Full wwPDB EM Validation Report

Jul 19, 2026 – 12:15 AM JST

PDB ID	:	23PI / pdb_000023pi
EMDB ID	:	EMD-69145
Title	:	Cryo-EM structure of the human ABCB7 in occluded state
Authors	:	Ju, S.; Choi, S.H.; Lee, H.Y.; Jin, M.S.
Deposited on	:	2026-02-12
Resolution	:	2.33 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

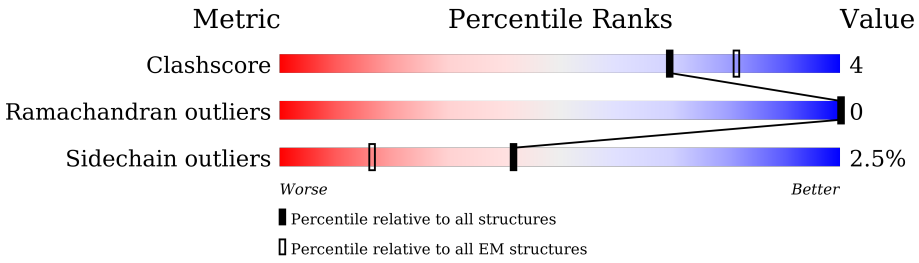
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

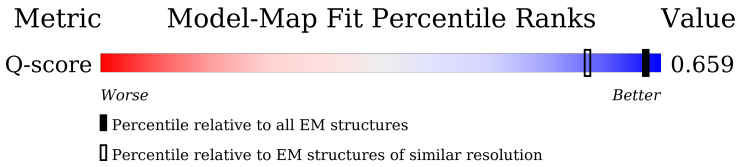
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.33 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	4434 (1.83 - 2.83)

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	682	5% 75% 8% 17%
1	B	682	74% 8% 17%

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
4	COH	A	803	X	-	-	-
4	COH	A	804	X	-	-	-
4	COH	A	805	X	-	-	-
4	COH	B	801	X	-	-	-
4	COH	B	802	X	-	-	-
4	COH	B	803	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8942 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.

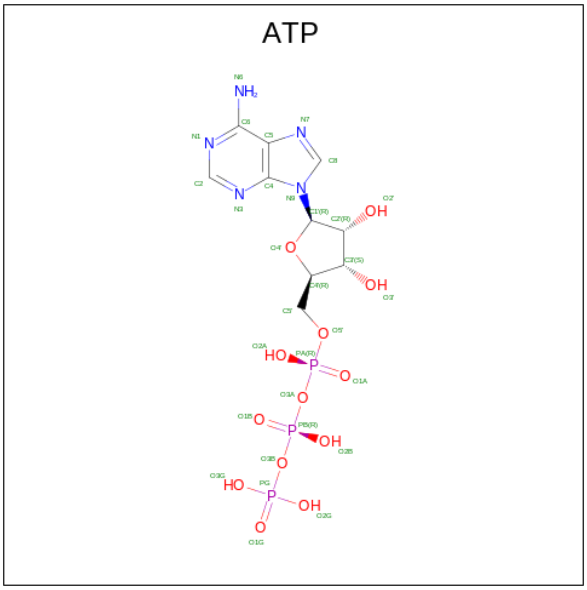
- Molecule 1 is a protein called Iron-sulfur clusters transporter ABCB7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	564	Total	C	N	O	S	0	0
			4303	2756	743	789	15		
1	B	564	Total	C	N	O	S	0	0
			4313	2762	743	793	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	634	GLN	GLU	engineered mutation	UNP O75027
B	634	GLN	GLU	engineered mutation	UNP O75027

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

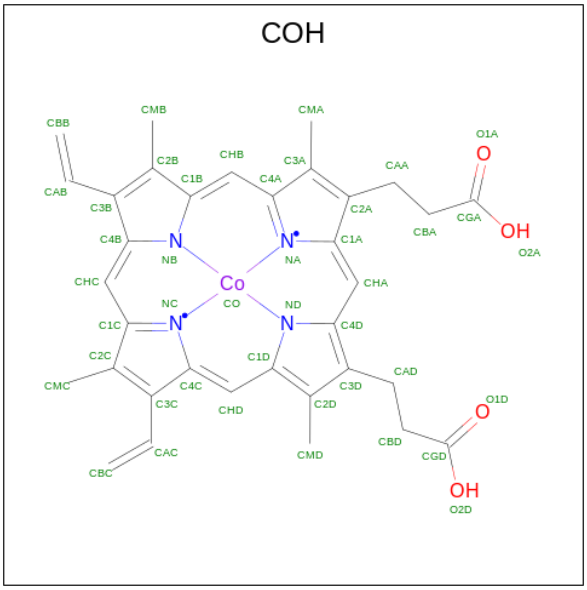


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING CO (CCD ID: COH) (formula: $C_{34}H_{32}CoN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C Co N O 43 34 1 4 4	0
4	A	1	Total C Co N O 43 34 1 4 4	0
4	A	1	Total C Co N O 43 34 1 4 4	0
4	B	1	Total C Co N O 43 34 1 4 4	0
4	B	1	Total C Co N O 43 34 1 4 4	0
4	B	1	Total C Co N O 43 34 1 4 4	0

- Molecule 5 is water.

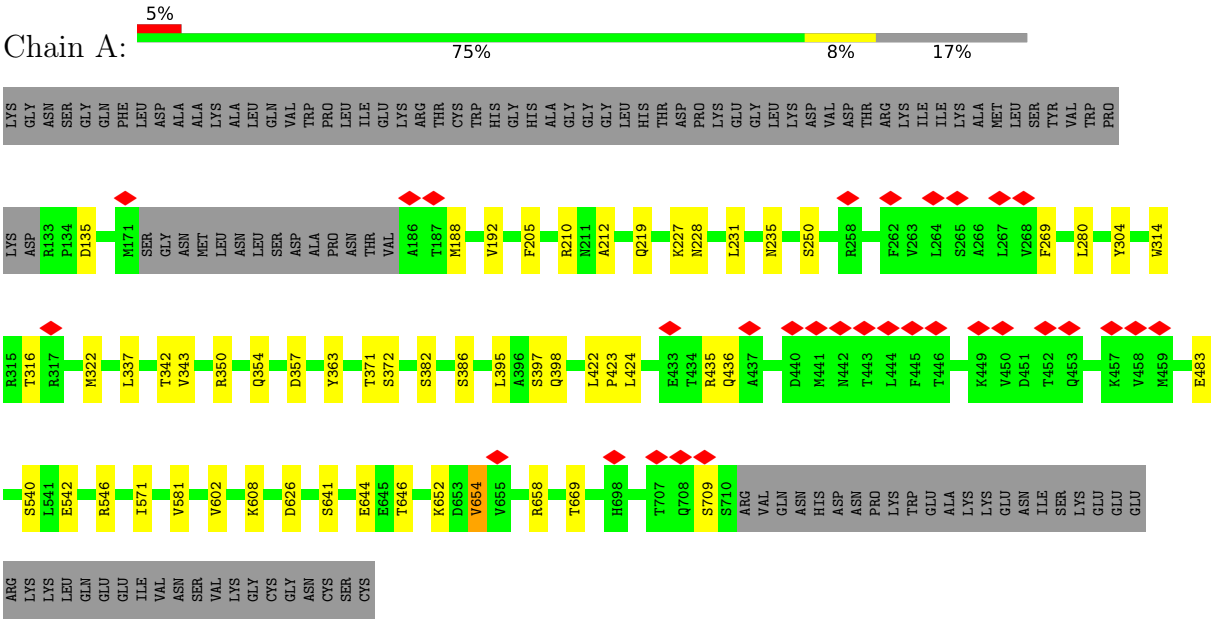
Mol	Chain	Residues	Atoms	AltConf
5	A	2	Total O 2 2	0
5	B	2	Total O 2 2	0

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.

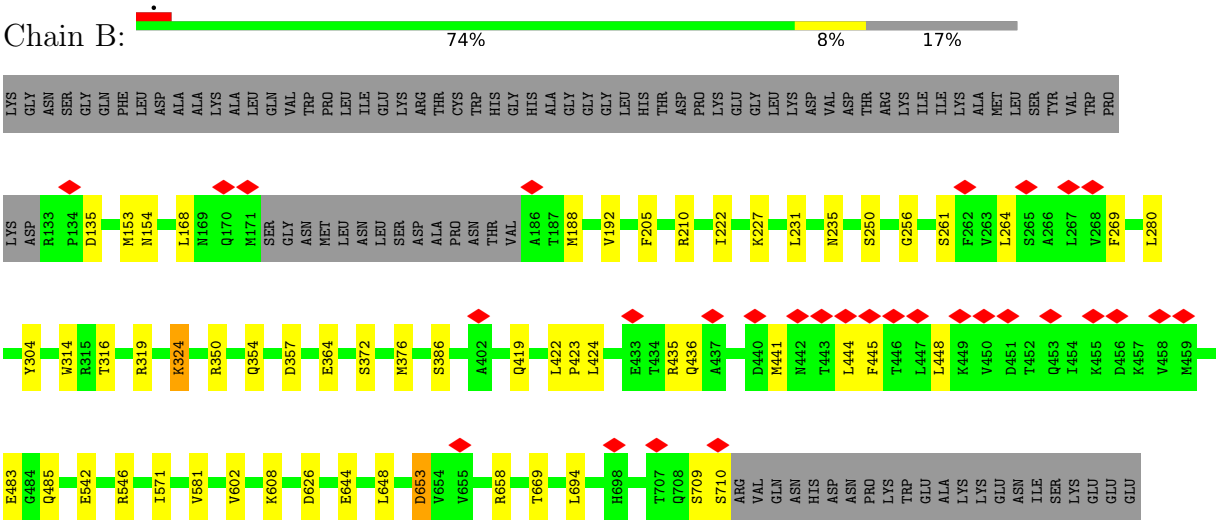
• Molecule 1: Iron-sulfur clusters transporter ABCB7, mitochondrial

Chain A:



• Molecule 1: Iron-sulfur clusters transporter ABCB7, mitochondrial

Chain B:



ARG
LYS
LYS
LEU
GLN
GLU
GLU
ILE
VAL
ASN
SER
VAL
LYS
GLY
CYS
GLY
ASN
CYS
SER
CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	425646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.329	Depositor
Minimum map value	-3.005	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.534	Depositor
Map size (Å)	242.28, 242.28, 242.28	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.673, 0.673, 0.673	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, COH

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	0.24	1/4381 (0.0%)	0.32	0/5940
1	B	0.19	0/4391	0.32	0/5954
All	All	0.22	1/8772 (0.0%)	0.32	0/11894

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	VAL	CA-CB	8.57	1.64	1.54

There are no bond angle outliers.

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	4303	0	4336	31	0
1	B	4313	0	4357	38	0
2	A	31	0	11	0	0
2	B	31	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	129	0	90	5	0
4	B	129	0	90	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	2	0	0	0	0
All	All	8942	0	8895	65	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 4.

All (65) 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:B:485:GLN:HE22	2:B:804:ATP:H8	1.26	0.81
1:A:641:SER:HB3	1:B:710:SER:HB2	1.67	0.76
1:A:316:THR:HG21	1:A:435:ARG:HH21	1.61	0.64
1:B:483:GLU:H	1:B:483:GLU:CD	2.06	0.64
1:A:483:GLU:H	1:A:483:GLU:CD	2.07	0.63
1:B:256:GLY:HA3	1:B:444:LEU:HD21	1.82	0.62
1:A:644:GLU:OE1	1:A:669:THR:OG1	2.19	0.59
1:A:709:SER:HG	1:B:709:SER:HG	1.48	0.59
1:B:653:ASP:N	1:B:653:ASP:OD1	2.35	0.57
1:B:448:LEU:HD13	4:B:803:COH:HBC1	1.86	0.57
1:B:135:ASP:N	1:B:135:ASP:OD1	2.38	0.56
1:B:314:TRP:HH2	4:B:802:COH:HAD2	1.70	0.56
1:B:372:SER:HB3	4:B:802:COH:HMD2	1.88	0.56
1:A:652:LYS:HD2	1:A:654:VAL:HG23	1.89	0.53
1:B:205:PHE:HE1	4:B:801:COH:HBC2	1.74	0.53
1:A:357:ASP:HB2	1:B:227:LYS:HE3	1.91	0.52
1:A:135:ASP:N	1:A:135:ASP:OD1	2.39	0.52
1:A:314:TRP:HH2	4:A:804:COH:HAD1	1.75	0.52
1:B:154:ASN:O	1:B:419:GLN:NE2	2.42	0.51
1:B:188:MET:O	1:B:192:VAL:HG22	2.12	0.50
1:A:205:PHE:HZ	4:A:805:COH:HBC2	1.77	0.50
1:B:205:PHE:CE1	4:B:801:COH:HBC2	2.47	0.50
1:A:397:SER:HB2	1:B:168:LEU:HD11	1.94	0.50
1:A:188:MET:O	1:A:192:VAL:HG22	2.12	0.49
1:B:376:MET:HE3	4:B:802:COH:HMB2	1.95	0.49
1:A:205:PHE:CZ	4:A:805:COH:HBC2	2.47	0.49
1:A:210:ARG:HD3	1:A:269:PHE:CE2	2.48	0.48
1:A:227:LYS:HE3	1:B:357:ASP:HB2	1.94	0.48
1:B:304:TYR:CD1	1:B:424:LEU:HD13	2.48	0.48
1:B:319:ARG:HG2	1:B:436:GLN:NE2	2.29	0.48
1:B:316:THR:HG21	1:B:435:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASP:OD1	1:A:658:ARG:NH2	2.48	0.46
4:B:802:COH:HHB	4:B:802:COH:HMA1	1.74	0.46
1:A:212:ALA:CB	4:B:802:COH:HBC2	2.46	0.45
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.83	0.45
1:B:210:ARG:HD3	1:B:269:PHE:CE2	2.52	0.45
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.85	0.45
1:B:153:MET:HA	1:B:153:MET:HE2	1.98	0.44
1:A:304:TYR:CD1	1:A:424:LEU:HD13	2.52	0.44
4:A:804:COH:HBC1	4:A:804:COH:HMC3	1.99	0.44
1:A:372:SER:HB3	4:A:804:COH:HMD2	2.00	0.44
1:B:324:LYS:HE3	1:B:324:LYS:HB3	1.90	0.44
1:A:337:LEU:HD12	1:A:337:LEU:HA	1.82	0.43
1:A:350:ARG:O	1:A:354:GLN:HG2	2.19	0.43
1:A:322:MET:HG2	1:A:363:TYR:CE1	2.53	0.43
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.85	0.43
1:B:350:ARG:O	1:B:354:GLN:HG2	2.19	0.43
1:B:441:MET:O	1:B:445:PHE:HB2	2.19	0.43
1:B:648:LEU:HD23	1:B:648:LEU:HA	1.90	0.42
1:A:422:LEU:HB2	1:A:423:PRO:HD3	2.01	0.42
1:B:231:LEU:HD12	1:B:231:LEU:HA	1.84	0.42
1:B:280:LEU:HD23	1:B:280:LEU:HA	1.84	0.42
1:B:424:LEU:HD23	1:B:424:LEU:HA	1.85	0.42
1:B:626:ASP:OD1	1:B:658:ARG:NH2	2.49	0.42
1:B:542:GLU:OE1	1:B:546:ARG:NE	2.46	0.42
1:A:542:GLU:OE1	1:A:546:ARG:NE	2.36	0.41
1:A:602:VAL:O	1:A:608:LYS:HB2	2.21	0.41
1:A:219:GLN:HB3	1:B:364:GLU:HG3	2.03	0.41
1:A:210:ARG:HD3	1:A:269:PHE:HE2	1.86	0.41
1:B:602:VAL:O	1:B:608:LYS:HB2	2.21	0.41
1:B:571:ILE:HD13	1:B:571:ILE:HA	1.91	0.41
1:B:314:TRP:HH2	4:B:802:COH:CAD	2.33	0.40
1:B:644:GLU:OE1	1:B:669:THR:HG22	2.20	0.40
1:B:422:LEU:HB2	1:B:423:PRO:HD3	2.02	0.40
1:A:571:ILE:HD13	1:A:571:ILE:HA	1.89	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	560/682 (82%)	551 (98%)	9 (2%)	0	100	100
1	B	560/682 (82%)	549 (98%)	11 (2%)	0	100	100
All	All	1120/1364 (82%)	1100 (98%)	20 (2%)	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	450/565 (80%)	437 (97%)	13 (3%)	37	48
1	B	454/565 (80%)	444 (98%)	10 (2%)	45	58
All	All	904/1130 (80%)	881 (98%)	23 (2%)	42	54

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	235	ASN
1	A	250	SER
1	A	342	THR
1	A	371	THR
1	A	382	SER
1	A	386	SER
1	A	398	GLN

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Mol	Chain	Res	Type
1	A	436	GLN
1	A	540	SER
1	A	581	VAL
1	A	646	THR
1	A	654	VAL
1	B	222	ILE
1	B	235	ASN
1	B	250	SER
1	B	261	SER
1	B	264	LEU
1	B	324	LYS
1	B	386	SER
1	B	581	VAL
1	B	653	ASP
1	B	694	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	ASN
1	A	537	GLN
1	B	476	ASN

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	COH	B	803	1	50,50,50	1.92	16 (32%)	68,82,82	1.85	9 (13%)
4	COH	A	804	-	50,50,50	1.96	15 (30%)	68,82,82	1.81	12 (17%)
2	ATP	A	801	3	29,33,33	3.57	14 (48%)	44,52,52	2.64	13 (29%)
4	COH	A	803	1	50,50,50	1.95	14 (28%)	68,82,82	1.86	12 (17%)
4	COH	B	801	-	50,50,50	1.98	15 (30%)	68,82,82	1.84	14 (20%)
4	COH	A	805	-	50,50,50	1.93	14 (28%)	68,82,82	1.82	13 (19%)
2	ATP	B	804	3	29,33,33	3.57	14 (48%)	44,52,52	2.64	15 (34%)
4	COH	B	802	-	50,50,50	2.01	16 (32%)	68,82,82	2.98	24 (35%)

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
4	COH	B	803	1	1/1/3/9	5/14/54/54	-
4	COH	A	804	-	1/1/3/9	5/14/54/54	-
2	ATP	A	801	3	-	1/22/38/38	0/3/3/3
4	COH	A	803	1	1/1/3/9	6/14/54/54	-
4	COH	B	801	-	1/1/3/9	3/14/54/54	-
4	COH	A	805	-	1/1/3/9	8/14/54/54	-
2	ATP	B	804	3	-	2/22/38/38	0/3/3/3
4	COH	B	802	-	1/1/3/9	5/14/54/54	-

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	804	ATP	C2'-C3'	-10.61	1.24	1.53
2	A	801	ATP	C2'-C3'	-10.58	1.24	1.53
2	B	804	ATP	C3'-C4'	6.96	1.70	1.53
2	A	801	ATP	C3'-C4'	6.95	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	COH	C1D-ND	-6.91	1.27	1.38
4	B	802	COH	C1D-ND	-6.81	1.27	1.38
2	A	801	ATP	O4'-C4'	-6.71	1.30	1.45
2	B	804	ATP	O4'-C4'	-6.67	1.30	1.45
4	A	804	COH	C1D-ND	-6.57	1.28	1.38
4	A	805	COH	C1D-ND	-6.47	1.28	1.38
4	A	803	COH	C1D-ND	-6.37	1.28	1.38
2	A	801	ATP	C6-N6	6.21	1.49	1.34
2	B	804	ATP	C6-N6	6.21	1.49	1.34
4	B	803	COH	C1D-ND	-6.16	1.28	1.38
2	B	804	ATP	C1'-N9	-5.25	1.31	1.46
2	A	801	ATP	C1'-N9	-5.21	1.31	1.46
2	B	804	ATP	O4'-C1'	4.91	1.53	1.42
2	A	801	ATP	O4'-C1'	4.88	1.53	1.42
4	B	801	COH	C4B-NB	-3.98	1.32	1.38
4	B	803	COH	C4B-NB	-3.88	1.32	1.38
4	B	802	COH	C4B-NB	-3.86	1.32	1.38
4	A	804	COH	C4B-NB	-3.80	1.32	1.38
4	A	805	COH	C4B-NB	-3.73	1.32	1.38
4	A	804	COH	CO-ND	3.62	2.09	1.96
4	B	802	COH	C1D-C2D	3.58	1.51	1.43
4	A	803	COH	CO-ND	3.54	2.09	1.96
4	B	803	COH	CO-ND	3.52	2.09	1.96
4	A	803	COH	C4B-NB	-3.51	1.33	1.38
4	A	804	COH	C1D-C2D	3.51	1.51	1.43
4	A	805	COH	CO-ND	3.51	2.09	1.96
4	B	801	COH	CO-ND	3.50	2.09	1.96
2	B	804	ATP	O2'-C2'	3.50	1.51	1.43
2	A	801	ATP	O2'-C2'	3.49	1.51	1.43
4	A	803	COH	C1D-C2D	3.41	1.51	1.43
2	B	804	ATP	PA-O2A	-3.41	1.39	1.55
2	A	801	ATP	PA-O2A	-3.40	1.39	1.55
4	B	802	COH	C1C-NC	-3.38	1.32	1.38
4	B	801	COH	C1D-C2D	3.38	1.51	1.43
4	B	803	COH	C1D-C2D	3.36	1.51	1.43
4	A	805	COH	C1D-C2D	3.34	1.51	1.43
4	B	802	COH	CO-ND	3.26	2.08	1.96
4	A	803	COH	C1C-NC	-3.13	1.32	1.38
4	A	803	COH	CMB-C2B	2.99	1.57	1.50
4	A	805	COH	C1C-NC	-2.95	1.32	1.38
4	B	803	COH	C1C-NC	-2.90	1.32	1.38
4	A	805	COH	CMB-C2B	2.89	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	COH	CMB-C2B	2.87	1.56	1.50
4	B	801	COH	C1C-NC	-2.84	1.33	1.38
4	B	801	COH	CMB-C2B	2.83	1.56	1.50
4	A	804	COH	CMB-C2B	2.80	1.56	1.50
2	A	801	ATP	C5-C4	-2.78	1.33	1.39
4	A	804	COH	C1C-NC	-2.73	1.33	1.38
4	A	803	COH	C1A-NA	2.69	1.44	1.39
4	A	804	COH	C3C-C2C	2.68	1.42	1.37
2	B	804	ATP	C5-C4	-2.66	1.34	1.39
4	B	801	COH	C3C-C2C	2.65	1.42	1.37
4	B	802	COH	CHD-C4C	-2.61	1.33	1.38
2	B	804	ATP	PG-O3G	-2.60	1.44	1.54
4	B	803	COH	CBC-CAC	2.59	1.43	1.30
2	B	804	ATP	C2'-C1'	2.59	1.61	1.53
2	A	801	ATP	C2'-C1'	2.56	1.61	1.53
4	B	802	COH	C1A-NA	2.55	1.44	1.39
4	A	803	COH	CBC-CAC	2.54	1.42	1.30
2	A	801	ATP	PG-O3G	-2.54	1.45	1.54
4	A	805	COH	C3C-C2C	2.53	1.42	1.37
4	B	801	COH	CBC-CAC	2.52	1.42	1.30
4	B	801	COH	CHB-C1B	2.52	1.43	1.38
4	B	802	COH	CMB-C2B	2.52	1.56	1.50
4	B	802	COH	C3C-C2C	2.52	1.42	1.37
4	A	804	COH	CBC-CAC	2.51	1.42	1.30
4	A	803	COH	C4C-NC	-2.51	1.35	1.39
4	A	803	COH	C3C-C2C	2.50	1.42	1.37
4	A	805	COH	C1A-NA	2.47	1.43	1.39
4	A	805	COH	CBC-CAC	2.46	1.42	1.30
4	B	802	COH	CHB-C1B	2.45	1.43	1.38
4	A	805	COH	CHB-C1B	2.42	1.43	1.38
4	A	804	COH	C1A-NA	2.40	1.43	1.39
4	B	803	COH	C3C-C2C	2.40	1.42	1.37
4	B	803	COH	CHB-C1B	2.38	1.43	1.38
4	B	802	COH	CBC-CAC	2.37	1.42	1.30
4	B	801	COH	C1A-NA	2.36	1.43	1.39
4	B	802	COH	CAB-C3B	-2.36	1.41	1.47
4	A	804	COH	CHD-C1D	2.35	1.44	1.39
2	B	804	ATP	PB-O1B	2.34	1.59	1.50
4	A	803	COH	CHB-C1B	2.34	1.42	1.38
2	A	801	ATP	PB-O1B	2.32	1.59	1.50
4	A	805	COH	C4C-NC	-2.31	1.35	1.39
4	A	804	COH	CHB-C1B	2.30	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	COH	C4C-NC	-2.30	1.35	1.39
4	B	803	COH	CHD-C1D	2.30	1.44	1.39
2	A	801	ATP	PB-O2B	-2.28	1.44	1.55
2	B	804	ATP	PB-O2B	-2.27	1.44	1.55
4	A	803	COH	CHD-C1D	2.23	1.44	1.39
4	B	803	COH	C1A-NA	2.23	1.43	1.39
4	B	801	COH	C4C-NC	-2.22	1.35	1.39
4	B	803	COH	C4D-ND	2.21	1.42	1.38
4	B	802	COH	O2D-CGD	-2.21	1.23	1.30
4	B	801	COH	C4D-ND	2.18	1.42	1.38
4	A	804	COH	C4C-NC	-2.17	1.35	1.39
4	A	803	COH	CHD-C4C	-2.17	1.34	1.38
2	B	804	ATP	PA-O5'	2.16	1.68	1.59
4	B	803	COH	CHD-C4C	-2.15	1.34	1.38
2	A	801	ATP	PA-O5'	2.15	1.68	1.59
4	B	802	COH	CHD-C1D	2.15	1.44	1.39
4	B	801	COH	O2D-CGD	-2.14	1.23	1.30
4	A	805	COH	CHD-C4C	-2.13	1.34	1.38
4	A	805	COH	O2D-CGD	-2.11	1.23	1.30
4	A	804	COH	O2D-CGD	-2.11	1.23	1.30
4	B	801	COH	CHD-C4C	-2.11	1.34	1.38
4	A	805	COH	CHD-C1D	2.11	1.44	1.39
4	B	802	COH	C4C-NC	-2.10	1.35	1.39
4	A	803	COH	O2D-CGD	-2.10	1.23	1.30
4	B	802	COH	C1B-C2B	-2.10	1.41	1.45
4	B	803	COH	O2D-CGD	-2.09	1.23	1.30
4	B	801	COH	CHD-C1D	2.08	1.44	1.39
4	A	804	COH	CMD-C2D	2.05	1.55	1.50
4	B	803	COH	CMD-C2D	2.02	1.55	1.50
4	A	804	COH	CO-NB	-2.01	1.88	1.96

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	802	COH	C3B-C2B-C1B	-11.69	95.91	107.08
2	B	804	ATP	C1'-N9-C8	-9.06	106.67	127.14
2	A	801	ATP	C1'-N9-C8	-8.61	107.69	127.14
2	B	804	ATP	C4-N9-C1'	8.24	146.22	126.59
4	B	802	COH	C4B-C3B-C2B	-7.78	100.36	106.75
4	B	802	COH	C4C-C3C-C2C	-7.73	100.98	107.11
2	A	801	ATP	C4-N9-C1'	7.61	144.72	126.59
4	B	803	COH	C3B-C2B-C1B	-7.28	100.12	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	802	COH	C3C-C4C-NC	6.89	116.81	109.67
4	B	802	COH	C2B-C1B-NB	-6.28	105.40	110.81
4	A	804	COH	C3B-C2B-C1B	-5.62	101.70	107.08
2	A	801	ATP	N3-C2-N1	-5.47	120.05	128.60
4	A	805	COH	C4C-C3C-C2C	-5.26	102.94	107.11
4	A	803	COH	C4C-C3C-C2C	-5.23	102.96	107.11
4	B	801	COH	C3B-C2B-C1B	-5.22	102.09	107.08
2	A	801	ATP	C5-C4-N3	-5.20	119.96	126.75
4	A	804	COH	C4C-C3C-C2C	-5.18	103.00	107.11
4	B	801	COH	C4C-C3C-C2C	-5.07	103.09	107.11
4	B	802	COH	CHB-C1B-NB	-5.07	118.03	124.83
4	A	803	COH	C3B-C2B-C1B	-5.04	102.27	107.08
2	B	804	ATP	N3-C2-N1	-5.03	120.73	128.60
4	B	803	COH	C4C-C3C-C2C	-5.01	103.14	107.11
4	A	803	COH	C2B-C1B-NB	4.91	115.04	110.81
4	A	804	COH	C3C-C4C-NC	4.85	114.69	109.67
4	A	805	COH	C2B-C1B-NB	4.84	114.97	110.81
4	A	805	COH	C3B-C2B-C1B	-4.84	102.46	107.08
4	A	805	COH	C3C-C4C-NC	4.83	114.67	109.67
2	B	804	ATP	C5-C4-N3	-4.80	120.49	126.75
4	A	803	COH	C1A-NA-C4A	-4.69	100.14	105.05
4	B	802	COH	C3D-C4D-ND	-4.61	106.31	110.68
4	B	803	COH	C3C-C4C-NC	4.61	114.44	109.67
4	B	801	COH	C3C-C4C-NC	4.57	114.40	109.67
4	A	803	COH	C3C-C4C-NC	4.55	114.38	109.67
4	B	802	COH	CAD-CBD-CGD	-4.49	103.94	113.60
4	B	802	COH	C1D-C2D-C3D	-4.36	101.72	106.83
4	B	802	COH	CMB-C2B-C1B	-4.22	117.28	124.71
4	B	801	COH	C2B-C1B-NB	4.19	114.42	110.81
2	A	801	ATP	N9-C8-N7	-3.98	108.47	113.91
2	A	801	ATP	N6-C6-N1	-3.87	109.87	118.35
4	B	802	COH	CMA-C3A-C4A	-3.84	119.19	125.04
4	B	802	COH	C1A-NA-C4A	-3.83	101.04	105.05
2	B	804	ATP	N6-C6-N1	-3.70	110.26	118.35
4	A	804	COH	C1A-NA-C4A	-3.67	101.21	105.05
4	B	801	COH	C1A-NA-C4A	-3.62	101.26	105.05
4	B	801	COH	CMC-C2C-C1C	-3.57	119.60	125.04
2	A	801	ATP	C2-N3-C4	3.55	120.13	111.75
4	A	805	COH	C1A-NA-C4A	-3.53	101.35	105.05
4	B	803	COH	C1A-NA-C4A	-3.41	101.48	105.05
2	B	804	ATP	N9-C8-N7	-3.37	109.30	113.91
4	A	804	COH	CMC-C2C-C1C	-3.35	119.94	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	802	COH	CMD-C2D-C1D	-3.35	120.27	125.37
4	B	802	COH	C2D-C1D-ND	3.27	112.87	109.69
4	B	802	COH	CHC-C4B-C3B	-3.26	119.69	125.26
2	B	804	ATP	C5-C6-N6	3.21	130.41	123.43
4	A	803	COH	CMC-C2C-C1C	-3.18	120.19	125.04
4	A	805	COH	CMC-C2C-C1C	-3.17	120.21	125.04
2	B	804	ATP	C2-N3-C4	3.13	119.14	111.75
2	A	801	ATP	C5-C6-N6	3.07	130.12	123.43
4	A	804	COH	C2B-C1B-NB	3.06	113.44	110.81
2	A	801	ATP	C5-N7-C8	3.03	107.81	103.51
4	B	802	COH	CHD-C4C-NC	-2.99	119.80	124.39
4	B	803	COH	CMC-C2C-C1C	-2.94	120.56	125.04
2	A	801	ATP	N3-C4-N9	2.93	131.91	127.08
4	B	801	COH	CMC-C2C-C3C	2.76	135.05	128.30
4	B	803	COH	C2B-C1B-NB	2.74	113.17	110.81
4	B	802	COH	CHB-C4A-C3A	-2.68	120.79	124.98
4	A	804	COH	CMC-C2C-C3C	2.67	134.84	128.30
2	B	804	ATP	N3-C4-N9	2.58	131.34	127.08
4	A	803	COH	C3D-C4D-ND	-2.51	108.30	110.68
4	A	803	COH	CMC-C2C-C3C	2.51	134.44	128.30
4	A	805	COH	CMC-C2C-C3C	2.50	134.43	128.30
4	B	802	COH	CAC-C3C-C2C	2.48	136.77	128.60
4	A	803	COH	CHB-C4A-C3A	-2.46	121.14	124.98
4	B	802	COH	CMA-C3A-C2A	2.43	132.71	126.12
4	B	801	COH	CHB-C4A-C3A	-2.42	121.20	124.98
2	B	804	ATP	C5-N7-C8	2.42	106.95	103.51
4	B	801	COH	CHC-C1C-NC	-2.41	120.39	124.82
4	A	804	COH	CHB-C4A-C3A	-2.41	121.22	124.98
4	B	803	COH	CMC-C2C-C3C	2.40	134.16	128.30
4	A	803	COH	C1D-C2D-C3D	-2.37	104.06	106.83
4	B	801	COH	C3A-C4A-NA	2.29	113.46	110.83
2	B	804	ATP	C2'-C3'-C4'	2.28	107.08	102.64
4	A	804	COH	CHC-C1C-NC	-2.28	120.62	124.82
4	A	805	COH	CHB-C4A-C3A	-2.27	121.43	124.98
2	A	801	ATP	C2'-C3'-C4'	2.27	107.05	102.64
4	A	805	COH	CHC-C1C-NC	-2.24	120.69	124.82
4	A	805	COH	CMD-C2D-C3D	2.22	130.40	125.61
4	B	801	COH	CMB-C2B-C3B	2.21	133.72	128.30
4	B	801	COH	C2D-C1D-ND	2.20	111.83	109.69
4	B	802	COH	CHA-C4D-C3D	-2.17	120.61	125.36
4	B	802	COH	O1D-CGD-CBD	-2.17	116.11	123.08
2	B	804	ATP	C6-C5-C4	2.17	120.10	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	ATP	C4-C5-N7	-2.15	108.00	110.62
4	A	803	COH	CMD-C2D-C3D	2.12	130.20	125.61
4	B	803	COH	CHA-C1A-NA	-2.11	121.15	124.39
4	B	803	COH	CHC-C1C-NC	-2.11	120.94	124.82
4	B	801	COH	CHB-C1B-NB	-2.11	122.00	124.83
4	B	801	COH	CMD-C2D-C3D	2.10	130.15	125.61
2	B	804	ATP	C4'-O4'-C1'	-2.08	104.88	109.47
4	A	803	COH	CHC-C4B-C3B	-2.08	121.70	125.26
4	B	802	COH	CHC-C1C-NC	-2.07	121.01	124.82
4	A	804	COH	C2D-C1D-ND	2.06	111.69	109.69
2	B	804	ATP	C5-C4-N9	2.06	108.17	105.78
4	A	805	COH	C3A-C4A-NA	2.04	113.18	110.83
4	A	805	COH	C3D-C4D-ND	-2.03	108.75	110.68
4	A	804	COH	C1D-C2D-C3D	-2.03	104.46	106.83
2	A	801	ATP	C5-C4-N9	2.02	108.13	105.78
4	B	802	COH	C3B-C4B-NB	-2.02	106.23	109.27
2	B	804	ATP	O4'-C1'-N9	2.01	112.03	108.06
4	B	802	COH	O1A-CGA-CBA	-2.01	116.64	123.08
4	A	804	COH	CHB-C1B-C2B	-2.01	121.27	125.48
4	A	805	COH	C1D-C2D-C3D	-2.00	104.49	106.83

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	803	COH	NB
4	A	804	COH	NB
4	A	805	COH	NB
4	B	801	COH	NB
4	B	802	COH	NB
4	B	803	COH	NB

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	COH	C2B-C3B-CAB-CBB
4	A	803	COH	C4B-C3B-CAB-CBB
4	A	805	COH	C2B-C3B-CAB-CBB
4	B	802	COH	C4B-C3B-CAB-CBB
4	B	803	COH	C2C-C3C-CAC-CBC
4	B	803	COH	C4C-C3C-CAC-CBC
4	B	802	COH	C4D-C3D-CAD-CBD
4	B	803	COH	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
4	B	801	COH	C2B-C3B-CAB-CBB
4	A	805	COH	C4B-C3B-CAB-CBB
4	A	804	COH	C3A-C2A-CAA-CBA
4	A	804	COH	C2B-C3B-CAB-CBB
4	B	802	COH	C2B-C3B-CAB-CBB
4	A	805	COH	C2D-C3D-CAD-CBD
2	B	804	ATP	PA-O3A-PB-O1B
2	A	801	ATP	PA-O3A-PB-O1B
4	A	803	COH	C3D-CAD-CBD-CGD
4	A	804	COH	CAD-CBD-CGD-O2D
4	B	802	COH	CAD-CBD-CGD-O2D
4	A	803	COH	CAD-CBD-CGD-O1D
4	A	805	COH	CAA-CBA-CGA-O1A
4	A	805	COH	CAD-CBD-CGD-O2D
4	B	801	COH	CAA-CBA-CGA-O1A
4	A	804	COH	CAD-CBD-CGD-O1D
4	A	803	COH	CAD-CBD-CGD-O2D
4	A	805	COH	CAA-CBA-CGA-O2A
4	A	805	COH	CAD-CBD-CGD-O1D
4	A	804	COH	CAA-CBA-CGA-O1A
4	B	803	COH	CAA-CBA-CGA-O1A
2	B	804	ATP	PA-O3A-PB-O2B
4	A	805	COH	C3D-CAD-CBD-CGD
4	B	801	COH	CAA-CBA-CGA-O2A
4	A	803	COH	CAA-CBA-CGA-O2A
4	B	802	COH	CAD-CBD-CGD-O1D
4	B	803	COH	CAA-CBA-CGA-O2A

There are no ring outliers.

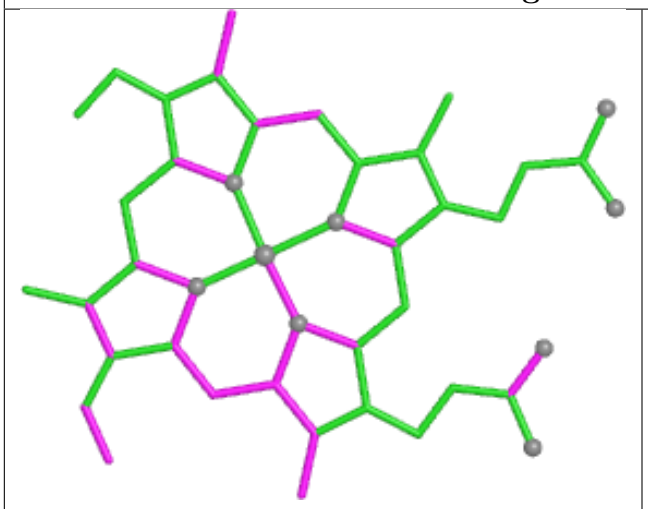
6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	COH	1	0
4	A	804	COH	3	0
4	B	801	COH	2	0
4	A	805	COH	2	0
2	B	804	ATP	1	0
4	B	802	COH	6	0

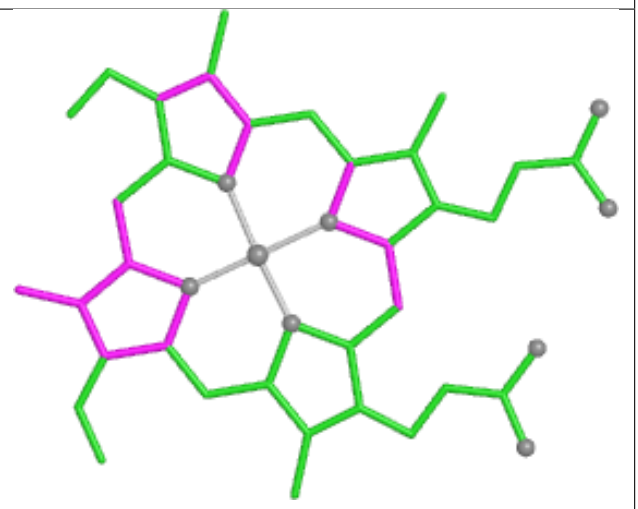
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

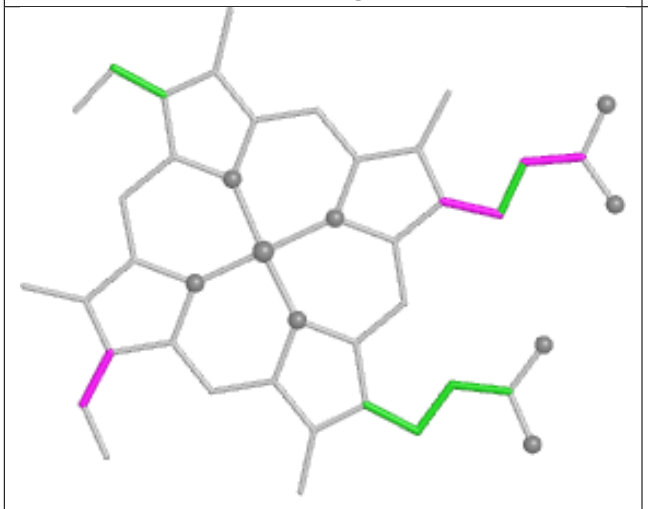
Ligand COH B 803



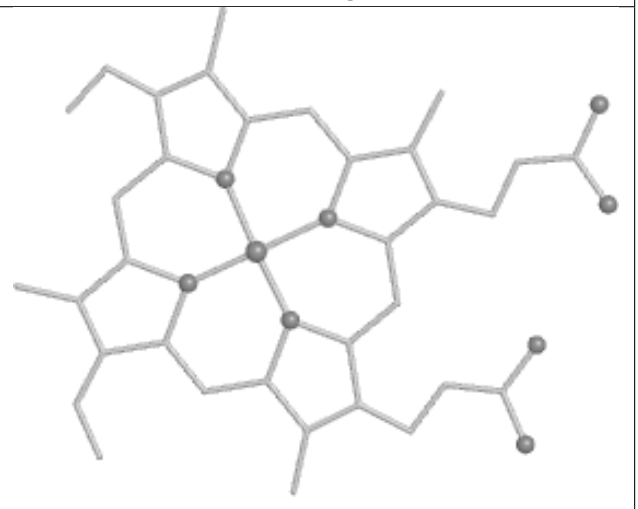
Bond lengths



Bond angles

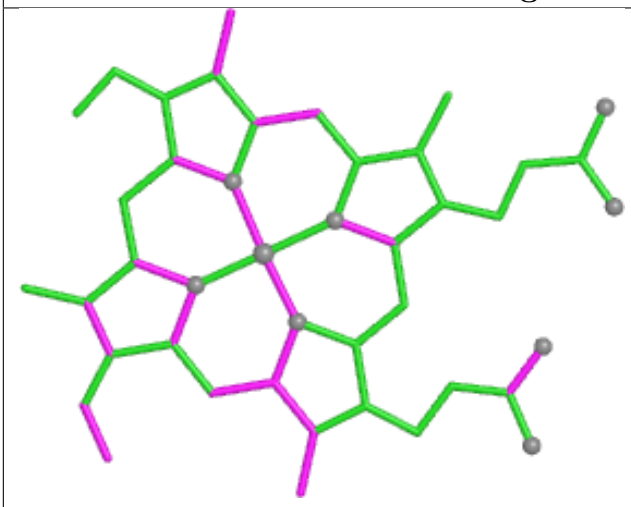


Torsions

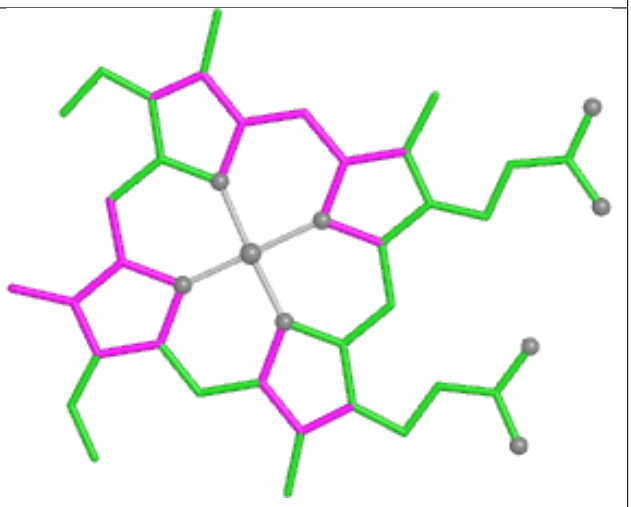


Rings

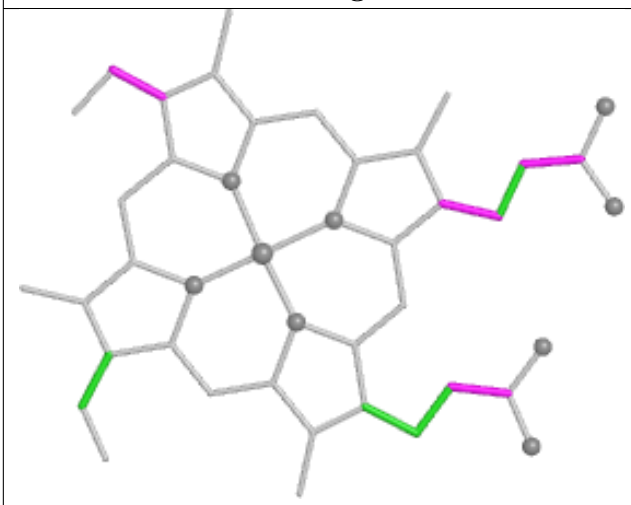
Ligand COH A 804



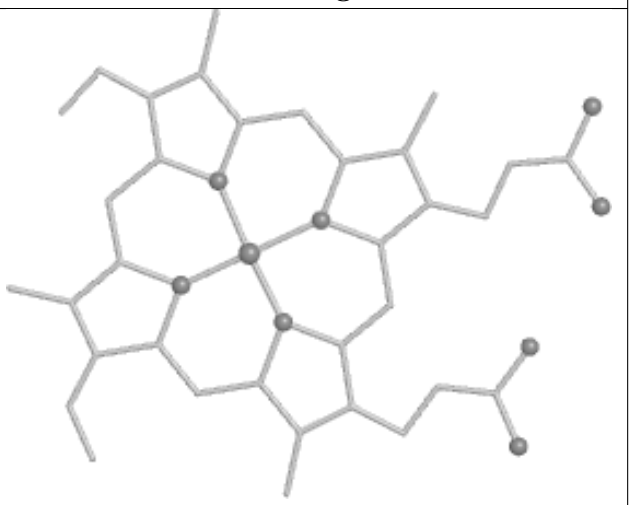
Bond lengths



Bond angles

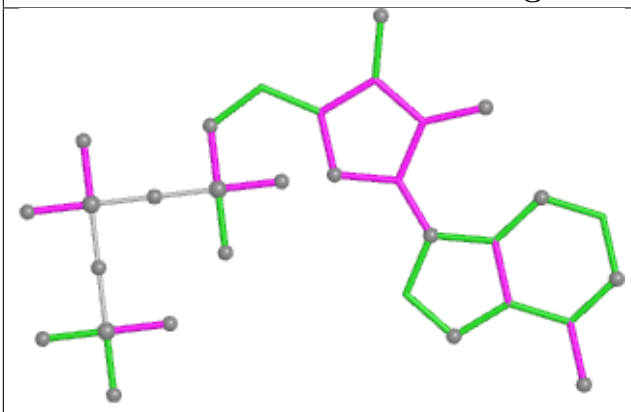


Torsions

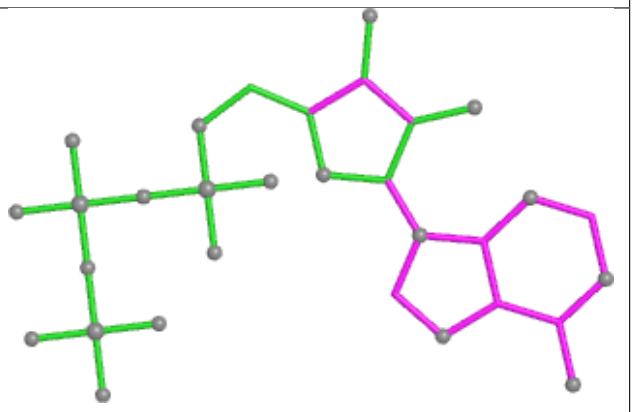


Rings

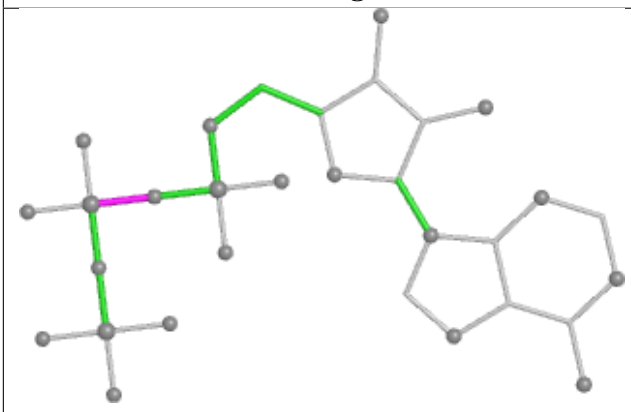
Ligand ATP A 801



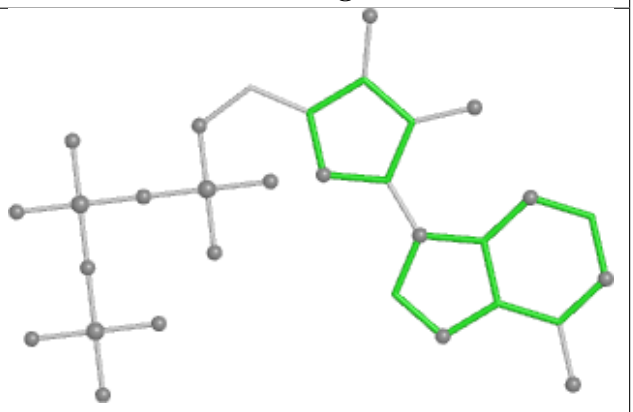
Bond lengths



Bond angles

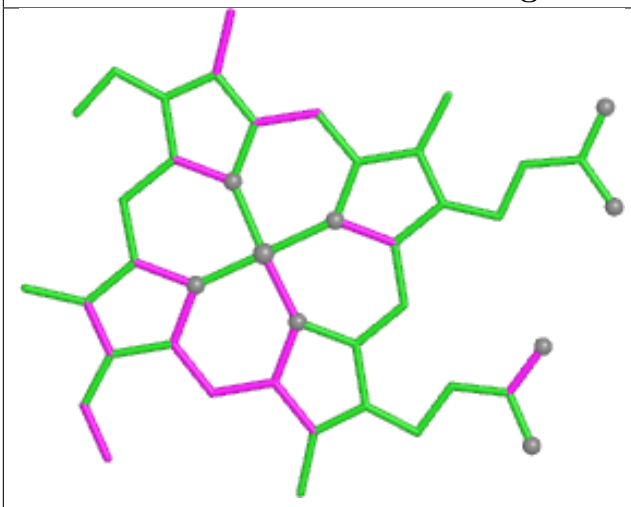


Torsions

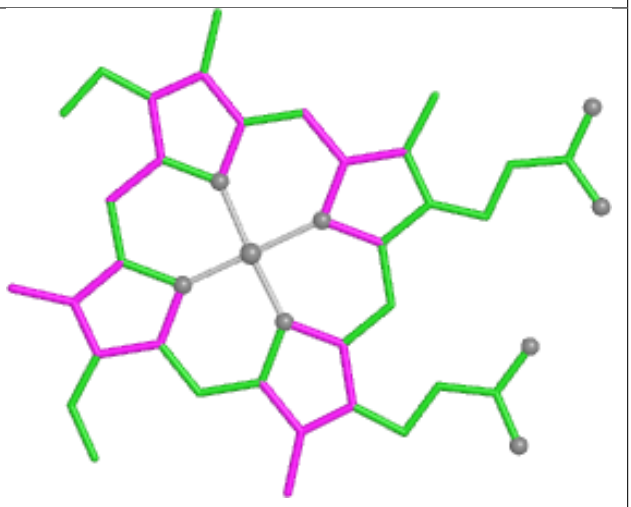


Rings

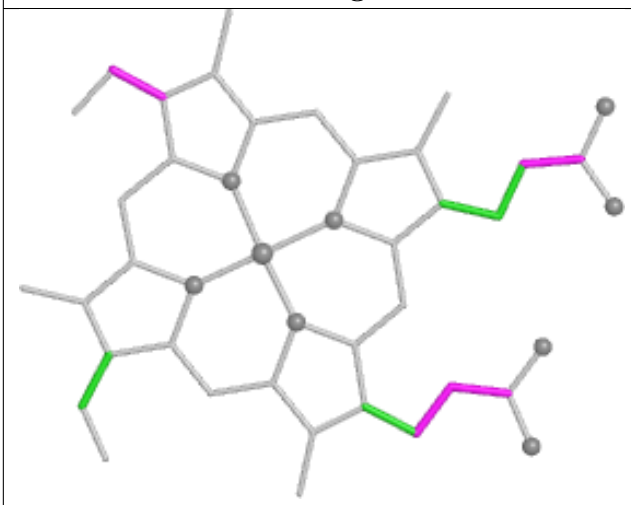
Ligand COH A 803



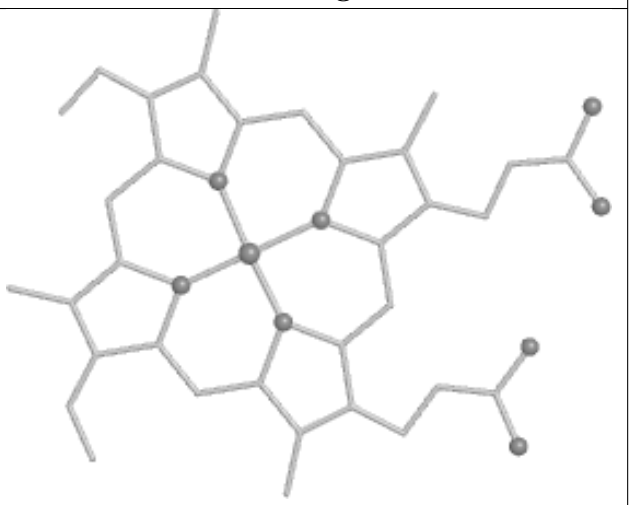
Bond lengths



Bond angles

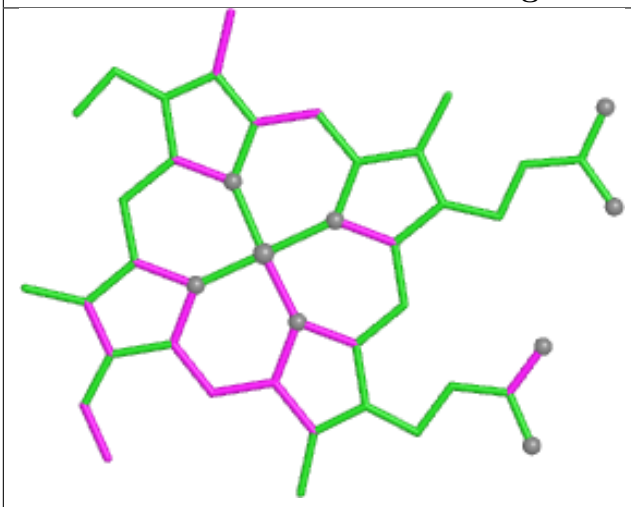


Torsions

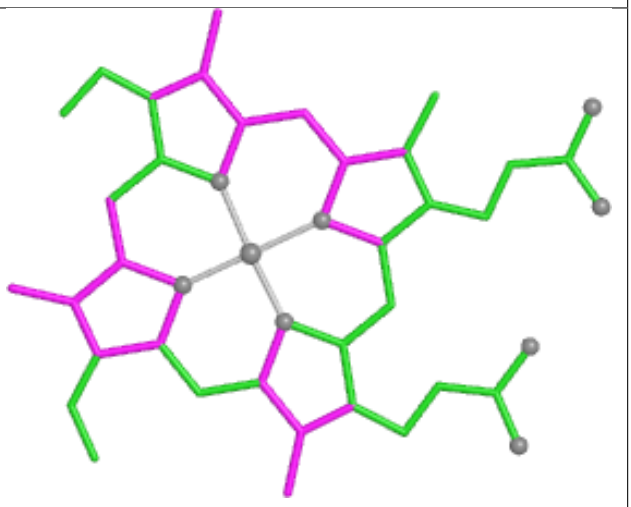


Rings

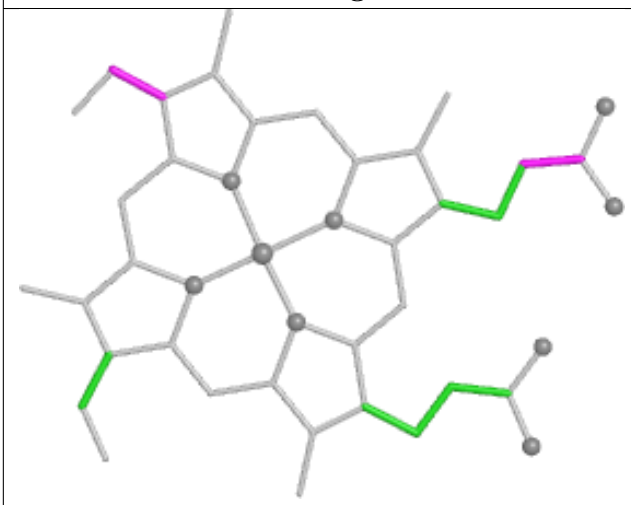
Ligand COH B 801



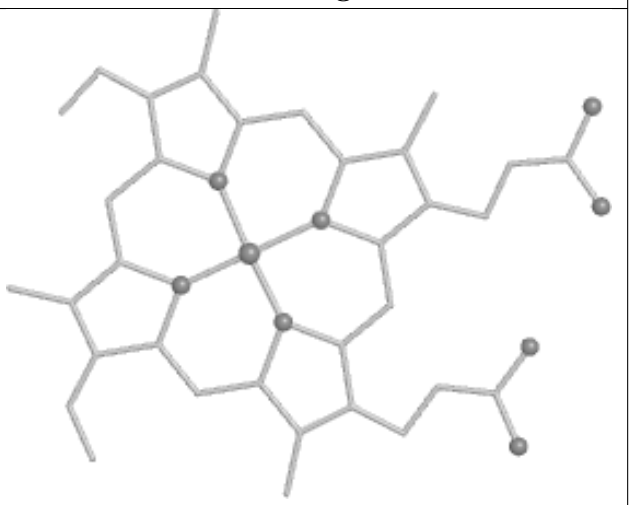
Bond lengths



Bond angles

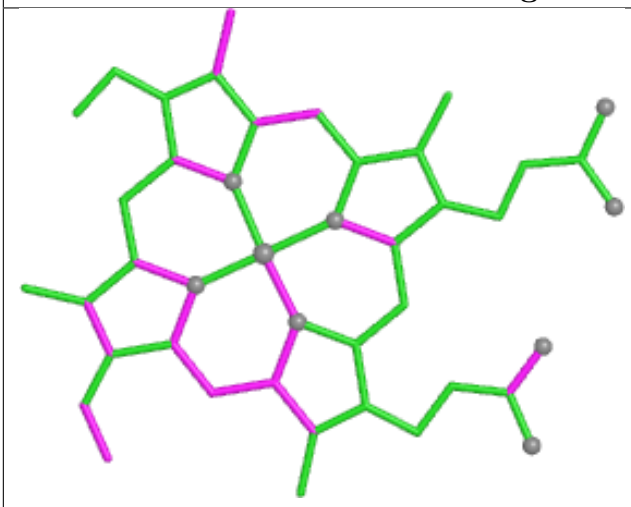


Torsions

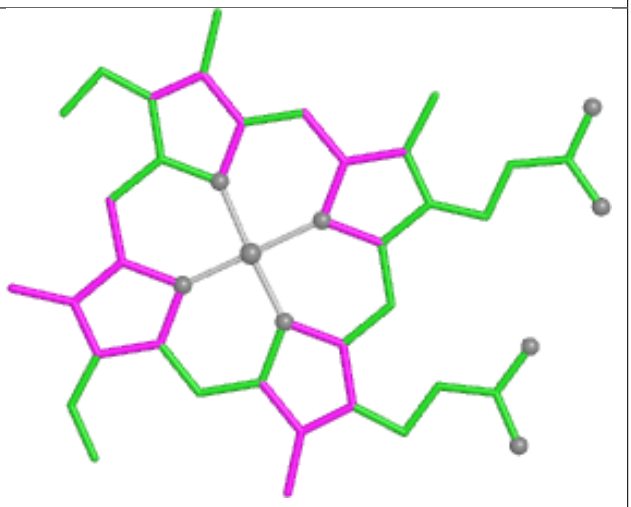


Rings

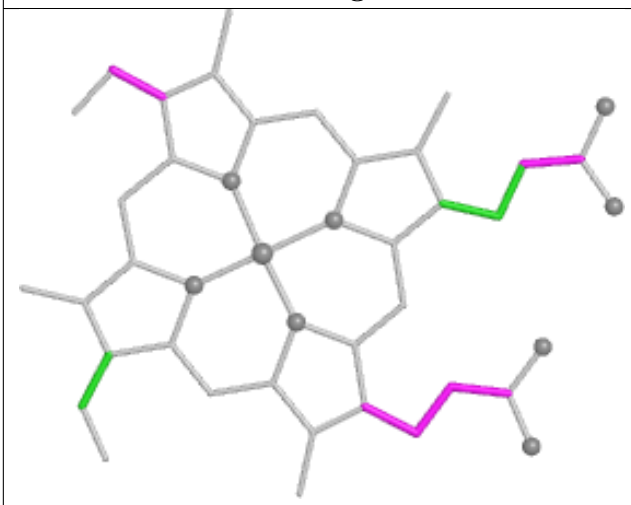
Ligand COH A 805



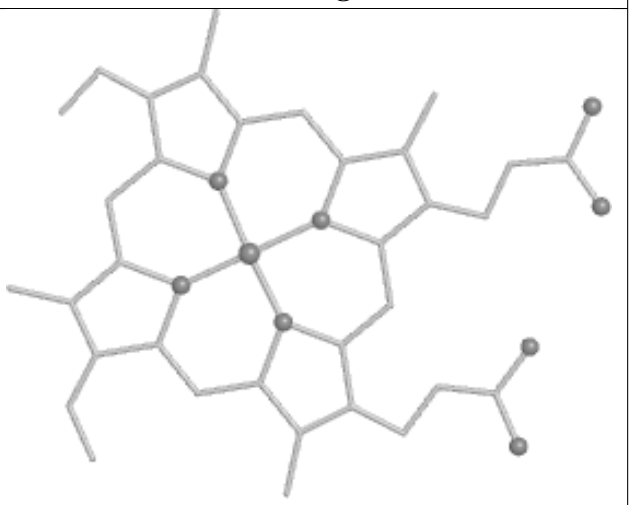
Bond lengths



Bond angles

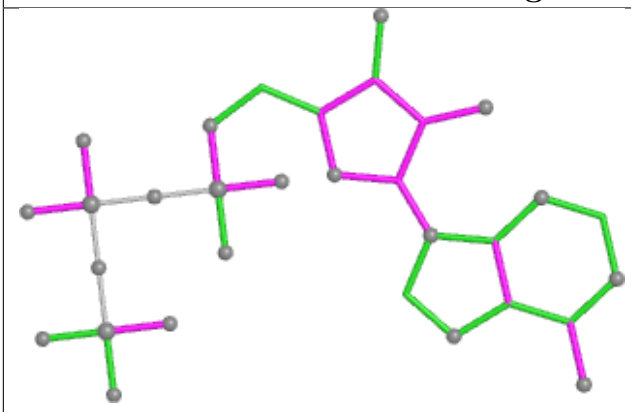


Torsions

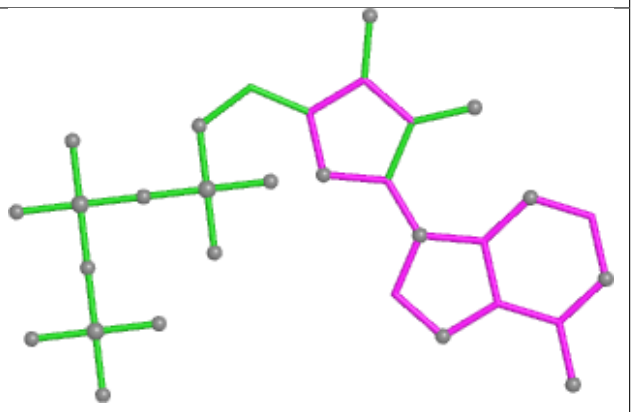


Rings

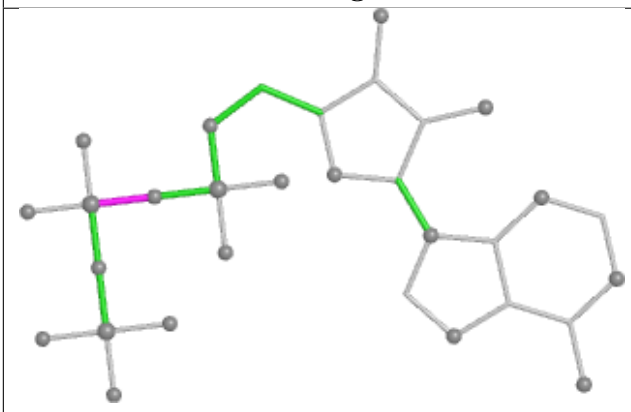
Ligand ATP B 804



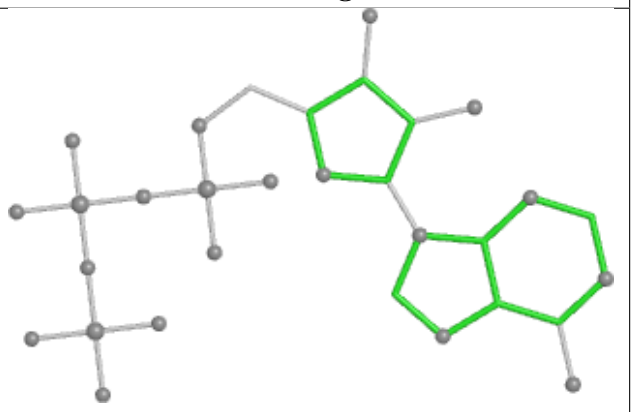
Bond lengths



Bond angles

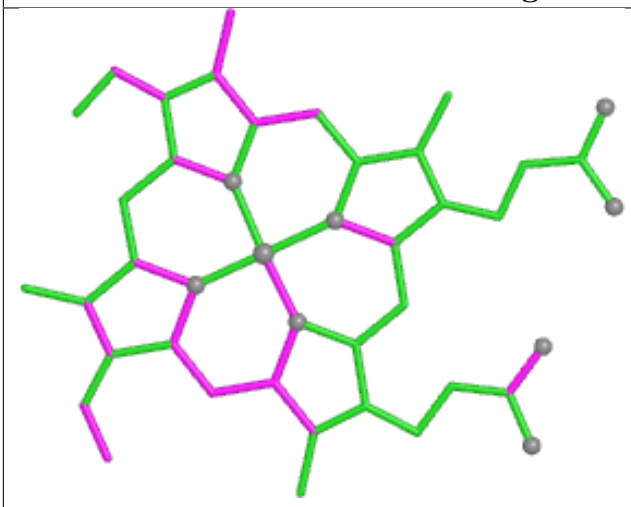


Torsions

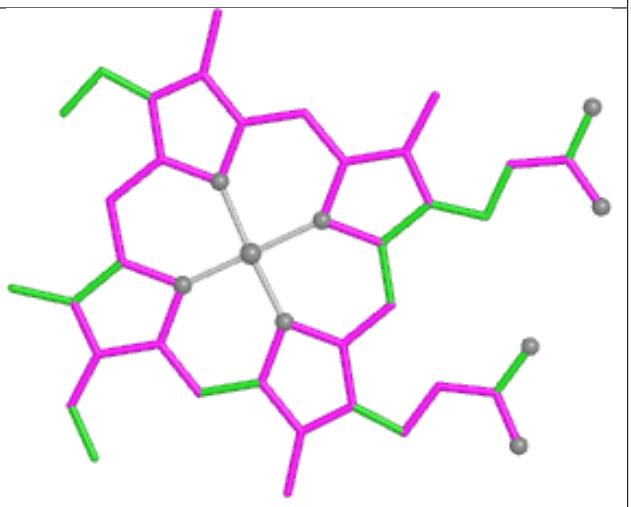


Rings

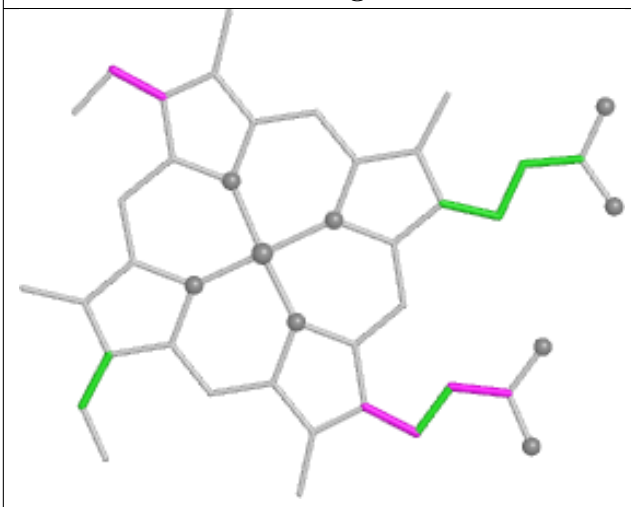
Ligand COH B 802



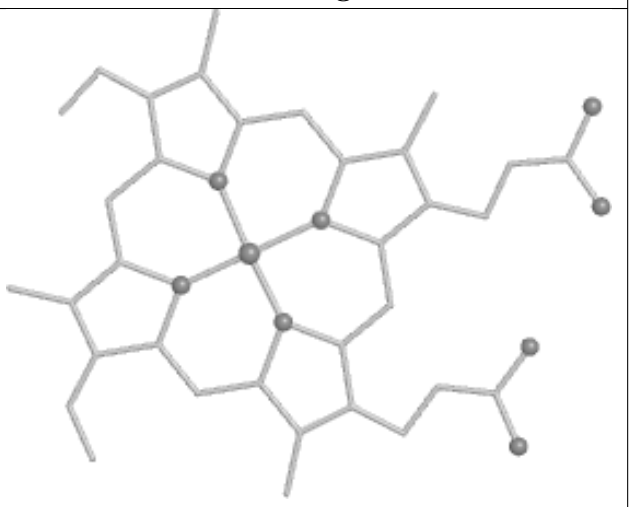
Bond lengths



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.

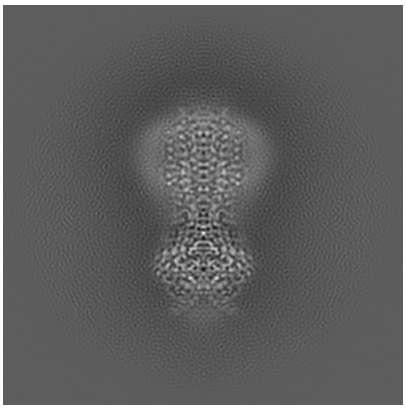
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-69145. These allow visual inspection of the internal detail of the map and identification of artifacts.

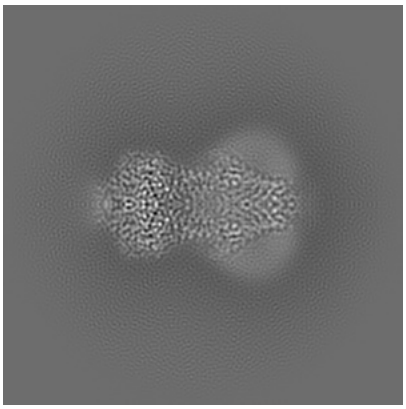
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

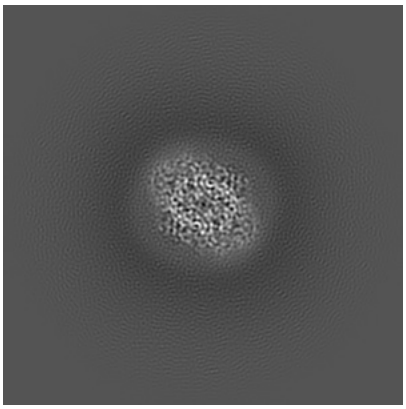
6.1.1 Primary map



X

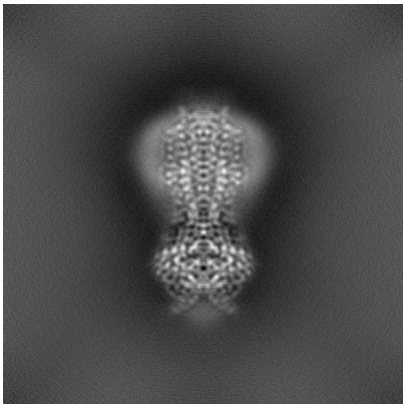


Y

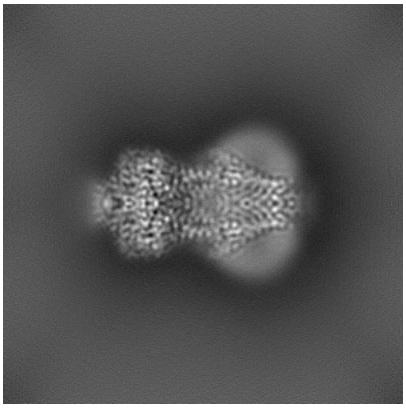


Z

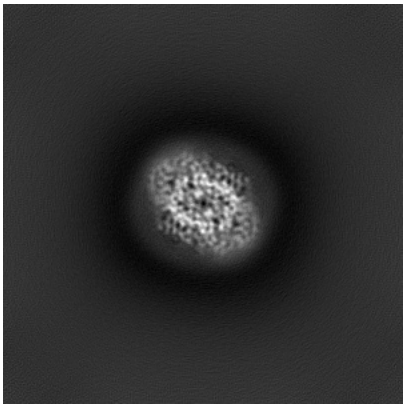
6.1.2 Raw map



X



Y

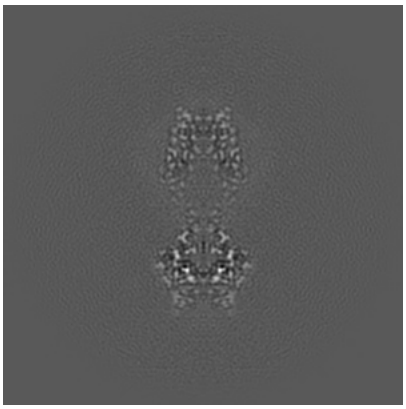


Z

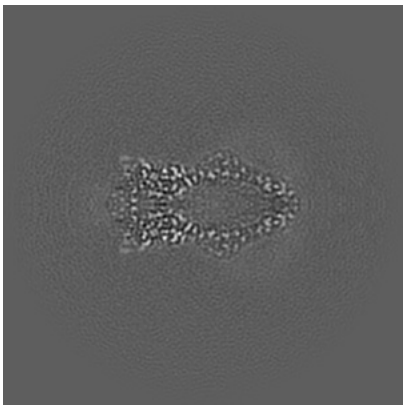
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

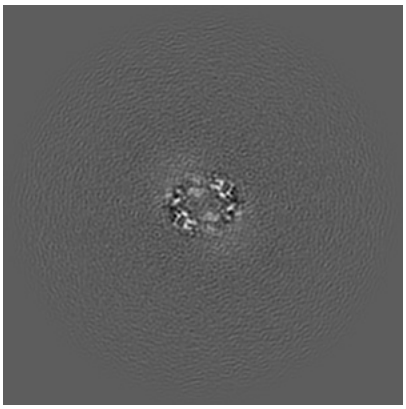
6.2.1 Primary map



X Index: 180

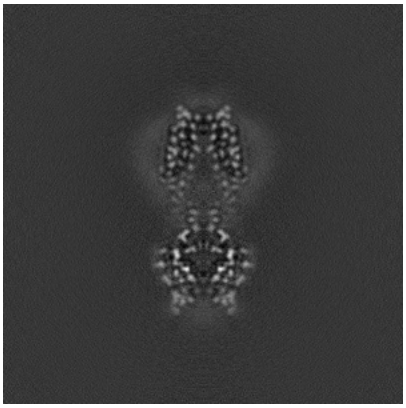


Y Index: 180

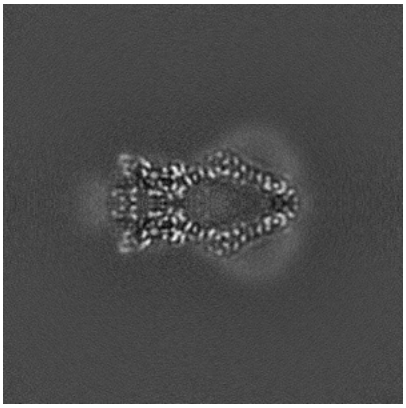


Z Index: 180

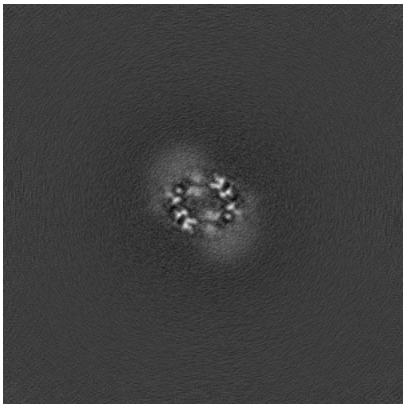
6.2.2 Raw map



X Index: 180



Y Index: 180

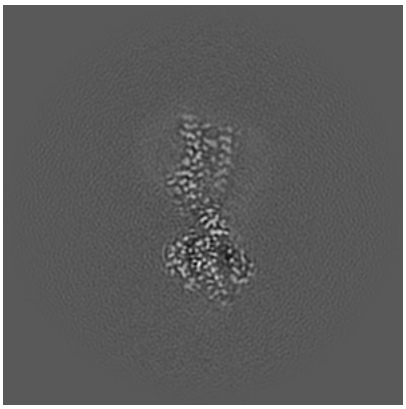


Z Index: 180

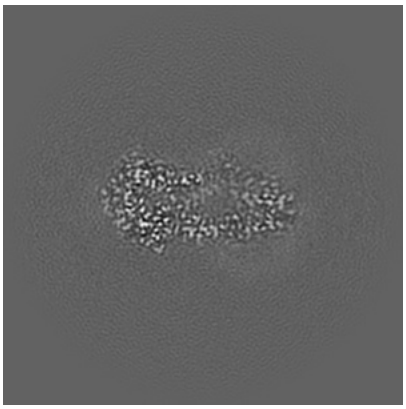
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

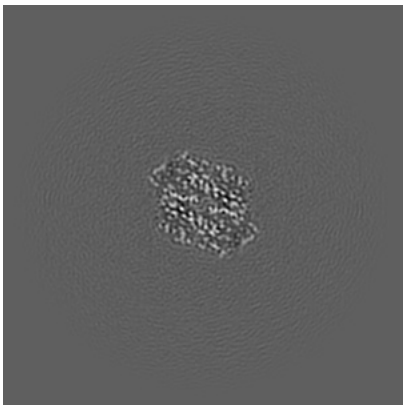
6.3.1 Primary map



X Index: 160

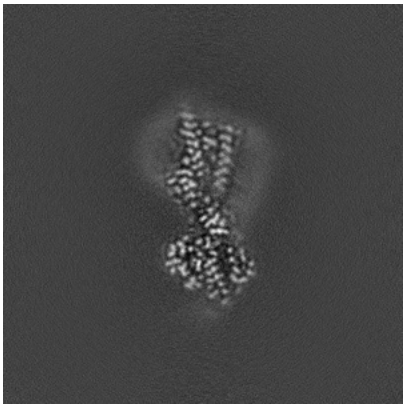


Y Index: 170

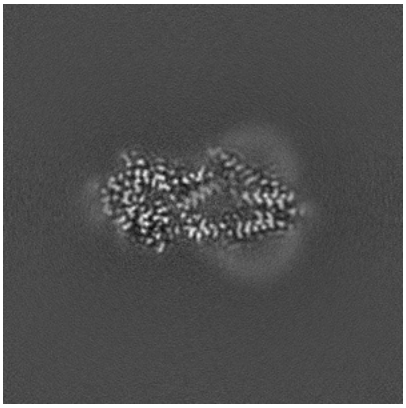


Z Index: 127

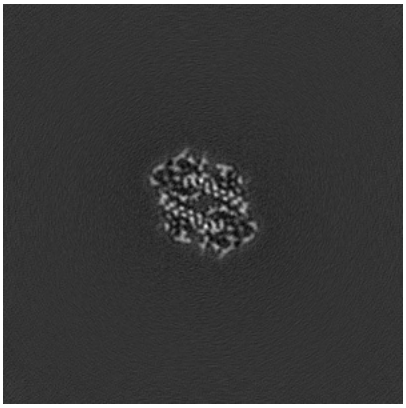
6.3.2 Raw map



X Index: 160



Y Index: 171

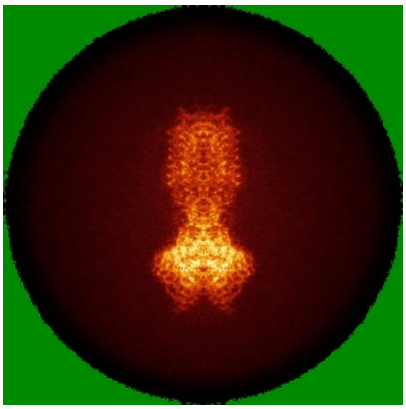


Z Index: 126

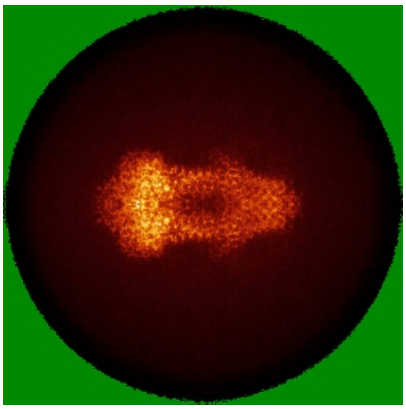
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

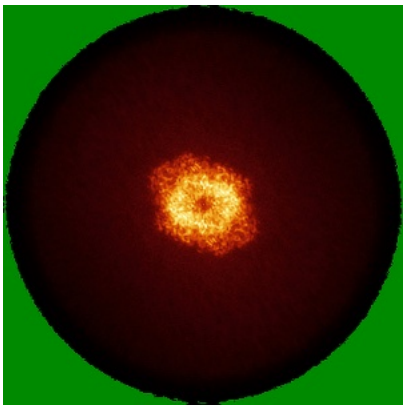
6.4.1 Primary map



X

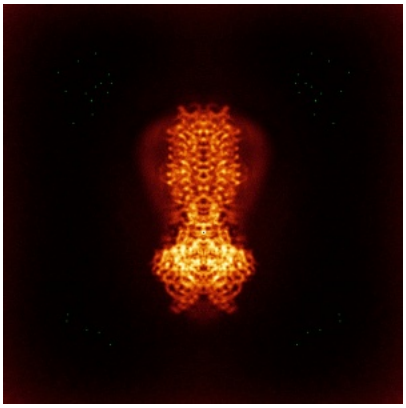


Y

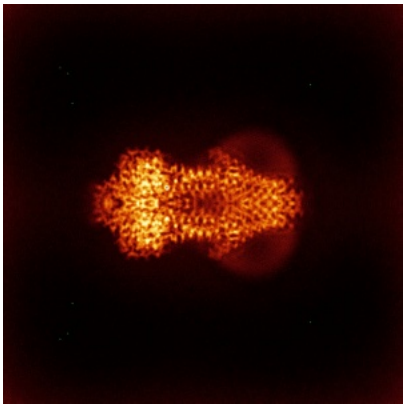


Z

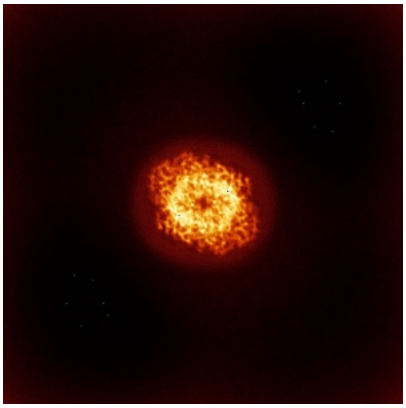
6.4.2 Raw map



X



Y



Z

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

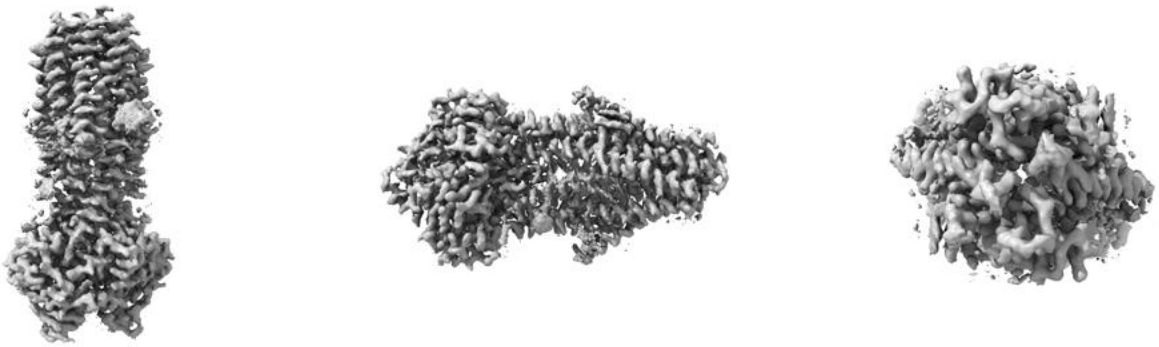
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.534. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

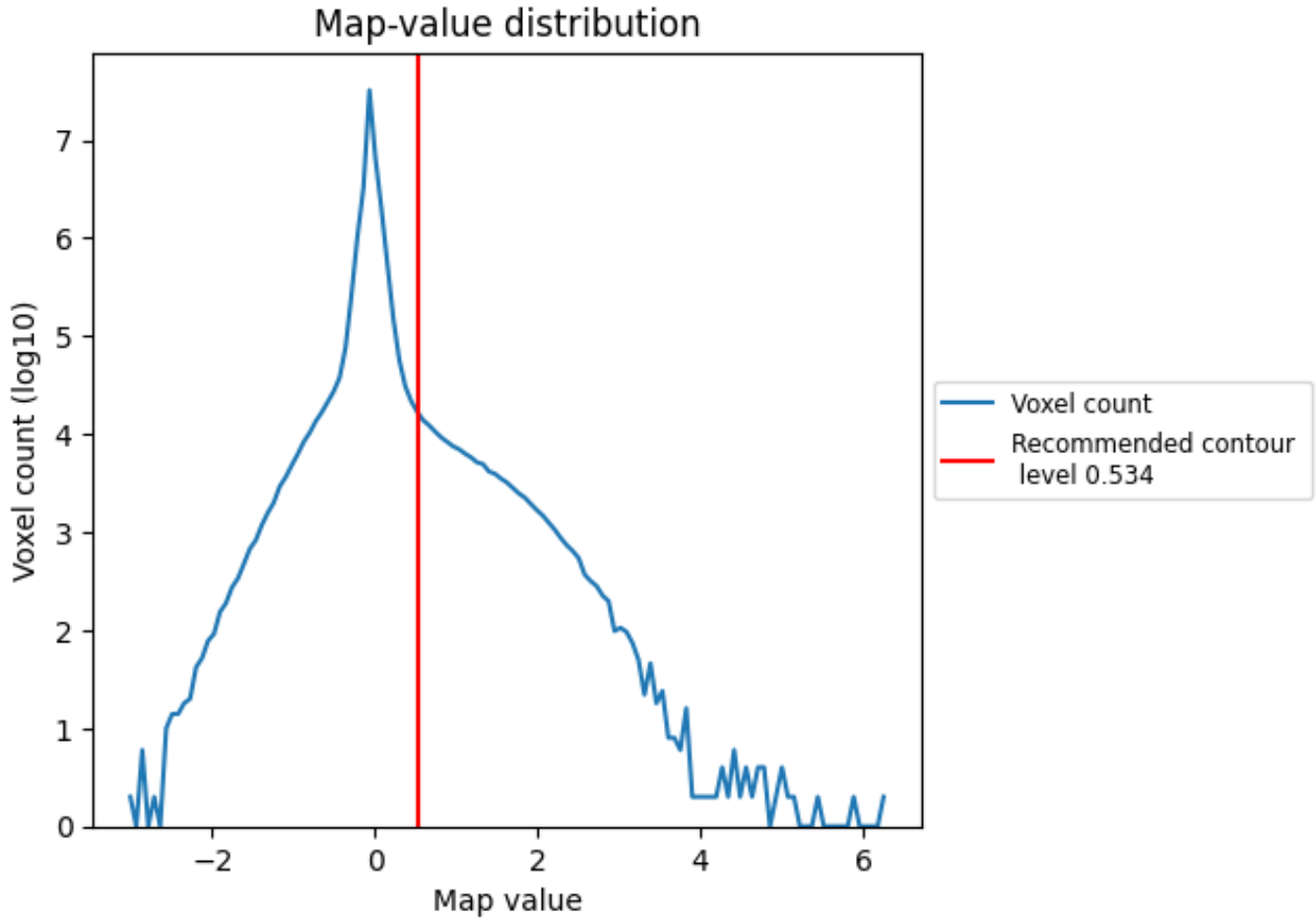
6.6 Mask visualisation (i)

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

7 Map analysis

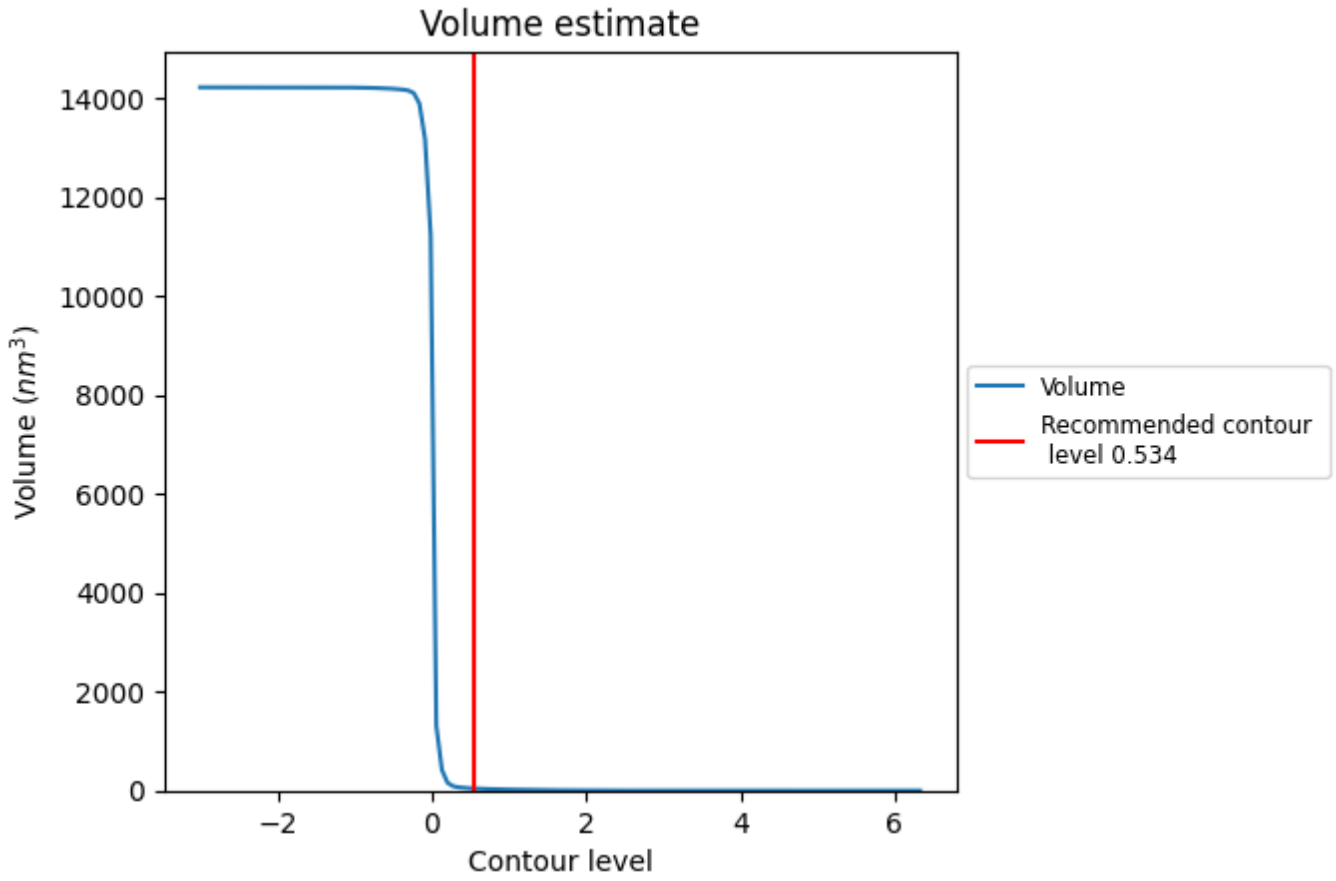
This section contains the results of statistical analysis of the map.

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.

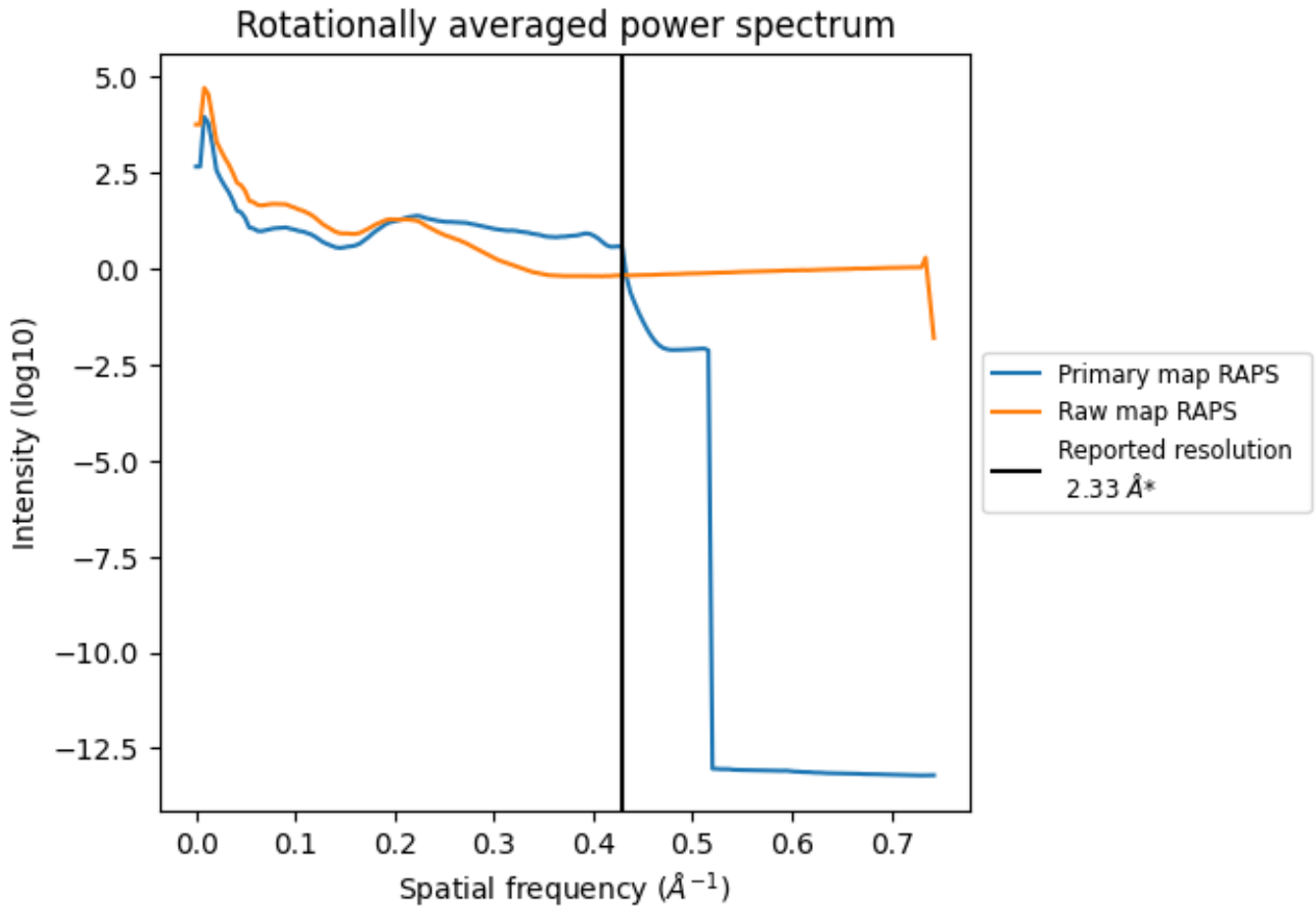
7.2 Volume estimate



The volume at the recommended contour level is 43 nm^3; this corresponds to an approximate mass of 39 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)

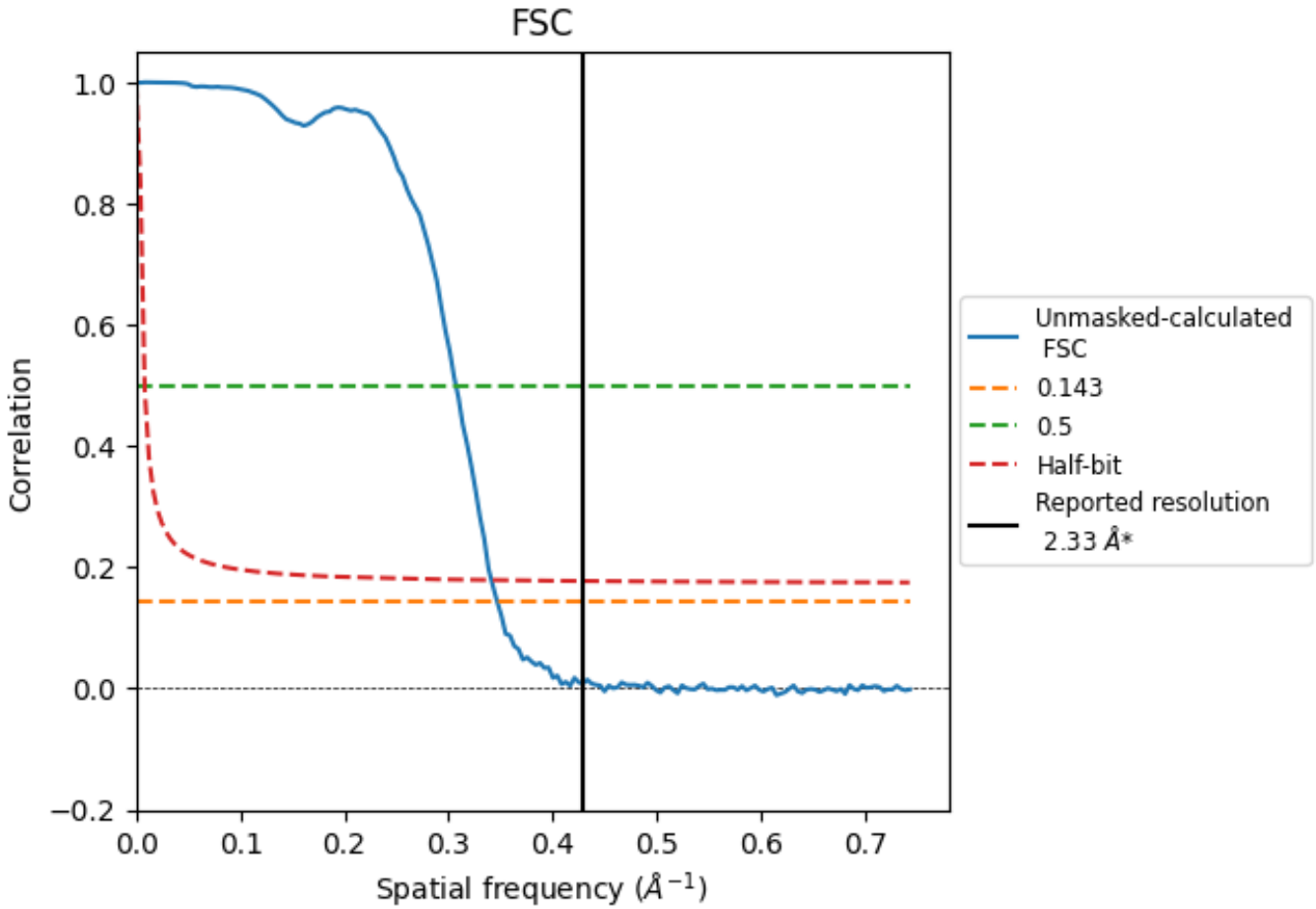


*Reported resolution corresponds to spatial frequency of 0.429 Å^{-1}

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 0.429 Å^{-1}

8.2 Resolution estimates (i)

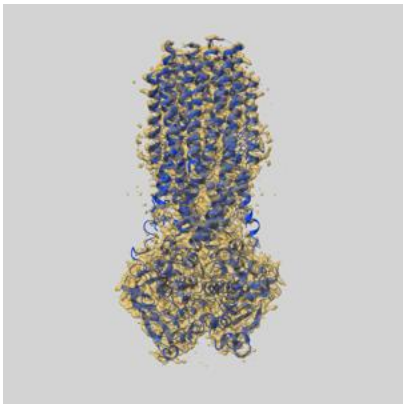
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.88	3.26	2.93

*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 2.88 differs from the reported value 2.33 by more than 10 %

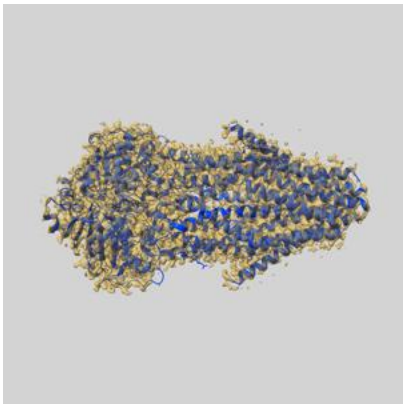
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-69145 and PDB model 23PI. Per-residue inclusion information can be found in section 3 on page 7.

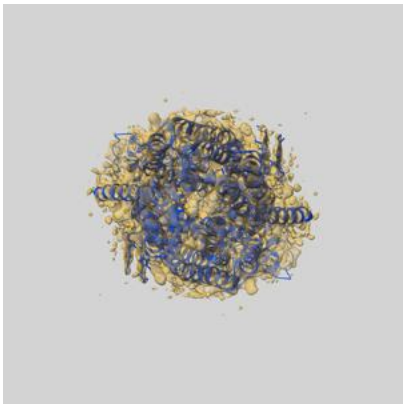
9.1 Map-model overlay



X



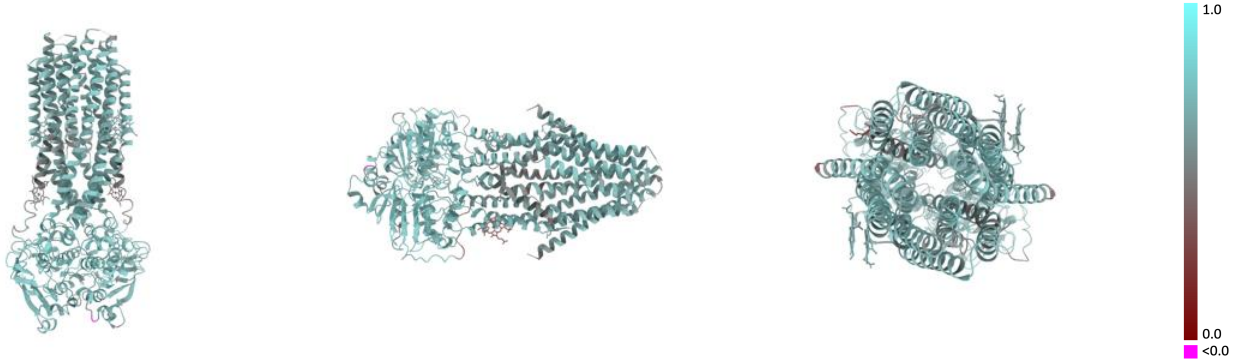
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.534 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.

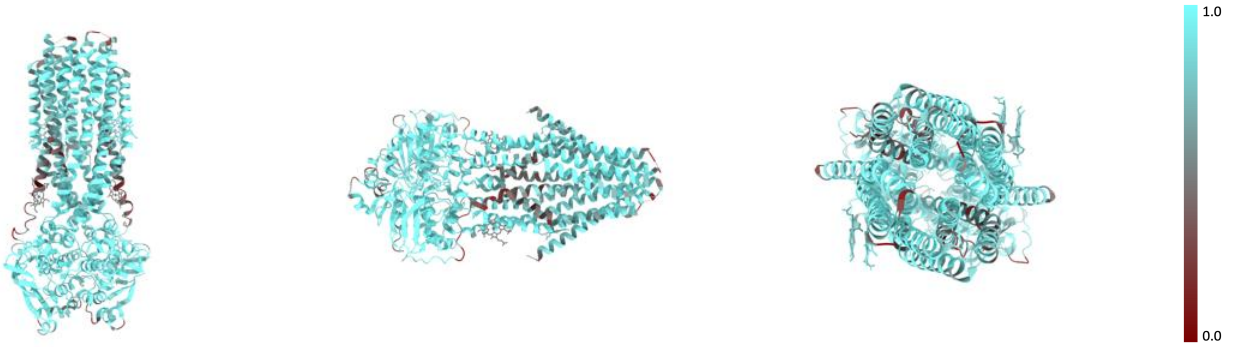
9.2 Q-score mapped to coordinate model (i)



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.

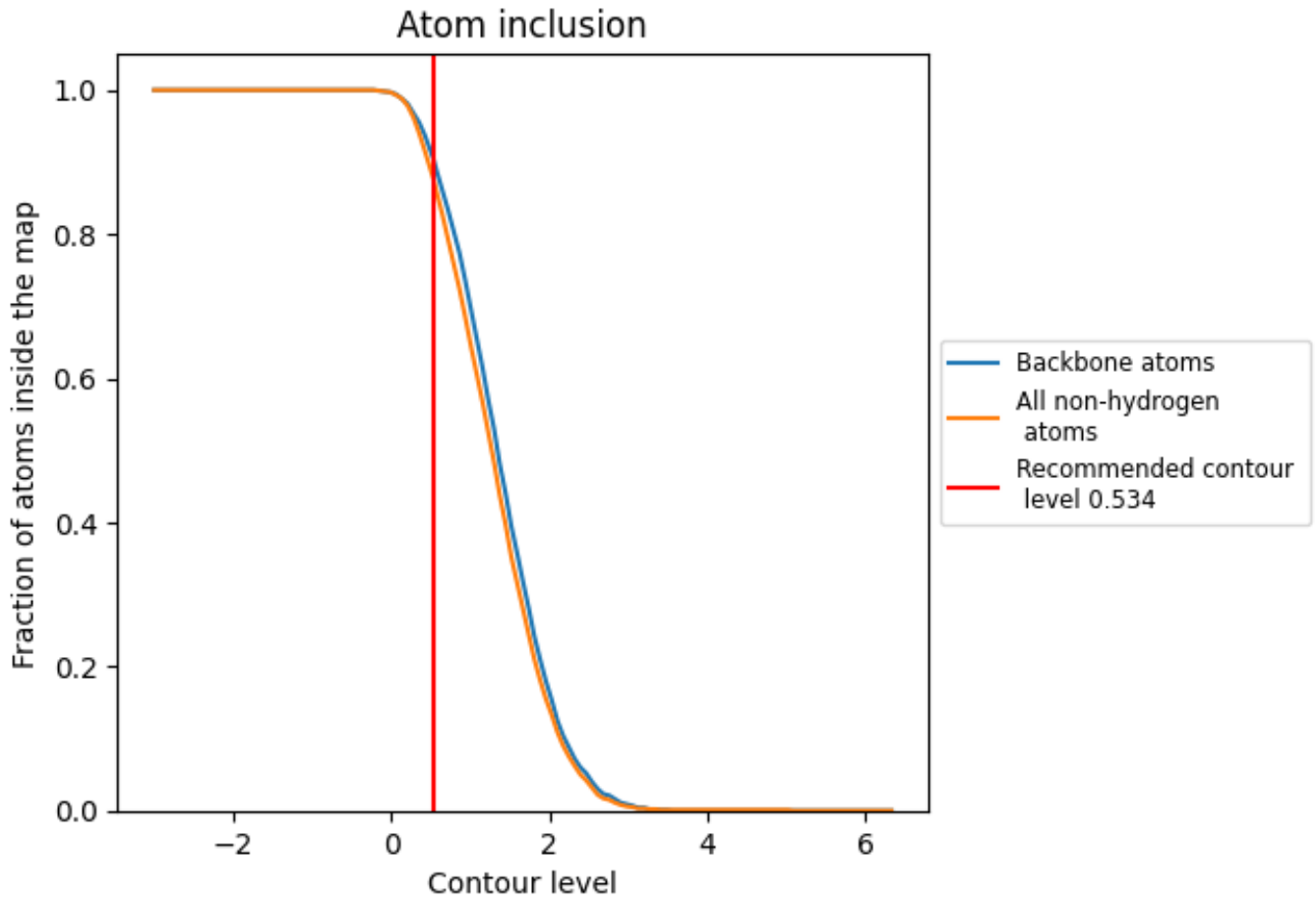
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.534).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.534) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8750	0.6590
A	0.8770	0.6610
B	0.8760	0.6570