



## Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 07:13 pm GMT

PDB ID : 7AU6  
EMDB ID : EMD-11925  
Title : Cytochrome c oxidase structure in O-state  
Authors : Kolbe, F.; Safarian, S.; Michel, H.  
Deposited on : 2020-11-02  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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

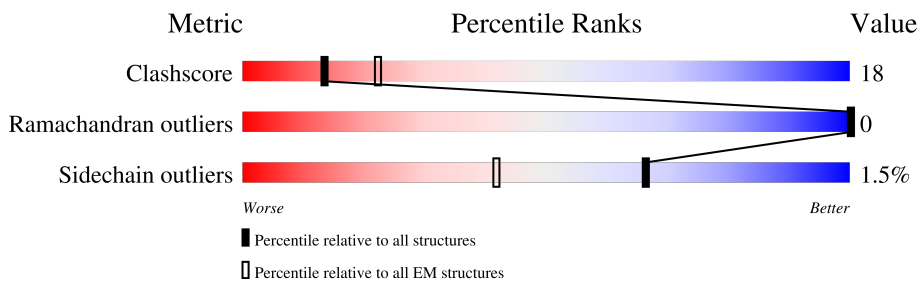
# 1 Overall quality at a glance

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

Mol	Chain	Length	Quality of chain
1	A	558	
2	B	298	
3	C	274	
4	D	50	

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
5	HEA	A	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEA	A	602	X	-	-	-
8	OXY	A	609	-	-	X	-

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 9024 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	248	1947	1278	314	347	8	0	0

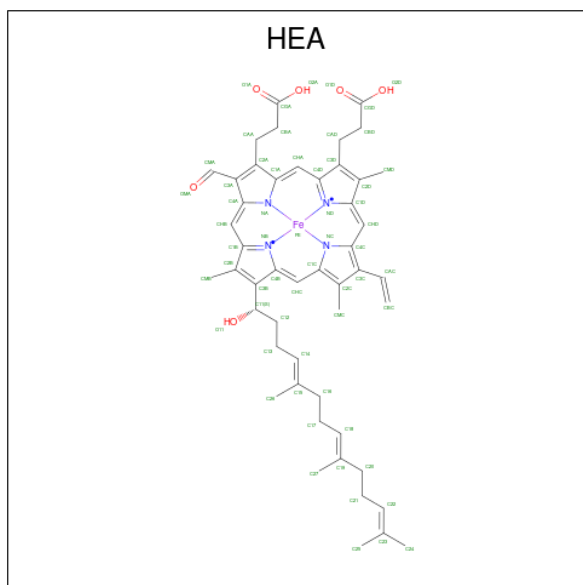
- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

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	38	288	188	48	51	1	0	0

- Molecule 5 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

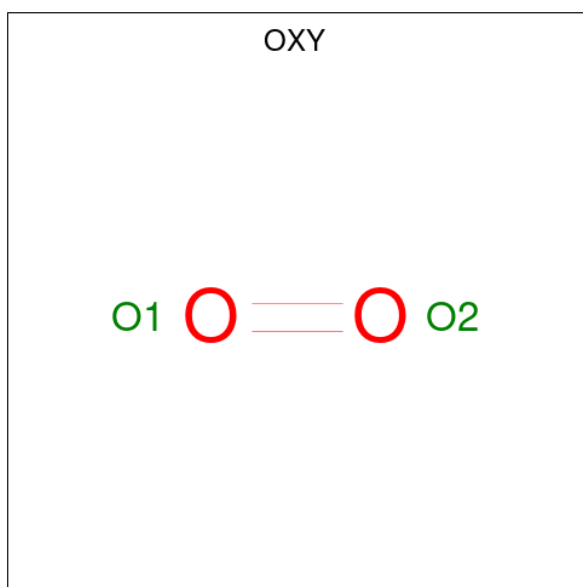
- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

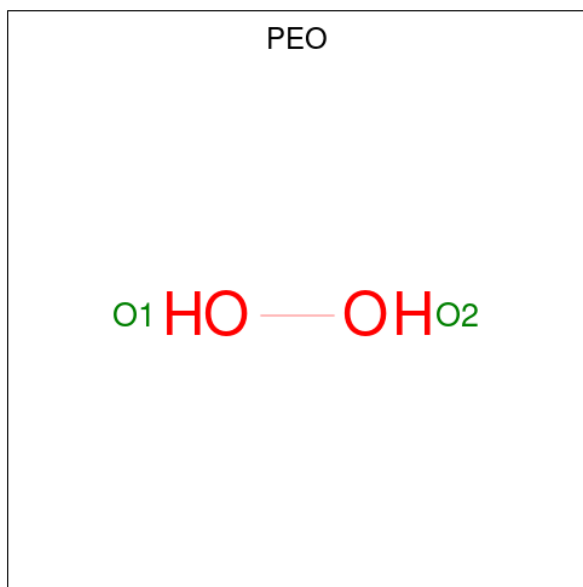
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
7	A	1	1	1	0

- Molecule 8 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total O 12 12	0
8	A	1	Total O 12 12	0
8	A	1	Total O 12 12	0
8	A	1	Total O 12 12	0
8	A	1	Total O 12 12	0
8	A	1	Total O 12 12	0

- Molecule 9 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H<sub>2</sub>O<sub>2</sub>).

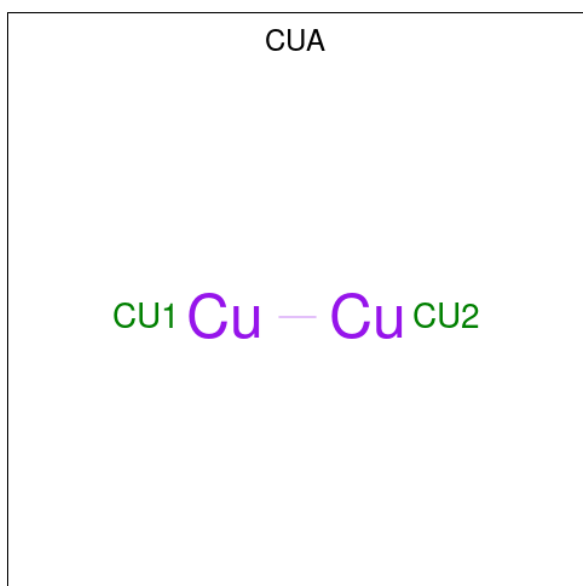


Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total O 2 2	0

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

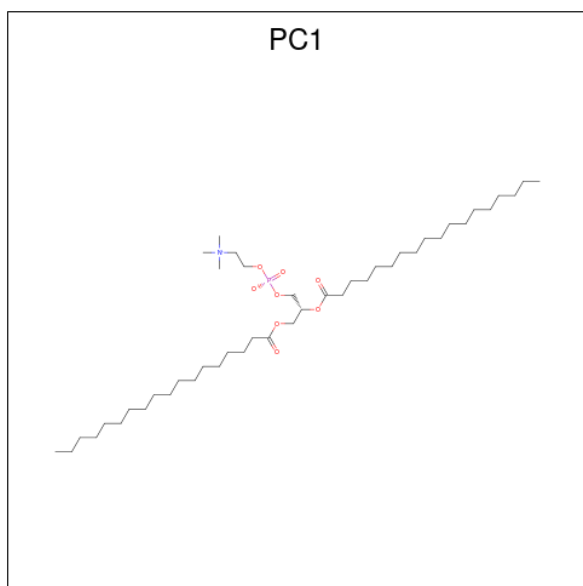
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total Mn 1 1	0

- Molecule 11 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 12 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	
12	C	1	Total	C	N	O	P	0
			95	75	2	16	2	
12	C	1	Total	C	N	O	P	0
			95	75	2	16	2	

- Molecule 13 is water.

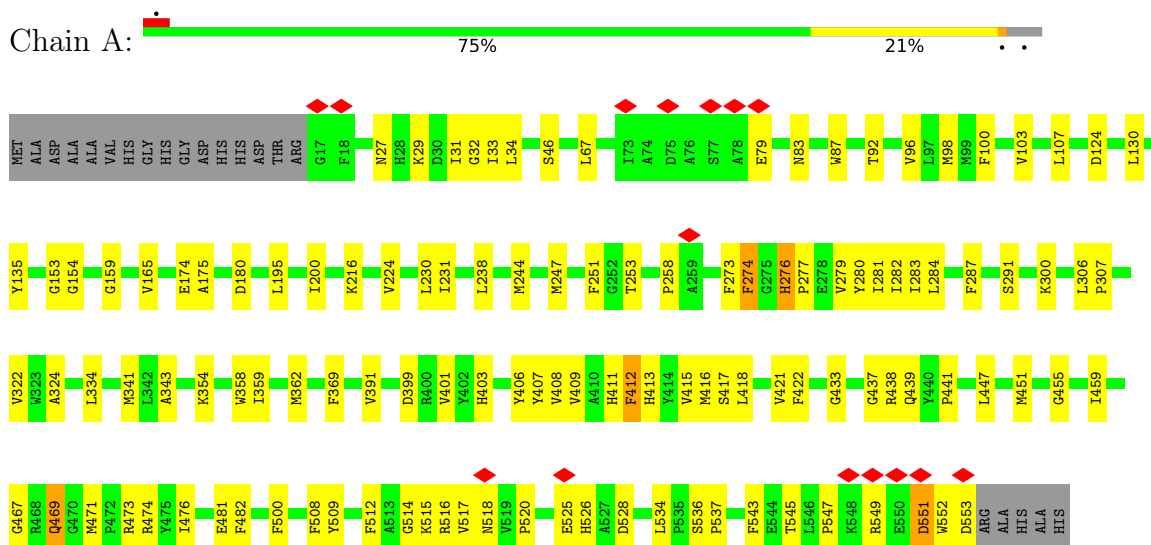
Mol	Chain	Residues	Atoms		AltConf
13	A	98	Total	O	0
			98	98	
13	B	40	Total	O	0
			40	40	
13	C	8	Total	O	0
			8	8	
13	D	2	Total	O	0
			2	2	



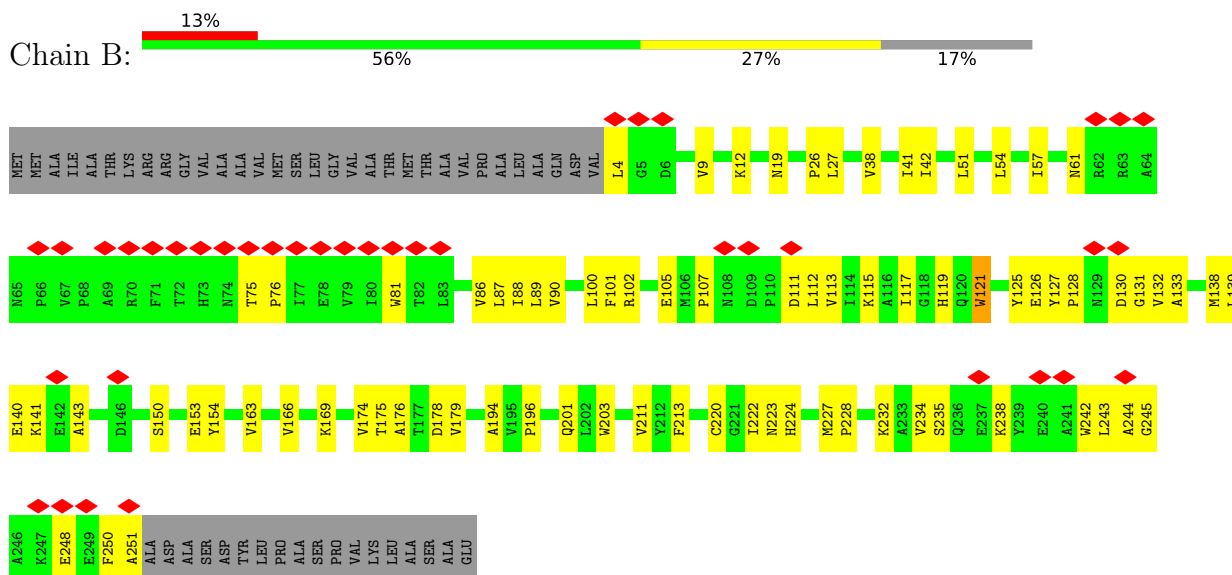
### 3 Residue-property plots

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

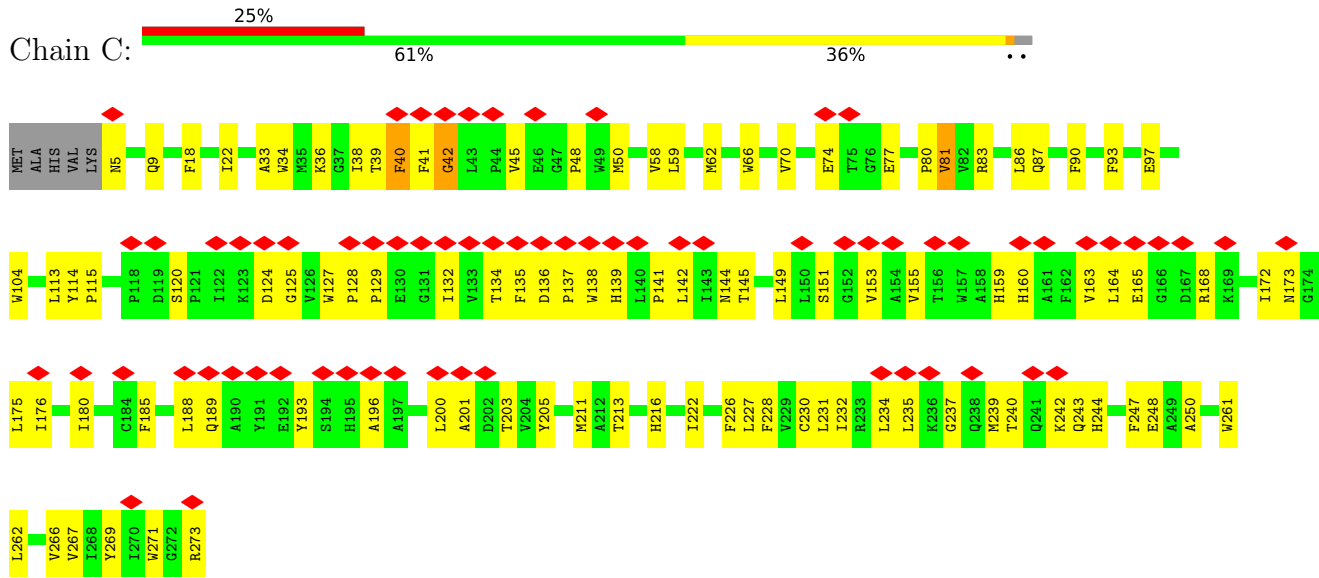
- Molecule 1: Cytochrome c oxidase subunit 1-beta



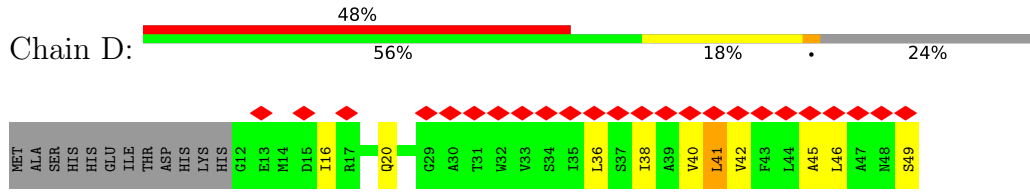
- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 4: Cytochrome c oxidase subunit 4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	321273	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 ( $e^-/\text{\AA}^2$ )	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	47.432	Depositor
Minimum map value	-25.651	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.512	Depositor
Recommended contour level	1.75	Depositor
Map size (Å)	98.294, 114.954, 137.445	wwPDB
Map dimensions	118, 138, 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: PEO, OXY, CA, MN, CUA, PC1, HEA, CU

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	0.78	12/4416 (0.3%)	0.81	4/6028 (0.1%)
2	B	0.51	1/2004 (0.0%)	0.63	3/2747 (0.1%)
3	C	0.38	0/2235	0.50	1/3060 (0.0%)
4	D	0.51	0/293	0.75	1/395 (0.3%)
All	All	0.63	13/8948 (0.1%)	0.70	9/12230 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ILE	C-O	-12.79	0.99	1.23
1	A	34	LEU	C-O	-11.12	1.02	1.23
1	A	33	ILE	C-O	-8.81	1.06	1.23
1	A	33	ILE	N-CA	-8.78	1.28	1.46
1	A	31	ILE	N-CA	-8.48	1.29	1.46
1	A	32	GLY	N-CA	-7.81	1.34	1.46
1	A	34	LEU	N-CA	-7.58	1.31	1.46
1	A	135	TYR	C-O	-6.63	1.10	1.23
1	A	32	GLY	C-O	-6.51	1.13	1.23
2	B	179	VAL	C-O	-5.93	1.12	1.23
1	A	31	ILE	C-N	5.78	1.43	1.33
1	A	469	GLN	C-O	-5.60	1.12	1.23
1	A	273	PHE	C-O	-5.49	1.12	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	THR	O-C-N	-11.55	104.21	122.70
1	A	276	HIS	CA-CB-CG	-8.57	99.02	113.60
2	B	175	THR	CA-C-N	7.50	133.69	117.20
3	C	42	GLY	C-N-CA	-6.62	105.15	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	41	LEU	CA-CB-CG	-6.40	100.58	115.30
1	A	324	ALA	CB-CA-C	6.14	119.31	110.10
2	B	178	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	369	PHE	CB-CA-C	5.67	121.75	110.40
1	A	412	PHE	CB-CA-C	5.57	121.54	110.40

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	130	0
2	B	1947	0	1934	73	0
3	C	2150	0	2113	108	0
4	D	288	0	293	16	0
5	A	120	0	107	17	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	12	0	0	5	0
9	A	2	0	0	0	0
10	A	1	0	0	0	0
11	B	2	0	0	0	0
12	C	95	0	144	13	0
13	A	98	0	0	39	0
13	B	40	0	0	5	0
13	C	8	0	0	4	0
13	D	2	0	0	0	0
All	All	9024	0	8762	317	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 18.

All (317) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:HD21	2:B:101:PHE:CD1	1.66	1.31
1:A:103:VAL:HB	13:A:782:HOH:O	1.23	1.27
3:C:114:TYR:CE1	12:C:301:PC1:H133	1.78	1.18
1:A:334:LEU:HD21	2:B:101:PHE:CE1	1.81	1.16
3:C:240:THR:HG22	3:C:242:LYS:H	1.12	1.08
1:A:276:HIS:NE2	1:A:280:TYR:HE2	1.57	1.02
5:A:602:HEA:H263	13:A:729:HOH:O	1.61	1.00
12:C:301:PC1:H352	12:C:301:PC1:H251	1.44	0.97
3:C:173:ASN:HA	3:C:176:ILE:HD12	1.46	0.97
1:A:334:LEU:HD21	2:B:101:PHE:HD1	1.29	0.95
1:A:276:HIS:NE2	1:A:280:TYR:CE2	2.32	0.94
1:A:438:ARG:NH1	1:A:514:GLY:O	1.99	0.94
1:A:154:GLY:N	1:A:174:GLU:OE2	2.01	0.92
1:A:334:LEU:CD2	2:B:101:PHE:CE1	2.53	0.91
5:A:602:HEA:H132	13:A:729:HOH:O	1.71	0.91
1:A:276:HIS:HE2	1:A:280:TYR:HE2	0.91	0.86
3:C:114:TYR:CD1	12:C:301:PC1:H133	2.10	0.86
1:A:153:GLY:C	1:A:174:GLU:OE2	2.16	0.84
2:B:121:TRP:CG	2:B:223:ASN:HB2	2.12	0.84
3:C:9:GLN:NE2	3:C:77:GLU:OE1	2.11	0.83
1:A:391:VAL:HG23	13:A:729:HOH:O	1.78	0.83
3:C:59:LEU:HD23	3:C:62:MET:CE	2.08	0.83
1:A:124:ASP:HB2	13:A:783:HOH:O	1.79	0.83
5:A:602:HEA:HBC1	5:A:602:HEA:HMC1	1.60	0.82
3:C:240:THR:HG22	3:C:242:LYS:N	1.93	0.82
3:C:172:ILE:HD13	3:C:235:LEU:HG	1.60	0.82
1:A:180:ASP:OD2	3:C:36:LYS:HE3	1.82	0.79
1:A:341:MET:HE1	2:B:100:LEU:HD22	1.63	0.79
1:A:447:LEU:O	1:A:451:MET:HG3	1.83	0.78
1:A:416:MET:SD	13:A:796:HOH:O	2.42	0.77
1:A:238:LEU:CD1	13:A:787:HOH:O	2.33	0.77
1:A:437:GLY:O	1:A:516:ARG:HD2	1.84	0.76
1:A:334:LEU:CD2	2:B:101:PHE:CD1	2.59	0.76
1:A:153:GLY:CA	1:A:174:GLU:OE2	2.34	0.76
3:C:127:TRP:HB3	3:C:128:PRO:HD3	1.68	0.75
4:D:38:ILE:O	4:D:42:VAL:HG23	1.85	0.74
3:C:70:VAL:O	3:C:74:GLU:HG2	1.86	0.74
2:B:88:ILE:HG22	13:B:440:HOH:O	1.86	0.74
1:A:279:VAL:HG11	8:A:605:OXY:O2	1.88	0.74
3:C:244:HIS:O	3:C:248:GLU:HG3	1.87	0.73
3:C:81:VAL:HG13	4:D:16:ILE:CG2	2.19	0.73
2:B:75:THR:N	2:B:76:PRO:HD2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:LEU:HD23	3:C:62:MET:HE3	1.72	0.72
1:A:282:ILE:HG21	13:A:798:HOH:O	1.89	0.72
1:A:455:GLY:O	1:A:459:ILE:HG13	1.90	0.71
3:C:164:LEU:HD13	3:C:164:LEU:O	1.89	0.71
4:D:45:ALA:HA	4:D:49:SER:OG	1.90	0.71
1:A:230:LEU:HB3	13:A:791:HOH:O	1.90	0.71
3:C:45:VAL:HG11	3:C:50:MET:HE3	1.73	0.70
1:A:174:GLU:OE2	1:A:175:ALA:O	2.09	0.70
4:D:42:VAL:O	4:D:46:LEU:HD13	1.91	0.70
3:C:176:ILE:HG22	3:C:180:ILE:HD11	1.73	0.70
2:B:132:VAL:HA	2:B:250:PHE:O	1.92	0.70
3:C:81:VAL:HG13	4:D:16:ILE:HG21	1.72	0.70
1:A:439:GLN:HB3	1:A:515:LYS:HZ3	1.57	0.69
1:A:391:VAL:HG13	13:A:794:HOH:O	1.91	0.69
5:A:601:HEA:HMC1	5:A:601:HEA:HBC1	1.76	0.68
3:C:144:ASN:ND2	3:C:188:LEU:HB3	2.10	0.67
3:C:136:ASP:OD1	3:C:138:TRP:N	2.23	0.66
1:A:238:LEU:HD12	13:A:787:HOH:O	1.93	0.66
3:C:149:LEU:O	3:C:153:VAL:HG23	1.94	0.66
1:A:551:ASP:OD1	1:A:551:ASP:N	2.27	0.66
3:C:227:LEU:HD12	3:C:250:ALA:HB1	1.78	0.65
1:A:334:LEU:CD2	2:B:101:PHE:HE1	2.07	0.65
1:A:180:ASP:OD2	3:C:36:LYS:CE	2.43	0.65
1:A:354:LYS:HD3	13:A:793:HOH:O	1.97	0.65
3:C:172:ILE:HG23	3:C:231:LEU:CD1	2.27	0.65
2:B:141:LYS:HG2	2:B:154:TYR:CD1	2.33	0.64
3:C:87:GLN:HA	3:C:90:PHE:CE2	2.33	0.64
1:A:98:MET:HB3	5:A:601:HEA:CAC	2.28	0.64
3:C:80:PRO:HB2	4:D:16:ILE:HD13	1.80	0.63
1:A:153:GLY:HA2	1:A:174:GLU:OE2	1.98	0.63
3:C:230:CYS:O	3:C:234:LEU:HD12	1.99	0.63
1:A:174:GLU:CD	1:A:175:ALA:O	2.36	0.62
3:C:216:HIS:CE1	3:C:261:TRP:HB2	2.34	0.62
3:C:144:ASN:OD1	3:C:185:PHE:HA	2.00	0.62
3:C:93:PHE:O	3:C:97:GLU:HG2	2.00	0.61
2:B:140:GLU:O	2:B:143:ALA:N	2.32	0.61
2:B:4:LEU:HD22	2:B:234:VAL:HG11	1.82	0.61
3:C:127:TRP:CZ2	3:C:205:TYR:HD2	2.18	0.60
1:A:408:VAL:HB	13:A:702:HOH:O	2.02	0.60
3:C:168:ARG:NH2	3:C:234:LEU:HA	2.17	0.60
1:A:543:PHE:CD1	1:A:547:PRO:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:THR:CG2	3:C:242:LYS:H	2.00	0.59
3:C:176:ILE:O	3:C:180:ILE:HD12	2.02	0.59
3:C:86:LEU:HD13	12:C:302:PC1:O22	2.01	0.59
12:C:301:PC1:H352	12:C:301:PC1:C25	2.27	0.59
2:B:166:VAL:HG22	2:B:234:VAL:O	2.02	0.59
1:A:277:PRO:HB3	13:A:791:HOH:O	2.03	0.58
1:A:238:LEU:HD13	13:A:787:HOH:O	1.97	0.58
3:C:127:TRP:CB	3:C:128:PRO:HD3	2.34	0.58
3:C:163:VAL:HG23	3:C:164:LEU:H	1.68	0.58
2:B:245:GLY:O	2:B:248:GLU:HG2	2.04	0.58
3:C:160:HIS:HA	3:C:163:VAL:CG2	2.34	0.58
3:C:228:PHE:O	3:C:232:ILE:HG12	2.03	0.58
1:A:276:HIS:CE1	1:A:280:TYR:HE2	2.20	0.57
3:C:159:HIS:O	3:C:163:VAL:HG22	2.04	0.57
2:B:138:MET:HG3	2:B:228:PRO:CD	2.34	0.57
3:C:115:PRO:HD2	3:C:124:ASP:HB3	1.86	0.57
1:A:282:ILE:HD12	13:A:796:HOH:O	2.05	0.56
3:C:134:THR:HG22	3:C:205:TYR:CZ	2.40	0.56
2:B:130:ASP:O	2:B:132:VAL:HG23	2.05	0.56
3:C:115:PRO:HG3	3:C:127:TRP:HA	1.87	0.56
3:C:175:LEU:HD21	3:C:247:PHE:CE1	2.41	0.56
1:A:473:ARG:CD	13:A:702:HOH:O	2.54	0.56
3:C:45:VAL:HG11	3:C:50:MET:CE	2.36	0.56
3:C:164:LEU:HD12	3:C:165:GLU:OE2	2.06	0.56
1:A:515:LYS:O	1:A:515:LYS:HG3	2.05	0.55
2:B:126:GLU:O	2:B:128:PRO:HD3	2.05	0.55
3:C:115:PRO:CG	3:C:127:TRP:HA	2.37	0.55
3:C:160:HIS:HA	3:C:163:VAL:HG22	1.89	0.55
2:B:139:LEU:HD22	2:B:143:ALA:HB1	1.89	0.55
1:A:334:LEU:CG	2:B:101:PHE:CE1	2.90	0.55
1:A:27:ASN:HD21	1:A:29:LYS:HB2	1.72	0.55
2:B:86:VAL:O	2:B:90:VAL:HG23	2.05	0.55
1:A:516:ARG:NH2	1:A:518:ASN:OD1	2.40	0.55
1:A:276:HIS:CD2	1:A:276:HIS:C	2.81	0.55
2:B:111:ASP:HB2	2:B:169:LYS:O	2.07	0.54
1:A:276:HIS:CE1	1:A:280:TYR:CE2	2.94	0.54
1:A:247:MET:HE3	1:A:251:PHE:HB2	1.88	0.54
1:A:358:TRP:HZ3	13:A:797:HOH:O	1.90	0.54
1:A:418:LEU:C	13:A:703:HOH:O	2.45	0.54
3:C:58:VAL:HG12	3:C:62:MET:HE2	1.90	0.54
3:C:45:VAL:CG1	3:C:50:MET:HE3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:ILE:HG22	3:C:176:ILE:HD11	1.90	0.54
1:A:231:ILE:HG13	1:A:281:ILE:HG12	1.89	0.54
4:D:36:LEU:O	4:D:40:VAL:HG23	2.08	0.54
1:A:200:ILE:HG21	1:A:224:VAL:HG12	1.90	0.53
1:A:216:LYS:HE3	1:A:549:ARG:HH21	1.72	0.53
1:A:341:MET:CE	2:B:100:LEU:HD22	2.34	0.53
3:C:222:ILE:HD13	12:C:302:PC1:H3C2	1.89	0.53
3:C:40:PHE:O	3:C:41:PHE:HB2	2.08	0.53
1:A:276:HIS:O	1:A:279:VAL:HG22	2.08	0.53
3:C:137:PRO:HD3	3:C:273:ARG:HD3	1.91	0.53
1:A:471:MET:HB2	1:A:482:PHE:CE1	2.44	0.53
13:A:794:HOH:O	2:B:89:LEU:HD22	2.09	0.53
3:C:139:HIS:O	3:C:142:LEU:N	2.42	0.52
2:B:220:CYS:SG	2:B:224:HIS:HA	2.49	0.52
1:A:253:THR:HA	13:C:404:HOH:O	2.08	0.52
1:A:422:PHE:HD1	13:A:703:HOH:O	1.94	0.51
2:B:101:PHE:O	2:B:105:GLU:HG3	2.11	0.51
3:C:135:PHE:HZ	3:C:196:ALA:CB	2.24	0.51
3:C:200:LEU:O	3:C:201:ALA:HB3	2.09	0.51
3:C:136:ASP:OD1	3:C:136:ASP:C	2.49	0.51
5:A:602:HEA:C13	13:A:729:HOH:O	2.44	0.51
2:B:121:TRP:HA	2:B:227:MET:SD	2.50	0.50
1:A:359:ILE:HA	1:A:362:MET:HE2	1.93	0.50
1:A:549:ARG:HG2	1:A:553:ASP:HB3	1.93	0.50
1:A:417:SER:O	1:A:421:VAL:HB	2.11	0.50
1:A:500:PHE:HB2	5:A:601:HEA:H261	1.92	0.50
2:B:57:ILE:O	2:B:61:ASN:ND2	2.32	0.50
1:A:334:LEU:HD11	2:B:101:PHE:CD1	2.46	0.50
1:A:67:LEU:HA	1:A:83:ASN:HB2	1.94	0.50
2:B:9:VAL:CG1	2:B:12:LYS:HE2	2.41	0.50
1:A:247:MET:HE3	1:A:251:PHE:CD2	2.46	0.50
3:C:81:VAL:HG22	13:C:407:HOH:O	2.12	0.49
1:A:549:ARG:HG3	1:A:552:TRP:CZ2	2.47	0.49
2:B:9:VAL:HG11	2:B:12:LYS:HE2	1.93	0.49
2:B:201:GLN:HB2	13:B:414:HOH:O	2.13	0.49
2:B:211:VAL:HG22	2:B:232:LYS:HG2	1.95	0.49
3:C:168:ARG:NH2	3:C:237:GLY:HA2	2.28	0.49
1:A:401:VAL:HA	13:A:790:HOH:O	2.13	0.49
1:A:306:LEU:HB3	1:A:307:PRO:HD3	1.95	0.49
3:C:144:ASN:HD21	3:C:188:LEU:HB3	1.77	0.49
3:C:33:ALA:HA	3:C:38:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:TYR:CD1	12:C:301:PC1:C13	2.90	0.48
1:A:473:ARG:NH1	13:A:702:HOH:O	2.36	0.48
1:A:415:VAL:HG11	13:A:795:HOH:O	2.13	0.48
3:C:172:ILE:O	3:C:176:ILE:HG13	2.13	0.48
1:A:27:ASN:HA	13:A:713:HOH:O	2.14	0.48
1:A:87:TRP:HB2	1:A:476:ILE:HG13	1.95	0.48
2:B:26:PRO:HB3	2:B:102:ARG:HH12	1.77	0.48
2:B:112:LEU:HD12	2:B:113:VAL:H	1.78	0.48
3:C:135:PHE:HZ	3:C:196:ALA:HB2	1.79	0.48
2:B:121:TRP:CD1	2:B:223:ASN:HB2	2.49	0.47
3:C:189:GLN:OE1	3:C:189:GLN:HA	2.14	0.47
1:A:545:THR:HA	3:C:5:ASN:HB3	1.96	0.47
1:A:92:THR:O	1:A:96:VAL:HG23	2.15	0.47
1:A:258:PRO:HG2	2:B:196:PRO:HB2	1.95	0.47
3:C:193:TYR:OH	3:C:213:THR:OG1	2.13	0.47
1:A:481:GLU:OE2	2:B:12:LYS:HD3	2.14	0.47
2:B:150:SER:N	2:B:153:GLU:OE2	2.32	0.47
3:C:172:ILE:CD1	3:C:235:LEU:HG	2.39	0.47
3:C:176:ILE:HG22	3:C:180:ILE:CD1	2.43	0.47
12:C:301:PC1:H292	4:D:41:LEU:HD11	1.97	0.47
2:B:119:HIS:O	2:B:121:TRP:N	2.48	0.47
1:A:549:ARG:HG3	1:A:552:TRP:CH2	2.50	0.47
2:B:238:LYS:HB3	2:B:238:LYS:HZ2	1.80	0.47
2:B:87:LEU:HD23	2:B:87:LEU:N	2.29	0.46
3:C:127:TRP:CE3	3:C:127:TRP:O	2.68	0.46
3:C:244:HIS:CD2	3:C:248:GLU:HG2	2.49	0.46
1:A:247:MET:HE2	3:C:211:MET:HE3	1.96	0.46
2:B:75:THR:N	2:B:76:PRO:CD	2.77	0.46
3:C:81:VAL:HG13	4:D:16:ILE:HG22	1.94	0.46
1:A:247:MET:HE2	3:C:211:MET:CE	2.46	0.46
3:C:129:PRO:HB2	3:C:203:THR:HG21	1.97	0.46
1:A:525:GLU:HG2	1:A:526:HIS:N	2.31	0.46
5:A:601:HEA:HBC2	13:A:798:HOH:O	2.15	0.46
1:A:107:LEU:HD12	13:A:782:HOH:O	2.15	0.46
5:A:601:HEA:C4C	13:A:773:HOH:O	2.64	0.46
5:A:602:HEA:H241	13:B:440:HOH:O	2.14	0.46
2:B:27:LEU:HD22	13:B:429:HOH:O	2.16	0.46
2:B:150:SER:OG	2:B:153:GLU:OE2	2.34	0.46
2:B:174:VAL:CG1	2:B:194:ALA:HB2	2.46	0.46
1:A:341:MET:HE2	1:A:341:MET:HB2	1.75	0.46
2:B:138:MET:HG3	2:B:228:PRO:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:MET:HE2	1:A:362:MET:HB2	1.84	0.45
3:C:66:TRP:CG	12:C:302:PC1:H332	2.51	0.45
4:D:45:ALA:O	4:D:49:SER:OG	2.34	0.45
2:B:9:VAL:HG13	2:B:213:PHE:HE2	1.81	0.45
1:A:441:PRO:HG3	1:A:509:TYR:CE1	2.51	0.45
3:C:172:ILE:HG23	3:C:231:LEU:HD13	1.98	0.45
3:C:18:PHE:CZ	3:C:22:ILE:HD11	2.51	0.45
3:C:132:ILE:HD13	3:C:132:ILE:HA	1.86	0.45
1:A:284:LEU:HD22	13:A:789:HOH:O	2.16	0.45
1:A:474:ARG:O	2:B:224:HIS:HD2	1.99	0.45
2:B:113:VAL:O	2:B:128:PRO:HD2	2.16	0.45
1:A:469:GLN:NE2	2:B:19:ASN:O	2.33	0.45
1:A:516:ARG:HH12	1:A:518:ASN:HA	1.81	0.45
13:A:794:HOH:O	2:B:89:LEU:CD2	2.64	0.45
3:C:34:TRP:CE2	3:C:48:PRO:HB3	2.51	0.45
3:C:201:ALA:HA	13:C:404:HOH:O	2.16	0.45
1:A:244:MET:HG2	3:C:104:TRP:CZ3	2.52	0.45
4:D:16:ILE:HG13	4:D:20:GLN:OE1	2.17	0.45
3:C:168:ARG:HH21	3:C:234:LEU:HA	1.82	0.45
3:C:230:CYS:SG	3:C:247:PHE:HA	2.56	0.45
3:C:231:LEU:HD12	3:C:231:LEU:O	2.17	0.45
4:D:46:LEU:N	4:D:46:LEU:HD12	2.32	0.44
1:A:287:PHE:CE2	13:A:793:HOH:O	2.57	0.44
1:A:300:LYS:HB3	1:A:300:LYS:HE2	1.53	0.44
2:B:176:ALA:O	2:B:196:PRO:HA	2.16	0.44
1:A:406:TYR:O	1:A:409:VAL:HB	2.17	0.44
3:C:163:VAL:HG23	3:C:164:LEU:N	2.30	0.44
3:C:70:VAL:HG22	12:C:302:PC1:H32	2.00	0.44
5:A:602:HEA:HAC	13:A:796:HOH:O	2.17	0.44
2:B:51:LEU:HD23	2:B:51:LEU:HA	1.84	0.44
1:A:416:MET:SD	5:A:602:HEA:HAC	2.58	0.44
1:A:517:VAL:HG23	1:A:517:VAL:O	2.18	0.44
3:C:81:VAL:CG1	4:D:16:ILE:HG22	2.47	0.44
3:C:141:PRO:O	3:C:145:THR:OG1	2.26	0.44
5:A:601:HEA:HMC1	5:A:601:HEA:CBC	2.47	0.44
2:B:125:TYR:O	2:B:133:ALA:HA	2.18	0.44
3:C:266:VAL:HG23	3:C:267:VAL:HG23	2.00	0.44
1:A:433:GLY:HA2	1:A:438:ARG:O	2.18	0.43
3:C:135:PHE:CZ	3:C:196:ALA:HA	2.53	0.43
2:B:235:SER:OG	2:B:238:LYS:HG3	2.18	0.43
3:C:137:PRO:HG2	3:C:138:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:HD2	13:A:702:HOH:O	2.17	0.43
3:C:80:PRO:HD2	13:C:407:HOH:O	2.18	0.43
1:A:543:PHE:CE1	1:A:547:PRO:HG3	2.53	0.43
2:B:131:GLY:O	2:B:251:ALA:HA	2.18	0.43
3:C:113:LEU:HD13	3:C:271:TRP:CH2	2.53	0.43
1:A:67:LEU:CA	1:A:83:ASN:HB2	2.49	0.43
1:A:130:LEU:HD11	1:A:195:LEU:HD22	2.00	0.43
2:B:115:LYS:HG2	2:B:117:ILE:HD11	2.00	0.43
1:A:96:VAL:HG22	8:A:609:OXY:O1	2.18	0.43
4:D:41:LEU:HA	4:D:41:LEU:HD23	1.67	0.43
1:A:334:LEU:HG	2:B:101:PHE:CE1	2.54	0.43
1:A:549:ARG:HA	1:A:552:TRP:NE1	2.34	0.43
3:C:83:ARG:HD3	3:C:243:GLN:HG3	2.01	0.43
3:C:115:PRO:HG2	3:C:125:GLY:O	2.19	0.43
1:A:549:ARG:HA	1:A:552:TRP:CE2	2.54	0.42
12:C:302:PC1:H2I3	12:C:302:PC1:H3C1	2.00	0.42
2:B:121:TRP:CZ2	2:B:222:ILE:HG22	2.55	0.42
1:A:508:PHE:O	1:A:512:PHE:HD1	2.02	0.42
2:B:245:GLY:O	2:B:248:GLU:CG	2.65	0.42
4:D:45:ALA:CA	4:D:49:SER:OG	2.64	0.42
1:A:411:HIS:O	1:A:415:VAL:HG22	2.20	0.42
5:A:602:HEA:H122	13:A:795:HOH:O	2.19	0.42
1:A:280:TYR:HA	1:A:283:ILE:HG22	2.00	0.42
3:C:127:TRP:CB	3:C:128:PRO:CD	2.97	0.42
3:C:127:TRP:CD2	3:C:127:TRP:C	2.91	0.42
1:A:238:LEU:HB2	1:A:274:PHE:CG	2.54	0.42
3:C:175:LEU:HD21	3:C:247:PHE:HE1	1.82	0.42
1:A:96:VAL:HG11	8:A:606:OXY:O1	2.19	0.42
1:A:418:LEU:CA	13:A:703:HOH:O	2.68	0.42
1:A:528:ASP:OD1	1:A:528:ASP:N	2.48	0.42
1:A:165:VAL:HA	8:A:610:OXY:O1	2.19	0.42
1:A:407:TYR:HB2	1:A:467:GLY:HA3	2.02	0.42
2:B:54:LEU:HD13	2:B:54:LEU:HA	1.72	0.42
2:B:88:ILE:CG2	13:B:440:HOH:O	2.57	0.42
3:C:262:LEU:O	3:C:266:VAL:HG13	2.19	0.42
1:A:409:VAL:HG13	1:A:413:HIS:CE1	2.55	0.41
3:C:239:MET:HA	12:C:302:PC1:H142	2.01	0.41
1:A:399:ASP:OD2	1:A:403:HIS:HB2	2.21	0.41
2:B:41:ILE:HG21	2:B:88:ILE:HG23	2.02	0.41
3:C:175:LEU:CD1	3:C:234:LEU:HD13	2.50	0.41
1:A:100:PHE:CE2	8:A:609:OXY:O2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:TRP:CD2	2:B:223:ASN:HB2	2.53	0.41
3:C:243:GLN:O	12:C:302:PC1:H143	2.20	0.41
3:C:39:THR:HG23	3:C:42:GLY:C	2.40	0.41
5:A:601:HEA:HBC1	5:A:601:HEA:CMC	2.49	0.41
1:A:153:GLY:HA3	1:A:159:GLY:O	2.21	0.41
2:B:243:LEU:O	2:B:244:ALA:C	2.57	0.41
3:C:62:MET:HB3	3:C:66:TRP:CZ3	2.56	0.41
3:C:137:PRO:HB3	3:C:269:TYR:HB3	2.01	0.41
1:A:282:ILE:HD13	13:A:798:HOH:O	2.21	0.41
2:B:140:GLU:O	2:B:141:LYS:C	2.58	0.41
2:B:163:VAL:HG21	2:B:242:TRP:CE2	2.56	0.41
4:D:46:LEU:N	4:D:46:LEU:CD1	2.84	0.41
1:A:98:MET:HB3	5:A:601:HEA:HAC	2.00	0.41
1:A:276:HIS:HB3	1:A:277:PRO:HD3	2.02	0.41
1:A:322:VAL:HG12	1:A:343:ALA:HB1	2.02	0.41
1:A:536:SER:HA	1:A:537:PRO:HA	1.91	0.41
2:B:174:VAL:HG12	2:B:194:ALA:HB2	2.03	0.41
2:B:107:PRO:HD3	2:B:203:TRP:CG	2.56	0.41
1:A:230:LEU:CB	13:A:791:HOH:O	2.61	0.40
1:A:409:VAL:HA	1:A:412:PHE:CE2	2.56	0.40
1:A:473:ARG:HD3	13:A:702:HOH:O	2.20	0.40
1:A:516:ARG:NH1	1:A:518:ASN:HA	2.36	0.40
1:A:520:PRO:HA	1:A:534:LEU:O	2.22	0.40
1:A:471:MET:HB2	1:A:482:PHE:CD1	2.56	0.40
1:A:549:ARG:HG2	1:A:553:ASP:CB	2.51	0.40
2:B:38:VAL:O	2:B:42:ILE:HG12	2.21	0.40
5:A:602:HEA:HMB1	5:A:602:HEA:H11	1.85	0.40
3:C:142:LEU:HD12	3:C:142:LEU:HA	1.78	0.40
2:B:127:TYR:HB2	2:B:132:VAL:HB	2.03	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%)	518 (97%)	17 (3%)	0	100	100
2	B	246/298 (83%)	237 (96%)	9 (4%)	0	100	100
3	C	267/274 (97%)	256 (96%)	11 (4%)	0	100	100
4	D	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
All	All	1084/1180 (92%)	1046 (96%)	38 (4%)	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%)	435 (99%)	5 (1%)	73	87
2	B	208/243 (86%)	206 (99%)	2 (1%)	76	88
3	C	217/221 (98%)	211 (97%)	6 (3%)	43	63
4	D	29/40 (72%)	29 (100%)	0	100	100
All	All	894/958 (93%)	881 (98%)	13 (2%)	66	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	79	GLU
1	A	274	PHE
1	A	291	SER
1	A	551	ASP
2	B	81	TRP
2	B	121	TRP
3	C	40	PHE
3	C	81	VAL
3	C	120	SER
3	C	151	SER
3	C	155	VAL
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 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	$\# Z  > 2$
8	OXY	A	605	-	1,1,1	0.26	0	-		
9	PEO	A	611	6,5	1,1,1	0.03	0	-		
8	OXY	A	608	-	1,1,1	0.41	0	-		
11	CUA	B	301	2	0,1,1	-	-	-		
8	OXY	A	607	-	1,1,1	0.28	0	-		
8	OXY	A	610	-	1,1,1	0.22	0	-		
5	HEA	A	601	1	57,67,67	1.90	13 (22%)	61,103,103	2.95	28 (45%)
12	PC1	C	302	-	53,53,53	0.37	0	59,61,61	0.62	2 (3%)
5	HEA	A	602	9,1	57,67,67	1.67	9 (15%)	61,103,103	2.63	22 (36%)
8	OXY	A	606	-	1,1,1	0.25	0	-		
12	PC1	C	301	-	40,40,53	1.27	3 (7%)	46,48,61	3.01	17 (36%)
8	OXY	A	609	-	1,1,1	0.26	0	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEA	A	601	1	3/3/7/16	10/32/76/76	-
12	PC1	C	301	-	-	20/44/44/57	-
5	HEA	A	602	9,1	3/3/7/16	10/32/76/76	-
12	PC1	C	302	-	-	20/57/57/57	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEA	C3A-C2A	-4.98	1.33	1.40
5	A	601	HEA	C1B-NB	-4.85	1.28	1.38
5	A	602	HEA	C1D-ND	-4.83	1.32	1.40
5	A	601	HEA	C4B-NB	-4.65	1.32	1.40
5	A	601	HEA	C3C-C2C	-4.59	1.34	1.40
5	A	602	HEA	C3C-C2C	-4.50	1.34	1.40
5	A	601	HEA	FE-NB	4.25	2.17	1.96
5	A	602	HEA	C3A-C2A	-4.21	1.34	1.40
12	C	301	PC1	O31-C31	4.20	1.45	1.33
12	C	301	PC1	O21-C2	-4.15	1.36	1.46
5	A	602	HEA	FE-NB	4.02	2.16	1.96
5	A	602	HEA	C4D-ND	-3.83	1.30	1.38
5	A	601	HEA	C4D-ND	-3.82	1.30	1.38
5	A	601	HEA	FE-ND	3.56	2.14	1.96
5	A	602	HEA	FE-ND	2.99	2.11	1.96
5	A	601	HEA	C4C-CHD	-2.76	1.33	1.41
5	A	602	HEA	C3C-CAC	2.72	1.53	1.47
5	A	601	HEA	C1D-ND	-2.65	1.35	1.40
5	A	602	HEA	C4B-NB	-2.61	1.35	1.40
5	A	601	HEA	C1B-C2B	-2.53	1.39	1.44
5	A	601	HEA	C3C-CAC	2.32	1.52	1.47
12	C	301	PC1	O22-C21	-2.25	1.15	1.22
5	A	602	HEA	O2A-CGA	-2.20	1.23	1.30
5	A	601	HEA	O2D-CGD	-2.05	1.23	1.30
5	A	601	HEA	C3D-C2D	-2.05	1.32	1.36

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEA	C4B-NB-C1B	10.37	115.78	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEA	C4A-CHB-C1B	9.60	135.23	122.56
5	A	602	HEA	C4D-CHA-C1A	9.01	134.45	122.56
12	C	301	PC1	C15-N-C13	-8.65	86.73	108.97
12	C	301	PC1	O21-C2-C1	-8.17	78.82	108.40
12	C	301	PC1	C15-N-C14	-7.73	89.09	108.97
5	A	602	HEA	C1D-ND-C4D	7.51	112.83	105.07
12	C	301	PC1	O21-C21-C22	6.68	125.89	111.50
5	A	601	HEA	C3B-C4B-NB	-6.08	102.64	109.84
12	C	301	PC1	O21-C21-O22	-5.79	109.72	123.70
5	A	602	HEA	C4B-NB-C1B	5.78	111.05	105.07
5	A	602	HEA	CAD-CBD-CGD	-5.71	101.32	113.60
5	A	601	HEA	C4D-CHA-C1A	5.39	129.67	122.56
5	A	602	HEA	C4A-CHB-C1B	5.13	129.32	122.56
5	A	601	HEA	C3A-C4A-NA	-5.02	101.46	110.94
12	C	301	PC1	C14-N-C13	4.89	121.53	108.97
5	A	601	HEA	CMC-C2C-C1C	-4.48	121.58	128.46
5	A	602	HEA	CMC-C2C-C1C	-4.10	122.16	128.46
12	C	301	PC1	C34-C33-C32	-3.86	99.31	113.19
12	C	301	PC1	C3-O31-C31	3.64	130.60	117.12
5	A	602	HEA	C3D-C4D-ND	-3.62	106.85	110.36
5	A	602	HEA	CAA-CBA-CGA	-3.60	103.67	113.76
5	A	601	HEA	C24-C23-C22	-3.40	112.82	122.65
5	A	601	HEA	CHC-C4B-C3B	3.37	134.47	125.80
5	A	601	HEA	C1D-ND-C4D	3.36	108.55	105.07
5	A	601	HEA	C2B-C1B-NB	-3.36	105.86	109.88
5	A	601	HEA	O11-C11-C12	3.36	118.80	109.42
5	A	601	HEA	OMA-CMA-C3A	-3.21	117.91	124.91
5	A	602	HEA	C3B-C4B-NB	-3.14	106.12	109.84
5	A	601	HEA	CMC-C2C-C3C	3.12	130.52	124.68
5	A	601	HEA	C13-C12-C11	-3.11	109.68	114.35
5	A	601	HEA	CHB-C1B-C2B	3.10	129.82	124.98
5	A	602	HEA	C2D-C1D-ND	-3.07	106.20	109.84
5	A	601	HEA	CMB-C2B-C1B	-3.01	120.46	125.04
5	A	602	HEA	C24-C23-C22	-2.99	114.00	122.65
12	C	301	PC1	O21-C2-C3	2.96	119.13	108.40
5	A	601	HEA	C17-C16-C15	2.92	122.58	112.98
5	A	602	HEA	CBA-CAA-C2A	-2.89	107.73	112.60
5	A	601	HEA	C13-C14-C15	-2.86	120.77	127.66
5	A	602	HEA	C3A-C4A-NA	-2.86	105.55	110.94
12	C	301	PC1	C15-N-C12	-2.74	98.72	109.92
5	A	601	HEA	CAA-CBA-CGA	-2.67	106.28	113.76
5	A	602	HEA	O2A-CGA-O1A	-2.64	116.72	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEA	CMC-C2C-C3C	2.62	129.59	124.68
5	A	602	HEA	C2B-C1B-NB	-2.62	106.75	109.88
12	C	301	PC1	C11-C12-N	-2.61	107.06	115.78
5	A	601	HEA	C21-C22-C23	-2.58	118.92	127.75
5	A	601	HEA	C16-C17-C18	2.58	120.35	111.88
12	C	301	PC1	C36-C35-C34	-2.56	101.42	114.42
5	A	602	HEA	CHA-C4D-C3D	2.48	128.48	124.84
5	A	601	HEA	CHD-C1D-ND	2.45	127.41	124.38
12	C	301	PC1	C33-C32-C31	-2.43	104.78	113.62
12	C	302	PC1	O21-C21-C22	2.39	116.64	111.50
5	A	602	HEA	CAD-C3D-C4D	-2.35	120.56	124.66
12	C	302	PC1	O21-C21-O22	-2.34	118.04	123.70
5	A	601	HEA	CBA-CAA-C2A	2.34	116.55	112.60
5	A	602	HEA	C17-C18-C19	-2.34	122.02	127.66
12	C	301	PC1	C23-C22-C21	-2.30	105.25	113.62
12	C	301	PC1	C13-N-C12	2.28	119.25	109.92
5	A	601	HEA	O2D-CGD-O1D	-2.27	117.64	123.30
12	C	301	PC1	C14-N-C12	2.23	119.03	109.92
5	A	602	HEA	CAD-C3D-C2D	2.15	131.89	127.88
5	A	601	HEA	C26-C15-C14	-2.12	118.25	123.68
5	A	601	HEA	C12-C13-C14	2.09	117.76	112.23
5	A	601	HEA	CBD-CAD-C3D	-2.09	106.81	112.63
5	A	602	HEA	CMB-C2B-C3B	-2.08	126.37	130.34
5	A	601	HEA	O2A-CGA-CBA	2.05	120.61	114.03
12	C	301	PC1	C35-C34-C33	-2.02	104.15	114.42
5	A	602	HEA	CBD-CAD-C3D	2.02	118.24	112.63

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601	HEA	ND
5	A	601	HEA	NB
5	A	601	HEA	NA
5	A	602	HEA	ND
5	A	602	HEA	NB
5	A	602	HEA	NA

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	301	PC1	C1-O11-P-O14
12	C	301	PC1	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
12	C	301	PC1	O13-C11-C12-N
12	C	301	PC1	O22-C21-O21-C2
12	C	301	PC1	C22-C21-O21-C2
12	C	302	PC1	O13-C11-C12-N
12	C	302	PC1	O11-C1-C2-O21
12	C	302	PC1	O22-C21-O21-C2
12	C	302	PC1	C22-C21-O21-C2
12	C	302	PC1	O32-C31-O31-C3
12	C	302	PC1	C32-C31-O31-C3
5	A	601	HEA	C21-C22-C23-C24
12	C	301	PC1	C11-C12-N-C14
5	A	602	HEA	C2D-C3D-CAD-CBD
5	A	601	HEA	C15-C16-C17-C18
12	C	302	PC1	C11-O13-P-O11
12	C	301	PC1	C11-C12-N-C15
12	C	302	PC1	C35-C36-C37-C38
12	C	302	PC1	C24-C25-C26-C27
12	C	302	PC1	C25-C26-C27-C28
12	C	301	PC1	C23-C24-C25-C26
12	C	301	PC1	C32-C33-C34-C35
5	A	602	HEA	C4D-C3D-CAD-CBD
5	A	601	HEA	C26-C15-C16-C17
12	C	302	PC1	C28-C29-C2A-C2B
12	C	302	PC1	C36-C37-C38-C39
5	A	601	HEA	C17-C18-C19-C27
12	C	301	PC1	C22-C23-C24-C25
12	C	301	PC1	C2-C1-O11-P
5	A	602	HEA	C27-C19-C20-C21
12	C	302	PC1	C29-C2A-C2B-C2C
12	C	302	PC1	O11-C1-C2-C3
12	C	301	PC1	C26-C27-C28-C29
5	A	602	HEA	C21-C22-C23-C24
12	C	301	PC1	C24-C25-C26-C27
12	C	302	PC1	C23-C24-C25-C26
12	C	302	PC1	C34-C35-C36-C37
12	C	302	PC1	C11-O13-P-O14
12	C	301	PC1	C27-C28-C29-C2A
12	C	301	PC1	O21-C2-C3-O31
12	C	301	PC1	C38-C39-C3A-C3B
5	A	601	HEA	C21-C22-C23-C25
5	A	601	HEA	C14-C15-C16-C17
12	C	301	PC1	C11-O13-P-O11

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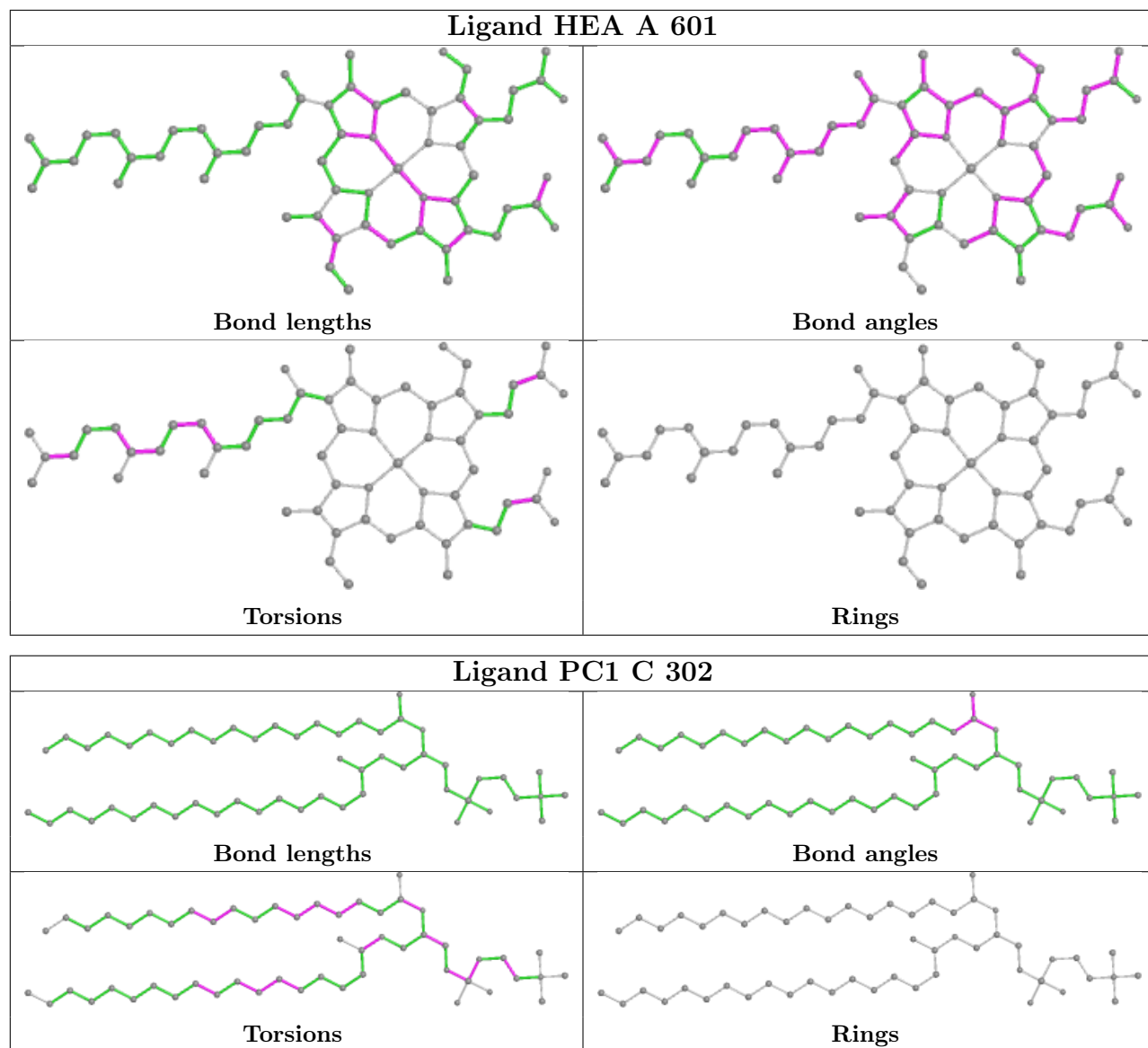
Mol	Chain	Res	Type	Atoms
12	C	301	PC1	C1-O11-P-O13
12	C	302	PC1	C1-O11-P-O13
5	A	602	HEA	CAD-CBD-CGD-O2D
12	C	302	PC1	C38-C39-C3A-C3B
12	C	301	PC1	C34-C35-C36-C37
5	A	601	HEA	CAA-CBA-CGA-O1A
5	A	602	HEA	C19-C20-C21-C22
12	C	301	PC1	C1-C2-O21-C21
5	A	602	HEA	CAD-CBD-CGD-O1D
12	C	302	PC1	C22-C23-C24-C25
5	A	602	HEA	CAA-CBA-CGA-O1A
5	A	601	HEA	C18-C19-C20-C21
5	A	602	HEA	CAA-CBA-CGA-O2A
5	A	602	HEA	C18-C19-C20-C21
5	A	601	HEA	CAD-CBD-CGD-O1D
5	A	601	HEA	CAA-CBA-CGA-O2A

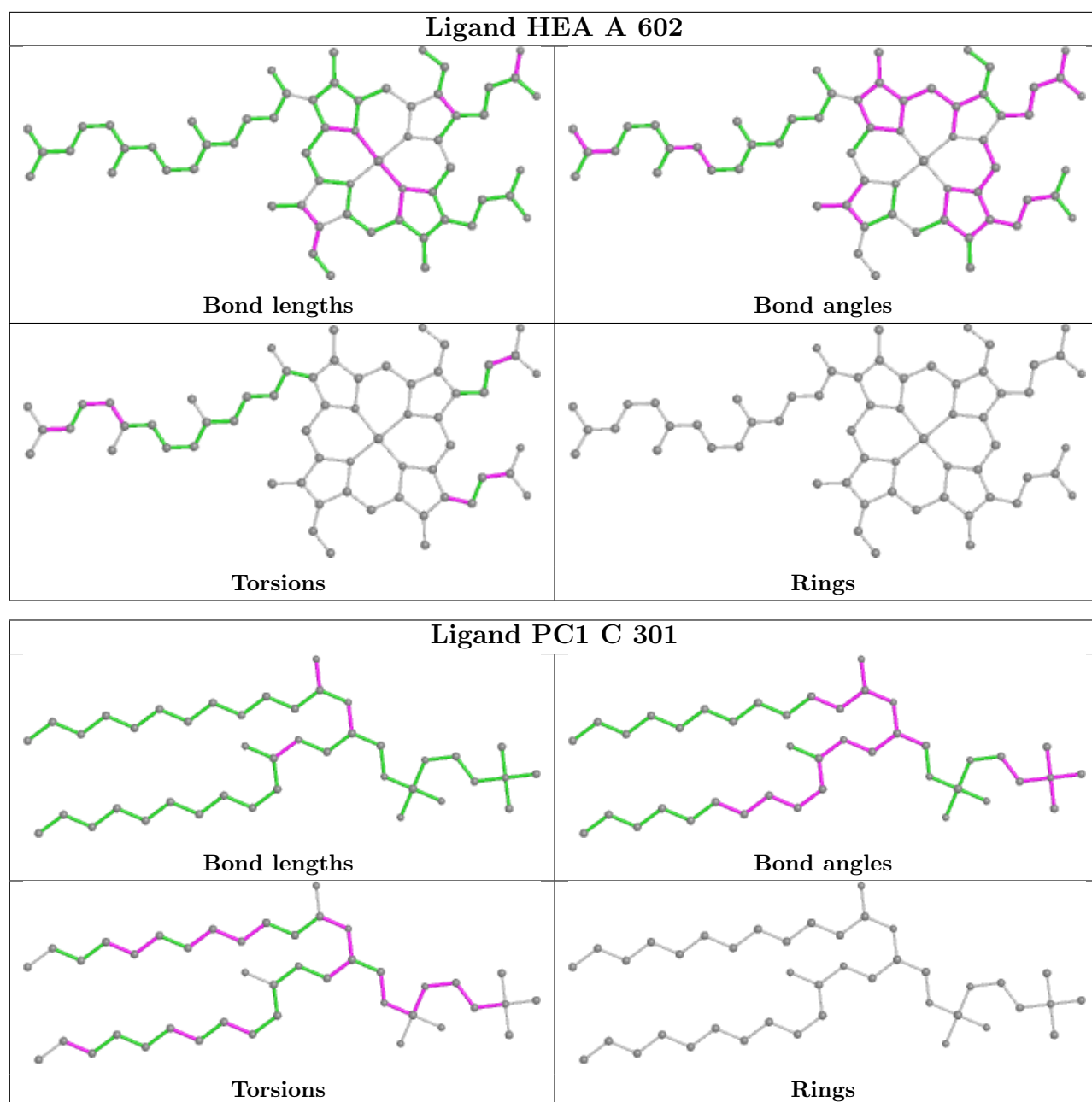
There are no ring outliers.

8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	605	OXY	1	0
8	A	610	OXY	1	0
5	A	601	HEA	8	0
12	C	302	PC1	7	0
5	A	602	HEA	9	0
8	A	606	OXY	1	0
12	C	301	PC1	6	0
8	A	609	OXY	2	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

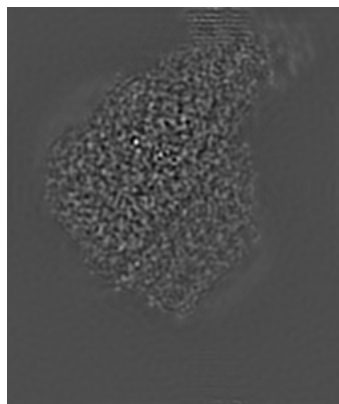
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11925. These allow visual inspection of the internal detail of the map and identification of artifacts.

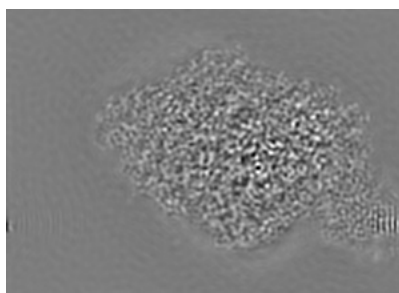
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

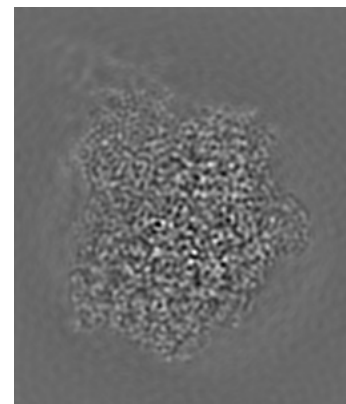
#### 6.1.1 Primary map



X

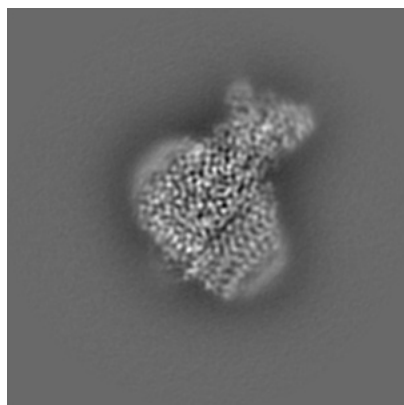


Y

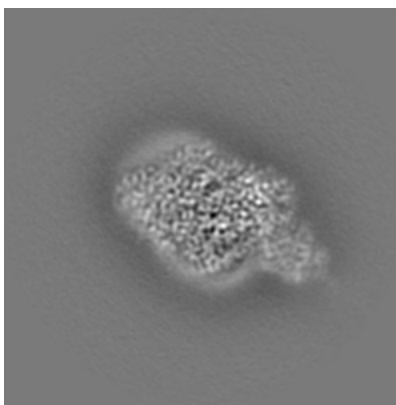


Z

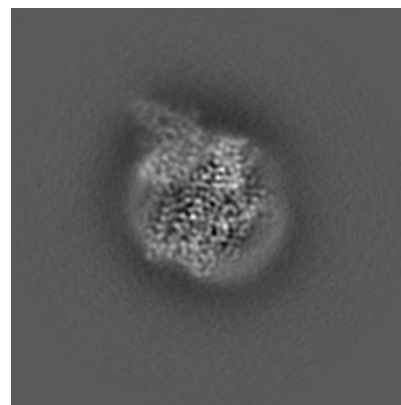
#### 6.1.2 Raw map



X



Y

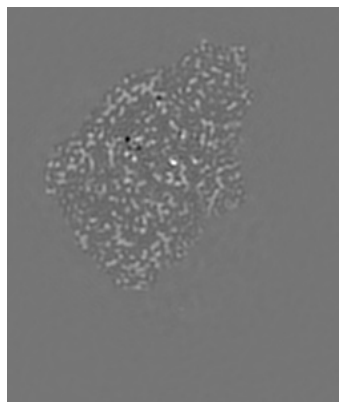


Z

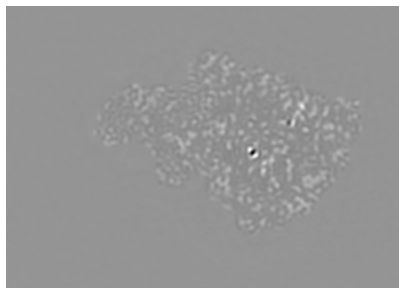
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

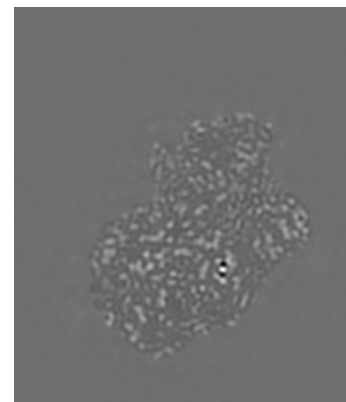
### 6.2.1 Primary map



X Index: 59

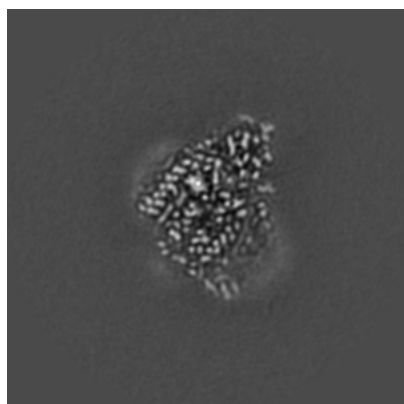


Y Index: 69

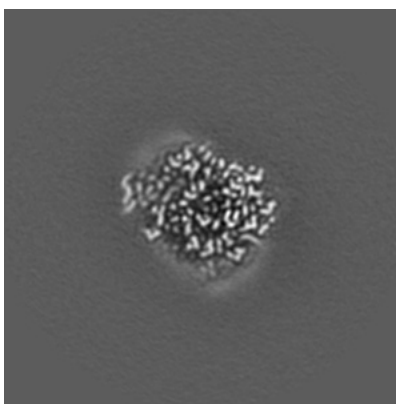


Z Index: 82

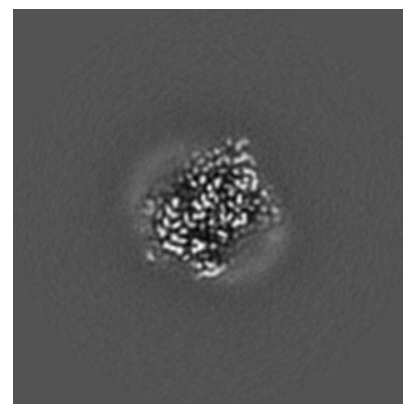
### 6.2.2 Raw map



X Index: 128



Y Index: 128



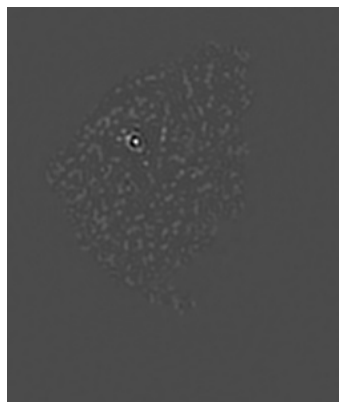
Z Index: 128

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

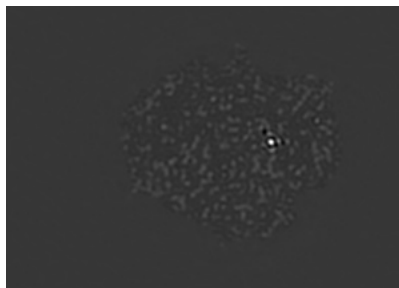


## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 61

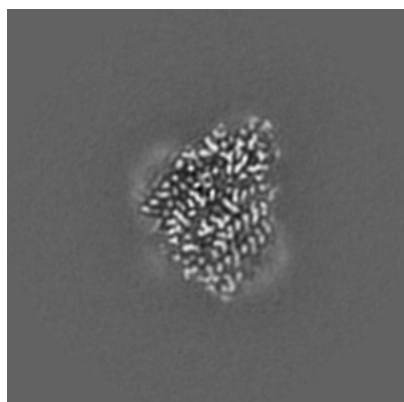


Y Index: 53

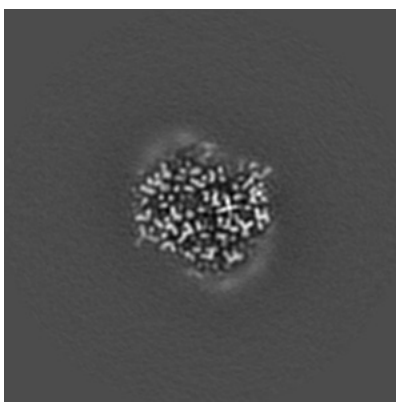


Z Index: 109

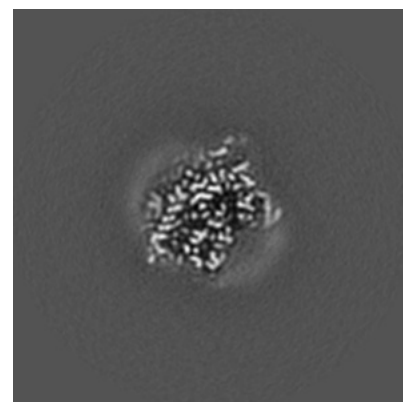
### 6.3.2 Raw map



X Index: 131



Y Index: 121

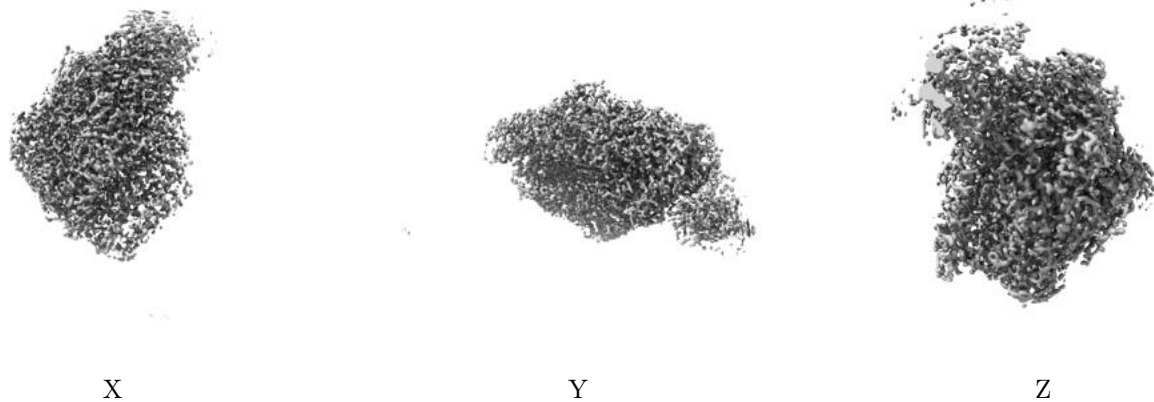


Z Index: 131

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

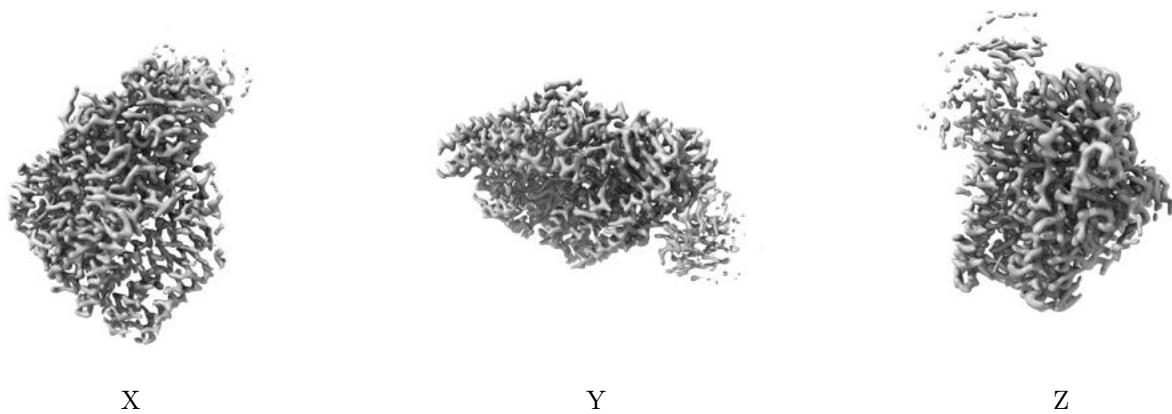
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.75. 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



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.

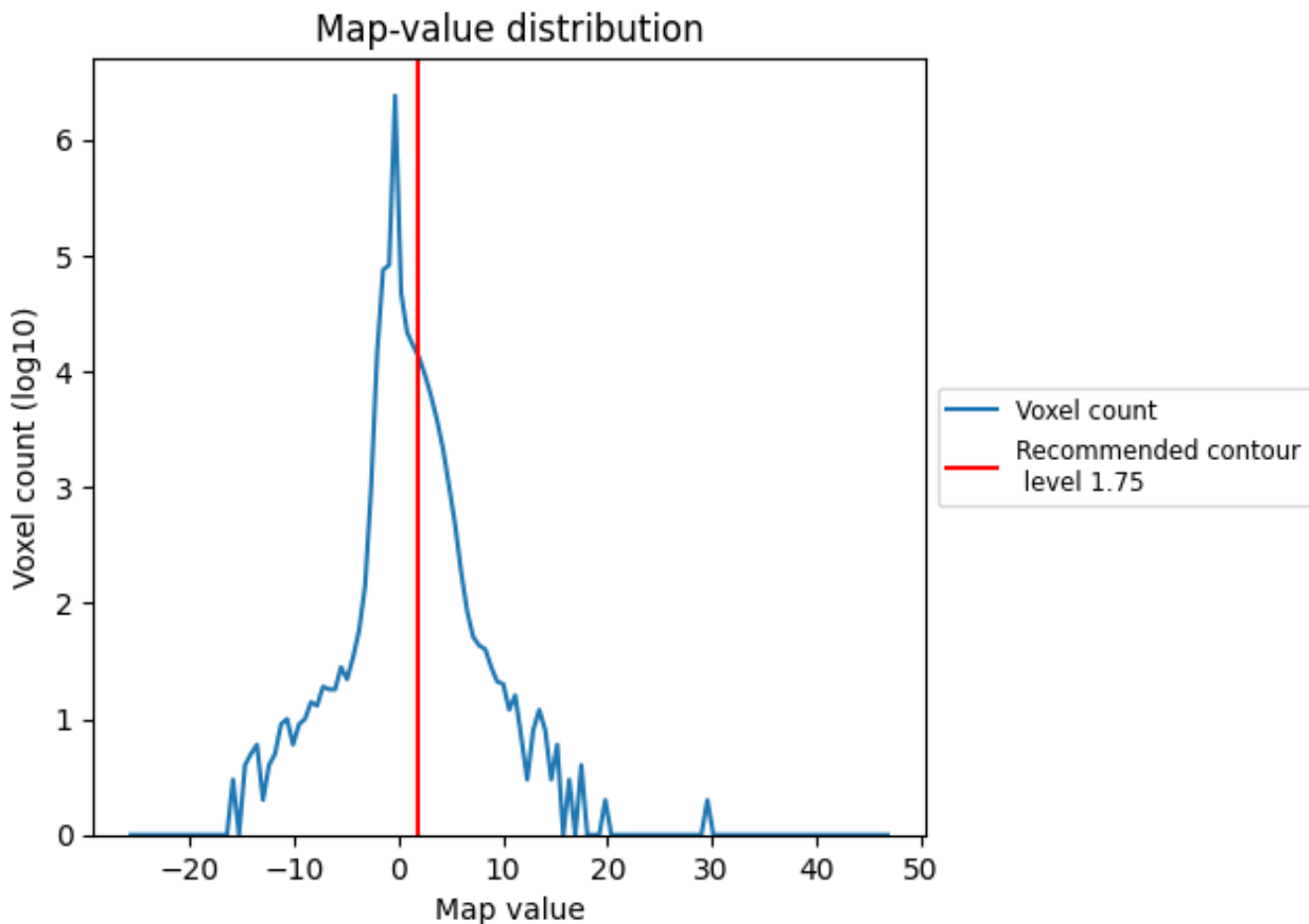
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

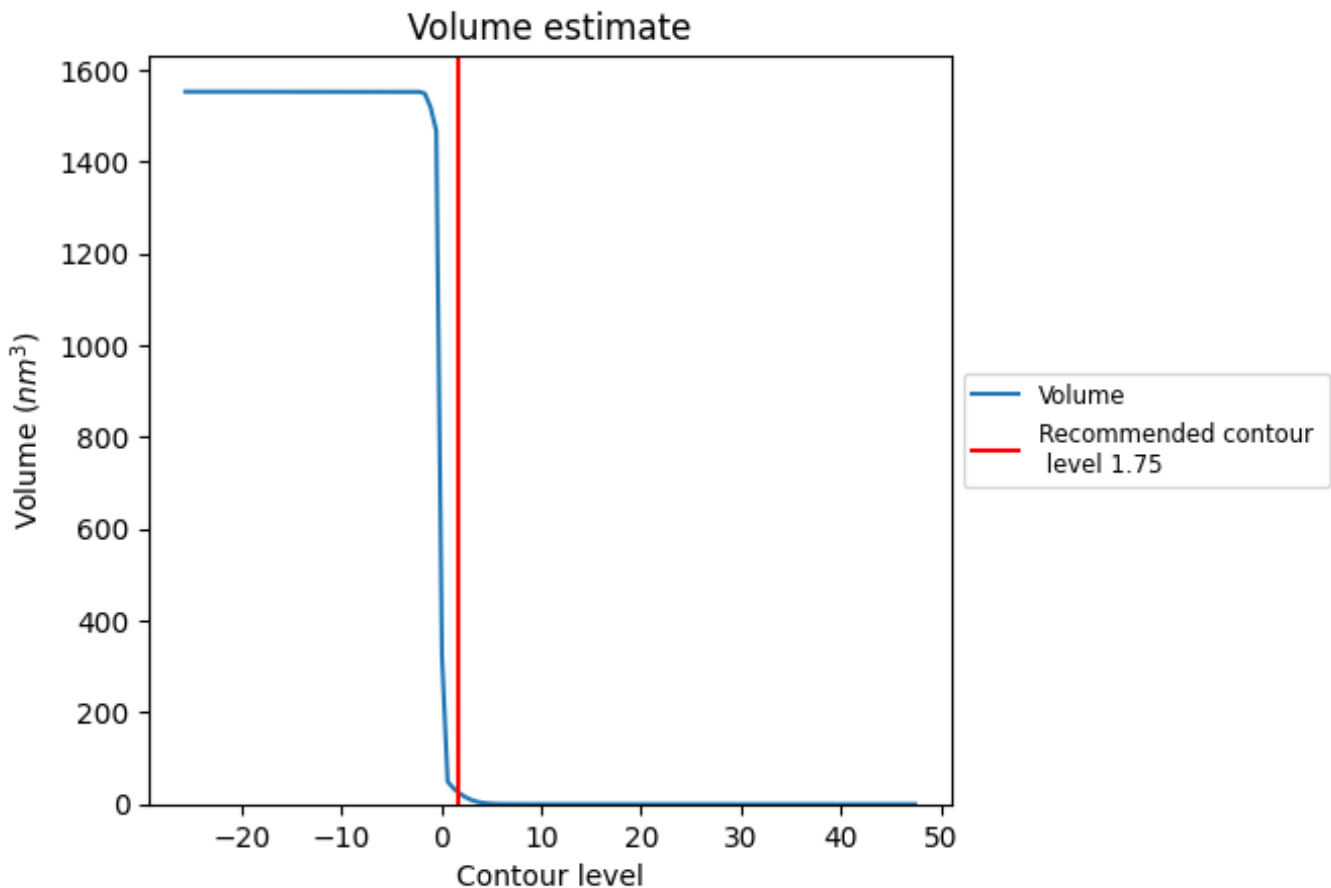
This section contains the results of statistical analysis of the map.

### 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 24 nm<sup>3</sup>; this corresponds to an approximate mass of 22 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.

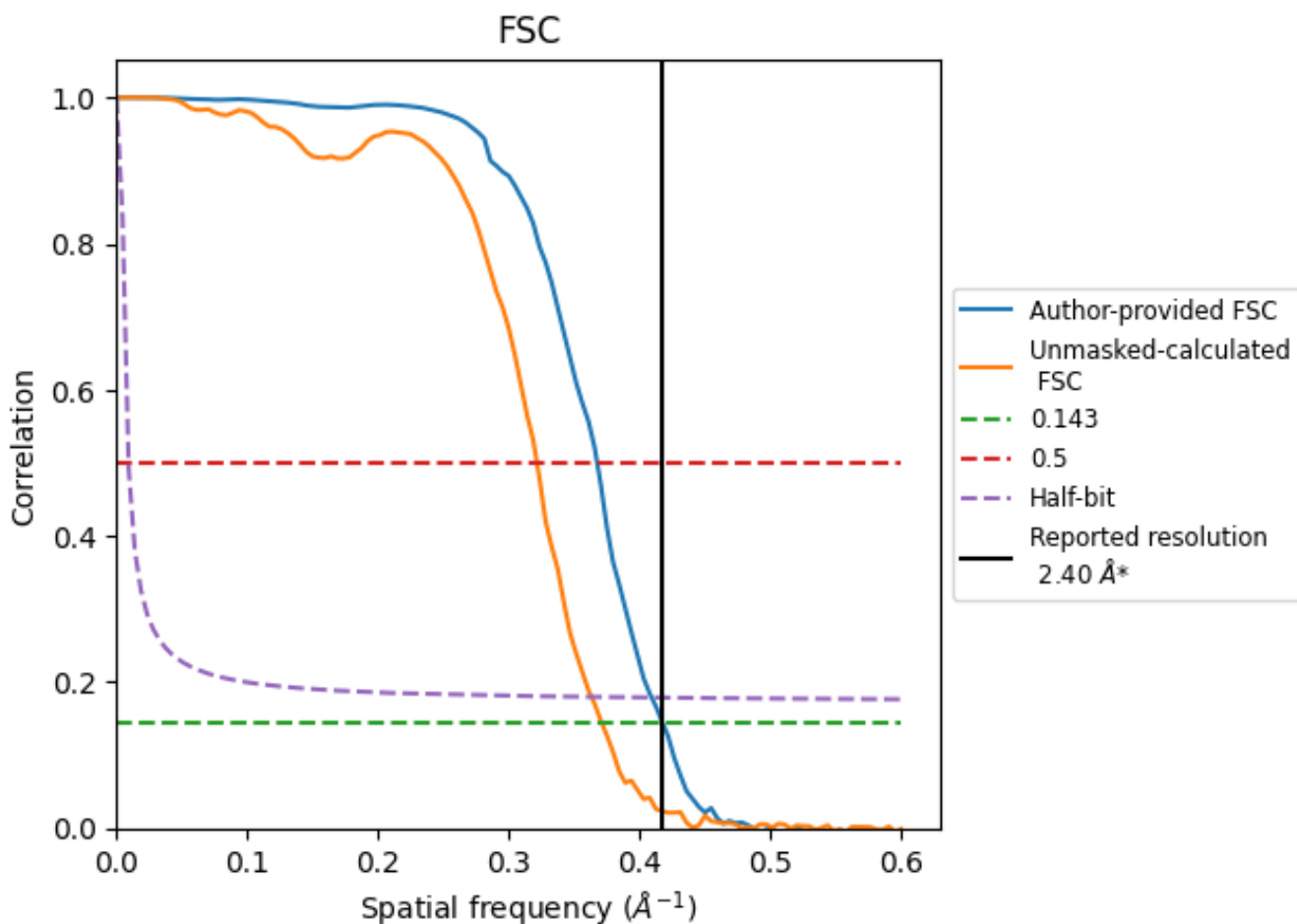
## 7.3 Rotationally averaged power spectrum [i](#)

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 0.417 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

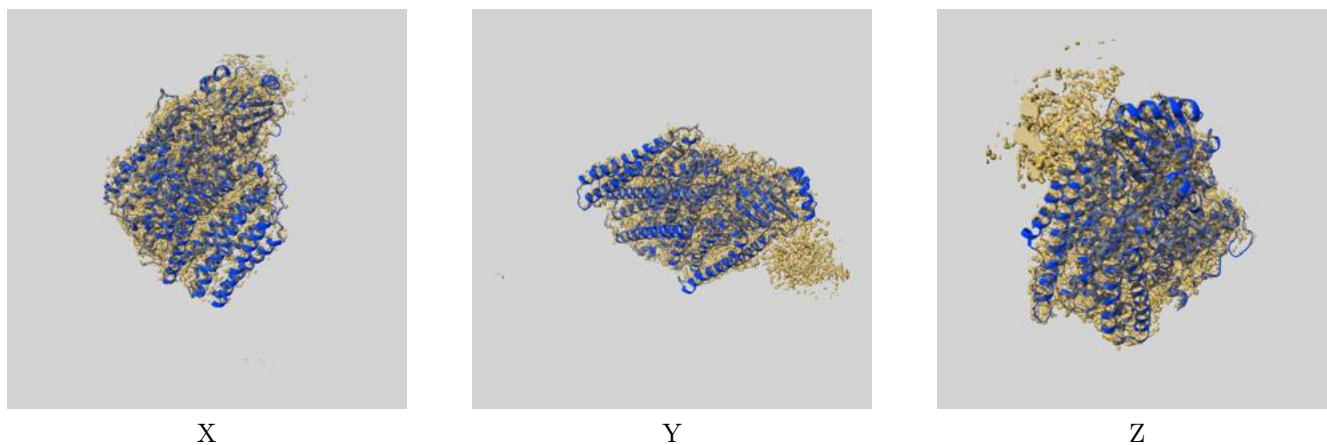
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.39	2.72	2.44
Unmasked-calculated*	2.69	3.11	2.75

\*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 [i](#)

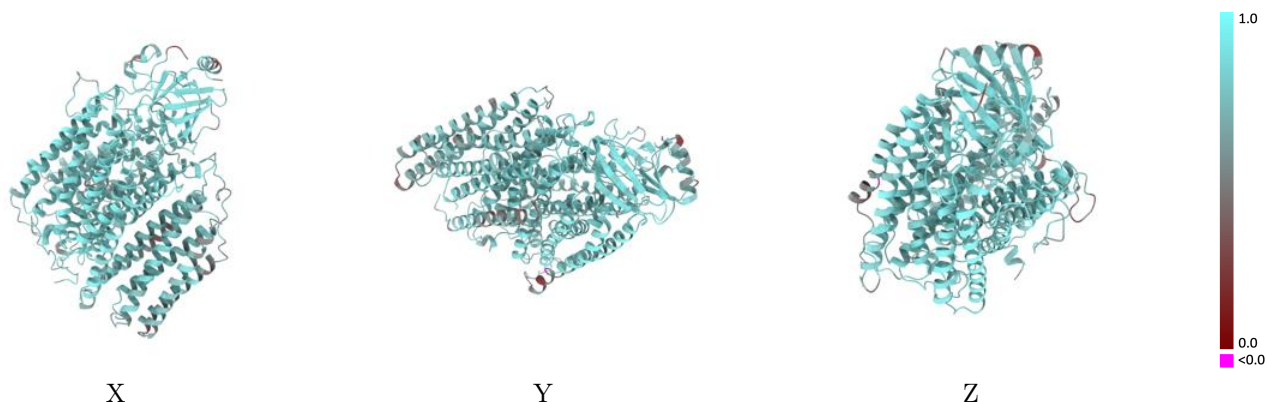
This section contains information regarding the fit between EMDB map EMD-11925 and PDB model 7AU6. Per-residue inclusion information can be found in section 3 on page 9.

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



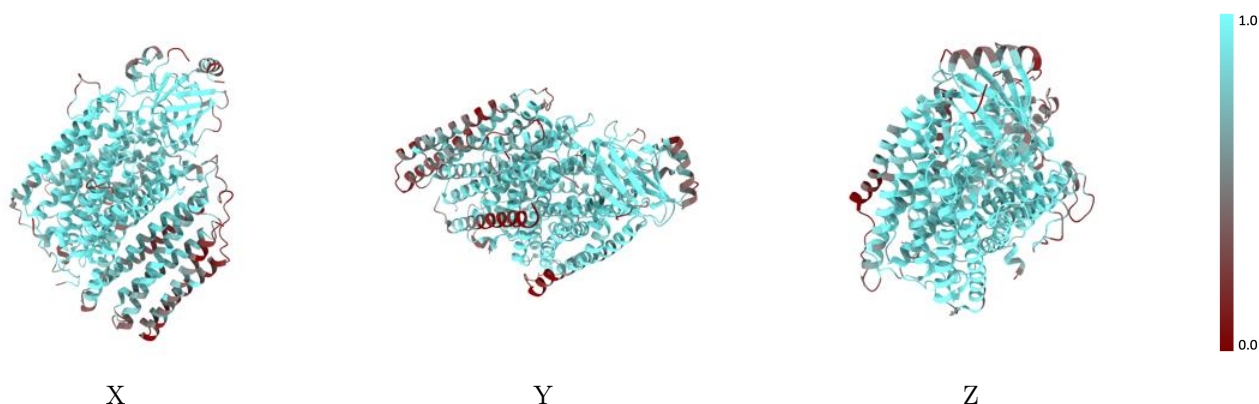
The images above show the 3D surface view of the map at the recommended contour level 1.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

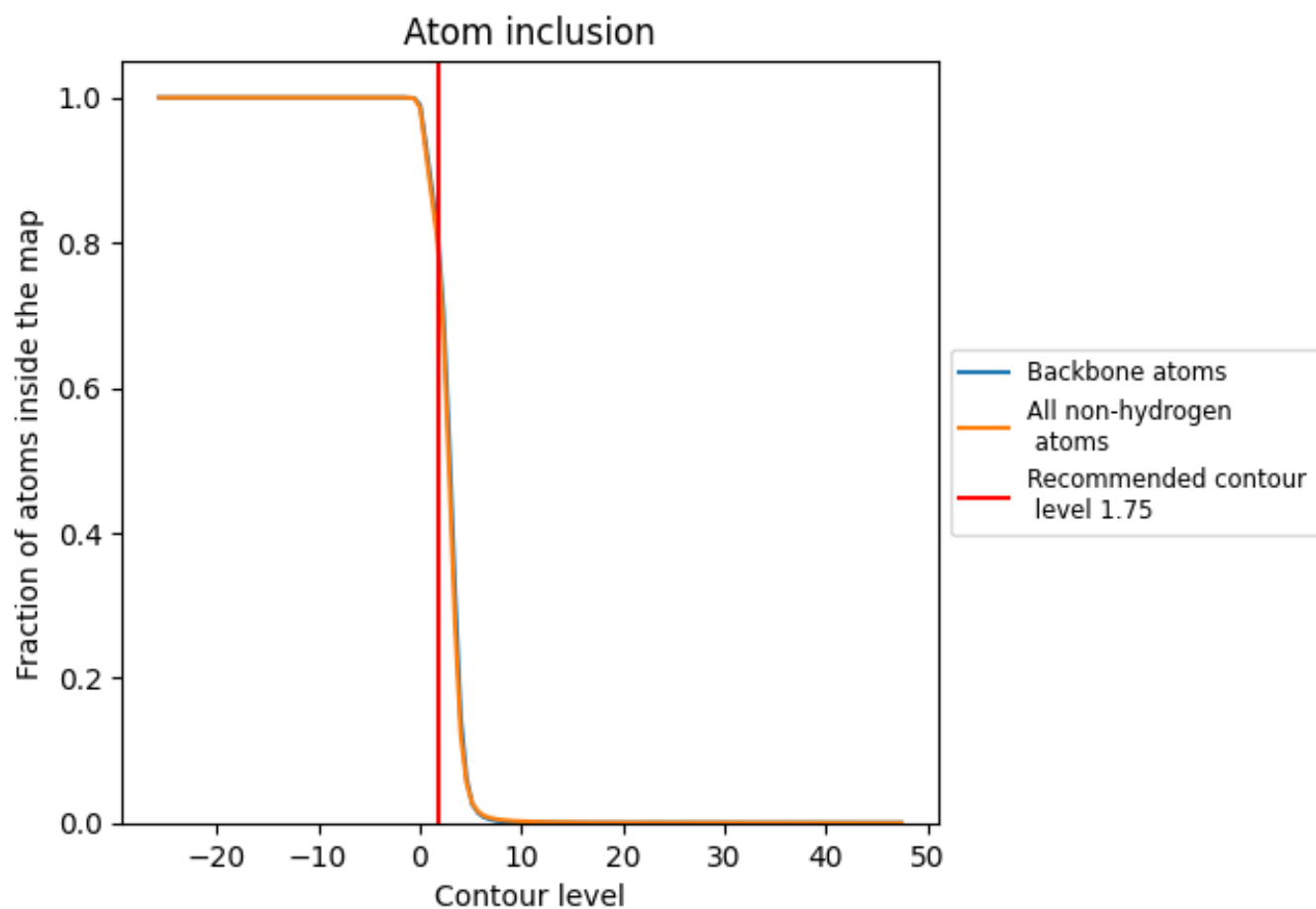
## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.75).













## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (1.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8028	 0.7510
A	 0.9293	 0.7950
B	 0.7678	 0.7360
C	 0.6477	 0.6980
D	 0.3684	 0.5980

