



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:01 PM UTC

PDB ID : 6SK5 / pdb_00006sk5
EMDB ID : EMD-10220
Title : Cryo-EM structure of rhinovirus-B5 complexed to antiviral OBR-5-340
Authors : Wald, J.; Goessweiner-Mohr, N.; Blaas, D.; Pasin, M.
Deposited on : 2019-08-14
Resolution : 3.60 Å(reported)
Based on initial model : 1AYM

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:

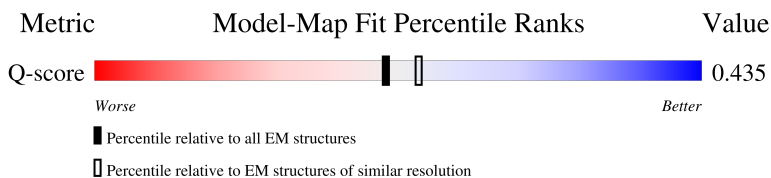
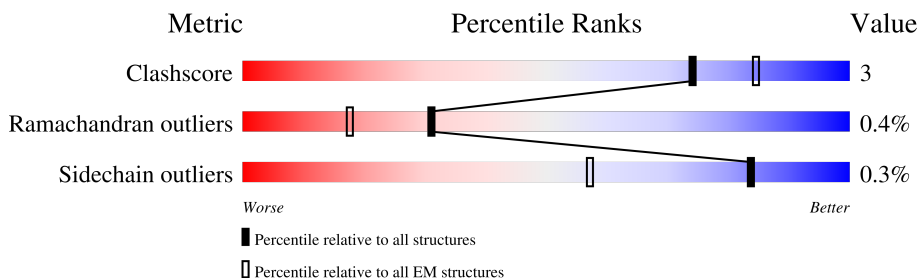
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 3.60 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	12797 (3.10 - 4.10)

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	D	69	58% 51% 42%
2	B	252	100% 93% 6%
3	A	288	95% 85% 8% 5%
4	C	230	100% 88% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12366 atoms, of which 6126 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 Rhinovirus B5 VP4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	40	Total	C	H	N	O	S	0	0
			589	188	290	47	62	2		

- Molecule 2 is a protein called Rhinovirus B5 VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	252	Total	C	H	N	O	S	0	0
			3826	1218	1899	320	375	14		

- Molecule 3 is a protein called Rhinovirus B5 VP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	273	Total	C	H	N	O	S	0	0
			4340	1383	2147	392	410	8		

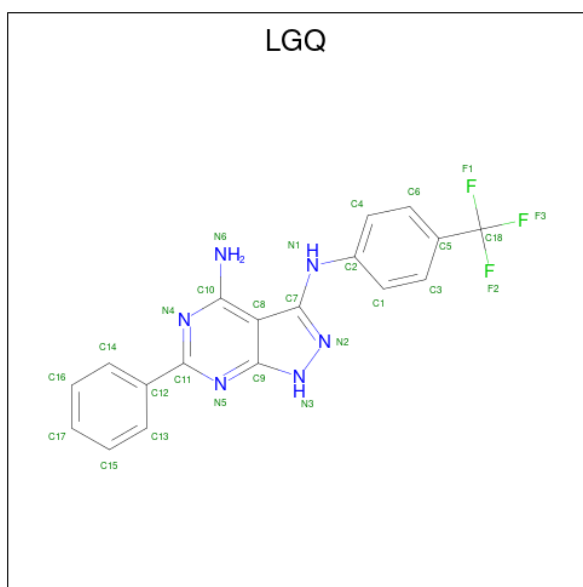
- Molecule 4 is a protein called Rhinovirus B5 VP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	230	Total	C	H	N	O	S	0	0
			3583	1154	1789	293	337	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	THR	ALA	conflict	UNP B9V433

- Molecule 5 is 6-phenyl- {N}3-[4-(trifluoromethyl)phenyl]-1 {H}-pyrazolo[3,4-d]pyrimidine-3,4-diamine (CCD ID: LGQ) (formula: C₁₈H₁₃F₃N₆) (labeled as "Ligand of Interest" by depositor).

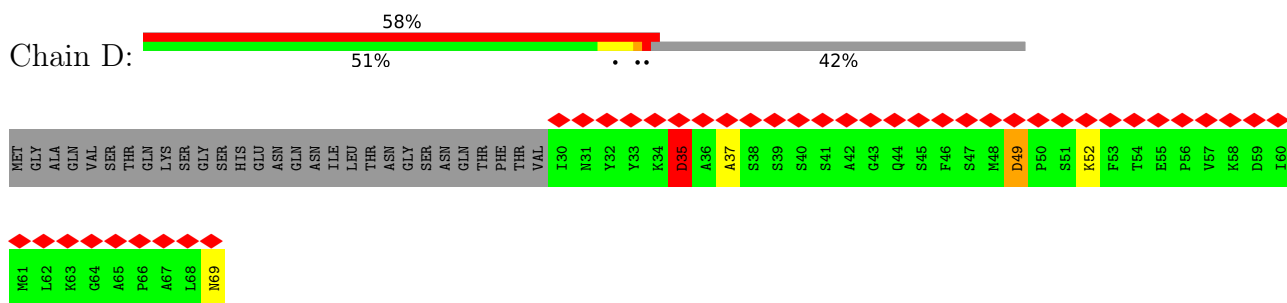


Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	H	N	
5	A	1	28	18	3	1	6	0

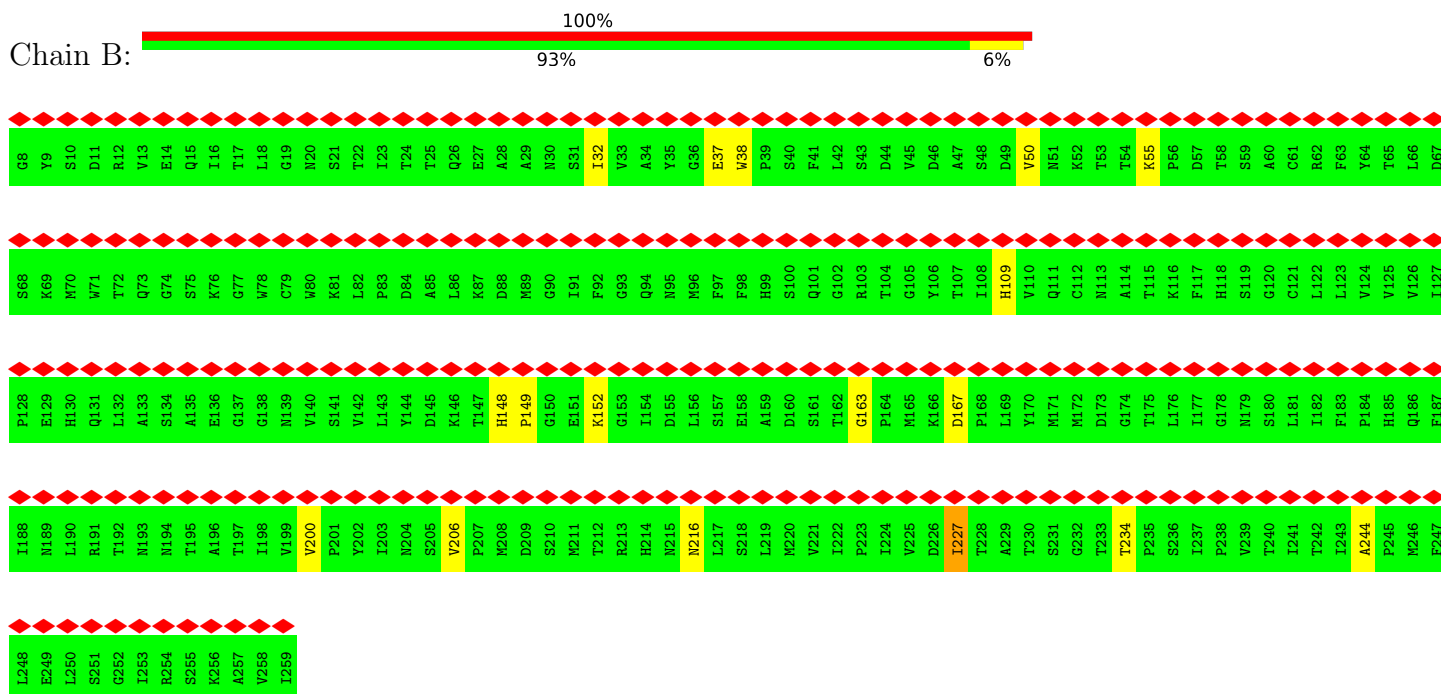
3 Residue-property plots

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.

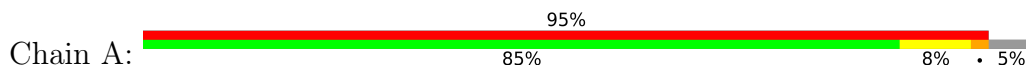
• Molecule 1: Rhinovirus B5 VP4



• Molecule 2: Rhinovirus B5 VP2

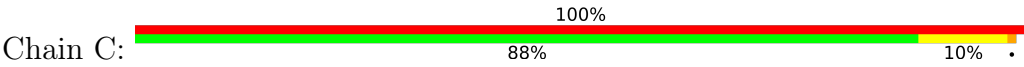


• Molecule 3: Rhinovirus B5 VP1



GLY	LEU	ASP	ASP	LEU	VAL	VAL	ILE	VAL	ASP	LYS	ALA	GLN	Q16	T17	L18	A19	S20	I21	K22	S23	D24	S25	K26	H27	T28	Q29	K30	V31	P32	S33	L34	T35	A36	N37	E38	T39	G40	A41	T42	L43	P44	T45	T46	P47	S48	D49	S50	V51	E52	T53	R54	T55	T56	L57	M58	H59	V60																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
T61	G62	S63	E64	T65	T66	L67	E68	N69	F70	L71	G72	R73		A74	A75	C76	V77	H78	V79	V80	E81	I82	V83	N84	K85	R86	L146	P87	T88	D89	T90	E91	E92	H93	R94	M95	Q96	L97	L98	F99	N100	N101	W102	K103	I104	N105	L106	S107	S108	L109	V110	Q111	L112	R113	R114	K115	L116	E117	M118	F119	T120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
Y121	V122	R123	F124	D125	S126	E127	Y128	T129	I130	I131	A132	T133	S134	S135	Q136	P137	N138	E139	A140	K141	F142	S143	S144	M145	L146	T147	I148	Q149	A150	M151	F152	I153	P154	P155	G156	A157	P158	N159	P160	K161	K162	W163	D164	D165	Y166	T167	W168	Q169	S170	A171	T172	M173	P174	S175	V176	F177	F178	M179	V180																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G181	K182	S183	A184	R185	F186	S187	V188	P189	Y190	L191	G192	I193	A194	S195	A196	Y197	N198	C199	F200	Y201	D202	G203	Y204	S205	H206	D207	N208	S209	T210	T211	P212	Y213	G214	I215	N216	V217	L218	N219	H220	M221	G222	S223	M224	A225	F226	R227	V228	V229	N230	E231	H232	D233	N234	H235	T236	T237	H238	V239	K240																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
V241	R242	V243	Y244	H245	R246	A247	K248	H249	T250	R251	A252	W253	V254	P255	R256	A257	P258	R259	A260	L261	E262	Y263	L264	H265	I266	G267	R268	T269	N270	Y271	K272	Q273	S274	P275	Q276	N277	T278	I279	K280	T281	R282	K283	T284	I285	S286	T287	Y288																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													

● Molecule 4: Rhinovirus B5 VP3



G1	L2	P3	T4	V5	L6	T7	P8	G9	S10	E11	Q12	F13	L14	T15	T16	D17	D18	R19	Q20	S21	S22	S23	A24	M25	P26	H27	Y28	E29	P30	T31	P32	L33	I34	H35	I36	P37	G38	E39	V40	K41	M42	L43	L44	E45	L46	A47	O48	V49	D50	T51	L52	I53	P54	L55	N56	M57	T58	T59	N60
T61	T62	G63	L64	G65	M66	G67	R68	I69	P70	L71	V72	Q73	N74	M75	Q76	G77	E78	Q79	V80	F81	G82	F83	R84	L85	Y86	L87	G88	D89	G90	V91	L92	K93	T94	T95	L96	L97	G98	E99	L100	C101	Q102	Y103	F104	T105	H106	W107	A108	G109	S110	L111	R112	L113	S114	F115	M116	Y117	T118	G119	P120
A121	L122	S123	S124	A125	K126	L127	L128	I129	A130	Y131	T132	P133	P134	G135	A136	Q137	G138	P139	T140	K141	R142	K143	E144	A145	M146	L147	G148	T149	H150	V151	V152	W153	D154	I155	G156	L157	Q158	S159	T160	V161	V162	L163	M164	I165	P166	W167	T168	S169	G170	V171	Q172	Y173	R174	Y175	T176	D177	P178	D179	T180
Y181	T182	S183	A184	G185	F186	V187	S188	C189	W190	Y191	Q192	T193	S194	L195	V196	L197	P198	P199	Q200	T201	Q202	Q203	T204	V205	Y206	M207	L208	G209	F210	I211	S212	A213	C214	P215	D216	F217	K218	L219	R220	L221	M222	K223	D224	T225	Q226	S227	I228	H229	Q230										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C60	Depositor
Number of particles used	46070	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	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	0.077	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0478	Depositor
Map size ($\text{\AA}$)	436.5, 436.5, 436.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.97, 0.97, 0.97	Depositor

5 Model quality

5.1 Standard geometry

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

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	D	1.09	0/305	1.08	3/409 (0.7%)
2	B	1.31	3/1971 (0.2%)	1.07	19/2684 (0.7%)
3	A	1.25	1/2252 (0.0%)	0.96	12/3064 (0.4%)
4	C	1.24	4/1842 (0.2%)	1.12	21/2518 (0.8%)
All	All	1.26	8/6370 (0.1%)	1.05	55/8675 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	B	0	1
3	A	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	227	ILE	CB-CG1	-11.17	1.31	1.53
3	A	34	LEU	CB-CG	-6.32	1.40	1.53
4	C	97	LEU	CB-CG	-6.08	1.41	1.53
2	B	32	ILE	CB-CG1	-5.98	1.41	1.53
2	B	109	HIS	CB-CG	-5.79	1.42	1.50
4	C	69	ILE	CB-CG1	-5.77	1.42	1.53
4	C	28	TYR	CB-CG	-5.21	1.40	1.51
4	C	53	ILE	CB-CG1	-5.11	1.43	1.53

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	25	MET	CA-C-N	8.09	128.85	119.47
4	C	25	MET	C-N-CA	8.09	128.85	119.47
2	B	55	LYS	CA-C-N	7.20	126.90	119.56
2	B	55	LYS	C-N-CA	7.20	126.90	119.56
4	C	119	GLY	CA-C-N	6.98	126.97	119.78
4	C	119	GLY	C-N-CA	6.98	126.97	119.78
4	C	133	PRO	CA-C-N	6.94	126.98	119.90
4	C	133	PRO	C-N-CA	6.94	126.98	119.90
2	B	206	VAL	CA-C-N	6.69	126.20	119.24
2	B	206	VAL	C-N-CA	6.69	126.20	119.24
2	B	167	ASP	CA-C-N	6.61	126.30	119.56
2	B	167	ASP	C-N-CA	6.61	126.30	119.56
4	C	29	GLU	CA-C-N	6.48	126.45	119.78
4	C	29	GLU	C-N-CA	6.48	126.45	119.78
4	C	31	THR	CA-C-N	6.36	126.33	119.78
4	C	31	THR	C-N-CA	6.36	126.33	119.78
2	B	163	GLY	CA-C-N	6.31	126.50	120.31
2	B	163	GLY	C-N-CA	6.31	126.50	120.31
2	B	200	VAL	CA-C-N	6.29	126.26	120.03
2	B	200	VAL	C-N-CA	6.29	126.26	120.03
4	C	36	ILE	CA-C-N	6.27	126.24	119.78
4	C	36	ILE	C-N-CA	6.27	126.24	119.78
2	B	38	TRP	CA-C-N	6.14	126.15	119.89
2	B	38	TRP	C-N-CA	6.14	126.15	119.89
4	C	198	PRO	CA-C-N	6.13	126.15	119.90
4	C	198	PRO	C-N-CA	6.13	126.15	119.90
1	D	49	ASP	CA-C-N	6.11	126.23	119.87
1	D	49	ASP	C-N-CA	6.11	126.23	119.87
2	B	234	THR	CA-C-N	6.06	126.03	120.03
2	B	234	THR	C-N-CA	6.06	126.03	120.03
1	D	35	ASP	CA-C-O	-6.03	114.01	120.46
3	A	257	ALA	CA-C-N	6.00	125.91	119.85
3	A	257	ALA	C-N-CA	6.00	125.91	119.85
4	C	21	SER	CA-C-N	5.91	125.85	119.76
4	C	21	SER	C-N-CA	5.91	125.85	119.76
3	A	31	VAL	CA-C-N	5.71	125.32	119.56
3	A	31	VAL	C-N-CA	5.71	125.32	119.56
4	C	132	THR	CA-C-N	5.69	126.25	120.38
4	C	132	THR	C-N-CA	5.69	126.25	120.38
2	B	227	ILE	CB-CA-C	-5.69	102.85	111.33
2	B	244	ALA	CA-C-N	5.63	125.56	119.76
2	B	244	ALA	C-N-CA	5.63	125.56	119.76
3	A	274	SER	CA-C-N	5.49	125.39	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	274	SER	C-N-CA	5.49	125.39	119.85
3	A	211	THR	CA-C-N	5.48	125.49	119.90
3	A	211	THR	C-N-CA	5.48	125.49	119.90
2	B	148	HIS	CA-C-N	5.43	126.48	120.45
2	B	148	HIS	C-N-CA	5.43	126.48	120.45
4	C	53	ILE	CB-CA-C	-5.37	104.62	110.37
4	C	165	ILE	CA-C-N	5.12	125.10	120.03
4	C	165	ILE	C-N-CA	5.12	125.10	120.03
3	A	159	ASN	CA-C-N	5.09	125.09	119.90
3	A	159	ASN	C-N-CA	5.09	125.09	119.90
3	A	188	VAL	CA-C-N	5.02	125.00	120.03
3	A	188	VAL	C-N-CA	5.02	125.00	120.03

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	61	THR	Mainchain
2	B	216	ASN	Mainchain
1	D	35	ASP	Mainchain

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	D	299	290	290	7	0
2	B	1927	1899	1899	4	0
3	A	2193	2147	2147	19	0
4	C	1794	1789	1789	11	0
5	A	27	1	0	6	0
All	All	6240	6126	6125	40	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 3.

All (40) 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:69:ASN:OD1	1:D:69:ASN:O	2.00	0.79
3:A:230:ASN:OD1	3:A:231:GLU:N	2.16	0.77
3:A:210:THR:O	3:A:211:THR:HG23	1.91	0.71
3:A:198:ASN:O	5:A:301:LGQ:N3	2.33	0.62
3:A:198:ASN:OD1	5:A:301:LGQ:C15	2.51	0.59
4:C:230:GLN:O	4:C:230:GLN:HG3	2.02	0.58
3:A:210:THR:O	3:A:211:THR:CG2	2.53	0.57
3:A:210:THR:C	3:A:211:THR:HG23	2.31	0.56
1:D:35:ASP:OD1	1:D:35:ASP:C	2.49	0.54
3:A:233:ASP:O	3:A:234:ASN:CB	2.56	0.54
4:C:105:THR:CB	4:C:221:LEU:HD23	2.39	0.53
3:A:155:PRO:HB3	3:A:220:HIS:CE1	2.45	0.52
2:B:37:GLU:OE1	4:C:37:PRO:HG3	2.10	0.52
3:A:221:MET:HE2	5:A:301:LGQ:F2	2.00	0.52
2:B:50:VAL:HG12	2:B:50:VAL:O	2.10	0.51
3:A:219:ASN:OD1	3:A:219:ASN:C	2.55	0.50
4:C:126:LYS:NZ	4:C:154:ASP:OD1	2.38	0.49
4:C:177:ASP:OD1	4:C:223:LYS:NZ	2.46	0.49
4:C:105:THR:HB	4:C:221:LEU:HD23	1.95	0.48
3:A:206:HIS:CE1	3:A:211:THR:HG21	2.49	0.48
1:D:35:ASP:CG	1:D:35:ASP:O	2.54	0.47
3:A:198:ASN:OD1	5:A:301:LGQ:C13	2.63	0.47
4:C:216:ASP:OD1	4:C:218:LYS:NZ	2.45	0.47
1:D:35:ASP:OD1	1:D:35:ASP:O	2.35	0.45
3:A:105:ASN:HA	5:A:301:LGQ:C4	2.48	0.44
2:B:227:ILE:HD13	2:B:227:ILE:HG21	1.77	0.43
3:A:233:ASP:O	3:A:234:ASN:HB3	2.16	0.43
4:C:198:PRO:HA	4:C:199:PRO:HD3	1.86	0.43
3:A:136:GLN:OE1	3:A:235:HIS:NE2	2.52	0.42
3:A:31:VAL:O	3:A:31:VAL:HG12	2.20	0.42
1:D:35:ASP:O	1:D:37:ALA:N	2.53	0.42
1:D:69:ASN:O	1:D:69:ASN:CG	2.58	0.41
3:A:215:ILE:O	3:A:215:ILE:HG13	2.20	0.41
4:C:161:VAL:O	4:C:161:VAL:HG13	2.19	0.41
4:C:55:LEU:HD23	4:C:55:LEU:HA	1.89	0.41
3:A:104:ILE:HG22	5:A:301:LGQ:C6	2.51	0.41
2:B:149:PRO:O	2:B:152:LYS:HG2	2.21	0.41
3:A:208:ASN:OD1	3:A:209:SER:N	2.53	0.41
1:D:49:ASP:OD2	1:D:52:LYS:NZ	2.49	0.40
4:C:97:LEU:HD23	4:C:97:LEU:HA	1.84	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	D	38/69 (55%)	37 (97%)	1 (3%)	0	100	100
2	B	250/252 (99%)	242 (97%)	8 (3%)	0	100	100
3	A	271/288 (94%)	265 (98%)	4 (2%)	2 (1%)	18	51
4	C	228/230 (99%)	223 (98%)	4 (2%)	1 (0%)	30	61
All	All	787/839 (94%)	767 (98%)	17 (2%)	3 (0%)	31	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	221	LEU
3	A	234	ASN
3	A	254	VAL

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	D	33/58 (57%)	33 (100%)	0	100	100
2	B	219/219 (100%)	219 (100%)	0	100	100
3	A	245/258 (95%)	243 (99%)	2 (1%)	73	77
4	C	201/201 (100%)	201 (100%)	0	100	100
All	All	698/736 (95%)	696 (100%)	2 (0%)	84	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	220	HIS
3	A	235	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	179	ASN
3	A	16	GLN
3	A	59	HIS
3	A	78	HIS

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$
5	LGQ	A	301	-	30,30,30	2.27	5 (16%)	39,44,44	2.16	10 (25%)

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
5	LGQ	A	301	-	-	2/14/14/14	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	LGQ	C8-C10	-6.33	1.35	1.42
5	A	301	LGQ	C8-C9	-5.85	1.33	1.41
5	A	301	LGQ	N3-N2	-4.82	1.24	1.36
5	A	301	LGQ	C9-N3	-3.98	1.32	1.35
5	A	301	LGQ	C8-C7	-2.21	1.35	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	LGQ	C10-C8-C9	7.98	121.67	115.71
5	A	301	LGQ	C2-N1-C7	-4.34	119.53	128.24
5	A	301	LGQ	N3-C9-N5	3.89	128.84	125.64
5	A	301	LGQ	C9-N3-N2	-3.80	109.07	111.18
5	A	301	LGQ	N6-C10-N4	2.98	121.05	117.03
5	A	301	LGQ	N5-C11-N4	-2.70	120.68	125.13
5	A	301	LGQ	C8-C9-N5	-2.62	122.41	126.54
5	A	301	LGQ	C12-C11-N4	2.54	121.60	117.40
5	A	301	LGQ	C10-N4-C11	2.47	120.34	117.36
5	A	301	LGQ	C8-C10-N4	-2.30	117.66	121.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

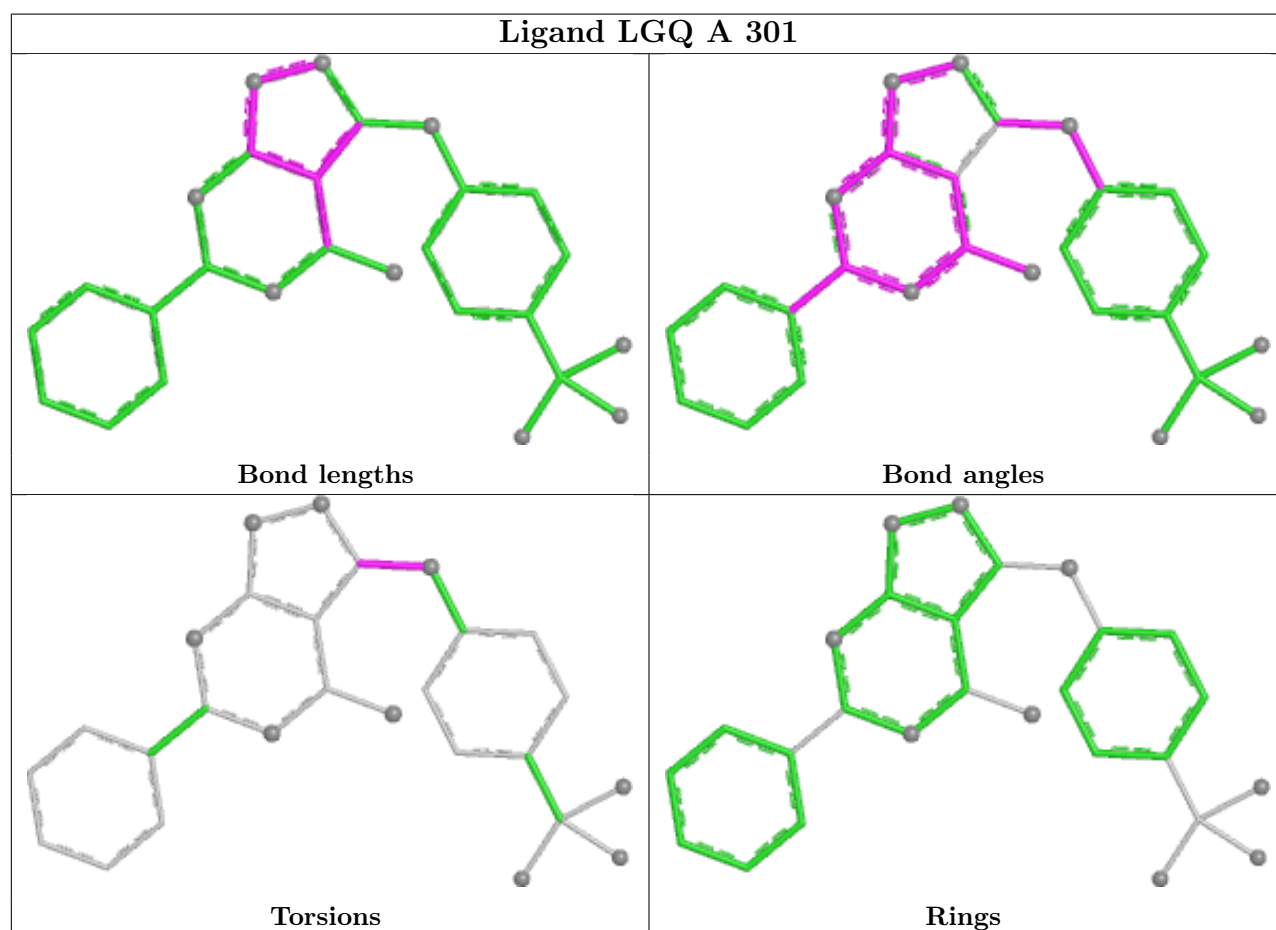
Mol	Chain	Res	Type	Atoms
5	A	301	LGQ	C8-C7-N1-C2
5	A	301	LGQ	N2-C7-N1-C2

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	LGQ	6	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.



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.

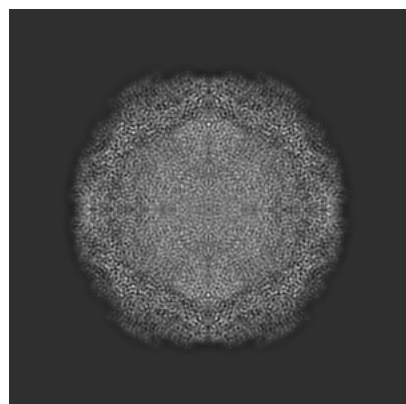
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10220. These allow visual inspection of the internal detail of the map and identification of artifacts.

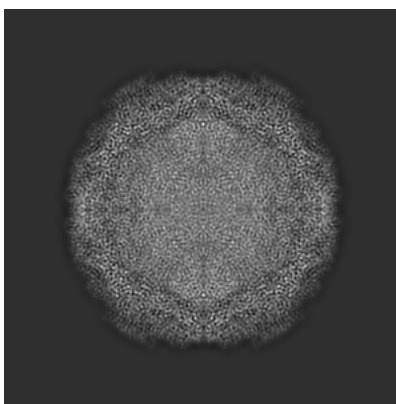
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

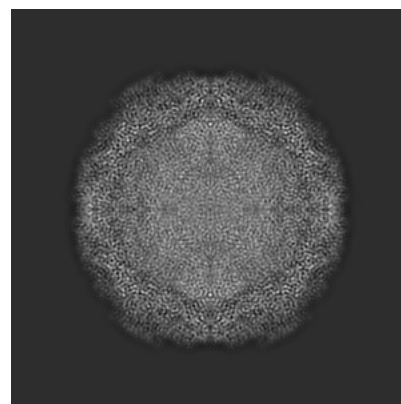
6.1.1 Primary map



X

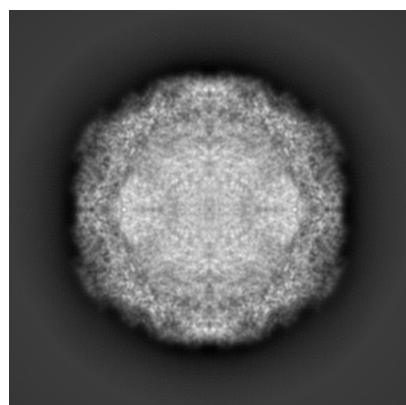


Y

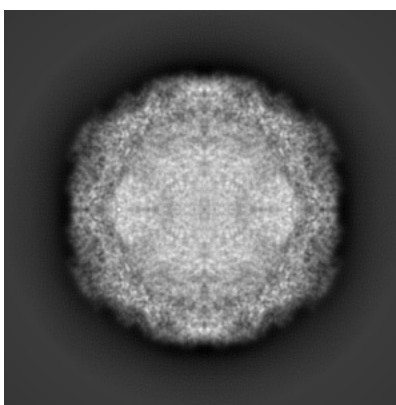


Z

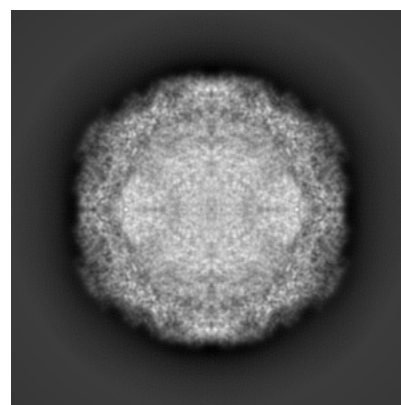
6.1.2 Raw map



X



Y

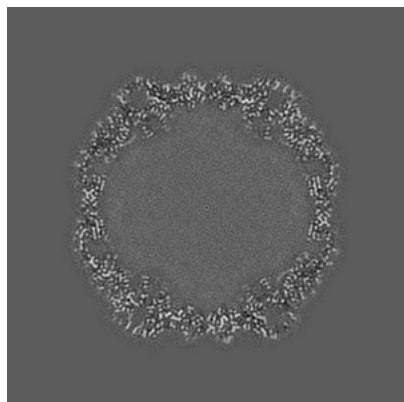


Z

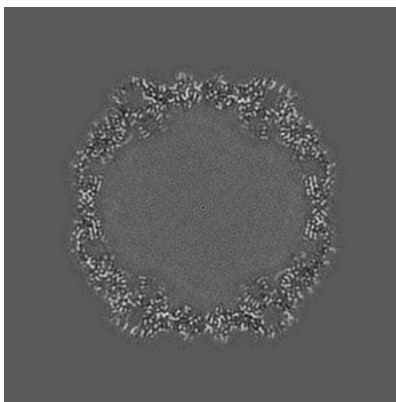
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

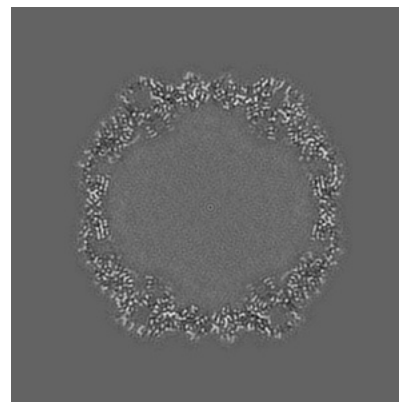
6.2.1 Primary map



X Index: 225

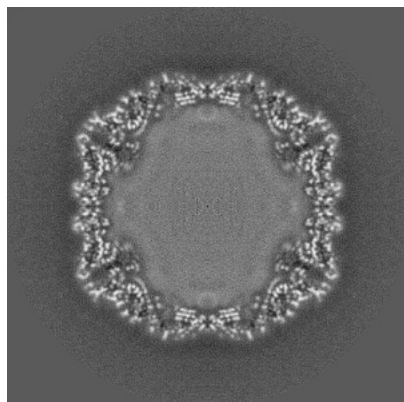


Y Index: 225

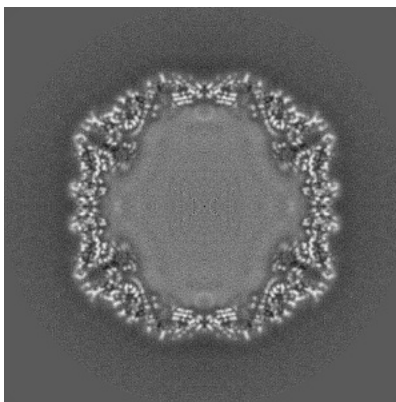


Z Index: 225

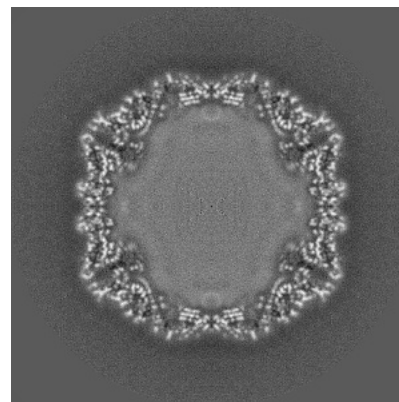
6.2.2 Raw map



X Index: 225



Y Index: 225

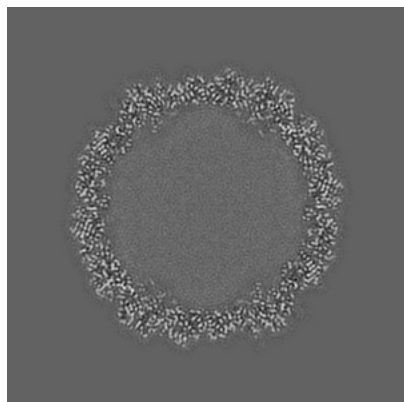


Z Index: 225

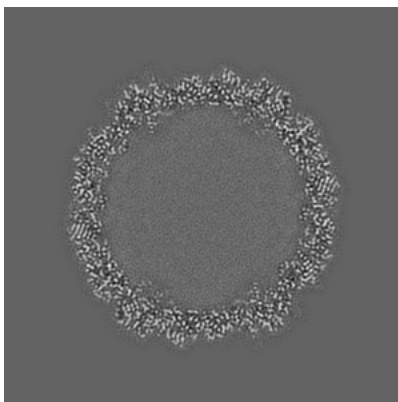
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

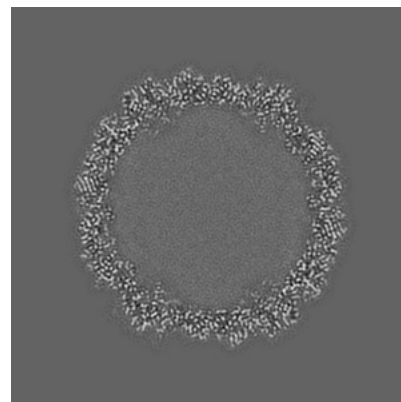
6.3.1 Primary map



X Index: 206

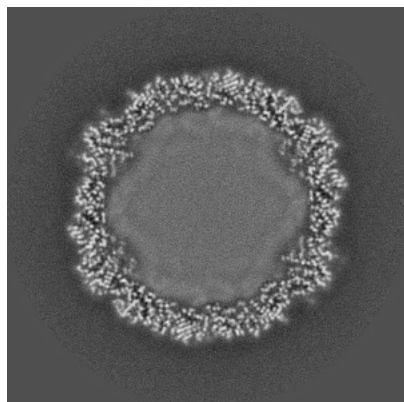


Y Index: 207

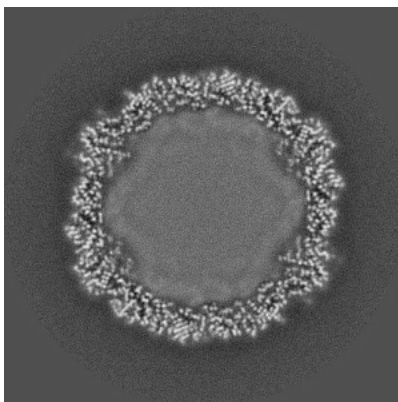


Z Index: 241

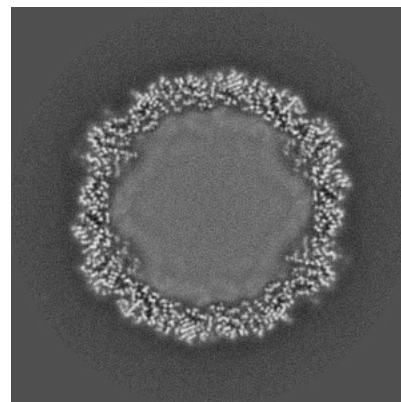
6.3.2 Raw map



X Index: 208



Y Index: 208

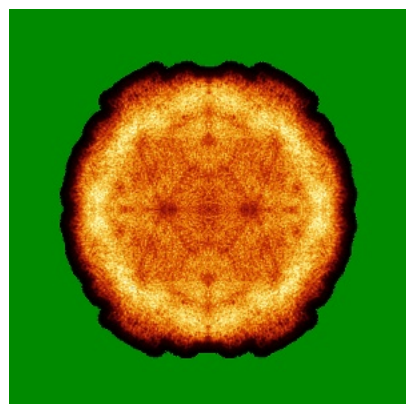


Z Index: 208

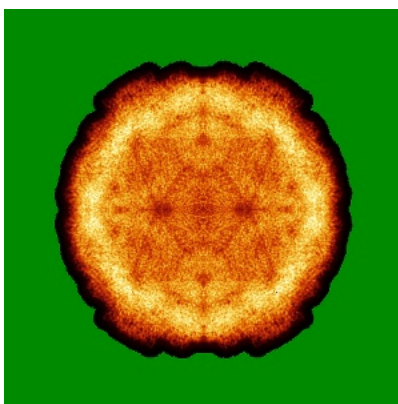
The images above show the largest variance slices of the map in three orthogonal directions.

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

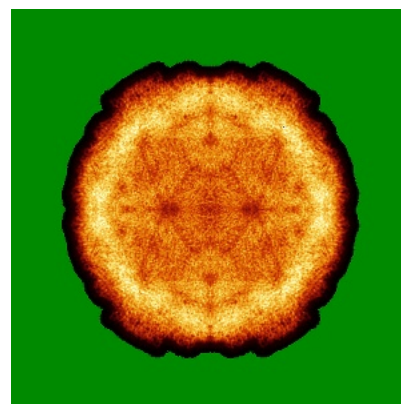
6.4.1 Primary map



X

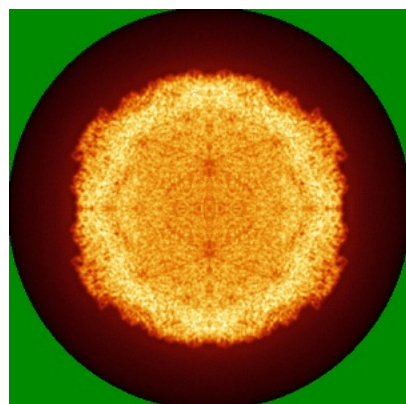


Y

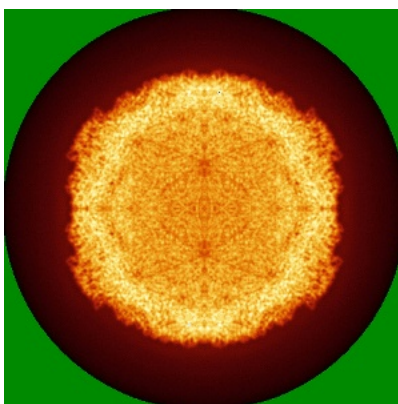


Z

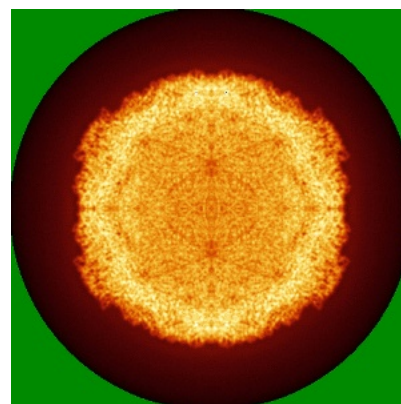
6.4.2 Raw map



X



Y

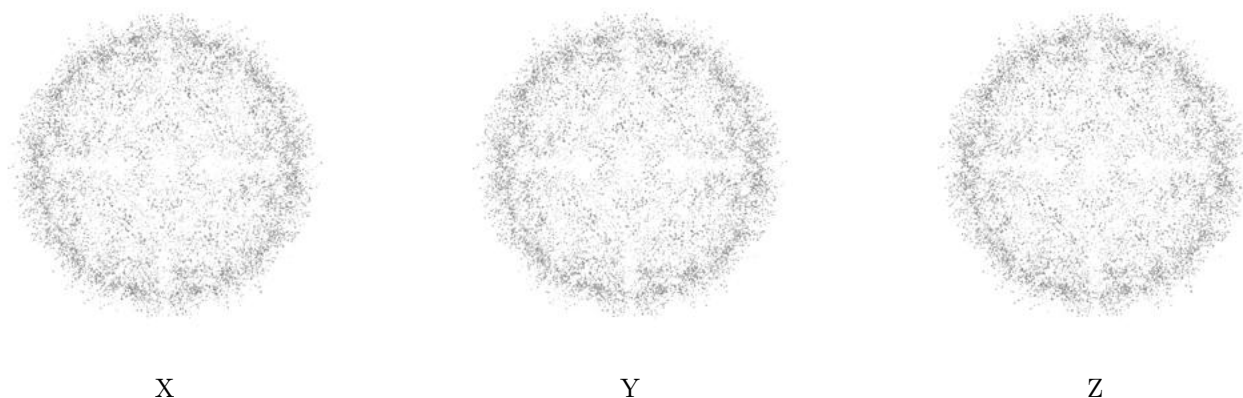


Z

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.

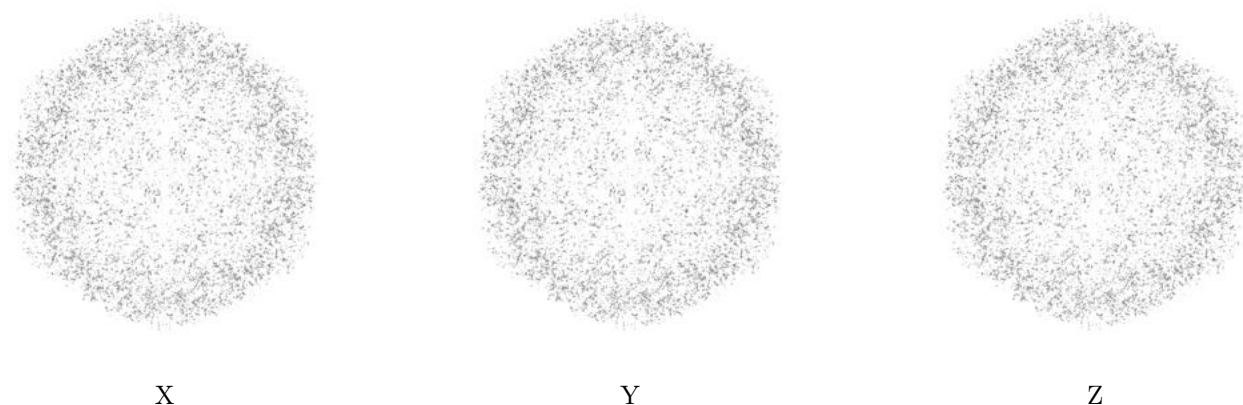
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0478. 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.

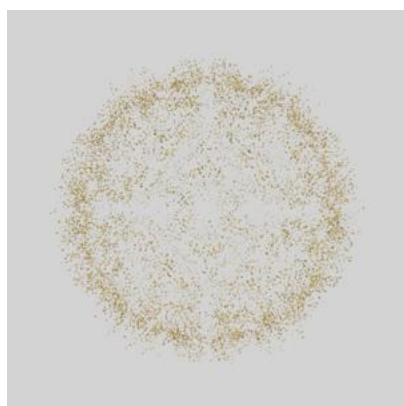
6.6 Mask visualisation [i](#)

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_10220_msk_1.map [i](#)



X



Y

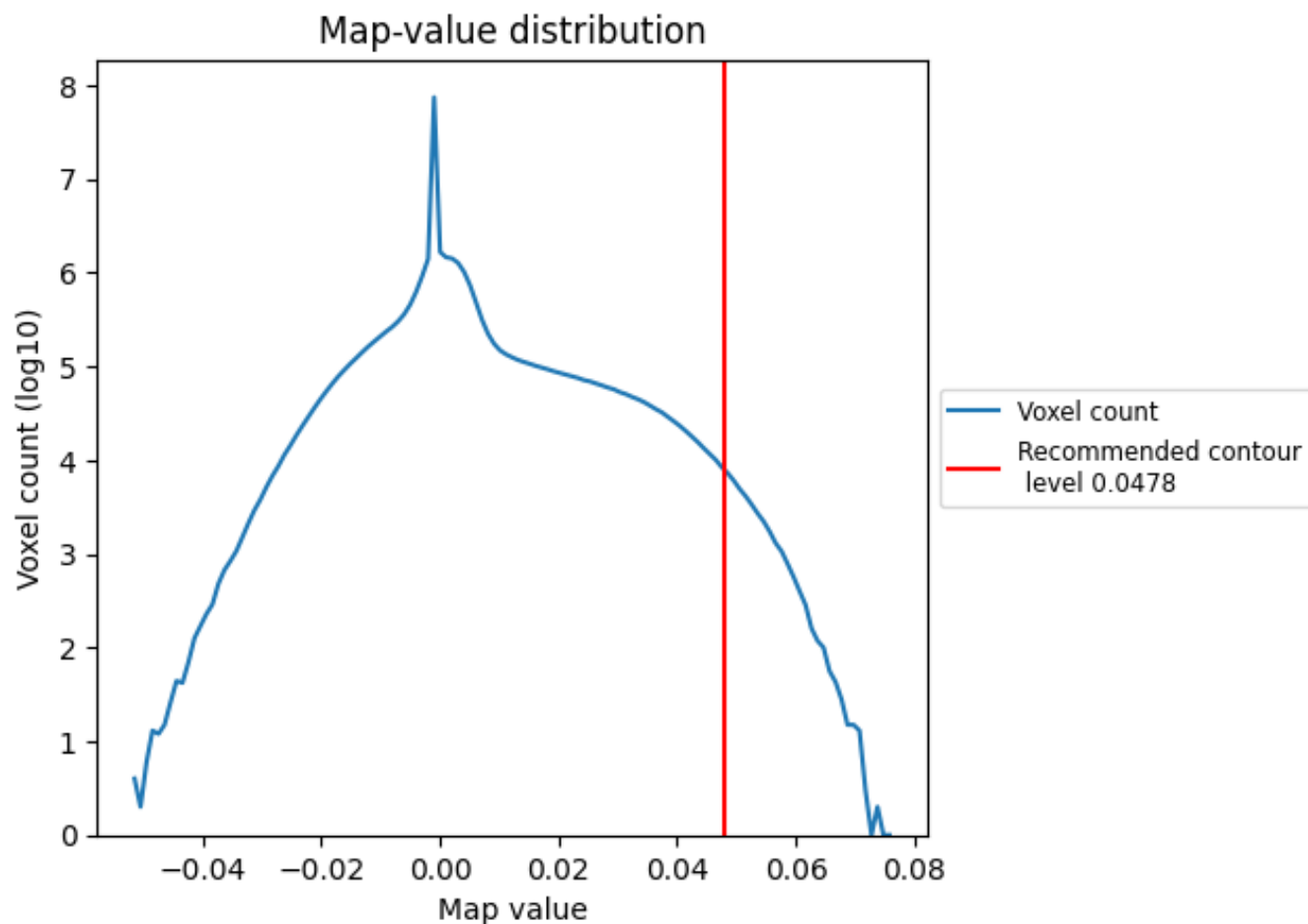


Z

7 Map analysis [i](#)

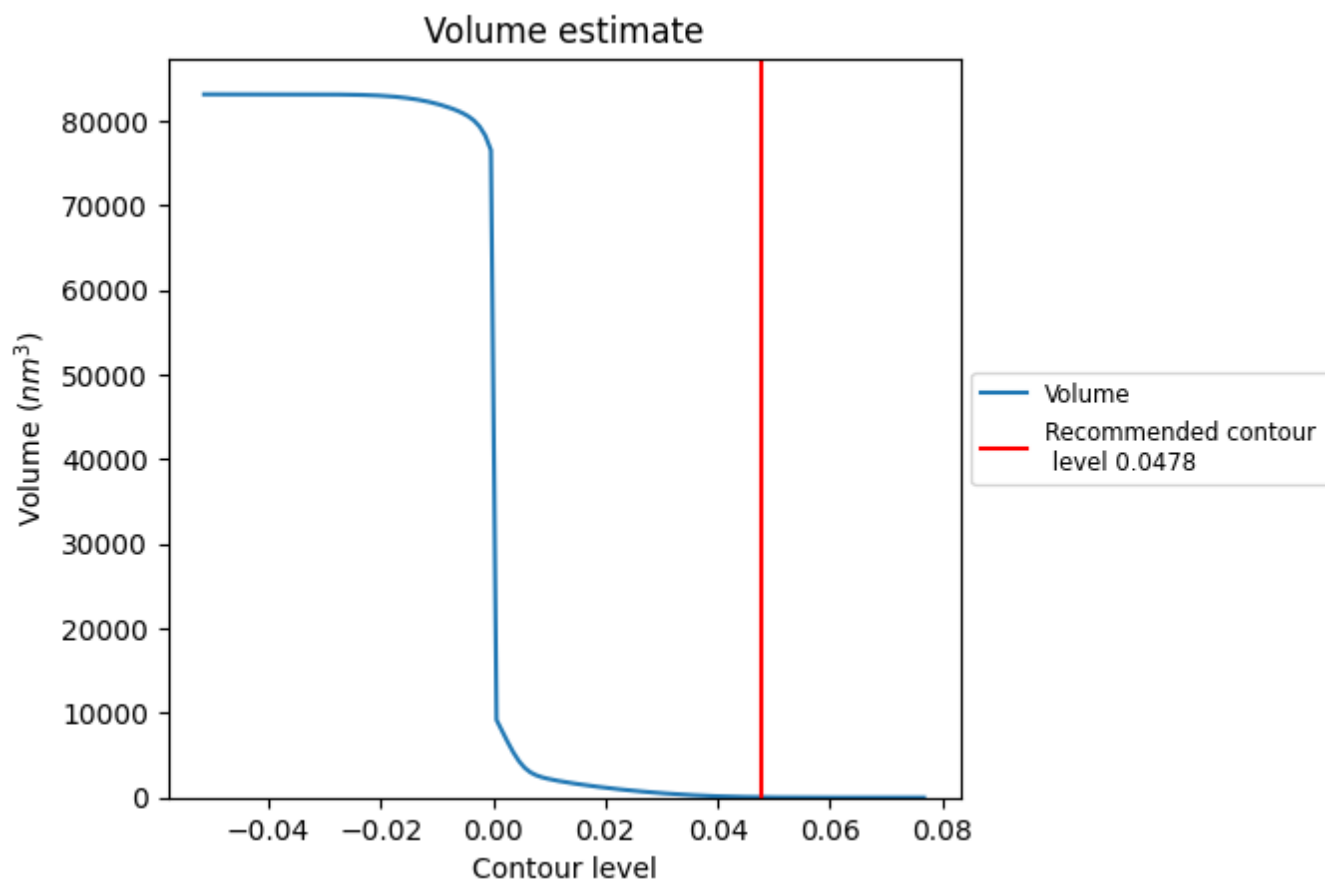
This section contains the results of statistical analysis of the map.

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.

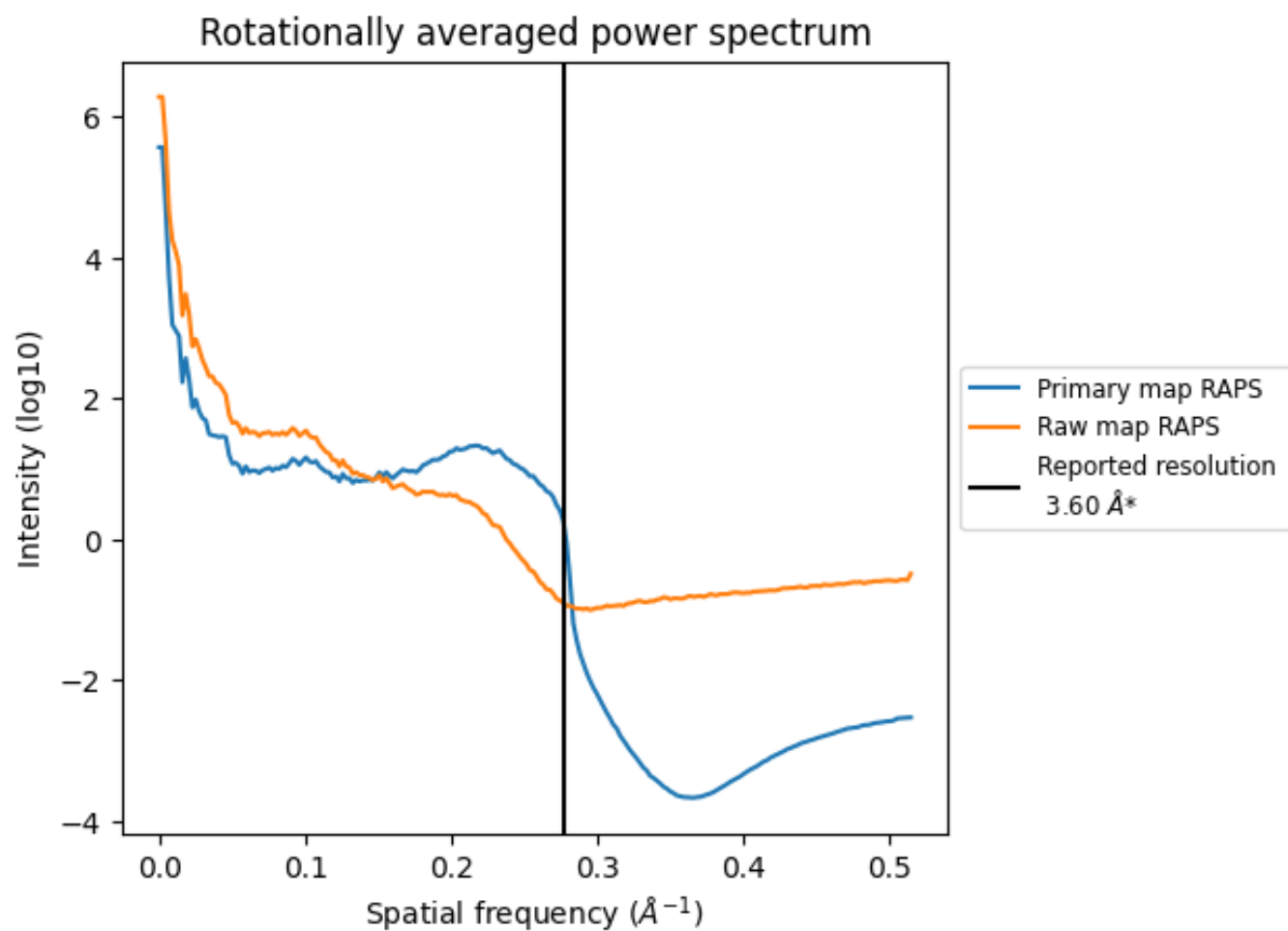
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm³; this corresponds to an approximate mass of 36 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 ⓘ

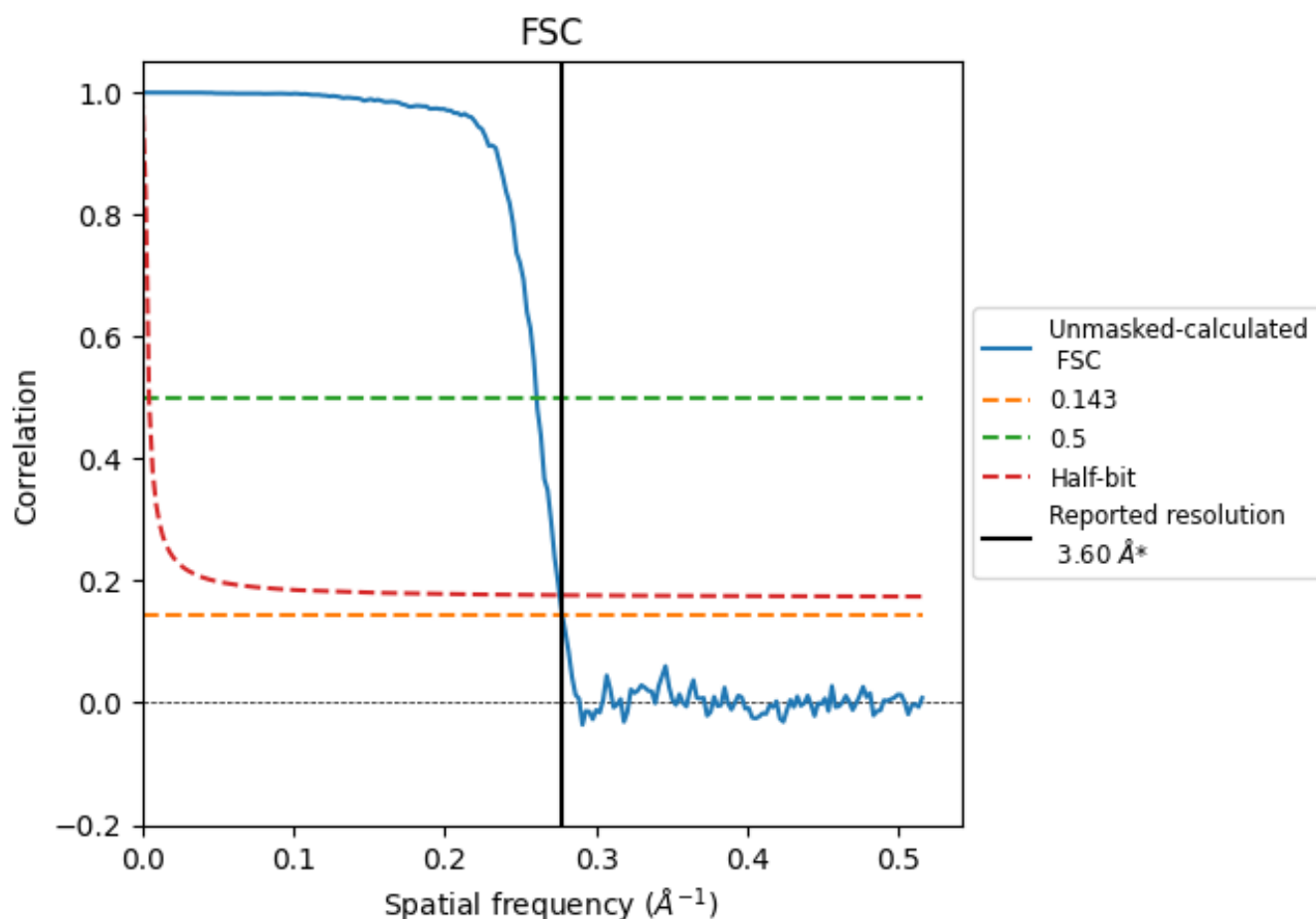


*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.60	3.84	3.62

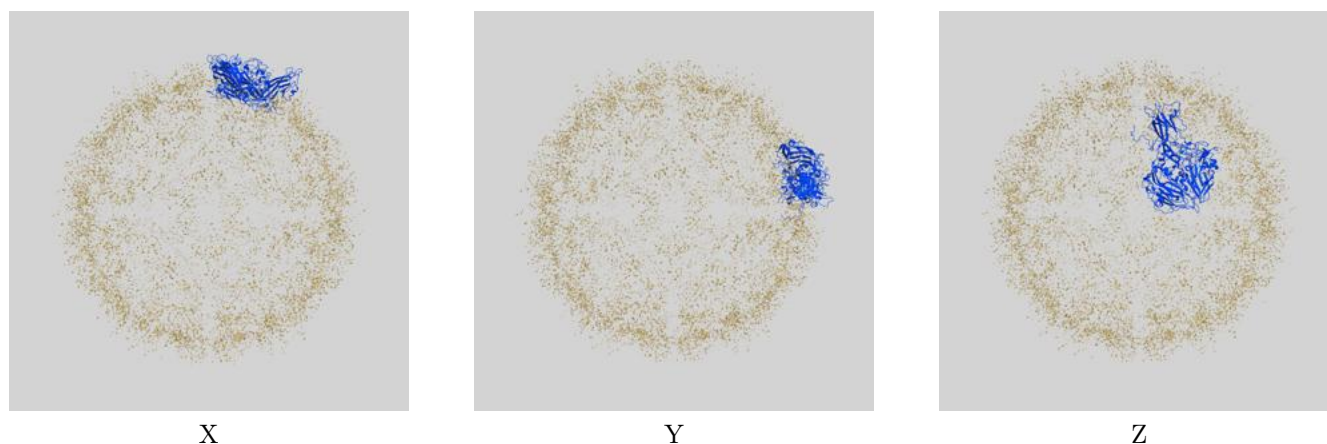
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

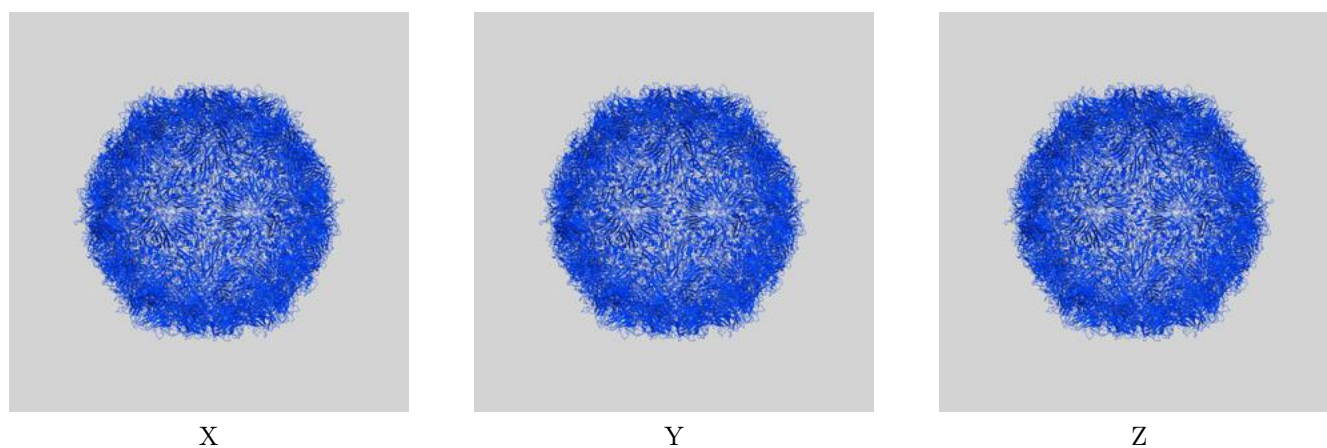
This section contains information regarding the fit between EMDB map EMD-10220 and PDB model 6SK5. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

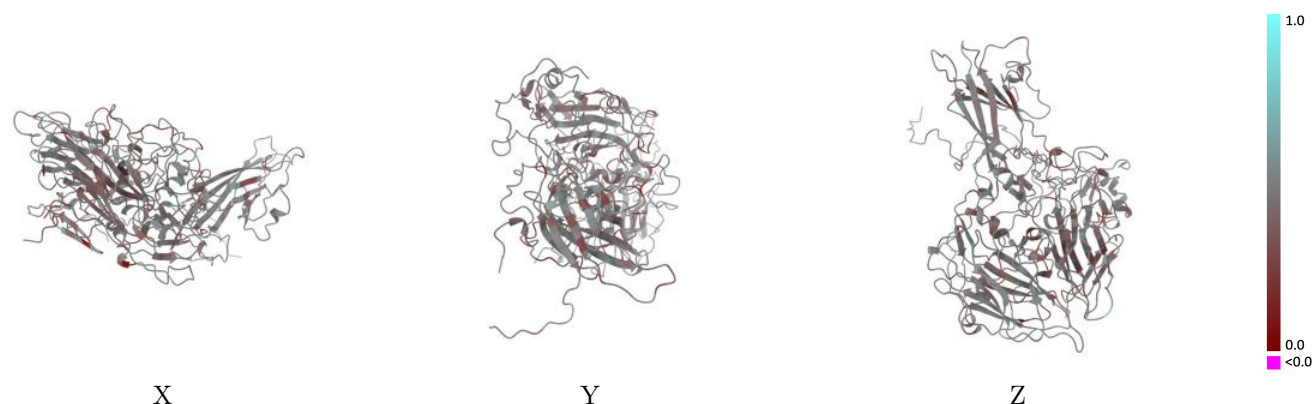


9.1.2 Map-model assembly overlay [i](#)



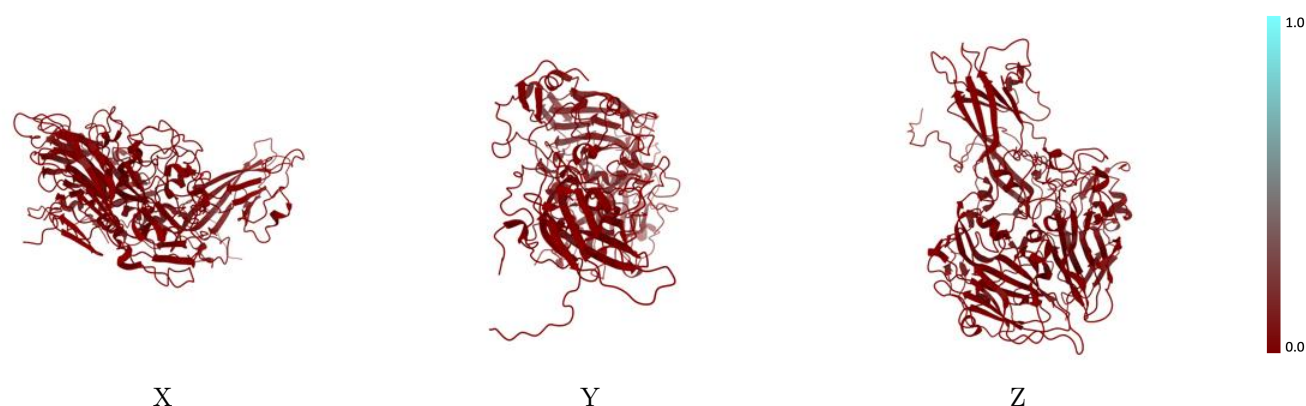
The images above show the 3D surface view of the map at the recommended contour level 0.0478 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



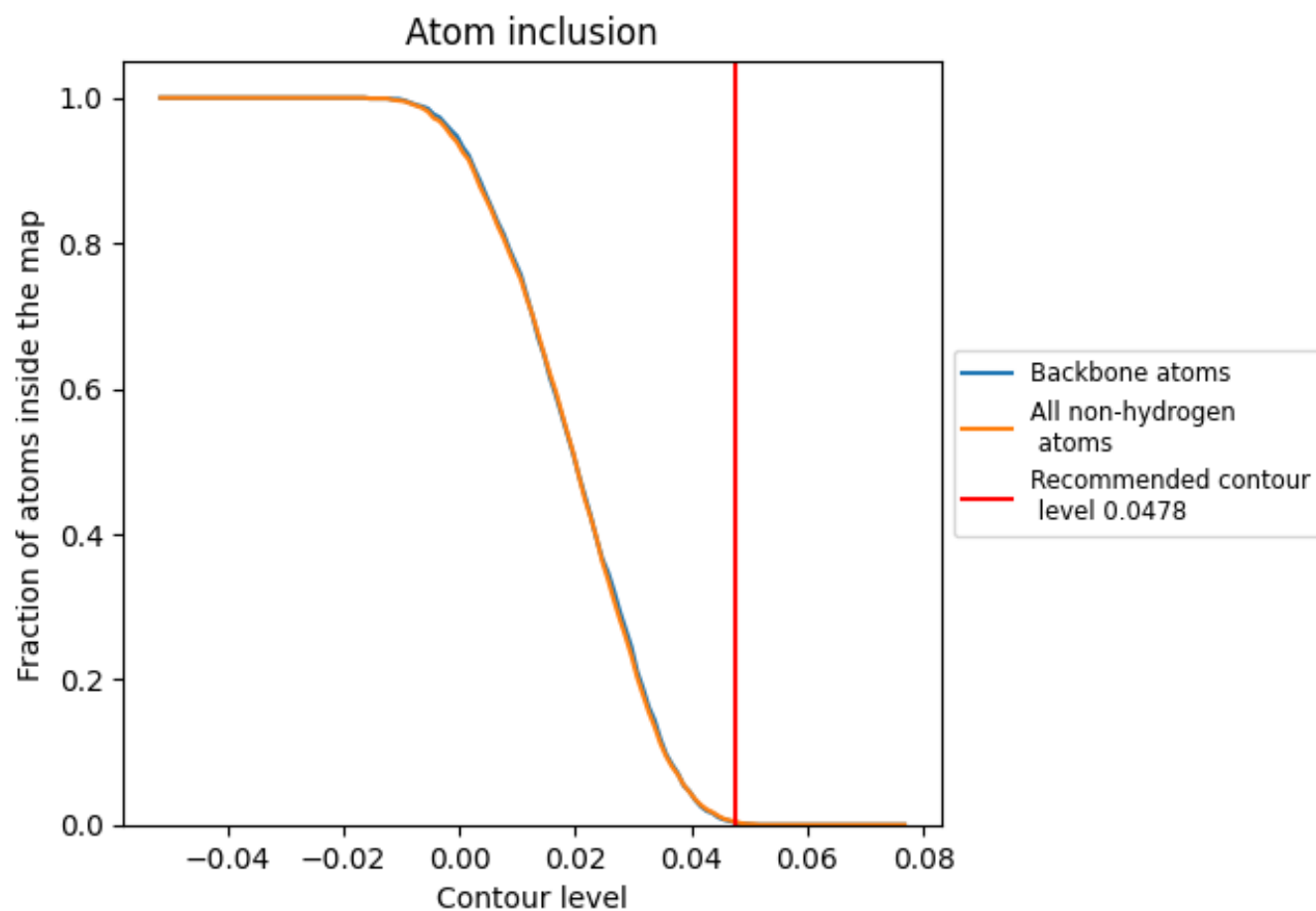
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0478).

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.0478) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0040	0.4350
A	0.0040	0.4430
B	0.0050	0.4260
C	0.0060	0.4410
D	0.0000	0.4060

