Full wwPDB EM Validation Report ⓘ

Sep 5, 2026 – 07:58 am BST

PDB ID	:	9TZ3 / pdb_00009tz3
EMDB ID	:	EMD-56458
Title	:	Cryo-EM structure of human VPS34-CI with ADP:MgF3
Authors	:	Dessus, A.N.; Williams, R.L.
Deposited on	:	2026-01-22
Resolution	:	3.66 Å(reported)
Based on initial model	:	9TW2

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:

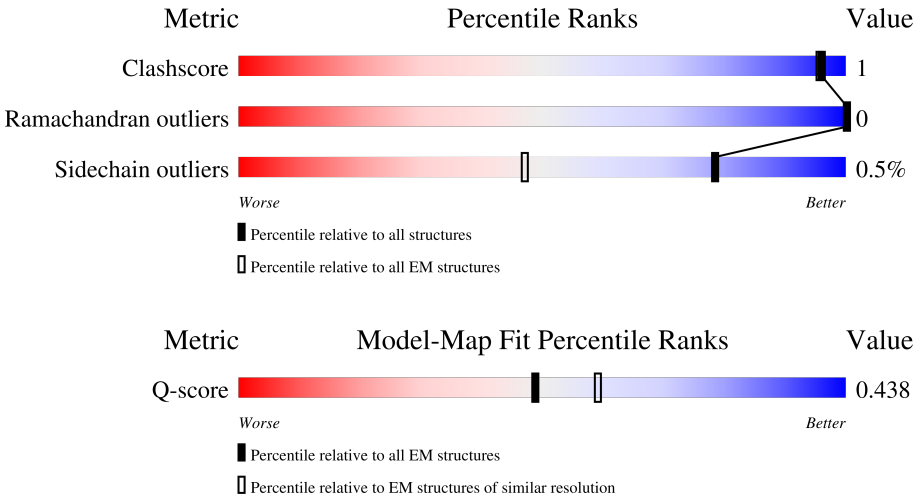
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.66 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.



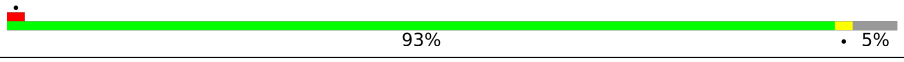
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11491 (3.16 - 4.16)

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	A	887	90% · 8%
2	B	1371	85% · 13%
3	C	450	14% 72% · 24%
3	F	450	· 97%

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Mol	Chain	Length	Quality of chain
4	D	493	
5	E	84	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22318 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 Phosphatidylinositol 3-kinase catalytic subunit type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	813	Total	C	N	O	S	0	0
			6583	4202	1115	1228	38		

- Molecule 2 is a protein called Phosphoinositide 3-kinase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1192	Total	C	N	O	S	0	0
			9481	6042	1651	1740	48		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1359	SER	-	expression tag	UNP Q99570
B	1360	ARG	-	expression tag	UNP Q99570
B	1361	PRO	-	expression tag	UNP Q99570
B	1362	THR	-	expression tag	UNP Q99570
B	1363	THR	-	expression tag	UNP Q99570
B	1364	ALA	-	expression tag	UNP Q99570
B	1365	SER	-	expression tag	UNP Q99570
B	1366	GLU	-	expression tag	UNP Q99570
B	1367	ASN	-	expression tag	UNP Q99570
B	1368	LEU	-	expression tag	UNP Q99570
B	1369	TYR	-	expression tag	UNP Q99570
B	1370	PHE	-	expression tag	UNP Q99570
B	1371	GLN	-	expression tag	UNP Q99570

- Molecule 3 is a protein called Beclin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	341	Total	C	N	O	S	0	0
			2812	1767	478	552	15		
3	F	13	Total	C	N	O	S	0	0
			103	65	19	17	2		

- Molecule 4 is a protein called Beclin 1-associated autophagy-related key regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	321	Total	C	N	O	S	0	0
			2621	1642	476	487	16		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	THR	-	insertion	UNP Q6ZNE5
D	256	SER	ASN	conflict	UNP Q6ZNE5

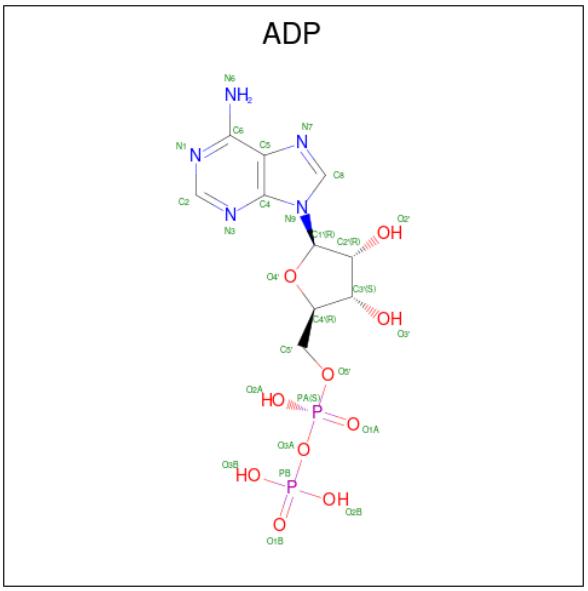
- Molecule 5 is a protein called Nuclear receptor-binding factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	80	Total	C	N	O	S	0	0
			644	398	122	119	5		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	SER	-	expression tag	UNP Q96F24
E	-3	HIS	-	expression tag	UNP Q96F24
E	-2	MET	-	expression tag	UNP Q96F24
E	-1	GLU	-	expression tag	UNP Q96F24
E	0	VAL	-	expression tag	UNP Q96F24

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

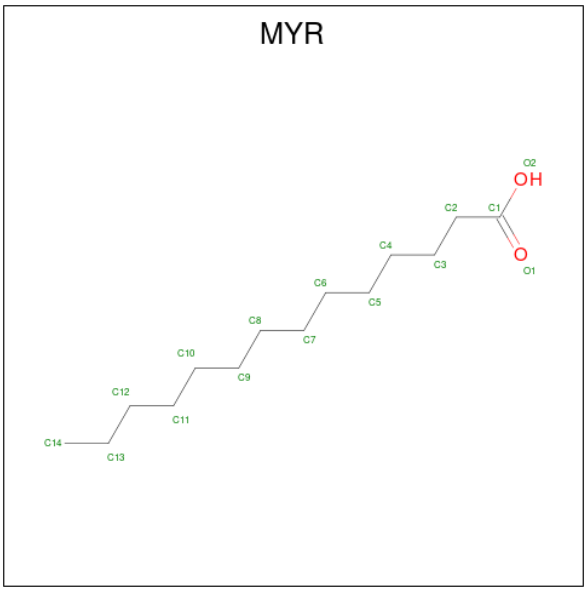


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

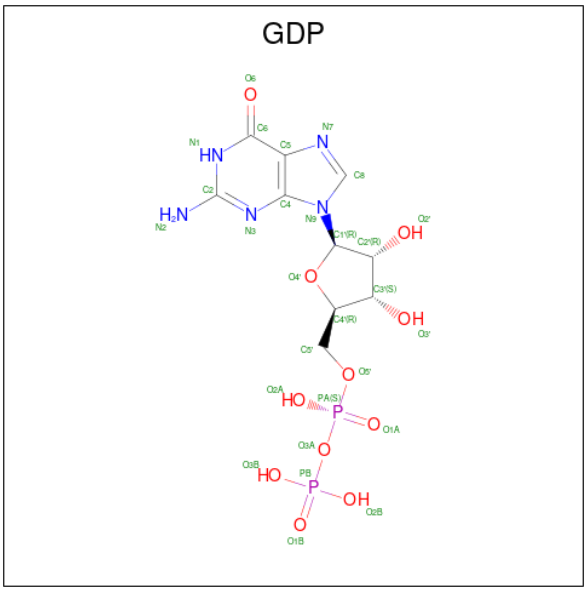
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	

- Molecule 8 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	C	O	0
			15	14	1	

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

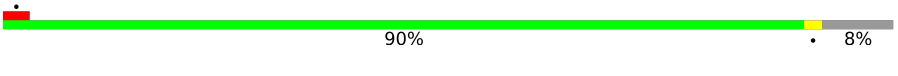
Mol	Chain	Residues	Atoms	AltConf
10	C	1	Total Zn 1 1	0
10	F	1	Total Zn 1 1	0

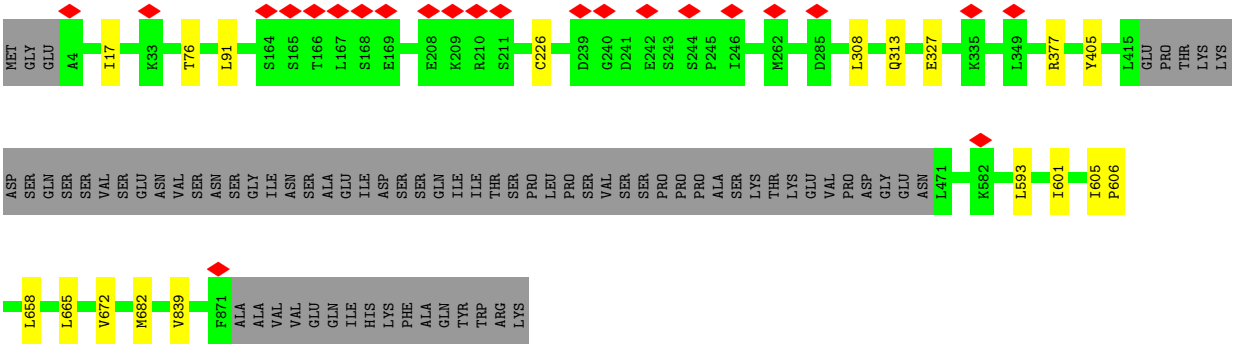
3 Residue-property plots (i)

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: Phosphatidylinositol 3-kinase catalytic subunit type 3

Chain A:

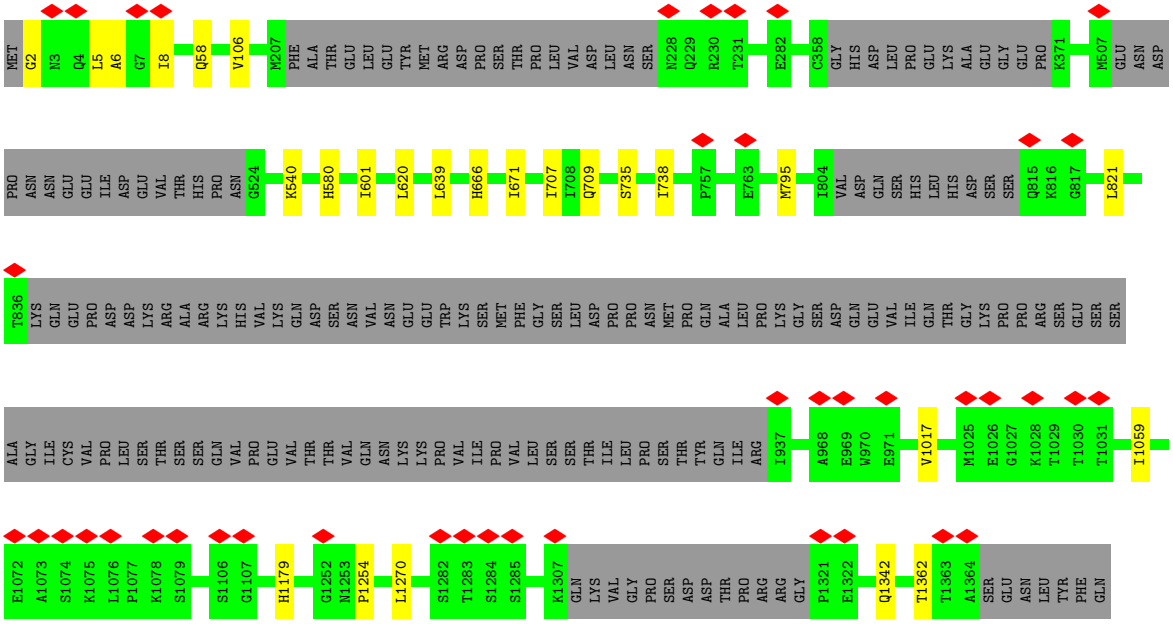




• Molecule 2: Phosphoinositide 3-kinase regulatory subunit 4

Chain B:

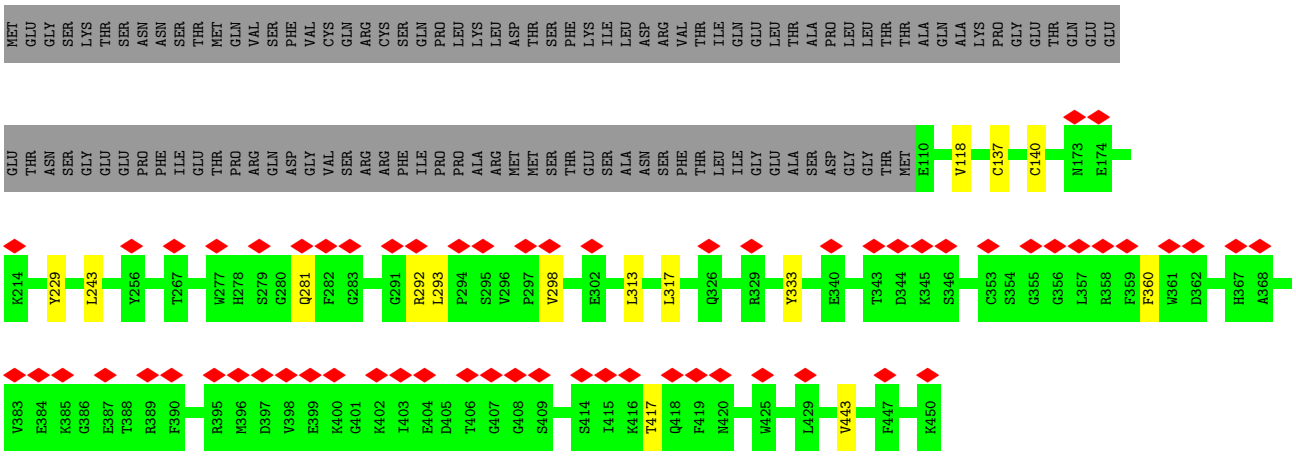




• Molecule 3: Beclin-1

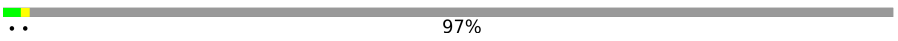
Chain C:

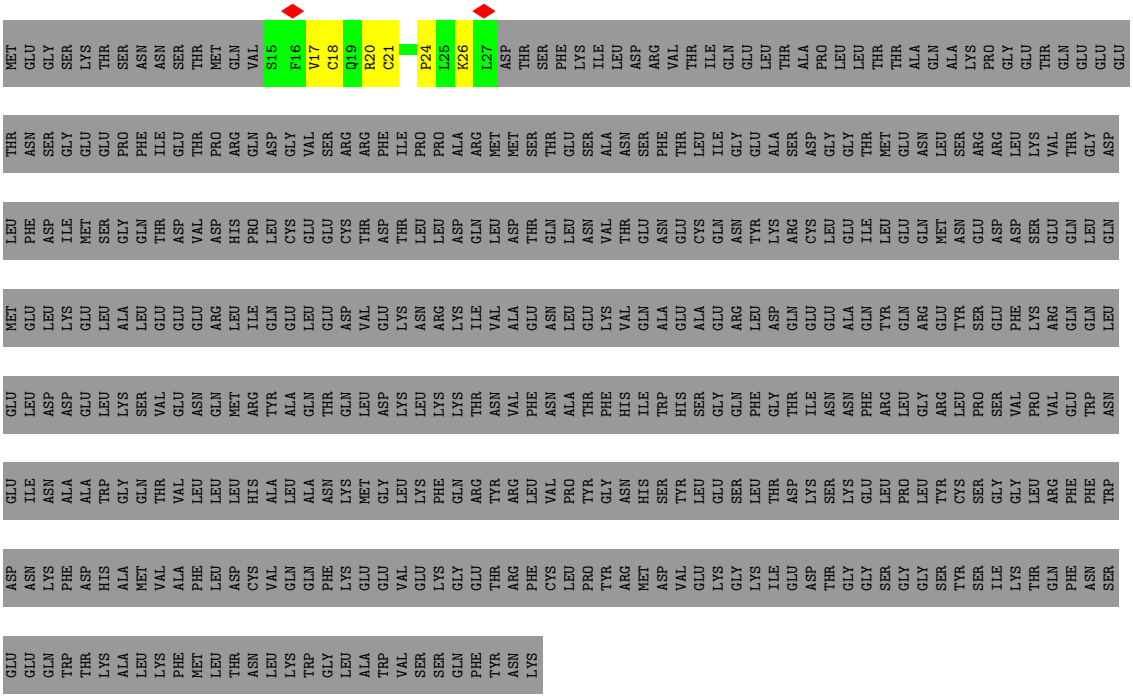




• Molecule 3: Beclin-1

Chain F:

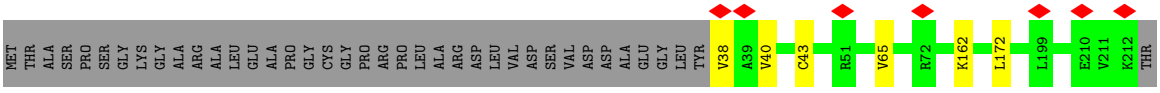


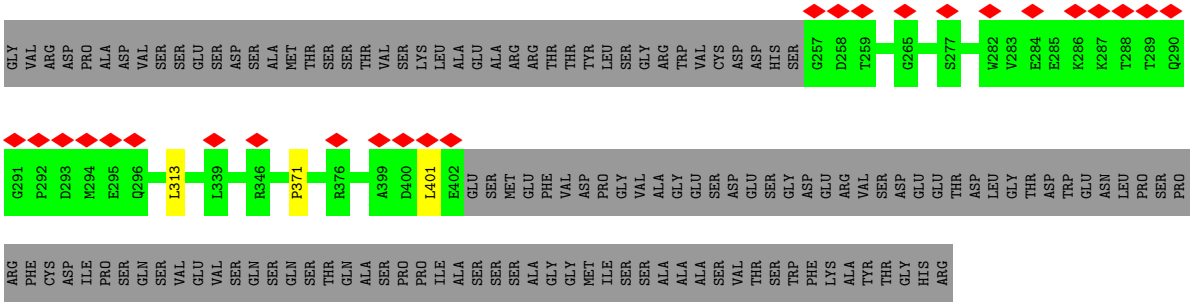


• Molecule 4: Beclin 1-associated autophagy-related key regulator

Chain D:

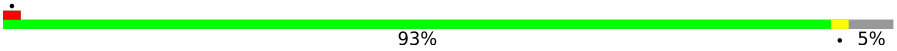


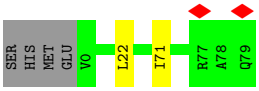




• Molecule 5: Nuclear receptor-binding factor 2

Chain E:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT	Depositor
Number of particles used	186859, 186859, 186859, 186859, 186859, 186859, 186859, 186859, 186859, 186859, 186859, 186859, 186859, 186859, 186859, 186859	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.638	Depositor
Minimum map value	-0.398	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.053	Depositor
Map size (Å)	327.7, 327.7, 327.7	wwPDB
Map dimensions	452, 452, 452	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.14	0/6724	0.36	0/9086
2	B	0.22	1/9684 (0.0%)	0.38	0/13121
3	C	0.16	0/2864	0.33	0/3856
3	F	0.14	0/104	0.42	0/138
4	D	0.16	0/2664	0.39	0/3575
5	E	0.14	0/652	0.28	0/870
All	All	0.18	1/22692 (0.0%)	0.37	0/30646

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GLY	N-CA	-14.80	1.21	1.45

There are no bond angle outliers.

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	6583	0	6610	8	0
2	B	9481	0	9551	13	0
3	C	2812	0	2718	9	0
3	F	103	0	106	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2621	0	2662	7	0
5	E	644	0	658	1	0
6	A	27	0	12	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	15	0	27	1	0
9	B	28	0	12	0	0
10	C	1	0	0	0	0
10	F	1	0	0	0	0
All	All	22318	0	22356	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 1.

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)
3:F:18:CYS:HB3	3:F:21:CYS:SG	2.32	0.70
6:A:900:ADP:O2B	6:A:900:ADP:O2A	2.14	0.65
1:A:672:VAL:HG22	1:A:682:MET:HG2	1.83	0.60
3:C:137:CYS:SG	4:D:43:CYS:CB	2.91	0.57
2:B:1254:PRO:HB2	2:B:1270:LEU:HD12	1.88	0.55
2:B:735:SER:HB3	2:B:738:ILE:HG22	1.90	0.53
3:C:137:CYS:SG	4:D:43:CYS:HB2	2.48	0.53
3:C:137:CYS:HB2	3:C:140:CYS:SG	2.49	0.52
2:B:1017:VAL:HG21	2:B:1059:ILE:HD13	1.95	0.48
3:C:243:LEU:HB3	4:D:172:LEU:HD23	1.95	0.48
3:C:360:PHE:HD1	3:C:417:THR:HB	1.79	0.48
1:A:658:LEU:HD13	1:A:665:LEU:HD12	1.95	0.48
4:D:65:VAL:HG22	3:F:20:ARG:HD2	1.95	0.48
1:A:308:LEU:HB2	1:A:313:GLN:HE21	1.79	0.47
3:C:229:TYR:HE1	4:D:162:LYS:HB2	1.79	0.47
3:F:18:CYS:CB	3:F:21:CYS:SG	2.97	0.45
1:A:226:CYS:HB2	2:B:821:LEU:HB2	1.98	0.45
3:C:292:ARG:HB3	3:C:298:VAL:HB	2.00	0.44
4:D:371:PRO:HD3	4:D:401:LEU:HD11	1.98	0.44
2:B:738:ILE:HD11	2:B:795:MET:HA	1.99	0.44
2:B:8:ILE:HG12	2:B:58:GLN:HB3	1.99	0.44
3:C:317:LEU:HD22	3:C:443:VAL:HG21	2.00	0.43
2:B:5:LEU:HB3	2:B:6:ALA:H	1.68	0.43
2:B:620:LEU:HD13	2:B:639:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ARG:HH22	1:A:405:TYR:HB2	1.83	0.43
4:D:401:LEU:HD12	4:D:401:LEU:HA	1.94	0.43
5:E:22:LEU:HD11	5:E:71:ILE:HD11	2.01	0.42
3:F:26:LYS:HD2	3:F:26:LYS:HA	1.85	0.42
2:B:707:ILE:HG22	2:B:709:GLN:H	1.83	0.42
2:B:601:ILE:HD12	2:B:601:ILE:HA	1.94	0.42
2:B:540:LYS:HA	2:B:540:LYS:HD3	1.90	0.42
1:A:605:ILE:HA	1:A:606:PRO:HD3	1.95	0.41
2:B:1342:GLN:HE22	2:B:1362:THR:HG21	1.85	0.41
3:C:281:GLN:HB2	3:C:293:LEU:HD11	2.02	0.41
8:B:1401:MYR:H91	8:B:1401:MYR:H121	1.93	0.41
1:A:76:THR:HG22	1:A:91:LEU:HD21	2.03	0.41
1:A:593:LEU:HD13	1:A:601:ILE:HG21	2.03	0.41
2:B:666:HIS:CG	2:B:671:ILE:HD11	2.56	0.41
3:F:17:VAL:HA	3:F:24:PRO:HA	2.03	0.41

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	809/887 (91%)	785 (97%)	24 (3%)	0	100	100
2	B	1178/1371 (86%)	1146 (97%)	32 (3%)	0	100	100
3	C	339/450 (75%)	334 (98%)	5 (2%)	0	100	100
3	F	11/450 (2%)	11 (100%)	0	0	100	100
4	D	317/493 (64%)	303 (96%)	14 (4%)	0	100	100
5	E	78/84 (93%)	78 (100%)	0	0	100	100
All	All	2732/3735 (73%)	2657 (97%)	75 (3%)	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	A	733/799 (92%)	730 (100%)	3 (0%)	84 79
2	B	1047/1213 (86%)	1044 (100%)	3 (0%)	86 81
3	C	309/405 (76%)	306 (99%)	3 (1%)	68 72
3	F	13/405 (3%)	13 (100%)	0	100 100
4	D	295/435 (68%)	292 (99%)	3 (1%)	68 72
5	E	67/71 (94%)	67 (100%)	0	100 100
All	All	2464/3328 (74%)	2452 (100%)	12 (0%)	78 79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	327	GLU
1	A	839	VAL
2	B	106	VAL
2	B	580	HIS
2	B	1179	HIS
3	C	118	VAL
3	C	313	LEU
3	C	333	TYR
4	D	38	VAL
4	D	40	VAL
4	D	313	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	141	HIS
1	A	184	GLN
1	A	289	ASN
1	A	560	GLN

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Continued from previous page...

Mol	Chain	Res	Type
1	A	637	HIS
2	B	45	HIS
2	B	121	ASN
2	B	153	ASN
2	B	311	GLN
2	B	457	ASN
2	B	472	GLN
2	B	538	GLN
2	B	554	GLN
2	B	1063	ASN
2	B	1067	GLN
2	B	1240	HIS
3	C	309	GLN
3	C	363	ASN
3	C	449	ASN
4	D	312	GLN
4	D	319	HIS
4	D	331	ASN
4	D	338	ASN

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

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ADP	A	900	7	27,29,29	1.36	4 (14%)	42,45,45	1.97	10 (23%)
8	MYR	B	1401	2	14,14,15	0.49	0	13,13,15	0.83	1 (7%)
9	GDP	B	1402	7	28,30,30	1.16	3 (10%)	44,47,47	1.80	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	A	900	7	-	5/16/32/32	0/3/3/3
8	MYR	B	1401	2	-	8/11/12/13	-
9	GDP	B	1402	7	-	4/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	900	ADP	C5-C4	4.57	1.47	1.39
9	B	1402	GDP	C5-C4	3.04	1.47	1.38
9	B	1402	GDP	C6-N1	-2.66	1.33	1.38
6	A	900	ADP	C5-C6	2.61	1.48	1.41
6	A	900	ADP	C8-N7	2.34	1.36	1.31
9	B	1402	GDP	C5-N7	-2.27	1.34	1.39
6	A	900	ADP	C5-N7	-2.25	1.34	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	900	ADP	C5-C4-N3	-6.17	118.70	126.75
9	B	1402	GDP	C5-C4-N3	-5.96	118.79	128.46
6	A	900	ADP	N3-C4-N9	4.91	135.17	127.08
9	B	1402	GDP	C2-N3-C4	4.75	120.76	112.30
9	B	1402	GDP	N9-C4-N3	4.45	134.87	125.94
6	A	900	ADP	C2-N3-C4	3.84	120.83	111.75
6	A	900	ADP	PA-O3A-PB	-3.48	120.88	132.83
9	B	1402	GDP	PA-O3A-PB	-3.43	121.05	132.83
6	A	900	ADP	N3-C2-N1	-3.17	123.64	128.60
6	A	900	ADP	C4-C5-N7	-3.15	106.78	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1402	GDP	C6-C5-N7	3.09	136.00	130.25
6	A	900	ADP	C5-N7-C8	2.71	107.36	103.51
6	A	900	ADP	C4-N9-C8	2.57	108.52	105.73
9	B	1402	GDP	C4-C5-N7	-2.50	106.77	110.72
6	A	900	ADP	C3'-C2'-C1'	2.49	106.16	101.43
9	B	1402	GDP	C3'-C2'-C1'	2.34	105.86	101.43
8	B	1401	MYR	C4-C3-C2	-2.18	104.30	113.79
6	A	900	ADP	C6-C5-N7	2.10	135.94	132.02
9	B	1402	GDP	O6-C6-C5	-2.09	121.05	126.60

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1401	MYR	C1-C2-C3-C4
9	B	1402	GDP	C5'-O5'-PA-O3A
9	B	1402	GDP	C3'-C4'-C5'-O5'
9	B	1402	GDP	O4'-C4'-C5'-O5'
8	B	1401	MYR	C3-C4-C5-C6
8	B	1401	MYR	C2-C3-C4-C5
8	B	1401	MYR	C10-C11-C12-C13
6	A	900	ADP	PB-O3A-PA-O1A
8	B	1401	MYR	C6-C7-C8-C9
6	A	900	ADP	PA-O3A-PB-O2B
6	A	900	ADP	PA-O3A-PB-O3B
8	B	1401	MYR	C5-C6-C7-C8
9	B	1402	GDP	C5'-O5'-PA-O1A
6	A	900	ADP	PB-O3A-PA-O2A
6	A	900	ADP	O4'-C4'-C5'-O5'
8	B	1401	MYR	C7-C8-C9-C10
8	B	1401	MYR	C9-C10-C11-C12

There are no ring outliers.

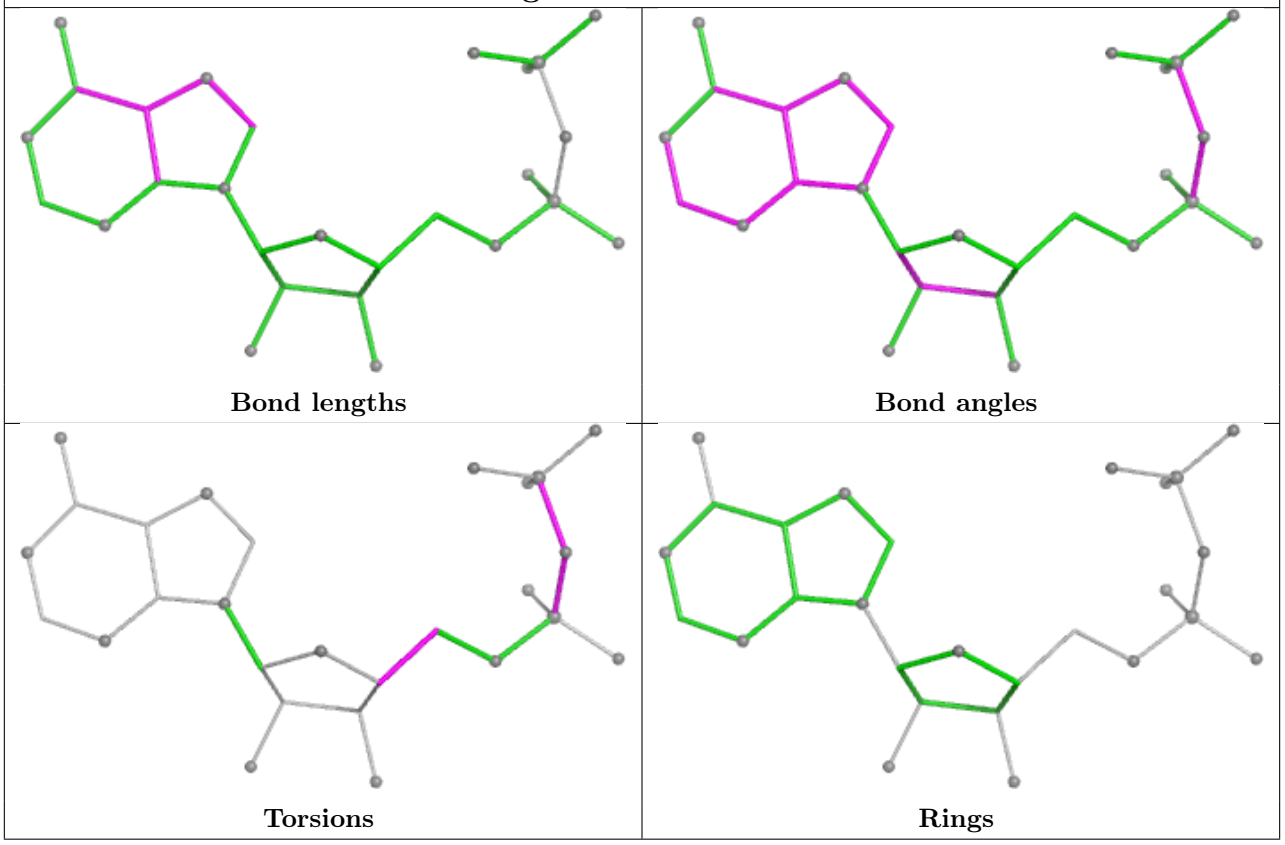
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	900	ADP	1	0
8	B	1401	MYR	1	0

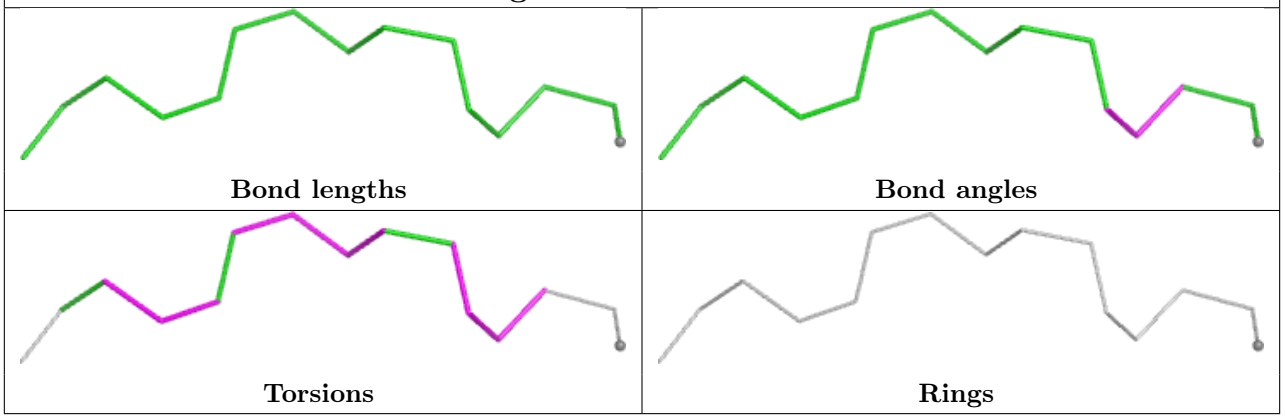
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

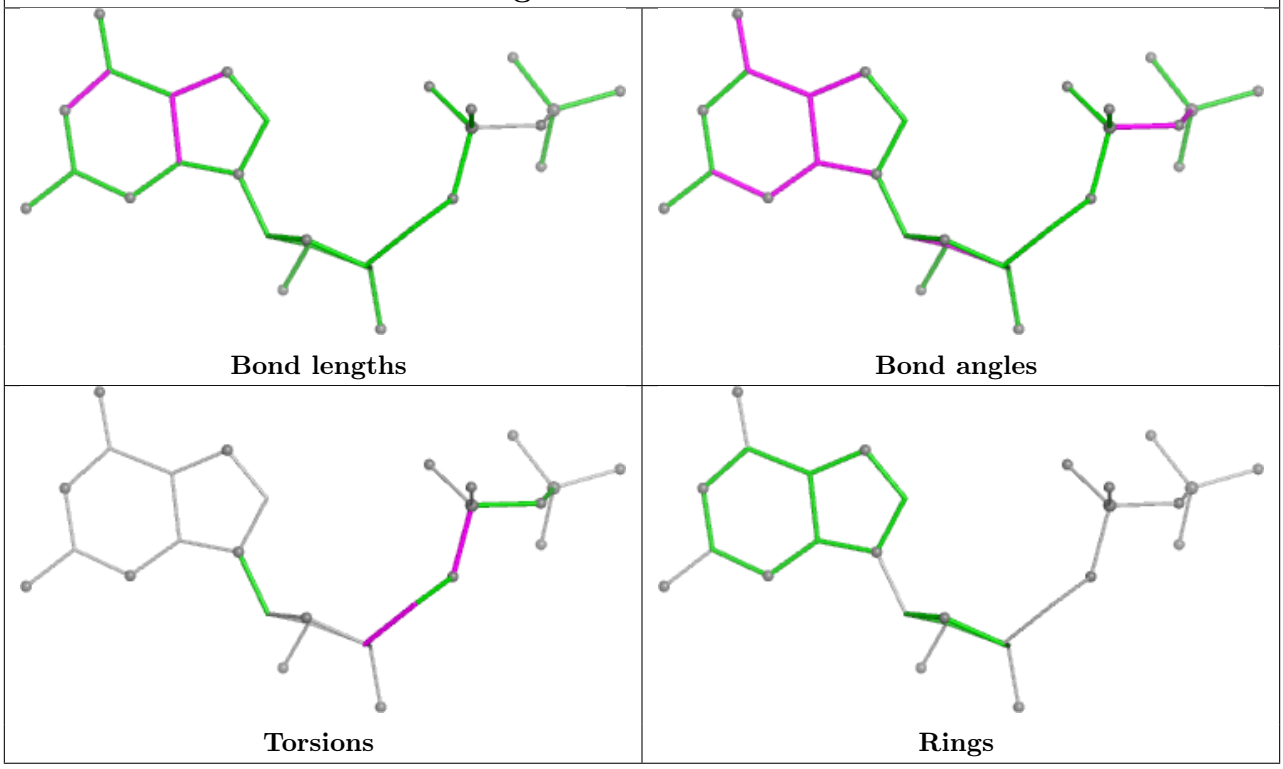
Ligand ADP A 900



Ligand MYR B 1401



Ligand GDP B 1402



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.

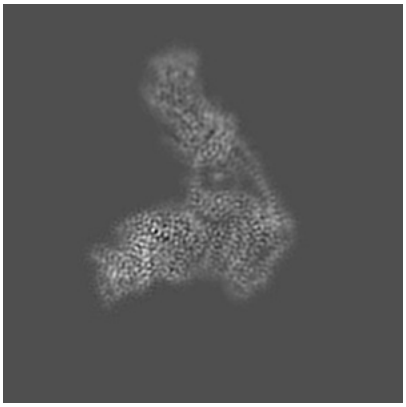
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56458. These allow visual inspection of the internal detail of the map and identification of artifacts.

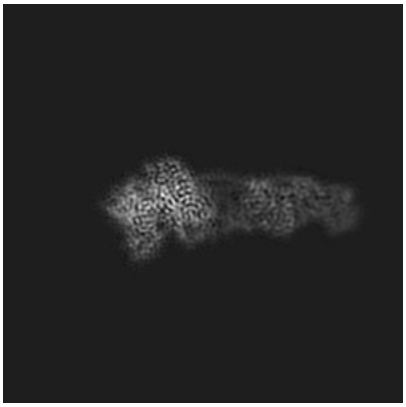
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

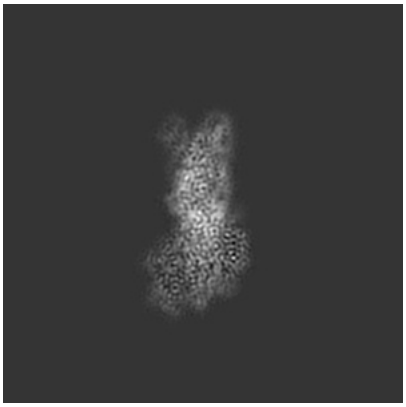
6.1.1 Primary map



X



Y

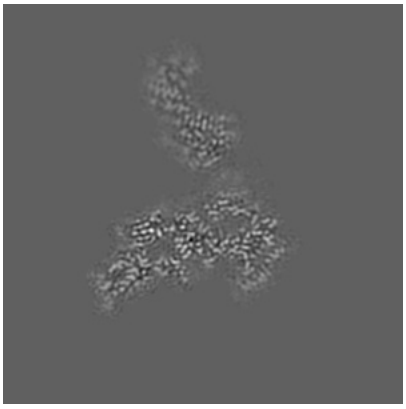


Z

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

6.2 Central slices

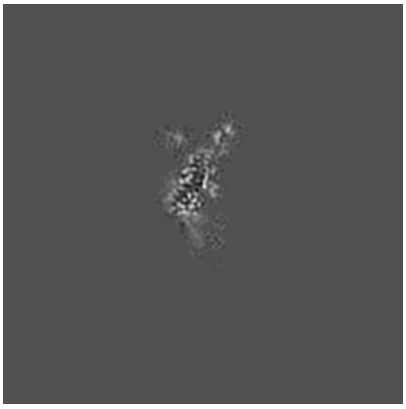
6.2.1 Primary map



X Index: 226



Y Index: 226

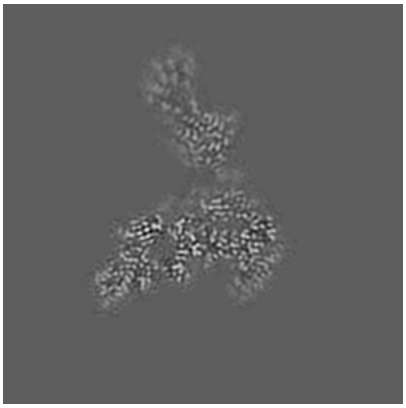


Z Index: 226

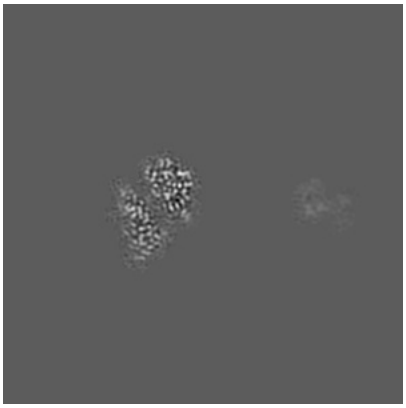
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

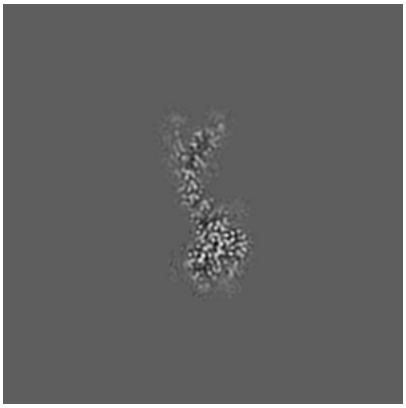
6.3.1 Primary map



X Index: 222



Y Index: 164

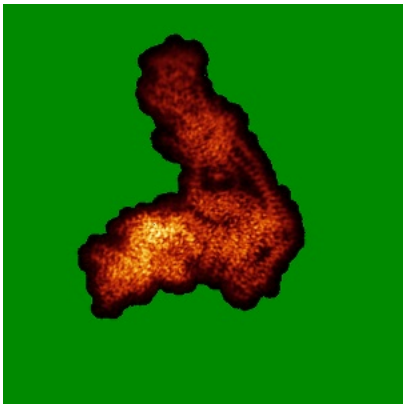


Z Index: 196

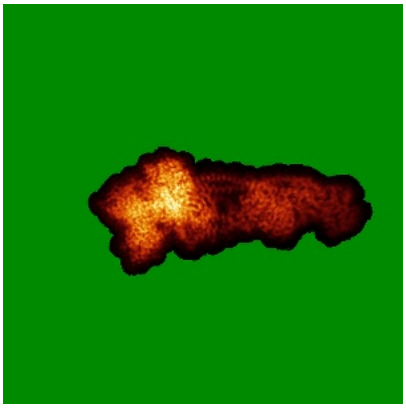
The images above show the largest variance slices of the map in three orthogonal directions.

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

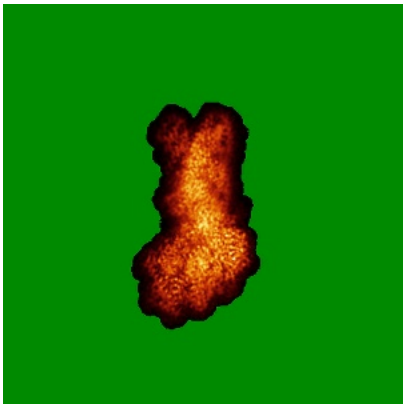
6.4.1 Primary map



X



Y

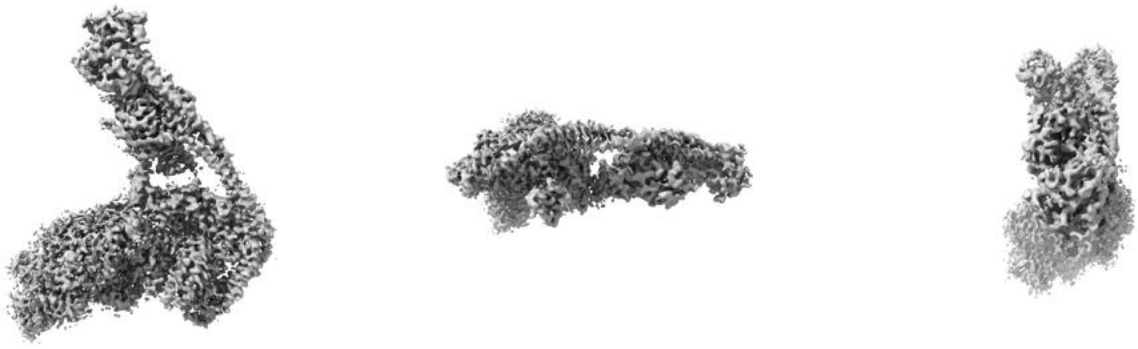


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.053. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

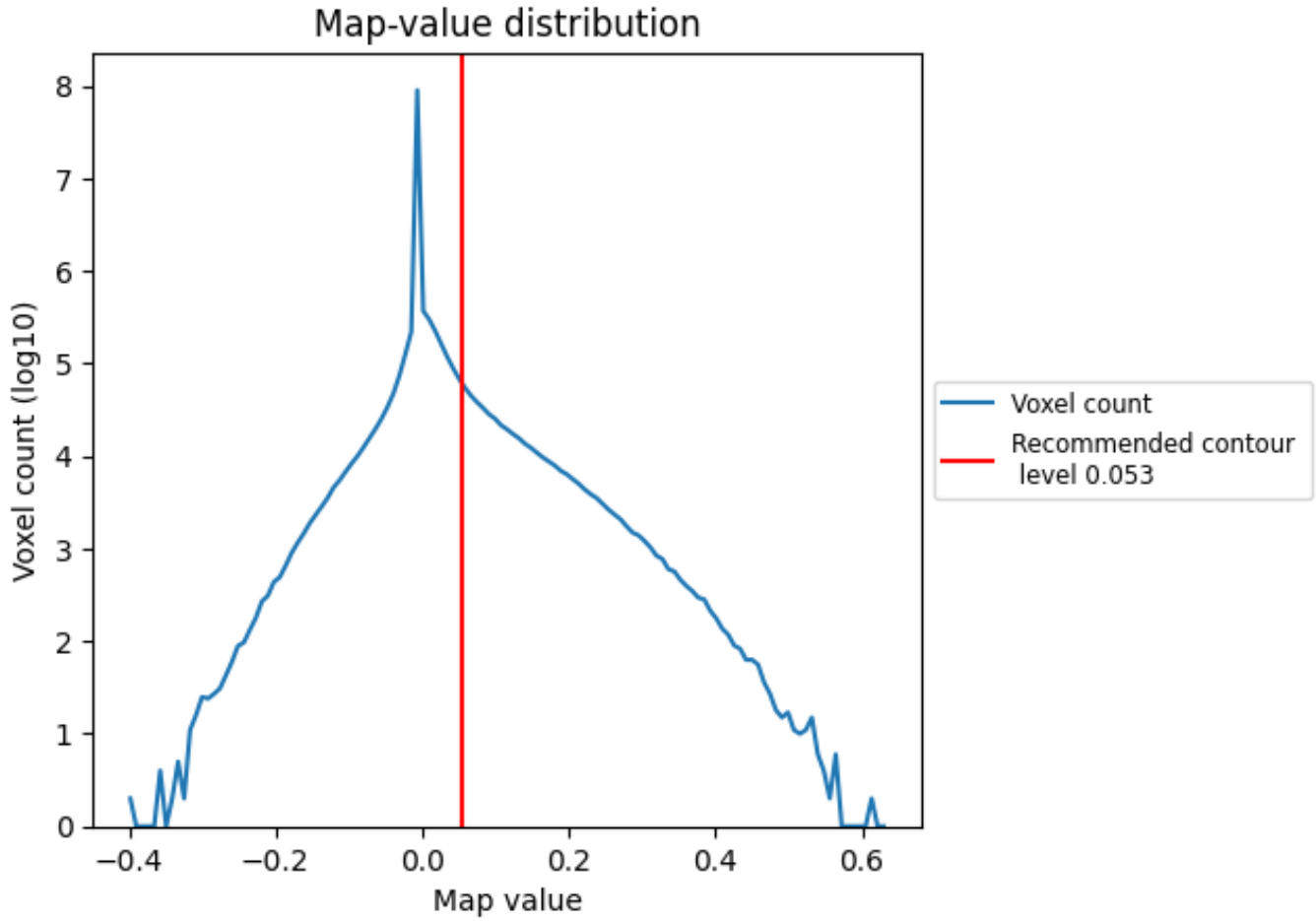
6.6 Mask visualisation (i)

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

7 Map analysis

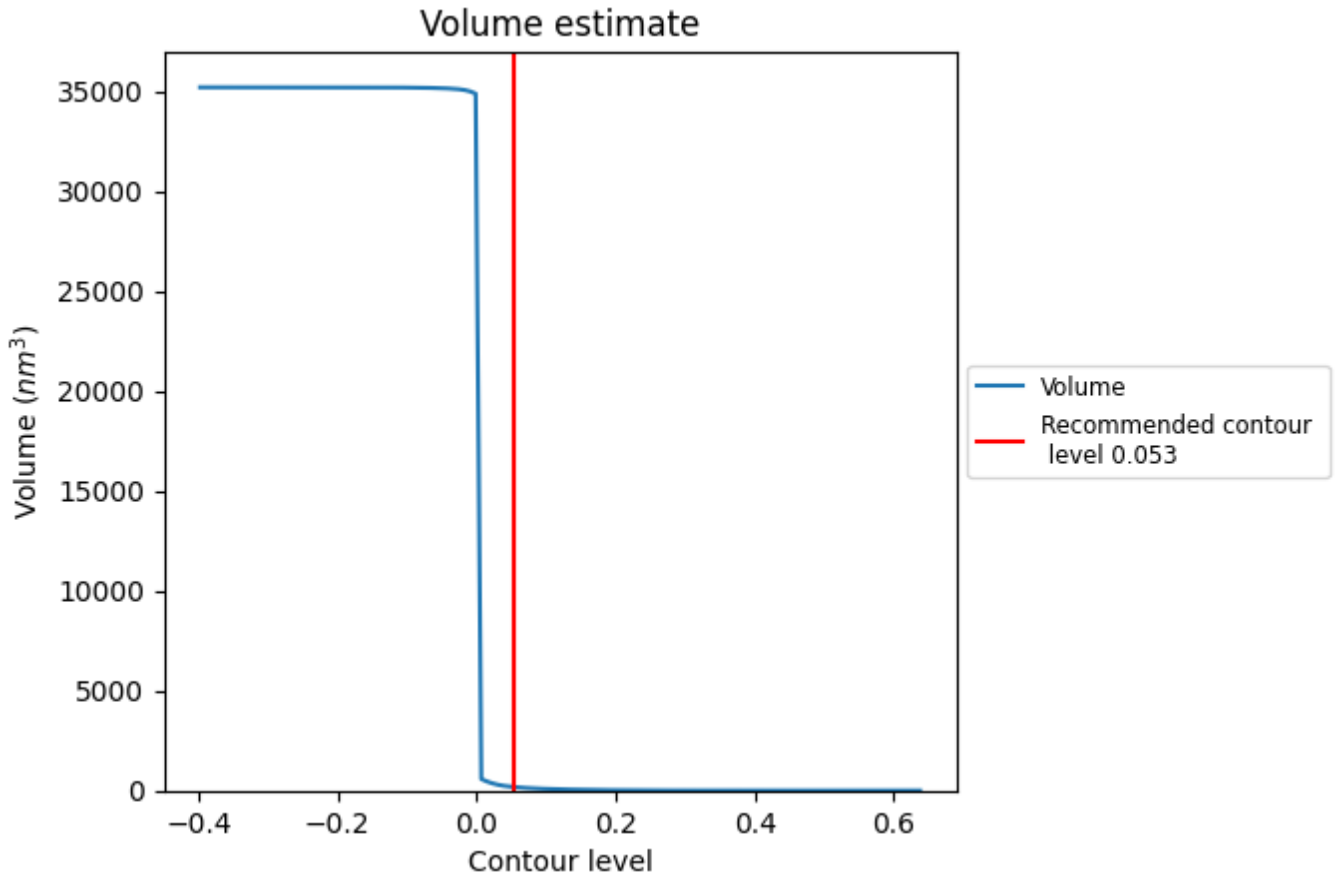
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

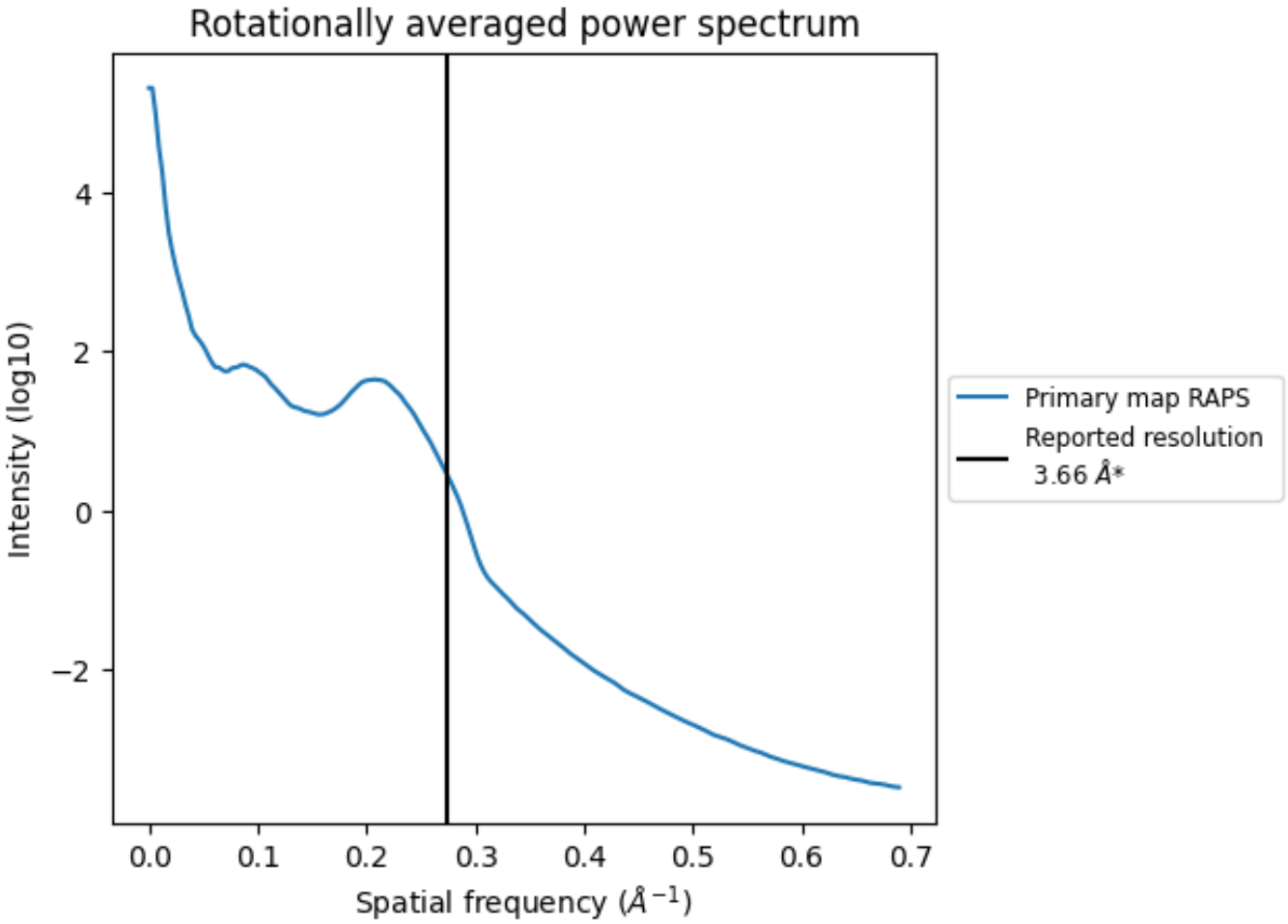
7.2 Volume estimate



The volume at the recommended contour level is 179 nm^3; this corresponds to an approximate mass of 161 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 0.273 Å^{-1}

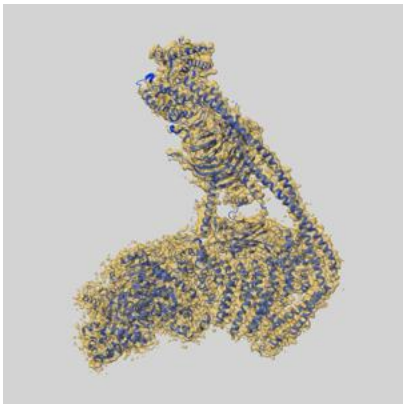
8 Fourier-Shell correlation (i)

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

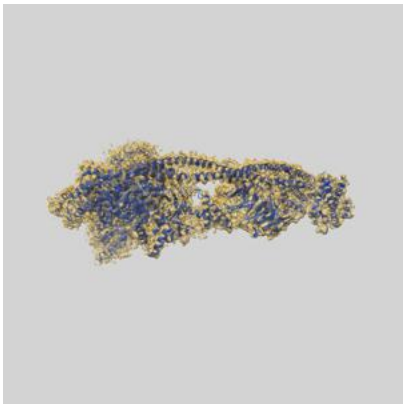
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56458 and PDB model 9TZ3. Per-residue inclusion information can be found in section 3 on page 9.

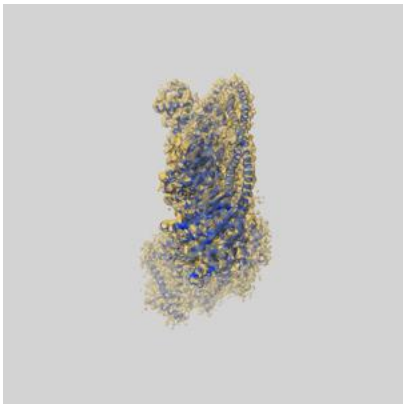
9.1 Map-model overlay



X



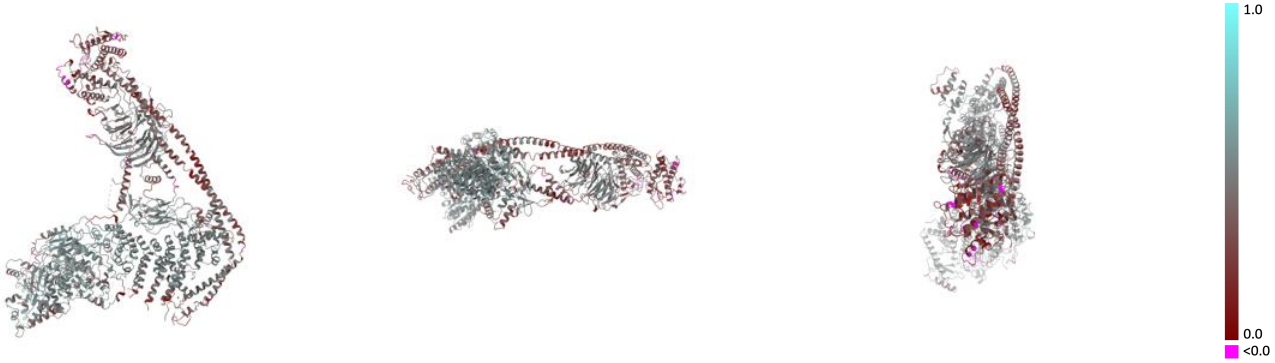
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.053 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.

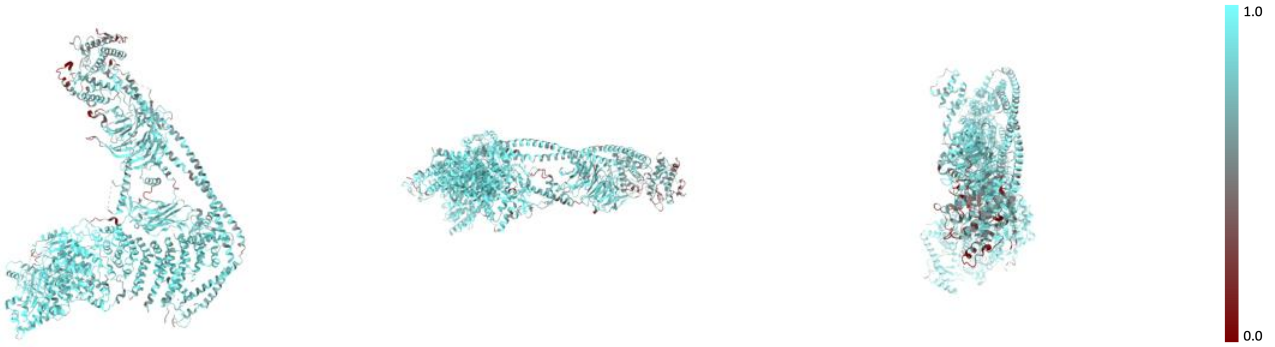
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

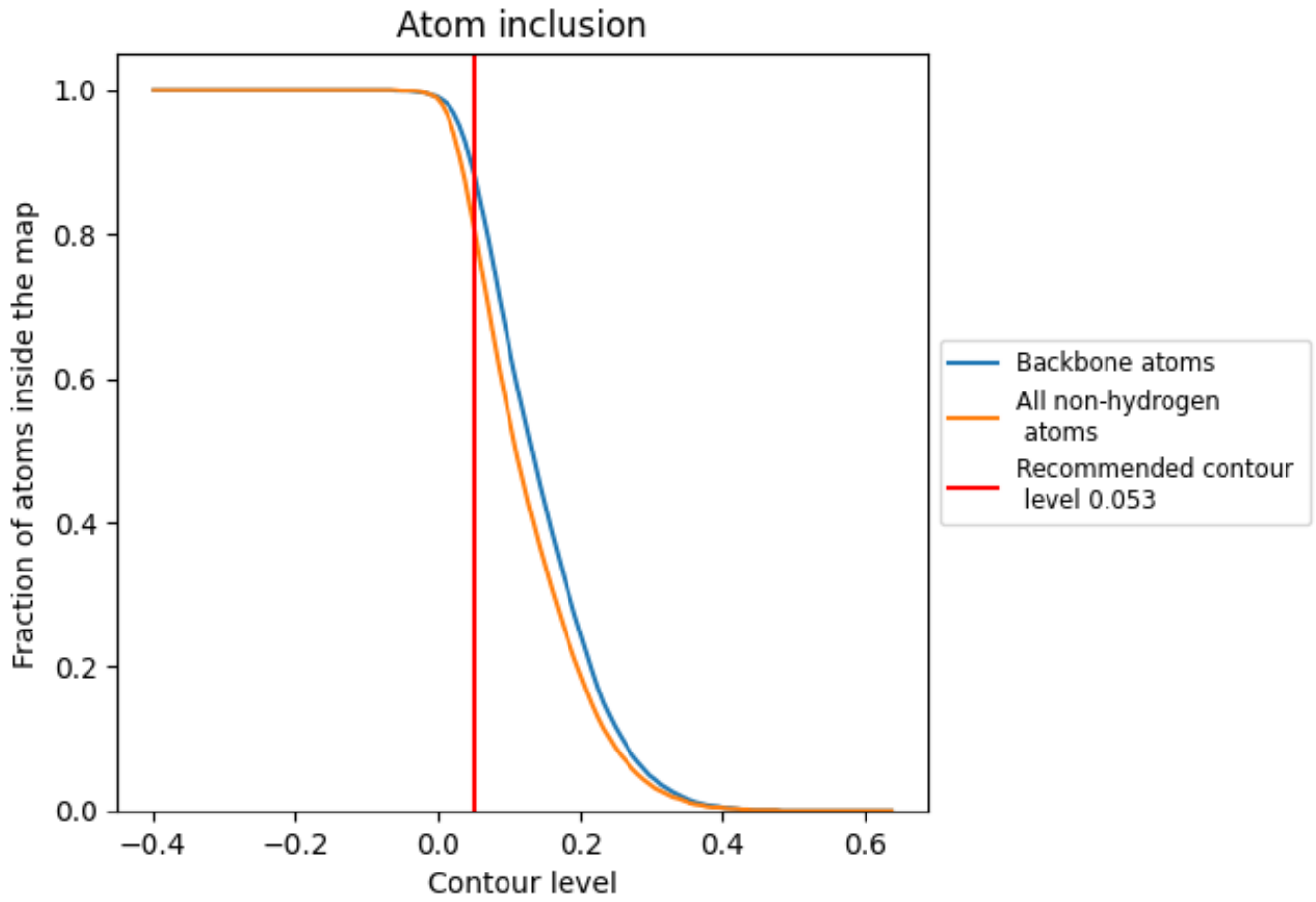
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.053).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.053) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.4380
A	0.8520	0.4780
B	0.8430	0.4710
C	0.6330	0.3210
D	0.6920	0.3450
E	0.8380	0.4630
F	0.6180	0.2620

