	-5.82	116.25	124.40
1	1	267	GLY	CA-C-N	-5.82	113.04	122.81
1	1	267	GLY	C-N-CA	-5.82	113.04	122.81
2	2	198	THR	O-C-N	5.82	130.11	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	197	LEU	CB-CA-C	5.81	117.23	108.86
2	2	105	GLY	CA-C-O	-5.80	112.99	122.56
3	3	33	ARG	CB-CG-CD	-5.80	97.96	111.30
3	3	93	LYS	N-CA-C	5.80	118.38	111.71
2	2	54	SER	CA-C-N	-5.80	115.03	122.98
2	2	54	SER	C-N-CA	-5.80	115.03	122.98
3	3	59	HIS	CA-CB-CG	-5.80	108.00	113.80
2	2	255	ARG	NE-CZ-NH1	5.79	127.29	121.50
4	4	65	PRO	CA-C-O	-5.79	114.74	121.34
1	1	145	ASN	CB-CG-ND2	-5.78	107.73	116.40
1	1	175	SER	CA-CB-OG	5.77	122.63	111.10
2	2	235	THR	OG1-CB-CG2	5.76	120.83	109.30
1	1	68	GLU	CG-CD-OE2	-5.74	105.20	118.40
2	2	189	ILE	CA-C-O	-5.73	113.24	120.69
2	2	210	ASP	N-CA-CB	-5.73	100.56	110.87
1	1	182	ASP	CA-C-N	5.72	131.55	122.62
1	1	182	ASP	C-N-CA	5.72	131.55	122.62
1	1	94	ARG	CG-CD-NE	-5.71	99.43	112.00
2	2	86	LEU	CA-C-O	-5.71	112.88	119.56
1	1	149	GLN	CB-CA-C	-5.70	102.01	110.62
3	3	38	GLY	N-CA-C	5.69	123.74	115.32
3	3	66	SER	N-CA-C	-5.69	106.00	113.17
1	1	83	GLN	CB-CG-CD	-5.68	102.94	112.60
3	3	45	GLU	CG-CD-OE1	5.68	131.47	118.40
3	3	137	ARG	O-C-N	5.68	129.64	122.65
1	1	129	THR	CA-C-O	-5.68	114.57	120.70
3	3	112	ARG	CA-CB-CG	5.68	125.45	114.10
1	1	139	SER	CA-CB-OG	-5.67	99.77	111.10
2	2	190	ASN	CB-CA-C	5.66	120.01	110.79
3	3	161	ILE	CA-CB-CG1	-5.66	100.79	110.40
2	2	199	ILE	CA-C-O	-5.65	114.37	120.36
1	1	28	THR	N-CA-C	5.64	118.08	109.95
1	1	232	HIS	CA-CB-CG	-5.64	108.16	113.80
1	1	94	ARG	NH1-CZ-NH2	5.63	126.62	119.30
3	3	235	THR	CA-CB-OG1	-5.61	101.18	109.60
1	1	208	ASP	CA-C-O	-5.61	114.66	121.28
3	3	42	ASN	CB-CG-ND2	5.60	124.80	116.40
2	2	99	HIS	CA-CB-CG	-5.58	108.22	113.80
1	1	241	ILE	N-CA-CB	-5.58	104.29	110.99
1	1	27	HIS	CA-CB-CG	5.58	119.38	113.80
2	2	217	ASN	CB-CA-C	5.58	118.92	109.55
2	2	251	PHE	CA-C-O	-5.58	114.81	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	58	ASP	CA-C-N	5.57	129.02	121.05
4	4	58	ASP	C-N-CA	5.57	129.02	121.05
2	2	262	GLN	OE1-CD-NE2	-5.57	117.03	122.60
2	2	106	TYR	CA-C-O	-5.56	115.33	121.33
2	2	215	HIS	CA-C-O	-5.55	112.50	120.11
1	1	273	LYS	CG-CD-CE	-5.55	98.54	111.30
3	3	166	PRO	CB-CA-C	5.55	118.62	111.46
2	2	9	TYR	CA-CB-CG	-5.54	103.93	113.90
3	3	190	TRP	CA-C-O	-5.54	115.14	121.40
2	2	94	GLN	CG-CD-NE2	-5.54	108.10	116.40
2	2	68	SER	N-CA-CB	-5.53	101.88	110.29
2	2	168	ASP	CA-C-N	5.53	127.52	120.56
2	2	168	ASP	C-N-CA	5.53	127.52	120.56
3	3	107	TRP	CA-C-O	-5.53	115.16	121.40
1	1	198	ASN	CA-C-O	-5.52	114.09	120.49
2	2	99	HIS	CA-C-N	5.51	128.22	120.28
2	2	99	HIS	C-N-CA	5.51	128.22	120.28
2	2	188	PHE	CA-C-O	-5.51	114.93	121.66
1	1	64	GLU	CA-CB-CG	5.51	125.12	114.10
3	3	175	TYR	CB-CA-C	-5.51	99.32	109.46
1	1	235	HIS	CA-CB-CG	-5.51	108.29	113.80
3	3	57	ASN	CA-C-N	5.51	132.08	121.18
3	3	57	ASN	C-N-CA	5.51	132.08	121.18
3	3	76	GLN	CA-C-O	-5.50	115.18	121.68
2	2	192	ARG	CA-C-O	-5.49	111.92	119.05
3	3	140	GLN	CA-CB-CG	-5.49	103.12	114.10
1	1	186	PHE	O-C-N	5.48	128.86	122.99
1	1	63	SER	O-C-N	5.48	127.92	122.12
3	3	63	GLU	CG-CD-OE2	-5.47	105.83	118.40
2	2	123	LEU	CA-C-O	-5.46	114.47	120.43
2	2	43	PRO	N-CD-CG	-5.46	95.01	103.20
2	2	167	LYS	CA-C-O	5.46	126.11	119.78
1	1	144	SER	CA-C-N	-5.45	115.37	123.11
1	1	144	SER	C-N-CA	-5.45	115.37	123.11
2	2	26	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	2	92	PHE	N-CA-C	-5.45	105.03	110.97
2	2	258	SER	O-C-N	5.45	129.51	122.81
2	2	38	TRP	CB-CA-C	5.45	116.25	108.68
3	3	164	THR	CB-CA-C	5.45	119.14	109.72
2	2	187	GLN	CA-C-O	-5.44	114.89	120.99
3	3	34	ILE	CA-C-O	-5.44	113.97	120.78
3	3	168	THR	CA-CB-OG1	-5.44	101.43	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	21	ILE	CA-CB-CG1	-5.44	101.15	110.40
3	3	84	ASN	OD1-CG-ND2	5.44	128.04	122.60
2	2	53	THR	CA-C-O	-5.43	115.54	121.89
1	1	50	SER	CB-CA-C	5.42	117.48	109.29
4	4	50	SER	CA-CB-OG	-5.42	100.26	111.10
2	2	13	VAL	CA-C-O	-5.42	114.56	120.84
2	2	232	THR	CA-CB-OG1	-5.42	101.48	109.60
2	2	63	PHE	CA-CB-CG	5.41	119.21	113.80
3	3	78	GLU	CA-CB-CG	5.40	124.91	114.10
1	1	166	TYR	N-CA-C	-5.40	105.55	111.82
2	2	219	SER	N-CA-C	-5.40	100.89	109.59
3	3	90	GLY	CA-C-O	-5.40	114.87	121.68
2	2	129	GLU	CB-CA-C	-5.40	104.22	111.89
2	2	221	MET	CA-C-O	-5.38	114.34	120.32
2	2	81	LYS	CB-CG-CD	5.37	123.66	111.30
3	3	112	ARG	CB-CA-C	5.37	119.08	110.16
1	1	231	GLU	N-CA-C	-5.37	102.94	110.35
3	3	38	GLY	O-C-N	-5.36	116.00	122.38
3	3	116	MET	CB-CG-SD	-5.36	96.63	112.70
1	1	92	ASN	O-C-N	5.36	129.49	123.28
1	1	117	GLU	CG-CD-OE2	-5.35	106.09	118.40
1	1	288	SER	CA-CB-OG	-5.35	100.41	111.10
2	2	120	GLY	CA-C-O	-5.35	114.41	122.54
3	3	195	LEU	CA-C-O	-5.34	114.97	121.05
2	2	210	ASP	CA-CB-CG	-5.33	107.27	112.60
1	1	286	ILE	O-C-N	5.33	127.82	121.80
2	2	177	LEU	N-CA-CB	-5.33	101.60	110.23
1	1	174	PRO	CA-C-O	-5.33	115.53	121.23
1	1	282	ARG	O-C-N	5.32	129.35	122.81
3	3	226	GLN	N-CA-C	-5.32	106.74	113.18
2	2	102	GLY	CA-C-O	-5.31	115.46	121.68
3	3	221	LEU	O-C-N	5.31	129.66	122.59
4	4	58	ASP	N-CA-CB	5.31	119.08	110.42
1	1	26	LYS	CG-CD-CE	-5.30	99.10	111.30
2	2	12	ARG	CB-CG-CD	-5.30	99.11	111.30
3	3	161	ILE	N-CA-CB	5.30	118.72	111.41
3	3	222	MET	CB-CG-SD	-5.30	96.80	112.70
2	2	72	THR	CA-CB-OG1	-5.28	101.68	109.60
3	3	143	ARG	O-C-N	5.28	128.17	122.15
2	2	262	GLN	CG-CD-NE2	5.28	124.32	116.40
3	3	16	THR	OG1-CB-CG2	5.28	119.85	109.30
3	3	86	PHE	CB-CA-C	5.28	120.49	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	204	GLN	CA-C-O	-5.28	115.03	121.36
3	3	192	GLN	N-CA-C	-5.27	105.13	112.45
1	1	60	PHE	N-CA-CB	-5.27	102.17	111.39
3	3	56	ASN	CA-C-N	5.27	131.60	121.54
3	3	56	ASN	C-N-CA	5.27	131.60	121.54
2	2	76	LYS	CA-C-O	-5.27	113.46	119.41
2	2	195	ASN	N-CA-C	-5.26	106.64	114.64
1	1	229	VAL	N-CA-C	-5.26	104.94	112.35
2	2	122	LEU	CA-C-O	-5.26	115.08	121.28
2	2	257	LYS	N-CA-CB	5.25	119.36	110.49
4	4	53	THR	CA-CB-OG1	-5.25	101.73	109.60
3	3	77	ASN	CA-CB-CG	-5.25	107.35	112.60
2	2	168	ASP	OD1-CG-OD2	5.24	135.49	122.90
3	3	94	THR	CA-C-O	-5.24	113.18	119.15
1	1	201	TYR	CA-C-N	-5.23	114.79	122.06
1	1	201	TYR	C-N-CA	-5.23	114.79	122.06
3	3	208	LEU	CA-C-O	-5.23	114.99	120.80
1	1	279	ILE	CA-C-N	5.23	128.76	121.02
1	1	279	ILE	C-N-CA	5.23	128.76	121.02
2	2	20	ASN	CA-CB-CG	5.23	117.83	112.60
3	3	28	TYR	N-CA-CB	-5.23	102.29	109.97
1	1	127	GLU	CA-C-O	-5.22	114.58	120.32
3	3	144	GLU	CA-CB-CG	5.22	124.54	114.10
1	1	136	GLN	OE1-CD-NE2	5.22	127.82	122.60
2	2	75	SER	N-CA-CB	-5.22	101.95	109.83
1	1	63	SER	N-CA-C	5.21	116.96	111.28
3	3	158	GLN	CG-CD-OE1	5.21	131.22	120.80
2	2	243	THR	CA-C-O	-5.21	114.70	120.38
2	2	127	ILE	CA-C-O	-5.21	114.21	119.89
1	1	187	SER	O-C-N	-5.20	117.03	123.33
2	2	214	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	1	282	ARG	CB-CA-C	-5.20	100.31	109.62
3	3	67	TYR	N-CA-C	-5.20	106.78	113.23
1	1	259	ARG	N-CA-CB	5.20	117.59	109.85
1	1	268	ARG	CB-CA-C	5.20	119.74	109.66
2	2	8	GLY	CA-C-N	-5.19	113.50	120.87
2	2	8	GLY	C-N-CA	-5.19	113.50	120.87
3	3	138	GLY	N-CA-C	-5.19	101.75	112.34
2	2	18	LEU	N-CA-CB	-5.18	102.78	110.71
2	2	38	TRP	CA-CB-CG	-5.18	103.77	113.60
2	2	213	THR	CA-CB-OG1	-5.17	101.84	109.60
1	1	257	ALA	N-CA-CB	-5.17	101.86	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	259	ILE	CA-C-O	-5.17	115.01	120.39
3	3	233	ALA	O-C-N	5.17	129.23	122.87
3	3	215	PRO	CB-CA-C	5.17	119.24	111.44
2	2	127	ILE	O-C-N	5.16	125.67	120.92
3	3	186	PHE	O-C-N	5.16	129.85	123.15
3	3	45	GLU	CG-CD-OE2	-5.15	106.55	118.40
1	1	23	SER	CA-C-O	-5.15	115.09	121.06
1	1	145	ASN	O-C-N	5.14	129.61	123.13
2	2	181	LEU	N-CA-C	-5.14	106.27	112.54
2	2	165	PRO	CA-C-O	-5.14	115.37	122.15
3	3	186	PHE	CA-CB-CG	-5.14	108.66	113.80
3	3	231	THR	CA-C-N	-5.14	115.39	122.69
3	3	231	THR	C-N-CA	-5.14	115.39	122.69
2	2	152	ARG	CD-NE-CZ	-5.13	117.22	124.40
2	2	143	LYS	CA-C-N	5.12	131.32	121.54
2	2	143	LYS	C-N-CA	5.12	131.32	121.54
1	1	204	TYR	CA-C-O	-5.12	115.64	121.58
3	3	125	ALA	CA-C-O	-5.11	115.48	121.10
1	1	170	SER	CA-C-O	-5.11	115.80	122.14
2	2	259	ILE	CA-C-N	-5.11	112.68	122.13
2	2	259	ILE	C-N-CA	-5.11	112.68	122.13
3	3	109	GLY	N-CA-C	5.11	117.50	111.63
2	2	119	SER	O-C-N	5.10	129.34	123.17
1	1	110	VAL	O-C-N	-5.10	117.23	122.23
1	1	27	HIS	CA-C-O	-5.10	113.09	122.62
1	1	285	ASP	CA-C-N	-5.09	111.95	120.30
1	1	285	ASP	C-N-CA	-5.09	111.95	120.30
2	2	32	VAL	O-C-N	5.09	128.33	123.14
3	3	82	GLY	N-CA-C	-5.09	103.03	110.87
3	3	32	PRO	CA-C-O	-5.08	115.67	121.56
2	2	126	VAL	CA-C-O	-5.08	115.09	120.53
2	2	65	THR	CA-CB-OG1	-5.08	101.98	109.60
3	3	1	GLY	N-CA-C	5.07	128.01	113.30
1	1	40	GLY	N-CA-C	-5.07	108.12	115.27
2	2	119	SER	CA-C-O	-5.07	115.67	121.40
2	2	215	HIS	CA-CB-CG	5.07	118.87	113.80
2	2	235	THR	CA-C-O	5.07	125.44	120.17
2	2	25	THR	CA-C-O	5.07	126.49	120.66
3	3	75	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	1	165	ASP	CB-CG-OD1	5.06	130.04	118.40
3	3	217	PHE	N-CA-C	5.06	117.57	110.23
2	2	168	ASP	CB-CG-OD2	-5.06	106.76	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	133	THR	CA-C-O	-5.06	115.39	121.11
1	1	83	GLN	OE1-CD-NE2	5.06	127.66	122.60
3	3	95	THR	CA-CB-OG1	-5.05	102.02	109.60
2	2	170	LEU	N-CA-C	-5.05	106.81	112.87
3	3	158	GLN	CB-CA-C	5.05	118.34	110.67
1	1	270	ASN	N-CA-CB	5.04	117.71	109.69
1	1	66	ASP	CA-C-O	-5.04	115.64	121.19
3	3	146	MET	CB-CA-C	5.03	120.43	110.17
2	2	261	PRO	CA-C-N	5.03	130.75	121.70
2	2	261	PRO	C-N-CA	5.03	130.75	121.70
1	1	65	THR	N-CA-C	-5.03	106.07	113.61
1	1	76	CYS	CA-C-O	-5.03	115.03	120.81
1	1	282	ARG	CG-CD-NE	-5.02	100.95	112.00
2	2	121	CYS	N-CA-CB	-5.02	102.31	110.59
3	3	217	PHE	CA-C-O	-5.02	115.67	121.19
1	1	189	PRO	CB-CA-C	-5.01	103.68	111.40
1	1	68	GLU	N-CA-C	-5.01	106.01	111.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	259	ARG	Sidechain
1	1	268	ARG	Sidechain
2	2	12	ARG	Sidechain
2	2	255	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2170	0	2107	163	0
2	2	1952	0	1926	132	0
3	3	1849	0	1832	154	0
4	4	297	0	294	36	0
5	1	26	0	27	8	0
6	1	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	2	1	0	0	0	0
All	All	6302	0	6186	410	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (410) 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
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.14
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.07
1:1:285:ASP:CA	1:1:285:ASP:OD2	2.00	1.07
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.36	1.06
1:1:47:PRO:HA	3:3:164:THR:HG21	1.34	1.05
2:2:12:ARG:NH1	2:2:12:ARG:HG3	1.69	1.05
2:2:255:ARG:HG2	2:2:256:SER:H	1.24	1.03
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.41	1.02
1:1:99:PHE:O	1:1:99:PHE:CD2	2.15	1.00
3:3:179:ASP:HB3	3:3:182:THR:HG22	1.44	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	0.96
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	1.27	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.90
1:1:77:VAL:C	1:1:109:LEU:HD12	1.95	0.90
1:1:58:MET:HE1	3:3:216:ASP:O	1.71	0.90
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
3:3:57:ASN:CA	3:3:57:ASN:CG	2.45	0.89
1:1:285:ASP:OD2	1:1:285:ASP:HA	1.73	0.88
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:20:ASN:ND2	2:2:62:ARG:HE	1.72	0.87
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	0.87
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.91	0.86
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.85
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.57	0.85
1:1:90:ILE:HD13	1:1:90:ILE:N	1.92	0.84
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.84
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.82
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.82
2:2:30:ASN:HD22	2:2:31:ALA:H	1.27	0.82
2:2:52:LYS:NZ	2:2:52:LYS:CD	2.43	0.82
1:1:248:LYS:HE3	4:4:38:THR:O	1.80	0.82
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.82
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.61	0.81
1:1:38:GLU:CD	3:3:116:MET:HE2	2.05	0.81
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.80
2:2:9:TYR:HD1	2:2:9:TYR:N	1.77	0.80
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.79
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.48	0.79
2:2:9:TYR:N	2:2:9:TYR:CD1	2.43	0.79
1:1:58:MET:HE1	3:3:216:ASP:C	2.08	0.78
2:2:262:GLN:HE21	2:2:262:GLN:C	1.91	0.78
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.13	0.77
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
1:1:188:VAL:HG21	5:1:900:W84:H2C2	1.66	0.77
1:1:94:ARG:CZ	1:1:101:ASP:OD2	2.33	0.77
2:2:255:ARG:HG2	2:2:256:SER:N	2.00	0.77
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.19	0.76
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.75
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.68	0.74
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	0.74
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.74
4:4:43:GLN:HG2	4:4:45:LEU:HB2	1.70	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.73
1:1:92:ASN:OD1	1:1:95:GLU:HB2	1.87	0.73
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.72
1:1:58:MET:HE1	3:3:216:ASP:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.71
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.71
1:1:99:PHE:CD2	1:1:99:PHE:C	2.68	0.71
1:1:201:TYR:HD2	1:1:214:GLY:O	1.73	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
1:1:94:ARG:NH2	1:1:101:ASP:OD2	2.23	0.71
2:2:195:ASN:HD22	2:2:195:ASN:C	1.99	0.71
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.71
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.71
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	0.70
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.69
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.69
1:1:82:ILE:HG22	1:1:100:ASN:H	1.57	0.69
4:4:29:ILE:HG22	4:4:29:ILE:O	1.94	0.68
3:3:20:GLN:HE22	4:4:31:TYR:H	1.42	0.68
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.67
1:1:278:VAL:HG12	3:3:62:ASP:OD1	1.95	0.67
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.67
3:3:61:LYS:HD3	3:3:63:GLU:OE1	1.95	0.67
1:1:152:TYR:O	1:1:154:PRO:HD3	1.94	0.67
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.77	0.66
2:2:155:ASP:OD2	2:2:155:ASP:C	2.37	0.66
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.66
1:1:107: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	2.09	0.65
2:2:190:ASN:HD21	3:3:118:THR:HA	1.62	0.65
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.64
1:1:58:MET:HE1	3:3:216:ASP:CA	2.27	0.64
1:1:77:VAL:C	1:1:109:LEU:CD1	2.69	0.64
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64
2:2:30:ASN:HD22	2:2:31:ALA:N	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.64
2:2:12:ARG:NH1	4:4:68:ASN:O	2.31	0.64
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.33	0.64
3:3:179:ASP:OD2	3:3:180:THR:N	2.32	0.63
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.63
2:2:39:PRO:CG	2:2:247:MET:HE2	2.29	0.63
2:2:205:ASN:ND2	2:2:206:SER:H	1.96	0.63
2:2:187:GLN:HE21	2:2:197:ALA:HA	1.63	0.63
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.80	0.63
3:3:75:ARG:O	3:3:194:SER:HB2	1.99	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62
3:3:84:ASN:ND2	3:3:86:PHE:H	1.98	0.62
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.61
1:1:188:VAL:HG11	5:1:900: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
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
3:3:55:MET:HG3	3:3:55:MET:O	1.99	0.61
1:1:90:ILE:N	1:1:90:ILE:CD1	2.62	0.61
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
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
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.59
1:1:94:ARG:NH1	1:1:94:ARG:CG	2.60	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE2	2.38	0.59
3:3:84:ASN:HD22	3:3:86:PHE:H	1.49	0.59
1:1:188:VAL:HG21	5:1:900:W84:C2C	2.33	0.59
2:2:30:ASN:HD21	4:4:58:ASP:H	1.51	0.59
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
3:3:179:ASP:HB3	3:3:182:THR:HB	1.85	0.58
1:1:151:MET:SD	1:1:170:SER:HB2	2.43	0.58
1:1:43:MET:HE3	1:1:43:MET:HA	1.85	0.57
3:3:175:TYR:HD1	3:3:182:THR:HG21	1.68	0.57
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.57
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	0.57
2:2:64:TYR:CD2	2:2:89:MET:HB3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.57
2:2:221:MET:HE2	2:2:223:ILE:HD11	1.87	0.57
2:2:52:LYS:NZ	2:2:52:LYS:HD3	2.20	0.57
3:3:57:ASN:HB3	3:3:57:ASN:C	2.28	0.57
1:1:188:VAL:HG21	5:1:900:W84:H3C1	1.86	0.57
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.56
1:1:58:MET:HE3	3:3:216:ASP:HA	1.85	0.56
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
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
3:3:31:THR:CG2	3:3:32:PRO:HD2	2.34	0.56
1:1:102:TRP:O	1:1:223:SER:HB2	2.05	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.56
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.56
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.56
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
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.55
1:1:215:ILE:O	1:1:218:LEU:N	2.35	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
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.55
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
1:1:266:ILE:HD12	3:3:235:THR:HA	1.88	0.54
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.54
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.87	0.54
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.54
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.54
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.54
3:3:20:GLN:HE22	4:4:31:TYR:N	2.04	0.54
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.54
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.54
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.54
2:2:170:LEU:CD2	3:3:64:VAL:HA	2.38	0.54
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.54
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.54
3:3:117:TYR:CD2	3:3:155:ILE:HD13	2.44	0.53
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:195:ASN:ND2	2:2:195:ASN:C	2.66	0.53
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.53
3:3:175:TYR:CD1	3:3:182:THR:HG21	2.43	0.53
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
3:3:18:ASP:OD1	4:4:40:SER:HB2	2.09	0.53
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.52
1:1:88:THR:O	1:1:90:ILE:HD13	2.10	0.52
1:1:188:VAL:HG21	5:1:900:W84:C3C	2.39	0.52
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.52
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
1:1:77: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
1:1:92:ASN:C	1:1:92:ASN:ND2	2.67	0.52
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.52
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.52
2:2:66:LEU:HD12	2:2:89:MET:HE3	1.91	0.52
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.45	0.51
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.51
4:4:44:SER:C	4:4:46:SER:N	2.68	0.51
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.51
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.51
3:3:75:ARG:NH1	3:3:78:GLU:OE1	2.41	0.51
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.51
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
3:3:84:ASN:ND2	3:3:84:ASN:C	2.69	0.51
1:1:38:GLU:OE1	3:3:116:MET:HE2	2.10	0.51
3:3:101:VAL:HG13	3:3:176:THR:CG2	2.41	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.51
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.51
1:1:105:ASN:HD21	1:1:108:SER:HB2	1.74	0.51
3:3:84:ASN:HD22	3:3:86:PHE:N	2.08	0.51
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE1	2.44	0.50
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.50
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
2:2:255:ARG:CG	2:2:256:SER:H	2.00	0.50

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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
2:2:158:SER:HG	2:2:167:LYS:HE2	1.71	0.50
3:3:84:ASN:HD22	3:3:84:ASN:C	2.20	0.49
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.49
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.49
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	0.49
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.49
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.94	0.49
3:3:20:GLN:NE2	4:4:31:TYR:H	2.11	0.49
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.49
2:2:30:ASN:ND2	2:2:31:ALA:H	2.05	0.48
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.48
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
1:1:82:ILE:CG2	1:1:100:ASN:H	2.23	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.48
1:1:280:LYS:HE3	3:3:89:ASP:OD2	2.13	0.48
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.48
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.96	0.48
1:1:122:VAL:O	1:1:197:TYR:HB2	2.13	0.48
3:3:61:LYS:O	3:3:61:LYS:HG2	2.07	0.48
3:3:175:TYR:H	3:3:182:THR:HG21	1.78	0.48
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.48
1:1:158:PRO:HB2	1:1:167:THR:HG22	1.96	0.48
3:3:112:ARG:NH1	3:3:112:ARG:HG2	2.28	0.48
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.96	0.48
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.79	0.48
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.47
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.43	0.47
1:1:215:ILE:O	1:1:216:THR:C	2.57	0.47
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.47
1:1:165:ASP:HB3	1:1:167:THR:H	1.79	0.47
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:268:ARG:CZ	2:2:139:ASN:HB2	2.44	0.47
2:2:13:VAL:HA	2:2:25:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
1:1:206:HIS:ND1	1:1:206:HIS:N	2.62	0.47
2:2:63:PHE:CD2	2:2:245:ALA:HB2	2.50	0.47
1:1:188:VAL:CG2	5:1:900:W84:H2C2	2.40	0.47
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.47
1:1:102:TRP:CZ3	1:1:224:MET:HE2	2.51	0.47
1:1:268:ARG:HH11	1:1:268:ARG:HD3	1.50	0.47
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.43	0.46
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.46
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.46
1:1:110:VAL:O	1:1:111:GLN:C	2.53	0.46
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.46
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.62	0.46
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.46
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.46
1:1:104:ILE:HG13	1:1:223:SER:HA	1.98	0.46
1:1:236:LYS:HE2	1:1:236:LYS:HB3	1.83	0.46
2:2:158:SER:HG	2:2:167:LYS:CE	2.26	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
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
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.45
3:3:57:ASN:CB	3:3:57:ASN:H	2.26	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.45
4:4:30:ASN:HA	4:4:30:ASN:HD22	1.40	0.45
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.45
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.97	0.45
1:1:77:VAL:CA	1:1:109:LEU:HD12	2.46	0.45
2:2:170:LEU:HD23	3:3:64:VAL:HG22	1.99	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.98	0.45
1:1:152:TYR:O	1:1:173:ASN:ND2	2.50	0.45
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
1:1:215:ILE:C	1:1:217:VAL:N	2.73	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
3:3:179:ASP:HB3	3:3:182:THR:CB	2.45	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.81	0.45
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.45
3:3:192:GLN:HE21	3:3:192:GLN:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.44
1:1:43:MET:HA	1:1:43:MET:CE	2.46	0.44
1:1:92:ASN:C	1:1:92:ASN:HD22	2.26	0.44
1:1:198:ASN:HB3	1:1:200:PHE:O	2.17	0.44
1:1:207:ASP:HA	2:2:144:TYR:CE1	2.52	0.44
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.44
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.17	0.44
1:1:289:TYR:CE1	3:3:138:GLY:HA3	2.53	0.44
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.44
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.44
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
3:3:221:LEU:C	3:3:221:LEU:HD23	2.43	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.44
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.44
3:3:101:VAL:HG13	3:3:176:THR:HG22	1.99	0.44
1:1:289:TYR:CD1	3:3:138:GLY:HA3	2.53	0.44
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.43
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.43
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.43
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.48	0.43
1:1:159:ASN:HA	1:1:160:PRO:HD3	1.65	0.43
2:2:190:ASN:O	2:2:191:LEU:C	2.61	0.43
1:1:38:GLU:N	3:3:116:MET:HE1	2.34	0.43
1:1:132:ALA:O	1:1:181:GLY:N	2.41	0.43
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	0.43
1:1:82:ILE:HG22	1:1:100:ASN:HB2	2.00	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
2:2:10:SER:CB	2:2:12:ARG:HB2	2.48	0.43
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.43
1:1:285:ASP:C	1:1:285:ASP:HB3	2.38	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:43:GLN:C	4:4:45:LEU:N	2.74	0.42
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.42
1:1:89:GLY:C	1:1:90:ILE:CD1	2.89	0.42
1:1:187:SER:HB3	3:3:21:SER:HB3	2.01	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	0.42
3:3:153:TRP:CD1	3:3:153:TRP:C	2.97	0.42
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.19	0.42
3:3:226:GLN:HE21	3:3:226:GLN:HB2	1.21	0.42
2:2:40:GLU:O	2:2:40:GLU:CG	2.61	0.42
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.42
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.38	0.42
1:1:201:TYR:H	2:2:131:GLN:HE21	1.68	0.42
1:1:215:ILE:O	1:1:217:VAL:N	2.53	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42
3:3:44:LEU:HA	3:3:44:LEU:HD23	1.79	0.42
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.42
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.42
1:1:97:LYS:C	1:1:99:PHE:H	2.27	0.41
1:1:261:LEU:HD11	2:2:171:TYR:CD1	2.55	0.41
1:1:286:ILE:HD13	1:1:286:ILE:HG21	1.77	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.41
3:3:113:PHE:CE1	3:3:115:LEU:HD13	2.55	0.41
1:1:86:ASP:OD2	1:1:88:THR:HB	2.21	0.41
1:1:87:ALA:C	1:1:90:ILE:HG12	2.45	0.41
5:1:900:W84:H7C1	5:1:900:W84:H6B	1.86	0.41
1:1:221:MET:HE3	5:1:900:W84:C2B	2.50	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.02	0.41
1:1:98:LEU:O	1:1:99:PHE:HB3	2.19	0.41
3:3:137:ARG:HH11	3:3:137:ARG:HD3	1.22	0.41
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.20	0.41
1:1:165:ASP:CB	1:1:167:THR:OG1	2.69	0.41
3:3:179:ASP:CB	3:3:182:THR:CG2	2.88	0.41
1:1:54:ARG:HH11	1:1:54:ARG:HD2	1.55	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
3:3:64:VAL:O	3:3:64:VAL:HG12	2.21	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
3:3:231:THR:C	3:3:232:VAL:HG13	2.45	0.40
3:3:20:GLN:NE2	4:4:30:ASN:HA	2.36	0.40
1:1:208:ASP:HB3	1:1:211:THR:HB	2.04	0.40
1:1:265:SER:OG	2:2:139:ASN:HB3	2.21	0.40
2:2:172:ASN:CG	2:2:181:LEU:HD13	2.47	0.40
3:3:175:TYR:CD1	3:3:179:ASP:HB2	2.57	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%)	252 (93%)	14 (5%)	5 (2%)	6	31
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%)	735 (92%)	50 (6%)	11 (1%)	9	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	SER
3	3	57	ASN
3	3	77	ASN
1	1	99	PHE
1	1	165	ASP
1	1	216	THR

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Mol	Chain	Res	Type
2	2	255	ARG
2	2	257	LYS
4	4	47	MET
1	1	104	ILE
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%)	183 (77%)	56 (23%)	1	4
2	2	223/229 (97%)	176 (79%)	47 (21%)	1	6
3	3	209/209 (100%)	171 (82%)	38 (18%)	2	9
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	1
All	All	704/748 (94%)	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

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Mol	Chain	Res	Type
1	1	101	ASP
1	1	103	LYS
1	1	105	ASN
1	1	106	LEU
1	1	107	SER
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	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	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

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Mol	Chain	Res	Type
2	2	26	GLN
2	2	30	ASN
2	2	49	ASP
2	2	52	LYS
2	2	66	LEU
2	2	69	LYS
2	2	73	THR
2	2	76	LYS
2	2	81	LYS
2	2	87	LYS
2	2	88	ASP
2	2	103	ARG
2	2	116	LYS
2	2	119	SER
2	2	136	GLU
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

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Mol	Chain	Res	Type
2	2	256	SER
2	2	259	ILE
2	2	262	GLN
3	3	12	GLN
3	3	16	THR
3	3	33	ARG
3	3	42	ASN
3	3	46	ILE
3	3	55	MET
3	3	60	THR
3	3	61	LYS
3	3	65	ASN
3	3	84	ASN
3	3	91	VAL
3	3	94	THR
3	3	101	VAL
3	3	112	ARG
3	3	114	SER
3	3	115	LEU
3	3	137	ARG
3	3	146	MET
3	3	157	LEU
3	3	158	GLN
3	3	159	SER
3	3	164	THR
3	3	172	GLN
3	3	174	ARG
3	3	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

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Mol	Chain	Res	Type
4	4	33	LYS
4	4	40	SER
4	4	43	GLN
4	4	45	LEU
4	4	46	SER
4	4	47	MET
4	4	50	SER
4	4	51	LYS
4	4	59	LEU
4	4	61	LEU
4	4	67	LEU
4	4	68	ASN

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

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

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Mol	Chain	Res	Type
3	3	84	ASN
3	3	140	GLN
3	3	192	GLN
3	3	226	GLN
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	900	-	28,28,28	2.76	4 (14%)	34,36,36	2.51	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	900	-	-	5/15/24/24	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	900	W84	C2A-N3A	11.08	1.43	1.27
5	1	900	W84	C4A-N3A	-7.39	1.35	1.48
5	1	900	W84	O1A-C2A	-4.24	1.29	1.36
5	1	900	W84	O1A-C5A	-3.75	1.38	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	900	W84	CM1-C4A-N3A	7.97	133.43	111.59
5	1	900	W84	O1A-C2A-N3A	-6.90	110.16	118.10
5	1	900	W84	O1A-C2A-C4B	6.54	124.12	115.85
5	1	900	W84	O1A-C5A-C4A	5.51	111.50	104.88
5	1	900	W84	C5A-C4A-N3A	-3.95	98.54	103.71
5	1	900	W84	CM1-C4A-C5A	-2.59	104.72	114.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	900	W84	C2C-C1C-C5-O1
5	1	900	W84	C3C-C4C-C5C-C6C
5	1	900	W84	C1C-C2C-C3C-C4C
5	1	900	W84	C2C-C1C-C5-C4
5	1	900	W84	C5-C1C-C2C-C3C

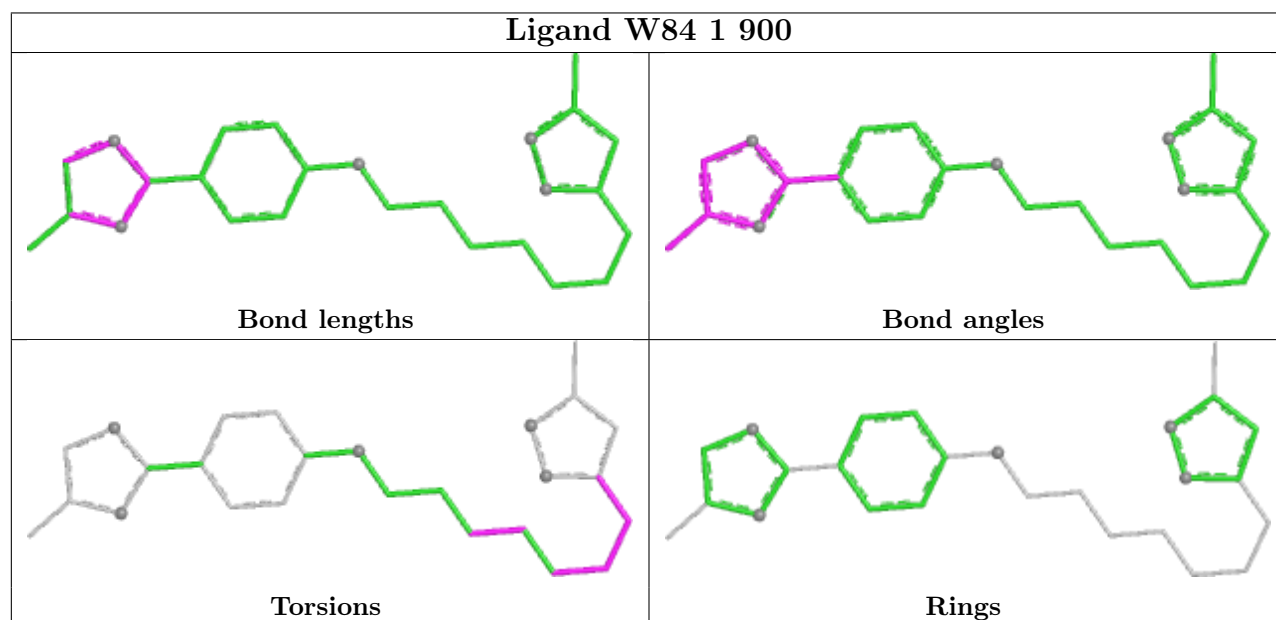
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	900	W84	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	25.26	273 (100%) 0 0	1, 1, 1, 1	0
2	2	255/262 (97%)	24.92	255 (100%) 0 0	1, 1, 1, 1	0
3	3	236/236 (100%)	25.20	236 (100%) 0 0	1, 1, 1, 1	0
4	4	40/68 (58%)	25.12	40 (100%) 0 0	1, 1, 1, 1	0
All	All	804/855 (94%)	25.13	804 (100%) 0 0	1, 1, 1, 1	0

All (804) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	2	139	ASN	32.3
3	3	74	ASN	31.7
1	1	61	ASN	31.6
2	2	104	SER	31.3
2	2	68	SER	30.9
3	3	188	SER	30.9
4	4	46	SER	30.8
3	3	18	ASP	30.8
1	1	143	SER	30.7
1	1	63	SER	30.6
3	3	214	CYS	30.6
3	3	31	THR	30.5
2	2	206	SER	30.4
3	3	229	SER	30.4
4	4	44	SER	30.3
1	1	233	ASP	30.3
3	3	177	ASP	30.3
1	1	230	ASN	30.3
2	2	121	CYS	30.2
2	2	100	SER	30.2
3	3	21	SER	30.2

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Mol	Chain	Res	Type	RSRZ
1	1	195	SER	30.1
1	1	29	GLN	30.0
1	1	198	ASN	29.9
1	1	50	SER	29.7
1	1	184	SER	29.6
4	4	68	ASN	29.5
2	2	256	SER	29.4
1	1	145	ASN	29.4
1	1	22	SER	29.2
1	1	141	ASN	29.2
1	1	69	CYS	29.2
3	3	78	GLU	29.2
1	1	175	SER	29.2
3	3	27	ASN	29.2
3	3	154	ASP	29.2
3	3	22	PRO	29.1
2	2	20	ASN	29.1
1	1	170	SER	29.1
2	2	79	CYS	29.0
1	1	49	ASP	29.0
3	3	9	GLY	29.0
1	1	48	SER	29.0
2	2	134	SER	28.9
4	4	58	ASP	28.9
3	3	180	THR	28.9
1	1	56	THR	28.9
2	2	158	SER	28.9
3	3	105	THR	28.9
2	2	195	ASN	28.9
1	1	23	SER	28.8
3	3	124	SER	28.8
3	3	189	CYS	28.8
2	2	59	SER	28.8
2	2	157	SER	28.8
1	1	76	CYS	28.8
2	2	219	SER	28.7
1	1	37	ASN	28.7
3	3	79	GLN	28.7
3	3	216	ASP	28.7
3	3	72	ASN	28.6
4	4	39	SER	28.6
1	1	275	THR	28.6

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Mol	Chain	Res	Type	RSRZ
2	2	112	CYS	28.6
2	2	61	CYS	28.6
1	1	270	ASN	28.5
3	3	114	SER	28.5
1	1	285	ASP	28.5
3	3	62	ASP	28.5
2	2	196	THR	28.4
2	2	203	TYR	28.4
1	1	288	SER	28.4
2	2	34	CYS	28.4
1	1	28	THR	28.4
3	3	42	ASN	28.4
2	2	248	CYS	28.3
2	2	88	ASP	28.3
1	1	216	THR	28.3
1	1	125	ASP	28.3
1	1	91	ASP	28.3
2	2	241	THR	28.2
1	1	199	CYS	28.2
4	4	50	SER	28.2
1	1	126	SER	28.2
2	2	70	THR	28.2
3	3	132	THR	28.2
3	3	231	THR	28.2
1	1	173	ASN	28.2
3	3	77	ASN	28.2
1	1	192	GLY	28.1
1	1	223	SER	28.1
2	2	10	SER	28.0
2	2	174	ASN	28.0
1	1	265	SER	28.0
2	2	147	THR	28.0
2	2	30	ASN	27.9
2	2	65	THR	27.9
1	1	207	ASP	27.9
2	2	21	SER	27.9
1	1	139	SER	27.9
1	1	72	GLY	27.8
1	1	107	SER	27.8
2	2	258	SER	27.8
1	1	211	THR	27.8
1	1	159	ASN	27.8

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Mol	Chain	Res	Type	RSRZ
3	3	10	SER	27.7
2	2	11	ASP	27.7
3	3	84	ASN	27.7
2	2	204	ILE	27.7
3	3	66	SER	27.7
2	2	237	SER	27.7
1	1	101	ASP	27.6
2	2	216	ASN	27.6
2	2	113	ASN	27.6
1	1	190	TYR	27.6
1	1	120	THR	27.6
1	1	158	PRO	27.6
3	3	169	SER	27.6
1	1	164	ASP	27.6
2	2	155	ASP	27.6
3	3	193	THR	27.6
2	2	46	ASP	27.5
1	1	197	TYR	27.5
1	1	208	ASP	27.5
2	2	73	THR	27.5
3	3	83	THR	27.5
1	1	172	SER	27.5
3	3	209	SER	27.5
2	2	194	ASN	27.5
3	3	141	ASP	27.5
2	2	111	GLN	27.5
1	1	80	THR	27.5
1	1	210	GLU	27.5
3	3	179	ASP	27.4
2	2	160	ASN	27.4
3	3	164	THR	27.4
3	3	89	ASP	27.4
1	1	213	TYR	27.4
1	1	86	ASP	27.4
2	2	49	ASP	27.4
1	1	165	ASP	27.3
2	2	84	ASP	27.3
1	1	187	SER	27.3
1	1	27	HIS	27.3
3	3	29	GLU	27.3
1	1	221	MET	27.3
3	3	183	SER	27.2

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Mol	Chain	Res	Type	RSRZ
1	1	65	THR	27.2
1	1	100	ASN	27.2
3	3	67	TYR	27.2
2	2	205	ASN	27.1
3	3	28	TYR	27.1
2	2	261	PRO	27.1
1	1	202	ASP	27.1
1	1	47	PRO	27.1
1	1	66	ASP	27.0
3	3	17	ASP	27.0
4	4	38	THR	27.0
1	1	269	THR	27.0
2	2	168	ASP	27.0
1	1	169	GLN	27.0
2	2	48	SER	27.0
2	2	163	GLY	27.0
1	1	277	PRO	27.0
3	3	178	PRO	27.0
1	1	163	TRP	27.0
1	1	167	THR	27.0
1	1	128	TYR	27.0
3	3	98	GLY	26.9
1	1	129	THR	26.9
1	1	133	THR	26.9
3	3	145	ALA	26.9
1	1	105	ASN	26.9
2	2	131	GLN	26.9
3	3	23	SER	26.9
3	3	204	GLN	26.9
3	3	138	GLY	26.9
1	1	205	SER	26.9
1	1	264	THR	26.9
3	3	58	THR	26.9
3	3	95	THR	26.9
2	2	172	ASN	26.9
1	1	272	PRO	26.9
2	2	57	ASP	26.9
4	4	30	ASN	26.8
1	1	89	GLY	26.8
2	2	105	GLY	26.8
4	4	31	TYR	26.8
2	2	44	ASP	26.8

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Mol	Chain	Res	Type	RSRZ
1	1	75	ALA	26.8
1	1	32	PRO	26.8
1	1	84	ASN	26.8
2	2	9	TYR	26.8
3	3	194	SER	26.8
3	3	167	TRP	26.7
2	2	119	SER	26.7
2	2	24	THR	26.7
3	3	107	TRP	26.7
3	3	12	GLN	26.7
3	3	35	HIS	26.7
1	1	289	TYR	26.7
4	4	37	SER	26.7
2	2	72	THR	26.6
2	2	145	THR	26.6
2	2	210	ASP	26.6
3	3	168	THR	26.6
3	3	99	GLU	26.6
1	1	284	GLY	26.6
2	2	208	PRO	26.6
3	3	76	GLN	26.6
2	2	115	THR	26.6
1	1	183	THR	26.6
2	2	239	PRO	26.5
1	1	35	THR	26.5
2	2	40	GLU	26.5
1	1	274	ASN	26.5
3	3	212	SER	26.5
1	1	95	GLU	26.5
3	3	133	PRO	26.5
1	1	25	PRO	26.5
4	4	43	GLN	26.5
2	2	141	SER	26.5
1	1	59	HIS	26.5
3	3	56	ASN	26.4
3	3	226	GLN	26.5
2	2	211	SER	26.4
2	2	78	TRP	26.4
3	3	140	GLN	26.4
3	3	175	TYR	26.4
3	3	200	GLU	26.4
1	1	149	GLN	26.4

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Mol	Chain	Res	Type	RSRZ
3	3	82	GLY	26.4
1	1	142	TYR	26.4
1	1	152	TYR	26.4
1	1	249	HIS	26.4
3	3	150	HIS	26.4
3	3	172	GLN	26.4
3	3	192	GLN	26.4
2	2	8	GLY	26.4
3	3	149	THR	26.4
3	3	148	GLY	26.3
1	1	219	ASN	26.3
2	2	51	ASN	26.3
1	1	144	SER	26.3
2	2	75	SER	26.3
4	4	40	SER	26.3
3	3	73	ALA	26.3
1	1	203	GLY	26.3
3	3	102	GLN	26.3
3	3	60	THR	26.3
3	3	159	SER	26.3
2	2	58	THR	26.3
2	2	106	TYR	26.3
3	3	230	GLN	26.3
3	3	131	TYR	26.3
2	2	149	PRO	26.2
3	3	123	SER	26.2
3	3	202	THR	26.2
1	1	191	VAL	26.2
1	1	189	PRO	26.2
3	3	206	TYR	26.2
2	2	80	TRP	26.1
2	2	64	TYR	26.1
1	1	64	GLU	26.1
3	3	57	ASN	26.1
2	2	213	THR	26.1
1	1	92	ASN	26.1
3	3	108	SER	26.1
2	2	243	THR	26.1
3	3	153	TRP	26.1
3	3	8	PRO	26.1
3	3	217	PHE	26.0
2	2	175	GLY	26.0

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Mol	Chain	Res	Type	RSRZ
2	2	162	VAL	26.0
3	3	203	GLY	26.0
2	2	176	THR	26.0
3	3	110	SER	26.0
2	2	171	TYR	26.0
2	2	229	THR	26.0
2	2	161	GLU	26.0
1	1	55	THR	26.0
1	1	201	TYR	26.0
1	1	237	THR	26.0
1	1	127	GLU	25.9
1	1	276	GLU	25.9
1	1	206	HIS	25.9
3	3	11	GLY	25.9
2	2	67	ASP	25.9
3	3	135	GLY	25.9
2	2	35	TYR	25.9
3	3	117	TYR	25.9
3	3	15	THR	25.9
1	1	78	HIS	25.9
3	3	88	GLY	25.9
3	3	160	THR	25.8
2	2	47	ALA	25.8
3	3	121	ALA	25.8
1	1	53	THR	25.8
4	4	53	THR	25.8
3	3	136	ALA	25.8
3	3	191	TYR	25.8
1	1	135	SER	25.8
1	1	17	THR	25.8
3	3	182	THR	25.8
1	1	228	ILE	25.8
1	1	181	GLY	25.8
2	2	90	GLY	25.8
2	2	190	ASN	25.8
3	3	104	TYR	25.8
1	1	262	PRO	25.8
2	2	71	TRP	25.8
2	2	94	GLN	25.7
4	4	54	GLU	25.7
2	2	22	THR	25.7
2	2	31	ALA	25.7

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Mol	Chain	Res	Type	RSRZ
2	2	41	TYR	25.7
2	2	159	ALA	25.7
1	1	263	TYR	25.7
1	1	102	TRP	25.7
1	1	271	TYR	25.7
2	2	138	GLY	25.7
3	3	94	THR	25.7
3	3	176	THR	25.7
1	1	117	GLU	25.7
1	1	96	ALA	25.6
2	2	186	HIS	25.6
1	1	267	GLY	25.6
4	4	48	ASP	25.6
1	1	177	PHE	25.6
2	2	252	SER	25.6
1	1	21	ILE	25.6
2	2	246	PRO	25.6
3	3	30	PRO	25.6
3	3	32	PRO	25.6
4	4	42	GLY	25.6
1	1	245	HIS	25.6
1	1	162	GLU	25.5
1	1	155	PRO	25.5
3	3	80	VAL	25.5
1	1	138	ASP	25.5
3	3	20	GLN	25.5
3	3	205	VAL	25.5
1	1	194	ALA	25.5
2	2	233	GLY	25.5
1	1	182	ASP	25.5
2	2	198	THR	25.5
1	1	212	GLN	25.5
2	2	202	PRO	25.5
2	2	227	PRO	25.5
2	2	217	ASN	25.5
3	3	190	TRP	25.5
2	2	17	THR	25.5
3	3	16	THR	25.5
2	2	114	ALA	25.5
2	2	27	GLU	25.5
1	1	174	PRO	25.5
3	3	37	PRO	25.5

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Mol	Chain	Res	Type	RSRZ
3	3	156	GLY	25.5
3	3	166	PRO	25.5
3	3	86	PHE	25.5
3	3	118	THR	25.4
1	1	74	ALA	25.4
2	2	235	THR	25.4
4	4	65	PRO	25.4
1	1	204	TYR	25.4
2	2	130	HIS	25.4
1	1	253	TRP	25.4
2	2	15	GLN	25.4
3	3	181	TYR	25.4
1	1	188	VAL	25.4
4	4	47	MET	25.4
3	3	130	ALA	25.4
1	1	154	PRO	25.4
3	3	81	PHE	25.4
3	3	45	GLU	25.3
2	2	140	VAL	25.3
3	3	69	ILE	25.3
1	1	278	VAL	25.3
1	1	224	MET	25.3
3	3	103	TYR	25.3
2	2	146	PHE	25.3
1	1	46	LEU	25.3
1	1	251	GLU	25.3
1	1	244	TYR	25.3
1	1	247	ALA	25.3
2	2	109	HIS	25.3
3	3	227	THR	25.2
2	2	250	GLU	25.2
2	2	259	ILE	25.2
1	1	24	GLY	25.2
1	1	231	GLU	25.2
1	1	132	ALA	25.2
3	3	26	PRO	25.2
3	3	70	PRO	25.2
1	1	180	VAL	25.2
2	2	107	THR	25.2
1	1	81	GLU	25.2
3	3	65	ASN	25.2
1	1	39	THR	25.2

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Mol	Chain	Res	Type	RSRZ
3	3	163	MET	25.2
1	1	166	TYR	25.2
3	3	139	PRO	25.2
1	1	38	GLU	25.2
2	2	135	HIS	25.1
2	2	249	THR	25.1
1	1	41	ALA	25.1
4	4	66	ALA	25.1
1	1	121	TYR	25.1
2	2	95	ASN	25.1
2	2	151	GLU	25.1
3	3	151	VAL	25.1
1	1	252	ALA	25.1
2	2	85	ALA	25.1
3	3	50	ASP	25.1
2	2	97	PHE	25.0
2	2	136	GLU	25.0
3	3	224	ASP	25.0
3	3	207	LEU	25.0
2	2	236	PRO	25.0
1	1	168	TRP	25.0
2	2	43	PRO	25.0
2	2	56	PRO	25.0
1	1	176	VAL	25.0
2	2	39	PRO	25.0
2	2	197	ALA	25.0
1	1	60	PHE	25.0
2	2	193	THR	25.0
2	2	215	HIS	24.9
3	3	106	HIS	24.9
3	3	233	ALA	24.9
2	2	188	PHE	24.9
1	1	226	PHE	24.9
1	1	108	SER	24.9
1	1	131	LEU	24.9
2	2	180	ASN	24.9
1	1	286	ILE	24.9
1	1	157	ALA	24.9
1	1	58	MET	24.9
1	1	151	MET	24.9
2	2	83	PRO	24.8
3	3	215	PRO	24.8

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Mol	Chain	Res	Type	RSRZ
1	1	57	TYR	24.8
2	2	262	GLN	24.8
1	1	178	PHE	24.8
2	2	165	PRO	24.8
4	4	29	ILE	24.8
1	1	225	ALA	24.8
2	2	232	THR	24.8
3	3	59	HIS	24.8
1	1	52	GLU	24.8
3	3	92	PHE	24.7
2	2	14	GLN	24.7
3	3	225	THR	24.7
3	3	13	PHE	24.7
2	2	221	MET	24.7
1	1	68	GLU	24.7
3	3	51	THR	24.7
3	3	219	LEU	24.7
2	2	245	ALA	24.7
3	3	171	VAL	24.7
3	3	146	MET	24.7
1	1	147	VAL	24.7
2	2	26	GLN	24.6
2	2	16	ILE	24.6
3	3	36	ILE	24.6
2	2	120	GLY	24.6
2	2	226	ALA	24.6
1	1	44	PRO	24.6
4	4	49	PRO	24.6
3	3	127	LEU	24.6
2	2	91	VAL	24.6
3	3	210	PHE	24.6
1	1	90	ILE	24.6
1	1	42	THR	24.6
1	1	234	GLU	24.6
3	3	235	THR	24.6
2	2	184	PHE	24.6
3	3	134	PRO	24.6
1	1	232	HIS	24.6
2	2	144	TYR	24.5
2	2	240	ILE	24.5
1	1	255	PRO	24.5
3	3	63	GLU	24.5

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Mol	Chain	Res	Type	RSRZ
2	2	164	GLY	24.5
2	2	102	GLY	24.4
2	2	122	LEU	24.4
1	1	268	ARG	24.4
1	1	111	GLN	24.4
1	1	20	SER	24.4
2	2	110	VAL	24.4
1	1	19	ALA	24.4
2	2	93	GLY	24.4
2	2	153	GLY	24.4
3	3	48	GLN	24.4
1	1	45	VAL	24.4
1	1	148	VAL	24.4
3	3	128	ILE	24.3
3	3	162	VAL	24.3
3	3	199	PRO	24.3
1	1	40	GLY	24.3
3	3	100	ILE	24.3
1	1	214	GLY	24.3
2	2	118	HIS	24.3
3	3	201	THR	24.3
1	1	209	ALA	24.3
2	2	189	ILE	24.3
1	1	109	LEU	24.2
2	2	234	ALA	24.2
4	4	36	ALA	24.2
4	4	41	ALA	24.2
3	3	34	ILE	24.2
1	1	62	GLY	24.2
2	2	247	MET	24.2
4	4	45	LEU	24.2
2	2	25	THR	24.2
1	1	153	VAL	24.2
1	1	106	LEU	24.2
3	3	158	GLN	24.2
2	2	128	PRO	24.2
3	3	41	HIS	24.2
2	2	77	GLY	24.2
2	2	187	GLN	24.1
3	3	38	GLY	24.1
2	2	166	VAL	24.1
3	3	111	LEU	24.1

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Mol	Chain	Res	Type	RSRZ
2	2	37	GLU	24.1
2	2	92	PHE	24.1
2	2	129	GLU	24.1
1	1	70	PHE	24.1
3	3	196	ILE	24.1
1	1	222	GLY	24.1
1	1	124	PHE	24.1
1	1	186	PHE	24.1
3	3	90	GLY	24.1
2	2	137	GLY	24.1
2	2	45	VAL	24.0
2	2	132	LEU	24.0
2	2	260	VAL	24.0
3	3	1	GLY	24.0
3	3	115	LEU	24.0
3	3	198	PRO	24.0
1	1	217	VAL	24.0
2	2	19	GLY	24.0
4	4	63	GLY	24.0
3	3	165	ILE	24.0
2	2	191	LEU	24.0
3	3	109	GLY	24.0
1	1	250	VAL	23.9
3	3	120	PRO	23.9
3	3	116	MET	23.9
2	2	23	ILE	23.9
2	2	133	ALA	23.9
2	2	50	VAL	23.9
1	1	215	ILE	23.9
3	3	54	PRO	23.9
1	1	43	MET	23.9
3	3	187	LEU	23.9
3	3	25	LEU	23.9
1	1	122	VAL	23.9
4	4	55	PRO	23.9
1	1	99	PHE	23.9
2	2	228	LEU	23.8
3	3	236	GLU	23.8
2	2	224	PRO	23.8
4	4	52	PHE	23.8
4	4	35	ALA	23.8
1	1	136	GLN	23.8

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Mol	Chain	Res	Type	RSRZ
1	1	93	HIS	23.8
1	1	229	VAL	23.8
3	3	55	MET	23.8
2	2	108	VAL	23.7
4	4	34	ASP	23.7
1	1	134	ALA	23.7
3	3	125	ALA	23.7
2	2	225	ILE	23.7
3	3	208	LEU	23.7
4	4	64	ALA	23.7
2	2	103	ARG	23.7
2	2	82	LEU	23.7
2	2	38	TRP	23.7
2	2	207	VAL	23.6
1	1	97	LYS	23.6
3	3	126	LYS	23.6
1	1	112	LEU	23.6
3	3	170	GLY	23.6
4	4	32	TYR	23.6
2	2	201	ILE	23.6
4	4	56	VAL	23.6
1	1	88	THR	23.6
3	3	3	PRO	23.6
1	1	218	LEU	23.6
1	1	51	ILE	23.6
3	3	186	PHE	23.5
2	2	173	MET	23.5
3	3	19	ARG	23.5
3	3	185	GLY	23.5
1	1	171	ALA	23.5
3	3	157	LEU	23.5
3	3	47	ILE	23.5
1	1	240	LYS	23.5
1	1	104	ILE	23.4
2	2	66	LEU	23.4
1	1	26	LYS	23.4
1	1	239	VAL	23.4
3	3	101	VAL	23.4
2	2	96	MET	23.4
2	2	179	GLY	23.4
1	1	83	GLN	23.4
3	3	113	PHE	23.3

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Mol	Chain	Res	Type	RSRZ
2	2	242	VAL	23.3
2	2	29	ALA	23.3
1	1	116	LEU	23.3
1	1	71	LEU	23.3
3	3	49	VAL	23.3
1	1	130	ILE	23.3
1	1	279	ILE	23.3
3	3	64	VAL	23.2
1	1	33	ILE	23.2
4	4	59	LEU	23.2
2	2	200	VAL	23.2
3	3	232	VAL	23.2
2	2	13	VAL	23.2
1	1	196	ALA	23.2
3	3	147	LEU	23.2
2	2	150	GLY	23.1
3	3	7	LEU	23.1
4	4	61	LEU	23.1
1	1	150	ALA	23.1
3	3	93	LYS	23.1
1	1	261	LEU	23.1
3	3	234	LEU	23.1
1	1	77	VAL	23.1
1	1	137	PRO	23.1
4	4	60	MET	23.1
3	3	195	LEU	23.1
3	3	211	ILE	23.1
1	1	140	ALA	23.1
2	2	220	LEU	23.1
3	3	43	LEU	23.1
2	2	33	VAL	23.1
1	1	82	ILE	23.1
3	3	46	ILE	23.1
3	3	155	ILE	23.1
2	2	255	ARG	23.0
2	2	244	ILE	23.0
1	1	220	HIS	23.0
1	1	146	LEU	23.0
2	2	86	LEU	23.0
3	3	129	LEU	23.0
3	3	213	ALA	23.0
3	3	144	GLU	22.9

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Mol	Chain	Res	Type	RSRZ
1	1	67	VAL	22.9
2	2	98	PHE	22.9
1	1	254	ILE	22.9
3	3	87	ILE	22.9
1	1	34	LEU	22.9
3	3	221	LEU	22.9
1	1	260	ALA	22.9
2	2	28	ALA	22.9
1	1	200	PHE	22.9
3	3	85	LEU	22.9
1	1	258	PRO	22.9
1	1	79	VAL	22.9
3	3	152	VAL	22.9
3	3	222	MET	22.9
1	1	243	VAL	22.8
2	2	154	ILE	22.8
2	2	177	LEU	22.8
1	1	257	ALA	22.8
2	2	18	LEU	22.8
1	1	266	ILE	22.8
2	2	209	ILE	22.8
3	3	112	ARG	22.8
1	1	30	LYS	22.7
2	2	181	LEU	22.7
2	2	54	SER	22.7
2	2	212	MET	22.7
3	3	184	ALA	22.7
2	2	199	ILE	22.7
3	3	24	ALA	22.7
2	2	76	LYS	22.7
3	3	197	LEU	22.7
4	4	67	LEU	22.7
1	1	123	ARG	22.6
2	2	117	PHE	22.6
3	3	228	ILE	22.6
1	1	31	VAL	22.6
2	2	142	VAL	22.6
2	2	156	LEU	22.6
1	1	73	ARG	22.6
1	1	259	ARG	22.6
2	2	238	LEU	22.6
2	2	254	ILE	22.5

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Mol	Chain	Res	Type	RSRZ
1	1	160	PRO	22.5
3	3	44	LEU	22.5
2	2	222	VAL	22.5
1	1	235	HIS	22.5
3	3	14	LEU	22.5
1	1	36	ALA	22.5
2	2	63	PHE	22.5
2	2	89	MET	22.5
3	3	143	ARG	22.5
3	3	161	ILE	22.4
3	3	137	ARG	22.4
2	2	126	VAL	22.4
2	2	185	PRO	22.4
1	1	248	LYS	22.3
1	1	18	VAL	22.3
3	3	91	VAL	22.3
2	2	99	HIS	22.3
3	3	4	THR	22.3
1	1	185	ARG	22.3
3	3	71	LEU	22.3
3	3	39	LYS	22.3
1	1	246	ARG	22.3
1	1	241	ILE	22.2
3	3	2	LEU	22.2
1	1	161	LYS	22.2
3	3	119	GLY	22.1
2	2	223	ILE	22.1
2	2	69	LYS	22.1
4	4	57	LYS	22.1
1	1	227	ARG	22.1
2	2	32	VAL	22.1
2	2	218	VAL	22.1
2	2	170	LEU	22.1
2	2	231	PRO	22.1
1	1	179	LYS	22.0
2	2	169	VAL	22.0
1	1	282	ARG	22.0
3	3	40	VAL	22.0
2	2	81	LYS	22.0
2	2	60	VAL	22.0
1	1	119	PHE	22.0
2	2	257	LYS	22.0

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Mol	Chain	Res	Type	RSRZ
3	3	68	LEU	22.0
3	3	5	THR	21.9
3	3	97	LEU	21.9
2	2	12	ARG	21.8
1	1	87	ALA	21.8
3	3	52	LEU	21.8
2	2	167	LYS	21.8
2	2	253	GLY	21.7
1	1	98	LEU	21.7
1	1	110	VAL	21.7
1	1	113	ARG	21.7
3	3	142	ARG	21.7
2	2	127	ILE	21.7
2	2	183	ILE	21.7
1	1	287	LYS	21.7
2	2	192	ARG	21.7
1	1	118	LEU	21.7
2	2	74	GLY	21.6
2	2	251	PHE	21.6
1	1	54	ARG	21.6
1	1	94	ARG	21.6
3	3	53	ILE	21.5
3	3	174	ARG	21.5
2	2	148	HIS	21.5
1	1	114	LYS	21.4
2	2	62	ARG	21.4
3	3	173	PHE	21.4
2	2	42	LEU	21.4
3	3	61	LYS	21.4
1	1	115	LYS	21.3
1	1	193	LEU	21.2
1	1	256	ARG	21.2
2	2	53	THR	21.2
2	2	214	ARG	21.2
2	2	124	VAL	21.2
3	3	220	ARG	21.2
3	3	218	LYS	21.2
2	2	125	VAL	21.2
3	3	75	ARG	21.2
2	2	123	LEU	21.2
4	4	33	LYS	21.2
3	3	122	LEU	21.1

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Mol	Chain	Res	Type	RSRZ
2	2	182	LEU	21.1
2	2	87	LYS	21.1
3	3	96	LEU	21.0
1	1	273	LYS	21.0
1	1	281	LYS	21.0
1	1	156	GLY	21.0
4	4	51	LYS	21.0
3	3	33	ARG	21.0
2	2	230	VAL	21.0
3	3	223	LYS	21.0
2	2	52	LYS	20.9
1	1	242	ARG	20.9
2	2	152	ARG	20.8
4	4	62	LYS	20.8
3	3	6	THR	20.7
1	1	280	LYS	20.6
2	2	116	LYS	20.6
1	1	238	LEU	20.6
1	1	85	LYS	20.5
1	1	103	LYS	20.4
2	2	101	LEU	20.3
2	2	178	LEU	20.3
2	2	55	LYS	20.1
1	1	283	LYS	20.1
1	1	236	LYS	19.6
2	2	143	LYS	19.3
2	2	36	ALA	19.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

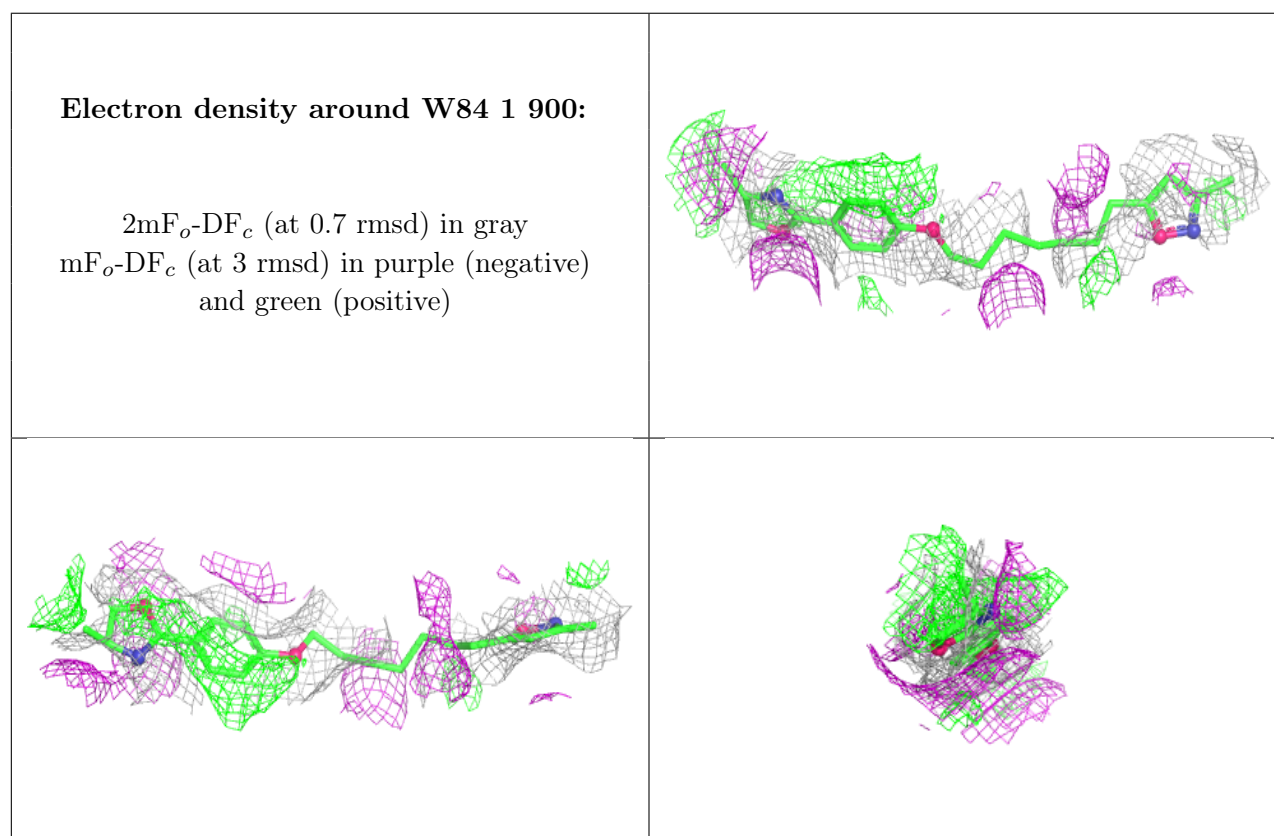
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	W84	1	900	26/26	-0.82	1.25	1,1,1,1	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.