wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 12:35 pm BST

PDB ID	:	9I6F / pdb_00009i6f
EMDB ID	:	EMD-52654
Title	:	Cryo-EM structure of HIGD2A bound complex IV
Authors	:	Nguyen, M.D.; Rorbach, J.; Singh, V.
Deposited on	:	2025-01-30
Resolution	:	2.95 Å(reported)
Based on initial model	:	5Z62

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

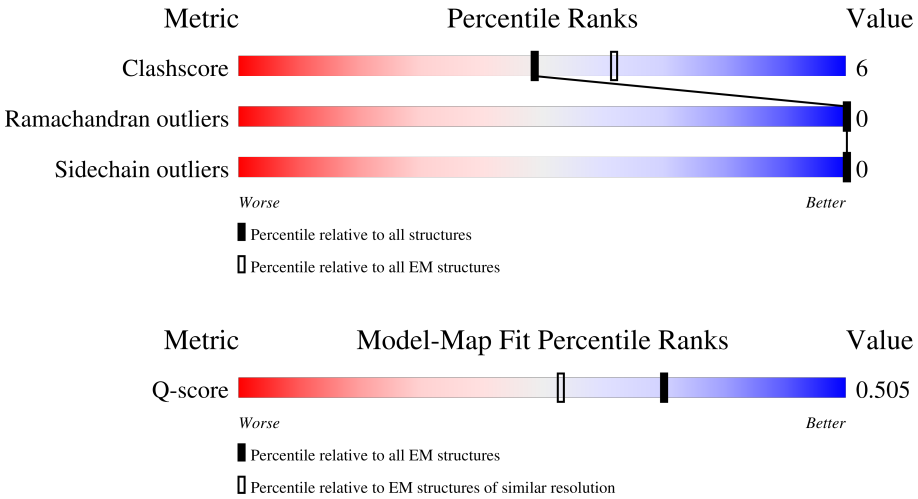
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.95 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	13114 (2.45 - 3.45)

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	N	106	58% 13% 28%
2	A	513	83% 17%
3	B	227	82% 16% •
4	C	261	85% 14%

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Mol	Chain	Length	Quality of chain
5	D	169	
6	E	150	
7	F	129	
8	G	109	
9	H	86	
10	I	75	
11	J	83	
12	K	80	
13	L	63	
14	M	69	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 30444 atoms, of which 15281 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 HIG1 domain family member 2A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	N	76	1196	370	612	109	101	4	0	0

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A	513	8055	2700	4025	622	675	33	0	0

- Molecule 3 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	B	222	3542	1151	1785	274	319	13	0	0

- Molecule 4 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	C	261	4200	1423	2071	340	354	12	0	0

- Molecule 5 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	D	139	2301	746	1147	195	206	7	0	0

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	E	105	1710	546	854	143	165	2	0	0

- Molecule 7 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	92	Total	C	H	N	O	S	0	0
			1389	436	689	126	133	5		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6A1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	75	Total	C	H	N	O	S	0	0
			1214	402	598	110	102	2		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	83	Total	C	H	N	O	S	0	0
			1335	434	642	122	131	6		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	71	Total	C	H	N	O	S	0	0
			1198	377	612	111	94	4		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	58	Total	C	H	N	O	S	0	0
			926	301	469	72	83	1		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	51	Total	C	H	N	O	S	0	0
			808	264	400	71	72	1		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	47	Total	C	H	N	O	S	0	0
			758	250	380	62	64	2		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	M	43	Total	C	H	N	O	S	0	0
			684	222	349	55	56	2		

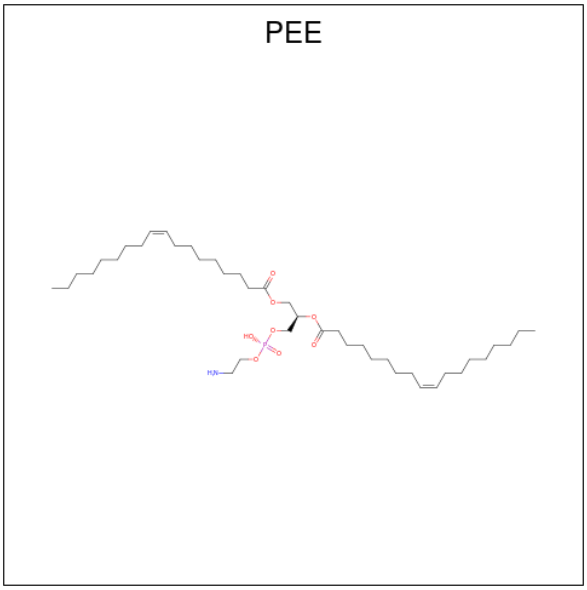
- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Cu	0
			1	1	
15	B	2	Total	Cu	0
			2	2	

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	

- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
17	A	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
17	C	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
17	C	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	

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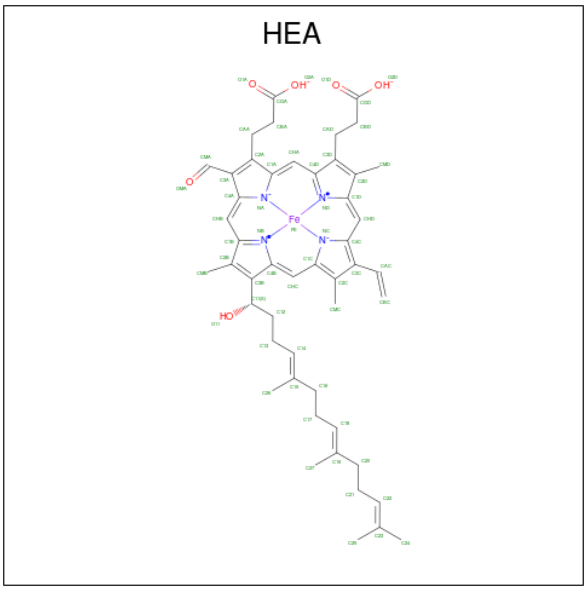
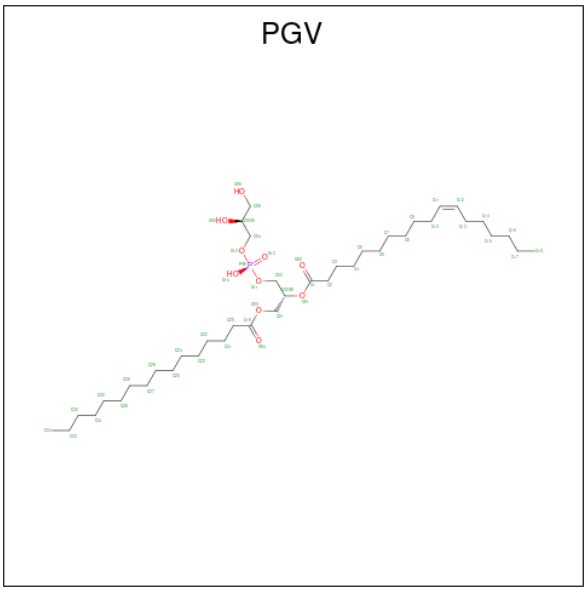
Mol	Chain	Residues	Atoms						AltConf
17	G	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



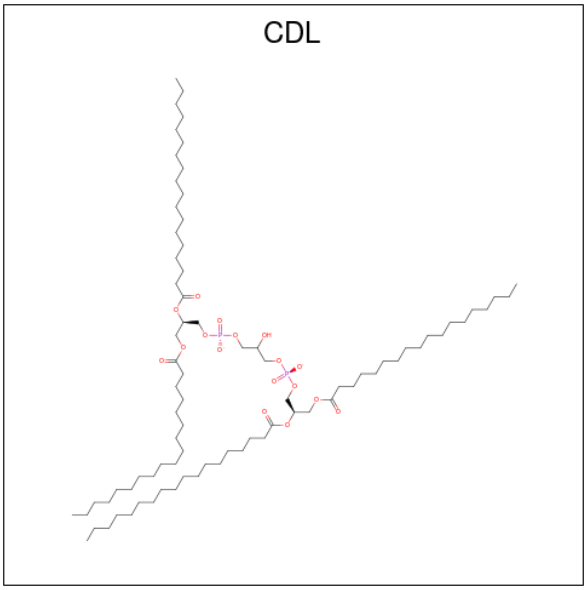
Mol	Chain	Residues	Atoms						AltConf
18	A	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
18	A	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	H	O	P	0
			127	40	76	10	1	

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	F	1	Total	Zn	0
			1	1	

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: HIG1 domain family member 2A, mitochondrial

Chain N:

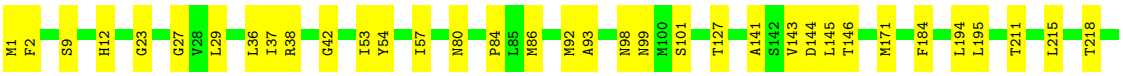




• Molecule 2: Cytochrome c oxidase subunit 1

Chain A:





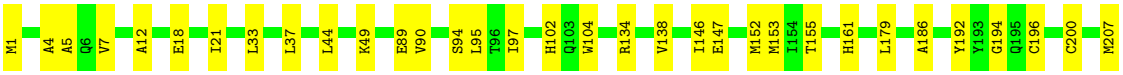


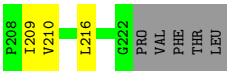


• Molecule 3: Cytochrome c oxidase subunit 2

Chain B:



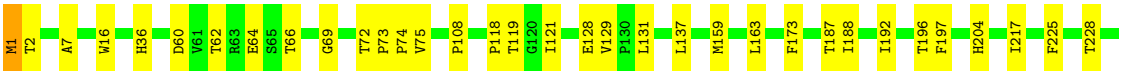


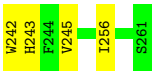


• Molecule 4: Cytochrome c oxidase subunit 3

Chain C:



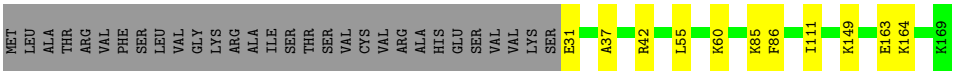




• Molecule 5: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:

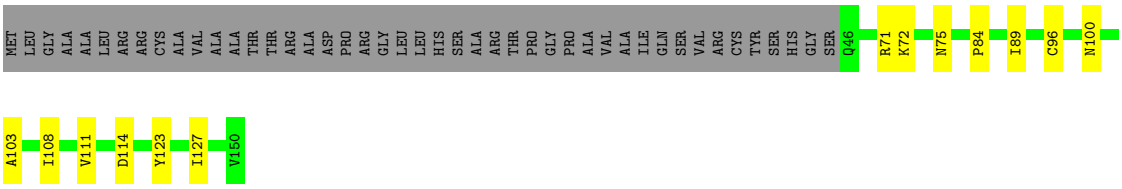




• Molecule 6: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:





• Molecule 7: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:





• Molecule 8: Cytochrome c oxidase subunit 6A1, mitochondrial

Chain G:

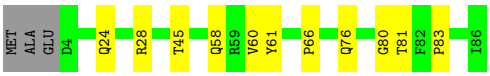




• Molecule 9: Cytochrome c oxidase subunit 6B1

Chain H:





• Molecule 10: Cytochrome c oxidase subunit 6C

Chain I:

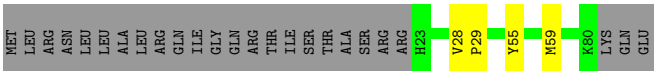




• Molecule 11: Cytochrome c oxidase subunit 7A2, mitochondrial

Chain J:





• Molecule 12: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:





• Molecule 13: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:





• Molecule 14: Cytochrome c oxidase subunit 8A, mitochondrial

Chain M:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	59.084	Depositor
Minimum map value	-37.883	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, PGV, CDL, MG, FME, CU, PEE, ZN

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	N	0.10	0/594	0.31	0/800
2	A	0.11	0/4161	0.36	2/5685 (0.0%)
3	B	0.09	0/1802	0.24	0/2466
4	C	0.10	0/2206	0.27	0/3018
5	D	0.07	0/1187	0.22	0/1594
6	E	0.07	0/874	0.21	0/1187
7	F	0.11	0/715	0.31	0/969
8	G	0.09	0/642	0.26	0/877
9	H	0.10	0/713	0.34	0/964
10	I	0.08	0/597	0.20	0/794
11	J	0.08	0/467	0.23	0/631
12	K	0.08	0/421	0.23	0/576
13	L	0.09	0/390	0.26	0/527
14	M	0.08	0/345	0.21	0/470
All	All	0.10	0/15114	0.29	2/20558 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	328	HIS	CA-C-N	9.59	137.46	120.77
2	A	328	HIS	C-N-CA	9.59	137.46	120.77

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	N	584	612	610	10	0
2	A	4030	4025	4014	59	0
3	B	1757	1785	1780	26	0
4	C	2129	2071	2057	33	0
5	D	1154	1147	1142	10	0
6	E	856	854	852	13	0
7	F	700	689	689	10	0
8	G	616	598	590	7	0
9	H	693	642	640	9	0
10	I	586	612	609	4	0
11	J	457	469	467	2	0
12	K	408	400	398	6	0
13	L	378	380	377	5	0
14	M	335	349	346	2	0
15	A	1	0	0	0	0
15	B	2	0	0	0	0
16	A	1	0	0	0	0
17	A	51	77	82	1	0
17	C	102	154	160	3	0
17	G	51	77	82	2	0
18	A	120	108	108	2	0
19	A	51	76	76	0	0
20	A	100	156	156	0	0
21	F	1	0	0	0	0
All	All	15163	15281	15235	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 177 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:B:200:CYS:SG	3:B:207:MET:SD	2.71	0.88
2:A:440:TYR:OH	3:B:196:CYS:O	1.94	0.85
7:F:91:CYS:SG	7:F:113:CYS:SG	2.46	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:449:THR:OG1	12:K:65:ASN:O	1.97	0.82
4:C:72:THR:O	4:C:75:VAL:N	2.27	0.67

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	N	74/106 (70%)	73 (99%)	1 (1%)	0	100	100
2	A	511/513 (100%)	472 (92%)	39 (8%)	0	100	100
3	B	220/227 (97%)	206 (94%)	14 (6%)	0	100	100
4	C	259/261 (99%)	247 (95%)	12 (5%)	0	100	100
5	D	137/169 (81%)	130 (95%)	7 (5%)	0	100	100
6	E	103/150 (69%)	100 (97%)	3 (3%)	0	100	100
7	F	90/129 (70%)	83 (92%)	7 (8%)	0	100	100
8	G	73/109 (67%)	69 (94%)	4 (6%)	0	100	100
9	H	81/86 (94%)	74 (91%)	7 (9%)	0	100	100
10	I	69/75 (92%)	66 (96%)	3 (4%)	0	100	100
11	J	56/83 (68%)	53 (95%)	3 (5%)	0	100	100
12	K	49/80 (61%)	46 (94%)	3 (6%)	0	100	100
13	L	45/63 (71%)	43 (96%)	2 (4%)	0	100	100
14	M	41/69 (59%)	38 (93%)	3 (7%)	0	100	100
All	All	1808/2120 (85%)	1700 (94%)	108 (6%)	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	N	61/88 (69%)	61 (100%)	0	100	100
2	A	426/426 (100%)	426 (100%)	0	100	100
3	B	197/202 (98%)	197 (100%)	0	100	100
4	C	226/226 (100%)	226 (100%)	0	100	100
5	D	123/149 (83%)	123 (100%)	0	100	100
6	E	94/126 (75%)	94 (100%)	0	100	100
7	F	75/97 (77%)	75 (100%)	0	100	100
8	G	66/92 (72%)	66 (100%)	0	100	100
9	H	75/77 (97%)	75 (100%)	0	100	100
10	I	58/62 (94%)	58 (100%)	0	100	100
11	J	47/69 (68%)	47 (100%)	0	100	100
12	K	43/70 (61%)	43 (100%)	0	100	100
13	L	41/56 (73%)	41 (100%)	0	100	100
14	M	37/59 (63%)	37 (100%)	0	100	100
All	All	1569/1799 (87%)	1569 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
4	C	177	GLN
7	F	111	GLN
10	I	21	ASN
9	H	33	ASN
4	C	38	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	A	1	2	8,9,10	0.51	0	7,9,11	0.96	1 (14%)
4	FME	C	1	4	8,9,10	0.51	0	7,9,11	1.12	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	A	1	2	-	0/7/9/11	-
4	FME	C	1	4	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1	FME	O-C-CA	-2.55	118.10	124.78
2	A	1	FME	O-C-CA	-2.38	118.55	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	FME	O1-CN-N-CA
4	C	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
17	PEE	C	302	-	50,50,50	0.31	0	53,55,55	0.29	0
18	HEA	A	604	2	66,67,67	2.46	26 (39%)	78,103,103	2.41	30 (38%)
17	PEE	C	301	-	50,50,50	0.32	0	53,55,55	0.39	0
17	PEE	A	603	-	50,50,50	0.31	0	53,55,55	0.77	2 (3%)
18	HEA	A	605	2	66,67,67	2.45	26 (39%)	78,103,103	2.39	33 (42%)
17	PEE	G	201	-	50,50,50	0.30	0	53,55,55	0.44	0
20	CDL	A	607	-	99,99,99	0.26	0	105,111,111	0.36	0
19	PGV	A	606	-	50,50,50	0.29	0	53,56,56	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PEE	C	302	-	-	10/54/54/54	-
18	HEA	A	604	2	-	12/36/76/76	-
17	PEE	C	301	-	-	6/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PEE	A	603	-	-	18/54/54/54	-
18	HEA	A	605	2	-	6/36/76/76	-
17	PEE	G	201	-	-	11/54/54/54	-
20	CDL	A	607	-	-	20/110/110/110	-
19	PGV	A	606	-	-	13/55/55/55	-

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	604	HEA	C3A-C2A	5.58	1.48	1.36
18	A	605	HEA	C3A-C2A	5.47	1.48	1.36
18	A	604	HEA	C3B-C2B	5.44	1.47	1.34
18	A	605	HEA	FE-ND	5.42	2.11	1.94
18	A	604	HEA	FE-ND	5.39	2.11	1.94

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	604	HEA	C3C-C4C-NC	7.10	114.61	110.25
18	A	605	HEA	C3C-C4C-NC	6.69	114.36	110.25
18	A	605	HEA	C3D-C4D-ND	6.56	116.71	110.36
18	A	604	HEA	C3D-C4D-ND	6.29	116.44	110.36
18	A	604	HEA	C2B-C1B-NB	5.33	116.27	109.88

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	603	PEE	C11-C10-O2-C2
17	A	603	PEE	O4-C10-O2-C2
17	A	603	PEE	C1-O3P-P-O1P
17	C	301	PEE	O5-C30-O3-C3
17	C	301	PEE	C31-C30-O3-C3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	302	PEE	2	0
18	A	604	HEA	1	0

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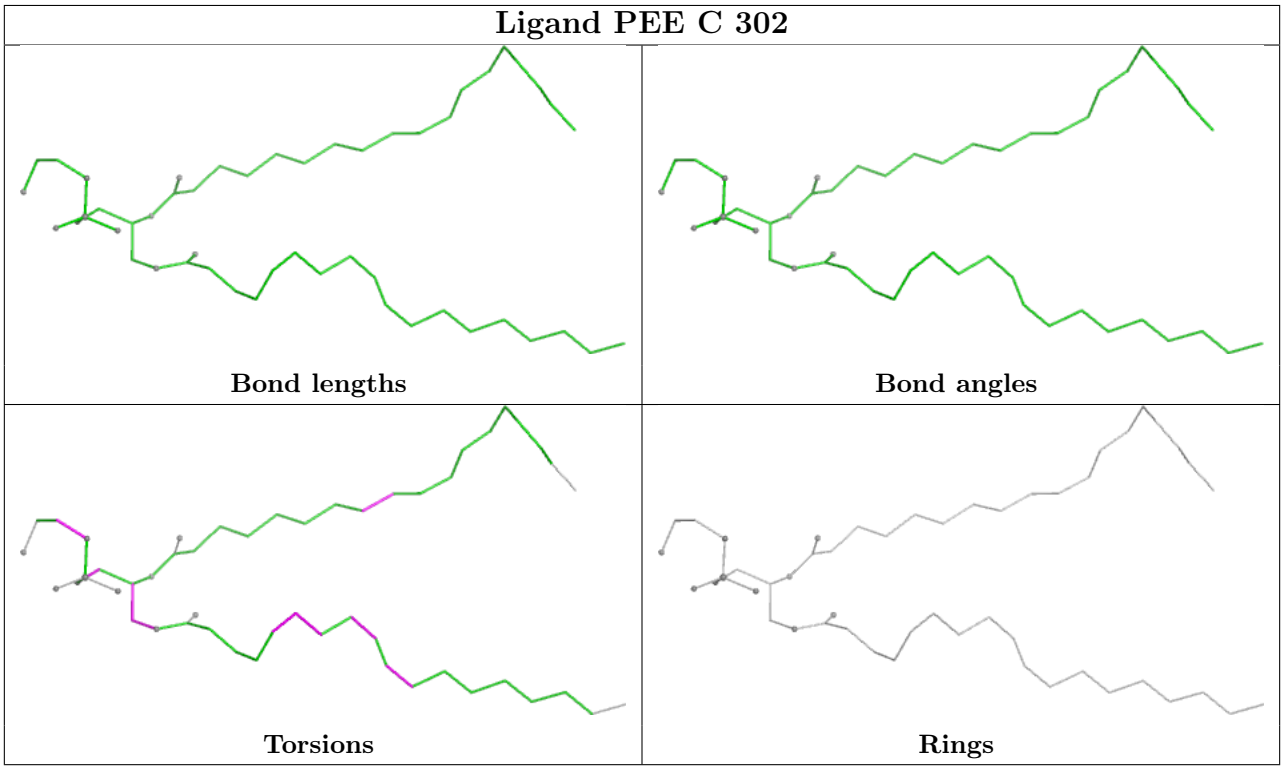
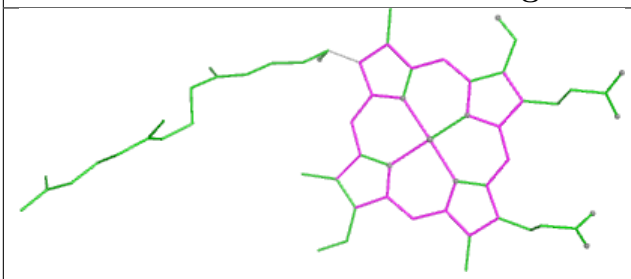
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	301	PEE	1	0
17	A	603	PEE	1	0
18	A	605	HEA	1	0
17	G	201	PEE	2	0

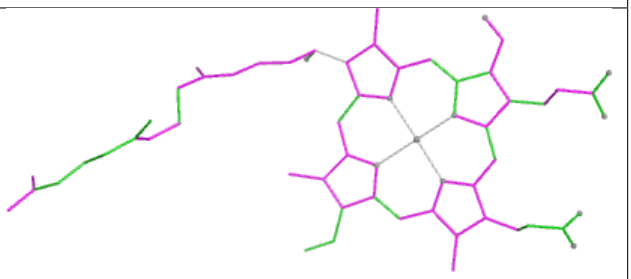
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



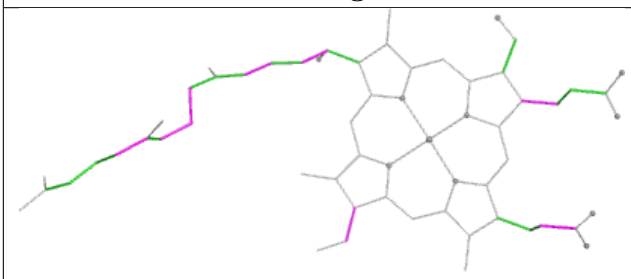
Ligand HEA A 604



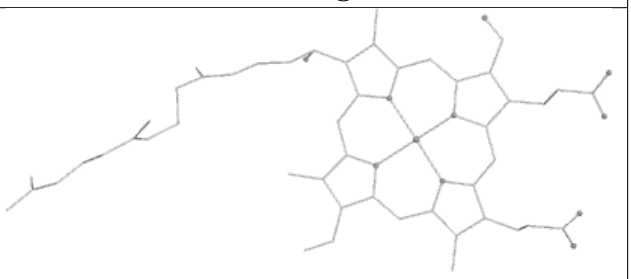
Bond lengths



Bond angles

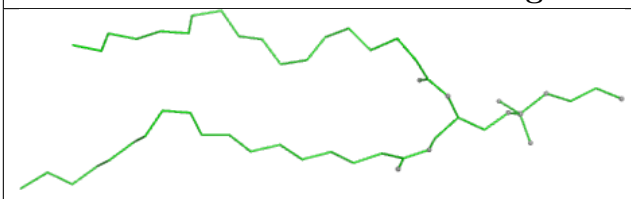


Torsions

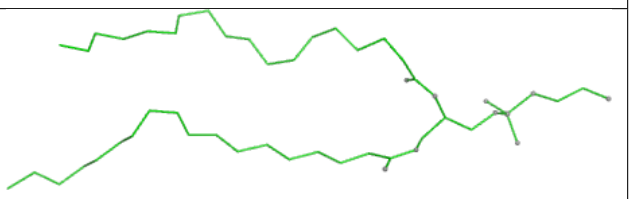


Rings

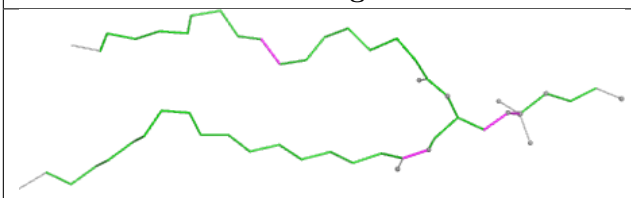
Ligand PEE C 301



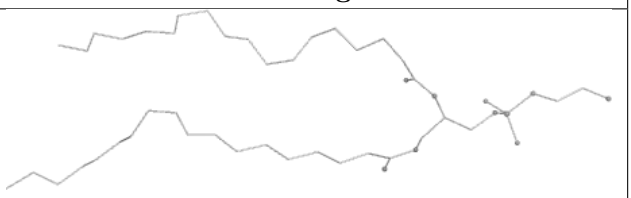
Bond lengths



Bond angles

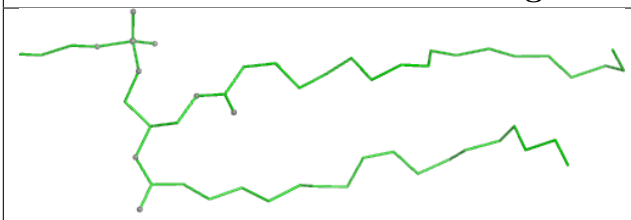


Torsions

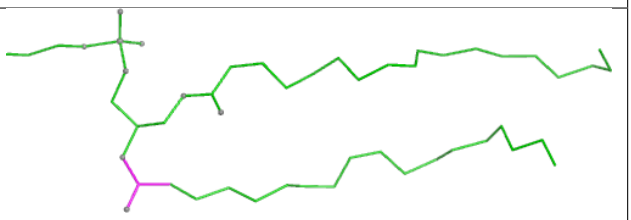


Rings

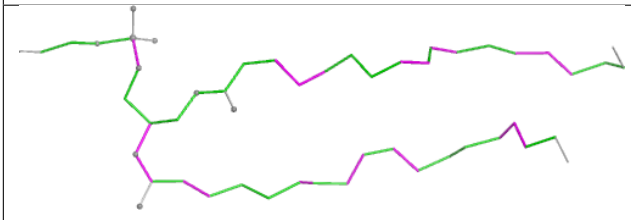
Ligand PEE A 603



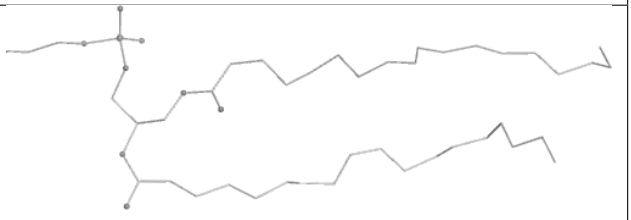
Bond lengths



Bond angles

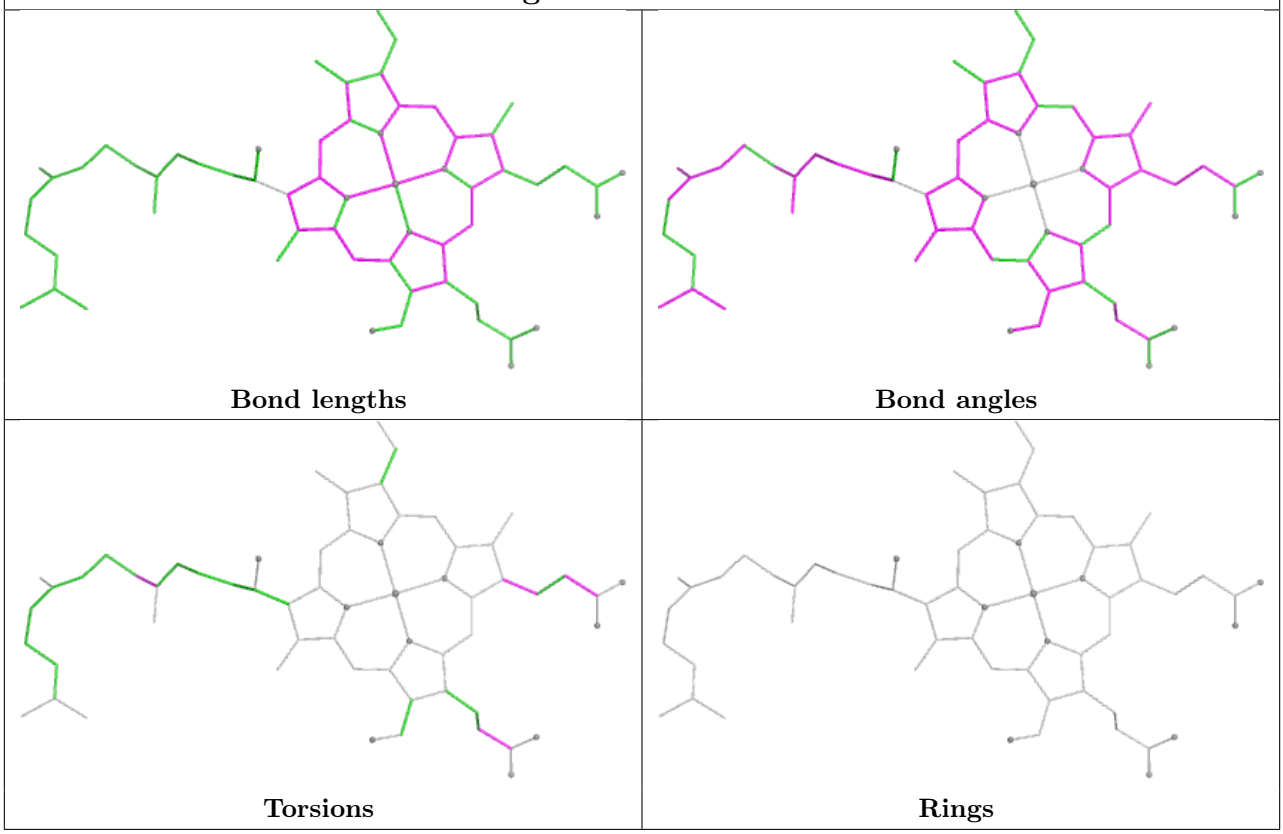


Torsions

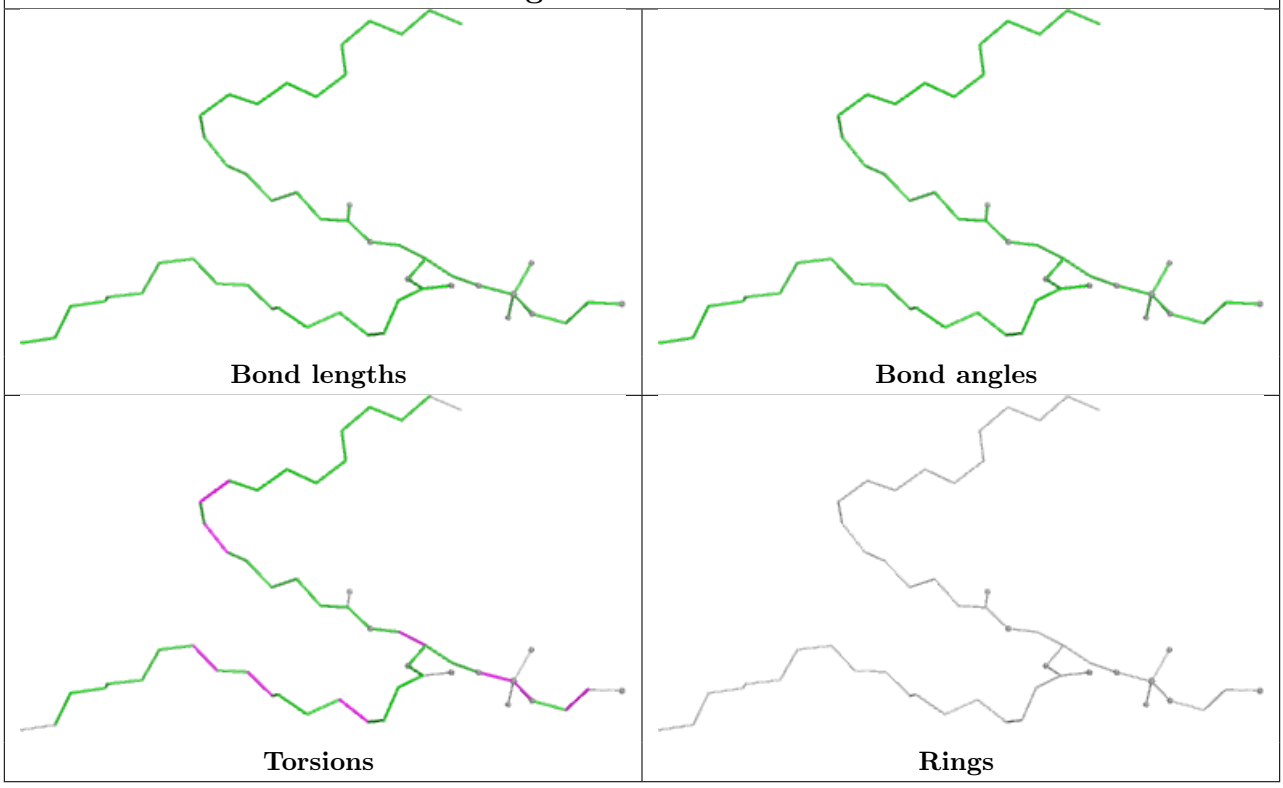


Rings

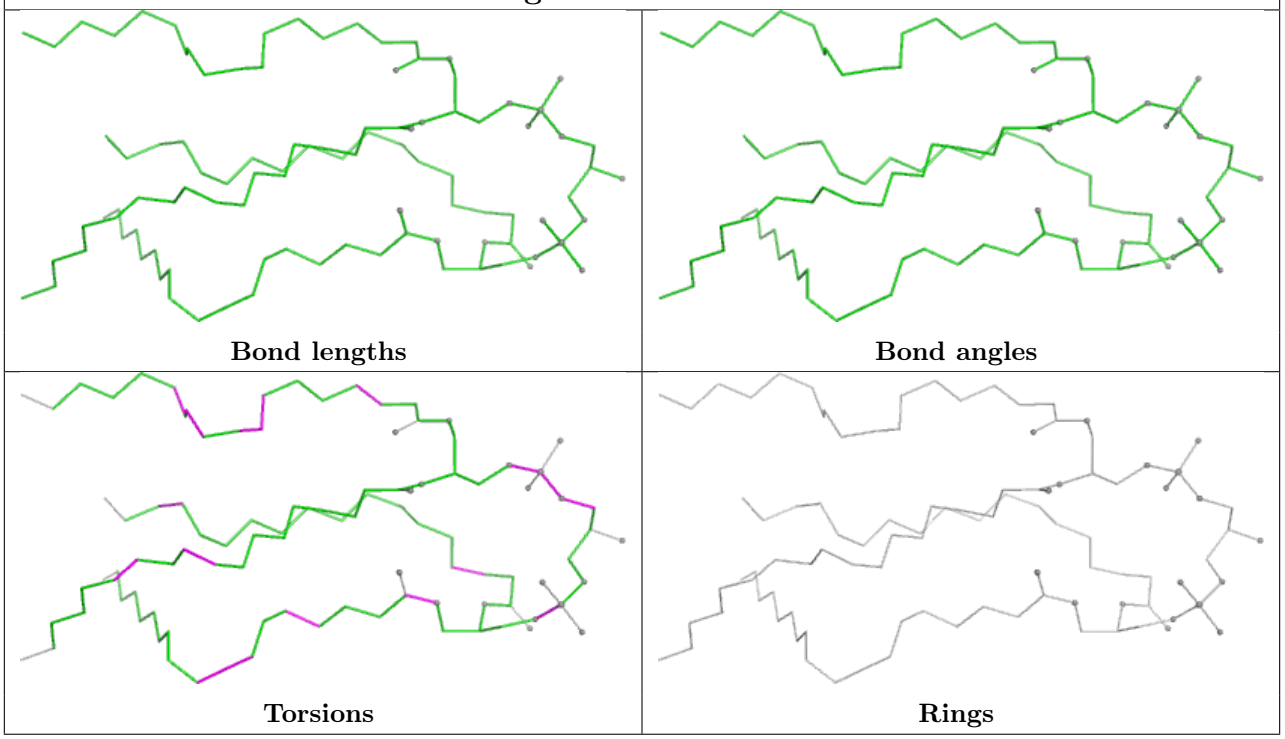
Ligand HEA A 605



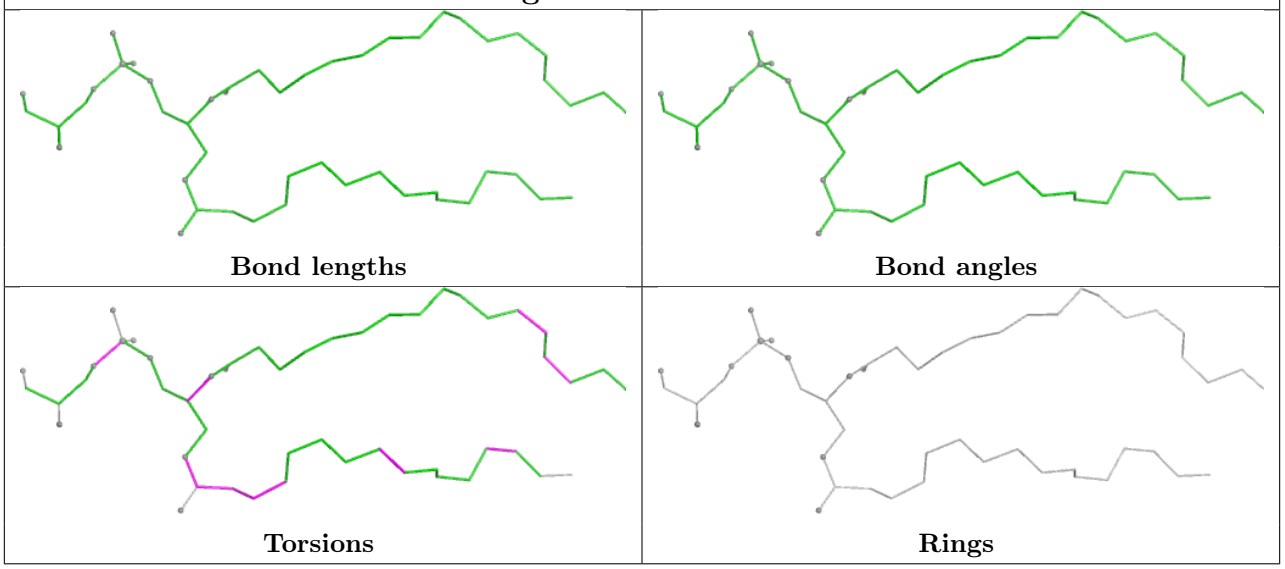
Ligand PEE G 201



Ligand CDL A 607



Ligand PGV A 606



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.

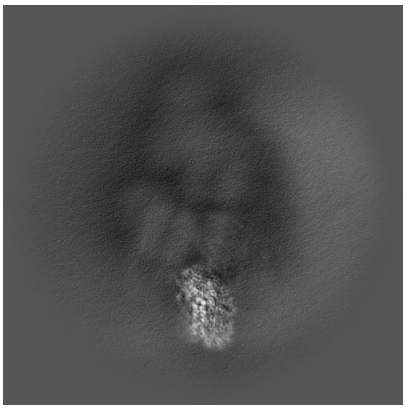
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52654. These allow visual inspection of the internal detail of the map and identification of artifacts.

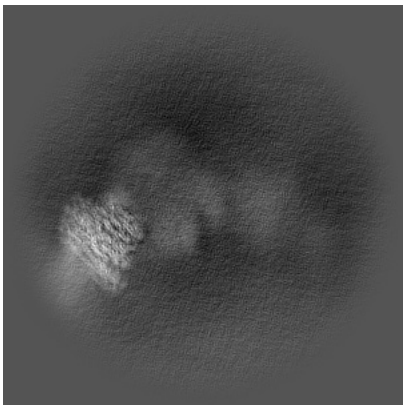
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

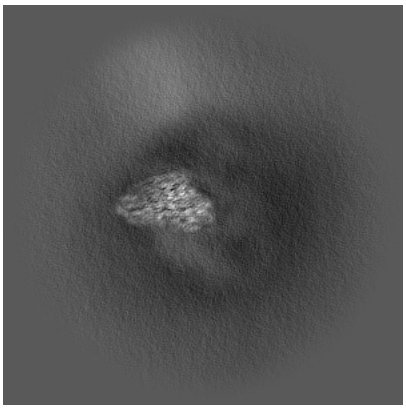
6.1.1 Primary map



X

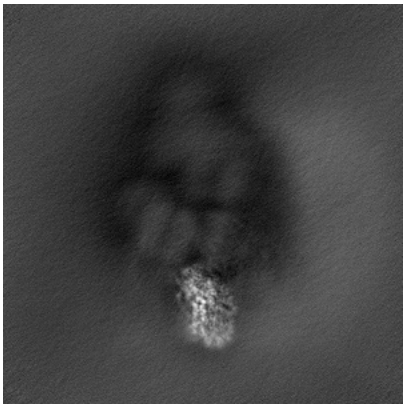


Y

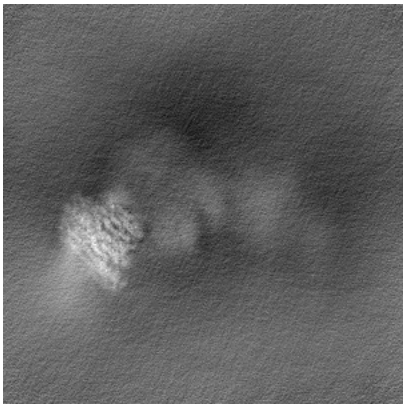


Z

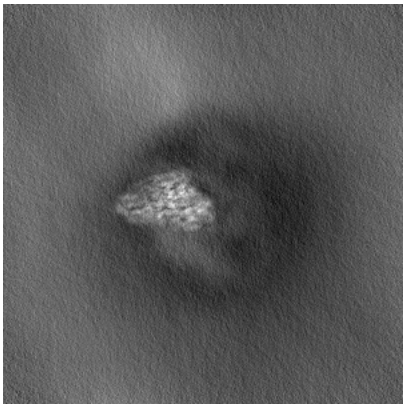
6.1.2 Raw map



X



Y

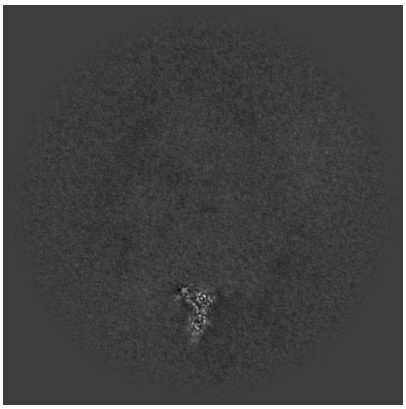


Z

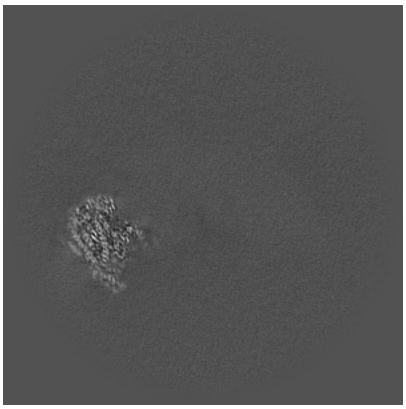
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

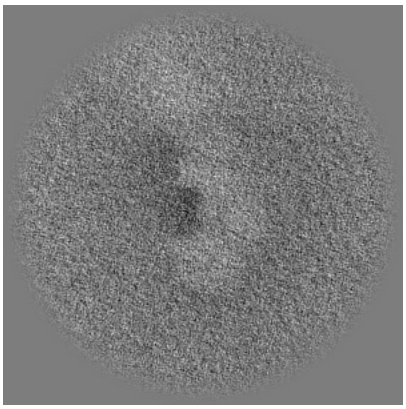
6.2.1 Primary map



X Index: 300

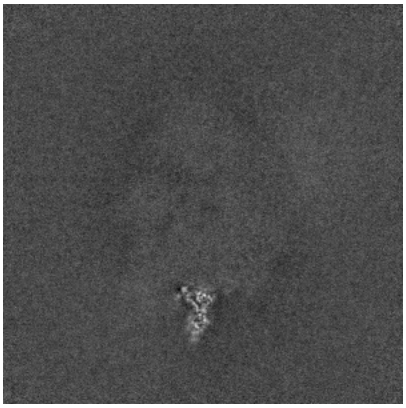


Y Index: 300

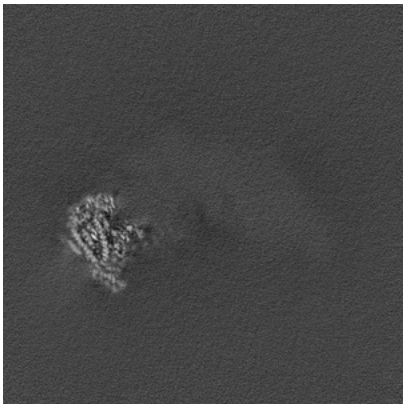


Z Index: 300

6.2.2 Raw map



X Index: 300



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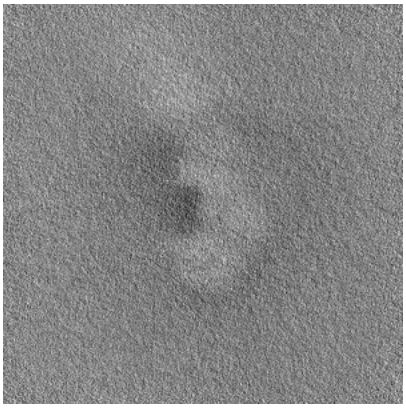
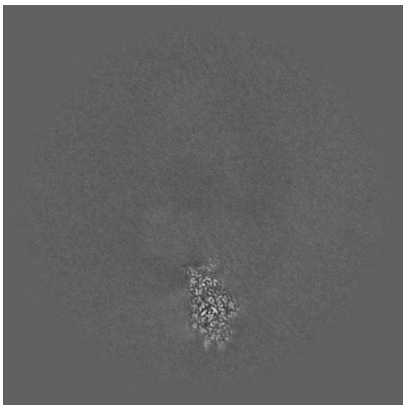


Z Index: 300

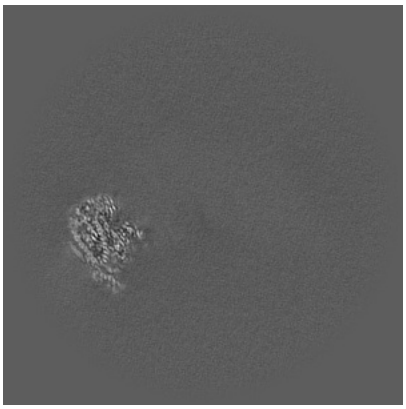
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

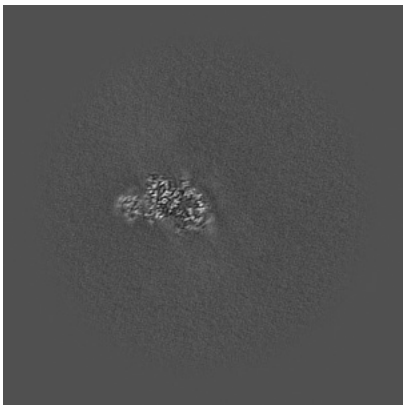
6.3.1 Primary map



X Index: 249

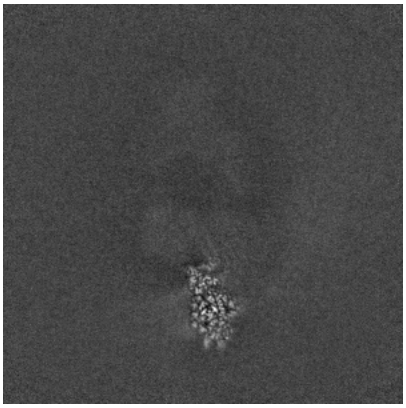


Y Index: 299

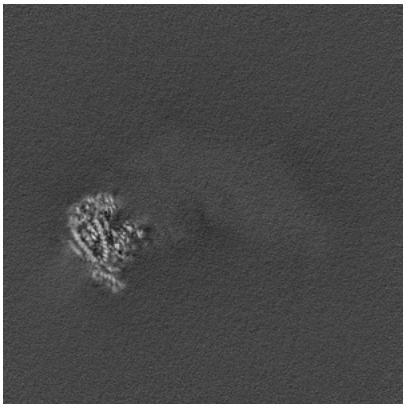


Z Index: 165

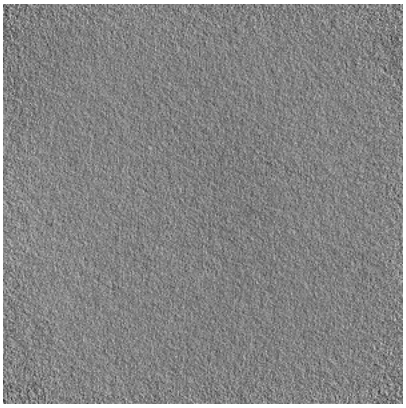
6.3.2 Raw map



X Index: 249



Y Index: 299

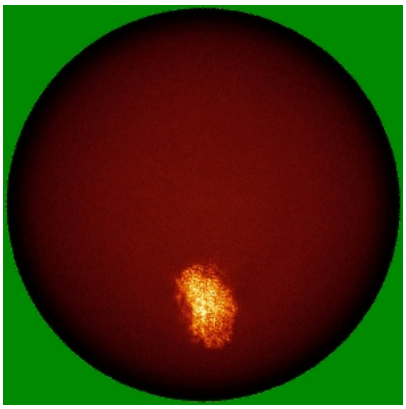


Z Index: 0

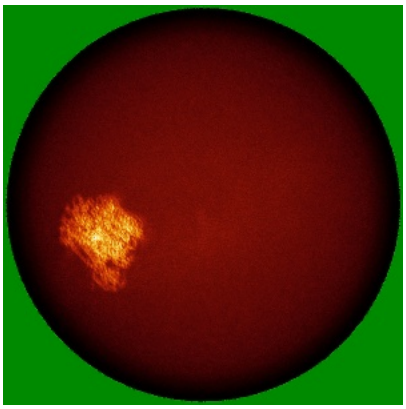
The images above show the largest variance slices of the map in three orthogonal directions.

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

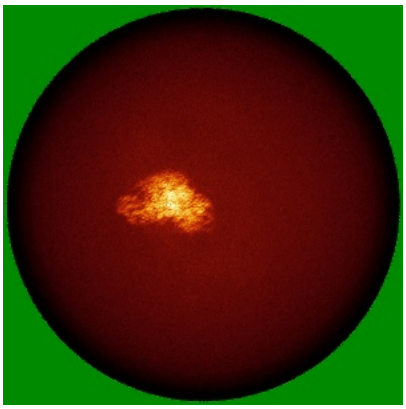
6.4.1 Primary map



X

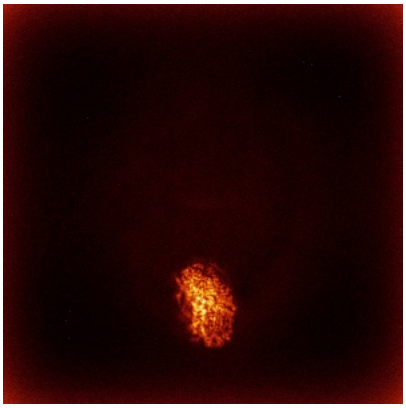


Y

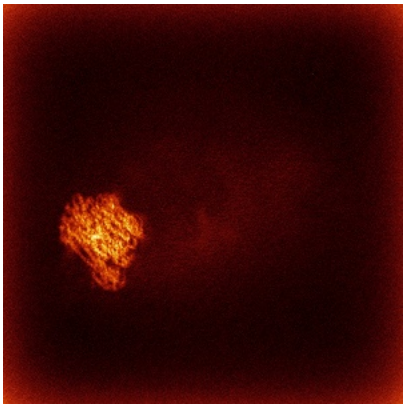


Z

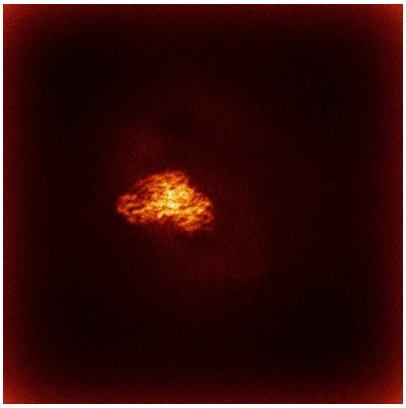
6.4.2 Raw map



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)

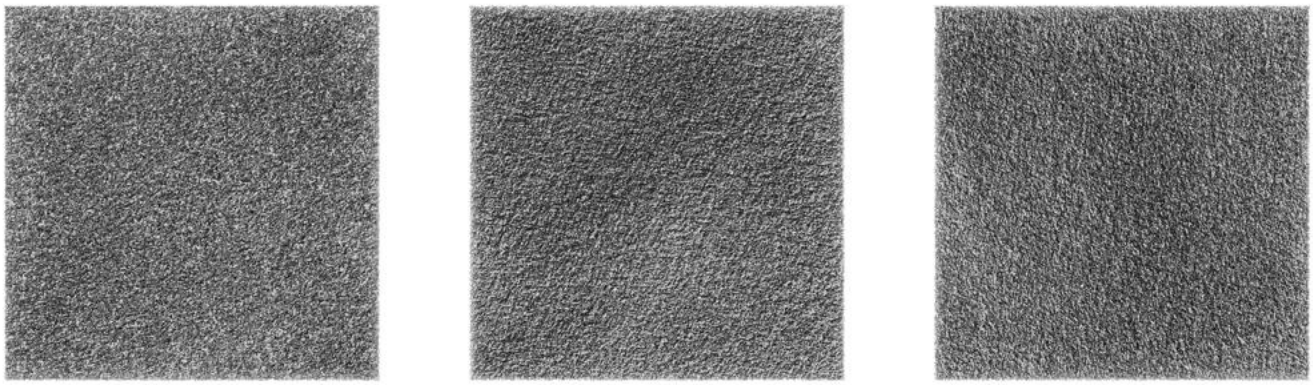
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. 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



X Y Z

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.

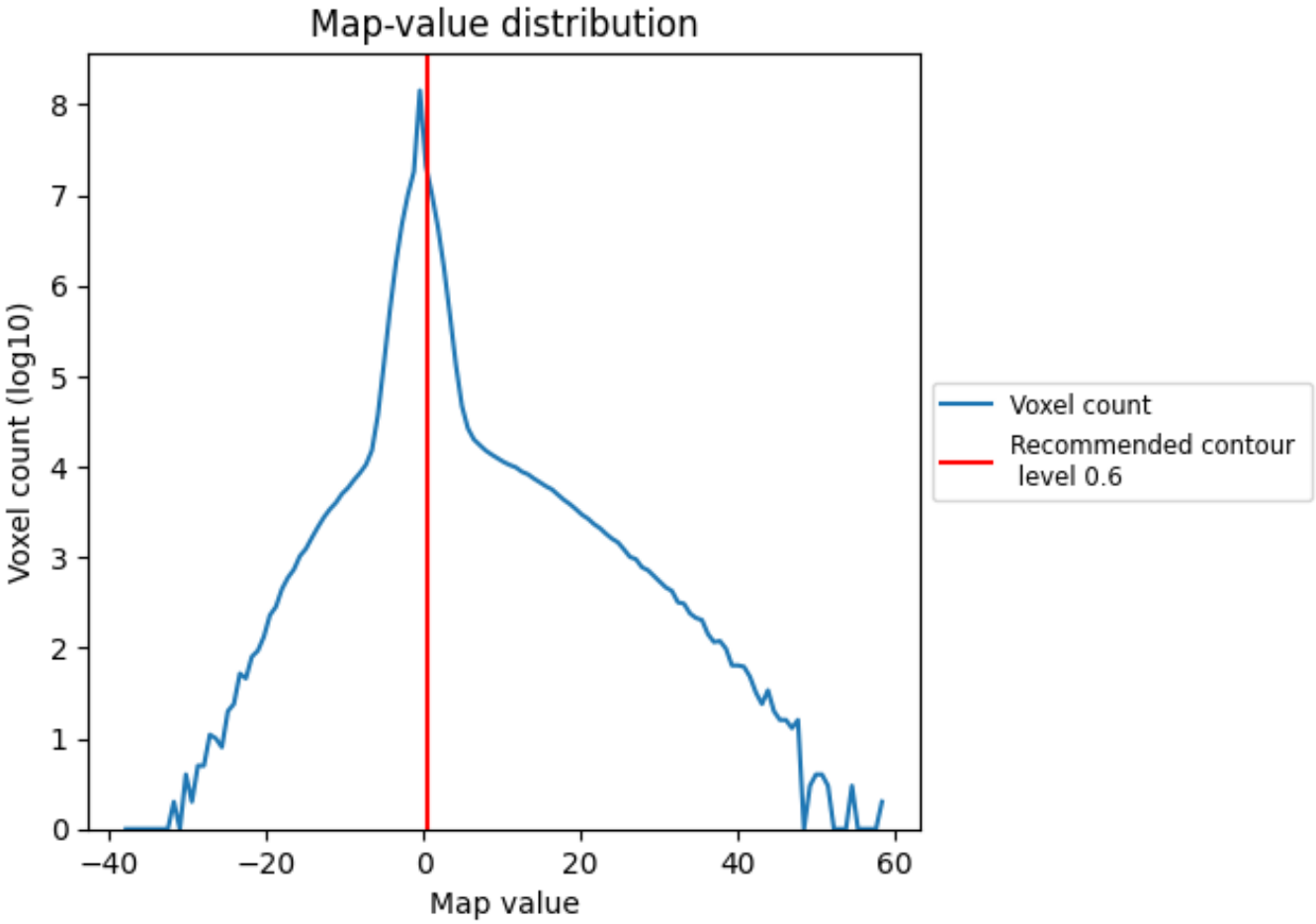
6.6 Mask visualisation (i)

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

7 Map analysis

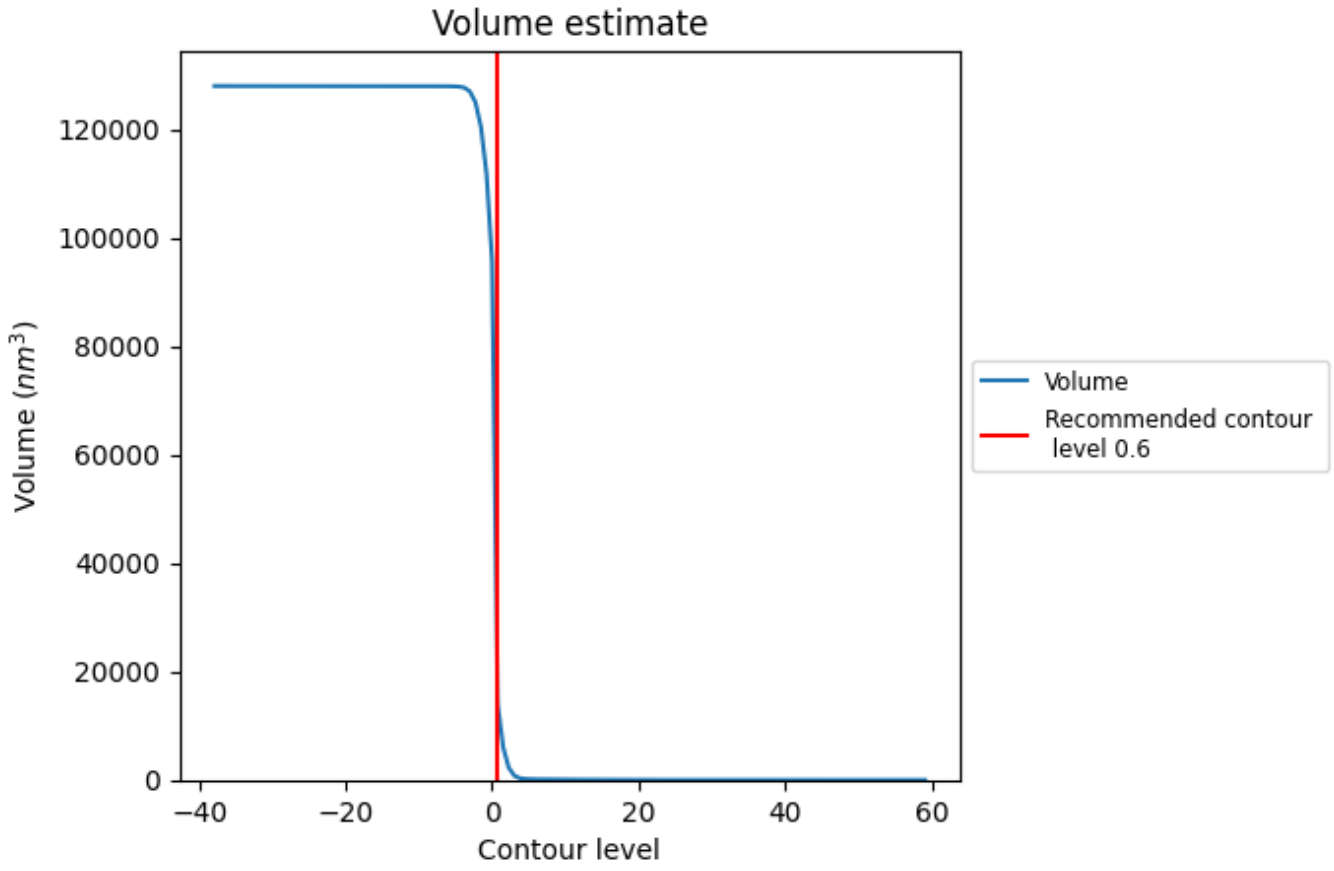
This section contains the results of statistical analysis of the map.

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.

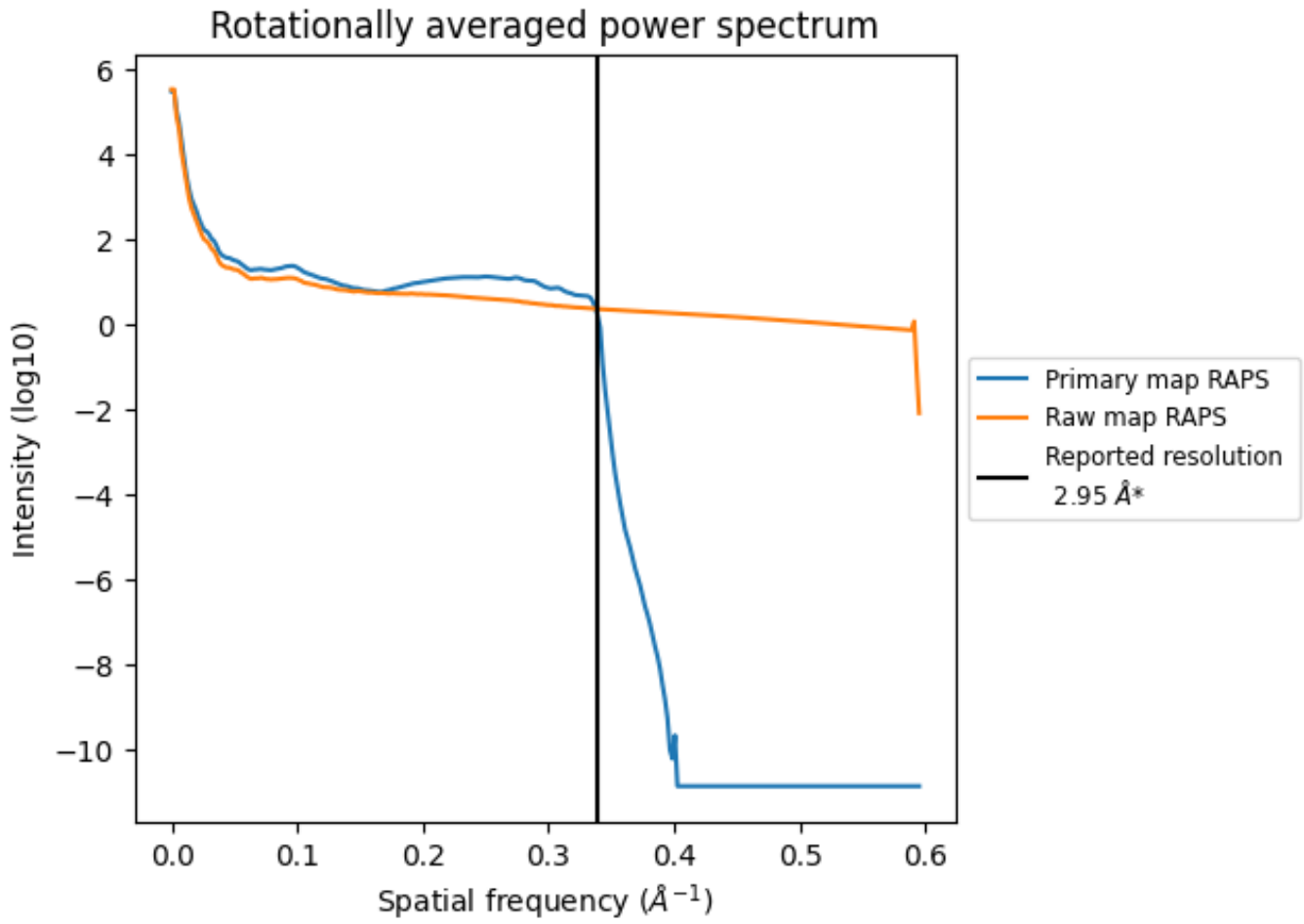
7.2 Volume estimate (i)



The volume at the recommended contour level is 30375 nm^3; this corresponds to an approximate mass of 27439 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)

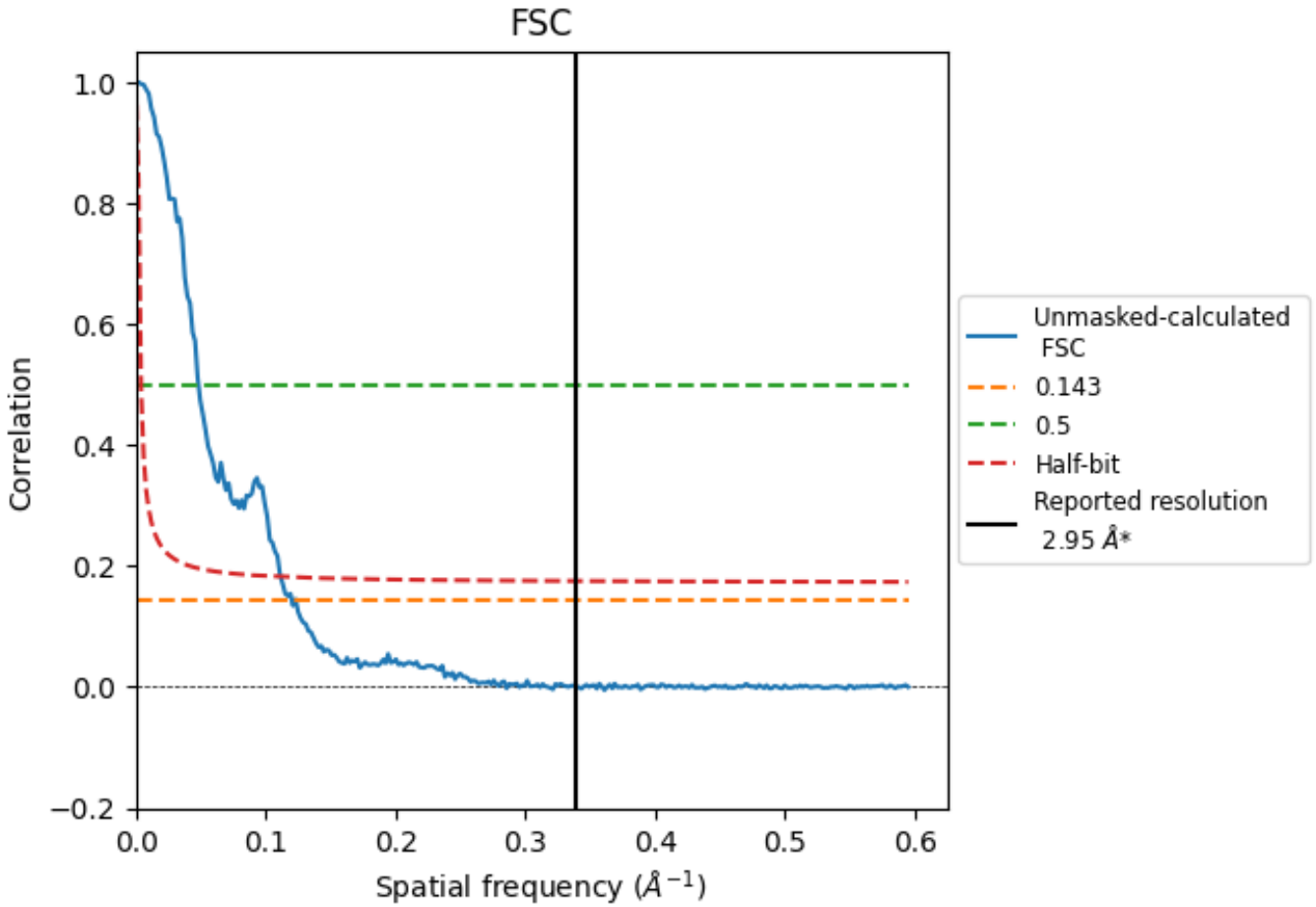


*Reported resolution corresponds to spatial frequency of 0.339 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.339 Å^{-1}

8.2 Resolution estimates (i)

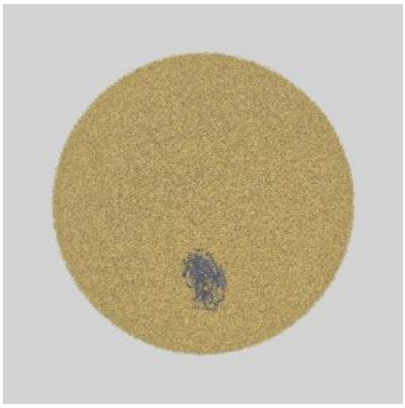
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.32	20.75	8.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.32 differs from the reported value 2.95 by more than 10 %

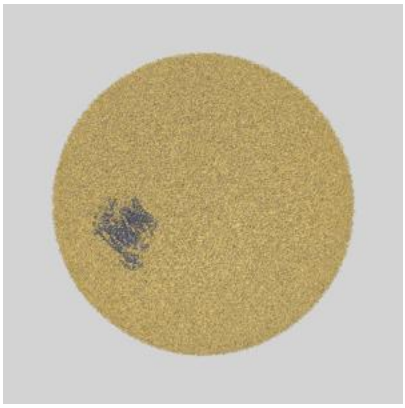
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52654 and PDB model 9I6F. Per-residue inclusion information can be found in section 3 on page 10.

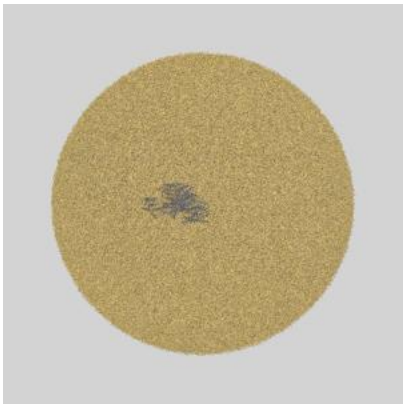
9.1 Map-model overlay



X



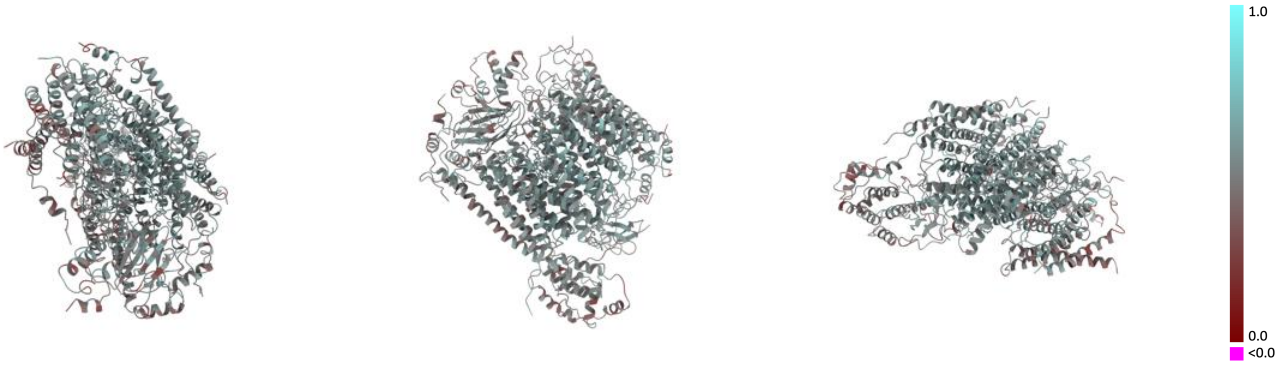
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

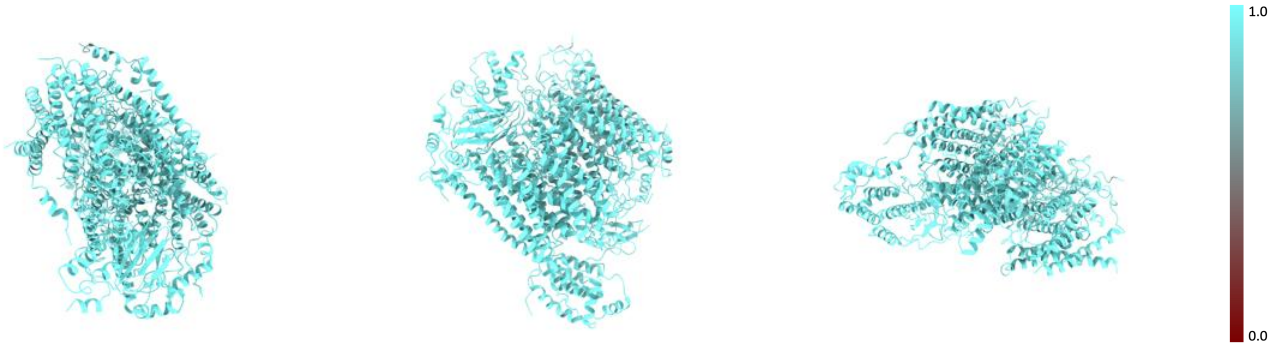
9.2 Q-score mapped to coordinate model



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.

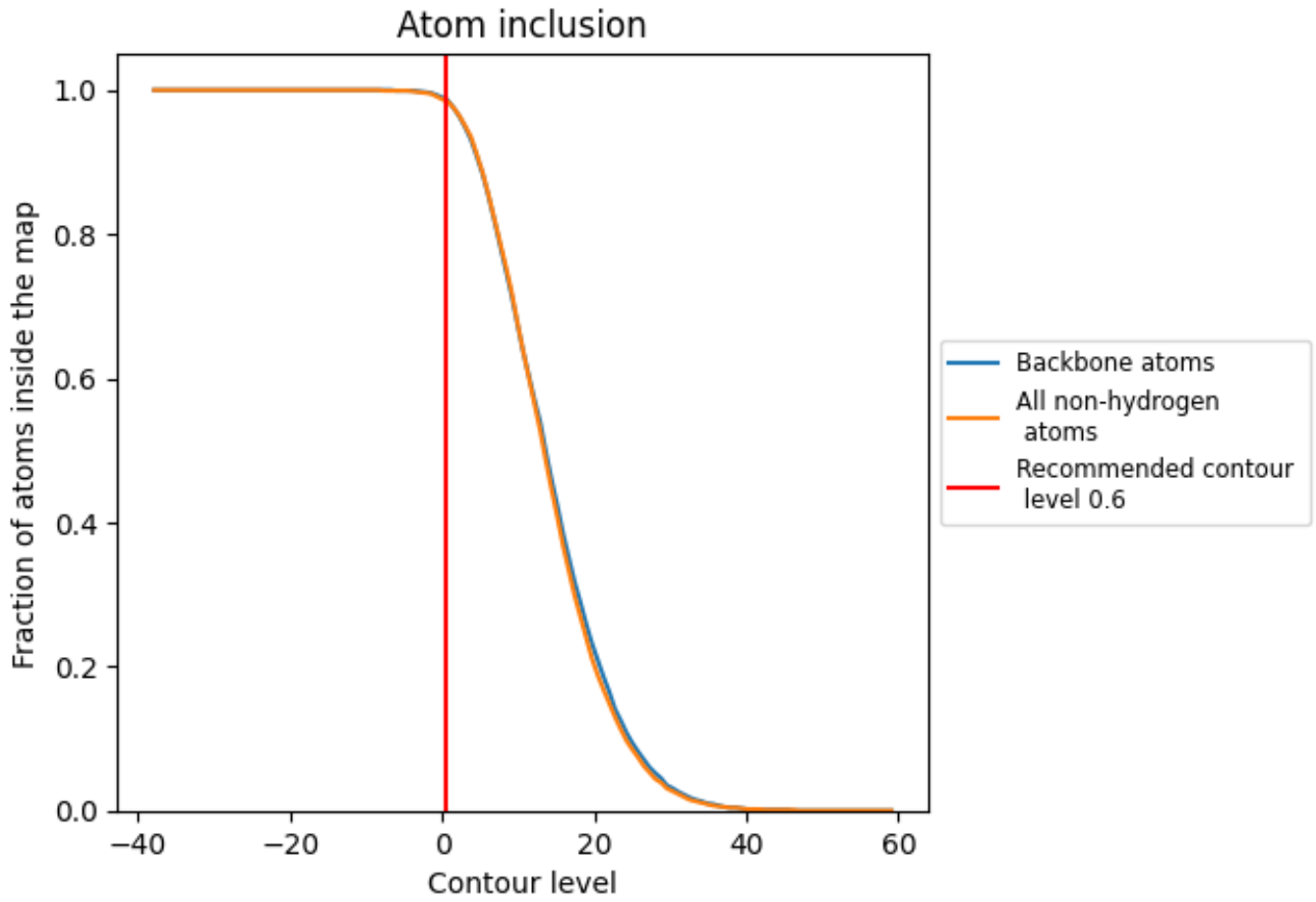
9.3 Atom inclusion mapped to coordinate model



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9840	0.5050
A	0.9900	0.5480
B	0.9910	0.4830
C	0.9800	0.5330
D	0.9940	0.4740
E	0.9940	0.4610
F	0.9960	0.4970
G	0.9690	0.4680
H	0.9970	0.4670
I	0.9980	0.4570
J	0.9490	0.4890
K	0.9950	0.4870
L	0.9970	0.5300
M	0.9820	0.5040
N	0.9510	0.4180

