



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:18 PM UTC

PDB ID : 3J1P / pdb_00003j1p
EMDB ID : EMD-5410
Title : Atomic model of rabbit hemorrhagic disease virus
Authors : Wang, X.; Liu, Y.; Sun, F.
Deposited on : 2012-04-09
Resolution : 6.50 Å(reported)
Based on initial models : 4EJR, 4EGT

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

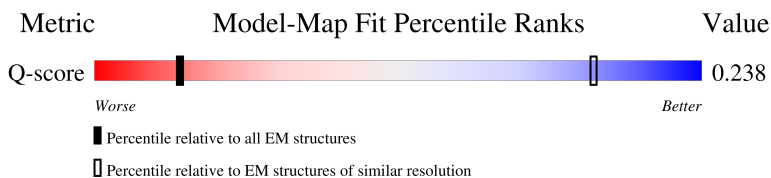
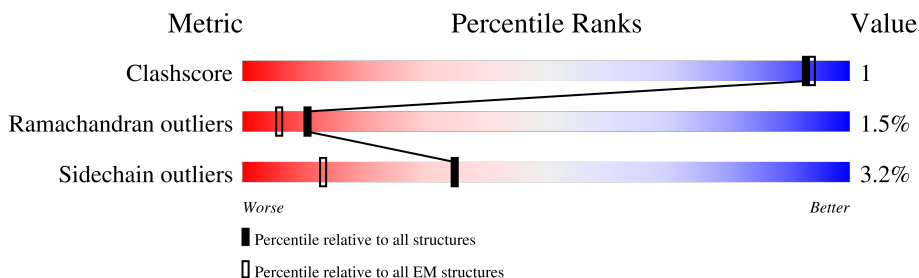
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	556 (6.00 - 7.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	579	10% 45% 42% 9%
1	B	579	18% 45% 42% 9%
1	C	579	7% 47% 40% 9%

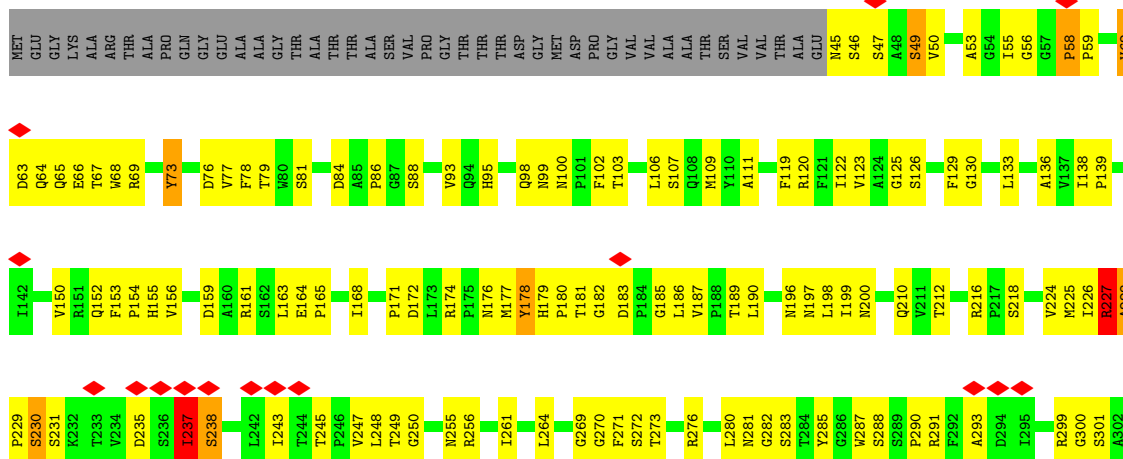
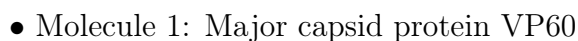
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11703 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Major capsid protein VP60.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	525	Total	C	N	O	S	0	0
			3901	2473	663	754	11		
1	B	525	Total	C	N	O	S	0	0
			3901	2473	663	754	11		
1	C	525	Total	C	N	O	S	0	0
			3901	2473	663	754	11		





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	26000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	CTF correction of each whole micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	160770	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	16.738	Depositor
Minimum map value	-8.733	Depositor
Average map value	0.120	Depositor
Map value standard deviation	1.836	Depositor
Recommended contour level	2.6	Depositor
Map size ($\text{\AA}$)	447.84003, 447.84003, 447.84003	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.933, 0.933, 0.933	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.11	113/4013 (2.8%)	2.43	271/5514 (4.9%)
1	B	2.14	119/4013 (3.0%)	2.36	232/5514 (4.2%)
1	C	2.14	116/4013 (2.9%)	2.38	226/5514 (4.1%)
All	All	2.13	348/12039 (2.9%)	2.39	729/16542 (4.4%)

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	A	0	12
1	B	0	15
1	C	0	11
All	All	0	38

All (348) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	VAL	N-CA	-12.68	1.36	1.46
1	B	514	VAL	CA-C	12.20	1.67	1.52
1	A	264	LEU	CA-CB	11.06	1.70	1.53
1	A	139	PRO	CA-C	10.90	1.57	1.51
1	B	238	SER	CA-C	9.68	1.63	1.52
1	B	560	PRO	CA-C	8.88	1.63	1.52
1	A	400	VAL	N-CA	8.43	1.55	1.46
1	C	187	VAL	CA-C	8.30	1.61	1.52
1	C	535	TYR	CA-C	8.30	1.62	1.52
1	A	263	GLY	CA-C	8.28	1.60	1.51
1	C	493	PRO	N-CD	-8.27	1.36	1.47
1	C	559	ARG	CD-NE	8.22	1.57	1.46
1	C	138	ILE	N-CA	-7.91	1.36	1.46
1	A	142	ILE	CA-CB	-7.91	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	556	VAL	CA-CB	-7.72	1.46	1.54
1	C	300	GLY	N-CA	7.72	1.52	1.45
1	C	409	THR	CA-C	-7.71	1.43	1.52
1	B	318	ALA	N-CA	-7.68	1.36	1.45
1	C	197	ASN	CA-CB	7.62	1.66	1.53
1	A	549	GLU	C-N	7.61	1.44	1.33
1	A	442	ARG	C-N	7.58	1.42	1.33
1	C	282	GLY	CA-C	7.52	1.62	1.51
1	C	454	PRO	CA-C	7.51	1.63	1.52
1	C	243	ILE	CA-CB	7.50	1.63	1.54
1	A	258	ASP	CA-C	7.47	1.62	1.53
1	B	497	GLY	C-N	7.46	1.44	1.33
1	A	216	ARG	CD-NE	7.44	1.56	1.46
1	C	210	GLN	CA-C	-7.43	1.44	1.52
1	B	552	ASP	CA-CB	7.34	1.66	1.53
1	C	424	GLY	CA-C	-7.31	1.45	1.51
1	A	154	PRO	N-CA	-7.24	1.38	1.47
1	A	372	THR	CA-C	-7.21	1.42	1.52
1	A	499	SER	N-CA	7.17	1.55	1.46
1	C	218	SER	CA-C	-7.16	1.43	1.53
1	B	373	VAL	CA-CB	7.16	1.62	1.53
1	C	381	ALA	CA-C	-7.12	1.43	1.52
1	C	63	ASP	CA-C	7.09	1.63	1.53
1	B	126	SER	CA-CB	7.03	1.65	1.53
1	A	491	PRO	N-CD	-7.01	1.38	1.47
1	B	143	GLU	CA-CB	7.01	1.64	1.53
1	C	516	GLN	CA-CB	6.95	1.64	1.53
1	A	351	THR	CA-CB	-6.94	1.44	1.53
1	A	97	PRO	CA-CB	6.91	1.64	1.53
1	A	361	TRP	CA-CB	6.90	1.64	1.53
1	C	106	LEU	CA-CB	6.89	1.64	1.53
1	B	313	LEU	CA-CB	6.89	1.62	1.53
1	C	403	SER	C-O	-6.88	1.15	1.23
1	B	172	ASP	CA-C	-6.87	1.44	1.52
1	B	63	ASP	CA-C	-6.87	1.46	1.53
1	C	183	ASP	CA-C	6.87	1.60	1.52
1	C	47	SER	CA-C	-6.81	1.43	1.52
1	B	438	PRO	N-CD	-6.80	1.38	1.47
1	B	414	ASN	CA-C	6.80	1.60	1.52
1	B	103	THR	CA-C	6.80	1.62	1.52
1	A	375	ALA	CA-C	6.79	1.61	1.52
1	C	337	PRO	CA-C	-6.78	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	ILE	C-N	6.77	1.42	1.33
1	B	356	GLY	CA-C	-6.76	1.45	1.52
1	B	374	GLN	N-CA	-6.75	1.38	1.46
1	B	341	PHE	C-N	-6.74	1.26	1.33
1	C	78	PHE	CA-C	-6.69	1.44	1.52
1	A	258	ASP	CA-CB	6.66	1.63	1.53
1	A	566	VAL	N-CA	6.66	1.54	1.46
1	A	68	TRP	CA-CB	6.66	1.64	1.53
1	C	109	MET	N-CA	-6.66	1.37	1.46
1	B	357	PHE	C-N	6.65	1.39	1.33
1	C	367	ALA	CA-C	6.64	1.59	1.52
1	A	499	SER	CA-CB	6.64	1.63	1.53
1	B	282	GLY	CA-C	-6.64	1.42	1.51
1	C	409	THR	N-CA	6.62	1.54	1.46
1	B	214	GLU	CA-C	-6.59	1.44	1.52
1	A	498	LEU	CA-CB	6.59	1.63	1.53
1	B	235	ASP	C-N	6.58	1.43	1.33
1	A	227	ARG	CD-NE	6.57	1.55	1.46
1	C	425	VAL	N-CA	6.55	1.53	1.46
1	C	46	SER	CA-C	-6.54	1.44	1.53
1	A	339	MET	N-CA	-6.52	1.37	1.46
1	C	398	GLN	CA-C	-6.51	1.44	1.52
1	A	114	ALA	N-CA	-6.48	1.38	1.46
1	A	92	THR	C-N	6.46	1.41	1.33
1	C	68	TRP	C-N	-6.43	1.25	1.33
1	C	155	HIS	CA-C	-6.43	1.45	1.52
1	C	412	ASN	CA-C	-6.42	1.44	1.52
1	C	81	SER	C-N	6.41	1.41	1.34
1	B	70	THR	CA-CB	-6.41	1.43	1.53
1	C	183	ASP	CA-CB	6.39	1.61	1.53
1	A	227	ARG	CA-C	-6.39	1.44	1.52
1	B	328	ILE	CA-CB	6.38	1.61	1.54
1	C	95	HIS	ND1-CE1	6.38	1.39	1.32
1	A	183	ASP	CA-CB	6.37	1.61	1.53
1	A	368	PRO	N-CA	-6.35	1.39	1.47
1	B	223	PHE	N-CA	-6.35	1.37	1.45
1	A	113	TRP	C-N	6.34	1.41	1.33
1	A	143	GLU	C-N	6.31	1.41	1.33
1	A	364	ASN	CA-CB	6.30	1.63	1.53
1	B	347	PRO	C-N	6.29	1.41	1.33
1	C	392	THR	CA-C	-6.25	1.44	1.52
1	C	406	ALA	N-CA	6.25	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	HIS	CD2-NE2	6.24	1.44	1.37
1	C	328	ILE	CA-CB	-6.23	1.47	1.54
1	B	226	ILE	C-O	-6.23	1.16	1.24
1	B	65	GLN	CA-C	-6.22	1.44	1.52
1	A	244	THR	C-O	6.22	1.31	1.23
1	B	76	ASP	CA-C	6.21	1.60	1.52
1	B	237	ILE	CA-CB	6.20	1.61	1.54
1	B	61	GLN	CA-C	-6.19	1.44	1.53
1	B	534	PHE	CA-CB	6.14	1.63	1.53
1	A	377	GLU	CA-CB	6.13	1.62	1.53
1	A	455	VAL	CA-C	-6.13	1.44	1.52
1	C	549	GLU	C-N	6.12	1.42	1.33
1	C	331	VAL	CA-CB	-6.11	1.46	1.54
1	B	276	ARG	CZ-NH2	-6.11	1.25	1.33
1	B	277	HIS	CD2-NE2	6.10	1.44	1.37
1	B	277	HIS	CA-C	6.09	1.60	1.52
1	C	538	THR	CA-CB	-6.09	1.43	1.53
1	A	388	LEU	C-N	6.06	1.40	1.33
1	A	175	PRO	N-CD	-6.06	1.39	1.47
1	B	493	PRO	N-CA	-6.06	1.39	1.47
1	B	323	ALA	N-CA	6.04	1.54	1.46
1	B	496	ILE	C-N	6.04	1.41	1.33
1	C	374	GLN	N-CA	-6.02	1.39	1.46
1	C	172	ASP	C-N	6.02	1.41	1.33
1	C	200	ASN	CA-C	6.02	1.61	1.52
1	C	564	THR	C-N	-6.02	1.25	1.33
1	B	403	SER	C-N	6.01	1.40	1.33
1	A	140	PRO	C-N	6.01	1.41	1.33
1	B	410	GLY	C-N	5.99	1.41	1.33
1	B	389	GLN	C-N	-5.98	1.25	1.33
1	C	507	LEU	CA-C	5.97	1.59	1.52
1	B	116	GLY	CA-C	-5.96	1.45	1.52
1	C	196	ASN	CA-C	-5.96	1.45	1.52
1	B	178	TYR	CA-C	-5.94	1.45	1.52
1	C	161	ARG	C-N	5.93	1.41	1.33
1	A	519	PHE	N-CA	5.93	1.53	1.45
1	B	473	VAL	CA-CB	-5.91	1.46	1.54
1	B	232	LYS	N-CA	5.91	1.53	1.45
1	C	358	GLY	C-N	5.91	1.40	1.33
1	C	414	ASN	CA-CB	5.90	1.62	1.53
1	C	273	THR	N-CA	5.90	1.53	1.46
1	C	469	ARG	CA-C	-5.90	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	TYR	C-N	5.89	1.42	1.33
1	B	259	GLY	C-N	5.89	1.41	1.33
1	C	319	ASN	CA-C	-5.87	1.45	1.52
1	C	354	TRP	CA-CB	5.87	1.61	1.53
1	A	102	PHE	CA-CB	5.87	1.62	1.53
1	C	492	LEU	CA-C	5.87	1.60	1.52
1	C	346	SER	CA-C	5.86	1.59	1.53
1	B	131	GLY	C-N	5.86	1.40	1.33
1	B	312	ALA	CA-C	5.86	1.60	1.52
1	C	247	VAL	CA-CB	-5.84	1.47	1.54
1	A	95	HIS	ND1-CE1	5.84	1.38	1.32
1	C	153	PHE	N-CA	-5.84	1.36	1.45
1	B	284	THR	C-N	5.84	1.42	1.33
1	B	546	ASP	CA-CB	5.82	1.61	1.53
1	C	168	ILE	CA-CB	-5.82	1.47	1.54
1	C	122	ILE	CA-C	5.80	1.60	1.52
1	B	546	ASP	N-CA	-5.79	1.39	1.46
1	C	56	GLY	CA-C	-5.79	1.44	1.51
1	B	97	PRO	N-CA	-5.79	1.40	1.47
1	A	510	GLY	CA-C	5.78	1.59	1.51
1	B	203	GLY	C-N	5.78	1.42	1.33
1	C	313	LEU	CA-C	-5.76	1.45	1.52
1	A	191	VAL	CA-C	-5.76	1.45	1.52
1	B	564	THR	N-CA	5.76	1.53	1.46
1	C	76	ASP	CA-CB	5.75	1.63	1.53
1	B	235	ASP	CA-CB	5.74	1.62	1.53
1	A	224	VAL	C-N	5.74	1.41	1.33
1	C	542	THR	CA-CB	-5.74	1.46	1.54
1	A	127	GLY	C-N	5.73	1.39	1.33
1	B	120	ARG	CD-NE	-5.72	1.38	1.46
1	A	92	THR	CA-C	-5.71	1.45	1.52
1	A	541	SER	CA-C	5.71	1.59	1.52
1	A	427	SER	N-CA	-5.70	1.39	1.46
1	C	303	SER	C-N	-5.70	1.26	1.33
1	A	355	VAL	N-CA	-5.69	1.39	1.46
1	C	62	VAL	N-CA	5.69	1.52	1.46
1	A	506	ALA	N-CA	-5.65	1.39	1.46
1	B	270	GLY	CA-C	-5.65	1.44	1.52
1	B	465	SER	CA-C	-5.65	1.45	1.52
1	A	140	PRO	N-CA	-5.64	1.40	1.47
1	A	469	ARG	NE-CZ	5.64	1.39	1.33
1	A	566	VAL	CA-C	5.63	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	TYR	C-N	5.62	1.41	1.33
1	A	349	ILE	N-CA	-5.62	1.39	1.46
1	B	96	SER	CA-CB	5.62	1.62	1.54
1	C	269	GLY	C-N	5.60	1.41	1.33
1	C	177	MET	C-N	5.60	1.41	1.33
1	A	305	SER	C-O	-5.58	1.16	1.24
1	C	489	SER	CA-C	-5.58	1.45	1.52
1	A	558	PRO	CA-C	5.58	1.59	1.52
1	C	287	TRP	CD2-CE3	-5.58	1.31	1.40
1	A	491	PRO	N-CA	-5.57	1.40	1.46
1	B	95	HIS	ND1-CE1	5.55	1.38	1.32
1	C	365	ASN	C-N	5.55	1.40	1.33
1	C	528	LEU	CA-C	-5.55	1.46	1.52
1	B	485	TYR	CA-C	-5.54	1.45	1.52
1	B	376	TYR	CA-C	-5.54	1.45	1.52
1	A	265	GLN	C-O	-5.53	1.18	1.24
1	C	362	ASN	CA-CB	5.53	1.61	1.53
1	A	111	ALA	CA-C	-5.53	1.45	1.52
1	B	119	PHE	C-N	5.52	1.41	1.33
1	C	183	ASP	N-CA	5.52	1.52	1.46
1	B	524	MET	CA-C	-5.52	1.45	1.52
1	C	301	SER	CA-C	-5.52	1.45	1.52
1	A	407	VAL	CA-C	-5.51	1.45	1.52
1	B	122	ILE	CA-C	-5.51	1.45	1.52
1	C	270	GLY	CA-C	5.51	1.59	1.52
1	B	271	PHE	CA-CB	5.50	1.62	1.53
1	B	401	ALA	CA-C	-5.50	1.45	1.52
1	B	145	GLY	CA-C	-5.50	1.44	1.51
1	C	331	VAL	N-CA	5.50	1.53	1.46
1	A	215	THR	C-N	5.49	1.40	1.33
1	A	68	TRP	NE1-CE2	5.47	1.43	1.37
1	B	113	TRP	CA-C	5.47	1.59	1.52
1	A	280	LEU	C-N	-5.46	1.25	1.33
1	A	177	MET	CA-C	5.46	1.59	1.52
1	A	121	PHE	C-N	-5.46	1.26	1.33
1	B	494	VAL	CA-CB	5.46	1.61	1.54
1	B	90	LEU	N-CA	5.46	1.53	1.46
1	A	376	TYR	CA-C	5.45	1.59	1.52
1	C	163	LEU	CA-C	-5.45	1.45	1.52
1	C	514	VAL	CA-CB	-5.45	1.47	1.54
1	A	68	TRP	N-CA	-5.45	1.40	1.46
1	C	520	ALA	C-N	5.45	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	321	GLY	CA-C	5.44	1.59	1.51
1	A	56	GLY	CA-C	-5.43	1.45	1.51
1	B	100	ASN	CA-CB	5.42	1.60	1.54
1	C	513	PHE	CA-CB	5.42	1.61	1.53
1	A	423	SER	N-CA	5.42	1.52	1.45
1	B	128	VAL	CA-CB	5.42	1.60	1.54
1	A	410	GLY	N-CA	5.41	1.52	1.44
1	A	350	PRO	CA-C	-5.40	1.46	1.52
1	A	457	LYS	CA-C	5.40	1.59	1.52
1	B	70	THR	CA-C	5.40	1.59	1.52
1	A	330	GLN	CA-C	-5.39	1.47	1.53
1	C	156	VAL	CA-C	-5.39	1.46	1.52
1	C	198	LEU	N-CA	-5.39	1.39	1.46
1	C	376	TYR	N-CA	-5.39	1.39	1.45
1	A	553	VAL	C-O	-5.39	1.18	1.24
1	B	101	PRO	C-N	5.38	1.41	1.33
1	B	196	ASN	C-O	-5.38	1.17	1.23
1	B	442	ARG	NE-CZ	5.38	1.39	1.33
1	A	62	VAL	C-N	5.36	1.41	1.33
1	B	495	THR	CA-C	5.35	1.59	1.52
1	B	287	TRP	C-N	5.35	1.40	1.33
1	B	119	PHE	N-CA	-5.35	1.39	1.46
1	C	355	VAL	CA-C	-5.35	1.46	1.52
1	C	369	ALA	CA-C	-5.35	1.46	1.52
1	C	180	PRO	N-CA	-5.34	1.40	1.47
1	C	181	THR	C-N	5.34	1.39	1.33
1	C	430	ASN	CA-C	5.34	1.59	1.52
1	C	552	ASP	CA-CB	5.33	1.62	1.53
1	A	133	LEU	CA-C	5.33	1.59	1.52
1	C	494	VAL	N-CA	-5.32	1.40	1.46
1	A	328	ILE	C-O	-5.32	1.18	1.24
1	B	60	GLN	C-N	5.31	1.39	1.32
1	A	166	VAL	CA-CB	-5.31	1.48	1.54
1	A	485	TYR	C-N	5.31	1.39	1.33
1	A	504	SER	N-CA	5.31	1.52	1.46
1	A	549	GLU	CA-C	-5.31	1.44	1.52
1	C	528	LEU	N-CA	-5.31	1.39	1.46
1	B	479	SER	CA-CB	5.30	1.61	1.53
1	B	77	VAL	CA-C	5.29	1.59	1.52
1	A	393	ASN	C-N	5.29	1.41	1.33
1	B	354	TRP	C-N	5.29	1.41	1.33
1	C	176	ASN	CA-C	-5.29	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	385	PRO	C-N	5.29	1.42	1.33
1	B	303	SER	CA-C	-5.28	1.46	1.52
1	A	424	GLY	CA-C	-5.27	1.45	1.52
1	B	544	LEU	C-O	5.27	1.30	1.24
1	C	129	PHE	CA-C	-5.26	1.46	1.52
1	A	196	ASN	C-N	5.25	1.40	1.33
1	A	319	ASN	C-N	5.25	1.40	1.33
1	B	324	ILE	C-O	-5.24	1.17	1.24
1	B	169	THR	C-N	5.24	1.42	1.33
1	A	234	VAL	CA-C	5.23	1.61	1.52
1	B	118	GLN	CA-CB	5.23	1.61	1.53
1	B	68	TRP	CA-CB	5.22	1.60	1.53
1	C	93	VAL	C-N	5.21	1.40	1.33
1	A	311	ASN	C-N	5.21	1.40	1.33
1	C	130	GLY	N-CA	5.21	1.51	1.45
1	C	491	PRO	CA-CB	5.20	1.60	1.53
1	C	300	GLY	CA-C	5.20	1.57	1.52
1	B	121	PHE	CA-C	5.20	1.58	1.52
1	C	273	THR	CA-CB	-5.19	1.45	1.53
1	B	441	ASP	C-O	-5.18	1.17	1.24
1	B	217	PRO	CA-C	-5.18	1.45	1.52
1	A	226	ILE	C-O	-5.18	1.18	1.24
1	A	556	VAL	CA-CB	5.18	1.61	1.54
1	A	411	THR	N-CA	5.17	1.52	1.46
1	B	220	ASP	N-CA	-5.17	1.39	1.46
1	C	434	VAL	CA-C	5.17	1.59	1.52
1	C	189	THR	N-CA	-5.17	1.39	1.46
1	A	560	PRO	CA-CB	5.16	1.60	1.53
1	B	144	ILE	N-CA	-5.16	1.40	1.46
1	C	62	VAL	CA-C	5.16	1.58	1.52
1	B	535	TYR	N-CA	5.15	1.52	1.45
1	B	409	THR	CA-C	-5.15	1.46	1.52
1	B	124	ALA	CA-C	-5.14	1.46	1.52
1	C	199	ILE	CA-CB	-5.14	1.47	1.54
1	B	468	ARG	CA-C	5.14	1.59	1.52
1	C	86	PRO	N-CA	-5.13	1.41	1.47
1	A	177	MET	C-N	5.13	1.40	1.33
1	B	365	ASN	CA-C	-5.13	1.46	1.52
1	B	179	HIS	CB-CG	-5.12	1.43	1.50
1	B	399	THR	N-CA	-5.12	1.39	1.46
1	B	464	ALA	CA-C	-5.12	1.46	1.52
1	A	222	GLU	C-O	-5.11	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	ASN	CA-C	-5.11	1.46	1.52
1	A	209	ILE	C-N	5.11	1.40	1.33
1	B	381	ALA	CA-C	-5.10	1.46	1.52
1	B	542	THR	C-N	5.10	1.40	1.33
1	A	167	THR	CA-C	5.09	1.58	1.52
1	C	524	MET	C-N	5.09	1.40	1.33
1	A	473	VAL	CA-CB	5.09	1.60	1.54
1	C	554	ARG	CD-NE	5.09	1.53	1.46
1	C	460	PRO	C-N	5.09	1.40	1.33
1	C	123	VAL	CA-CB	5.08	1.60	1.54
1	C	282	GLY	N-CA	5.08	1.52	1.45
1	B	146	PRO	C-N	5.07	1.39	1.33
1	A	295	ILE	CA-C	-5.07	1.47	1.52
1	A	429	PRO	CA-CB	-5.07	1.46	1.53
1	C	62	VAL	CA-CB	-5.07	1.47	1.55
1	B	107	SER	CA-CB	5.07	1.61	1.53
1	A	291	ARG	CA-CB	5.06	1.59	1.53
1	B	198	LEU	CA-C	-5.06	1.46	1.52
1	B	73	TYR	C-N	5.06	1.40	1.33
1	B	483	THR	N-CA	5.06	1.52	1.46
1	A	292	PHE	CG-CD1	5.06	1.49	1.38
1	B	181	THR	C-N	5.05	1.40	1.33
1	C	283	SER	CA-C	-5.05	1.46	1.52
1	A	179	HIS	CG-CD2	5.05	1.41	1.35
1	A	146	PRO	N-CD	5.04	1.54	1.47
1	A	520	ALA	C-N	5.04	1.40	1.33
1	A	496	ILE	CA-CB	-5.04	1.48	1.54
1	B	177	MET	CA-C	-5.04	1.46	1.52
1	B	467	VAL	CA-C	-5.03	1.46	1.52
1	A	440	PRO	N-CA	5.03	1.54	1.47
1	A	148	LEU	C-O	5.03	1.30	1.24
1	A	228	ALA	CA-C	5.02	1.58	1.53
1	B	418	LEU	CA-C	-5.02	1.46	1.52
1	B	169	THR	CA-C	-5.02	1.46	1.52
1	C	320	ALA	CA-C	5.01	1.59	1.52
1	A	396	GLY	CA-C	5.00	1.58	1.51
1	A	484	GLN	N-CA	-5.00	1.39	1.46
1	B	170	MET	SD-CE	-5.00	1.67	1.79
1	B	560	PRO	CA-CB	5.00	1.60	1.53
1	A	133	LEU	N-CA	5.00	1.51	1.45

All (729) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	PRO	N-CA-C	13.63	127.33	110.70
1	A	238	SER	CA-C-O	-12.13	107.17	118.33
1	C	226	ILE	N-CA-C	11.02	123.19	110.62
1	A	414	ASN	O-C-N	-10.78	109.44	122.16
1	B	255	ASN	OD1-CG-ND2	-10.14	112.46	122.60
1	A	519	PHE	CA-CB-CG	-10.13	103.67	113.80
1	C	348	ASN	CA-CB-CG	-9.86	102.74	112.60
1	A	517	LEU	CA-C-O	9.72	131.03	120.43
1	B	108	GLN	CA-C-N	9.61	133.16	120.28
1	B	108	GLN	C-N-CA	9.61	133.16	120.28
1	A	506	ALA	N-CA-C	9.56	121.70	111.28
1	A	320	ALA	CA-C-O	9.32	130.43	120.55
1	C	492	LEU	O-C-N	-9.28	111.99	120.71
1	B	53	ALA	CA-C-N	9.22	130.22	119.98
1	B	53	ALA	C-N-CA	9.22	130.22	119.98
1	C	486	GLY	O-C-N	-9.10	112.29	123.21
1	A	422	ALA	N-CA-C	9.09	122.02	111.11
1	C	272	SER	O-C-N	-9.03	112.79	123.27
1	B	176	ASN	OD1-CG-ND2	-9.01	113.59	122.60
1	A	53	ALA	CA-C-N	8.98	129.95	119.98
1	A	53	ALA	C-N-CA	8.98	129.95	119.98
1	B	556	VAL	N-CA-CB	-8.93	102.39	112.21
1	A	102	PHE	CA-CB-CG	-8.88	104.92	113.80
1	B	453	ALA	O-C-N	-8.79	116.08	121.71
1	C	559	ARG	O-C-N	-8.67	115.73	121.88
1	A	254	ASP	CA-CB-CG	8.59	121.19	112.60
1	B	292	PHE	CA-CB-CG	-8.56	105.23	113.80
1	C	398	GLN	OE1-CD-NE2	-8.55	114.05	122.60
1	B	554	ARG	O-C-N	-8.53	115.88	121.85
1	A	187	VAL	CA-C-N	8.49	128.43	119.85
1	A	187	VAL	C-N-CA	8.49	128.43	119.85
1	C	512	PHE	CA-CB-CG	8.46	122.25	113.80
1	C	511	GLN	OE1-CD-NE2	-8.40	114.20	122.60
1	C	488	GLY	O-C-N	-8.39	115.77	123.57
1	B	233	THR	CA-C-N	8.38	134.35	120.62
1	B	233	THR	C-N-CA	8.38	134.35	120.62
1	B	289	SER	O-C-N	-8.29	112.81	121.60
1	A	139	PRO	CA-C-O	-8.25	114.96	120.90
1	B	253	ASN	CA-C-O	-8.22	112.67	121.38
1	A	463	PHE	CA-CB-CG	-8.18	105.62	113.80
1	A	454	PRO	N-CA-C	8.11	123.91	111.34
1	A	459	THR	CA-C-N	8.08	128.01	119.85
1	A	459	THR	C-N-CA	8.08	128.01	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	441	ASP	CA-CB-CG	8.05	120.65	112.60
1	C	49	SER	CA-C-N	8.00	131.42	120.46
1	C	49	SER	C-N-CA	8.00	131.42	120.46
1	A	485	TYR	CA-C-N	7.99	129.74	120.71
1	A	485	TYR	C-N-CA	7.99	129.74	120.71
1	A	220	ASP	CA-CB-CG	7.94	120.54	112.60
1	A	490	GLN	O-C-N	-7.94	113.97	122.06
1	C	103	THR	N-CA-CB	7.93	121.78	110.12
1	A	367	ALA	CA-C-N	7.91	127.81	120.21
1	A	367	ALA	C-N-CA	7.91	127.81	120.21
1	B	224	VAL	CA-C-N	7.88	133.31	122.19
1	B	224	VAL	C-N-CA	7.88	133.31	122.19
1	C	107	SER	CA-C-N	7.88	131.18	120.38
1	C	107	SER	C-N-CA	7.88	131.18	120.38
1	B	538	THR	CA-C-O	7.87	129.18	119.11
1	B	176	ASN	N-CA-C	7.86	121.97	112.38
1	A	247	VAL	CB-CA-C	-7.85	101.92	111.97
1	A	57	GLY	CA-C-N	7.84	128.46	120.38
1	A	57	GLY	C-N-CA	7.84	128.46	120.38
1	B	245	THR	N-CA-C	7.83	123.42	113.25
1	A	369	ALA	CA-C-N	7.81	130.75	120.28
1	A	369	ALA	C-N-CA	7.81	130.75	120.28
1	B	54	GLY	O-C-N	-7.78	114.72	122.19
1	A	245	THR	O-C-N	-7.77	113.41	120.71
1	C	248	LEU	CA-C-N	7.76	130.52	120.44
1	C	248	LEU	C-N-CA	7.76	130.52	120.44
1	C	355	VAL	CA-CB-CG1	7.71	123.52	110.40
1	A	107	SER	N-CA-C	7.71	121.78	112.38
1	A	216	ARG	O-C-N	-7.66	116.49	121.85
1	C	389	GLN	O-C-N	-7.62	116.47	121.88
1	C	435	THR	CA-C-O	-7.62	112.85	120.70
1	C	150	VAL	N-CA-C	-7.61	105.30	112.83
1	B	498	LEU	CA-C-O	7.60	128.48	120.42
1	C	529	SER	CA-C-N	7.58	131.22	120.53
1	C	529	SER	C-N-CA	7.58	131.22	120.53
1	B	224	VAL	O-C-N	-7.57	113.11	122.57
1	C	139	PRO	N-CA-C	7.56	119.92	110.70
1	B	93	VAL	CA-C-O	-7.52	112.85	120.90
1	A	462	MET	O-C-N	-7.51	113.04	123.11
1	B	387	ASN	O-C-N	7.51	131.28	122.19
1	C	430	ASN	CA-CB-CG	7.51	120.11	112.60
1	A	559	ARG	NE-CZ-NH2	7.38	125.84	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ALA	N-CA-C	7.33	120.62	110.35
1	A	113	TRP	O-C-N	-7.28	115.61	123.26
1	A	386	ASN	N-CA-C	7.28	121.42	112.54
1	B	458	ASN	CA-CB-CG	-7.27	105.33	112.60
1	C	69	ARG	N-CA-C	7.26	122.27	111.81
1	B	534	PHE	CA-C-O	7.26	129.84	121.28
1	A	45	ASN	CA-C-N	7.25	131.00	120.71
1	A	45	ASN	C-N-CA	7.25	131.00	120.71
1	A	475	ALA	CA-C-N	7.25	131.00	120.71
1	A	475	ALA	C-N-CA	7.25	131.00	120.71
1	A	175	PRO	CA-C-N	7.25	130.72	120.28
1	A	175	PRO	C-N-CA	7.25	130.72	120.28
1	B	496	ILE	N-CA-C	-7.23	103.42	110.72
1	C	322	SER	CB-CA-C	-7.23	98.02	110.09
1	A	99	ASN	CB-CG-ND2	7.22	127.22	116.40
1	B	414	ASN	CA-CB-CG	7.21	119.81	112.60
1	A	389	GLN	CA-C-O	-7.20	112.86	120.28
1	C	183	ASP	O-C-N	7.17	126.42	121.19
1	C	68	TRP	CG-CD2-CE3	-7.17	126.73	133.90
1	C	460	PRO	CB-CA-C	7.16	120.36	110.98
1	B	148	LEU	CA-C-N	7.16	135.22	121.54
1	B	148	LEU	C-N-CA	7.16	135.22	121.54
1	A	474	ASN	OD1-CG-ND2	-7.12	115.47	122.60
1	C	288	SER	N-CA-CB	7.12	121.11	110.29
1	C	482	GLY	CA-C-N	7.11	135.12	121.54
1	C	482	GLY	C-N-CA	7.11	135.12	121.54
1	C	455	VAL	N-CA-CB	-7.10	102.16	111.82
1	B	70	THR	N-CA-C	7.09	120.41	111.69
1	C	319	ASN	CA-CB-CG	-7.05	105.55	112.60
1	A	365	ASN	CA-CB-CG	-7.05	105.55	112.60
1	A	466	VAL	CA-C-O	7.04	128.67	120.71
1	C	212	THR	O-C-N	-7.02	115.19	123.06
1	A	240	ALA	CA-C-O	7.02	128.07	120.20
1	A	95	HIS	CE1-NE2-CD2	-7.01	101.99	109.00
1	A	370	ALA	N-CA-C	6.99	118.90	111.28
1	A	57	GLY	O-C-N	-6.99	114.78	121.77
1	C	503	TYR	CA-C-O	6.99	126.13	118.65
1	C	458	ASN	CA-CB-CG	-6.96	105.64	112.60
1	B	164	GLU	N-CA-CB	6.96	119.43	110.04
1	A	114	ALA	N-CA-CB	-6.96	100.75	111.46
1	C	100	ASN	CA-C-N	6.95	126.93	119.28
1	C	100	ASN	C-N-CA	6.95	126.93	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	HIS	CE1-NE2-CD2	-6.93	102.07	109.00
1	B	383	GLY	O-C-N	-6.91	114.25	122.33
1	A	63	ASP	CA-CB-CG	-6.89	105.71	112.60
1	C	395	SER	CB-CA-C	-6.89	99.92	110.26
1	B	69	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	B	561	SER	N-CA-C	6.88	118.78	111.28
1	C	50	VAL	CA-C-O	6.88	128.11	120.95
1	A	257	TRP	CE2-CD2-CE3	6.87	125.67	118.80
1	B	567	PHE	CA-CB-CG	-6.86	106.94	113.80
1	C	73	TYR	CA-CB-CG	-6.86	101.56	113.90
1	B	368	PRO	N-CA-C	6.83	121.93	111.34
1	B	285	TYR	N-CA-C	-6.82	104.57	113.17
1	B	493	PRO	N-CA-CB	6.82	110.83	103.33
1	B	137	VAL	CA-C-N	-6.82	115.93	123.43
1	B	137	VAL	C-N-CA	-6.82	115.93	123.43
1	B	218	SER	CA-C-N	6.82	129.41	120.28
1	B	218	SER	C-N-CA	6.82	129.41	120.28
1	C	64	GLN	CG-CD-NE2	6.82	126.62	116.40
1	B	168	ILE	CA-C-N	-6.81	113.32	122.72
1	B	168	ILE	C-N-CA	-6.81	113.32	122.72
1	A	386	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	B	115	GLY	CA-C-N	6.81	128.22	120.53
1	B	115	GLY	C-N-CA	6.81	128.22	120.53
1	C	88	SER	CB-CA-C	-6.79	98.06	109.53
1	A	124	ALA	N-CA-C	6.79	118.75	111.36
1	C	55	ILE	CA-C-N	6.78	128.83	120.22
1	C	55	ILE	C-N-CA	6.78	128.83	120.22
1	C	168	ILE	O-C-N	-6.78	116.23	123.14
1	B	488	GLY	CA-C-N	6.77	129.65	120.44
1	B	488	GLY	C-N-CA	6.77	129.65	120.44
1	B	534	PHE	O-C-N	-6.76	115.32	123.10
1	C	98	GLN	OE1-CD-NE2	-6.75	115.84	122.60
1	A	95	HIS	ND1-CE1-NE2	6.74	115.14	108.40
1	C	200	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	C	99	ASN	N-CA-C	6.74	118.71	111.36
1	C	155	HIS	CE1-NE2-CD2	-6.74	102.26	109.00
1	B	459	THR	CA-C-N	6.74	126.72	119.78
1	B	459	THR	C-N-CA	6.74	126.72	119.78
1	A	122	ILE	N-CA-CB	6.72	120.38	111.64
1	C	237	ILE	O-C-N	-6.72	114.17	122.57
1	C	349	ILE	CA-CB-CG1	6.69	121.78	110.40
1	B	296	ASP	CA-C-O	6.69	127.33	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	PRO	N-CA-CB	6.68	110.61	103.39
1	A	465	SER	N-CA-C	6.68	119.33	109.24
1	C	435	THR	N-CA-C	6.68	118.35	111.14
1	B	94	GLN	CA-C-O	-6.67	113.44	121.05
1	A	47	SER	CA-C-N	6.67	130.18	120.71
1	A	47	SER	C-N-CA	6.67	130.18	120.71
1	B	71	ASN	O-C-N	6.67	131.82	123.15
1	C	216	ARG	NE-CZ-NH2	-6.67	113.20	119.20
1	A	67	THR	N-CA-C	-6.66	102.27	112.99
1	A	484	GLN	N-CA-C	-6.66	98.60	108.79
1	B	71	ASN	OD1-CG-ND2	6.66	129.26	122.60
1	B	52	THR	N-CA-C	6.65	118.61	111.36
1	B	192	LEU	CB-CA-C	6.65	121.21	110.16
1	B	196	ASN	CA-C-O	6.65	128.31	120.66
1	B	197	ASN	N-CA-C	6.65	119.87	110.50
1	C	255	ASN	O-C-N	-6.65	113.82	122.39
1	B	207	ASN	CA-CB-CG	6.64	119.24	112.60
1	A	510	GLY	CA-C-O	6.63	126.69	119.06
1	C	100	ASN	O-C-N	-6.62	111.94	121.54
1	A	299	ARG	CA-C-N	6.62	130.50	122.03
1	A	299	ARG	C-N-CA	6.62	130.50	122.03
1	A	455	VAL	O-C-N	-6.61	116.62	123.03
1	B	75	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	A	407	VAL	CA-C-N	6.60	128.87	120.56
1	A	407	VAL	C-N-CA	6.60	128.87	120.56
1	B	534	PHE	CA-CB-CG	-6.59	107.20	113.80
1	C	235	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	144	ILE	O-C-N	-6.59	115.94	122.99
1	C	352	ALA	CA-C-N	6.59	127.25	120.60
1	C	352	ALA	C-N-CA	6.59	127.25	120.60
1	C	73	TYR	CA-C-N	6.58	130.10	120.82
1	C	73	TYR	C-N-CA	6.58	130.10	120.82
1	C	153	PHE	CA-C-N	6.57	128.05	119.84
1	C	153	PHE	C-N-CA	6.57	128.05	119.84
1	A	396	GLY	CA-C-O	6.57	126.31	119.02
1	B	421	MET	CA-C-N	6.56	130.66	120.82
1	B	421	MET	C-N-CA	6.56	130.66	120.82
1	B	57	GLY	O-C-N	-6.56	115.21	121.77
1	A	393	ASN	CA-C-N	6.55	131.82	120.68
1	A	393	ASN	C-N-CA	6.55	131.82	120.68
1	A	391	THR	O-C-N	-6.54	115.94	123.33
1	A	364	ASN	O-C-N	-6.53	114.48	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	PRO	CA-C-O	-6.53	111.09	120.56
1	B	65	GLN	O-C-N	-6.53	115.31	123.27
1	A	125	GLY	N-CA-C	6.52	123.02	111.73
1	A	296	ASP	O-C-N	-6.52	114.52	123.12
1	B	486	GLY	O-C-N	-6.51	116.70	123.48
1	C	77	VAL	CA-CB-CG2	6.50	121.45	110.40
1	C	93	VAL	O-C-N	-6.50	115.55	123.09
1	A	387	ASN	CA-CB-CG	-6.50	106.11	112.60
1	A	334	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	291	ARG	CA-C-O	6.48	127.52	120.58
1	C	182	GLY	O-C-N	-6.48	115.82	121.97
1	A	138	ILE	O-C-N	-6.46	117.30	121.37
1	C	306	GLY	O-C-N	-6.46	116.91	124.15
1	A	173	LEU	CA-C-O	6.44	126.99	119.32
1	C	333	PRO	CA-C-N	6.44	129.90	120.82
1	C	333	PRO	C-N-CA	6.44	129.90	120.82
1	A	277	HIS	CG-CD2-NE2	6.44	113.64	107.20
1	A	448	GLY	N-CA-C	6.44	121.75	114.67
1	B	79	THR	N-CA-CB	6.43	121.05	110.69
1	B	232	LYS	CA-C-N	6.43	133.82	121.54
1	B	232	LYS	C-N-CA	6.43	133.82	121.54
1	A	209	ILE	O-C-N	-6.41	115.92	123.04
1	C	45	ASN	CA-CB-CG	-6.41	106.19	112.60
1	B	49	SER	CA-C-N	6.41	129.24	120.46
1	B	49	SER	C-N-CA	6.41	129.24	120.46
1	B	389	GLN	CA-C-O	-6.40	113.69	120.28
1	C	163	LEU	N-CA-CB	-6.40	101.26	110.80
1	B	179	HIS	CG-CD2-NE2	6.39	113.59	107.20
1	C	99	ASN	CA-CB-CG	-6.38	106.22	112.60
1	A	561	SER	CA-C-O	6.38	127.31	119.97
1	A	538	THR	CA-C-O	6.37	126.42	119.15
1	B	552	ASP	CA-C-N	6.37	131.80	122.94
1	B	552	ASP	C-N-CA	6.37	131.80	122.94
1	C	428	THR	O-C-N	-6.37	114.64	122.16
1	C	53	ALA	O-C-N	-6.36	115.37	122.12
1	B	474	ASN	CA-CB-CG	-6.36	106.24	112.60
1	C	179	HIS	ND1-CE1-NE2	6.35	114.75	108.40
1	B	445	THR	N-CA-C	6.35	118.83	109.24
1	A	431	ALA	CA-C-N	6.34	133.66	121.54
1	A	431	ALA	C-N-CA	6.34	133.66	121.54
1	B	408	VAL	N-CA-C	6.34	116.51	110.42
1	A	127	GLY	CA-C-N	-6.34	115.00	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	GLY	C-N-CA	-6.34	115.00	122.36
1	C	67	THR	O-C-N	-6.34	115.40	122.12
1	A	254	ASP	CA-C-O	-6.33	114.25	121.72
1	B	115	GLY	CA-C-O	6.33	129.17	122.59
1	A	453	ALA	O-C-N	-6.33	117.66	121.71
1	B	196	ASN	CA-CB-CG	-6.33	106.27	112.60
1	C	281	ASN	CA-CB-CG	-6.33	106.27	112.60
1	B	459	THR	N-CA-C	-6.32	100.59	110.14
1	C	159	ASP	O-C-N	-6.32	115.80	123.19
1	B	422	ALA	N-CA-C	6.31	121.78	111.37
1	C	179	HIS	CB-CA-C	-6.30	98.97	108.61
1	A	474	ASN	O-C-N	-6.29	114.22	122.59
1	B	252	GLY	O-C-N	-6.29	114.78	122.71
1	B	51	ALA	CA-C-N	6.29	129.22	120.29
1	B	51	ALA	C-N-CA	6.29	129.22	120.29
1	B	48	ALA	N-CA-CB	6.29	120.83	110.39
1	B	66	GLU	CA-C-N	6.29	133.55	121.54
1	B	66	GLU	C-N-CA	6.29	133.55	121.54
1	C	323	ALA	N-CA-CB	6.29	119.63	110.58
1	A	562	LYS	CG-CD-CE	6.28	125.74	111.30
1	C	344	PHE	CA-CB-CG	6.27	120.07	113.80
1	B	420	VAL	CA-C-O	-6.27	114.64	121.28
1	B	106	LEU	CA-C-O	6.26	127.08	119.38
1	C	49	SER	N-CA-C	6.24	124.09	110.80
1	C	102	PHE	CA-C-N	6.24	128.64	120.28
1	C	102	PHE	C-N-CA	6.24	128.64	120.28
1	B	172	ASP	O-C-N	-6.23	115.97	123.13
1	A	50	VAL	O-C-N	-6.22	115.42	121.83
1	B	352	ALA	CA-C-N	6.22	128.47	120.64
1	B	352	ALA	C-N-CA	6.22	128.47	120.64
1	B	426	ILE	CA-C-N	6.21	130.69	122.30
1	B	426	ILE	C-N-CA	6.21	130.69	122.30
1	A	223	PHE	O-C-N	-6.21	115.33	123.16
1	C	249	THR	N-CA-C	6.21	117.71	111.07
1	C	431	ALA	CA-C-N	6.21	131.13	121.26
1	C	431	ALA	C-N-CA	6.21	131.13	121.26
1	A	245	THR	CA-C-N	6.20	126.10	119.28
1	A	245	THR	C-N-CA	6.20	126.10	119.28
1	B	325	ASP	CA-CB-CG	-6.20	106.40	112.60
1	A	64	GLN	N-CA-C	6.18	123.97	110.80
1	C	424	GLY	O-C-N	-6.18	117.93	123.37
1	A	560	PRO	CA-C-N	6.17	129.69	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	560	PRO	C-N-CA	6.17	129.69	120.31
1	C	529	SER	O-C-N	-6.17	115.46	122.68
1	A	466	VAL	CB-CA-C	-6.16	103.27	110.91
1	A	248	LEU	N-CA-C	6.16	119.99	112.23
1	C	186	LEU	CA-C-O	-6.15	114.25	120.96
1	B	253	ASN	O-C-N	6.14	129.71	123.26
1	A	559	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	C	459	THR	CA-C-N	6.13	126.04	119.85
1	C	459	THR	C-N-CA	6.13	126.04	119.85
1	B	66	GLU	N-CA-C	-6.13	104.68	111.36
1	A	70	THR	O-C-N	-6.12	114.74	122.27
1	C	237	ILE	N-CA-CB	6.12	121.32	111.23
1	A	308	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	C	228	ALA	CA-C-O	6.11	125.37	119.62
1	A	158	ILE	CB-CA-C	-6.11	102.10	110.77
1	C	119	PHE	CA-CB-CG	-6.11	107.69	113.80
1	B	153	PHE	CA-C-O	-6.10	114.34	120.63
1	B	49	SER	N-CA-C	6.10	119.56	111.75
1	B	538	THR	O-C-N	-6.09	113.53	122.43
1	A	355	VAL	CA-CB-CG1	6.09	120.76	110.40
1	C	59	PRO	CA-C-N	6.09	128.44	120.28
1	C	59	PRO	C-N-CA	6.09	128.44	120.28
1	C	102	PHE	N-CA-C	-6.09	104.20	111.69
1	B	414	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	B	164	GLU	CA-C-N	6.08	126.42	119.92
1	B	164	GLU	C-N-CA	6.08	126.42	119.92
1	B	279	ASN	O-C-N	-6.08	114.01	122.76
1	A	173	LEU	N-CA-C	-6.07	105.16	113.30
1	C	489	SER	CA-C-O	6.07	126.41	119.18
1	A	77	VAL	CA-CB-CG2	6.07	120.72	110.40
1	A	406	ALA	N-CA-C	6.06	119.05	110.50
1	B	196	ASN	O-C-N	-6.06	115.88	123.27
1	B	479	SER	CA-C-N	6.06	128.40	120.28
1	B	479	SER	C-N-CA	6.06	128.40	120.28
1	A	46	SER	CA-C-N	6.05	129.30	120.71
1	A	46	SER	C-N-CA	6.05	129.30	120.71
1	A	385	PRO	CA-C-N	6.05	130.82	120.72
1	A	385	PRO	C-N-CA	6.05	130.82	120.72
1	A	110	TYR	CA-C-O	6.04	127.11	120.71
1	A	277	HIS	N-CA-C	-6.02	98.59	108.76
1	C	325	ASP	N-CA-C	-6.01	105.87	112.72
1	B	388	LEU	N-CA-C	6.01	119.19	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ALA	CA-C-O	-6.01	113.75	120.66
1	C	65	GLN	N-CA-C	6.00	119.27	107.98
1	A	82	VAL	CA-C-N	5.99	128.80	120.29
1	A	82	VAL	C-N-CA	5.99	128.80	120.29
1	C	534	PHE	CA-CB-CG	-5.99	107.81	113.80
1	B	473	VAL	CA-CB-CG2	5.99	120.58	110.40
1	B	179	HIS	N-CA-C	-5.98	102.06	110.31
1	B	83	ALA	CA-C-N	5.97	129.19	120.71
1	B	83	ALA	C-N-CA	5.97	129.19	120.71
1	A	115	GLY	CA-C-O	-5.96	116.36	122.26
1	C	155	HIS	CA-CB-CG	-5.96	107.84	113.80
1	C	50	VAL	CB-CA-C	-5.96	104.09	112.14
1	A	379	GLY	O-C-N	-5.96	116.87	123.66
1	C	506	ALA	N-CA-CB	-5.95	101.32	110.42
1	A	47	SER	O-C-N	-5.95	115.56	122.87
1	A	183	ASP	CA-C-N	5.95	126.10	119.32
1	A	183	ASP	C-N-CA	5.95	126.10	119.32
1	B	553	VAL	O-C-N	-5.95	116.74	123.10
1	A	308	ASN	CA-CB-CG	-5.94	106.66	112.60
1	A	486	GLY	O-C-N	-5.94	116.90	122.96
1	B	429	PRO	CA-C-N	5.94	132.88	121.54
1	B	429	PRO	C-N-CA	5.94	132.88	121.54
1	C	563	SER	N-CA-CB	5.93	118.89	109.51
1	C	281	ASN	N-CA-C	-5.93	105.35	113.30
1	C	190	LEU	N-CA-CB	-5.93	100.38	110.16
1	C	328	ILE	N-CA-C	5.92	116.09	110.53
1	C	326	ASN	CA-C-O	5.92	125.72	119.69
1	C	237	ILE	CA-C-O	5.91	128.16	120.78
1	C	111	ALA	O-C-N	-5.90	114.96	122.34
1	C	555	PRO	CA-C-O	-5.90	114.23	121.31
1	B	354	TRP	CB-CG-CD1	-5.89	118.06	126.90
1	C	159	ASP	CA-C-O	5.89	127.34	120.80
1	B	160	ALA	N-CA-CB	-5.89	101.15	110.28
1	B	384	ALA	N-CA-C	5.88	118.20	110.08
1	B	48	ALA	CA-C-N	5.88	128.96	120.38
1	B	48	ALA	C-N-CA	5.88	128.96	120.38
1	A	494	VAL	O-C-N	-5.88	115.78	121.83
1	B	50	VAL	CA-CB-CG2	5.87	120.38	110.40
1	B	189	THR	O-C-N	-5.87	115.60	123.23
1	B	82	VAL	CA-C-N	5.86	128.14	120.28
1	B	82	VAL	C-N-CA	5.86	128.14	120.28
1	C	432	SER	N-CA-C	5.86	119.09	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	LEU	O-C-N	-5.86	116.65	123.27
1	A	414	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	C	100	ASN	CA-C-O	5.86	124.47	119.66
1	C	180	PRO	CA-C-O	-5.86	114.28	121.31
1	A	223	PHE	CA-CB-CG	-5.86	107.94	113.80
1	A	369	ALA	N-CA-CB	-5.84	100.36	110.17
1	B	64	GLN	CA-C-O	-5.83	114.93	121.81
1	B	249	THR	N-CA-CB	5.83	118.79	110.16
1	C	547	LEU	CA-C-N	5.83	128.41	120.54
1	C	547	LEU	C-N-CA	5.83	128.41	120.54
1	A	275	ASN	CA-CB-CG	-5.83	106.77	112.60
1	C	228	ALA	O-C-N	-5.82	113.39	121.12
1	B	138	ILE	N-CA-CB	-5.80	105.40	111.61
1	C	347	PRO	N-CA-CB	-5.80	96.22	102.60
1	A	487	THR	N-CA-C	5.80	118.99	109.72
1	B	367	ALA	CA-C-O	-5.79	114.14	119.76
1	A	530	VAL	CA-C-O	5.79	127.31	121.17
1	A	303	SER	N-CA-C	-5.79	100.57	108.38
1	B	73	TYR	CB-CG-CD1	-5.78	112.12	120.80
1	B	421	MET	N-CA-C	5.78	118.16	110.53
1	C	370	ALA	CA-C-N	5.77	128.59	120.28
1	C	370	ALA	C-N-CA	5.77	128.59	120.28
1	B	266	PRO	N-CA-CB	-5.77	97.98	103.34
1	A	336	PHE	N-CA-C	5.76	117.78	109.48
1	B	299	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	C	150	VAL	CA-C-N	5.76	127.92	120.44
1	C	150	VAL	C-N-CA	5.76	127.92	120.44
1	C	293	ALA	CA-C-N	5.75	129.97	120.94
1	C	293	ALA	C-N-CA	5.75	129.97	120.94
1	A	59	PRO	CA-C-N	5.75	131.84	122.81
1	A	59	PRO	C-N-CA	5.75	131.84	122.81
1	A	488	GLY	O-C-N	-5.75	118.19	123.42
1	A	216	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	C	448	GLY	CA-C-O	-5.74	112.84	119.10
1	B	84	ASP	N-CA-C	5.74	118.55	110.23
1	A	75	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	331	VAL	CB-CA-C	-5.74	101.88	111.29
1	B	57	GLY	CA-C-N	5.74	126.29	120.38
1	B	57	GLY	C-N-CA	5.74	126.29	120.38
1	A	139	PRO	CA-C-N	5.74	125.50	119.76
1	A	139	PRO	C-N-CA	5.74	125.50	119.76
1	C	68	TRP	CE2-CD2-CE3	5.72	124.52	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	465	SER	O-C-N	-5.72	115.71	123.15
1	B	286	GLY	O-C-N	-5.72	117.89	122.81
1	A	223	PHE	CB-CA-C	-5.72	98.90	109.37
1	A	483	THR	N-CA-C	5.72	122.98	110.80
1	B	525	GLU	CA-C-N	5.72	130.89	122.94
1	B	525	GLU	C-N-CA	5.72	130.89	122.94
1	C	183	ASP	CA-C-O	-5.72	115.97	121.34
1	C	563	SER	CA-C-O	-5.72	114.13	120.70
1	C	559	ARG	CA-C-N	5.71	125.73	119.90
1	C	559	ARG	C-N-CA	5.71	125.73	119.90
1	B	275	ASN	CA-CB-CG	-5.71	106.89	112.60
1	C	161	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	B	138	ILE	O-C-N	-5.70	116.28	121.41
1	B	308	ASN	CA-CB-CG	-5.70	106.91	112.60
1	B	121	PHE	CA-CB-CG	-5.69	108.11	113.80
1	A	341	PHE	CA-CB-CG	5.69	119.49	113.80
1	B	440	PRO	CA-C-N	5.69	128.47	120.28
1	B	440	PRO	C-N-CA	5.69	128.47	120.28
1	B	217	PRO	N-CA-CB	5.68	108.61	103.33
1	C	358	GLY	O-C-N	-5.68	118.49	123.88
1	B	413	GLN	CB-CG-CD	-5.67	102.96	112.60
1	B	327	PRO	CA-C-N	5.67	127.70	120.56
1	B	327	PRO	C-N-CA	5.67	127.70	120.56
1	A	49	SER	CA-C-O	5.67	126.56	120.55
1	A	471	GLY	CA-C-N	5.67	128.76	120.71
1	A	471	GLY	C-N-CA	5.67	128.76	120.71
1	B	242	LEU	O-C-N	5.67	128.13	122.12
1	C	245	THR	O-C-N	-5.67	114.80	121.32
1	C	474	ASN	CB-CA-C	5.66	119.76	111.73
1	C	290	PRO	CA-C-O	-5.64	111.11	119.18
1	A	260	GLN	OE1-CD-NE2	5.64	128.24	122.60
1	A	122	ILE	O-C-N	-5.64	117.22	123.20
1	B	219	ASP	N-CA-CB	5.63	118.39	110.12
1	C	327	PRO	CB-CA-C	-5.62	103.90	112.11
1	B	552	ASP	N-CA-CB	-5.62	102.28	111.66
1	C	513	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	155	HIS	ND1-CE1-NE2	5.62	114.02	108.40
1	A	530	VAL	N-CA-CB	5.61	117.12	110.55
1	B	429	PRO	O-C-N	5.61	130.12	122.99
1	C	261	ILE	CA-C-N	5.61	129.51	120.82
1	C	261	ILE	C-N-CA	5.61	129.51	120.82
1	C	541	SER	N-CA-C	5.60	117.96	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	490	GLN	OE1-CD-NE2	5.59	128.19	122.60
1	A	155	HIS	CE1-NE2-CD2	-5.59	103.41	109.00
1	B	230	SER	N-CA-CB	5.59	120.96	111.57
1	A	379	GLY	N-CA-C	5.58	119.82	110.56
1	C	448	GLY	O-C-N	5.57	129.72	122.42
1	B	500	LEU	N-CA-C	5.56	117.15	111.14
1	A	325	ASP	CA-CB-CG	-5.56	107.04	112.60
1	A	95	HIS	CG-CD2-NE2	5.56	112.76	107.20
1	C	501	ASN	OD1-CG-ND2	5.55	128.16	122.60
1	C	548	THR	N-CA-C	5.55	117.78	111.11
1	C	171	PRO	CA-C-O	-5.55	115.24	122.12
1	C	501	ASN	O-C-N	-5.55	115.94	123.15
1	B	428	THR	CA-C-O	-5.54	115.36	120.13
1	C	218	SER	N-CA-C	5.54	117.22	110.41
1	B	559	ARG	O-C-N	-5.53	116.46	121.66
1	C	177	MET	CA-C-N	5.53	128.70	120.90
1	C	177	MET	C-N-CA	5.53	128.70	120.90
1	A	448	GLY	CA-C-N	5.53	128.74	120.83
1	A	448	GLY	C-N-CA	5.53	128.74	120.83
1	B	544	LEU	O-C-N	-5.53	115.65	123.01
1	C	47	SER	CA-C-O	5.53	125.90	119.32
1	A	86	PRO	N-CA-CB	5.52	108.24	103.27
1	A	513	PHE	CA-C-O	-5.50	114.32	120.54
1	B	172	ASP	CA-C-O	5.50	126.59	120.43
1	B	126	SER	CA-C-O	5.50	127.11	121.23
1	C	355	VAL	O-C-N	-5.50	117.24	123.18
1	B	294	ASP	N-CA-C	5.50	117.82	110.35
1	C	521	SER	CB-CA-C	-5.50	101.68	110.14
1	A	266	PRO	CB-CA-C	5.49	118.49	110.63
1	C	84	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	151	ARG	CD-NE-CZ	5.49	132.09	124.40
1	A	568	ASN	CA-C-N	5.49	131.59	121.70
1	A	568	ASN	C-N-CA	5.49	131.59	121.70
1	C	161	ARG	CB-CA-C	5.48	120.13	110.37
1	A	85	ALA	CA-C-N	5.47	125.73	119.83
1	A	85	ALA	C-N-CA	5.47	125.73	119.83
1	A	58	PRO	CA-C-O	-5.46	112.64	120.56
1	B	58	PRO	O-C-N	-5.46	115.02	121.46
1	B	238	SER	CA-C-O	-5.46	113.72	119.50
1	B	214	GLU	O-C-N	-5.46	116.53	123.24
1	C	449	THR	O-C-N	-5.45	115.05	121.32
1	A	389	GLN	CA-C-N	5.45	125.36	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	GLN	C-N-CA	5.45	125.36	119.85
1	C	325	ASP	O-C-N	-5.45	115.65	122.35
1	A	257	TRP	CB-CG-CD2	-5.45	119.17	126.80
1	B	498	LEU	O-C-N	-5.45	115.94	122.15
1	C	543	THR	CA-C-O	5.45	127.18	121.19
1	B	384	ALA	O-C-N	-5.44	115.55	121.53
1	C	469	ARG	CA-C-O	5.44	127.47	121.11
1	B	179	HIS	CA-CB-CG	5.44	119.24	113.80
1	A	552	ASP	N-CA-CB	-5.43	103.14	111.56
1	C	531	ASP	O-C-N	-5.43	115.86	122.22
1	A	91	TYR	CD1-CG-CD2	5.43	126.25	118.10
1	B	559	ARG	CA-C-O	-5.43	113.52	120.04
1	C	69	ARG	CA-C-N	5.43	127.56	120.28
1	C	69	ARG	C-N-CA	5.43	127.56	120.28
1	C	506	ALA	CB-CA-C	5.43	118.52	109.56
1	A	320	ALA	O-C-N	-5.43	116.36	122.12
1	B	320	ALA	CA-C-N	5.43	129.33	122.00
1	B	320	ALA	C-N-CA	5.43	129.33	122.00
1	B	446	THR	N-CA-CB	5.43	115.62	109.49
1	A	342	VAL	CA-C-N	5.42	126.62	119.84
1	A	342	VAL	C-N-CA	5.42	126.62	119.84
1	B	245	THR	CA-C-N	5.42	125.25	119.28
1	B	245	THR	C-N-CA	5.42	125.25	119.28
1	A	81	SER	O-C-N	-5.42	116.90	123.03
1	A	154	PRO	CA-C-O	-5.42	115.58	121.27
1	B	194	VAL	O-C-N	-5.41	116.77	122.83
1	B	550	LEU	O-C-N	-5.41	115.39	122.59
1	C	299	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	A	277	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	C	519	PHE	CA-C-N	5.40	128.06	120.28
1	C	519	PHE	C-N-CA	5.40	128.06	120.28
1	B	92	THR	CA-CB-OG1	5.40	117.70	109.60
1	A	501	ASN	CA-C-O	5.40	126.78	120.20
1	C	562	LYS	N-CA-C	-5.40	106.54	113.23
1	A	60	GLN	CB-CG-CD	5.39	121.77	112.60
1	A	495	THR	CB-CA-C	-5.39	102.41	110.88
1	B	295	ILE	CB-CA-C	-5.39	104.44	110.96
1	A	374	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	566	VAL	N-CA-CB	5.39	122.01	110.64
1	B	196	ASN	CB-CA-C	5.39	120.02	109.35
1	A	338	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	239	PRO	CA-C-N	5.38	127.49	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	PRO	C-N-CA	5.38	127.49	120.28
1	A	143	GLU	CB-CG-CD	5.38	121.74	112.60
1	A	334	ASP	CA-C-N	5.38	131.78	122.05
1	A	334	ASP	C-N-CA	5.38	131.78	122.05
1	C	271	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	403	SER	N-CA-C	5.37	118.23	110.28
1	A	481	ASN	CA-CB-CG	-5.37	107.23	112.60
1	B	93	VAL	N-CA-C	5.37	115.44	108.35
1	C	197	ASN	N-CA-C	5.37	118.22	110.28
1	A	138	ILE	CA-C-N	5.37	123.58	119.66
1	A	138	ILE	C-N-CA	5.37	123.58	119.66
1	C	380	PHE	O-C-N	-5.37	116.91	123.19
1	B	55	ILE	N-CA-C	5.36	116.61	109.37
1	C	566	VAL	N-CA-C	5.36	116.93	109.80
1	B	206	THR	N-CA-C	-5.35	100.17	108.90
1	B	427	SER	CA-C-O	-5.35	114.43	120.43
1	C	100	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	203	GLY	CA-C-N	5.35	131.90	121.41
1	A	203	GLY	C-N-CA	5.35	131.90	121.41
1	A	123	VAL	CA-CB-CG1	-5.35	101.31	110.40
1	B	135	ALA	O-C-N	-5.34	117.23	123.27
1	C	566	VAL	CA-CB-CG1	-5.34	101.31	110.40
1	A	216	ARG	CA-C-N	5.34	125.25	119.85
1	A	216	ARG	C-N-CA	5.34	125.25	119.85
1	A	306	GLY	CA-C-N	5.33	131.42	123.05
1	A	306	GLY	C-N-CA	5.33	131.42	123.05
1	B	267	VAL	CA-C-N	5.33	124.96	119.05
1	B	267	VAL	C-N-CA	5.33	124.96	119.05
1	B	552	ASP	N-CA-C	5.33	117.16	109.07
1	B	105	VAL	CA-C-O	-5.32	115.21	120.85
1	A	324	ILE	N-CA-C	5.32	117.73	111.09
1	B	138	ILE	N-CA-C	5.31	113.68	107.89
1	A	457	LYS	CA-C-O	5.31	125.20	119.15
1	C	490	GLN	CA-C-O	-5.31	115.46	120.34
1	C	556	VAL	N-CA-C	-5.31	107.64	113.43
1	C	133	LEU	O-C-N	-5.30	116.29	123.19
1	A	355	VAL	CA-C-N	5.30	126.81	121.35
1	A	355	VAL	C-N-CA	5.30	126.81	121.35
1	A	206	THR	N-CA-CB	5.29	119.43	110.49
1	A	207	ASN	N-CA-C	-5.29	106.72	114.39
1	A	364	ASN	OD1-CG-ND2	5.29	127.89	122.60
1	A	458	ASN	CB-CG-ND2	-5.29	108.47	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	VAL	O-C-N	-5.29	117.75	123.14
1	A	382	THR	O-C-N	-5.28	116.74	123.24
1	B	432	SER	N-CA-C	5.28	117.89	109.96
1	A	90	LEU	CA-C-O	5.28	126.09	120.24
1	C	389	GLN	CA-C-N	5.27	125.73	120.14
1	C	389	GLN	C-N-CA	5.27	125.73	120.14
1	C	439	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	253	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	383	GLY	CA-C-N	5.26	128.66	120.60
1	A	383	GLY	C-N-CA	5.26	128.66	120.60
1	A	478	GLY	CA-C-N	5.26	131.17	122.33
1	A	478	GLY	C-N-CA	5.26	131.17	122.33
1	A	348	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	C	507	LEU	CA-C-O	5.26	126.11	120.38
1	A	336	PHE	CA-C-O	-5.24	114.83	119.75
1	B	552	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	387	ASN	CA-C-N	5.23	128.53	121.05
1	C	387	ASN	C-N-CA	5.23	128.53	121.05
1	A	470	THR	CA-C-O	5.23	126.71	120.28
1	C	280	LEU	N-CA-C	-5.23	106.68	113.16
1	B	307	ASN	N-CA-C	5.22	118.65	111.54
1	B	299	ARG	NH1-CZ-NH2	-5.22	112.51	119.30
1	A	299	ARG	NH1-CZ-NH2	-5.21	112.52	119.30
1	C	439	GLN	CG-CD-NE2	5.21	124.22	116.40
1	A	138	ILE	N-CA-C	-5.21	102.39	107.55
1	B	374	GLN	O-C-N	-5.21	118.08	123.29
1	A	491	PRO	N-CA-CB	5.21	108.20	103.15
1	A	508	MET	CA-C-N	5.20	126.34	119.84
1	A	508	MET	C-N-CA	5.20	126.34	119.84
1	C	336	PHE	CA-CB-CG	-5.20	108.60	113.80
1	C	256	ARG	CA-C-O	-5.20	113.08	120.51
1	A	225	MET	N-CA-C	5.20	121.87	110.80
1	B	319	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	B	359	GLY	O-C-N	-5.19	117.42	123.44
1	B	169	THR	CA-C-O	5.19	126.09	120.43
1	A	555	PRO	CA-C-N	5.18	128.85	120.55
1	A	555	PRO	C-N-CA	5.18	128.85	120.55
1	A	470	THR	O-C-N	-5.18	117.04	123.36
1	C	309	SER	N-CA-CB	5.18	118.84	110.40
1	A	289	SER	CA-C-O	-5.18	115.94	120.60
1	A	277	HIS	CB-CG-ND1	5.18	130.47	122.70
1	C	67	THR	N-CA-C	5.18	116.92	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	PRO	CA-C-O	-5.17	113.06	120.56
1	C	489	SER	O-C-N	-5.17	115.07	122.41
1	C	487	THR	CA-CB-CG2	-5.17	101.72	110.50
1	C	383	GLY	CA-C-O	5.17	124.75	118.86
1	C	238	SER	N-CA-CB	5.16	117.54	110.11
1	C	291	ARG	CD-NE-CZ	5.16	131.63	124.40
1	B	436	TYR	CB-CG-CD1	-5.16	113.06	120.80
1	A	501	ASN	CA-C-N	5.16	128.17	120.95
1	A	501	ASN	C-N-CA	5.16	128.17	120.95
1	B	177	MET	O-C-N	-5.16	117.09	123.33
1	B	149	GLU	CA-C-N	5.15	131.25	121.97
1	B	149	GLU	C-N-CA	5.15	131.25	121.97
1	B	50	VAL	CA-C-O	-5.15	115.59	120.95
1	C	154	PRO	CA-N-CD	-5.15	104.78	112.00
1	A	104	ALA	N-CA-C	-5.15	105.56	111.07
1	B	344	PHE	CA-C-N	-5.15	115.21	122.94
1	B	344	PHE	C-N-CA	-5.15	115.21	122.94
1	A	143	GLU	O-C-N	-5.15	116.61	122.89
1	A	166	VAL	CG1-CB-CG2	-5.15	99.48	110.80
1	B	136	ALA	O-C-N	-5.15	117.30	123.27
1	B	184	PRO	N-CA-CB	5.15	108.09	103.20
1	B	284	THR	CA-CB-OG1	5.15	117.32	109.60
1	A	408	VAL	O-C-N	5.14	126.95	121.91
1	A	497	GLY	O-C-N	-5.14	117.25	122.19
1	C	58	PRO	N-CA-C	5.14	116.98	110.70
1	B	399	THR	CA-C-O	-5.14	114.67	120.43
1	A	382	THR	CA-C-N	5.14	130.27	121.07
1	A	382	THR	C-N-CA	5.14	130.27	121.07
1	B	132	ARG	CD-NE-CZ	-5.14	117.20	124.40
1	A	300	GLY	O-C-N	-5.14	119.21	123.73
1	A	101	PRO	CA-N-CD	-5.13	104.81	112.00
1	A	314	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	556	VAL	N-CA-C	-5.13	105.41	111.00
1	B	523	PHE	CB-CG-CD2	5.13	129.42	120.70
1	B	297	HIS	CG-CD2-NE2	5.13	112.33	107.20
1	A	86	PRO	O-C-N	-5.13	117.11	123.01
1	C	129	PHE	CA-C-O	-5.12	114.79	120.38
1	A	83	ALA	N-CA-C	5.12	116.94	111.36
1	C	345	ASN	CA-CB-CG	-5.12	107.48	112.60
1	C	516	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	121	PHE	O-C-N	-5.11	117.22	123.30
1	C	360	ILE	CA-CB-CG2	5.11	119.19	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	562	LYS	CA-C-O	-5.11	113.29	119.27
1	A	126	SER	N-CA-CB	5.11	119.12	110.49
1	A	561	SER	N-CA-CB	5.11	118.19	110.28
1	B	179	HIS	ND1-CE1-NE2	5.11	113.51	108.40
1	B	202	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	153	PHE	O-C-N	-5.10	115.45	121.32
1	B	535	TYR	CA-C-N	5.09	130.70	122.29
1	B	535	TYR	C-N-CA	5.09	130.70	122.29
1	C	547	LEU	O-C-N	-5.09	115.82	122.39
1	A	377	GLU	CB-CA-C	-5.09	101.45	109.80
1	C	479	SER	N-CA-CB	5.09	120.41	111.55
1	A	356	GLY	O-C-N	-5.09	118.84	123.57
1	C	66	GLU	N-CA-CB	-5.09	102.64	110.42
1	A	272	SER	O-C-N	-5.08	117.37	123.27
1	B	552	ASP	O-C-N	-5.08	117.46	123.25
1	A	361	TRP	O-C-N	-5.07	117.33	123.27
1	B	332	ALA	CA-C-O	5.07	125.08	120.26
1	A	524	MET	CG-SD-CE	-5.07	89.74	100.90
1	A	277	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
1	C	79	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	544	LEU	CA-C-O	-5.07	114.98	120.81
1	C	65	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	C	503	TYR	CB-CG-CD2	5.07	128.40	120.80
1	A	435	THR	O-C-N	-5.07	117.29	123.27
1	A	511	GLN	CA-CB-CG	-5.07	103.97	114.10
1	B	474	ASN	CB-CG-ND2	5.06	124.00	116.40
1	B	60	GLN	CB-CG-CD	-5.06	104.00	112.60
1	B	459	THR	CA-C-O	-5.05	113.98	120.04
1	C	474	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	B	546	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	164	GLU	CA-C-O	-5.04	115.45	120.64
1	C	125	GLY	O-C-N	5.04	129.25	122.70
1	A	196	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	A	487	THR	CB-CA-C	-5.04	99.41	109.33
1	C	103	THR	CB-CA-C	-5.04	102.43	110.79
1	C	154	PRO	N-CA-CB	5.04	108.54	103.25
1	C	185	GLY	CA-C-N	5.03	128.25	121.05
1	C	185	GLY	C-N-CA	5.03	128.25	121.05
1	A	244	THR	OG1-CB-CG2	-5.02	99.25	109.30
1	C	93	VAL	N-CA-C	5.02	114.98	108.35
1	C	264	LEU	CA-C-O	5.02	125.79	120.36
1	C	307	ASN	OD1-CG-ND2	-5.02	117.58	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	VAL	N-CA-C	5.02	115.81	108.53
1	A	328	ILE	CB-CA-C	-5.02	105.44	112.02
1	B	342	VAL	N-CA-C	5.02	113.46	107.73
1	C	136	ALA	CA-C-N	5.02	128.76	122.43
1	C	136	ALA	C-N-CA	5.02	128.76	122.43
1	A	551	ILE	N-CA-C	-5.02	106.78	111.45
1	A	216	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	A	403	SER	CA-C-O	-5.01	115.55	121.16
1	A	535	TYR	CA-CB-CG	-5.01	104.88	113.90
1	C	66	GLU	N-CA-C	5.01	119.38	113.12
1	B	111	ALA	CA-C-N	5.00	125.46	121.61
1	B	111	ALA	C-N-CA	5.00	125.46	121.61
1	A	461	ILE	N-CA-CB	5.00	121.18	111.93
1	B	502	ASN	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Sidechain
1	A	216	ARG	Sidechain
1	A	298	ARG	Sidechain
1	A	299	ARG	Sidechain
1	A	304	TYR	Sidechain
1	A	436	TYR	Sidechain
1	A	468	ARG	Sidechain
1	A	485	TYR	Sidechain
1	A	523	PHE	Sidechain
1	A	533	TYR	Sidechain
1	A	69	ARG	Sidechain
1	A	73	TYR	Sidechain
1	B	151	ARG	Sidechain
1	B	161	ARG	Sidechain
1	B	223	PHE	Sidechain
1	B	227	ARG	Sidechain
1	B	276	ARG	Sidechain
1	B	298	ARG	Sidechain
1	B	341	PHE	Sidechain
1	B	376	TYR	Sidechain
1	B	405	TYR	Sidechain
1	B	468	ARG	Sidechain
1	B	533	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	62	VAL	Peptide,Mainchain
1	B	78	PHE	Sidechain
1	B	91	TYR	Sidechain
1	C	120	ARG	Sidechain
1	C	227	ARG	Sidechain
1	C	229	PRO	Peptide
1	C	231	SER	Peptide
1	C	276	ARG	Sidechain
1	C	285	TYR	Sidechain
1	C	376	TYR	Sidechain
1	C	405	TYR	Sidechain
1	C	469	ARG	Sidechain
1	C	554	ARG	Sidechain
1	C	73	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	A	3901	0	3756	10	0
1	B	3901	0	3756	13	0
1	C	3901	0	3756	11	0
All	All	11703	0	11268	32	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 1.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:HG11	1:B:193:SER:HB3	1.81	0.61
1:C:224:VAL:HG22	1:C:225:MET:H	1.70	0.56
1:B:150:VAL:HG11	1:B:193:SER:CB	2.41	0.51
1:B:446:THR:HB	1:B:447:PRO:HD2	1.93	0.50
1:C:227:ARG:HG2	1:C:228:ALA:H	1.78	0.49
1:B:297:HIS:CD2	1:B:333:PRO:HD3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ALA:HB2	1:A:416:THR:HG21	1.94	0.48
1:B:92:THR:HG23	1:B:191:VAL:HG22	1.96	0.48
1:A:278:TRP:CE2	1:A:284:THR:HB	2.50	0.47
1:B:97:PRO:HA	1:B:117:MET:HE1	1.97	0.46
1:B:110:TYR:CE1	1:B:226:ILE:HD12	2.50	0.46
1:B:354:TRP:CE2	1:B:424:GLY:HA3	2.51	0.46
1:A:154:PRO:HB3	1:B:61:GLN:HE22	1.81	0.46
1:B:153:PHE:CD1	1:C:227:ARG:HB2	2.51	0.45
1:C:164:GLU:HG2	1:C:165:PRO:HD2	1.99	0.45
1:B:379:GLY:O	1:B:400:VAL:HG12	2.17	0.44
1:C:336:PHE:CG	1:C:337:PRO:HD2	2.53	0.44
1:A:517:LEU:HG	1:A:553:VAL:HG22	2.00	0.43
1:C:469:ARG:HD2	1:C:484:GLN:HB2	1.99	0.43
1:B:332:ALA:HB1	1:B:333:PRO:HD2	2.00	0.42
1:A:246:PRO:HA	1:A:249:THR:HG22	2.02	0.42
1:A:392:THR:HG21	1:A:441:ASP:O	2.20	0.42
1:A:331:VAL:O	1:A:332:ALA:HB2	2.19	0.42
1:A:151:ARG:HD2	1:A:195:TYR:CZ	2.55	0.41
1:B:316:TRP:CE2	1:B:418:LEU:HB2	2.55	0.41
1:C:237:ILE:HD13	1:C:237:ILE:HA	1.84	0.41
1:A:57:GLY:N	1:A:58:PRO:CD	2.84	0.41
1:C:436:TYR:CD1	1:C:487:THR:HG21	2.56	0.41
1:A:492:LEU:N	1:A:493:PRO:HD2	2.36	0.40
1:C:224:VAL:HG22	1:C:225:MET:N	2.36	0.40
1:C:62:VAL:HB	1:C:224:VAL:HG23	2.03	0.40
1:C:178:TYR:CE1	1:C:224:VAL:HG12	2.56	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 PDB entries followed by that with respect to all EM entries.

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	A	523/579 (90%)	486 (93%)	31 (6%)	6 (1%)	11	46
1	B	523/579 (90%)	486 (93%)	31 (6%)	6 (1%)	11	46
1	C	523/579 (90%)	491 (94%)	20 (4%)	12 (2%)	5	28
All	All	1569/1737 (90%)	1463 (93%)	82 (5%)	24 (2%)	11	40

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	B	228	ALA
1	C	49	SER
1	A	64	GLN
1	A	332	ALA
1	A	343	PRO
1	B	473	VAL
1	C	126	SER
1	C	434	VAL
1	C	483	THR
1	B	46	SER
1	B	150	VAL
1	B	250	GLY
1	C	230	SER
1	C	250	GLY
1	B	435	THR
1	C	237	ILE
1	A	206	THR
1	A	509	PRO
1	C	227	ARG
1	C	430	ASN
1	C	472	ASP
1	C	174	ARG
1	C	447	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 PDB entries followed by that with respect to all EM entries.

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	A	421/457 (92%)	408 (97%)	13 (3%)	35	56
1	B	421/457 (92%)	402 (96%)	19 (4%)	24	46
1	C	421/457 (92%)	412 (98%)	9 (2%)	47	65
All	All	1263/1371 (92%)	1222 (97%)	41 (3%)	35	56

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	65	GLN
1	A	90	LEU
1	A	122	ILE
1	A	157	VAL
1	A	173	LEU
1	A	224	VAL
1	A	244	THR
1	A	268	PRO
1	A	403	SER
1	A	425	VAL
1	A	454	PRO
1	A	483	THR
1	B	50	VAL
1	B	76	ASP
1	B	86	PRO
1	B	93	VAL
1	B	95	HIS
1	B	105	VAL
1	B	128	VAL
1	B	134	VAL
1	B	142	ILE
1	B	151	ARG
1	B	218	SER
1	B	227	ARG
1	B	268	PRO
1	B	341	PHE
1	B	349	ILE
1	B	355	VAL
1	B	371	THR
1	B	469	ARG
1	B	516	GLN
1	C	58	PRO
1	C	152	GLN

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Mol	Chain	Res	Type
1	C	178	TYR
1	C	227	ARG
1	C	230	SER
1	C	238	SER
1	C	341	PHE
1	C	382	THR
1	C	444	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	210	GLN
1	A	279	ASN
1	A	297	HIS
1	A	365	ASN
1	B	61	GLN
1	B	71	ASN
1	B	176	ASN
1	B	281	ASN
1	B	297	HIS
1	B	326	ASN
1	B	484	GLN
1	B	501	ASN
1	B	516	GLN
1	C	75	ASN
1	C	99	ASN
1	C	100	ASN
1	C	207	ASN
1	C	319	ASN
1	C	365	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

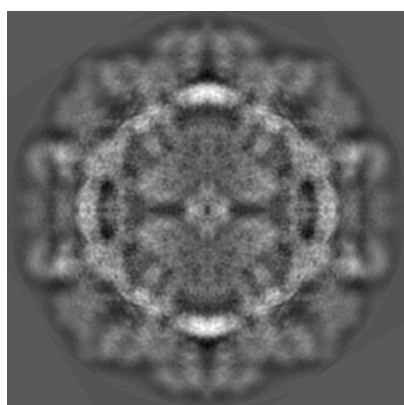
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5410. These allow visual inspection of the internal detail of the map and identification of artifacts.

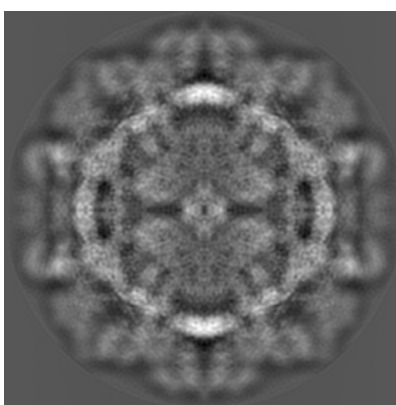
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

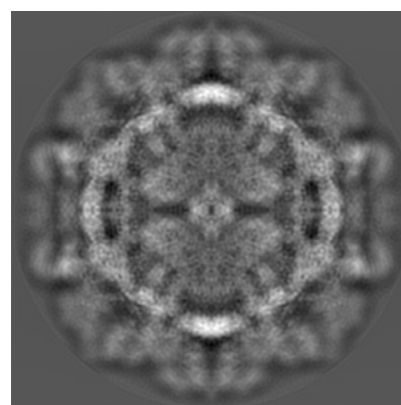
6.1.1 Primary map



X



Y

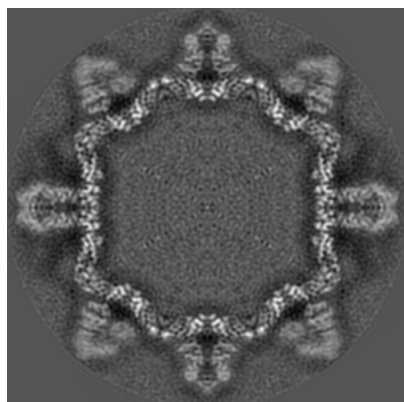


Z

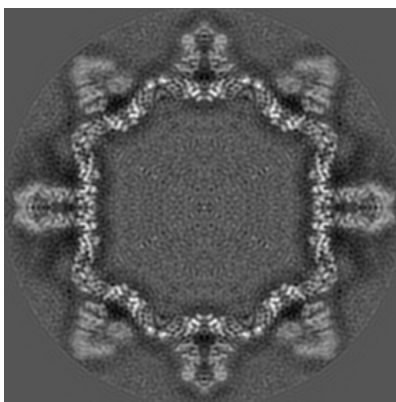
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

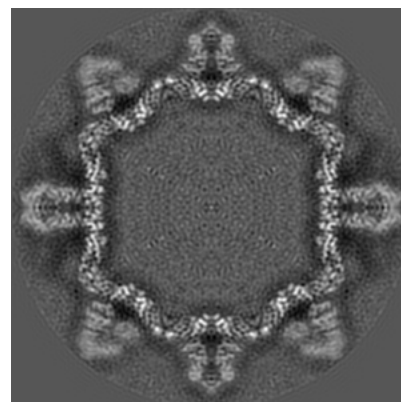
6.2.1 Primary map



X Index: 240



Y Index: 240

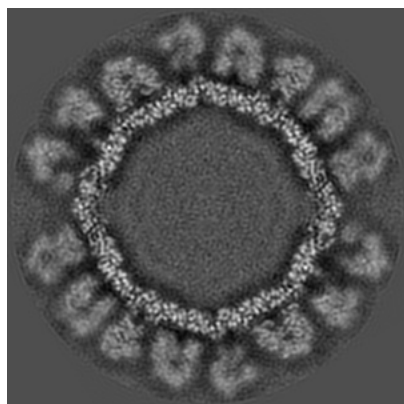


Z Index: 240

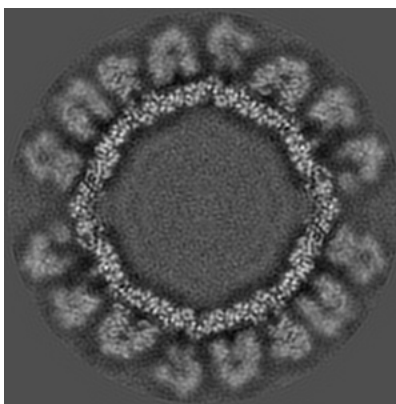
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

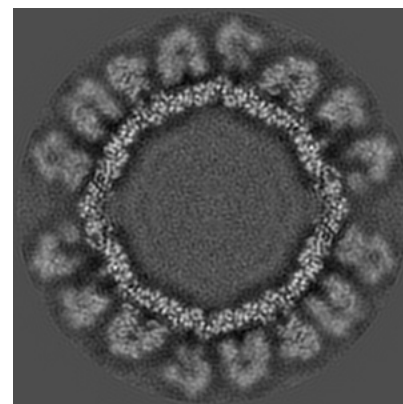
6.3.1 Primary map



X Index: 288



Y Index: 192

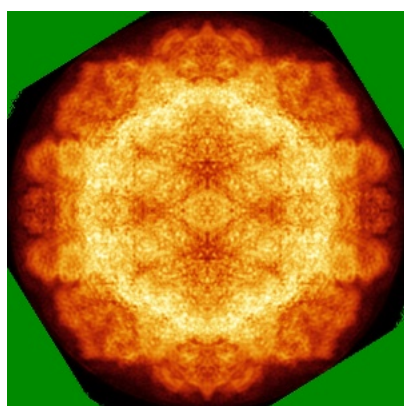


Z Index: 192

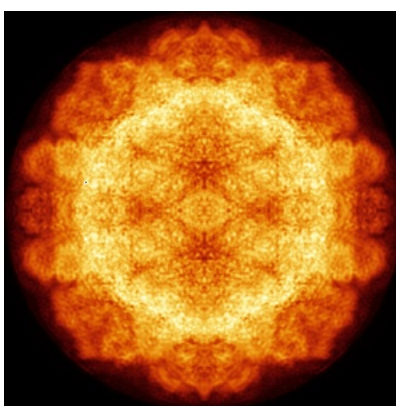
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

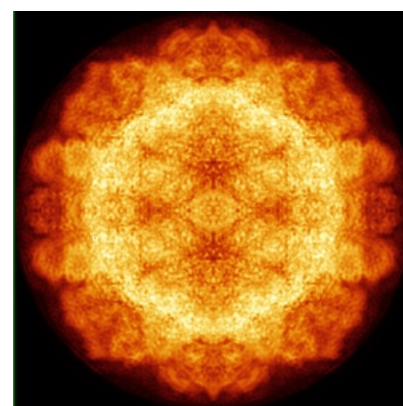
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

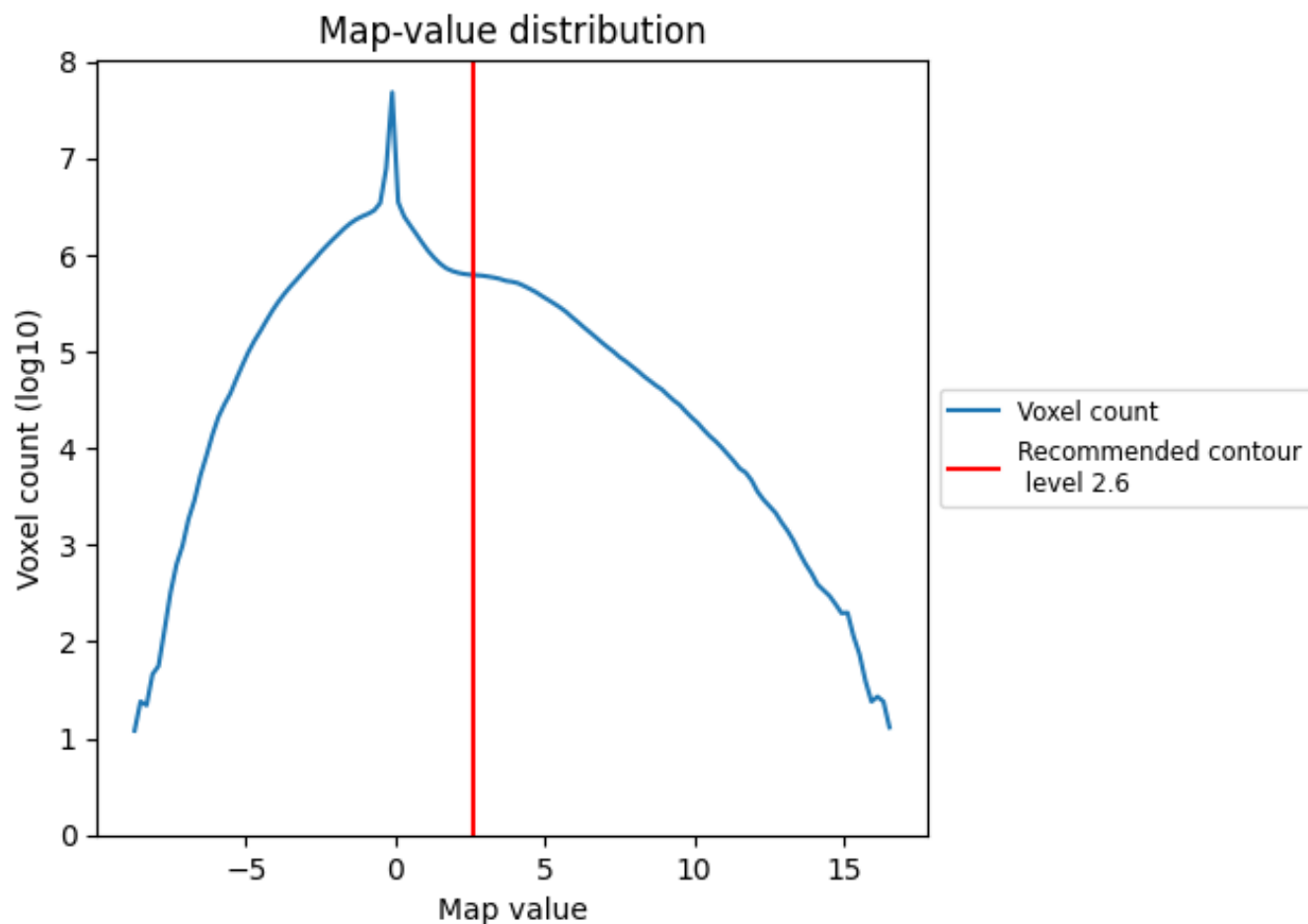
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

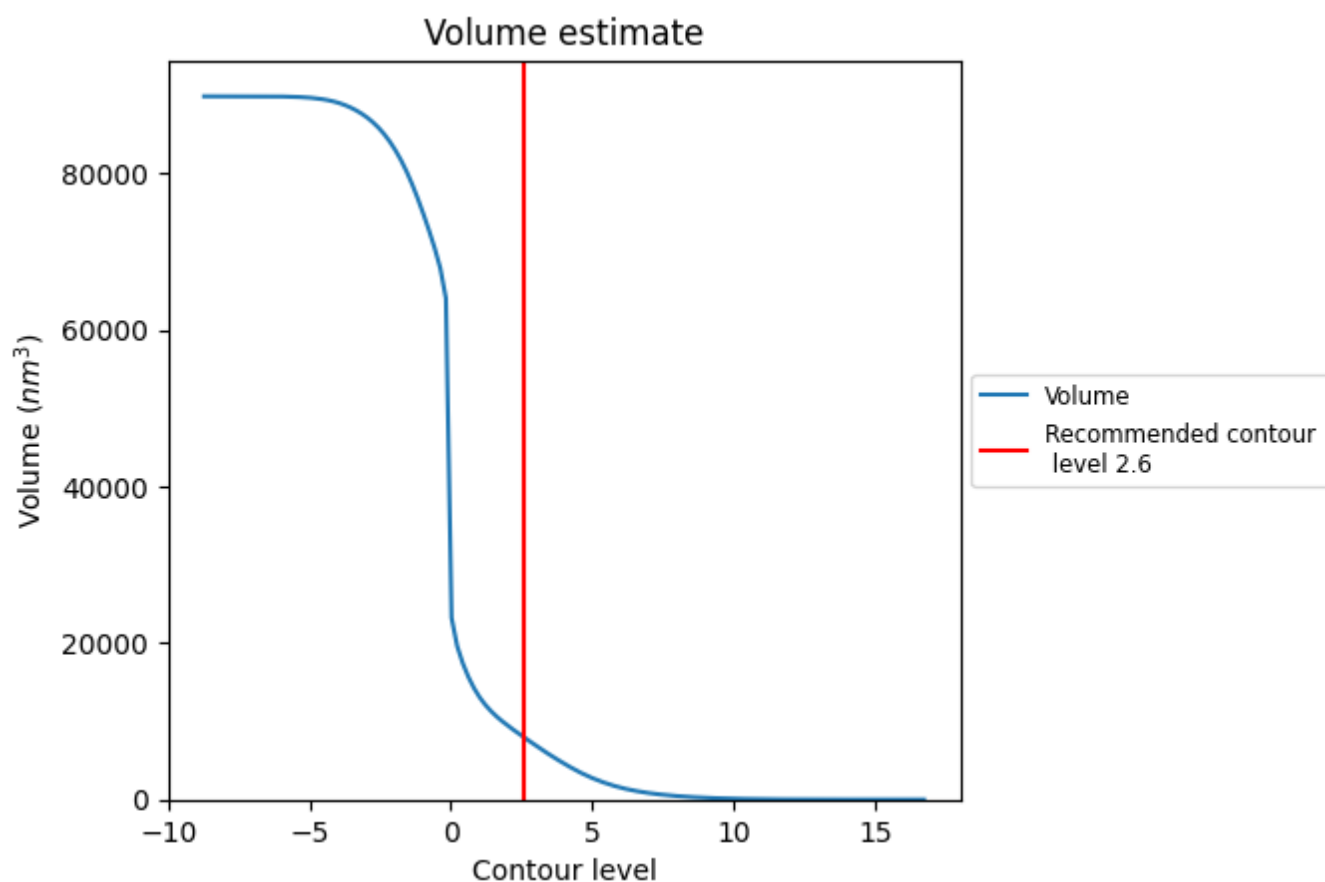
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

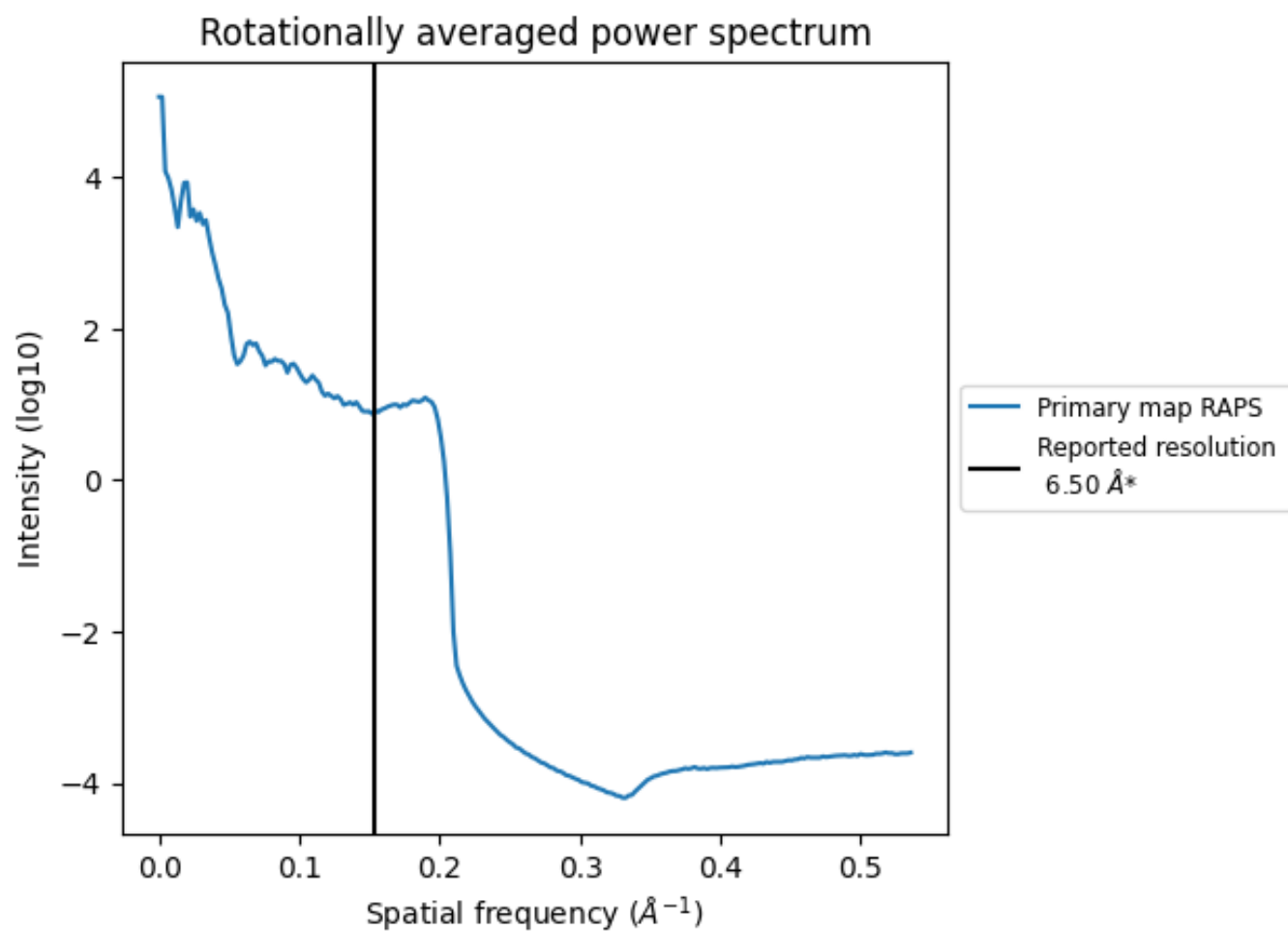
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7913 nm³; this corresponds to an approximate mass of 7148 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.154 Å⁻¹

8 Fourier-Shell correlation ⓘ

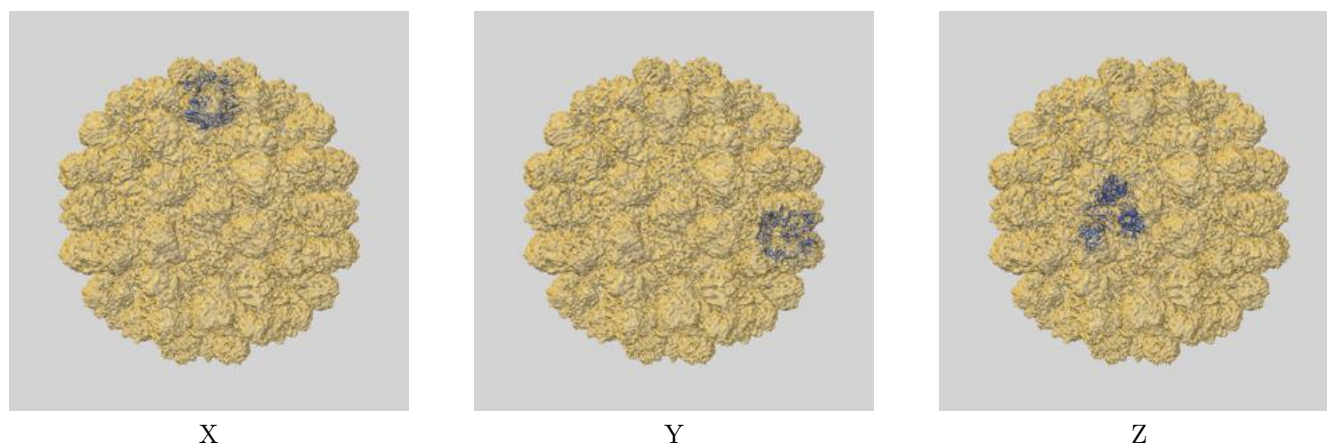
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

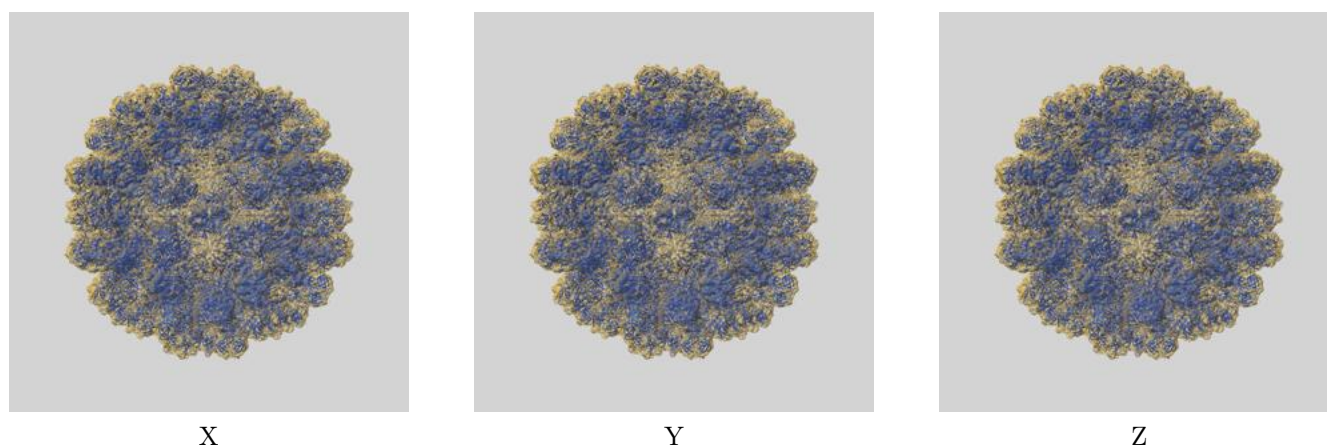
This section contains information regarding the fit between EMDB map EMD-5410 and PDB model 3J1P. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

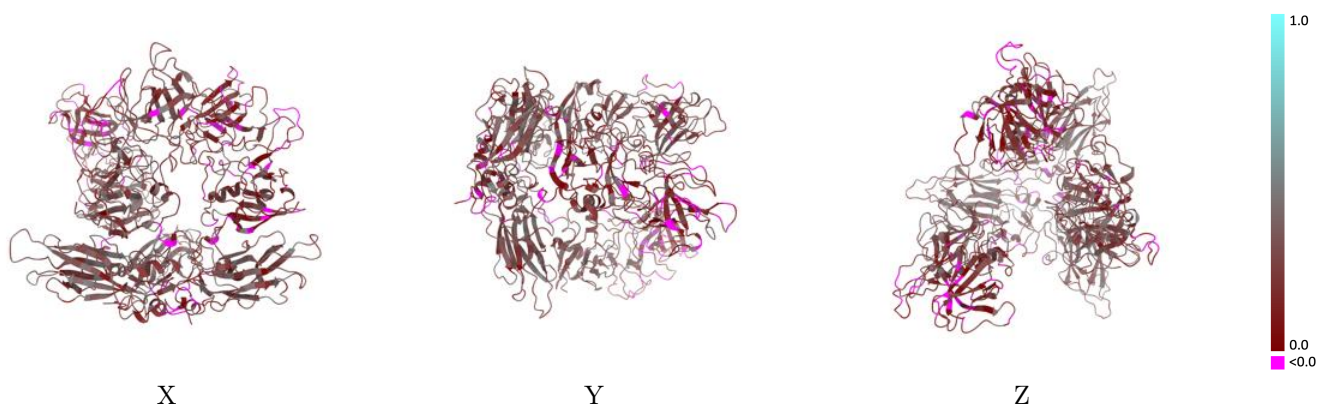


9.1.2 Map-model assembly overlay [i](#)



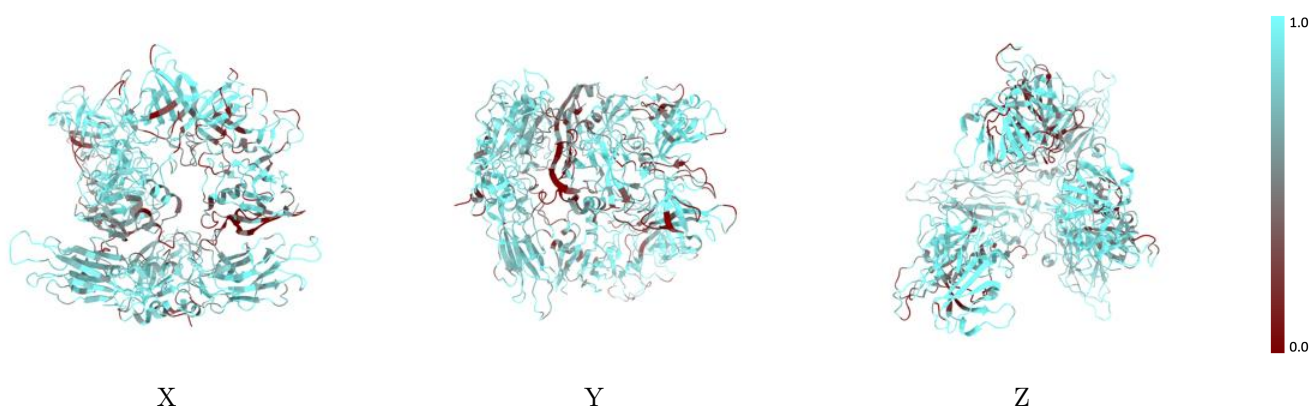
The images above show the 3D surface view of the map at the recommended contour level 2.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



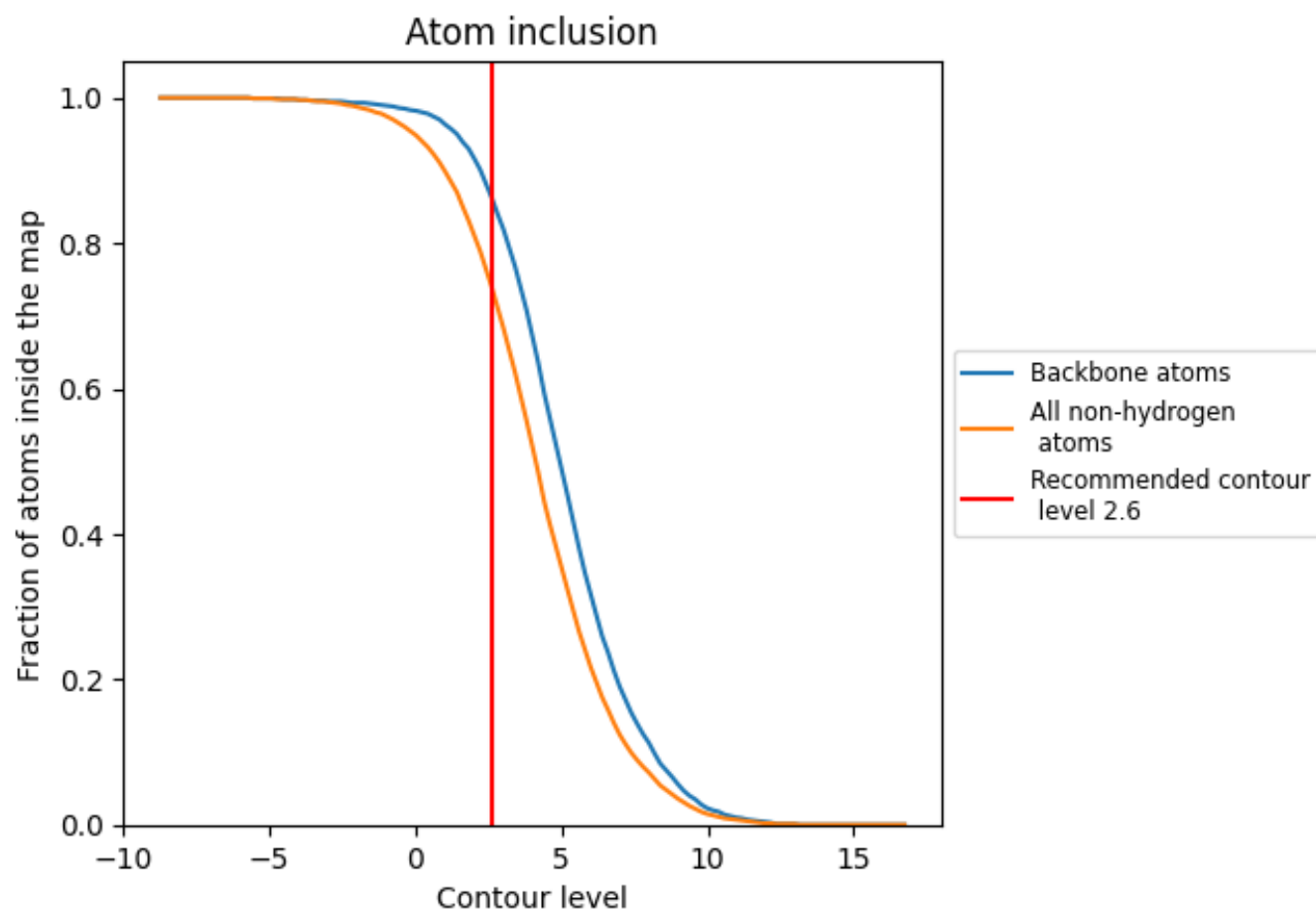
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7410	0.2380
A	0.7590	0.2350
B	0.6920	0.2040
C	0.7710	0.2740

