



Full wwPDB EM Validation Report ⓘ

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PDB ID : 7YJN / pdb_00007yjn
EMDB ID : EMD-33875
Title : Cryo-EM structure of the monomeric atSPT-ORM1 (ORM1-N17A) complex
Authors : Xie, T.; Liu, P.; Gong, X.
Deposited on : 2022-07-20
Resolution : 3.40 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:

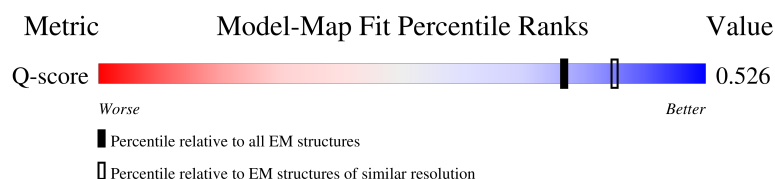
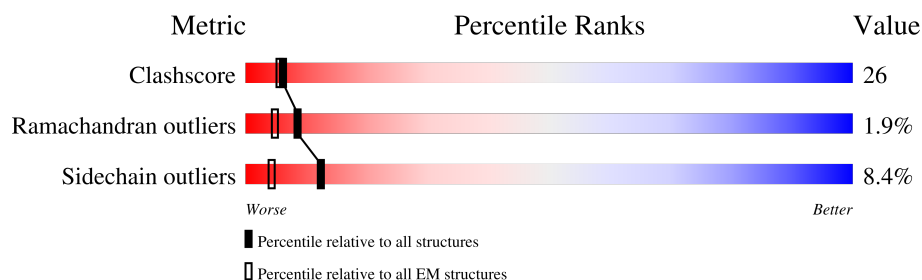
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	420	
2	B	489	
3	D	157	
4	E	62	

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Mol	Chain	Length	Quality of chain
5	C	77	25% 19% 17% 39%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8528 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 Long chain base biosynthesis protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	418	Total	C	N	O	S	0	0
			3230	2051	545	618	16		

- Molecule 2 is a protein called Long chain base biosynthesis protein 2a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	465	Total	C	N	O	S	0	0
			3592	2291	624	656	21		

- Molecule 3 is a protein called ORMDL family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	138	Total	C	N	O	S	0	0
			1122	746	181	186	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	17	ALA	ASN	engineered mutation	UNP Q9C5I0

- Molecule 4 is a protein called Long chain base biosynthesis protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	27	Total	C	N	O	0	0
			186	122	32	32		

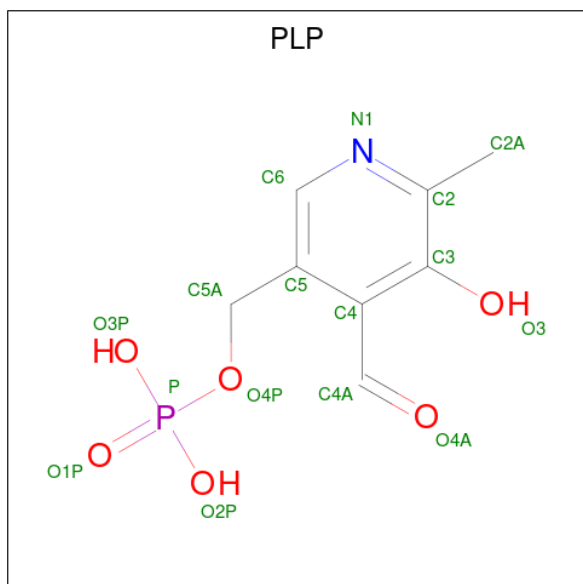
- Molecule 5 is a protein called Transmembrane protein, putative (DUF3317).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	47	Total	C	N	O	S	0	0
			383	258	62	60	3		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	initiating methionine	UNP A8MSB8
C	-19	ALA	-	expression tag	UNP A8MSB8
C	-18	ASP	-	expression tag	UNP A8MSB8
C	-17	TYR	-	expression tag	UNP A8MSB8
C	-16	LYS	-	expression tag	UNP A8MSB8
C	-15	ASP	-	expression tag	UNP A8MSB8
C	-14	ASP	-	expression tag	UNP A8MSB8
C	-13	ASP	-	expression tag	UNP A8MSB8
C	-12	ASP	-	expression tag	UNP A8MSB8
C	-11	LYS	-	expression tag	UNP A8MSB8
C	-10	SER	-	expression tag	UNP A8MSB8
C	-9	GLY	-	expression tag	UNP A8MSB8
C	-8	PRO	-	expression tag	UNP A8MSB8
C	-7	ASP	-	expression tag	UNP A8MSB8
C	-6	GLU	-	expression tag	UNP A8MSB8
C	-5	VAL	-	expression tag	UNP A8MSB8
C	-4	ASP	-	expression tag	UNP A8MSB8
C	-3	ALA	-	expression tag	UNP A8MSB8
C	-2	SER	-	expression tag	UNP A8MSB8
C	-1	GLY	-	expression tag	UNP A8MSB8
C	0	ARG	-	expression tag	UNP A8MSB8

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).

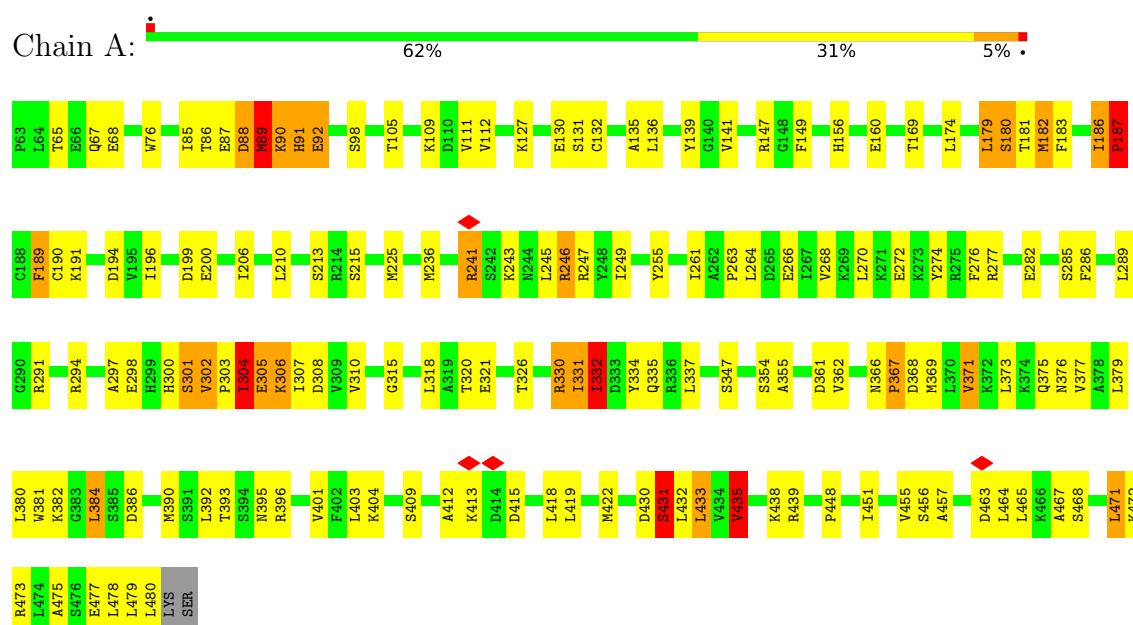


Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			15	8	1	5	1	

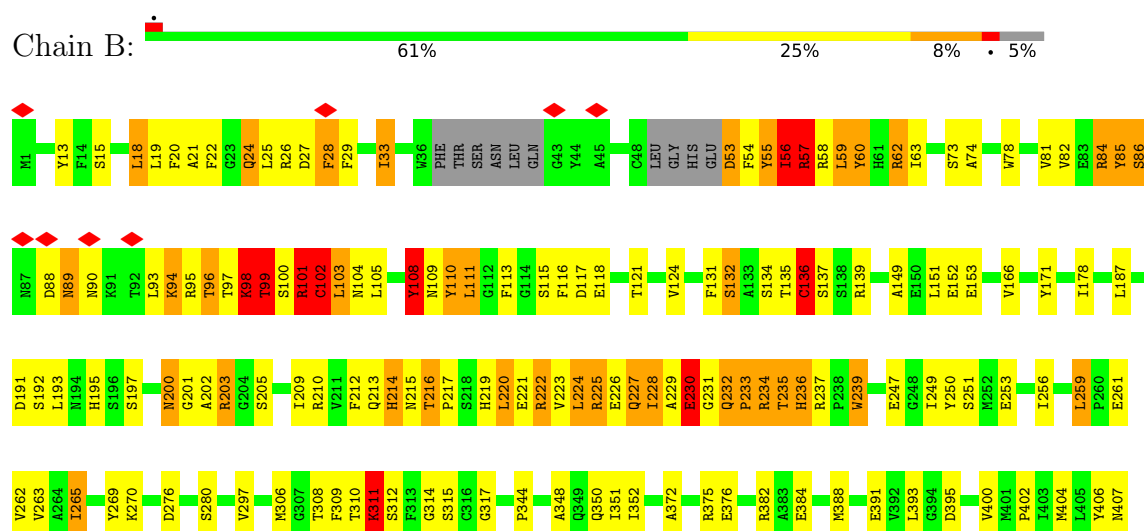
3 Residue-property plots

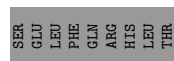
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Long chain base biosynthesis protein 1



• Molecule 2: Long chain base biosynthesis protein 2a





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58458	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.085	Depositor
Minimum map value	-2.455	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.94	9/3289 (0.3%)	0.94	19/4445 (0.4%)
2	B	1.28	40/3667 (1.1%)	1.08	28/4958 (0.6%)
3	D	1.47	8/1165 (0.7%)	1.37	19/1598 (1.2%)
4	E	0.22	0/188	0.56	0/255
5	C	1.83	6/394 (1.5%)	1.54	6/538 (1.1%)
All	All	1.21	63/8703 (0.7%)	1.09	72/11794 (0.6%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	64	THR	CA-C	-9.20	1.40	1.52
2	B	103	LEU	C-N	-9.18	1.20	1.33
2	B	103	LEU	C-O	-9.12	1.13	1.23
2	B	103	LEU	CA-C	-8.88	1.41	1.52
2	B	102	CYS	C-O	-8.15	1.13	1.24
2	B	227	GLN	CA-C	-7.73	1.42	1.52
1	A	180	SER	N-CA	-7.60	1.37	1.46
2	B	259	LEU	C-O	-7.39	1.17	1.24
3	D	61	PHE	CA-C	-7.35	1.43	1.52
2	B	259	LEU	CA-C	-7.25	1.44	1.52
2	B	24	GLN	CA-C	-7.16	1.43	1.52
2	B	317	GLY	C-O	-7.12	1.18	1.24
2	B	20	PHE	C-O	-6.91	1.16	1.24
3	D	65	TYR	CA-C	-6.86	1.43	1.52
2	B	101	ARG	C-O	-6.74	1.15	1.24
2	B	227	GLN	C-O	-6.71	1.16	1.24
1	A	435	VAL	C-O	-6.61	1.17	1.24
1	A	186	ILE	CA-CB	-6.56	1.45	1.54
1	A	186	ILE	CA-C	-6.56	1.46	1.52
2	B	265	ILE	C-O	-6.34	1.16	1.24
1	A	180	SER	CA-C	-6.32	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	259	LEU	N-CA	-6.27	1.41	1.46
5	C	8	ILE	CA-C	-6.22	1.45	1.52
2	B	262	VAL	CA-C	-6.21	1.44	1.52
2	B	195	HIS	N-CA	-6.13	1.37	1.45
2	B	55	TYR	CA-C	-6.04	1.45	1.52
2	B	109	ASN	C-O	-6.00	1.18	1.24
5	C	12	ASN	CA-C	-5.98	1.45	1.52
2	B	262	VAL	C-O	-5.91	1.17	1.24
2	B	223	VAL	CA-CB	-5.91	1.47	1.54
2	B	223	VAL	C-O	-5.89	1.17	1.24
2	B	57	ARG	CA-C	-5.85	1.45	1.52
2	B	312	SER	CA-C	-5.84	1.45	1.52
2	B	60	TYR	CA-C	-5.81	1.44	1.52
3	D	71	MET	CA-C	-5.68	1.46	1.53
2	B	137	SER	C-O	-5.60	1.19	1.24
2	B	234	ARG	C-O	-5.57	1.18	1.24
2	B	99	THR	CA-C	-5.55	1.45	1.52
2	B	18	LEU	CA-CB	-5.53	1.43	1.53
5	C	18	TYR	CA-C	-5.51	1.46	1.52
2	B	315	SER	CA-CB	-5.49	1.46	1.53
5	C	16	GLY	C-O	-5.46	1.18	1.24
1	A	335	GLN	CA-C	-5.45	1.45	1.52
1	A	433	LEU	C-O	-5.42	1.17	1.23
2	B	18	LEU	C-O	-5.41	1.17	1.24
2	B	56	ILE	CA-C	-5.36	1.46	1.52
2	B	18	LEU	CB-CG	-5.35	1.42	1.53
1	A	182	MET	CA-C	-5.34	1.46	1.52
5	C	27	LEU	CA-C	-5.32	1.46	1.52
2	B	108	TYR	CA-C	-5.26	1.46	1.52
5	C	13	VAL	C-O	-5.23	1.17	1.24
3	D	66	HIS	CA-C	-5.21	1.46	1.52
2	B	230	GLU	CA-C	-5.18	1.45	1.52
2	B	235	THR	C-O	-5.16	1.17	1.24
2	B	56	ILE	C-O	-5.15	1.18	1.24
3	D	27	TRP	C-O	-5.14	1.18	1.24
2	B	262	VAL	CA-CB	-5.13	1.47	1.54
2	B	220	LEU	C-O	-5.13	1.18	1.24
3	D	33	ILE	CA-CB	-5.12	1.48	1.54
2	B	236	HIS	CA-C	-5.06	1.46	1.53
1	A	335	GLN	CA-CB	-5.03	1.45	1.53
2	B	228	ILE	CA-CB	-5.01	1.48	1.54
3	D	67	SER	CA-C	-5.00	1.46	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	PHE	N-CA-C	13.84	130.32	113.16
5	C	8	ILE	CB-CA-C	-10.83	98.11	111.97
3	D	71	MET	CA-C-N	-8.89	109.66	122.19
3	D	71	MET	C-N-CA	-8.89	109.66	122.19
3	D	142	PHE	CA-C-N	8.64	130.64	119.84
3	D	142	PHE	C-N-CA	8.64	130.64	119.84
2	B	223	VAL	CB-CA-C	-8.23	101.03	112.14
2	B	259	LEU	N-CA-C	8.12	123.51	112.55
2	B	136	CYS	N-CA-C	8.11	121.88	108.49
2	B	102	CYS	N-CA-C	8.00	127.83	110.80
3	D	33	ILE	CB-CA-C	-7.91	101.46	112.14
1	A	92	GLU	N-CA-C	7.91	119.73	109.93
3	D	26	VAL	CB-CA-C	-7.65	102.09	111.88
1	A	187	PRO	CA-N-CD	-7.42	101.61	112.00
3	D	23	TYR	CA-C-N	7.36	129.04	119.84
3	D	23	TYR	C-N-CA	7.36	129.04	119.84
1	A	306	LYS	N-CA-C	-7.19	103.38	111.14
2	B	20	PHE	N-CA-C	-7.14	103.43	111.07
3	D	62	VAL	CB-CA-C	-7.02	102.90	111.88
2	B	135	THR	CB-CA-C	-6.92	96.55	111.78
1	A	302	VAL	CA-C-N	6.77	128.30	119.84
1	A	302	VAL	C-N-CA	6.77	128.30	119.84
2	B	21	ALA	N-CA-C	6.74	118.62	111.28
3	D	70	TRP	CA-C-N	-6.70	112.85	122.77
3	D	70	TRP	C-N-CA	-6.70	112.85	122.77
3	D	64	THR	CB-CA-C	-6.67	96.01	109.55
1	A	304	ILE	N-CA-C	6.57	123.01	109.34
5	C	20	LEU	CA-C-N	-6.54	110.88	122.07
5	C	20	LEU	C-N-CA	-6.54	110.88	122.07
1	A	183	PHE	N-CA-C	6.35	118.28	111.36
2	B	84	ARG	N-CA-C	6.31	118.71	107.80
2	B	216	THR	CA-C-N	6.28	127.69	119.84
2	B	216	THR	C-N-CA	6.28	127.69	119.84
2	B	237	ARG	N-CA-C	-6.27	102.91	110.13
1	A	371	VAL	CB-CA-C	-6.23	103.73	112.14
3	D	124	HIS	N-CA-C	6.22	123.55	109.81
5	C	39	VAL	N-CA-C	6.20	116.37	110.42
3	D	61	PHE	N-CA-C	-6.17	104.25	110.97
1	A	331	ILE	CB-CA-C	-6.10	103.89	111.70
2	B	259	LEU	CA-CB-CG	-6.08	95.02	116.30
2	B	86	SER	N-CA-C	6.07	120.84	113.38
2	B	103	LEU	CA-C-O	5.97	128.26	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	LEU	N-CA-C	-5.89	97.88	108.48
3	D	25	GLY	N-CA-C	5.87	119.86	113.58
2	B	132	SER	N-CA-C	5.83	123.22	110.80
1	A	182	MET	CA-C-N	-5.81	112.04	120.29
1	A	182	MET	C-N-CA	-5.81	112.04	120.29
2	B	89	ASN	N-CA-C	5.74	123.02	110.80
3	D	44	VAL	CB-CA-C	-5.69	104.45	112.14
2	B	311	LYS	N-CA-C	5.64	119.69	113.21
2	B	236	HIS	N-CA-C	5.56	119.06	111.39
1	A	367	PRO	CA-C-O	5.55	125.90	118.90
3	D	129	LEU	CA-CB-CG	-5.55	96.88	116.30
1	A	433	LEU	CB-CA-C	-5.55	101.25	109.90
5	C	24	GLU	N-CA-C	-5.46	105.25	111.14
1	A	332	ILE	N-CA-C	5.44	116.07	110.36
1	A	186	ILE	CA-C-N	-5.36	114.09	119.56
1	A	186	ILE	C-N-CA	-5.36	114.09	119.56
2	B	103	LEU	CD1-CG-CD2	-5.30	99.15	110.80
2	B	225	ARG	CB-CA-C	-5.28	102.58	110.88
2	B	99	THR	N-CA-C	5.26	117.19	109.24
3	D	41	VAL	CB-CA-C	-5.18	105.23	112.02
2	B	220	LEU	N-CA-C	-5.18	105.53	111.07
3	D	123	ARG	N-CA-C	-5.17	99.79	110.80
1	A	89	MET	N-CA-C	5.11	121.69	110.80
1	A	335	GLN	CB-CA-C	-5.10	102.65	110.81
5	C	5	GLN	CB-CA-C	-5.09	102.66	110.81
2	B	135	THR	CA-C-N	-5.09	116.22	123.03
2	B	135	THR	C-N-CA	-5.09	116.22	123.03
2	B	224	LEU	CA-CB-CG	-5.06	98.60	116.30
2	B	110	TYR	N-CA-C	5.05	121.56	110.80
2	B	62	ARG	CB-CA-C	5.05	120.37	110.67

There are no chirality outliers.

There are no planarity outliers.

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	3230	0	3284	173	0
2	B	3592	0	3609	181	0
3	D	1122	0	1076	72	0
4	E	186	0	186	10	0
5	C	383	0	364	35	0
6	B	15	0	6	0	0
All	All	8528	0	8525	443	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 26.

All (443) 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:B:232:GLN:HB3	2:B:233:PRO:CD	1.45	1.40
2:B:24:GLN:OE1	2:B:54:PHE:CE1	1.91	1.23
2:B:24:GLN:OE1	2:B:54:PHE:HE1	1.16	1.22
2:B:26:ARG:NH1	5:C:23:TRP:CH2	2.10	1.18
1:A:194:ASP:OD2	1:A:246:ARG:HD3	1.45	1.17
1:A:422:MET:HE1	1:A:475:ALA:CB	1.74	1.14
1:A:291:ARG:HG2	1:A:298:GLU:OE1	1.48	1.14
3:D:123:ARG:O	3:D:127:LEU:HD21	1.48	1.14
2:B:27:ASP:OD1	2:B:58:ARG:NH1	1.87	1.08
2:B:232:GLN:CB	2:B:233:PRO:CD	2.32	1.08
1:A:194:ASP:OD2	1:A:246:ARG:CD	2.02	1.06
2:B:82:VAL:HA	2:B:99:THR:HG22	1.36	1.06
2:B:232:GLN:HB3	2:B:233:PRO:HD3	1.28	1.06
2:B:78:TRP:CE3	2:B:102:CYS:O	2.10	1.04
2:B:229:ALA:O	2:B:231:GLY:N	1.91	1.04
2:B:232:GLN:HB3	2:B:233:PRO:HD2	1.34	1.03
3:D:28:THR:O	3:D:29:THR:C	1.95	1.03
2:B:26:ARG:NH1	5:C:23:TRP:CZ2	2.22	1.03
2:B:82:VAL:HA	2:B:99:THR:CG2	1.86	1.03
3:D:120:THR:HG21	3:D:126:TRP:HD1	1.25	1.02
1:A:380:LEU:HD23	1:A:401:VAL:HG21	1.40	1.01
2:B:314:GLY:O	2:B:350:GLN:OE1	1.78	1.00
1:A:422:MET:HE1	1:A:475:ALA:CA	1.93	0.99
1:A:422:MET:CE	1:A:475:ALA:HA	1.93	0.98
1:A:422:MET:HE1	1:A:475:ALA:HB2	1.44	0.95
2:B:232:GLN:CB	2:B:233:PRO:HD3	1.90	0.94
2:B:229:ALA:C	2:B:231:GLY:H	1.76	0.94
2:B:84:ARG:HG2	2:B:95:ARG:HA	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:PHE:HE1	5:C:24:GLU:CB	1.83	0.91
1:A:291:ARG:CG	1:A:298:GLU:OE1	2.18	0.90
2:B:26:ARG:HH12	5:C:23:TRP:HZ2	1.15	0.90
2:B:93:LEU:HD12	2:B:93:LEU:H	1.35	0.90
1:A:377:VAL:HG22	1:A:455:VAL:HG11	1.53	0.89
1:A:422:MET:HE1	1:A:475:ALA:HA	1.52	0.89
1:A:422:MET:CE	1:A:475:ALA:CA	2.51	0.89
1:A:380:LEU:CD2	1:A:401:VAL:HG21	2.03	0.88
3:D:51:MET:O	3:D:55:VAL:HG23	1.73	0.88
2:B:26:ARG:NH1	5:C:23:TRP:HH2	1.67	0.88
1:A:305:GLU:OE1	1:A:305:GLU:N	2.08	0.87
3:D:28:THR:O	3:D:30:TYR:N	2.08	0.86
1:A:422:MET:CE	1:A:475:ALA:HB2	2.06	0.86
5:C:5:GLN:HA	5:C:8:ILE:HD12	1.58	0.85
2:B:26:ARG:HH11	5:C:23:TRP:HH2	1.18	0.85
3:D:140:ALA:O	3:D:141:LYS:O	1.95	0.84
2:B:98:LYS:HE2	2:B:98:LYS:HA	1.59	0.84
3:D:89:TRP:CZ2	3:D:141:LYS:HG3	2.14	0.82
1:A:422:MET:CE	1:A:475:ALA:CB	2.58	0.82
3:D:123:ARG:O	3:D:127:LEU:CD2	2.26	0.82
3:D:120:THR:HG21	3:D:126:TRP:CD1	2.14	0.82
1:A:366:ASN:HB2	1:A:369:MET:HE2	1.60	0.82
1:A:390:MET:HE2	1:A:403:LEU:HB3	1.62	0.82
3:D:28:THR:HG22	3:D:29:THR:N	1.95	0.81
1:A:330:ARG:NH2	1:A:330:ARG:HB2	1.96	0.80
5:C:10:LEU:HD12	5:C:10:LEU:O	1.82	0.80
2:B:311:LYS:H	2:B:311:LYS:HD3	1.46	0.80
2:B:261:GLU:OE2	2:B:261:GLU:N	2.12	0.79
2:B:311:LYS:HD3	2:B:311:LYS:N	1.97	0.79
2:B:22:PHE:CE1	5:C:24:GLU:CB	2.66	0.79
5:C:35:LEU:O	5:C:35:LEU:HD12	1.83	0.78
1:A:422:MET:HE3	1:A:475:ALA:HA	1.65	0.78
1:A:384:LEU:CD2	1:A:468:SER:HB2	2.13	0.78
2:B:111:LEU:N	2:B:111:LEU:HD23	1.99	0.78
1:A:194:ASP:OD2	1:A:246:ARG:CG	2.31	0.78
2:B:98:LYS:HA	2:B:98:LYS:CE	2.14	0.78
2:B:249:ILE:HG22	2:B:256:ILE:HG13	1.67	0.77
1:A:241:ARG:HH21	1:A:241:ARG:HG3	1.50	0.77
1:A:147:ARG:HH12	1:A:156:HIS:HB3	1.49	0.76
3:D:123:ARG:C	3:D:127:LEU:CD2	2.58	0.76
1:A:247:ARG:HB3	1:A:276:PHE:CD1	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ASN:O	2:B:105:LEU:HD23	1.87	0.75
1:A:179:LEU:N	1:A:179:LEU:HD23	2.00	0.74
1:A:182:MET:HE3	1:A:182:MET:HA	1.68	0.74
3:D:123:ARG:N	3:D:127:LEU:HD23	2.04	0.73
1:A:379:LEU:HD12	1:A:379:LEU:O	1.87	0.73
2:B:239:TRP:H	2:B:239:TRP:CD1	2.05	0.73
1:A:247:ARG:HB3	1:A:276:PHE:CE1	2.24	0.72
1:A:478:LEU:C	1:A:478:LEU:HD23	2.15	0.72
2:B:62:ARG:HD2	5:C:19:MET:O	1.90	0.71
5:C:10:LEU:HD12	5:C:10:LEU:C	2.16	0.71
5:C:35:LEU:HD12	5:C:35:LEU:C	2.15	0.71
1:A:241:ARG:H	1:A:241:ARG:HD2	1.55	0.71
1:A:373:LEU:C	1:A:373:LEU:HD23	2.16	0.71
2:B:434:PRO:HG2	2:B:437:LEU:HD12	1.72	0.71
1:A:236:MET:HE2	1:A:274:TYR:HB3	1.73	0.70
3:D:123:ARG:C	3:D:127:LEU:HD23	2.15	0.70
1:A:418:LEU:HD13	1:A:418:LEU:O	1.91	0.70
1:A:199:ASP:OD2	1:A:255:TYR:OH	2.06	0.70
1:A:384:LEU:HD23	1:A:468:SER:HB2	1.72	0.69
1:A:182:MET:HA	1:A:182:MET:CE	2.20	0.69
1:A:245:LEU:HD23	1:A:245:LEU:N	2.07	0.69
3:D:13:ASP:OD2	3:D:22:MET:CE	2.40	0.69
2:B:82:VAL:CA	2:B:99:THR:HG22	2.19	0.69
2:B:94:LYS:HB3	2:B:94:LYS:HZ2	1.56	0.69
5:C:2:ASN:OD1	5:C:2:ASN:N	2.25	0.69
2:B:232:GLN:OE1	2:B:233:PRO:HD3	1.93	0.68
1:A:330:ARG:CZ	1:A:330:ARG:HA	2.24	0.68
1:A:371:VAL:HG12	1:A:375:GLN:HE21	1.56	0.68
2:B:84:ARG:HG2	2:B:95:ARG:CA	2.23	0.68
1:A:330:ARG:HA	1:A:330:ARG:NE	2.09	0.68
1:A:377:VAL:CG2	1:A:455:VAL:HG11	2.24	0.67
1:A:418:LEU:HD13	1:A:418:LEU:C	2.19	0.67
1:A:478:LEU:HD23	1:A:478:LEU:O	1.94	0.67
2:B:81:VAL:O	2:B:99:THR:HG22	1.95	0.67
2:B:382:ARG:NH2	2:B:393:LEU:O	2.27	0.67
4:E:44:LEU:O	4:E:48:ILE:HD12	1.93	0.67
2:B:98:LYS:HE2	2:B:98:LYS:CA	2.24	0.67
3:D:124:HIS:HA	3:D:127:LEU:HG	1.77	0.67
1:A:418:LEU:HD21	1:A:478:LEU:HD21	1.75	0.67
2:B:232:GLN:CG	2:B:233:PRO:HD3	2.24	0.66
2:B:221:GLU:HB2	2:B:265:ILE:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:ARG:HG2	2:B:225:ARG:NH2	2.10	0.65
5:C:20:LEU:N	5:C:20:LEU:HD23	2.10	0.65
5:C:36:MET:N	5:C:36:MET:SD	2.70	0.65
2:B:85:TYR:CD1	2:B:96:THR:HG21	2.33	0.64
2:B:384:GLU:HG2	2:B:457:LEU:HD13	1.79	0.64
3:D:122:TYR:C	3:D:127:LEU:CD2	2.70	0.64
3:D:114:LEU:HD21	4:E:44:LEU:HD12	1.80	0.64
1:A:182:MET:HE3	1:A:182:MET:CA	2.26	0.64
2:B:249:ILE:HG12	2:B:280:SER:HB3	1.80	0.64
1:A:264:LEU:H	1:A:300:HIS:HD2	1.45	0.63
1:A:88:ASP:N	1:A:88:ASP:OD1	2.29	0.63
1:A:246:ARG:CD	1:A:246:ARG:H	2.09	0.63
3:D:120:THR:O	3:D:120:THR:HG22	1.99	0.63
2:B:95:ARG:HD2	2:B:95:ARG:O	1.99	0.63
1:A:304:ILE:HD13	1:A:304:ILE:O	1.98	0.62
1:A:393:THR:HG21	1:A:404:LYS:HE3	1.80	0.62
1:A:366:ASN:CB	1:A:369:MET:HE2	2.28	0.62
2:B:191:ASP:OD1	2:B:192:SER:N	2.33	0.62
1:A:386:ASP:O	1:A:472:LYS:CE	2.49	0.61
1:A:465:LEU:HD23	1:A:465:LEU:C	2.27	0.60
3:D:44:VAL:HG13	3:D:45:SER:N	2.17	0.60
1:A:379:LEU:HD12	1:A:379:LEU:C	2.26	0.60
1:A:418:LEU:HD11	1:A:479:LEU:CD1	2.31	0.60
2:B:227:GLN:HA	2:B:227:GLN:NE2	2.15	0.60
2:B:259:LEU:HB3	2:B:297:VAL:HG21	1.84	0.60
1:A:321:GLU:OE2	2:B:134:SER:OG	2.13	0.59
2:B:29:PHE:HD2	2:B:29:PHE:N	1.99	0.59
2:B:225:ARG:HG2	2:B:225:ARG:HH21	1.65	0.59
1:A:111:VAL:HG12	1:A:431:SER:HB3	1.84	0.59
2:B:391:GLU:OE2	2:B:406:TYR:OH	2.19	0.59
1:A:435:VAL:HG13	1:A:435:VAL:O	2.02	0.59
3:D:68:PHE:CD1	3:D:68:PHE:N	2.69	0.59
3:D:81:GLY:O	3:D:84:ASN:N	2.36	0.59
2:B:28:PHE:N	2:B:28:PHE:HD1	2.01	0.59
2:B:193:LEU:HD11	2:B:214:HIS:HE1	1.68	0.59
1:A:463:ASP:OD1	1:A:464:LEU:N	2.35	0.58
2:B:85:TYR:C	2:B:85:TYR:HD2	2.11	0.58
3:D:32:LEU:C	3:D:32:LEU:HD23	2.28	0.58
1:A:136:LEU:HD11	1:A:141:VAL:HG22	1.85	0.58
1:A:361:ASP:OD2	1:A:362:VAL:N	2.36	0.58
2:B:261:GLU:H	2:B:261:GLU:CD	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:130:ASN:O	3:D:134:VAL:HG12	2.04	0.58
2:B:24:GLN:OE1	2:B:54:PHE:CZ	2.51	0.58
1:A:190:CYS:SG	1:A:196:ILE:HD11	2.44	0.58
3:D:13:ASP:OD2	3:D:22:MET:HE1	2.04	0.58
3:D:130:ASN:OD1	3:D:130:ASN:N	2.35	0.58
2:B:232:GLN:OE1	2:B:233:PRO:CD	2.51	0.57
1:A:304:ILE:O	1:A:304:ILE:HG23	2.03	0.57
2:B:85:TYR:C	2:B:85:TYR:CD2	2.82	0.57
2:B:308:THR:HG22	2:B:310:THR:H	1.70	0.57
2:B:28:PHE:N	2:B:28:PHE:CD1	2.72	0.57
3:D:68:PHE:O	3:D:87:THR:HB	2.05	0.57
2:B:225:ARG:HH21	2:B:225:ARG:CG	2.18	0.57
2:B:149:ALA:O	2:B:153:GLU:HG3	2.04	0.56
2:B:314:GLY:O	2:B:350:GLN:CD	2.49	0.56
1:A:307:ILE:HD12	1:A:307:ILE:N	2.20	0.56
3:D:64:THR:O	3:D:64:THR:HG22	2.05	0.56
2:B:29:PHE:N	2:B:29:PHE:CD2	2.72	0.56
2:B:151:LEU:HD23	2:B:166:VAL:HG21	1.87	0.56
3:D:61:PHE:C	3:D:61:PHE:CD1	2.80	0.56
1:A:246:ARG:H	1:A:246:ARG:HD2	1.71	0.56
2:B:63:ILE:HG23	5:C:19:MET:SD	2.46	0.56
2:B:85:TYR:HD2	2:B:85:TYR:O	1.89	0.56
2:B:192:SER:OG	2:B:212:PHE:O	2.22	0.56
2:B:213:GLN:O	2:B:216:THR:HG22	2.06	0.56
3:D:68:PHE:N	3:D:68:PHE:HD1	2.04	0.56
1:A:366:ASN:O	1:A:369:MET:HE2	2.06	0.56
3:D:23:TYR:N	3:D:23:TYR:CD2	2.72	0.56
2:B:33:ILE:HD12	2:B:33:ILE:O	2.05	0.55
1:A:98:SER:HB3	1:A:105:THR:HG22	1.88	0.55
1:A:266:GLU:O	1:A:270:LEU:HG	2.05	0.55
1:A:384:LEU:HD21	1:A:468:SER:HA	1.87	0.55
2:B:402:PRO:HA	2:B:441:ARG:HA	1.88	0.55
2:B:101:ARG:O	2:B:101:ARG:HG3	2.06	0.55
1:A:330:ARG:HB2	1:A:330:ARG:HH21	1.71	0.55
2:B:118:GLU:OE1	2:B:118:GLU:N	2.40	0.55
2:B:234:ARG:HG3	2:B:234:ARG:O	2.05	0.55
1:A:135:ALA:O	1:A:139:TYR:HB2	2.07	0.55
2:B:54:PHE:C	2:B:54:PHE:CD2	2.85	0.55
1:A:307:ILE:HD12	1:A:307:ILE:H	1.72	0.54
1:A:330:ARG:CZ	1:A:330:ARG:CA	2.85	0.54
1:A:330:ARG:CZ	1:A:330:ARG:CB	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:44:VAL:CG1	3:D:45:SER:N	2.71	0.54
5:C:9:TYR:C	5:C:9:TYR:CD2	2.85	0.54
2:B:276:ASP:OD2	2:B:306:MET:HE3	2.08	0.54
1:A:98:SER:O	2:B:131:PHE:CD1	2.61	0.54
3:D:110:VAL:HG11	4:E:48:ILE:HD11	1.89	0.54
1:A:303:PRO:HG2	1:A:306:LYS:HG2	1.90	0.54
2:B:58:ARG:HD3	2:B:58:ARG:N	2.22	0.53
3:D:85:GLY:O	3:D:86:LEU:HD12	2.08	0.53
1:A:132:CYS:SG	1:A:355:ALA:HB2	2.49	0.53
1:A:332:ILE:CD1	1:A:332:ILE:N	2.72	0.53
1:A:384:LEU:HD21	1:A:468:SER:HB2	1.91	0.53
3:D:66:HIS:CE1	3:D:71:MET:HE2	2.44	0.53
1:A:366:ASN:HB2	1:A:369:MET:CE	2.35	0.53
5:C:3:TRP:CD1	5:C:3:TRP:C	2.85	0.53
5:C:19:MET:C	5:C:20:LEU:HD23	2.33	0.53
1:A:386:ASP:O	1:A:472:LYS:HE3	2.07	0.53
2:B:171:TYR:CD2	2:B:197:SER:HB3	2.44	0.53
2:B:247:GLU:HB2	2:B:250:TYR:CE2	2.43	0.53
1:A:131:SER:OG	1:A:354:SER:OG	2.26	0.52
2:B:187:LEU:HD11	2:B:210:ARG:HG2	1.92	0.52
1:A:243:LYS:HD2	1:A:243:LYS:C	2.34	0.52
1:A:330:ARG:HB2	1:A:330:ARG:CZ	2.39	0.52
3:D:92:MET:O	3:D:102:ARG:NH2	2.42	0.52
5:C:28:PHE:C	5:C:28:PHE:CD2	2.88	0.52
2:B:93:LEU:HD12	2:B:93:LEU:N	2.16	0.52
1:A:241:ARG:HG3	1:A:241:ARG:NH2	2.21	0.51
3:D:13:ASP:OD2	3:D:22:MET:HE3	2.09	0.51
2:B:203:ARG:O	2:B:205:SER:N	2.43	0.51
3:D:61:PHE:C	3:D:61:PHE:HD1	2.18	0.51
5:C:40:LEU:N	5:C:40:LEU:CD2	2.74	0.51
1:A:182:MET:HE2	1:A:206:ILE:HG12	1.91	0.51
1:A:439:ARG:HG3	1:A:439:ARG:HH11	1.76	0.51
3:D:21:PHE:HB3	3:D:92:MET:HE1	1.91	0.51
1:A:282:GLU:HB2	1:A:285:SER:OG	2.10	0.51
2:B:404:MET:HE2	2:B:406:TYR:CE1	2.46	0.51
2:B:221:GLU:HB2	2:B:265:ILE:CD1	2.41	0.51
2:B:98:LYS:HD3	2:B:99:THR:H	1.76	0.50
2:B:228:ILE:HG22	2:B:228:ILE:O	2.10	0.50
2:B:57:ARG:HD3	2:B:57:ARG:N	2.26	0.50
3:D:28:THR:O	3:D:31:MET:N	2.44	0.50
3:D:122:TYR:CA	3:D:127:LEU:HD22	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TRP:HE3	1:A:396:ARG:NH1	2.10	0.50
1:A:404:LYS:HD2	1:A:448:PRO:HG2	1.94	0.50
3:D:12:PRO:C	3:D:14:MET:H	2.20	0.50
3:D:140:ALA:C	3:D:141:LYS:O	2.55	0.50
1:A:286:PHE:HE2	1:A:318:LEU:HD11	1.76	0.50
2:B:219:HIS:HD1	2:B:219:HIS:C	2.19	0.50
1:A:432:LEU:HD23	1:A:432:LEU:O	2.12	0.50
3:D:128:PHE:CD1	3:D:128:PHE:C	2.85	0.50
2:B:382:ARG:NH1	2:B:400:VAL:O	2.42	0.49
3:D:51:MET:O	3:D:54:THR:HG22	2.12	0.49
2:B:78:TRP:HE3	2:B:102:CYS:O	1.83	0.49
1:A:334:TYR:C	1:A:334:TYR:CD2	2.85	0.49
1:A:418:LEU:C	1:A:418:LEU:CD1	2.86	0.49
2:B:235:THR:O	2:B:235:THR:HG22	2.12	0.49
1:A:98:SER:O	2:B:131:PHE:CE1	2.65	0.49
1:A:381:TRP:CE2	1:A:392:LEU:HD23	2.47	0.49
1:A:456:SER:OG	1:A:457:ALA:N	2.45	0.49
2:B:311:LYS:N	2:B:311:LYS:CD	2.73	0.49
1:A:305:GLU:H	1:A:305:GLU:CD	2.14	0.49
1:A:386:ASP:O	1:A:472:LYS:HE2	2.12	0.49
1:A:430:ASP:O	1:A:431:SER:O	2.29	0.49
2:B:230:GLU:HG3	2:B:230:GLU:O	2.11	0.49
2:B:236:HIS:N	2:B:236:HIS:ND1	2.59	0.49
2:B:117:ASP:OD1	2:B:117:ASP:N	2.40	0.49
5:C:23:TRP:CD1	5:C:23:TRP:H	2.31	0.49
1:A:471:LEU:CD1	1:A:471:LEU:C	2.84	0.49
2:B:116:PHE:CD1	2:B:121:THR:HG21	2.48	0.49
3:D:124:HIS:H	3:D:125:PRO:HD2	1.78	0.49
1:A:243:LYS:C	1:A:243:LYS:CD	2.86	0.48
2:B:57:ARG:N	2:B:57:ARG:CD	2.75	0.48
2:B:73:SER:OG	2:B:74:ALA:N	2.44	0.48
1:A:213:SER:OG	1:A:213:SER:O	2.31	0.48
2:B:84:ARG:CG	2:B:95:ARG:HA	2.33	0.48
2:B:94:LYS:HB3	2:B:94:LYS:NZ	2.22	0.48
1:A:422:MET:HE3	1:A:475:ALA:CA	2.33	0.48
2:B:63:ILE:CG2	2:B:412:PRO:HG3	2.44	0.48
3:D:93:ASP:OD2	3:D:99:THR:OG1	2.31	0.48
1:A:307:ILE:HG21	1:A:310:VAL:HG23	1.95	0.48
1:A:373:LEU:C	1:A:373:LEU:CD2	2.84	0.48
2:B:53:ASP:HA	2:B:57:ARG:NH1	2.29	0.48
4:E:58:LYS:HE3	4:E:59:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TRP:CE3	1:A:396:ARG:NH1	2.82	0.48
2:B:139:ARG:NH1	2:B:152:GLU:OE2	2.36	0.48
1:A:169:THR:HG21	1:A:326:THR:HG22	1.95	0.48
2:B:18:LEU:HG	2:B:18:LEU:O	2.12	0.48
3:D:39:LEU:HD23	3:D:39:LEU:HA	1.53	0.48
1:A:147:ARG:HG3	1:A:347:SER:HB3	1.96	0.48
2:B:388:MET:HE3	2:B:461:SER:HB2	1.96	0.48
1:A:225:MET:HE3	1:A:263:PRO:HG2	1.95	0.47
1:A:315:GLY:HA2	1:A:320:THR:O	2.14	0.47
2:B:232:GLN:CD	2:B:233:PRO:HD3	2.38	0.47
2:B:256:ILE:HB	2:B:395:ASP:OD2	2.14	0.47
2:B:178:ILE:HD12	2:B:201:GLY:HA3	1.96	0.47
1:A:246:ARG:HD2	1:A:246:ARG:N	2.29	0.47
1:A:432:LEU:HD11	1:A:467:ALA:HA	1.96	0.47
2:B:202:ALA:HB1	2:B:209:ILE:HD11	1.94	0.47
2:B:239:TRP:CD1	2:B:239:TRP:N	2.72	0.47
2:B:372:ALA:O	2:B:376:GLU:HG3	2.15	0.47
5:C:21:ASP:O	5:C:22:TRP:C	2.58	0.47
2:B:78:TRP:CZ3	2:B:102:CYS:O	2.63	0.47
2:B:116:PHE:C	2:B:116:PHE:CD2	2.93	0.47
2:B:171:TYR:OH	2:B:200:ASN:OD1	2.28	0.47
1:A:65:THR:HG23	1:A:68:GLU:H	1.80	0.47
1:A:337:LEU:HD21	2:B:60:TYR:CD2	2.50	0.47
3:D:32:LEU:C	3:D:32:LEU:CD2	2.87	0.47
3:D:64:THR:CG2	3:D:68:PHE:CZ	2.98	0.47
5:C:31:LEU:HD12	5:C:31:LEU:HA	1.57	0.47
2:B:226:GLU:C	2:B:226:GLU:CD	2.83	0.47
1:A:147:ARG:NH2	1:A:160:GLU:OE2	2.48	0.47
2:B:104:ASN:C	2:B:105:LEU:HD23	2.40	0.47
3:D:122:TYR:C	3:D:127:LEU:HD23	2.39	0.47
3:D:143:PRO:HB3	4:E:57:TYR:OH	2.14	0.47
2:B:63:ILE:HG21	2:B:412:PRO:HG3	1.96	0.46
5:C:28:PHE:CD2	5:C:28:PHE:O	2.68	0.46
2:B:15:SER:O	2:B:19:LEU:HG	2.15	0.46
2:B:18:LEU:HA	2:B:18:LEU:HD12	1.62	0.46
2:B:82:VAL:CA	2:B:99:THR:CG2	2.77	0.46
2:B:56:ILE:HD13	2:B:56:ILE:HA	1.51	0.46
2:B:78:TRP:NE1	2:B:452:ASP:OD1	2.45	0.46
1:A:373:LEU:HD23	1:A:373:LEU:O	2.14	0.46
2:B:227:GLN:NE2	2:B:227:GLN:CA	2.73	0.46
3:D:123:ARG:N	3:D:127:LEU:CD2	2.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:124:HIS:ND1	3:D:124:HIS:C	2.73	0.46
1:A:213:SER:O	1:A:215:SER:N	2.48	0.46
1:A:261:ILE:HD12	1:A:395:ASN:ND2	2.31	0.46
1:A:418:LEU:HD11	1:A:479:LEU:HD13	1.98	0.46
1:A:87:GLU:C	1:A:87:GLU:CD	2.84	0.45
1:A:241:ARG:NH2	1:A:241:ARG:CG	2.77	0.45
2:B:116:PHE:CD2	2:B:116:PHE:O	2.69	0.45
2:B:85:TYR:CD2	2:B:85:TYR:O	2.68	0.45
2:B:225:ARG:NH2	2:B:269:TYR:OH	2.49	0.45
3:D:122:TYR:OH	4:E:37:HIS:CB	2.65	0.45
2:B:62:ARG:CD	5:C:19:MET:O	2.62	0.45
3:D:28:THR:C	3:D:30:TYR:N	2.72	0.45
1:A:91:HIS:CD2	1:A:91:HIS:N	2.84	0.45
1:A:268:VAL:O	1:A:272:GLU:HG2	2.17	0.45
3:D:44:VAL:O	3:D:44:VAL:HG22	2.16	0.45
4:E:43:LEU:O	4:E:47:VAL:HG23	2.17	0.45
5:C:7:LYS:HD3	5:C:7:LYS:HA	1.77	0.45
1:A:149:PHE:HE2	2:B:441:ARG:HH21	1.64	0.45
2:B:105:LEU:HD23	2:B:105:LEU:HA	1.66	0.45
2:B:219:HIS:C	2:B:219:HIS:ND1	2.75	0.45
1:A:189:PHE:CZ	1:A:331:ILE:HG23	2.51	0.45
1:A:382:LYS:HZ3	1:A:382:LYS:HB3	1.80	0.45
1:A:105:THR:OG1	1:A:109:LYS:O	2.29	0.45
2:B:203:ARG:C	2:B:205:SER:H	2.25	0.45
3:D:64:THR:HG23	3:D:68:PHE:CZ	2.52	0.45
4:E:58:LYS:HE3	4:E:58:LYS:HB3	1.63	0.45
1:A:307:ILE:HG22	1:A:308:ASP:N	2.28	0.44
1:A:377:VAL:CG2	1:A:455:VAL:CG1	2.94	0.44
2:B:462:LYS:HE3	2:B:462:LYS:HB2	1.62	0.44
2:B:93:LEU:N	2:B:93:LEU:CD1	2.79	0.44
1:A:249:ILE:N	1:A:277:ARG:O	2.49	0.44
1:A:89:MET:H	1:A:89:MET:HG2	1.39	0.44
1:A:264:LEU:HD21	1:A:307:ILE:HD11	1.99	0.44
3:D:99:THR:O	3:D:103:LYS:HG3	2.18	0.44
3:D:129:LEU:HD23	3:D:129:LEU:HA	1.55	0.44
2:B:193:LEU:HD12	2:B:193:LEU:O	2.18	0.44
2:B:213:GLN:O	2:B:214:HIS:C	2.58	0.44
2:B:13:TYR:CZ	2:B:436:LEU:HD11	2.53	0.44
2:B:348:ALA:O	2:B:352:ILE:HG13	2.18	0.44
5:C:40:LEU:N	5:C:40:LEU:HD23	2.32	0.44
2:B:224:LEU:HD23	2:B:269:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:LEU:HD12	2:B:466:LEU:O	2.18	0.44
1:A:90:LYS:HE2	1:A:90:LYS:HB3	1.56	0.44
1:A:291:ARG:N	1:A:298:GLU:OE1	2.50	0.44
2:B:203:ARG:C	2:B:205:SER:N	2.75	0.44
1:A:67:GLN:O	1:A:67:GLN:NE2	2.46	0.43
1:A:409:SER:OG	1:A:415:ASP:OD1	2.31	0.43
1:A:246:ARG:CD	1:A:246:ARG:N	2.79	0.43
1:A:189:PHE:HZ	1:A:331:ILE:HG23	1.82	0.43
2:B:81:VAL:C	2:B:99:THR:HG22	2.43	0.43
3:D:137:LEU:HD12	3:D:137:LEU:HA	1.61	0.43
3:D:145:MET:HE2	3:D:145:MET:HB3	1.68	0.43
1:A:85:ILE:N	1:A:85:ILE:HD13	2.33	0.43
1:A:112:VAL:HG11	1:A:463:ASP:HB2	2.00	0.43
2:B:57:ARG:HA	2:B:57:ARG:HD2	1.75	0.43
2:B:234:ARG:HH22	4:E:62:ARG:CB	2.31	0.43
3:D:111:VAL:O	3:D:115:ILE:HG12	2.19	0.43
5:C:35:LEU:HG	5:C:36:MET:SD	2.58	0.43
1:A:332:ILE:N	1:A:332:ILE:HD13	2.34	0.43
2:B:216:THR:HG23	2:B:216:THR:O	2.18	0.43
2:B:216:THR:HA	2:B:217:PRO:HD2	1.68	0.43
1:A:315:GLY:O	2:B:136:CYS:SG	2.77	0.43
2:B:224:LEU:HD12	2:B:224:LEU:HA	1.56	0.43
3:D:133:ALA:O	3:D:134:VAL:C	2.58	0.43
1:A:332:ILE:HA	1:A:332:ILE:HD12	1.73	0.42
2:B:404:MET:HE1	2:B:437:LEU:HD22	2.02	0.42
3:D:65:TYR:O	3:D:65:TYR:CG	2.70	0.42
5:C:39:VAL:HG12	5:C:40:LEU:CD2	2.49	0.42
1:A:191:LYS:HD2	3:D:80:GLN:O	2.19	0.42
1:A:379:LEU:C	1:A:379:LEU:CD1	2.86	0.42
1:A:430:ASP:O	1:A:431:SER:C	2.61	0.42
2:B:116:PHE:CE1	2:B:121:THR:HG21	2.53	0.42
1:A:321:GLU:HG3	2:B:344:PRO:HG3	2.00	0.42
3:D:89:TRP:CH2	3:D:141:LYS:HG3	2.53	0.42
1:A:136:LEU:HD21	2:B:124:VAL:HG12	2.00	0.42
1:A:297:ALA:O	1:A:301:SER:N	2.52	0.42
1:A:412:ALA:HB3	1:A:413:LYS:NZ	2.34	0.42
1:A:294:ARG:HB2	1:A:298:GLU:HG3	2.02	0.42
1:A:361:ASP:OD2	1:A:361:ASP:C	2.63	0.42
2:B:214:HIS:O	2:B:215:ASN:C	2.61	0.42
2:B:375:ARG:HD2	2:B:375:ARG:HA	1.85	0.42
3:D:124:HIS:HA	3:D:127:LEU:CG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:39:VAL:HG12	5:C:40:LEU:HD22	2.02	0.42
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.88	0.42
3:D:122:TYR:C	3:D:127:LEU:HD22	2.43	0.42
3:D:142:PHE:HA	3:D:143:PRO:HD3	1.81	0.42
1:A:76:TRP:O	2:B:270:LYS:HE3	2.19	0.42
2:B:108:TYR:CD2	2:B:108:TYR:N	2.72	0.42
5:C:10:LEU:C	5:C:10:LEU:CD1	2.84	0.42
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.92	0.41
2:B:102:CYS:HB3	2:B:103:LEU:H	1.57	0.41
2:B:105:LEU:HB2	2:B:424:ALA:O	2.20	0.41
3:D:122:TYR:HB3	3:D:127:LEU:HD22	2.02	0.41
1:A:289:LEU:HA	1:A:289:LEU:HD12	1.85	0.41
1:A:366:ASN:N	1:A:367:PRO:HD3	2.34	0.41
1:A:92:GLU:OE2	1:A:92:GLU:HA	2.19	0.41
1:A:418:LEU:HD21	1:A:478:LEU:CD2	2.47	0.41
2:B:59:LEU:HA	2:B:59:LEU:HD12	1.67	0.41
1:A:307:ILE:CG2	1:A:308:ASP:N	2.79	0.41
3:D:81:GLY:O	3:D:83:TYR:N	2.54	0.41
1:A:127:LYS:O	1:A:130:GLU:HG3	2.19	0.41
1:A:186:ILE:HB	1:A:187:PRO:HD2	2.03	0.41
2:B:219:HIS:ND1	2:B:219:HIS:O	2.52	0.41
2:B:228:ILE:O	2:B:228:ILE:CG2	2.68	0.41
2:B:391:GLU:CD	2:B:406:TYR:HH	2.24	0.41
3:D:98:LEU:HD21	4:E:54:ARG:HB2	2.03	0.41
1:A:419:LEU:HD22	1:A:451:ILE:HG23	2.02	0.41
1:A:181:THR:H	1:A:181:THR:HG23	1.66	0.41
1:A:200:GLU:O	1:A:200:GLU:HG2	2.20	0.41
2:B:55:TYR:HD1	2:B:55:TYR:HA	1.53	0.41
2:B:59:LEU:N	2:B:59:LEU:CD1	2.82	0.41
2:B:229:ALA:C	2:B:231:GLY:N	2.41	0.41
1:A:384:LEU:HD21	1:A:468:SER:CB	2.50	0.41
1:A:478:LEU:C	1:A:478:LEU:CD2	2.85	0.41
2:B:251:SER:C	2:B:253:GLU:H	2.28	0.41
2:B:407:ASN:HB2	2:B:410:LYS:CG	2.51	0.41
2:B:13:TYR:OH	2:B:436:LEU:HD11	2.22	0.40
2:B:230:GLU:OE1	2:B:230:GLU:HA	2.22	0.40
1:A:98:SER:H	2:B:131:PHE:HE1	1.70	0.40
1:A:381:TRP:CE3	1:A:396:ARG:CZ	3.04	0.40
2:B:222:ARG:HH11	2:B:222:ARG:HD3	1.72	0.40
2:B:249:ILE:O	2:B:249:ILE:HG13	2.21	0.40
2:B:309:PHE:HB3	2:B:351:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TYR:CD2	1:A:334:TYR:O	2.74	0.40
2:B:351:ILE:HA	2:B:351:ILE:HD13	1.81	0.40
1:A:98:SER:N	2:B:131:PHE:CE1	2.90	0.40
5:C:40:LEU:HD22	5:C:40:LEU:HA	1.75	0.40
5:C:2:ASN:HD22	5:C:4:VAL:HG13	1.87	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	416/420 (99%)	373 (90%)	42 (10%)	1 (0%)	43	71
2	B	459/489 (94%)	392 (85%)	53 (12%)	14 (3%)	3	18
3	D	136/157 (87%)	109 (80%)	21 (15%)	6 (4%)	2	13
4	E	25/62 (40%)	24 (96%)	1 (4%)	0	100	100
5	C	45/77 (58%)	42 (93%)	3 (7%)	0	100	100
All	All	1081/1205 (90%)	940 (87%)	120 (11%)	21 (2%)	8	26

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	89	ASN
2	B	110	TYR
2	B	230	GLU
2	B	232	GLN
3	D	141	LYS
2	B	88	ASP
2	B	101	ARG
2	B	214	HIS
3	D	29	THR

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Mol	Chain	Res	Type
3	D	121	ASP
1	A	431	SER
2	B	98	LYS
2	B	132	SER
2	B	233	PRO
3	D	124	HIS
2	B	100	SER
2	B	102	CYS
2	B	115	SER
3	D	142	PHE
2	B	96	THR
3	D	122	TYR

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	361/363 (99%)	334 (92%)	27 (8%)	12	38
2	B	386/414 (93%)	361 (94%)	25 (6%)	15	42
3	D	119/138 (86%)	105 (88%)	14 (12%)	5	20
4	E	17/54 (32%)	17 (100%)	0	100	100
5	C	37/71 (52%)	26 (70%)	11 (30%)	0	1
All	All	920/1040 (88%)	843 (92%)	77 (8%)	12	34

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	THR
1	A	88	ASP
1	A	89	MET
1	A	90	LYS
1	A	91	HIS
1	A	179	LEU
1	A	180	SER

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Mol	Chain	Res	Type
1	A	187	PRO
1	A	241	ARG
1	A	246	ARG
1	A	301	SER
1	A	302	VAL
1	A	304	ILE
1	A	305	GLU
1	A	330	ARG
1	A	332	ILE
1	A	368	ASP
1	A	376	ASN
1	A	384	LEU
1	A	431	SER
1	A	433	LEU
1	A	435	VAL
1	A	438	LYS
1	A	471	LEU
1	A	473	ARG
1	A	477	GLU
1	A	480	LEU
2	B	25	LEU
2	B	28	PHE
2	B	33	ILE
2	B	53	ASP
2	B	56	ILE
2	B	57	ARG
2	B	59	LEU
2	B	85	TYR
2	B	86	SER
2	B	90	ASN
2	B	94	LYS
2	B	97	THR
2	B	98	LYS
2	B	99	THR
2	B	108	TYR
2	B	111	LEU
2	B	113	PHE
2	B	136	CYS
2	B	200	ASN
2	B	203	ARG
2	B	220	LEU
2	B	222	ARG

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Mol	Chain	Res	Type
2	B	239	TRP
2	B	263	VAL
2	B	311	LYS
3	D	24	PRO
3	D	28	THR
3	D	30	TYR
3	D	61	PHE
3	D	64	THR
3	D	84	ASN
3	D	122	TYR
3	D	128	PHE
3	D	130	ASN
3	D	131	THR
3	D	132	LEU
3	D	134	VAL
3	D	137	LEU
3	D	142	PHE
5	C	2	ASN
5	C	4	VAL
5	C	10	LEU
5	C	13	VAL
5	C	14	THR
5	C	17	LEU
5	C	31	LEU
5	C	33	VAL
5	C	35	LEU
5	C	36	MET
5	C	40	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	300	HIS
1	A	316	HIS
1	A	375	GLN
2	B	90	ASN
2	B	214	HIS
2	B	227	GLN
2	B	328	GLN
2	B	350	GLN
3	D	94	ASN

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Mol	Chain	Res	Type
5	C	29	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PLP	B	501	2	15,15,16	2.47	3 (20%)	21,22,23	1.20	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLP	B	501	2	-	2/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	PLP	C5-C4	6.53	1.47	1.40
6	B	501	PLP	C3-C2	5.30	1.46	1.41
6	B	501	PLP	C3-C4	3.22	1.46	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	PLP	C3-C4-C5	-2.21	115.93	118.59
6	B	501	PLP	O2P-P-O4P	-2.04	101.34	106.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	501	PLP	C5A-O4P-P-O1P
6	B	501	PLP	C5A-O4P-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

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.

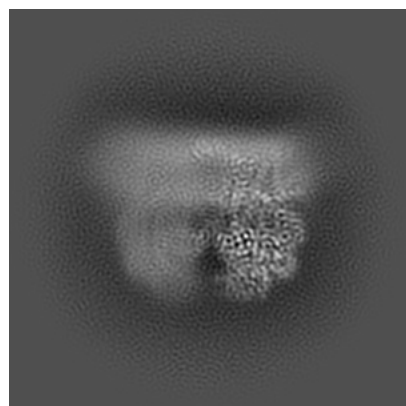
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33875. These allow visual inspection of the internal detail of the map and identification of artifacts.

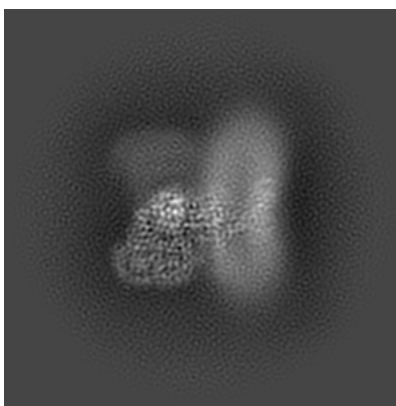
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

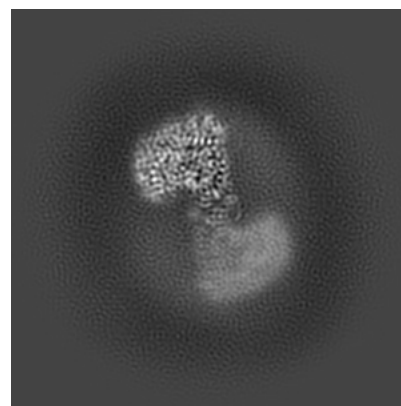
6.1.1 Primary map



X

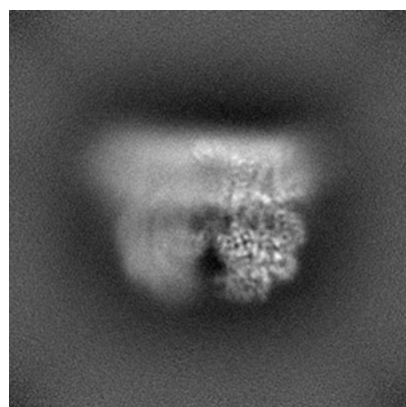


Y

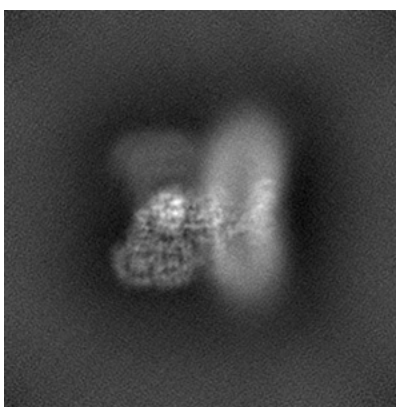


Z

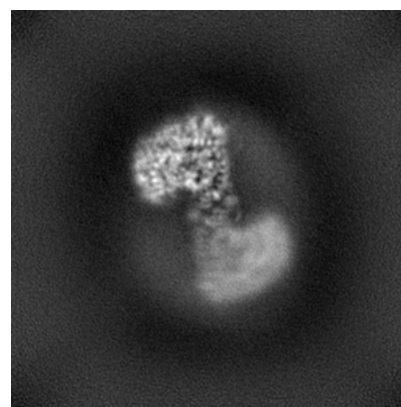
6.1.2 Raw map



X



Y

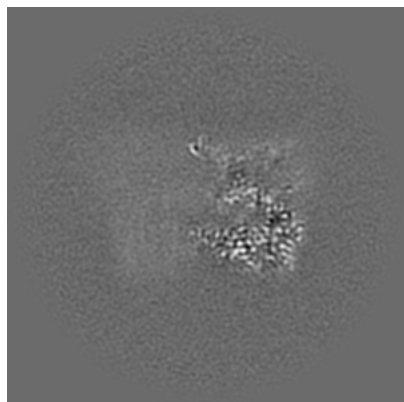


Z

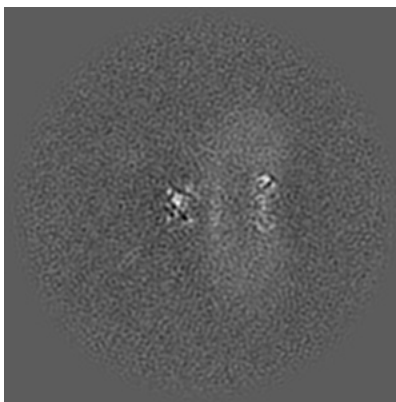
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

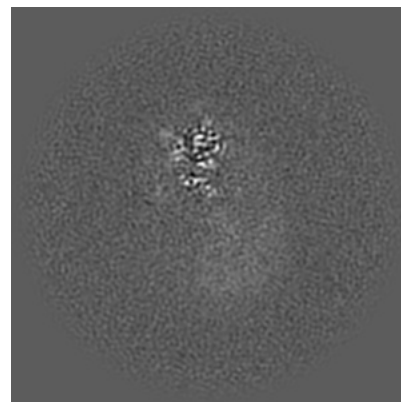
6.2.1 Primary map



X Index: 128

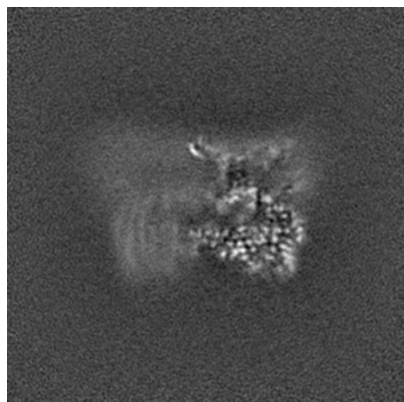


Y Index: 128

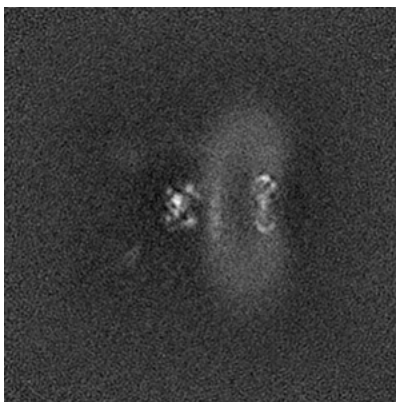


Z Index: 128

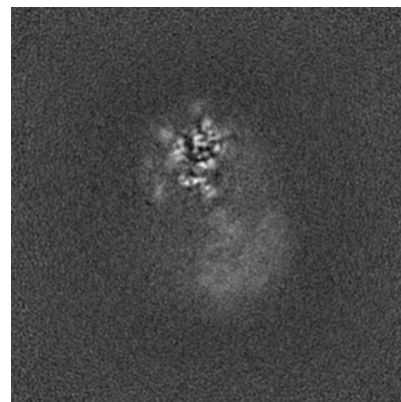
6.2.2 Raw map



X Index: 128



Y Index: 128

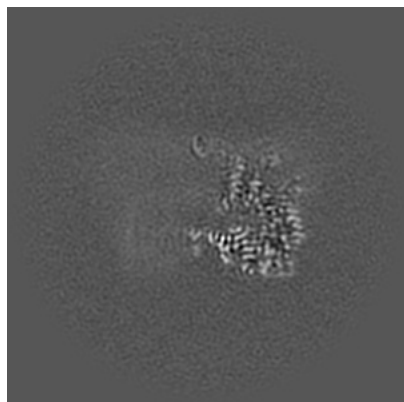


Z Index: 128

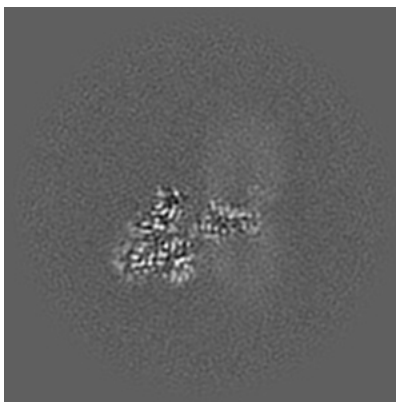
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

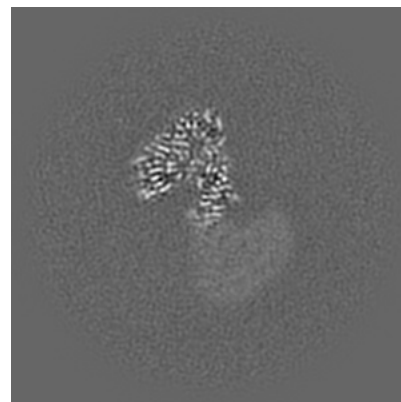
6.3.1 Primary map



X Index: 125

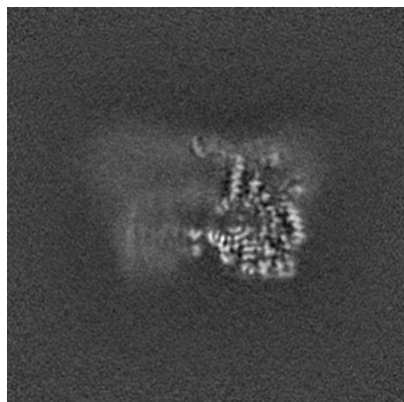


Y Index: 146

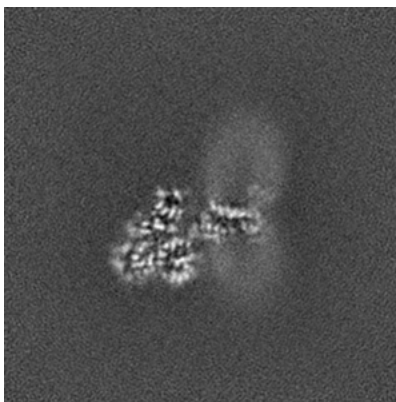


Z Index: 110

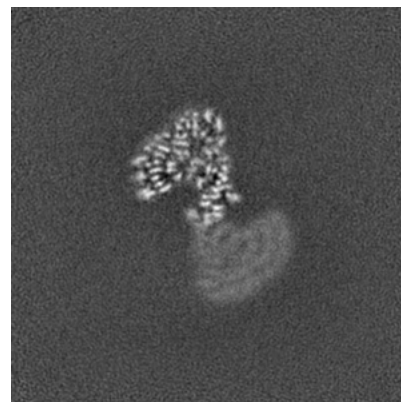
6.3.2 Raw map



X Index: 125



Y Index: 146

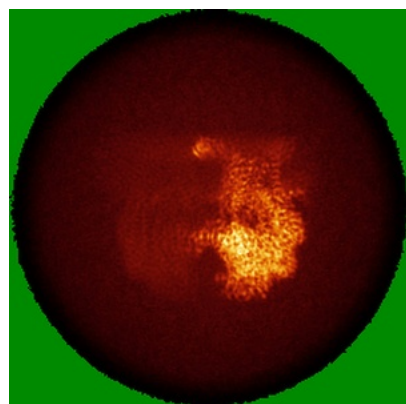


Z Index: 110

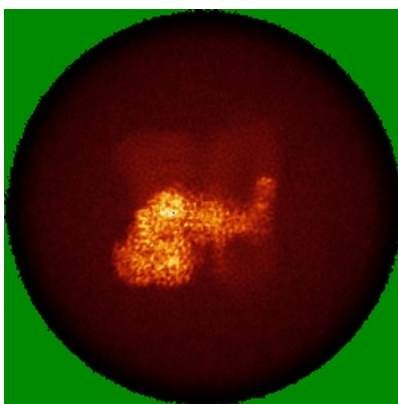
The images above show the largest variance slices of the map in three orthogonal directions.

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

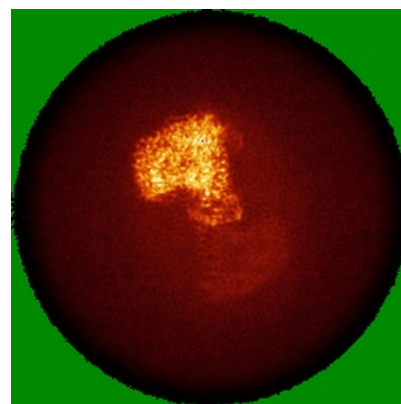
6.4.1 Primary map



X

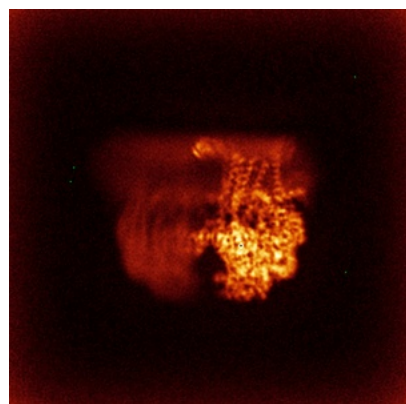


Y

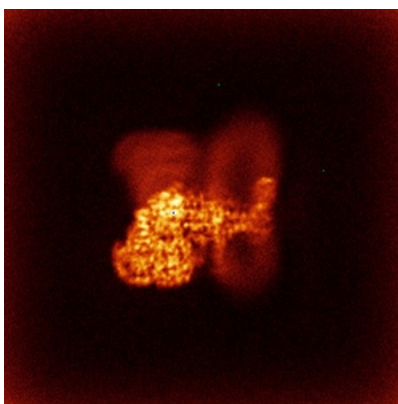


Z

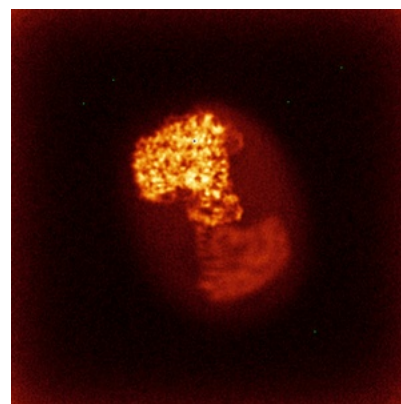
6.4.2 Raw map



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.

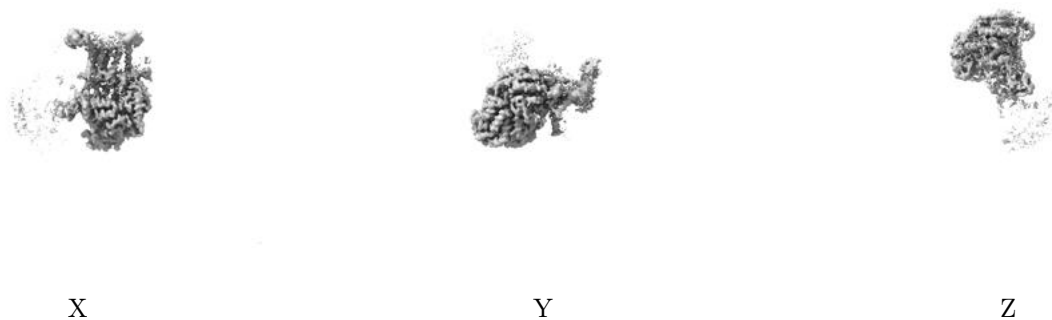
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

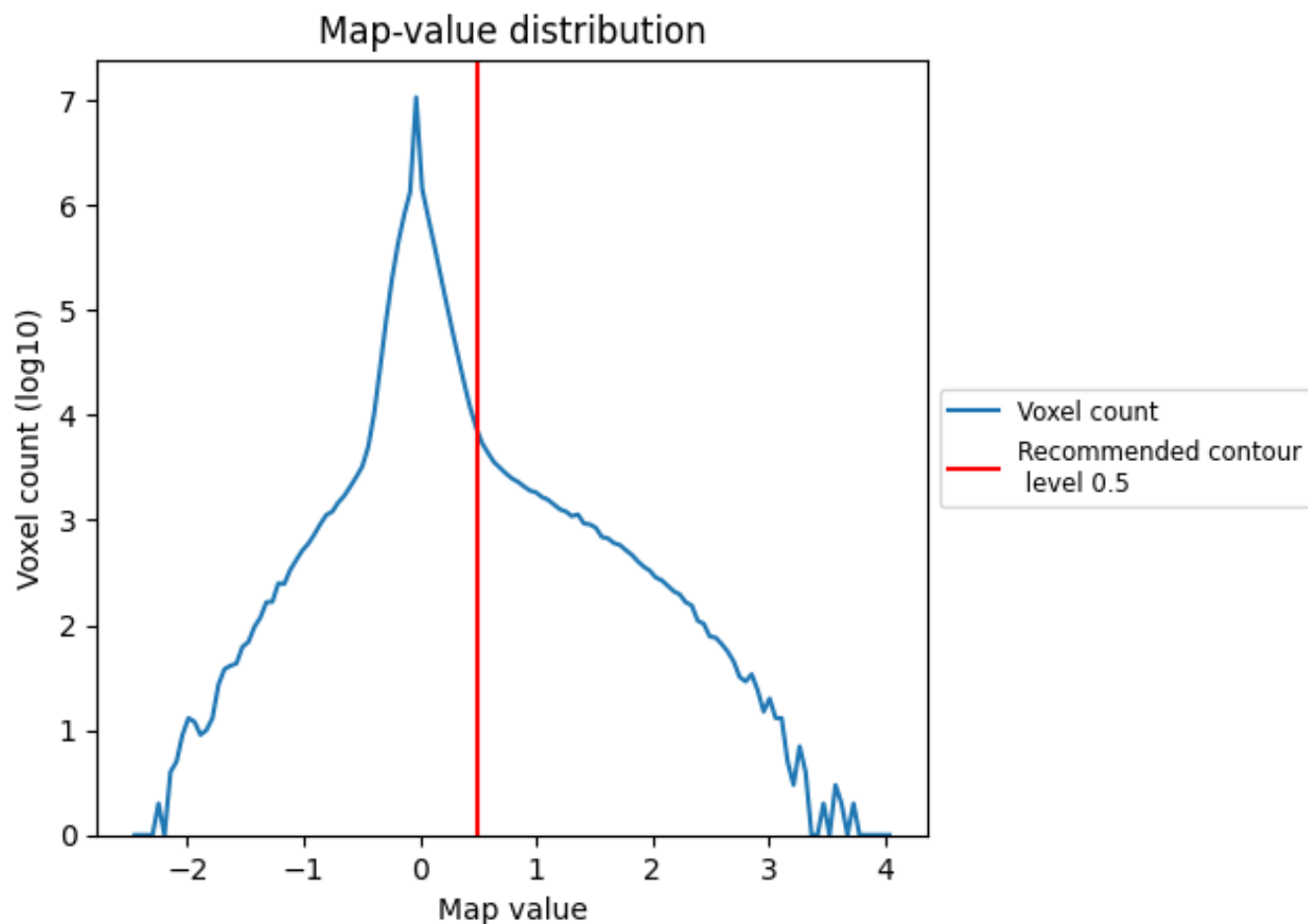
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

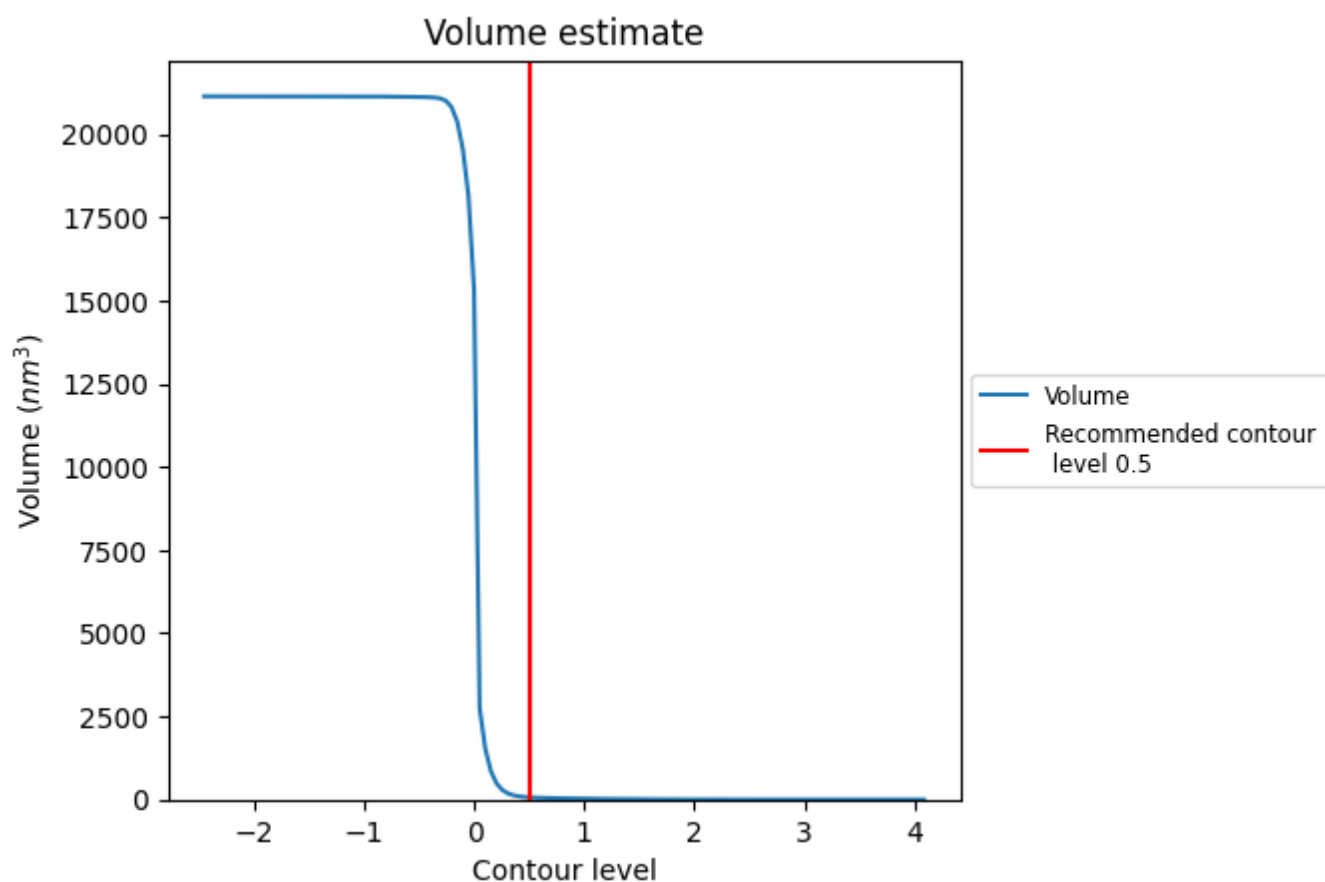
This section contains the results of statistical analysis of the map.

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.

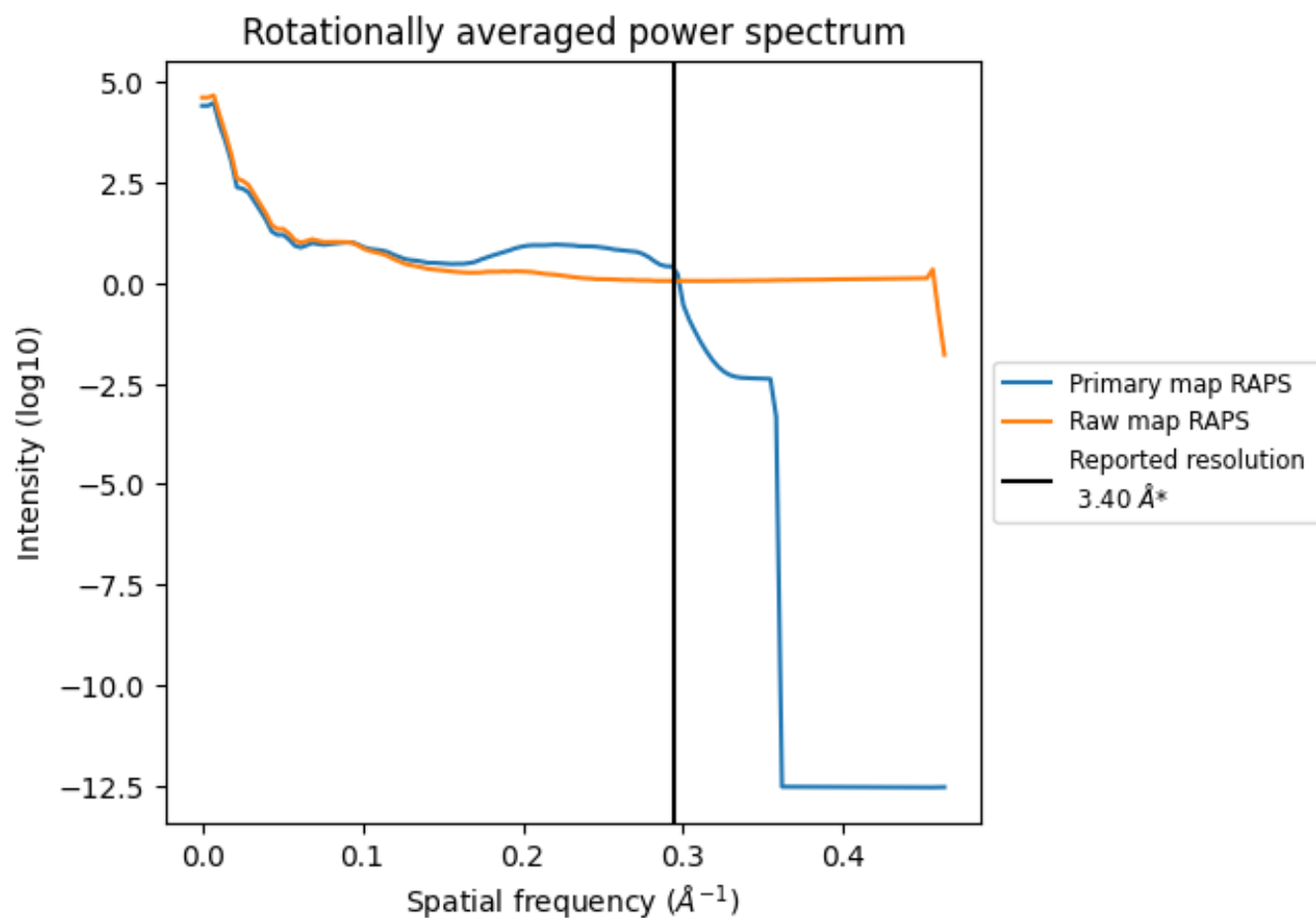
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm^3 ; this corresponds to an approximate mass of 61 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 ⓘ

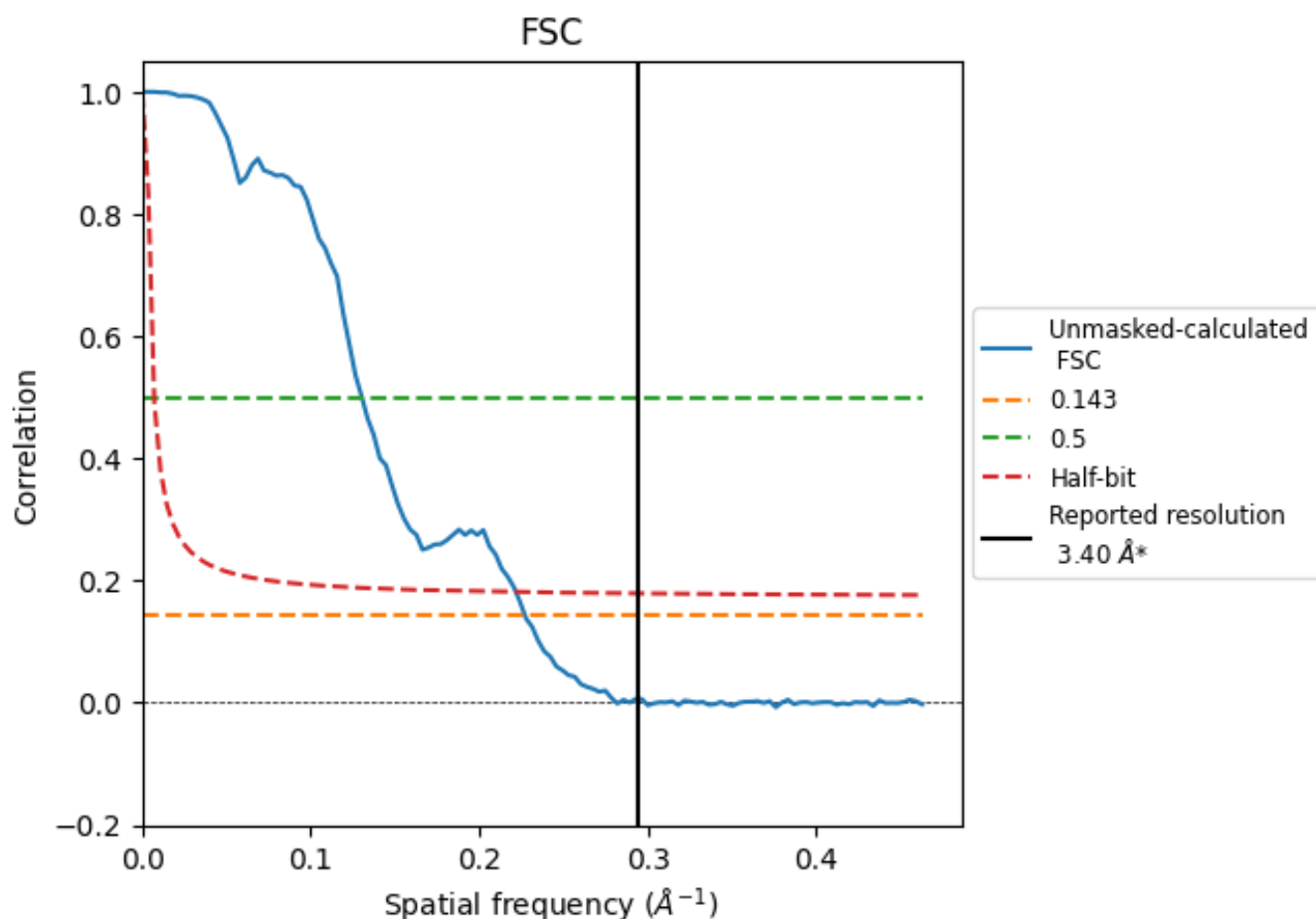


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

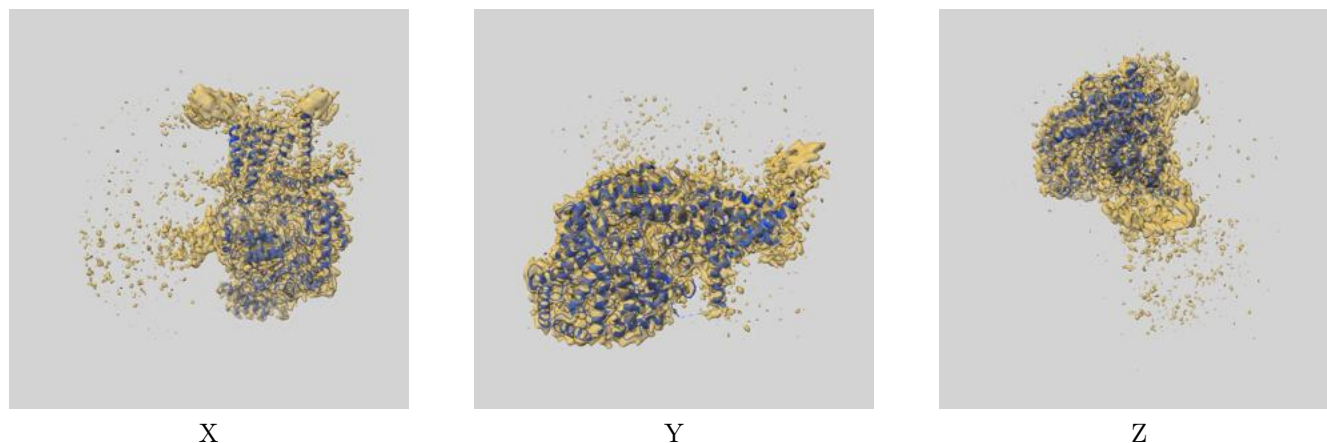
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.40	7.67	4.51

*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 4.40 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

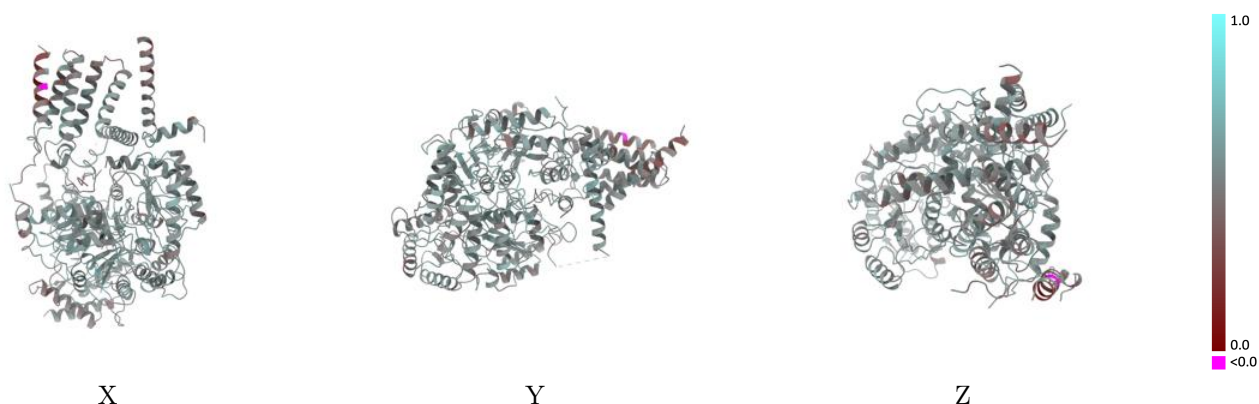
This section contains information regarding the fit between EMDB map EMD-33875 and PDB model 7YJN. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.5 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](#)



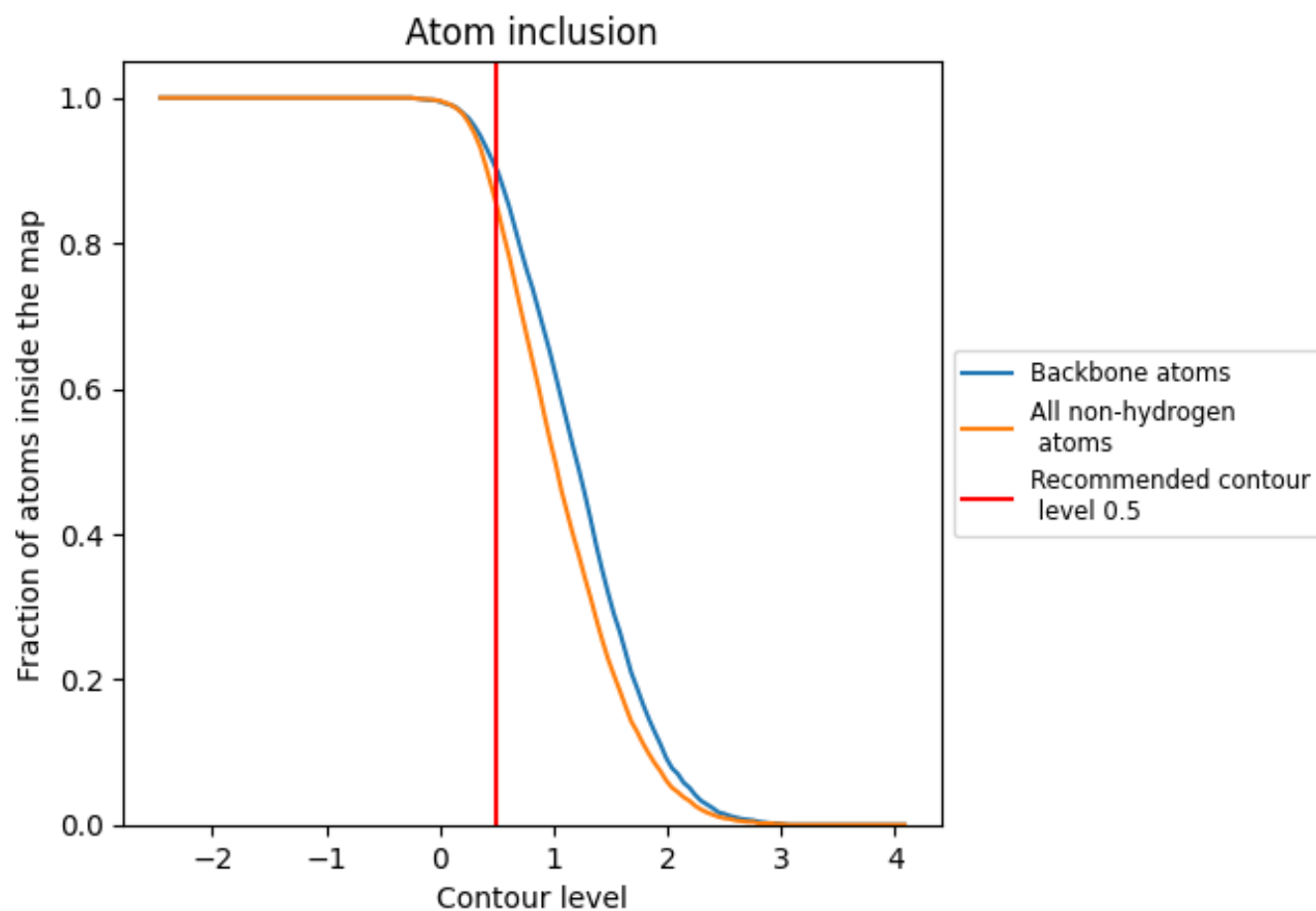
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8520	0.5260
A	0.8630	0.5260
B	0.8610	0.5420
C	0.8660	0.4880
D	0.8270	0.5070
E	0.6070	0.3850

