



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 07:30 AM EST

PDB ID : 7MHY
EMDB ID : EMD-23836
Title : Human Hedgehog acyltransferase (HHAT) in complex with palmitoyl-CoA and two Fab antibody fragments
Authors : Long, S.B.; Jiang, Y.
Deposited on : 2021-04-16
Resolution : 2.70 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

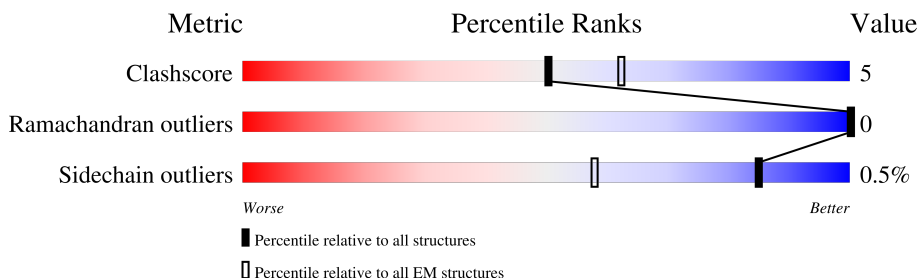
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	493	
2	M	211	
3	N	207	
4	O	211	
5	P	207	

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	-	-	-
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	-	-	-
8	AJP	A	515	X	-	-	-
8	AJP	A	516	X	-	-	-
8	AJP	A	517	X	-	-	-
8	AJP	A	518	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7904 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 Protein-cysteine N-palmitoyltransferase HHAT.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	491	Total	C	N	O	S	0	0
			4003	2669	638	665	31		

- Molecule 2 is a protein called 1C06 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	118	Total	C	N	O	S	0	0
			887	565	144	174	4		

- Molecule 3 is a protein called 1C06 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	109	Total	C	N	O	S	0	0
			812	523	136	150	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	100	Total	C	N	O	S	0	0
			805	528	128	144	5		

- Molecule 5 is a protein called 3H02 Fab light chain.

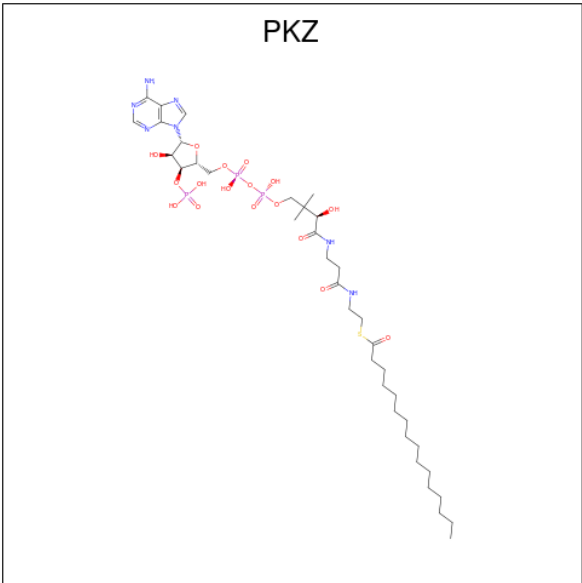
Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	94	Total	C	N	O	S	0	0
			683	441	113	126	3		

- 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).



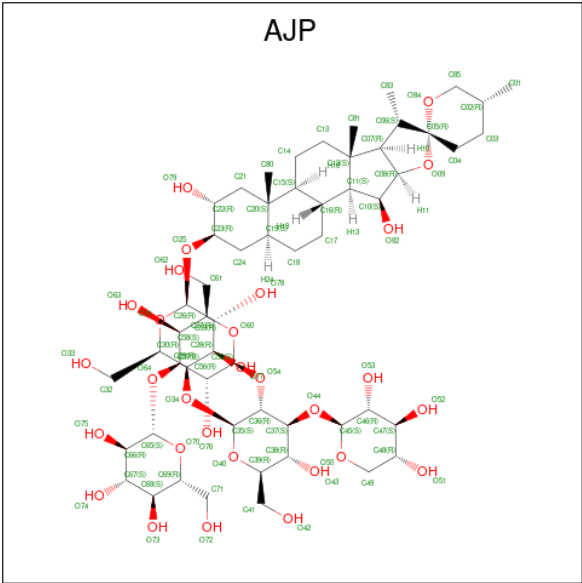
Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	N	O	P	S	0
			65	37	7	17	3	1	
7	A	1	Total	C	N	O	P	S	0
			65	37	7	17	3	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	C	0
			15	15	

- Molecule 8 is Digitonin (three-letter code: AJP) (formula: C₅₆H₉₂O₂₉).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			54	39	15	
8	A	1	Total	C	O	0
			43	33	10	
8	A	1	Total	C	O	0
			32	27	5	
8	A	1	Total	C	O	0
			43	33	10	
8	A	1	Total	C	O	0
			43	33	10	
8	A	1	Total	C	O	0
			33	28	5	
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
			43	33	10	
8	A	1	Total	C	O	0
			30	27	3	

Continued on next page...

Continued from previous page...

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
			31	27	4	
8	A	1	Total	C	O	0
			32	27	5	

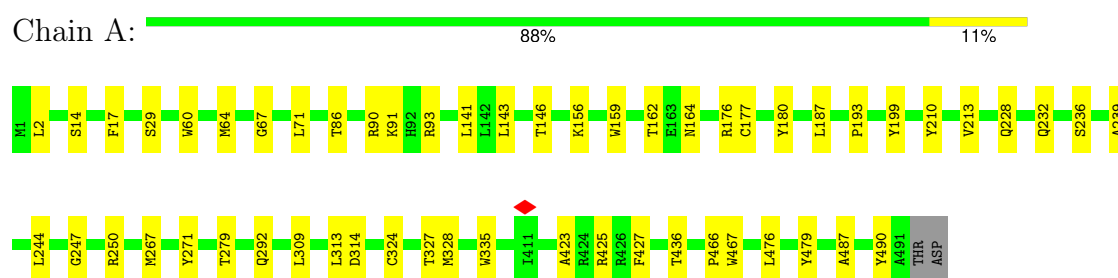
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	15	Total	O	0
			15	15	

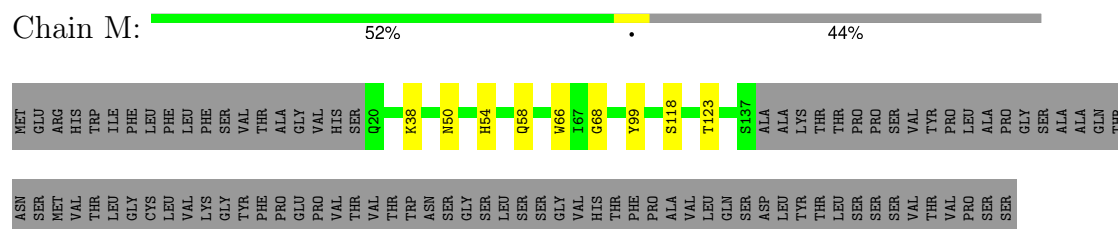
3 Residue-property plots

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

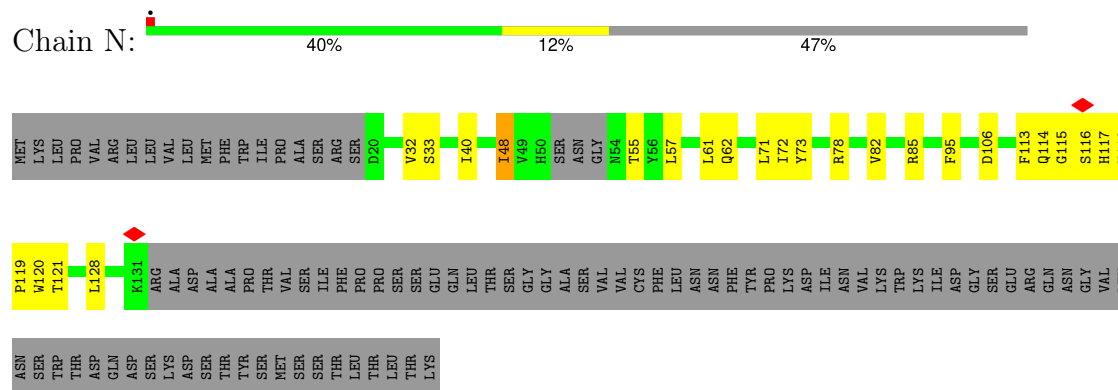
- Molecule 1: Protein-cysteine N-palmitoyltransferase HHAT



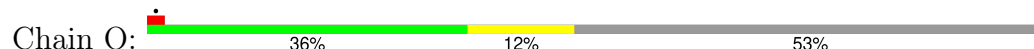
- Molecule 2: 1C06 Fab heavy chain



- Molecule 3: 1C06 Fab light chain



- Molecule 4: 3H02 Fab heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	174058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26.5	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	18.682	Depositor
Minimum map value	-10.477	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.402	Depositor
Recommended contour level	1.65	Depositor
Map size (Å)	220.78, 220.78, 220.78	wwPDB
Map dimensions	415, 415, 415	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.532, 0.532, 0.532	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/4143	0.46	0/5655
2	M	0.45	0/911	0.54	0/1242
3	N	0.43	0/834	0.55	0/1137
4	O	0.39	0/830	0.50	0/1127
5	P	0.40	0/700	0.49	0/952
All	All	0.42	0/7418	0.49	0/10113

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4003	0	3921	31	0
2	M	887	0	823	6	0
3	N	812	0	762	17	0
4	O	805	0	738	20	0
5	P	683	0	609	7	0
6	A	43	0	30	3	0
7	A	145	0	0	1	0
8	A	511	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	15	0	0	0	0
All	All	7904	0	6883	79	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 5.

All (79) 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)
4:O:25:GLN:H	4:O:130:GLN:HE22	1.10	0.94
4:O:25:GLN:NE2	4:O:115:CYS:H	1.90	0.70
3:N:114:GLN:HE21	3:N:121:THR:HG22	1.60	0.66
5:P:59:TRP:HD1	5:P:72:ILE:HD11	1.60	0.65
1:A:210:TYR:OH	1:A:314:ASP:OD2	2.16	0.62
4:O:47:THR:HG23	4:O:50:ASN:HB2	1.81	0.62
5:P:59:TRP:CD1	5:P:72:ILE:HD11	2.37	0.59
1:A:91:LYS:HA	1:A:232:GLN:HE21	1.66	0.59
2:M:58:GLN:HE22	3:N:62:GLN:HE22	1.52	0.58
4:O:123:TYR:HB3	5:P:73:TYR:HB2	1.86	0.57
1:A:162:THR:HG23	1:A:164:ASN:H	1.68	0.57
4:O:25:GLN:HE22	4:O:115:CYS:H	1.52	0.57
6:A:501:HEM:HHA	6:A:501:HEM:HBA1	1.86	0.56
4:O:39:ILE:HB	4:O:102:ILE:HG22	1.87	0.56
2:M:54:HIS:NE2	2:M:118:SER:OG	2.38	0.56
1:A:436:THR:HG23	1:A:476:LEU:HD13	1.87	0.55
4:O:118:VAL:HA	4:O:124:TYR:O	2.08	0.54
1:A:176:ARG:NH2	1:A:213:VAL:O	2.40	0.54
1:A:279:THR:HG21	2:M:50:ASN:HB2	1.91	0.53
1:A:271:TYR:CE2	1:A:292:GLN:HG3	2.44	0.53
1:A:466:PRO:HB2	1:A:467:TRP:CD1	2.44	0.53
1:A:156:LYS:HD3	1:A:159:TRP:CZ3	2.43	0.52
1:A:423:ALA:O	1:A:427:PHE:HD1	1.93	0.51
7:A:502:PKZ:O2B	7:A:502:PKZ:O7A	2.28	0.51
3:N:57:LEU:HD22	3:N:95:PHE:CG	2.46	0.51
1:A:93:ARG:NH2	1:A:228:GLN:OE1	2.43	0.51
4:O:57:ARG:HH22	4:O:109:ASP:HA	1.74	0.50
3:N:113:PHE:CE1	3:N:120:TRP:HB3	2.46	0.50
1:A:67:GLY:HA2	1:A:71:LEU:HB2	1.94	0.50
1:A:247:GLY:HA3	1:A:309:LEU:HD13	1.93	0.49
1:A:267:MET:HG3	1:A:292:GLN:OE1	2.13	0.49
3:N:113:PHE:CZ	3:N:120:TRP:CD1	3.02	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:O	1:A:146:THR:OG1	2.33	0.47
4:O:70:ILE:HG21	4:O:100:LEU:HD11	1.96	0.47
4:O:110:MET:SD	4:O:135:THR:HA	2.55	0.46
1:A:86:THR:HG23	1:A:90:ARG:HD2	1.97	0.46
1:A:244:LEU:HD13	1:A:313:LEU:HD11	1.98	0.46
1:A:187:LEU:HD12	1:A:199:TYR:HB3	1.98	0.45
1:A:236:SER:O	1:A:239:ALA:N	2.43	0.44
3:N:61:LEU:HD12	3:N:62:GLN:N	2.32	0.44
4:O:72:THR:HA	4:O:91:LEU:HD11	2.00	0.44
4:O:81:ASP:N	4:O:81:ASP:OD1	2.50	0.44
3:N:118:VAL:HG13	3:N:119:PRO:HD2	2.00	0.44
1:A:324:CYS:O	1:A:327:THR:OG1	2.34	0.44
3:N:40:ILE:HD11	3:N:128:LEU:HD11	2.00	0.43
1:A:487:ALA:HA	1:A:490:TYR:CE2	2.54	0.43
3:N:116:SER:O	3:N:116:SER:OG	2.34	0.43
5:P:109:VAL:HG12	5:P:127:LYS:HA	2.00	0.43
2:M:123:THR:HG22	3:N:116:SER:HB2	2.00	0.43
3:N:85:ARG:HH21	3:N:106:ASP:CG	2.21	0.43
1:A:328:MET:O	1:A:479:TYR:OH	2.27	0.43
4:O:65:LYS:HE3	4:O:65:LYS:HB2	1.71	0.42
4:O:25:GLN:NE2	4:O:115:CYS:SG	2.76	0.42
1:A:2:LEU:HD21	1:A:425:ARG:HG2	2.01	0.42
5:P:127:LYS:HE3	5:P:127:LYS:HB3	1.89	0.42
4:O:70:ILE:CG2	4:O:100:LEU:HD11	2.49	0.42
1:A:177:CYS:HA	1:A:180:TYR:CZ	2.55	0.42
1:A:193:PRO:HA	4:O:120:ASN:O	2.20	0.42
2:M:38:LYS:HE2	2:M:99:TYR:CD2	2.55	0.42
4:O:89:PHE:HE1	4:O:102:ILE:HD12	1.85	0.42
3:N:48:ILE:HD11	3:N:95:PHE:CE2	2.54	0.42
3:N:61:LEU:HB2	3:N:71:LEU:CD1	2.50	0.42
4:O:25:GLN:N	4:O:130:GLN:HE22	1.95	0.42
1:A:60:TRP:O	1:A:64:MET:HG2	2.19	0.42
3:N:115:GLY:O	3:N:117:HIS:N	2.53	0.42
1:A:250:ARG:HH21	6:A:501:HEM:CGD	2.33	0.41
6:A:501:HEM:HAA1	8:A:515:AJP:C21	2.50	0.41
3:N:71:LEU:HD22	3:N:82:VAL:HG11	2.03	0.41
5:P:72:ILE:O	5:P:72:ILE:HG13	2.20	0.41
3:N:72:ILE:HD13	3:N:78:ARG:HA	2.01	0.41
4:O:25:GLN:HE22	4:O:114:PHE:HA	1.86	0.41
4:O:56:VAL:HG12	4:O:66:TRP:HA	2.03	0.41
1:A:14:SER:HA	1:A:17:PHE:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.88	0.40
1:A:335:TRP:HA	1:A:335:TRP:CE3	2.56	0.40
2:M:66:TRP:CZ2	2:M:68:GLY:HA2	2.56	0.40
5:P:76:SER:HA	5:P:88:GLY:O	2.21	0.40
3:N:32:VAL:HG22	3:N:33:SER:O	2.22	0.40
1:A:162:THR:C	1:A:164:ASN:H	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	A	489/493 (99%)	473 (97%)	16 (3%)	0	100	100
2	M	116/211 (55%)	112 (97%)	4 (3%)	0	100	100
3	N	105/207 (51%)	101 (96%)	4 (4%)	0	100	100
4	O	92/211 (44%)	88 (96%)	4 (4%)	0	100	100
5	P	86/207 (42%)	85 (99%)	1 (1%)	0	100	100
All	All	888/1329 (67%)	859 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	418/429 (97%)	417 (100%)	1 (0%)	92	98
2	M	90/177 (51%)	90 (100%)	0	100	100
3	N	86/185 (46%)	83 (96%)	3 (4%)	31	60
4	O	79/177 (45%)	79 (100%)	0	100	100
5	P	68/185 (37%)	68 (100%)	0	100	100
All	All	741/1153 (64%)	737 (100%)	4 (0%)	85	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
3	N	48	ILE
3	N	55	THR
3	N	73	TYR

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

Mol	Chain	Res	Type
2	M	58	GLN
3	N	114	GLN
4	O	130	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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$
7	PKZ	A	502	-	61,67,67	0.55	0	74,93,93	1.07	5 (6%)
8	AJP	A	506	-	49,49,95	0.41	0	75,80,149	0.86	2 (2%)
8	AJP	A	518	-	37,37,95	0.44	0	58,62,149	0.73	2 (3%)
8	AJP	A	505	-	61,61,95	0.39	0	93,98,149	0.67	1 (1%)
8	AJP	A	514	-	35,35,95	0.45	0	54,58,149	0.66	1 (1%)
8	AJP	A	507	-	37,37,95	0.43	0	58,62,149	0.73	1 (1%)
8	AJP	A	517	-	36,36,95	0.43	0	56,60,149	0.71	0
8	AJP	A	516	-	37,37,95	0.45	0	58,62,149	0.92	2 (3%)
6	HEM	A	501	-	42,50,50	1.44	5 (11%)	46,82,82	1.49	8 (17%)
7	PKZ	A	504	-	14,14,67	0.16	0	13,13,93	0.11	0
7	PKZ	A	503	-	61,67,67	0.55	0	74,93,93	1.03	5 (6%)
8	AJP	A	509	-	49,49,95	0.41	0	75,80,149	0.72	1 (1%)
8	AJP	A	511	-	37,37,95	0.45	0	58,62,149	0.77	2 (3%)
8	AJP	A	512	-	37,37,95	0.44	0	58,62,149	0.71	1 (1%)
8	AJP	A	513	-	49,49,95	0.40	0	75,80,149	0.79	3 (4%)
8	AJP	A	515	-	36,36,95	0.48	0	56,60,149	1.28	5 (8%)
8	AJP	A	508	-	49,49,95	0.40	0	75,80,149	0.73	2 (2%)
8	AJP	A	510	-	38,38,95	0.42	0	58,63,149	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PKZ	A	502	-	-	14/62/82/82	0/3/3/3
8	AJP	A	506	-	14/14/19/38	2/6/121/220	0/7/7/11
8	AJP	A	505	-	15/15/24/38	7/12/147/220	0/8/8/11
8	AJP	A	514	-	9/9/12/38	-	0/6/6/11
8	AJP	A	507	-	10/10/14/38	-	0/6/6/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	AJP	A	517	-	10/10/13/38	-	0/6/6/11
8	AJP	A	516	-	10/10/14/38	-	0/6/6/11
8	AJP	A	512	-	10/10/14/38	-	0/6/6/11
6	HEM	A	501	-	-	3/12/54/54	-
8	AJP	A	513	-	12/12/19/38	2/6/121/220	0/7/7/11
8	AJP	A	509	-	13/13/19/38	4/6/121/220	0/7/7/11
8	AJP	A	511	-	10/10/14/38	-	0/6/6/11
7	PKZ	A	503	-	-	11/62/82/82	0/3/3/3
8	AJP	A	518	-	10/10/14/38	-	0/6/6/11
8	AJP	A	515	-	10/10/13/38	-	0/6/6/11
7	PKZ	A	504	-	-	1/12/12/82	-
8	AJP	A	508	-	12/12/19/38	3/6/121/220	0/7/7/11
8	AJP	A	510	-	11/11/14/38	0/2/97/220	0/6/6/11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	501	HEM	C3C-C2C	-4.55	1.34	1.40
6	A	501	HEM	C3C-CAC	3.21	1.54	1.47
6	A	501	HEM	CAB-C3B	2.72	1.54	1.47
6	A	501	HEM	C3C-C4C	2.04	1.44	1.41
6	A	501	HEM	CMD-C2D	2.02	1.54	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	502	PKZ	C4B-O4B-C1B	-5.95	104.47	109.92
7	A	503	PKZ	P3B-O3B-C3B	-4.61	111.13	123.43
7	A	503	PKZ	C4B-O4B-C1B	-4.06	106.21	109.92
7	A	502	PKZ	P3B-O3B-C3B	-3.76	113.40	123.43
8	A	513	AJP	C26-O25-C23	3.32	120.82	115.27
8	A	515	AJP	C06-C07-C08	-3.31	98.95	104.28
8	A	506	AJP	C26-O25-C23	3.31	120.80	115.27
8	A	515	AJP	O09-C08-C10	3.25	116.79	110.20
6	A	501	HEM	CAD-CBD-CGD	-3.23	105.09	113.67
8	A	515	AJP	C12-C07-C06	3.22	130.01	120.50
7	A	503	PKZ	OAP-CAP-CBP	-3.19	102.80	110.18
8	A	515	AJP	C05-C06-C07	-3.07	98.84	103.37
8	A	516	AJP	C83-C06-C05	2.89	119.59	114.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	501	HEM	C4A-C3A-C2A	2.84	108.97	107.00
8	A	515	AJP	C11-C12-C07	-2.79	95.95	100.16
8	A	506	AJP	C83-C06-C05	2.61	119.13	114.94
6	A	501	HEM	C3D-C4D-ND	-2.46	107.47	110.17
7	A	502	PKZ	C5A-C6A-N6A	2.44	124.03	120.31
8	A	513	AJP	O25-C23-C24	2.43	114.37	109.64
8	A	508	AJP	C21-C20-C19	2.34	109.47	107.23
8	A	512	AJP	C21-C20-C19	2.34	109.46	107.23
8	A	509	AJP	C24-C23-C22	2.33	113.50	111.07
7	A	503	PKZ	C5A-C6A-N6A	2.30	123.81	120.31
7	A	503	PKZ	C7P-C6P-C5P	2.30	116.22	112.39
6	A	501	HEM	C4D-ND-C1D	2.29	107.92	105.21
8	A	514	AJP	C83-C06-C05	2.29	118.62	114.94
6	A	501	HEM	C4C-CHD-C1D	2.29	125.58	122.56
8	A	505	AJP	C24-C23-C22	2.23	113.40	111.07
6	A	501	HEM	CMC-C2C-C3C	2.22	129.11	124.68
6	A	501	HEM	CMA-C3A-C4A	-2.21	125.22	128.46
8	A	508	AJP	C24-C23-C22	2.20	113.37	111.07
8	A	511	AJP	C24-C23-C22	2.16	113.05	110.38
7	A	502	PKZ	O6A-CCP-CBP	-2.13	107.12	110.55
8	A	513	AJP	C21-C20-C19	2.09	109.22	107.23
8	A	518	AJP	C24-C23-C22	2.09	112.96	110.38
8	A	516	AJP	C24-C23-C22	2.09	112.96	110.38
6	A	501	HEM	C1B-NB-C4B	2.03	107.61	105.21
8	A	518	AJP	C21-C20-C19	2.02	109.16	107.23
8	A	511	AJP	C21-C20-C19	2.02	109.16	107.23
8	A	507	AJP	C21-C20-C19	2.01	109.15	107.23
7	A	502	PKZ	C7P-C6P-C5P	-2.01	109.05	112.39

All (156) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	505	AJP	C38
8	A	505	AJP	C35
8	A	505	AJP	C20
8	A	505	AJP	C36
8	A	505	AJP	C11
8	A	505	AJP	C10
8	A	505	AJP	C08
8	A	505	AJP	C16
8	A	505	AJP	C15
8	A	505	AJP	C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
8	A	505	AJP	C22
8	A	505	AJP	C30
8	A	505	AJP	C12
8	A	505	AJP	C07
8	A	505	AJP	C27
8	A	506	AJP	C26
8	A	506	AJP	C20
8	A	506	AJP	C11
8	A	506	AJP	C10
8	A	506	AJP	C08
8	A	506	AJP	C16
8	A	506	AJP	C15
8	A	506	AJP	C19
8	A	506	AJP	C22
8	A	506	AJP	C23
8	A	506	AJP	C12
8	A	506	AJP	C30
8	A	506	AJP	C07
8	A	506	AJP	C27
8	A	507	AJP	C20
8	A	507	AJP	C11
8	A	507	AJP	C10
8	A	507	AJP	C08
8	A	507	AJP	C16
8	A	507	AJP	C15
8	A	507	AJP	C19
8	A	507	AJP	C22
8	A	507	AJP	C12
8	A	507	AJP	C07
8	A	508	AJP	C20
8	A	508	AJP	C11
8	A	508	AJP	C10
8	A	508	AJP	C08
8	A	508	AJP	C16
8	A	508	AJP	C15
8	A	508	AJP	C19
8	A	508	AJP	C22
8	A	508	AJP	C30
8	A	508	AJP	C12
8	A	508	AJP	C07
8	A	508	AJP	C27
8	A	509	AJP	C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
8	A	509	AJP	C20
8	A	509	AJP	C11
8	A	509	AJP	C10
8	A	509	AJP	C08
8	A	509	AJP	C16
8	A	509	AJP	C15
8	A	509	AJP	C19
8	A	509	AJP	C22
8	A	509	AJP	C30
8	A	509	AJP	C12
8	A	509	AJP	C07
8	A	509	AJP	C27
8	A	510	AJP	C20
8	A	510	AJP	C11
8	A	510	AJP	C10
8	A	510	AJP	C08
8	A	510	AJP	C16
8	A	510	AJP	C15
8	A	510	AJP	C19
8	A	510	AJP	C22
8	A	510	AJP	C23
8	A	510	AJP	C12
8	A	510	AJP	C07
8	A	511	AJP	C20
8	A	511	AJP	C11
8	A	511	AJP	C10
8	A	511	AJP	C08
8	A	511	AJP	C16
8	A	511	AJP	C15
8	A	511	AJP	C19
8	A	511	AJP	C22
8	A	511	AJP	C12
8	A	511	AJP	C07
8	A	512	AJP	C20
8	A	512	AJP	C11
8	A	512	AJP	C10
8	A	512	AJP	C08
8	A	512	AJP	C16
8	A	512	AJP	C15
8	A	512	AJP	C19
8	A	512	AJP	C22
8	A	512	AJP	C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
8	A	512	AJP	C07
8	A	513	AJP	C20
8	A	513	AJP	C11
8	A	513	AJP	C10
8	A	513	AJP	C08
8	A	513	AJP	C16
8	A	513	AJP	C15
8	A	513	AJP	C19
8	A	513	AJP	C22
8	A	513	AJP	C30
8	A	513	AJP	C12
8	A	513	AJP	C07
8	A	513	AJP	C27
8	A	514	AJP	C20
8	A	514	AJP	C11
8	A	514	AJP	C10
8	A	514	AJP	C08
8	A	514	AJP	C16
8	A	514	AJP	C15
8	A	514	AJP	C19
8	A	514	AJP	C12
8	A	514	AJP	C07
8	A	515	AJP	C20
8	A	515	AJP	C11
8	A	515	AJP	C10
8	A	515	AJP	C16
8	A	515	AJP	C15
8	A	515	AJP	C19
8	A	515	AJP	C22
8	A	515	AJP	C02
8	A	515	AJP	C12
8	A	515	AJP	C07
8	A	516	AJP	C20
8	A	516	AJP	C11
8	A	516	AJP	C10
8	A	516	AJP	C08
8	A	516	AJP	C16
8	A	516	AJP	C15
8	A	516	AJP	C19
8	A	516	AJP	C22
8	A	516	AJP	C12
8	A	516	AJP	C07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
8	A	517	AJP	C20
8	A	517	AJP	C11
8	A	517	AJP	C10
8	A	517	AJP	C08
8	A	517	AJP	C16
8	A	517	AJP	C15
8	A	517	AJP	C19
8	A	517	AJP	C22
8	A	517	AJP	C12
8	A	517	AJP	C07
8	A	518	AJP	C20
8	A	518	AJP	C11
8	A	518	AJP	C10
8	A	518	AJP	C08
8	A	518	AJP	C16
8	A	518	AJP	C15
8	A	518	AJP	C19
8	A	518	AJP	C22
8	A	518	AJP	C12
8	A	518	AJP	C07

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	HEM	C1A-C2A-CAA-CBA
6	A	501	HEM	C3A-C2A-CAA-CBA
7	A	502	PKZ	OAP-CAP-CBP-CCP
7	A	502	PKZ	C9P-CAP-CBP-CCP
7	A	502	PKZ	C9P-CAP-CBP-CDP
7	A	502	PKZ	OAP-CAP-CBP-CEP
7	A	502	PKZ	C9P-CAP-CBP-CEP
7	A	503	PKZ	O1-C1-S1P-C2P
7	A	503	PKZ	C2-C1-S1P-C2P
7	A	503	PKZ	CCP-O6A-P2A-O5A
7	A	503	PKZ	O9P-C9P-CAP-CBP
7	A	503	PKZ	N8P-C9P-CAP-OAP
7	A	503	PKZ	CAP-C9P-N8P-C7P
8	A	509	AJP	C22-C23-O25-C26
8	A	513	AJP	C22-C23-O25-C26
7	A	503	PKZ	O9P-C9P-N8P-C7P
8	A	506	AJP	O31-C26-O25-C23
8	A	506	AJP	C27-C26-O25-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	503	PKZ	C4B-C5B-O5B-P1A
8	A	505	AJP	O40-C35-O34-C29
8	A	505	AJP	C36-C35-O34-C29
8	A	505	AJP	C30-C29-O34-C35
8	A	509	AJP	C24-C23-O25-C26
8	A	505	AJP	C28-C29-O34-C35
7	A	502	PKZ	S1P-C2P-C3P-N4P
8	A	513	AJP	O31-C30-C32-O33
8	A	505	AJP	O31-C30-C32-O33
7	A	502	PKZ	O9P-C9P-CAP-OAP
7	A	503	PKZ	O9P-C9P-CAP-OAP
7	A	502	PKZ	OAP-CAP-CBP-CDP
8	A	508	AJP	O31-C26-O25-C23
7	A	504	PKZ	C9-C10-C11-C12
7	A	503	PKZ	N8P-C9P-CAP-CBP
7	A	502	PKZ	N8P-C9P-CAP-OAP
7	A	502	PKZ	O1-C1-S1P-C2P
7	A	502	PKZ	C2-C1-S1P-C2P
7	A	502	PKZ	C5P-C6P-C7P-N8P
7	A	503	PKZ	C2-C3-C4-C5
8	A	508	AJP	C27-C26-O25-C23
8	A	505	AJP	O31-C26-O25-C23
8	A	508	AJP	C22-C23-O25-C26
8	A	509	AJP	O31-C26-O25-C23
8	A	509	AJP	C27-C26-O25-C23
8	A	505	AJP	C27-C26-O25-C23
7	A	502	PKZ	C2-C3-C4-C5
7	A	502	PKZ	C2P-C3P-N4P-C5P
6	A	501	HEM	CAA-CBA-CGA-O2A

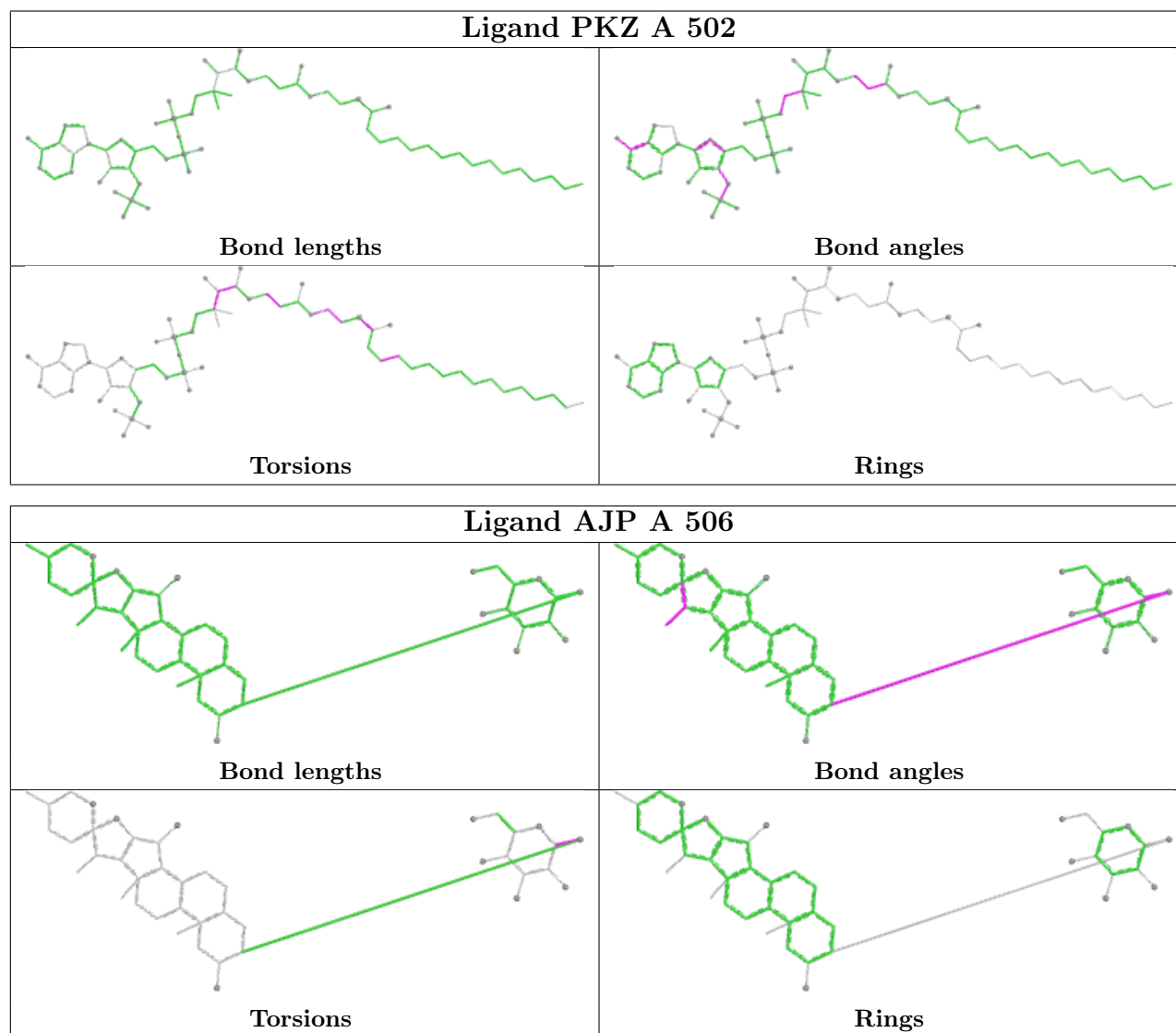
There are no ring outliers.

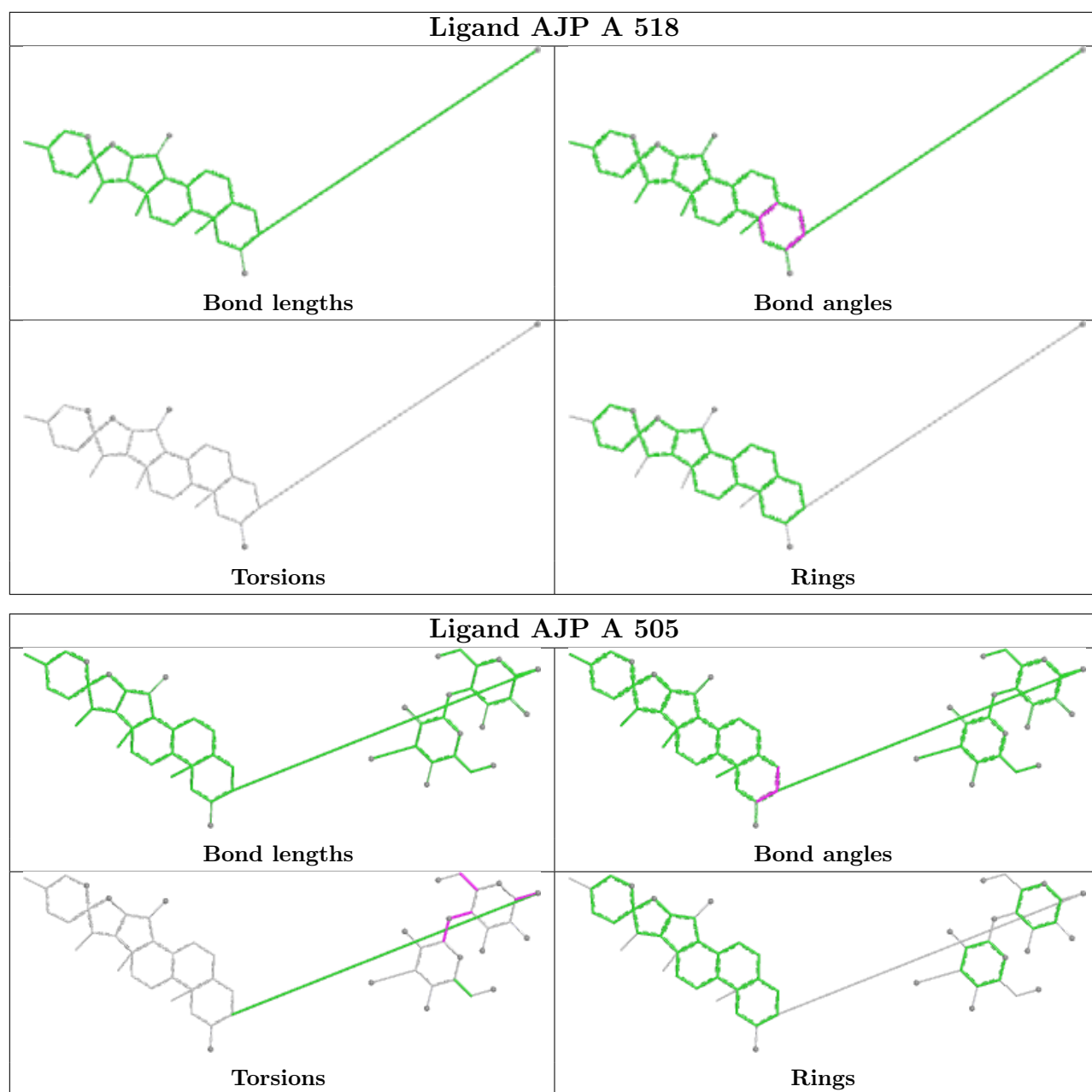
3 monomers are involved in 4 short contacts:

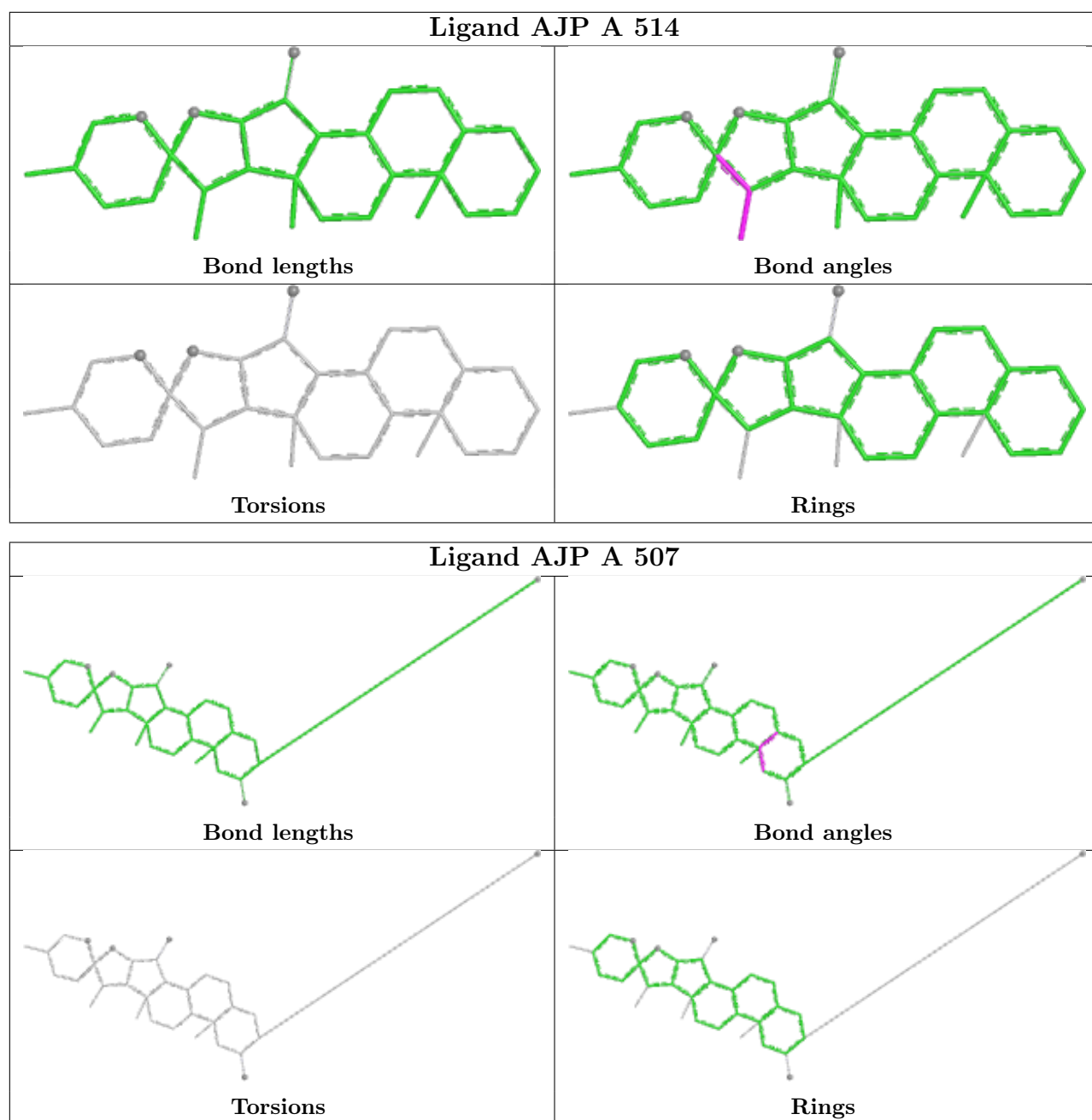
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	502	PKZ	1	0
6	A	501	HEM	3	0
8	A	515	AJP	1	0

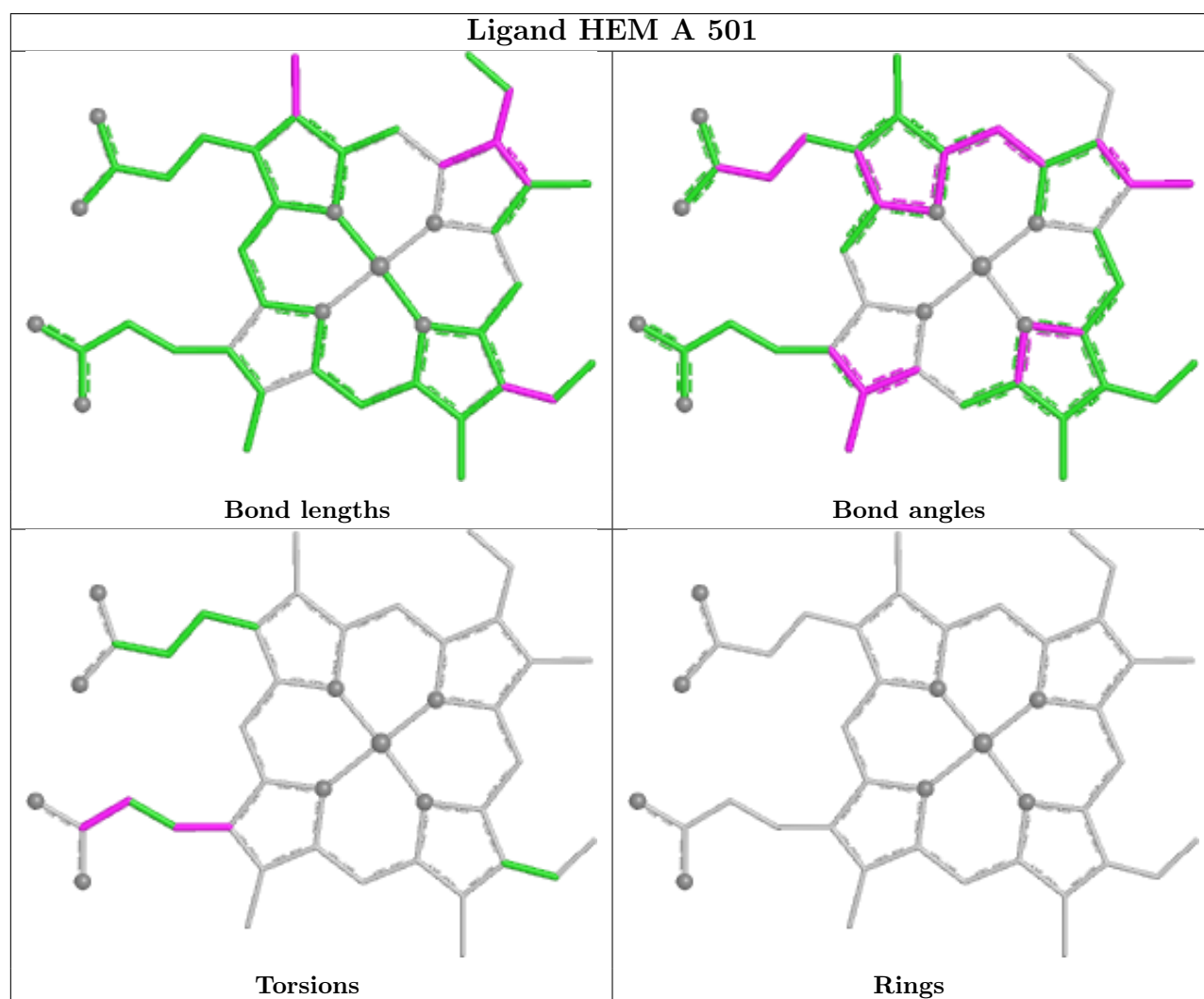
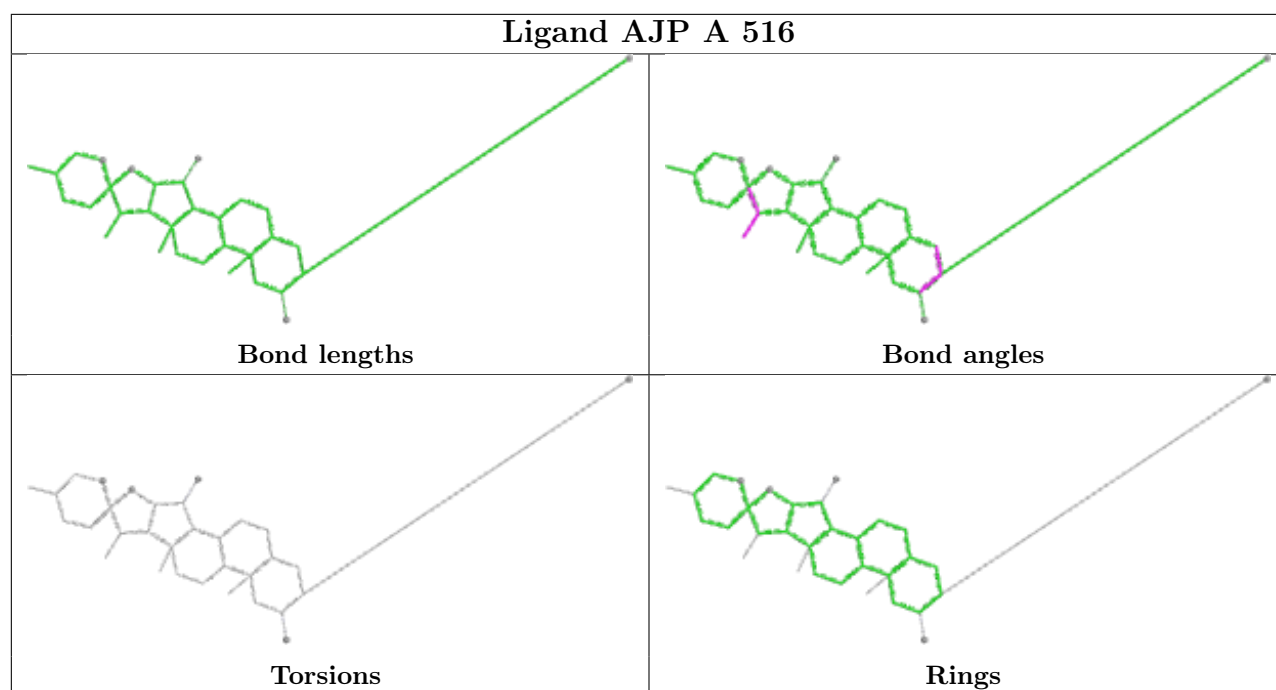
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

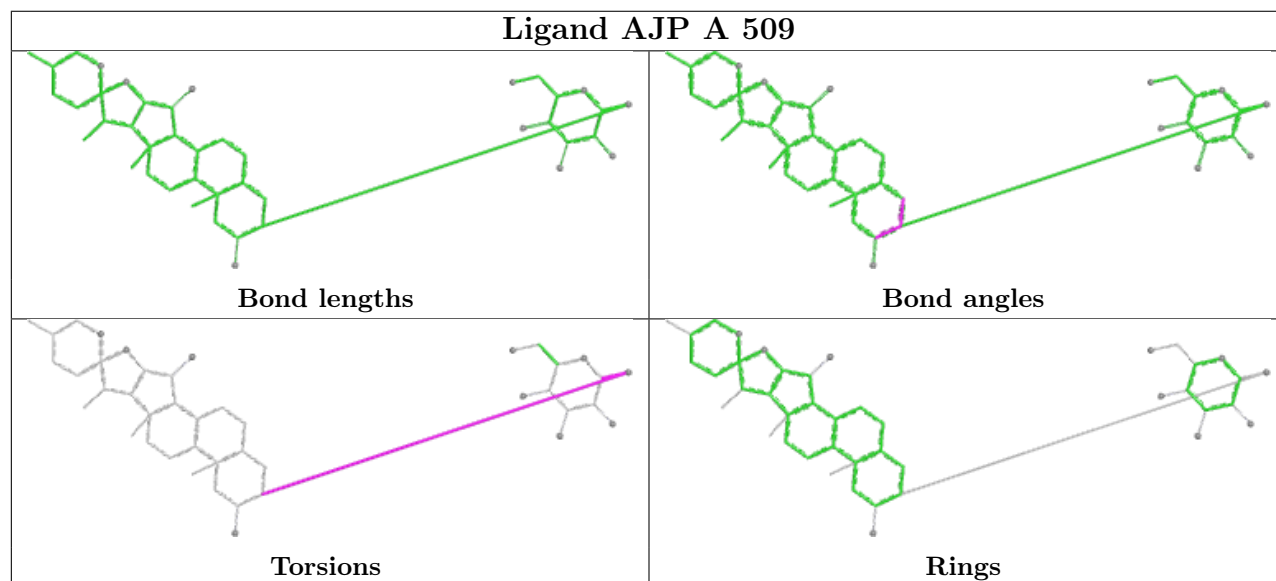
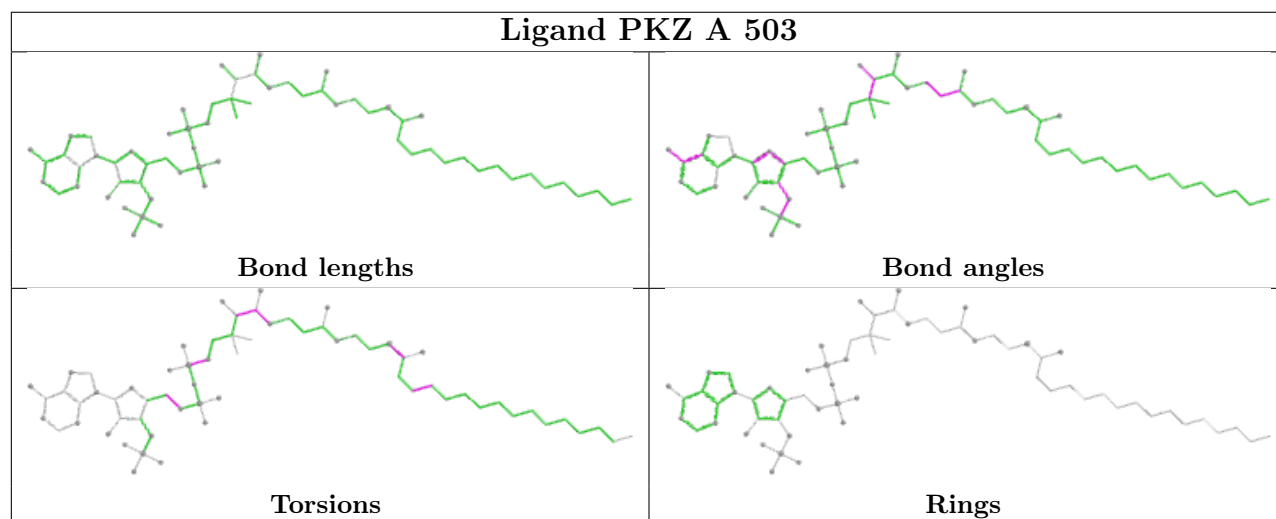
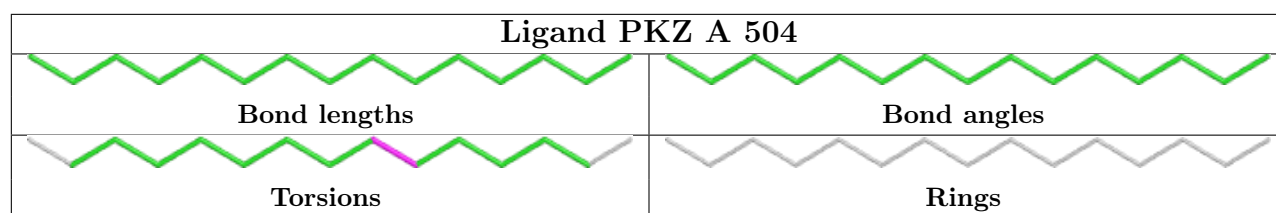
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

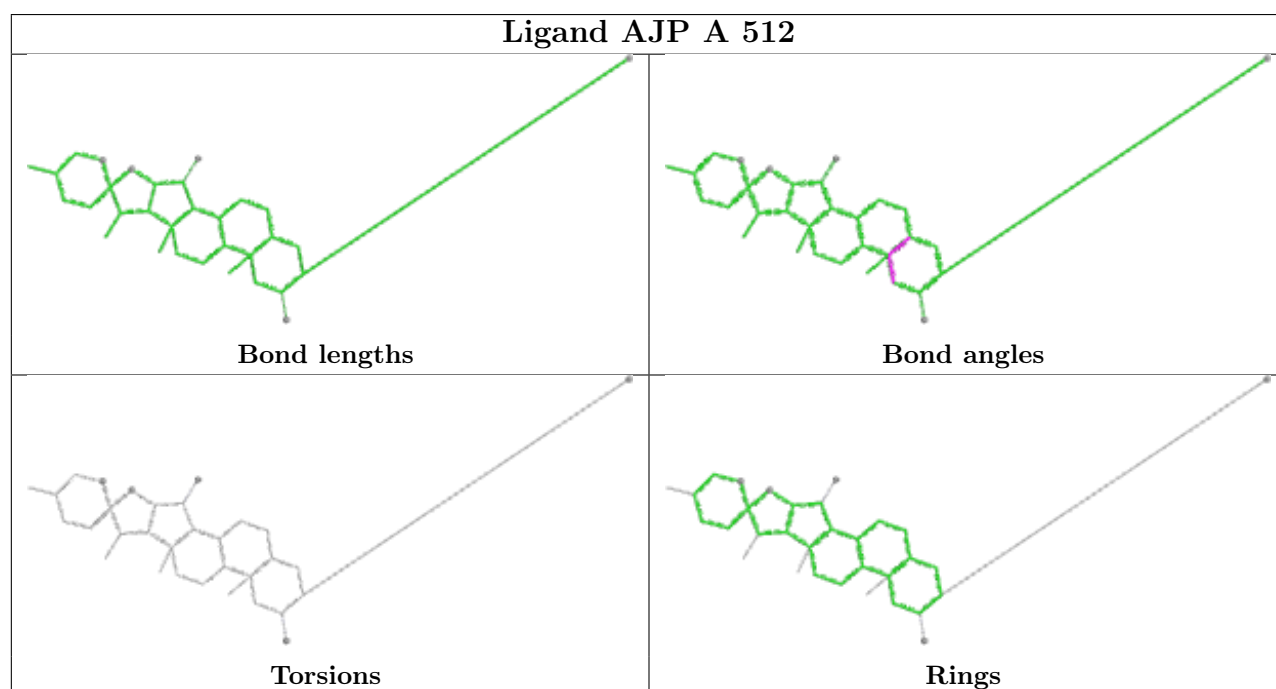
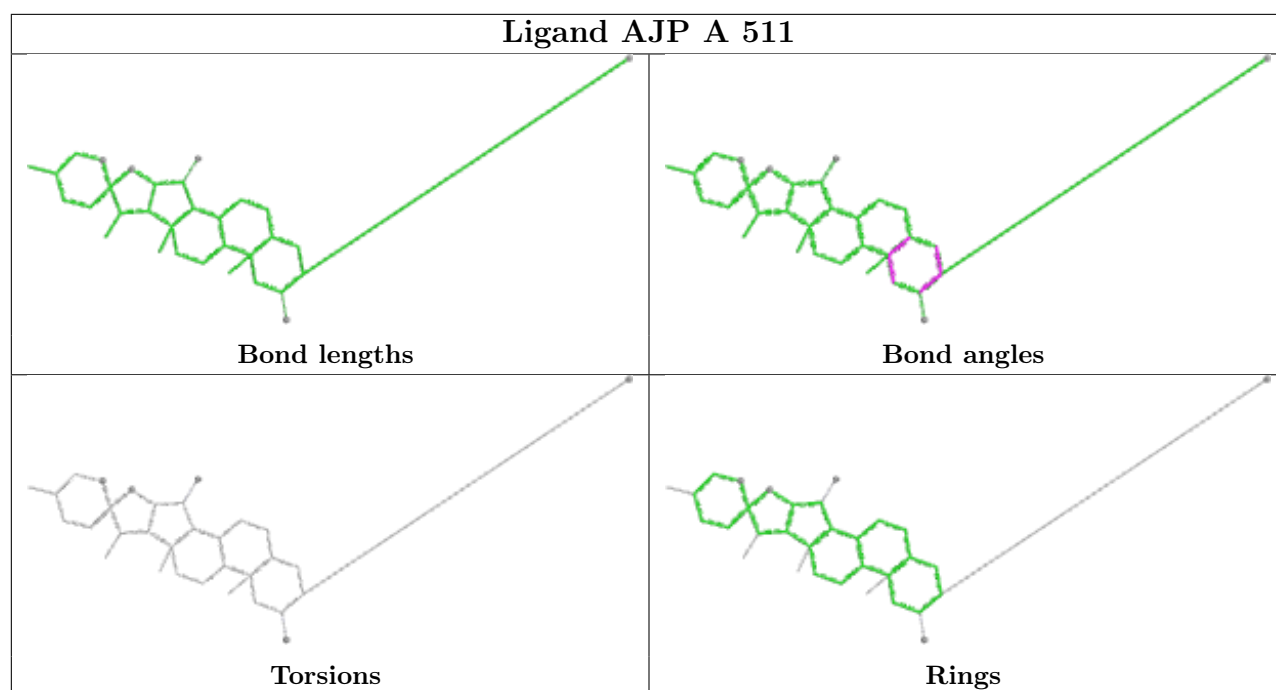




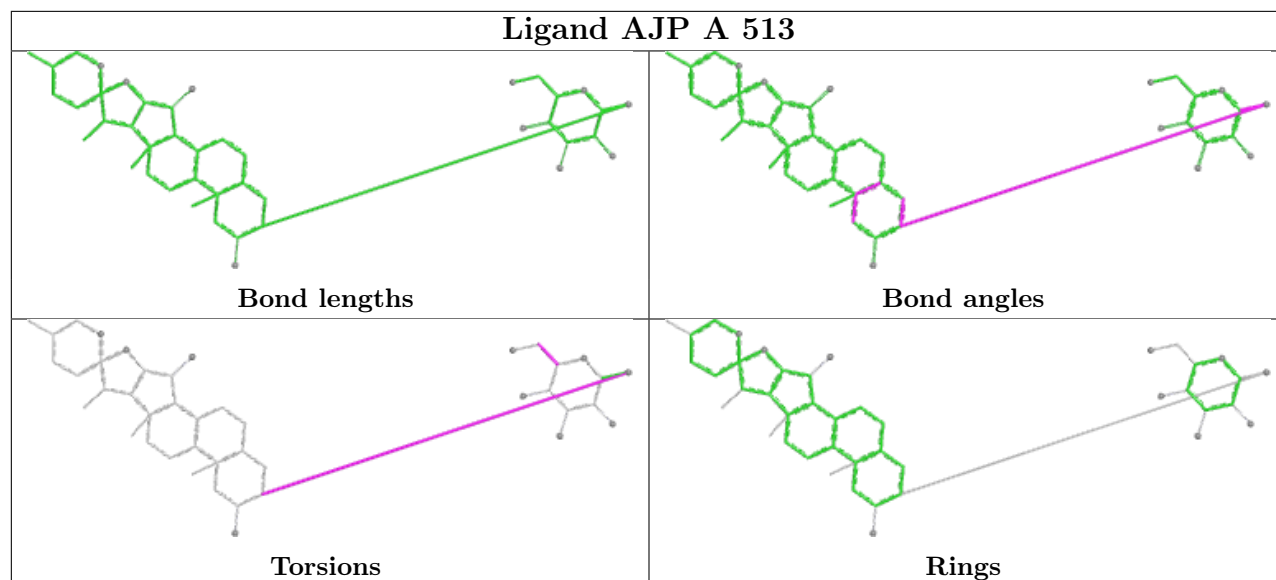




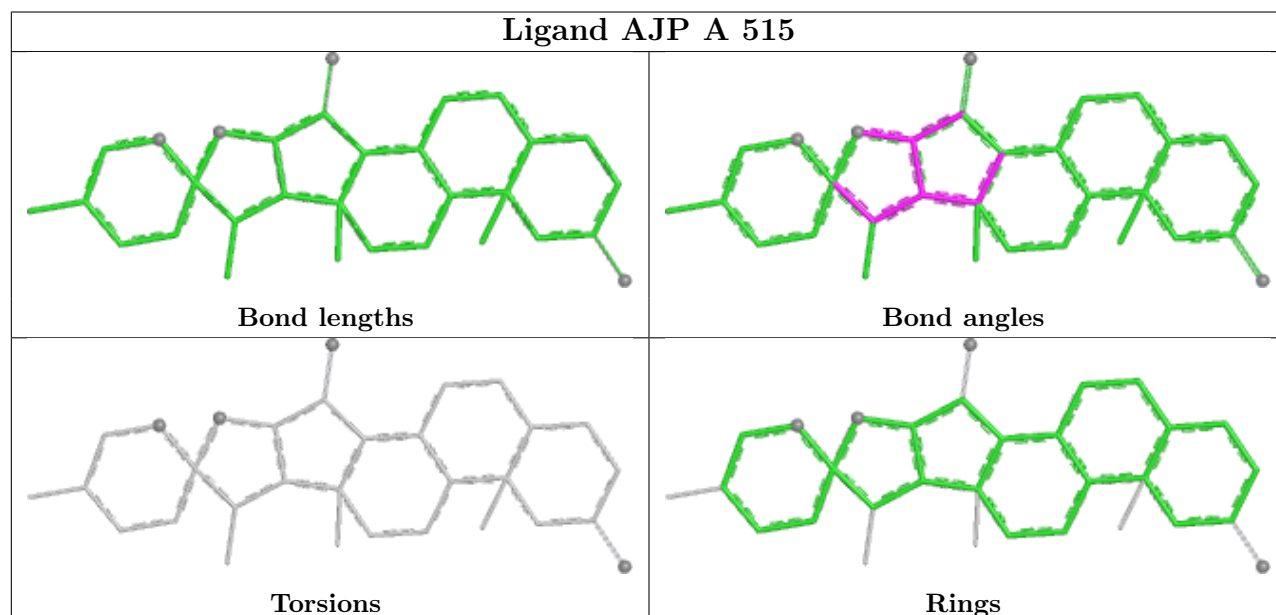




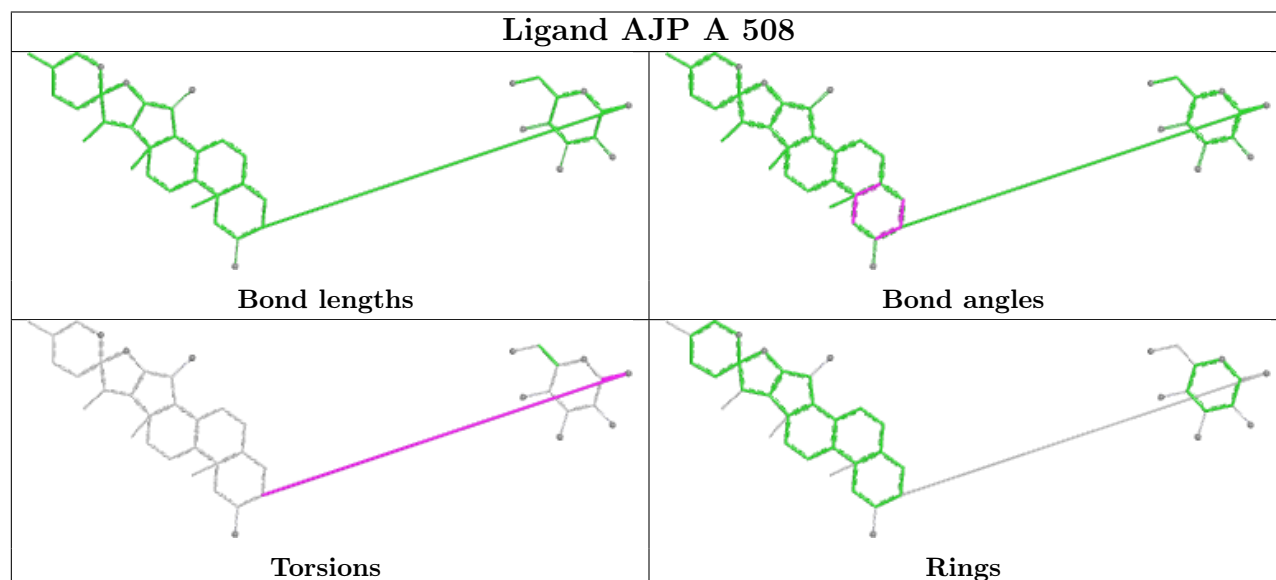
Ligand AJP A 513



Ligand AJP A 515



Ligand AJP A 508



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

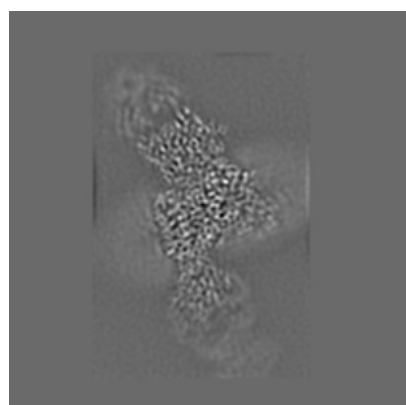
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23836. These allow visual inspection of the internal detail of the map and identification of artifacts.

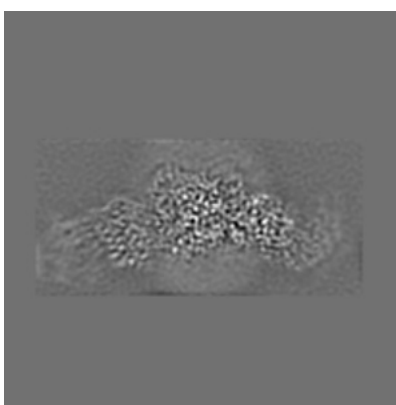
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

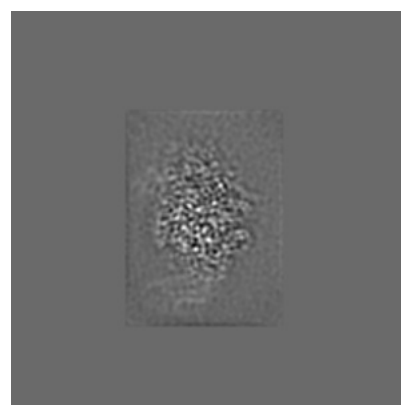
6.1.1 Primary map



X



Y

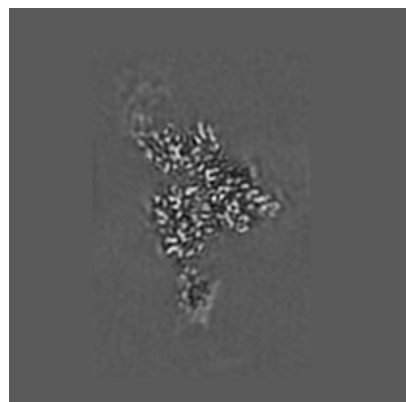


Z

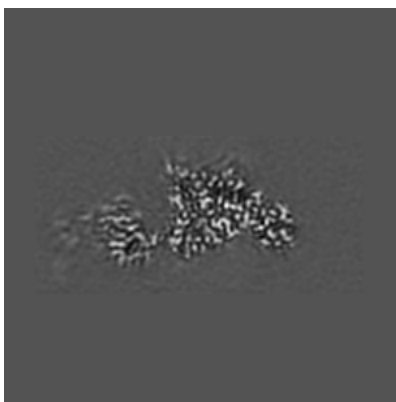
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

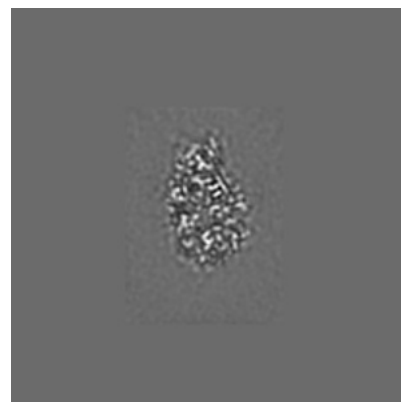
6.2.1 Primary map



X Index: 207



Y Index: 207

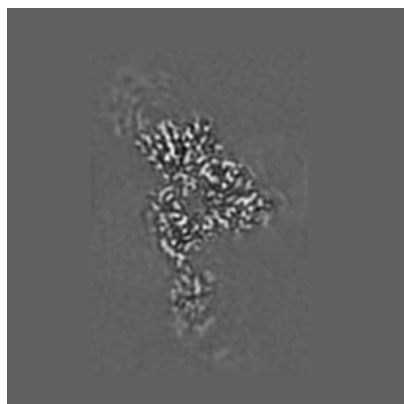


Z Index: 207

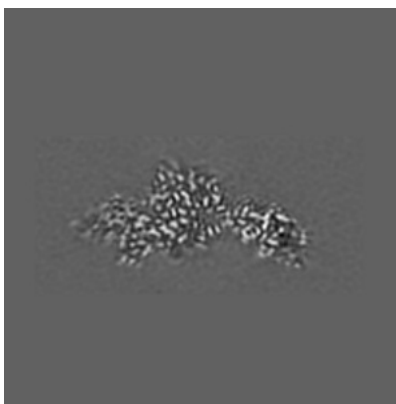
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

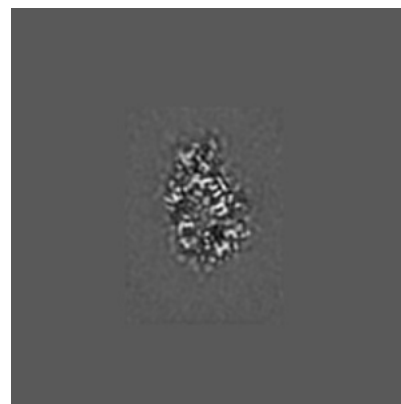
6.3.1 Primary map



X Index: 199



Y Index: 187

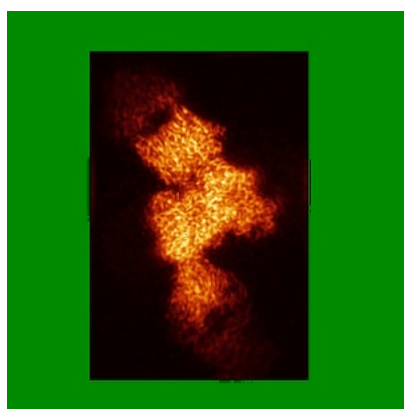


Z Index: 205

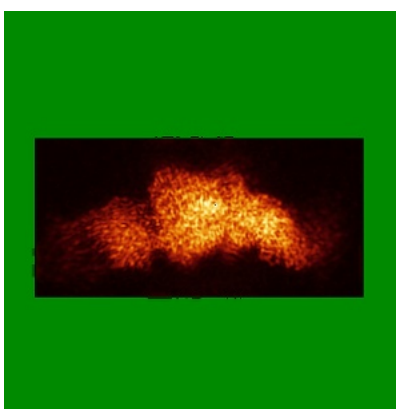
The images above show the largest variance slices of the map in three orthogonal directions.

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

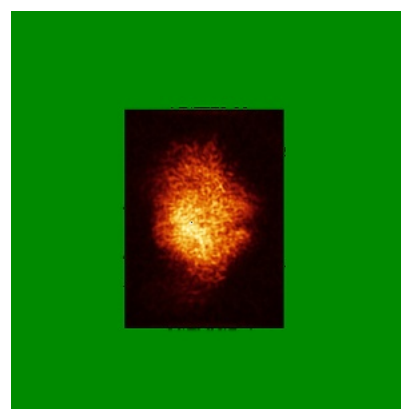
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

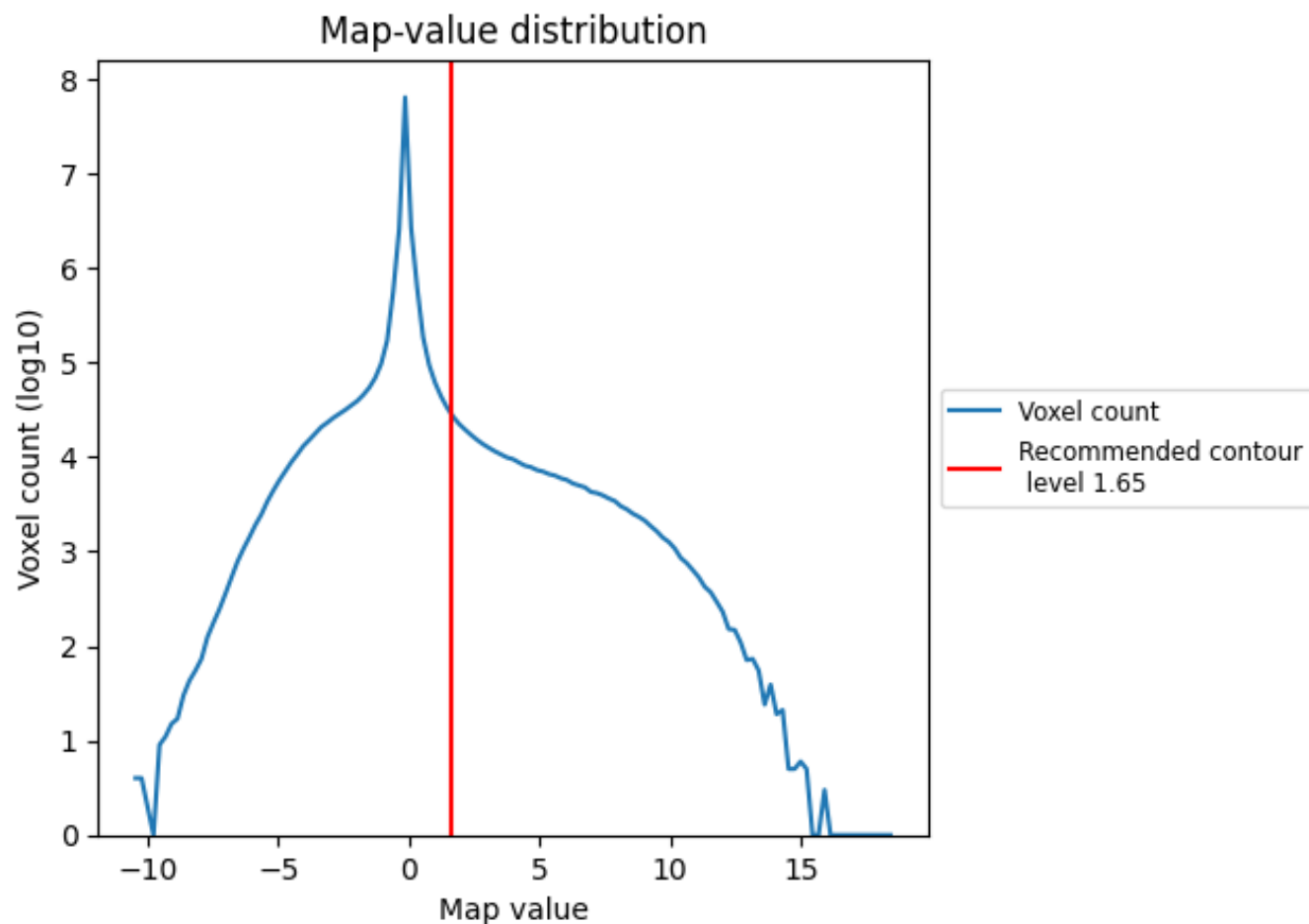
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

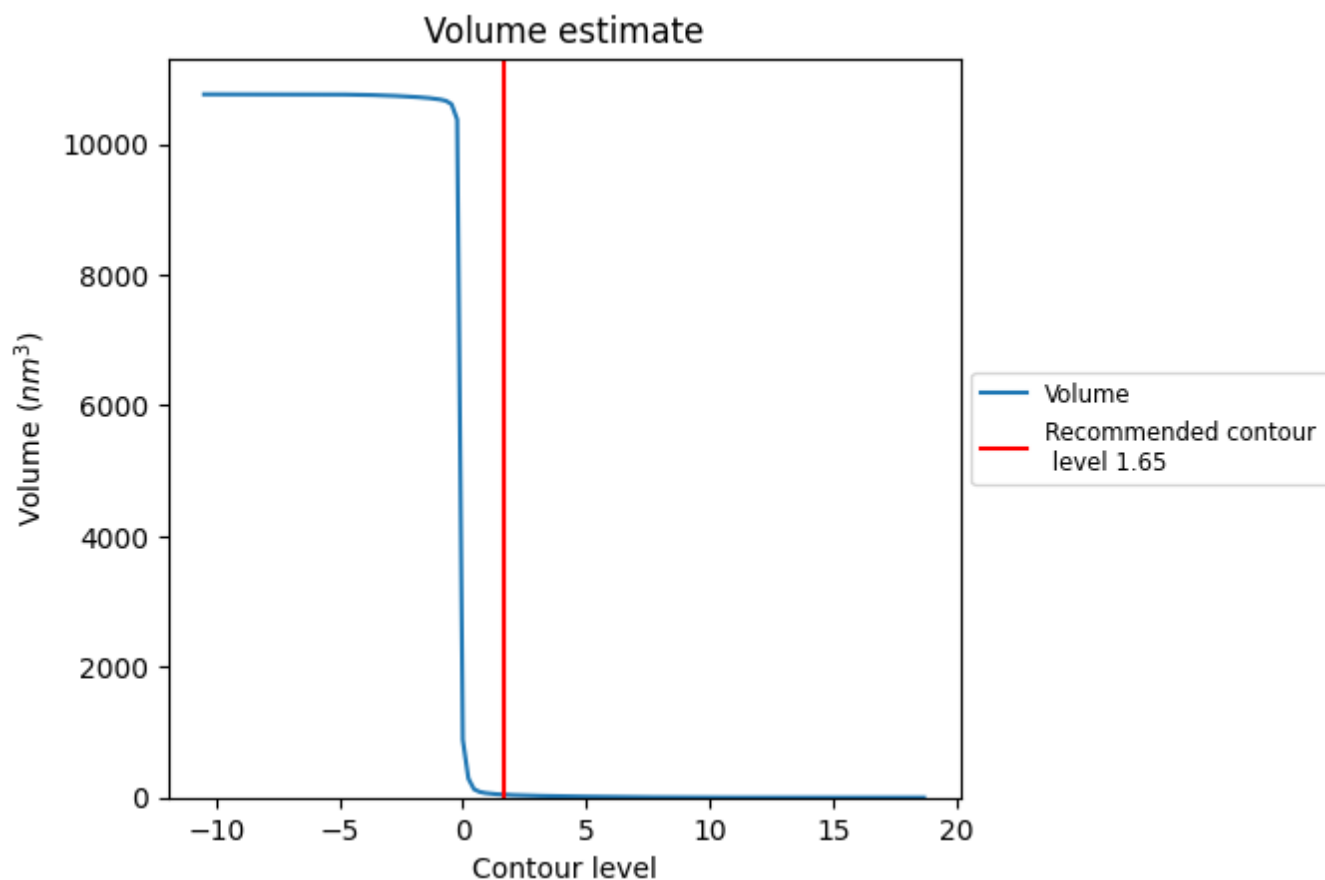
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

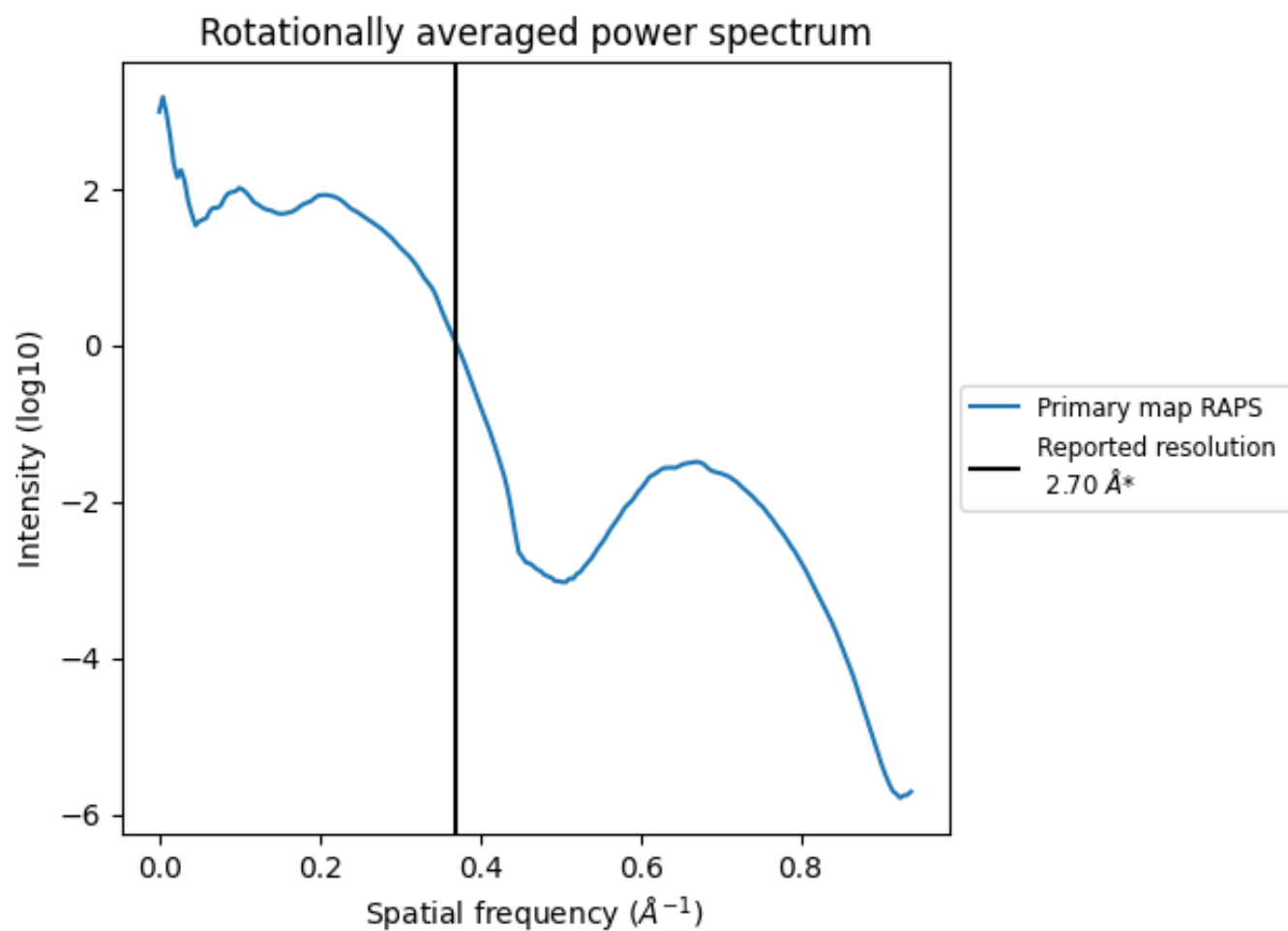
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

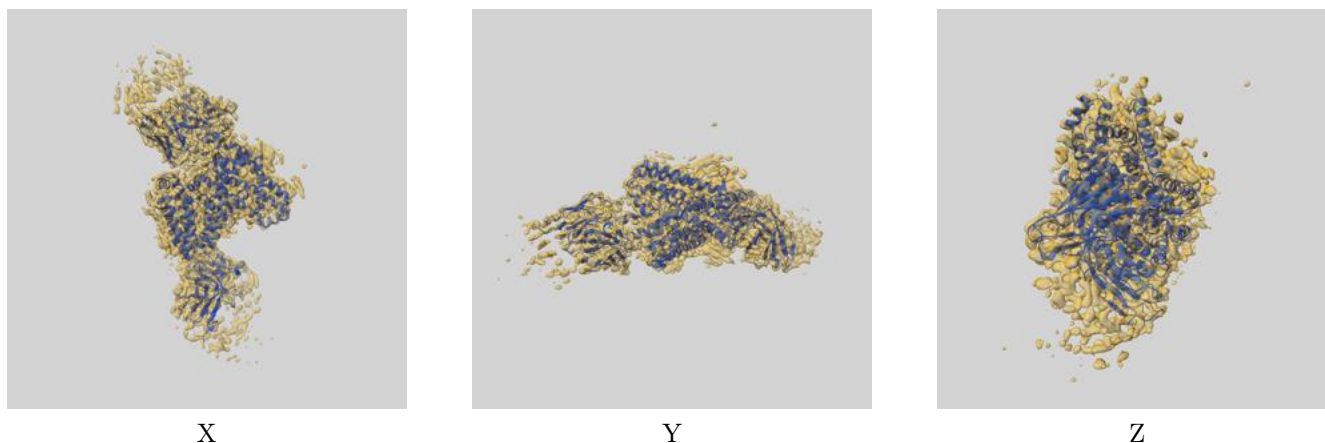
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

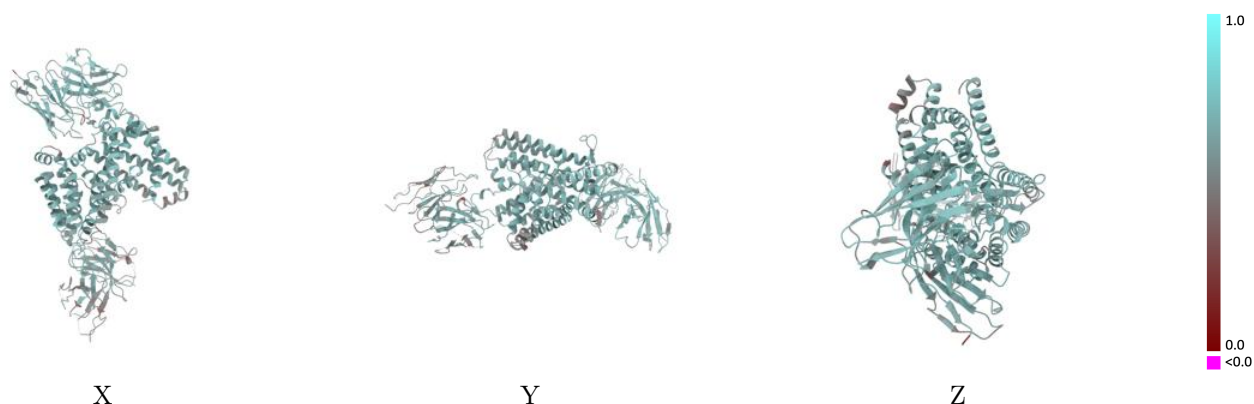
This section contains information regarding the fit between EMDB map EMD-23836 and PDB model 7MHY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



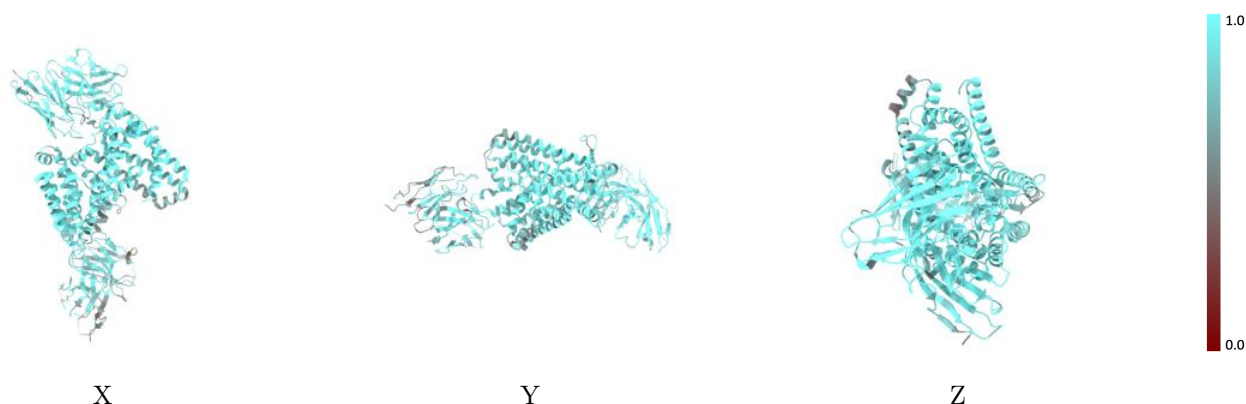
The images above show the 3D surface view of the map at the recommended contour level 1.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



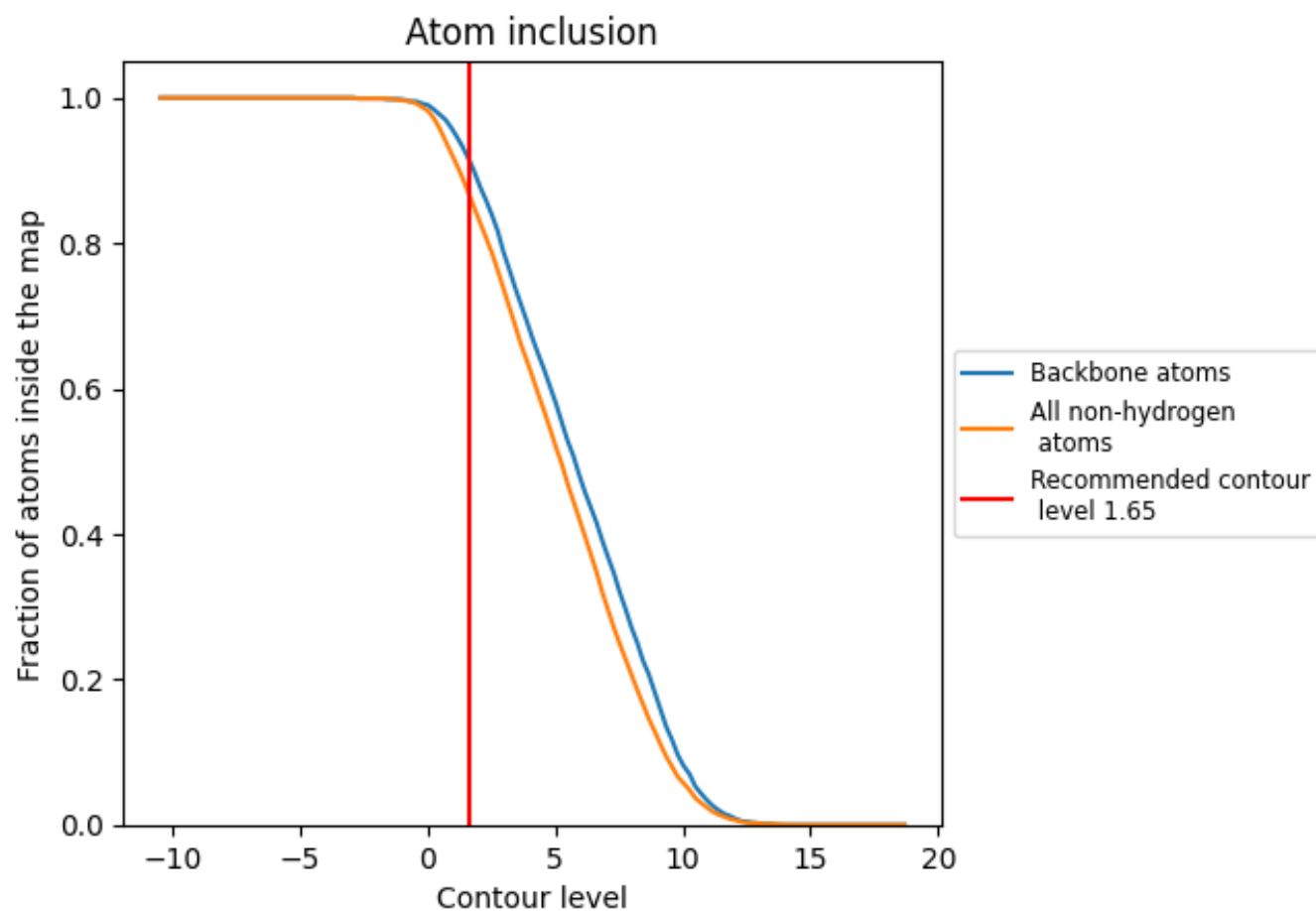
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.65).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8640	<div><div></div></div> 0.5990
A	<div><div></div></div> 0.8730	<div><div></div></div> 0.6060
M	<div><div></div></div> 0.9440	<div><div></div></div> 0.6340
N	<div><div></div></div> 0.8850	<div><div></div></div> 0.6050
O	<div><div></div></div> 0.8150	<div><div></div></div> 0.5630
P	<div><div></div></div> 0.7540	<div><div></div></div> 0.5370

