Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 12:39 PM EDT

PDB ID	:	7MHZ
EMDB ID	:	EMD-23837
Title	:	Human Hedgehog acyltransferase (HHAT) in complex with a palmitoylated Hedgehog peptide product and a Fab antibody fragment
Authors	:	Long, S.B.; Jiang, Y.
Deposited on	:	2021-04-16
Resolution	:	3.20 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:

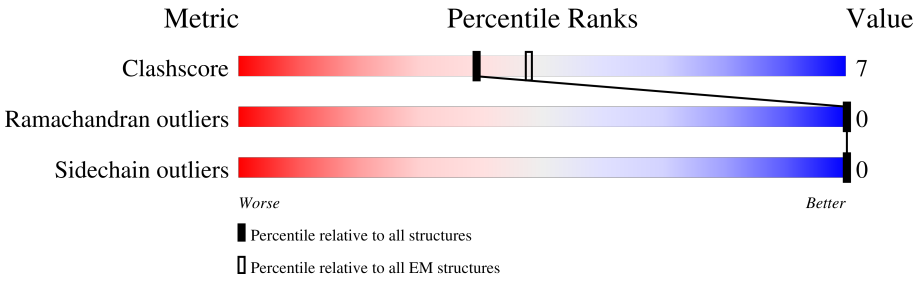
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	8	62% 38%
2	A	493	85% 15%
3	O	462	18% 6% 76%
4	P	207	44% 10% 46%

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
8	AJP	A	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	AJP	A	506	X	-	-	-
8	AJP	A	507	X	-	-	-
8	AJP	A	508	X	-	-	-
8	AJP	A	509	X	-	-	-
8	AJP	A	510	X	-	-	-
8	AJP	A	511	X	-	-	-
8	AJP	A	512	X	-	-	-
8	AJP	A	513	X	-	-	-
8	AJP	A	514	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6189 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 Sonic hedgehog protein N-product peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	8	51	31	11	8	1	0	0

- Molecule 2 is a protein called Protein-cysteine N-palmitoyltransferase HHAT.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	491	3980	2655	632	662	31	0	0

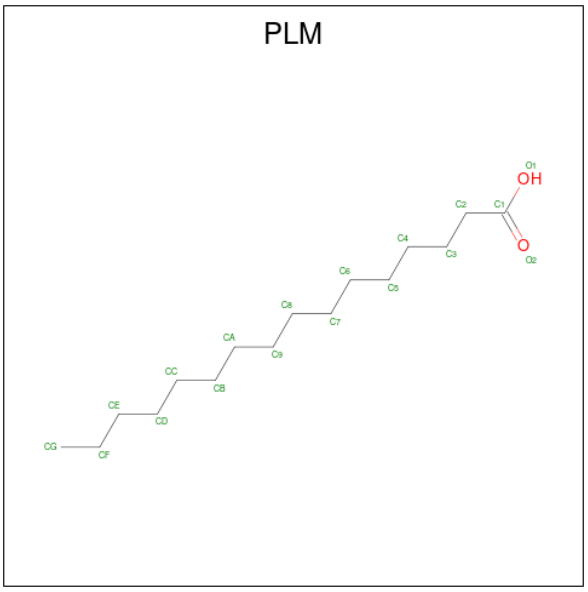
- Molecule 3 is a protein called 3H02 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	O	113	872	568	142	157	5	0	0

- Molecule 4 is a protein called 3H02 Fab light chain.

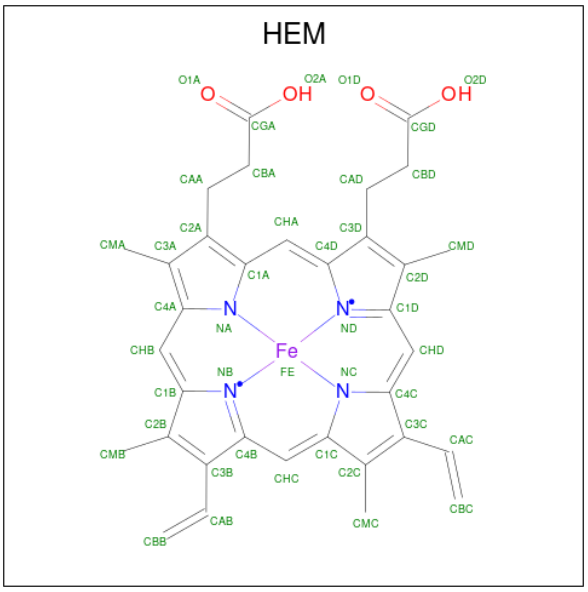
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P	111	793	508	135	147	3	0	0

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



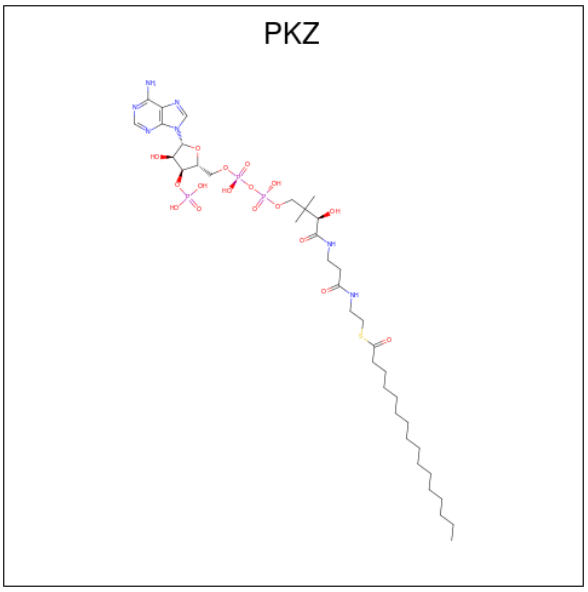
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			17	16	1	

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



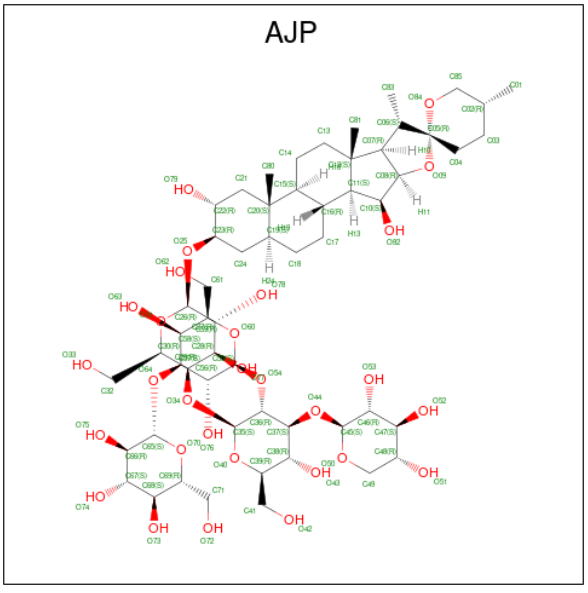
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 7 is Palmitoyl-CoA (three-letter code: PKZ) (formula: $C_{37}H_{66}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O P S 65 37 7 17 3 1	0
7	A	1	Total C N O P 33 13 2 15 3	0
7	A	1	Total C 15 15	0

- Molecule 8 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).



Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C O 43 33 10	0

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Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			31	27	4	
8	A	1	Total	C	O	0
			32	27	5	
8	A	1	Total	C	O	0
			26	23	3	
8	A	1	Total	C	O	0
			32	27	5	
8	A	1	Total	C	O	0
			32	27	5	
8	A	1	Total	C	O	0
			30	27	3	
8	A	1	Total	C	O	0
			31	27	4	
8	A	1	Total	C	O	0
			31	27	4	
8	A	1	Total	C	O	0
			32	27	5	

3 Residue-property plots (i)

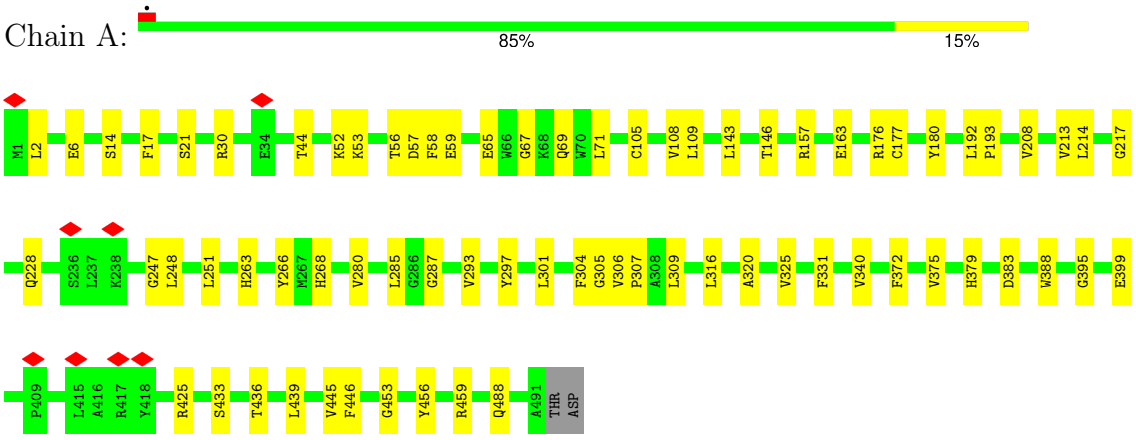
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sonic hedgehog protein N-product peptide

Chain B:

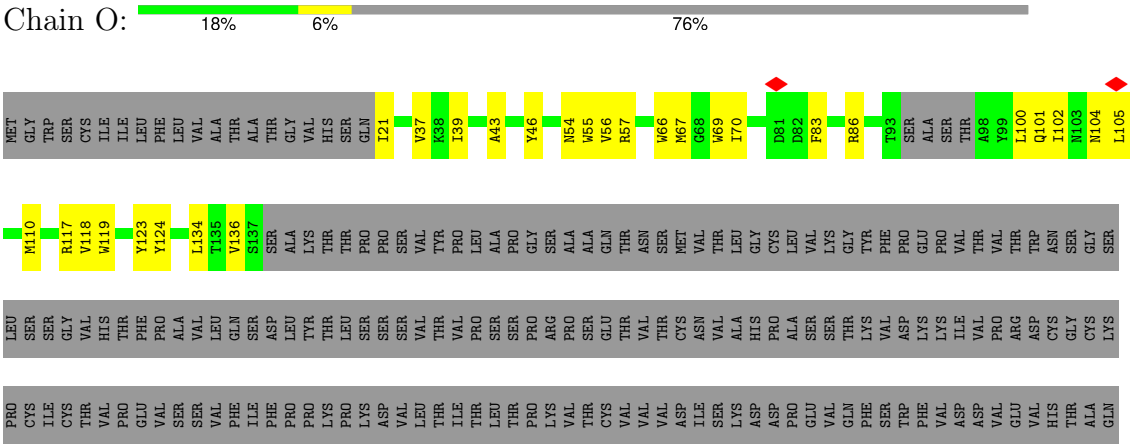
• Molecule 2: Protein-cysteine N-palmitoyltransferase HHAT

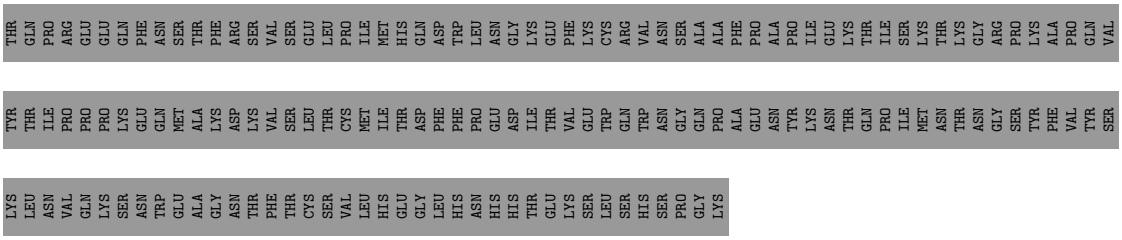
Chain A:



• Molecule 3: 3H02 Fab heavy chain

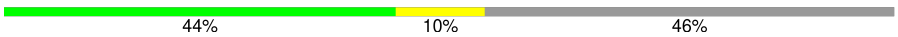
Chain O:

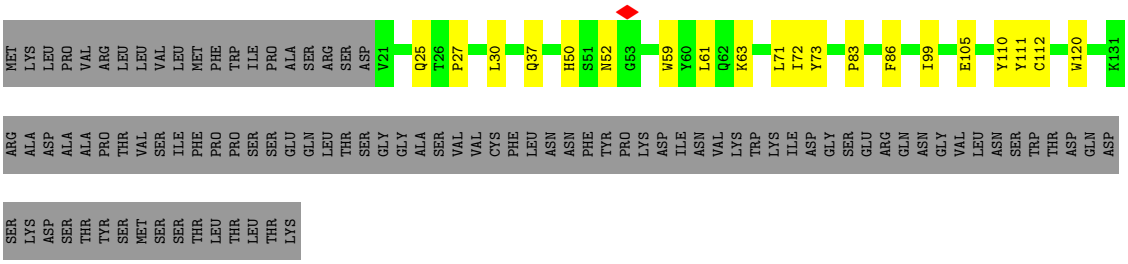




• Molecule 4: 3H02 Fab light chain

Chain P:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142121	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.960	Depositor
Minimum map value	-1.921	Depositor
Average map value	0.079	Depositor
Map value standard deviation	0.156	Depositor
Recommended contour level	0.877	Depositor
Map size (Å)	200.564, 200.564, 200.564	wwPDB
Map dimensions	377, 377, 377	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.532, 0.532, 0.532	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PKZ, HEM, AJP, PLM

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	B	0.31	0/52	0.45	0/67
2	A	0.28	0/4120	0.40	0/5630
3	O	0.29	0/899	0.46	0/1227
4	P	0.30	0/814	0.45	0/1113
All	All	0.28	0/5885	0.42	0/8037

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	51	0	45	3	0
2	A	3980	0	3879	44	0
3	O	872	0	791	22	0
4	P	793	0	711	15	0
5	B	17	0	31	3	0
6	A	43	0	30	2	0
7	A	113	0	0	3	0
8	A	320	0	0	0	0
All	All	6189	0	5487	82	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.

All (82) 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:A:502:PKZ:O4B	7:A:502:PKZ:C1B	1.65	1.17
7:A:503:PKZ:O4B	7:A:503:PKZ:C1B	1.65	1.17
4:P:63:LYS:NZ	4:P:105:GLU:O	2.21	0.72
2:A:176:ARG:NH2	2:A:213:VAL:O	2.25	0.68
3:O:123:TYR:HB3	4:P:73:TYR:HB2	1.77	0.66
2:A:67:GLY:HA2	2:A:71:LEU:HB2	1.78	0.65
2:A:192:LEU:HD11	4:P:120:TRP:HH2	1.62	0.64
3:O:55:TRP:HE1	3:O:100:LEU:HD22	1.63	0.63
3:O:117:ARG:HH12	3:O:119:TRP:HE3	1.47	0.62
2:A:176:ARG:NH1	2:A:208:VAL:O	2.33	0.62
2:A:30:ARG:NH2	2:A:266:TYR:OH	2.34	0.61
2:A:177:CYS:HA	2:A:180:TYR:CZ	2.37	0.59
2:A:213:VAL:HG12	2:A:217:GLY:HA3	1.85	0.59
3:O:118:VAL:HA	3:O:124:TYR:O	2.03	0.59
1:B:24:CYS:HB3	2:A:304:PHE:HZ	1.67	0.58
6:A:501:HEM:HBC2	6:A:501:HEM:HMC1	1.84	0.58
2:A:280:VAL:O	2:A:459:ARG:NH1	2.31	0.58
6:A:501:HEM:HBB2	6:A:501:HEM:HMB2	1.86	0.57
2:A:157:ARG:NH1	2:A:163:GLU:OE2	2.37	0.57
1:B:24:CYS:SG	1:B:25:GLY:N	2.77	0.57
1:B:28:ARG:NH2	2:A:59:GLU:OE1	2.38	0.55
2:A:57:ASP:HB2	2:A:268:HIS:CD2	2.42	0.54
2:A:57:ASP:OD1	2:A:58:PHE:N	2.42	0.53
3:O:86:ARG:NH1	3:O:105:LEU:O	2.42	0.52
2:A:297:TYR:CZ	2:A:301:LEU:HD11	2.45	0.52
2:A:251:LEU:HD21	2:A:305:GLY:HA3	1.92	0.52
2:A:436:THR:HA	2:A:439:LEU:HB3	1.92	0.52
2:A:56:THR:HB	2:A:268:HIS:HB2	1.92	0.52
3:O:56:VAL:HG12	3:O:66:TRP:HA	1.93	0.51
2:A:247:GLY:HA3	2:A:309:LEU:HD13	1.93	0.50
4:P:61:LEU:HB2	4:P:71:LEU:HD11	1.94	0.50
2:A:108:VAL:HG13	2:A:109:LEU:HG	1.92	0.50
2:A:445:VAL:HG22	2:A:453:GLY:HA3	1.94	0.49
3:O:110:MET:HG2	3:O:136:VAL:HG12	1.94	0.49
5:B:101:PLM:HC2	2:A:325:VAL:HB	1.95	0.48
4:P:61:LEU:HD13	4:P:110:TYR:CZ	2.48	0.48
3:O:66:TRP:CZ2	3:O:69:TRP:HD1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:37:VAL:HG11	3:O:134:LEU:HD11	1.96	0.48
3:O:39:ILE:HB	3:O:102:ILE:HG22	1.97	0.47
3:O:66:TRP:HZ2	3:O:69:TRP:HD1	1.62	0.47
2:A:399:GLU:HG2	7:A:502:PKZ:OAP	2.14	0.47
3:O:54:ASN:OD1	3:O:69:TRP:HB3	2.14	0.47
3:O:123:TYR:HB3	4:P:73:TYR:CB	2.45	0.46
3:O:21:ILE:HG12	3:O:46:TYR:HB3	1.96	0.46
5:B:101:PLM:HB1	2:A:293:VAL:HB	1.97	0.46
2:A:320:ALA:HB3	2:A:340:VAL:HG21	1.97	0.46
4:P:50:HIS:ND1	4:P:52:ASN:OD1	2.48	0.46
4:P:37:GLN:HA	4:P:99:ILE:O	2.15	0.45
2:A:425:ARG:HH22	2:A:488:GLN:NE2	2.14	0.45
2:A:105:CYS:HB2	2:A:214:LEU:HD21	1.99	0.45
3:O:57:ARG:HD3	3:O:83:PHE:CE1	2.52	0.45
4:P:25:GLN:HE22	4:P:111:TYR:HA	1.82	0.45
2:A:143:LEU:O	2:A:146:THR:OG1	2.36	0.44
4:P:25:GLN:NE2	4:P:112:CYS:H	2.15	0.44
2:A:65:GLU:OE2	2:A:69:GLN:NE2	2.51	0.44
2:A:306:VAL:HB	2:A:307:PRO:HD3	2.00	0.44
2:A:433:SER:HA	2:A:436:THR:HG22	1.99	0.44
4:P:83:PRO:HD2	4:P:86:PHE:HD2	1.82	0.44
4:P:27:PRO:HG2	4:P:30:LEU:HB2	2.00	0.44
3:O:57:ARG:HB3	3:O:67:MET:SD	2.58	0.43
3:O:54:ASN:HD22	3:O:118:VAL:HB	1.83	0.43
2:A:14:SER:HA	2:A:17:PHE:CD1	2.54	0.43
2:A:44:THR:OG1	2:A:52:LYS:NZ	2.51	0.43
2:A:285:LEU:O	2:A:456:TYR:OH	2.29	0.43
2:A:2:LEU:HB3	2:A:6:GLU:OE2	2.19	0.42
5:B:101:PLM:O2	2:A:379:HIS:NE2	2.51	0.42
2:A:21:SER:HB2	2:A:287:GLY:CA	2.47	0.42
2:A:372:PHE:O	2:A:375:VAL:HG12	2.18	0.42
2:A:228:GLN:HG2	2:A:316:LEU:HA	2.01	0.42
2:A:331:PHE:CE2	2:A:395:GLY:HA3	2.55	0.42
2:A:383:ASP:N	2:A:383:ASP:OD1	2.48	0.42
4:P:83:PRO:HD2	4:P:86:PHE:CD2	2.55	0.41
4:P:59:TRP:CD1	4:P:72:ILE:HD11	2.55	0.41
2:A:388:TRP:CD1	2:A:446:PHE:HB2	2.55	0.41
2:A:53:LYS:HB2	2:A:263:HIS:NE2	2.36	0.41
2:A:193:PRO:HG3	3:O:119:TRP:O	2.21	0.41
2:A:248:LEU:HD23	2:A:248:LEU:HA	1.82	0.41
4:P:59:TRP:HB2	4:P:72:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:39:ILE:O	3:O:101:GLN:HA	2.22	0.40
3:O:43:ALA:HB1	3:O:46:TYR:CE1	2.57	0.40
3:O:70:ILE:HG21	3:O:100:LEU:HD21	2.02	0.40
3:O:86:ARG:O	3:O:104:ASN:HA	2.22	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	B	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	A	489/493 (99%)	478 (98%)	11 (2%)	0	100	100
3	O	109/462 (24%)	104 (95%)	5 (5%)	0	100	100
4	P	109/207 (53%)	102 (94%)	7 (6%)	0	100	100
All	All	713/1170 (61%)	689 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	4/4 (100%)	4 (100%)	0	100	100
2	A	414/429 (96%)	414 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	83/411 (20%)	83 (100%)	0	100	100
4	P	77/185 (42%)	77 (100%)	0	100	100
All	All	578/1029 (56%)	578 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

15 ligands are modelled in this entry.

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	AJP	A	512	-	36,36,95	0.47	0	56,60,149	1.32	8 (14%)
8	AJP	A	506	-	36,36,95	0.46	0	56,60,149	0.72	0
8	AJP	A	508	-	30,30,95	0.58	0	45,49,149	0.73	0
7	PKZ	A	502	-	61,67,67	3.47	19 (31%)	74,93,93	2.32	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	AJP	A	511	-	35,35,95	0.44	0	54,58,149	0.62	1 (1%)
8	AJP	A	505	-	49,49,95	0.40	0	75,80,149	0.70	2 (2%)
8	AJP	A	514	-	37,37,95	0.46	0	58,62,149	0.75	2 (3%)
8	AJP	A	513	-	36,36,95	0.45	0	56,60,149	0.74	0
7	PKZ	A	504	-	14,14,67	0.79	0	13,13,93	0.91	0
8	AJP	A	509	-	37,37,95	0.44	0	58,62,149	0.73	2 (3%)
8	AJP	A	510	-	37,37,95	0.45	0	58,62,149	0.73	2 (3%)
5	PLM	B	101	1	15,16,17	0.24	0	14,15,17	0.50	0
6	HEM	A	501	-	42,50,50	1.45	5 (11%)	46,82,82	1.35	5 (10%)
8	AJP	A	507	-	37,37,95	0.45	0	58,62,149	0.74	2 (3%)
7	PKZ	A	503	-	30,33,67	3.72	14 (46%)	43,51,93	0.93	2 (4%)

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
8	AJP	A	512	-	10/10/13/38	-	0/6/6/11
8	AJP	A	508	-	7/7/11/38	-	0/5/5/11
8	AJP	A	506	-	10/10/13/38	-	0/6/6/11
8	AJP	A	511	-	9/9/12/38	-	0/6/6/11
7	PKZ	A	502	-	-	21/62/82/82	0/3/3/3
8	AJP	A	505	-	12/12/19/38	3/6/121/220	0/7/7/11
8	AJP	A	514	-	10/10/14/38	-	0/6/6/11
8	AJP	A	513	-	10/10/13/38	-	0/6/6/11
7	PKZ	A	504	-	-	3/12/12/82	-
8	AJP	A	509	-	10/10/14/38	-	0/6/6/11
8	AJP	A	510	-	10/10/14/38	-	0/6/6/11
8	AJP	A	507	-	10/10/14/38	-	0/6/6/11
5	PLM	B	101	1	-	10/14/14/15	-
6	HEM	A	501	-	-	1/12/54/54	-
7	PKZ	A	503	-	-	10/37/53/82	0/1/1/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	502	PKZ	O4B-C1B	18.53	1.65	1.40
7	A	503	PKZ	O4B-C1B	10.40	1.65	1.42
7	A	502	PKZ	P1A-O3A	7.97	1.68	1.59
7	A	503	PKZ	P1A-O3A	7.91	1.68	1.59
7	A	502	PKZ	P2A-O3A	7.72	1.67	1.59
7	A	503	PKZ	P2A-O3A	7.60	1.67	1.59
7	A	502	PKZ	C9P-N8P	6.75	1.49	1.33
7	A	503	PKZ	C9P-N8P	6.43	1.48	1.33
7	A	503	PKZ	C2B-C1B	-6.41	1.33	1.53
7	A	503	PKZ	O4B-C4B	-6.35	1.30	1.45
7	A	502	PKZ	O4B-C4B	-6.31	1.31	1.45
7	A	502	PKZ	C5P-N4P	5.63	1.46	1.33
7	A	502	PKZ	C2-C1	4.69	1.55	1.50
6	A	501	HEM	C3C-C2C	-3.97	1.35	1.40
7	A	502	PKZ	P3B-O3B	3.40	1.65	1.59
6	A	501	HEM	C3C-CAC	3.39	1.55	1.47
7	A	503	PKZ	P3B-O3B	3.39	1.65	1.59
7	A	502	PKZ	C1-S1P	3.35	1.84	1.76
7	A	502	PKZ	C1B-N9A	-3.28	1.41	1.49
7	A	502	PKZ	C6A-N6A	3.26	1.45	1.34
7	A	502	PKZ	O3B-C3B	-3.11	1.33	1.44
7	A	503	PKZ	O3B-C3B	-3.10	1.33	1.44
6	A	501	HEM	CAB-C3B	2.96	1.55	1.47
7	A	502	PKZ	OAP-CAP	-2.65	1.37	1.42
6	A	501	HEM	C3C-C4C	2.59	1.45	1.41
7	A	502	PKZ	C2A-N3A	2.55	1.36	1.32
7	A	503	PKZ	OAP-CAP	-2.53	1.37	1.42
7	A	503	PKZ	O9P-C9P	-2.52	1.18	1.23
7	A	502	PKZ	O9P-C9P	-2.43	1.18	1.23
7	A	502	PKZ	C3B-C4B	2.36	1.59	1.52
7	A	503	PKZ	CCP-CBP	2.31	1.56	1.52
7	A	503	PKZ	P2A-O6A	2.29	1.68	1.59
7	A	502	PKZ	CCP-CBP	2.26	1.56	1.52
7	A	502	PKZ	P2A-O6A	2.26	1.68	1.59
7	A	503	PKZ	C3B-C4B	2.22	1.58	1.52
7	A	503	PKZ	O2B-C2B	2.16	1.48	1.43
7	A	502	PKZ	O2B-C2B	2.13	1.48	1.43
6	A	501	HEM	CMB-C2B	2.09	1.55	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	502	PKZ	C5A-C6A-N6A	10.83	136.81	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	502	PKZ	N6A-C6A-N1A	-7.07	103.22	118.33
7	A	502	PKZ	C4B-O4B-C1B	-6.97	103.54	109.92
7	A	502	PKZ	N3A-C2A-N1A	-6.37	120.02	128.67
7	A	502	PKZ	C2-C1-S1P	5.70	120.19	113.40
8	A	512	AJP	O09-C08-C10	4.53	119.36	110.20
7	A	502	PKZ	O1-C1-C2	-3.55	119.88	123.98
8	A	512	AJP	C83-C06-C05	3.44	120.47	114.94
8	A	512	AJP	C11-C12-C07	-3.19	95.35	100.16
7	A	502	PKZ	O9P-C9P-N8P	-3.02	116.58	122.98
8	A	512	AJP	C12-C07-C06	2.89	129.05	120.50
7	A	503	PKZ	C3B-C2B-C1B	2.85	106.19	99.91
6	A	501	HEM	CBA-CAA-C2A	-2.67	108.05	112.54
7	A	502	PKZ	CAP-C9P-N8P	2.61	121.44	116.48
6	A	501	HEM	C4B-CHC-C1C	2.60	125.99	122.56
7	A	502	PKZ	C2P-S1P-C1	2.54	109.36	101.84
8	A	512	AJP	C85-O84-C05	2.51	118.01	113.69
8	A	512	AJP	C06-C07-C08	-2.28	100.61	104.28
6	A	501	HEM	C4D-ND-C1D	2.27	107.89	105.21
7	A	502	PKZ	C6P-C5P-N4P	2.25	120.44	116.34
8	A	507	AJP	C24-C23-C22	2.24	113.14	110.38
7	A	502	PKZ	CEP-CBP-CAP	2.21	112.54	108.77
6	A	501	HEM	CMC-C2C-C3C	2.21	129.10	124.68
7	A	502	PKZ	O1-C1-S1P	-2.16	119.93	122.68
8	A	509	AJP	C24-C23-C22	2.16	113.04	110.38
8	A	510	AJP	C24-C23-C22	2.14	113.03	110.38
8	A	514	AJP	C24-C23-C22	2.11	112.98	110.38
8	A	507	AJP	C21-C20-C19	2.08	109.22	107.23
8	A	514	AJP	C21-C20-C19	2.08	109.22	107.23
8	A	505	AJP	C21-C20-C19	2.07	109.21	107.23
8	A	512	AJP	C21-C20-C19	2.05	109.19	107.23
8	A	511	AJP	C83-C06-C05	2.05	118.24	114.94
7	A	503	PKZ	P3B-O3B-C3B	-2.04	117.97	123.43
8	A	509	AJP	C21-C20-C19	2.03	109.17	107.23
8	A	512	AJP	O09-C08-C07	-2.03	99.42	104.08
8	A	510	AJP	C21-C20-C19	2.02	109.16	107.23
6	A	501	HEM	CMA-C3A-C4A	-2.02	125.50	128.46
8	A	505	AJP	C83-C06-C05	2.02	118.18	114.94

All (98) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	505	AJP	C22

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Mol	Chain	Res	Type	Atom
8	A	505	AJP	C27
8	A	505	AJP	C30
8	A	505	AJP	C15
8	A	505	AJP	C19
8	A	505	AJP	C16
8	A	505	AJP	C08
8	A	505	AJP	C11
8	A	505	AJP	C20
8	A	505	AJP	C12
8	A	505	AJP	C07
8	A	505	AJP	C10
8	A	506	AJP	C22
8	A	506	AJP	C15
8	A	506	AJP	C19
8	A	506	AJP	C16
8	A	506	AJP	C08
8	A	506	AJP	C11
8	A	506	AJP	C20
8	A	506	AJP	C12
8	A	506	AJP	C07
8	A	506	AJP	C10
8	A	507	AJP	C22
8	A	507	AJP	C15
8	A	507	AJP	C19
8	A	507	AJP	C16
8	A	507	AJP	C08
8	A	507	AJP	C11
8	A	507	AJP	C20
8	A	507	AJP	C12
8	A	507	AJP	C07
8	A	507	AJP	C10
8	A	508	AJP	C15
8	A	508	AJP	C16
8	A	508	AJP	C08
8	A	508	AJP	C11
8	A	508	AJP	C12
8	A	508	AJP	C07
8	A	508	AJP	C10
8	A	509	AJP	C22
8	A	509	AJP	C15
8	A	509	AJP	C19
8	A	509	AJP	C16

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Mol	Chain	Res	Type	Atom
8	A	509	AJP	C08
8	A	509	AJP	C11
8	A	509	AJP	C20
8	A	509	AJP	C12
8	A	509	AJP	C07
8	A	509	AJP	C10
8	A	510	AJP	C22
8	A	510	AJP	C15
8	A	510	AJP	C19
8	A	510	AJP	C16
8	A	510	AJP	C08
8	A	510	AJP	C11
8	A	510	AJP	C20
8	A	510	AJP	C12
8	A	510	AJP	C07
8	A	510	AJP	C10
8	A	511	AJP	C15
8	A	511	AJP	C19
8	A	511	AJP	C16
8	A	511	AJP	C08
8	A	511	AJP	C11
8	A	511	AJP	C20
8	A	511	AJP	C12
8	A	511	AJP	C07
8	A	511	AJP	C10
8	A	512	AJP	C22
8	A	512	AJP	C15
8	A	512	AJP	C19
8	A	512	AJP	C16
8	A	512	AJP	C02
8	A	512	AJP	C11
8	A	512	AJP	C20
8	A	512	AJP	C12
8	A	512	AJP	C07
8	A	512	AJP	C10
8	A	513	AJP	C22
8	A	513	AJP	C15
8	A	513	AJP	C19
8	A	513	AJP	C16
8	A	513	AJP	C08
8	A	513	AJP	C11
8	A	513	AJP	C20

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Mol	Chain	Res	Type	Atom
8	A	513	AJP	C12
8	A	513	AJP	C07
8	A	513	AJP	C10
8	A	514	AJP	C22
8	A	514	AJP	C15
8	A	514	AJP	C19
8	A	514	AJP	C16
8	A	514	AJP	C08
8	A	514	AJP	C11
8	A	514	AJP	C20
8	A	514	AJP	C12
8	A	514	AJP	C07
8	A	514	AJP	C10

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	101	PLM	O2-C1-C2-C3
7	A	502	PKZ	O1-C1-S1P-C2P
7	A	502	PKZ	C2-C1-S1P-C2P
7	A	502	PKZ	C5B-O5B-P1A-O2A
7	A	502	PKZ	CCP-O6A-P2A-O3A
7	A	502	PKZ	CCP-O6A-P2A-O4A
7	A	502	PKZ	N8P-C9P-CAP-OAP
7	A	502	PKZ	CAP-C9P-N8P-C7P
7	A	503	PKZ	C5B-O5B-P1A-O1A
7	A	503	PKZ	C5B-O5B-P1A-O2A
7	A	503	PKZ	C5B-O5B-P1A-O3A
7	A	503	PKZ	CCP-O6A-P2A-O3A
7	A	503	PKZ	CCP-O6A-P2A-O4A
7	A	503	PKZ	CCP-O6A-P2A-O5A
7	A	503	PKZ	CDP-CBP-CCP-O6A
7	A	503	PKZ	CEP-CBP-CCP-O6A
7	A	503	PKZ	CAP-CBP-CCP-O6A
7	A	502	PKZ	O9P-C9P-N8P-C7P
7	A	502	PKZ	C7-C8-C9-C10
7	A	502	PKZ	C2-C3-C4-C5
5	B	101	PLM	C3-C4-C5-C6
5	B	101	PLM	CB-CC-CD-CE
7	A	502	PKZ	C5P-C6P-C7P-N8P
5	B	101	PLM	C5-C6-C7-C8
7	A	502	PKZ	O9P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
8	A	505	AJP	O31-C26-O25-C23
5	B	101	PLM	C7-C8-C9-CA
7	A	502	PKZ	C4-C5-C6-C7
5	B	101	PLM	C2-C3-C4-C5
7	A	504	PKZ	C11-C10-C9-C8
7	A	502	PKZ	C6-C7-C8-C9
7	A	504	PKZ	C10-C11-C12-C13
7	A	502	PKZ	O9P-C9P-CAP-CBP
7	A	502	PKZ	C4B-C5B-O5B-P1A
7	A	502	PKZ	S1P-C2P-C3P-N4P
7	A	502	PKZ	N8P-C9P-CAP-CBP
7	A	502	PKZ	C11-C10-C9-C8
7	A	504	PKZ	C9-C10-C11-C12
5	B	101	PLM	C1-C2-C3-C4
7	A	502	PKZ	CCP-O6A-P2A-O5A
5	B	101	PLM	C9-CA-CB-CC
8	A	505	AJP	C27-C26-O25-C23
5	B	101	PLM	CD-CE-CF-CG
5	B	101	PLM	CC-CD-CE-CF
8	A	505	AJP	C22-C23-O25-C26
6	A	501	HEM	C4D-C3D-CAD-CBD
7	A	503	PKZ	C3B-O3B-P3B-O9A
7	A	502	PKZ	P1A-O3A-P2A-O4A

There are no ring outliers.

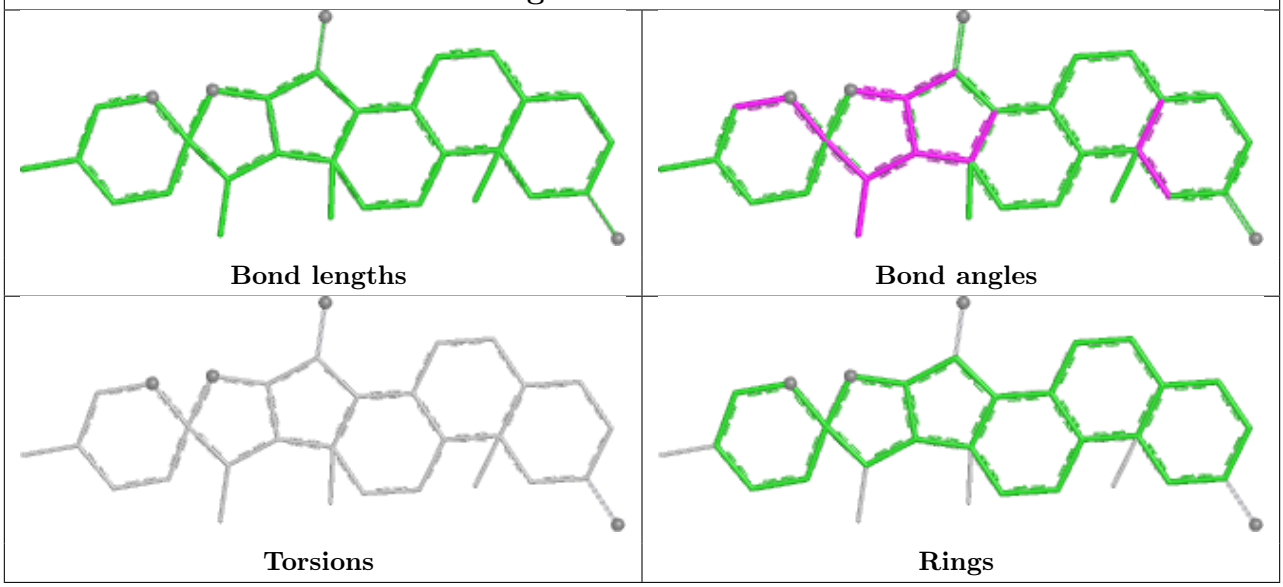
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	502	PKZ	2	0
5	B	101	PLM	3	0
6	A	501	HEM	2	0
7	A	503	PKZ	1	0

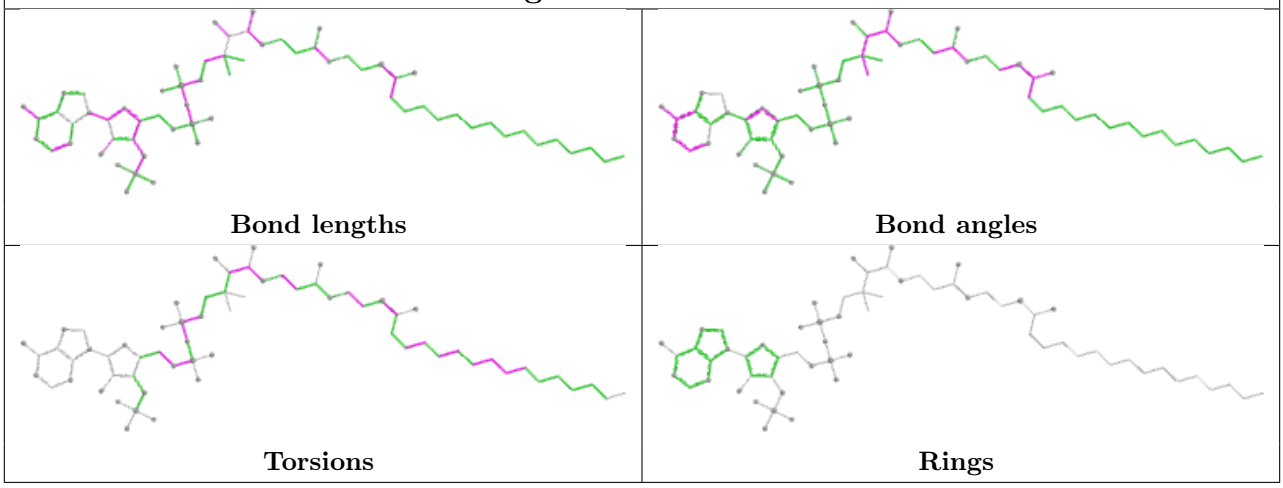
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

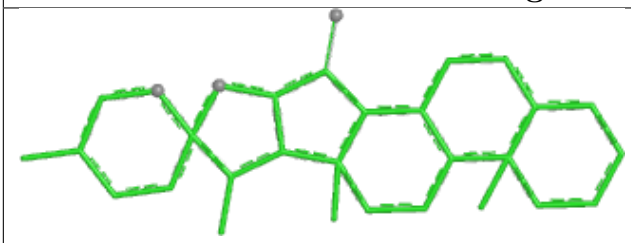
Ligand AJP A 512



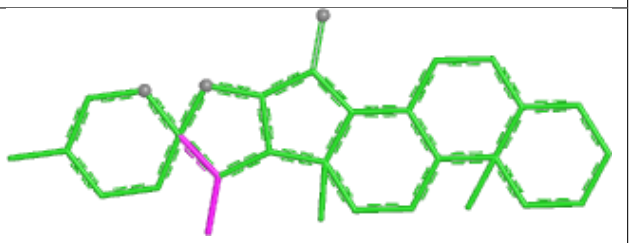
Ligand PKZ A 502



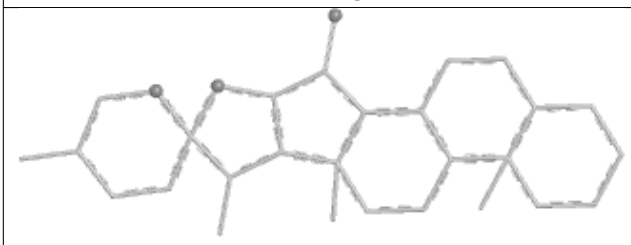
Ligand AJP A 511



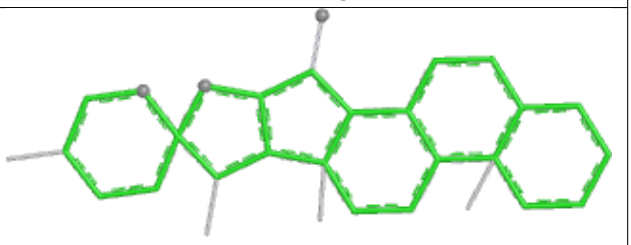
Bond lengths



Bond angles

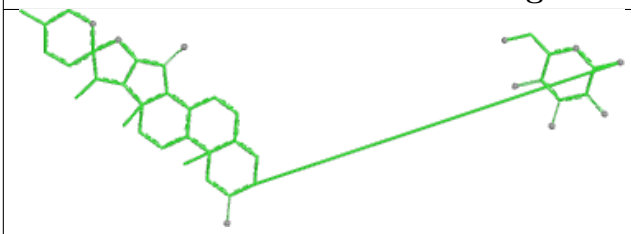


Torsions

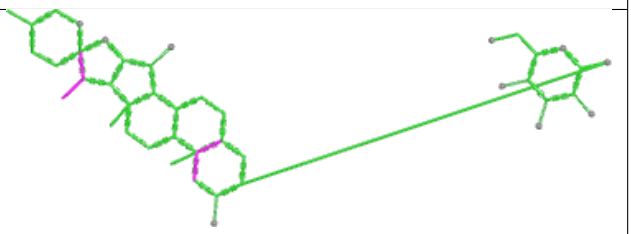


Rings

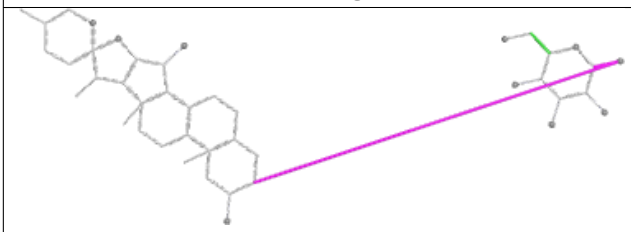
Ligand AJP A 505



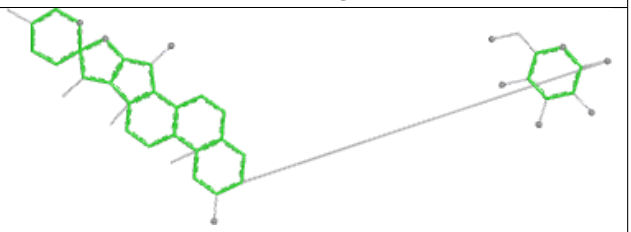
Bond lengths



Bond angles

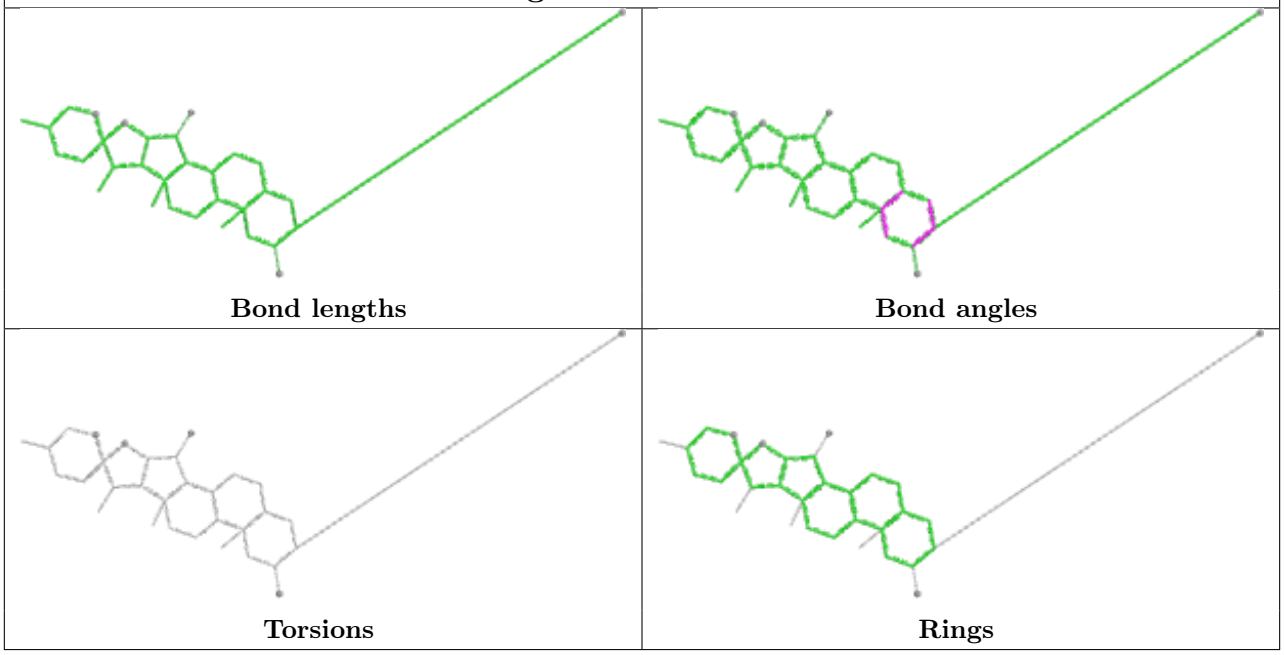


Torsions

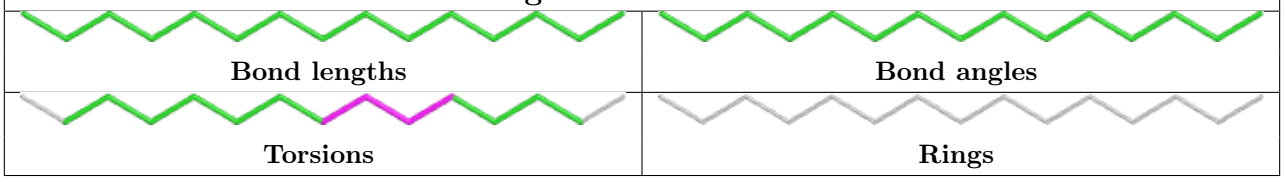


Rings

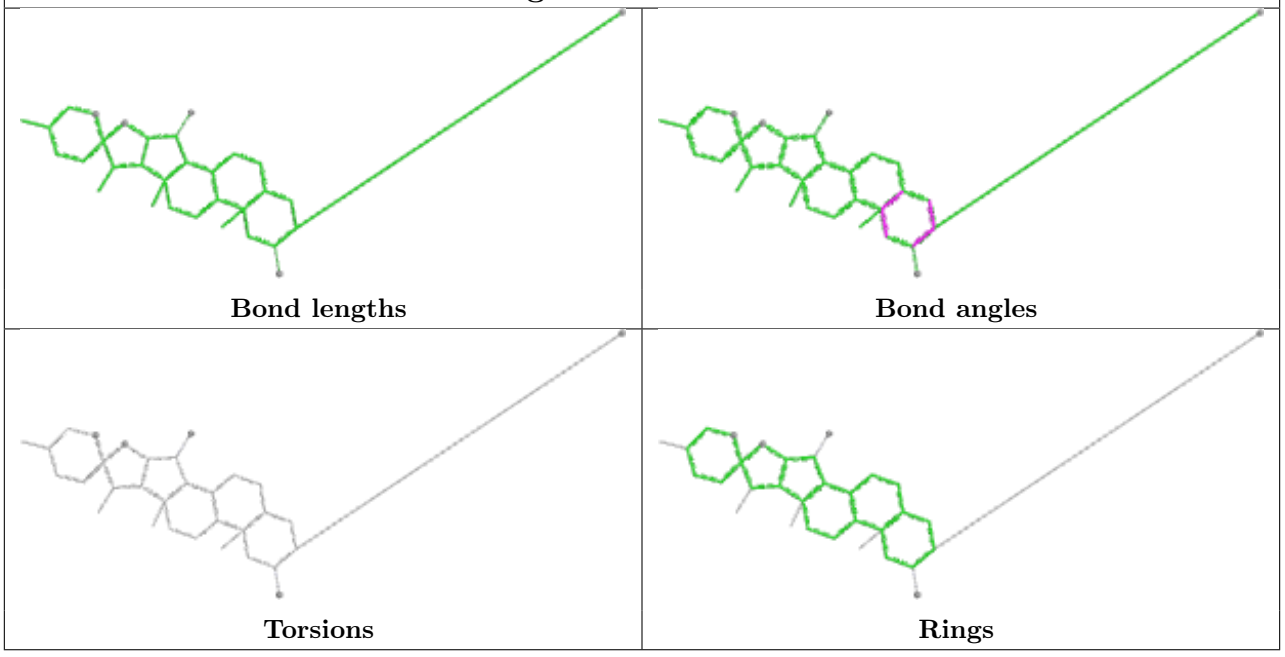
Ligand AJP A 514



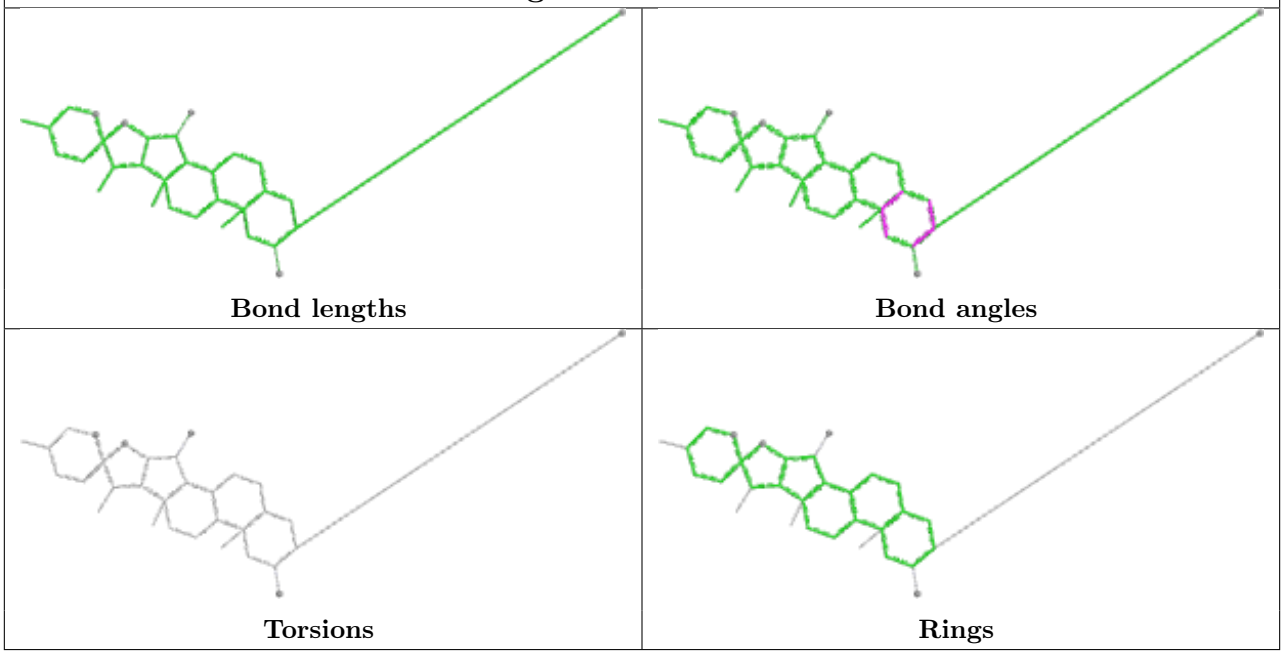
Ligand PKZ A 504



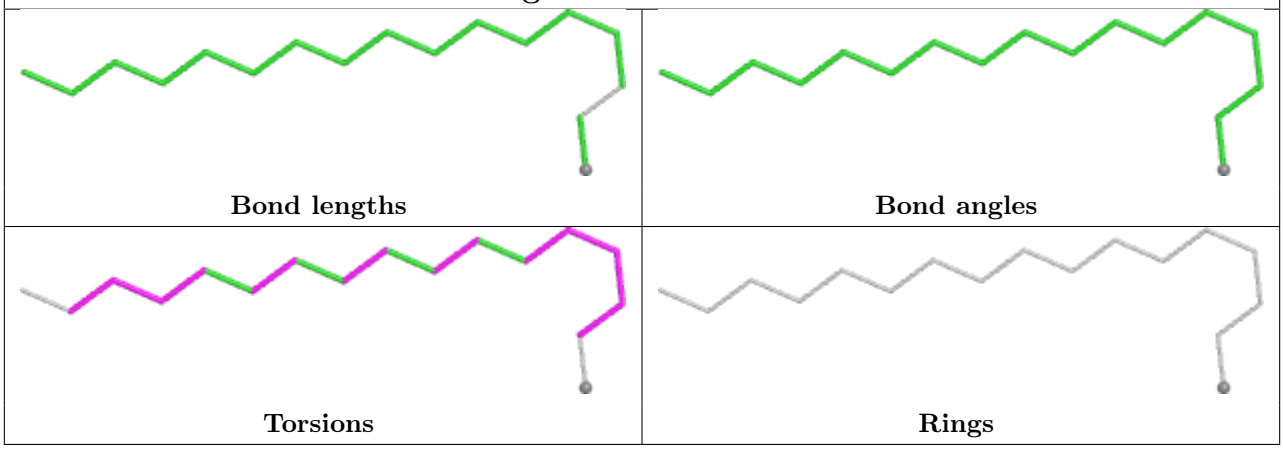
Ligand AJP A 509



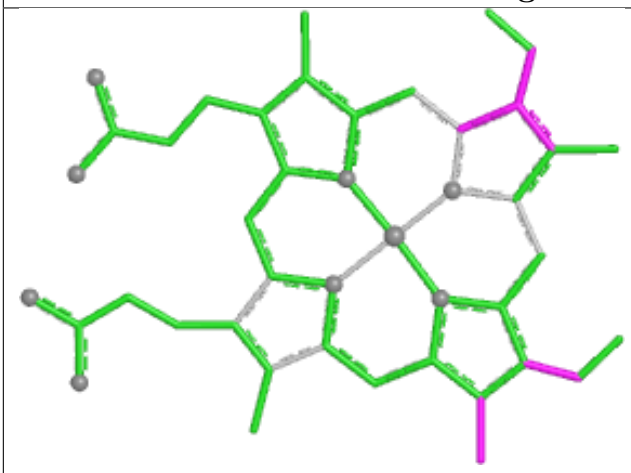
Ligand AJP A 510



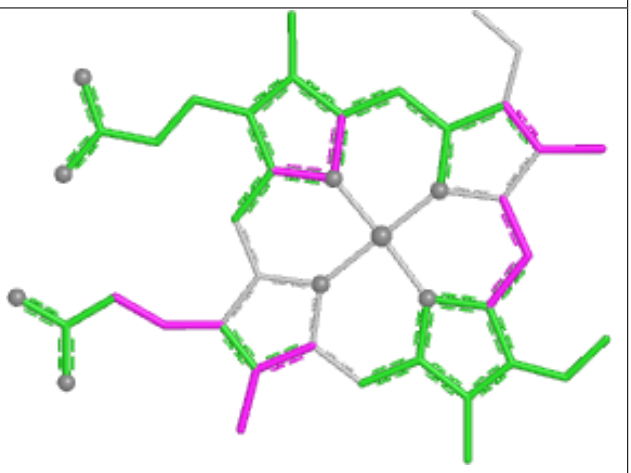
Ligand PLM B 101



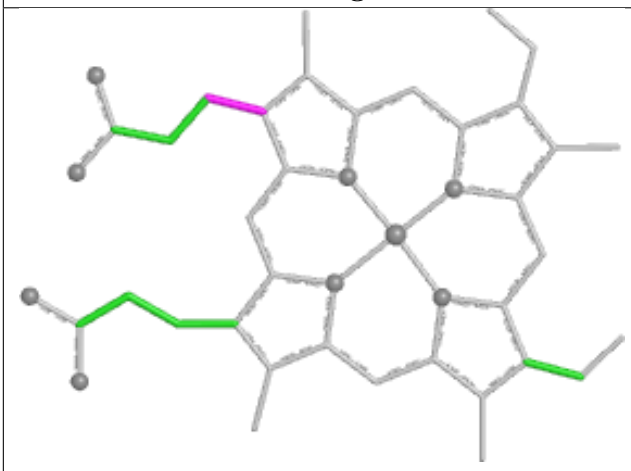
Ligand HEM A 501



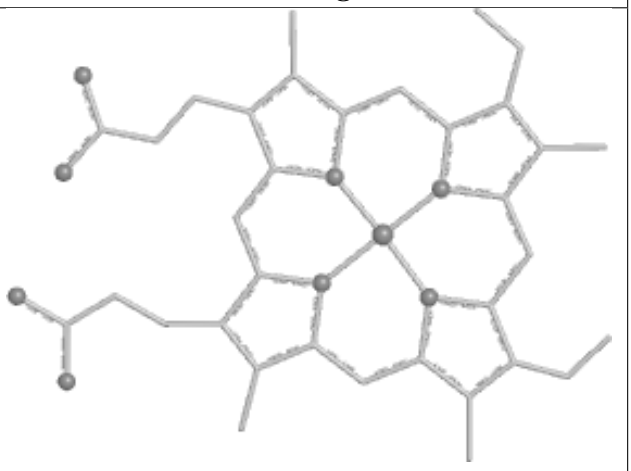
Bond lengths



Bond angles

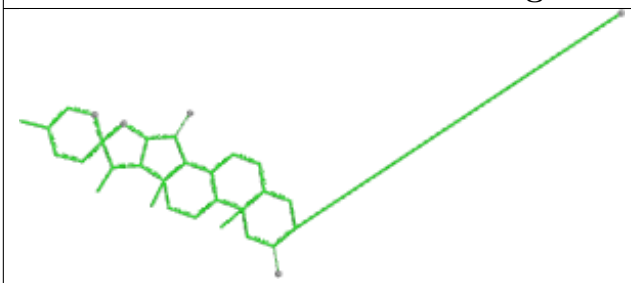


Torsions

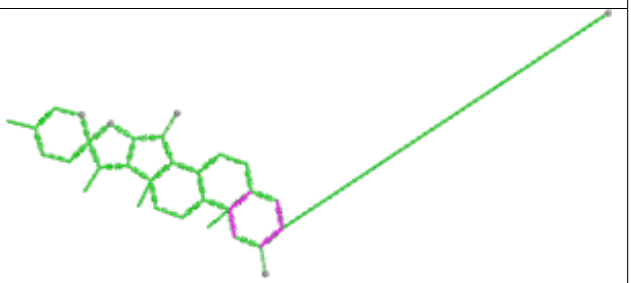


Rings

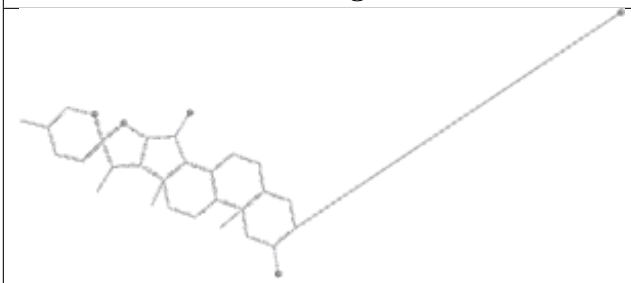
Ligand AJP A 507



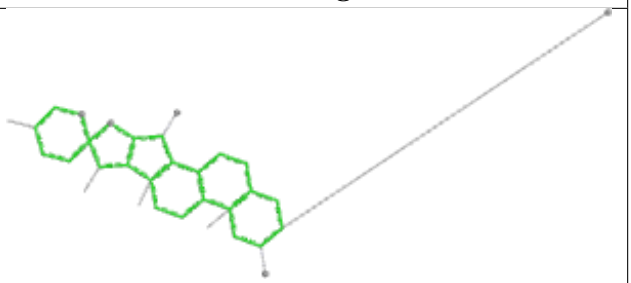
Bond lengths



Bond angles

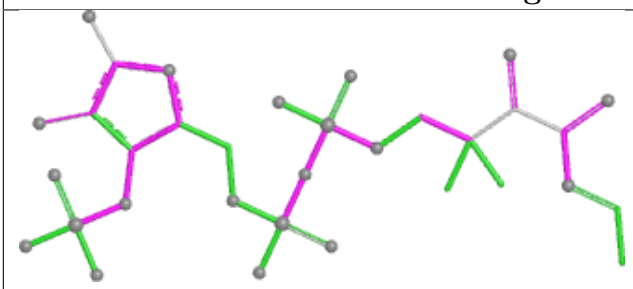


Torsions

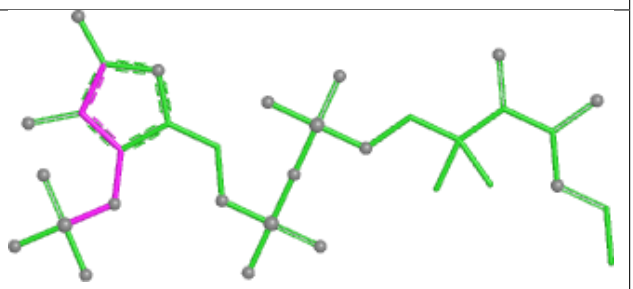


Rings

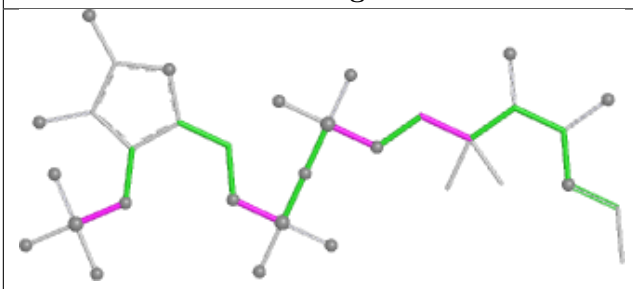
Ligand PKZ A 503



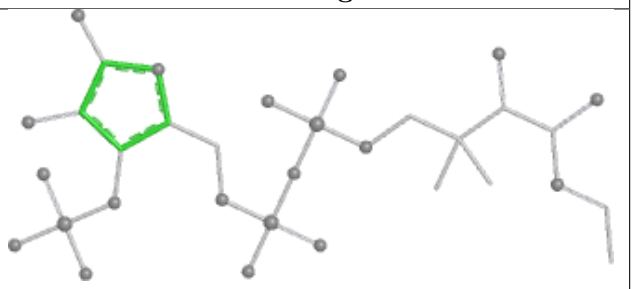
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

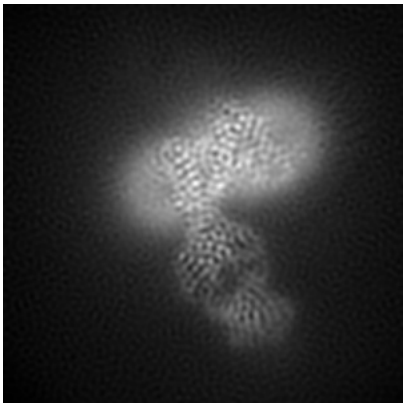
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23837. These allow visual inspection of the internal detail of the map and identification of artifacts.

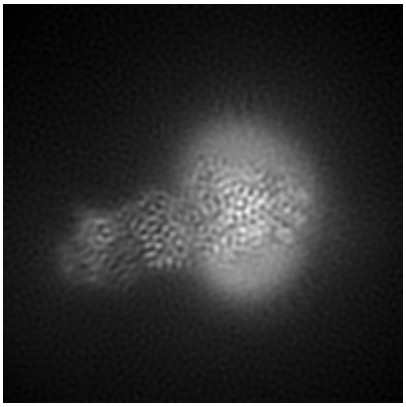
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

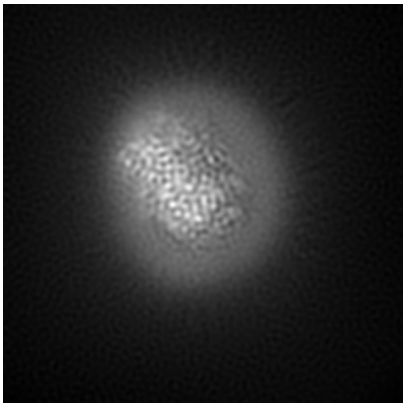
6.1.1 Primary map



X



Y

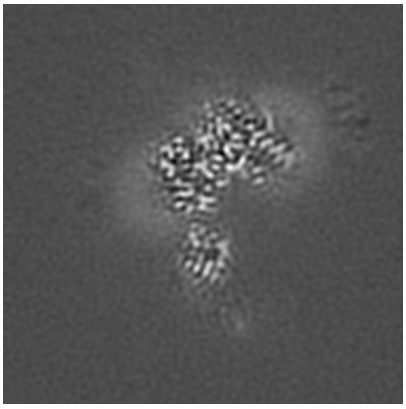


Z

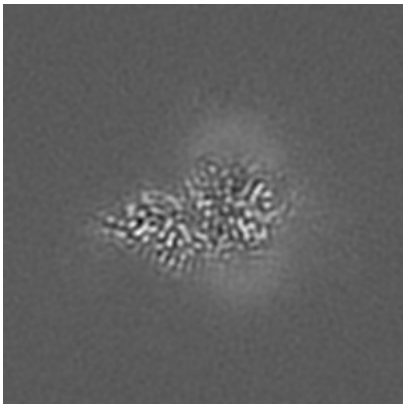
The images above show the map projected in three orthogonal directions.

6.2 Central slices

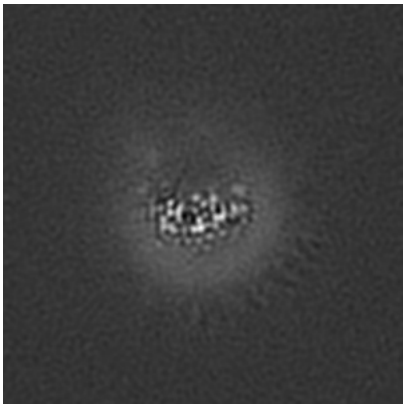
6.2.1 Primary map



X Index: 188



Y Index: 188

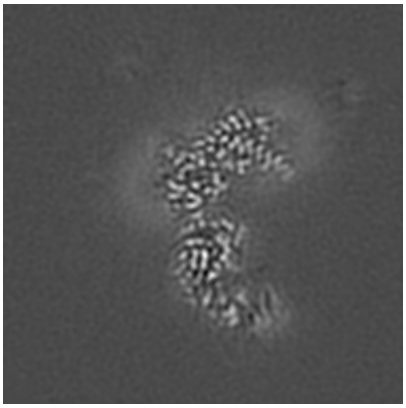


Z Index: 188

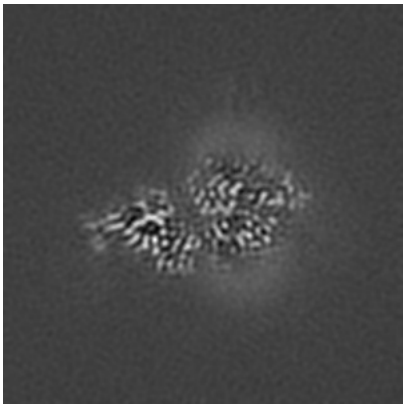
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

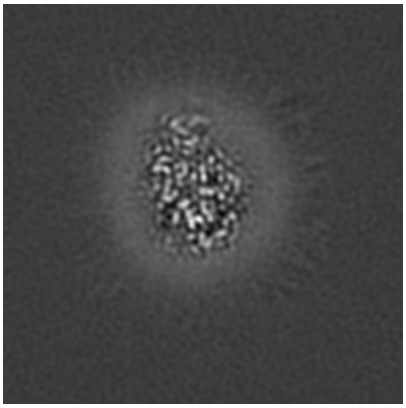
6.3.1 Primary map



X Index: 164



Y Index: 194

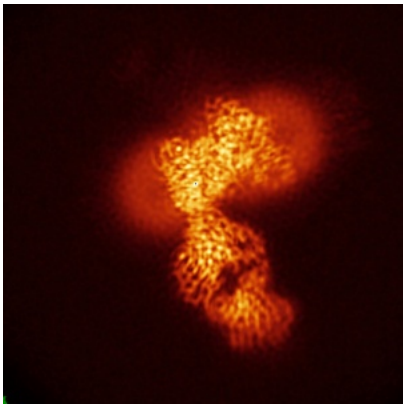


Z Index: 223

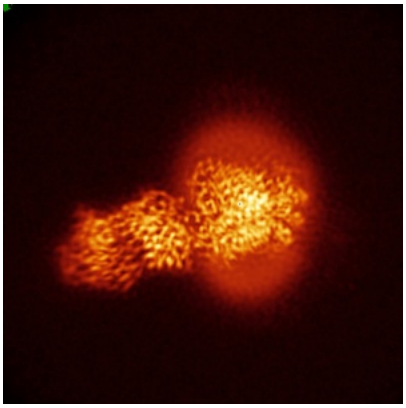
The images above show the largest variance slices of the map in three orthogonal directions.

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

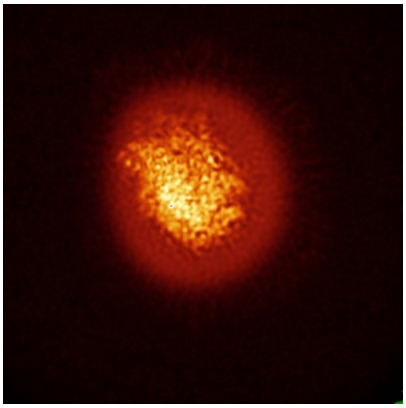
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.877. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

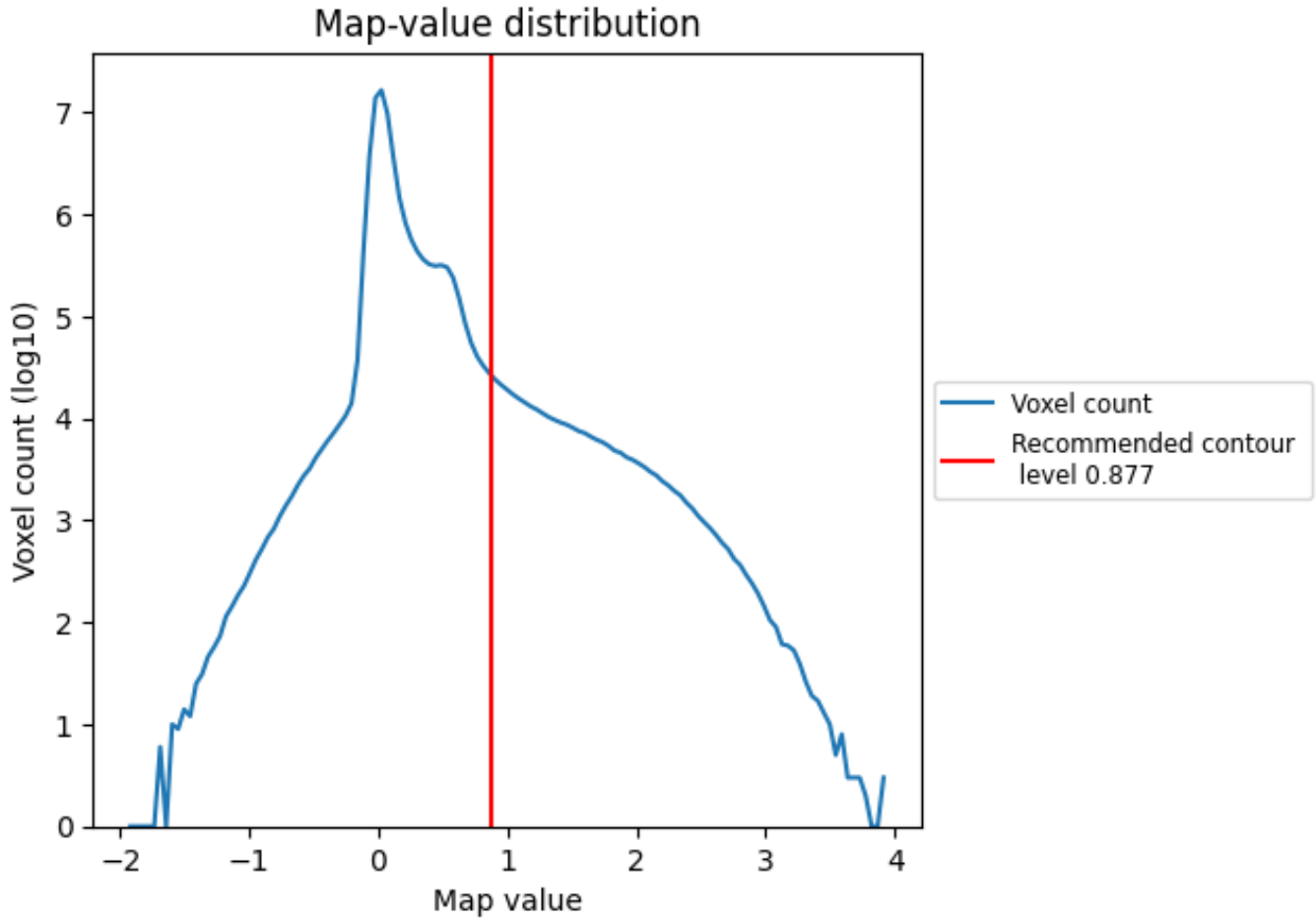
6.6 Mask visualisation (i)

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

7 Map analysis

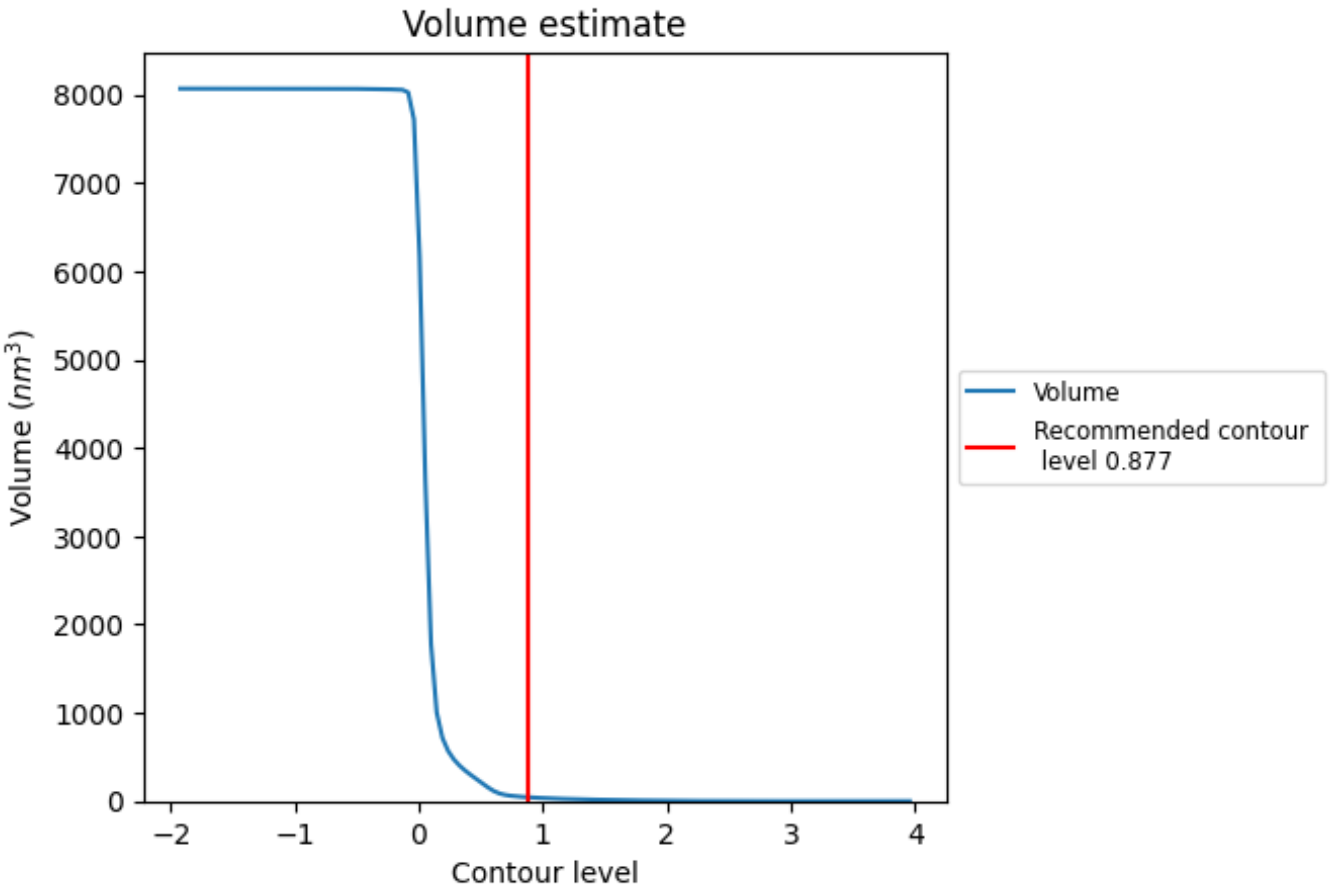
This section contains the results of statistical analysis of the map.

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.

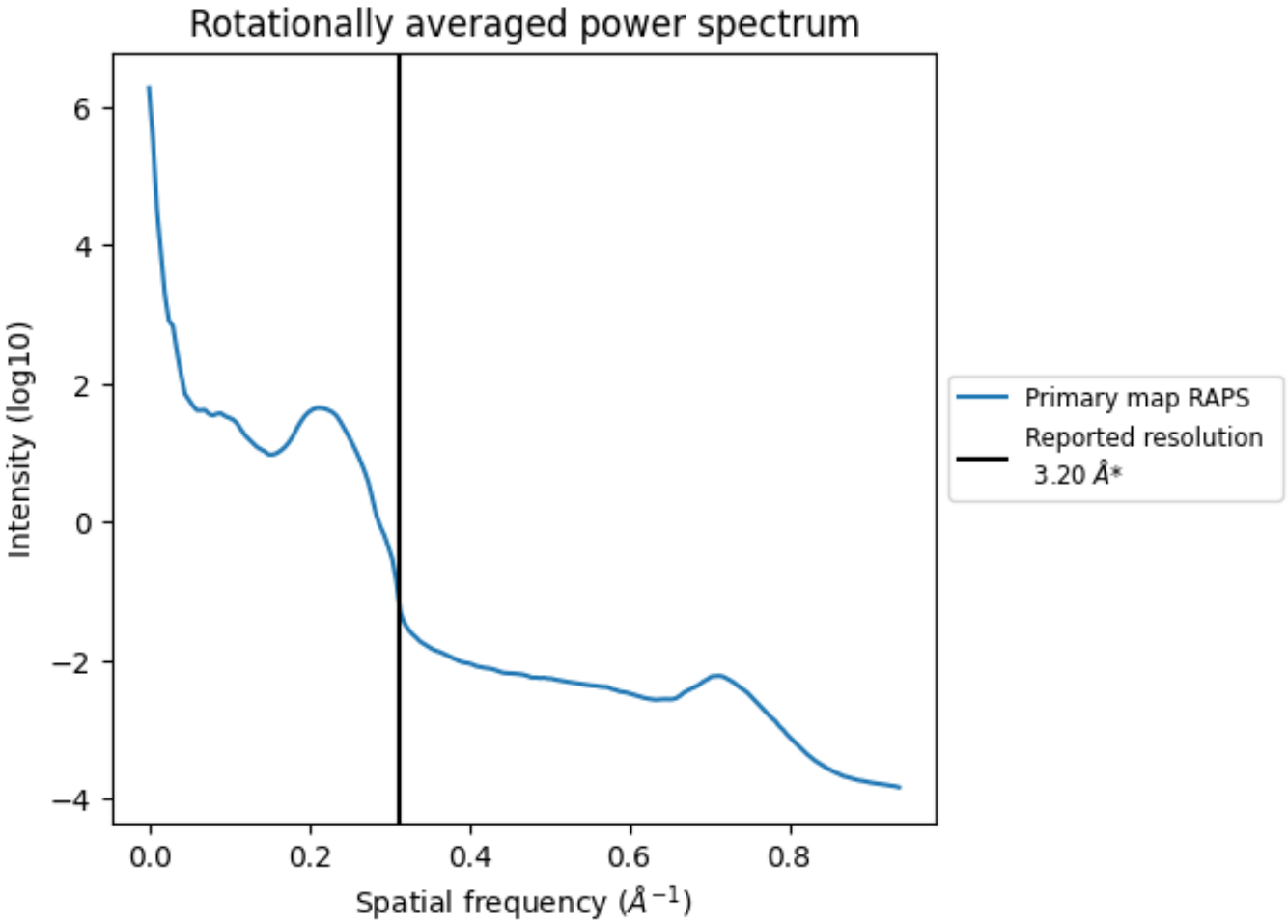
7.2 Volume estimate



The volume at the recommended contour level is 45 nm^3; this corresponds to an approximate mass of 40 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 0.312 $Å^{-1}$

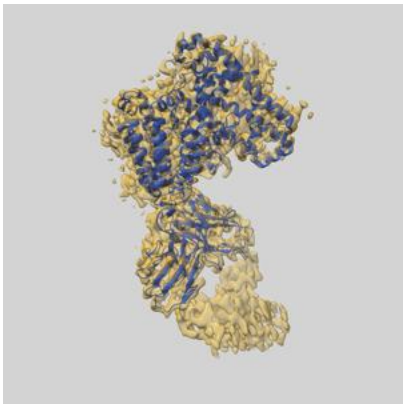
8 Fourier-Shell correlation (i)

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

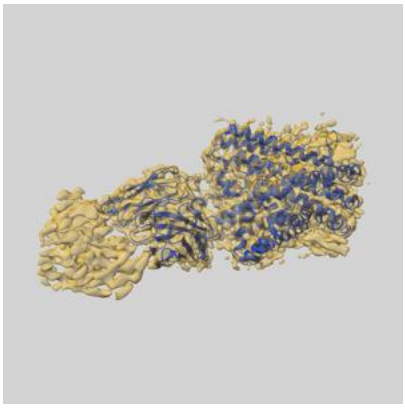
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23837 and PDB model 7MHZ. Per-residue inclusion information can be found in section 3 on page 8.

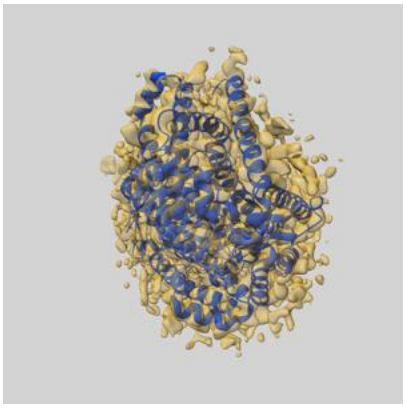
9.1 Map-model overlay



X



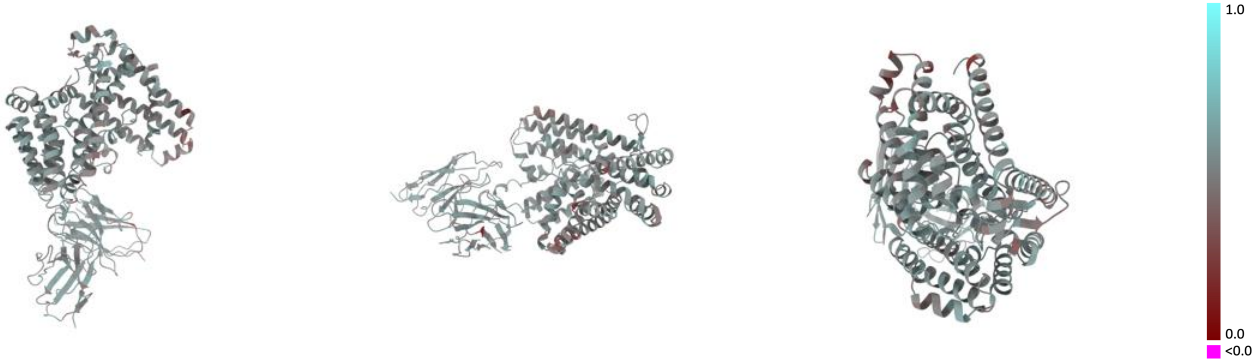
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.877 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.

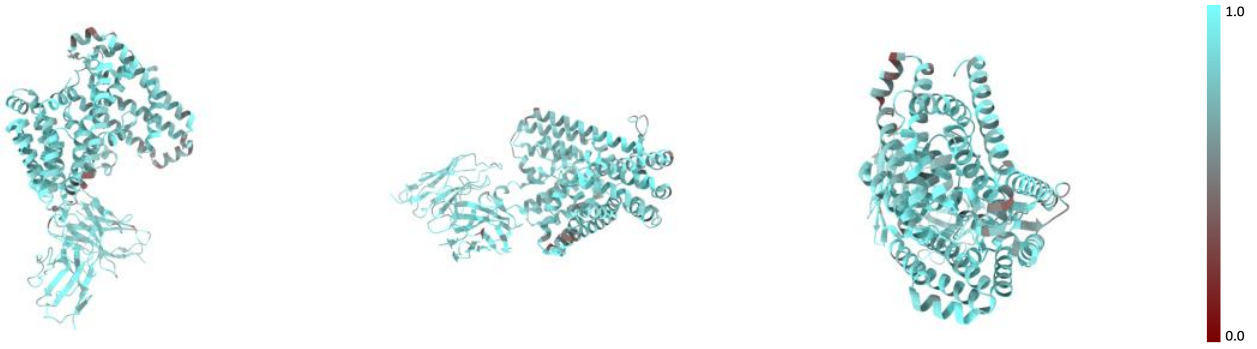
9.2 Q-score mapped to coordinate model (i)



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.

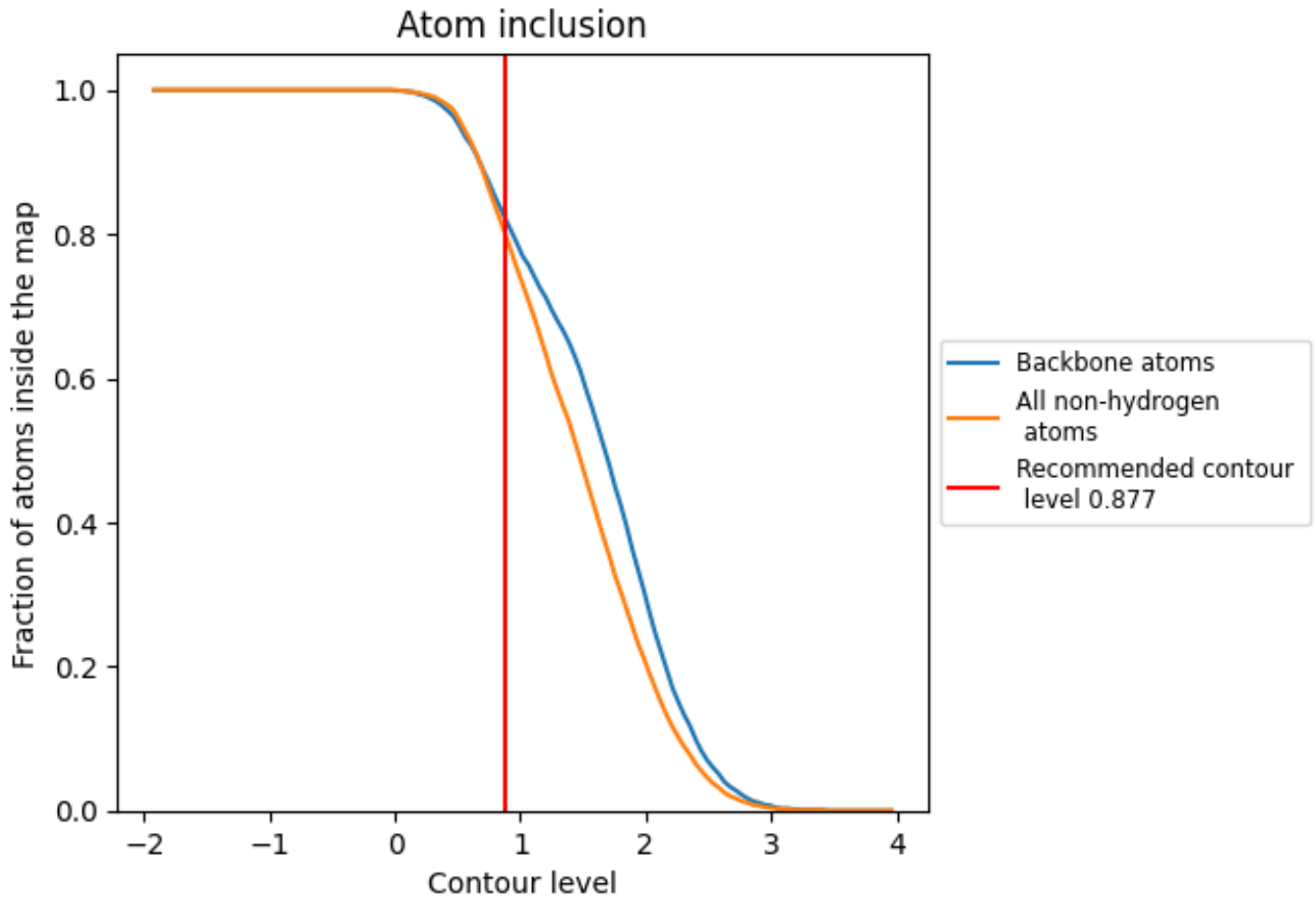
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.877).

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

The table lists the average atom inclusion at the recommended contour level (0.877) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8010	0.5090
A	0.7860	0.5030
B	0.8490	0.5410
O	0.8460	0.5240
P	0.8320	0.5220