Full wwPDB EM Validation Report (i)

Dec 18, 2022 – 07:04 pm GMT

PDB ID	:	7ATN
EMDB ID	:	EMD-11922
Title	:	Cytochrome c oxidase structure in R-state
Authors	:	Kolbe, F.; Safarian, S.; Michel, H.
Deposited on	:	2020-10-30
Resolution	:	2.66 Å(reported)
Based on initial model	:	3HB3

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

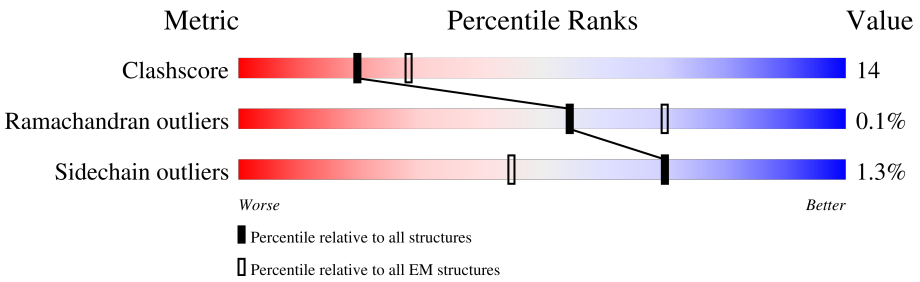
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.66 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	558	80% 16%
2	B	298	9% 63% 21% 15%
3	C	274	28% 63% 35%
4	D	50	52% 60% 20% 20%

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
10	PC1	C	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HEA	A	602	X	-	-	-
6	HEA	A	605	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 8944 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	537	4257	2854	667	703	33	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	252	1975	1294	318	355	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	269	2150	1463	332	344	11	0	0

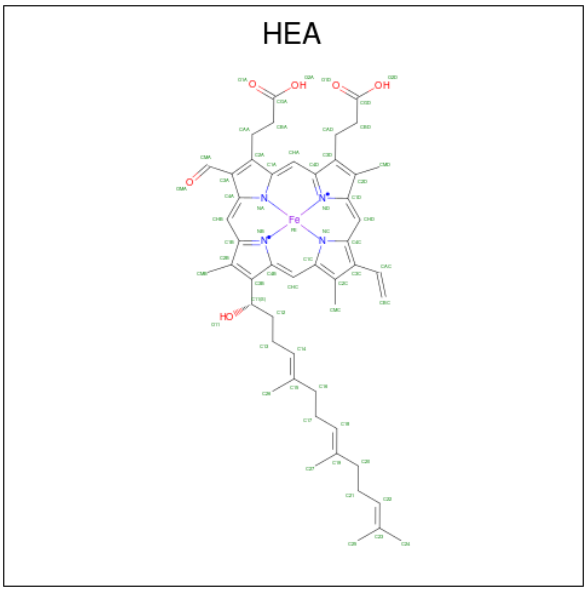
- Molecule 4 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	40	307	200	53	53	1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
5	A	1	1	1	0

- Molecule 6 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
6	A	1	120	98	2	8	12	0
			Total	C	Fe	N	O	
6	A	1	120	98	2	8	12	0

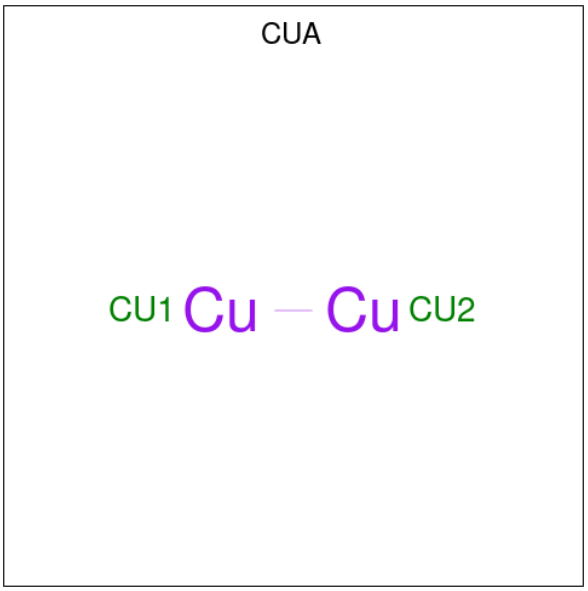
- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
7	A	1	1	1	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

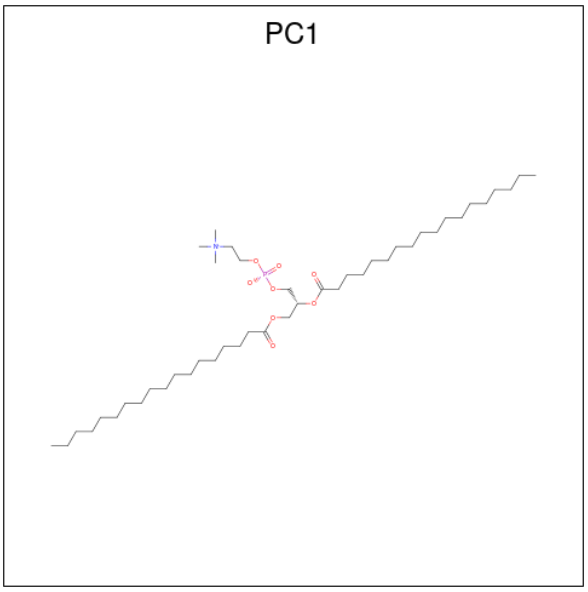
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
8	A	1	1	1	0

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
9	B	1	2	2	0

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	C	1	47	37	1	8	1	0

- Molecule 11 is water.

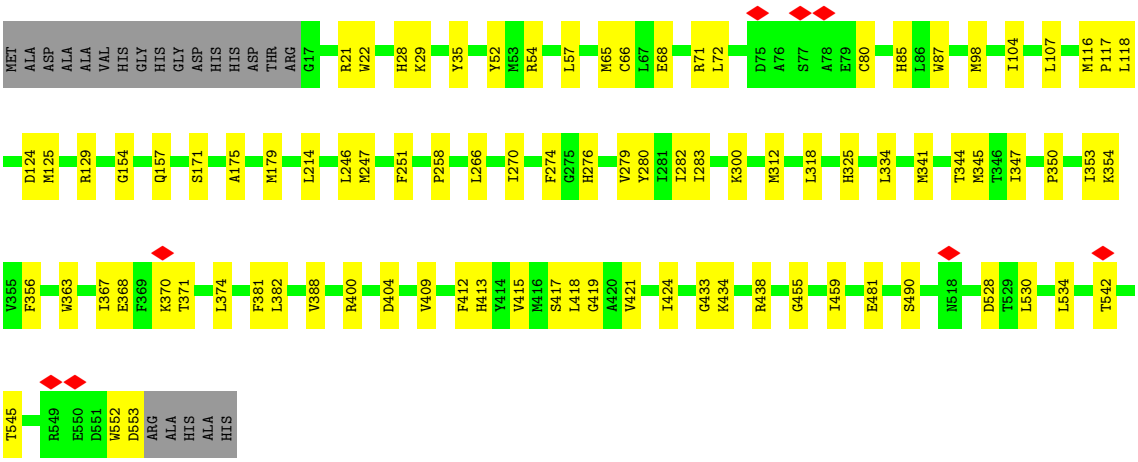
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
11	A	48	48	48	0
			Total	O	
11	B	27	27	27	0
			Total	O	
11	C	7	7	7	0
			Total	O	
11	D	1	1	1	0

3 Residue-property plots (i)

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

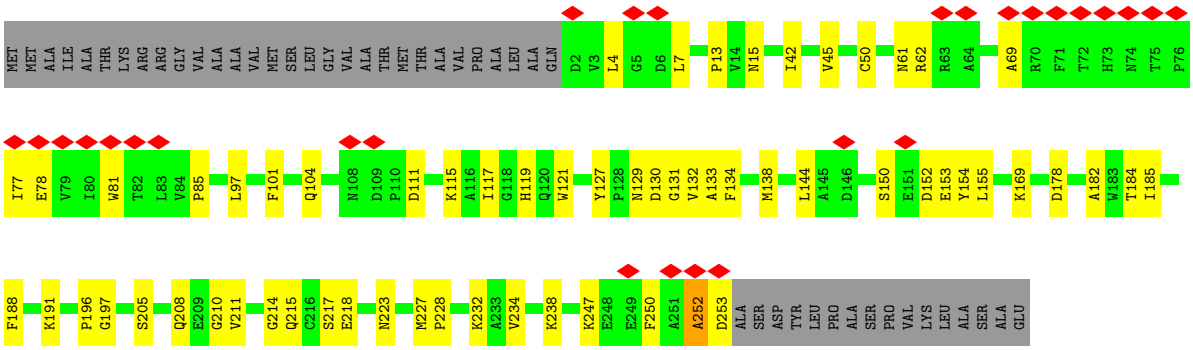
• Molecule 1: Cytochrome c oxidase subunit 1-beta

Chain A:



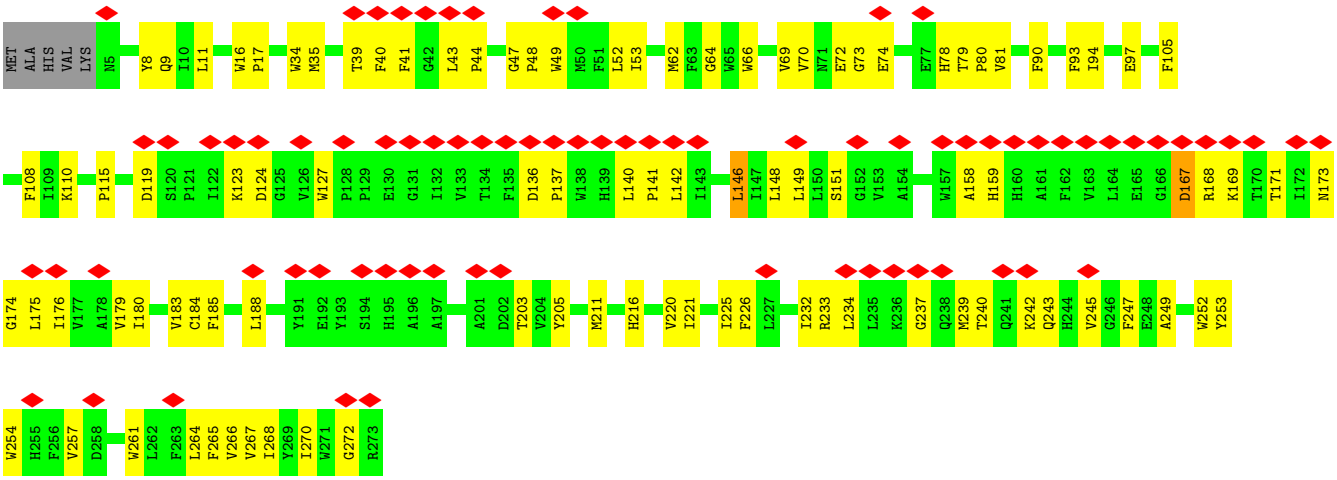
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



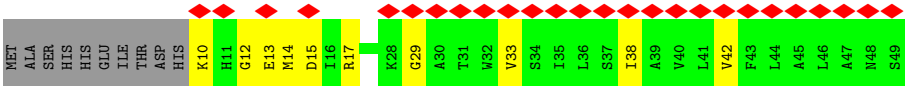
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



- Molecule 4: Cytochrome c oxidase subunit 4

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	289627	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	21.302	Depositor
Minimum map value	-12.403	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.362	Depositor
Recommended contour level	1.15	Depositor
Map size (Å)	107.457, 120.785, 137.445	wwPDB
Map dimensions	129, 145, 165	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.83300006	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CU, CA, HEA, CUA, PC1

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	0.60	0/4416	0.57	0/6028
2	B	0.54	0/2032	0.58	0/2786
3	C	0.47	0/2235	0.51	0/3060
4	D	0.32	0/313	0.40	0/421
All	All	0.55	0/8996	0.55	0/12295

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4257	0	4171	85	0
2	B	1975	0	1958	50	0
3	C	2150	0	2114	122	0
4	D	307	0	313	7	0
5	A	1	0	0	0	0
6	A	120	0	108	9	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	47	0	71	22	0
11	A	48	0	0	2	0
11	B	27	0	0	1	0
11	C	7	0	0	1	0
11	D	1	0	0	0	0
All	All	8944	0	8735	247	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 14.

All (247) 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:C:40:PHE:CE2	3:C:41:PHE:CD2	1.75	1.70
3:C:40:PHE:CE2	3:C:41:PHE:CE2	1.77	1.64
3:C:40:PHE:CZ	3:C:41:PHE:CE2	2.04	1.44
1:A:368:GLU:OE2	1:A:370:LYS:HE2	1.50	1.11
2:B:81:TRP:O	2:B:85:PRO:CD	1.98	1.10
3:C:40:PHE:CD2	3:C:41:PHE:CD2	2.40	1.09
1:A:247:MET:HG3	3:C:211:MET:CE	1.82	1.07
3:C:40:PHE:HE2	3:C:41:PHE:CE2	1.37	1.07
1:A:368:GLU:CD	1:A:370:LYS:HE2	1.75	1.05
1:A:247:MET:CE	3:C:211:MET:HE1	1.87	1.05
2:B:81:TRP:O	2:B:85:PRO:HD2	1.58	1.02
3:C:233:ARG:HH12	10:C:301:PC1:H111	1.25	1.00
3:C:203:THR:O	11:C:401:HOH:O	1.83	0.96
3:C:40:PHE:CD2	3:C:41:PHE:HD2	1.80	0.96
1:A:247:MET:SD	3:C:211:MET:HE1	2.08	0.94
3:C:40:PHE:CE2	3:C:41:PHE:HE2	1.64	0.91
1:A:368:GLU:OE2	1:A:370:LYS:CE	2.23	0.87
2:B:81:TRP:O	2:B:85:PRO:CG	2.22	0.87
3:C:239:MET:HA	10:C:301:PC1:H132	1.57	0.86
1:A:247:MET:CG	3:C:211:MET:HE1	2.04	0.86
3:C:40:PHE:CE2	3:C:41:PHE:HD2	1.59	0.86
1:A:247:MET:HG3	3:C:211:MET:HE1	1.54	0.86
3:C:90:PHE:HE2	3:C:252:TRP:CB	1.89	0.84
3:C:74:GLU:OE2	10:C:301:PC1:H122	1.80	0.82
1:A:247:MET:HG3	3:C:211:MET:HE3	1.61	0.82
3:C:40:PHE:HZ	3:C:41:PHE:CE2	1.90	0.81
1:A:247:MET:CE	3:C:211:MET:CE	2.59	0.80
3:C:142:LEU:O	3:C:142:LEU:HD23	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:ASP:O	3:C:141:PRO:HD2	1.82	0.78
1:A:247:MET:HE2	3:C:211:MET:HE1	1.64	0.78
3:C:140:LEU:HD11	3:C:188:LEU:HD12	1.68	0.75
1:A:312:MET:HG3	1:A:354:LYS:HE3	1.68	0.75
3:C:265:PHE:CE2	3:C:270:ILE:HD11	2.22	0.75
3:C:40:PHE:CZ	3:C:41:PHE:CZ	2.73	0.74
6:A:605:HEA:HHA	6:A:605:HEA:HBA2	1.70	0.74
2:B:81:TRP:O	2:B:85:PRO:HG2	1.85	0.74
1:A:247:MET:CG	3:C:211:MET:CE	2.59	0.73
2:B:7:LEU:HB3	2:B:210:GLY:HA2	1.70	0.73
3:C:171:THR:HB	3:C:234:LEU:HD21	1.69	0.73
3:C:40:PHE:CZ	3:C:41:PHE:CD2	2.54	0.72
3:C:90:PHE:HE2	3:C:252:TRP:HB3	1.53	0.72
3:C:90:PHE:HE2	3:C:252:TRP:HB2	1.54	0.72
3:C:40:PHE:HE2	3:C:41:PHE:CD2	1.54	0.72
3:C:90:PHE:CZ	3:C:249:ALA:O	2.43	0.71
3:C:90:PHE:HZ	3:C:253:TYR:HB2	1.55	0.71
3:C:127:TRP:CZ2	3:C:205:TYR:HD2	2.07	0.71
3:C:90:PHE:CE2	3:C:252:TRP:HB2	2.26	0.71
3:C:93:PHE:CE2	3:C:97:GLU:OE2	2.44	0.70
3:C:243:GLN:HG2	10:C:301:PC1:H142	1.72	0.70
3:C:40:PHE:HE2	3:C:41:PHE:HE2	1.09	0.69
3:C:70:VAL:HG22	10:C:301:PC1:H32	1.74	0.69
3:C:140:LEU:HD11	3:C:188:LEU:CD1	2.22	0.69
1:A:276:HIS:NE2	1:A:280:TYR:HE2	1.90	0.68
3:C:169:LYS:O	3:C:173:ASN:ND2	2.24	0.68
6:A:605:HEA:HBC1	6:A:605:HEA:HMC1	1.76	0.68
2:B:133:ALA:HB3	2:B:252:ALA:HB3	1.74	0.68
4:D:10:LYS:HE3	4:D:13:GLU:HG3	1.76	0.67
3:C:176:ILE:O	3:C:180:ILE:HG13	1.95	0.67
1:A:356:PHE:CD2	2:B:81:TRP:HB2	2.30	0.66
3:C:49:TRP:O	3:C:53:ILE:HG13	1.95	0.66
1:A:54:ARG:HD3	1:A:490:SER:HA	1.77	0.66
1:A:154:GLY:HA2	1:A:175:ALA:HB3	1.76	0.66
1:A:247:MET:HE2	3:C:211:MET:CE	2.22	0.65
3:C:90:PHE:CZ	3:C:253:TYR:HB2	2.31	0.65
3:C:110:LYS:C	3:C:110:LYS:HD3	2.16	0.65
2:B:131:GLY:HA2	2:B:253:ASP:HA	1.78	0.64
3:C:136:ASP:OD1	3:C:137:PRO:HD2	1.97	0.64
3:C:136:ASP:O	3:C:141:PRO:CD	2.45	0.64
3:C:159:HIS:HD1	3:C:247:PHE:HE2	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:VAL:HG22	2:B:232:LYS:HG2	1.79	0.64
3:C:110:LYS:HD3	3:C:110:LYS:O	1.98	0.64
3:C:136:ASP:O	3:C:141:PRO:HG2	1.98	0.64
3:C:48:PRO:O	3:C:52:LEU:HG	1.97	0.64
1:A:344:THR:O	1:A:347:ILE:HG22	1.99	0.63
2:B:127:TYR:HB2	2:B:132:VAL:HG22	1.80	0.63
1:A:300:LYS:HE2	1:A:363:TRP:O	1.99	0.63
10:C:301:PC1:H361	10:C:301:PC1:H292	1.79	0.62
3:C:137:PRO:HA	3:C:141:PRO:HB2	1.80	0.62
2:B:215:GLN:NE2	11:B:401:HOH:O	2.11	0.62
3:C:233:ARG:NH1	10:C:301:PC1:H111	2.07	0.61
1:A:356:PHE:CD2	2:B:81:TRP:CB	2.84	0.61
1:A:368:GLU:CG	1:A:370:LYS:HG3	2.29	0.61
1:A:368:GLU:HG2	1:A:370:LYS:HG3	1.81	0.61
3:C:141:PRO:HB2	3:C:265:PHE:HE1	1.67	0.60
3:C:119:ASP:HB2	3:C:123:LYS:HB2	1.83	0.60
4:D:13:GLU:OE2	4:D:13:GLU:HA	2.01	0.60
1:A:85:HIS:CD2	1:A:157:GLN:HB2	2.37	0.59
3:C:266:VAL:HA	3:C:270:ILE:HD12	1.84	0.59
1:A:276:HIS:HE2	1:A:280:TYR:HE2	1.49	0.58
3:C:90:PHE:CZ	3:C:94:ILE:HD11	2.39	0.58
10:C:301:PC1:O14	10:C:301:PC1:H121	2.01	0.58
3:C:79:THR:HB	3:C:80:PRO:HD2	1.85	0.58
1:A:71:ARG:NH1	1:A:80:CYS:HB2	2.19	0.58
3:C:79:THR:HB	3:C:80:PRO:CD	2.34	0.58
1:A:350:PRO:HA	1:A:353:ILE:HD12	1.85	0.58
6:A:605:HEA:HMD1	6:A:605:HEA:HBD2	1.84	0.58
2:B:132:VAL:HG12	2:B:247:LYS:HA	1.85	0.58
3:C:90:PHE:CE2	3:C:252:TRP:CB	2.80	0.58
3:C:243:GLN:HG2	10:C:301:PC1:C14	2.35	0.57
1:A:455:GLY:O	1:A:459:ILE:HG13	2.05	0.57
2:B:121:TRP:CG	2:B:223:ASN:HB2	2.40	0.57
2:B:185:ILE:HG21	2:B:188:PHE:CD2	2.40	0.57
2:B:111:ASP:OD2	2:B:169:LYS:N	2.34	0.56
1:A:356:PHE:HB3	2:B:81:TRP:CE3	2.40	0.56
2:B:78:GLU:HA	2:B:81:TRP:CE2	2.39	0.56
3:C:40:PHE:HZ	3:C:41:PHE:CZ	2.20	0.56
3:C:240:THR:HG23	3:C:242:LYS:H	1.70	0.55
3:C:216:HIS:CE1	3:C:261:TRP:HB2	2.42	0.55
2:B:138:MET:HB2	2:B:228:PRO:HD2	1.89	0.55
2:B:127:TYR:HB3	2:B:130:ASP:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:MET:HA	10:C:301:PC1:C13	2.35	0.54
3:C:243:GLN:O	10:C:301:PC1:H133	2.06	0.54
1:A:382:LEU:HD13	1:A:418:LEU:HB3	1.90	0.54
3:C:267:VAL:O	3:C:272:GLY:N	2.40	0.54
1:A:129:ARG:NH1	3:C:72:GLU:OE1	2.41	0.54
1:A:434:LYS:NZ	1:A:534:LEU:O	2.41	0.53
3:C:179:VAL:O	3:C:183:VAL:HG23	2.07	0.53
1:A:66:CYS:HB3	1:A:68:GLU:OE2	2.08	0.53
2:B:184:THR:HB	2:B:191:LYS:HG3	1.90	0.53
3:C:62:MET:O	3:C:66:TRP:CD1	2.61	0.53
3:C:148:LEU:HD22	3:C:185:PHE:CE2	2.44	0.53
1:A:276:HIS:CD2	1:A:280:TYR:HE2	2.27	0.53
3:C:80:PRO:HD2	4:D:12:GLY:HA2	1.90	0.53
3:C:151:SER:HG	3:C:254:TRP:HE1	1.52	0.53
3:C:245:VAL:HG12	10:C:301:PC1:H221	1.91	0.52
4:D:29:GLY:O	4:D:33:VAL:HG23	2.09	0.52
3:C:220:VAL:HG22	3:C:257:VAL:CG1	2.39	0.52
3:C:142:LEU:HD23	3:C:146:LEU:HD23	1.91	0.52
3:C:136:ASP:O	3:C:141:PRO:CG	2.57	0.52
1:A:528:ASP:OD1	1:A:528:ASP:N	2.43	0.52
1:A:341:MET:O	1:A:345:MET:HG3	2.10	0.51
3:C:16:TRP:HB2	3:C:17:PRO:HD3	1.92	0.51
3:C:39:THR:HA	3:C:44:PRO:HA	1.91	0.51
2:B:119:HIS:O	2:B:121:TRP:N	2.44	0.51
1:A:334:LEU:HD13	2:B:104:GLN:HB2	1.91	0.51
1:A:276:HIS:O	1:A:279:VAL:HG22	2.11	0.51
6:A:602:HEA:HBC1	6:A:602:HEA:HMC1	1.91	0.51
6:A:605:HEA:H252	6:A:605:HEA:H201	1.92	0.51
2:B:182:ALA:HB3	2:B:217:SER:H	1.76	0.51
3:C:265:PHE:CD2	3:C:270:ILE:HD11	2.45	0.51
3:C:127:TRP:CZ2	3:C:205:TYR:CD2	2.96	0.50
1:A:417:SER:O	1:A:421:VAL:HB	2.11	0.50
3:C:167:ASP:OD1	3:C:167:ASP:N	2.38	0.50
1:A:400:ARG:NH1	11:A:703:HOH:O	2.39	0.50
3:C:151:SER:OG	3:C:254:TRP:NE1	2.45	0.49
2:B:178:ASP:OD1	2:B:178:ASP:N	2.44	0.49
3:C:105:PHE:CZ	3:C:264:LEU:HD23	2.47	0.49
2:B:133:ALA:O	2:B:250:PHE:HB3	2.13	0.49
2:B:134:PHE:HB3	2:B:250:PHE:CD1	2.47	0.48
1:A:356:PHE:HD2	2:B:81:TRP:HB2	1.77	0.48
1:A:371:THR:HA	1:A:374:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:O	2:B:101:PHE:HD1	1.96	0.48
3:C:140:LEU:N	3:C:141:PRO:CD	2.76	0.48
2:B:144:LEU:HD11	2:B:154:TYR:HB2	1.96	0.48
1:A:481:GLU:HG2	2:B:13:PRO:O	2.13	0.48
3:C:115:PRO:HD2	3:C:124:ASP:HB3	1.96	0.47
2:B:121:TRP:HA	2:B:227:MET:SD	2.54	0.47
3:C:168:ARG:NE	3:C:237:GLY:HA2	2.29	0.47
2:B:238:LYS:HB2	2:B:238:LYS:HE3	1.63	0.47
1:A:300:LYS:HZ3	2:B:69:ALA:C	2.17	0.47
3:C:69:VAL:HG12	10:C:301:PC1:H2	1.97	0.47
1:A:552:TRP:CZ3	1:A:553:ASP:HB2	2.49	0.47
3:C:175:LEU:HD11	3:C:247:PHE:HE1	1.79	0.47
3:C:168:ARG:HE	3:C:237:GLY:HA2	1.80	0.46
10:C:301:PC1:H361	10:C:301:PC1:C29	2.44	0.46
1:A:279:VAL:HA	1:A:282:ILE:HD12	1.96	0.46
2:B:4:LEU:HD22	2:B:234:VAL:HG11	1.97	0.46
3:C:81:VAL:HG21	4:D:14:MET:HE1	1.97	0.46
1:A:276:HIS:NE2	1:A:280:TYR:CE2	2.79	0.46
1:A:367:ILE:HB	2:B:61:ASN:HA	1.98	0.46
1:A:481:GLU:O	2:B:15:ASN:HA	2.16	0.46
4:D:15:ASP:OD1	4:D:17:ARG:HG3	2.14	0.46
3:C:243:GLN:CG	10:C:301:PC1:H142	2.42	0.46
3:C:140:LEU:HB3	3:C:141:PRO:HD3	1.96	0.46
1:A:98:MET:HB3	6:A:602:HEA:CAC	2.45	0.46
1:A:409:VAL:HG13	1:A:413:HIS:CE1	2.51	0.46
1:A:29:LYS:HD3	1:A:118:LEU:HD11	1.98	0.46
1:A:246:LEU:HD11	3:C:35:MET:HE1	1.98	0.45
1:A:65:MET:SD	1:A:87:TRP:HE3	2.40	0.45
1:A:412:PHE:HA	1:A:415:VAL:HG22	1.98	0.45
3:C:16:TRP:CE3	3:C:16:TRP:HA	2.52	0.45
1:A:28:HIS:HB3	1:A:125:MET:HG3	1.98	0.45
1:A:247:MET:HE3	3:C:211:MET:CE	2.45	0.45
2:B:185:ILE:HG21	2:B:188:PHE:CE2	2.52	0.45
3:C:245:VAL:N	10:C:301:PC1:O12	2.34	0.45
2:B:184:THR:HG22	2:B:215:GLN:O	2.17	0.44
1:A:276:HIS:CE1	1:A:325:HIS:CE1	3.05	0.44
1:A:258:PRO:HB3	2:B:197:GLY:HA3	1.99	0.44
1:A:318:LEU:HB2	1:A:347:ILE:HD12	2.00	0.43
3:C:110:LYS:C	3:C:110:LYS:CD	2.85	0.43
3:C:8:TYR:CE1	3:C:81:VAL:HG21	2.53	0.43
3:C:141:PRO:CB	3:C:265:PHE:HE1	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PRO:HG3	2:B:196:PRO:O	2.18	0.43
3:C:149:LEU:HD23	3:C:149:LEU:HA	1.74	0.43
3:C:34:TRP:CD1	3:C:47:GLY:HA2	2.54	0.43
3:C:78:HIS:HB2	3:C:243:GLN:HE22	1.84	0.43
3:C:158:ALA:HB2	3:C:174:GLY:HA3	2.00	0.43
3:C:188:LEU:HD13	3:C:188:LEU:HA	1.88	0.43
1:A:530:LEU:HG	1:A:552:TRP:HB3	2.01	0.43
4:D:38:ILE:O	4:D:42:VAL:HG13	2.19	0.42
1:A:280:TYR:HA	1:A:283:ILE:HG22	2.01	0.42
1:A:116:MET:HB3	1:A:117:PRO:HD3	2.00	0.42
2:B:152:ASP:OD1	2:B:153:GLU:HG2	2.19	0.42
3:C:232:ILE:N	3:C:232:ILE:HD13	2.34	0.42
1:A:247:MET:HE1	1:A:251:PHE:CD2	2.54	0.42
1:A:368:GLU:OE1	2:B:62:ARG:NH1	2.53	0.42
3:C:70:VAL:O	3:C:74:GLU:HG2	2.20	0.42
3:C:16:TRP:CZ2	3:C:64:GLY:HA3	2.55	0.42
1:A:54:ARG:HH11	1:A:57:LEU:HB3	1.85	0.42
1:A:171:SER:HB2	1:A:179:MET:CE	2.49	0.42
3:C:74:GLU:OE2	10:C:301:PC1:C15	2.68	0.42
3:C:221:ILE:O	3:C:225:ILE:HG13	2.19	0.42
10:C:301:PC1:H132	10:C:301:PC1:H112	1.54	0.42
1:A:29:LYS:HE2	1:A:542:THR:CG2	2.50	0.42
6:A:605:HEA:HMB1	6:A:605:HEA:H11	1.71	0.42
3:C:74:GLU:OE2	10:C:301:PC1:H153	2.20	0.42
1:A:171:SER:HB2	1:A:179:MET:HE1	2.02	0.41
1:A:107:LEU:HD21	1:A:424:ILE:HG13	2.03	0.41
2:B:184:THR:O	2:B:214:GLY:HA3	2.20	0.41
3:C:171:THR:CB	3:C:234:LEU:HD21	2.43	0.41
1:A:247:MET:HE1	1:A:251:PHE:CG	2.55	0.41
3:C:216:HIS:O	3:C:220:VAL:HG23	2.20	0.41
1:A:433:GLY:HA2	1:A:438:ARG:O	2.21	0.41
1:A:52:TYR:CE1	1:A:72:LEU:HD13	2.55	0.41
1:A:415:VAL:O	1:A:419:GLY:HA3	2.21	0.41
3:C:226:PHE:CD1	10:C:301:PC1:H362	2.56	0.41
1:A:381:PHE:CE1	2:B:50:CYS:SG	3.14	0.41
6:A:605:HEA:H212	6:A:605:HEA:H18	1.70	0.41
1:A:21:ARG:HG2	1:A:22:TRP:CE2	2.56	0.41
2:B:115:LYS:HD3	2:B:117:ILE:HD11	2.02	0.41
1:A:388:VAL:HB	2:B:42:ILE:HB	2.02	0.41
3:C:9:GLN:HG2	3:C:11:LEU:HD22	2.02	0.41
3:C:73:GLY:O	10:C:301:PC1:H143	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:HB	11:A:744:HOH:O	2.21	0.41
2:B:77:ILE:HD12	2:B:77:ILE:HA	1.87	0.41
1:A:29:LYS:HE2	1:A:542:THR:HG23	2.03	0.41
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.93	0.40
1:A:368:GLU:HG3	1:A:370:LYS:HG3	2.01	0.40
3:C:90:PHE:CE2	3:C:94:ILE:HD11	2.55	0.40
3:C:184:CYS:O	3:C:188:LEU:HD23	2.21	0.40
10:C:301:PC1:H342	10:C:301:PC1:H281	2.02	0.40
1:A:412:PHE:HA	1:A:415:VAL:CG2	2.51	0.40
2:B:154:TYR:CE2	2:B:155:LEU:HG	2.55	0.40
6:A:605:HEA:H252	2:B:45:VAL:HG11	2.04	0.40
3:C:108:PHE:CE1	3:C:268:ILE:HG12	2.55	0.40
1:A:124:ASP:OD1	1:A:125:MET:N	2.52	0.40
1:A:266:LEU:O	1:A:270:ILE:HG13	2.21	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	535/558 (96%)	515 (96%)	20 (4%)	0	100	100
2	B	250/298 (84%)	238 (95%)	11 (4%)	1 (0%)	34	48
3	C	267/274 (97%)	261 (98%)	6 (2%)	0	100	100
4	D	38/50 (76%)	38 (100%)	0	0	100	100
All	All	1090/1180 (92%)	1052 (96%)	37 (3%)	1 (0%)	54	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	252	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/454 (97%)	436 (99%)	4 (1%)	78	87
2	B	211/243 (87%)	206 (98%)	5 (2%)	49	67
3	C	217/221 (98%)	214 (99%)	3 (1%)	67	81
4	D	31/40 (78%)	31 (100%)	0	100	100
All	All	899/958 (94%)	887 (99%)	12 (1%)	70	82

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

Mol	Chain	Res	Type
1	A	35	TYR
1	A	274	PHE
1	A	404	ASP
1	A	545	THR
2	B	129	ASN
2	B	150	SER
2	B	205	SER
2	B	208	GLN
2	B	218	GLU
3	C	43	LEU
3	C	146	LEU
3	C	167	ASP

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

Mol	Chain	Res	Type
1	A	85	HIS
3	C	243	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
10	PC1	C	301	-	46,46,53	0.98	2 (4%)	52,54,61	1.04	5 (9%)
6	HEA	A	602	1	57,67,67	1.55	12 (21%)	61,103,103	2.60	24 (39%)
9	CUA	B	301	2	0,1,1	-	-	-		
6	HEA	A	605	1	57,67,67	1.54	10 (17%)	61,103,103	2.60	22 (36%)

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
10	PC1	C	301	-	-	19/50/50/57	-
6	HEA	A	602	1	3/3/7/16	7/32/76/76	-
6	HEA	A	605	1	3/3/7/16	12/32/76/76	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	HEA	C3A-C2A	-5.73	1.32	1.40
6	A	602	HEA	FE-NB	4.25	2.17	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	HEA	FE-NB	4.07	2.17	1.96
6	A	602	HEA	C3A-C2A	-3.92	1.34	1.40
10	C	301	PC1	C14-N	-3.84	1.38	1.50
6	A	602	HEA	C4B-NB	-3.33	1.34	1.40
10	C	301	PC1	C13-N	-3.10	1.40	1.50
6	A	605	HEA	C3C-CAC	3.00	1.54	1.47
6	A	602	HEA	C3C-C2C	-2.97	1.36	1.40
6	A	602	HEA	FE-ND	2.93	2.11	1.96
6	A	605	HEA	C3C-C2C	-2.87	1.36	1.40
6	A	602	HEA	C3C-CAC	2.74	1.53	1.47
6	A	602	HEA	C1B-NB	-2.68	1.33	1.38
6	A	602	HEA	O2D-CGD	-2.58	1.22	1.30
6	A	605	HEA	C3A-CMA	2.54	1.52	1.46
6	A	602	HEA	C1D-ND	-2.48	1.36	1.40
6	A	605	HEA	O2D-CGD	-2.43	1.22	1.30
6	A	602	HEA	C4C-CHD	-2.20	1.34	1.41
6	A	605	HEA	FE-ND	2.13	2.07	1.96
6	A	605	HEA	CMD-C2D	2.07	1.55	1.50
6	A	602	HEA	C4D-ND	-2.06	1.34	1.38
6	A	605	HEA	CHD-C1D	2.05	1.40	1.35
6	A	605	HEA	O2A-CGA	-2.03	1.23	1.30
6	A	602	HEA	O2A-CGA	-2.01	1.24	1.30

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	602	HEA	C4B-NB-C1B	8.37	113.72	105.07
6	A	605	HEA	C1D-ND-C4D	7.58	112.90	105.07
6	A	602	HEA	C4A-CHB-C1B	6.93	131.70	122.56
6	A	605	HEA	CAD-CBD-CGD	-6.46	99.69	113.60
6	A	605	HEA	CAA-CBA-CGA	-6.19	96.40	113.76
6	A	602	HEA	C1D-ND-C4D	6.10	111.37	105.07
6	A	605	HEA	C3D-C4D-ND	-5.41	105.11	110.36
6	A	605	HEA	C2D-C1D-ND	-4.86	104.08	109.84
6	A	602	HEA	C4D-CHA-C1A	4.59	128.62	122.56
6	A	605	HEA	O1A-CGA-CBA	-4.47	108.73	123.08
6	A	602	HEA	C3B-C4B-NB	-4.18	104.89	109.84
6	A	605	HEA	CAA-C2A-C3A	-4.12	116.70	126.86
6	A	605	HEA	C4A-CHB-C1B	4.09	127.95	122.56
6	A	602	HEA	C27-C19-C20	3.95	121.92	115.27
6	A	605	HEA	CMC-C2C-C1C	-3.90	122.47	128.46
6	A	602	HEA	C3A-C4A-NA	-3.67	104.01	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	605	HEA	C4D-CHA-C1A	3.66	127.39	122.56
6	A	602	HEA	CBA-CAA-C2A	3.65	118.76	112.60
6	A	602	HEA	CAA-CBA-CGA	-3.63	103.58	113.76
6	A	605	HEA	CHA-C4D-ND	3.63	128.37	124.43
6	A	602	HEA	C2D-C1D-ND	-3.60	105.58	109.84
6	A	602	HEA	CMC-C2C-C1C	-3.50	123.08	128.46
10	C	301	PC1	O11-P-O14	-3.49	95.44	109.07
6	A	602	HEA	OMA-CMA-C3A	-3.44	117.42	124.91
6	A	602	HEA	CHB-C1B-C2B	3.44	130.35	124.98
6	A	602	HEA	C3D-C4D-ND	-3.42	107.04	110.36
6	A	602	HEA	C2B-C1B-NB	-3.37	105.85	109.88
6	A	602	HEA	CAD-CBD-CGD	-3.33	106.44	113.60
6	A	605	HEA	C4B-NB-C1B	3.15	108.32	105.07
6	A	602	HEA	C20-C19-C18	-3.08	114.89	121.12
6	A	605	HEA	C3B-C4B-NB	-3.00	106.28	109.84
6	A	605	HEA	CBA-CAA-C2A	2.97	117.62	112.60
6	A	602	HEA	C26-C15-C16	2.86	120.08	115.27
6	A	605	HEA	CMB-C2B-C3B	-2.84	124.94	130.34
6	A	605	HEA	CAD-C3D-C4D	-2.79	119.79	124.66
10	C	301	PC1	C15-N-C12	2.79	121.32	109.92
6	A	605	HEA	C3A-C4A-NA	-2.66	105.92	110.94
10	C	301	PC1	O21-C2-C1	-2.55	99.16	108.40
10	C	301	PC1	C15-N-C14	-2.49	102.57	108.97
6	A	602	HEA	CAA-C2A-C3A	2.48	132.97	126.86
6	A	602	HEA	CHA-C4D-ND	2.35	126.98	124.43
6	A	605	HEA	CMC-C2C-C3C	2.33	129.04	124.68
6	A	605	HEA	C24-C23-C22	-2.29	116.03	122.65
6	A	602	HEA	C13-C14-C15	-2.22	122.32	127.66
10	C	301	PC1	O12-P-O11	2.20	117.95	107.75
6	A	605	HEA	C3C-C4C-NC	-2.14	106.44	109.21
6	A	605	HEA	C25-C23-C24	2.14	119.32	114.60
6	A	602	HEA	CAD-C3D-C4D	-2.08	121.03	124.66
6	A	605	HEA	CBD-CAD-C3D	2.07	118.37	112.63
6	A	602	HEA	CMC-C2C-C3C	2.02	128.45	124.68
6	A	602	HEA	O2A-CGA-O1A	-2.01	118.30	123.30

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	602	HEA	NA
6	A	602	HEA	NB
6	A	602	HEA	ND

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Mol	Chain	Res	Type	Atom
6	A	605	HEA	NA
6	A	605	HEA	NB
6	A	605	HEA	ND

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	HEA	C1A-C2A-CAA-CBA
6	A	602	HEA	C3A-C2A-CAA-CBA
6	A	605	HEA	C1A-C2A-CAA-CBA
6	A	605	HEA	C3A-C2A-CAA-CBA
6	A	605	HEA	C2A-CAA-CBA-CGA
6	A	605	HEA	C2D-C3D-CAD-CBD
6	A	605	HEA	C4D-C3D-CAD-CBD
10	C	301	PC1	C12-C11-O13-P
10	C	301	PC1	O13-C11-C12-N
6	A	605	HEA	C19-C20-C21-C22
6	A	605	HEA	C21-C22-C23-C24
10	C	301	PC1	C11-O13-P-O11
10	C	301	PC1	C11-C12-N-C13
10	C	301	PC1	C11-C12-N-C14
10	C	301	PC1	C31-C32-C33-C34
10	C	301	PC1	C23-C24-C25-C26
10	C	301	PC1	C11-C12-N-C15
10	C	301	PC1	C2A-C2B-C2C-C2D
6	A	602	HEA	C21-C22-C23-C24
10	C	301	PC1	C22-C21-O21-C2
10	C	301	PC1	C27-C28-C29-C2A
10	C	301	PC1	O22-C21-O21-C2
10	C	301	PC1	C21-C22-C23-C24
10	C	301	PC1	O11-C1-C2-O21
10	C	301	PC1	C33-C34-C35-C36
10	C	301	PC1	C11-O13-P-O12
10	C	301	PC1	C34-C35-C36-C37
6	A	605	HEA	C20-C21-C22-C23
6	A	602	HEA	C21-C22-C23-C25
6	A	602	HEA	CAA-CBA-CGA-O1A
10	C	301	PC1	C36-C37-C38-C39
6	A	602	HEA	CAA-CBA-CGA-O2A
6	A	605	HEA	C18-C19-C20-C21
6	A	605	HEA	CAD-CBD-CGD-O2D
6	A	605	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	A	605	HEA	CAD-CBD-CGD-O1D
10	C	301	PC1	O11-C1-C2-C3
6	A	602	HEA	CAD-CBD-CGD-O1D

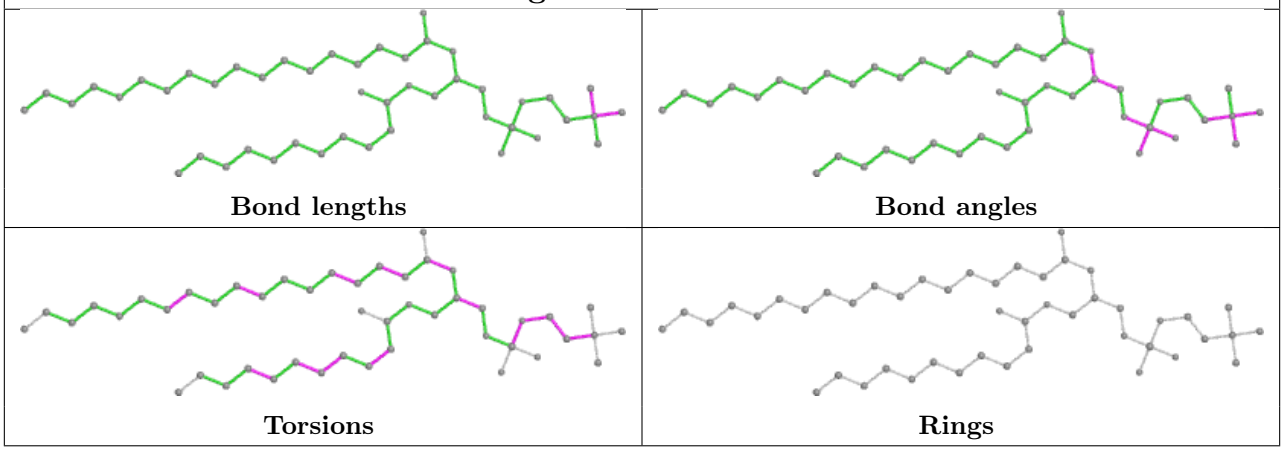
There are no ring outliers.

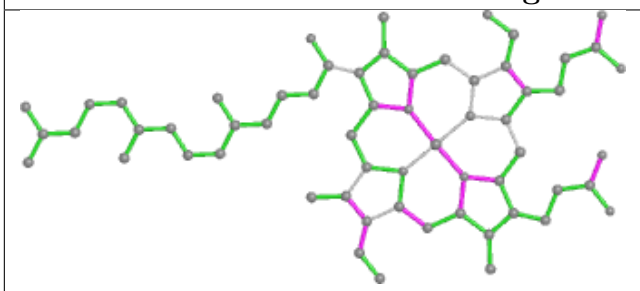
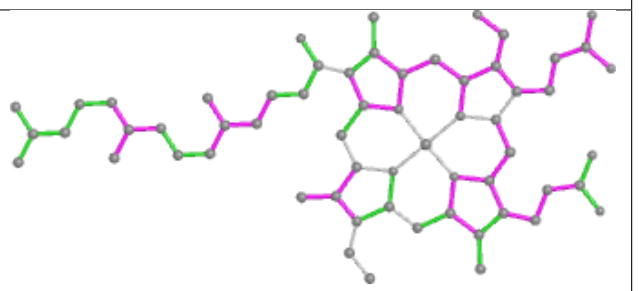
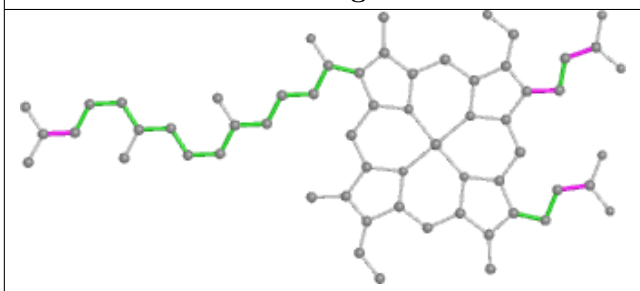
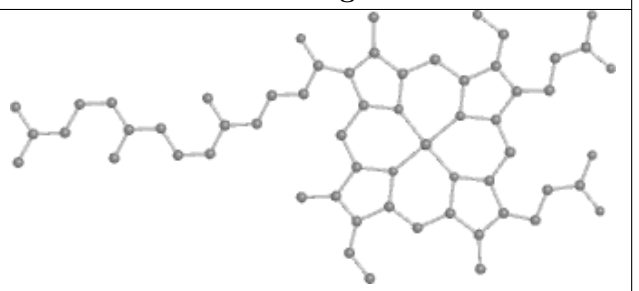
3 monomers are involved in 31 short contacts:

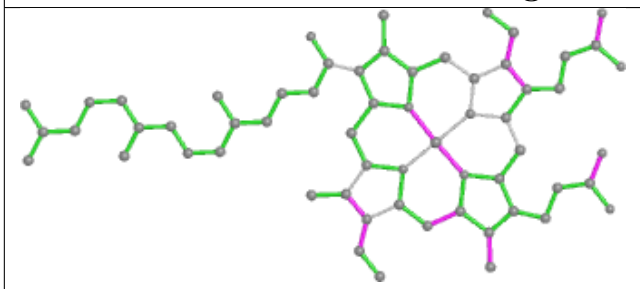
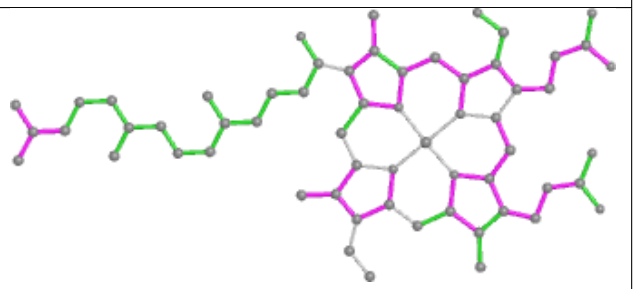
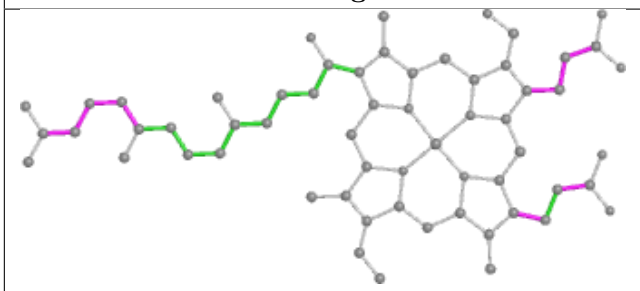
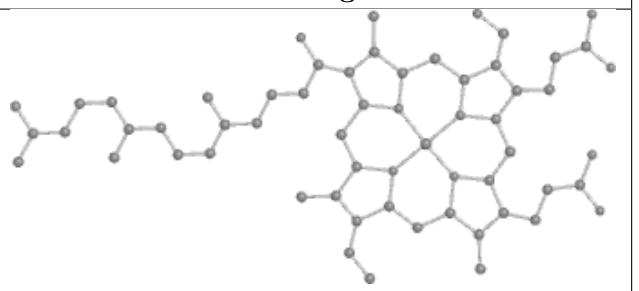
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	301	PC1	22	0
6	A	602	HEA	2	0
6	A	605	HEA	7	0

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 PC1 C 301



Ligand HEA A 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA A 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

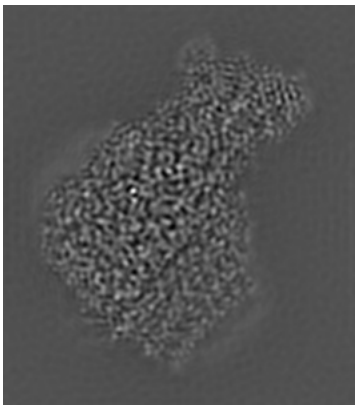
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11922. These allow visual inspection of the internal detail of the map and identification of artifacts.

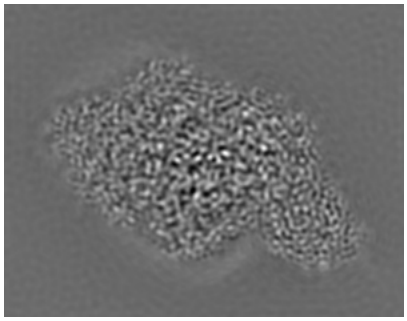
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

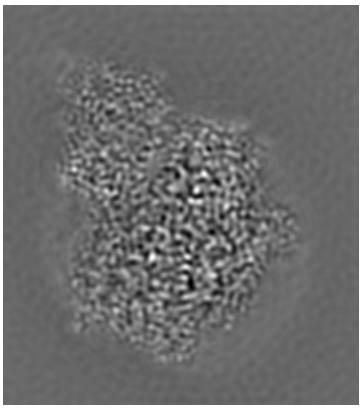
6.1.1 Primary map



X

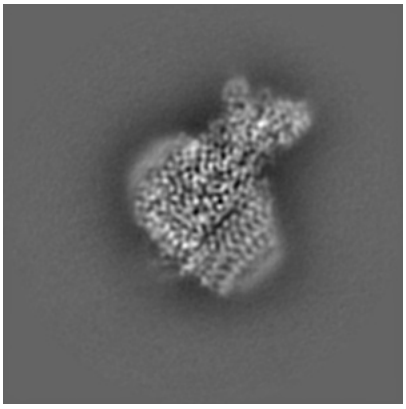


Y

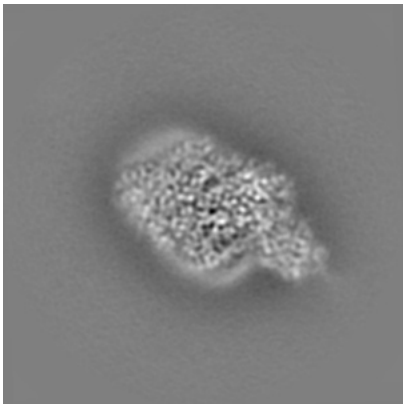


Z

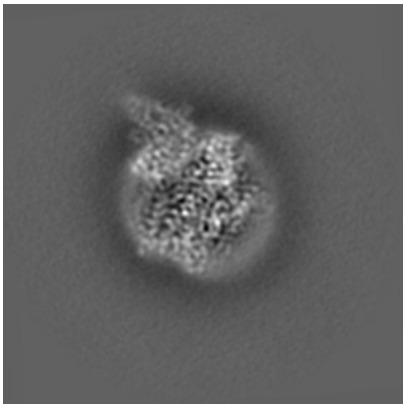
6.1.2 Raw map



X



Y

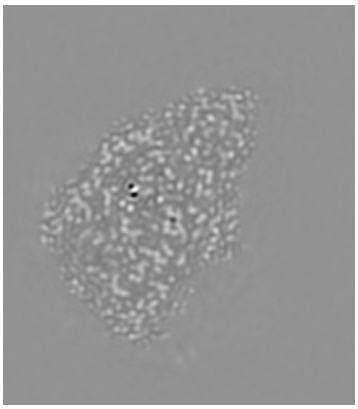


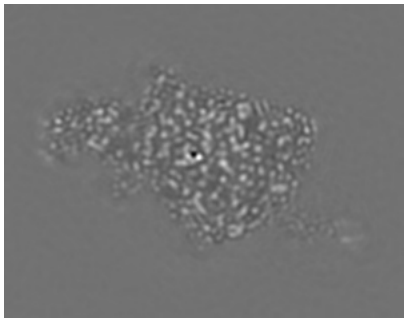
Z

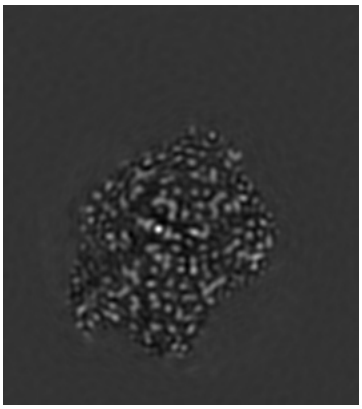
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

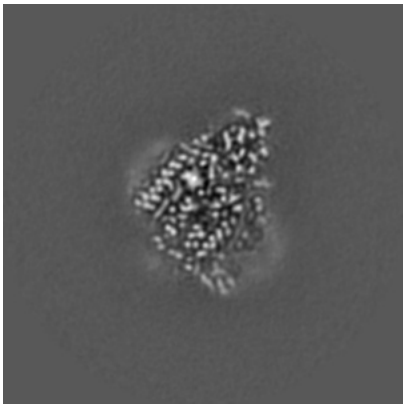
6.2.1 Primary map

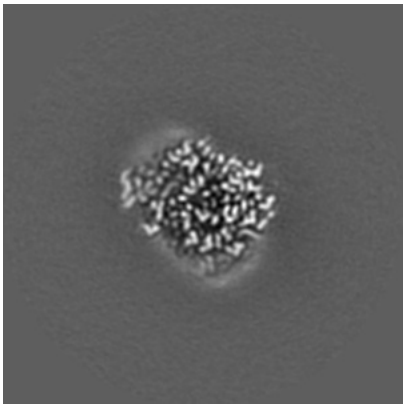

X Index: 64

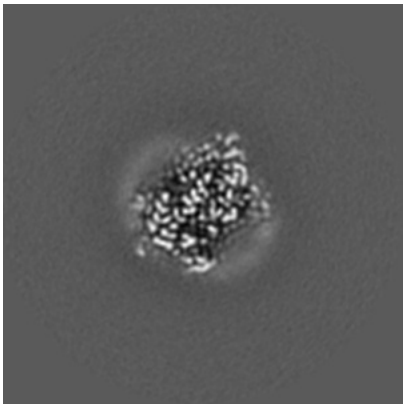

Y Index: 72


Z Index: 82

6.2.2 Raw map


X Index: 128

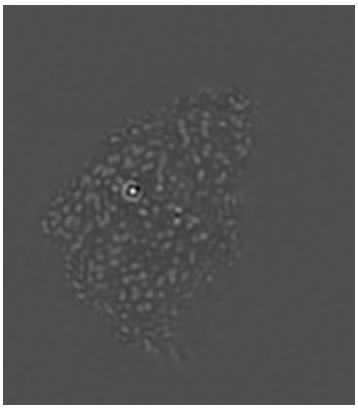

Y Index: 128


Z Index: 128

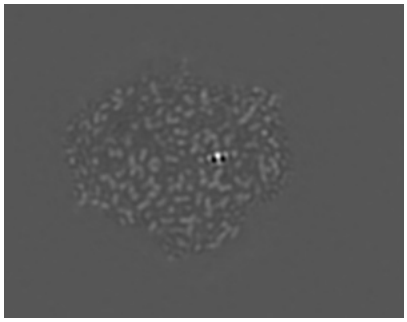
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



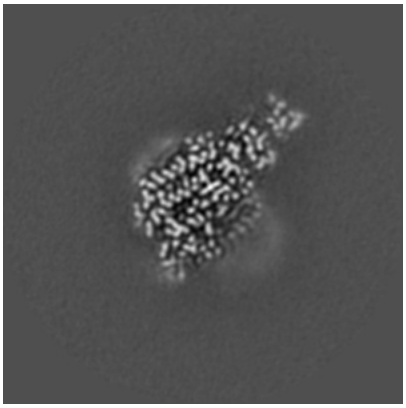
X Index: 66



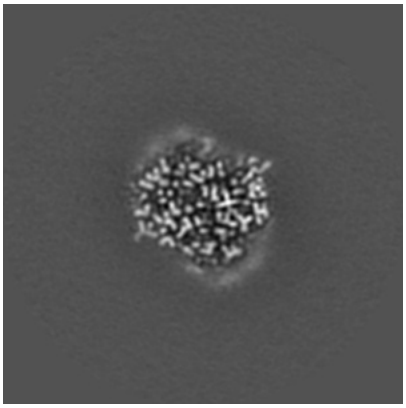
Y Index: 53

Z Index: 88

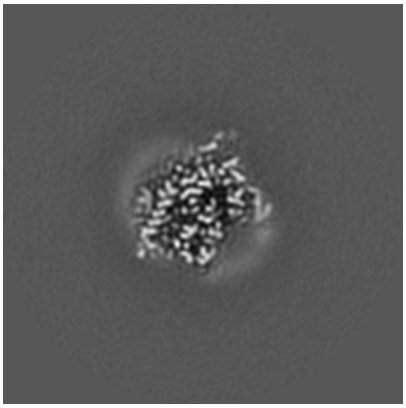
6.3.2 Raw map



X Index: 118



Y Index: 121



Z Index: 131

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

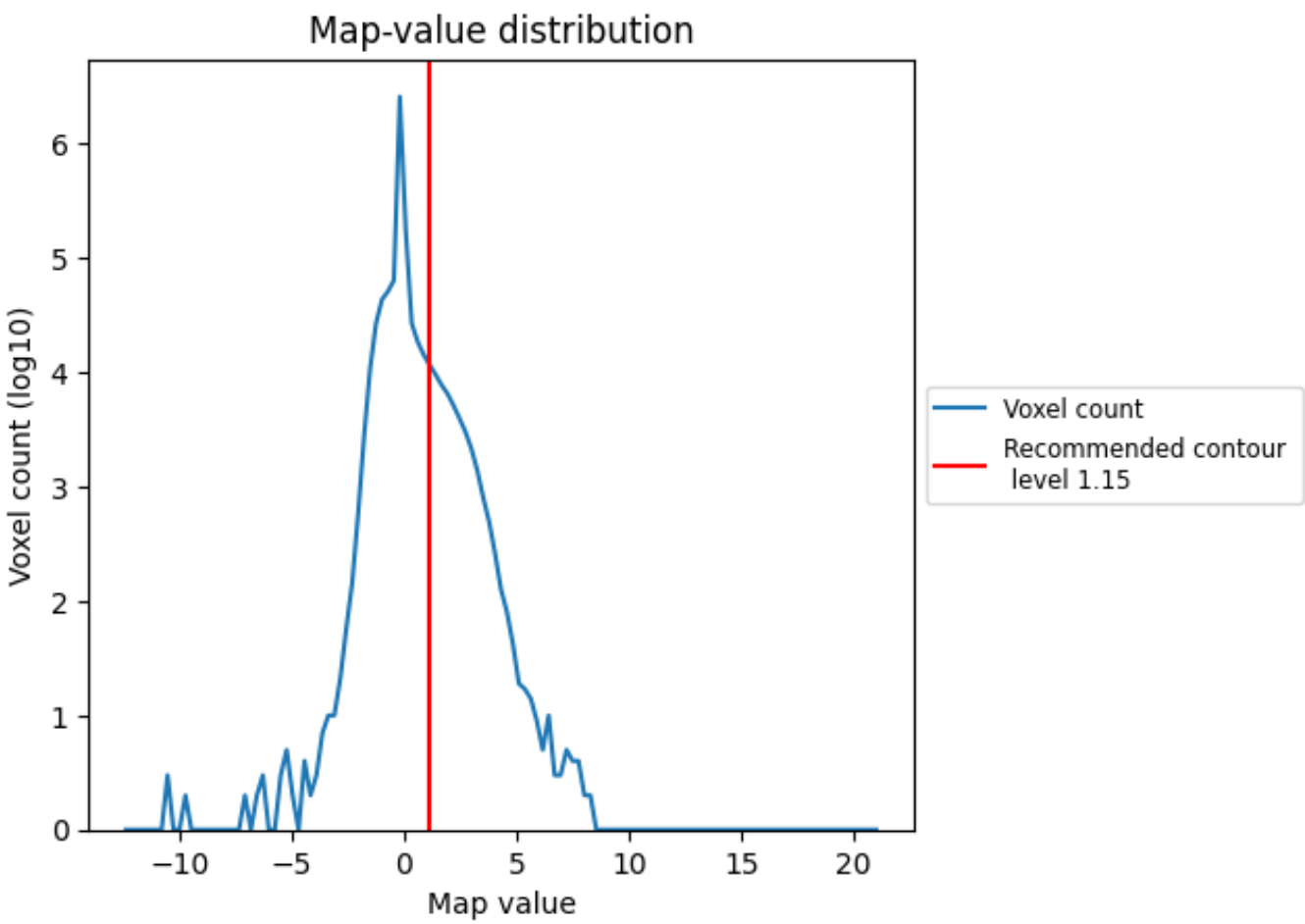
6.5 Mask visualisation (i)

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

7 Map analysis (i)

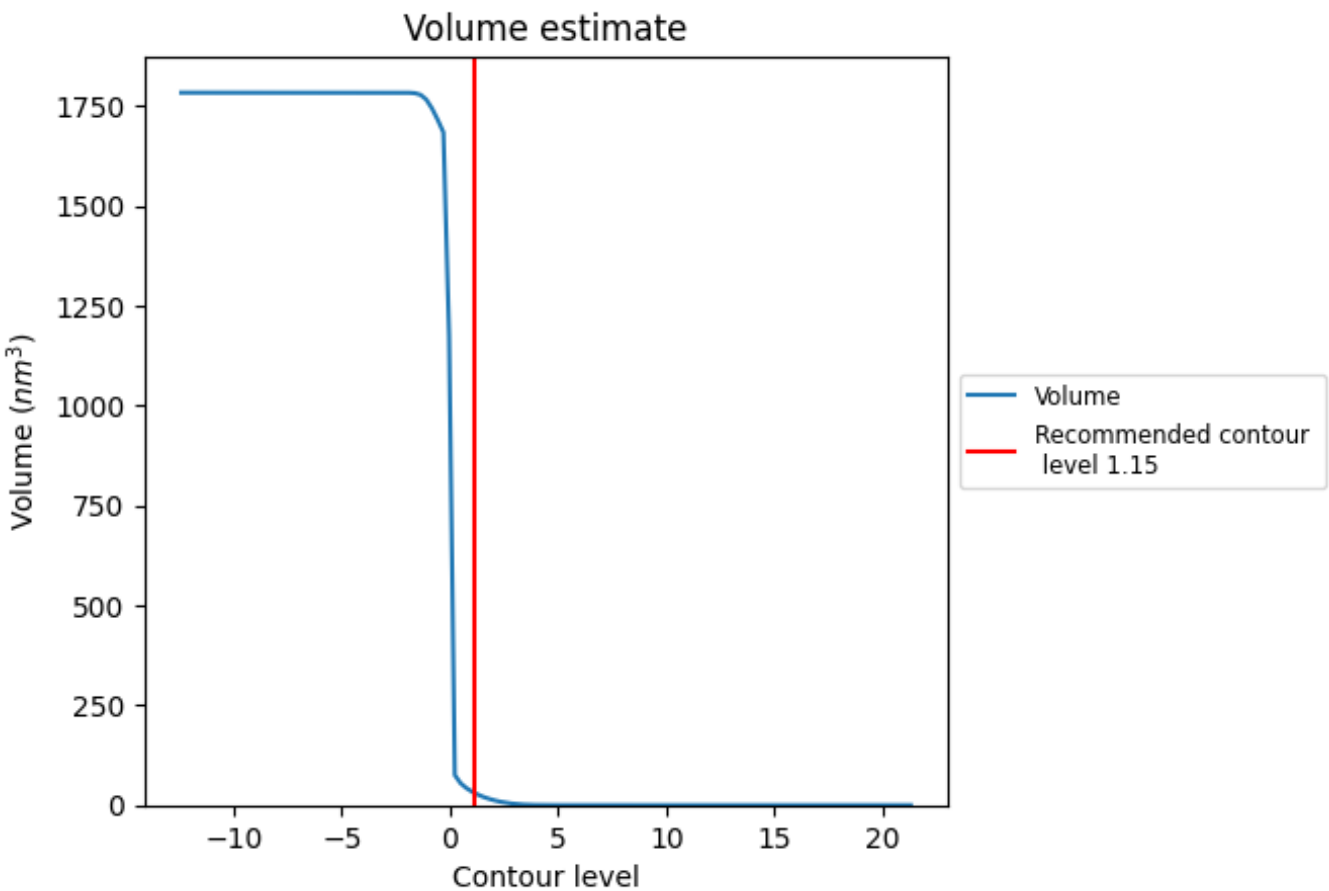
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 31 nm^3; this corresponds to an approximate mass of 28 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.

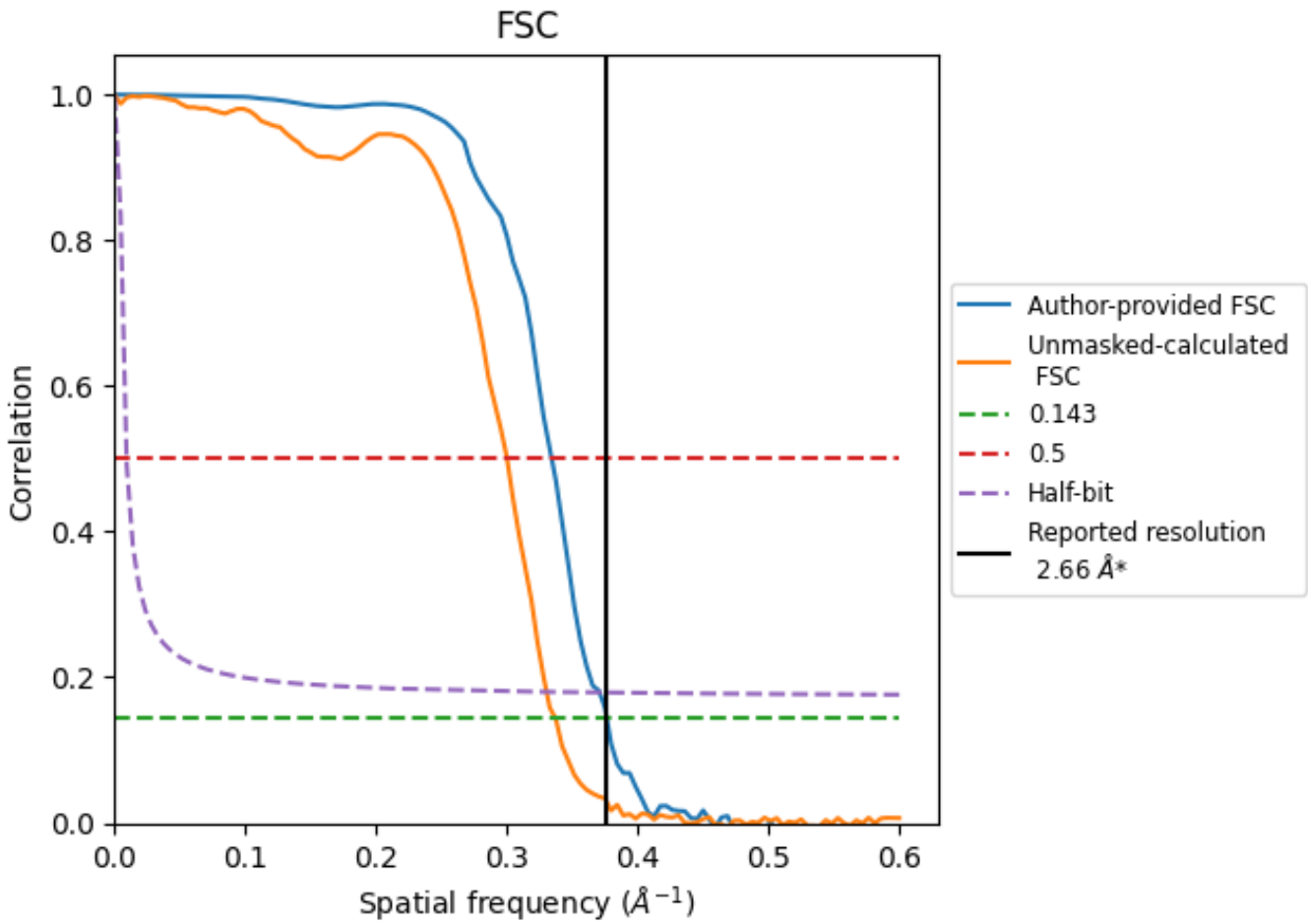
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.376 Å^{-1}

8.2 Resolution estimates (i)

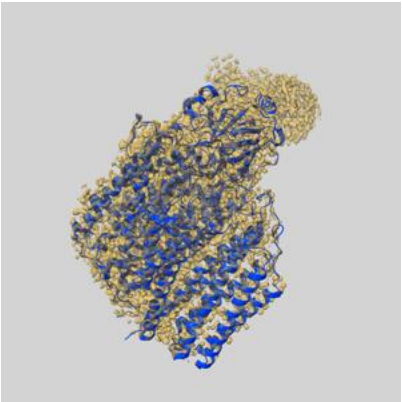
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.66	2.99	2.70
Unmasked-calculated*	2.96	3.33	3.03

*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 2.96 differs from the reported value 2.66 by more than 10 %

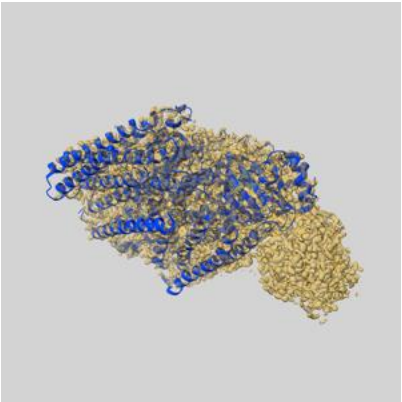
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11922 and PDB model 7ATN. Per-residue inclusion information can be found in section 3 on page 8.

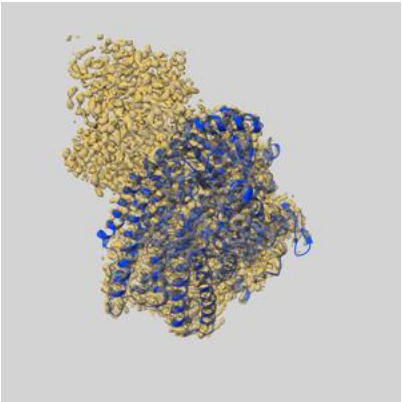
9.1 Map-model overlay (i)



X



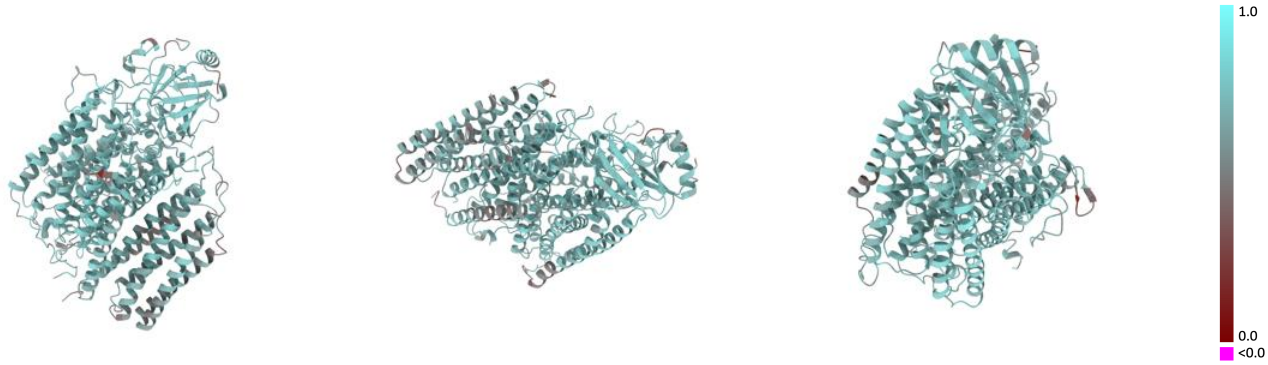
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

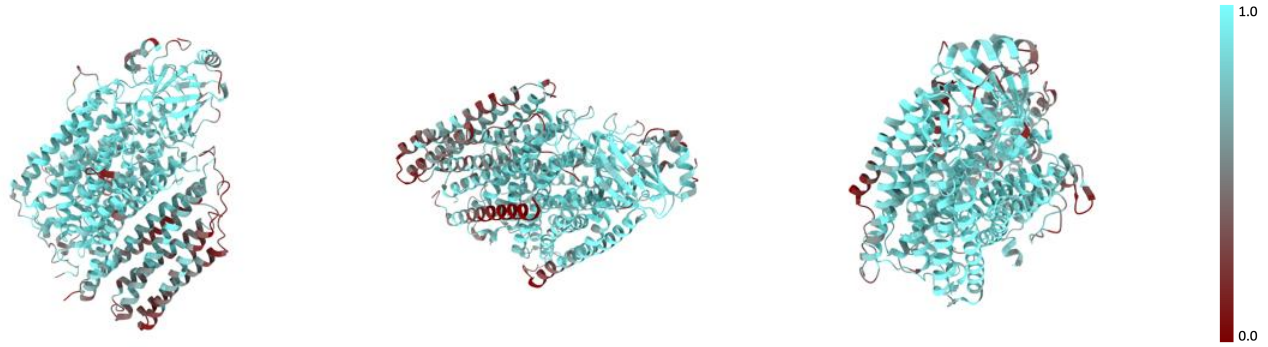
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

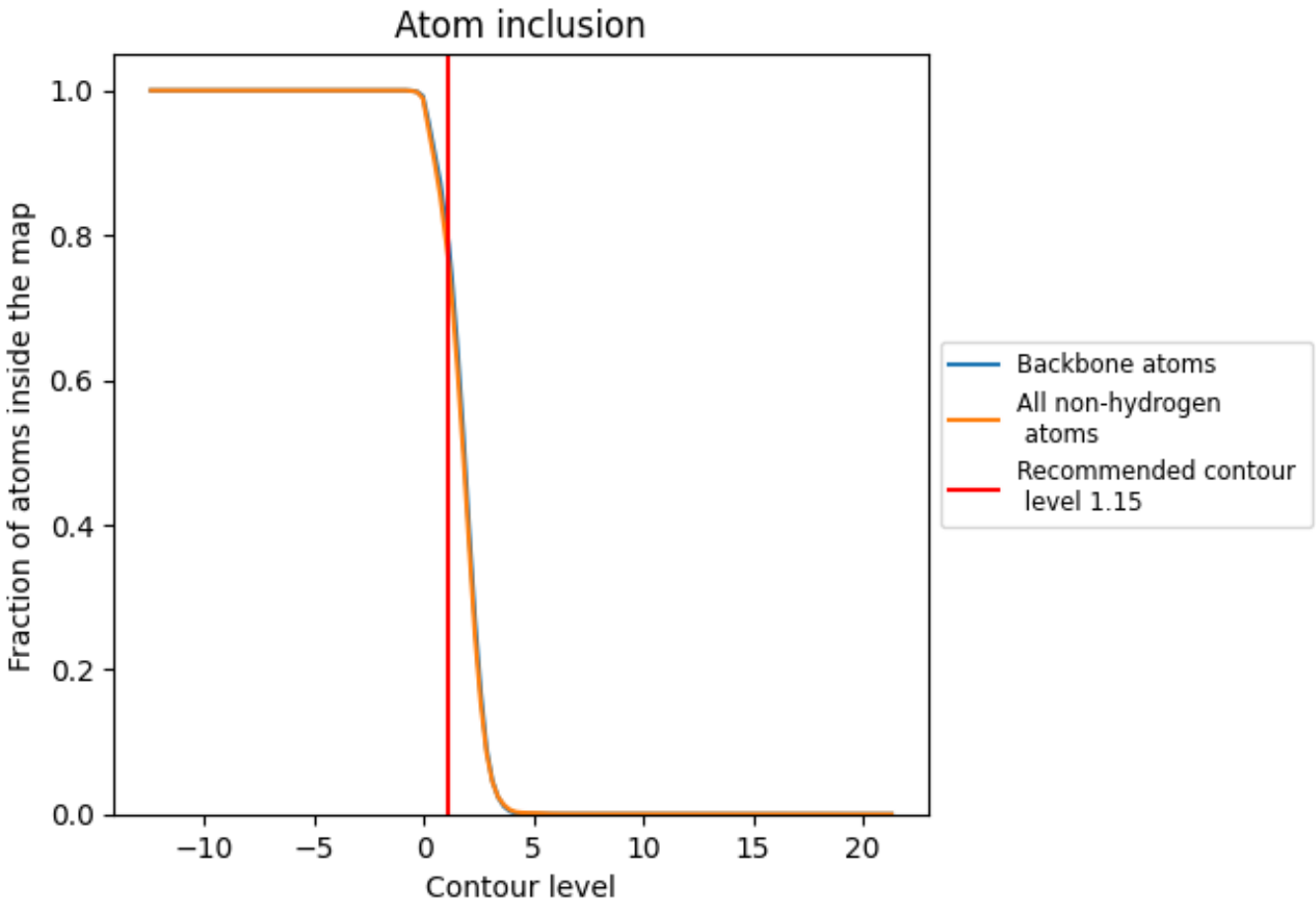
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.15).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7615	0.6650
A	0.8896	0.7020
B	0.7645	0.6640
C	0.5767	0.6100
D	0.2862	0.5330