



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:47 AM UTC

PDB ID : 5JZC / pdb_00005jzc
EMDB ID : EMD-8183
Title : helical filament
Authors : Short, J.; Liu, Y.
Deposited on : 2016-05-16
Resolution : 4.20 Å(reported)

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:

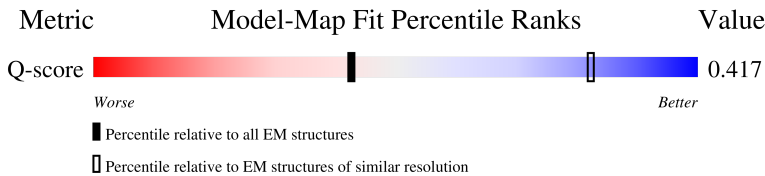
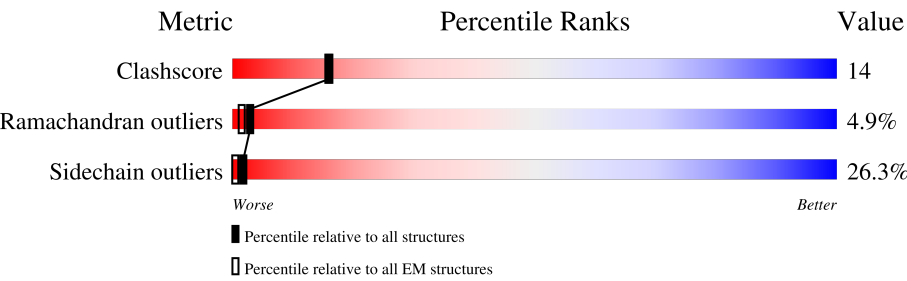
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

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	339	17% 59% 27% 5% • 8%
1	B	339	15% 57% 29% 5% • 8%
1	C	339	14% 58% 28% 5% • 8%
1	D	339	15% 56% 29% 5% • 8%

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Mol	Chain	Length	Quality of chain
1	E	339	14% 57% 28% 6% 8%
1	F	339	14% 59% 26% 5% 8%
1	G	339	15% 59% 27% 5% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11935 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.

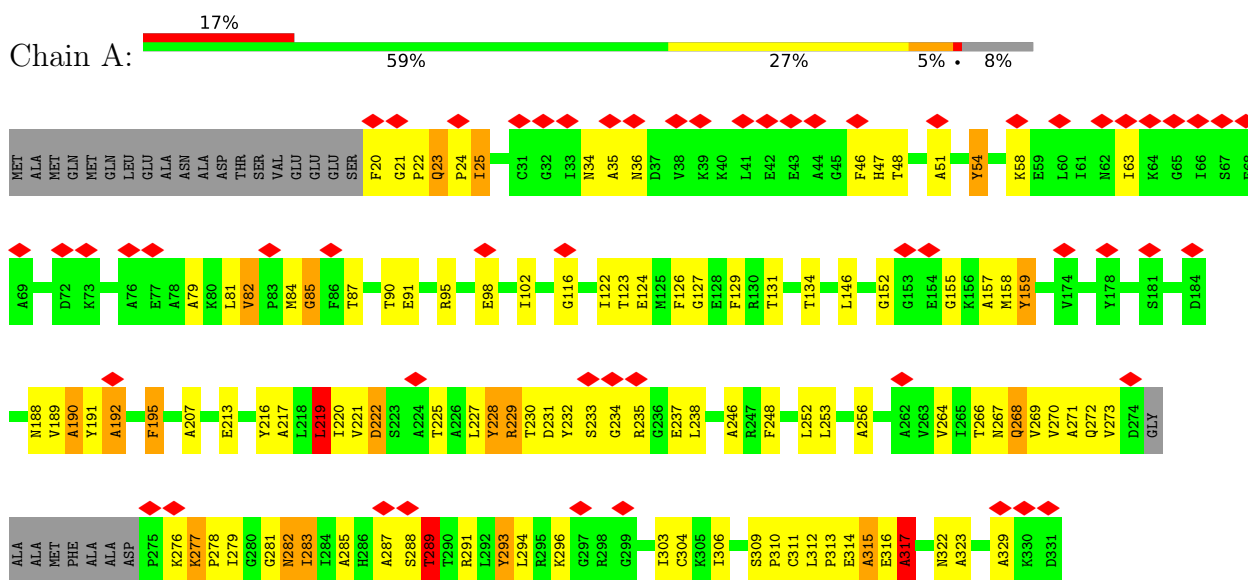
- Molecule 1 is a protein called DNA repair protein RAD51 homolog 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	B	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	C	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	D	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	E	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	F	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	G	312	Total	C	N	O	4	0
			1705	1043	332	330		

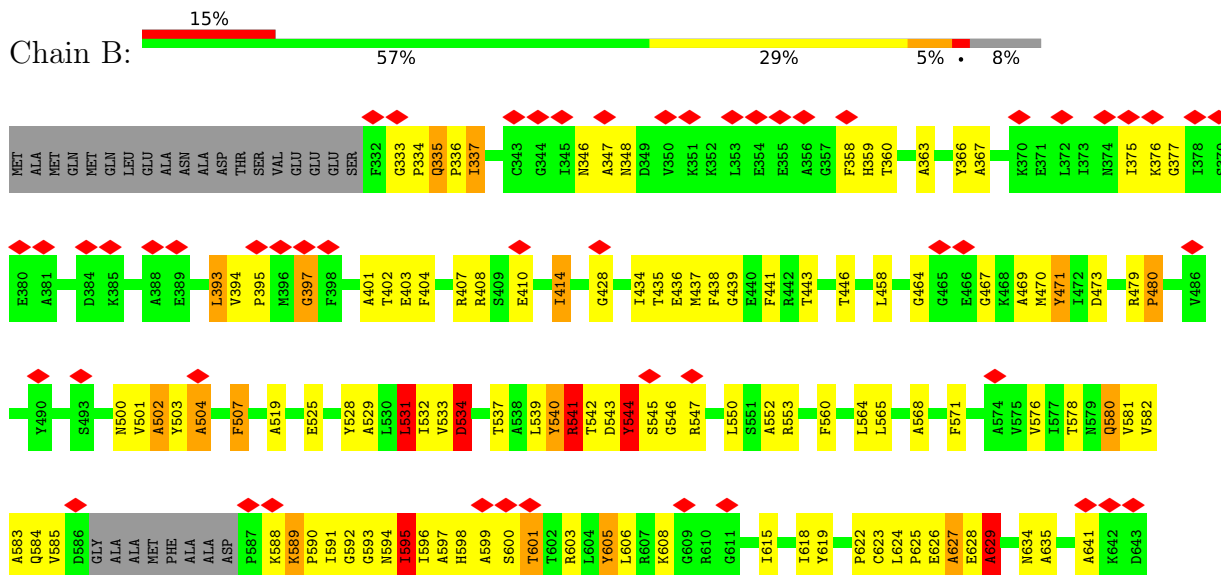
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

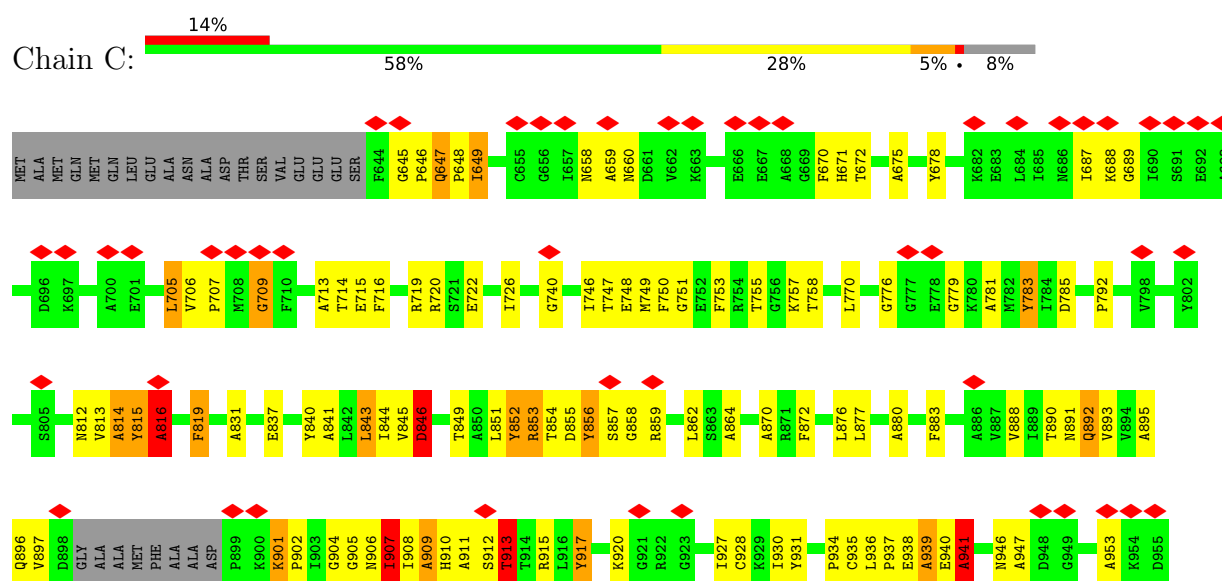
- Molecule 1: DNA repair protein RAD51 homolog 1



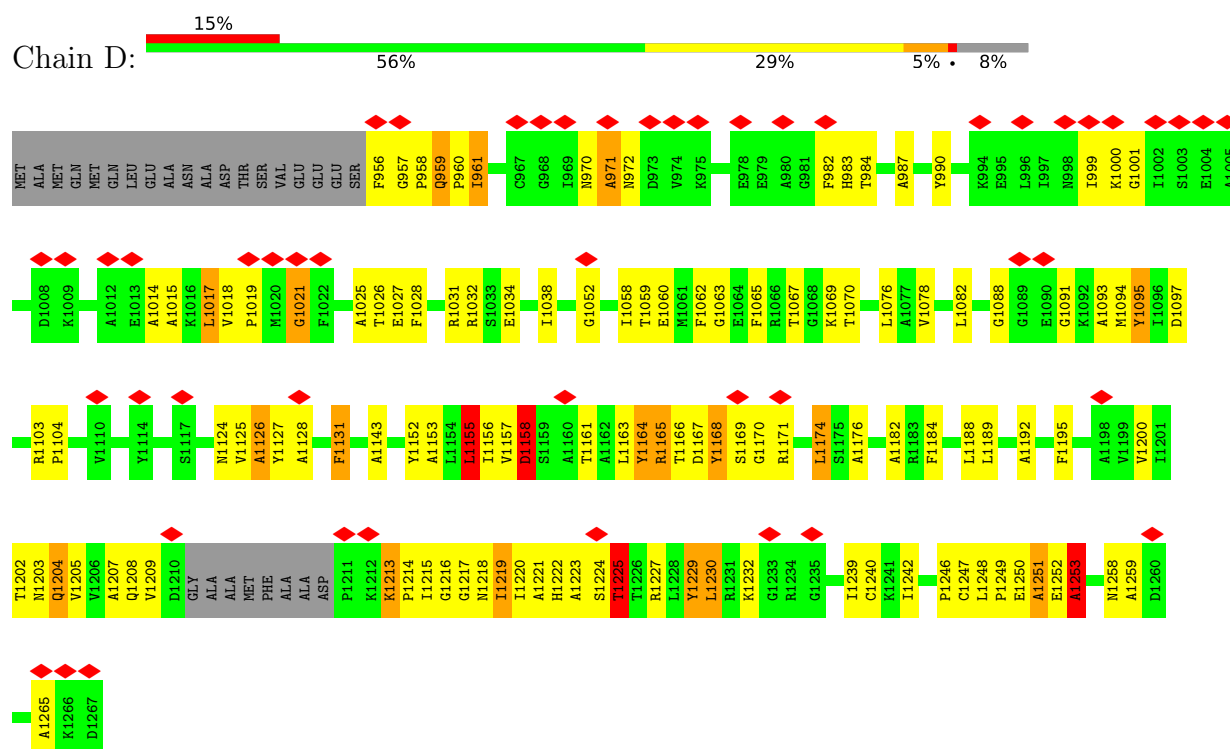
- Molecule 1: DNA repair protein RAD51 homolog 1



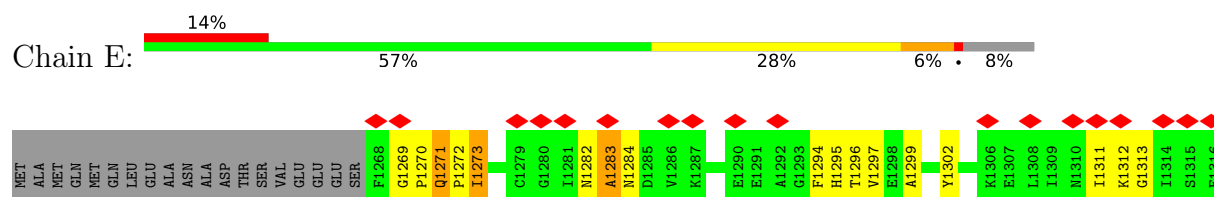
- Molecule 1: DNA repair protein RAD51 homolog 1

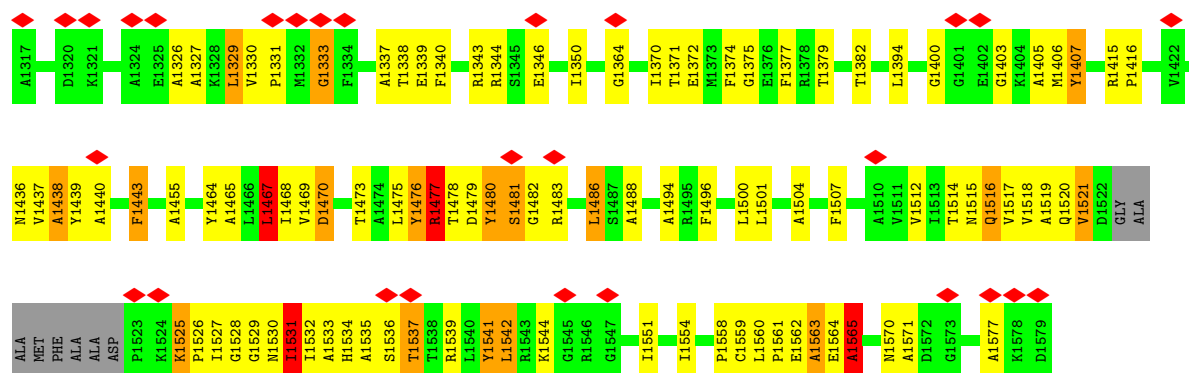


• Molecule 1: DNA repair protein RAD51 homolog 1



• Molecule 1: DNA repair protein RAD51 homolog 1





• Molecule 1: DNA repair protein RAD51 homolog 1



• Molecule 1: DNA repair protein RAD51 homolog 1



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=56.2°, rise=16.05 Å, axial sym=C1	Depositor
Number of segments used	69000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.511	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	1.74	32/1725 (1.9%)	1.97	53/2388 (2.2%)
1	B	1.70	27/1725 (1.6%)	2.02	57/2388 (2.4%)
1	C	1.72	29/1725 (1.7%)	2.01	61/2388 (2.6%)
1	D	1.73	28/1725 (1.6%)	2.01	60/2388 (2.5%)
1	E	1.73	28/1725 (1.6%)	2.00	64/2388 (2.7%)
1	F	1.87	38/1725 (2.2%)	2.01	62/2388 (2.6%)
1	G	1.86	38/1725 (2.2%)	1.99	60/2388 (2.5%)
All	All	1.76	220/12075 (1.8%)	2.00	417/16716 (2.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	4
1	E	0	4
1	F	0	4
1	G	0	4
All	All	0	31

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	2101	ARG	CD-NE	15.87	1.68	1.46
1	F	1789	ARG	CD-NE	14.32	1.66	1.46
1	F	1833	VAL	CA-CB	12.85	1.72	1.54
1	G	2145	VAL	CA-CB	12.27	1.71	1.54
1	G	2101	ARG	N-CA	11.97	1.60	1.46
1	G	2101	ARG	NE-CZ	11.78	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1843	ILE	CA-CB	11.34	1.66	1.54
1	F	1789	ARG	N-CA	11.29	1.60	1.46
1	F	1789	ARG	NE-CZ	10.59	1.44	1.33
1	A	287	ALA	N-CA	10.48	1.59	1.46
1	F	1789	ARG	CZ-NH2	10.04	1.46	1.33
1	F	1833	VAL	N-CA	9.75	1.58	1.46
1	A	285	ALA	CA-C	9.41	1.65	1.52
1	E	1533	ALA	CA-C	9.41	1.65	1.52
1	C	909	ALA	CA-C	9.28	1.65	1.52
1	G	2145	VAL	N-CA	9.22	1.57	1.46
1	B	597	ALA	CA-C	9.16	1.65	1.52
1	G	1996	GLU	N-CA	9.14	1.56	1.45
1	A	314	GLU	N-CA	8.98	1.56	1.46
1	G	2101	ARG	CZ-NH2	8.74	1.44	1.33
1	E	1437	VAL	N-CA	8.61	1.56	1.46
1	F	1845	ALA	CA-C	8.58	1.64	1.52
1	G	2157	ALA	CA-C	8.53	1.64	1.52
1	D	1221	ALA	CA-C	8.35	1.64	1.52
1	D	1125	VAL	N-CA	8.32	1.55	1.46
1	B	501	VAL	N-CA	8.29	1.55	1.46
1	F	1684	GLU	N-CA	8.28	1.55	1.45
1	C	813	VAL	N-CA	8.24	1.55	1.46
1	G	2186	GLU	N-CA	8.21	1.56	1.46
1	F	1749	VAL	N-CA	8.19	1.55	1.46
1	F	1694	THR	CA-C	8.16	1.63	1.52
1	F	1789	ARG	CZ-NH1	8.13	1.44	1.32
1	G	2101	ARG	CZ-NH1	8.13	1.44	1.32
1	F	1874	GLU	N-CA	8.04	1.55	1.46
1	A	189	VAL	N-CA	8.03	1.55	1.46
1	C	748	GLU	N-CA	8.01	1.55	1.45
1	D	1250	GLU	N-CA	7.99	1.56	1.46
1	A	134	THR	CA-C	7.96	1.63	1.52
1	E	1372	GLU	N-CA	7.92	1.55	1.45
1	G	2006	THR	CA-C	7.91	1.63	1.52
1	C	758	THR	CA-C	7.89	1.63	1.52
1	D	1060	GLU	N-CA	7.87	1.55	1.45
1	G	2101	ARG	CA-CB	7.87	1.65	1.53
1	E	1382	THR	CA-C	7.85	1.63	1.52
1	G	2155	ILE	CA-CB	7.68	1.62	1.54
1	D	1176	ALA	N-CA	-7.66	1.36	1.46
1	E	1488	ALA	N-CA	-7.54	1.36	1.46
1	B	436	GLU	N-CA	7.53	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	446	THR	CA-C	7.52	1.62	1.52
1	E	1531	ILE	CA-CB	7.51	1.62	1.54
1	F	1789	ARG	CA-CB	7.50	1.65	1.53
1	A	124	GLU	N-CA	7.49	1.54	1.45
1	C	938	GLU	N-CA	7.47	1.55	1.46
1	E	1532	ILE	C-O	-7.46	1.15	1.24
1	B	626	GLU	N-CA	7.38	1.55	1.46
1	F	1843	ILE	CA-C	7.38	1.61	1.52
1	C	908	ILE	C-O	-7.33	1.15	1.24
1	E	1562	GLU	N-CA	7.30	1.55	1.46
1	G	1998	PHE	N-CA	7.27	1.55	1.46
1	F	1686	PHE	N-CA	7.23	1.55	1.46
1	C	864	ALA	N-CA	-7.21	1.36	1.46
1	G	2062	ALA	N-CA	7.20	1.54	1.45
1	F	1832	GLN	CA-C	7.18	1.61	1.52
1	F	1800	ALA	N-CA	-7.14	1.37	1.46
1	D	1070	THR	CA-C	7.13	1.62	1.52
1	F	1844	ILE	C-O	-7.13	1.15	1.24
1	D	1158	ASP	N-CA	7.08	1.54	1.46
1	D	1220	ILE	C-O	-7.08	1.15	1.24
1	C	846	ASP	N-CA	7.07	1.54	1.46
1	D	1062	PHE	N-CA	7.00	1.55	1.46
1	A	222	ASP	N-CA	6.99	1.54	1.46
1	F	1843	ILE	N-CA	6.97	1.54	1.46
1	G	2155	ILE	CB-CG1	6.95	1.67	1.53
1	B	534	ASP	N-CA	6.93	1.54	1.46
1	C	909	ALA	N-CA	6.79	1.54	1.46
1	C	750	PHE	N-CA	6.77	1.54	1.46
1	E	1470	ASP	N-CA	6.69	1.54	1.46
1	B	438	PHE	N-CA	6.67	1.54	1.46
1	B	552	ALA	N-CA	-6.64	1.37	1.46
1	F	1836	LYS	N-CA	6.59	1.54	1.46
1	A	283	ILE	N-CA	6.54	1.54	1.46
1	A	268	GLN	CG-CD	6.50	1.68	1.52
1	G	2067	PHE	CA-C	6.49	1.61	1.52
1	D	1204	GLN	CG-CD	6.48	1.68	1.52
1	E	1374	PHE	N-CA	6.47	1.54	1.46
1	G	2061	VAL	N-CA	6.47	1.53	1.46
1	F	1684	GLU	CA-C	6.44	1.62	1.53
1	G	2094	ASP	N-CA	6.44	1.54	1.46
1	A	229	ARG	NE-CZ	6.40	1.40	1.33
1	F	1689	PHE	N-CA	6.39	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1377	PHE	N-CA	6.38	1.53	1.46
1	G	1996	GLU	CA-C	6.38	1.62	1.53
1	B	580	GLN	CG-CD	6.35	1.68	1.52
1	A	287	ALA	CA-CB	6.32	1.63	1.53
1	F	1828	GLN	CG-CD	6.31	1.67	1.52
1	D	1219	ILE	N-CA	6.28	1.53	1.46
1	E	1313	GLY	N-CA	6.28	1.51	1.44
1	G	2144	GLN	CA-C	6.28	1.61	1.53
1	C	892	GLN	CG-CD	6.27	1.67	1.52
1	G	2152	GLY	C-O	-6.22	1.19	1.24
1	D	1065	PHE	N-CA	6.21	1.54	1.45
1	E	1516	GLN	CG-CD	6.21	1.67	1.52
1	D	1001	GLY	N-CA	6.21	1.52	1.45
1	G	2156	ILE	C-O	-6.21	1.17	1.24
1	E	1528	GLY	N-CA	6.11	1.53	1.45
1	E	1531	ILE	N-CA	6.08	1.53	1.46
1	C	689	GLY	N-CA	6.04	1.51	1.45
1	C	911	ALA	N-CA	6.02	1.53	1.46
1	B	596	ILE	C-O	-5.99	1.17	1.24
1	B	595	ILE	N-CA	5.99	1.53	1.46
1	B	588	LYS	N-CA	5.97	1.53	1.46
1	A	126	PHE	N-CA	5.96	1.53	1.46
1	D	1251	ALA	N-CA	5.95	1.53	1.46
1	B	592	GLY	N-CA	5.94	1.53	1.45
1	B	436	GLU	CA-C	5.92	1.60	1.52
1	A	276	LYS	N-CA	5.92	1.53	1.46
1	E	1372	GLU	CA-C	5.90	1.61	1.53
1	E	1533	ALA	N-CA	5.89	1.53	1.46
1	G	2063	TYR	CA-C	-5.89	1.45	1.52
1	B	437	MET	CA-C	5.89	1.59	1.52
1	A	283	ILE	CA-CB	5.88	1.60	1.54
1	D	1060	GLU	CA-C	5.88	1.61	1.53
1	A	129	PHE	N-CA	5.86	1.53	1.45
1	A	54	TYR	CE1-CZ	5.81	1.52	1.38
1	A	85	GLY	N-CA	5.81	1.53	1.45
1	E	1535	ALA	N-CA	5.80	1.53	1.46
1	D	1223	ALA	N-CA	5.79	1.53	1.46
1	F	1847	ALA	N-CA	5.79	1.53	1.46
1	F	1845	ALA	N-CA	5.79	1.53	1.46
1	A	267	ASN	CA-C	5.77	1.61	1.53
1	C	907	ILE	CA-CB	5.77	1.62	1.54
1	A	188	ASN	CA-C	5.75	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	441	PHE	N-CA	5.73	1.53	1.45
1	F	1782	ASP	N-CA	5.72	1.53	1.46
1	A	266	THR	CA-C	5.71	1.59	1.52
1	D	1216	GLY	N-CA	5.71	1.53	1.45
1	C	748	GLU	CA-C	5.71	1.61	1.53
1	G	2140	GLN	CG-CD	5.62	1.66	1.52
1	C	907	ILE	N-CA	5.61	1.53	1.46
1	E	1436	ASN	CA-C	5.61	1.60	1.52
1	D	1124	ASN	CA-C	5.60	1.60	1.52
1	C	890	THR	CA-C	5.60	1.59	1.52
1	D	1221	ALA	N-CA	5.58	1.53	1.46
1	A	315	ALA	N-CA	5.57	1.53	1.46
1	A	124	GLU	CA-C	5.57	1.61	1.53
1	C	753	PHE	N-CA	5.55	1.53	1.45
1	A	289	THR	CA-C	5.55	1.60	1.52
1	C	904	GLY	N-CA	5.53	1.53	1.45
1	G	2093	VAL	CA-CB	-5.53	1.47	1.54
1	B	377	GLY	N-CA	5.50	1.51	1.45
1	B	606	LEU	CA-C	5.48	1.59	1.52
1	F	1875	ALA	N-CA	5.48	1.53	1.46
1	F	1826	THR	CA-C	5.47	1.59	1.52
1	C	853	ARG	NE-CZ	5.46	1.39	1.33
1	G	2138	THR	CA-C	5.46	1.59	1.52
1	B	578	THR	CA-C	5.43	1.59	1.52
1	G	2096	ALA	C-O	5.42	1.30	1.24
1	F	1854	LEU	CA-C	5.41	1.59	1.52
1	G	2004	GLY	N-CA	5.41	1.53	1.45
1	G	2158	HIS	CA-C	-5.39	1.45	1.52
1	E	1514	THR	CA-C	5.38	1.59	1.52
1	G	1937	GLY	N-CA	5.38	1.50	1.45
1	B	593	GLY	N-CA	5.38	1.52	1.45
1	E	1542	LEU	CA-C	5.37	1.59	1.52
1	C	812	ASN	CA-C	5.36	1.59	1.52
1	G	2007	GLN	N-CA	5.34	1.52	1.46
1	C	939	ALA	N-CA	5.33	1.53	1.46
1	E	1438	ALA	N-CA	5.31	1.52	1.45
1	G	2187	ALA	N-CA	5.30	1.53	1.46
1	F	1750	ALA	N-CA	5.29	1.52	1.45
1	G	2143	ALA	CA-C	5.29	1.59	1.52
1	C	915	ARG	N-CA	5.27	1.52	1.46
1	A	229	ARG	CZ-NH2	5.27	1.40	1.33
1	A	291	ARG	N-CA	5.26	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	907	ILE	CA-C	5.25	1.59	1.52
1	D	1126	ALA	N-CA	5.25	1.52	1.45
1	A	229	ARG	CD-NE	5.25	1.53	1.46
1	E	1563	ALA	N-CA	5.22	1.52	1.46
1	A	79	ALA	CA-C	5.22	1.59	1.52
1	B	627	ALA	N-CA	5.21	1.52	1.46
1	B	500	ASN	CA-C	5.21	1.59	1.52
1	B	598	HIS	C-O	5.21	1.30	1.23
1	G	2112	ALA	N-CA	-5.21	1.39	1.46
1	D	1230	LEU	CA-C	5.20	1.59	1.52
1	B	595	ILE	CA-CB	5.19	1.61	1.54
1	A	279	ILE	CA-C	5.18	1.59	1.52
1	A	317	ALA	N-CA	5.18	1.52	1.46
1	D	1202	THR	CA-C	5.17	1.59	1.52
1	D	1217	GLY	N-CA	5.17	1.53	1.45
1	A	282	ASN	CA-C	5.16	1.59	1.52
1	F	1789	ARG	CG-CD	5.15	1.68	1.52
1	F	1828	GLN	CD-OE1	5.14	1.33	1.23
1	C	749	MET	CA-C	5.13	1.58	1.52
1	D	1222	HIS	CA-C	-5.13	1.46	1.52
1	B	414	ILE	CA-C	5.12	1.59	1.52
1	E	1515	ASN	N-CA	5.12	1.51	1.45
1	E	1527	ILE	C-N	5.12	1.38	1.33
1	B	599	ALA	N-CA	5.12	1.52	1.46
1	D	1215	ILE	CA-C	5.12	1.59	1.52
1	C	913	THR	CA-C	5.11	1.59	1.52
1	B	502	ALA	N-CA	5.10	1.52	1.45
1	F	1692	GLY	N-CA	5.09	1.52	1.45
1	D	1225	THR	CA-C	5.07	1.59	1.52
1	A	90	THR	CA-C	5.07	1.60	1.53
1	G	2088	TYR	CA-C	5.06	1.59	1.52
1	C	941	ALA	N-CA	5.06	1.52	1.46
1	D	1182	ALA	CA-C	-5.05	1.46	1.52
1	F	1846	HIS	C-O	5.05	1.30	1.23
1	F	1781	VAL	CA-CB	-5.05	1.48	1.54
1	E	1494	ALA	CA-C	-5.04	1.46	1.52
1	E	1531	ILE	CA-C	5.03	1.58	1.52
1	D	1203	ASN	N-CA	5.03	1.51	1.45
1	E	1529	GLY	N-CA	5.03	1.52	1.45
1	F	1877	ALA	N-CA	5.03	1.52	1.46
1	C	891	ASN	N-CA	5.02	1.51	1.45
1	F	1851	ARG	N-CA	5.01	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	870	ALA	CA-C	-5.01	1.46	1.52
1	G	2163	ARG	N-CA	5.01	1.52	1.46
1	A	246	ALA	CA-C	-5.01	1.46	1.52
1	G	2139	ASN	N-CA	5.00	1.51	1.45

All (417) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	901	LYS	N-CA-C	14.54	121.30	108.22
1	A	229	ARG	NE-CZ-NH2	14.09	131.88	119.20
1	F	1837	LYS	N-CA-C	13.92	124.15	108.14
1	B	589	LYS	N-CA-C	13.82	124.28	108.25
1	D	1213	LYS	N-CA-C	13.40	120.28	108.22
1	E	1525	LYS	N-CA-C	12.75	119.70	108.22
1	B	541	ARG	NE-CZ-NH2	12.68	130.61	119.20
1	G	2101	ARG	CD-NE-CZ	12.08	141.32	124.40
1	F	1789	ARG	CD-NE-CZ	11.35	140.28	124.40
1	G	1895	GLN	CA-C-N	11.20	133.83	119.84
1	G	1895	GLN	C-N-CA	11.20	133.83	119.84
1	C	853	ARG	NE-CZ-NH2	11.10	129.19	119.20
1	F	1789	ARG	N-CA-CB	10.92	126.18	110.12
1	G	2101	ARG	N-CA-CB	10.89	126.13	110.12
1	B	335	GLN	CA-C-N	10.84	133.39	119.84
1	B	335	GLN	C-N-CA	10.84	133.39	119.84
1	E	1271	GLN	CA-C-N	10.77	133.31	119.84
1	E	1271	GLN	C-N-CA	10.77	133.31	119.84
1	C	647	GLN	CA-C-N	10.75	133.28	119.84
1	C	647	GLN	C-N-CA	10.75	133.28	119.84
1	F	1583	GLN	CA-C-N	10.54	133.01	119.84
1	F	1583	GLN	C-N-CA	10.54	133.01	119.84
1	G	2149	LYS	N-CA-C	10.52	120.45	108.25
1	D	959	GLN	CA-C-N	10.51	132.97	119.84
1	D	959	GLN	C-N-CA	10.51	132.97	119.84
1	A	23	GLN	CA-C-N	10.43	132.87	119.84
1	A	23	GLN	C-N-CA	10.43	132.87	119.84
1	D	1027	GLU	N-CA-C	-10.26	100.89	113.41
1	A	191	TYR	N-CA-C	10.23	126.45	109.06
1	C	815	TYR	N-CA-C	10.17	126.23	109.24
1	B	403	GLU	N-CA-C	-10.16	101.01	113.41
1	E	1339	GLU	N-CA-C	-10.07	101.12	113.41
1	F	1651	GLU	N-CA-C	-10.06	101.14	113.41
1	C	715	GLU	N-CA-C	-10.04	101.17	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1127	TYR	N-CA-C	9.90	125.89	109.06
1	E	1439	TYR	N-CA-C	9.83	125.78	109.06
1	D	1060	GLU	N-CA-C	9.77	124.76	110.59
1	F	1751	TYR	N-CA-C	9.75	125.63	109.06
1	B	503	TYR	N-CA-C	9.73	125.61	109.06
1	C	748	GLU	N-CA-C	9.72	124.68	110.59
1	F	1684	GLU	N-CA-C	9.71	124.68	110.59
1	G	1963	GLU	N-CA-C	-9.66	101.62	113.41
1	B	541	ARG	NE-CZ-NH1	-9.66	111.84	121.50
1	E	1477	ARG	NE-CZ-NH2	9.56	127.81	119.20
1	F	1789	ARG	CB-CG-CD	9.51	133.17	111.30
1	E	1372	GLU	N-CA-C	9.47	124.32	110.59
1	A	124	GLU	N-CA-C	9.44	124.28	110.59
1	G	1996	GLU	N-CA-C	9.28	124.18	110.17
1	C	819	PHE	N-CA-C	9.21	121.08	111.14
1	D	1131	PHE	N-CA-C	9.21	121.08	111.14
1	G	2029	ALA	N-CA-C	9.09	123.98	108.25
1	F	1788	TYR	N-CA-C	9.06	124.12	112.89
1	B	507	PHE	N-CA-C	9.00	120.86	111.14
1	A	195	PHE	N-CA-C	8.92	120.77	111.14
1	F	1755	PHE	N-CA-C	8.92	120.93	111.03
1	G	2101	ARG	CB-CG-CD	8.91	131.79	111.30
1	D	1093	ALA	N-CA-C	8.73	122.97	108.47
1	F	1829	VAL	CB-CA-C	-8.70	98.03	111.26
1	E	1443	PHE	N-CA-C	8.70	120.53	111.14
1	G	2100	TYR	N-CA-C	8.69	123.66	112.89
1	A	269	VAL	CB-CA-C	-8.61	98.17	111.26
1	F	1833	VAL	N-CA-CB	8.60	125.43	111.23
1	G	2093	VAL	N-CA-C	-8.59	97.53	109.21
1	B	436	GLU	N-CA-C	8.56	123.68	110.42
1	C	893	VAL	CB-CA-C	-8.55	99.20	111.34
1	B	469	ALA	N-CA-C	8.46	122.87	108.25
1	B	581	VAL	CB-CA-C	-8.45	98.41	111.26
1	F	1781	VAL	N-CA-C	-8.36	97.84	109.21
1	E	1405	ALA	N-CA-C	8.29	122.59	108.25
1	B	533	VAL	N-CA-C	-8.28	97.95	109.21
1	A	157	ALA	N-CA-C	8.26	122.54	108.25
1	G	2141	VAL	CB-CA-C	-8.19	98.81	111.26
1	C	781	ALA	N-CA-C	8.19	122.41	108.25
1	E	1469	VAL	N-CA-C	-8.14	98.13	109.21
1	A	221	VAL	N-CA-C	-8.04	98.27	109.21
1	D	1205	VAL	CB-CA-C	-8.02	99.06	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	896	GLN	CA-C-O	-8.00	112.20	120.84
1	D	1157	VAL	N-CA-C	-8.00	98.33	109.21
1	F	1717	ALA	N-CA-C	7.90	121.91	108.25
1	A	63	ILE	N-CA-C	7.87	120.79	107.18
1	E	1517	VAL	CB-CA-C	-7.85	99.32	111.26
1	G	2101	ARG	N-CA-C	-7.81	102.77	111.28
1	F	1789	ARG	N-CA-C	-7.76	102.82	111.28
1	C	845	VAL	N-CA-C	-7.74	98.69	109.21
1	B	375	ILE	N-CA-C	7.62	120.37	107.18
1	B	584	GLN	CA-C-O	-7.59	112.05	120.70
1	A	228	TYR	N-CA-C	7.58	120.62	111.82
1	B	592	GLY	CA-C-O	-7.56	114.03	120.30
1	D	1216	GLY	CA-C-O	-7.55	114.03	120.30
1	A	229	ARG	NE-CZ-NH1	-7.40	114.10	121.50
1	G	2109	GLU	N-CA-C	-7.39	105.14	112.97
1	E	1529	GLY	N-CA-C	7.35	125.51	115.30
1	F	1846	HIS	N-CA-C	-7.34	99.04	110.42
1	C	751	GLY	N-CA-C	7.33	121.51	111.54
1	D	1248	LEU	N-CA-C	-7.28	100.27	110.31
1	E	1375	GLY	N-CA-C	7.21	121.34	111.54
1	G	2145	VAL	N-CA-CB	7.20	123.11	111.23
1	E	1528	GLY	CA-C-O	-7.19	114.33	120.30
1	D	1063	GLY	N-CA-C	7.06	121.14	111.54
1	E	1436	ASN	N-CA-C	7.03	118.94	111.28
1	E	1476	TYR	N-CA-C	7.00	119.94	111.82
1	B	595	ILE	CB-CA-C	-6.97	99.85	111.29
1	F	1687	GLY	N-CA-C	6.95	120.99	111.54
1	G	2184	LEU	N-CA-C	-6.89	100.81	110.31
1	G	2142	VAL	CB-CA-C	6.88	119.71	110.42
1	F	1872	LEU	N-CA-C	-6.87	100.83	110.31
1	C	688	LYS	CA-C-N	6.87	127.98	121.46
1	C	688	LYS	C-N-CA	6.87	127.98	121.46
1	B	439	GLY	N-CA-C	6.86	120.87	111.54
1	G	2189	ALA	N-CA-C	6.82	125.33	110.80
1	G	1936	LYS	CA-C-N	6.82	126.86	121.61
1	G	1936	LYS	C-N-CA	6.82	126.86	121.61
1	D	1253	ALA	N-CA-C	6.80	125.28	110.80
1	E	1520	GLN	CA-C-O	-6.77	113.52	120.84
1	E	1530	ASN	CA-C-N	6.76	129.63	120.77
1	E	1530	ASN	C-N-CA	6.76	129.63	120.77
1	C	941	ALA	N-CA-C	6.73	125.13	110.80
1	C	812	ASN	N-CA-C	6.72	118.61	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1164	TYR	N-CA-C	6.72	119.61	111.82
1	C	910	HIS	N-CA-C	-6.68	100.07	110.42
1	B	540	TYR	N-CA-C	6.66	119.55	111.82
1	A	283	ILE	N-CA-CB	6.64	117.59	110.62
1	F	1877	ALA	N-CA-C	6.64	124.95	110.80
1	C	936	LEU	N-CA-C	-6.63	100.31	110.32
1	C	852	TYR	CB-CA-C	-6.60	98.00	110.67
1	G	2155	ILE	CA-CB-CG1	6.54	121.51	110.40
1	A	317	ALA	N-CA-C	6.53	124.70	110.80
1	C	904	GLY	CA-C-O	-6.53	114.88	120.30
1	A	127	GLY	N-CA-C	6.51	120.39	111.54
1	B	540	TYR	CB-CA-C	-6.50	98.19	110.67
1	B	624	LEU	N-CA-C	-6.49	100.53	110.32
1	D	1208	GLN	CA-C-O	-6.48	113.80	120.54
1	B	629	ALA	N-CA-C	6.47	124.59	110.80
1	B	500	ASN	N-CA-C	6.46	118.32	111.28
1	B	629	ALA	CA-C-N	-6.44	111.23	121.86
1	B	629	ALA	C-N-CA	-6.44	111.23	121.86
1	D	1164	TYR	CB-CA-C	-6.42	98.33	110.67
1	D	1124	ASN	N-CA-C	6.42	118.28	111.28
1	F	1843	ILE	CA-CB-CG1	6.42	121.31	110.40
1	D	1218	ASN	CA-C-N	6.41	128.87	120.60
1	D	1218	ASN	C-N-CA	6.41	128.87	120.60
1	F	1841	GLY	N-CA-C	6.40	124.20	115.30
1	B	502	ALA	N-CA-C	6.39	119.13	109.23
1	D	1126	ALA	N-CA-C	6.39	119.13	109.23
1	E	1438	ALA	N-CA-C	6.37	119.11	109.23
1	E	1532	ILE	CA-C-O	-6.36	112.83	120.78
1	G	2093	VAL	CB-CA-C	-6.36	102.31	111.34
1	C	915	ARG	N-CA-C	6.33	118.73	108.41
1	E	1382	THR	CB-CA-C	6.33	121.34	110.84
1	E	1312	LYS	CA-C-N	6.29	126.99	121.58
1	E	1312	LYS	C-N-CA	6.29	126.99	121.58
1	G	2158	HIS	N-CA-C	-6.29	100.67	110.42
1	D	1165	ARG	NE-CZ-NH1	-6.26	115.23	121.50
1	E	1565	ALA	CA-C-N	-6.26	111.52	121.86
1	E	1565	ALA	C-N-CA	-6.26	111.52	121.86
1	F	1750	ALA	N-CA-C	6.26	118.93	109.23
1	C	852	TYR	N-CA-C	6.26	119.08	111.82
1	A	288	SER	N-CA-C	6.25	117.76	111.07
1	A	291	ARG	N-CA-C	6.24	118.58	108.41
1	B	367	ALA	N-CA-C	6.24	116.77	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1476	TYR	CB-CA-C	-6.23	98.71	110.67
1	D	1253	ALA	CA-C-N	-6.22	111.60	121.86
1	D	1253	ALA	C-N-CA	-6.22	111.60	121.86
1	E	1565	ALA	N-CA-C	6.22	124.05	110.80
1	D	1188	LEU	N-CA-C	-6.21	104.59	111.36
1	E	1534	HIS	N-CA-C	-6.19	100.83	110.42
1	F	1691	THR	CA-C-N	6.18	133.53	121.41
1	F	1691	THR	C-N-CA	6.18	133.53	121.41
1	F	1848	SER	N-CA-C	6.18	117.68	111.07
1	D	1000	LYS	CA-C-N	6.17	127.32	121.46
1	D	1000	LYS	C-N-CA	6.17	127.32	121.46
1	A	188	ASN	N-CA-C	6.15	117.99	111.28
1	C	853	ARG	CB-CG-CD	6.14	125.41	111.30
1	F	1851	ARG	N-CA-C	6.12	118.39	108.41
1	E	1560	LEU	N-CA-C	-6.11	101.10	110.32
1	F	1748	ASN	N-CA-C	6.11	118.73	111.71
1	F	1846	HIS	O-C-N	6.09	129.91	123.03
1	A	317	ALA	CA-C-N	-6.08	111.82	121.86
1	A	317	ALA	C-N-CA	-6.08	111.82	121.86
1	G	2003	THR	CA-C-N	6.08	133.32	121.41
1	G	2003	THR	C-N-CA	6.08	133.32	121.41
1	C	904	GLY	O-C-N	6.07	126.93	122.62
1	E	1477	ARG	NE-CZ-NH1	-6.07	115.43	121.50
1	C	883	PHE	CB-CA-C	6.05	119.72	109.55
1	E	1539	ARG	N-CA-C	6.03	118.23	108.41
1	D	1195	PHE	CB-CA-C	6.02	119.67	109.55
1	F	1615	ALA	N-CA-C	6.01	116.52	109.60
1	E	1521	VAL	CG1-CB-CG2	-6.01	97.58	110.80
1	D	1227	ARG	N-CA-C	6.00	118.19	108.41
1	B	598	HIS	O-C-N	5.99	129.80	123.03
1	A	312	LEU	N-CA-C	-5.99	101.28	110.32
1	D	1239	ILE	CA-C-O	-5.97	114.12	120.39
1	D	1222	HIS	O-C-N	5.96	129.96	123.10
1	E	1528	GLY	O-C-N	5.96	126.86	122.62
1	E	1534	HIS	O-C-N	5.96	129.76	123.03
1	G	2155	ILE	N-CA-CB	5.96	117.12	110.51
1	C	851	LEU	CA-C-N	5.94	129.34	120.31
1	C	851	LEU	C-N-CA	5.94	129.34	120.31
1	C	814	ALA	N-CA-C	5.94	119.16	109.24
1	E	1536	SER	N-CA-C	5.94	117.42	111.07
1	F	1842	ASN	CA-C-N	5.93	128.54	120.77
1	F	1842	ASN	C-N-CA	5.93	128.54	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	941	ALA	CA-C-N	-5.93	112.08	121.86
1	C	941	ALA	C-N-CA	-5.93	112.08	121.86
1	D	1216	GLY	O-C-N	5.92	126.83	122.62
1	C	755	THR	O-C-N	5.92	130.02	122.39
1	C	910	HIS	O-C-N	5.92	129.71	123.03
1	A	82	VAL	CA-C-N	5.90	125.59	119.05
1	A	82	VAL	C-N-CA	5.90	125.59	119.05
1	B	594	ASN	N-CA-C	5.89	118.04	108.08
1	C	910	HIS	CA-C-N	5.89	129.65	120.82
1	C	910	HIS	C-N-CA	5.89	129.65	120.82
1	C	783	TYR	N-CA-CB	5.88	120.09	110.50
1	C	927	ILE	CA-C-O	-5.88	114.22	120.39
1	D	1218	ASN	N-CA-C	5.86	118.45	108.67
1	C	876	LEU	N-CA-C	-5.85	104.99	111.36
1	G	2158	HIS	O-C-N	5.84	129.63	123.03
1	G	2144	GLN	CA-C-O	-5.84	113.93	121.11
1	B	615	ILE	CA-C-O	-5.84	114.26	120.39
1	B	564	LEU	N-CA-C	-5.83	105.01	111.36
1	D	1163	LEU	CA-C-N	5.83	129.17	120.31
1	D	1163	LEU	C-N-CA	5.83	129.17	120.31
1	G	2006	THR	CA-C-N	5.80	128.37	120.54
1	G	2006	THR	C-N-CA	5.80	128.37	120.54
1	G	2160	SER	N-CA-C	5.77	118.03	111.11
1	E	1551	ILE	CA-C-O	-5.76	114.34	120.39
1	D	1070	THR	CB-CA-C	5.75	120.39	110.84
1	A	287	ALA	N-CA-CB	5.75	119.15	109.78
1	A	252	LEU	N-CA-C	-5.75	105.10	111.36
1	D	1219	ILE	N-CA-C	5.74	116.38	110.36
1	A	190	ALA	N-CA-C	5.72	118.78	109.06
1	A	159	TYR	N-CA-CB	5.71	119.81	110.50
1	E	1527	ILE	CA-C-O	-5.71	115.08	121.36
1	G	2156	ILE	CA-C-O	-5.70	112.15	119.39
1	A	277	LYS	CA-C-N	5.69	125.70	119.89
1	A	277	LYS	C-N-CA	5.69	125.70	119.89
1	D	999	ILE	N-CA-C	5.69	121.17	109.34
1	D	1155	LEU	CA-C-N	-5.69	115.13	123.10
1	D	1155	LEU	C-N-CA	-5.69	115.13	123.10
1	G	2031	TYR	N-CA-CB	5.69	119.77	110.50
1	A	229	ARG	CB-CG-CD	5.69	124.38	111.30
1	D	1222	HIS	N-CA-C	-5.68	101.02	110.17
1	B	471	TYR	N-CA-CB	5.68	119.76	110.50
1	D	1155	LEU	CA-CB-CG	5.67	136.16	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1694	THR	CA-C-N	5.67	128.20	120.54
1	F	1694	THR	C-N-CA	5.67	128.20	120.54
1	B	443	THR	O-C-N	5.67	129.70	122.39
1	G	2101	ARG	CG-CD-NE	5.66	124.45	112.00
1	G	2145	VAL	CA-CB-CG2	5.65	120.01	110.40
1	G	2163	ARG	N-CA-C	5.65	118.11	108.90
1	A	216	TYR	CB-CA-C	5.65	118.97	109.48
1	A	227	LEU	CA-C-N	5.65	128.90	120.31
1	A	227	LEU	C-N-CA	5.65	128.90	120.31
1	G	2091	LEU	CA-C-N	-5.65	115.43	123.11
1	G	2091	LEU	C-N-CA	-5.65	115.43	123.11
1	E	1527	ILE	N-CA-CB	-5.65	100.64	110.13
1	C	905	GLY	N-CA-C	5.64	123.14	115.30
1	D	1067	THR	CA-C-N	5.63	132.44	121.41
1	D	1067	THR	C-N-CA	5.63	132.44	121.41
1	G	2145	VAL	CG1-CB-CG2	-5.62	98.43	110.80
1	D	1222	HIS	CA-C-N	5.62	129.24	120.82
1	D	1222	HIS	C-N-CA	5.62	129.24	120.82
1	C	906	ASN	N-CA-C	5.61	118.04	108.67
1	G	1935	ILE	N-CA-C	5.61	121.00	109.34
1	A	131	THR	O-C-N	5.60	130.10	122.37
1	G	2149	LYS	CA-C-N	5.60	125.61	119.89
1	G	2149	LYS	C-N-CA	5.60	125.61	119.89
1	D	1095	TYR	N-CA-CB	5.60	119.63	110.50
1	B	528	TYR	CB-CA-C	5.59	118.88	109.48
1	E	1407	TYR	N-CA-CB	5.59	119.62	110.50
1	F	1623	ILE	N-CA-C	5.59	120.96	109.34
1	A	219	LEU	CA-C-N	-5.58	115.28	123.10
1	A	219	LEU	C-N-CA	-5.58	115.28	123.10
1	B	600	SER	N-CA-C	5.58	117.81	111.11
1	E	1507	PHE	CB-CA-C	5.58	118.93	109.55
1	B	591	ILE	CA-C-O	-5.58	115.27	121.23
1	B	598	HIS	N-CA-C	-5.58	101.78	110.42
1	G	2124	LEU	N-CA-C	-5.55	105.31	111.36
1	F	1837	LYS	CA-C-N	5.55	125.55	119.89
1	F	1837	LYS	C-N-CA	5.55	125.55	119.89
1	F	1812	LEU	N-CA-C	-5.54	105.32	111.36
1	G	1999	GLY	N-CA-C	5.54	119.08	111.54
1	E	1500	LEU	N-CA-C	-5.54	105.33	111.36
1	F	1719	TYR	N-CA-CB	5.53	119.52	110.50
1	G	2079	ALA	N-CA-C	-5.53	105.15	111.07
1	A	207	ALA	N-CA-C	-5.53	105.16	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1836	LYS	CA-C-N	-5.52	114.12	122.07
1	F	1836	LYS	C-N-CA	-5.52	114.12	122.07
1	C	912	SER	N-CA-C	5.51	116.97	111.07
1	E	1530	ASN	N-CA-C	5.51	117.87	108.67
1	A	272	GLN	CA-C-O	-5.50	114.34	121.11
1	G	2155	ILE	CB-CG1-CD1	5.50	125.35	113.80
1	B	539	LEU	CA-C-N	5.50	128.66	120.31
1	B	539	LEU	C-N-CA	5.50	128.66	120.31
1	E	1311	ILE	N-CA-C	5.50	120.77	109.34
1	G	2175	ILE	CA-C-O	-5.49	114.62	120.39
1	C	840	TYR	CB-CA-C	5.49	118.70	109.48
1	G	2189	ALA	CA-C-N	-5.49	111.05	121.54
1	G	2189	ALA	C-N-CA	-5.49	111.05	121.54
1	E	1312	LYS	N-CA-C	5.48	118.95	111.39
1	E	1534	HIS	CA-C-N	5.48	129.04	120.82
1	E	1534	HIS	C-N-CA	5.48	129.04	120.82
1	G	2101	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	B	531	LEU	CA-CB-CG	5.47	135.45	116.30
1	C	843	LEU	CA-C-N	-5.47	115.45	123.10
1	C	843	LEU	C-N-CA	-5.47	115.45	123.10
1	F	1693	LYS	N-CA-C	-5.46	105.40	111.36
1	C	928	CYS	N-CA-C	5.46	119.12	107.70
1	A	237	GLU	N-CA-C	-5.46	105.30	112.72
1	A	304	CYS	N-CA-C	5.46	119.11	107.70
1	G	2088	TYR	CB-CA-C	5.46	118.65	109.48
1	B	598	HIS	CA-C-N	5.46	129.00	120.82
1	B	598	HIS	C-N-CA	5.46	129.00	120.82
1	A	134	THR	CB-CA-C	5.45	121.27	110.42
1	A	91	GLU	N-CA-C	-5.45	107.18	113.88
1	E	1464	TYR	CB-CA-C	5.45	118.63	109.48
1	G	2152	GLY	CA-C-O	-5.45	115.78	120.30
1	D	1240	CYS	N-CA-C	5.44	119.07	107.70
1	C	853	ARG	NH1-CZ-NH2	-5.43	112.24	119.30
1	D	1217	GLY	N-CA-C	5.43	122.85	115.30
1	E	1475	LEU	CA-C-N	5.43	128.56	120.31
1	E	1475	LEU	C-N-CA	5.43	128.56	120.31
1	F	1776	TYR	CB-CA-C	5.42	118.58	109.48
1	B	531	LEU	CA-C-N	-5.41	115.52	123.10
1	B	531	LEU	C-N-CA	-5.41	115.52	123.10
1	B	592	GLY	O-C-N	5.41	126.46	122.62
1	A	58	LYS	CA-C-N	5.41	127.97	120.29
1	A	58	LYS	C-N-CA	5.41	127.97	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1936	LYS	N-CA-C	5.40	118.84	111.39
1	D	1067	THR	O-C-N	5.40	130.38	122.39
1	A	283	ILE	N-CA-C	5.39	115.84	110.23
1	C	831	ALA	N-CA-C	-5.39	105.30	111.07
1	B	519	ALA	N-CA-C	-5.39	105.30	111.07
1	D	1220	ILE	CA-C-O	-5.39	114.04	120.78
1	D	1152	TYR	CB-CA-C	5.38	118.51	109.48
1	E	1379	THR	CA-C-N	5.36	131.91	121.41
1	E	1379	THR	C-N-CA	5.36	131.91	121.41
1	A	228	TYR	CB-CA-C	-5.35	100.40	110.67
1	B	376	LYS	N-CA-C	5.34	118.76	111.39
1	G	2003	THR	O-C-N	5.34	131.02	122.42
1	G	2131	PHE	CB-CA-C	5.34	118.52	109.55
1	E	1467	LEU	CA-C-N	-5.33	115.63	123.10
1	E	1467	LEU	C-N-CA	-5.33	115.63	123.10
1	B	571	PHE	CB-CA-C	5.33	118.51	109.55
1	C	687	ILE	N-CA-C	5.32	120.40	109.34
1	D	1069	LYS	N-CA-C	-5.29	105.59	111.36
1	C	755	THR	CA-C-N	5.29	131.78	121.41
1	C	755	THR	C-N-CA	5.29	131.78	121.41
1	F	1846	HIS	CA-C-N	5.29	128.76	120.82
1	F	1846	HIS	C-N-CA	5.29	128.76	120.82
1	E	1297	VAL	O-C-N	5.29	127.09	121.91
1	G	2005	LYS	N-CA-C	-5.27	105.61	111.36
1	E	1382	THR	CA-C-N	5.27	127.66	120.54
1	E	1382	THR	C-N-CA	5.27	127.66	120.54
1	D	1143	ALA	N-CA-C	-5.27	105.43	111.07
1	F	1624	LYS	CA-C-N	5.26	126.77	121.35
1	F	1624	LYS	C-N-CA	5.26	126.77	121.35
1	F	1839	ILE	CA-C-O	-5.25	116.18	121.59
1	E	1455	ALA	N-CA-C	-5.25	105.46	111.07
1	F	1842	ASN	N-CA-C	5.25	117.43	108.67
1	G	2153	GLY	N-CA-C	5.23	122.81	115.43
1	A	134	THR	CA-C-N	5.23	127.60	120.54
1	A	134	THR	C-N-CA	5.23	127.60	120.54
1	B	603	ARG	N-CA-C	5.23	117.42	108.90
1	D	1165	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	F	1767	ALA	N-CA-C	-5.22	105.48	111.07
1	F	1832	GLN	CA-C-O	-5.22	115.00	120.58
1	C	758	THR	CB-CA-C	5.21	120.78	110.42
1	F	1694	THR	CB-CA-C	5.21	120.78	110.42
1	C	816	ALA	N-CA-C	5.20	116.99	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1224	SER	N-CA-C	5.18	116.61	111.07
1	F	1779	LEU	CA-C-N	-5.17	115.86	123.10
1	F	1779	LEU	C-N-CA	-5.17	115.86	123.10
1	B	443	THR	CA-C-N	5.17	131.55	121.41
1	B	443	THR	C-N-CA	5.17	131.55	121.41
1	A	131	THR	CA-C-N	5.16	131.53	121.41
1	A	131	THR	C-N-CA	5.16	131.53	121.41
1	F	1789	ARG	CG-CD-NE	5.16	123.36	112.00
1	A	281	GLY	N-CA-C	5.14	123.00	115.08
1	B	593	GLY	CA-C-O	5.14	126.12	119.44
1	B	525	GLU	N-CA-C	5.14	116.88	111.28
1	C	758	THR	CA-C-N	5.13	127.47	120.54
1	C	758	THR	C-N-CA	5.13	127.47	120.54
1	E	1467	LEU	CA-CB-CG	5.13	134.26	116.30
1	E	1407	TYR	CB-CA-C	5.13	118.21	109.75
1	D	1215	ILE	CA-C-O	-5.12	116.31	121.59
1	F	1863	ILE	CA-C-O	-5.12	114.68	120.67
1	F	1833	VAL	CG1-CB-CG2	-5.11	99.55	110.80
1	D	971	ALA	N-CA-C	5.11	121.69	110.80
1	F	1843	ILE	N-CA-C	5.11	115.54	110.23
1	G	2176	CYS	N-CA-C	5.10	118.36	107.70
1	B	446	THR	CA-C-N	5.09	127.41	120.54
1	B	446	THR	C-N-CA	5.09	127.41	120.54
1	C	907	ILE	CA-CB-CG1	5.09	119.05	110.40
1	C	897	VAL	CB-CA-C	5.09	119.63	111.29
1	C	837	GLU	N-CA-C	5.08	116.81	111.28
1	B	581	VAL	CA-C-O	-5.08	115.80	121.23
1	E	1283	ALA	N-CA-C	5.07	121.61	110.80
1	E	1531	ILE	CA-CB-CG1	5.06	119.01	110.40
1	B	480	PRO	CA-C-N	5.05	127.36	120.54
1	B	480	PRO	C-N-CA	5.05	127.36	120.54
1	C	688	LYS	N-CA-C	5.05	118.35	111.39
1	F	1719	TYR	CB-CA-C	5.04	118.07	109.75
1	E	1531	ILE	CB-CA-C	-5.04	105.25	111.70
1	F	1779	LEU	CA-CB-CG	5.04	133.93	116.30
1	E	1531	ILE	N-CA-C	5.04	115.47	110.23
1	G	2085	GLU	N-CA-C	5.03	116.76	111.28
1	A	303	ILE	CA-C-O	-5.03	114.79	120.67
1	G	2031	TYR	CB-CA-C	5.02	118.04	109.75
1	D	1070	THR	CA-C-N	5.02	127.32	120.54
1	D	1070	THR	C-N-CA	5.02	127.32	120.54
1	C	757	LYS	N-CA-C	-5.02	105.89	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1877	ALA	CA-C-N	-5.02	111.95	121.54
1	F	1877	ALA	C-N-CA	-5.02	111.95	121.54
1	C	792	PRO	CA-C-N	5.01	127.31	120.54
1	C	792	PRO	C-N-CA	5.01	127.31	120.54
1	A	213	GLU	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ALA	Peptide
1	A	222	ASP	Peptide
1	A	282	ASN	Peptide
1	A	296	LYS	Peptide
1	A	81	LEU	Peptide
1	B	393	LEU	Peptide
1	B	504	ALA	Peptide
1	B	534	ASP	Peptide
1	B	544	TYR	Peptide
1	B	608	LYS	Peptide
1	C	705	LEU	Peptide
1	C	816	ALA	Peptide
1	C	846	ASP	Peptide
1	C	856	TYR	Peptide
1	C	920	LYS	Peptide
1	D	1017	LEU	Peptide
1	D	1158	ASP	Peptide
1	D	1168	TYR	Peptide
1	D	1232	LYS	Peptide
1	E	1329	LEU	Peptide
1	E	1470	ASP	Peptide
1	E	1480	TYR	Peptide
1	E	1544	LYS	Peptide
1	F	1641	LEU	Peptide
1	F	1782	ASP	Peptide
1	F	1792	TYR	Peptide
1	F	1831	ALA	Peptide
1	G	1953	LEU	Peptide
1	G	2094	ASP	Peptide
1	G	2104	TYR	Peptide
1	G	2168	LYS	Peptide

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	A	1705	0	991	35	0
1	B	1705	0	991	48	0
1	C	1705	0	991	44	0
1	D	1705	0	991	54	0
1	E	1705	0	991	51	0
1	F	1705	0	991	49	0
1	G	1705	0	991	39	0
All	All	11935	0	6937	273	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 14.

All (273) 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:G:2101:ARG:NE	1:G:2101:ARG:CD	1.68	1.54
1:B:541:ARG:HH12	1:B:582:VAL:HG11	1.33	0.94
1:G:1994:ILE:O	1:G:2161:THR:HA	1.70	0.92
1:B:434:ILE:O	1:B:601:THR:HA	1.72	0.88
1:D:1091:GLY:HA3	1:D:1153:ALA:HB2	1.58	0.86
1:B:583:ALA:HB3	1:C:907:ILE:HD11	1.61	0.83
1:E:1403:GLY:HA3	1:E:1465:ALA:HB2	1.63	0.79
1:E:1438:ALA:HB2	1:F:1649:ALA:HB2	1.65	0.79
1:C:814:ALA:HB2	1:D:1025:ALA:HB2	1.64	0.78
1:F:1682:ILE:O	1:F:1849:THR:HA	1.83	0.78
1:A:155:GLY:HA3	1:A:217:ALA:HB2	1.66	0.78
1:F:1750:ALA:HB2	1:G:1961:ALA:HB2	1.66	0.78
1:B:502:ALA:HB2	1:C:713:ALA:HB2	1.64	0.77
1:A:190:ALA:HB2	1:B:401:ALA:HB2	1.66	0.77
1:C:779:GLY:HA3	1:C:841:ALA:HB2	1.67	0.76
1:B:467:GLY:HA3	1:B:529:ALA:HB2	1.68	0.76
1:D:1126:ALA:HB2	1:E:1337:ALA:HB2	1.68	0.74
1:E:1370:ILE:O	1:E:1537:THR:HA	1.87	0.73
1:F:1715:GLY:HA3	1:F:1777:ALA:HB2	1.70	0.73
1:A:271:ALA:HB3	1:B:595:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1837:LYS:CB	1:F:1838:PRO:HD2	2.18	0.72
1:D:1161:THR:O	1:D:1164:TYR:HB2	1.89	0.72
1:A:25:ILE:HA	1:A:48:THR:HA	1.71	0.72
1:E:1473:THR:O	1:E:1476:TYR:HB2	1.89	0.70
1:C:649:ILE:HA	1:C:672:THR:HA	1.72	0.70
1:G:2027:GLY:HA3	1:G:2089:ALA:HB2	1.72	0.70
1:B:537:THR:O	1:B:540:TYR:HB2	1.93	0.69
1:D:961:ILE:HA	1:D:984:THR:HA	1.73	0.69
1:A:225:THR:O	1:A:228:TYR:HB2	1.92	0.69
1:B:337:ILE:HA	1:B:360:THR:HA	1.73	0.69
1:E:1443:PHE:H	1:F:1614:TYR:HE2	1.41	0.69
1:F:1585:ILE:HA	1:F:1608:THR:HA	1.74	0.69
1:C:746:ILE:O	1:C:913:THR:HA	1.93	0.69
1:C:849:THR:O	1:C:852:TYR:HB2	1.93	0.68
1:G:1897:ILE:HA	1:G:1920:THR:HA	1.75	0.67
1:D:1058:ILE:O	1:D:1225:THR:HA	1.94	0.67
1:F:1853:TYR:HD1	1:F:1853:TYR:C	2.03	0.66
1:A:102:ILE:O	1:A:116:GLY:HA3	1.95	0.66
1:G:2165:TYR:C	1:G:2165:TYR:CD1	2.74	0.66
1:B:628:GLU:O	1:B:629:ALA:CB	2.43	0.66
1:D:1038:ILE:O	1:D:1052:GLY:HA3	1.96	0.66
1:C:726:ILE:O	1:C:740:GLY:HA3	1.95	0.65
1:E:1273:ILE:HA	1:E:1296:THR:HA	1.78	0.65
1:G:2188:GLU:O	1:G:2189:ALA:CB	2.43	0.65
1:A:277:LYS:CB	1:A:278:PRO:HD2	2.27	0.65
1:B:414:ILE:O	1:B:428:GLY:HA3	1.96	0.65
1:F:1853:TYR:C	1:F:1853:TYR:CD1	2.75	0.65
1:D:1252:GLU:O	1:D:1253:ALA:CB	2.44	0.64
1:A:46:PHE:CB	1:A:51:ALA:HB1	2.27	0.64
1:E:1541:TYR:CD1	1:E:1541:TYR:C	2.76	0.64
1:D:1131:PHE:H	1:E:1302:TYR:HE2	1.46	0.64
1:F:1876:GLU:O	1:F:1877:ALA:CB	2.45	0.63
1:G:1974:ILE:O	1:G:1988:GLY:HA3	1.97	0.63
1:A:316:GLU:O	1:A:317:ALA:CB	2.46	0.62
1:G:1918:PHE:CB	1:G:1923:ALA:HB1	2.29	0.62
1:G:2165:TYR:C	1:G:2165:TYR:HD1	2.07	0.62
1:E:1564:GLU:O	1:E:1565:ALA:CB	2.48	0.62
1:B:589:LYS:CB	1:B:590:PRO:HD2	2.29	0.62
1:F:1662:ILE:O	1:F:1676:GLY:HA3	2.00	0.61
1:F:1755:PHE:H	1:G:1926:TYR:HE2	1.46	0.61
1:C:819:PHE:CB	1:D:990:TYR:CE2	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1350:ILE:O	1:E:1364:GLY:HA3	2.01	0.61
1:D:1229:TYR:CD1	1:D:1229:TYR:C	2.78	0.61
1:A:293:TYR:C	1:A:293:TYR:CD1	2.79	0.61
1:B:585:VAL:HG12	1:B:585:VAL:O	2.00	0.60
1:C:819:PHE:CB	1:D:990:TYR:CD2	2.84	0.60
1:G:2188:GLU:O	1:G:2189:ALA:HB2	2.00	0.60
1:B:435:THR:O	1:B:576:VAL:HA	2.01	0.60
1:B:605:TYR:CD1	1:B:605:TYR:C	2.80	0.60
1:E:1521:VAL:HG12	1:E:1521:VAL:O	2.03	0.59
1:C:917:TYR:CD1	1:C:917:TYR:C	2.80	0.59
1:F:1683:THR:O	1:F:1824:VAL:HA	2.03	0.59
1:C:940:GLU:O	1:C:941:ALA:CB	2.50	0.59
1:E:1541:TYR:C	1:E:1541:TYR:HD1	2.11	0.59
1:E:1371:THR:O	1:E:1512:VAL:HA	2.03	0.58
1:E:1519:ALA:HB3	1:F:1843:ILE:HD11	1.86	0.58
1:C:670:PHE:CB	1:C:675:ALA:HB1	2.34	0.57
1:C:747:THR:O	1:C:888:VAL:HA	2.04	0.57
1:D:1252:GLU:O	1:D:1253:ALA:HB2	2.04	0.57
1:G:2029:ALA:O	1:G:2061:VAL:CB	2.52	0.57
1:F:1785:THR:O	1:F:1788:TYR:HB2	2.04	0.56
1:A:195:PHE:CB	1:B:366:TYR:CE2	2.89	0.56
1:D:982:PHE:CB	1:D:987:ALA:HB1	2.35	0.56
1:G:2105:SER:O	1:G:2107:ARG:N	2.39	0.56
1:A:195:PHE:CB	1:B:366:TYR:CD2	2.89	0.55
1:F:1606:PHE:CB	1:F:1611:ALA:HB1	2.36	0.55
1:B:507:PHE:H	1:C:678:TYR:HE2	1.54	0.55
1:D:1131:PHE:CB	1:E:1302:TYR:CD2	2.90	0.55
1:G:2097:THR:O	1:G:2100:TYR:HB2	2.06	0.55
1:E:1519:ALA:H	1:F:1843:ILE:HD13	1.71	0.55
1:B:628:GLU:O	1:B:629:ALA:HB2	2.07	0.55
1:E:1481:SER:O	1:E:1483:ARG:N	2.41	0.54
1:A:123:THR:O	1:A:264:VAL:HA	2.07	0.54
1:B:507:PHE:CB	1:C:678:TYR:CE2	2.91	0.54
1:C:716:PHE:O	1:C:720:ARG:N	2.39	0.54
1:E:1443:PHE:CB	1:F:1614:TYR:CD2	2.91	0.54
1:E:1564:GLU:O	1:E:1565:ALA:HB2	2.08	0.54
1:G:2027:GLY:HA3	1:G:2089:ALA:CB	2.37	0.54
1:D:1207:ALA:HB3	1:E:1531:ILE:HD11	1.90	0.53
1:E:1340:PHE:O	1:E:1344:ARG:N	2.40	0.53
1:C:857:SER:O	1:C:859:ARG:N	2.42	0.53
1:G:2030[A]:MET:CB	1:G:2091:LEU:HD13	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1876:GLU:O	1:F:1877:ALA:HB2	2.07	0.53
1:D:1184:PHE:CD1	1:D:1184:PHE:C	2.86	0.53
1:D:1131:PHE:CB	1:E:1302:TYR:CE2	2.92	0.53
1:D:1229:TYR:C	1:D:1229:TYR:HD1	2.15	0.53
1:F:1793:SER:O	1:F:1795:ARG:N	2.43	0.52
1:D:1028:PHE:O	1:D:1032:ARG:N	2.41	0.52
1:C:645:GLY:N	1:C:646:PRO:HD2	2.24	0.52
1:C:895:ALA:HB3	1:D:1219:ILE:HD11	1.91	0.52
1:F:1719:TYR:HA	1:F:1780[A]:ILE:O	2.10	0.52
1:A:233:SER:O	1:A:235:ARG:N	2.42	0.52
1:B:404:PHE:O	1:B:408:ARG:N	2.40	0.52
1:D:1169:SER:O	1:D:1171:ARG:N	2.43	0.52
1:D:1059:THR:O	1:D:1200:VAL:HA	2.09	0.51
1:F:1755:PHE:CB	1:G:1926:TYR:CD2	2.93	0.51
1:B:560:PHE:CD1	1:B:560:PHE:C	2.88	0.51
1:E:1496:PHE:CD1	1:E:1496:PHE:C	2.88	0.51
1:B:583:ALA:CB	1:C:907:ILE:HD11	2.37	0.51
1:B:507:PHE:CB	1:C:678:TYR:CD2	2.93	0.51
1:E:1294:PHE:CB	1:E:1299:ALA:HB1	2.40	0.51
1:G:1964:PHE:O	1:G:1968:ARG:N	2.40	0.51
1:A:195:PHE:H	1:B:366:TYR:HE2	1.59	0.51
1:G:2033:ASP:O	1:G:2065:ARG:HA	2.11	0.51
1:A:248:PHE:C	1:A:248:PHE:CD1	2.88	0.50
1:B:545:SER:O	1:B:547:ARG:N	2.45	0.50
1:C:872:PHE:CD1	1:C:872:PHE:C	2.88	0.50
1:B:358:PHE:CB	1:B:363:ALA:HB1	2.41	0.50
1:F:1808:PHE:CD1	1:F:1808:PHE:C	2.88	0.50
1:F:1652:PHE:O	1:F:1656:ARG:N	2.41	0.50
1:F:1719:TYR:HA	1:F:1780[B]:ILE:O	2.11	0.49
1:F:1581:GLY:N	1:F:1582:PRO:HD2	2.28	0.49
1:F:1837:LYS:CB	1:F:1838:PRO:CD	2.90	0.49
1:E:1443:PHE:CB	1:F:1614:TYR:CE2	2.96	0.49
1:C:819:PHE:H	1:D:990:TYR:HE2	1.61	0.49
1:D:1017:LEU:HA	1:D:1019:PRO:N	2.28	0.49
1:D:1213:LYS:CB	1:D:1214:PRO:HD2	2.43	0.49
1:G:1893:GLY:N	1:G:1894:PRO:HD2	2.28	0.49
1:D:1095:TYR:HA	1:D:1156[A]:ILE:O	2.14	0.48
1:E:1403:GLY:HA3	1:E:1465:ALA:CB	2.41	0.48
1:E:1519:ALA:HA	1:E:1525:LYS:CB	2.43	0.48
1:B:333:GLY:N	1:B:334:PRO:HD2	2.29	0.48
1:A:192:ALA:HB2	1:B:397:GLY:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:895:ALA:H	1:D:1219:ILE:HD13	1.76	0.48
1:F:1715:GLY:HA3	1:F:1777:ALA:CB	2.42	0.48
1:G:1906:ASN:O	1:G:1908:ASN:N	2.47	0.48
1:C:901:LYS:CB	1:C:902:PRO:HD2	2.42	0.48
1:G:2120:PHE:CD1	1:G:2120:PHE:C	2.90	0.48
1:A:158[A]:MET:O	1:A:219:LEU:HA	2.14	0.48
1:B:634:ASN:O	1:B:635:ALA:C	2.56	0.48
1:F:1594:ASN:O	1:F:1596:ASN:N	2.47	0.48
1:C:719:ARG:O	1:C:722:GLU:N	2.47	0.48
1:E:1407:TYR:HA	1:E:1468[A]:ILE:O	2.14	0.47
1:B:407:ARG:O	1:B:410:GLU:N	2.46	0.47
1:B:504:ALA:HB2	1:C:709:GLY:C	2.39	0.47
1:B:541:ARG:NH1	1:B:582:VAL:HG11	2.15	0.47
1:C:770:LEU:O	1:C:776:GLY:HA3	2.14	0.47
1:C:895:ALA:H	1:D:1219:ILE:CD1	2.28	0.47
1:F:1706:LEU:O	1:F:1712:GLY:HA3	2.14	0.47
1:G:1953:LEU:HA	1:G:1955:PRO:N	2.30	0.47
1:A:21:GLY:N	1:A:22:PRO:HD2	2.30	0.47
1:A:293:TYR:C	1:A:293:TYR:HD1	2.22	0.47
1:D:1095:TYR:HA	1:D:1156[B]:ILE:O	2.15	0.47
1:D:1128:ALA:HB2	1:E:1333:GLY:C	2.39	0.47
1:D:1082:LEU:O	1:D:1088:GLY:HA3	2.14	0.47
1:E:1343:ARG:O	1:E:1346:GLU:N	2.48	0.47
1:E:1407:TYR:HA	1:E:1468[B]:ILE:O	2.15	0.47
1:G:1995:THR:O	1:G:2136:VAL:HA	2.14	0.47
1:G:2018:LEU:O	1:G:2024:GLY:HA3	2.15	0.47
1:D:1031:ARG:O	1:D:1034:GLU:N	2.48	0.47
1:D:1166:THR:OG1	1:D:1167:ASP:N	2.48	0.47
1:E:1394:LEU:O	1:E:1400:GLY:HA3	2.14	0.47
1:F:1751:TYR:HE2	1:G:1964:PHE:CB	2.27	0.47
1:C:658:ASN:O	1:C:660:ASN:N	2.48	0.47
1:F:1831:ALA:HA	1:F:1837:LYS:CB	2.45	0.46
1:E:1282:ASN:O	1:E:1284:ASN:N	2.48	0.46
1:C:917:TYR:C	1:C:917:TYR:HD1	2.23	0.46
1:E:1501:LEU:O	1:E:1504:ALA:HB3	2.15	0.46
1:B:605:TYR:C	1:B:605:TYR:HD1	2.24	0.46
1:D:957:GLY:N	1:D:958:PRO:HD2	2.30	0.46
1:C:705:LEU:HA	1:C:707:PRO:N	2.30	0.46
1:D:970:ASN:O	1:D:972:ASN:N	2.49	0.46
1:E:1329:LEU:HA	1:E:1331:PRO:N	2.30	0.46
1:D:1189:LEU:O	1:D:1192:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1655:ARG:O	1:F:1658:GLU:N	2.49	0.46
1:A:316:GLU:O	1:A:317:ALA:HB2	2.15	0.45
1:B:458:LEU:O	1:B:464:GLY:HA3	2.16	0.45
1:B:393:LEU:HA	1:B:395:PRO:N	2.30	0.45
1:A:146:LEU:O	1:A:152:GLY:HA3	2.17	0.45
1:B:471:TYR:HA	1:B:532[A]:ILE:O	2.17	0.45
1:C:816:ALA:HB2	1:D:1021:GLY:C	2.41	0.45
1:C:815:TYR:HE2	1:D:1028:PHE:CB	2.29	0.45
1:F:1641:LEU:HA	1:F:1643:PRO:N	2.32	0.45
1:A:253:LEU:O	1:A:256:ALA:HB3	2.17	0.45
1:F:1752:ALA:HB2	1:G:1957:GLY:C	2.42	0.45
1:E:1570:ASN:O	1:E:1571:ALA:C	2.60	0.45
1:F:1813:LEU:O	1:F:1816:ALA:HB3	2.17	0.45
1:E:1518:VAL:HA	1:F:1843:ILE:HG21	1.99	0.44
1:F:1798:LEU:O	1:F:1798:LEU:HG	2.17	0.44
1:E:1486:LEU:O	1:E:1486:LEU:HG	2.17	0.44
1:E:1440:ALA:HB2	1:F:1645:GLY:C	2.42	0.44
1:G:2091:LEU:HB3	1:G:2134:ALA:O	2.18	0.44
1:D:956:PHE:O	1:D:956:PHE:CG	2.71	0.44
1:A:34:ASN:O	1:A:36:ASN:N	2.51	0.44
1:G:1918:PHE:CB	1:G:1923:ALA:CB	2.96	0.44
1:A:122:ILE:O	1:A:289:THR:HA	2.17	0.44
1:B:471:TYR:HA	1:B:532[B]:ILE:O	2.18	0.44
1:C:854:THR:OG1	1:C:855:ASP:N	2.50	0.44
1:E:1415:ARG:HA	1:E:1416:PRO:HD3	1.91	0.44
1:F:1882:ASN:O	1:F:1883:ALA:C	2.61	0.44
1:D:1094[A]:MET:CB	1:D:1155:LEU:HD13	2.48	0.43
1:G:2063:TYR:CG	1:G:2063:TYR:O	2.69	0.43
1:G:2165:TYR:HD1	1:G:2166:LEU:N	2.16	0.43
1:A:159:TYR:HA	1:A:220[A]:ILE:O	2.18	0.43
1:E:1269:GLY:N	1:E:1270:PRO:HD2	2.33	0.43
1:G:2125:LEU:O	1:G:2128:ALA:HB3	2.19	0.43
1:B:542:THR:OG1	1:B:543:ASP:N	2.51	0.43
1:G:1967:ARG:O	1:G:1970:GLU:N	2.50	0.43
1:A:322:ASN:O	1:A:323:ALA:C	2.60	0.43
1:A:95:ARG:O	1:A:98:GLU:N	2.52	0.43
1:C:783:TYR:HA	1:C:844[A]:ILE:O	2.18	0.43
1:E:1478:THR:OG1	1:E:1479:ASP:N	2.51	0.43
1:F:1718[A]:MET:CB	1:F:1779:LEU:HD13	2.49	0.43
1:F:1779:LEU:HB3	1:F:1822:ALA:O	2.19	0.43
1:G:2110:LEU:O	1:G:2110:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:CB	1:A:278:PRO:CD	2.96	0.43
1:B:565:LEU:O	1:B:568:ALA:HB3	2.19	0.43
1:E:1443:PHE:N	1:F:1614:TYR:HE2	2.13	0.42
1:B:346:ASN:O	1:B:348:ASN:N	2.52	0.42
1:G:1991:THR:HA	1:G:2134:ALA:HA	2.00	0.42
1:C:819:PHE:CB	1:D:990:TYR:HE2	2.30	0.42
1:B:470[A]:MET:O	1:B:531:LEU:HA	2.20	0.42
1:D:1258:ASN:O	1:D:1259:ALA:C	2.61	0.42
1:G:2108:GLY:C	1:G:2110:LEU:H	2.27	0.42
1:C:946:ASN:O	1:C:947:ALA:C	2.62	0.42
1:A:159:TYR:HA	1:A:220[B]:ILE:O	2.20	0.42
1:B:583:ALA:H	1:C:907:ILE:HD13	1.83	0.42
1:G:2194:ASN:O	1:G:2195:ALA:C	2.61	0.42
1:E:1541:TYR:HD1	1:E:1542:LEU:N	2.18	0.42
1:F:1791:ASP:O	1:F:1792:TYR:HB2	2.20	0.42
1:C:746:ILE:O	1:C:913:THR:CA	2.66	0.42
1:C:877:LEU:O	1:C:880:ALA:HB3	2.19	0.42
1:E:1406[A]:MET:O	1:E:1467:LEU:HA	2.20	0.42
1:F:1790:THR:OG1	1:F:1791:ASP:N	2.53	0.42
1:D:1091:GLY:HA3	1:D:1153:ALA:CB	2.38	0.41
1:D:1229:TYR:HD1	1:D:1230:LEU:N	2.18	0.41
1:F:1606:PHE:CB	1:F:1611:ALA:CB	2.98	0.41
1:C:783:TYR:HA	1:C:844[B]:ILE:O	2.19	0.41
1:E:1525:LYS:CB	1:E:1526:PRO:HD2	2.50	0.41
1:A:46:PHE:CB	1:A:51:ALA:CB	2.96	0.41
1:D:1207:ALA:H	1:E:1531:ILE:HD13	1.85	0.41
1:E:1326:ALA:O	1:E:1327:ALA:C	2.64	0.41
1:A:230:THR:OG1	1:A:231:ASP:N	2.53	0.41
1:B:589:LYS:CB	1:B:590:PRO:CD	2.97	0.41
1:E:1477:ARG:HH11	1:E:1477:ARG:HD2	1.67	0.41
1:F:1580:PHE:O	1:F:1580:PHE:CG	2.74	0.41
1:B:479:ARG:HA	1:B:480:PRO:HD3	1.92	0.41
1:D:1174:LEU:O	1:D:1174:LEU:HG	2.21	0.41
1:C:785:ASP:HA	1:C:846:ASP:O	2.21	0.41
1:D:1097:ASP:HA	1:D:1158:ASP:O	2.21	0.41
1:A:20:PHE:O	1:A:20:PHE:CG	2.73	0.41
1:A:293:TYR:HD1	1:A:294:LEU:N	2.19	0.41
1:D:956:PHE:O	1:D:956:PHE:CD2	2.74	0.41
1:D:1076:LEU:C	1:D:1078:VAL:N	2.79	0.41
1:B:473:ASP:HA	1:B:534:ASP:O	2.21	0.40
1:A:84:MET:O	1:A:87:THR:N	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:TYR:CE2	1:B:553:ARG:HA	2.57	0.40
1:D:1014:ALA:O	1:D:1015:ALA:C	2.65	0.40
1:D:1103:ARG:HA	1:D:1104:PRO:HD3	1.92	0.40
1:D:1131:PHE:N	1:E:1302:TYR:HE2	2.15	0.40
1:B:541:ARG:HH12	1:B:582:VAL:CG1	2.18	0.40
1:D:1209:VAL:HG12	1:D:1209:VAL:O	2.21	0.40
1:F:1755:PHE:CB	1:G:1926:TYR:CE2	3.05	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	312/339 (92%)	264 (85%)	33 (11%)	15 (5%)	2	17
1	B	312/339 (92%)	259 (83%)	38 (12%)	15 (5%)	2	17
1	C	312/339 (92%)	261 (84%)	35 (11%)	16 (5%)	1	16
1	D	312/339 (92%)	265 (85%)	32 (10%)	15 (5%)	2	17
1	E	312/339 (92%)	263 (84%)	34 (11%)	15 (5%)	2	17
1	F	312/339 (92%)	264 (85%)	33 (11%)	15 (5%)	2	17
1	G	312/339 (92%)	260 (83%)	37 (12%)	15 (5%)	2	17
All	All	2184/2373 (92%)	1836 (84%)	242 (11%)	106 (5%)	3	16

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	24	PRO
1	A	35	ALA
1	A	82	VAL

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Mol	Chain	Res	Type
1	A	85	GLY
1	A	311	CYS
1	A	317	ALA
1	B	335	GLN
1	B	336	PRO
1	B	347	ALA
1	B	394	VAL
1	B	618	ILE
1	B	623	CYS
1	B	629	ALA
1	C	647	GLN
1	C	648	PRO
1	C	659	ALA
1	C	706	VAL
1	C	930	ILE
1	C	935	CYS
1	C	941	ALA
1	D	959	GLN
1	D	960	PRO
1	D	971	ALA
1	D	1018	VAL
1	D	1242	ILE
1	D	1247	CYS
1	D	1253	ALA
1	E	1271	GLN
1	E	1272	PRO
1	E	1283	ALA
1	E	1330	VAL
1	E	1333	GLY
1	E	1559	CYS
1	E	1565	ALA
1	F	1583	GLN
1	F	1584	PRO
1	F	1595	ALA
1	F	1642	VAL
1	F	1645	GLY
1	F	1866	ILE
1	F	1871	CYS
1	F	1877	ALA
1	G	1895	GLN
1	G	1896	PRO
1	G	1907	ALA

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Mol	Chain	Res	Type
1	G	1954	VAL
1	G	2178	ILE
1	G	2183	CYS
1	G	2189	ALA
1	A	232	TYR
1	A	234	GLY
1	A	306	ILE
1	B	397	GLY
1	B	402	THR
1	B	544	TYR
1	B	546	GLY
1	B	627	ALA
1	B	641	ALA
1	C	709	GLY
1	C	714	THR
1	C	856	TYR
1	C	858	GLY
1	C	913	THR
1	D	1021	GLY
1	D	1026	THR
1	D	1168	TYR
1	D	1170	GLY
1	D	1251	ALA
1	E	1338	THR
1	E	1482	GLY
1	E	1554	ILE
1	E	1563	ALA
1	F	1650	THR
1	F	1792	TYR
1	F	1794	GLY
1	F	1849	THR
1	G	1957	GLY
1	G	1962	THR
1	G	2104	TYR
1	G	2106	GLY
1	G	2187	ALA
1	G	2201	ALA
1	A	289	THR
1	A	315	ALA
1	A	329	ALA
1	B	601	THR
1	C	939	ALA

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Mol	Chain	Res	Type
1	C	953	ALA
1	D	1225	THR
1	D	1265	ALA
1	E	1480	TYR
1	E	1537	THR
1	E	1577	ALA
1	F	1875	ALA
1	F	1889	ALA
1	G	2161	THR
1	A	25	ILE
1	A	309	SER
1	B	337	ILE
1	C	649	ILE
1	D	961	ILE
1	E	1273	ILE
1	F	1585	ILE
1	G	1897	ILE
1	C	909	ALA

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	37/269 (14%)	25 (68%)	12 (32%)	0	2
1	B	37/269 (14%)	27 (73%)	10 (27%)	0	3
1	C	37/269 (14%)	27 (73%)	10 (27%)	0	3
1	D	37/269 (14%)	29 (78%)	8 (22%)	1	6
1	E	37/269 (14%)	27 (73%)	10 (27%)	0	3
1	F	37/269 (14%)	28 (76%)	9 (24%)	1	5
1	G	37/269 (14%)	28 (76%)	9 (24%)	1	5
All	All	259/1883 (14%)	191 (74%)	68 (26%)	2	3

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	54	TYR
1	A	219	LEU
1	A	229	ARG
1	A	238	LEU
1	A	268	GLN
1	A	270	VAL
1	A	273	VAL
1	A	283	ILE
1	A	293	TYR
1	A	310	PRO
1	A	313	PRO
1	B	359	HIS
1	B	531	LEU
1	B	541	ARG
1	B	550	LEU
1	B	580	GLN
1	B	595	ILE
1	B	605	TYR
1	B	619	TYR
1	B	622	PRO
1	B	625	PRO
1	C	671	HIS
1	C	843	LEU
1	C	853	ARG
1	C	862	LEU
1	C	892	GLN
1	C	907	ILE
1	C	917	TYR
1	C	931	TYR
1	C	934	PRO
1	C	937	PRO
1	D	983	HIS
1	D	1155	LEU
1	D	1165	ARG
1	D	1174	LEU
1	D	1204	GLN
1	D	1229	TYR
1	D	1246	PRO
1	D	1249	PRO
1	E	1295	HIS
1	E	1467	LEU
1	E	1477	ARG

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Mol	Chain	Res	Type
1	E	1481	SER
1	E	1486	LEU
1	E	1516	GLN
1	E	1531	ILE
1	E	1541	TYR
1	E	1558	PRO
1	E	1561	PRO
1	F	1607	HIS
1	F	1779	LEU
1	F	1789	ARG
1	F	1798	LEU
1	F	1828	GLN
1	F	1843	ILE
1	F	1853	TYR
1	F	1870	PRO
1	F	1873	PRO
1	G	1919	HIS
1	G	2065	ARG
1	G	2101	ARG
1	G	2110	LEU
1	G	2140	GLN
1	G	2155	ILE
1	G	2165	TYR
1	G	2182	PRO
1	G	2185	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	580	GLN
1	E	1516	GLN

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.

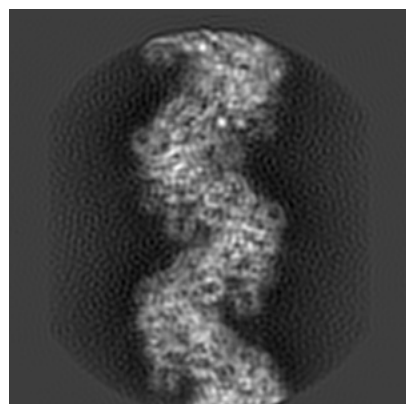
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8183. These allow visual inspection of the internal detail of the map and identification of artifacts.

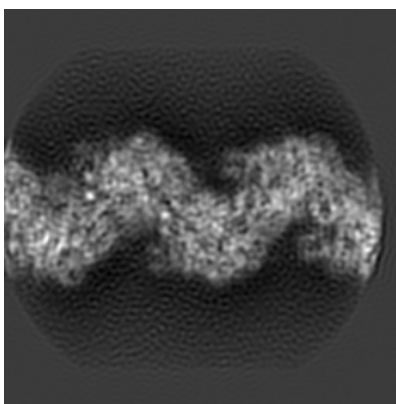
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

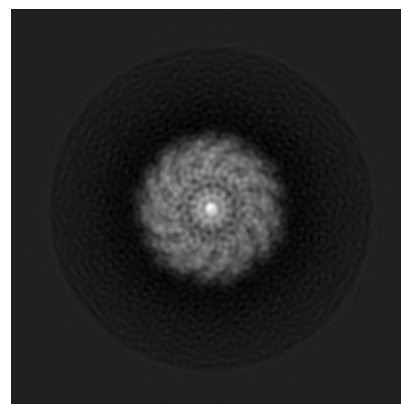
6.1.1 Primary map



X

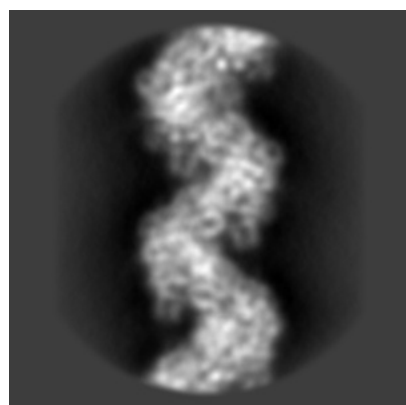


Y

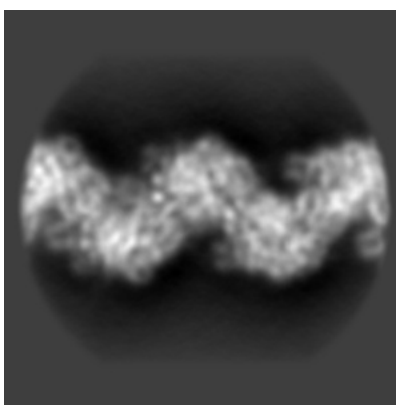


Z

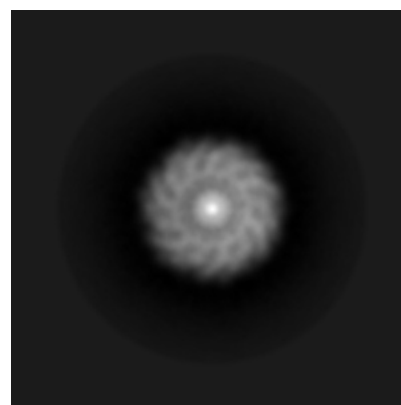
6.1.2 Raw map



X



Y

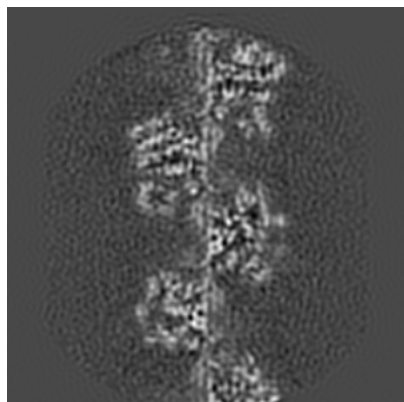


Z

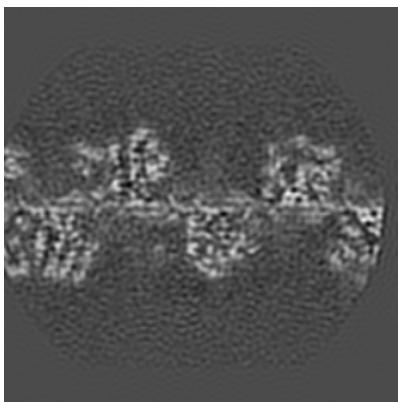
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

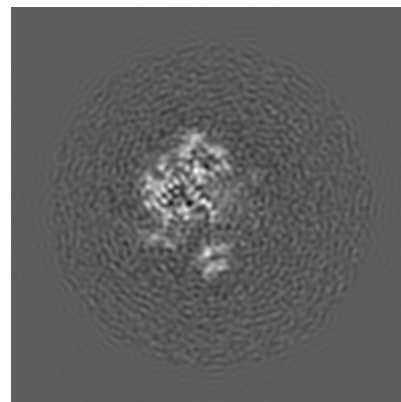
6.2.1 Primary map



X Index: 128

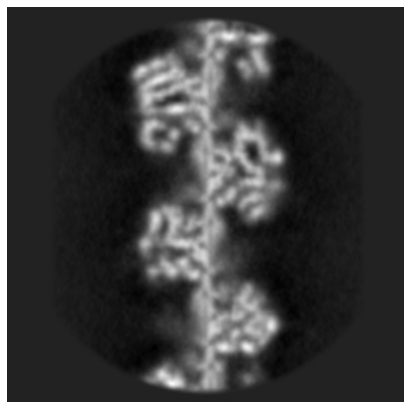


Y Index: 128

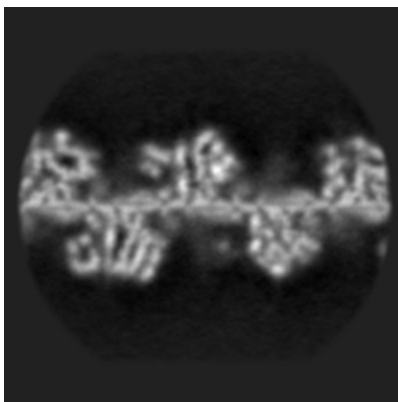


Z Index: 128

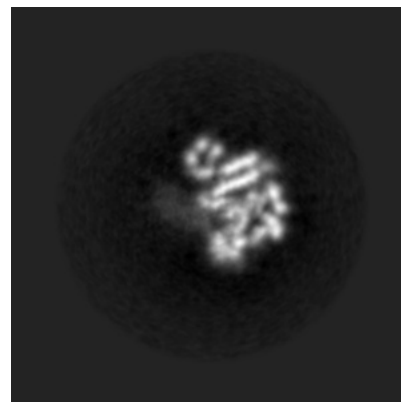
6.2.2 Raw map



X Index: 100



Y Index: 100

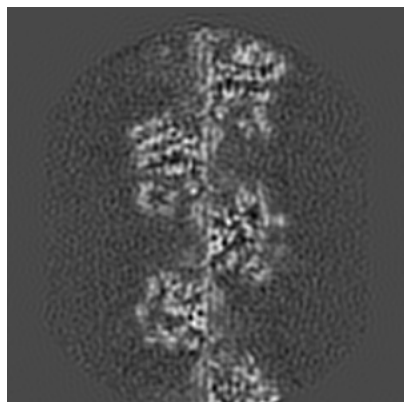


Z Index: 100

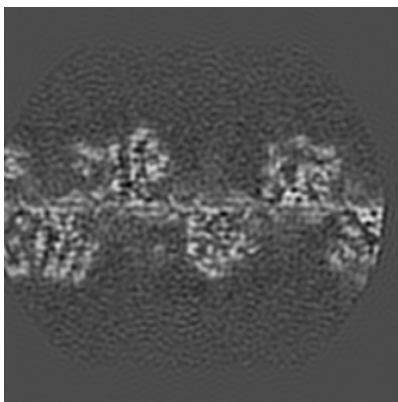
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

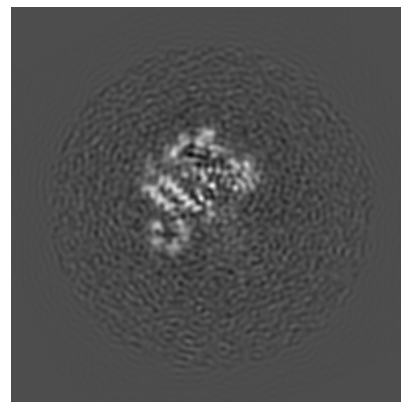
6.3.1 Primary map



X Index: 128

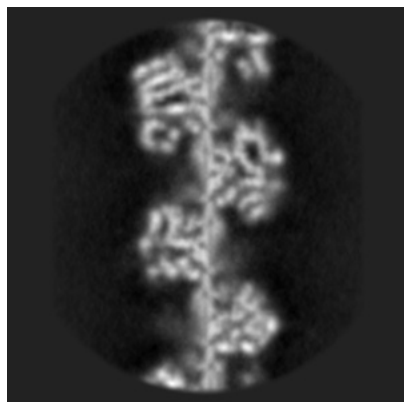


Y Index: 128

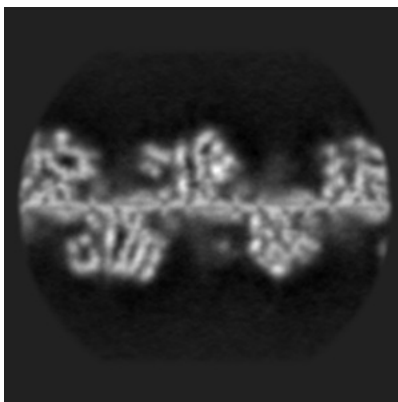


Z Index: 118

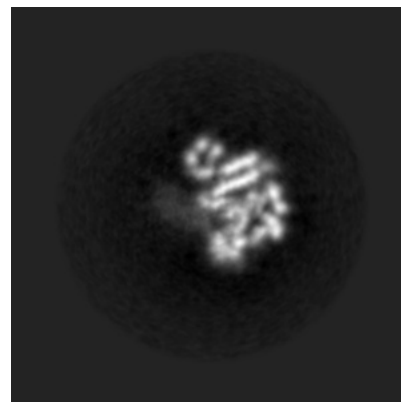
6.3.2 Raw map



X Index: 100



Y Index: 100

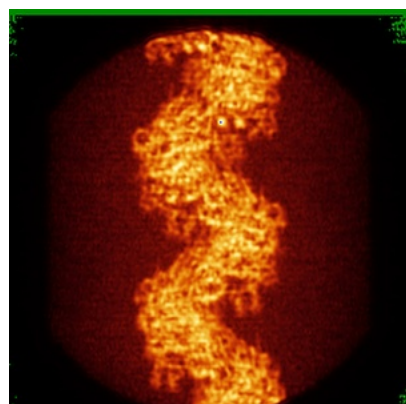


Z Index: 100

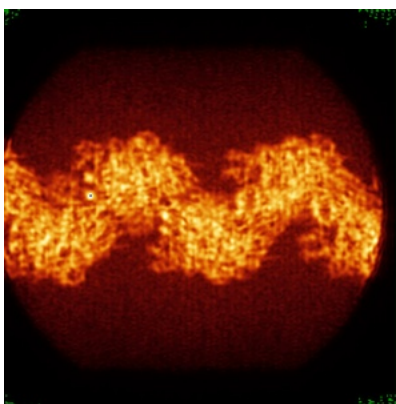
The images above show the largest variance slices of the map in three orthogonal directions.

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

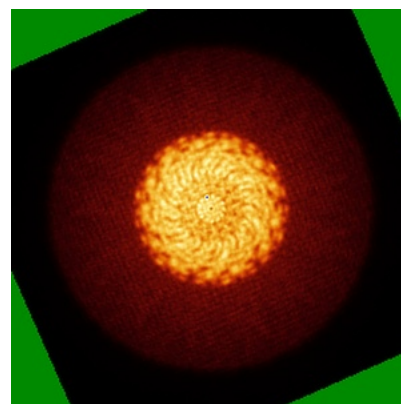
6.4.1 Primary map



X



Y

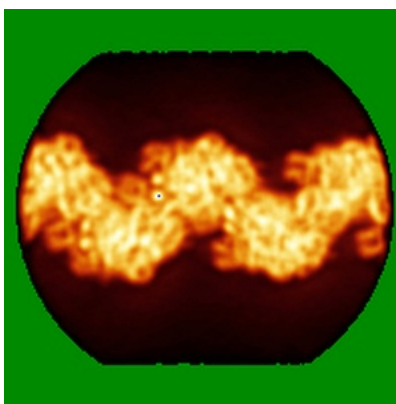


Z

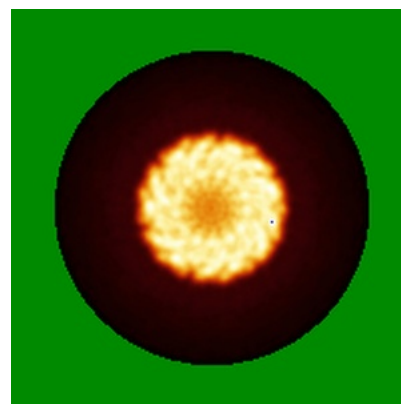
6.4.2 Raw map



X



Y

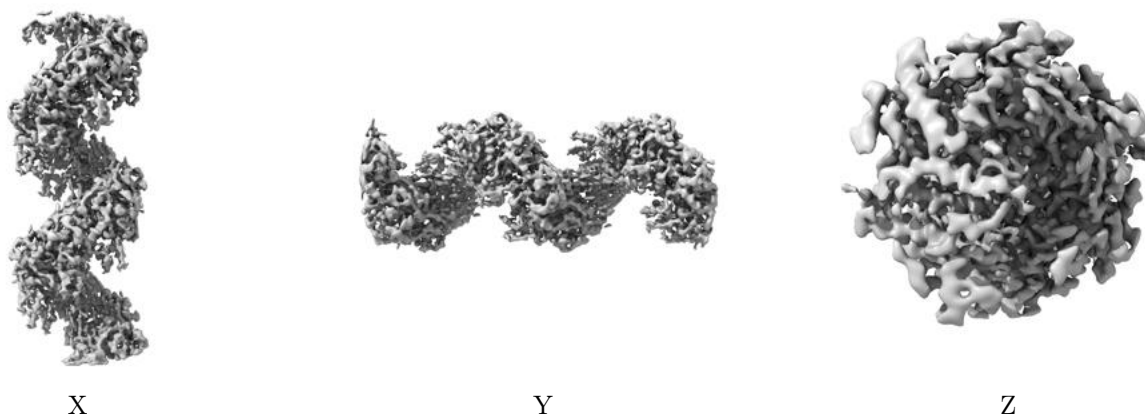


Z

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.

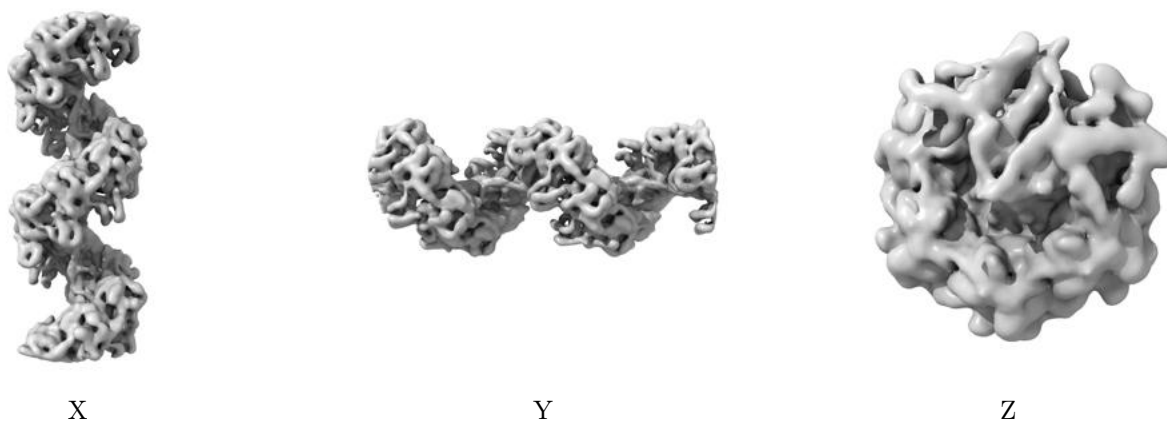
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

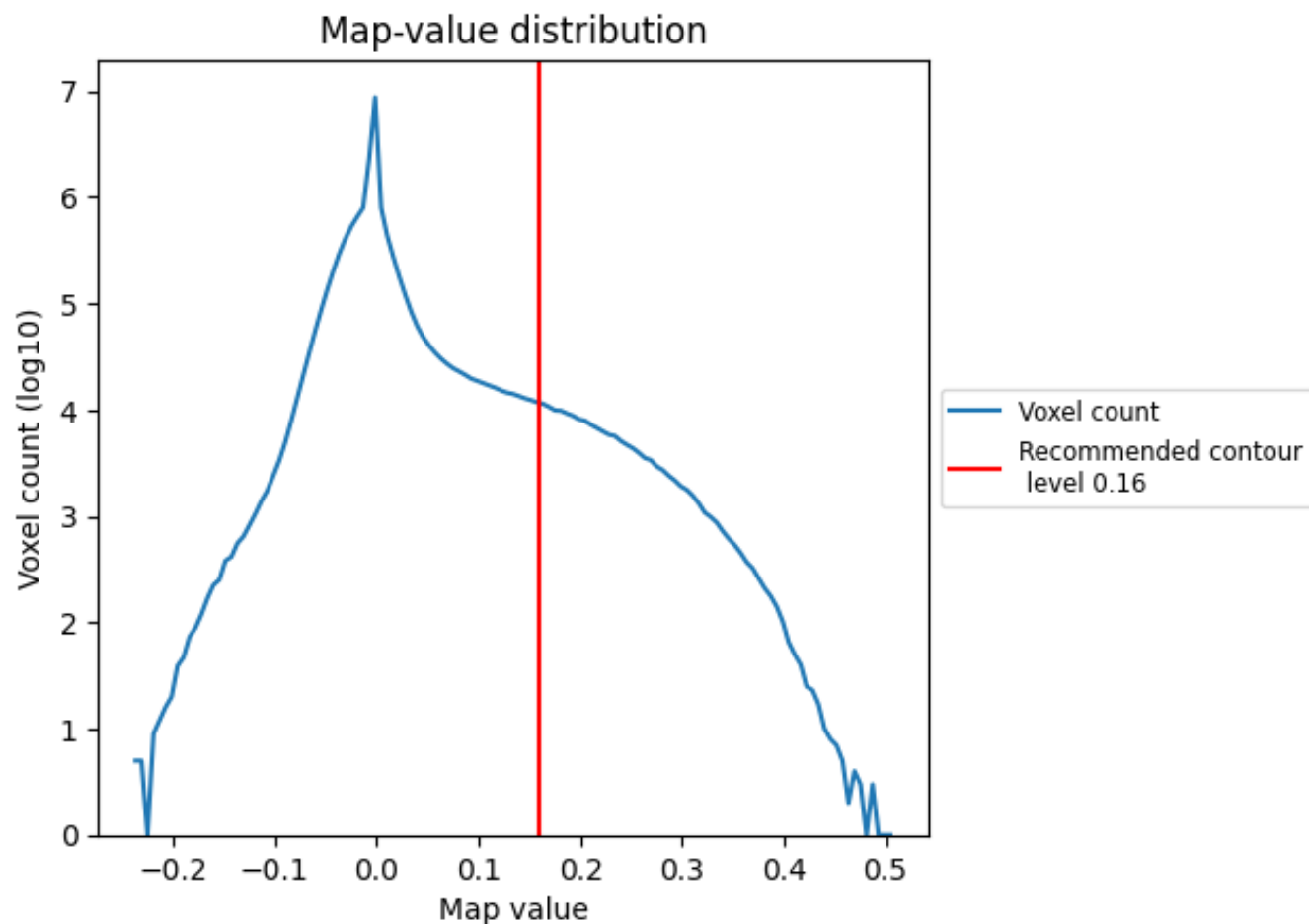
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

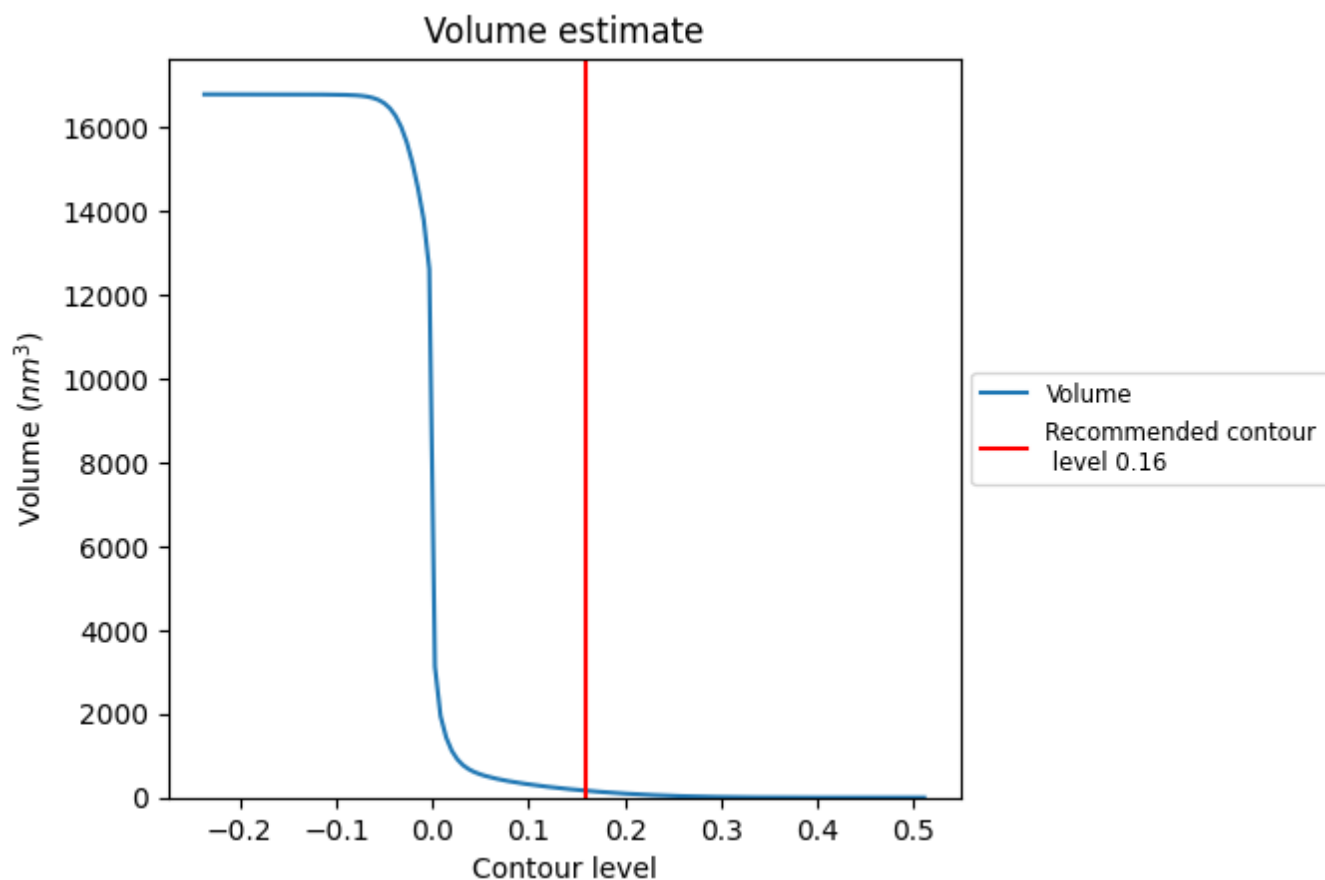
This section contains the results of statistical analysis of the map.

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.

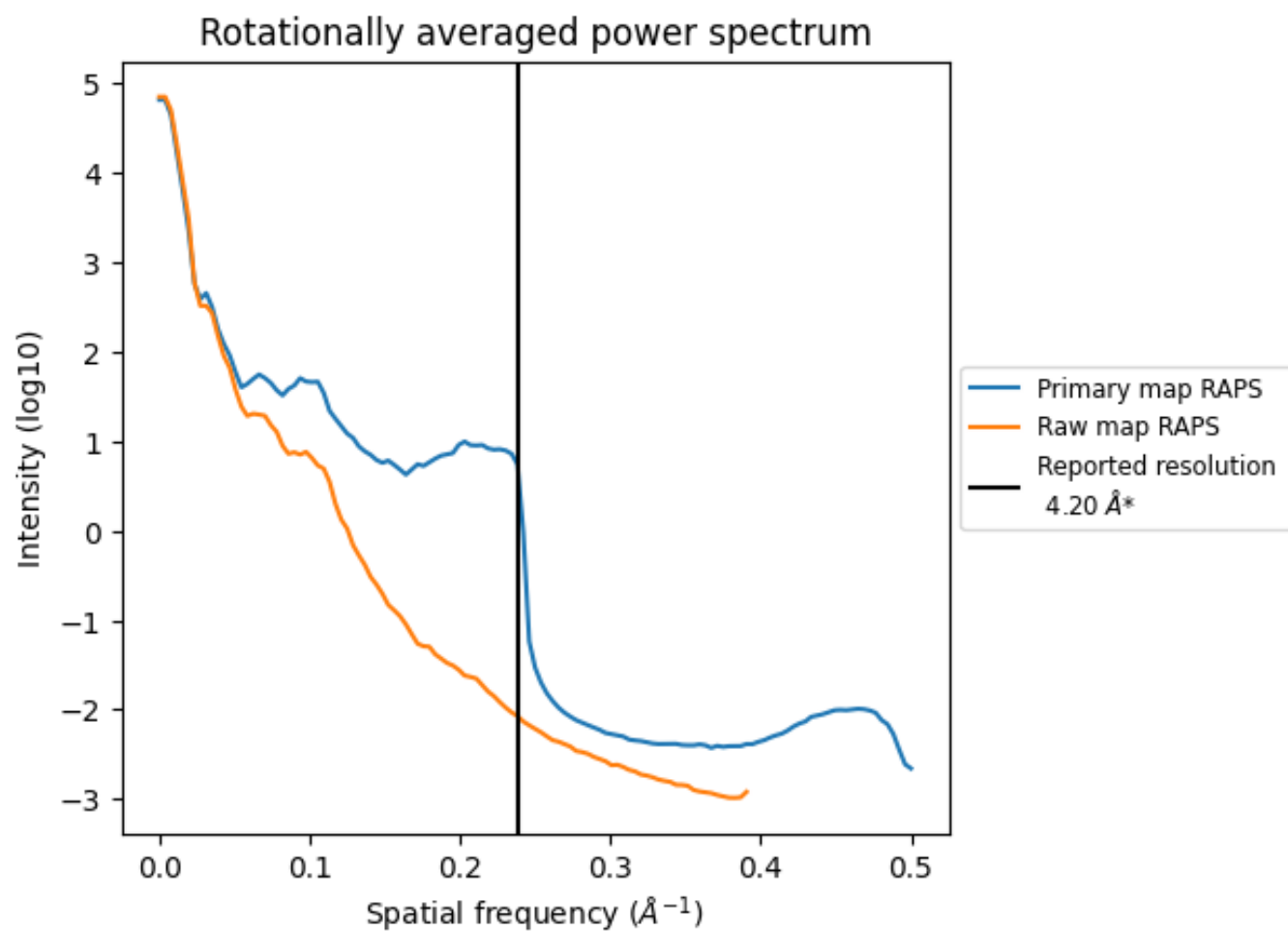
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm³; this corresponds to an approximate mass of 148 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 ⓘ

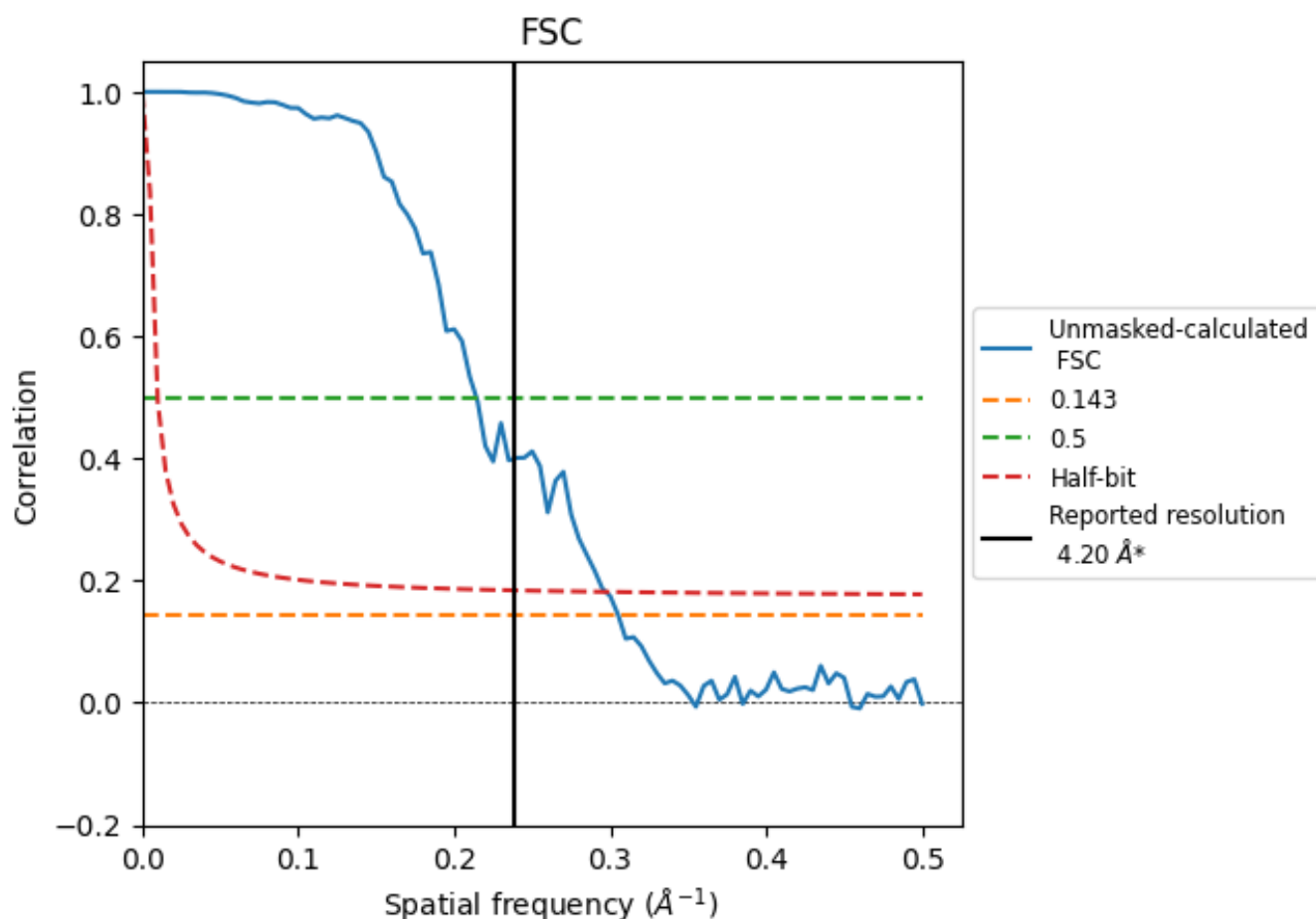


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

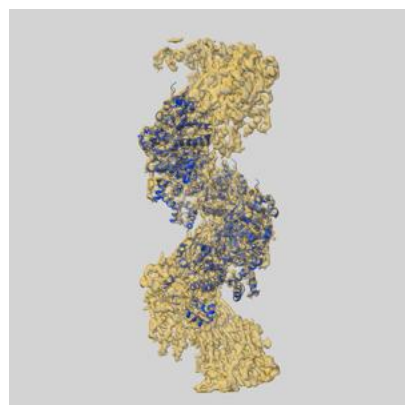
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.67	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 4.2 by more than 10 %

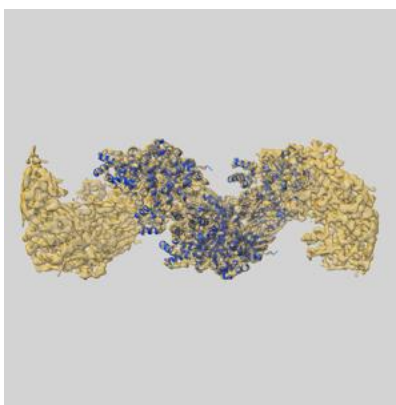
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8183 and PDB model 5JZC. Per-residue inclusion information can be found in section [3](#) on page [5](#).

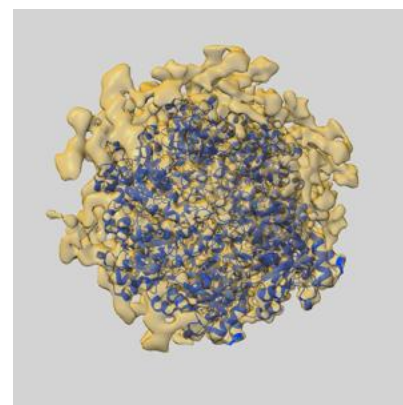
9.1 Map-model overlay [i](#)



X



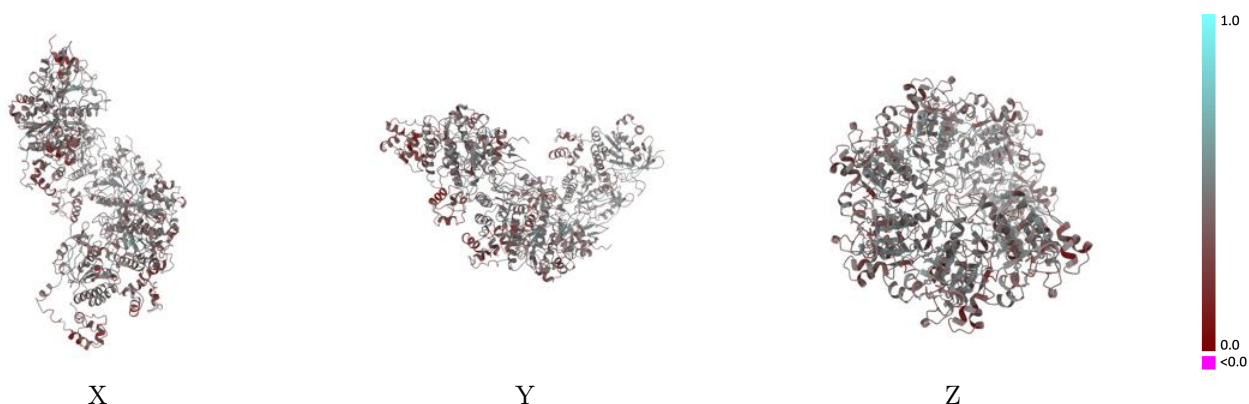
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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](#)

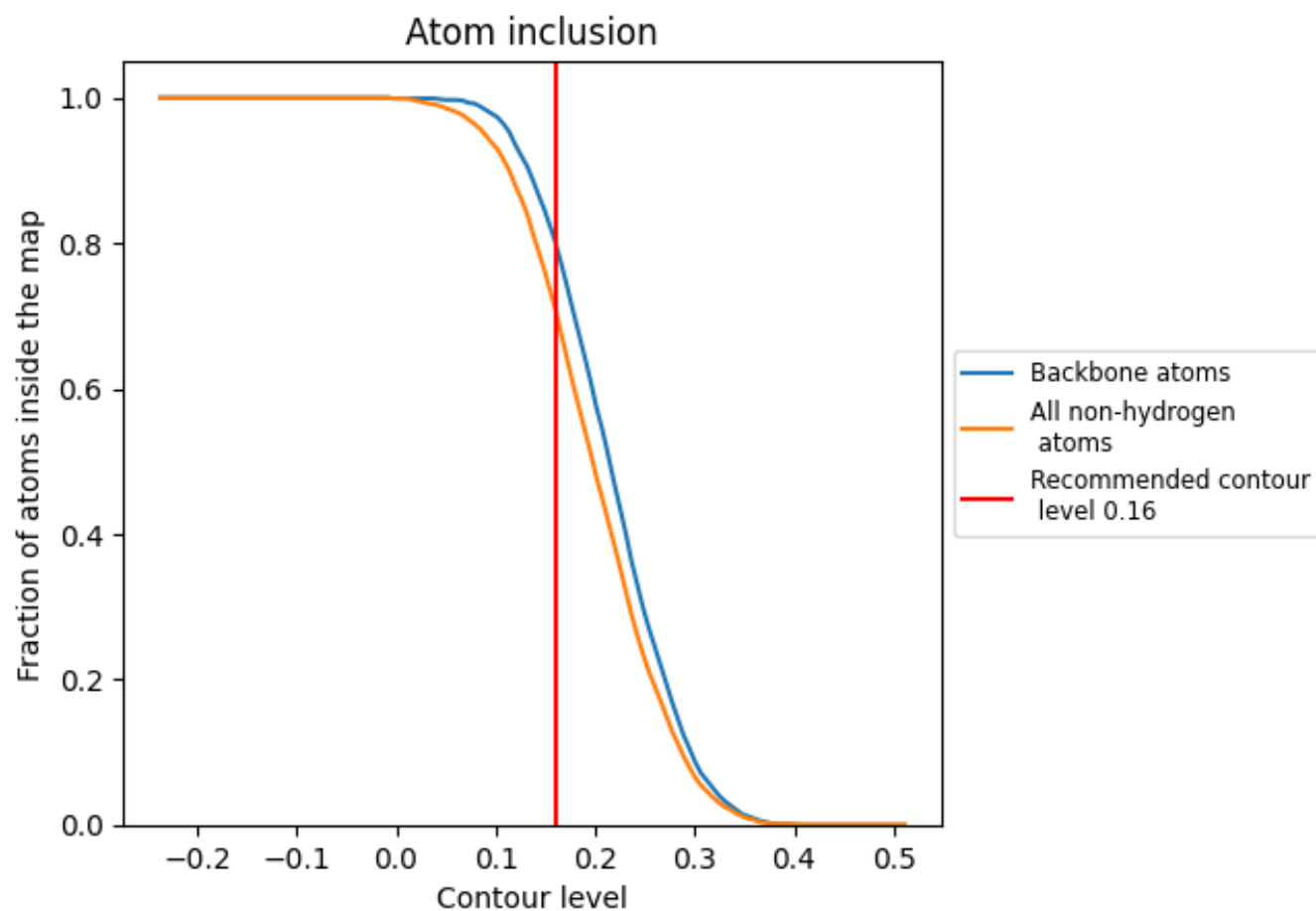


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.4170
A	0.7030	0.4150
B	0.7090	0.4180
C	0.7150	0.4180
D	0.7120	0.4200
E	0.7150	0.4200
F	0.7090	0.4160
G	0.7080	0.4140

1.0

0.0

<0.0