



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:58 AM UTC

PDB ID : 6BDF / pdb_00006bdf
EMDB ID : EMD-6287
Title : 2.8 Å resolution reconstruction of the Thermoplasma acidophilum 20S proteasome using cryo-electron microscopy
Authors : Campbell, M.G.; Veesler, D.; Cheng, A.; Potter, C.S.; Carragher, B.
Deposited on : 2017-10-23
Resolution : 2.80 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:

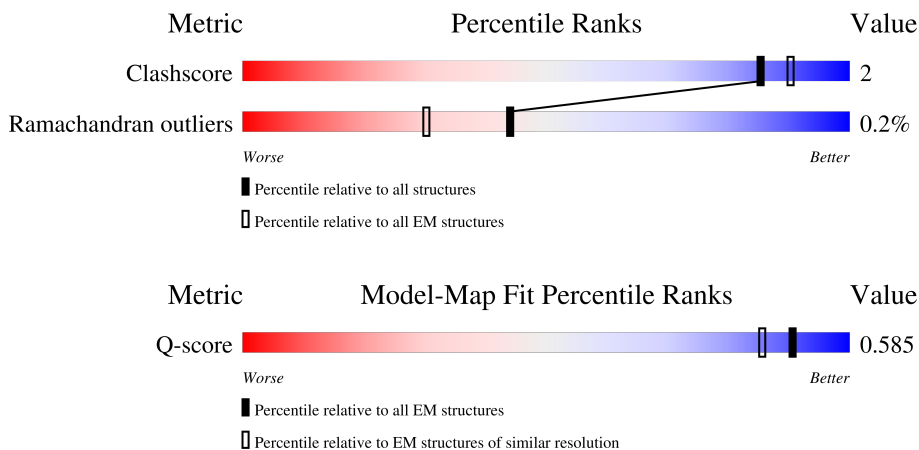
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.80 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	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	0	233	 8% 90% . . 5%
1	A	233	 9% 90% . . 5%
1	C	233	 9% 90% . . 5%
1	E	233	 9% 90% . . 5%
1	G	233	 9% 90% . . 5%

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Mol	Chain	Length	Quality of chain
1	I	233	9% 90% 5%
1	K	233	9% 90% 5%
1	M	233	9% 90% 5%
1	O	233	8% 90% 5%
1	Q	233	9% 90% 5%
1	S	233	9% 90% 5%
1	U	233	9% 90% 5%
1	W	233	9% 90% 5%
1	Y	233	9% 91% 5%
2	1	211	86% 9% 5%
2	B	211	86% 9% 5%
2	D	211	86% 9% 5%
2	F	211	86% 9% 5%
2	H	211	86% 9% 5%
2	J	211	86% 9% 5%
2	L	211	86% 9% 5%
2	N	211	86% 9% 5%
2	P	211	86% 9% 5%
2	R	211	86% 9% 5%
2	T	211	86% 9% 5%
2	V	211	86% 9% 5%
2	X	211	86% 9% 5%
2	Z	211	86% 9% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 46382 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	221	1720	1092	290	335	3	0	0
1	C	221	1720	1092	290	335	3	0	0
1	E	221	1720	1092	290	335	3	0	0
1	G	221	1720	1092	290	335	3	0	0
1	I	221	1720	1092	290	335	3	0	0
1	K	221	1720	1092	290	335	3	0	0
1	M	221	1720	1092	290	335	3	0	0
1	O	221	1720	1092	290	335	3	0	0
1	Q	221	1720	1092	290	335	3	0	0
1	S	221	1720	1092	290	335	3	0	0
1	U	221	1720	1092	290	335	3	0	0
1	W	221	1720	1092	290	335	3	0	0
1	Y	221	1720	1092	290	335	3	0	0
1	0	221	1720	1092	290	335	3	0	0

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	201	1541	973	262	295	11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	F	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	H	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	J	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	L	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	N	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	P	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	R	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	T	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	V	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	X	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	Z	201	Total 1541	C 973	N 262	O 295	S 11	0	0
2	1	201	Total 1541	C 973	N 262	O 295	S 11	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	21	Total 21	O 21	0
3	B	31	Total 31	O 31	0
3	C	21	Total 21	O 21	0
3	D	31	Total 31	O 31	0
3	E	21	Total 21	O 21	0
3	F	31	Total 31	O 31	0

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Mol	Chain	Residues	Atoms		AltConf
3	G	21	Total 21	O 21	0
3	H	31	Total 31	O 31	0
3	I	21	Total 21	O 21	0
3	J	31	Total 31	O 31	0
3	K	21	Total 21	O 21	0
3	L	31	Total 31	O 31	0
3	M	21	Total 21	O 21	0
3	N	31	Total 31	O 31	0
3	O	21	Total 21	O 21	0
3	P	31	Total 31	O 31	0
3	Q	21	Total 21	O 21	0
3	R	31	Total 31	O 31	0
3	S	21	Total 21	O 21	0
3	T	31	Total 31	O 31	0
3	U	21	Total 21	O 21	0
3	V	31	Total 31	O 31	0
3	W	21	Total 21	O 21	0
3	X	31	Total 31	O 31	0
3	Y	21	Total 21	O 21	0
3	Z	31	Total 31	O 31	0
3	0	21	Total 21	O 21	0

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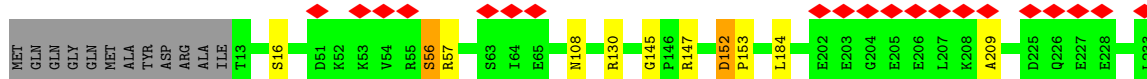
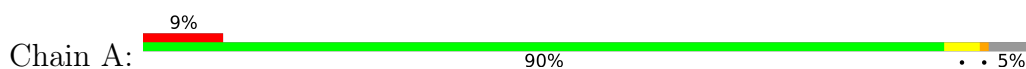
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Mol	Chain	Residues	Atoms		AltConf
3	1	31	Total	O	0
			31	31	

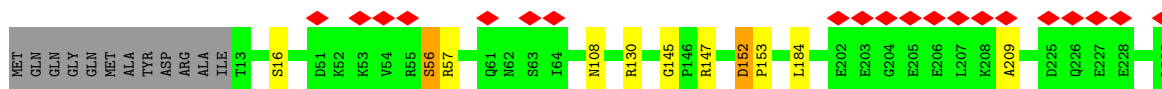
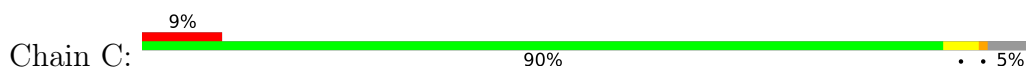
3 Residue-property plots [i](#)

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.

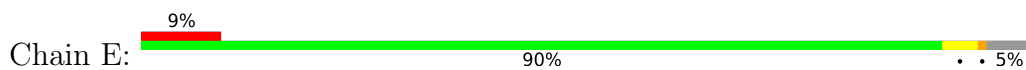
- Molecule 1: Proteasome subunit alpha



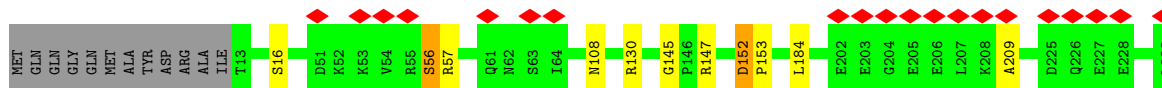
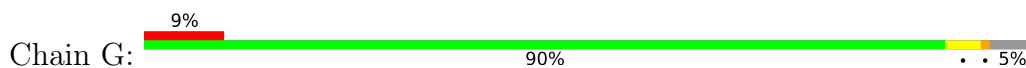
- Molecule 1: Proteasome subunit alpha



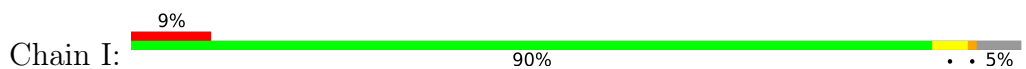
- Molecule 1: Proteasome subunit alpha



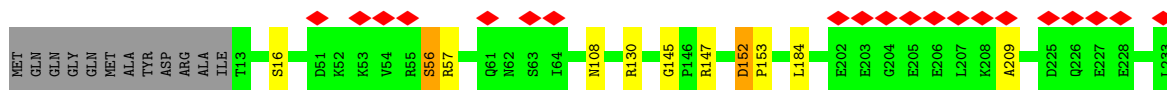
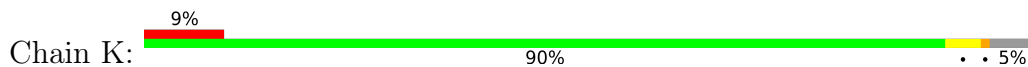
- Molecule 1: Proteasome subunit alpha



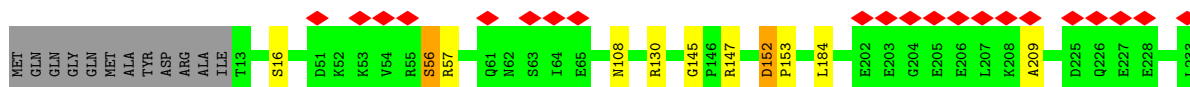
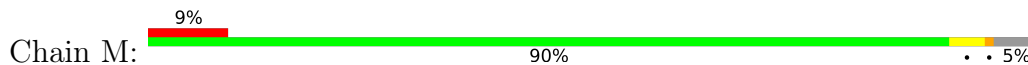
- Molecule 1: Proteasome subunit alpha



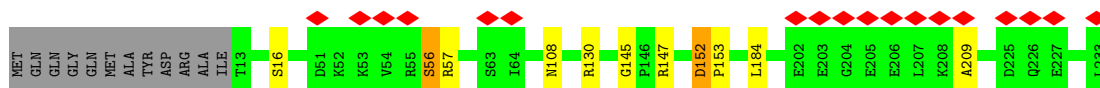
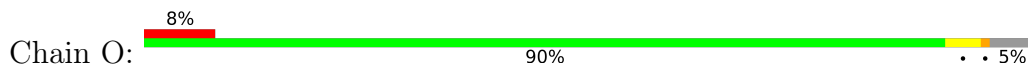
• Molecule 1: Proteasome subunit alpha



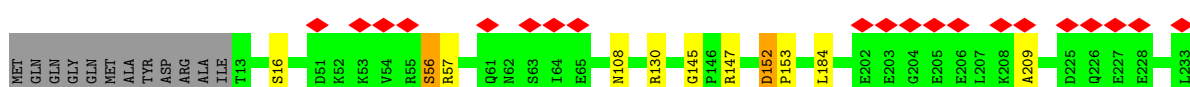
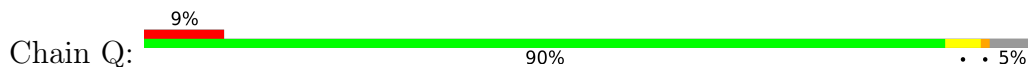
• Molecule 1: Proteasome subunit alpha



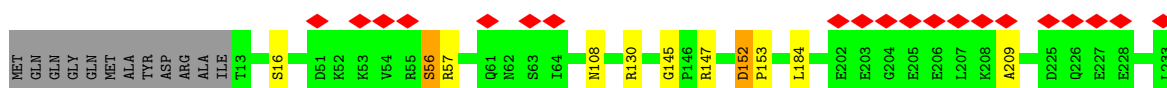
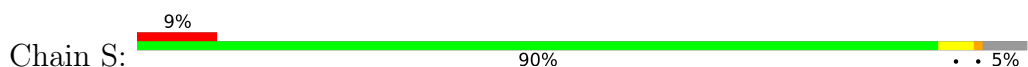
• Molecule 1: Proteasome subunit alpha



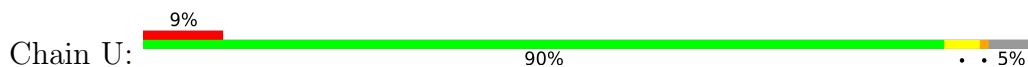
• Molecule 1: Proteasome subunit alpha



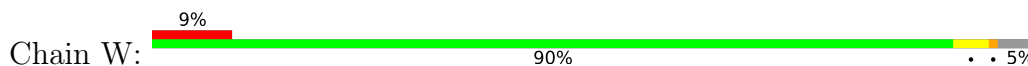
• Molecule 1: Proteasome subunit alpha

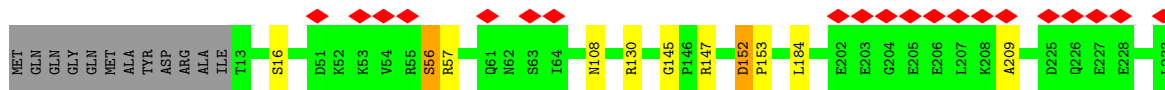


• Molecule 1: Proteasome subunit alpha

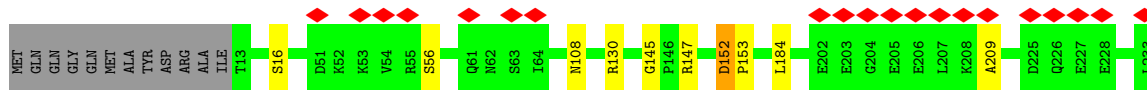
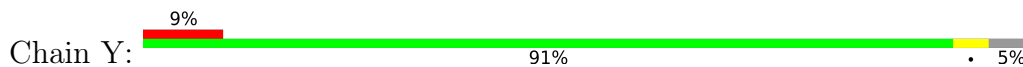


• Molecule 1: Proteasome subunit alpha

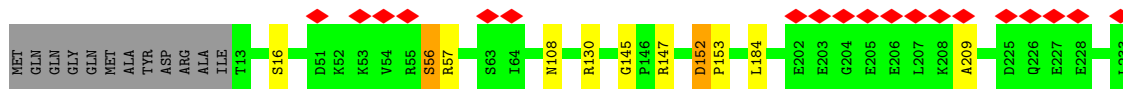
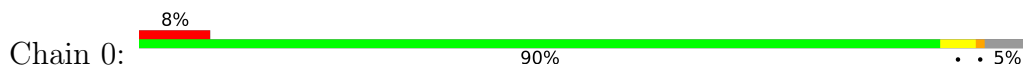




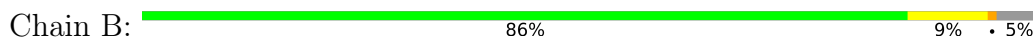
• Molecule 1: Proteasome subunit alpha



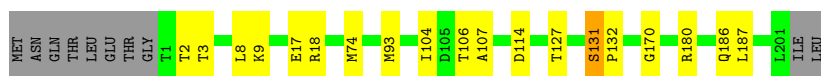
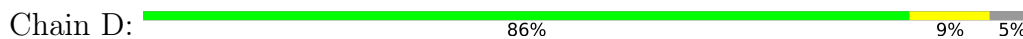
• Molecule 1: Proteasome subunit alpha



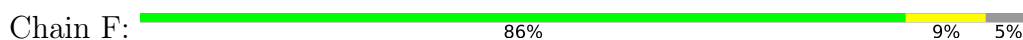
• Molecule 2: Proteasome subunit beta



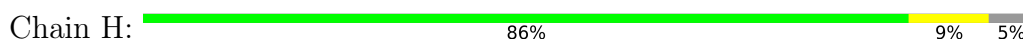
• Molecule 2: Proteasome subunit beta



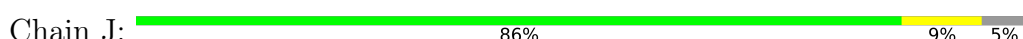
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

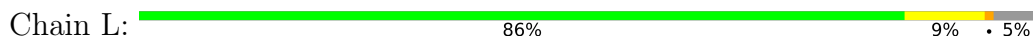


• Molecule 2: Proteasome subunit beta

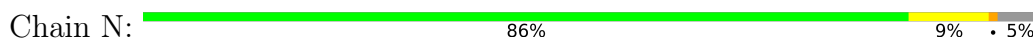




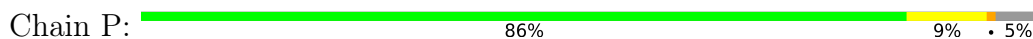
- Molecule 2: Proteasome subunit beta



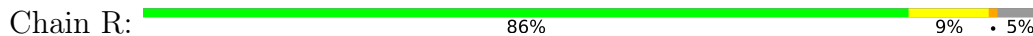
- Molecule 2: Proteasome subunit beta



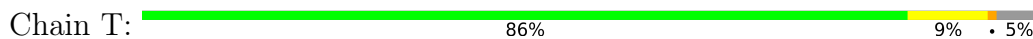
- Molecule 2: Proteasome subunit beta



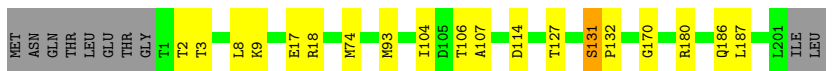
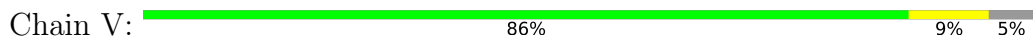
- Molecule 2: Proteasome subunit beta



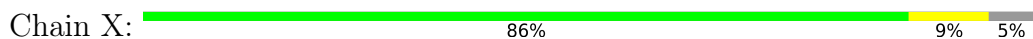
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta





- Molecule 2: Proteasome subunit beta

Chain Z: 86% 9% 5%



- Molecule 2: Proteasome subunit beta

Chain 1: 86% 9% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	49954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	294.6, 294.6, 294.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.982, 0.982, 0.982	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	O	0.87	0/1743	0.86	12/2348 (0.5%)
1	A	0.87	0/1743	0.86	12/2348 (0.5%)
1	C	0.87	0/1743	0.86	12/2348 (0.5%)
1	E	0.87	0/1743	0.86	12/2348 (0.5%)
1	G	0.87	0/1743	0.86	12/2348 (0.5%)
1	I	0.87	0/1743	0.86	12/2348 (0.5%)
1	K	0.87	0/1743	0.86	12/2348 (0.5%)
1	M	0.87	0/1743	0.86	12/2348 (0.5%)
1	O	0.87	0/1743	0.86	12/2348 (0.5%)
1	Q	0.87	0/1743	0.86	12/2348 (0.5%)
1	S	0.87	0/1743	0.86	12/2348 (0.5%)
1	U	0.87	0/1743	0.86	12/2348 (0.5%)
1	W	0.87	0/1743	0.86	12/2348 (0.5%)
1	Y	0.87	0/1743	0.86	12/2348 (0.5%)
2	1	0.92	0/1560	0.88	11/2107 (0.5%)
2	B	0.92	0/1560	0.88	11/2107 (0.5%)
2	D	0.92	0/1560	0.88	11/2107 (0.5%)
2	F	0.92	0/1560	0.88	11/2107 (0.5%)
2	H	0.92	0/1560	0.88	11/2107 (0.5%)
2	J	0.92	0/1560	0.88	11/2107 (0.5%)
2	L	0.92	0/1560	0.88	11/2107 (0.5%)
2	N	0.92	0/1560	0.88	11/2107 (0.5%)
2	P	0.92	0/1560	0.88	11/2107 (0.5%)
2	R	0.92	0/1560	0.88	11/2107 (0.5%)
2	T	0.92	0/1560	0.88	11/2107 (0.5%)
2	V	0.92	0/1560	0.88	11/2107 (0.5%)
2	X	0.92	0/1560	0.88	11/2107 (0.5%)
2	Z	0.92	0/1560	0.88	11/2107 (0.5%)
All	All	0.90	0/46242	0.87	322/62370 (0.5%)

There are no bond length outliers.

All (322) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	93	MET	CA-C-N	7.72	127.68	120.03
2	L	93	MET	C-N-CA	7.72	127.68	120.03
2	H	93	MET	CA-C-N	7.70	127.65	120.03
2	H	93	MET	C-N-CA	7.70	127.65	120.03
2	Z	93	MET	CA-C-N	7.69	127.65	120.03
2	Z	93	MET	C-N-CA	7.69	127.65	120.03
2	J	93	MET	CA-C-N	7.69	127.64	120.03
2	J	93	MET	C-N-CA	7.69	127.64	120.03
2	V	93	MET	CA-C-N	7.68	127.63	120.03
2	V	93	MET	C-N-CA	7.68	127.63	120.03
2	T	93	MET	CA-C-N	7.68	127.63	120.03
2	T	93	MET	C-N-CA	7.68	127.63	120.03
2	B	93	MET	CA-C-N	7.67	127.62	120.03
2	B	93	MET	C-N-CA	7.67	127.62	120.03
2	D	93	MET	CA-C-N	7.67	127.62	120.03
2	D	93	MET	C-N-CA	7.67	127.62	120.03
2	P	93	MET	CA-C-N	7.67	127.62	120.03
2	P	93	MET	C-N-CA	7.67	127.62	120.03
2	1	93	MET	CA-C-N	7.67	127.62	120.03
2	1	93	MET	C-N-CA	7.67	127.62	120.03
2	F	93	MET	CA-C-N	7.64	127.60	120.03
2	F	93	MET	C-N-CA	7.64	127.60	120.03
2	X	93	MET	CA-C-N	7.64	127.60	120.03
2	X	93	MET	C-N-CA	7.64	127.60	120.03
2	R	93	MET	CA-C-N	7.64	127.60	120.03
2	R	93	MET	C-N-CA	7.64	127.60	120.03
2	N	93	MET	CA-C-N	7.62	127.58	120.03
2	N	93	MET	C-N-CA	7.62	127.58	120.03
1	Y	152	ASP	CA-C-N	7.01	127.31	119.32
1	Y	152	ASP	C-N-CA	7.01	127.31	119.32
1	M	152	ASP	CA-C-N	7.00	127.30	119.32
1	M	152	ASP	C-N-CA	7.00	127.30	119.32
1	S	152	ASP	CA-C-N	6.99	127.29	119.32
1	S	152	ASP	C-N-CA	6.99	127.29	119.32
1	K	152	ASP	CA-C-N	6.99	127.29	119.32
1	K	152	ASP	C-N-CA	6.99	127.29	119.32
1	W	152	ASP	CA-C-N	6.99	127.29	119.32
1	W	152	ASP	C-N-CA	6.99	127.29	119.32
1	C	152	ASP	CA-C-N	6.99	127.28	119.32
1	C	152	ASP	C-N-CA	6.99	127.28	119.32
1	A	152	ASP	CA-C-N	6.98	127.28	119.32
1	A	152	ASP	C-N-CA	6.98	127.28	119.32
1	Q	152	ASP	CA-C-N	6.98	127.27	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	152	ASP	C-N-CA	6.98	127.27	119.32
1	O	152	ASP	CA-C-N	6.97	127.27	119.32
1	O	152	ASP	C-N-CA	6.97	127.27	119.32
1	O	152	ASP	CA-C-N	6.96	127.25	119.32
1	O	152	ASP	C-N-CA	6.96	127.25	119.32
1	U	152	ASP	CA-C-N	6.96	127.25	119.32
1	U	152	ASP	C-N-CA	6.96	127.25	119.32
1	I	152	ASP	CA-C-N	6.95	127.25	119.32
1	I	152	ASP	C-N-CA	6.95	127.25	119.32
1	G	152	ASP	CA-C-N	6.95	127.24	119.32
1	G	152	ASP	C-N-CA	6.95	127.24	119.32
1	E	152	ASP	CA-C-N	6.94	127.23	119.32
1	E	152	ASP	C-N-CA	6.94	127.23	119.32
2	P	74	MET	CA-C-N	6.85	126.88	119.90
2	P	74	MET	C-N-CA	6.85	126.88	119.90
2	L	74	MET	CA-C-N	6.83	126.87	119.90
2	L	74	MET	C-N-CA	6.83	126.87	119.90
2	R	74	MET	CA-C-N	6.83	126.86	119.90
2	R	74	MET	C-N-CA	6.83	126.86	119.90
2	N	74	MET	CA-C-N	6.82	126.85	119.90
2	N	74	MET	C-N-CA	6.82	126.85	119.90
2	H	74	MET	CA-C-N	6.81	126.85	119.90
2	H	74	MET	C-N-CA	6.81	126.85	119.90
2	D	74	MET	CA-C-N	6.81	126.84	119.90
2	D	74	MET	C-N-CA	6.81	126.84	119.90
2	B	74	MET	CA-C-N	6.80	126.84	119.90
2	B	74	MET	C-N-CA	6.80	126.84	119.90
2	T	74	MET	CA-C-N	6.79	126.83	119.90
2	T	74	MET	C-N-CA	6.79	126.83	119.90
2	J	74	MET	CA-C-N	6.79	126.82	119.90
2	J	74	MET	C-N-CA	6.79	126.82	119.90
2	F	74	MET	CA-C-N	6.78	126.82	119.90
2	F	74	MET	C-N-CA	6.78	126.82	119.90
2	V	74	MET	CA-C-N	6.78	126.82	119.90
2	V	74	MET	C-N-CA	6.78	126.82	119.90
2	1	74	MET	CA-C-N	6.77	126.81	119.90
2	1	74	MET	C-N-CA	6.77	126.81	119.90
2	Z	74	MET	CA-C-N	6.76	126.79	119.90
2	Z	74	MET	C-N-CA	6.76	126.79	119.90
2	X	74	MET	CA-C-N	6.74	126.78	119.90
2	X	74	MET	C-N-CA	6.74	126.78	119.90
2	R	187	LEU	CA-C-N	6.57	126.55	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	187	LEU	C-N-CA	6.57	126.55	119.78
2	V	187	LEU	CA-C-N	6.56	126.54	119.78
2	V	187	LEU	C-N-CA	6.56	126.54	119.78
2	F	187	LEU	CA-C-N	6.55	126.53	119.78
2	F	187	LEU	C-N-CA	6.55	126.53	119.78
2	X	187	LEU	CA-C-N	6.55	126.53	119.78
2	X	187	LEU	C-N-CA	6.55	126.53	119.78
2	Z	187	LEU	CA-C-N	6.55	126.53	119.78
2	Z	187	LEU	C-N-CA	6.55	126.53	119.78
2	D	187	LEU	CA-C-N	6.55	126.53	119.78
2	D	187	LEU	C-N-CA	6.55	126.53	119.78
2	H	187	LEU	CA-C-N	6.55	126.53	119.78
2	H	187	LEU	C-N-CA	6.55	126.53	119.78
2	B	187	LEU	CA-C-N	6.54	126.52	119.78
2	B	187	LEU	C-N-CA	6.54	126.52	119.78
2	N	187	LEU	CA-C-N	6.54	126.52	119.78
2	N	187	LEU	C-N-CA	6.54	126.52	119.78
2	J	187	LEU	CA-C-N	6.54	126.51	119.78
2	J	187	LEU	C-N-CA	6.54	126.51	119.78
2	T	187	LEU	CA-C-N	6.52	126.50	119.78
2	T	187	LEU	C-N-CA	6.52	126.50	119.78
2	P	187	LEU	CA-C-N	6.51	126.48	119.78
2	P	187	LEU	C-N-CA	6.51	126.48	119.78
2	1	187	LEU	CA-C-N	6.50	126.48	119.78
2	1	187	LEU	C-N-CA	6.50	126.48	119.78
2	L	187	LEU	CA-C-N	6.49	126.46	119.78
2	L	187	LEU	C-N-CA	6.49	126.46	119.78
1	Y	16	SER	CA-C-N	6.48	126.17	119.56
1	Y	16	SER	C-N-CA	6.48	126.17	119.56
1	S	16	SER	CA-C-N	6.47	126.17	119.56
1	S	16	SER	C-N-CA	6.47	126.17	119.56
1	G	16	SER	CA-C-N	6.47	126.16	119.56
1	G	16	SER	C-N-CA	6.47	126.16	119.56
1	Q	16	SER	CA-C-N	6.47	126.16	119.56
1	Q	16	SER	C-N-CA	6.47	126.16	119.56
1	I	16	SER	CA-C-N	6.46	126.15	119.56
1	I	16	SER	C-N-CA	6.46	126.15	119.56
1	K	16	SER	CA-C-N	6.46	126.15	119.56
1	K	16	SER	C-N-CA	6.46	126.15	119.56
1	A	16	SER	CA-C-N	6.45	126.14	119.56
1	A	16	SER	C-N-CA	6.45	126.14	119.56
1	O	16	SER	CA-C-N	6.45	126.13	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	16	SER	C-N-CA	6.45	126.13	119.56
1	C	16	SER	CA-C-N	6.44	126.13	119.56
1	C	16	SER	C-N-CA	6.44	126.13	119.56
1	E	16	SER	CA-C-N	6.44	126.13	119.56
1	E	16	SER	C-N-CA	6.44	126.13	119.56
1	0	16	SER	CA-C-N	6.43	126.12	119.56
1	0	16	SER	C-N-CA	6.43	126.12	119.56
1	U	16	SER	CA-C-N	6.42	126.11	119.56
1	U	16	SER	C-N-CA	6.42	126.11	119.56
1	M	16	SER	CA-C-N	6.42	126.11	119.56
1	M	16	SER	C-N-CA	6.42	126.11	119.56
1	W	16	SER	CA-C-N	6.40	126.09	119.56
1	W	16	SER	C-N-CA	6.40	126.09	119.56
1	G	209	ALA	CA-C-N	6.34	126.52	120.31
1	G	209	ALA	C-N-CA	6.34	126.52	120.31
1	0	209	ALA	CA-C-N	6.34	126.52	120.31
1	0	209	ALA	C-N-CA	6.34	126.52	120.31
1	M	209	ALA	CA-C-N	6.33	126.51	120.31
1	M	209	ALA	C-N-CA	6.33	126.51	120.31
1	C	209	ALA	CA-C-N	6.33	126.51	120.31
1	C	209	ALA	C-N-CA	6.33	126.51	120.31
1	K	209	ALA	CA-C-N	6.32	126.51	120.31
1	K	209	ALA	C-N-CA	6.32	126.51	120.31
1	S	209	ALA	CA-C-N	6.31	126.50	120.31
1	S	209	ALA	C-N-CA	6.31	126.50	120.31
1	W	209	ALA	CA-C-N	6.30	126.48	120.31
1	W	209	ALA	C-N-CA	6.30	126.48	120.31
1	U	209	ALA	CA-C-N	6.30	126.48	120.31
1	U	209	ALA	C-N-CA	6.30	126.48	120.31
1	A	209	ALA	CA-C-N	6.29	126.48	120.31
1	A	209	ALA	C-N-CA	6.29	126.48	120.31
1	I	209	ALA	CA-C-N	6.28	126.47	120.31
1	I	209	ALA	C-N-CA	6.28	126.47	120.31
1	E	209	ALA	CA-C-N	6.28	126.46	120.31
1	E	209	ALA	C-N-CA	6.28	126.46	120.31
1	Q	209	ALA	CA-C-N	6.27	126.46	120.31
1	Q	209	ALA	C-N-CA	6.27	126.46	120.31
1	O	209	ALA	CA-C-N	6.26	126.44	120.31
1	O	209	ALA	C-N-CA	6.26	126.44	120.31
1	Y	209	ALA	CA-C-N	6.23	126.41	120.31
1	Y	209	ALA	C-N-CA	6.23	126.41	120.31
1	O	184	LEU	CA-C-N	6.11	126.07	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	184	LEU	C-N-CA	6.11	126.07	119.78
1	G	145	GLY	CA-C-N	6.10	126.30	119.90
1	G	145	GLY	C-N-CA	6.10	126.30	119.90
1	G	184	LEU	CA-C-N	6.09	126.05	119.78
1	G	184	LEU	C-N-CA	6.09	126.05	119.78
1	K	184	LEU	CA-C-N	6.09	126.05	119.78
1	K	184	LEU	C-N-CA	6.09	126.05	119.78
1	O	145	GLY	CA-C-N	6.08	126.29	119.90
1	O	145	GLY	C-N-CA	6.08	126.29	119.90
1	E	184	LEU	CA-C-N	6.07	126.03	119.78
1	E	184	LEU	C-N-CA	6.07	126.03	119.78
1	A	184	LEU	CA-C-N	6.07	126.03	119.78
1	A	184	LEU	C-N-CA	6.07	126.03	119.78
1	S	184	LEU	CA-C-N	6.07	126.03	119.78
1	S	184	LEU	C-N-CA	6.07	126.03	119.78
1	M	184	LEU	CA-C-N	6.07	126.03	119.78
1	M	184	LEU	C-N-CA	6.07	126.03	119.78
1	0	184	LEU	CA-C-N	6.07	126.03	119.78
1	0	184	LEU	C-N-CA	6.07	126.03	119.78
1	W	145	GLY	CA-C-N	6.07	126.27	119.90
1	W	145	GLY	C-N-CA	6.07	126.27	119.90
1	Y	184	LEU	CA-C-N	6.07	126.03	119.78
1	Y	184	LEU	C-N-CA	6.07	126.03	119.78
1	U	145	GLY	CA-C-N	6.06	126.26	119.90
1	U	145	GLY	C-N-CA	6.06	126.26	119.90
1	W	184	LEU	CA-C-N	6.05	126.02	119.78
1	W	184	LEU	C-N-CA	6.05	126.02	119.78
1	Q	184	LEU	CA-C-N	6.05	126.01	119.78
1	Q	184	LEU	C-N-CA	6.05	126.01	119.78
1	U	184	LEU	CA-C-N	6.05	126.01	119.78
1	U	184	LEU	C-N-CA	6.05	126.01	119.78
1	K	145	GLY	CA-C-N	6.05	126.25	119.90
1	K	145	GLY	C-N-CA	6.05	126.25	119.90
1	Q	145	GLY	CA-C-N	6.05	126.25	119.90
1	Q	145	GLY	C-N-CA	6.05	126.25	119.90
1	C	184	LEU	CA-C-N	6.05	126.01	119.78
1	C	184	LEU	C-N-CA	6.05	126.01	119.78
1	Y	145	GLY	CA-C-N	6.05	126.25	119.90
1	Y	145	GLY	C-N-CA	6.05	126.25	119.90
1	A	145	GLY	CA-C-N	6.04	126.25	119.90
1	A	145	GLY	C-N-CA	6.04	126.25	119.90
1	0	145	GLY	CA-C-N	6.04	126.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	145	GLY	C-N-CA	6.04	126.25	119.90
1	M	145	GLY	CA-C-N	6.04	126.24	119.90
1	M	145	GLY	C-N-CA	6.04	126.24	119.90
1	I	145	GLY	CA-C-N	6.03	126.23	119.90
1	I	145	GLY	C-N-CA	6.03	126.23	119.90
1	E	145	GLY	CA-C-N	6.03	126.23	119.90
1	E	145	GLY	C-N-CA	6.03	126.23	119.90
1	I	184	LEU	CA-C-N	6.02	125.98	119.78
1	I	184	LEU	C-N-CA	6.02	125.98	119.78
1	S	145	GLY	CA-C-N	6.01	126.22	119.90
1	S	145	GLY	C-N-CA	6.01	126.22	119.90
1	C	145	GLY	CA-C-N	6.01	126.21	119.90
1	C	145	GLY	C-N-CA	6.01	126.21	119.90
2	R	107	ALA	CA-C-N	5.98	125.74	119.76
2	R	107	ALA	C-N-CA	5.98	125.74	119.76
2	X	107	ALA	CA-C-N	5.98	125.74	119.76
2	X	107	ALA	C-N-CA	5.98	125.74	119.76
2	N	107	ALA	CA-C-N	5.97	125.73	119.76
2	N	107	ALA	C-N-CA	5.97	125.73	119.76
1	O	130	ARG	CA-C-N	5.97	126.31	119.92
1	O	130	ARG	C-N-CA	5.97	126.31	119.92
2	Z	107	ALA	CA-C-N	5.97	125.73	119.76
2	Z	107	ALA	C-N-CA	5.97	125.73	119.76
1	0	130	ARG	CA-C-N	5.96	126.30	119.92
1	0	130	ARG	C-N-CA	5.96	126.30	119.92
2	L	107	ALA	CA-C-N	5.96	125.72	119.76
2	L	107	ALA	C-N-CA	5.96	125.72	119.76
1	G	130	ARG	CA-C-N	5.95	126.29	119.92
1	G	130	ARG	C-N-CA	5.95	126.29	119.92
1	M	130	ARG	CA-C-N	5.95	126.28	119.92
1	M	130	ARG	C-N-CA	5.95	126.28	119.92
1	Y	130	ARG	CA-C-N	5.94	126.28	119.92
1	Y	130	ARG	C-N-CA	5.94	126.28	119.92
2	J	107	ALA	CA-C-N	5.94	125.70	119.76
2	J	107	ALA	C-N-CA	5.94	125.70	119.76
2	B	107	ALA	CA-C-N	5.94	125.70	119.76
2	B	107	ALA	C-N-CA	5.94	125.70	119.76
2	D	107	ALA	CA-C-N	5.93	125.69	119.76
2	D	107	ALA	C-N-CA	5.93	125.69	119.76
2	H	107	ALA	CA-C-N	5.93	125.69	119.76
2	H	107	ALA	C-N-CA	5.93	125.69	119.76
2	1	107	ALA	CA-C-N	5.93	125.69	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	107	ALA	C-N-CA	5.93	125.69	119.76
2	P	107	ALA	CA-C-N	5.92	125.68	119.76
2	P	107	ALA	C-N-CA	5.92	125.68	119.76
1	A	130	ARG	CA-C-N	5.92	126.26	119.92
1	A	130	ARG	C-N-CA	5.92	126.26	119.92
1	Q	130	ARG	CA-C-N	5.92	126.26	119.92
1	Q	130	ARG	C-N-CA	5.92	126.26	119.92
1	S	130	ARG	CA-C-N	5.92	126.25	119.92
1	S	130	ARG	C-N-CA	5.92	126.25	119.92
1	U	130	ARG	CA-C-N	5.92	126.25	119.92
1	U	130	ARG	C-N-CA	5.92	126.25	119.92
1	W	130	ARG	CA-C-N	5.92	126.25	119.92
1	W	130	ARG	C-N-CA	5.92	126.25	119.92
2	F	107	ALA	CA-C-N	5.91	125.67	119.76
2	F	107	ALA	C-N-CA	5.91	125.67	119.76
1	I	130	ARG	CA-C-N	5.91	126.25	119.92
1	I	130	ARG	C-N-CA	5.91	126.25	119.92
1	C	130	ARG	CA-C-N	5.91	126.24	119.92
1	C	130	ARG	C-N-CA	5.91	126.24	119.92
2	T	107	ALA	CA-C-N	5.91	125.67	119.76
2	T	107	ALA	C-N-CA	5.91	125.67	119.76
1	K	130	ARG	CA-C-N	5.90	126.23	119.92
1	K	130	ARG	C-N-CA	5.90	126.23	119.92
2	V	107	ALA	CA-C-N	5.88	125.64	119.76
2	V	107	ALA	C-N-CA	5.88	125.64	119.76
2	Z	106	THR	N-CA-C	-5.88	105.95	114.12
1	E	130	ARG	CA-C-N	5.87	126.20	119.92
1	E	130	ARG	C-N-CA	5.87	126.20	119.92
2	B	106	THR	N-CA-C	-5.86	105.97	114.12
2	R	106	THR	N-CA-C	-5.86	105.97	114.12
2	J	106	THR	N-CA-C	-5.86	105.97	114.12
2	P	106	THR	N-CA-C	-5.86	105.98	114.12
2	H	106	THR	N-CA-C	-5.86	105.98	114.12
2	T	106	THR	N-CA-C	-5.86	105.98	114.12
2	1	106	THR	N-CA-C	-5.86	105.98	114.12
2	F	106	THR	N-CA-C	-5.85	105.98	114.12
2	X	106	THR	N-CA-C	-5.85	105.99	114.12
2	N	106	THR	N-CA-C	-5.85	105.99	114.12
2	V	106	THR	N-CA-C	-5.84	106.00	114.12
2	D	106	THR	N-CA-C	-5.83	106.02	114.12
2	L	106	THR	N-CA-C	-5.83	106.02	114.12
2	R	131	SER	CA-C-N	5.30	125.11	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	131	SER	C-N-CA	5.30	125.11	119.28
2	L	131	SER	CA-C-N	5.28	125.09	119.28
2	L	131	SER	C-N-CA	5.28	125.09	119.28
2	N	131	SER	CA-C-N	5.28	125.08	119.28
2	N	131	SER	C-N-CA	5.28	125.08	119.28
2	H	131	SER	CA-C-N	5.27	125.08	119.28
2	H	131	SER	C-N-CA	5.27	125.08	119.28
2	P	131	SER	CA-C-N	5.27	125.08	119.28
2	P	131	SER	C-N-CA	5.27	125.08	119.28
2	B	131	SER	CA-C-N	5.27	125.08	119.28
2	B	131	SER	C-N-CA	5.27	125.08	119.28
2	V	131	SER	CA-C-N	5.27	125.08	119.28
2	V	131	SER	C-N-CA	5.27	125.08	119.28
2	J	131	SER	CA-C-N	5.27	125.08	119.28
2	J	131	SER	C-N-CA	5.27	125.08	119.28
2	Z	131	SER	CA-C-N	5.27	125.07	119.28
2	Z	131	SER	C-N-CA	5.27	125.07	119.28
2	T	131	SER	CA-C-N	5.26	125.06	119.28
2	T	131	SER	C-N-CA	5.26	125.06	119.28
2	F	131	SER	CA-C-N	5.25	125.06	119.28
2	F	131	SER	C-N-CA	5.25	125.06	119.28
2	X	131	SER	CA-C-N	5.25	125.06	119.28
2	X	131	SER	C-N-CA	5.25	125.06	119.28
2	D	131	SER	CA-C-N	5.24	125.04	119.28
2	D	131	SER	C-N-CA	5.24	125.04	119.28
2	1	131	SER	CA-C-N	5.24	125.04	119.28
2	1	131	SER	C-N-CA	5.24	125.04	119.28

There are no chirality outliers.

There are no planarity outliers.

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	0	1720	0	1753	3	0
1	A	1720	0	1753	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1720	0	1753	4	0
1	E	1720	0	1753	3	0
1	G	1720	0	1753	4	0
1	I	1720	0	1753	4	0
1	K	1720	0	1753	4	0
1	M	1720	0	1753	4	0
1	O	1720	0	1753	4	0
1	Q	1720	0	1753	4	0
1	S	1720	0	1753	4	0
1	U	1720	0	1753	4	0
1	W	1720	0	1753	4	0
1	Y	1720	0	1753	2	0
2	1	1541	0	1587	11	0
2	B	1541	0	1587	11	0
2	D	1541	0	1587	10	0
2	F	1541	0	1587	10	0
2	H	1541	0	1587	10	0
2	J	1541	0	1587	10	0
2	L	1541	0	1587	11	0
2	N	1541	0	1587	11	0
2	P	1541	0	1587	11	0
2	R	1541	0	1587	11	0
2	T	1541	0	1587	11	0
2	V	1541	0	1587	10	0
2	X	1541	0	1587	10	0
2	Z	1541	0	1587	10	0
3	0	21	0	0	0	0
3	1	31	0	0	1	0
3	A	21	0	0	0	0
3	B	31	0	0	1	0
3	C	21	0	0	0	0
3	D	31	0	0	1	0
3	E	21	0	0	0	0
3	F	31	0	0	1	0
3	G	21	0	0	0	0
3	H	31	0	0	1	0
3	I	21	0	0	0	0
3	J	31	0	0	1	0
3	K	21	0	0	0	0
3	L	31	0	0	1	0
3	M	21	0	0	0	0
3	N	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	21	0	0	0	0
3	P	31	0	0	1	0
3	Q	21	0	0	0	0
3	R	31	0	0	1	0
3	S	21	0	0	0	0
3	T	31	0	0	1	0
3	U	21	0	0	0	0
3	V	31	0	0	1	0
3	W	21	0	0	0	0
3	X	31	0	0	1	0
3	Y	21	0	0	0	0
3	Z	31	0	0	1	0
All	All	46382	0	46760	199	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 2.

All (199) 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)
2:P:17:GLU:HG3	2:P:170:GLY:H	1.44	0.83
2:B:17:GLU:HG3	2:B:170:GLY:H	1.44	0.83
2:J:17:GLU:HG3	2:J:170:GLY:H	1.44	0.82
2:T:17:GLU:HG3	2:T:170:GLY:H	1.44	0.82
2:L:17:GLU:HG3	2:L:170:GLY:H	1.44	0.82
2:V:17:GLU:HG3	2:V:170:GLY:H	1.44	0.82
2:N:17:GLU:HG3	2:N:170:GLY:H	1.44	0.81
2:R:17:GLU:HG3	2:R:170:GLY:H	1.44	0.81
2:F:17:GLU:HG3	2:F:170:GLY:H	1.44	0.81
2:H:17:GLU:HG3	2:H:170:GLY:H	1.44	0.81
2:X:17:GLU:HG3	2:X:170:GLY:H	1.44	0.81
2:Z:17:GLU:HG3	2:Z:170:GLY:H	1.44	0.81
2:1:17:GLU:HG3	2:1:170:GLY:H	1.44	0.80
2:D:17:GLU:HG3	2:D:170:GLY:H	1.44	0.80
2:D:186:GLN:OE1	3:D:301:HOH:O	2.05	0.74
2:B:186:GLN:OE1	3:B:301:HOH:O	2.05	0.74
2:P:186:GLN:OE1	3:P:301:HOH:O	2.06	0.74
2:1:186:GLN:OE1	3:1:301:HOH:O	2.05	0.74
2:F:186:GLN:OE1	3:F:301:HOH:O	2.05	0.74
2:Z:186:GLN:OE1	3:Z:301:HOH:O	2.05	0.74
2:N:186:GLN:OE1	3:N:301:HOH:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:186:GLN:OE1	3:R:301:HOH:O	2.05	0.74
2:X:186:GLN:OE1	3:X:301:HOH:O	2.05	0.73
2:H:186:GLN:OE1	3:H:301:HOH:O	2.05	0.73
2:L:186:GLN:OE1	3:L:301:HOH:O	2.05	0.72
2:T:186:GLN:OE1	3:T:301:HOH:O	2.05	0.72
2:J:186:GLN:OE1	3:J:301:HOH:O	2.05	0.72
2:V:186:GLN:OE1	3:V:301:HOH:O	2.05	0.72
2:J:2:THR:N	2:J:17:GLU:OE2	2.33	0.61
2:V:2:THR:N	2:V:17:GLU:OE2	2.33	0.61
2:P:2:THR:N	2:P:17:GLU:OE2	2.33	0.61
2:H:2:THR:N	2:H:17:GLU:OE2	2.33	0.61
2:X:2:THR:N	2:X:17:GLU:OE2	2.33	0.61
2:B:2:THR:N	2:B:17:GLU:OE2	2.33	0.60
2:F:2:THR:N	2:F:17:GLU:OE2	2.33	0.60
2:D:2:THR:N	2:D:17:GLU:OE2	2.33	0.60
2:Z:2:THR:N	2:Z:17:GLU:OE2	2.33	0.60
2:1:2:THR:N	2:1:17:GLU:OE2	2.33	0.60
2:N:2:THR:N	2:N:17:GLU:OE2	2.33	0.56
2:R:2:THR:N	2:R:17:GLU:OE2	2.33	0.56
2:L:2:THR:N	2:L:17:GLU:OE2	2.33	0.55
2:1:131:SER:N	2:1:132:PRO:CD	2.70	0.55
2:D:131:SER:N	2:D:132:PRO:CD	2.70	0.55
2:T:2:THR:N	2:T:17:GLU:OE2	2.33	0.55
2:H:104:ILE:HG22	2:H:180:ARG:HD3	1.88	0.55
2:H:131:SER:N	2:H:132:PRO:CD	2.70	0.55
2:V:104:ILE:HG22	2:V:180:ARG:HD3	1.88	0.55
2:X:104:ILE:HG22	2:X:180:ARG:HD3	1.88	0.55
2:Z:104:ILE:HG22	2:Z:180:ARG:HD3	1.88	0.55
2:J:104:ILE:HG22	2:J:180:ARG:HD3	1.88	0.55
2:X:131:SER:N	2:X:132:PRO:CD	2.70	0.55
2:F:104:ILE:HG22	2:F:180:ARG:HD3	1.88	0.55
2:N:104:ILE:HG22	2:N:180:ARG:HD3	1.88	0.55
2:P:131:SER:N	2:P:132:PRO:CD	2.70	0.55
2:Z:131:SER:N	2:Z:132:PRO:CD	2.70	0.55
2:B:131:SER:N	2:B:132:PRO:CD	2.70	0.54
2:F:131:SER:N	2:F:132:PRO:CD	2.70	0.54
2:J:131:SER:N	2:J:132:PRO:CD	2.70	0.54
2:L:104:ILE:HG22	2:L:180:ARG:HD3	1.88	0.54
2:T:104:ILE:HG22	2:T:180:ARG:HD3	1.88	0.54
2:V:131:SER:N	2:V:132:PRO:CD	2.70	0.54
2:1:104:ILE:HG22	2:1:180:ARG:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:ILE:HG22	2:D:180:ARG:HD3	1.88	0.54
2:R:104:ILE:HG22	2:R:180:ARG:HD3	1.88	0.54
2:B:104:ILE:HG22	2:B:180:ARG:HD3	1.88	0.54
2:N:131:SER:N	2:N:132:PRO:CD	2.70	0.54
2:R:131:SER:N	2:R:132:PRO:CD	2.70	0.54
2:P:104:ILE:HG22	2:P:180:ARG:HD3	1.88	0.54
2:L:131:SER:N	2:L:132:PRO:CD	2.70	0.54
2:T:131:SER:N	2:T:132:PRO:CD	2.70	0.54
1:E:152:ASP:HB2	1:E:153:PRO:HD2	1.91	0.53
1:Y:152:ASP:HB2	1:Y:153:PRO:HD2	1.91	0.53
1:W:152:ASP:HB2	1:W:153:PRO:HD2	1.91	0.53
1:G:152:ASP:HB2	1:G:153:PRO:HD2	1.91	0.53
1:C:152:ASP:HB2	1:C:153:PRO:HD2	1.91	0.53
1:O:152:ASP:HB2	1:O:153:PRO:HD2	1.91	0.53
1:I:152:ASP:HB2	1:I:153:PRO:HD2	1.91	0.52
1:U:152:ASP:HB2	1:U:153:PRO:HD2	1.91	0.52
1:A:152:ASP:HB2	1:A:153:PRO:HD2	1.91	0.52
1:O:152:ASP:HB2	1:O:153:PRO:HD2	1.91	0.52
1:K:152:ASP:HB2	1:K:153:PRO:HD2	1.91	0.51
1:S:152:ASP:HB2	1:S:153:PRO:HD2	1.91	0.51
1:M:152:ASP:HB2	1:M:153:PRO:HD2	1.91	0.51
1:Q:152:ASP:HB2	1:Q:153:PRO:HD2	1.91	0.51
2:V:3:THR:OG1	2:V:127:THR:OG1	2.25	0.49
2:X:3:THR:OG1	2:X:127:THR:OG1	2.25	0.49
2:H:3:THR:OG1	2:H:127:THR:OG1	2.25	0.49
1:M:108:ASN:OD1	1:M:147:ARG:NH1	2.47	0.47
1:Q:108:ASN:OD1	1:Q:147:ARG:NH1	2.48	0.47
1:U:108:ASN:OD1	1:U:147:ARG:NH1	2.48	0.47
1:I:108:ASN:OD1	1:I:147:ARG:NH1	2.48	0.47
1:K:108:ASN:OD1	1:K:147:ARG:NH1	2.48	0.47
1:C:108:ASN:OD1	1:C:147:ARG:NH1	2.48	0.47
1:E:108:ASN:OD1	1:E:147:ARG:NH1	2.48	0.47
1:S:108:ASN:OD1	1:S:147:ARG:NH1	2.48	0.47
1:O:108:ASN:OD1	1:O:147:ARG:NH1	2.48	0.47
1:G:108:ASN:OD1	1:G:147:ARG:NH1	2.48	0.47
1:W:108:ASN:OD1	1:W:147:ARG:NH1	2.48	0.47
1:Y:108:ASN:OD1	1:Y:147:ARG:NH1	2.48	0.47
1:A:108:ASN:OD1	1:A:147:ARG:NH1	2.48	0.47
1:O:108:ASN:OD1	1:O:147:ARG:NH1	2.48	0.47
2:B:17:GLU:HG2	2:B:18:ARG:N	2.30	0.46
2:J:8:LEU:O	2:J:9:LYS:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:17:GLU:HG2	2:J:18:ARG:N	2.30	0.46
2:L:8:LEU:O	2:L:9:LYS:C	2.58	0.46
2:V:8:LEU:O	2:V:9:LYS:C	2.58	0.46
2:V:17:GLU:HG2	2:V:18:ARG:N	2.30	0.46
2:H:8:LEU:O	2:H:9:LYS:C	2.58	0.46
2:P:17:GLU:HG2	2:P:18:ARG:N	2.30	0.46
2:T:8:LEU:O	2:T:9:LYS:C	2.58	0.46
2:H:17:GLU:HG2	2:H:18:ARG:N	2.30	0.46
2:J:3:THR:OG1	2:J:127:THR:OG1	2.25	0.46
2:X:8:LEU:O	2:X:9:LYS:C	2.58	0.46
2:X:17:GLU:HG2	2:X:18:ARG:N	2.30	0.46
2:D:8:LEU:O	2:D:9:LYS:C	2.58	0.46
2:D:17:GLU:HG2	2:D:18:ARG:N	2.30	0.46
2:N:8:LEU:O	2:N:9:LYS:C	2.58	0.46
2:R:8:LEU:O	2:R:9:LYS:C	2.58	0.46
2:1:8:LEU:O	2:1:9:LYS:C	2.58	0.46
2:R:17:GLU:HG2	2:R:18:ARG:N	2.30	0.46
2:N:17:GLU:HG2	2:N:18:ARG:N	2.30	0.46
2:1:17:GLU:HG2	2:1:18:ARG:N	2.30	0.45
2:B:8:LEU:O	2:B:9:LYS:C	2.58	0.45
2:F:17:GLU:HG2	2:F:18:ARG:N	2.30	0.45
2:P:8:LEU:O	2:P:9:LYS:C	2.58	0.45
2:V:114:ASP:OD1	2:V:114:ASP:C	2.60	0.45
2:Z:17:GLU:HG2	2:Z:18:ARG:N	2.30	0.45
2:J:114:ASP:OD1	2:J:114:ASP:C	2.60	0.45
2:Z:8:LEU:O	2:Z:9:LYS:C	2.58	0.45
2:F:8:LEU:O	2:F:9:LYS:C	2.58	0.45
2:H:114:ASP:OD1	2:H:114:ASP:C	2.60	0.45
2:L:17:GLU:HG2	2:L:18:ARG:N	2.30	0.45
2:X:114:ASP:OD1	2:X:114:ASP:C	2.60	0.45
2:T:17:GLU:HG2	2:T:18:ARG:N	2.30	0.45
2:F:114:ASP:C	2:F:114:ASP:OD1	2.60	0.45
2:D:114:ASP:OD1	2:D:114:ASP:C	2.60	0.45
2:Z:114:ASP:OD1	2:Z:114:ASP:C	2.60	0.45
2:1:114:ASP:OD1	2:1:114:ASP:C	2.60	0.45
2:T:3:THR:OG1	2:T:127:THR:OG1	2.25	0.44
2:P:104:ILE:CG2	2:P:180:ARG:HD3	2.48	0.44
2:B:104:ILE:CG2	2:B:180:ARG:HD3	2.48	0.44
2:B:114:ASP:C	2:B:114:ASP:OD1	2.60	0.44
2:H:104:ILE:CG2	2:H:180:ARG:HD3	2.48	0.44
2:L:3:THR:OG1	2:L:127:THR:OG1	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:104:ILE:CG2	2:N:180:ARG:HD3	2.48	0.44
2:X:104:ILE:CG2	2:X:180:ARG:HD3	2.48	0.44
2:F:104:ILE:CG2	2:F:180:ARG:HD3	2.48	0.44
2:P:114:ASP:OD1	2:P:114:ASP:C	2.60	0.44
2:R:104:ILE:CG2	2:R:180:ARG:HD3	2.48	0.44
2:Z:104:ILE:CG2	2:Z:180:ARG:HD3	2.48	0.44
2:R:3:THR:OG1	2:R:127:THR:OG1	2.25	0.44
1:A:56:SER:OG	1:A:57:ARG:N	2.51	0.44
1:G:56:SER:OG	1:G:57:ARG:N	2.51	0.44
1:O:56:SER:OG	1:O:57:ARG:N	2.51	0.44
1:M:56:SER:OG	1:M:57:ARG:N	2.51	0.43
2:N:3:THR:OG1	2:N:127:THR:OG1	2.25	0.43
1:Q:56:SER:OG	1:Q:57:ARG:N	2.51	0.43
1:W:56:SER:OG	1:W:57:ARG:N	2.51	0.43
1:I:56:SER:OG	1:I:57:ARG:N	2.51	0.43
2:L:104:ILE:CG2	2:L:180:ARG:HD3	2.48	0.43
2:N:114:ASP:C	2:N:114:ASP:OD1	2.60	0.43
2:T:104:ILE:CG2	2:T:180:ARG:HD3	2.48	0.43
1:U:56:SER:OG	1:U:57:ARG:N	2.51	0.43
2:V:104:ILE:CG2	2:V:180:ARG:HD3	2.48	0.43
2:D:3:THR:OG1	2:D:127:THR:OG1	2.25	0.43
2:J:104:ILE:CG2	2:J:180:ARG:HD3	2.48	0.43
2:R:114:ASP:OD1	2:R:114:ASP:C	2.60	0.43
2:1:3:THR:OG1	2:1:127:THR:OG1	2.25	0.43
2:P:3:THR:OG1	2:P:127:THR:OG1	2.25	0.43
1:O:56:SER:OG	1:O:57:ARG:N	2.51	0.43
1:E:56:SER:OG	1:E:57:ARG:N	2.51	0.43
1:C:56:SER:OG	1:C:57:ARG:N	2.51	0.43
2:F:3:THR:OG1	2:F:127:THR:OG1	2.25	0.43
2:Z:3:THR:OG1	2:Z:127:THR:OG1	2.25	0.43
2:1:104:ILE:CG2	2:1:180:ARG:HD3	2.48	0.43
2:B:3:THR:OG1	2:B:127:THR:OG1	2.25	0.43
2:D:104:ILE:CG2	2:D:180:ARG:HD3	2.48	0.43
2:L:114:ASP:OD1	2:L:114:ASP:C	2.60	0.43
2:T:114:ASP:OD1	2:T:114:ASP:C	2.60	0.42
1:K:56:SER:OG	1:K:57:ARG:N	2.51	0.42
1:S:56:SER:OG	1:S:57:ARG:N	2.51	0.42
2:L:187:LEU:HA	2:L:188:PRO:HD3	1.92	0.42
2:T:187:LEU:HA	2:T:188:PRO:HD3	1.92	0.41
2:1:187:LEU:HA	2:1:188:PRO:HD3	1.92	0.41
1:K:152:ASP:HB2	1:K:153:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:152:ASP:HB2	1:M:153:PRO:CD	2.51	0.41
1:Q:152:ASP:HB2	1:Q:153:PRO:CD	2.51	0.41
1:S:152:ASP:HB2	1:S:153:PRO:CD	2.51	0.41
2:B:187:LEU:HA	2:B:188:PRO:HD3	1.92	0.41
1:I:152:ASP:HB2	1:I:153:PRO:CD	2.51	0.41
1:U:152:ASP:HB2	1:U:153:PRO:CD	2.51	0.41
1:A:152:ASP:HB2	1:A:153:PRO:CD	2.51	0.41
2:N:187:LEU:HA	2:N:188:PRO:HD3	1.92	0.41
1:O:152:ASP:HB2	1:O:153:PRO:CD	2.51	0.41
2:P:187:LEU:HA	2:P:188:PRO:HD3	1.92	0.40
2:R:187:LEU:HA	2:R:188:PRO:HD3	1.92	0.40
1:W:152:ASP:HB2	1:W:153:PRO:CD	2.51	0.40
1:C:152:ASP:HB2	1:C:153:PRO:CD	2.51	0.40
1:G:152:ASP:HB2	1:G:153:PRO:CD	2.51	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	0	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	A	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	C	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	E	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	G	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	I	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	K	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	M	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	O	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	S	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	U	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	W	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
1	Y	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	24	55
2	1	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	B	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	D	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	F	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	H	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	J	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	L	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	N	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	P	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	R	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	T	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	V	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	X	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
2	Z	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
All	All	5852/6216 (94%)	5754 (98%)	84 (1%)	14 (0%)	44	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	C	56	SER
1	E	56	SER
1	G	56	SER
1	I	56	SER
1	K	56	SER
1	M	56	SER
1	O	56	SER
1	Q	56	SER
1	S	56	SER
1	U	56	SER

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Mol	Chain	Res	Type
1	W	56	SER
1	Y	56	SER
1	0	56	SER

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

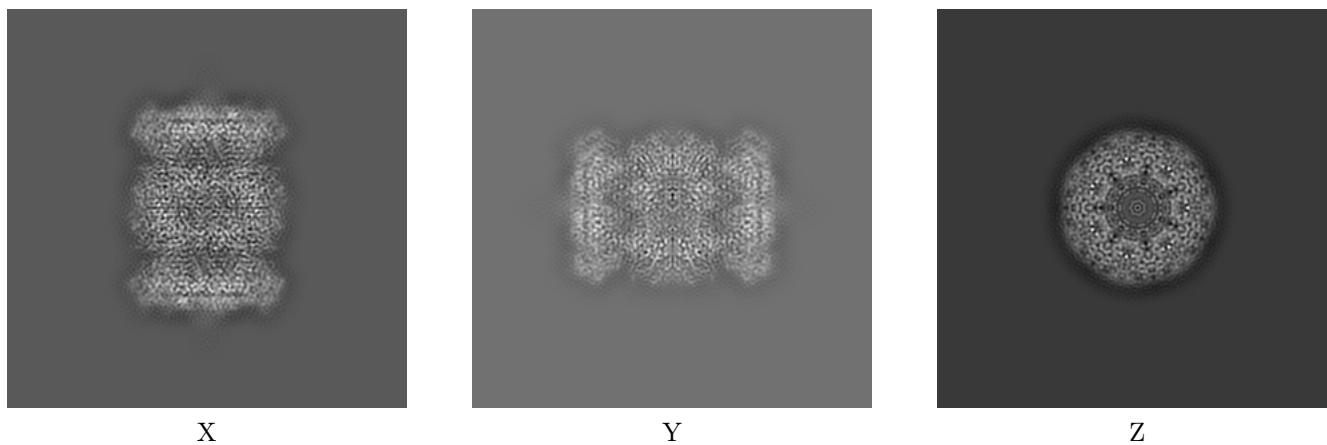
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6287. 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](#)

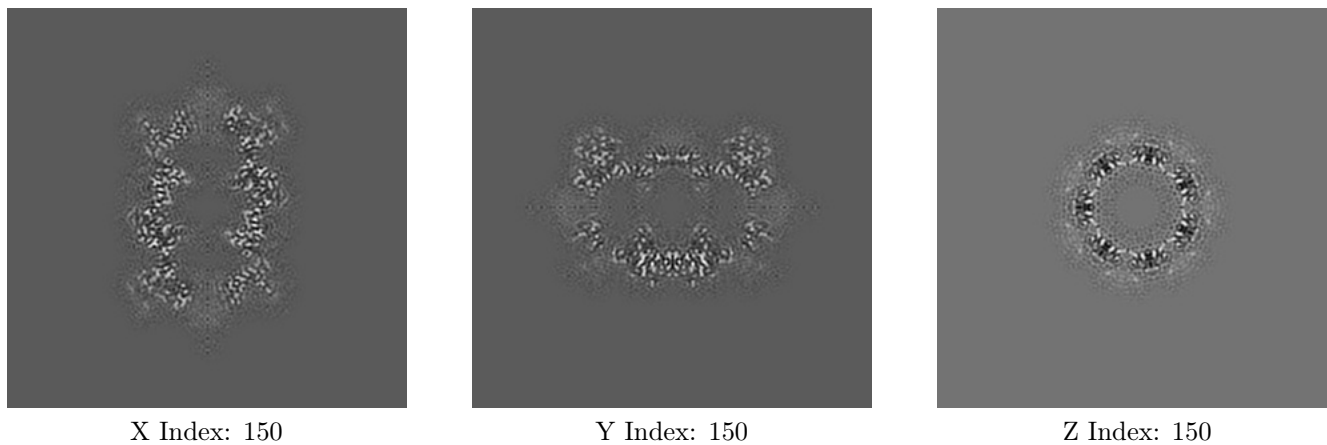
6.1.1 Primary map



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

6.2 Central slices [i](#)

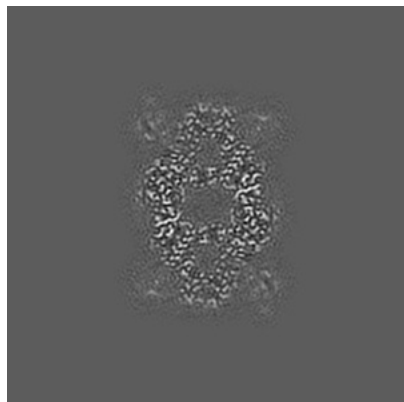
6.2.1 Primary map



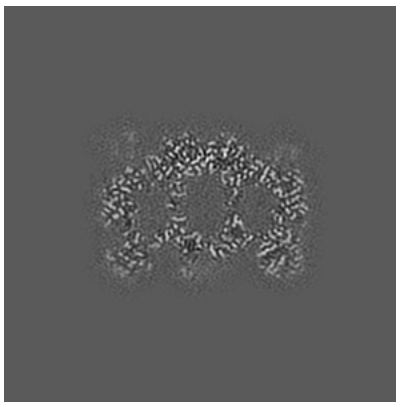
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

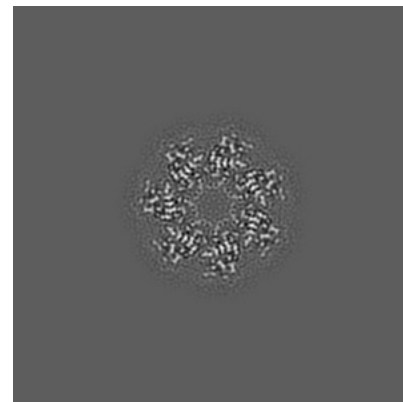
6.3.1 Primary map



X Index: 127



Y Index: 169

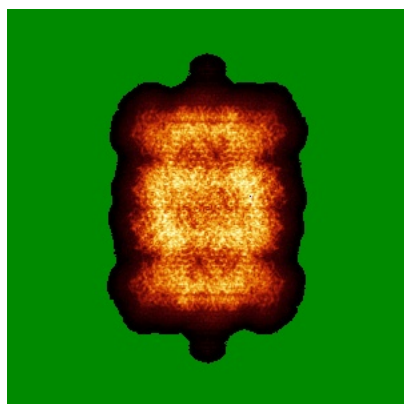


Z Index: 132

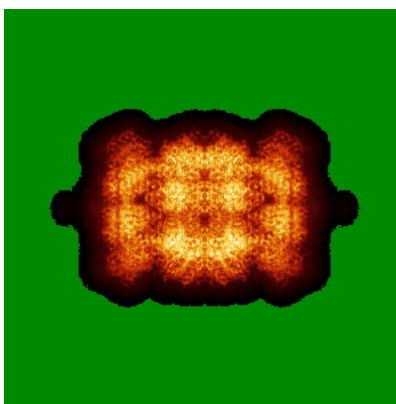
The images above show the largest variance slices of the map in three orthogonal directions.

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

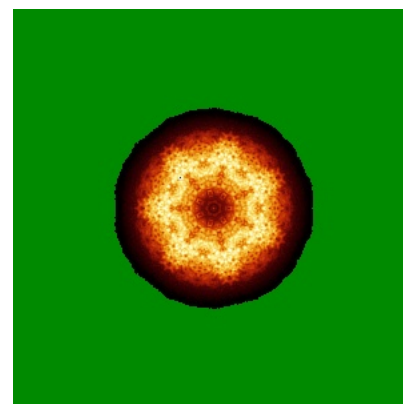
6.4.1 Primary map



X



Y

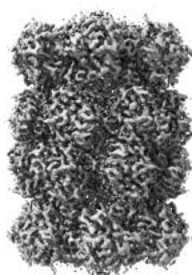


Z

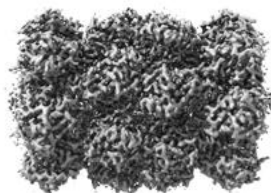
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

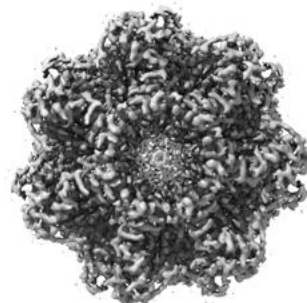
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

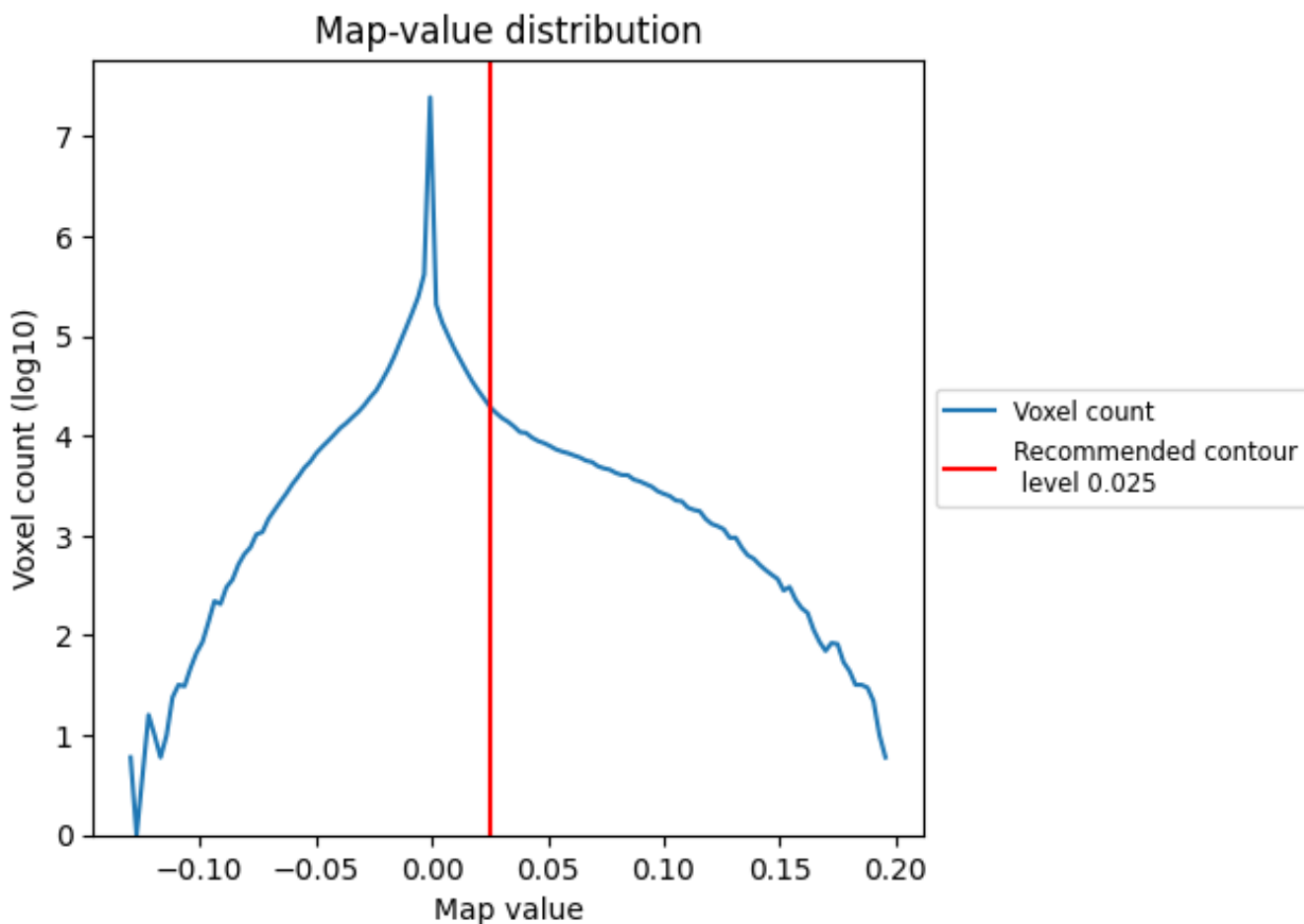
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

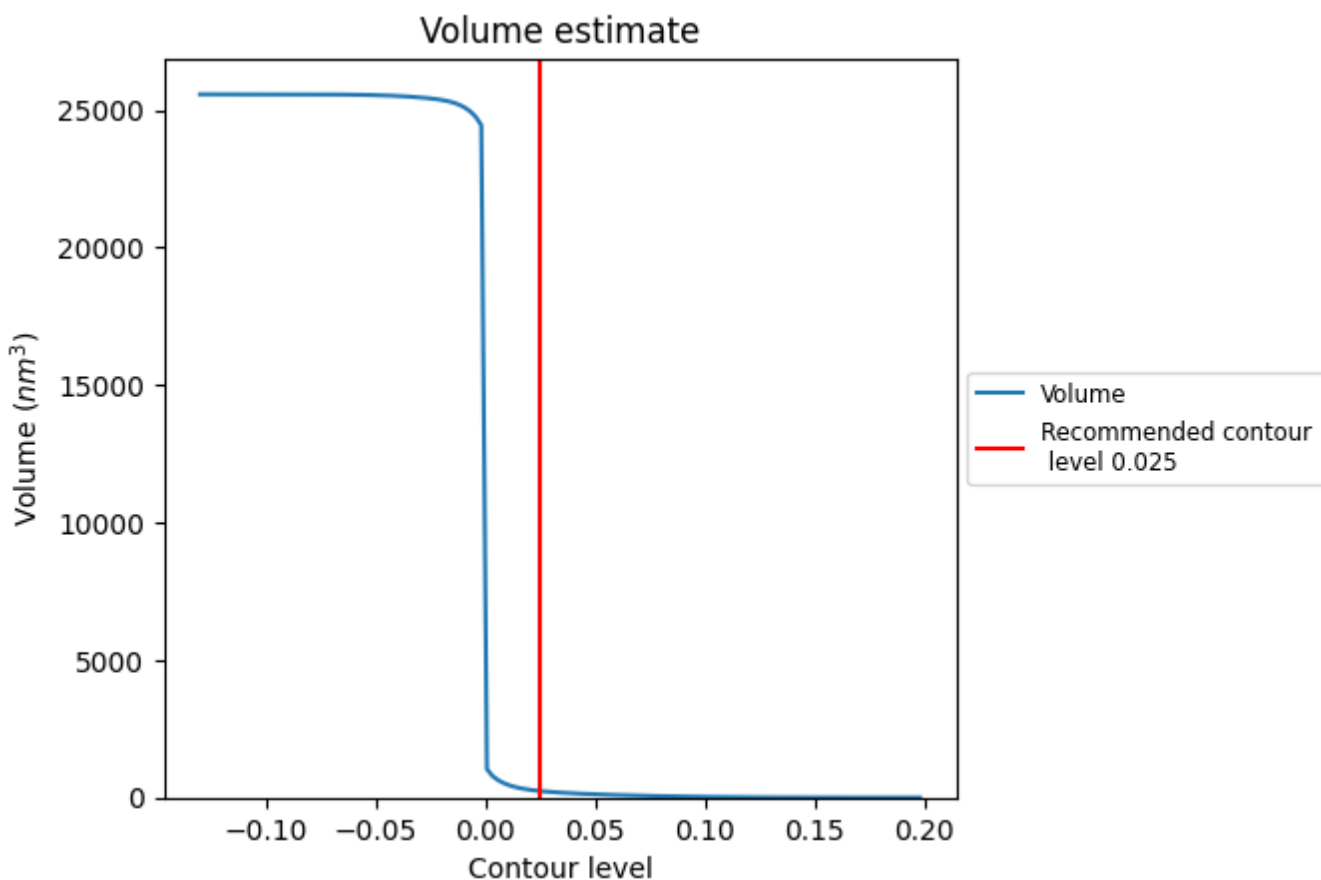
This section contains the results of statistical analysis of the map.

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.

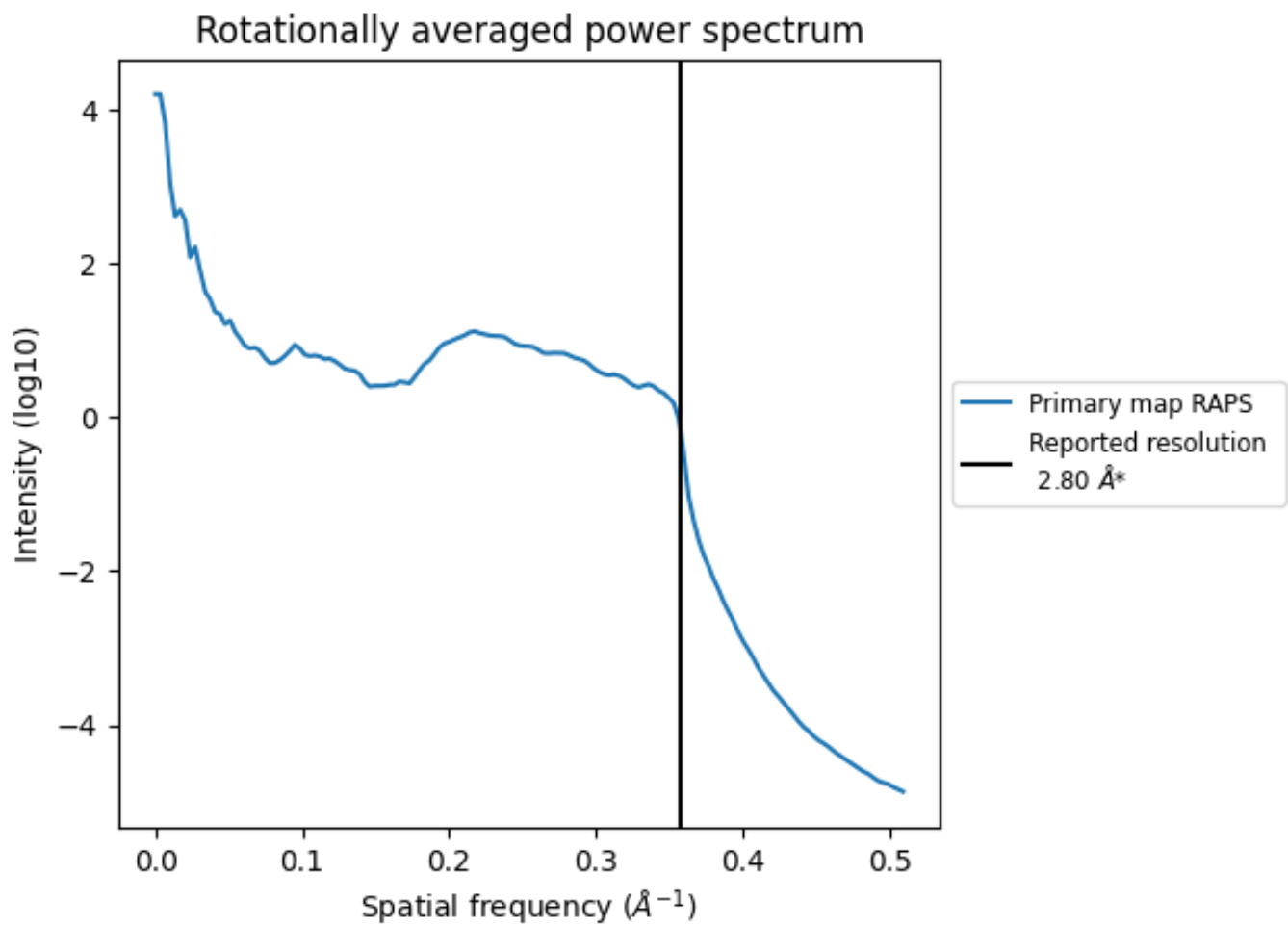
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm^3 ; this corresponds to an approximate mass of 215 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.357\AA^{-1}

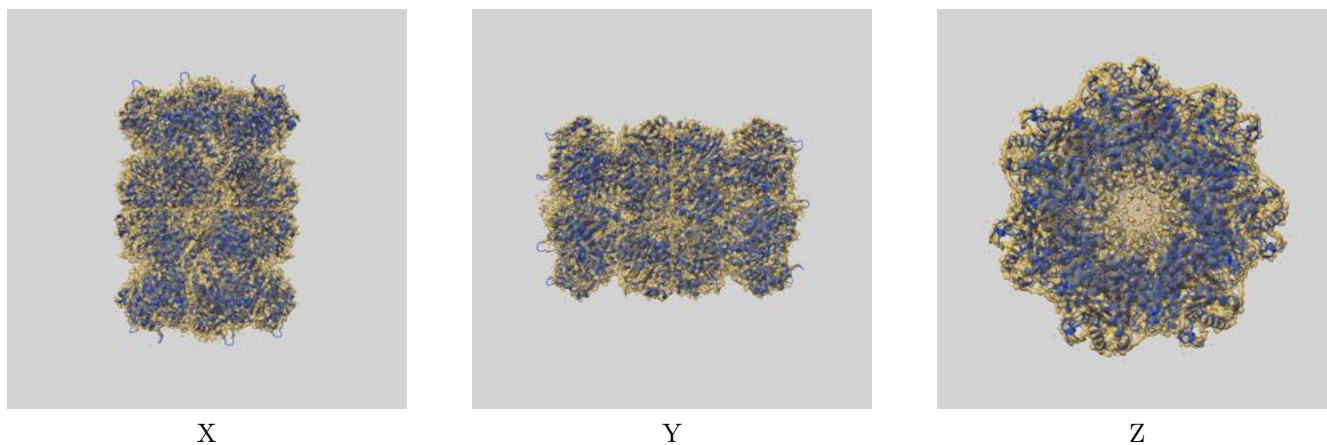
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

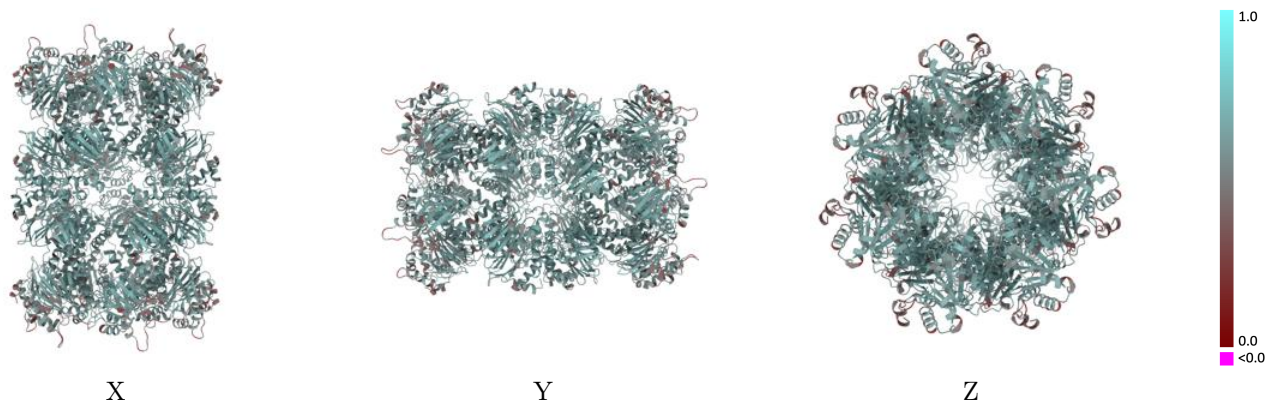
This section contains information regarding the fit between EMDB map EMD-6287 and PDB model 6BDF. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



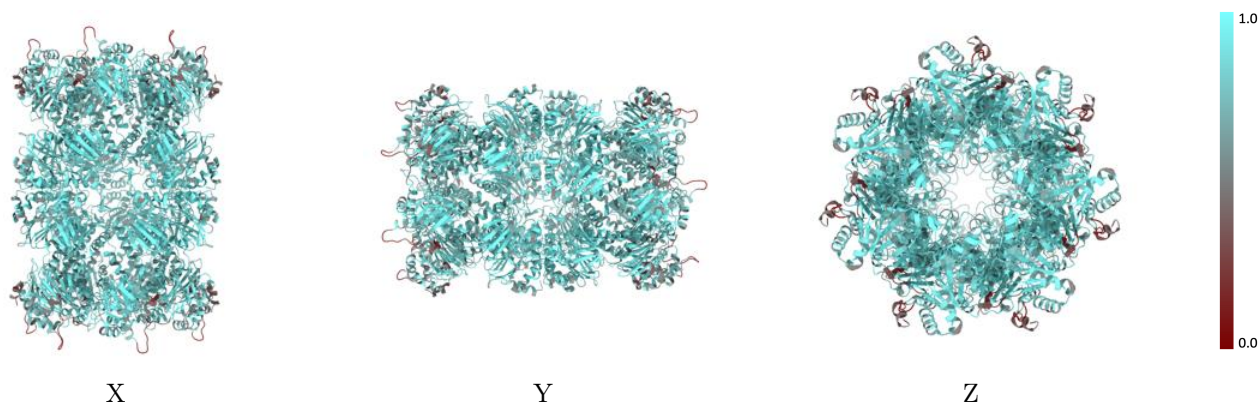
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



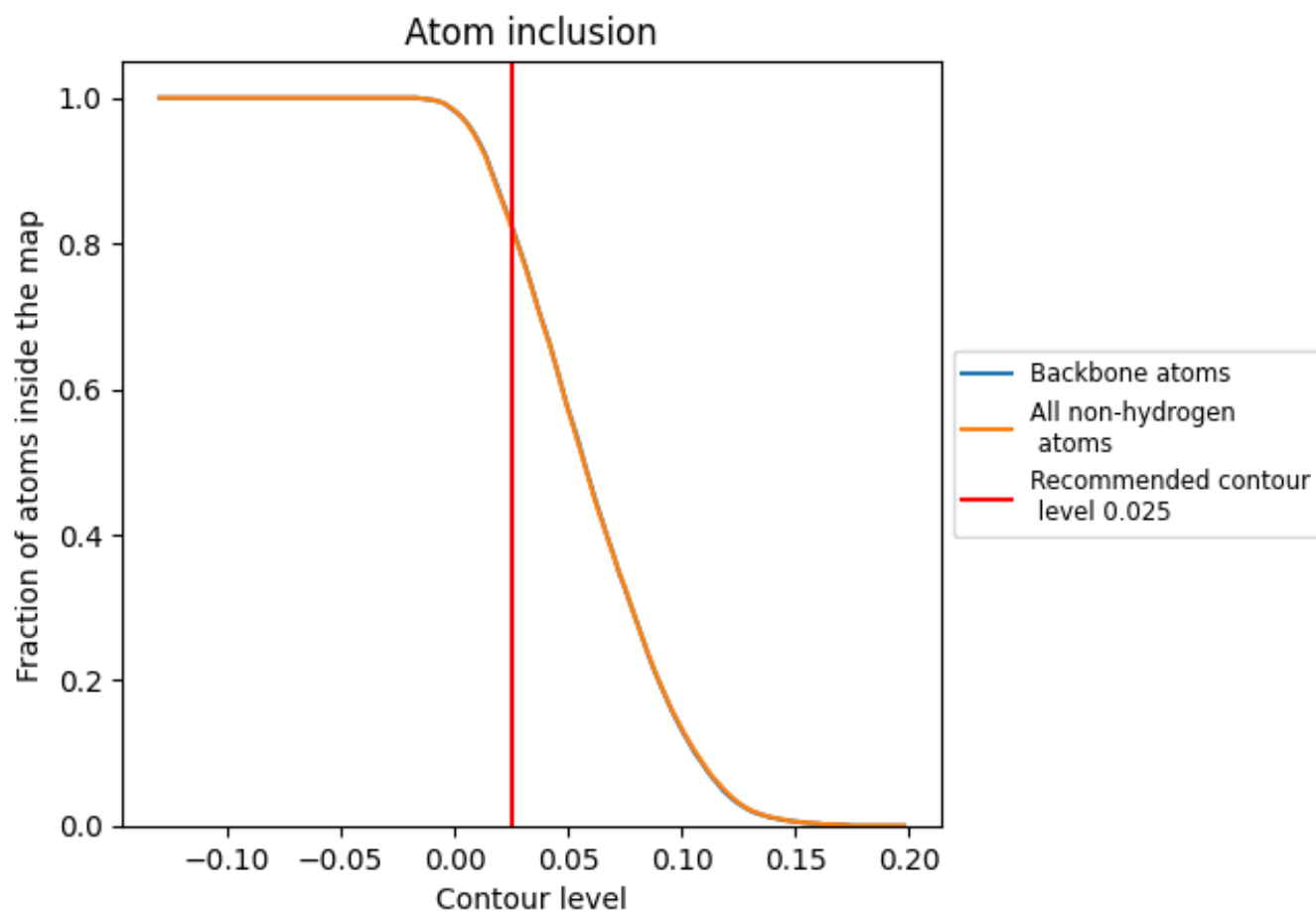
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.5850
0	 0.7730	 0.5600
1	 0.8870	 0.6140
A	 0.7750	 0.5590
B	 0.8870	 0.6120
C	 0.7770	 0.5610
D	 0.8860	 0.6130
E	 0.7720	 0.5600
F	 0.8850	 0.6150
G	 0.7760	 0.5590
H	 0.8920	 0.6150
I	 0.7730	 0.5580
J	 0.8870	 0.6120
K	 0.7770	 0.5590
L	 0.8850	 0.6130
M	 0.7750	 0.5610
N	 0.8890	 0.6120
O	 0.7730	 0.5600
P	 0.8890	 0.6140
Q	 0.7750	 0.5610
R	 0.8890	 0.6130
S	 0.7770	 0.5600
T	 0.8830	 0.6140
U	 0.7760	 0.5590
V	 0.8820	 0.6140
W	 0.7750	 0.5590
X	 0.8890	 0.6140
Y	 0.7720	 0.5590
Z	 0.8830	 0.6130

