



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 09:36 AM JST

PDB ID : 5Z62 / pdb_00005z62
EMDB ID : EMD-6896
Title : Structure of human cytochrome c oxidase
Authors : Gu, J.; Zong, S.; Wu, M.; Yang, M.
Deposited on : 2018-01-22
Resolution : 3.60 Å(reported)

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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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

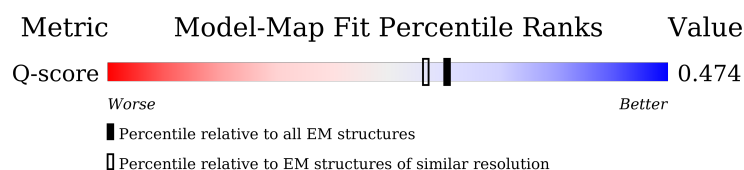
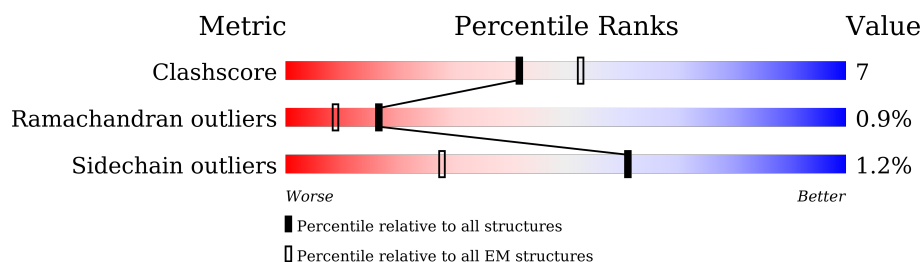
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	513	
2	B	227	
3	C	260	
4	D	144	

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Mol	Chain	Length	Quality of chain
5	E	109	
6	F	98	
7	G	75	
8	H	82	
9	I	73	
10	J	56	
11	K	49	
12	L	47	
13	M	43	
14	N	79	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	PEE	A	605	X	-	-	-
18	PEE	C	301	X	-	-	-
18	PEE	C	302	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 15037 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			4028	2699	622	674	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	227	Total	C	N	O	S	0	0
			1798	1180	279	326	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	260	Total	C	N	O	S	0	0
			2119	1417	339	352	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1189	768	201	213	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	109	Total	C	N	O	S	0	0
			882	560	149	171	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	98	Total	C	N	O	S	0	0
			744	462	135	142	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	75	Total	C	N	O	S	0	0
			616	402	110	102	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	82	Total	C	N	O	S	0	0
			662	415	118	124	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	73	Total	C	N	O	S	0	0
			604	389	113	98	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	56	Total	C	N	O	S	0	0
			436	286	68	81	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	49	Total	C	N	O	S	0	0
			388	252	65	70	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	43	Total	C	N	O	S	0	0
			335	222	55	56	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	79	Total	C	N	O	0	0
			480	309	86	85		

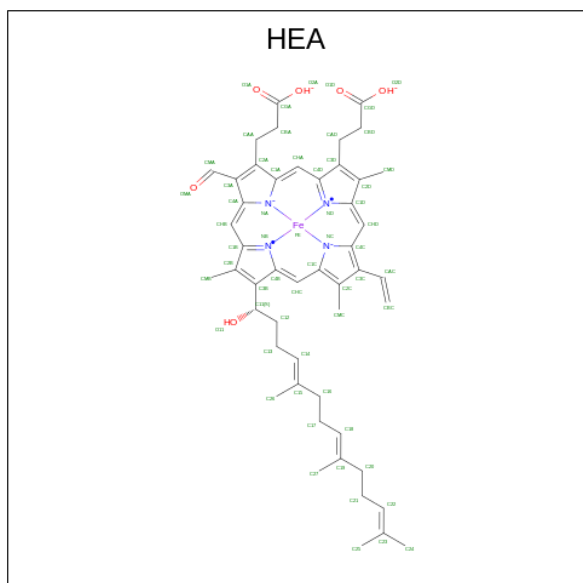
- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

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

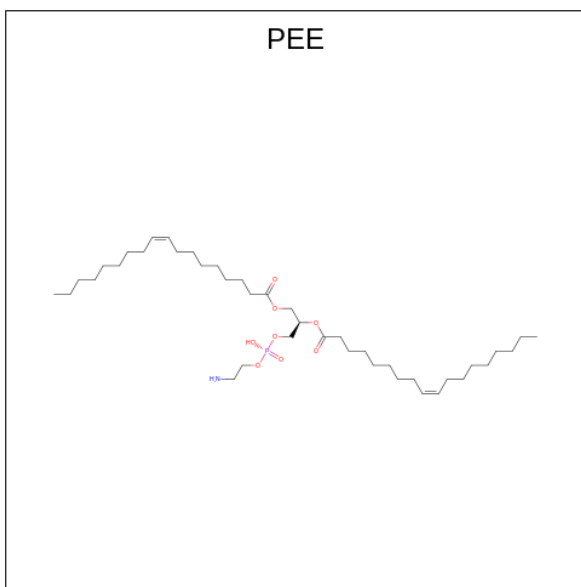
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



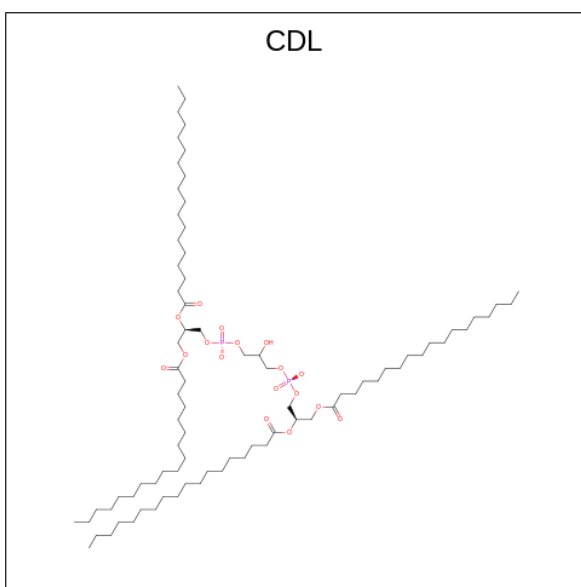
Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
17	A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 18 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	C	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 19 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
19	C	1	Total	C	O	P	0
			100	81	17	2	

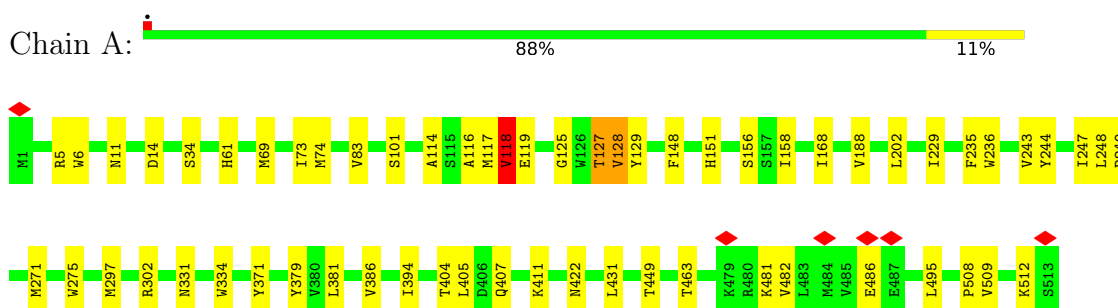
- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

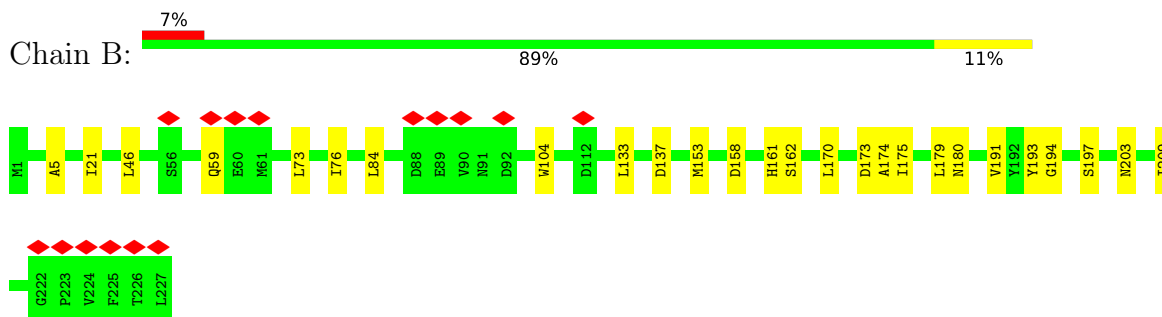
3 Residue-property plots [i](#)

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

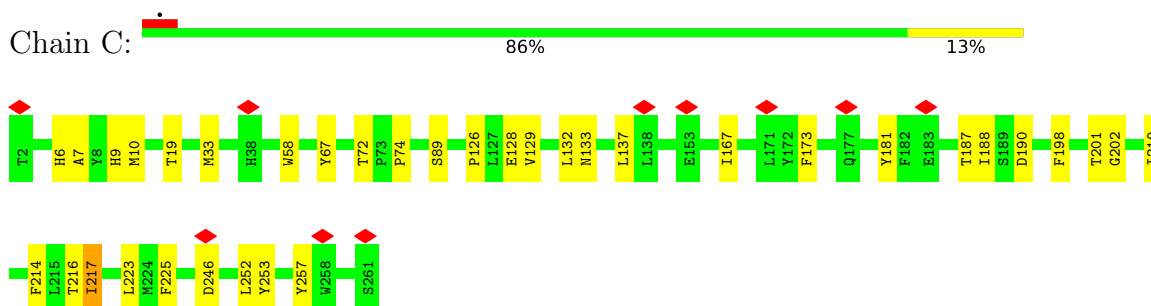
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2

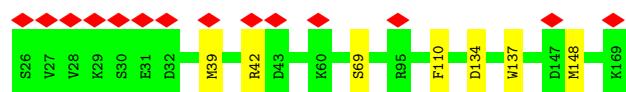


- Molecule 3: Cytochrome c oxidase subunit 3



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

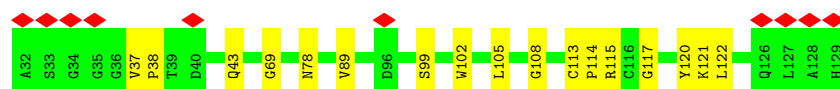
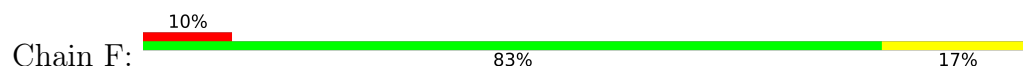




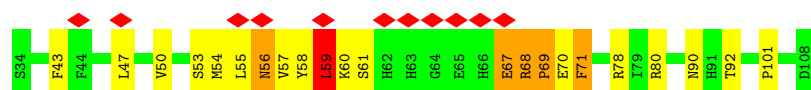
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



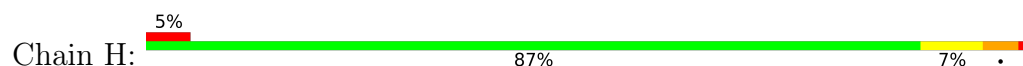
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



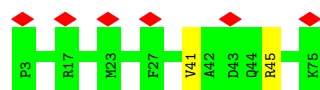
- Molecule 7: Cytochrome c oxidase subunit 6A1, mitochondrial



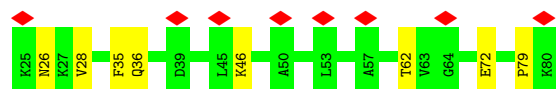
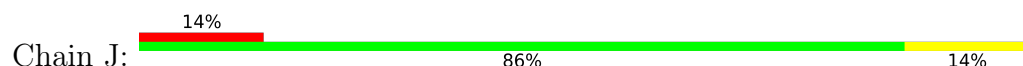
- Molecule 8: Cytochrome c oxidase subunit 6B1



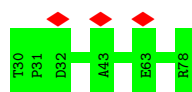
- Molecule 9: Cytochrome c oxidase subunit 6C



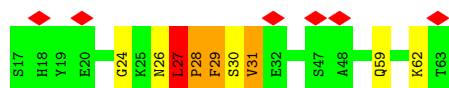
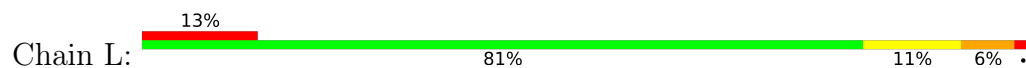
- Molecule 10: Cytochrome c oxidase subunit 7A2, mitochondrial



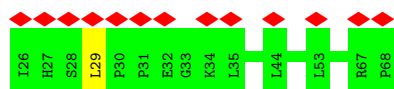
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



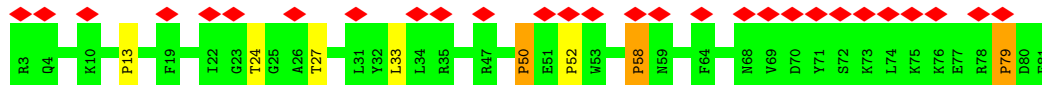
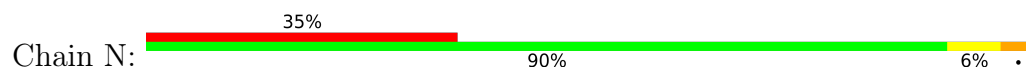
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



- Molecule 14: Cytochrome c oxidase subunit NDUF4A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1010000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.032	Depositor
Map size ($\text{\AA}$)	523.68, 523.68, 523.68	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/4169	0.62	1/5695 (0.0%)
2	B	0.31	0/1845	0.60	0/2525
3	C	0.30	0/2206	0.56	0/3018
4	D	0.22	0/1222	0.46	0/1641
5	E	0.23	0/901	0.45	0/1223
6	F	0.30	0/760	0.60	0/1029
7	G	0.27	0/642	0.57	0/877
8	H	0.25	0/682	0.56	1/926 (0.1%)
9	I	0.20	0/616	0.43	0/820
10	J	0.25	0/444	0.64	0/600
11	K	0.20	0/401	0.47	0/551
12	L	0.26	0/390	0.55	1/527 (0.2%)
13	M	0.24	0/345	0.57	0/470
14	N	0.30	0/489	0.94	4/677 (0.6%)
All	All	0.29	0/15112	0.58	7/20579 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	79	PRO	N-CA-CB	7.81	111.45	103.25
14	N	58	PRO	N-CA-CB	7.12	110.73	103.25
14	N	50	PRO	N-CA-CB	6.96	110.56	103.25
14	N	52	PRO	N-CA-CB	6.35	110.25	103.52
1	A	118	VAL	N-CA-C	5.95	117.25	109.58

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	4028	0	4015	45	0
2	B	1798	0	1823	17	0
3	C	2119	0	2046	29	0
4	D	1189	0	1183	8	0
5	E	882	0	872	4	0
6	F	744	0	729	14	0
7	G	616	0	590	65	0
8	H	662	0	586	13	0
9	I	604	0	630	1	0
10	J	436	0	451	8	0
11	K	388	0	372	0	0
12	L	378	0	377	18	0
13	M	335	0	346	1	0
14	N	480	0	347	3	0
15	A	1	0	0	0	0
15	B	2	0	0	0	0
16	A	1	0	0	0	0
17	A	120	0	108	6	0
18	A	51	0	82	4	0
18	C	102	0	164	13	0
19	C	100	0	156	3	0
20	F	1	0	0	0	0
All	All	15037	0	14877	203	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 7.

The worst 5 of 203 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)
7:G:57:VAL:HG23	7:G:61:SER:CB	1.38	1.51
1:A:6:TRP:CZ2	12:L:27:LEU:O	1.64	1.48
7:G:54:MET:HG3	7:G:58:TYR:CD2	1.54	1.41
7:G:57:VAL:CG2	7:G:61:SER:CB	2.07	1.30
7:G:57:VAL:CA	7:G:61:SER:HB2	1.63	1.28

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/513 (100%)	489 (96%)	21 (4%)	1 (0%)	43	72
2	B	225/227 (99%)	212 (94%)	13 (6%)	0	100	100
3	C	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
4	D	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
5	E	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
7	G	73/75 (97%)	58 (80%)	11 (15%)	4 (6%)	1	14
8	H	80/82 (98%)	72 (90%)	3 (4%)	5 (6%)	1	12
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
11	K	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
12	L	45/47 (96%)	42 (93%)	0	3 (7%)	1	11
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
14	N	77/79 (98%)	58 (75%)	16 (21%)	3 (4%)	2	20
All	All	1827/1855 (98%)	1717 (94%)	94 (5%)	16 (1%)	16	46

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	59	LEU
7	G	68	ARG
7	G	69	PRO
8	H	51	ILE
8	H	55	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/427 (100%)	421 (99%)	6 (1%)	59	71
2	B	202/202 (100%)	200 (99%)	2 (1%)	68	75
3	C	226/226 (100%)	224 (99%)	2 (1%)	70	76
4	D	128/128 (100%)	128 (100%)	0	100	100
5	E	97/97 (100%)	97 (100%)	0	100	100
6	F	79/79 (100%)	79 (100%)	0	100	100
7	G	66/66 (100%)	63 (96%)	3 (4%)	24	51
8	H	67/74 (90%)	64 (96%)	3 (4%)	24	51
9	I	61/61 (100%)	61 (100%)	0	100	100
10	J	45/45 (100%)	45 (100%)	0	100	100
11	K	41/41 (100%)	41 (100%)	0	100	100
12	L	41/41 (100%)	39 (95%)	2 (5%)	22	49
13	M	37/37 (100%)	37 (100%)	0	100	100
14	N	25/70 (36%)	25 (100%)	0	100	100
All	All	1542/1594 (97%)	1524 (99%)	18 (1%)	61	73

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	51	ILE
12	L	29	PHE
12	L	27	LEU
3	C	188	ILE
8	H	50	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	207	HIS

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Mol	Chain	Res	Type
12	L	59	GLN
4	D	141	GLN
13	M	61	HIS
8	H	26	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 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	$\# Z > 2$
18	PEE	A	605	-	50,50,50	1.14	4 (8%)	53,55,55	1.21	3 (5%)
17	HEA	A	604	1	66,67,67	2.31	25 (37%)	78,103,103	2.58	35 (44%)
18	PEE	C	302	-	50,50,50	1.16	4 (8%)	53,55,55	1.11	4 (7%)
18	PEE	C	301	-	50,50,50	1.19	4 (8%)	53,55,55	1.18	3 (5%)
19	CDL	C	303	-	99,99,99	0.92	4 (4%)	105,111,111	1.08	7 (6%)
17	HEA	A	603	1	66,67,67	2.31	25 (37%)	78,103,103	2.68	34 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PEE	A	605	-	1/1/4/8	14/54/54/54	-
17	HEA	A	604	1	-	8/36/76/76	-
18	PEE	C	302	-	1/1/4/8	24/54/54/54	-
18	PEE	C	301	-	1/1/4/8	17/54/54/54	-
19	CDL	C	303	-	-	48/110/110/110	-
17	HEA	A	603	1	-	14/36/76/76	-

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	604	HEA	FE-NB	5.34	2.11	1.94
17	A	604	HEA	FE-ND	5.24	2.11	1.94
17	A	603	HEA	C3B-C2B	5.24	1.46	1.34
17	A	603	HEA	FE-ND	5.23	2.11	1.94
17	A	603	HEA	FE-NB	5.20	2.11	1.94

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	603	HEA	C3C-C4C-NC	7.42	114.81	110.25
17	A	604	HEA	C3D-C4D-ND	7.02	117.16	110.36
17	A	603	HEA	C3D-C4D-ND	6.34	116.50	110.36
17	A	604	HEA	C3B-C4B-NB	6.03	116.98	109.84
17	A	603	HEA	C2B-C1B-NB	5.67	116.67	109.88

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	605	PEE	C2
18	C	301	PEE	C2
18	C	302	PEE	C2

5 of 125 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	HEA	C2A-C3A-CMA-OMA
18	A	605	PEE	C1-O3P-P-O2P
18	A	605	PEE	C1-O3P-P-O1P

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Continued from previous page...

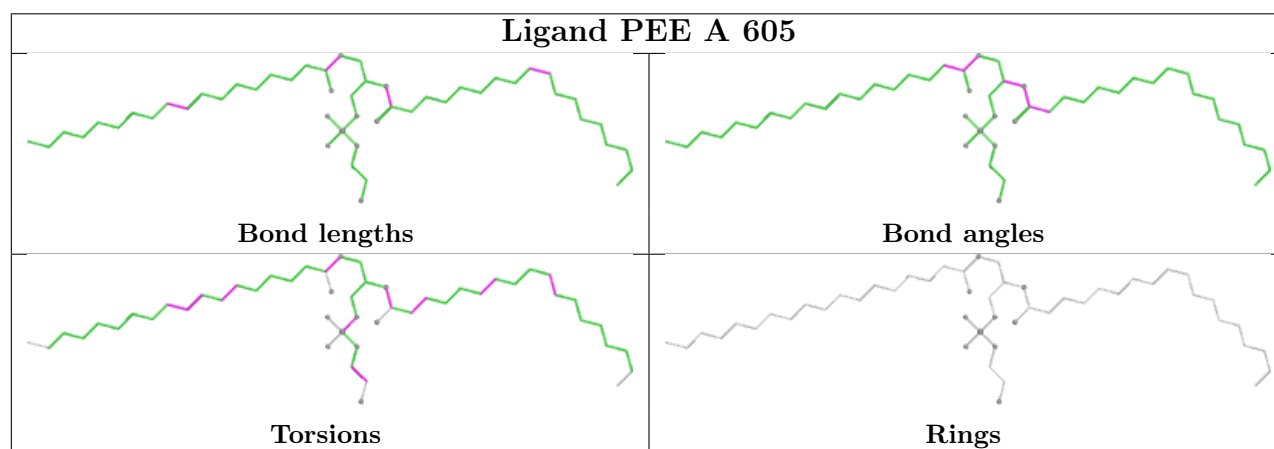
Mol	Chain	Res	Type	Atoms
18	A	605	PEE	O4P-C4-C5-N
18	C	301	PEE	C4-O4P-P-O2P

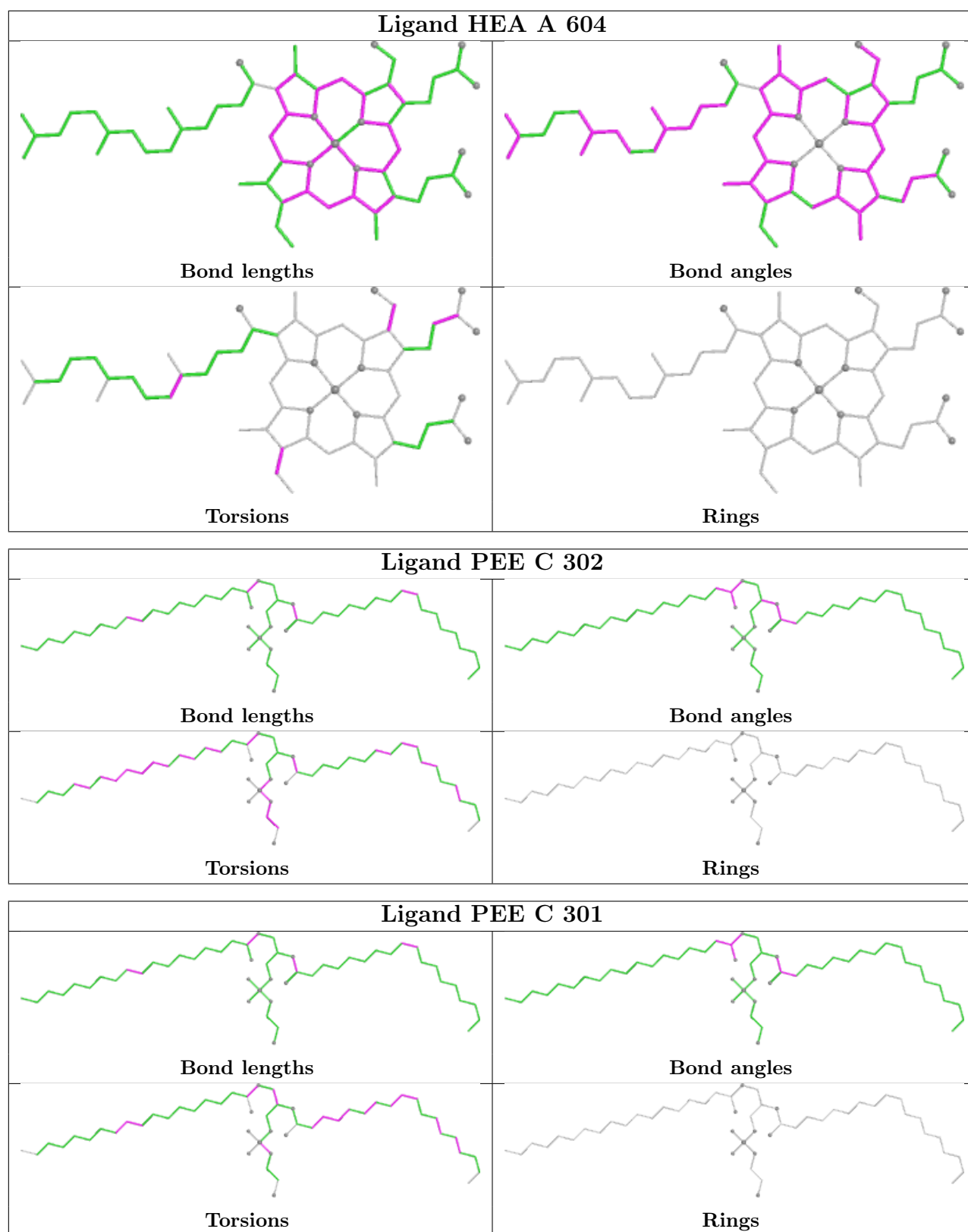
There are no ring outliers.

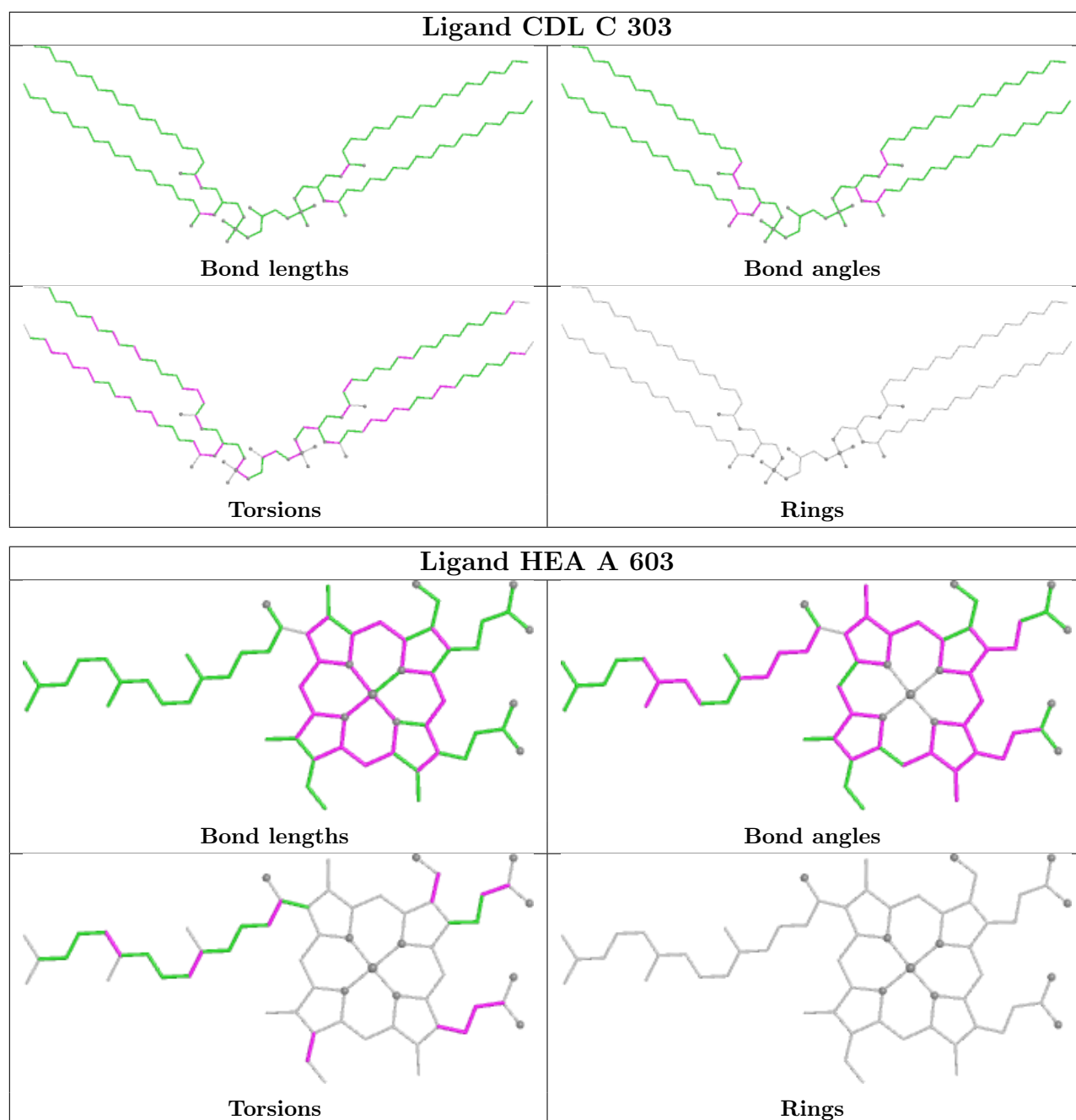
6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	605	PEE	4	0
17	A	604	HEA	2	0
18	C	302	PEE	6	0
18	C	301	PEE	9	0
19	C	303	CDL	3	0
17	A	603	HEA	4	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.

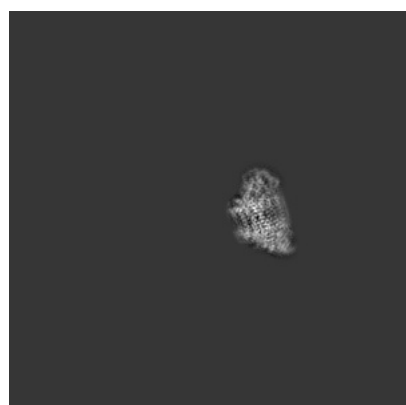
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6896. These allow visual inspection of the internal detail of the map and identification of artifacts.

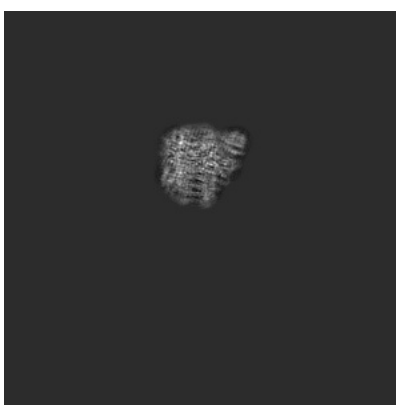
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

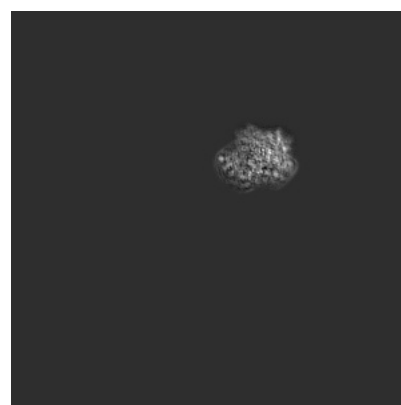
6.1.1 Primary map



X



Y

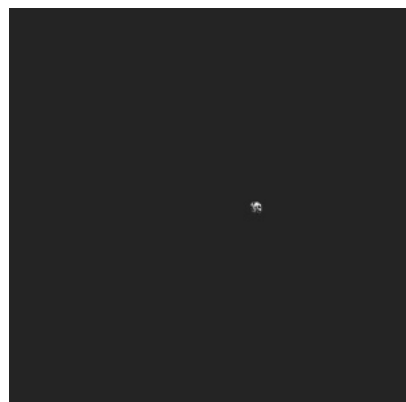


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240

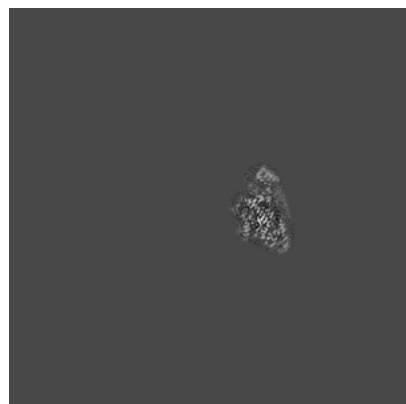


Z Index: 240

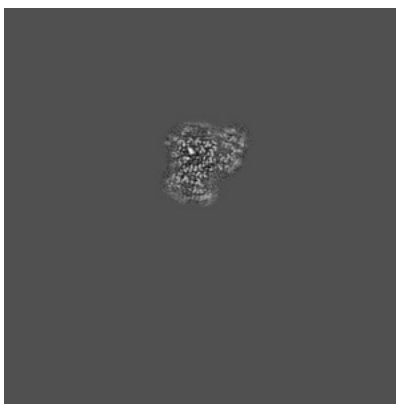
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 309



Y Index: 300

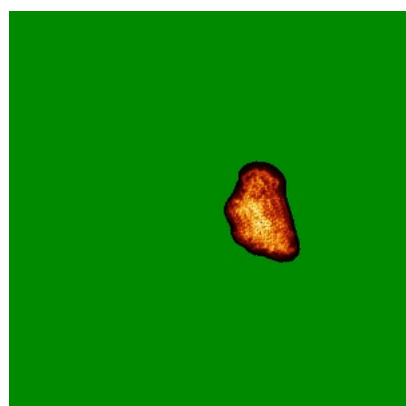


Z Index: 223

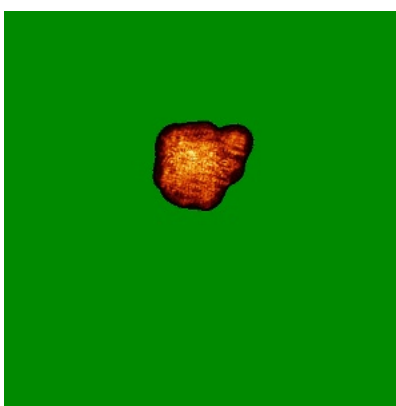
The images above show the largest variance slices of the map in three orthogonal directions.

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

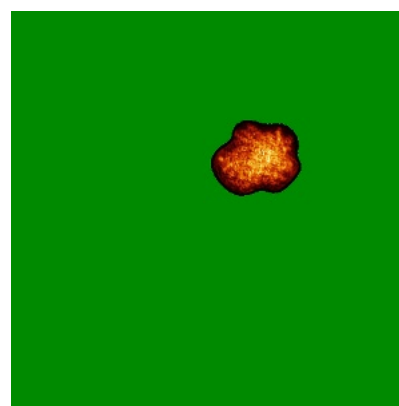
6.4.1 Primary map



X



Y

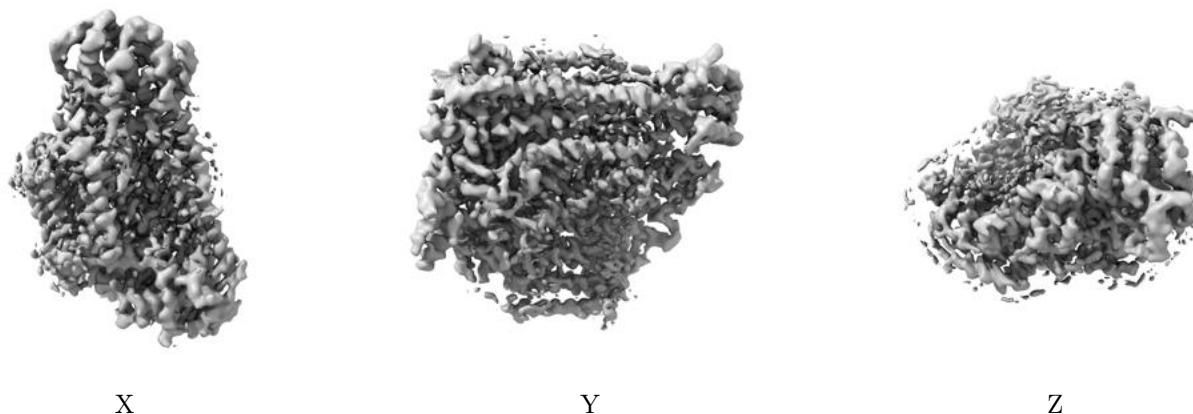


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

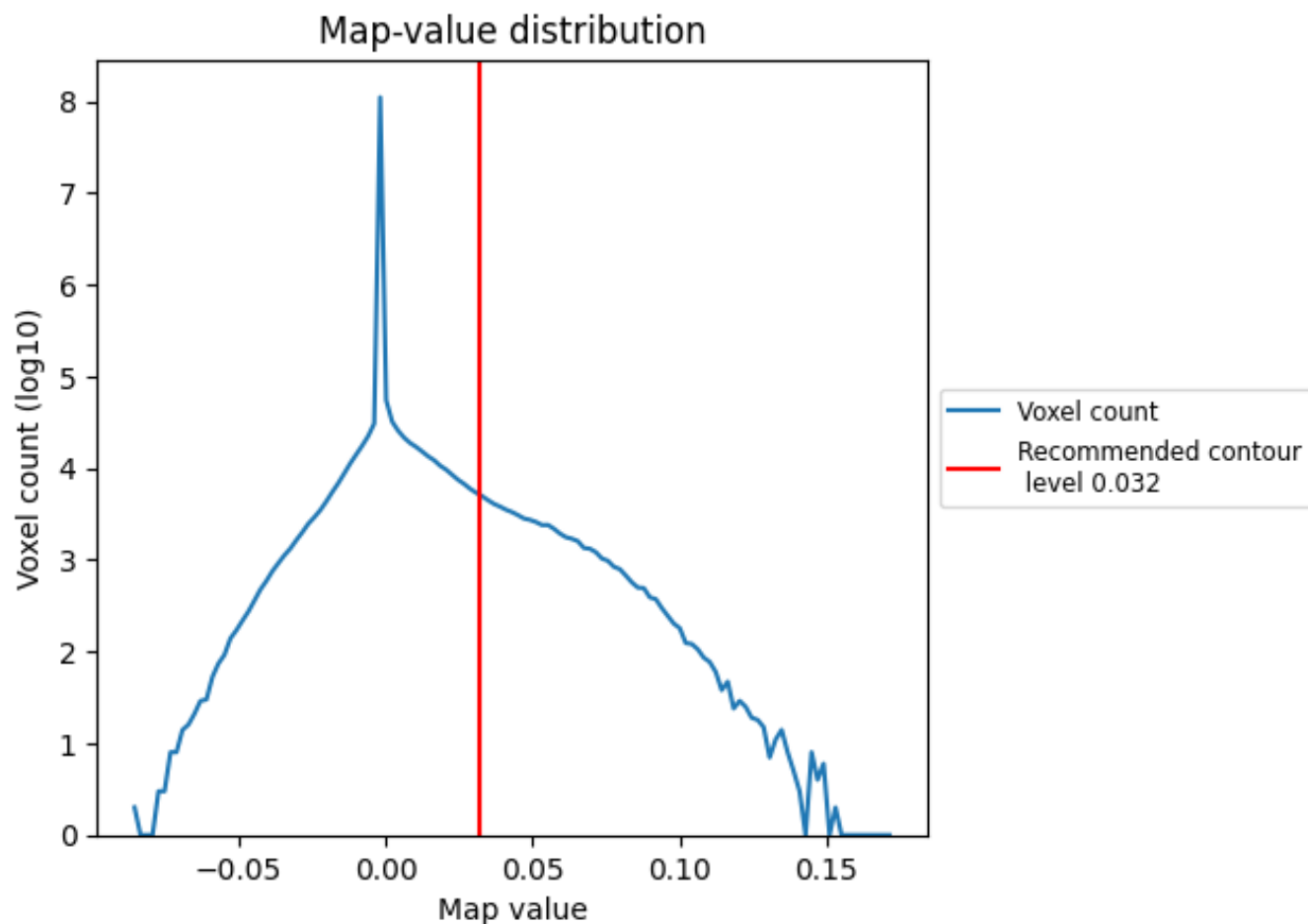
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

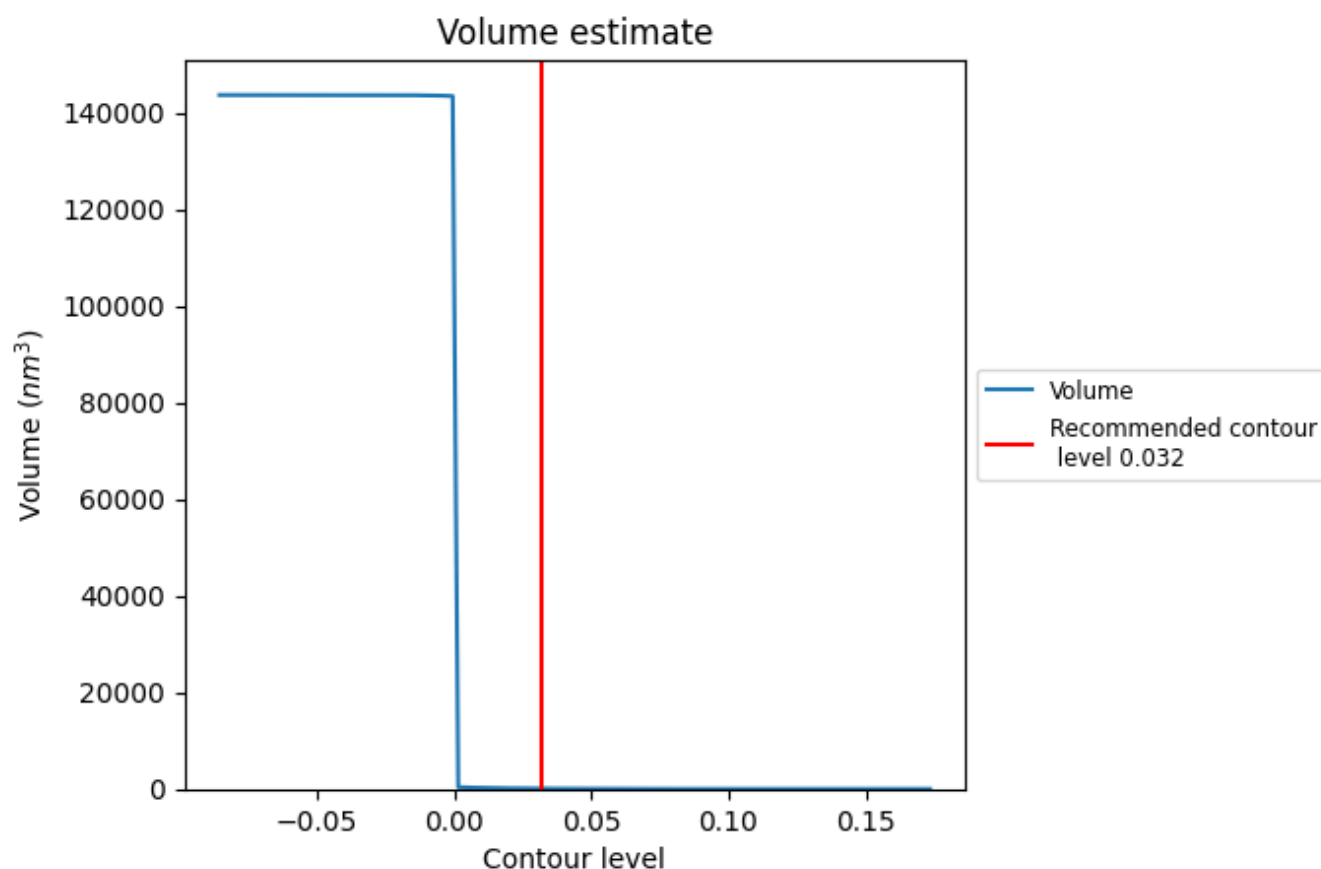
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

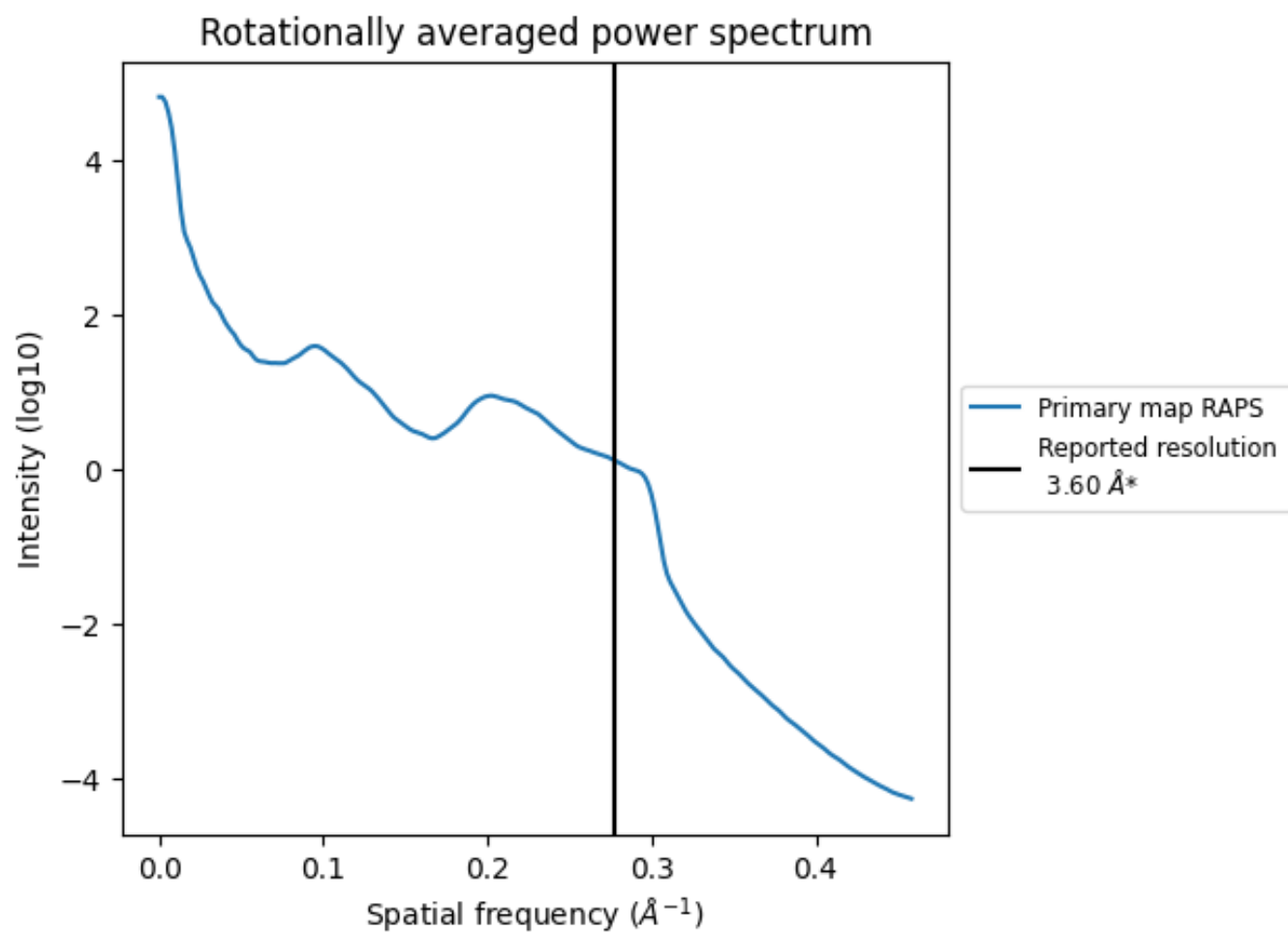
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm^3 ; this corresponds to an approximate mass of 74 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

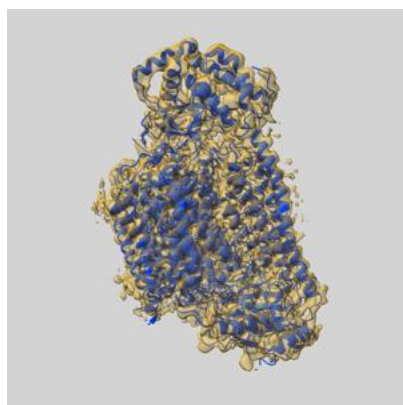
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

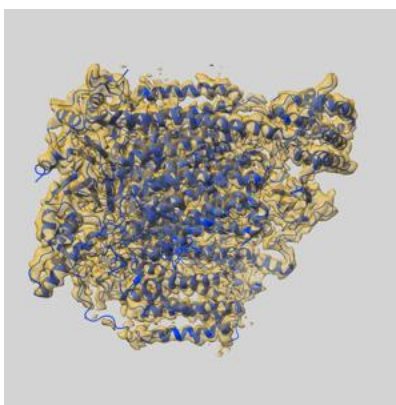
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6896 and PDB model 5Z62. Per-residue inclusion information can be found in section [3](#) on page [9](#).

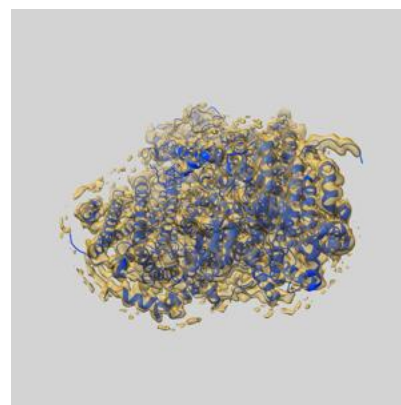
9.1 Map-model overlay [i](#)



X



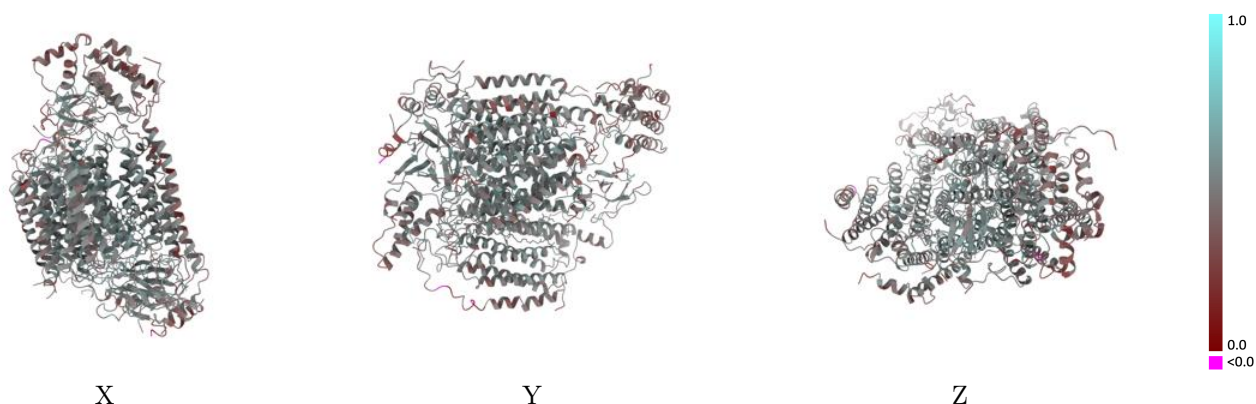
Y



Z

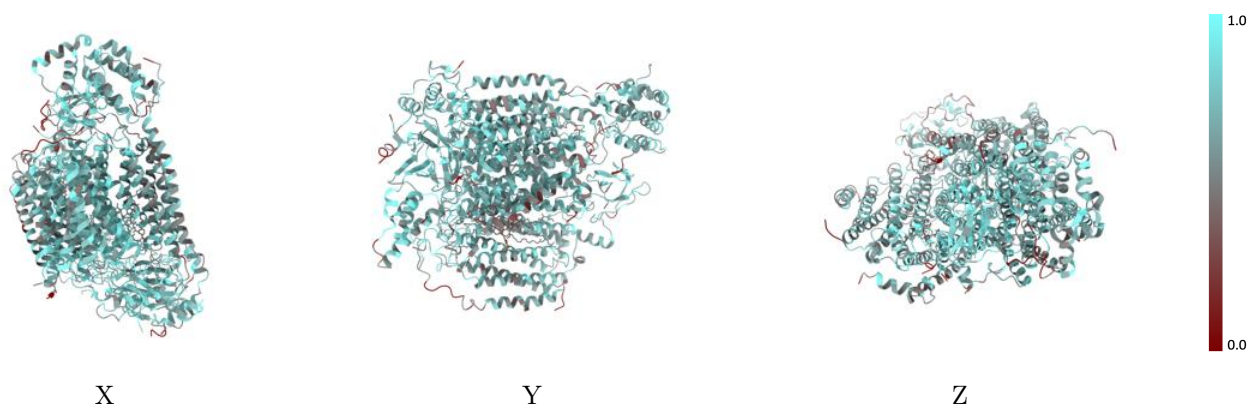
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



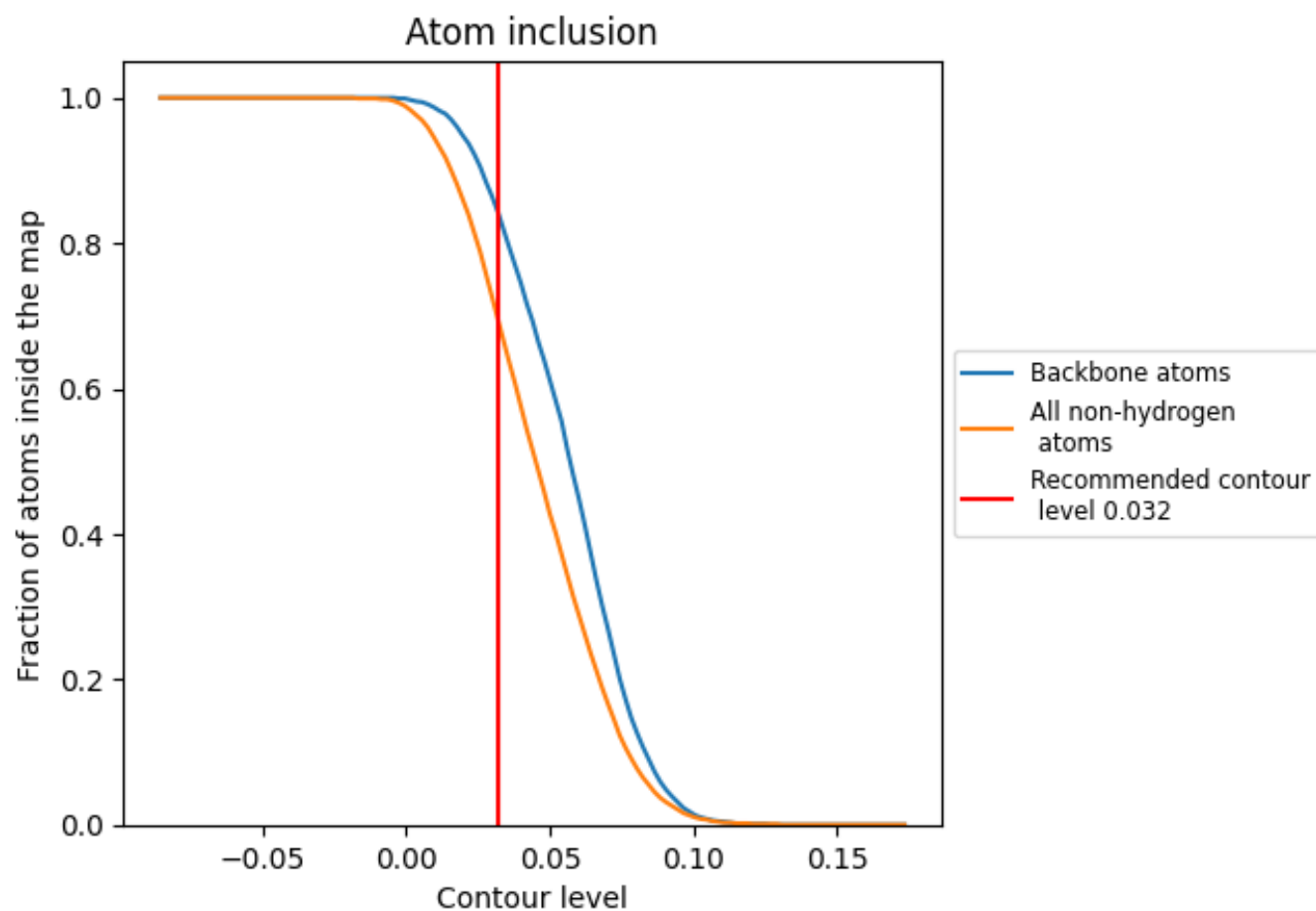
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6940	 0.4740
A	 0.7730	 0.5270
B	 0.6870	 0.4800
C	 0.6950	 0.4900
D	 0.6540	 0.4340
E	 0.6620	 0.4080
F	 0.6900	 0.4620
G	 0.6240	 0.4180
H	 0.7410	 0.4520
I	 0.6460	 0.4190
J	 0.6070	 0.4350
K	 0.7070	 0.4580
L	 0.6920	 0.4820
M	 0.4860	 0.3780
N	 0.5020	 0.4240

