Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 05:37 pm GMT

PDB ID	:	5O5P
EMDB ID	:	EMD-3749
Title	:	Poliovirus type 3 (strain Saukett) stabilized virus-like particle in complex with the pocket factor compound GPP3
Authors	:	Bahar, M.W.; Kotecha, A.; Fry, E.E.; Stuart, D.I.
Deposited on	:	2017-06-02
Resolution	:	4.10 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:

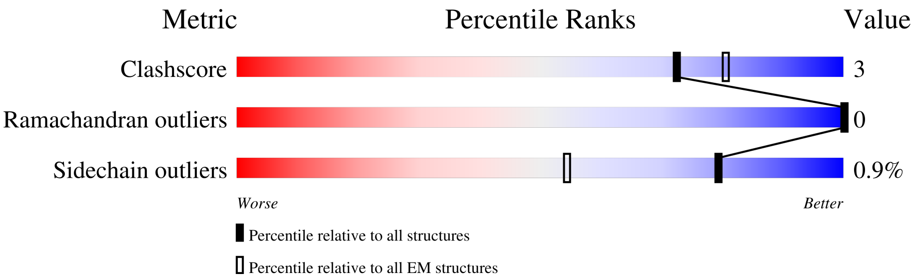
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1	300	29% 69% 9% 22%
2	2	271	42% 86% 10% •
3	3	238	26% 90% 9% •
4	4	69	20% 23% • 75%

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
5	9LW	1	401	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5922 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 Capsid proteins, VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	235	1897	1215	324	351	7	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	105	MET	THR	engineered mutation	UNP Q84895
1	132	LEU	PHE	engineered mutation	UNP Q84895

- Molecule 2 is a protein called Capsid proteins, VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	260	2047	1306	347	382	12	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	18	ILE	LEU	engineered mutation	UNP Q84895
2	215	MET	LEU	engineered mutation	UNP Q84895
2	241	GLU	ASP	engineered mutation	UNP Q84895

- Molecule 3 is a protein called Capsid proteins, VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	235	1814	1151	295	350	18	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	19	TYR	HIS	engineered mutation	UNP Q84895
3	85	PHE	LEU	engineered mutation	UNP Q84895

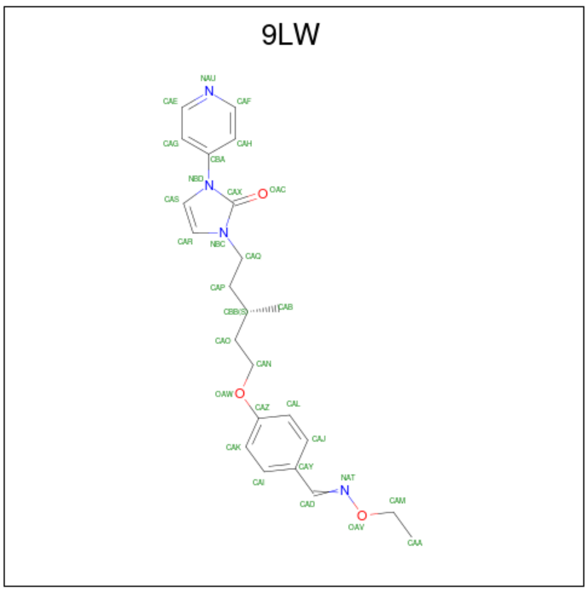
- Molecule 4 is a protein called Capsid proteins, VP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	4	17	134	84	21	29	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	67	ALA	UNK	engineered mutation	UNP Q84895

- Molecule 5 is 1-[5-[4-(ethoxyiminomethyl)phenoxy]-3-methyl-pentyl]-3-pyridin-4-yl-imidazol -2-one (three-letter code: 9LW) (formula: $C_{23}H_{28}N_4O_3$).



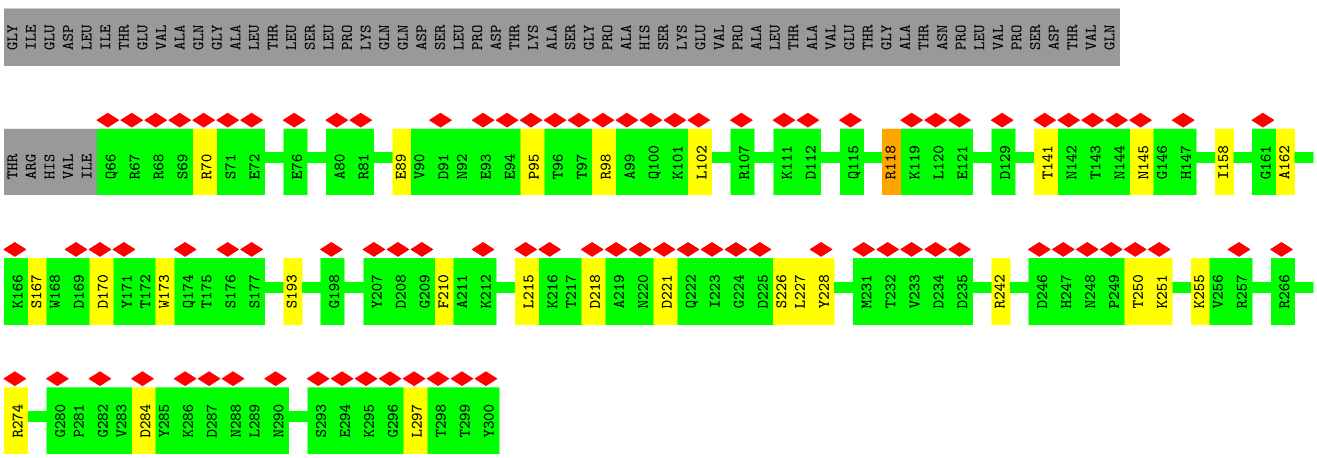
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	1	1	30	23	4	3	0

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.

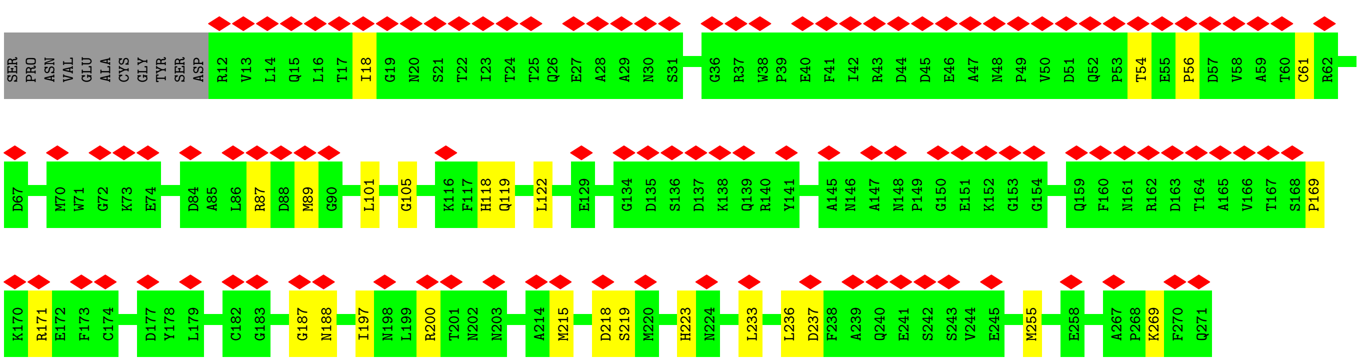
- Molecule 1: Capsid proteins, VP1

Chain 1:



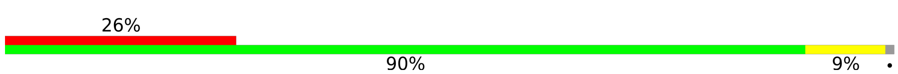
- Molecule 2: Capsid proteins, VP2

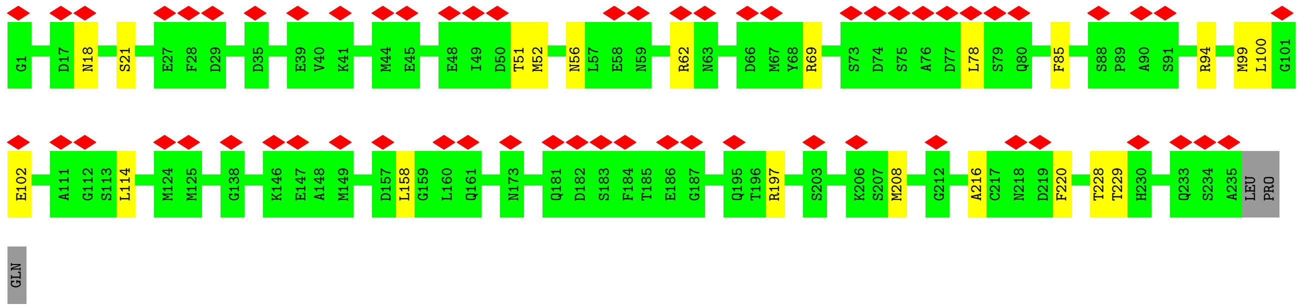
Chain 2:



- Molecule 3: Capsid proteins, VP3

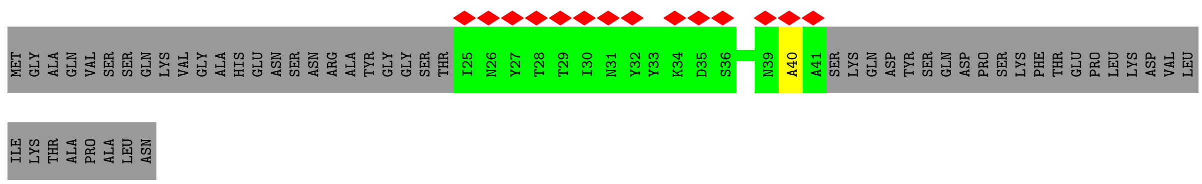
Chain 3:





- Molecule 4: Capsid proteins, VP4

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	2060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF parameters were estimated using CTFFIND3 as part of RELION 1.3.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.149	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0475	Depositor
Map size (Å)	691.2, 691.2, 691.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 9LW

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	1	0.38	0/1953	0.52	0/2662
2	2	0.38	0/2104	0.55	0/2868
3	3	0.36	0/1859	0.54	0/2536
4	4	0.31	0/136	0.44	0/185
All	All	0.37	0/6052	0.54	0/8251

There are no bond length outliers.

There are no bond angle outliers.

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	1	1897	0	1844	16	0
2	2	2047	0	1975	16	0
3	3	1814	0	1789	16	0
4	4	134	0	122	1	0
5	1	30	0	0	0	0
All	All	5922	0	5730	39	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 (39) 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)
1:1:193:SER:HG	3:3:21:SER:HG	1.41	0.69
2:2:54:THR:HG22	2:2:56:PRO:HD3	1.83	0.60
1:1:89:GLU:OE2	1:1:255:LYS:NZ	2.37	0.56
1:1:95:PRO:HG3	1:1:102:LEU:HD11	1.89	0.54
1:1:170:ASP:H	1:1:173:TRP:HD1	1.56	0.54
3:3:51:THR:HG21	3:3:99:MET:HB3	1.90	0.53
2:2:200:ARG:NH2	3:3:158:LEU:O	2.42	0.53
1:1:145:ASN:ND2	1:1:250:THR:OG1	2.41	0.53
1:1:70:ARG:NH2	3:3:220:PHE:O	2.42	0.52
1:1:158:ILE:HG23	1:1:162:ALA:HB3	1.91	0.51
1:1:274:ARG:NH2	1:1:284:ASP:O	2.40	0.51
3:3:85:PHE:HB3	3:3:94:ARG:HE	1.76	0.50
2:2:119:GLN:HE21	2:2:237:ASP:HB3	1.78	0.49
1:1:210:PHE:HE1	1:1:228:TYR:HD1	1.62	0.48
1:1:221:ASP:OD1	2:2:269:LYS:NZ	2.45	0.47
2:2:105:GLY:O	2:2:255:MET:N	2.46	0.46
2:2:218:ASP:OD1	2:2:219:SER:N	2.49	0.45
1:1:141:THR:HG21	1:1:251:LYS:HE3	1.98	0.45
3:3:208:MET:SD	3:3:208:MET:N	2.89	0.45
2:2:215:MET:SD	2:2:215:MET:N	2.90	0.45
2:2:218:ASP:OD2	2:2:223:HIS:ND1	2.49	0.45
2:2:233:LEU:O	3:3:69:ARG:NH2	2.42	0.45
2:2:122:LEU:HB2	2:2:197:ILE:HB	1.99	0.43
3:3:18:ASN:HB2	4:4:40:ALA:HB1	2.00	0.43
3:3:228:THR:OG1	3:3:229:THR:N	2.50	0.43
1:1:215:LEU:N	1:1:218:ASP:OD2	2.52	0.43
2:2:118:HIS:HD2	2:2:236:LEU:HD21	1.84	0.43
3:3:100:LEU:HD21	3:3:114:LEU:HD22	2.00	0.43
1:1:297:LEU:HD13	3:3:56:ASN:HA	2.01	0.42
2:2:187:GLY:HA2	3:3:52:MET:HB3	2.01	0.42
2:2:188:ASN:OD1	3:3:99:MET:N	2.52	0.42
1:1:226:SER:OG	1:1:227:LEU:N	2.53	0.42
2:2:169:PRO:HB2	2:2:171:ARG:HG3	2.03	0.41
2:2:18:ILE:HG22	2:2:61:CYS:HB3	2.02	0.41
2:2:101:LEU:HA	2:2:219:SER:HA	2.01	0.41
3:3:78:LEU:HD21	3:3:197:ARG:HB2	2.02	0.41
1:1:118:ARG:NH2	3:3:102:GLU:OE1	2.54	0.41
3:3:114:LEU:HA	3:3:216:ALA:HA	2.02	0.41
1:1:167:SER:OG	1:1:170:ASP:OD1	2.34	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	1	233/300 (78%)	205 (88%)	28 (12%)	0	100	100
2	2	258/271 (95%)	240 (93%)	18 (7%)	0	100	100
3	3	233/238 (98%)	220 (94%)	13 (6%)	0	100	100
4	4	15/69 (22%)	14 (93%)	1 (7%)	0	100	100
All	All	739/878 (84%)	679 (92%)	60 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	1	206/260 (79%)	203 (98%)	3 (2%)	65	79
2	2	220/229 (96%)	218 (99%)	2 (1%)	78	87
3	3	210/213 (99%)	209 (100%)	1 (0%)	88	93
4	4	14/57 (25%)	14 (100%)	0	100	100
All	All	650/759 (86%)	644 (99%)	6 (1%)	79	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	98	ARG
1	1	118	ARG
1	1	242	ARG
2	2	87	ARG
2	2	89	MET
3	3	62	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	222	GLN
2	2	119	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 monosaccharides 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	9LW	1	401	-	32,32,32	5.43	23 (71%)	34,41,41	8.31	26 (76%)

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	9LW	1	401	-	-	14/20/20/20	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	401	9LW	CAP-CAQ	-15.33	1.18	1.52
5	1	401	9LW	CAS-CAR	11.63	1.55	1.34
5	1	401	9LW	CAO-CAN	-9.29	1.18	1.50
5	1	401	9LW	OAV-CAM	-8.19	1.28	1.44
5	1	401	9LW	CAK-CAI	-7.09	1.25	1.38
5	1	401	9LW	CAX-NBC	7.05	1.45	1.37
5	1	401	9LW	CAL-CAJ	-6.73	1.26	1.38
5	1	401	9LW	CAD-NAT	-6.38	1.15	1.27
5	1	401	9LW	CAB-CBB	-6.03	1.33	1.52
5	1	401	9LW	CAQ-NBC	-5.70	1.33	1.47
5	1	401	9LW	CAG-CAE	-5.00	1.28	1.38
5	1	401	9LW	CAS-NBD	-4.29	1.33	1.39
5	1	401	9LW	CAY-CAD	-4.10	1.38	1.47
5	1	401	9LW	OAV-NAT	-3.77	1.34	1.41
5	1	401	9LW	CAX-NBD	3.70	1.43	1.39
5	1	401	9LW	OAW-CAN	-3.48	1.31	1.43
5	1	401	9LW	CAF-NAU	-3.34	1.24	1.33
5	1	401	9LW	CBA-NBD	-3.10	1.39	1.44
5	1	401	9LW	CAA-CAM	-2.83	1.24	1.46
5	1	401	9LW	CAO-CBB	-2.70	1.38	1.52
5	1	401	9LW	CAH-CAF	2.52	1.43	1.38
5	1	401	9LW	CAP-CBB	-2.43	1.39	1.52
5	1	401	9LW	CAR-NBC	-2.02	1.33	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	401	9LW	OAV-NAT-CAD	28.32	154.31	110.80
5	1	401	9LW	OAV-CAM-CAA	14.80	147.84	109.44
5	1	401	9LW	CAQ-CAP-CBB	13.97	153.34	114.20
5	1	401	9LW	CAY-CAD-NAT	12.30	157.74	120.50
5	1	401	9LW	CAE-CAG-CBA	11.01	131.55	119.03
5	1	401	9LW	CAK-CAZ-CAL	-10.69	103.71	120.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	401	9LW	CBA-NBD-CAS	10.05	138.92	124.42
5	1	401	9LW	CAJ-CAY-CAD	9.03	140.06	120.81
5	1	401	9LW	CAI-CAY-CAJ	-8.72	104.74	117.64
5	1	401	9LW	CAG-CAE-NAU	-7.78	110.08	123.62
5	1	401	9LW	CAJ-CAL-CAZ	7.75	129.21	119.73
5	1	401	9LW	CAQ-NBC-CAX	-7.21	112.59	122.32
5	1	401	9LW	CAI-CAK-CAZ	6.47	127.65	119.73
5	1	401	9LW	OAW-CAN-CAO	6.13	152.00	109.58
5	1	401	9LW	CAK-CAI-CAY	5.74	128.74	121.25
5	1	401	9LW	CAP-CBB-CAO	5.72	142.23	112.13
5	1	401	9LW	CAF-NAU-CAE	5.32	129.38	116.85
5	1	401	9LW	CAH-CAF-NAU	-5.23	114.51	123.62
5	1	401	9LW	CAH-CBA-CAG	-5.20	108.59	119.16
5	1	401	9LW	CAG-CBA-NBD	4.39	125.31	119.63
5	1	401	9LW	CAL-CAJ-CAY	3.60	125.94	121.25
5	1	401	9LW	CAS-CAR-NBC	-3.59	103.40	107.21
5	1	401	9LW	CAQ-NBC-CAR	3.49	133.69	124.98
5	1	401	9LW	OAW-CAZ-CAK	3.47	136.99	119.94
5	1	401	9LW	CAI-CAY-CAD	-2.63	115.21	120.81
5	1	401	9LW	NBD-CAX-NBC	-2.02	103.79	105.51

There are no chirality outliers.

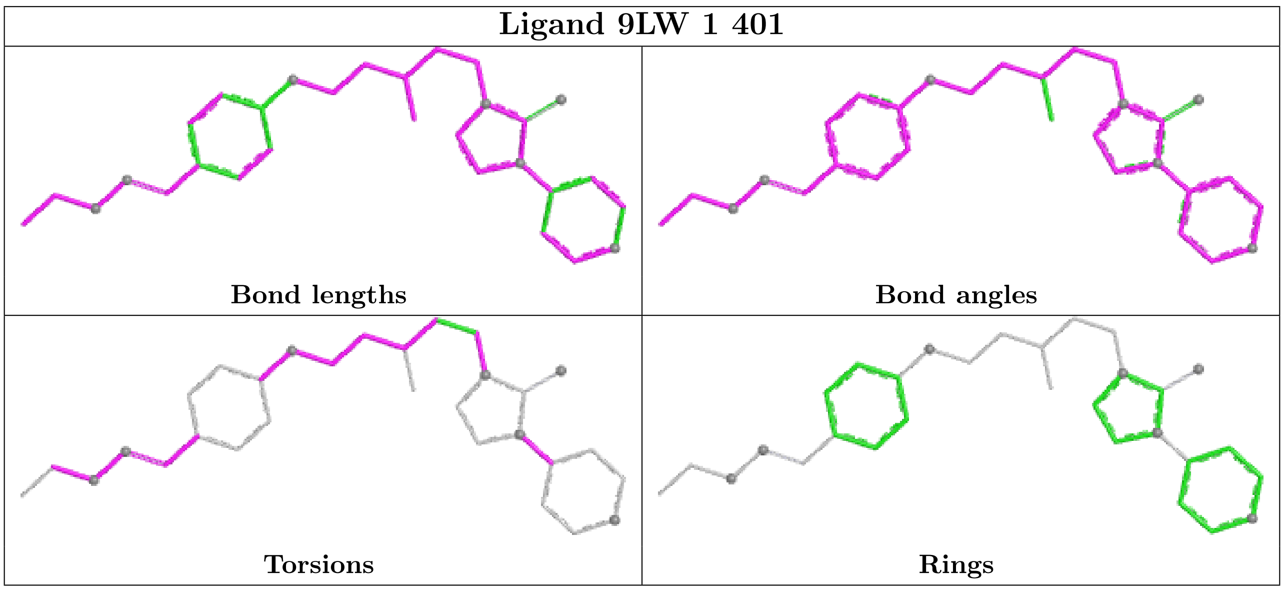
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	401	9LW	CAA-CAM-OAV-NAT
5	1	401	9LW	CAD-NAT-OAV-CAM
5	1	401	9LW	CAY-CAD-NAT-OAV
5	1	401	9LW	CAN-CAO-CBB-CAB
5	1	401	9LW	CAQ-CAP-CBB-CAB
5	1	401	9LW	CAH-CBA-NBD-CAX
5	1	401	9LW	CAL-CAZ-OAW-CAN
5	1	401	9LW	CAK-CAZ-OAW-CAN
5	1	401	9LW	OAW-CAN-CAO-CBB
5	1	401	9LW	CAO-CAN-OAW-CAZ
5	1	401	9LW	CAP-CAQ-NBC-CAR
5	1	401	9LW	NAT-CAD-CAY-CAI
5	1	401	9LW	CAQ-CAP-CBB-CAO
5	1	401	9LW	NAT-CAD-CAY-CAJ

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

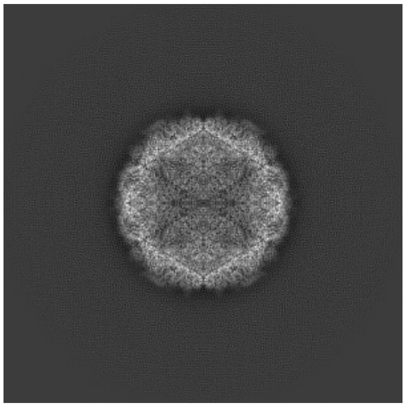
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3749. These allow visual inspection of the internal detail of the map and identification of artifacts.

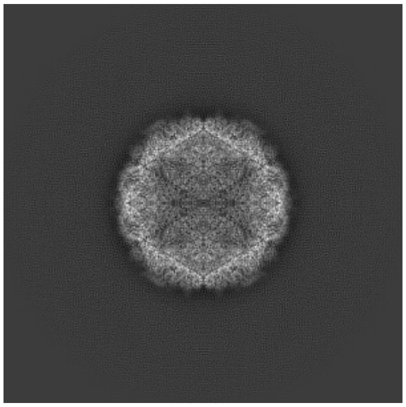
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

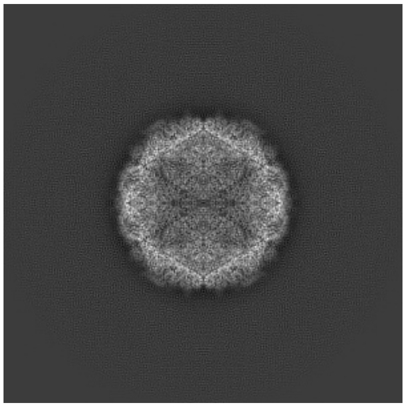
6.1.1 Primary map



X



Y

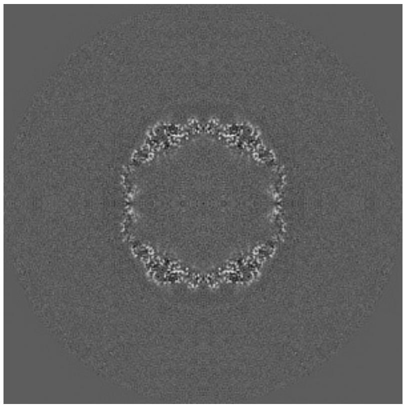


Z

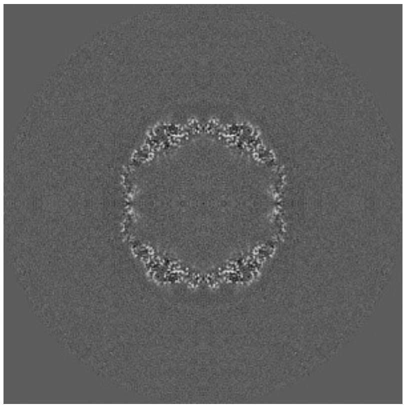
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

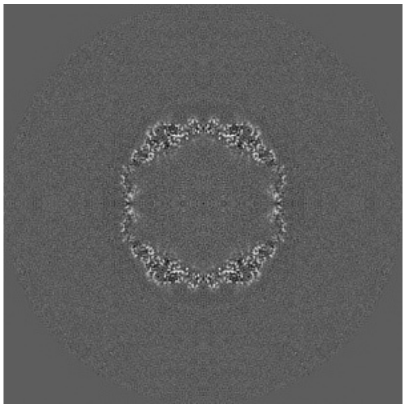
6.2.1 Primary map



X Index: 256



Y Index: 256

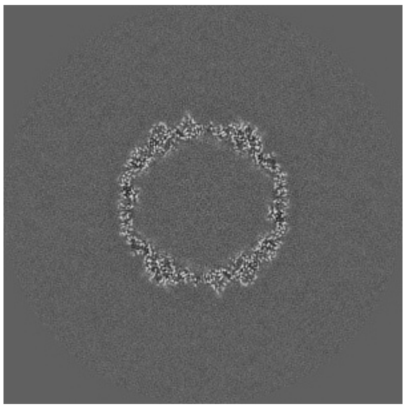


Z Index: 256

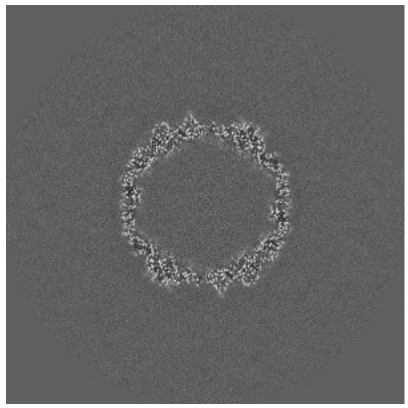
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

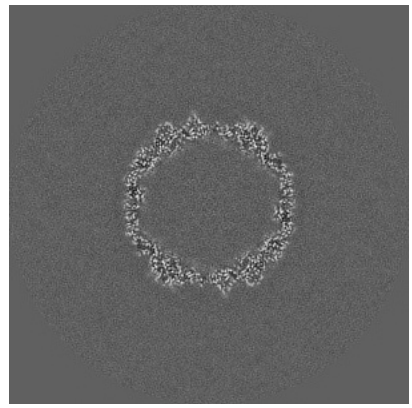
6.3.1 Primary map



X Index: 264



Y Index: 264

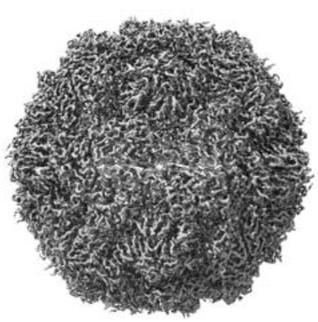


Z Index: 264

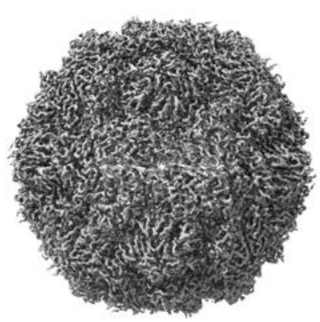
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

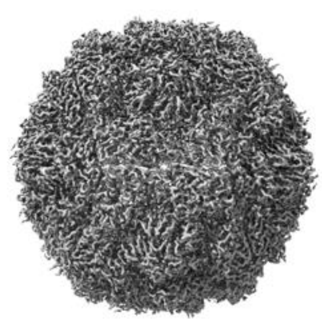
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0475. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

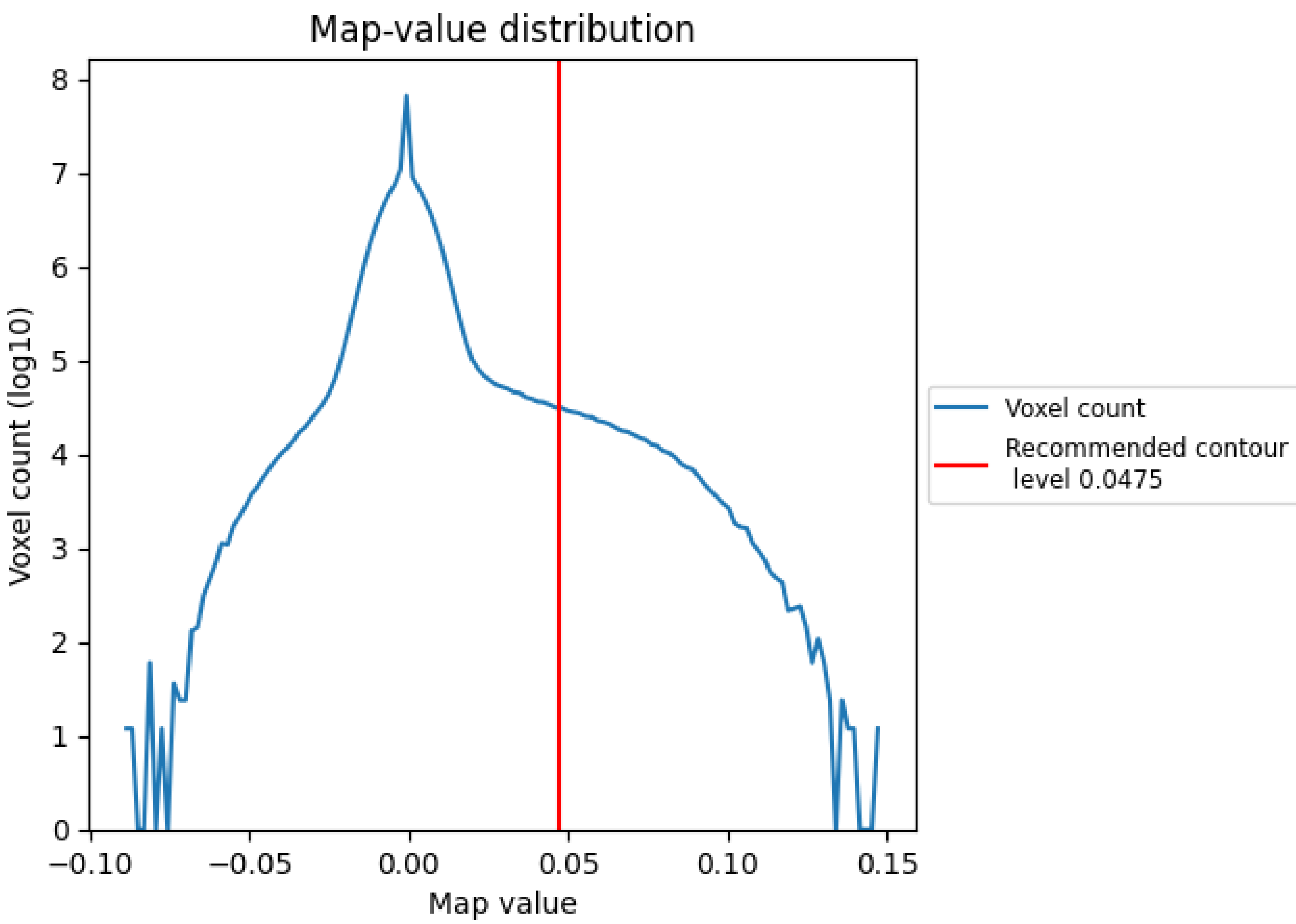
6.5 Mask visualisation (i)

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

7 Map analysis (i)

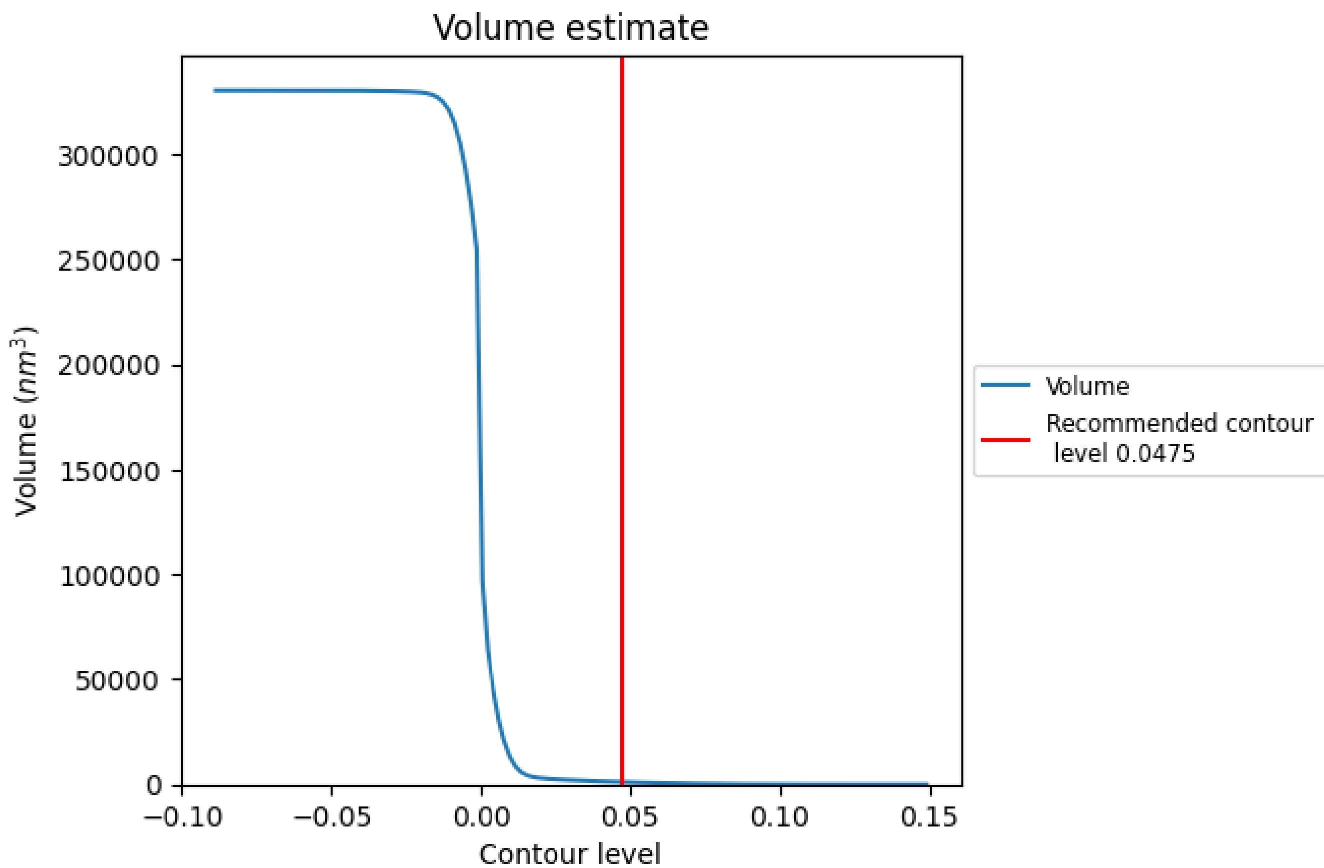
This section contains the results of statistical analysis of the map.

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.

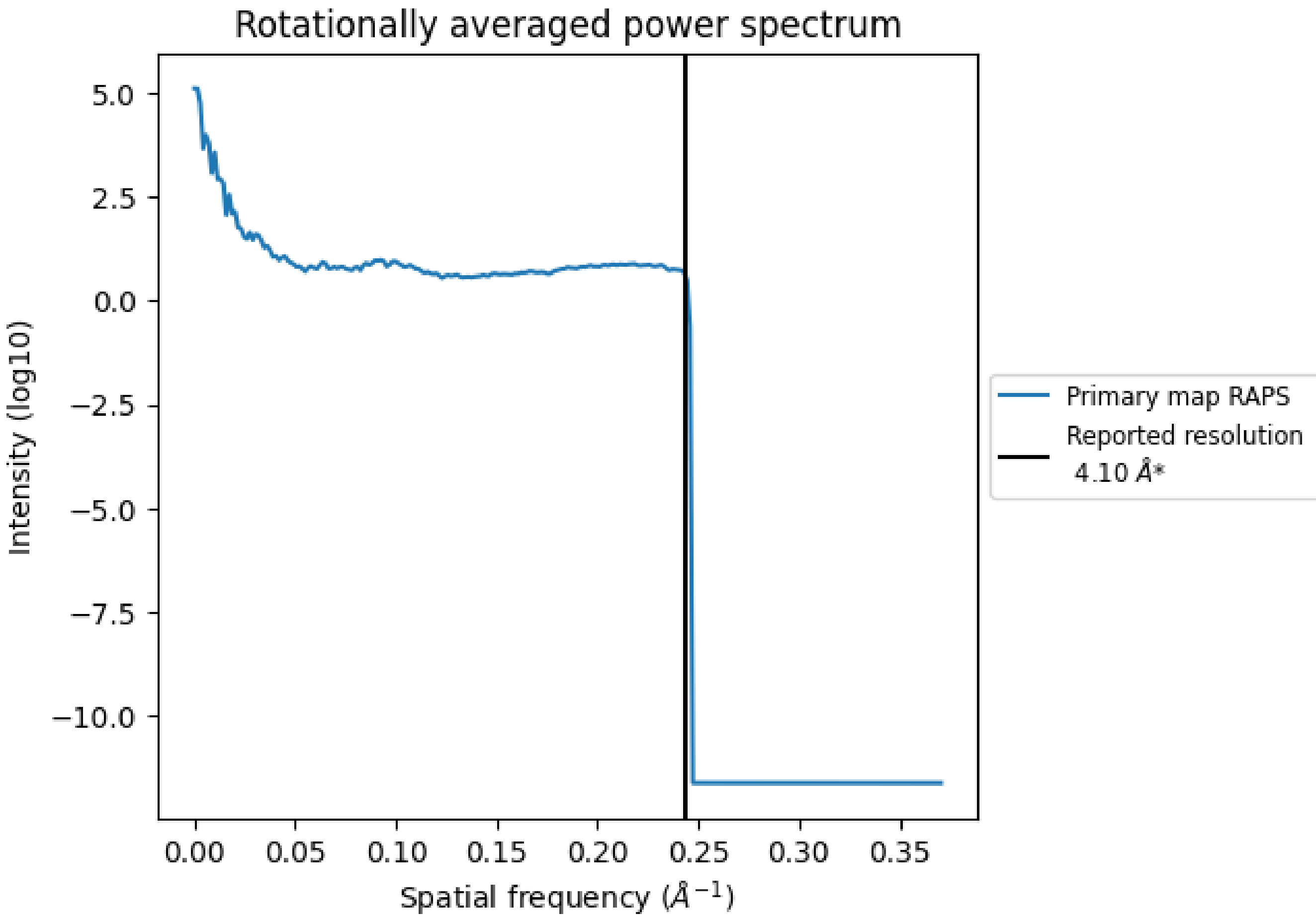
7.2 Volume estimate (i)



The volume at the recommended contour level is 1116 nm^3; this corresponds to an approximate mass of 1008 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

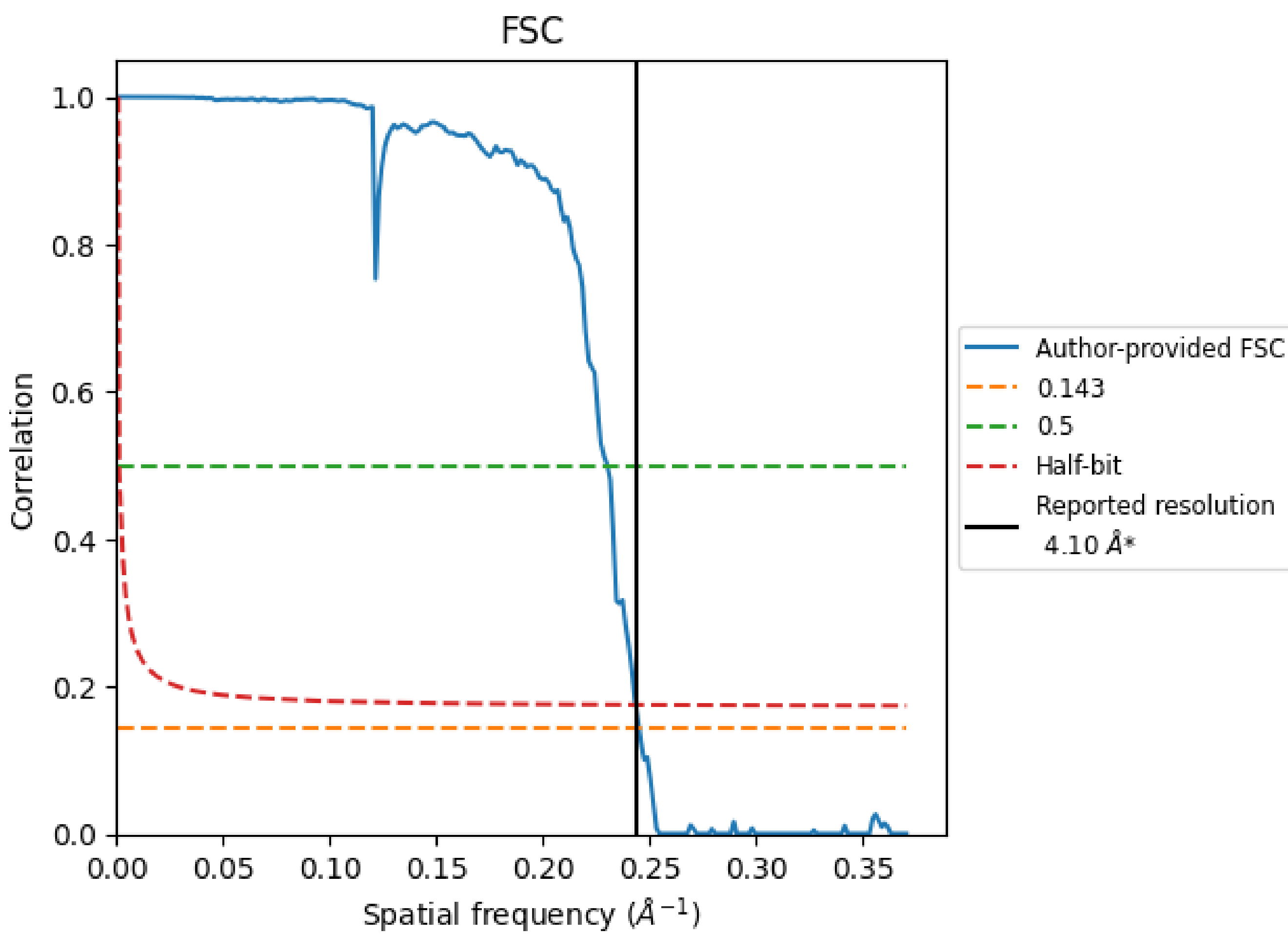


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	4.35	4.11
Unmasked-calculated*	-	-	-

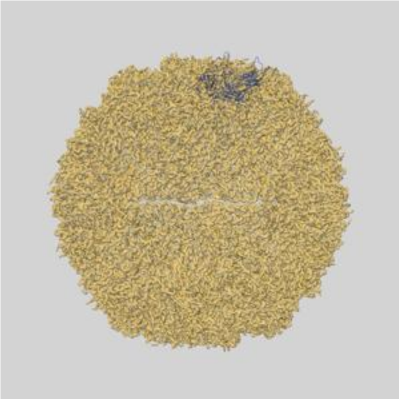
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

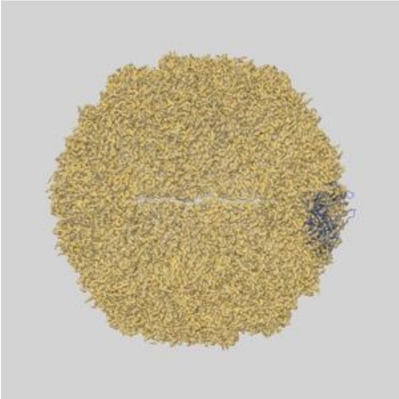
9 Map-model fit (i)

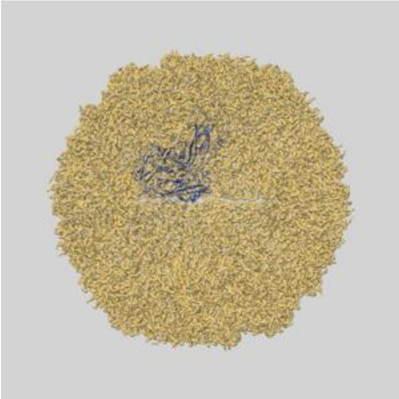
This section contains information regarding the fit between EMDB map EMD-3749 and PDB model 5O5P. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

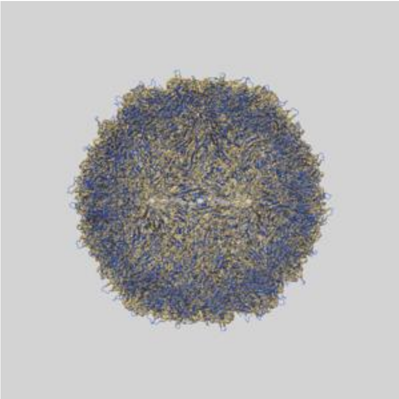
9.1.1 Map-model overlay (i)

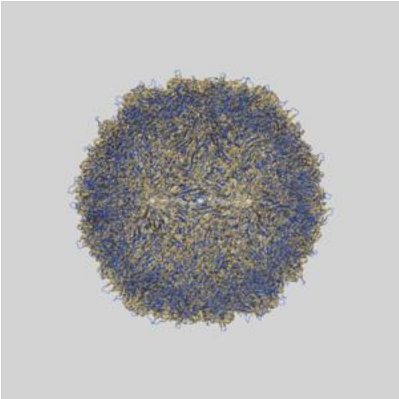

X

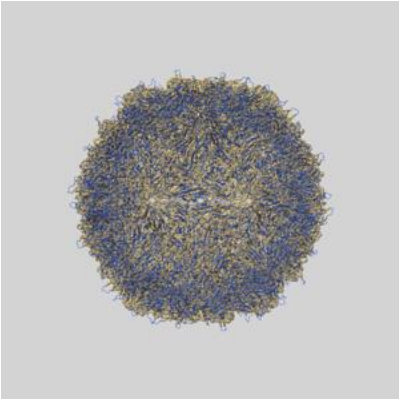

Y


Z

9.1.2 Map-model assembly overlay (i)

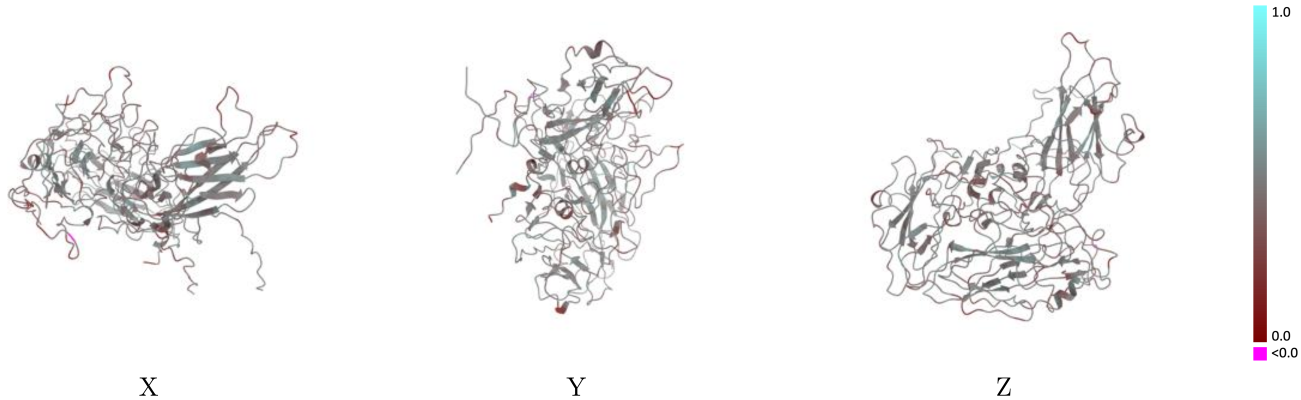

X


Y


Z

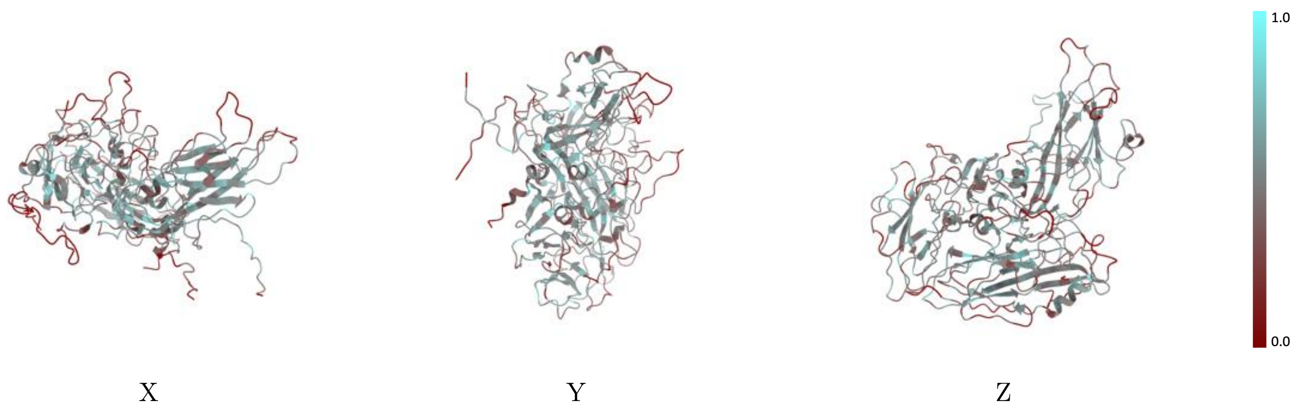
The images above show the 3D surface view of the map at the recommended contour level 0.0475 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



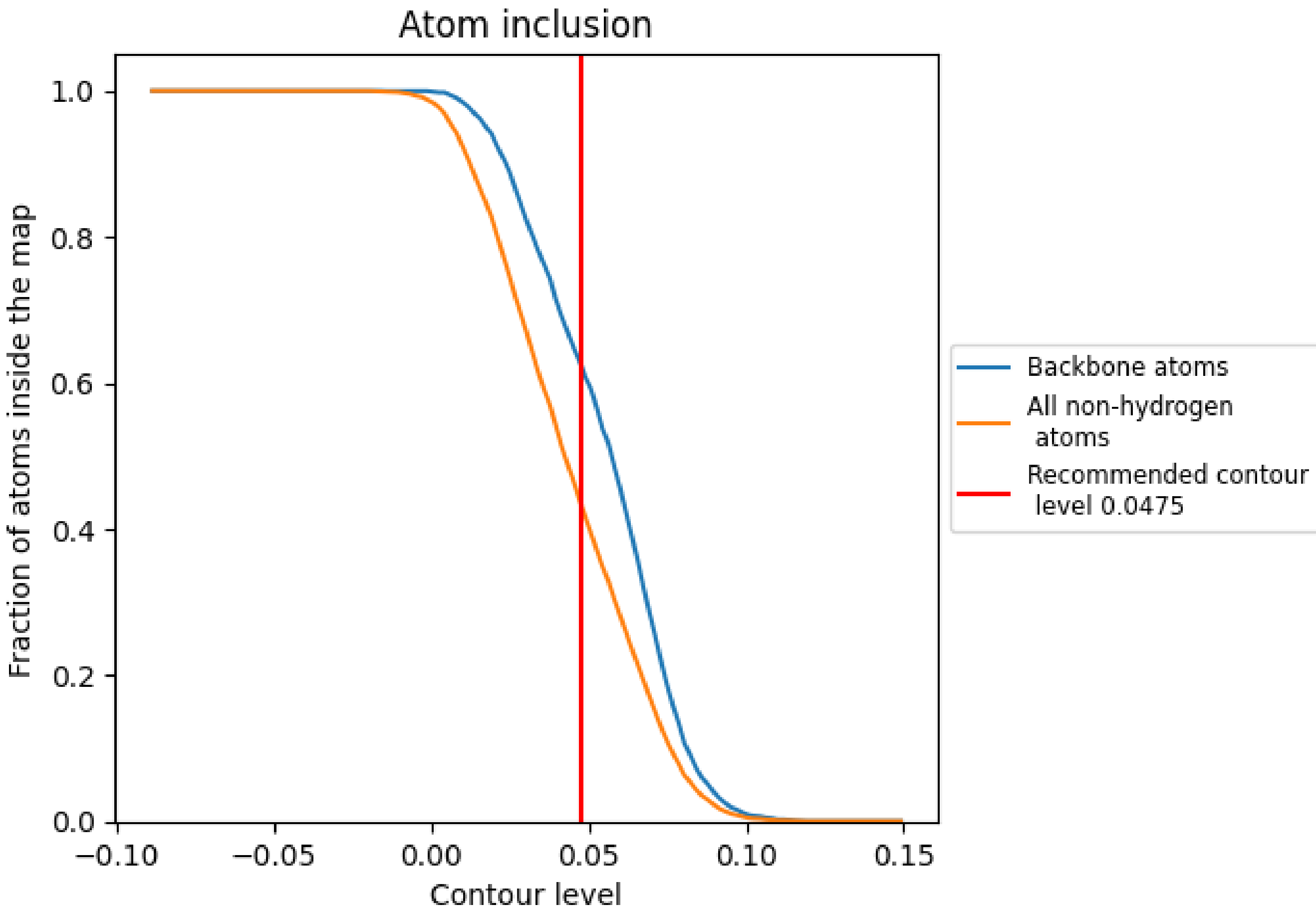
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0475).

9.4 Atom inclusion ⓘ



At the recommended contour level, 63% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0475) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4342	0.4400
1	0.4392	0.4400
2	0.4083	0.4330
3	0.4714	0.4500
4	0.2519	0.4250