



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:27 PM UTC

PDB ID : 6RAM / pdb_00006ram
EMDB ID : EMD-4780
Title : Heterodimeric ABC exporter TmrAB under turnover conditions in asymmetric unlocked return conformation with wider opened intracellular gate
Authors : Thomas, C.; Janulienė, D.; Mehdipour, A.R.; Hofmann, S.; Hummer, G.; Moeller, A.; Tampe, R.
Deposited on : 2019-04-06
Resolution : 3.80 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

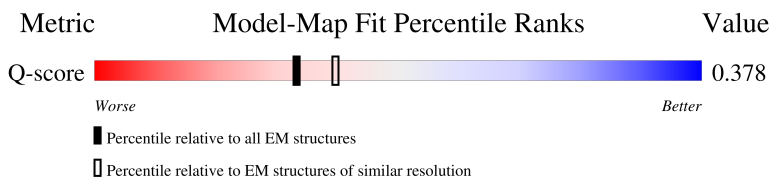
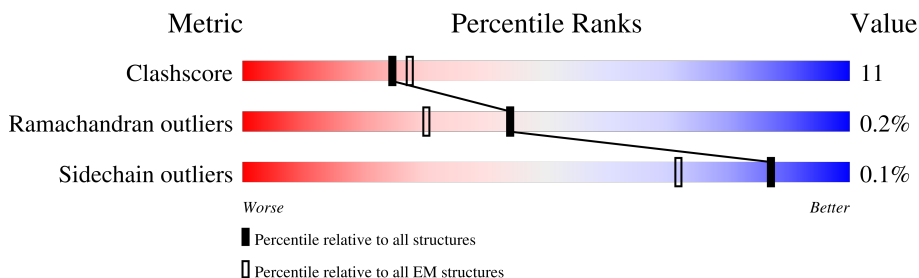
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	A	623	
2	B	578	
3	C	136	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10186 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 Multidrug resistance ABC transporter ATP-binding and permease protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	588	Total	C	N	O	S	0	0
			4710	3069	818	815	8		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	601	LYS	-	expression tag	UNP Q72J05
A	602	LEU	-	expression tag	UNP Q72J05
A	603	GLY	-	expression tag	UNP Q72J05
A	604	GLY	-	expression tag	UNP Q72J05
A	605	GLY	-	expression tag	UNP Q72J05
A	606	GLY	-	expression tag	UNP Q72J05
A	607	GLU	-	expression tag	UNP Q72J05
A	608	ASN	-	expression tag	UNP Q72J05
A	609	LEU	-	expression tag	UNP Q72J05
A	610	TYR	-	expression tag	UNP Q72J05
A	611	PHE	-	expression tag	UNP Q72J05
A	612	GLN	-	expression tag	UNP Q72J05
A	613	GLY	-	expression tag	UNP Q72J05
A	614	HIS	-	expression tag	UNP Q72J05
A	615	HIS	-	expression tag	UNP Q72J05
A	616	HIS	-	expression tag	UNP Q72J05
A	617	HIS	-	expression tag	UNP Q72J05
A	618	HIS	-	expression tag	UNP Q72J05
A	619	HIS	-	expression tag	UNP Q72J05
A	620	HIS	-	expression tag	UNP Q72J05
A	621	HIS	-	expression tag	UNP Q72J05
A	622	HIS	-	expression tag	UNP Q72J05
A	623	HIS	-	expression tag	UNP Q72J05

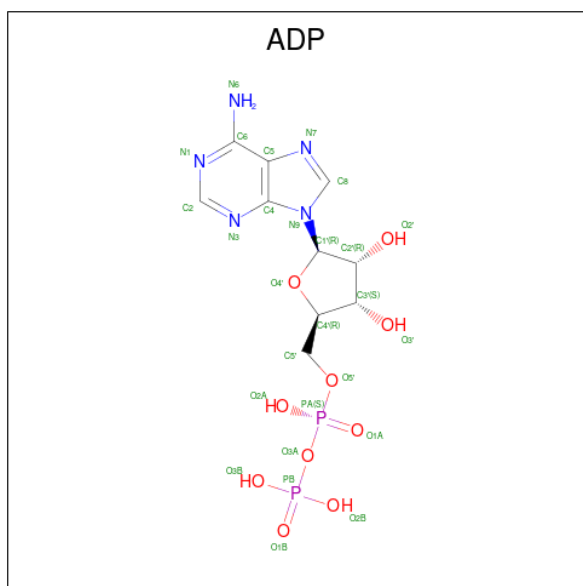
- Molecule 2 is a protein called Multidrug resistance ABC transporter ATP-binding and permease protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	572	Total	C	N	O	S	0	0
			4519	2920	810	777	12		

- Molecule 3 is a protein called Nanobody Nb9F10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	121	Total	C	N	O	S	0	0
			897	560	159	173	5		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

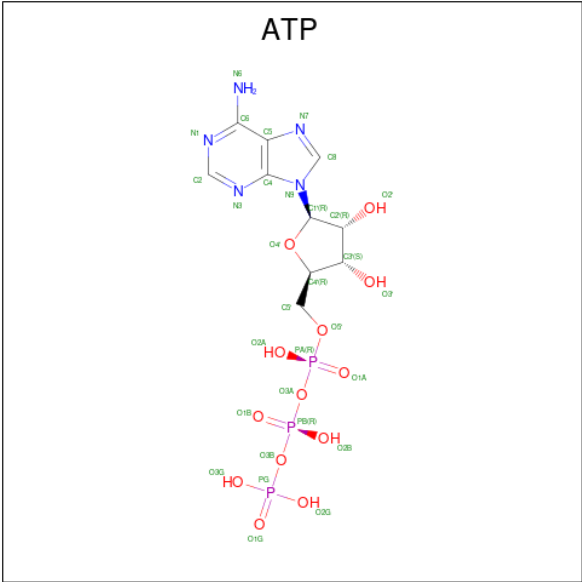


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

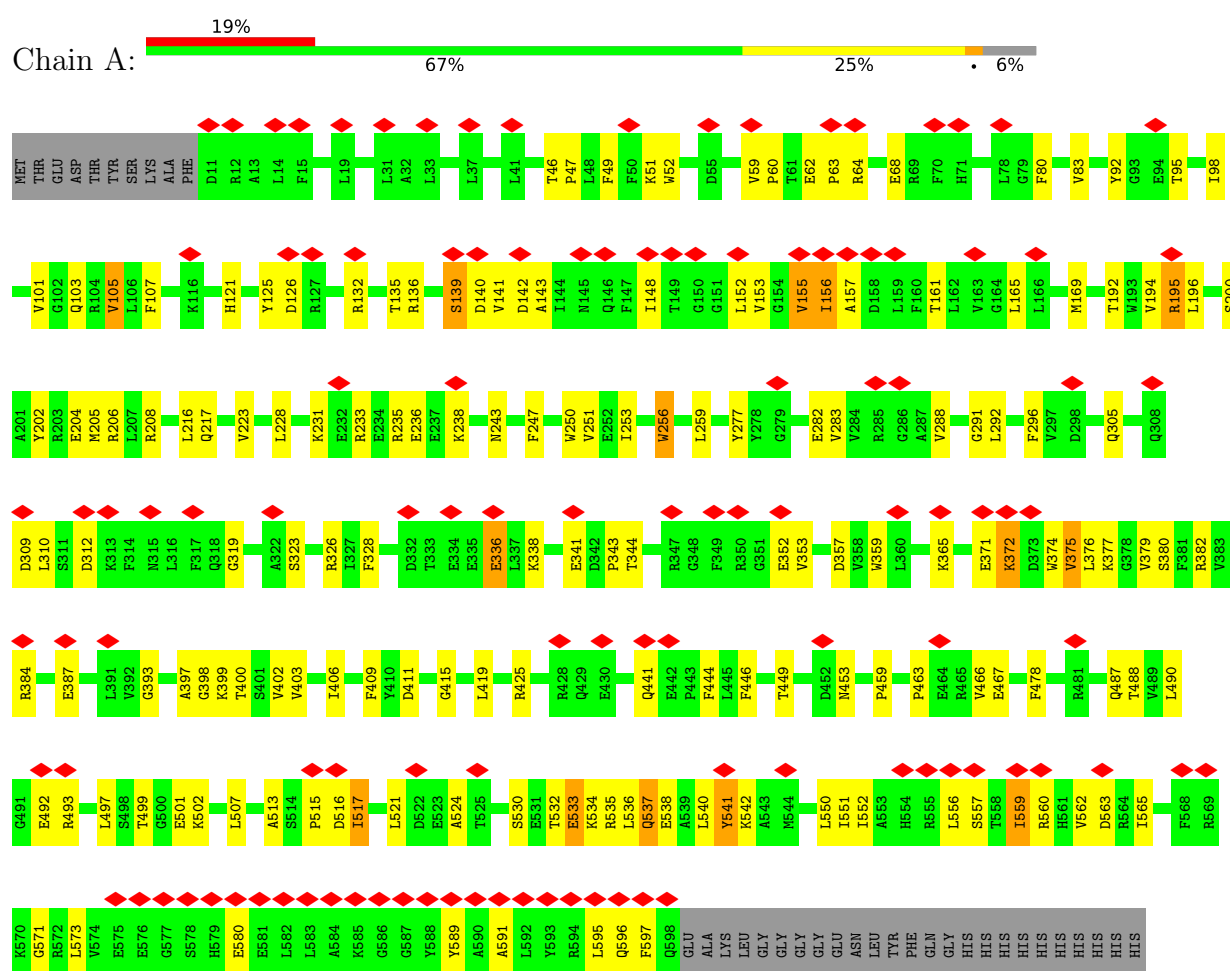


Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

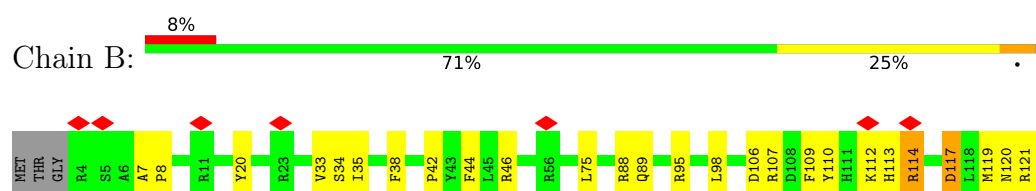
3 Residue-property plots

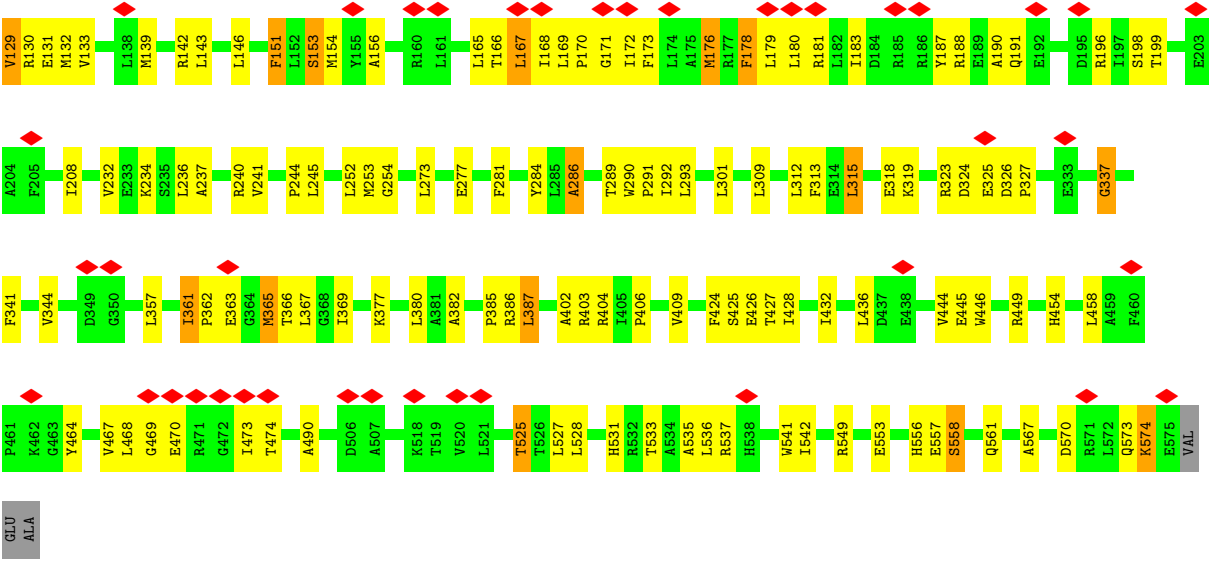
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Multidrug resistance ABC transporter ATP-binding and permease protein

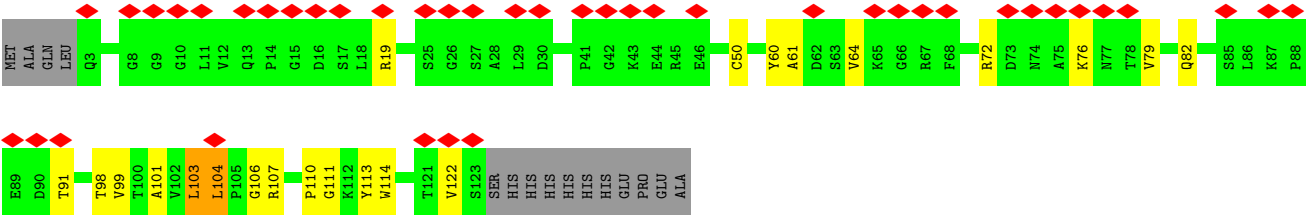


- Molecule 2: Multidrug resistance ABC transporter ATP-binding and permease protein





● Molecule 3: Nanobody Nb9F10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	97763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed within 3D reconstruction in RELION-3	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.078	Depositor
Minimum map value	-0.997	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	275.712, 275.712, 275.712	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.16	0/4815	1.43	66/6531 (1.0%)
2	B	1.20	0/4608	1.51	59/6238 (0.9%)
3	C	0.51	0/914	0.90	4/1242 (0.3%)
All	All	1.14	0/10337	1.43	129/14011 (0.9%)

There are no bond length outliers.

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	VAL	N-CA-C	-12.69	101.60	111.62
2	B	558	SER	N-CA-C	-10.21	100.23	111.36
2	B	473	ILE	N-CA-C	-10.09	103.64	113.53
1	A	217	GLN	N-CA-C	8.79	120.86	111.28
2	B	113	HIS	N-CA-C	8.76	122.80	108.52
1	A	139	SER	N-CA-C	8.75	120.59	111.14
2	B	557	GLU	N-CA-C	8.75	124.08	113.23
1	A	283	VAL	N-CA-C	8.52	120.61	111.58
2	B	558	SER	N-CA-CB	8.42	122.62	110.16
2	B	254	GLY	N-CA-C	-8.27	102.90	112.50
1	A	375	VAL	N-CA-C	-8.10	105.59	113.53
1	A	535	ARG	N-CA-C	-8.03	102.48	111.07
2	B	38	PHE	N-CA-C	-7.95	103.71	113.41
2	B	119	MET	N-CA-C	-7.85	102.67	111.07
1	A	60	PRO	N-CA-C	-7.82	102.92	113.40
1	A	156	ILE	N-CA-C	7.79	118.80	111.48
1	A	155	VAL	CA-C-N	-7.75	115.37	122.97
1	A	155	VAL	C-N-CA	-7.75	115.37	122.97
1	A	580	GLU	N-CA-C	-7.62	102.91	111.07
1	A	559	ILE	N-CA-C	-7.58	101.62	111.09
2	B	112	LYS	N-CA-C	-7.51	103.03	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	ILE	N-CA-C	7.51	115.34	107.76
1	A	64	ARG	N-CA-C	-7.50	101.47	108.22
2	B	106	ASP	N-CA-C	7.50	120.70	110.35
1	A	235	ARG	N-CA-C	-7.21	103.42	111.71
2	B	123	ASN	N-CA-C	7.20	120.04	111.33
1	A	466	VAL	N-CA-C	-7.15	103.50	110.72
1	A	256	TRP	N-CA-C	7.13	119.13	111.36
2	B	126	LEU	N-CA-C	-7.13	103.51	111.28
2	B	337	GLY	N-CA-C	7.11	121.50	112.83
2	B	574	LYS	N-CA-C	7.06	119.05	111.36
2	B	313	PHE	N-CA-C	-7.05	104.67	113.20
1	A	352	GLU	CA-C-N	-7.03	113.22	122.99
1	A	352	GLU	C-N-CA	-7.03	113.22	122.99
2	B	365	MET	N-CA-C	7.01	119.95	108.52
1	A	532	THR	N-CA-C	-6.98	103.72	111.82
2	B	425	SER	N-CA-C	-6.85	104.83	112.57
2	B	129	VAL	N-CA-C	-6.80	102.59	111.09
1	A	277	TYR	N-CA-C	6.75	118.64	111.28
1	A	238	LYS	N-CA-C	-6.74	103.86	111.07
1	A	533	GLU	N-CA-C	6.71	119.17	111.11
1	A	441	GLN	N-CA-C	6.69	121.18	112.89
1	A	515	PRO	N-CA-C	-6.65	104.29	113.53
2	B	404	ARG	N-CA-C	-6.59	104.87	113.17
2	B	469	GLY	O-C-N	6.57	128.49	122.18
1	A	537	GLN	N-CA-C	6.44	119.29	111.82
1	A	441	GLN	CA-C-N	6.38	128.30	122.37
1	A	441	GLN	C-N-CA	6.38	128.30	122.37
2	B	573	GLN	N-CA-C	-6.37	104.41	111.36
2	B	436	LEU	N-CA-C	6.30	119.36	110.23
2	B	180	LEU	N-CA-C	-6.28	104.51	111.36
1	A	589	TYR	N-CA-C	6.25	118.90	111.71
1	A	231	LYS	N-CA-C	-6.22	102.23	111.81
1	A	541	TYR	N-CA-C	-6.19	104.54	111.28
2	B	173	PHE	N-CA-C	6.16	117.66	111.07
2	B	286	ALA	N-CA-C	6.14	117.97	111.28
2	B	402	ALA	N-CA-C	6.10	117.93	111.28
1	A	52	TRP	N-CA-CB	6.07	119.15	110.16
1	A	478	PHE	CA-CB-CG	-6.04	107.76	113.80
3	C	113	TYR	CB-CA-C	-6.01	100.33	110.19
1	A	105	VAL	N-CA-C	-5.95	104.94	110.53
2	B	133	VAL	N-CA-C	-5.93	107.21	112.90
1	A	196	LEU	N-CA-C	5.91	119.55	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	42	PRO	N-CA-C	5.91	121.63	113.65
2	B	34	SER	N-CA-C	-5.89	104.77	111.07
1	A	153	VAL	N-CA-C	-5.88	107.08	112.96
1	A	141	VAL	N-CA-C	-5.87	103.72	111.05
3	C	104	LEU	N-CA-C	5.86	120.20	112.35
2	B	187	TYR	N-CA-C	5.84	117.45	111.14
2	B	127	SER	N-CA-C	-5.80	104.86	111.07
1	A	205	MET	N-CA-C	-5.75	104.62	111.69
1	A	200	SER	N-CA-C	-5.74	106.26	113.20
2	B	126	LEU	N-CA-CB	5.68	118.47	110.12
1	A	95	THR	N-CA-C	5.64	117.23	111.14
2	B	133	VAL	N-CA-CB	5.64	119.54	112.26
2	B	196	ARG	N-CA-C	-5.64	105.04	111.07
1	A	344	THR	CA-C-N	5.62	125.62	119.89
1	A	344	THR	C-N-CA	5.62	125.62	119.89
2	B	176	MET	N-CA-C	5.60	117.06	111.07
1	A	341	GLU	N-CA-C	-5.56	105.22	111.28
1	A	372	LYS	N-CA-C	5.54	118.03	111.33
3	C	103	LEU	N-CA-C	-5.52	100.70	109.59
2	B	236	LEU	N-CA-CB	5.50	118.76	110.30
2	B	151	PHE	CA-CB-CG	-5.49	108.31	113.80
2	B	199	THR	N-CA-C	5.45	118.14	111.82
1	A	161	THR	N-CA-C	5.41	117.93	111.71
1	A	243	ASN	N-CA-C	5.41	116.86	111.07
2	B	490	ALA	N-CA-C	5.41	117.17	111.28
2	B	146	LEU	N-CA-C	-5.40	105.47	111.36
1	A	411	ASP	N-CA-CB	5.39	116.55	110.03
2	B	117	ASP	N-CA-C	5.39	118.32	111.69
1	A	563	ASP	N-CA-C	-5.39	106.76	113.55
1	A	195	ARG	N-CA-C	5.38	117.59	111.02
1	A	194	VAL	N-CA-C	-5.38	105.28	110.72
1	A	228	LEU	N-CA-C	5.38	119.46	113.01
2	B	153	SER	N-CA-C	5.37	117.13	111.28
1	A	126	ASP	N-CA-C	-5.37	106.57	113.01
1	A	513	ALA	N-CA-C	-5.33	105.39	111.14
2	B	171	GLY	N-CA-C	-5.29	106.38	112.73
2	B	44	PHE	N-CA-CB	5.29	119.03	110.40
2	B	114	ARG	N-CA-CB	5.29	117.78	110.17
2	B	124	THR	N-CA-C	5.29	118.19	111.69
2	B	387	LEU	N-CA-C	-5.25	106.92	113.38
2	B	366	THR	N-CA-CB	5.24	118.20	109.60
2	B	198	SER	N-CA-C	5.23	117.06	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	167	LEU	N-CA-C	-5.23	105.58	111.28
3	C	113	TYR	N-CA-C	5.22	117.03	108.52
2	B	567	ALA	N-CA-C	-5.21	105.68	111.36
1	A	196	LEU	CB-CA-C	-5.21	101.81	110.81
1	A	382	ARG	N-CA-C	-5.20	101.40	109.72
2	B	178	PHE	N-CA-C	-5.19	105.70	111.36
1	A	103	GLN	N-CA-C	5.19	117.01	111.36
1	A	488	THR	N-CA-C	-5.18	102.38	110.10
1	A	596	GLN	N-CA-C	-5.18	106.81	113.23
1	A	415	GLY	N-CA-C	-5.17	104.33	112.61
1	A	409	PHE	N-CA-C	-5.17	107.00	113.72
2	B	253	MET	CB-CA-C	-5.14	100.81	110.67
2	B	561	GLN	CB-CA-C	-5.13	102.76	111.02
1	A	336	GLU	N-CA-C	-5.12	106.81	113.16
1	A	524	ALA	N-CA-C	-5.12	107.70	114.31
1	A	200	SER	N-CA-CB	5.12	118.71	110.42
1	A	68	GLU	N-CA-C	-5.10	106.22	112.90
2	B	315	LEU	N-CA-C	5.07	116.62	111.14
1	A	328	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	157	ALA	CA-C-N	5.06	127.57	120.28
1	A	157	ALA	C-N-CA	5.06	127.57	120.28
2	B	318	GLU	N-CA-C	5.06	117.56	110.23
1	A	343	PRO	N-CA-CB	-5.03	97.97	103.25
2	B	525	THR	N-CA-C	-5.00	102.29	110.20

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	A	4710	0	4836	108	0
2	B	4519	0	4686	113	0
3	C	897	0	887	15	0
4	A	27	0	12	2	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	B	31	0	12	0	0
All	All	10186	0	10433	218	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 11.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:VAL:HG21	1:A:565:ILE:HD11	1.41	0.98
1:A:336:GLU:HG3	1:A:365:LYS:HB2	1.52	0.89
1:A:140:ASP:HB3	1:A:323:SER:HB3	1.54	0.87
2:B:536:LEU:HD12	2:B:542:ILE:HG23	1.56	0.87
1:A:51:LYS:HD2	1:A:292:LEU:HG	1.58	0.85
2:B:131:GLU:HB3	2:B:301:LEU:HD11	1.60	0.83
3:C:50:CYS:HB3	3:C:99:VAL:HG21	1.59	0.82
2:B:35:ILE:HD11	2:B:142:ARG:HG3	1.61	0.82
2:B:361:ILE:HG12	2:B:367:LEU:HD13	1.63	0.81
3:C:98:THR:O	3:C:111:GLY:HA3	1.83	0.79
1:A:406:ILE:HG23	1:A:419:LEU:HD11	1.66	0.77
3:C:60:TYR:O	3:C:106:GLY:HA2	1.84	0.77
1:A:492:GLU:HB2	2:B:114:ARG:HG2	1.65	0.76
2:B:382:ALA:O	2:B:385:PRO:HD2	1.85	0.76
2:B:167:LEU:O	2:B:170:PRO:HD2	1.84	0.76
2:B:98:LEU:HD13	2:B:122:LEU:HG	1.69	0.75
2:B:428:ILE:O	2:B:432:ILE:HG13	1.87	0.74
1:A:562:VAL:HG21	1:A:565:ILE:CD1	2.17	0.73
1:A:556:LEU:HD22	1:A:597:PHE:HA	1.70	0.72
1:A:204:GLU:O	1:A:208:ARG:HG2	1.89	0.72
2:B:35:ILE:HD11	2:B:142:ARG:CG	2.20	0.71
1:A:591:ALA:O	1:A:595:LEU:HG	1.91	0.71
2:B:432:ILE:HG21	2:B:444:VAL:HG13	1.73	0.70
1:A:393:GLY:N	1:A:399:LYS:HD3	2.07	0.69
1:A:398:GLY:HA2	4:A:701:ADP:O5'	1.93	0.69
1:A:135:THR:HG23	1:A:139:SER:HB2	1.74	0.68
1:A:507:LEU:CD1	1:A:536:LEU:HD21	2.24	0.68
3:C:110:PRO:HB3	3:C:114:TRP:CZ2	2.29	0.67
1:A:379:VAL:HG23	1:A:573:LEU:HB2	1.76	0.67
2:B:154:MET:HE3	2:B:284:TYR:HB2	1.76	0.66
3:C:50:CYS:CB	3:C:99:VAL:HG21	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LEU:HD21	1:A:402:VAL:HG22	1.76	0.66
1:A:223:VAL:HG11	2:B:110:TYR:CE2	2.30	0.66
2:B:468:LEU:HD13	2:B:470:GLU:O	1.94	0.66
3:C:110:PRO:HB3	3:C:114:TRP:HZ2	1.59	0.66
1:A:507:LEU:CD1	1:A:536:LEU:HD11	2.26	0.65
1:A:59:VAL:HG21	1:A:62:GLU:HB3	1.77	0.65
1:A:556:LEU:HD12	1:A:559:ILE:CG2	2.26	0.65
1:A:338:LYS:HD2	1:A:425:ARG:HG2	1.78	0.64
1:A:309:ASP:HB2	2:B:290:TRP:HE1	1.62	0.64
1:A:384:ARG:HB2	1:A:387:GLU:CD	2.22	0.64
2:B:169:LEU:O	2:B:172:ILE:HB	1.97	0.64
1:A:449:THR:HB	1:A:487:GLN:HA	1.79	0.64
2:B:153:SER:O	2:B:156:ALA:HB3	1.98	0.64
2:B:528:LEU:HD21	2:B:535:ALA:HB1	1.80	0.63
1:A:233:ARG:O	1:A:236:GLU:HB3	1.98	0.63
1:A:223:VAL:HG21	2:B:110:TYR:OH	2.00	0.62
3:C:91:THR:HG22	3:C:122:VAL:H	1.65	0.62
1:A:507:LEU:HD11	1:A:536:LEU:HD21	1.82	0.62
1:A:98:ILE:CD1	1:A:152:LEU:HD23	2.31	0.61
1:A:463:PRO:O	1:A:467:GLU:HG3	2.00	0.61
2:B:361:ILE:HG12	2:B:367:LEU:CD1	2.29	0.61
2:B:324:ASP:OD2	2:B:327:PRO:HG3	2.00	0.61
1:A:51:LYS:CD	1:A:292:LEU:HG	2.30	0.59
2:B:121:ARG:O	2:B:125:ASP:HB2	2.03	0.59
1:A:98:ILE:HD12	1:A:152:LEU:HD23	1.83	0.59
1:A:101:VAL:O	1:A:105:VAL:HG23	2.03	0.58
2:B:179:LEU:O	2:B:183:ILE:HG13	2.04	0.58
2:B:88:ARG:CZ	2:B:130:ARG:HD2	2.34	0.58
1:A:192:THR:O	1:A:195:ARG:HB3	2.03	0.58
1:A:338:LYS:HD2	1:A:425:ARG:CG	2.33	0.57
1:A:155:VAL:HG12	1:A:156:ILE:HD13	1.85	0.57
2:B:341:PHE:HD1	2:B:344:VAL:HG21	1.69	0.57
2:B:446:TRP:O	2:B:449:ARG:HG2	2.05	0.57
1:A:507:LEU:HD12	1:A:536:LEU:HD11	1.87	0.57
2:B:533:THR:HG21	2:B:570:ASP:HA	1.87	0.57
2:B:377:LYS:HE3	2:B:531:HIS:CE1	2.40	0.57
2:B:20:TYR:CZ	2:B:89:GLN:HB3	2.40	0.56
2:B:290:TRP:HB3	2:B:291:PRO:HD3	1.87	0.56
2:B:361:ILE:CG1	2:B:367:LEU:HD13	2.34	0.56
1:A:256:TRP:O	1:A:259:LEU:HB3	2.05	0.56
2:B:122:LEU:O	2:B:126:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LEU:O	1:A:559:ILE:HG22	2.06	0.56
1:A:557:SER:O	1:A:560:ARG:HB3	2.05	0.56
1:A:59:VAL:HG13	1:A:59:VAL:O	2.06	0.56
2:B:188:ARG:O	2:B:191:GLN:HB3	2.06	0.56
2:B:117:ASP:O	2:B:121:ARG:HG2	2.06	0.55
1:A:398:GLY:HA2	4:A:701:ADP:PA	2.46	0.55
2:B:151:PHE:HE2	2:B:166:THR:HG1	1.53	0.55
1:A:492:GLU:HG2	1:A:493:ARG:HG3	1.87	0.55
2:B:369:ILE:HD13	2:B:380:LEU:HD22	1.89	0.55
2:B:468:LEU:HD12	2:B:468:LEU:O	2.06	0.54
1:A:446:PHE:HB2	1:A:453:ASN:ND2	2.22	0.54
1:A:376:LEU:HD23	1:A:379:VAL:HG12	1.90	0.54
1:A:492:GLU:HB2	2:B:114:ARG:CG	2.34	0.54
2:B:237:ALA:O	2:B:240:ARG:HG2	2.07	0.54
1:A:384:ARG:HD2	1:A:387:GLU:OE2	2.07	0.54
2:B:337:GLY:HA3	2:B:363:GLU:CB	2.38	0.54
2:B:445:GLU:HG2	2:B:464:TYR:CZ	2.43	0.53
1:A:516:ASP:O	1:A:517:ILE:HB	2.09	0.53
2:B:125:ASP:HB2	2:B:312:LEU:HD21	1.90	0.53
2:B:165:LEU:O	2:B:168:ILE:HG12	2.09	0.53
1:A:92:TYR:HE1	2:B:244:PRO:HG3	1.73	0.53
3:C:19:ARG:NH1	3:C:82:GLN:OE1	2.42	0.53
1:A:46:THR:HB	1:A:47:PRO:HD3	1.89	0.53
2:B:536:LEU:CD1	2:B:542:ILE:HG23	2.35	0.53
1:A:202:TYR:OH	1:A:319:GLY:HA2	2.09	0.52
2:B:169:LEU:HA	2:B:172:ILE:HD12	1.90	0.52
2:B:357:LEU:HD13	2:B:380:LEU:HD12	1.89	0.52
1:A:507:LEU:HD13	1:A:536:LEU:HD11	1.91	0.52
1:A:312:ASP:CG	2:B:139:MET:HE1	2.35	0.52
1:A:51:LYS:HG3	1:A:291:GLY:C	2.35	0.52
1:A:501:GLU:OE1	1:A:501:GLU:HA	2.10	0.52
2:B:428:ILE:HB	2:B:464:TYR:O	2.09	0.52
1:A:250:TRP:O	1:A:253:ILE:HG22	2.10	0.52
1:A:155:VAL:HG12	1:A:156:ILE:CD1	2.40	0.52
1:A:403:VAL:HG11	1:A:552:ILE:HD11	1.91	0.51
2:B:154:MET:HE3	2:B:284:TYR:CB	2.40	0.51
2:B:558:SER:HB2	3:C:101:ALA:HB2	1.93	0.51
2:B:169:LEU:HD23	2:B:172:ILE:HD12	1.91	0.51
1:A:46:THR:HG23	1:A:80:PHE:HE1	1.76	0.51
1:A:534:LYS:HA	1:A:537:GLN:HB2	1.92	0.51
1:A:534:LYS:HG2	1:A:534:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:MET:HE1	2:B:309:LEU:HD22	1.92	0.51
2:B:176:MET:SD	2:B:245:LEU:HD11	2.51	0.51
2:B:252:LEU:C	2:B:252:LEU:HD13	2.36	0.50
2:B:126:LEU:HA	2:B:129:VAL:HG12	1.93	0.50
2:B:273:LEU:HD12	2:B:277:GLU:OE1	2.11	0.50
1:A:538:GLU:HA	1:A:541:TYR:CD2	2.47	0.50
2:B:124:THR:O	2:B:127:SER:HB3	2.12	0.50
2:B:143:LEU:HD11	2:B:291:PRO:O	2.11	0.50
1:A:312:ASP:OD1	2:B:139:MET:HE1	2.12	0.49
2:B:432:ILE:CG2	2:B:444:VAL:HG13	2.41	0.49
1:A:140:ASP:CB	1:A:323:SER:HB3	2.34	0.49
2:B:154:MET:HB3	2:B:281:PHE:HE2	1.77	0.49
2:B:541:TRP:NE1	2:B:553:GLU:HB2	2.28	0.49
1:A:155:VAL:HG13	1:A:310:LEU:HD13	1.94	0.49
2:B:46:ARG:HD3	2:B:277:GLU:HA	1.93	0.49
2:B:109:PHE:HZ	2:B:315:LEU:CD2	2.26	0.49
3:C:61:ALA:HB3	3:C:64:VAL:HG22	1.93	0.49
2:B:558:SER:CB	3:C:101:ALA:HB2	2.43	0.48
2:B:172:ILE:HG12	2:B:252:LEU:HG	1.95	0.48
3:C:103:LEU:HB2	3:C:107:ARG:HB3	1.95	0.48
1:A:375:VAL:C	1:A:376:LEU:HD12	2.38	0.48
1:A:49:PHE:HZ	1:A:83:VAL:HG21	1.78	0.48
1:A:538:GLU:O	1:A:542:LYS:HG2	2.13	0.48
2:B:190:ALA:HB2	2:B:234:LYS:HB3	1.96	0.48
2:B:178:PHE:HA	2:B:181:ARG:NH2	2.29	0.47
2:B:361:ILE:HD13	2:B:527:LEU:HD11	1.96	0.47
1:A:223:VAL:HG11	2:B:110:TYR:CZ	2.48	0.47
1:A:125:TYR:CE2	2:B:208:ILE:HG12	2.49	0.47
2:B:33:VAL:CG1	2:B:75:LEU:HD22	2.44	0.47
2:B:286:ALA:O	2:B:289:THR:HG22	2.14	0.47
1:A:376:LEU:HD23	1:A:379:VAL:CG1	2.44	0.47
2:B:120:ASN:O	2:B:124:THR:HB	2.15	0.47
1:A:305:GLN:HG3	2:B:290:TRP:CD1	2.49	0.47
1:A:550:LEU:O	1:A:551:ILE:HG13	2.15	0.47
2:B:537:ARG:HG3	2:B:556:HIS:CD2	2.49	0.47
1:A:397:ALA:O	1:A:571:GLY:HA2	2.15	0.47
1:A:556:LEU:HD12	1:A:559:ILE:HG22	1.97	0.47
2:B:88:ARG:NE	2:B:130:ARG:HD2	2.30	0.47
2:B:154:MET:HB3	2:B:281:PHE:CE2	2.50	0.46
1:A:139:SER:O	1:A:142:ASP:HB3	2.16	0.46
1:A:216:LEU:HD12	2:B:123:ASN:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:THR:HG22	2:B:467:VAL:HG22	1.96	0.46
2:B:406:PRO:HB2	2:B:409:VAL:HG23	1.97	0.46
2:B:325:GLU:HG2	2:B:326:ASP:N	2.31	0.46
2:B:337:GLY:HA3	2:B:363:GLU:HB2	1.96	0.46
1:A:371:GLU:HA	1:A:374:TRP:CD1	2.50	0.46
1:A:169:MET:HE2	1:A:296:PHE:CE1	2.51	0.46
2:B:126:LEU:CA	2:B:129:VAL:HG12	2.46	0.46
2:B:95:ARG:HB2	2:B:126:LEU:HD13	1.97	0.46
2:B:386:ARG:NH1	2:B:403:ARG:HA	2.31	0.45
3:C:76:LYS:HB2	3:C:76:LYS:HE2	1.77	0.45
2:B:468:LEU:HA	2:B:474:THR:OG1	2.15	0.45
2:B:424:PHE:C	2:B:426:GLU:H	2.23	0.45
2:B:165:LEU:O	2:B:168:ILE:HG23	2.17	0.45
2:B:172:ILE:CG1	2:B:252:LEU:HG	2.47	0.45
1:A:556:LEU:HD23	2:B:574:LYS:O	2.17	0.45
2:B:151:PHE:HE2	2:B:166:THR:OG1	2.00	0.45
1:A:497:LEU:HD11	1:A:501:GLU:HG2	1.98	0.45
1:A:165:LEU:O	1:A:169:MET:HG3	2.17	0.45
1:A:107:PHE:HB2	2:B:232:VAL:HG21	1.99	0.45
1:A:400:THR:HA	1:A:403:VAL:HG22	1.98	0.45
1:A:444:PHE:HE1	1:A:493:ARG:HG2	1.81	0.45
1:A:206:ARG:O	1:A:206:ARG:HD3	2.17	0.44
2:B:172:ILE:HD11	2:B:252:LEU:CD1	2.47	0.44
2:B:468:LEU:HD12	2:B:468:LEU:C	2.42	0.44
1:A:121:HIS:CG	1:A:336:GLU:HB3	2.53	0.44
1:A:492:GLU:HB2	2:B:114:ARG:CD	2.47	0.44
1:A:148:ILE:HA	1:A:152:LEU:HB2	2.00	0.44
1:A:357:ASP:H	1:A:380:SER:HB3	1.83	0.44
2:B:362:PRO:HD2	2:B:365:MET:CE	2.48	0.44
1:A:453:ASN:OD1	1:A:490:LEU:HD12	2.18	0.43
2:B:33:VAL:HG12	2:B:75:LEU:HD22	2.00	0.43
2:B:536:LEU:HD12	2:B:542:ILE:HD12	1.98	0.43
1:A:359:TRP:CE3	1:A:377:LYS:HA	2.53	0.43
2:B:252:LEU:HD13	2:B:252:LEU:O	2.18	0.43
2:B:363:GLU:HA	2:B:525:THR:OG1	2.18	0.43
1:A:59:VAL:CG2	1:A:62:GLU:HB3	2.45	0.43
1:A:140:ASP:O	1:A:143:ALA:HB3	2.19	0.43
1:A:247:PHE:O	1:A:251:VAL:HG23	2.19	0.43
1:A:282:GLU:HB3	1:A:288:VAL:HG12	2.00	0.43
1:A:562:VAL:HG21	1:A:565:ILE:CG1	2.49	0.43
2:B:549:ARG:HH12	3:C:104:LEU:CD2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ARG:HH21	2:B:387:LEU:HD13	1.84	0.43
3:C:72:ARG:HB3	3:C:79:VAL:HG23	2.01	0.43
2:B:362:PRO:HD2	2:B:365:MET:HE2	2.00	0.43
1:A:49:PHE:CZ	1:A:83:VAL:HG21	2.54	0.43
1:A:206:ARG:CG	1:A:326:ARG:HH21	2.32	0.43
1:A:250:TRP:HA	1:A:253:ILE:HG22	2.00	0.43
2:B:289:THR:O	2:B:293:LEU:HG	2.19	0.42
2:B:7:ALA:HB3	2:B:8:PRO:HD3	2.01	0.42
1:A:530:SER:O	1:A:533:GLU:HB3	2.20	0.42
2:B:319:LYS:HE3	2:B:323:ARG:HH12	1.83	0.42
2:B:369:ILE:CD1	2:B:380:LEU:HD22	2.49	0.42
1:A:353:VAL:O	1:A:353:VAL:HG23	2.20	0.41
1:A:521:LEU:HD11	1:A:540:LEU:HD23	2.01	0.41
1:A:132:ARG:CZ	1:A:136:ARG:HH22	2.34	0.41
2:B:126:LEU:HA	2:B:129:VAL:CG1	2.50	0.41
1:A:336:GLU:O	1:A:336:GLU:HG2	2.21	0.41
2:B:289:THR:HA	2:B:292:ILE:HG22	2.01	0.41
2:B:454:HIS:CE1	2:B:458:LEU:HD11	2.56	0.41
1:A:135:THR:O	1:A:135:THR:HG22	2.22	0.40
1:A:499:THR:HA	1:A:502:LYS:HE2	2.02	0.40
1:A:393:GLY:H	1:A:399:LYS:HD3	1.85	0.40
1:A:530:SER:HA	1:A:533:GLU:HB3	2.03	0.40
2:B:35:ILE:CD1	2:B:142:ARG:HG3	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	586/623 (94%)	565 (96%)	18 (3%)	3 (0%)	24 57
2	B	570/578 (99%)	555 (97%)	15 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	119/136 (88%)	116 (98%)	3 (2%)	0	100	100
All	All	1275/1337 (95%)	1236 (97%)	36 (3%)	3 (0%)	44	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
1	A	459	PRO
1	A	517	ILE

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	493/521 (95%)	492 (100%)	1 (0%)	87	87
2	B	460/464 (99%)	460 (100%)	0	100	100
3	C	96/109 (88%)	96 (100%)	0	100	100
All	All	1049/1094 (96%)	1048 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	121	HIS
1	A	315	ASN
2	B	191	GLN
2	B	419	GLN
2	B	524	GLN

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Mol	Chain	Res	Type
2	B	531	HIS
2	B	556	HIS
2	B	561	GLN
3	C	3	GLN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ATP	B	601	5	32,33,33	1.36	4 (12%)	48,52,52	1.89	10 (20%)
4	ADP	A	701	5	28,29,29	1.36	5 (17%)	43,45,45	1.83	8 (18%)

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	ATP	B	601	5	-	7/22/38/38	0/3/3/3
4	ADP	A	701	5	-	1/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	ADP	C5-C4	4.09	1.46	1.39
6	B	601	ATP	C5-C4	4.06	1.46	1.39
6	B	601	ATP	C5-N7	-3.22	1.33	1.39
4	A	701	ADP	C5-N7	-2.88	1.33	1.39
6	B	601	ATP	C4-N9	-2.49	1.32	1.37
4	A	701	ADP	C4-N9	-2.38	1.32	1.37
4	A	701	ADP	C5-C6	2.17	1.47	1.41
6	B	601	ATP	C8-N9	-2.09	1.34	1.37
4	A	701	ADP	C8-N7	2.08	1.35	1.31

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	ATP	C5-C4-N3	-5.94	118.54	126.72
4	A	701	ADP	C5-C4-N3	-5.48	119.17	126.72
6	B	601	ATP	N3-C4-N9	5.01	135.69	127.17
4	A	701	ADP	N3-C4-N9	4.49	134.81	127.17
6	B	601	ATP	C2-N3-C4	3.57	120.55	111.83
4	A	701	ADP	C2-N3-C4	3.57	120.54	111.83
4	A	701	ADP	N3-C2-N1	-3.42	123.40	128.58
6	B	601	ATP	O4'-C1'-N9	3.37	114.56	108.09
6	B	601	ATP	N3-C2-N1	-3.16	123.80	128.58
4	A	701	ADP	C4-C5-N7	-2.98	107.18	110.58
4	A	701	ADP	C4-N9-C8	2.82	108.70	105.74
6	B	601	ATP	C4'-O4'-C1'	-2.55	103.84	109.47
6	B	601	ATP	C4-C5-N7	-2.54	107.68	110.58
6	B	601	ATP	C4-N9-C8	2.45	108.31	105.74
6	B	601	ATP	O3G-PG-O2G	2.26	116.29	107.80
4	A	701	ADP	C5-N7-C8	2.25	106.98	103.45
6	B	601	ATP	O2A-PA-O1A	2.16	122.47	112.44
4	A	701	ADP	C3'-C2'-C1'	2.01	105.27	101.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	ATP	C5'-O5'-PA-O1A
6	B	601	ATP	C5'-O5'-PA-O2A
6	B	601	ATP	O4'-C4'-C5'-O5'
6	B	601	ATP	O4'-C1'-N9-C8
6	B	601	ATP	O4'-C1'-N9-C4
6	B	601	ATP	C3'-C4'-C5'-O5'
6	B	601	ATP	C5'-O5'-PA-O3A
4	A	701	ADP	O4'-C4'-C5'-O5'

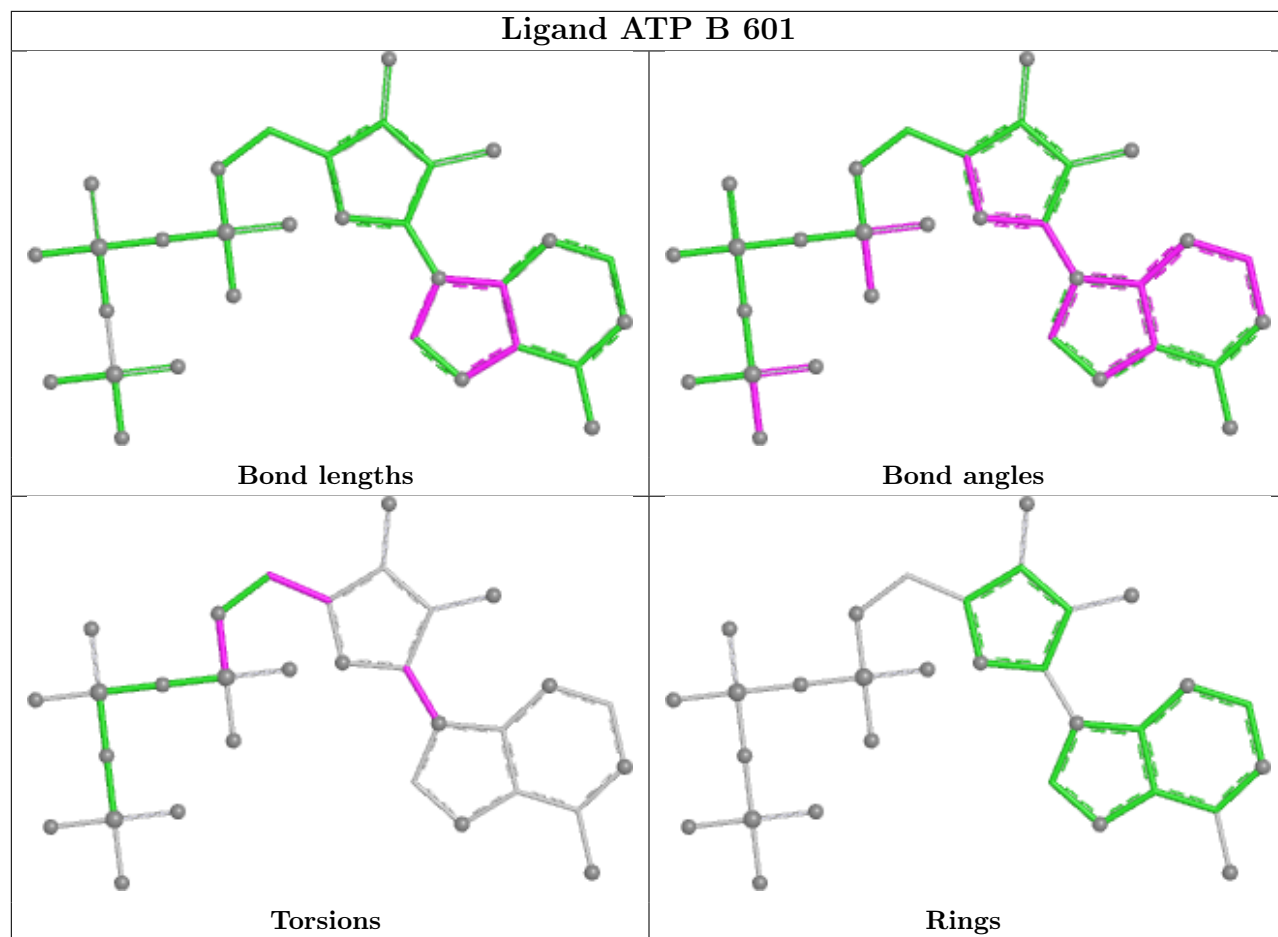
There are no ring outliers.

1 monomer is involved in 2 short contacts:

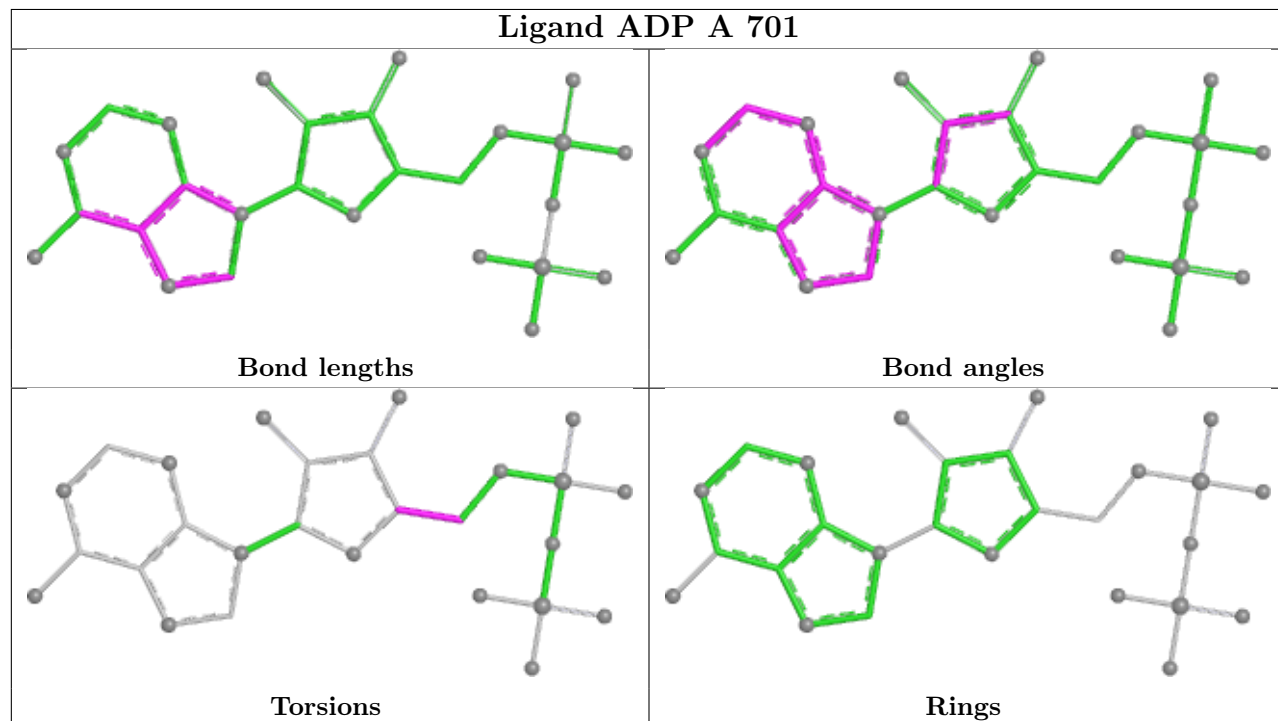
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP B 601



Ligand ADP A 701



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

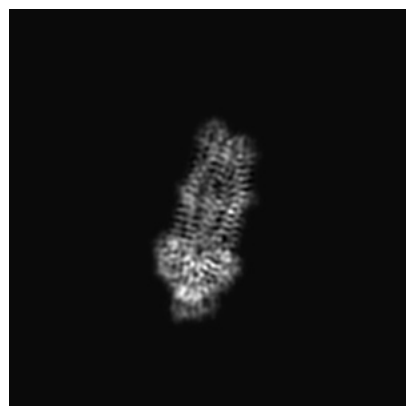
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4780. These allow visual inspection of the internal detail of the map and identification of artifacts.

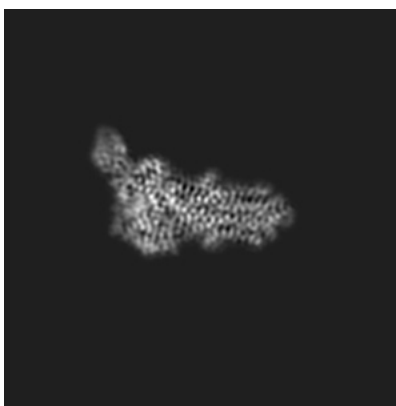
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

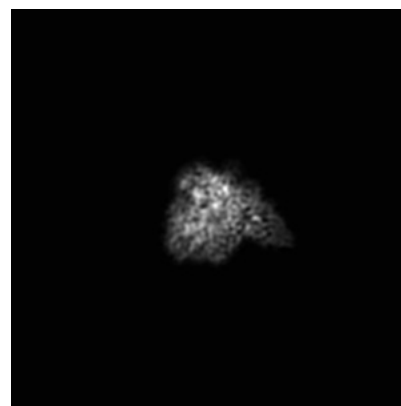
6.1.1 Primary map



X

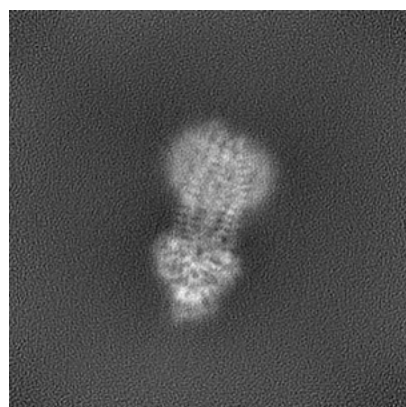


Y

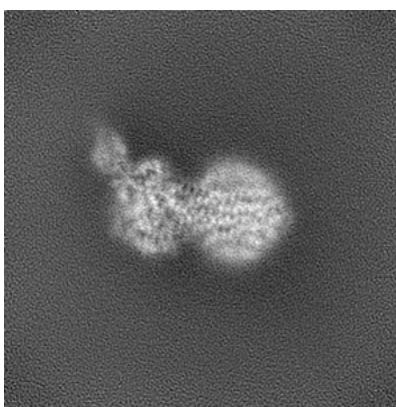


Z

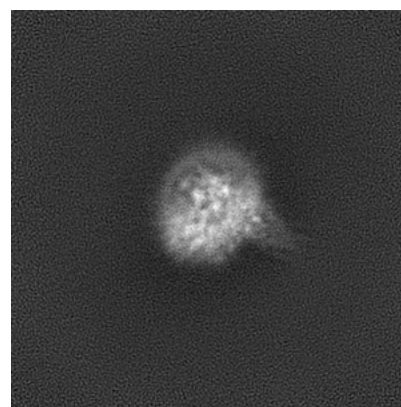
6.1.2 Raw map



X



Y

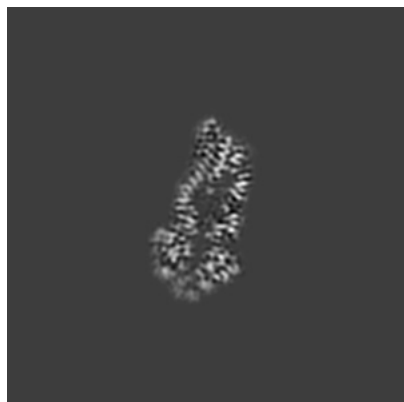


Z

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

6.2 Central slices [i](#)

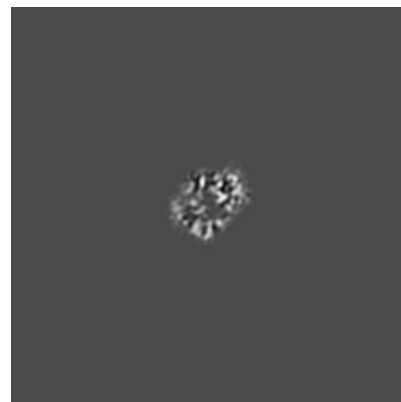
6.2.1 Primary map



X Index: 128

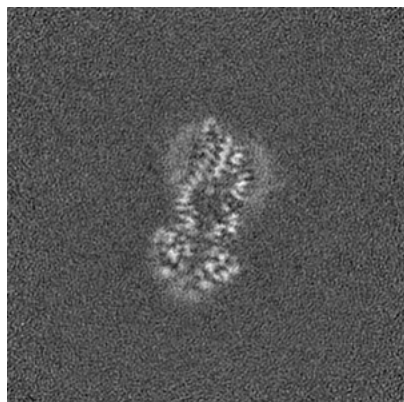


Y Index: 128

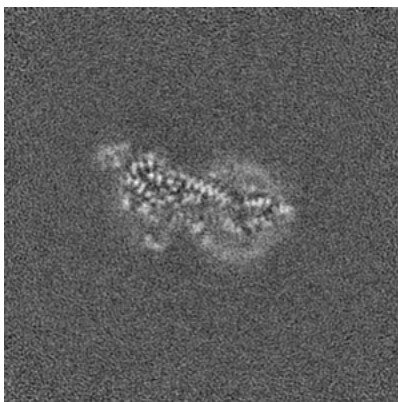


Z Index: 128

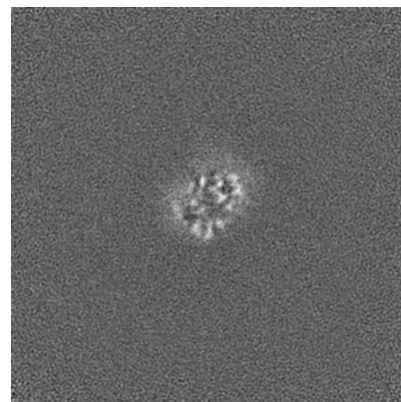
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

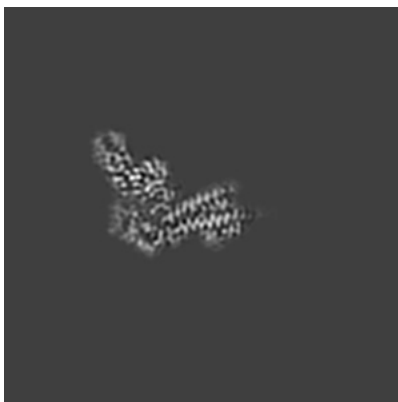
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

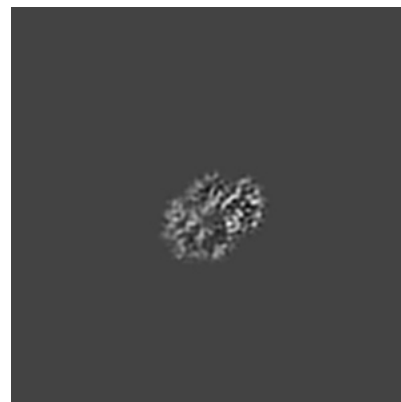
6.3.1 Primary map



X Index: 130

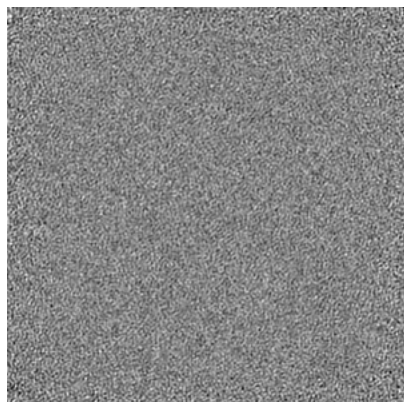


Y Index: 116

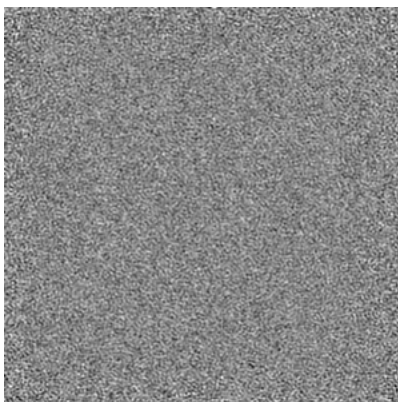


Z Index: 91

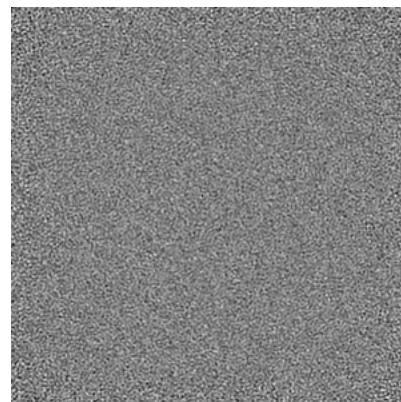
6.3.2 Raw map



X Index: 0



Y Index: 0

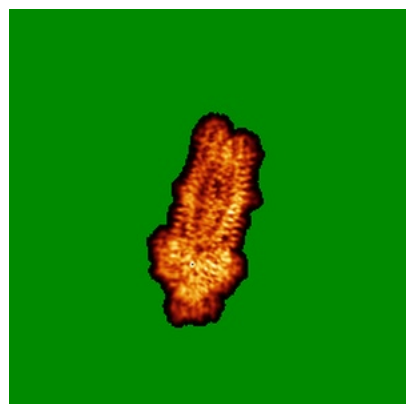


Z Index: 0

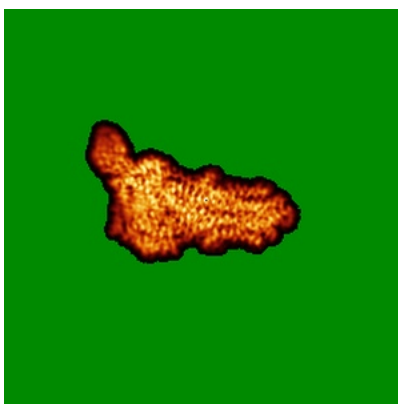
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

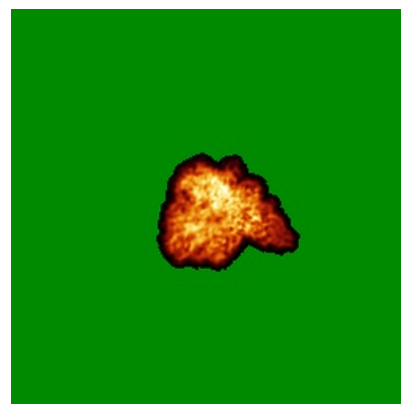
6.4.1 Primary map



X

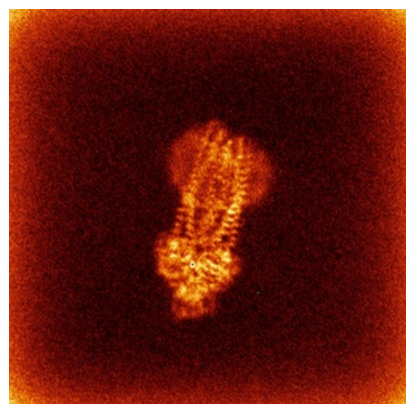


Y

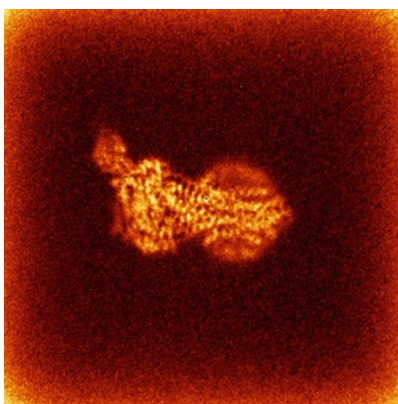


Z

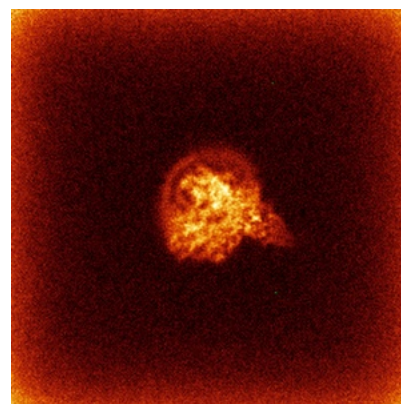
6.4.2 Raw map



X



Y

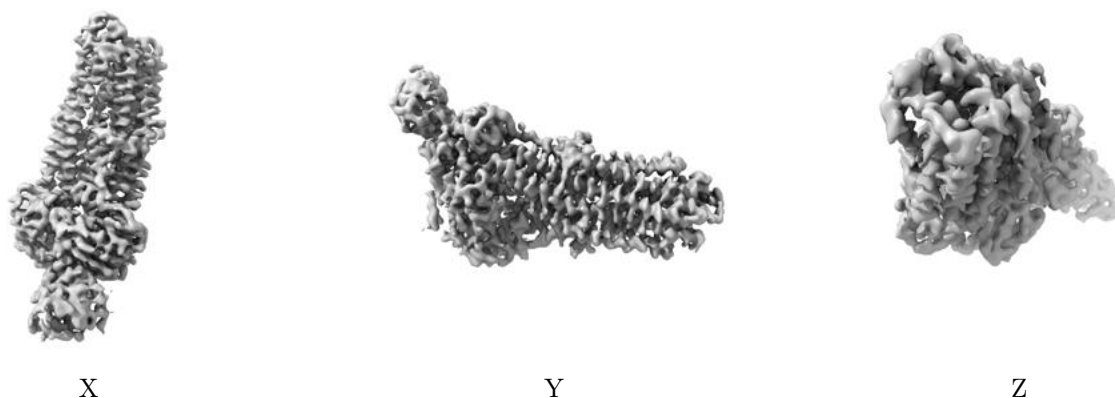


Z

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.

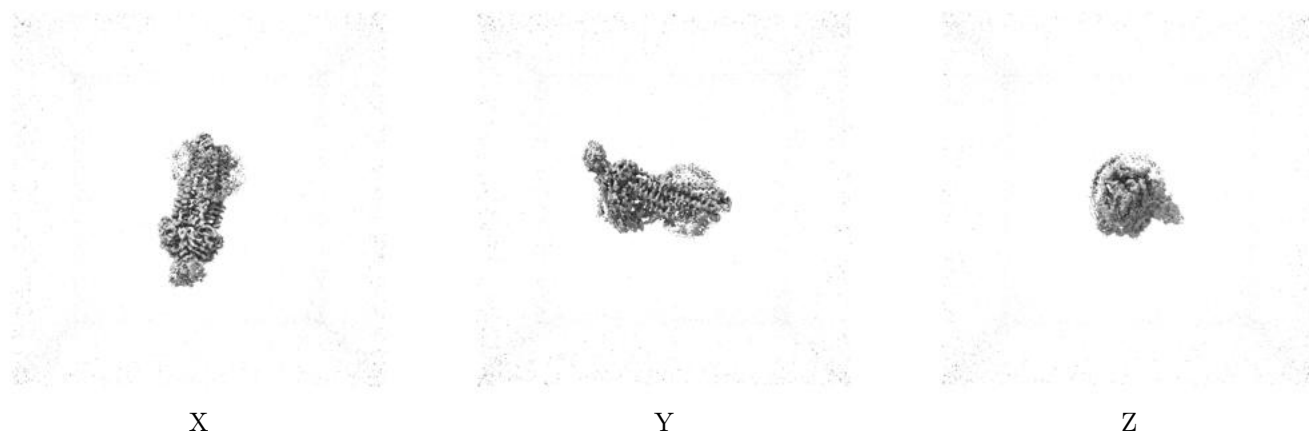
6.5 Orthogonal surface views [i](#)

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.

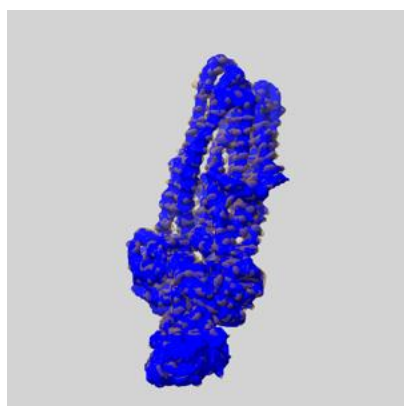
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

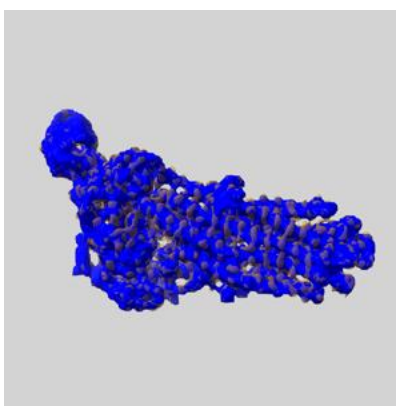
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

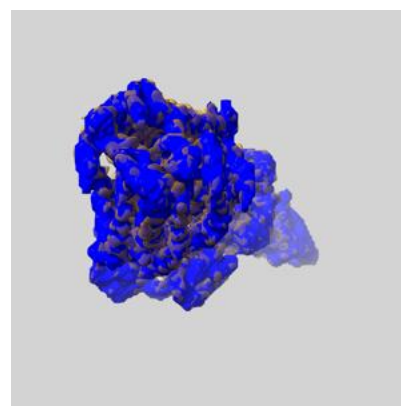
6.6.1 emd_4780_msk_1.map [i](#)



X



Y

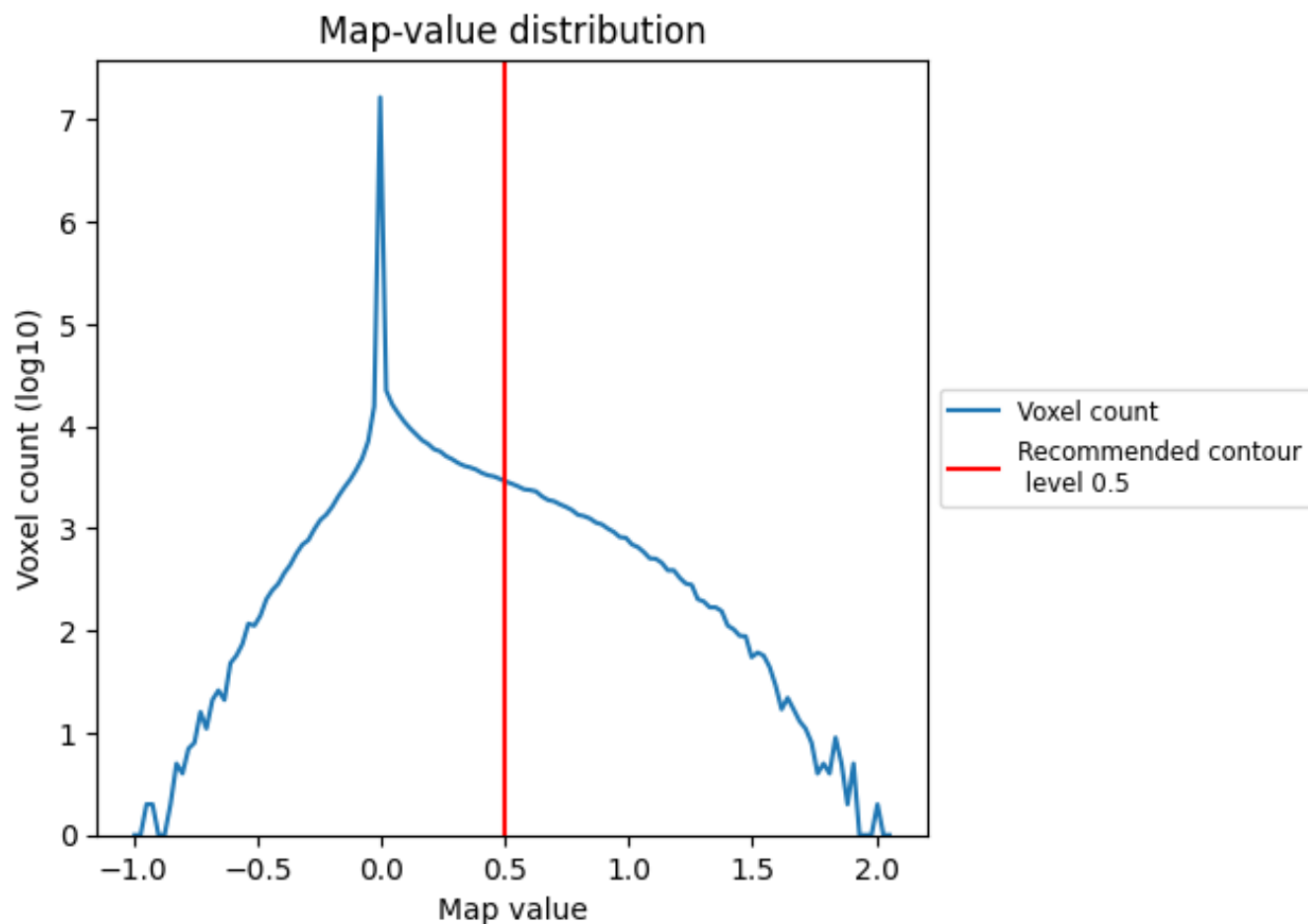


Z

7 Map analysis [i](#)

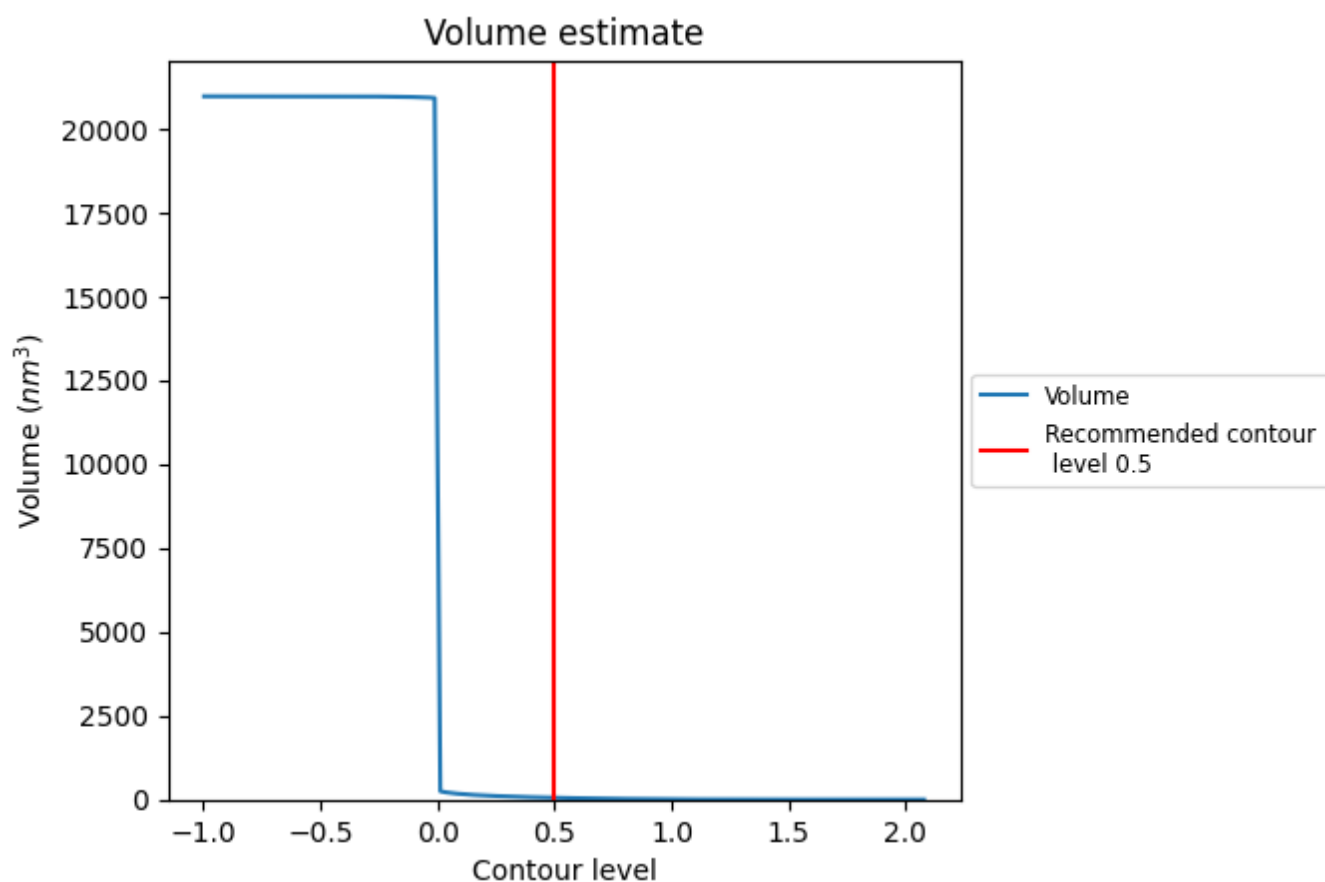
This section contains the results of statistical analysis of the map.

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.

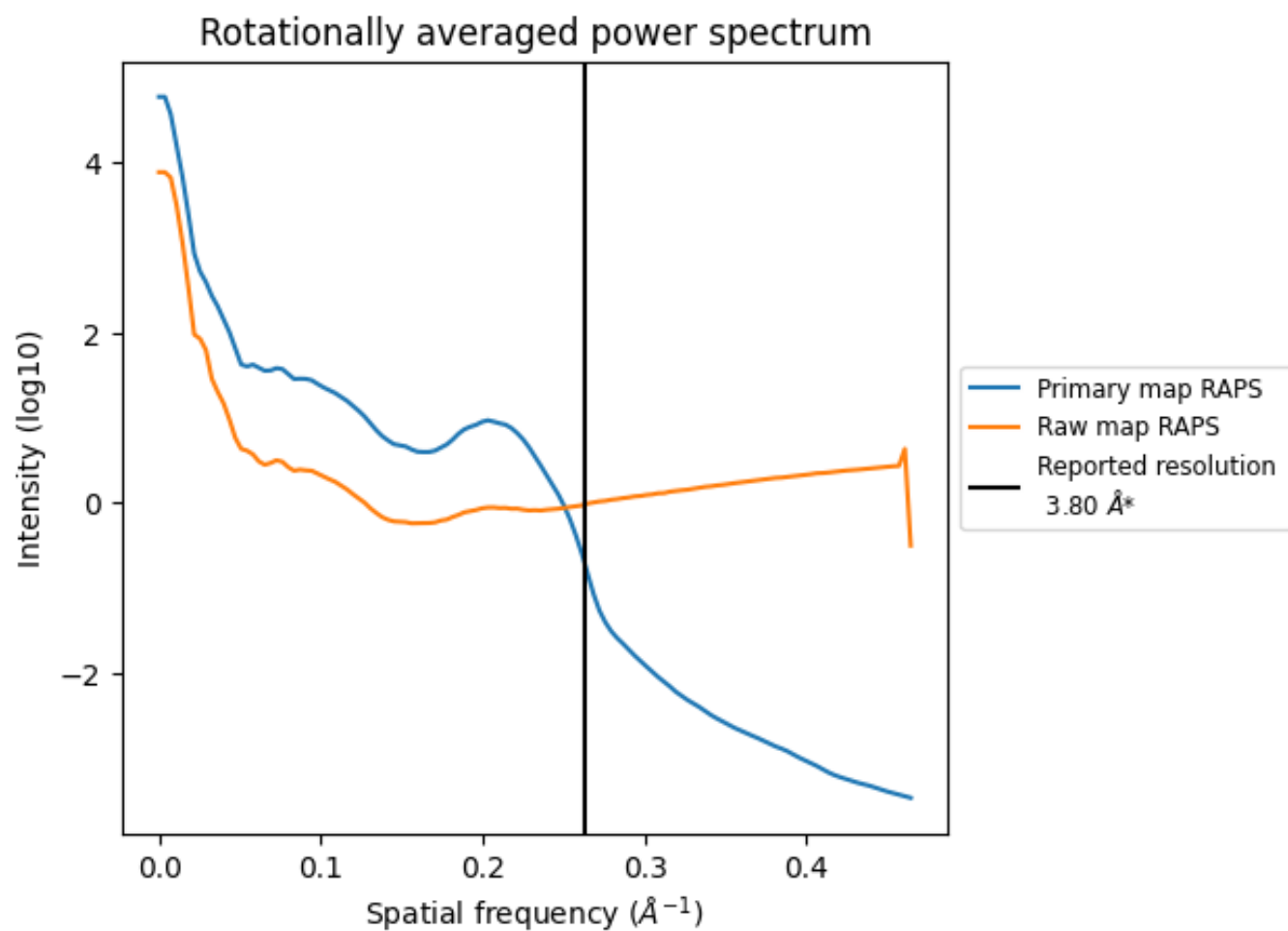
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm^3 ; this corresponds to an approximate mass of 48 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 ⓘ

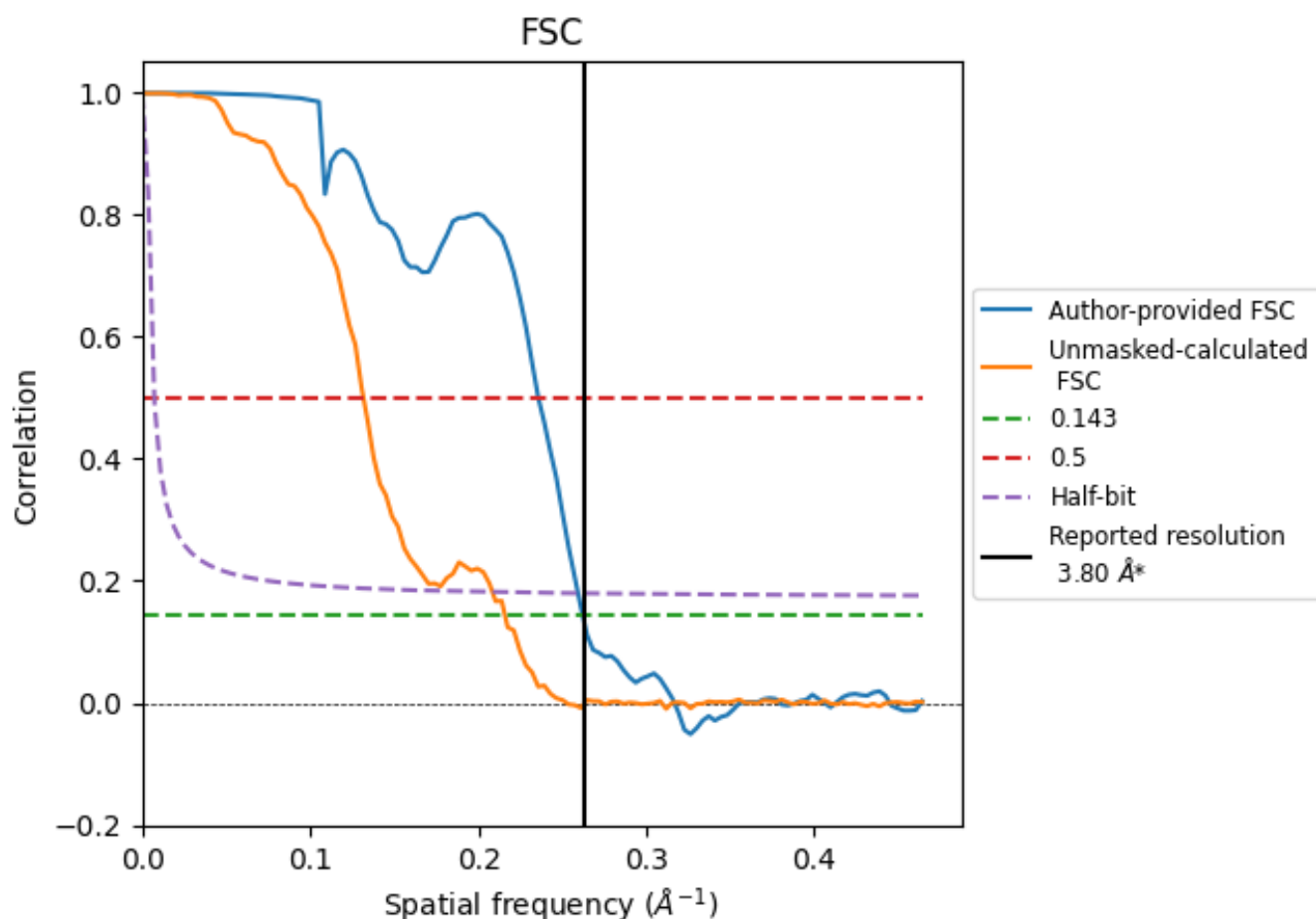


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

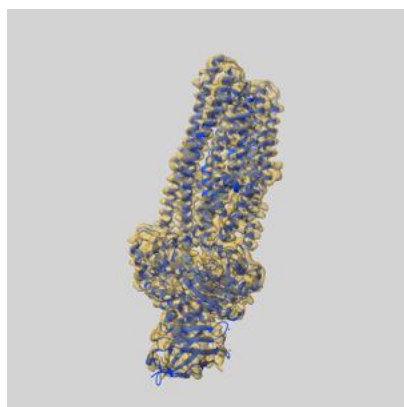
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.24	3.85
Unmasked-calculated*	4.63	7.59	4.80

*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 4.63 differs from the reported value 3.8 by more than 10 %

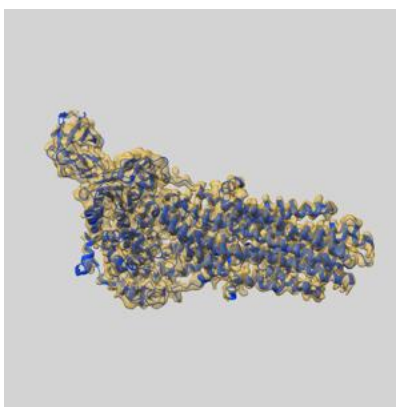
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4780 and PDB model 6RAM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

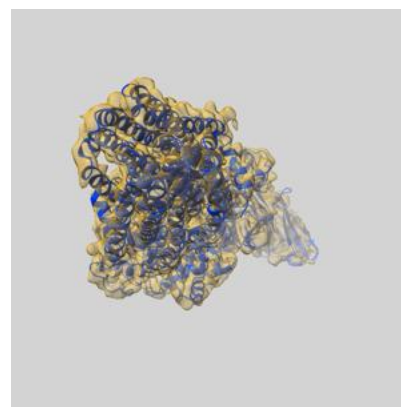
9.1 Map-model overlay [i](#)



X



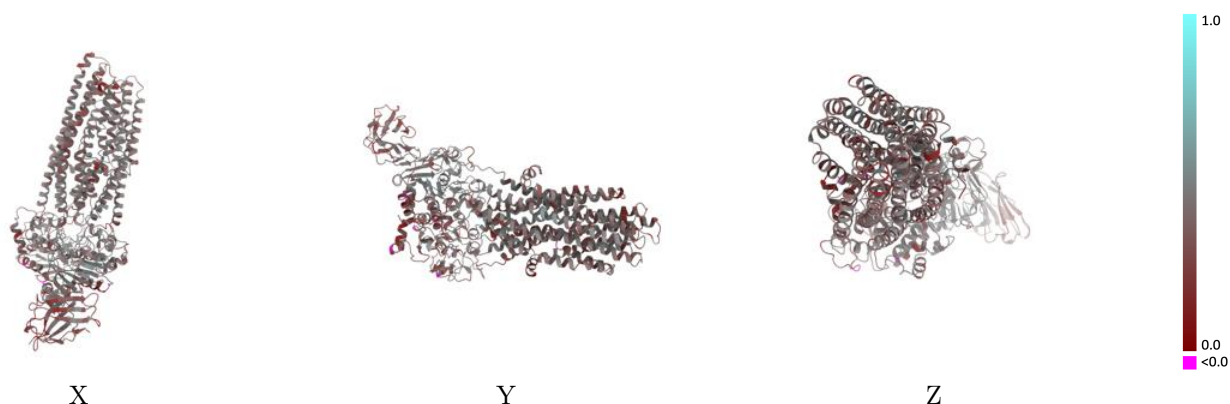
Y



Z

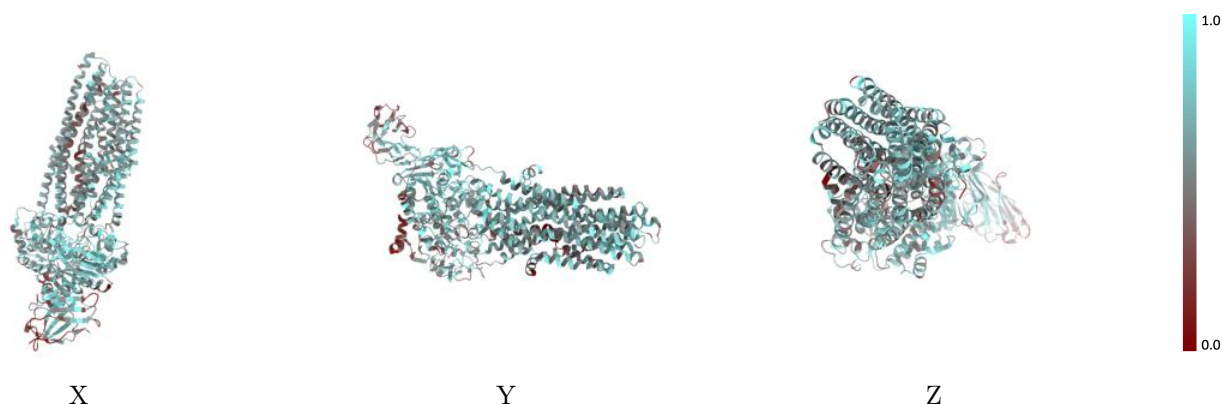
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



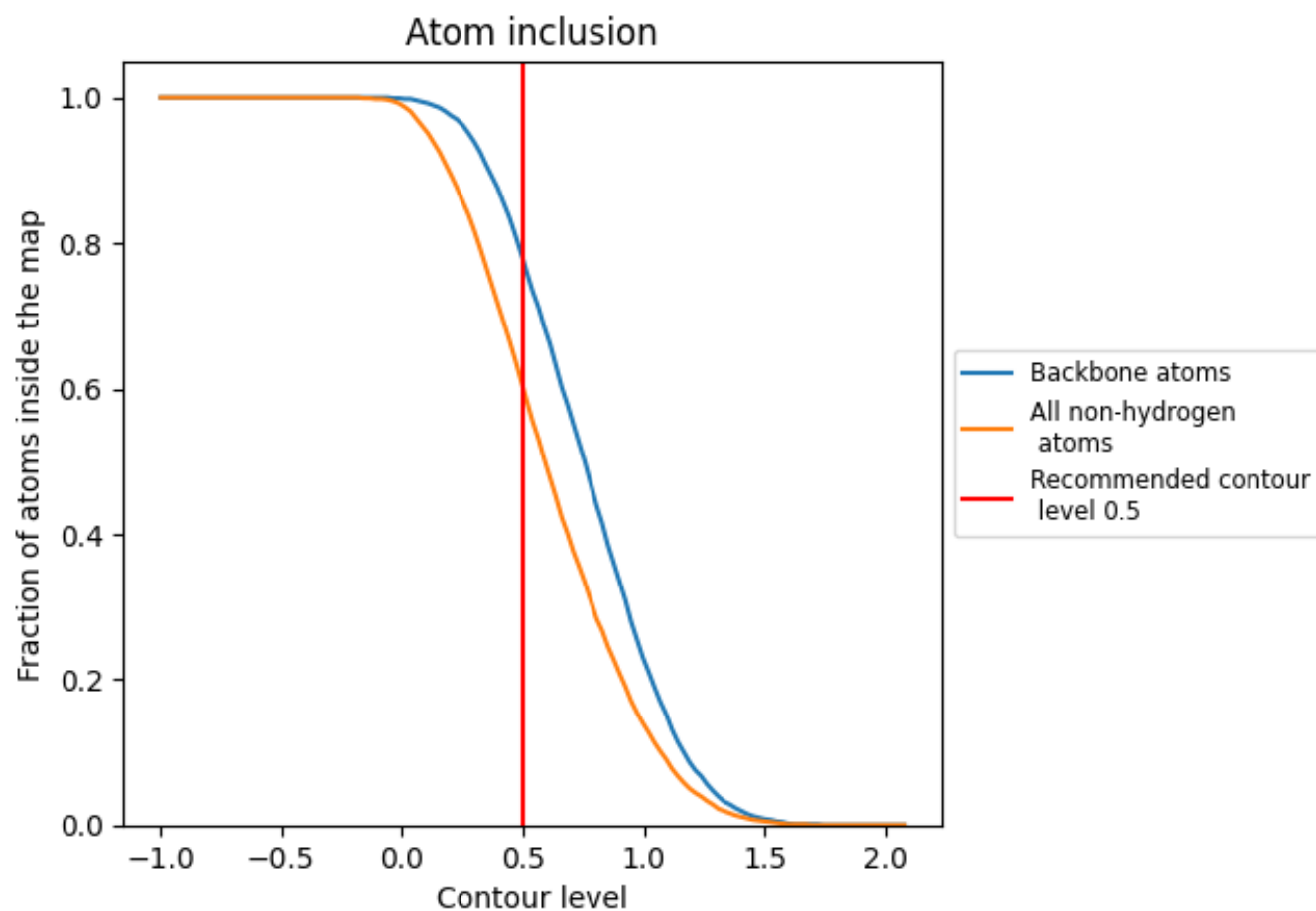
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 60% 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	0.6030	0.3780
A	0.5830	0.3660
B	0.6440	0.4000
C	0.4950	0.3280

