



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 11:55 pm BST

PDB ID : 6ZG1 / pdb_00006zg1
EMDB ID : EMD-11191
Title : SARM1 SAM1-2 domains
Authors : Sporny, M.; Guez-Haddad, J.; Khazma, T.; Yaron, A.; Dessau, M.; Mim, C.;
Isupov, M.N.; Zalk, R.; Hons, M.; Opatowsky, Y.
Deposited on : 2020-06-18
Resolution : 3.77 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

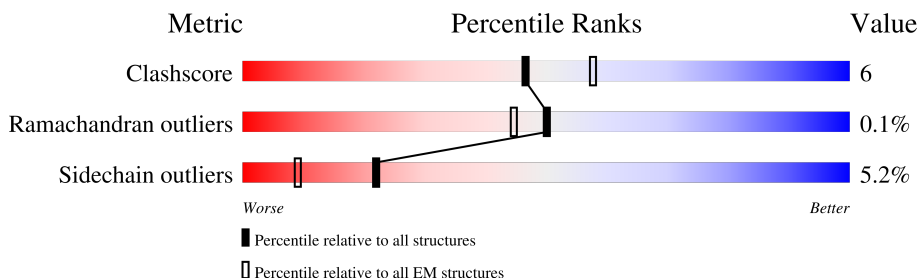
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.77 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	164	<div> <div>24%</div> <div>79%</div> <div>8%</div> <div>13%</div> </div>
1	B	164	<div> <div>27%</div> <div>78%</div> <div>17%</div> <div>•</div> </div>
1	C	164	<div> <div>23%</div> <div>80%</div> <div>9%</div> <div>•</div> <div>10%</div> </div>
1	D	164	<div> <div>27%</div> <div>73%</div> <div>16%</div> <div>•</div> <div>11%</div> </div>
1	E	164	<div> <div>22%</div> <div>80%</div> <div>9%</div> <div>•</div> <div>11%</div> </div>
1	F	164	<div> <div>21%</div> <div>79%</div> <div>7%</div> <div>•</div> <div>12%</div> </div>
1	G	164	<div> <div>21%</div> <div>77%</div> <div>12%</div> <div>12%</div> </div>
1	H	164	<div> <div>21%</div> <div>79%</div> <div>10%</div> <div>•</div> <div>11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	D	608	-	-	X	-
2	EDO	E	601	-	-	X	-
3	BME	D	603	-	-	X	-
3	BME	E	602	-	-	X	-
3	BME	H	601	-	-	X	-
4	PEG	D	602	-	-	X	-
5	PGE	B	605	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9931 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 Sterile alpha and TIR motif-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	143	Total	C	N	O	S	7	0
			1211	763	220	221	7		
1	B	157	Total	C	N	O	S	8	0
			1324	832	241	244	7		
1	C	148	Total	C	N	O	S	5	0
			1232	775	221	229	7		
1	D	146	Total	C	N	O	S	3	0
			1204	756	215	226	7		
1	E	146	Total	C	N	O	S	3	0
			1209	761	219	222	7		
1	F	144	Total	C	N	O	S	7	0
			1211	762	219	223	7		
1	G	145	Total	C	N	O	S	5	0
			1206	758	217	224	7		
1	H	146	Total	C	N	O	S	4	0
			1210	761	217	225	7		

There are 16 discrepancies between the modelled and reference sequences:

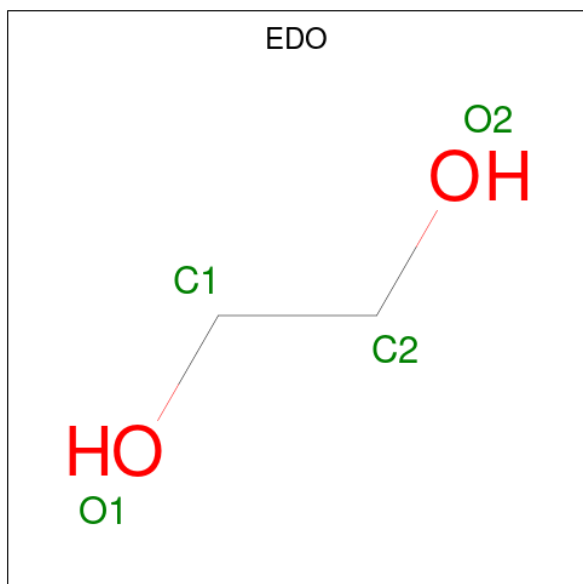
Chain	Residue	Modelled	Actual	Comment	Reference
A	385	GLY	-	expression tag	UNP Q6SZW1
A	386	SER	-	expression tag	UNP Q6SZW1
B	385	GLY	-	expression tag	UNP Q6SZW1
B	386	SER	-	expression tag	UNP Q6SZW1
C	385	GLY	-	expression tag	UNP Q6SZW1
C	386	SER	-	expression tag	UNP Q6SZW1
D	385	GLY	-	expression tag	UNP Q6SZW1
D	386	SER	-	expression tag	UNP Q6SZW1
E	385	GLY	-	expression tag	UNP Q6SZW1
E	386	SER	-	expression tag	UNP Q6SZW1
F	385	GLY	-	expression tag	UNP Q6SZW1
F	386	SER	-	expression tag	UNP Q6SZW1
G	385	GLY	-	expression tag	UNP Q6SZW1
G	386	SER	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	385	GLY	-	expression tag	UNP Q6SZW1
H	386	SER	-	expression tag	UNP Q6SZW1

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



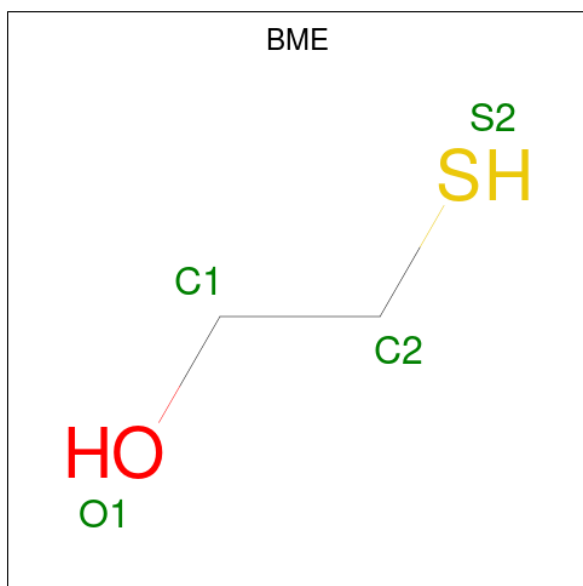
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			4	2	2	
2	A	1	Total	C	O	0
			4	2	2	
2	B	1	Total	C	O	0
			4	2	2	
2	B	1	Total	C	O	0
			4	2	2	
2	B	1	Total	C	O	0
			4	2	2	
2	C	1	Total	C	O	0
			4	2	2	
2	C	1	Total	C	O	0
			4	2	2	
2	C	1	Total	C	O	0
			4	2	2	
2	D	1	Total	C	O	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
2	D	1	Total	C	O	0
			4	2	2	
2	D	1	Total	C	O	0
			4	2	2	
2	D	1	Total	C	O	0
			4	2	2	
2	D	1	Total	C	O	0
			4	2	2	
2	D	1	Total	C	O	0
			4	2	2	
2	E	1	Total	C	O	0
			4	2	2	
2	F	1	Total	C	O	0
			4	2	2	

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



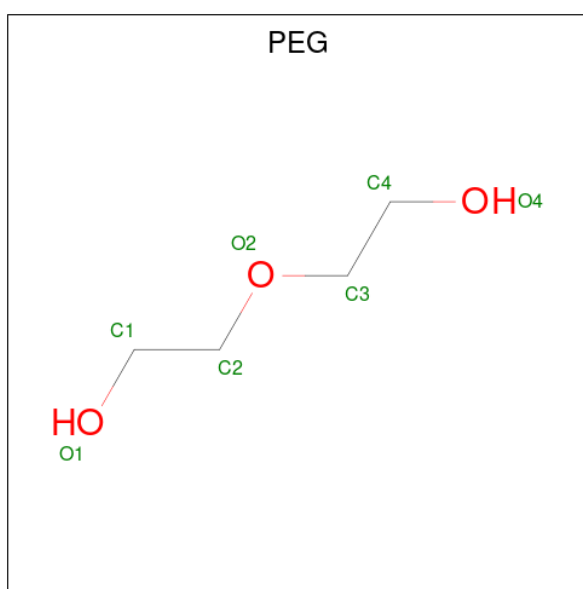
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	S	0
			4	2	1	1	
3	B	1	Total	C	O	S	0
			4	2	1	1	
3	C	1	Total	C	O	S	0
			4	2	1	1	
3	D	1	Total	C	O	S	0
			4	2	1	1	

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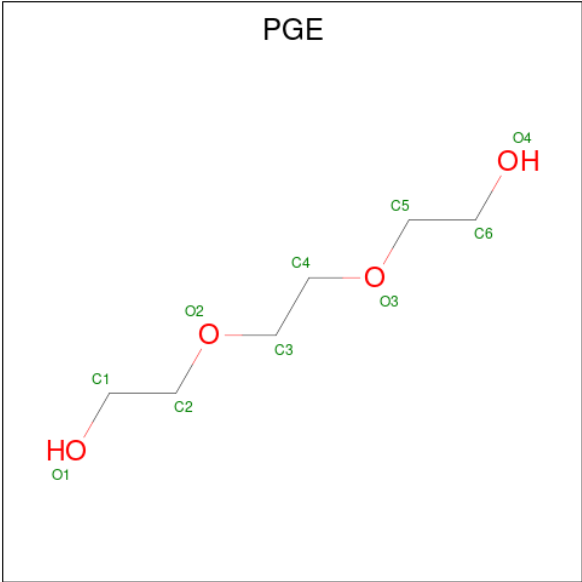
Mol	Chain	Residues	Atoms				AltConf
3	E	1	Total	C	O	S	0
			4	2	1	1	
3	F	1	Total	C	O	S	0
			4	2	1	1	
3	G	1	Total	C	O	S	0
			4	2	1	1	
3	H	1	Total	C	O	S	0
			4	2	1	1	

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			7	4	3	
4	D	1	Total	C	O	0
			7	4	3	

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

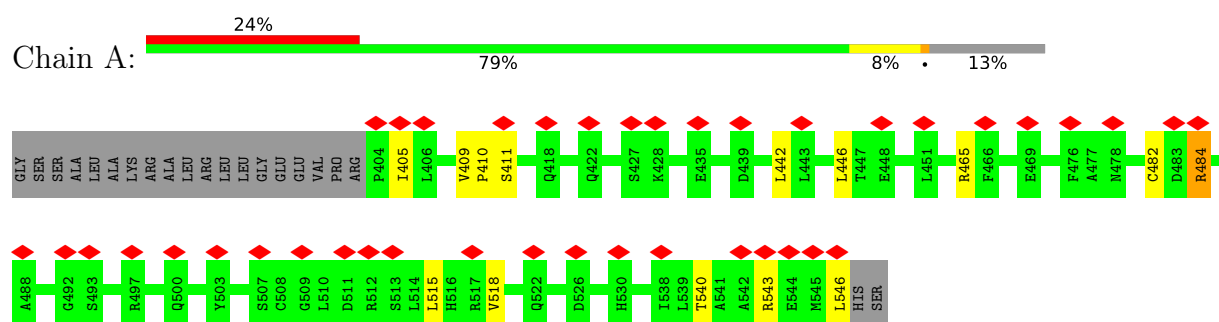


Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			10	6	4	

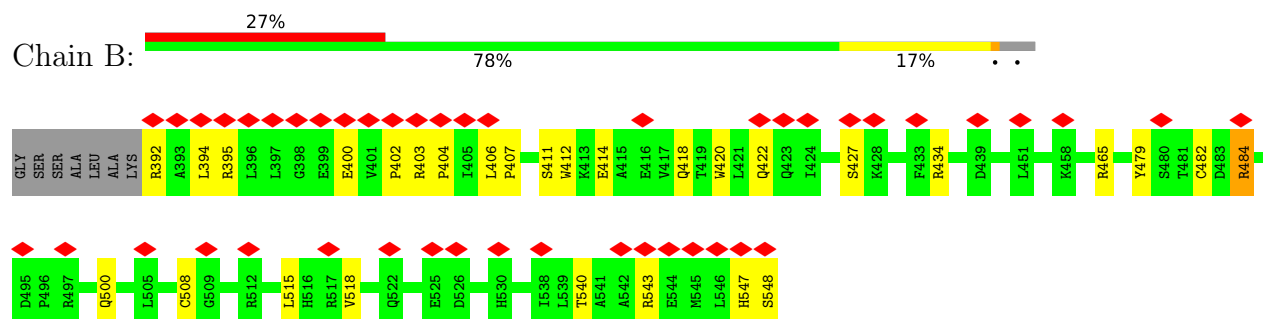
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

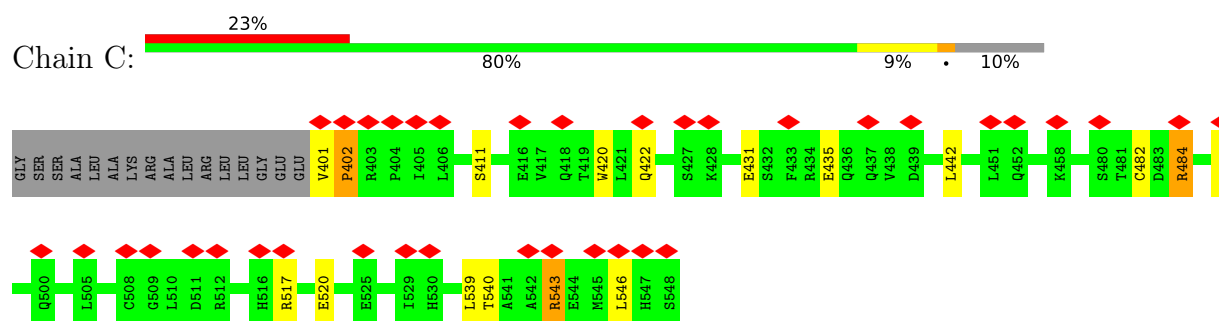
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



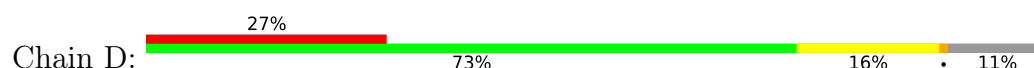
- Molecule 1: Sterile alpha and TIR motif-containing protein 1

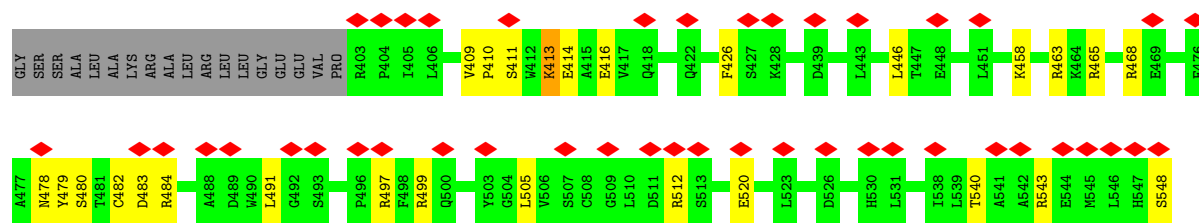


- Molecule 1: Sterile alpha and TIR motif-containing protein 1

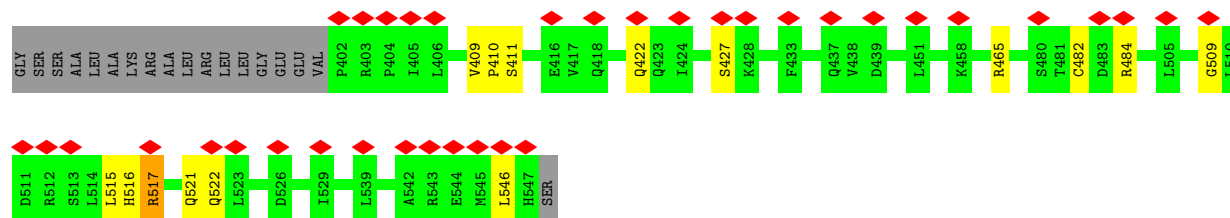
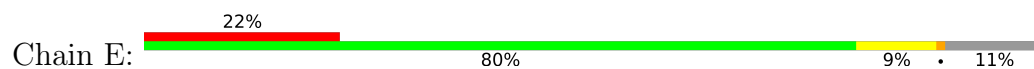


- Molecule 1: Sterile alpha and TIR motif-containing protein 1

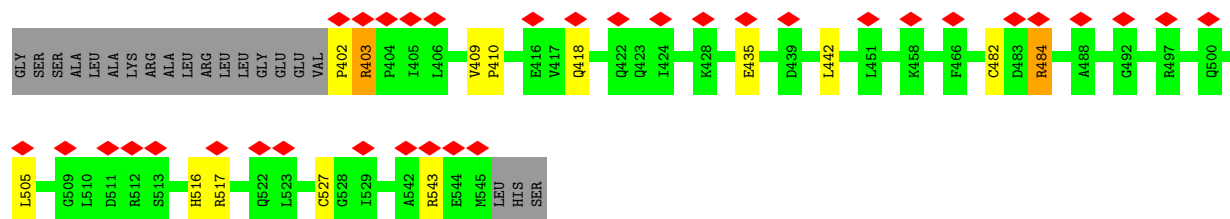
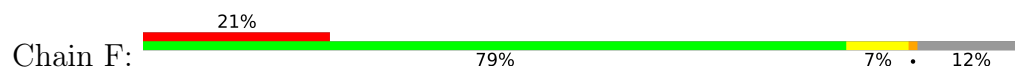




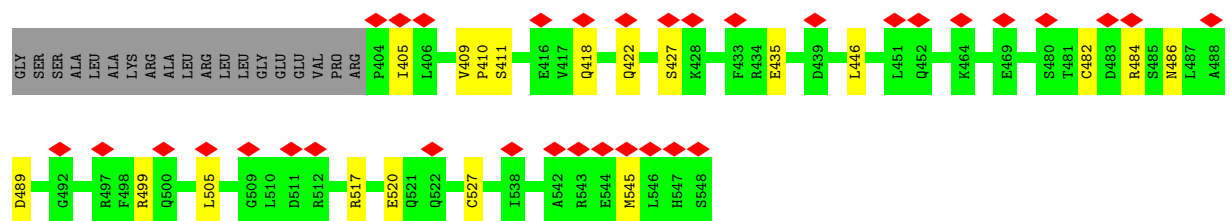
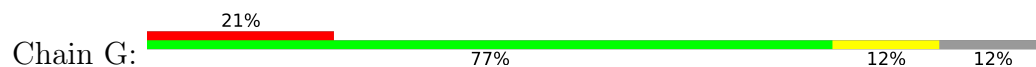
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



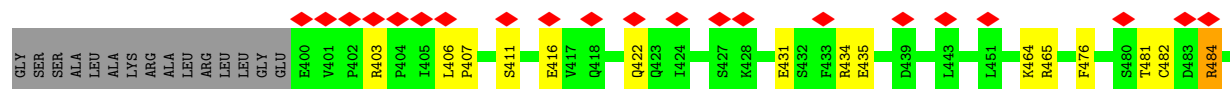
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



- Molecule 1: Sterile alpha and TIR motif-containing protein 1



- Molecule 1: Sterile alpha and TIR motif-containing protein 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43868	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.593	Depositor
Minimum map value	-0.303	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	165.0, 165.0, 165.0	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, PGE, BME

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	0.38	0/1254	0.69	0/1687
1	B	0.46	0/1372	0.80	1/1846 (0.1%)
1	C	0.46	0/1271	0.77	0/1713
1	D	0.47	0/1236	0.79	1/1665 (0.1%)
1	E	0.44	0/1242	0.72	0/1674
1	F	0.38	0/1256	0.73	1/1692 (0.1%)
1	G	0.39	0/1244	0.78	2/1674 (0.1%)
1	H	0.43	0/1245	0.72	0/1679
All	All	0.43	0/10120	0.75	5/13630 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	CYS	CB-CA-C	-7.05	96.31	110.40
1	D	414	GLU	CB-CG-CD	6.18	130.88	114.20
1	F	484	ARG	CG-CD-NE	-5.37	100.52	111.80
1	G	499[A]	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	G	499[B]	ARG	NE-CZ-NH2	-5.33	117.64	120.30

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	1211	0	1225	15	0
1	B	1324	0	1339	20	0
1	C	1232	0	1231	14	0
1	D	1204	0	1194	27	0
1	E	1209	0	1207	17	0
1	F	1211	0	1215	13	0
1	G	1206	0	1207	7	0
1	H	1210	0	1208	17	0
2	A	8	0	12	3	0
2	B	16	0	24	1	0
2	C	12	0	18	2	0
2	D	24	0	36	9	0
2	E	4	0	6	5	0
2	F	4	0	6	0	0
3	A	4	0	5	3	0
3	B	4	0	5	1	0
3	C	4	0	5	3	0
3	D	4	0	5	5	0
3	E	4	0	5	4	0
3	F	4	0	5	2	0
3	G	4	0	5	2	0
3	H	4	0	5	4	0
4	B	7	0	10	1	0
4	D	7	0	10	8	0
5	B	10	0	14	6	0
All	All	9931	0	10002	118	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 6.

All (118) 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:D:482[A]:CYS:HB3	3:D:603:BME:S2	2.06	0.96
1:B:402:PRO:HB2	5:B:605:PGE:H32	1.52	0.90
1:A:465[A]:ARG:HH12	2:A:603:EDO:H21	1.38	0.88
1:D:482[A]:CYS:CB	3:D:603:BME:S2	2.61	0.87
1:G:486:ASN:OD1	1:G:489:ASP:HB2	1.76	0.85
1:C:482[A]:CYS:HB3	3:C:601:BME:S2	2.19	0.83
1:D:465:ARG:HD2	2:D:608:EDO:H22	1.64	0.79
1:F:482[A]:CYS:HB3	3:F:602:BME:S2	2.23	0.79
1:H:521[B]:GLN:HA	1:H:521[B]:GLN:OE1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:ARG:HH12	3:D:603:BME:H11	1.51	0.76
1:B:404:PRO:HD2	5:B:605:PGE:H6	1.68	0.75
1:E:522:GLN:HG3	2:E:601:EDO:H22	1.71	0.73
1:A:482[A]:CYS:CB	3:A:602:BME:S2	2.77	0.72
1:A:482[A]:CYS:HB3	3:A:602:BME:S2	2.29	0.72
1:B:465[A]:ARG:HG2	1:C:442:LEU:HD11	1.71	0.72
1:D:413:LYS:HG3	1:D:416:GLU:OE2	1.89	0.71
1:B:482[A]:CYS:HB3	3:B:604:BME:S2	2.30	0.70
1:A:465[A]:ARG:HH12	2:A:603:EDO:C2	2.05	0.68
1:B:465[A]:ARG:CG	1:C:442:LEU:HD11	2.23	0.67
1:E:482[A]:CYS:HB3	3:E:602:BME:S2	2.33	0.67
1:C:482[A]:CYS:CB	3:C:601:BME:S2	2.80	0.67
1:D:465:ARG:CD	2:D:608:EDO:H22	2.25	0.66
1:B:412:TRP:CH2	5:B:605:PGE:H52	2.30	0.66
1:G:482[A]:CYS:HB3	3:G:601:BME:S2	2.35	0.66
1:E:522:GLN:CG	2:E:601:EDO:H22	2.25	0.65
1:A:482[A]:CYS:HB2	3:A:602:BME:S2	2.37	0.64
1:D:482[A]:CYS:HB2	3:D:603:BME:S2	2.33	0.63
1:D:463:ARG:HH12	2:D:607:EDO:H11	1.65	0.61
1:B:404:PRO:O	5:B:605:PGE:H4	2.01	0.61
1:D:479:TYR:HB2	4:D:602:PEG:C2	2.32	0.60
1:A:540:THR:O	1:A:543[B]:ARG:HG3	2.02	0.59
1:C:401:VAL:N	1:C:402:PRO:CD	2.65	0.59
1:D:497:ARG:HH12	1:E:509:GLY:HA2	1.66	0.59
1:D:465:ARG:HD2	2:D:608:EDO:C2	2.31	0.58
1:H:406:LEU:N	1:H:407:PRO:HD3	2.18	0.58
1:D:465:ARG:HH11	2:D:608:EDO:H11	1.69	0.57
1:H:482[A]:CYS:HB2	3:H:601:BME:H12	1.86	0.57
1:D:468:ARG:HH21	2:D:608:EDO:H12	1.70	0.57
1:E:482[A]:CYS:CB	3:E:602:BME:S2	2.90	0.56
1:H:482[A]:CYS:HB3	3:H:601:BME:S2	2.45	0.56
1:F:516[A]:HIS:HD2	1:F:517[A]:ARG:CZ	2.18	0.56
1:C:520:GLU:HB2	1:C:539:LEU:HD11	1.88	0.56
1:G:482[A]:CYS:CB	3:G:601:BME:S2	2.92	0.56
1:B:406:LEU:N	1:B:407:PRO:HD3	2.21	0.55
1:D:512:ARG:HH12	2:D:604:EDO:H22	1.72	0.55
1:D:480:SER:HA	4:D:602:PEG:C3	2.37	0.54
1:E:465:ARG:CG	1:F:442:LEU:HD11	2.38	0.54
1:D:468:ARG:NH2	2:D:608:EDO:H12	2.22	0.54
1:A:442:LEU:HD11	1:H:465[A]:ARG:CG	2.38	0.54
1:H:482[B]:CYS:HB3	3:H:601:BME:H12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:540:THR:HG21	1:E:517[A]:ARG:NH2	2.23	0.53
1:E:516:HIS:CE1	1:E:517[A]:ARG:HD2	2.44	0.52
1:E:482[A]:CYS:HB2	3:E:602:BME:H21	1.91	0.52
1:D:480:SER:HA	4:D:602:PEG:H31	1.90	0.52
1:C:546:LEU:HB3	2:C:602:EDO:H22	1.92	0.52
1:A:442:LEU:HD11	1:H:465[B]:ARG:HG2	1.92	0.51
1:D:479:TYR:HB2	4:D:602:PEG:H22	1.91	0.51
1:D:479:TYR:HB2	4:D:602:PEG:H21	1.92	0.51
1:B:500:GLN:HE22	4:B:603:PEG:H42	1.75	0.51
1:B:479:TYR:HB2	2:B:602:EDO:H21	1.91	0.51
1:F:516[A]:HIS:CD2	1:F:517[A]:ARG:CZ	2.94	0.50
1:B:406:LEU:N	1:B:407:PRO:CD	2.76	0.49
1:A:465[A]:ARG:NH1	2:A:603:EDO:H21	2.16	0.49
1:E:465:ARG:HG3	1:F:442:LEU:HD11	1.95	0.49
1:C:540:THR:O	1:C:543:ARG:HG2	2.12	0.49
1:H:406:LEU:N	1:H:407:PRO:CD	2.76	0.49
1:E:521:GLN:NE2	2:E:601:EDO:H21	2.28	0.48
1:E:521:GLN:HE21	2:E:601:EDO:H21	1.77	0.48
1:C:420:TRP:HE1	2:C:604:EDO:H12	1.78	0.48
1:B:402:PRO:HD2	5:B:605:PGE:H12	1.94	0.47
1:B:414:GLU:O	1:B:418:GLN:HG2	2.13	0.47
1:A:442:LEU:HD11	1:H:465[B]:ARG:CG	2.44	0.47
1:F:482[A]:CYS:CB	3:F:602:BME:S2	2.93	0.47
1:A:409:VAL:N	1:A:410:PRO:CD	2.78	0.47
1:D:499:ARG:NH2	4:D:602:PEG:H12	2.30	0.47
1:H:431:GLU:HG3	1:H:434:ARG:HH22	1.80	0.46
1:B:515:LEU:O	1:B:518:VAL:HG12	2.14	0.46
1:C:484:ARG:HD3	1:C:484:ARG:HA	1.63	0.46
1:H:406:LEU:HA	1:H:476:PHE:O	2.16	0.46
1:H:521[B]:GLN:OE1	1:H:521[B]:GLN:CA	2.57	0.46
1:F:516[A]:HIS:CD2	1:F:517[A]:ARG:NH2	2.84	0.46
1:D:540:THR:HG21	1:E:517[A]:ARG:HH22	1.81	0.45
1:F:403:ARG:H	1:F:403:ARG:CD	2.29	0.45
1:C:401:VAL:N	1:C:402:PRO:HD2	2.31	0.45
1:E:484:ARG:HD3	1:E:484:ARG:HA	1.64	0.45
1:G:409:VAL:N	1:G:410:PRO:CD	2.80	0.44
1:H:481:THR:O	1:H:484:ARG:NH1	2.50	0.44
1:F:403:ARG:H	1:F:403:ARG:HD3	1.82	0.44
1:A:442:LEU:HD11	1:H:465[A]:ARG:HG2	2.00	0.44
1:D:426:PHE:HA	2:D:601:EDO:H11	1.98	0.44
1:F:505:LEU:HD23	1:F:527:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:ARG:CD	1:F:403:ARG:N	2.81	0.44
1:H:431:GLU:HG3	1:H:434:ARG:NH2	2.33	0.44
1:E:522:GLN:HG2	2:E:601:EDO:H22	2.00	0.44
1:C:482[A]:CYS:HB2	3:C:601:BME:S2	2.53	0.43
1:B:484:ARG:HD3	1:B:484:ARG:HA	1.78	0.43
1:B:420:TRP:HB2	5:B:605:PGE:H5	2.01	0.43
1:E:482[A]:CYS:HB2	3:E:602:BME:C2	2.48	0.43
1:H:482[A]:CYS:CB	3:H:601:BME:S2	3.03	0.43
1:B:392:ARG:HG2	1:B:394:LEU:HD12	2.00	0.43
1:D:478:ASN:HA	4:D:602:PEG:O1	2.19	0.42
1:G:505:LEU:HD23	1:G:527:CYS:SG	2.59	0.42
1:G:486:ASN:OD1	1:G:489:ASP:CB	2.60	0.42
1:D:482[A]:CYS:HB2	3:D:603:BME:C2	2.49	0.42
1:B:547:HIS:O	1:B:548:SER:HB2	2.20	0.42
1:B:465[A]:ARG:HG3	1:C:442:LEU:HD11	2.01	0.42
1:B:540:THR:O	1:B:543[B]:ARG:HG2	2.20	0.41
1:A:484:ARG:HA	1:A:484:ARG:HD3	1.73	0.41
1:H:515:LEU:HD12	1:H:515:LEU:HA	1.94	0.41
1:D:483:ASP:O	4:D:602:PEG:H42	2.20	0.41
1:F:409:VAL:N	1:F:410:PRO:CD	2.84	0.41
1:D:409:VAL:N	1:D:410:PRO:CD	2.84	0.41
1:D:491:LEU:HD11	1:D:505:LEU:HD12	2.03	0.40
1:A:515:LEU:O	1:A:518:VAL:HG12	2.22	0.40
1:E:409:VAL:N	1:E:410:PRO:CD	2.84	0.40
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.94	0.40
1:F:402:PRO:HB3	1:F:403:ARG:HD3	2.02	0.40
1:G:446:LEU:HD12	1:G:446:LEU:HA	1.94	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	148/164 (90%)	146 (99%)	2 (1%)	0	100	100
1	B	163/164 (99%)	159 (98%)	4 (2%)	0	100	100
1	C	151/164 (92%)	147 (97%)	3 (2%)	1 (1%)	19	52
1	D	147/164 (90%)	145 (99%)	2 (1%)	0	100	100
1	E	147/164 (90%)	144 (98%)	3 (2%)	0	100	100
1	F	149/164 (91%)	147 (99%)	2 (1%)	0	100	100
1	G	148/164 (90%)	145 (98%)	3 (2%)	0	100	100
1	H	148/164 (90%)	144 (97%)	4 (3%)	0	100	100
All	All	1201/1312 (92%)	1177 (98%)	23 (2%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	402	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/144 (94%)	131 (97%)	4 (3%)	36	59
1	B	148/144 (103%)	138 (93%)	10 (7%)	13	39
1	C	138/144 (96%)	130 (94%)	8 (6%)	17	43
1	D	134/144 (93%)	126 (94%)	8 (6%)	16	43
1	E	134/144 (93%)	127 (95%)	7 (5%)	19	46
1	F	136/144 (94%)	131 (96%)	5 (4%)	29	54
1	G	135/144 (94%)	124 (92%)	11 (8%)	9	33
1	H	135/144 (94%)	127 (94%)	8 (6%)	16	43
All	All	1095/1152 (95%)	1034 (94%)	61 (6%)	22	44

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	ILE
1	A	411	SER
1	A	484	ARG
1	A	546	LEU
1	B	395	ARG
1	B	400	GLU
1	B	403	ARG
1	B	411	SER
1	B	422	GLN
1	B	427[A]	SER
1	B	427[B]	SER
1	B	434[A]	ARG
1	B	434[B]	ARG
1	B	484	ARG
1	C	411[A]	SER
1	C	411[B]	SER
1	C	422	GLN
1	C	431	GLU
1	C	435	GLU
1	C	484	ARG
1	C	517	ARG
1	C	543	ARG
1	D	411	SER
1	D	413	LYS
1	D	446	LEU
1	D	458	LYS
1	D	484	ARG
1	D	520	GLU
1	D	543	ARG
1	D	548	SER
1	E	411	SER
1	E	422	GLN
1	E	427	SER
1	E	515	LEU
1	E	517[A]	ARG
1	E	517[B]	ARG
1	E	546	LEU
1	F	403	ARG
1	F	418	GLN
1	F	435	GLU
1	F	484	ARG
1	F	543	ARG
1	G	405	ILE

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Mol	Chain	Res	Type
1	G	411	SER
1	G	418	GLN
1	G	422	GLN
1	G	427[A]	SER
1	G	427[B]	SER
1	G	435	GLU
1	G	484	ARG
1	G	517	ARG
1	G	520	GLU
1	G	545	MET
1	H	403	ARG
1	H	411[A]	SER
1	H	411[B]	SER
1	H	416	GLU
1	H	422	GLN
1	H	435	GLU
1	H	464	LYS
1	H	484	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	GLN
1	B	500	GLN
1	C	418	GLN
1	D	418	GLN
1	E	500	GLN
1	E	521	GLN
1	F	423	GLN
1	G	436	GLN
1	H	423	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

28 ligands are 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	$\# Z > 2$
2	EDO	B	602	-	3,3,3	0.23	0	2,2,2	0.28	0
2	EDO	C	602	-	3,3,3	0.34	0	2,2,2	0.88	0
2	EDO	D	604	-	3,3,3	0.18	0	2,2,2	0.07	0
2	EDO	D	607	-	3,3,3	0.10	0	2,2,2	0.32	0
3	BME	A	602	1	3,3,3	0.26	0	1,2,2	0.92	0
2	EDO	B	606	-	3,3,3	0.18	0	2,2,2	0.31	0
2	EDO	C	603	-	3,3,3	0.17	0	2,2,2	0.19	0
2	EDO	A	603	-	3,3,3	0.17	0	2,2,2	0.24	0
3	BME	F	602	1	3,3,3	0.14	0	1,2,2	0.47	0
2	EDO	F	601	-	3,3,3	0.04	0	2,2,2	0.04	0
3	BME	D	603	1	3,3,3	0.25	0	1,2,2	1.60	0
2	EDO	B	607	-	3,3,3	0.08	0	2,2,2	0.25	0
2	EDO	A	601	-	3,3,3	0.06	0	2,2,2	0.27	0
3	BME	E	602	1	3,3,3	0.34	0	1,2,2	0.95	0
3	BME	C	601	1	3,3,3	0.29	0	1,2,2	0.36	0
2	EDO	D	608	-	3,3,3	0.35	0	2,2,2	0.65	0
2	EDO	D	605	-	3,3,3	0.21	0	2,2,2	0.12	0
3	BME	B	604	1	3,3,3	0.41	0	1,2,2	0.66	0
2	EDO	D	606	-	3,3,3	0.27	0	2,2,2	0.44	0
2	EDO	E	601	-	3,3,3	0.18	0	2,2,2	0.76	0
3	BME	G	601	1	3,3,3	0.24	0	1,2,2	0.63	0
3	BME	H	601	1	3,3,3	0.21	0	1,2,2	-	0
4	PEG	D	602	-	6,6,6	0.34	0	5,5,5	0.38	0
4	PEG	B	603	-	6,6,6	0.16	0	5,5,5	0.12	0
5	PGE	B	605	-	9,9,9	0.31	0	8,8,8	0.36	0
2	EDO	D	601	-	3,3,3	0.31	0	2,2,2	0.79	0
2	EDO	B	601	-	3,3,3	0.50	0	2,2,2	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	604	-	3,3,3	0.17	0	2,2,2	0.02	0

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
2	EDO	B	602	-	-	1/1/1/1	-
2	EDO	C	602	-	-	0/1/1/1	-
2	EDO	D	604	-	-	0/1/1/1	-
2	EDO	D	607	-	-	1/1/1/1	-
3	BME	A	602	1	-	0/1/1/1	-
2	EDO	B	606	-	-	1/1/1/1	-
2	EDO	C	603	-	-	0/1/1/1	-
2	EDO	A	603	-	-	1/1/1/1	-
3	BME	F	602	1	-	1/1/1/1	-
2	EDO	F	601	-	-	1/1/1/1	-
3	BME	D	603	1	-	1/1/1/1	-
2	EDO	B	607	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
3	BME	E	602	1	-	0/1/1/1	-
3	BME	C	601	1	-	1/1/1/1	-
2	EDO	D	608	-	-	1/1/1/1	-
2	EDO	D	605	-	-	1/1/1/1	-
3	BME	B	604	1	-	0/1/1/1	-
2	EDO	D	606	-	-	0/1/1/1	-
2	EDO	E	601	-	-	1/1/1/1	-
3	BME	G	601	1	-	0/1/1/1	-
3	BME	H	601	1	-	1/1/1/1	-
4	PEG	D	602	-	-	3/4/4/4	-
4	PEG	B	603	-	-	0/4/4/4	-
5	PGE	B	605	-	-	6/7/7/7	-
2	EDO	D	601	-	-	1/1/1/1	-
2	EDO	B	601	-	-	1/1/1/1	-
2	EDO	C	604	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	BME	O1-C1-C2-S2
5	B	605	PGE	O2-C3-C4-O3
2	B	606	EDO	O1-C1-C2-O2
5	B	605	PGE	C1-C2-O2-C3
4	D	602	PEG	O1-C1-C2-O2
2	D	605	EDO	O1-C1-C2-O2
2	D	607	EDO	O1-C1-C2-O2
2	E	601	EDO	O1-C1-C2-O2
3	D	603	BME	O1-C1-C2-S2
3	F	602	BME	O1-C1-C2-S2
5	B	605	PGE	O3-C5-C6-O4
2	C	604	EDO	O1-C1-C2-O2
5	B	605	PGE	O1-C1-C2-O2
5	B	605	PGE	C3-C4-O3-C5
4	D	602	PEG	O2-C3-C4-O4
2	D	608	EDO	O1-C1-C2-O2
5	B	605	PGE	C6-C5-O3-C4
2	B	602	EDO	O1-C1-C2-O2
3	H	601	BME	O1-C1-C2-S2
2	A	603	EDO	O1-C1-C2-O2
4	D	602	PEG	C1-C2-O2-C3
2	B	601	EDO	O1-C1-C2-O2
2	D	601	EDO	O1-C1-C2-O2
2	F	601	EDO	O1-C1-C2-O2

There are no ring outliers.

20 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	EDO	1	0
2	C	602	EDO	1	0
2	D	604	EDO	1	0
2	D	607	EDO	1	0
3	A	602	BME	3	0
2	A	603	EDO	3	0
3	F	602	BME	2	0
3	D	603	BME	5	0
3	E	602	BME	4	0
3	C	601	BME	3	0
2	D	608	EDO	6	0
3	B	604	BME	1	0
2	E	601	EDO	5	0
3	G	601	BME	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	601	BME	4	0
4	D	602	PEG	8	0
4	B	603	PEG	1	0
5	B	605	PGE	6	0
2	D	601	EDO	1	0
2	C	604	EDO	1	0

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.

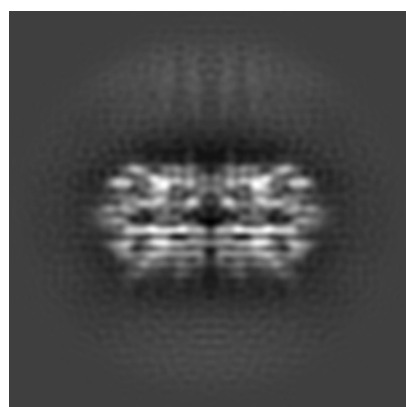
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11191. These allow visual inspection of the internal detail of the map and identification of artifacts.

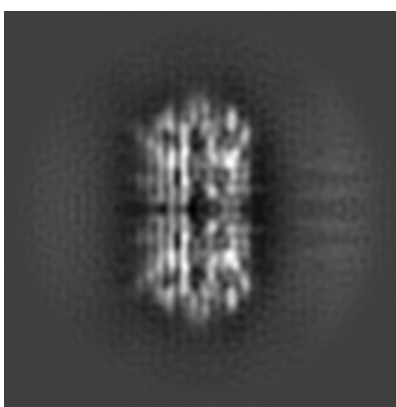
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

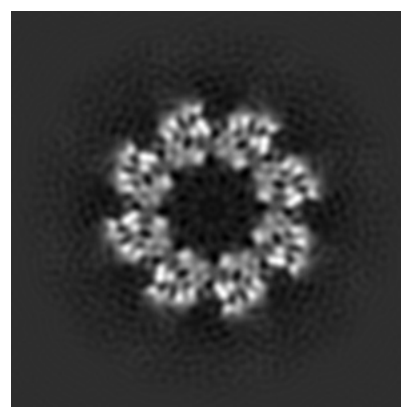
6.1.1 Primary map



X



Y

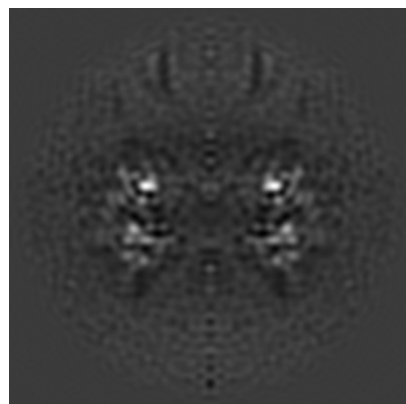


Z

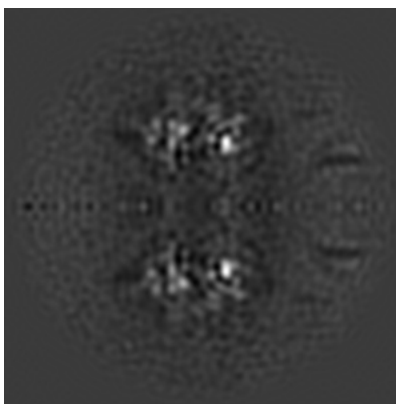
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

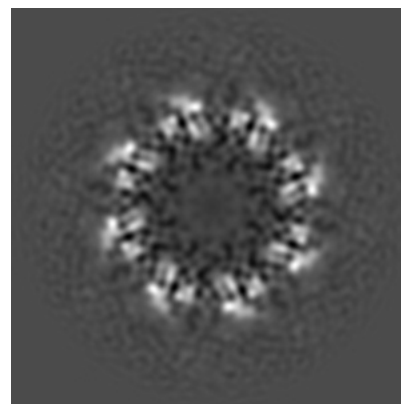
6.2.1 Primary map



X Index: 75



Y Index: 75

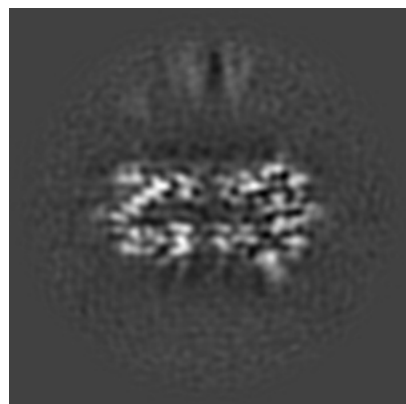


Z Index: 75

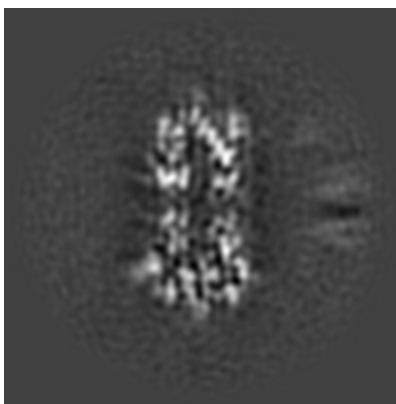
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

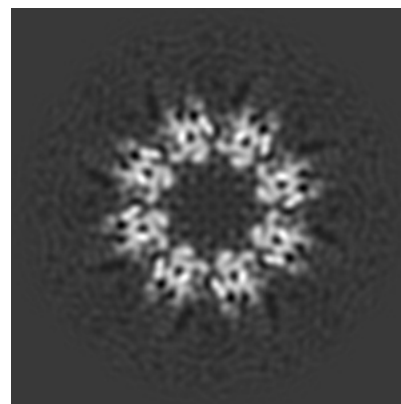
6.3.1 Primary map



X Index: 92



Y Index: 92

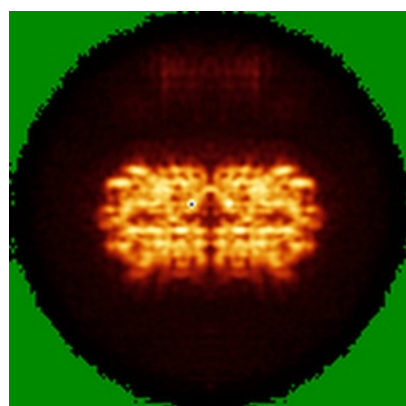


Z Index: 67

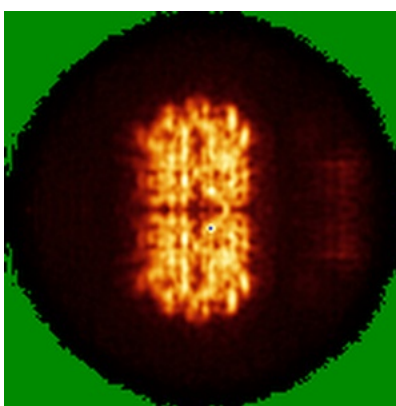
The images above show the largest variance slices of the map in three orthogonal directions.

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

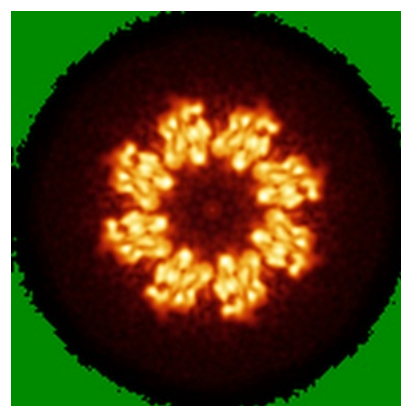
6.4.1 Primary map



X



Y

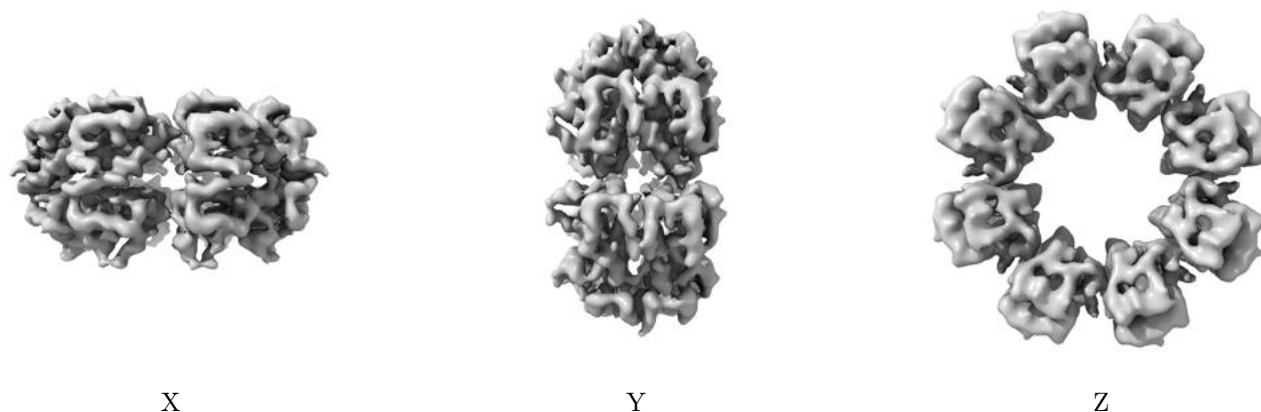


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

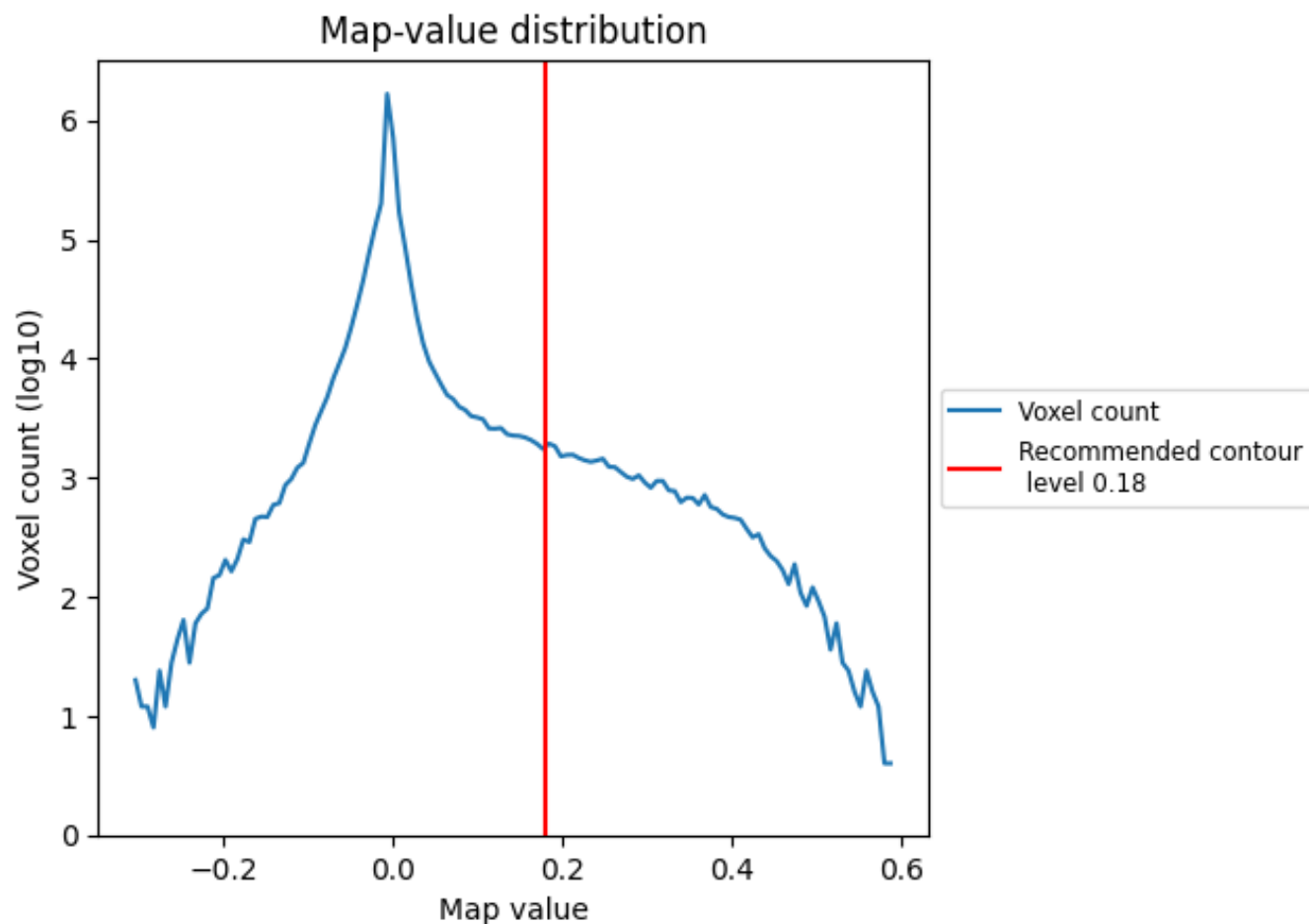
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

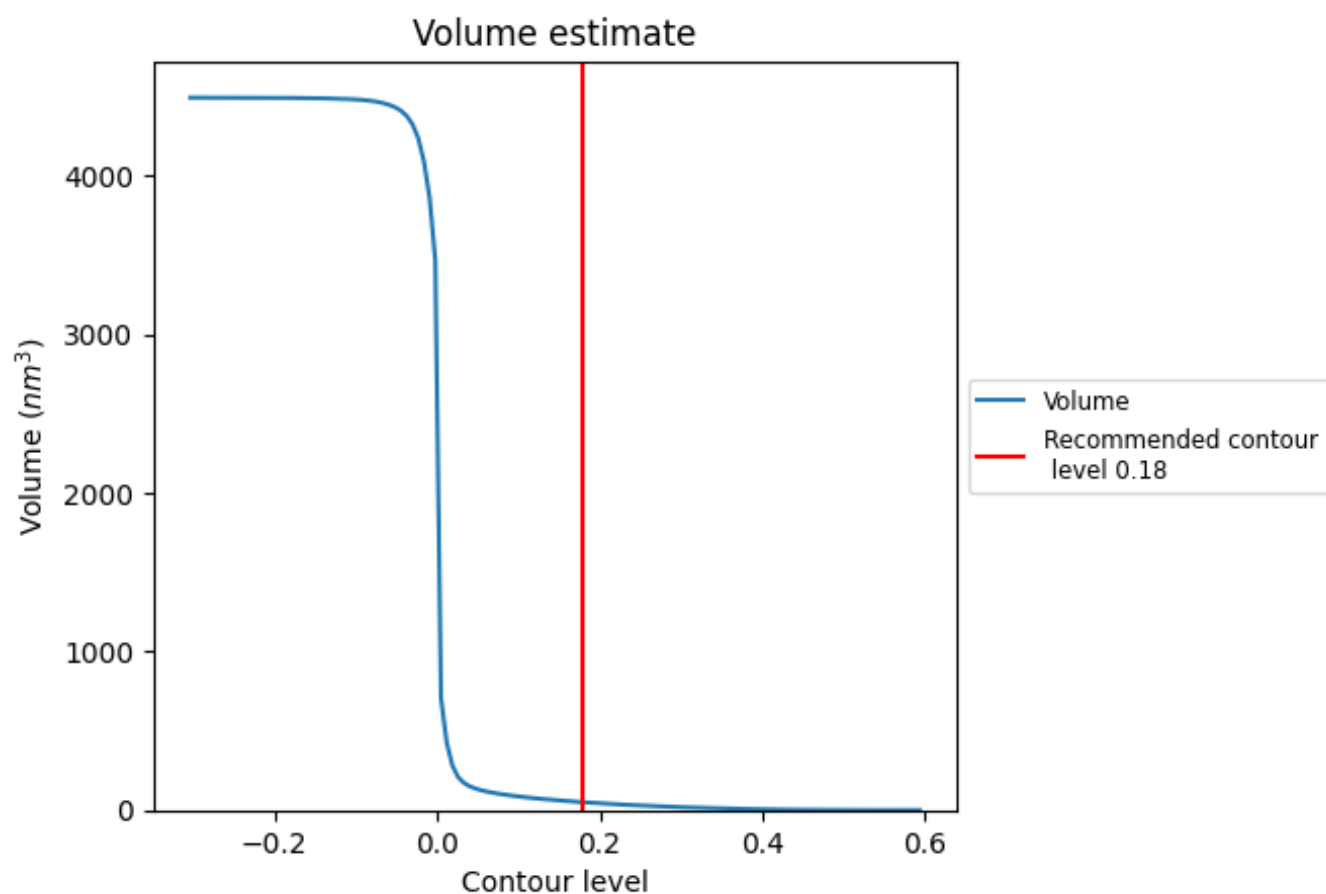
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

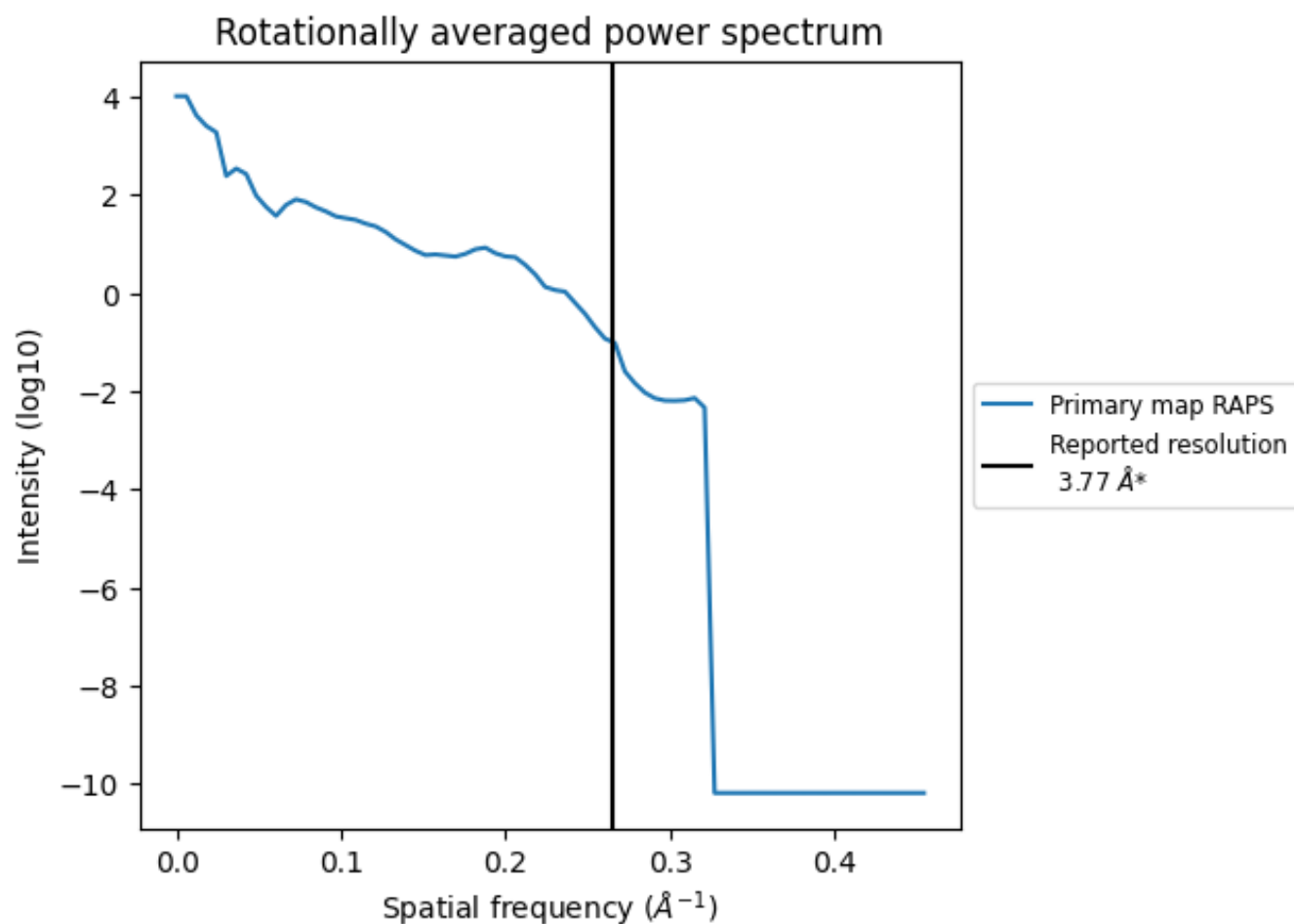
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50 nm^3 ; this corresponds to an approximate mass of 45 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 0.265 Å⁻¹

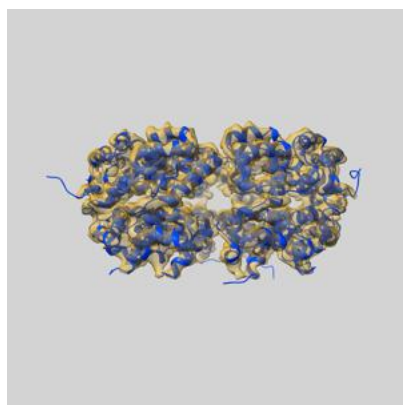
8 Fourier-Shell correlation

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

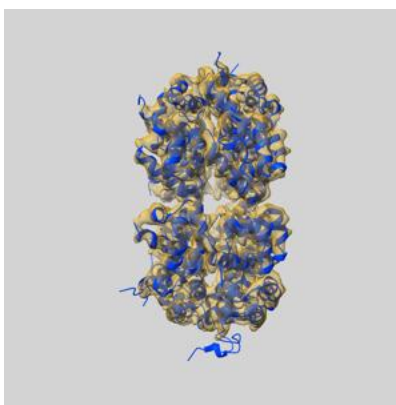
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11191 and PDB model 6ZG1. Per-residue inclusion information can be found in section [3](#) on page [9](#).

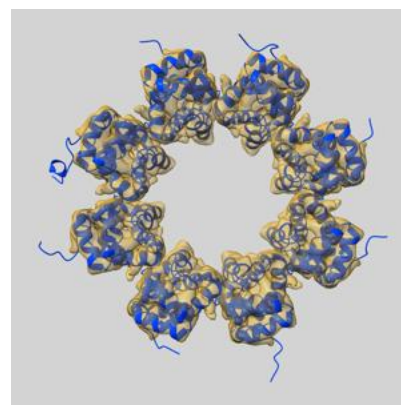
9.1 Map-model overlay [i](#)



X



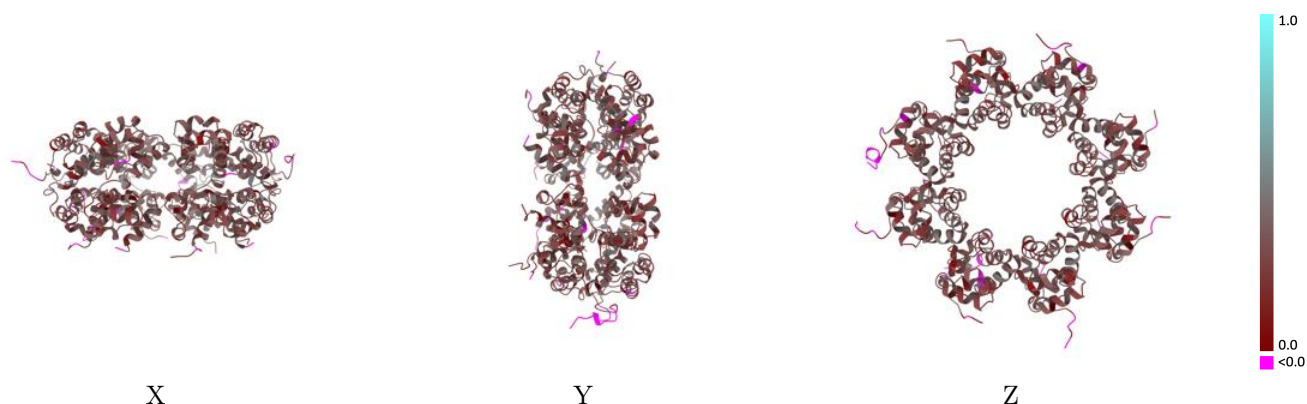
Y



Z

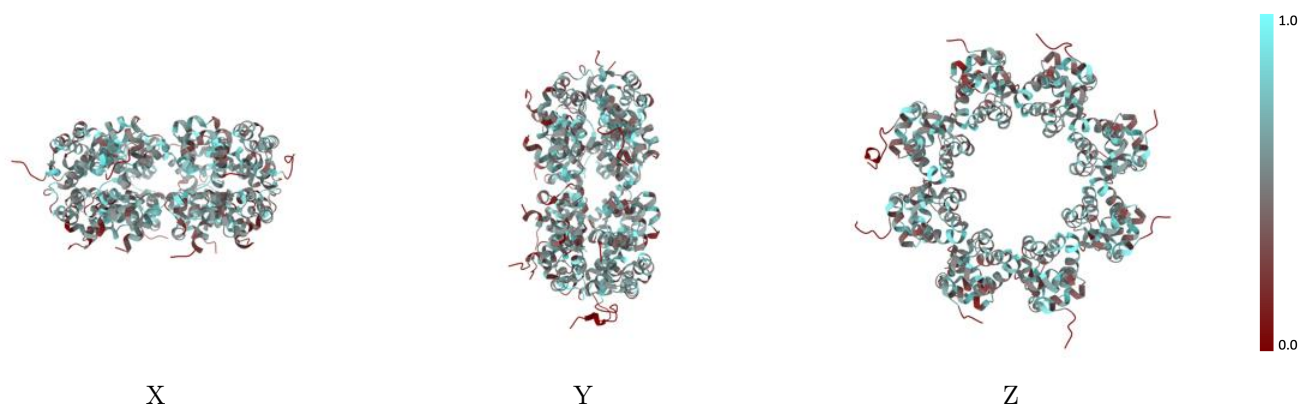
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



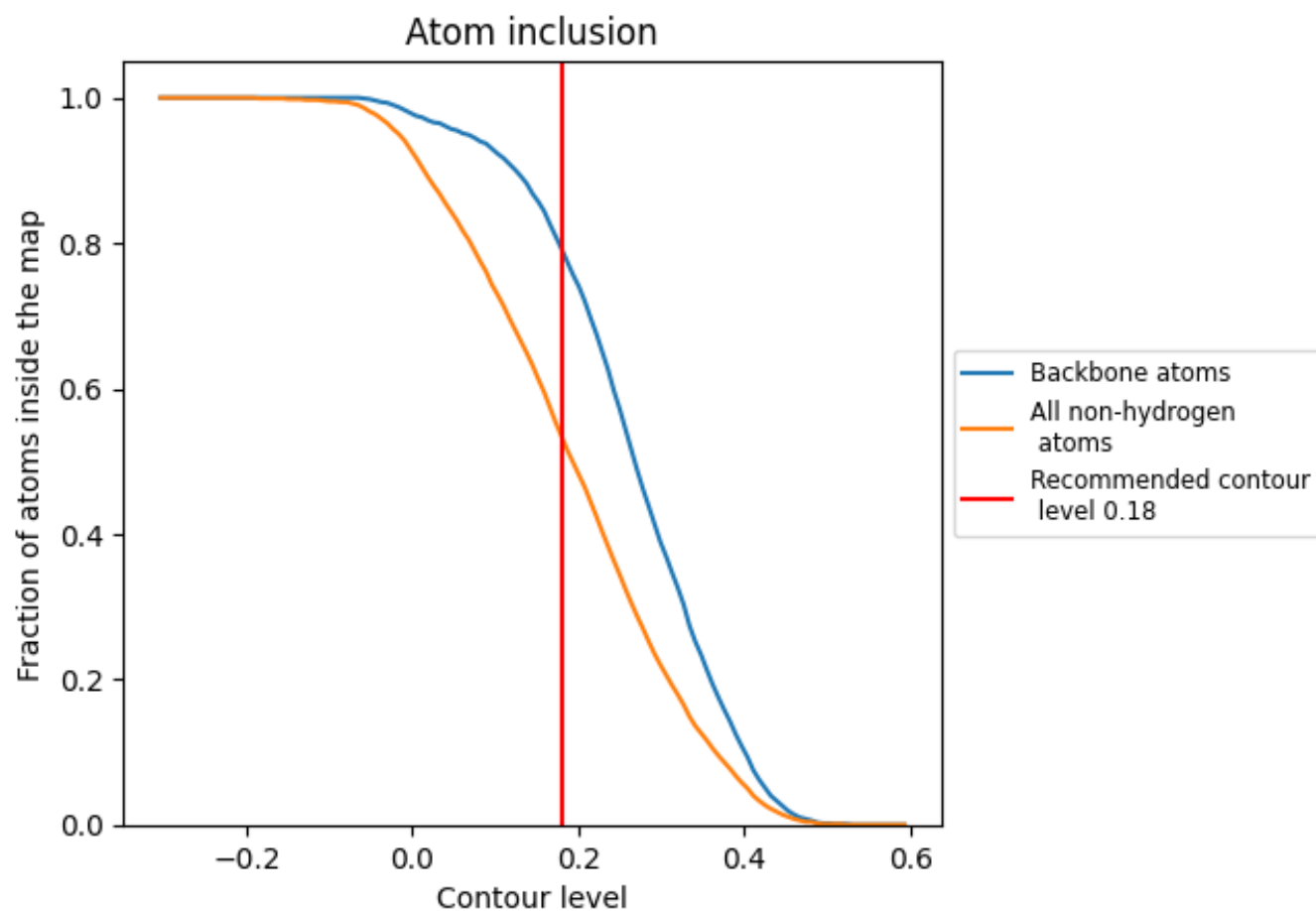
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 53% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5340	<div><div></div></div> 0.2810
A	<div><div></div></div> 0.5350	<div><div></div></div> 0.2850
B	<div><div></div></div> 0.5020	<div><div></div></div> 0.2550
C	<div><div></div></div> 0.5370	<div><div></div></div> 0.2860
D	<div><div></div></div> 0.5010	<div><div></div></div> 0.2530
E	<div><div></div></div> 0.5440	<div><div></div></div> 0.2770
F	<div><div></div></div> 0.5580	<div><div></div></div> 0.2890
G	<div><div></div></div> 0.5520	<div><div></div></div> 0.3050
H	<div><div></div></div> 0.5450	<div><div></div></div> 0.3030

1.0

0.0

<0.0