



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:05 PM UTC

PDB ID : 9I7U / pdb\_00009i7u  
EMDB ID : EMD-52662  
Title : Cryo-EM structure of NDUFA4 bound complex IV within the respirasome complex  
Authors : Nguyen, M.D.; Singh, V.; Rorbach, J.  
Deposited on : 2025-02-02  
Resolution : 3.15 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the 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) : 2.49

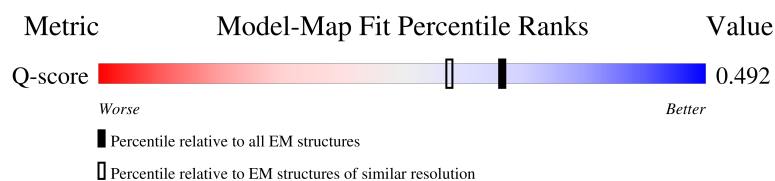
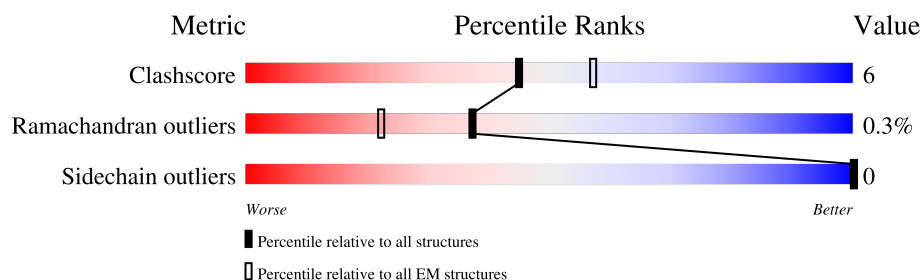
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.15 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.





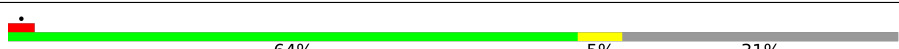
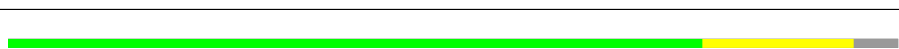
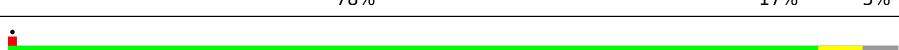
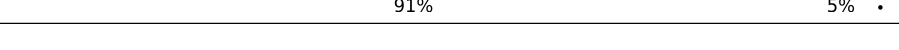
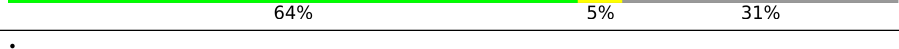

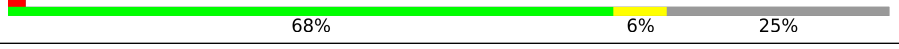

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14486 ( 2.65 - 3.65 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	513	
2	B	227	
3	C	261	
4	D	169	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	E	150	
6	F	129	
7	G	109	
8	H	86	
9	I	75	
10	J	83	
11	K	80	
12	L	63	
13	M	69	
14	N	81	

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
18	HEA	A	605	X	-	-	-

## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 30626 atoms, of which 15330 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	513	Total	C	H	N	O	S	0	0
			8046	2700	4016	622	675	33		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	222	Total	C	H	N	O	S	0	0
			3539	1151	1782	274	319	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	261	Total	C	H	N	O	S	0	0
			4187	1423	2058	340	354	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	139	Total	C	H	N	O	S	0	0
			2296	746	1142	195	206	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	105	Total	C	H	N	O	S	0	0
			1708	546	852	143	165	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	98	Total	C	H	N	O	S	0	0
			1471	462	727	135	142	5		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	75	Total	C	H	N	O	S	0	0
			1206	402	590	110	102	2		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	82	Total	C	H	N	O	S	0	0
			1321	430	636	121	128	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	72	Total	C	H	N	O	S	0	0
			1219	384	622	112	97	4		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	57	Total	C	H	N	O	S	0	0
			907	295	460	69	82	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	53	Total	C	H	N	O	S	0	0
			837	273	412	75	76	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	47	Total	C	H	N	O	S	0	0
			756	250	378	62	64	2		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	43	Total	C	H	N	O	S	0	0
			681	222	346	55	56	2		

- Molecule 14 is a protein called Cytochrome c oxidase subunit NDUFA4.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	81	Total	C	H	N	O	S	0	0
			1326	434	663	113	114	2		

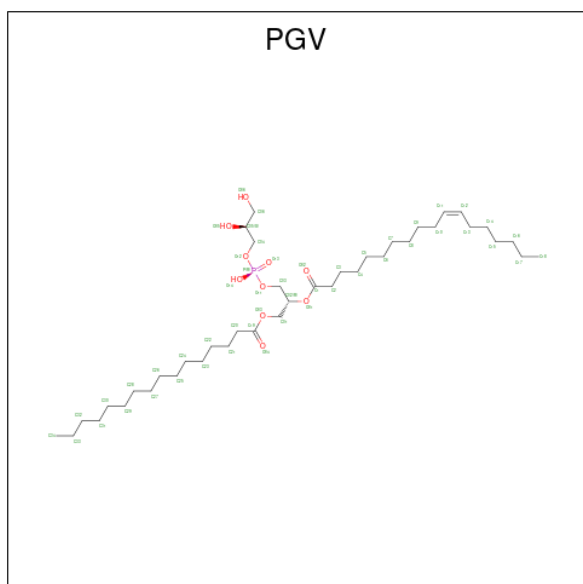
- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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) (labeled as "Ligand of Interest" by depositor).

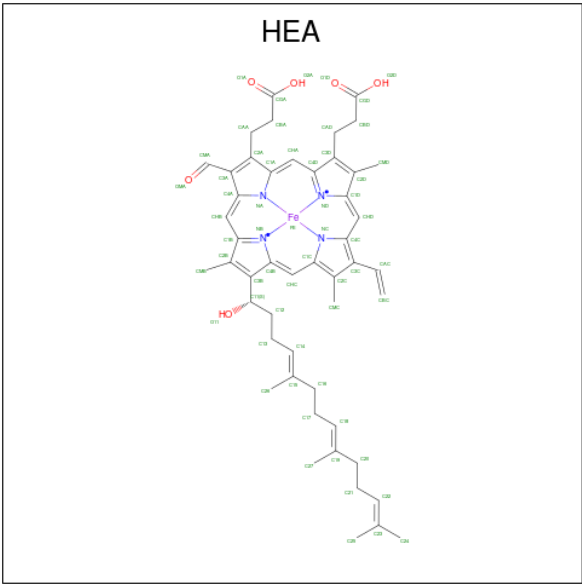
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	

- Molecule 17 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



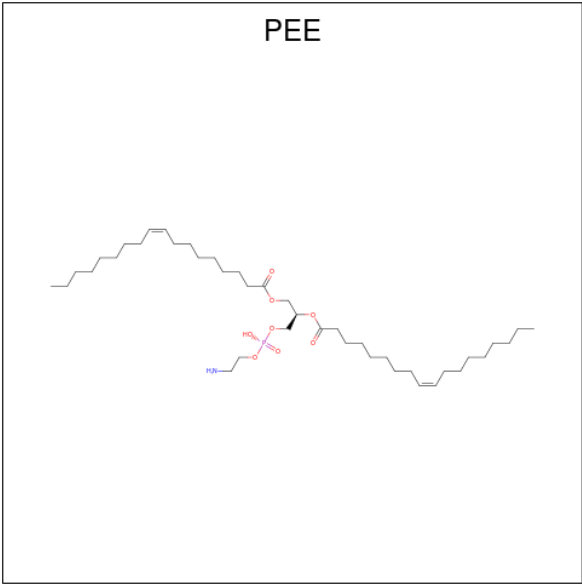
Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	H	O	P	0
			127	40	76	10	1	

- 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
			Total	C	Fe	H	N	O	
18	A	1	114	49	1	54	4	6	0
18	A	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 19 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).

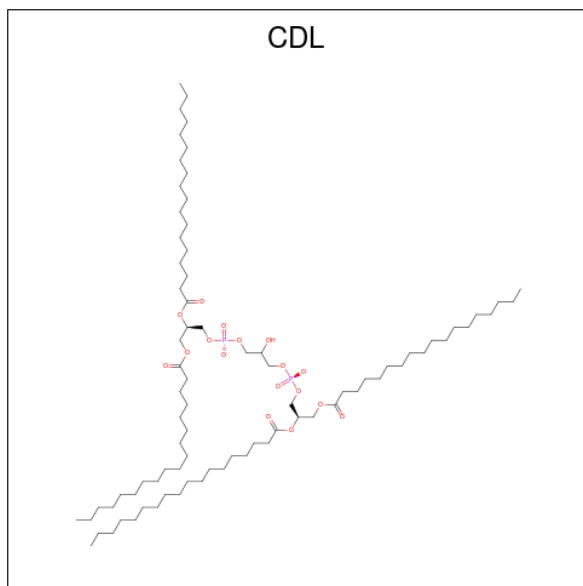


Mol	Chain	Residues	Atoms					AltConf	
19	C	1	Total 128	C 41	H 77	N 1	O 8	P 1	0
19	C	1	Total 128	C 41	H 77	N 1	O 8	P 1	0
19	C	1	Total 127	C 41	H 76	N 1	O 8	P 1	0
19	C	1	Total 127	C 41	H 76	N 1	O 8	P 1	0

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



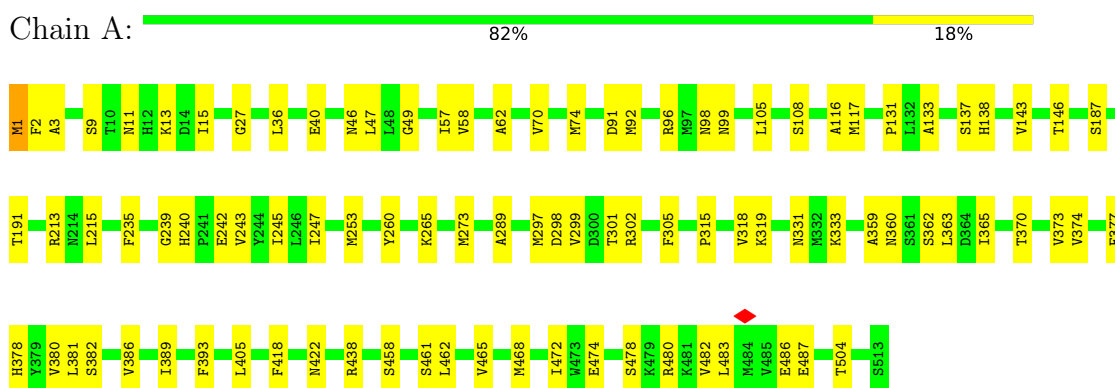
Mol	Chain	Residues	Atoms					AltConf
21	N	1	Total	C	H	O	P	0
			256	81	156	17	2	



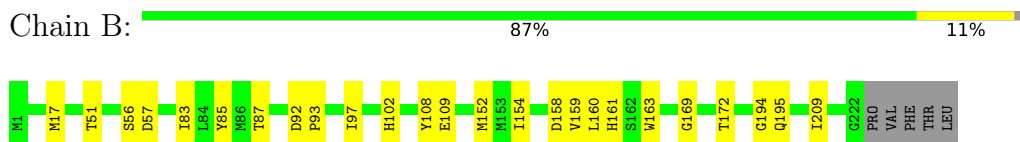
### 3 Residue-property plots

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

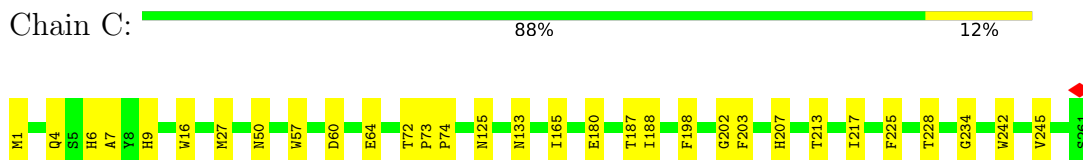
#### • Molecule 1: Cytochrome c oxidase subunit 1



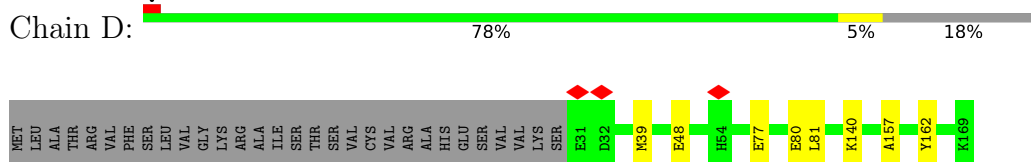
#### • Molecule 2: Cytochrome c oxidase subunit 2



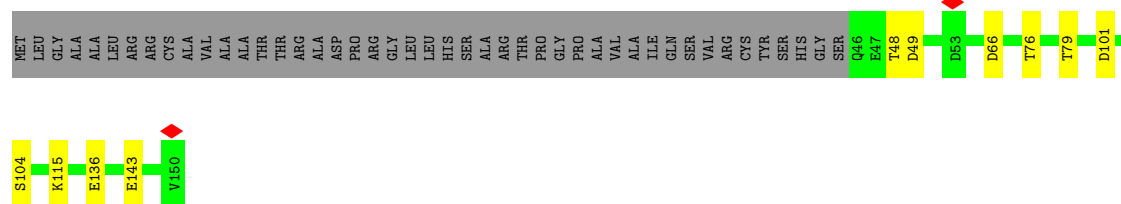
#### • Molecule 3: Cytochrome c oxidase subunit 3



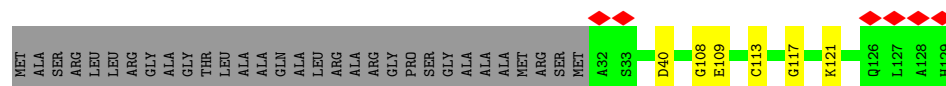
#### • Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



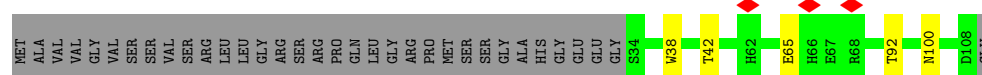
#### • Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



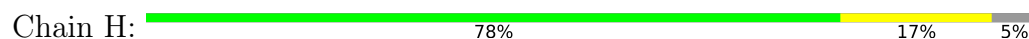
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



- Molecule 7: Cytochrome c oxidase subunit 6A1, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 9: Cytochrome c oxidase subunit 6C

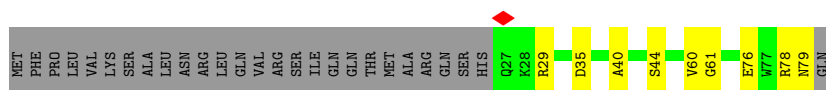


- Molecule 10: Cytochrome c oxidase subunit 7A2, mitochondrial

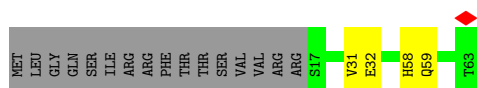


- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

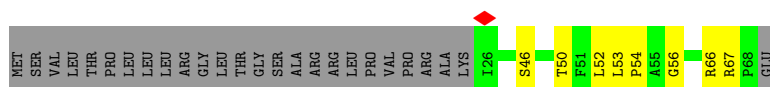




- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8A, mitochondrial



- Molecule 14: Cytochrome c oxidase subunit NDUFA4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109624	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	50.318	Depositor
Minimum map value	-33.846	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.08	Depositor
Map size ( $\text{\AA}$ )	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: FME, PEE, PGV, CDL, HEA, ZN, CU, 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	0.17	0/4161	0.29	0/5685
2	B	0.11	0/1802	0.27	0/2466
3	C	0.13	0/2206	0.26	0/3018
4	D	0.10	0/1187	0.25	0/1594
5	E	0.10	0/874	0.27	0/1187
6	F	0.11	0/760	0.26	0/1029
7	G	0.10	0/642	0.24	0/877
8	H	0.12	0/705	0.32	0/953
9	I	0.09	0/608	0.24	0/809
10	J	0.11	0/456	0.22	0/616
11	K	0.09	0/438	0.26	0/599
12	L	0.11	0/390	0.23	0/527
13	M	0.10	0/345	0.25	0/470
14	N	0.17	0/683	0.57	0/927
All	All	0.13	0/15257	0.29	0/20757

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	47	ARG	Sidechain
14	N	66	SER	Peptide

## 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	A	4030	4016	4014	74	0
2	B	1757	1782	1780	16	0
3	C	2129	2058	2057	22	0
4	D	1154	1142	1142	6	0
5	E	856	852	852	7	0
6	F	744	727	727	4	0
7	G	616	590	590	5	0
8	H	685	636	636	11	0
9	I	597	622	622	2	0
10	J	447	460	460	3	0
11	K	425	412	412	6	0
12	L	378	378	377	4	0
13	M	335	346	346	5	0
14	N	663	663	669	29	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	76	76	0	0
18	A	120	108	108	26	0
19	C	204	306	316	13	0
20	F	1	0	0	0	0
21	N	100	156	156	1	0
All	All	15296	15330	15340	193	0

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

All (193) 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:A:74:MET:HE1	1:A:253:MET:HE1	1.58	0.84
5:E:76:THR:O	5:E:79:THR:OG1	1.99	0.80
2:B:195:GLN:OE1	2:B:195:GLN:N	2.16	0.79
3:C:4:GLN:NE2	3:C:6:HIS:O	2.16	0.78
2:B:109:GLU:N	2:B:109:GLU:OE1	2.19	0.74
1:A:133:ALA:O	1:A:213:ARG:NH1	2.22	0.72
11:K:78:ARG:O	11:K:78:ARG:NE	2.24	0.70
12:L:32:GLU:N	12:L:32:GLU:OE1	2.25	0.69
9:I:27:PHE:O	9:I:30:SER:OG	2.12	0.67
14:N:35:ARG:NH2	14:N:64:PHE:O	2.29	0.66
4:D:48:GLU:N	4:D:48:GLU:OE1	2.28	0.65
2:B:102:HIS:O	2:B:161:HIS:NE2	2.29	0.65
3:C:203:PHE:O	3:C:207:HIS:ND1	2.29	0.65
19:C:303:PEE:H35	19:C:303:PEE:H63	1.79	0.65
2:B:83:ILE:O	2:B:87:THR:HG23	1.97	0.65
1:A:438:ARG:NH2	18:A:605:HEA:HAD1	2.12	0.64
1:A:27:GLY:C	18:A:605:HEA:H273	2.23	0.64
2:B:85:TYR:CD1	14:N:67:VAL:HG23	2.33	0.63
1:A:74:MET:HE3	1:A:389:ILE:HG12	1.80	0.63
1:A:215:LEU:HD11	19:C:303:PEE:H27	1.81	0.63
1:A:74:MET:HE3	1:A:389:ILE:CG1	2.29	0.62
1:A:91:ASP:OD1	1:A:92:MET:N	2.28	0.62
6:F:113:CYS:N	6:F:117:GLY:O	2.33	0.62
18:A:605:HEA:C18	18:A:605:HEA:H261	2.30	0.61
1:A:74:MET:HA	1:A:74:MET:HE2	1.83	0.61
3:C:234:GLY:N	19:C:302:PEE:O1P	2.29	0.61
6:F:108:GLY:O	6:F:121:LYS:NZ	2.30	0.61
1:A:359:ALA:HA	18:A:604:HEA:HBC2	1.83	0.60
2:B:85:TYR:CE1	14:N:67:VAL:HG23	2.37	0.60
1:A:98:ASN:OD1	1:A:99:ASN:N	2.34	0.59
12:L:31:VAL:HG23	12:L:31:VAL:O	2.02	0.58
1:A:359:ALA:HB2	18:A:604:HEA:HAC	1.84	0.58
1:A:438:ARG:NH2	18:A:605:HEA:O1D	2.30	0.58
14:N:65:TYR:HB3	14:N:67:VAL:HB	1.85	0.58
1:A:418:PHE:O	1:A:422:ASN:ND2	2.37	0.57
1:A:438:ARG:NH1	18:A:605:HEA:HBA1	2.19	0.57
1:A:116:ALA:O	12:L:59:GLN:NE2	2.37	0.57
1:A:117:MET:SD	12:L:58:HIS:ND1	2.78	0.56
3:C:16:TRP:NE1	3:C:60:ASP:OD2	2.38	0.56
1:A:240:HIS:O	1:A:243:VAL:HG22	2.06	0.56
1:A:265:LYS:NZ	1:A:487:GLU:OE1	2.40	0.55
18:A:604:HEA:HHD	18:A:604:HEA:HBC1	1.88	0.55

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:49:ASN:HB2	14:N:50:PRO:HD3	1.88	0.55
1:A:131:PRO:O	1:A:137:SER:OG	2.22	0.55
1:A:62:ALA:HB2	18:A:605:HEA:HBD1	1.89	0.55
5:E:136:GLU:N	5:E:136:GLU:OE1	2.41	0.53
1:A:105:LEU:O	1:A:108:SER:OG	2.24	0.53
8:H:9:ILE:HG22	8:H:9:ILE:O	2.08	0.53
11:K:29:ARG:NH2	11:K:35:ASP:OD2	2.42	0.53
8:H:32:GLN:HE21	14:N:56:LEU:HD21	1.74	0.53
14:N:71:TYR:O	14:N:72:SER:CB	2.56	0.53
1:A:359:ALA:HA	18:A:604:HEA:CBC	2.39	0.53
19:C:303:PEE:O1P	7:G:92:THR:OG1	2.11	0.53
1:A:46:ASN:ND2	1:A:49:GLY:O	2.38	0.52
1:A:393:PHE:CD2	18:A:605:HEA:H252	2.43	0.52
1:A:377:PHE:HB2	18:A:604:HEA:CMA	2.40	0.51
2:B:17:MET:SD	2:B:169:GLY:N	2.82	0.51
14:N:59:ASN:O	14:N:60:ASP:HB3	2.09	0.51
1:A:474:GLU:OE2	1:A:480:ARG:NH2	2.41	0.51
1:A:143:VAL:O	1:A:146:THR:OG1	2.24	0.51
1:A:468:MET:HE1	18:A:605:HEA:H253	1.92	0.51
2:B:159:VAL:HG12	2:B:160:LEU:N	2.26	0.50
14:N:59:ASN:OD1	14:N:60:ASP:N	2.45	0.50
7:G:38:TRP:O	7:G:42:THR:OG1	2.29	0.50
19:C:301:PEE:H5	19:C:301:PEE:P	2.35	0.50
14:N:69:VAL:HG22	14:N:70:ASP:N	2.26	0.50
4:D:77:GLU:O	4:D:81:LEU:HD12	2.12	0.49
3:C:27:MET:HE2	3:C:50:ASN:HD21	1.77	0.49
1:A:36:LEU:HD22	1:A:57:ILE:HD13	1.94	0.49
1:A:474:GLU:OE2	1:A:478:SER:OG	2.31	0.49
4:D:77:GLU:O	4:D:80:GLU:HG3	2.13	0.49
8:H:22:PRO:O	14:N:65:TYR:OH	2.31	0.49
3:C:188:ILE:N	19:C:303:PEE:O2P	2.45	0.49
2:B:158:ASP:OD1	2:B:159:VAL:N	2.46	0.48
18:A:605:HEA:HBC1	18:A:605:HEA:HMC1	1.96	0.48
3:C:7:ALA:O	3:C:72:THR:HG21	2.13	0.48
1:A:298:ASP:OD1	1:A:299:VAL:N	2.47	0.47
2:B:51:THR:O	5:E:115:LYS:NZ	2.46	0.47
1:A:260:TYR:OH	1:A:486:GLU:OE1	2.30	0.47
4:D:157:ALA:O	4:D:162:TYR:OH	2.26	0.47
8:H:21:PHE:HD1	14:N:55:LYS:HD3	1.79	0.47
14:N:55:LYS:O	14:N:56:LEU:HD23	2.14	0.47
1:A:13:LYS:NZ	1:A:504:THR:OG1	2.44	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ARG:HH21	18:A:605:HEA:HAD1	1.78	0.47
3:C:72:THR:OG1	3:C:73:PRO:HD2	2.14	0.47
7:G:65:GLU:N	7:G:65:GLU:OE1	2.47	0.47
14:N:42:ASP:HB3	14:N:55:LYS:HE2	1.95	0.47
1:A:393:PHE:CD2	18:A:605:HEA:C25	2.98	0.47
5:E:48:THR:O	5:E:49:ASP:HB2	2.15	0.47
14:N:47:ARG:HB3	14:N:50:PRO:HD2	1.97	0.46
1:A:360:ASN:HB2	1:A:363:LEU:HB3	1.98	0.46
1:A:11:ASN:O	1:A:15:ILE:HD12	2.15	0.46
8:H:58:GLN:HA	8:H:61:TYR:CE2	2.51	0.46
1:A:378:HIS:HE1	18:A:605:HEA:NB	2.14	0.46
5:E:66:ASP:C	5:E:66:ASP:OD1	2.58	0.46
13:M:52:LEU:O	13:M:56:GLY:N	2.39	0.46
1:A:482:VAL:HG12	1:A:483:LEU:O	2.16	0.46
3:C:198:PHE:O	3:C:202:GLY:N	2.43	0.46
14:N:63:LYS:HD2	14:N:67:VAL:CG1	2.46	0.46
1:A:486:GLU:HA	4:D:39:MET:HE1	1.98	0.46
1:A:187:SER:O	1:A:191:THR:OG1	2.27	0.45
2:B:92:ASP:N	2:B:93:PRO:HD3	2.31	0.45
13:M:66:ARG:O	13:M:67:ARG:HB2	2.16	0.45
1:A:40:GLU:OE1	1:A:47:LEU:HG	2.16	0.45
2:B:56:SER:OG	2:B:57:ASP:N	2.49	0.45
1:A:9:SER:O	1:A:99:ASN:ND2	2.50	0.45
10:J:40:GLU:N	10:J:40:GLU:OE1	2.49	0.45
14:N:67:VAL:HG22	14:N:68:ASN:N	2.32	0.45
1:A:2:PHE:O	1:A:2:PHE:CD2	2.70	0.45
1:A:438:ARG:CZ	18:A:605:HEA:HBA1	2.47	0.45
1:A:74:MET:HE3	1:A:389:ILE:HG13	1.98	0.45
1:A:289:ALA:HB3	1:A:305:PHE:CZ	2.52	0.45
18:A:604:HEA:C14	18:A:604:HEA:O11	2.65	0.45
3:C:9:HIS:NE2	3:C:64:GLU:OE1	2.50	0.45
19:C:303:PEE:C30	19:C:303:PEE:O4	2.65	0.45
3:C:202:GLY:HA3	19:C:303:PEE:H16	1.99	0.45
2:B:194:GLY:O	2:B:209:ILE:N	2.41	0.44
2:B:97:ILE:HB	2:B:152:MET:HE1	2.00	0.44
5:E:143:GLU:CD	5:E:143:GLU:H	2.26	0.44
8:H:34:TYR:OH	8:H:77:ARG:NH1	2.51	0.44
14:N:52:PRO:HB2	14:N:53:TRP:CE3	2.53	0.44
19:C:301:PEE:H63	19:C:301:PEE:H36	2.00	0.44
14:N:46:ASP:O	14:N:47:ARG:O	2.36	0.44
14:N:48:ASN:O	14:N:49:ASN:C	2.60	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:THR:O	3:C:217:ILE:HD12	2.18	0.43
1:A:405:LEU:H	1:A:405:LEU:HD23	1.82	0.43
3:C:72:THR:HG23	3:C:74:PRO:HD2	1.99	0.43
8:H:7:THR:OG1	8:H:8:LYS:N	2.51	0.43
14:N:67:VAL:HG11	14:N:69:VAL:HG12	1.99	0.43
4:D:140:LYS:NZ	11:K:76:GLU:O	2.48	0.43
11:K:40:ALA:O	11:K:44:SER:OG	2.36	0.43
1:A:138:HIS:O	1:A:138:HIS:ND1	2.51	0.43
3:C:187:THR:HG22	3:C:188:ILE:N	2.33	0.43
6:F:109:GLU:HA	6:F:109:GLU:OE1	2.17	0.43
1:A:247:ILE:HD12	18:A:604:HEA:CMB	2.49	0.43
1:A:380:VAL:HG23	1:A:381:LEU:N	2.34	0.43
3:C:228:THR:OG1	6:F:40:ASP:OD1	2.27	0.43
14:N:60:ASP:HB2	14:N:77:GLU:HB2	2.01	0.43
8:H:30:CYS:SG	8:H:61:TYR:HB2	2.58	0.43
1:A:235:PHE:O	1:A:239:GLY:N	2.50	0.42
2:B:108:TYR:OH	2:B:163:TRP:NE1	2.51	0.42
1:A:315:PRO:O	1:A:318:VAL:HG12	2.19	0.42
1:A:331:ASN:O	1:A:333:LYS:HD3	2.20	0.42
1:A:297:MET:O	1:A:302:ARG:NH2	2.53	0.42
1:A:465:VAL:O	1:A:468:MET:HG2	2.18	0.42
1:A:370:THR:O	1:A:373:VAL:HG12	2.20	0.42
13:M:66:ARG:HG3	13:M:67:ARG:H	1.85	0.42
14:N:43:VAL:HG13	14:N:43:VAL:O	2.20	0.42
10:J:32:GLN:O	10:J:36:GLN:HG3	2.20	0.42
1:A:362:SER:O	1:A:365:ILE:HG12	2.20	0.42
8:H:21:PHE:CD2	8:H:29:ASN:ND2	2.88	0.42
8:H:52:SER:O	8:H:53:VAL:C	2.62	0.42
14:N:49:ASN:HB2	14:N:50:PRO:CD	2.50	0.42
1:A:273:MET:SD	1:A:319:LYS:NZ	2.92	0.42
19:C:302:PEE:H36	19:C:302:PEE:H29	1.89	0.42
3:C:165:ILE:H	3:C:165:ILE:HD12	1.84	0.41
3:C:242:TRP:O	3:C:245:VAL:HG12	2.19	0.41
19:C:303:PEE:H6	7:G:100:ASN:CG	2.25	0.41
1:A:382:SER:O	1:A:386:VAL:HB	2.20	0.41
18:A:604:HEA:H132	18:A:604:HEA:HHC	2.01	0.41
19:C:303:PEE:N	7:G:100:ASN:OD1	2.37	0.41
18:A:605:HEA:H261	18:A:605:HEA:H18	2.01	0.41
1:A:58:VAL:HG21	18:A:605:HEA:HBA2	2.03	0.41
3:C:73:PRO:HB2	3:C:74:PRO:HD3	2.03	0.41
13:M:53:LEU:HB3	13:M:54:PRO:HD3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:MET:O	1:A:472:ILE:HG13	2.21	0.41
3:C:133:ASN:ND2	3:C:180:GLU:OE2	2.46	0.41
19:C:301:PEE:O3P	19:C:301:PEE:N	2.37	0.41
14:N:67:VAL:HG22	14:N:68:ASN:H	1.86	0.41
14:N:75:LYS:C	14:N:76:LYS:HD3	2.46	0.41
1:A:96:ARG:HH21	3:C:57:TRP:CD1	2.39	0.41
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.03	0.41
1:A:438:ARG:HH12	18:A:605:HEA:HBA1	1.83	0.41
1:A:462:LEU:O	1:A:465:VAL:HG22	2.20	0.41
3:C:225:PHE:CZ	10:J:26:ASN:HA	2.56	0.41
5:E:101:ASP:OD2	5:E:104:SER:OG	2.33	0.41
9:I:64:GLU:OE2	9:I:65:MET:HG3	2.20	0.41
1:A:70:VAL:HG21	18:A:605:HEA:HBC2	2.02	0.41
1:A:301:THR:HG21	21:N:101:CDL:OA4	2.21	0.41
1:A:458:SER:O	1:A:461:SER:OG	2.29	0.41
14:N:77:GLU:C	14:N:79:PRO:HD2	2.46	0.41
1:A:374:VAL:HA	1:A:377:PHE:CE1	2.56	0.41
2:B:154:ILE:HD13	2:B:172:THR:HB	2.03	0.41
3:C:125:ASN:OD1	3:C:125:ASN:C	2.64	0.41
1:A:393:PHE:CG	18:A:605:HEA:H251	2.56	0.40
14:N:53:TRP:HB2	14:N:56:LEU:HD12	2.04	0.40
11:K:60:VAL:HG12	11:K:61:GLY:N	2.37	0.40
11:K:76:GLU:OE2	11:K:79:ASN:N	2.54	0.40
14:N:68:ASN:O	14:N:68:ASN:CG	2.64	0.40
1:A:374:VAL:HG22	1:A:438:ARG:NH1	2.36	0.40
1:A:1:FME:C	1:A:3:ALA:H	2.34	0.40
8:H:44:MET:HE2	8:H:44:MET:N	2.36	0.40
13:M:46:SER:O	13:M:50:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/513 (100%)	489 (96%)	22 (4%)	0	100	100
2	B	220/227 (97%)	208 (94%)	12 (6%)	0	100	100
3	C	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
4	D	137/169 (81%)	130 (95%)	7 (5%)	0	100	100
5	E	103/150 (69%)	101 (98%)	2 (2%)	0	100	100
6	F	96/129 (74%)	88 (92%)	8 (8%)	0	100	100
7	G	73/109 (67%)	71 (97%)	2 (3%)	0	100	100
8	H	80/86 (93%)	68 (85%)	12 (15%)	0	100	100
9	I	70/75 (93%)	68 (97%)	2 (3%)	0	100	100
10	J	55/83 (66%)	52 (94%)	3 (6%)	0	100	100
11	K	51/80 (64%)	48 (94%)	3 (6%)	0	100	100
12	L	45/63 (71%)	40 (89%)	5 (11%)	0	100	100
13	M	41/69 (59%)	38 (93%)	3 (7%)	0	100	100
14	N	79/81 (98%)	59 (75%)	15 (19%)	5 (6%)	1	7
All	All	1820/2095 (87%)	1709 (94%)	106 (6%)	5 (0%)	37	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	47	ARG
14	N	72	SER
14	N	61	GLN
14	N	52	PRO
14	N	57	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	426 (100%)	0	100	100
2	B	197/202 (98%)	197 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	226/226 (100%)	226 (100%)	0	100	100
4	D	123/149 (83%)	123 (100%)	0	100	100
5	E	94/126 (75%)	94 (100%)	0	100	100
6	F	79/97 (81%)	79 (100%)	0	100	100
7	G	66/92 (72%)	66 (100%)	0	100	100
8	H	74/77 (96%)	74 (100%)	0	100	100
9	I	60/62 (97%)	60 (100%)	0	100	100
10	J	46/69 (67%)	46 (100%)	0	100	100
11	K	45/70 (64%)	45 (100%)	0	100	100
12	L	41/56 (73%)	41 (100%)	0	100	100
13	M	37/59 (63%)	37 (100%)	0	100	100
14	N	72/72 (100%)	72 (100%)	0	100	100
All	All	1586/1783 (89%)	1586 (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. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	413	HIS
4	D	123	HIS
5	E	119	HIS
6	F	129	HIS
7	G	66	HIS
8	H	26	GLN
8	H	32	GLN
14	N	40	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
1	FME	A	1	1	8,9,10	0.54	0	8,9,11	0.93	1 (12%)
3	FME	C	1	3	8,9,10	0.55	0	8,9,11	1.00	1 (12%)

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
1	FME	A	1	1	-	0/7/9/11	-
3	FME	C	1	3	-	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(°)	Ideal(°)
3	C	1	FME	O-C-CA	-2.66	117.92	124.77
1	A	1	FME	O-C-CA	-2.42	118.56	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	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
18	HEA	A	605	1	67,67,67	2.41	26 (38%)	81,103,103	2.62	36 (44%)
21	CDL	N	101	-	99,99,99	1.18	7 (7%)	105,111,111	0.79	2 (1%)
18	HEA	A	604	-	67,67,67	2.35	25 (37%)	81,103,103	2.44	33 (40%)
19	PEE	C	303	-	50,50,50	1.09	3 (6%)	53,55,55	0.73	1 (1%)
17	PGV	A	603	-	50,50,50	1.26	5 (10%)	53,56,56	1.09	2 (3%)
19	PEE	C	301	-	50,50,50	1.11	3 (6%)	53,55,55	1.20	3 (5%)
19	PEE	C	304	-	50,50,50	1.12	3 (6%)	53,55,55	0.84	1 (1%)
19	PEE	C	302	-	50,50,50	1.09	3 (6%)	53,55,55	1.01	3 (5%)

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
18	HEA	A	605	1	1/1/16/16	12/36/76/76	-
21	CDL	N	101	-	-	14/110/110/110	-
18	HEA	A	604	-	-	9/36/76/76	-
19	PEE	C	303	-	-	14/54/54/54	-
17	PGV	A	603	-	-	7/55/55/55	-
19	PEE	C	301	-	-	15/54/54/54	-
19	PEE	C	304	-	-	13/54/54/54	-
19	PEE	C	302	-	-	11/54/54/54	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	605	HEA	FE-NB	5.67	2.12	1.94
18	A	604	HEA	C3B-C2B	5.32	1.46	1.34
18	A	605	HEA	FE-ND	5.18	2.10	1.94
18	A	605	HEA	CHA-C1A	5.10	1.48	1.38
18	A	604	HEA	FE-NB	5.04	2.10	1.94
18	A	605	HEA	C3B-C2B	5.03	1.46	1.34
18	A	604	HEA	C3D-C2D	5.00	1.47	1.36
18	A	604	HEA	FE-ND	4.95	2.10	1.94
18	A	604	HEA	C3A-C2A	4.69	1.47	1.37
18	A	605	HEA	FE-NC	4.58	2.10	1.95
18	A	604	HEA	CHA-C1A	4.51	1.47	1.38
18	A	604	HEA	FE-NC	4.48	2.09	1.95
18	A	605	HEA	C3A-C2A	4.46	1.47	1.37
18	A	605	HEA	CHC-C4B	4.46	1.47	1.38
18	A	604	HEA	CHB-C4A	4.44	1.47	1.38
18	A	605	HEA	C3D-C2D	4.14	1.45	1.36
18	A	605	HEA	CHD-C1D	4.01	1.46	1.38
18	A	605	HEA	C1A-NA	4.00	1.47	1.39
18	A	605	HEA	CHA-C4D	3.97	1.48	1.39
18	A	605	HEA	C1A-C2A	3.93	1.52	1.45
17	A	603	PGV	O01-C1	3.83	1.45	1.34
18	A	604	HEA	CHD-C1D	3.76	1.46	1.38
18	A	604	HEA	CHC-C4B	3.72	1.45	1.38
18	A	604	HEA	C1D-ND	-3.70	1.33	1.40
18	A	604	HEA	C4A-NA	3.65	1.46	1.39
18	A	604	HEA	CHA-C4D	3.60	1.47	1.39
18	A	605	HEA	CHB-C4A	3.59	1.45	1.38
19	C	304	PEE	O3-C30	3.53	1.43	1.33
18	A	605	HEA	CHC-C1C	3.50	1.47	1.39
19	C	301	PEE	O2-C10	3.31	1.43	1.34
19	C	302	PEE	O3-C30	3.31	1.43	1.33
18	A	604	HEA	CHD-C4C	3.30	1.46	1.39
19	C	303	PEE	O3-C30	3.27	1.42	1.33
18	A	605	HEA	CHD-C4C	3.27	1.46	1.39
18	A	604	HEA	C4B-NB	-3.19	1.34	1.40
19	C	301	PEE	O3-C30	3.16	1.42	1.33
18	A	604	HEA	CHB-C1B	3.15	1.46	1.39
21	N	101	CDL	OA8-CA7	3.15	1.42	1.33
21	N	101	CDL	OA6-CA4	-3.10	1.39	1.46
18	A	605	HEA	C4B-C3B	3.10	1.50	1.44
21	N	101	CDL	OA6-CA5	3.04	1.42	1.34
21	N	101	CDL	OB8-CB7	3.03	1.42	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	605	HEA	C4D-C3D	3.02	1.50	1.45
18	A	605	HEA	C4A-NA	3.00	1.45	1.39
18	A	604	HEA	C1A-NA	2.96	1.45	1.39
21	N	101	CDL	OB6-CB4	-2.95	1.39	1.46
18	A	605	HEA	C1D-ND	-2.93	1.35	1.40
19	C	304	PEE	O2-C2	-2.92	1.39	1.46
19	C	302	PEE	O2-C2	-2.87	1.39	1.46
17	A	603	PGV	O03-C19	2.86	1.41	1.33
19	C	303	PEE	O2-C2	-2.84	1.39	1.46
19	C	304	PEE	O2-C10	2.82	1.42	1.34
18	A	604	HEA	CHC-C1C	2.80	1.45	1.39
19	C	303	PEE	O2-C10	2.72	1.41	1.34
21	N	101	CDL	OB6-CB5	2.67	1.41	1.34
18	A	605	HEA	CHB-C1B	2.66	1.45	1.39
19	C	302	PEE	O2-C10	2.57	1.41	1.34
19	C	301	PEE	O2-C2	-2.56	1.40	1.46
18	A	605	HEA	C4C-NC	-2.56	1.34	1.39
18	A	605	HEA	C11-C3B	-2.52	1.48	1.51
18	A	605	HEA	C1C-C2C	2.49	1.49	1.43
18	A	605	HEA	C4B-NB	-2.44	1.36	1.40
17	A	603	PGV	C2-C1	2.43	1.57	1.50
18	A	604	HEA	C11-C3B	-2.43	1.48	1.51
18	A	604	HEA	C4C-NC	-2.41	1.35	1.39
18	A	604	HEA	C1C-NC	-2.41	1.35	1.39
18	A	604	HEA	C4D-C3D	2.41	1.49	1.45
17	A	603	PGV	P-O12	2.35	1.68	1.59
17	A	603	PGV	C4-C3	2.24	1.62	1.51
18	A	604	HEA	C1B-NB	-2.17	1.34	1.38
21	N	101	CDL	PB2-OB2	2.16	1.67	1.59
18	A	605	HEA	C1C-NC	-2.08	1.35	1.39
18	A	604	HEA	C4D-ND	-2.07	1.34	1.38
18	A	605	HEA	C1B-NB	-2.05	1.34	1.38
18	A	604	HEA	C3C-C4C	2.03	1.48	1.42

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	605	HEA	C2B-C1B-NB	6.59	117.52	109.90
18	A	604	HEA	C3D-C4D-ND	6.33	116.47	110.35
18	A	604	HEA	C3B-C4B-NB	6.12	116.88	109.84
18	A	604	HEA	C2D-C1D-ND	6.08	116.83	109.84
18	A	605	HEA	C2D-C1D-ND	5.85	116.57	109.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	603	PGV	O01-C1-C2	5.71	123.84	111.48
18	A	605	HEA	C3C-C2C-C1C	-5.67	100.49	107.17
18	A	605	HEA	C3C-C4C-NC	5.67	114.57	109.80
19	C	301	PEE	O2-C10-C11	5.55	123.50	111.48
18	A	604	HEA	C3C-C2C-C1C	-5.53	100.65	107.17
18	A	605	HEA	CAA-C2A-C1A	5.22	135.47	124.85
18	A	604	HEA	C2B-C1B-NB	5.08	115.77	109.90
18	A	605	HEA	C26-C15-C16	4.81	123.57	115.23
18	A	605	HEA	C3B-C4B-NB	4.79	115.34	109.84
18	A	605	HEA	C13-C12-C11	-4.78	106.76	114.39
18	A	605	HEA	C3D-C4D-ND	4.55	114.75	110.35
18	A	604	HEA	C26-C15-C16	4.48	123.00	115.23
18	A	605	HEA	CAD-C3D-C4D	4.48	132.50	124.70
18	A	604	HEA	C2A-C1A-NA	4.40	114.57	110.32
18	A	604	HEA	C1D-C2D-C3D	-4.39	102.36	106.98
18	A	604	HEA	C3C-C4C-NC	4.29	113.41	109.80
18	A	604	HEA	C2C-C1C-NC	4.28	117.00	110.14
18	A	605	HEA	CHB-C1B-C2B	-4.19	118.42	125.03
18	A	605	HEA	C1D-C2D-C3D	-4.16	102.61	106.98
18	A	605	HEA	C2C-C1C-NC	3.98	116.52	110.14
18	A	604	HEA	C3A-C2A-C1A	-3.95	103.31	107.05
19	C	302	PEE	C40-C39-C38	3.93	154.25	124.83
19	C	301	PEE	C40-C39-C38	3.83	153.56	124.83
18	A	605	HEA	C1B-C2B-C3B	-3.72	102.49	106.80
18	A	604	HEA	C4D-C3D-C2D	-3.55	101.72	106.89
18	A	605	HEA	C12-C11-C3B	3.47	117.55	112.12
18	A	604	HEA	C4B-C3B-C2B	-3.39	101.74	107.44
18	A	604	HEA	C1B-C2B-C3B	-3.30	102.98	106.80
18	A	605	HEA	C16-C15-C14	-3.11	114.19	121.17
18	A	605	HEA	C25-C23-C24	3.02	121.54	114.59
18	A	604	HEA	CHC-C1C-C2C	-2.98	118.77	127.43
18	A	605	HEA	O11-C11-C3B	-2.94	105.86	111.26
18	A	605	HEA	C4B-C3B-C2B	-2.91	102.54	107.44
18	A	605	HEA	CHD-C1D-C2D	-2.90	118.71	126.95
18	A	605	HEA	CHC-C1C-C2C	-2.79	119.33	127.43
18	A	604	HEA	CHC-C4B-C3B	-2.76	118.85	125.80
18	A	605	HEA	C3A-C2A-C1A	-2.73	104.46	107.05
18	A	604	HEA	O11-C11-C3B	-2.71	106.30	111.26
18	A	604	HEA	OMA-CMA-C3A	-2.71	119.51	125.62
18	A	605	HEA	C25-C23-C22	-2.65	114.70	122.66
18	A	605	HEA	C4D-C3D-C2D	-2.64	103.06	106.89
18	A	604	HEA	CMC-C2C-C1C	2.63	129.43	125.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	605	HEA	C4B-NB-C1B	-2.62	102.11	105.21
18	A	604	HEA	CHD-C1D-C2D	-2.61	119.52	126.95
18	A	605	HEA	OMA-CMA-C3A	-2.61	119.72	125.62
18	A	605	HEA	C21-C20-C19	-2.61	104.53	113.19
18	A	605	HEA	CHB-C4A-NA	2.61	127.29	124.45
21	N	101	CDL	OB6-CB5-C51	2.56	117.03	111.48
18	A	605	HEA	C27-C19-C20	2.54	119.64	115.23
17	A	603	PGV	O01-C1-O02	-2.52	117.82	123.70
18	A	605	HEA	C17-C18-C19	-2.43	122.06	127.62
21	N	101	CDL	OA6-CA5-C11	2.42	116.72	111.48
18	A	605	HEA	CMD-C2D-C1D	2.41	128.81	125.03
18	A	605	HEA	C27-C19-C18	-2.36	117.57	123.63
19	C	304	PEE	O2-C10-C11	2.32	116.51	111.48
18	A	604	HEA	CHA-C4D-C3D	-2.28	121.45	124.77
18	A	604	HEA	C13-C14-C15	-2.27	122.43	127.62
18	A	604	HEA	CHA-C4D-ND	-2.26	121.99	124.42
18	A	605	HEA	CHA-C1A-NA	-2.25	122.00	124.45
18	A	604	HEA	C4A-NA-C1A	-2.25	102.15	105.82
18	A	605	HEA	CHB-C4A-C3A	-2.25	121.41	125.21
18	A	604	HEA	CMB-C2B-C1B	2.24	128.54	125.03
18	A	604	HEA	C27-C19-C18	-2.24	117.87	123.63
19	C	301	PEE	O2-C10-O4	-2.21	118.53	123.70
18	A	604	HEA	C1D-ND-C4D	-2.20	102.60	105.21
18	A	604	HEA	C16-C15-C14	-2.18	116.26	121.17
18	A	604	HEA	C4B-NB-C1B	-2.18	102.62	105.21
18	A	604	HEA	CAD-C3D-C2D	2.16	131.91	127.87
18	A	605	HEA	CMC-C2C-C3C	2.12	131.55	126.55
19	C	303	PEE	C40-C39-C38	2.12	140.74	124.83
18	A	604	HEA	C25-C23-C24	2.12	119.46	114.59
19	C	302	PEE	O2-C10-C11	2.10	116.02	111.48
18	A	605	HEA	CMB-C2B-C1B	2.09	128.31	125.03
18	A	604	HEA	CHB-C1B-NB	-2.06	122.21	124.42
19	C	302	PEE	C33-C32-C31	-2.05	105.61	113.13
18	A	604	HEA	C21-C22-C23	-2.01	120.95	127.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	605	HEA	C11

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	603	PGV	C05-C04-O12-P
17	A	603	PGV	O02-C1-O01-C02
17	A	603	PGV	C2-C1-O01-C02
18	A	604	HEA	C4D-C3D-CAD-CBD
18	A	604	HEA	C3B-C11-C12-C13
18	A	605	HEA	C1A-C2A-CAA-CBA
18	A	605	HEA	C3A-C2A-CAA-CBA
18	A	605	HEA	C12-C11-C3B-C2B
18	A	605	HEA	C12-C11-C3B-C4B
19	C	301	PEE	C11-C10-O2-C2
19	C	301	PEE	O4-C10-O2-C2
19	C	302	PEE	C2-C1-O3P-P
19	C	302	PEE	C1-O3P-P-O1P
19	C	303	PEE	C1-O3P-P-O2P
19	C	303	PEE	C1-O3P-P-O4P
19	C	303	PEE	C4-O4P-P-O1P
19	C	303	PEE	C5-C4-O4P-P
19	C	304	PEE	O2-C2-C3-O3
19	C	304	PEE	C1-O3P-P-O2P
19	C	304	PEE	C1-O3P-P-O1P
19	C	304	PEE	C1-O3P-P-O4P
19	C	304	PEE	C4-O4P-P-O2P
21	N	101	CDL	CA2-OA2-PA1-OA4
21	N	101	CDL	CA2-OA2-PA1-OA5
18	A	604	HEA	C26-C15-C16-C17
18	A	604	HEA	C14-C15-C16-C17
18	A	605	HEA	C19-C20-C21-C22
18	A	604	HEA	C2D-C3D-CAD-CBD
18	A	604	HEA	C2A-CAA-CBA-CGA
18	A	605	HEA	C26-C15-C16-C17
18	A	605	HEA	C14-C15-C16-C17
19	C	302	PEE	C10-C11-C12-C13
21	N	101	CDL	O1-C1-CA2-OA2
21	N	101	CDL	CB2-C1-CA2-OA2
18	A	604	HEA	O11-C11-C12-C13
18	A	605	HEA	O11-C11-C12-C13
21	N	101	CDL	C57-C58-C59-C60
17	A	603	PGV	C01-C02-C03-O11
19	C	303	PEE	C31-C32-C33-C34
17	A	603	PGV	C23-C24-C25-C26
19	C	303	PEE	C43-C44-C45-C46
19	C	301	PEE	C14-C15-C16-C17
21	N	101	CDL	C77-C78-C79-C80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	C	301	PEE	C43-C44-C45-C46
19	C	303	PEE	C2-C1-O3P-P
21	N	101	CDL	C53-C54-C55-C56
19	C	304	PEE	C30-C31-C32-C33
18	A	605	HEA	C3B-C11-C12-C13
19	C	304	PEE	C2-C1-O3P-P
19	C	304	PEE	O3P-C1-C2-C3
19	C	304	PEE	C1-C2-C3-O3
17	A	603	PGV	O01-C02-C03-O11
19	C	301	PEE	O3P-C1-C2-O2
19	C	302	PEE	C38-C39-C40-C41
21	N	101	CDL	C58-C59-C60-C61
19	C	302	PEE	C34-C35-C36-C37
19	C	304	PEE	O3P-C1-C2-O2
19	C	301	PEE	C5-C4-O4P-P
19	C	301	PEE	O3P-C1-C2-C3
21	N	101	CDL	CB4-CB3-OB5-PB2
19	C	301	PEE	O2-C2-C3-O3
19	C	303	PEE	O2-C2-C3-O3
21	N	101	CDL	CB7-C71-C72-C73
17	A	603	PGV	C03-O11-P-O13
19	C	301	PEE	C1-O3P-P-O1P
19	C	303	PEE	C1-O3P-P-O1P
19	C	304	PEE	C4-O4P-P-O3P
19	C	301	PEE	C11-C12-C13-C14
19	C	302	PEE	C40-C41-C42-C43
18	A	604	HEA	CAA-CBA-CGA-O2A
19	C	303	PEE	C36-C37-C38-C39
19	C	302	PEE	C14-C15-C16-C17
21	N	101	CDL	C15-C16-C17-C18
19	C	302	PEE	C1-C2-O2-C10
19	C	303	PEE	C1-C2-O2-C10
19	C	301	PEE	C36-C37-C38-C39
18	A	604	HEA	CAA-CBA-CGA-O1A
19	C	301	PEE	C18-C19-C20-C21
21	N	101	CDL	C31-C32-C33-C34
19	C	303	PEE	C1-C2-C3-O3
19	C	304	PEE	C16-C17-C18-C19
19	C	301	PEE	C2-C1-O3P-P
18	A	605	HEA	CAD-CBD-CGD-O2D
19	C	302	PEE	C18-C19-C20-C21
19	C	303	PEE	C38-C39-C40-C41

*Continued on next page...*

*Continued from previous page...*

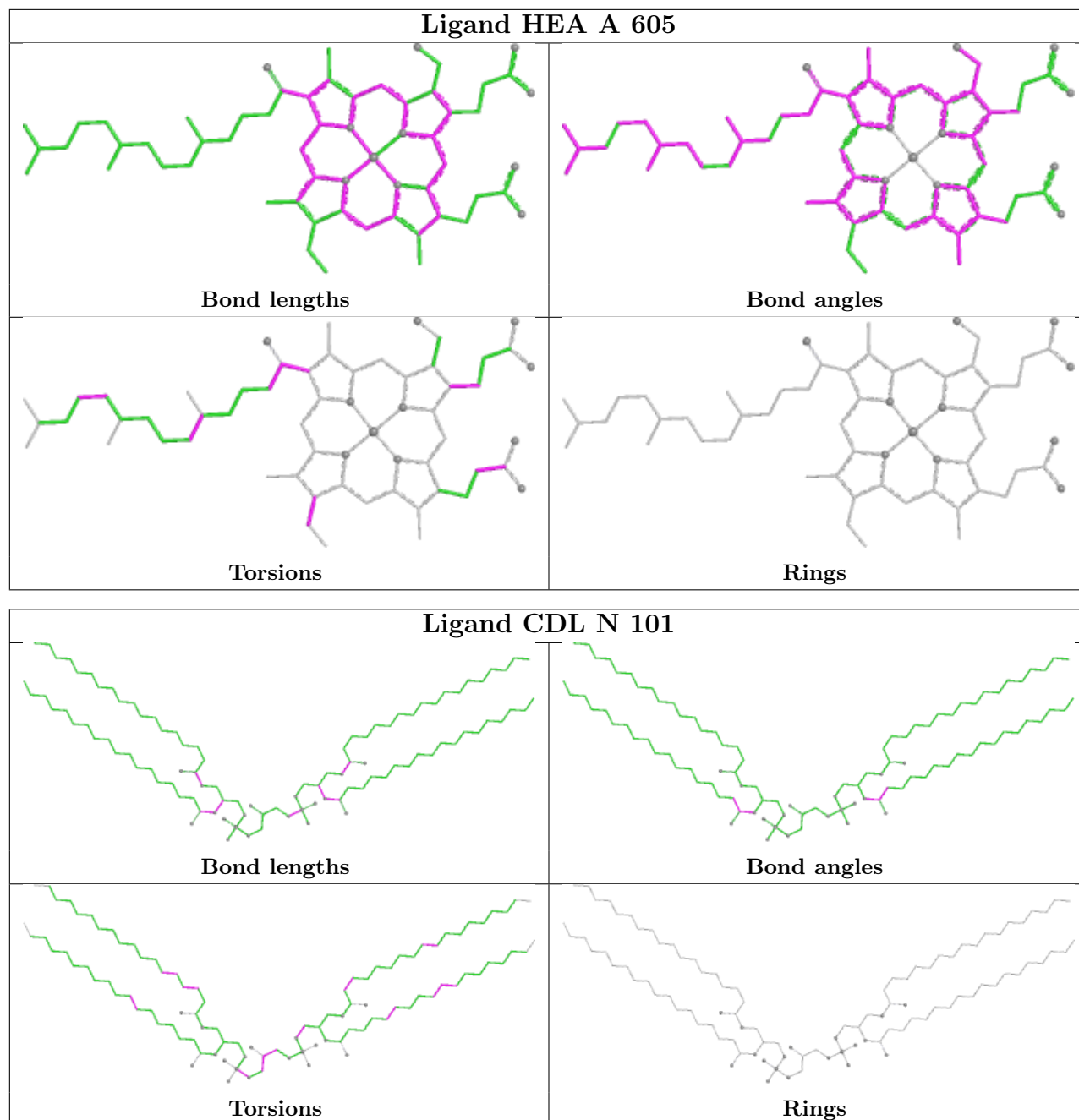
Mol	Chain	Res	Type	Atoms
19	C	301	PEE	C1-C2-C3-O3
18	A	605	HEA	C2C-C3C-CAC-CBC
21	N	101	CDL	C33-C34-C35-C36
18	A	605	HEA	CAD-CBD-CGD-O1D
19	C	304	PEE	C31-C32-C33-C34
19	C	302	PEE	C3-C2-O2-C10
19	C	303	PEE	C21-C22-C23-C24
21	N	101	CDL	O1-C1-CB2-OB2
19	C	302	PEE	C11-C12-C13-C14
19	C	301	PEE	O3-C30-C31-C32

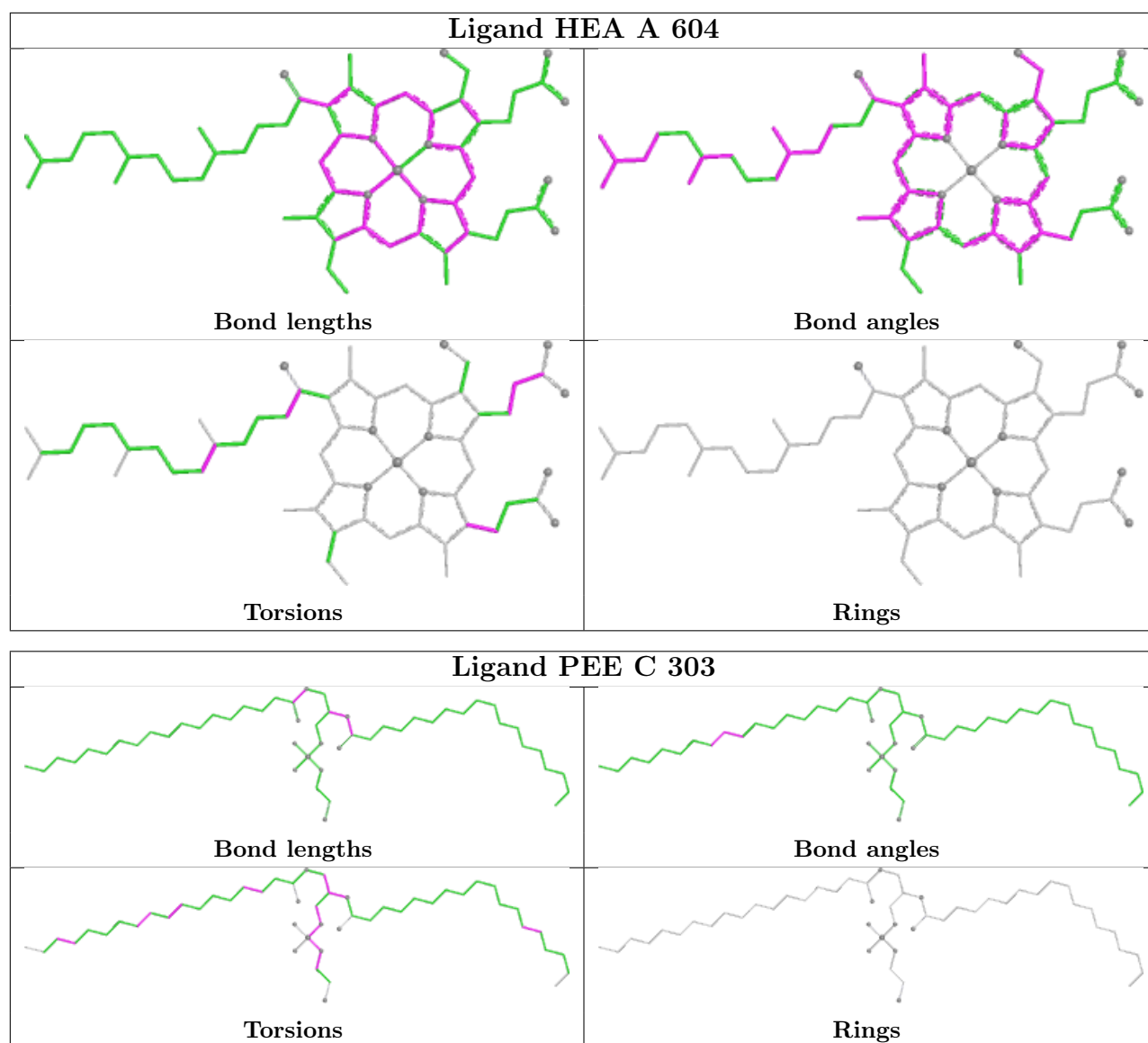
There are no ring outliers.

6 monomers are involved in 40 short contacts:

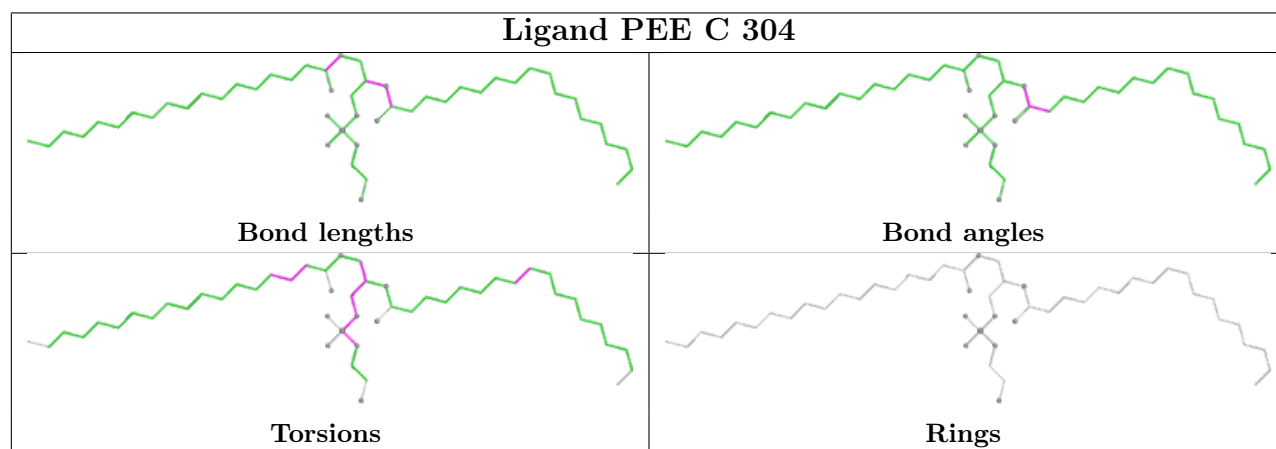
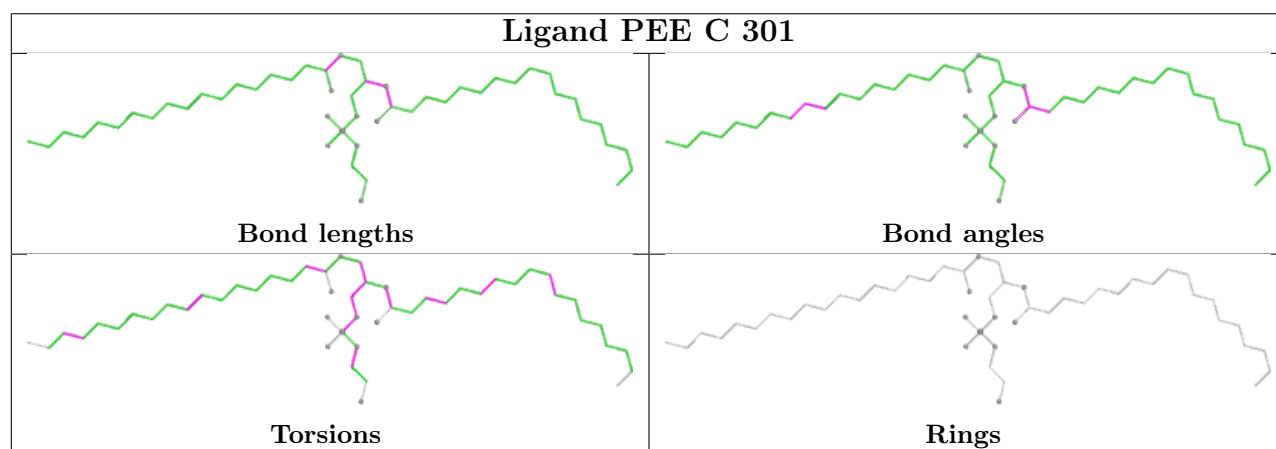
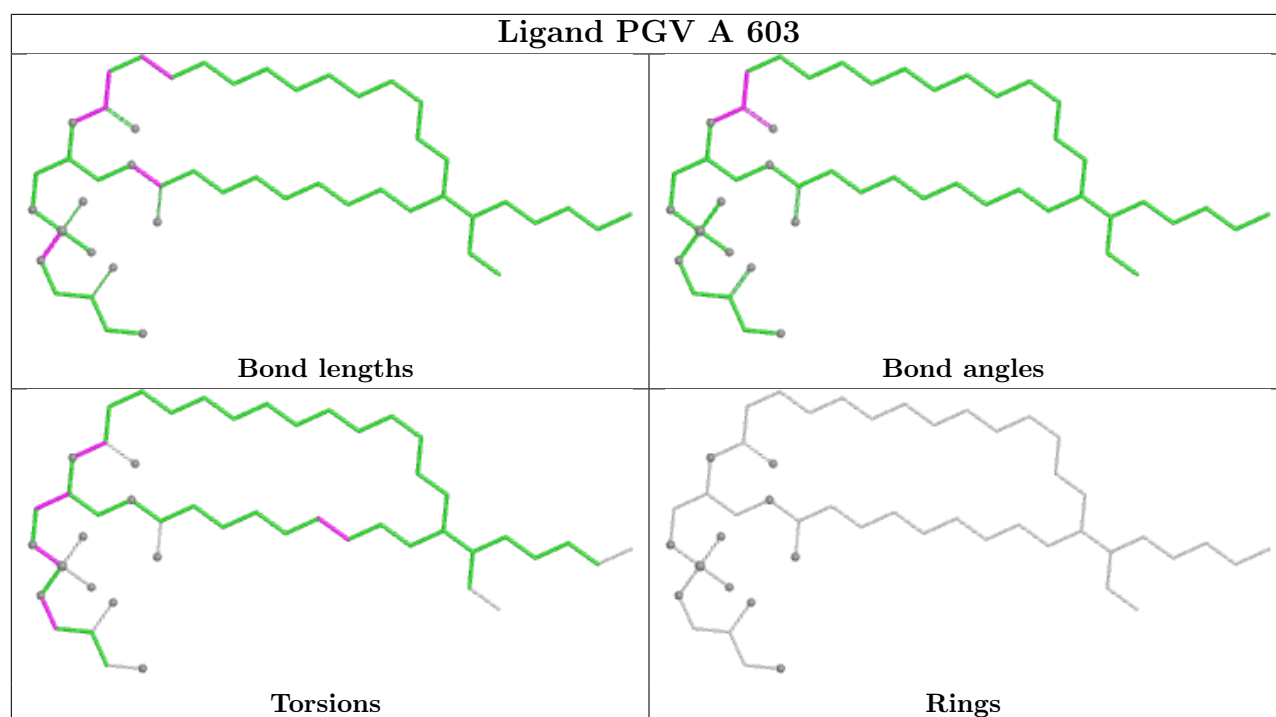
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	605	HEA	18	0
21	N	101	CDL	1	0
18	A	604	HEA	8	0
19	C	303	PEE	8	0
19	C	301	PEE	3	0
19	C	302	PEE	2	0

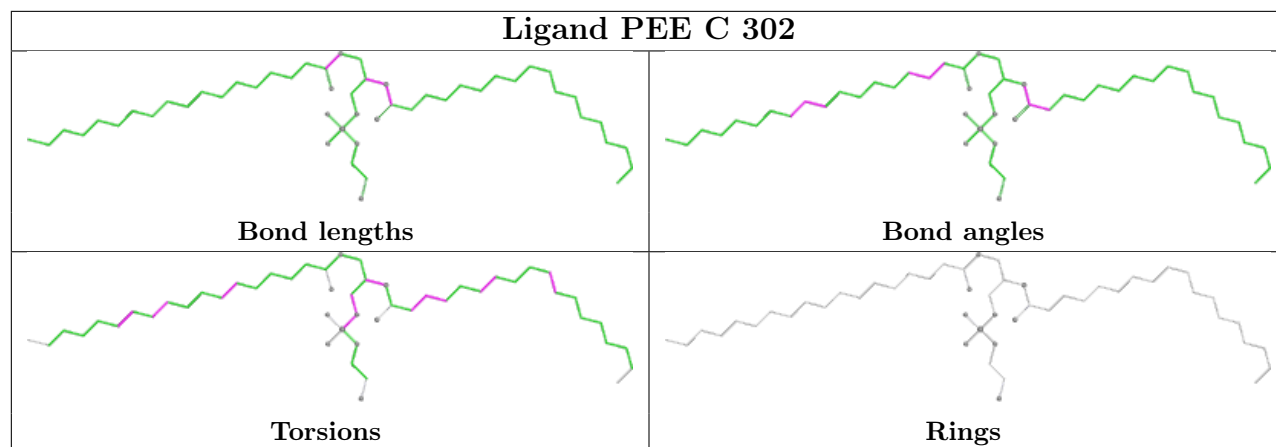
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

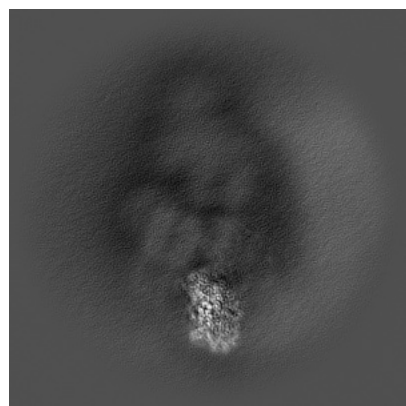
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52662. These allow visual inspection of the internal detail of the map and identification of artifacts.

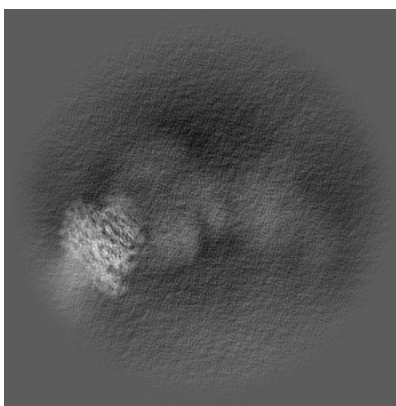
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

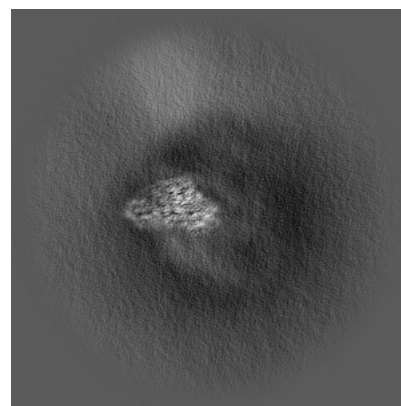
#### 6.1.1 Primary map



X

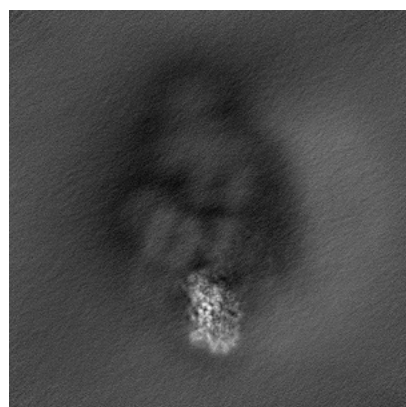


Y

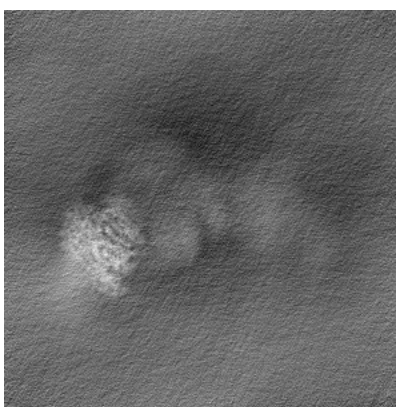


Z

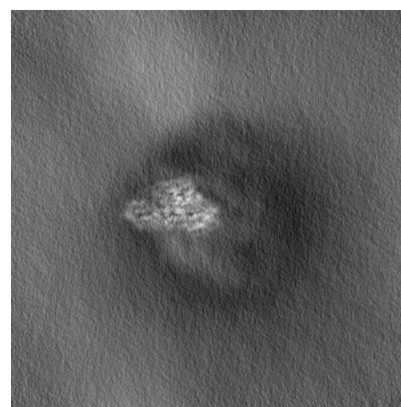
#### 6.1.2 Raw map



X



Y

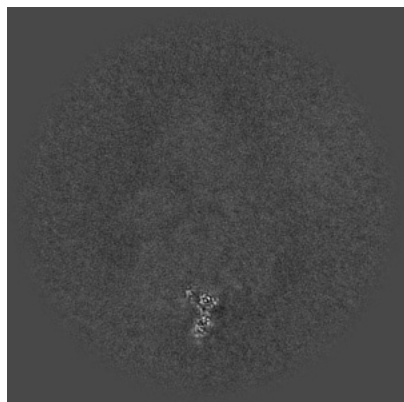


Z

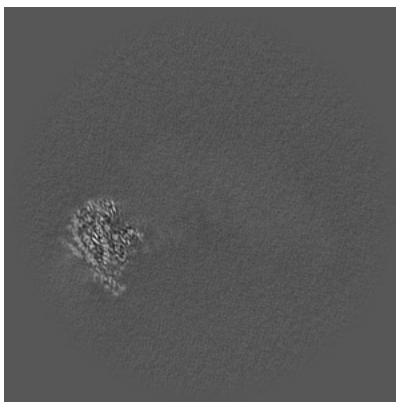
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

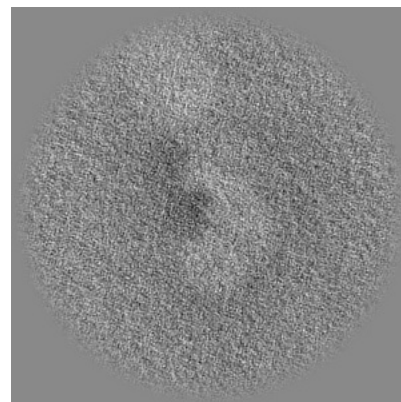
### 6.2.1 Primary map



X Index: 300

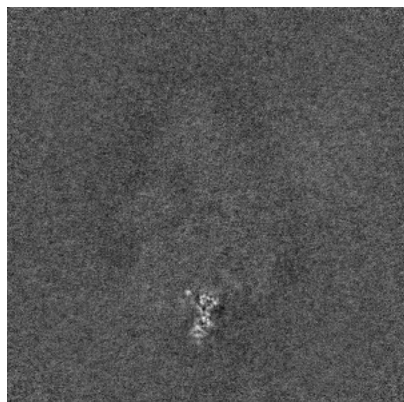


Y Index: 300

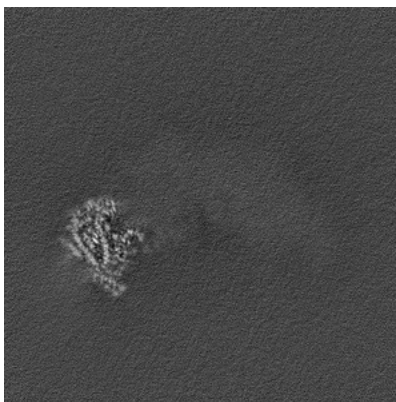


Z Index: 300

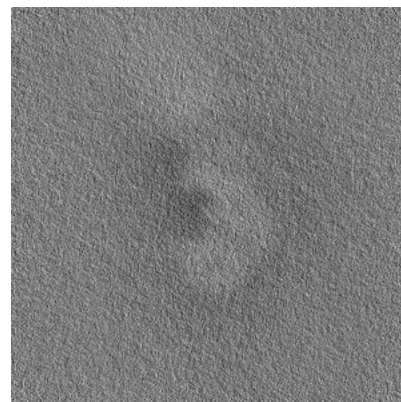
### 6.2.2 Raw map



X Index: 300



Y Index: 300

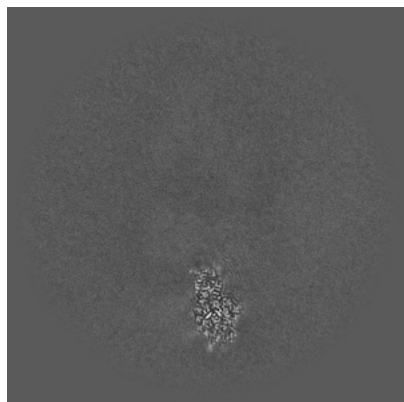


Z Index: 300

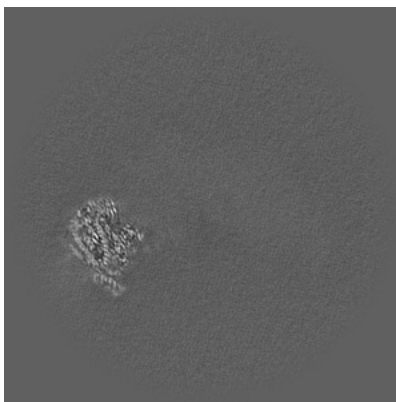
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

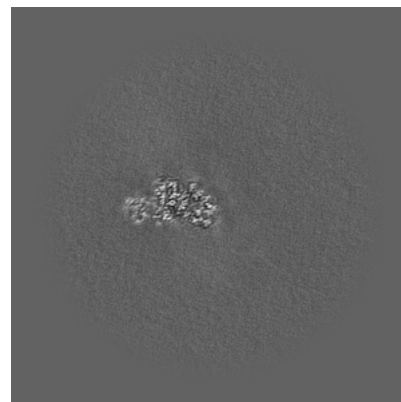
### 6.3.1 Primary map



X Index: 251

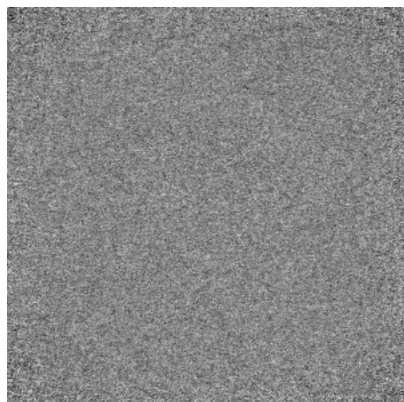


Y Index: 299

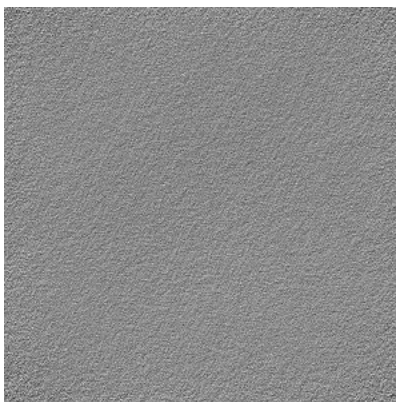


Z Index: 164

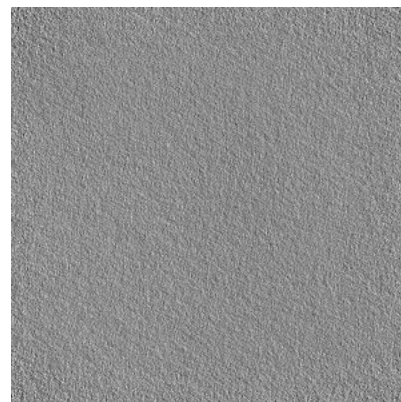
### 6.3.2 Raw map



X Index: 0



Y Index: 0



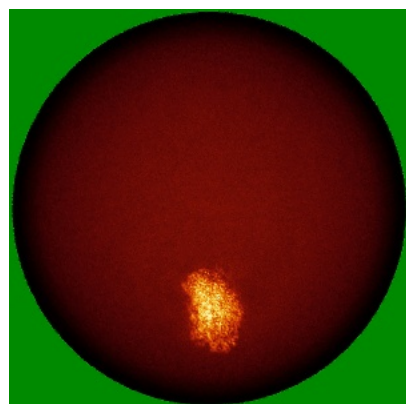
Z Index: 0

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

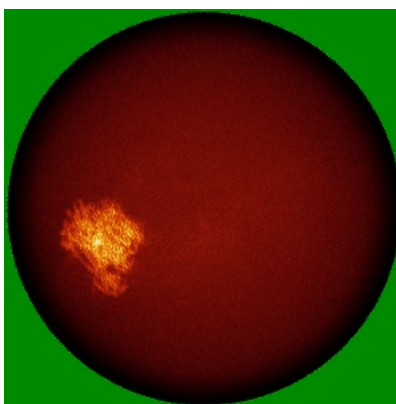


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

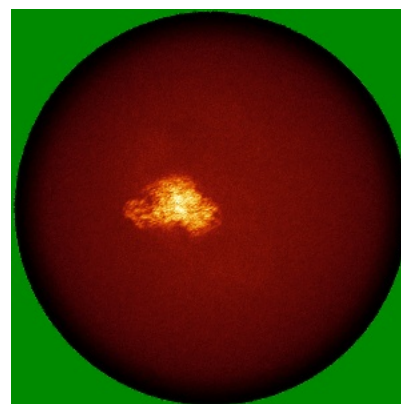
### 6.4.1 Primary map



X

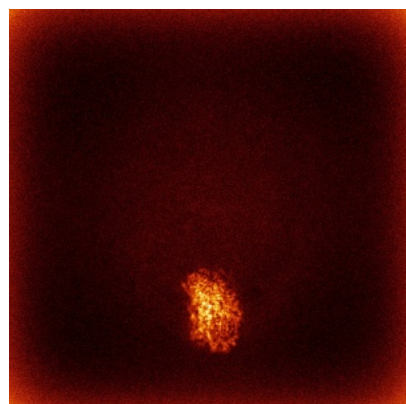


Y

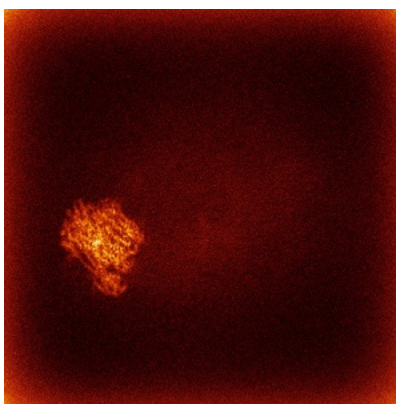


Z

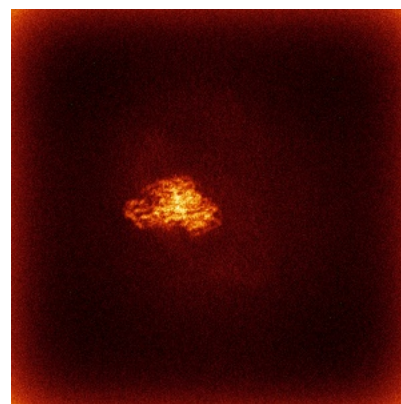
### 6.4.2 Raw map



X



Y

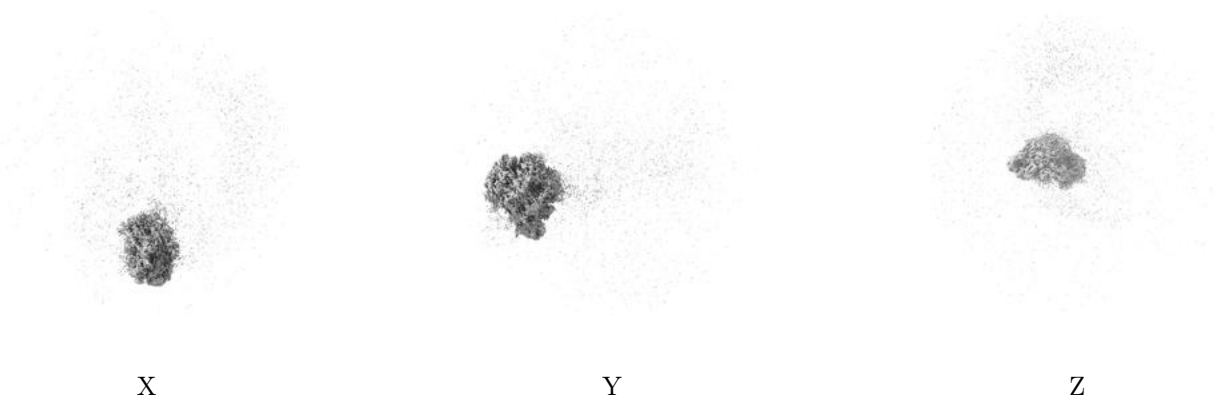


Z

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.

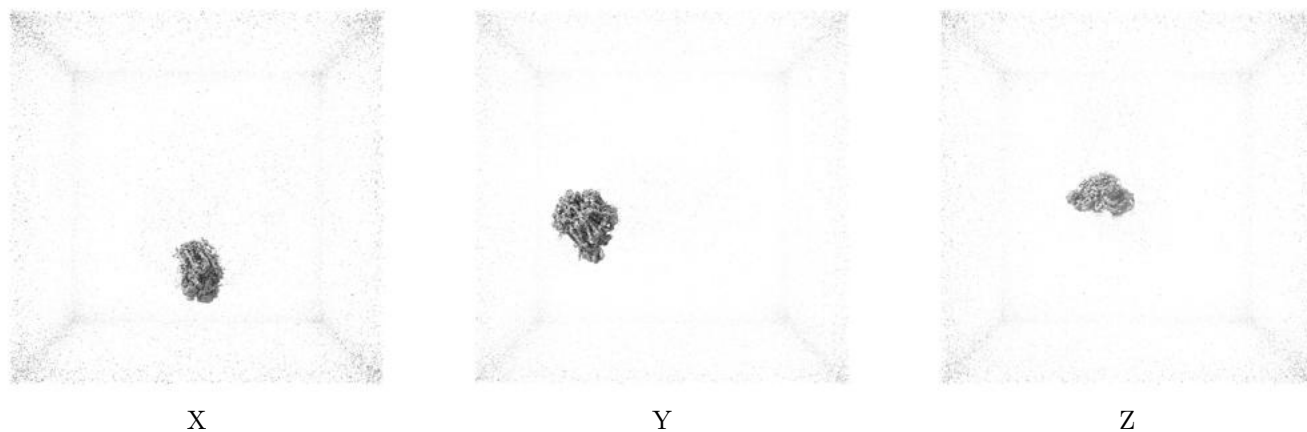
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

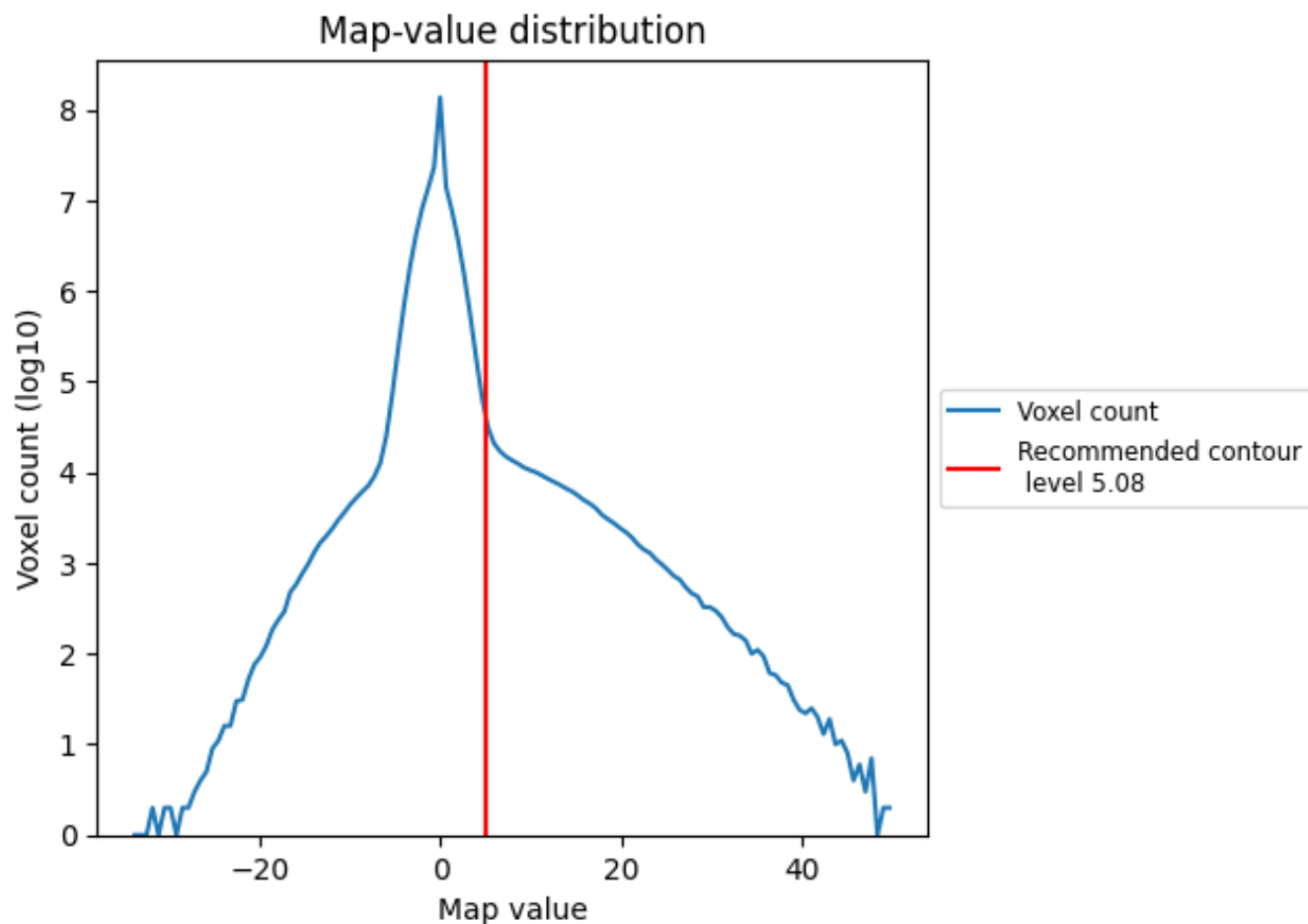
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

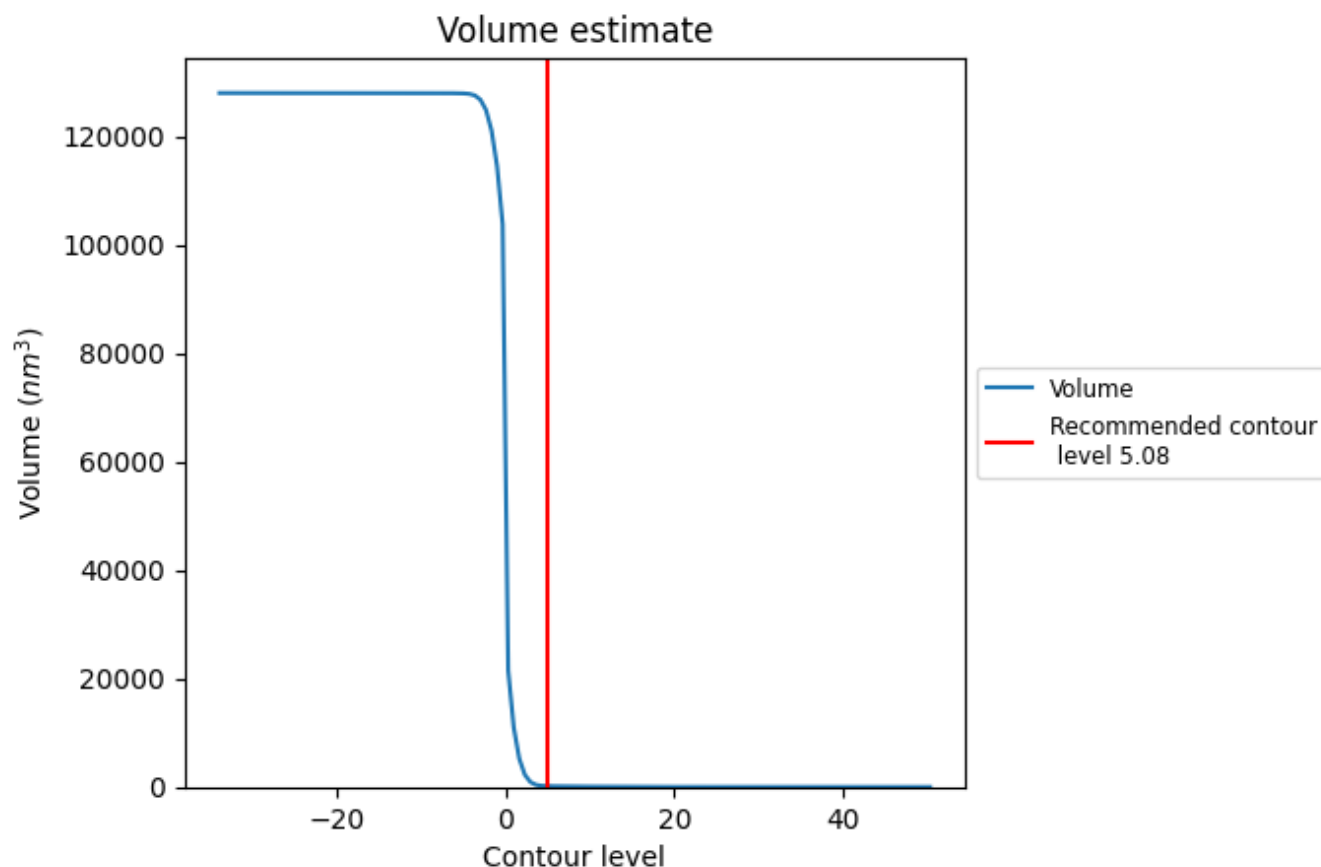
### 7.1 Map-value distribution [i](#)



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.



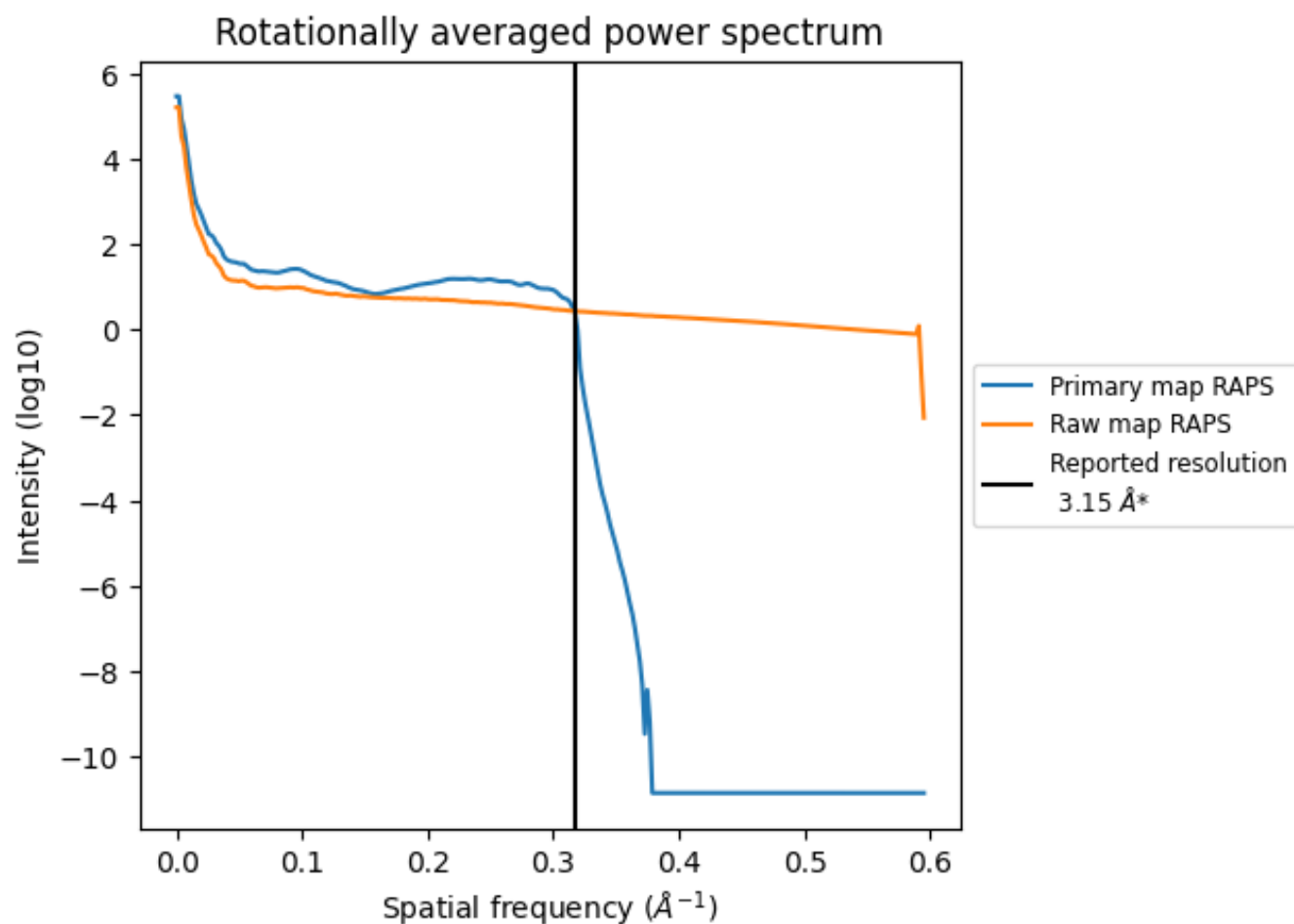
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm<sup>3</sup>; this corresponds to an approximate mass of 133 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

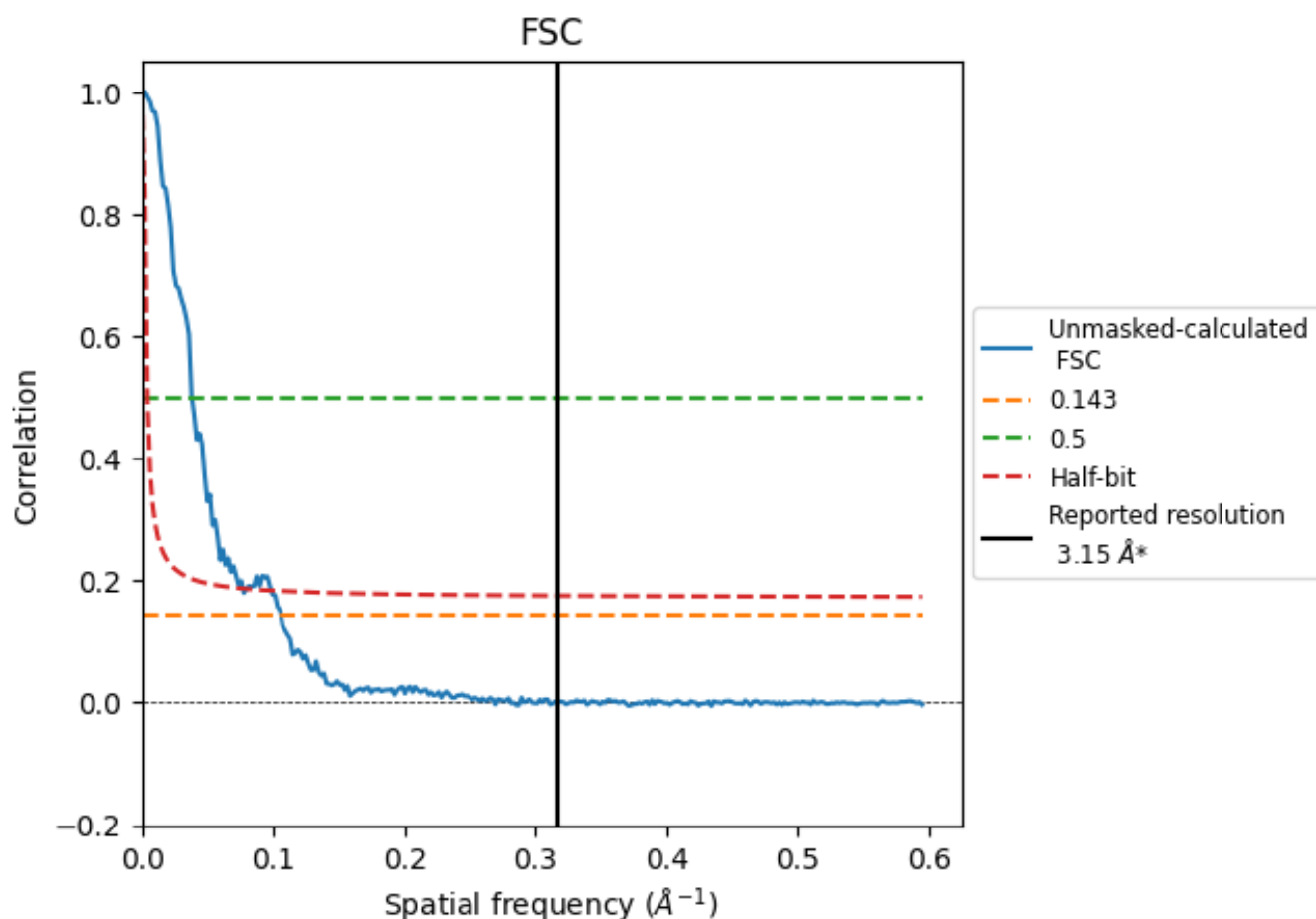


\*Reported resolution corresponds to spatial frequency of 0.317 Å<sup>-1</sup>

## 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 0.317 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

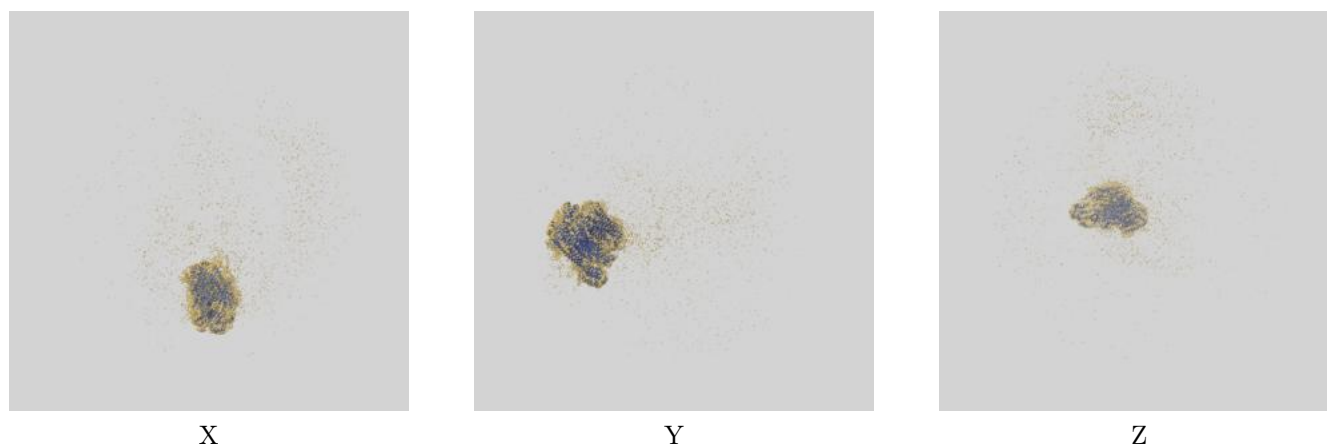
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.45	26.39	13.04

\*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 9.45 differs from the reported value 3.15 by more than 10 %

## 9 Map-model fit [i](#)

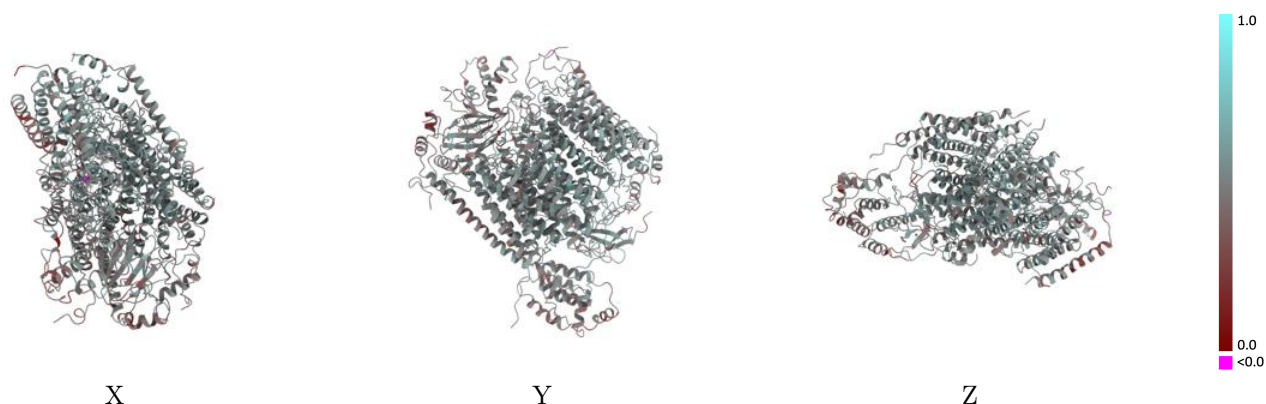
This section contains information regarding the fit between EMDB map EMD-52662 and PDB model 9I7U. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



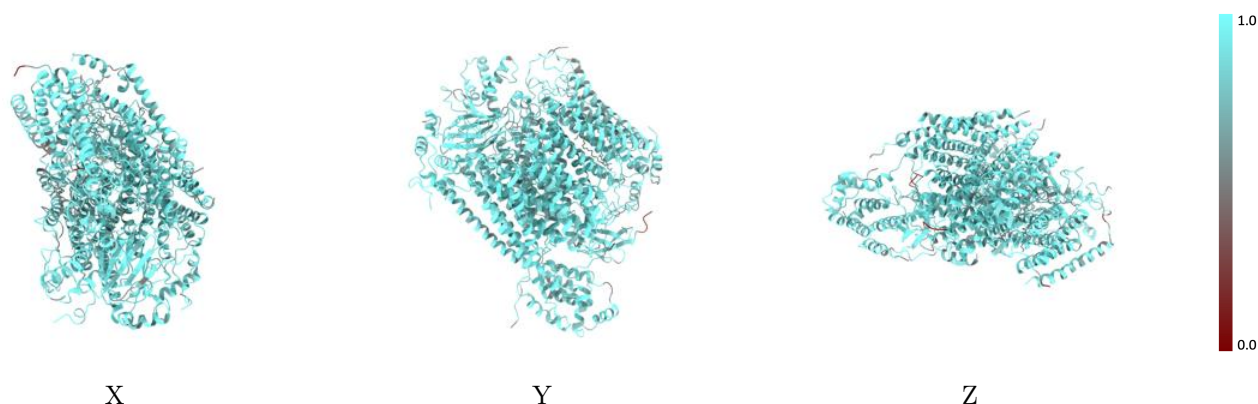
The images above show the 3D surface view of the map at the recommended contour level 5.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



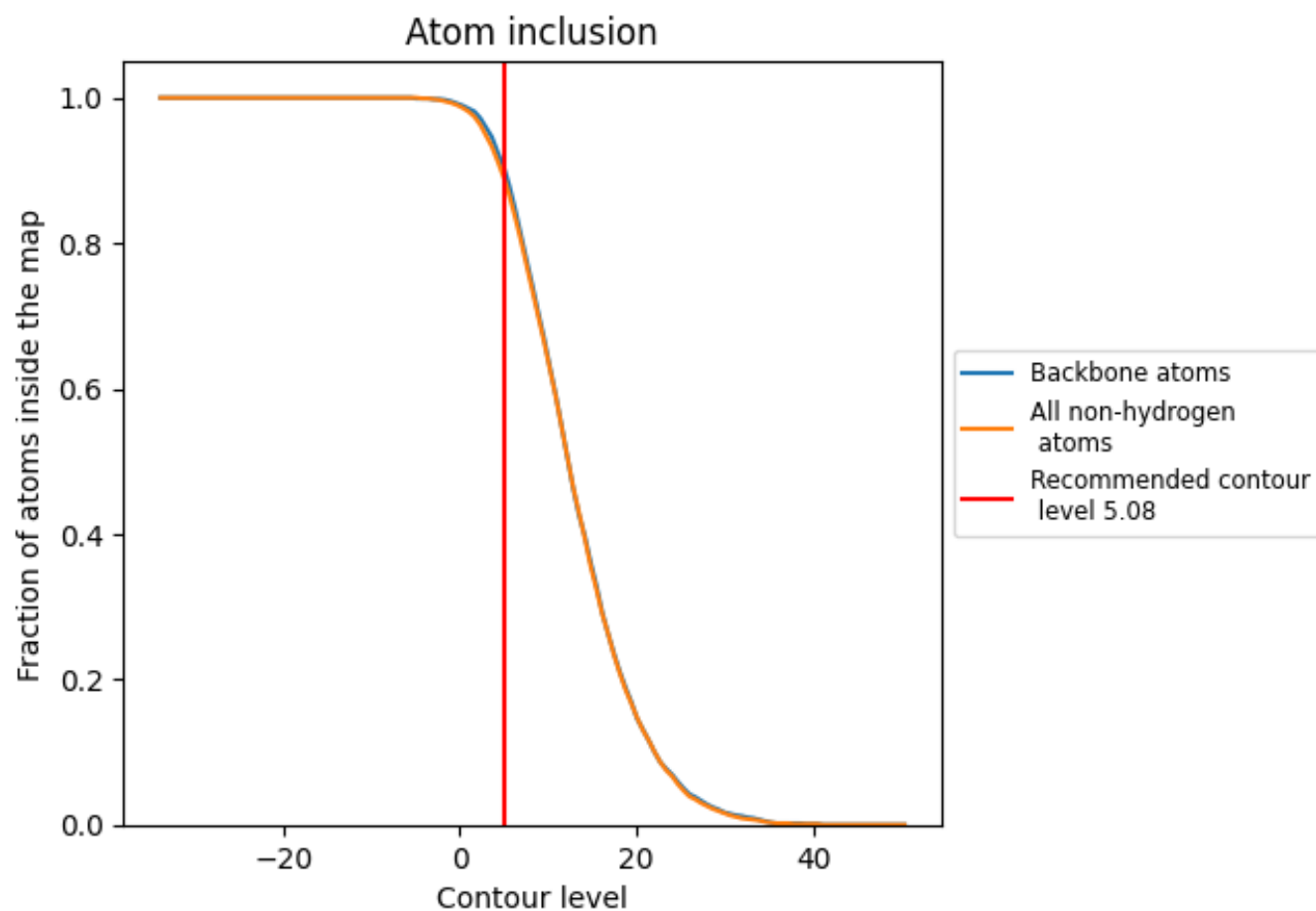
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.08).































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (5.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.4920
A	 0.9430	 0.5320
B	 0.9000	 0.4790
C	 0.9000	 0.5210
D	 0.8890	 0.4620
E	 0.8830	 0.4460
F	 0.8260	 0.4790
G	 0.8340	 0.4470
H	 0.8950	 0.4560
I	 0.8560	 0.4370
J	 0.8350	 0.4940
K	 0.8840	 0.4620
L	 0.9200	 0.5200
M	 0.8660	 0.4900
N	 0.7780	 0.4370

