Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 07:04 pm GMT

PDB ID	:	7ATE
EMDB ID	:	EMD-11921
Title	:	Cytochrome c oxidase structure in P-state
Authors	:	Kolbe, F.; Safarian, S.; Michel, H.
Deposited on	:	2020-10-30
Resolution	:	2.40 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

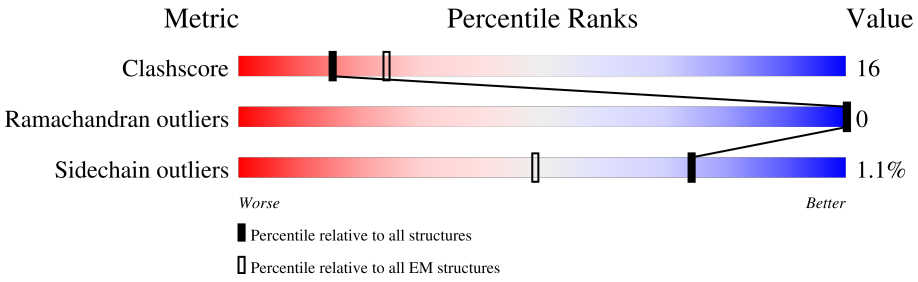
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

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 2.40 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	76% 20%
2	B	298	9% 61% 23% 16%
3	C	274	19% 65% 32%
4	D	50	48% 54% 28% 18%

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
6	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HEA	A	603	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 9056 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	251	1967	1290	317	352	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

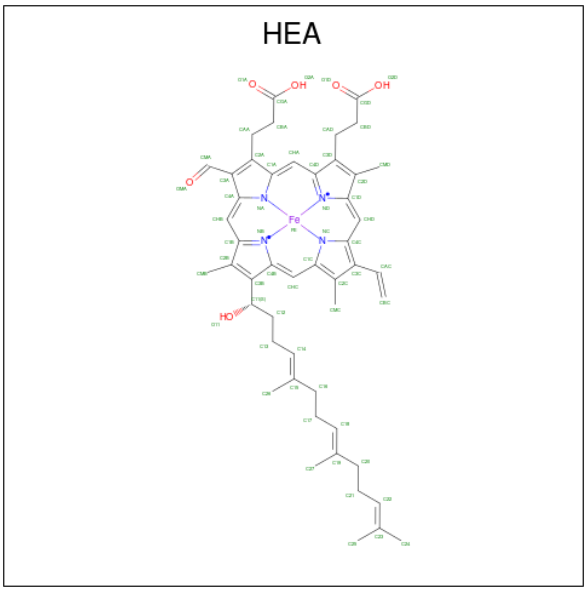
- Molecule 4 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	41	317	206	56	54	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
6	A	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
6	A	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

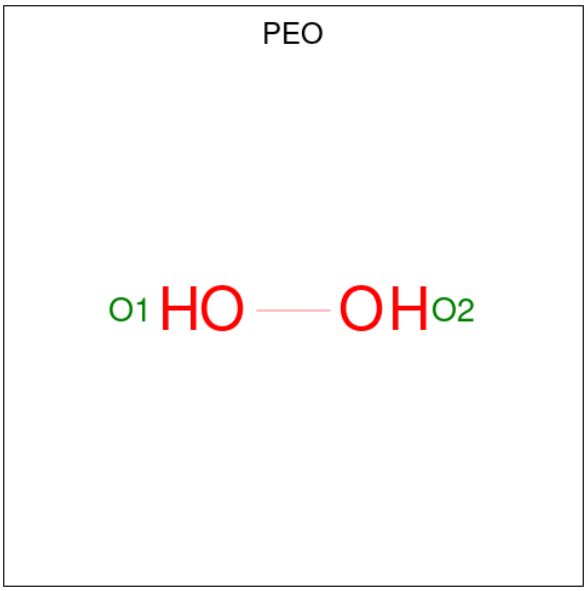
- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

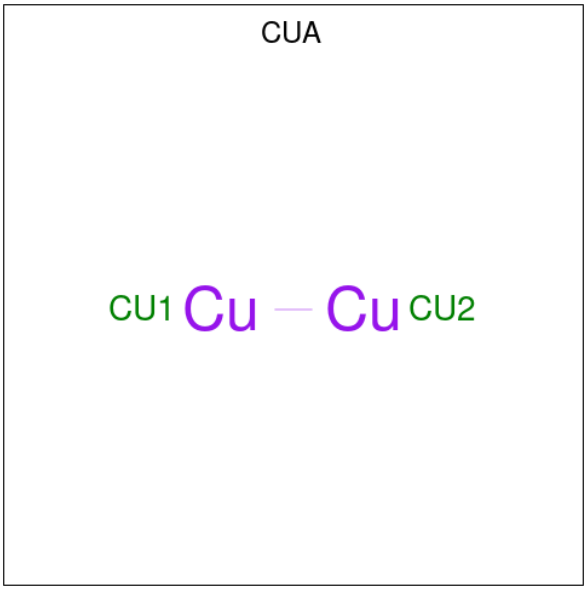
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Ca	0
			1	1	

- Molecule 9 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).



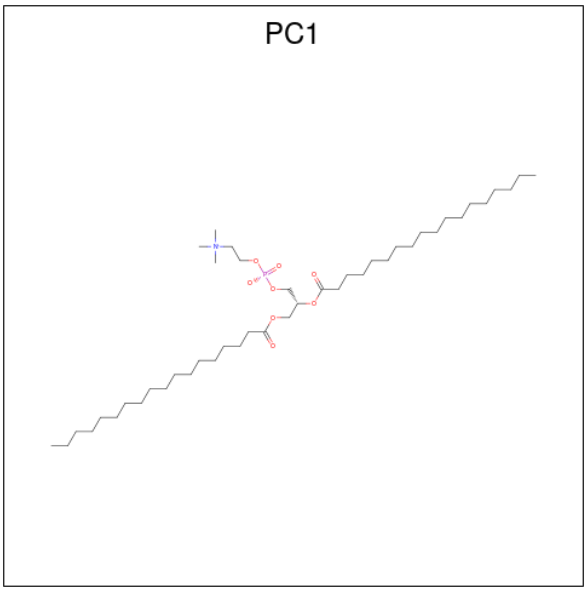
Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total O 2 2	0

- Molecule 10 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



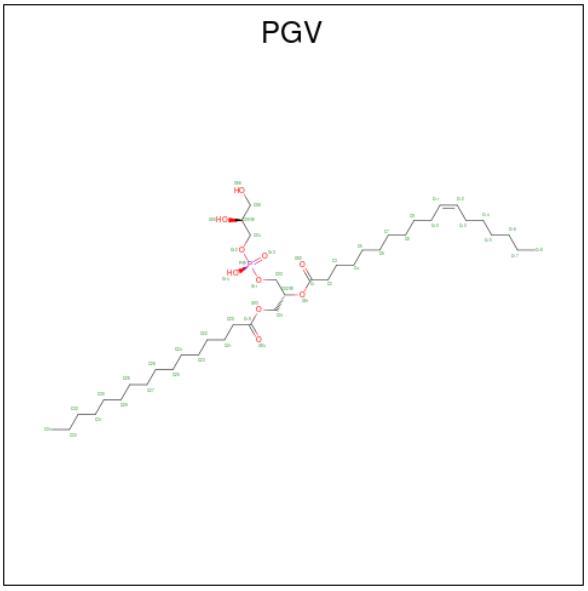
Mol	Chain	Residues	Atoms	AltConf
10	B	1	Total Cu 2 2	0

- Molecule 11 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 12 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total	C	O	P	0
			51	40	10	1	

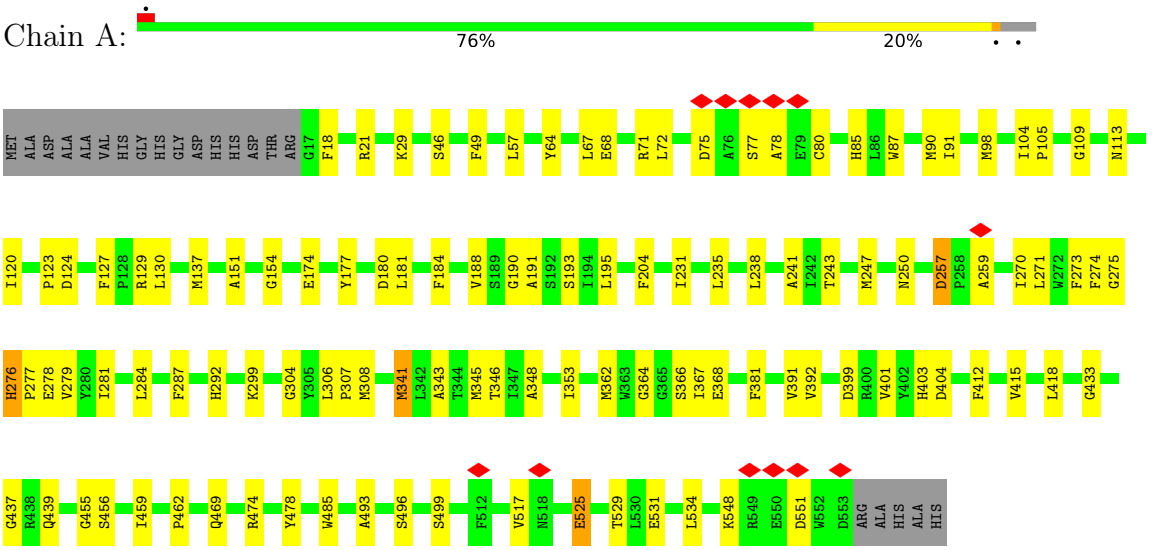
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	AltConf
13	A	93	Total O 93 93	0
13	B	42	Total O 42 42	0
13	C	10	Total O 10 10	0

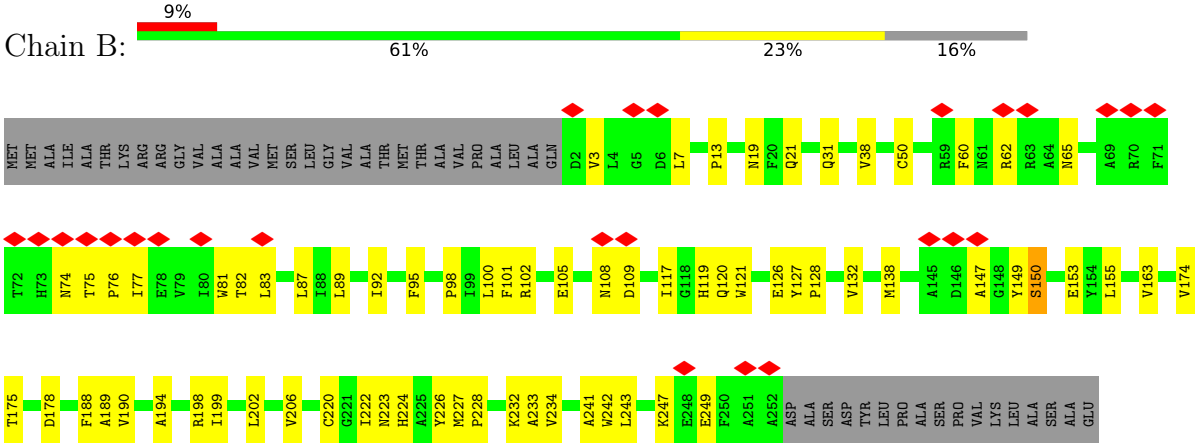
3 Residue-property plots (i)

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.

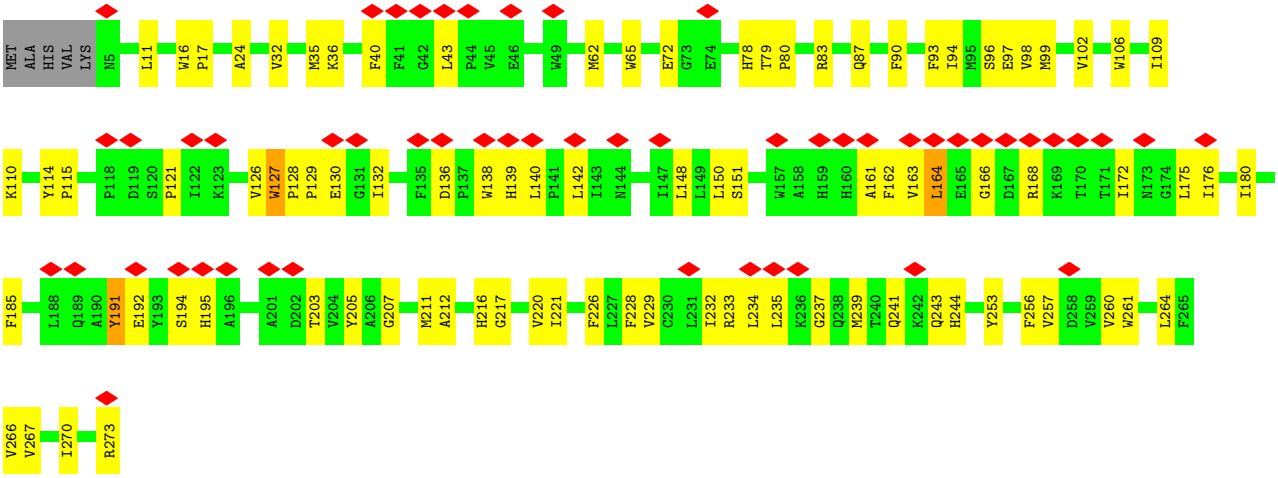
• Molecule 1: Cytochrome c oxidase subunit 1-beta



• Molecule 2: Cytochrome c oxidase subunit 2

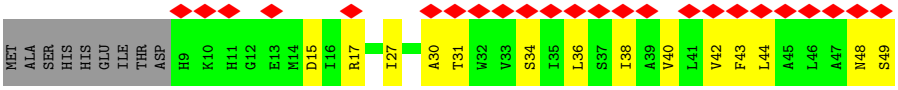


• Molecule 3: Cytochrome c oxidase subunit 3



• 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	268222	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	17.036	Depositor
Minimum map value	-6.270	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.153	Depositor
Recommended contour level	1.36	Depositor
Map size (Å)	213.248, 213.248, 213.248	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.56	1/4416 (0.0%)	0.58	3/6028 (0.0%)
2	B	0.40	0/2024	0.55	0/2775
3	C	0.47	1/2235 (0.0%)	0.52	0/3060
4	D	0.33	0/324	0.39	0/436
All	All	0.50	2/8999 (0.0%)	0.55	3/12299 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	HIS	C-O	-17.63	0.89	1.23
3	C	191	TYR	CB-CG	-5.10	1.44	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	276	HIS	N-CA-CB	6.68	122.62	110.60
1	A	18	PHE	N-CA-CB	-6.21	99.42	110.60
1	A	21	ARG	NE-CZ-NH1	-5.22	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4257	0	4170	117	0
2	B	1967	0	1952	64	0
3	C	2150	0	2114	113	0
4	D	317	0	320	12	0
5	A	1	0	0	0	0
6	A	120	0	108	7	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	2	0	0	0	0
10	B	2	0	0	0	0
11	C	42	0	58	16	0
12	C	51	0	75	13	0
13	A	93	0	0	18	0
13	B	42	0	0	4	0
13	C	10	0	0	1	0
All	All	9056	0	8797	290	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 16.

All (290) 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)
2:B:38:VAL:HB	13:B:438:HOH:O	1.31	1.28
13:A:788:HOH:O	2:B:92:ILE:HG21	1.35	1.27
3:C:172:ILE:HD13	3:C:235:LEU:CD2	1.69	1.20
3:C:172:ILE:CD1	3:C:235:LEU:HD23	1.70	1.20
1:A:415:VAL:HB	13:A:789:HOH:O	1.49	1.09
3:C:172:ILE:HD13	3:C:235:LEU:HD23	1.19	1.07
1:A:392:VAL:HA	13:A:786:HOH:O	1.51	1.06
1:A:174:GLU:OE1	13:A:701:HOH:O	1.76	1.02
1:A:71:ARG:HH12	1:A:78:ALA:CB	1.73	1.01
3:C:234:LEU:CD2	3:C:239:MET:HE3	1.91	1.00
3:C:234:LEU:HD23	3:C:239:MET:HE3	1.43	1.00
13:A:786:HOH:O	2:B:38:VAL:HG11	1.64	0.98
1:A:418:LEU:HD11	1:A:456:SER:HB3	1.41	0.98
3:C:176:ILE:O	3:C:180:ILE:HD12	1.65	0.97
1:A:68:GLU:OE2	1:A:68:GLU:N	2.01	0.93
1:A:129:ARG:HG3	3:C:11:LEU:HD23	1.49	0.92
1:A:204:PHE:HA	13:A:784:HOH:O	1.71	0.91
4:D:40:VAL:O	4:D:44:LEU:HD23	1.72	0.88
3:C:121:PRO:HB2	11:C:301:PC1:H143	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:HH12	1:A:78:ALA:HB3	1.39	0.87
1:A:275:GLY:O	1:A:278:GLU:HB3	1.76	0.86
1:A:404:ASP:OD1	13:A:702:HOH:O	1.93	0.86
1:A:120:ILE:HD13	13:A:784:HOH:O	1.76	0.85
1:A:91:ILE:HB	13:A:776:HOH:O	1.77	0.84
3:C:163:VAL:O	3:C:241:GLN:NE2	2.09	0.84
1:A:180:ASP:OD2	3:C:36:LYS:HE3	1.77	0.84
1:A:151:ALA:HB2	3:C:40:PHE:HZ	1.44	0.82
1:A:71:ARG:NH1	1:A:78:ALA:HB3	1.95	0.81
3:C:121:PRO:O	11:C:301:PC1:H151	1.80	0.81
1:A:154:GLY:N	1:A:174:GLU:OE1	2.15	0.80
4:D:34:SER:O	4:D:38:ILE:HG13	1.81	0.80
1:A:71:ARG:HH12	1:A:78:ALA:HB1	1.46	0.78
1:A:137:MET:CE	1:A:188:VAL:HG13	2.13	0.78
3:C:62:MET:HG2	12:C:302:PGV:H231	1.65	0.78
1:A:238:LEU:HD22	1:A:274:PHE:CE2	2.18	0.78
1:A:71:ARG:HH21	1:A:80:CYS:HB2	1.49	0.78
3:C:78:HIS:HE1	12:C:302:PGV:H061	1.49	0.78
1:A:71:ARG:NH1	1:A:78:ALA:CB	2.49	0.76
3:C:228:PHE:O	3:C:232:ILE:HG12	1.87	0.75
1:A:273:PHE:O	1:A:277:PRO:HD2	1.87	0.75
1:A:391:VAL:HG13	13:A:747:HOH:O	1.88	0.73
3:C:172:ILE:CD1	3:C:235:LEU:CD2	2.47	0.73
4:D:27:ILE:O	4:D:31:THR:HG23	1.88	0.73
2:B:74:ASN:HB3	2:B:77:ILE:HG22	1.69	0.73
2:B:74:ASN:O	2:B:77:ILE:HG22	1.90	0.71
3:C:172:ILE:HD13	3:C:235:LEU:HD21	1.68	0.70
3:C:140:LEU:HD11	3:C:191:TYR:HE2	1.58	0.68
2:B:150:SER:N	2:B:153:GLU:OE1	2.26	0.68
1:A:412:PHE:HA	1:A:415:VAL:HG22	1.75	0.68
4:D:38:ILE:O	4:D:42:VAL:HG23	1.93	0.68
3:C:78:HIS:CE1	12:C:302:PGV:H061	2.29	0.67
2:B:74:ASN:HB3	2:B:77:ILE:CG2	2.24	0.67
3:C:127:TRP:HB3	3:C:128:PRO:HD3	1.75	0.67
1:A:306:LEU:HB3	1:A:307:PRO:HD3	1.77	0.67
1:A:366:SER:OG	2:B:65:ASN:O	2.12	0.66
3:C:129:PRO:HB2	3:C:132:ILE:HD13	1.77	0.66
1:A:154:GLY:CA	1:A:174:GLU:OE1	2.43	0.66
1:A:154:GLY:HA3	1:A:174:GLU:OE1	1.97	0.65
1:A:548:LYS:N	1:A:551:ASP:OD2	2.30	0.65
1:A:257:ASP:OD1	1:A:259:ALA:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:VAL:O	3:C:233:ARG:HG3	1.98	0.64
3:C:32:VAL:HA	3:C:35:MET:HE3	1.79	0.63
3:C:132:ILE:HD11	3:C:203:THR:HG23	1.81	0.63
3:C:168:ARG:O	3:C:172:ILE:HG13	1.98	0.63
3:C:121:PRO:CB	11:C:301:PC1:H143	2.27	0.63
1:A:193:SER:HB2	1:A:235:LEU:CD2	2.29	0.63
1:A:124:ASP:HB2	13:A:779:HOH:O	1.99	0.63
1:A:273:PHE:O	1:A:277:PRO:CD	2.47	0.63
1:A:71:ARG:NH2	1:A:80:CYS:HB2	2.12	0.63
4:D:43:PHE:HD1	4:D:44:LEU:HD22	1.63	0.63
3:C:216:HIS:CE1	3:C:261:TRP:HB2	2.33	0.62
1:A:137:MET:HE3	1:A:188:VAL:HG13	1.80	0.62
1:A:231:ILE:HG13	1:A:281:ILE:HG12	1.82	0.61
13:A:743:HOH:O	2:B:31:GLN:HG3	1.98	0.61
1:A:299:LYS:NZ	1:A:368:GLU:OE1	2.32	0.61
1:A:353:ILE:HD11	2:B:82:THR:HG23	1.82	0.60
2:B:3:VAL:CG1	2:B:241:ALA:HB1	2.31	0.60
2:B:220:CYS:SG	2:B:224:HIS:HA	2.42	0.60
1:A:250:ASN:OD1	3:C:36:LYS:HE2	2.02	0.60
2:B:188:PHE:HB2	2:B:190:VAL:HG22	1.81	0.60
1:A:64:TYR:HE1	1:A:72:LEU:O	1.84	0.60
2:B:121:TRP:CG	2:B:223:ASN:HB2	2.37	0.60
3:C:142:LEU:HD12	3:C:142:LEU:O	2.02	0.59
1:A:64:TYR:CE1	1:A:72:LEU:O	2.55	0.59
3:C:175:LEU:CD1	3:C:234:LEU:HD12	2.32	0.59
2:B:119:HIS:O	2:B:121:TRP:N	2.36	0.59
1:A:531:GLU:HA	1:A:534:LEU:HD12	1.85	0.59
3:C:139:HIS:O	3:C:142:LEU:N	2.33	0.59
3:C:234:LEU:CG	3:C:239:MET:HE3	2.32	0.59
1:A:174:GLU:CD	13:A:701:HOH:O	2.33	0.59
1:A:496:SER:O	1:A:499:SER:OG	2.15	0.59
1:A:238:LEU:HD22	1:A:274:PHE:CZ	2.38	0.59
3:C:121:PRO:HB2	11:C:301:PC1:C15	2.34	0.58
1:A:109:GLY:O	1:A:113:ASN:HB2	2.03	0.58
2:B:126:GLU:O	2:B:128:PRO:HD3	2.03	0.58
3:C:121:PRO:HB2	11:C:301:PC1:C14	2.31	0.57
3:C:212:ALA:HB1	3:C:264:LEU:HD21	1.86	0.57
3:C:140:LEU:HB3	3:C:192:GLU:OE1	2.04	0.57
1:A:412:PHE:HA	1:A:415:VAL:CG2	2.34	0.57
1:A:433:GLY:O	1:A:437:GLY:N	2.37	0.57
3:C:270:ILE:O	3:C:273:ARG:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:SER:OG	3:C:195:HIS:ND1	2.38	0.57
2:B:198:ARG:NH1	3:C:121:PRO:HG3	2.20	0.57
3:C:87:GLN:HA	3:C:90:PHE:CE2	2.39	0.57
3:C:11:LEU:HD21	12:C:302:PGV:H041	1.87	0.56
1:A:257:ASP:OD1	1:A:259:ALA:HB3	2.05	0.56
1:A:343:ALA:O	1:A:346:THR:OG1	2.19	0.56
2:B:198:ARG:HD3	13:B:426:HOH:O	2.04	0.56
3:C:172:ILE:HG21	3:C:235:LEU:HD21	1.85	0.56
3:C:207:GLY:O	3:C:211:MET:HG2	2.05	0.56
1:A:137:MET:HE2	1:A:188:VAL:HG13	1.88	0.56
3:C:127:TRP:CZ2	3:C:205:TYR:HD2	2.24	0.56
2:B:249:GLU:O	2:B:249:GLU:HG2	2.05	0.56
1:A:75:ASP:OD1	1:A:77:SER:N	2.38	0.56
3:C:130:GLU:OE2	3:C:130:GLU:HA	2.05	0.55
3:C:194:SER:HG	3:C:195:HIS:HD1	1.52	0.55
1:A:190:GLY:HA2	1:A:235:LEU:HD23	1.89	0.55
3:C:24:ALA:HB2	12:C:302:PGV:H292	1.88	0.55
2:B:174:VAL:HG12	2:B:194:ALA:HB2	1.89	0.55
2:B:38:VAL:CG1	13:B:438:HOH:O	2.49	0.55
3:C:24:ALA:CB	12:C:302:PGV:H292	2.37	0.54
3:C:234:LEU:HG	3:C:239:MET:CE	2.37	0.54
1:A:367:ILE:HG13	2:B:60:PHE:O	2.07	0.54
4:D:15:ASP:OD1	4:D:17:ARG:HD2	2.08	0.53
3:C:127:TRP:O	3:C:129:PRO:HD3	2.08	0.53
3:C:121:PRO:HB2	11:C:301:PC1:H152	1.90	0.53
1:A:98:MET:HB3	6:A:602:HEA:HAC	1.91	0.53
3:C:140:LEU:CD1	3:C:191:TYR:HE2	2.22	0.53
1:A:279:VAL:HB	6:A:603:HEA:CAC	2.39	0.53
1:A:439:GLN:OE1	1:A:439:GLN:HA	2.09	0.53
1:A:120:ILE:HG21	13:A:784:HOH:O	2.09	0.52
3:C:136:ASP:OD1	3:C:138:TRP:N	2.34	0.52
1:A:401:VAL:HG23	13:A:743:HOH:O	2.10	0.52
2:B:13:PRO:HD3	2:B:21:GLN:NE2	2.25	0.52
2:B:108:ASN:OD1	2:B:109:ASP:N	2.41	0.52
13:A:743:HOH:O	2:B:189:ALA:HB1	2.09	0.52
3:C:163:VAL:HG12	3:C:164:LEU:CD2	2.40	0.52
1:A:98:MET:HB3	6:A:602:HEA:CAC	2.40	0.51
1:A:104:ILE:HB	1:A:105:PRO:HD3	1.92	0.51
1:A:304:GLY:O	1:A:307:PRO:HD2	2.10	0.51
3:C:253:TYR:O	3:C:257:VAL:HG23	2.11	0.51
2:B:38:VAL:CB	13:B:438:HOH:O	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:VAL:HG21	11:C:301:PC1:H2D2	1.93	0.51
2:B:3:VAL:CG1	2:B:241:ALA:CB	2.88	0.51
3:C:106:TRP:CD1	11:C:301:PC1:H341	2.45	0.51
1:A:284:LEU:O	1:A:287:PHE:HB2	2.11	0.51
1:A:469:GLN:NE2	2:B:19:ASN:O	2.30	0.50
3:C:140:LEU:HD11	3:C:191:TYR:CE2	2.43	0.50
2:B:175:THR:HB	2:B:199:ILE:HD13	1.94	0.50
1:A:341:MET:HE1	2:B:100:LEU:HD22	1.94	0.50
3:C:168:ARG:NH2	3:C:237:GLY:HA2	2.26	0.50
1:A:462:PRO:HB3	1:A:485:TRP:CE3	2.47	0.49
2:B:127:TYR:HB2	2:B:132:VAL:HB	1.94	0.49
3:C:83:ARG:CD	3:C:243:GLN:HG3	2.41	0.49
3:C:127:TRP:O	3:C:127:TRP:CE3	2.65	0.49
2:B:121:TRP:CD2	2:B:223:ASN:HB2	2.47	0.49
3:C:94:ILE:O	3:C:98:VAL:HG23	2.12	0.49
3:C:114:TYR:CD2	11:C:301:PC1:H112	2.48	0.49
1:A:57:LEU:HG	1:A:87:TRP:CH2	2.48	0.49
1:A:238:LEU:HB2	1:A:274:PHE:CG	2.48	0.49
1:A:130:LEU:HD11	1:A:195:LEU:HD22	1.95	0.48
3:C:65:TRP:CE2	12:C:302:PGV:O04	2.66	0.48
1:A:276:HIS:HB3	1:A:277:PRO:HD3	1.94	0.48
1:A:364:GLY:HA2	2:B:60:PHE:CE1	2.48	0.48
1:A:177:TYR:HE1	3:C:40:PHE:CZ	2.32	0.48
2:B:95:PHE:O	2:B:98:PRO:HD2	2.14	0.48
1:A:304:GLY:C	1:A:307:PRO:HD2	2.34	0.48
1:A:127:PHE:HD1	12:C:302:PGV:O13	1.96	0.48
1:A:517:VAL:HG23	1:A:517:VAL:O	2.13	0.48
6:A:602:HEA:HBC1	6:A:602:HEA:HMC1	1.96	0.48
4:D:48:ASN:O	4:D:49:SER:HB3	2.13	0.48
4:D:43:PHE:CD1	4:D:44:LEU:HD22	2.48	0.47
2:B:138:MET:HB2	2:B:228:PRO:HD2	1.96	0.47
2:B:121:TRP:HA	2:B:227:MET:SD	2.54	0.47
1:A:271:LEU:HD13	1:A:271:LEU:C	2.34	0.47
1:A:455:GLY:O	1:A:459:ILE:HG13	2.13	0.47
3:C:110:LYS:HE3	13:C:406:HOH:O	2.13	0.47
3:C:132:ILE:HD11	3:C:203:THR:CG2	2.44	0.47
1:A:181:LEU:HD11	3:C:40:PHE:CE2	2.49	0.47
3:C:136:ASP:OD1	3:C:136:ASP:C	2.52	0.47
2:B:121:TRP:N	2:B:121:TRP:CD1	2.83	0.46
3:C:148:LEU:HG	3:C:185:PHE:CD2	2.50	0.46
3:C:234:LEU:HD23	3:C:239:MET:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HD11	3:C:40:PHE:HE2	1.80	0.46
3:C:79:THR:O	3:C:83:ARG:HG3	2.15	0.46
3:C:126:VAL:O	3:C:127:TRP:C	2.54	0.46
6:A:602:HEA:H14	6:A:602:HEA:H11	1.58	0.46
2:B:7:LEU:HD12	2:B:232:LYS:HD3	1.97	0.46
1:A:341:MET:CE	2:B:100:LEU:HD22	2.46	0.46
1:A:151:ALA:HB2	3:C:40:PHE:CZ	2.36	0.46
1:A:29:LYS:HB2	1:A:29:LYS:HE2	1.78	0.45
2:B:101:PHE:O	2:B:105:GLU:HG3	2.16	0.45
2:B:138:MET:CE	2:B:226:TYR:HD1	2.29	0.45
3:C:114:TYR:CG	11:C:301:PC1:H112	2.51	0.45
2:B:150:SER:OG	2:B:153:GLU:OE1	2.34	0.45
3:C:161:ALA:O	3:C:166:GLY:N	2.47	0.45
3:C:43:LEU:HD23	3:C:43:LEU:H	1.81	0.45
3:C:79:THR:HB	3:C:80:PRO:HD2	1.98	0.45
3:C:98:VAL:HG22	3:C:256:PHE:HE1	1.82	0.45
3:C:115:PRO:HG3	3:C:127:TRP:HA	1.99	0.45
2:B:3:VAL:HG12	2:B:241:ALA:HB3	1.98	0.44
2:B:138:MET:HE1	2:B:226:TYR:HD1	1.83	0.44
6:A:603:HEA:CMC	13:A:789:HOH:O	2.65	0.44
3:C:62:MET:CG	12:C:302:PGV:H231	2.42	0.44
1:A:72:LEU:HD22	1:A:72:LEU:N	2.32	0.44
3:C:109:ILE:HD12	11:C:301:PC1:H362	1.99	0.44
3:C:139:HIS:O	3:C:140:LEU:C	2.55	0.44
3:C:163:VAL:HG22	3:C:244:HIS:CE1	2.53	0.44
3:C:150:LEU:HD23	3:C:150:LEU:HA	1.73	0.44
1:A:184:PHE:CE2	3:C:32:VAL:HG23	2.53	0.44
1:A:368:GLU:HG2	2:B:62:ARG:HH11	1.83	0.43
1:A:362:MET:HB2	1:A:362:MET:HE2	1.63	0.43
3:C:234:LEU:HG	3:C:239:MET:HE3	1.95	0.43
2:B:243:LEU:HD12	2:B:243:LEU:HA	1.83	0.43
1:A:193:SER:HB2	1:A:235:LEU:HD21	2.01	0.43
3:C:239:MET:HE3	3:C:239:MET:HB2	1.99	0.43
1:A:241:ALA:HB2	1:A:270:ILE:HG22	2.01	0.43
1:A:345:MET:HG2	13:A:747:HOH:O	2.17	0.43
1:A:348:ALA:HB3	2:B:89:LEU:HD11	2.00	0.43
2:B:3:VAL:HG12	2:B:241:ALA:CB	2.49	0.43
3:C:40:PHE:O	3:C:43:LEU:O	2.36	0.43
3:C:140:LEU:HD13	3:C:192:GLU:HG3	2.00	0.43
3:C:168:ARG:NH2	3:C:234:LEU:O	2.34	0.43
3:C:168:ARG:NH1	3:C:239:MET:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLY:O	1:A:437:GLY:CA	2.67	0.42
3:C:228:PHE:CE2	3:C:232:ILE:HD11	2.54	0.42
1:A:129:ARG:HG3	3:C:11:LEU:CD2	2.36	0.42
1:A:190:GLY:CA	1:A:235:LEU:HD23	2.49	0.42
1:A:525:GLU:H	1:A:525:GLU:HG3	1.61	0.42
2:B:147:ALA:HB3	2:B:149:TYR:HD2	1.84	0.42
12:C:302:PGV:O02	12:C:302:PGV:H032	2.19	0.42
2:B:202:LEU:HD12	2:B:202:LEU:C	2.40	0.42
3:C:266:VAL:CG2	3:C:267:VAL:N	2.82	0.42
1:A:433:GLY:O	1:A:437:GLY:HA2	2.20	0.42
1:A:46:SER:HB3	1:A:98:MET:CE	2.50	0.42
1:A:439:GLN:HB2	1:A:517:VAL:HG11	2.02	0.42
2:B:7:LEU:HD21	2:B:234:VAL:HG12	2.01	0.42
3:C:140:LEU:HD22	3:C:192:GLU:OE1	2.20	0.42
3:C:175:LEU:HD12	3:C:234:LEU:HD12	2.02	0.42
11:C:301:PC1:O32	11:C:301:PC1:C1	2.68	0.42
4:D:36:LEU:O	4:D:40:VAL:HG23	2.20	0.42
1:A:75:ASP:OD1	1:A:77:SER:OG	2.30	0.42
3:C:16:TRP:HB2	3:C:17:PRO:HD3	2.02	0.42
3:C:127:TRP:C	3:C:127:TRP:CD2	2.92	0.42
1:A:299:LYS:CE	1:A:368:GLU:OE1	2.68	0.41
12:C:302:PGV:H241	12:C:302:PGV:H212	1.75	0.41
1:A:85:HIS:HB2	2:B:222:ILE:HD12	2.02	0.41
6:A:603:HEA:HMD1	6:A:603:HEA:HBD2	2.02	0.41
3:C:217:GLY:O	3:C:221:ILE:HG13	2.20	0.41
1:A:243:THR:O	1:A:247:MET:HG2	2.20	0.41
3:C:114:TYR:OH	4:D:49:SER:HB3	2.19	0.41
4:D:30:ALA:O	4:D:34:SER:OG	2.33	0.41
1:A:478:TYR:C	2:B:155:LEU:HD12	2.40	0.41
11:C:301:PC1:O12	11:C:301:PC1:C3	2.68	0.41
1:A:137:MET:HE3	1:A:188:VAL:CG1	2.48	0.41
1:A:474:ARG:O	2:B:224:HIS:HD2	2.04	0.41
2:B:243:LEU:HG	2:B:247:LYS:HD2	2.01	0.41
4:D:15:ASP:OD1	4:D:17:ARG:CD	2.68	0.41
1:A:459:ILE:HG12	1:A:493:ALA:N	2.36	0.41
3:C:256:PHE:O	3:C:260:VAL:HG23	2.20	0.41
1:A:299:LYS:HZ1	1:A:368:GLU:CD	2.22	0.41
1:A:399:ASP:O	1:A:403:HIS:N	2.47	0.41
2:B:120:GLN:C	2:B:121:TRP:CG	2.92	0.41
2:B:206:VAL:HG11	2:B:233:ALA:CB	2.50	0.41
3:C:163:VAL:HG12	3:C:164:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD12	1:A:67:LEU:HA	1.79	0.41
1:A:177:TYR:HA	1:A:180:ASP:OD2	2.21	0.41
1:A:304:GLY:O	1:A:308:MET:HG2	2.21	0.41
2:B:102:ARG:HB2	2:B:102:ARG:NH2	2.36	0.41
2:B:178:ASP:OD1	2:B:178:ASP:N	2.54	0.41
3:C:72:GLU:OE2	12:C:302:PGV:H05	2.21	0.41
3:C:163:VAL:HG12	3:C:164:LEU:HD22	2.03	0.41
3:C:220:VAL:HG22	3:C:257:VAL:CG1	2.50	0.41
3:C:234:LEU:HG	3:C:239:MET:HE1	2.01	0.41
11:C:301:PC1:O32	11:C:301:PC1:H11	2.21	0.41
2:B:75:THR:N	2:B:76:PRO:HD2	2.36	0.40
3:C:93:PHE:O	3:C:97:GLU:HG2	2.20	0.40
1:A:292:HIS:HE1	1:A:529:THR:HG21	1.86	0.40
2:B:163:VAL:HG21	2:B:242:TRP:CE2	2.56	0.40
3:C:99:MET:O	3:C:102:VAL:HB	2.21	0.40
1:A:123:PRO:O	1:A:124:ASP:HB3	2.19	0.40
3:C:121:PRO:CB	11:C:301:PC1:C14	2.97	0.40
1:A:49:PHE:CG	1:A:90:MET:HE3	2.57	0.40
1:A:127:PHE:CD1	12:C:302:PGV:O13	2.73	0.40
1:A:191:ALA:O	1:A:195:LEU:HG	2.21	0.40
2:B:83:LEU:O	2:B:87:LEU:HG	2.22	0.40
3:C:162:PHE:O	3:C:166:GLY:HA2	2.22	0.40
1:A:381:PHE:CE1	2:B:50:CYS:SG	3.14	0.40
2:B:117:ILE:HA	2:B:175:THR:O	2.22	0.40
3:C:121:PRO:HB2	11:C:301:PC1:H151	2.02	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%)	519 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	249/298 (84%)	242 (97%)	7 (3%)	0	100	100
3	C	267/274 (97%)	260 (97%)	7 (3%)	0	100	100
4	D	39/50 (78%)	34 (87%)	5 (13%)	0	100	100
All	All	1090/1180 (92%)	1055 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/454 (97%)	437 (99%)	3 (1%)	84	92
2	B	210/243 (86%)	208 (99%)	2 (1%)	76	88
3	C	217/221 (98%)	212 (98%)	5 (2%)	50	70
4	D	32/40 (80%)	32 (100%)	0	100	100
All	All	899/958 (94%)	889 (99%)	10 (1%)	74	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ASP
1	A	341	MET
1	A	525	GLU
2	B	81	TRP
2	B	150	SER
3	C	96	SER
3	C	127	TRP
3	C	151	SER
3	C	164	LEU
3	C	226	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	HEA	A	602	1	57,67,67	1.57	9 (15%)	61,103,103	2.54	25 (40%)
12	PGV	C	302	-	50,50,50	0.92	2 (4%)	53,56,56	1.00	2 (3%)
9	PEO	A	606	7,6	1,1,1	0.97	0	-		
11	PC1	C	301	-	41,41,53	1.21	4 (9%)	47,49,61	3.03	16 (34%)
10	CUA	B	301	2	0,1,1	-	-	-		
6	HEA	A	603	9,1	57,67,67	1.57	8 (14%)	61,103,103	2.38	23 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEA	A	603	9,1	3/3/7/16	9/32/76/76	-
6	HEA	A	602	1	3/3/7/16	6/32/76/76	-
12	PGV	C	302	-	-	15/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PC1	C	301	-	-	24/45/45/57	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HEA	C3A-C2A	-6.05	1.32	1.40
6	A	602	HEA	C3A-C2A	-5.20	1.33	1.40
12	C	302	PGV	O03-C19	4.24	1.45	1.33
6	A	602	HEA	C3C-C2C	-4.19	1.34	1.40
12	C	302	PGV	O01-C1	4.12	1.45	1.34
11	C	301	PC1	O31-C31	3.80	1.44	1.33
11	C	301	PC1	O31-C3	-3.59	1.37	1.45
6	A	602	HEA	FE-NB	3.45	2.13	1.96
6	A	603	HEA	C3C-C2C	-3.39	1.35	1.40
11	C	301	PC1	O21-C21	3.38	1.43	1.34
6	A	603	HEA	C4B-NB	-3.37	1.34	1.40
6	A	603	HEA	FE-NB	3.36	2.13	1.96
6	A	602	HEA	FE-ND	3.10	2.12	1.96
6	A	602	HEA	C4B-NB	-3.04	1.35	1.40
6	A	603	HEA	C3C-CAC	3.01	1.54	1.47
6	A	602	HEA	C3C-CAC	2.95	1.53	1.47
6	A	603	HEA	FE-ND	2.89	2.11	1.96
6	A	602	HEA	C1D-ND	-2.80	1.35	1.40
11	C	301	PC1	O21-C2	-2.35	1.40	1.46
6	A	603	HEA	O2D-CGD	-2.33	1.22	1.30
6	A	602	HEA	C3A-CMA	2.11	1.51	1.46
6	A	603	HEA	CHD-C1D	2.04	1.40	1.35
6	A	602	HEA	O2D-CGD	-2.03	1.23	1.30

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	301	PC1	C15-N-C14	-11.15	80.32	108.97
11	C	301	PC1	C15-N-C13	-9.68	84.09	108.97
6	A	602	HEA	C4B-NB-C1B	8.30	113.65	105.07
11	C	301	PC1	C2-O21-C21	-7.72	98.78	117.79
6	A	602	HEA	C4A-CHB-C1B	6.55	131.20	122.56
6	A	603	HEA	C4B-NB-C1B	6.48	111.77	105.07
6	A	603	HEA	CMC-C2C-C1C	-6.03	119.20	128.46
6	A	603	HEA	CAD-CBD-CGD	-5.22	102.36	113.60
11	C	301	PC1	C24-C23-C22	-5.02	95.15	113.19
6	A	602	HEA	C3B-C4B-NB	-4.78	104.17	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	602	HEA	C1D-ND-C4D	4.76	109.98	105.07
6	A	603	HEA	C4A-CHB-C1B	4.72	128.79	122.56
6	A	602	HEA	C13-C12-C11	-4.67	107.33	114.35
6	A	602	HEA	CBA-CAA-C2A	4.30	119.85	112.60
11	C	301	PC1	C14-N-C13	4.20	119.78	108.97
6	A	602	HEA	C2B-C1B-NB	-4.20	104.86	109.88
6	A	603	HEA	C3B-C4B-NB	-4.13	104.95	109.84
12	C	302	PGV	O01-C1-C2	4.05	120.24	111.50
6	A	603	HEA	O2A-CGA-O1A	-4.05	113.21	123.30
6	A	603	HEA	CMC-C2C-C3C	3.88	131.94	124.68
6	A	603	HEA	C4D-CHA-C1A	3.66	127.39	122.56
6	A	602	HEA	C3A-C4A-NA	-3.56	104.22	110.94
6	A	603	HEA	C1D-ND-C4D	3.54	108.73	105.07
11	C	301	PC1	O31-C3-C2	-3.46	98.36	108.43
11	C	301	PC1	C3-C2-C1	3.42	119.89	111.79
6	A	602	HEA	CAA-CBA-CGA	-3.40	104.22	113.76
6	A	602	HEA	C4D-CHA-C1A	3.36	126.99	122.56
6	A	602	HEA	CHB-C1B-C2B	3.34	130.19	124.98
6	A	603	HEA	CBD-CAD-C3D	3.30	121.79	112.63
6	A	603	HEA	C27-C19-C20	3.29	120.81	115.27
11	C	301	PC1	C15-N-C12	-3.21	96.78	109.92
6	A	602	HEA	CMC-C2C-C1C	-3.14	123.64	128.46
6	A	602	HEA	C3D-C4D-ND	-3.09	107.36	110.36
6	A	602	HEA	O11-C11-C12	3.07	118.00	109.42
6	A	603	HEA	C3A-C4A-NA	-3.00	105.28	110.94
6	A	603	HEA	C2B-C1B-NB	-2.95	106.34	109.88
6	A	603	HEA	C13-C14-C15	-2.92	120.62	127.66
6	A	602	HEA	O2A-CGA-CBA	2.89	123.32	114.03
11	C	301	PC1	C23-C22-C21	2.81	123.85	113.62
11	C	301	PC1	C13-N-C12	2.78	121.30	109.92
6	A	602	HEA	CHA-C4D-ND	2.58	127.24	124.43
11	C	301	PC1	O21-C2-C3	2.49	117.43	108.40
6	A	602	HEA	C16-C15-C14	-2.48	116.11	121.12
6	A	603	HEA	CMB-C2B-C3B	-2.47	125.63	130.34
6	A	603	HEA	O11-C11-C12	2.47	116.31	109.42
12	C	302	PGV	O03-C19-C20	2.45	119.61	111.91
6	A	602	HEA	O2D-CGD-CBD	2.43	121.84	114.03
11	C	301	PC1	C33-C32-C31	-2.43	104.78	113.62
6	A	602	HEA	O2D-CGD-O1D	-2.40	117.31	123.30
6	A	603	HEA	C2D-C1D-ND	-2.37	107.03	109.84
11	C	301	PC1	C29-C28-C27	-2.33	102.59	114.42
6	A	602	HEA	C2D-C1D-ND	-2.29	107.13	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	602	HEA	C12-C13-C14	-2.27	106.24	112.23
11	C	301	PC1	O31-C31-C32	2.25	118.98	111.91
6	A	602	HEA	C26-C15-C16	2.21	118.99	115.27
6	A	603	HEA	CHB-C1B-C2B	2.18	128.38	124.98
6	A	603	HEA	CAD-C3D-C4D	-2.14	120.91	124.66
6	A	602	HEA	C17-C18-C19	-2.10	122.61	127.66
6	A	603	HEA	C17-C18-C19	-2.09	122.63	127.66
6	A	602	HEA	C24-C23-C22	-2.07	116.67	122.65
6	A	603	HEA	C24-C23-C22	-2.06	116.68	122.65
6	A	602	HEA	OMA-CMA-C3A	-2.06	120.42	124.91
11	C	301	PC1	C26-C25-C24	-2.04	104.06	114.42
6	A	603	HEA	CAD-C3D-C2D	2.03	131.66	127.88
6	A	603	HEA	O1D-CGD-CBD	-2.02	116.60	123.08
11	C	301	PC1	C14-N-C12	2.01	118.13	109.92

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	602	HEA	ND
6	A	602	HEA	NB
6	A	602	HEA	NA
6	A	603	HEA	ND
6	A	603	HEA	NB
6	A	603	HEA	NA

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	HEA	C13-C14-C15-C16
6	A	603	HEA	C2D-C3D-CAD-CBD
6	A	603	HEA	C4D-C3D-CAD-CBD
6	A	603	HEA	C21-C22-C23-C25
11	C	301	PC1	C11-O13-P-O14
11	C	301	PC1	C1-O11-P-O13
11	C	301	PC1	O22-C21-O21-C2
12	C	302	PGV	C03-O11-P-O13
12	C	302	PGV	C04-O12-P-O11
6	A	603	HEA	C21-C22-C23-C24
11	C	301	PC1	C22-C21-O21-C2
6	A	602	HEA	C13-C14-C15-C26
12	C	302	PGV	C2-C1-O01-C02
11	C	301	PC1	C2-C1-O11-P

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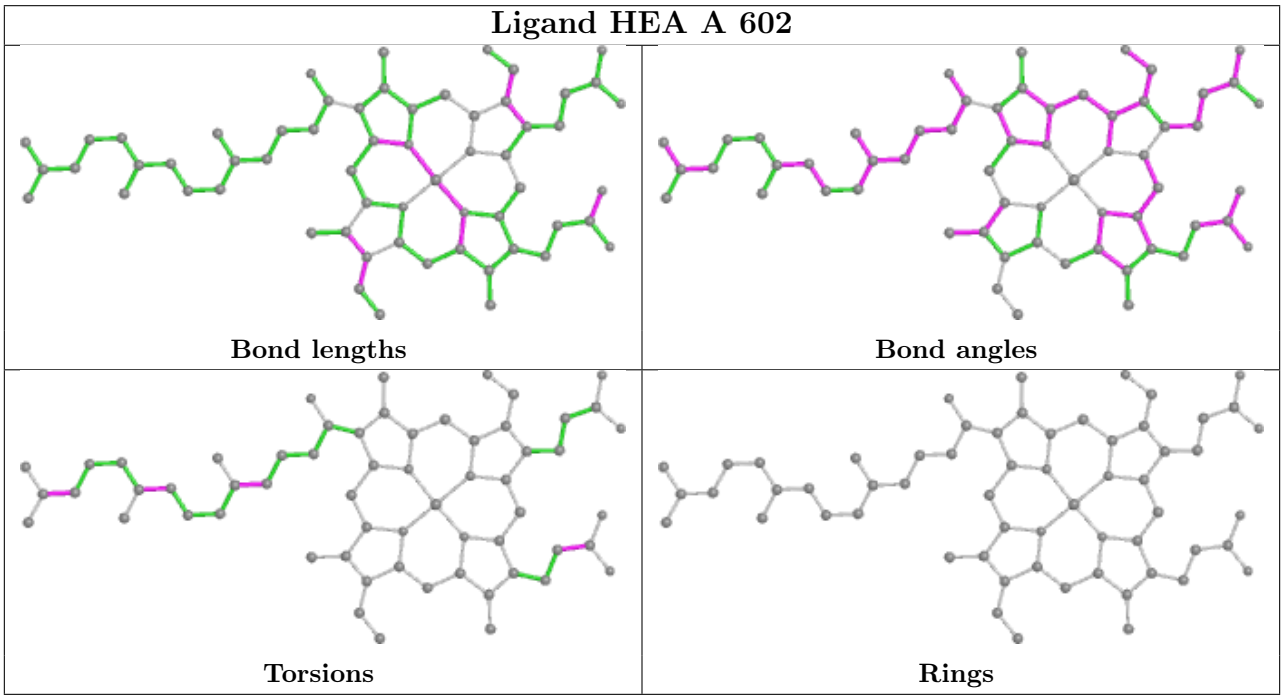
Mol	Chain	Res	Type	Atoms
12	C	302	PGV	C3-C4-C5-C6
11	C	301	PC1	C31-C32-C33-C34
12	C	302	PGV	O02-C1-O01-C02
12	C	302	PGV	C21-C22-C23-C24
11	C	301	PC1	C11-O13-P-O11
12	C	302	PGV	C03-O11-P-O12
11	C	301	PC1	C11-C12-N-C13
6	A	602	HEA	C21-C22-C23-C24
11	C	301	PC1	C36-C37-C38-C39
11	C	301	PC1	C1-C2-C3-O31
11	C	301	PC1	O11-C1-C2-C3
11	C	301	PC1	C29-C2A-C2B-C2C
11	C	301	PC1	O11-C1-C2-O21
11	C	301	PC1	C11-O13-P-O12
11	C	301	PC1	C1-O11-P-O12
12	C	302	PGV	C03-O11-P-O14
12	C	302	PGV	C04-O12-P-O14
11	C	301	PC1	C32-C31-O31-C3
11	C	301	PC1	O21-C2-C3-O31
12	C	302	PGV	O01-C1-C2-C3
6	A	603	HEA	C11-C12-C13-C14
11	C	301	PC1	C22-C23-C24-C25
12	C	302	PGV	C19-C20-C21-C22
11	C	301	PC1	O32-C31-O31-C3
11	C	301	PC1	C2B-C2C-C2D-C2E
6	A	603	HEA	CAD-CBD-CGD-O1D
6	A	603	HEA	CAA-CBA-CGA-O1A
11	C	301	PC1	C35-C36-C37-C38
6	A	602	HEA	CAD-CBD-CGD-O2D
12	C	302	PGV	C9-C10-C11-C12
11	C	301	PC1	C33-C34-C35-C36
6	A	602	HEA	CAD-CBD-CGD-O1D
6	A	603	HEA	CAD-CBD-CGD-O2D
11	C	301	PC1	O31-C31-C32-C33
12	C	302	PGV	C2-C3-C4-C5
11	C	301	PC1	O32-C31-C32-C33
6	A	602	HEA	C17-C18-C19-C27
6	A	603	HEA	CAA-CBA-CGA-O2A
12	C	302	PGV	C03-C02-O01-C1
12	C	302	PGV	C7-C8-C9-C10

There are no ring outliers.

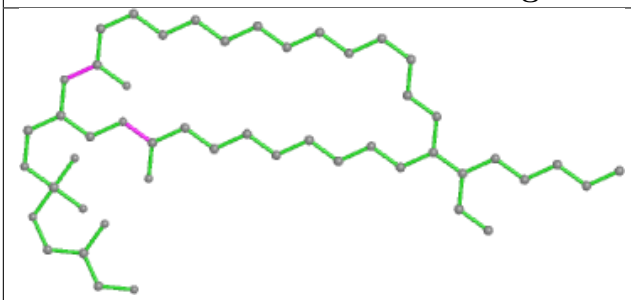
4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	HEA	4	0
12	C	302	PGV	13	0
11	C	301	PC1	16	0
6	A	603	HEA	3	0

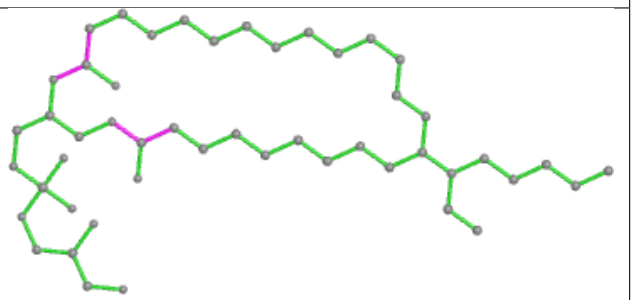
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



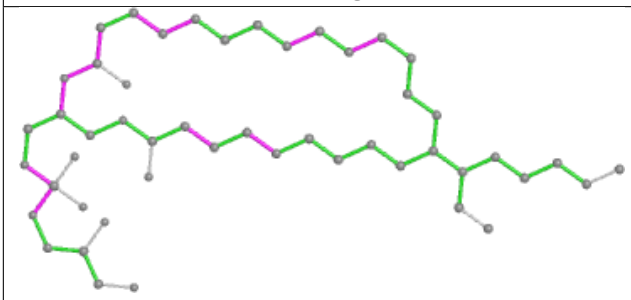
Ligand PGV C 302



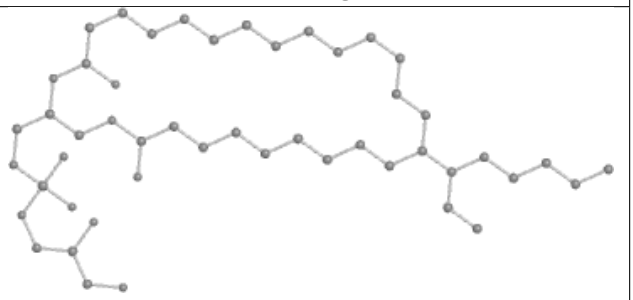
Bond lengths



Bond angles

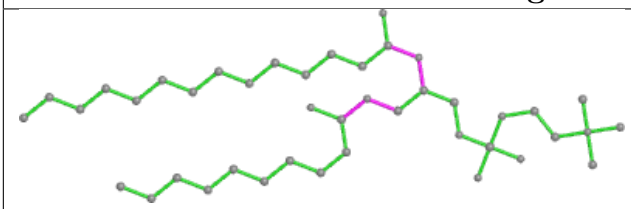


Torsions

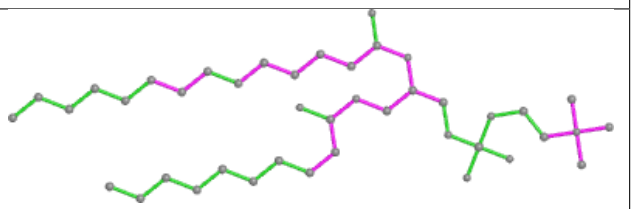


Rings

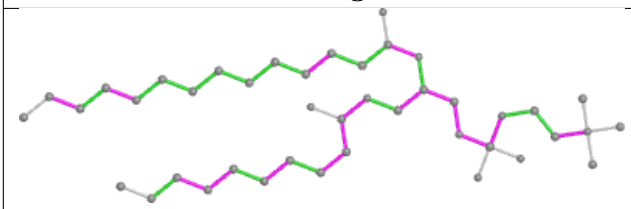
Ligand PC1 C 301



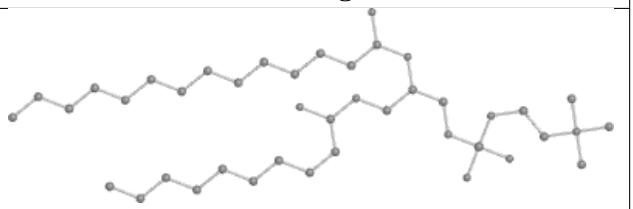
Bond lengths



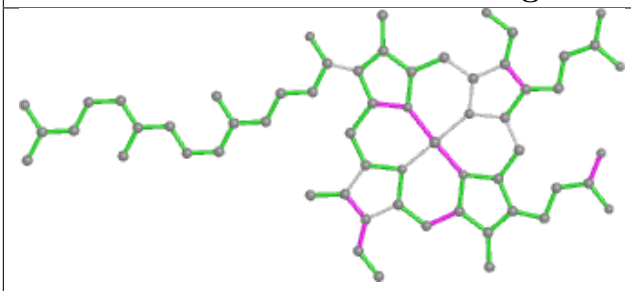
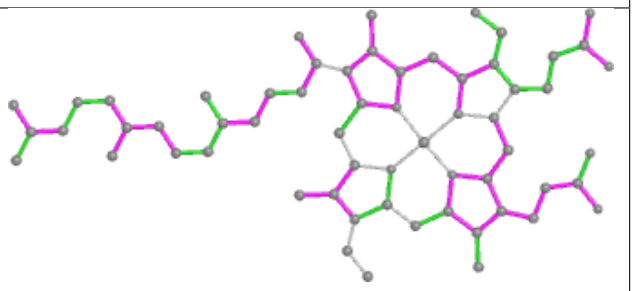
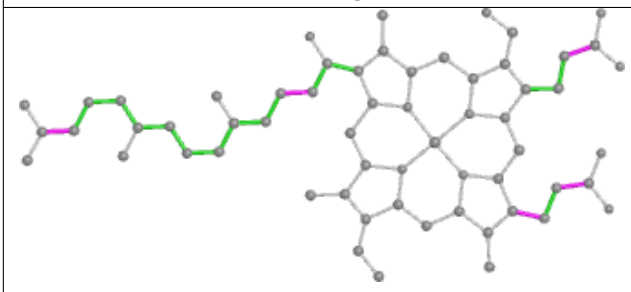
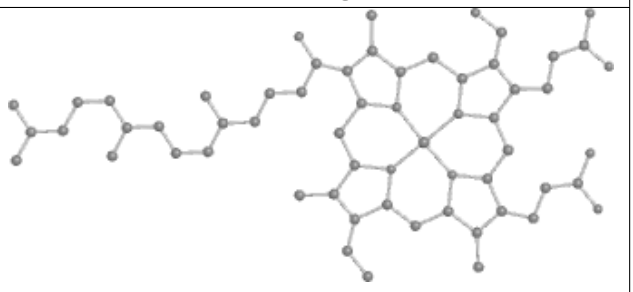
Bond angles



Torsions



Rings

Ligand HEA A 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

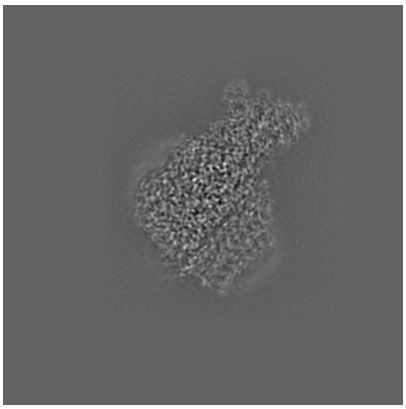
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11921. These allow visual inspection of the internal detail of the map and identification of artifacts.

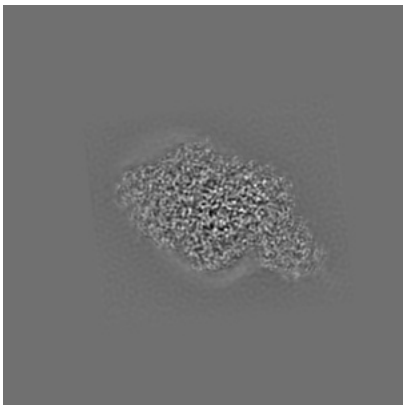
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

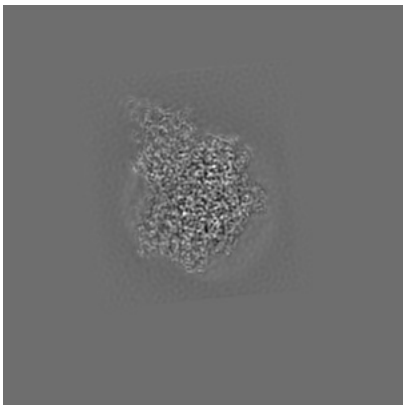
6.1.1 Primary map



X

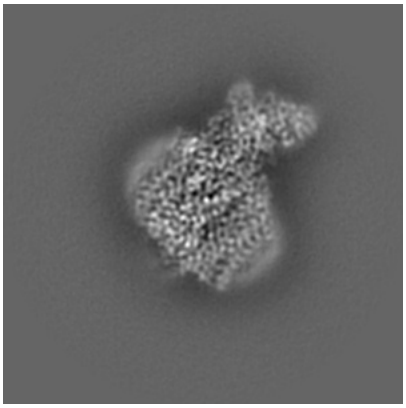


Y

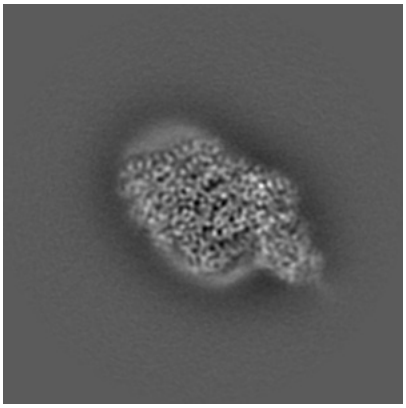


Z

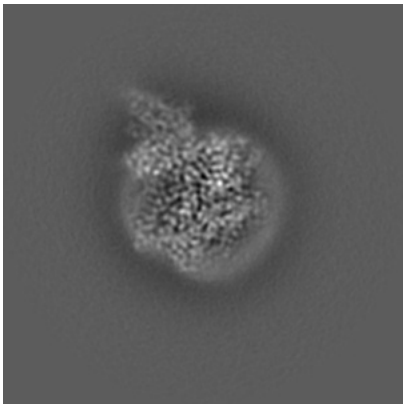
6.1.2 Raw map



X



Y



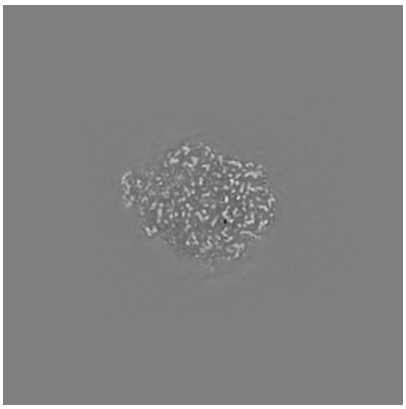
Z

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

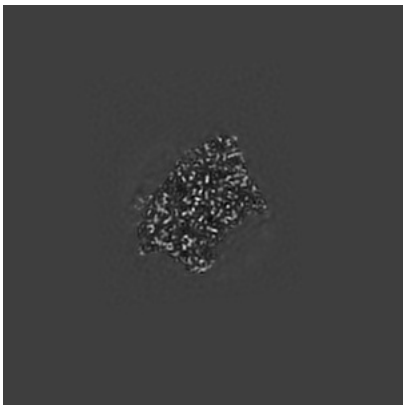
6.2 Central slices (i)

6.2.1 Primary map

X Index: 128

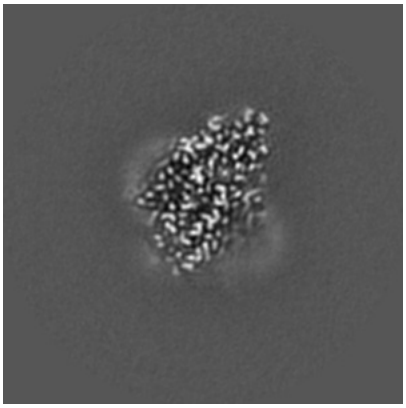


Y Index: 128

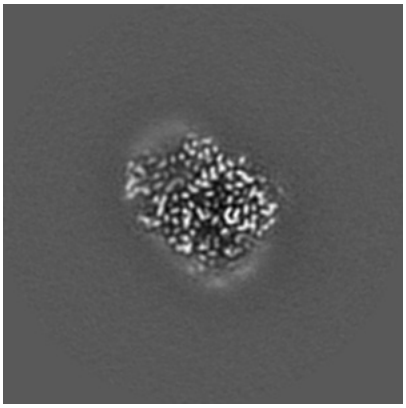


Z Index: 128

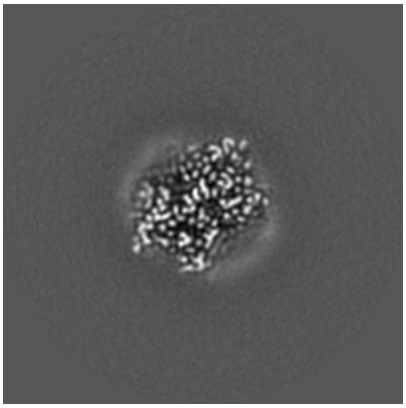
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

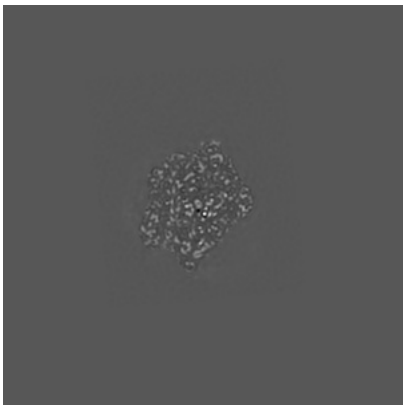
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

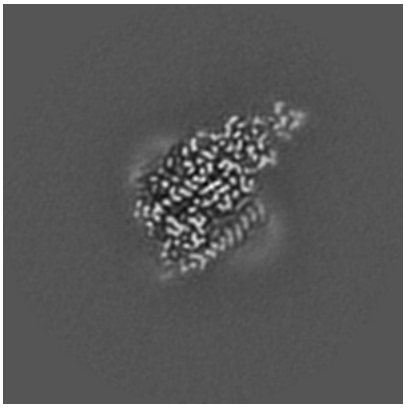
X Index: 134

Y Index: 122

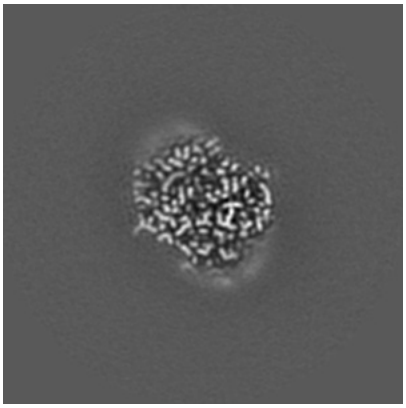


Z Index: 143

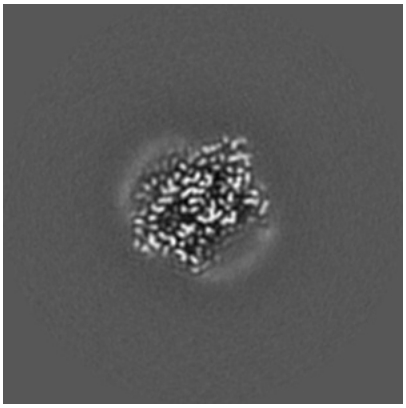
6.3.2 Raw map



X Index: 118



Y Index: 123



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 1.36. 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.

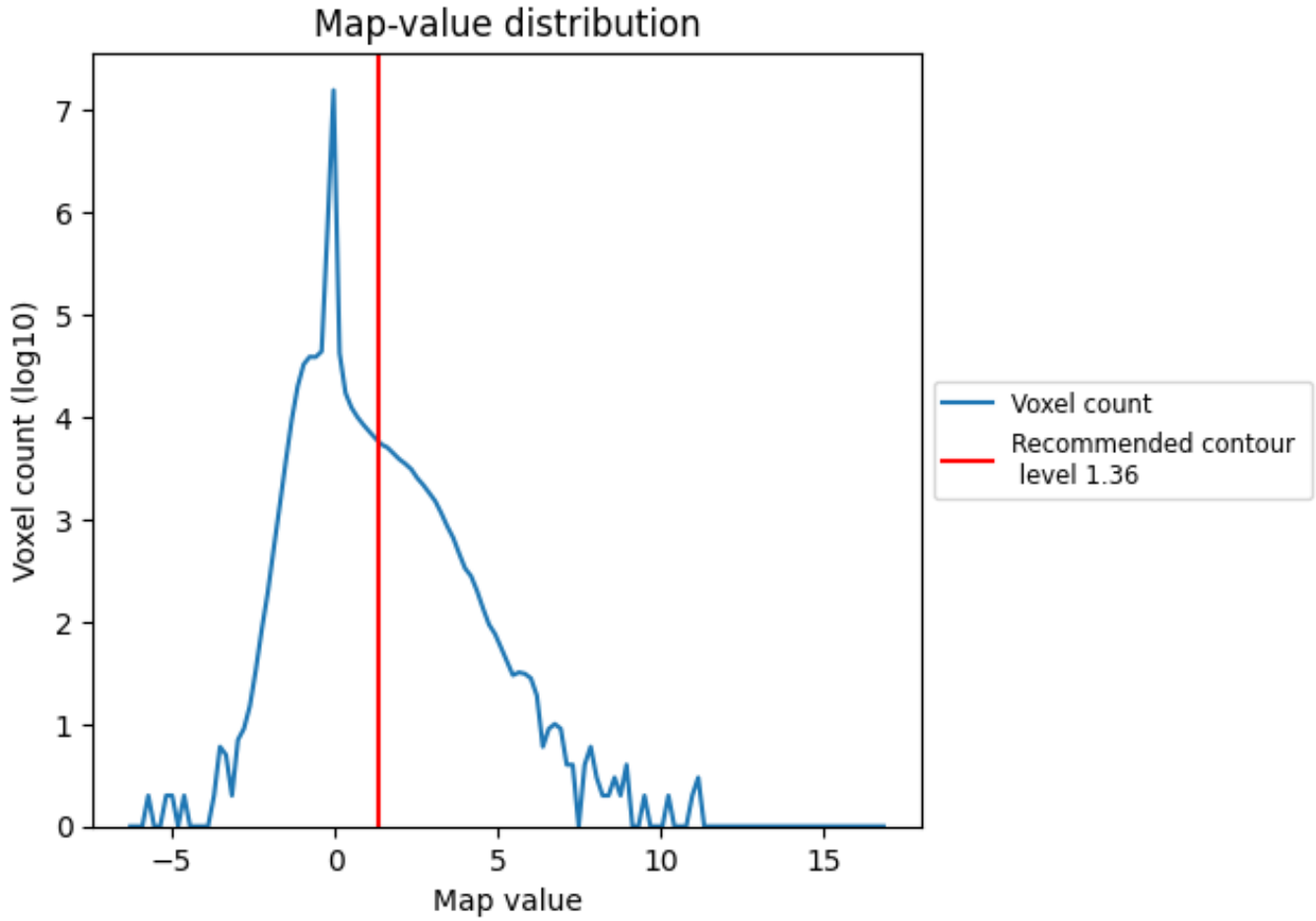
6.5 Mask visualisation (i)

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

7 Map analysis

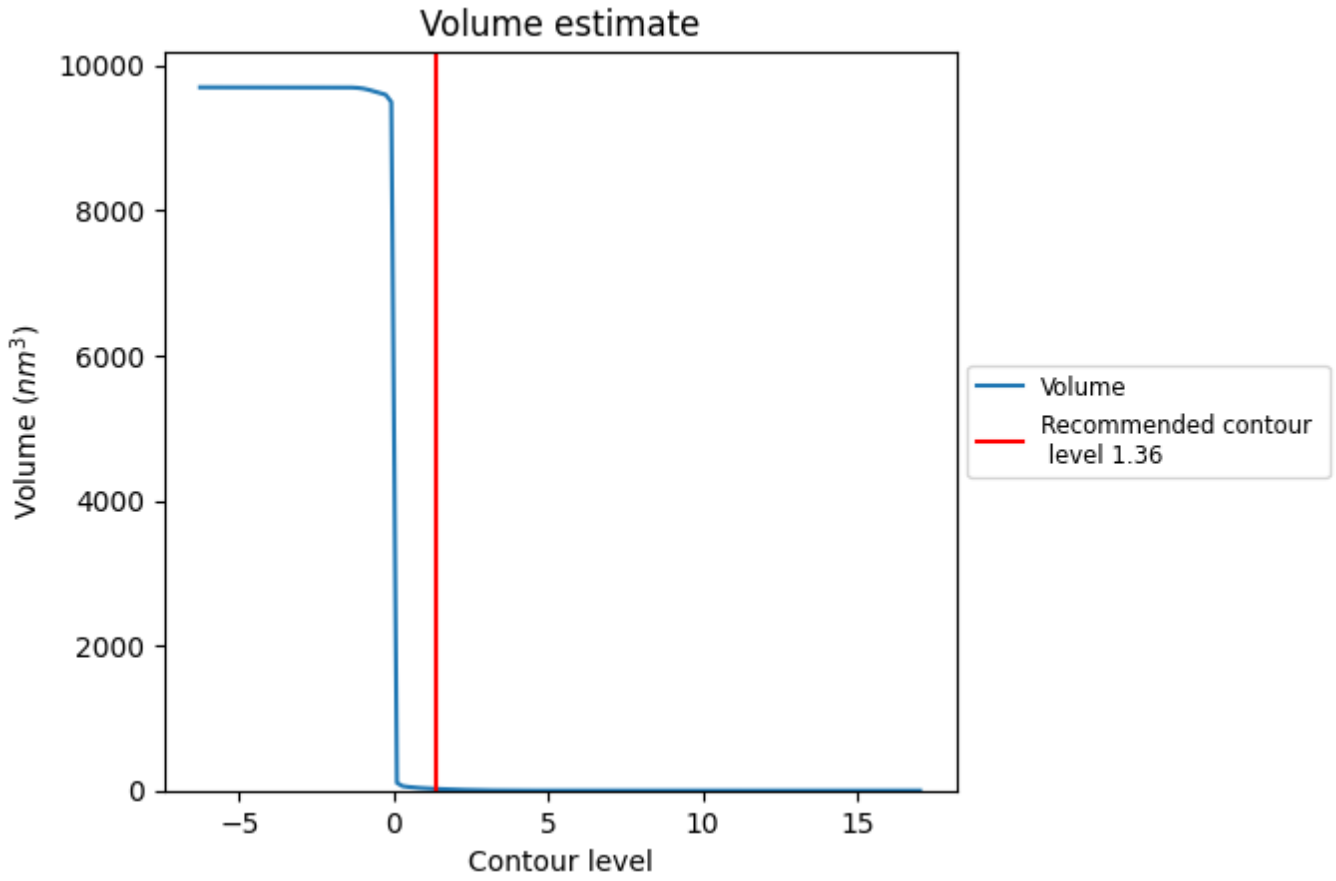
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

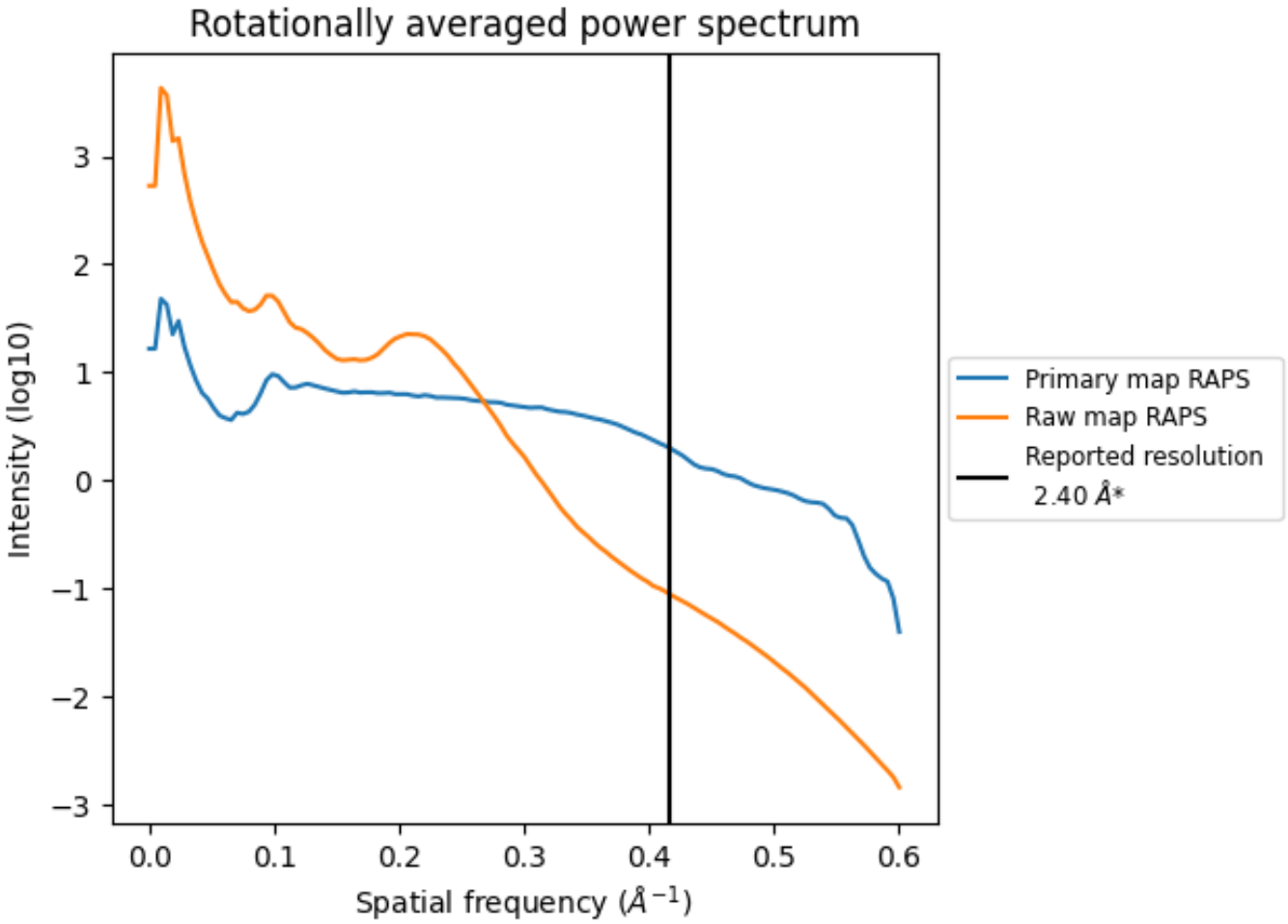
7.2 Volume estimate



The volume at the recommended contour level is 23 nm^3; this corresponds to an approximate mass of 21 kDa.

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

7.3 Rotationally averaged power spectrum (i)

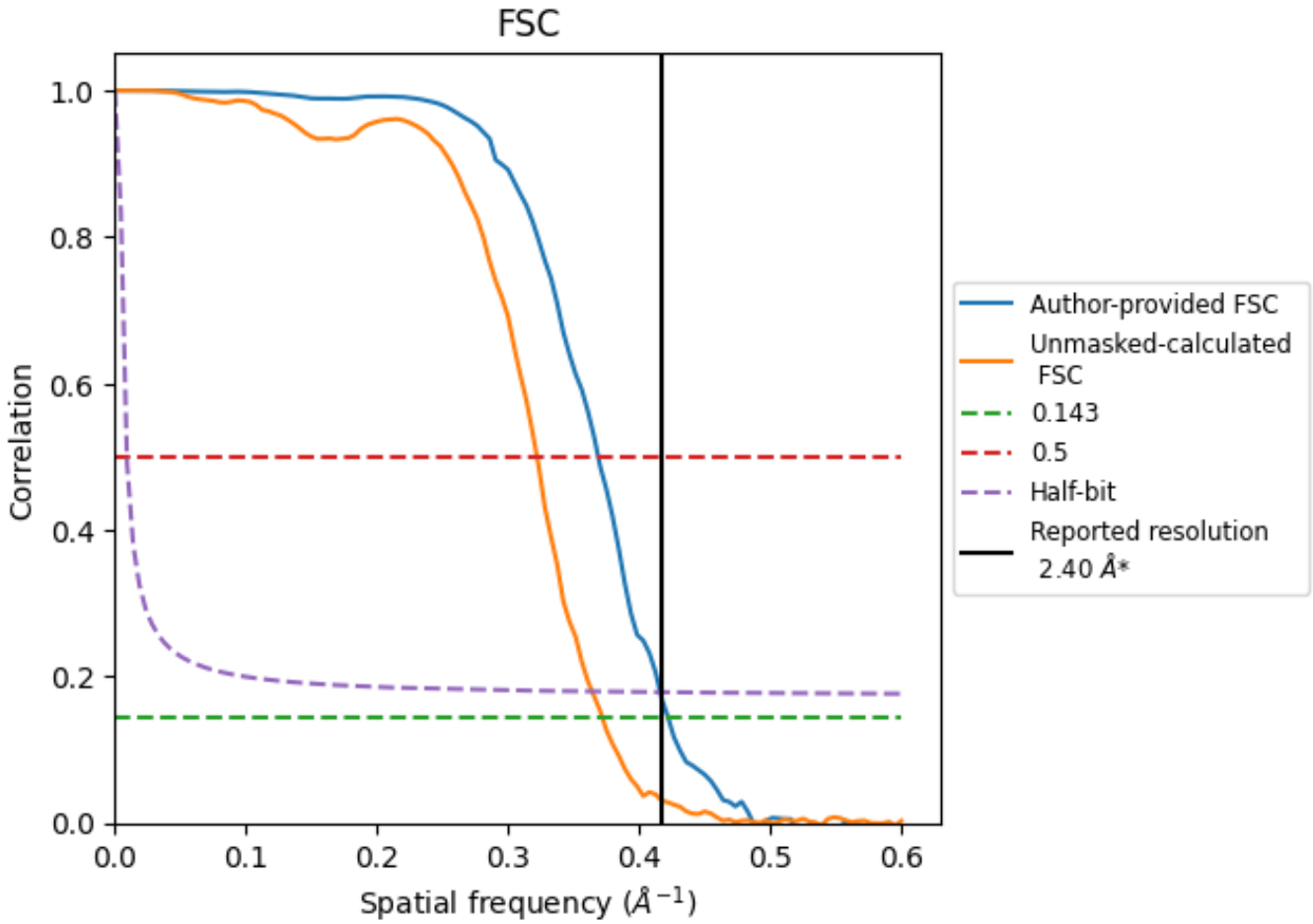


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8.2 Resolution estimates (i)

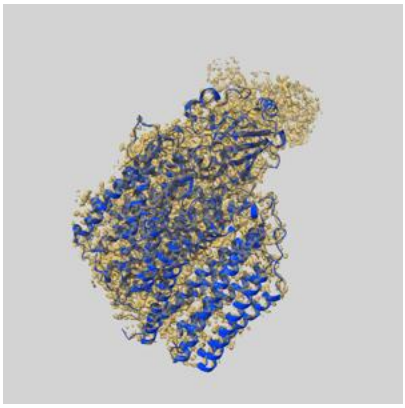
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.37	2.71	2.40
Unmasked-calculated*	2.69	3.10	2.74

*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 2.69 differs from the reported value 2.4 by more than 10 %

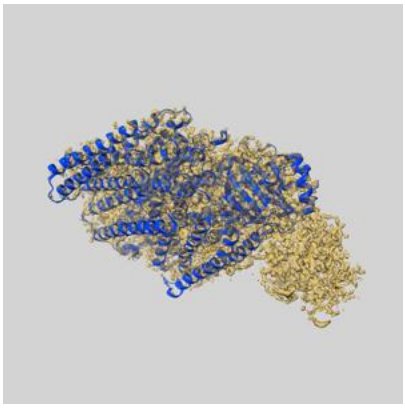
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11921 and PDB model 7ATE. Per-residue inclusion information can be found in section 3 on page 9.

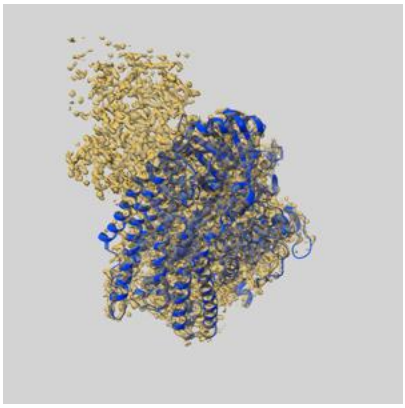
9.1 Map-model overlay



X



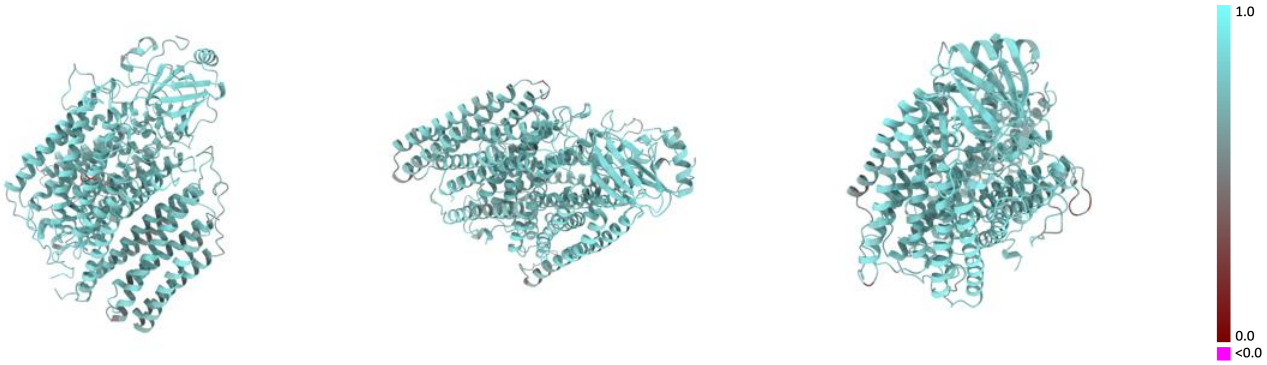
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.36 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.

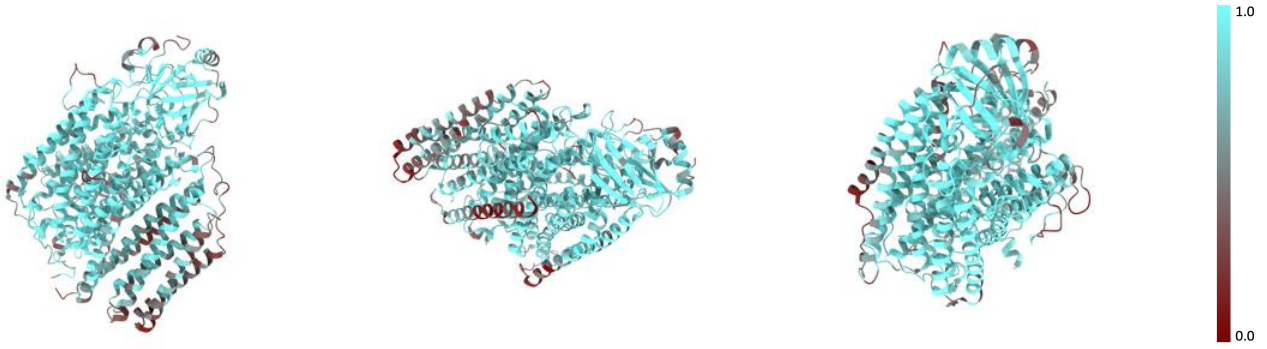
9.2 Q-score mapped to coordinate model (i)



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.

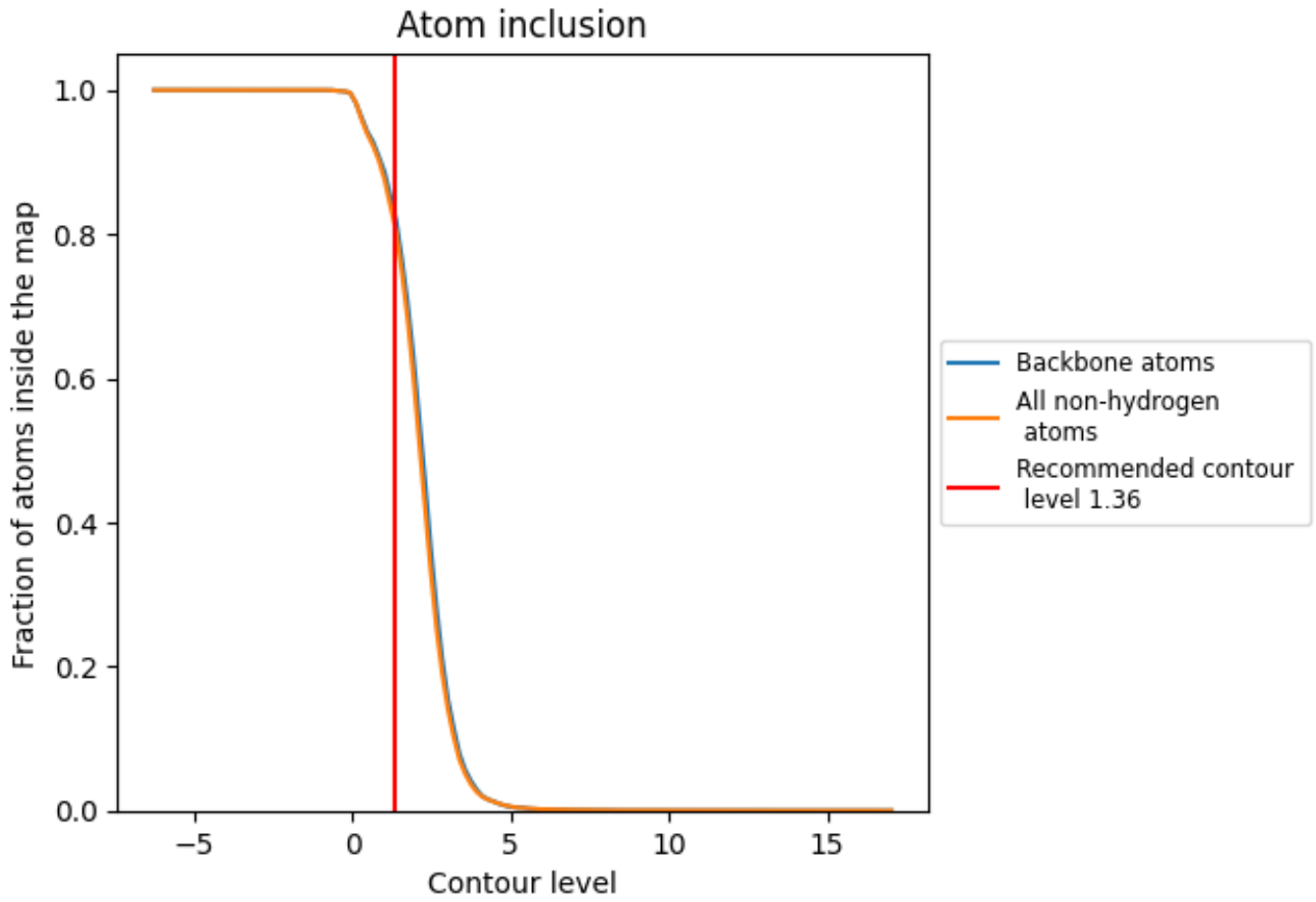
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.36).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (1.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8065	0.7490
A	0.9219	0.7810
B	0.7950	0.7470
C	0.6545	0.7000
D	0.3917	0.6670