



Full wwPDB EM Validation Report ⓘ

Nov 4, 2025 – 02:57 PM JST

PDB ID : 9VJX / pdb_00009vjx
EMDB ID : EMD-65126
Title : Structure of the plant diacylglycerol O-acyltransferase 1 H447A mutant
Authors : Liu, X.Y.; Li, J.J.; Song, D.F.; Liu, Z.F.
Deposited on : 2025-06-21
Resolution : 2.60 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

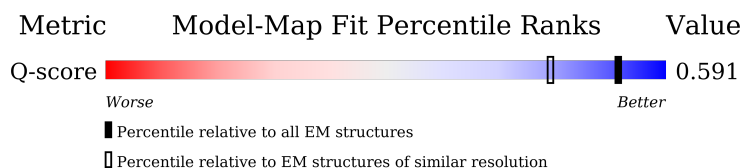
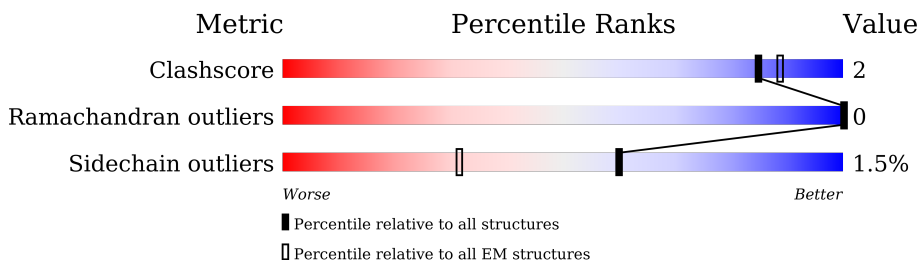
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	528	
1	B	528	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7556 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.

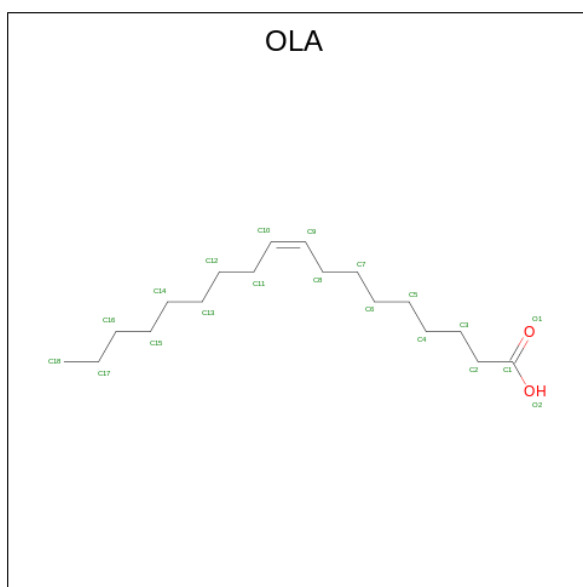
- Molecule 1 is a protein called Diacylglycerol O-acyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	421	Total	C	N	O	S	1	0
			3462	2309	565	558	30		
1	A	420	Total	C	N	O	S	2	0
			3466	2315	564	557	30		

There are 18 discrepancies between the modelled and reference sequences:

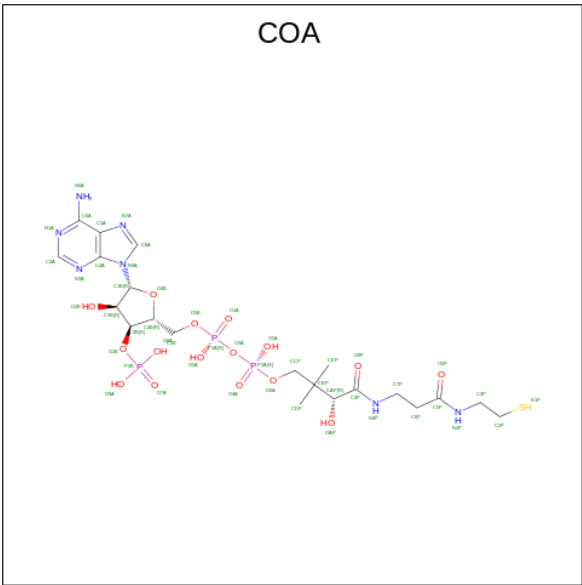
Chain	Residue	Modelled	Actual	Comment	Reference
B	447	ALA	HIS	engineered mutation	UNP Q9SLD2
B	521	GLY	-	expression tag	UNP Q9SLD2
B	522	PRO	-	expression tag	UNP Q9SLD2
B	523	HIS	-	expression tag	UNP Q9SLD2
B	524	HIS	-	expression tag	UNP Q9SLD2
B	525	HIS	-	expression tag	UNP Q9SLD2
B	526	HIS	-	expression tag	UNP Q9SLD2
B	527	HIS	-	expression tag	UNP Q9SLD2
B	528	HIS	-	expression tag	UNP Q9SLD2
A	447	ALA	HIS	engineered mutation	UNP Q9SLD2
A	521	GLY	-	expression tag	UNP Q9SLD2
A	522	PRO	-	expression tag	UNP Q9SLD2
A	523	HIS	-	expression tag	UNP Q9SLD2
A	524	HIS	-	expression tag	UNP Q9SLD2
A	525	HIS	-	expression tag	UNP Q9SLD2
A	526	HIS	-	expression tag	UNP Q9SLD2
A	527	HIS	-	expression tag	UNP Q9SLD2
A	528	HIS	-	expression tag	UNP Q9SLD2

- Molecule 2 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$) (labeled as "Ligand of Interest" by depositor).



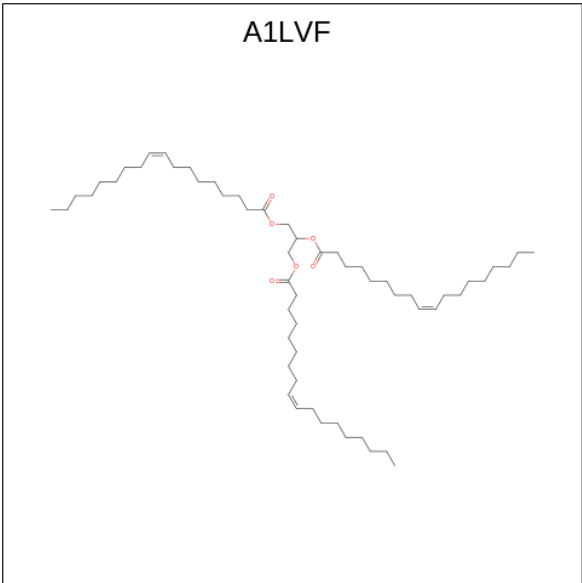
Mol	Chain	Residues	Atoms			AltConf
2	B	1	Total	C	O	0
			20	18	2	
2	B	1	Total	C	O	0
			20	18	2	
2	B	1	Total	C	O	0
			20	18	2	
2	B	1	Total	C	O	0
			20	18	2	
2	A	1	Total	C	O	0
			20	18	2	
2	A	1	Total	C	O	0
			20	18	2	
2	A	1	Total	C	O	0
			20	18	2	
2	A	1	Total	C	O	0
			20	18	2	

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	B	1	48	21	7	16	3	0

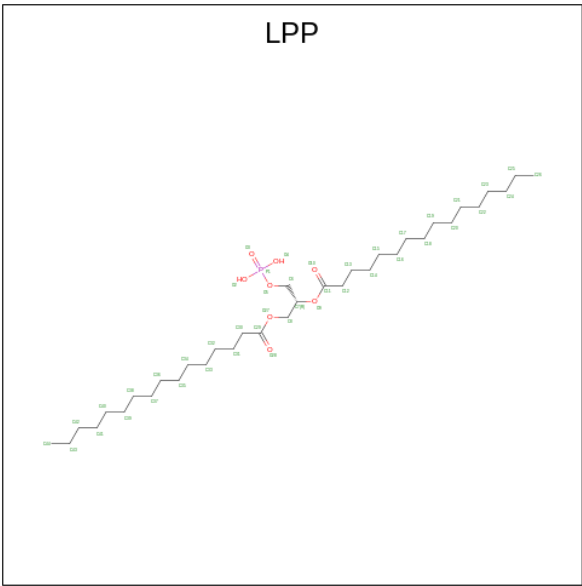
- Molecule 4 is 2,3-bis[[*(Z)*-octadec-9-enoyl]oxy]propyl (*(Z)*-octadec-9-enoate (CCD ID: A1LVF) (formula: C₅₇H₁₀₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	B	1	63	57	6	0

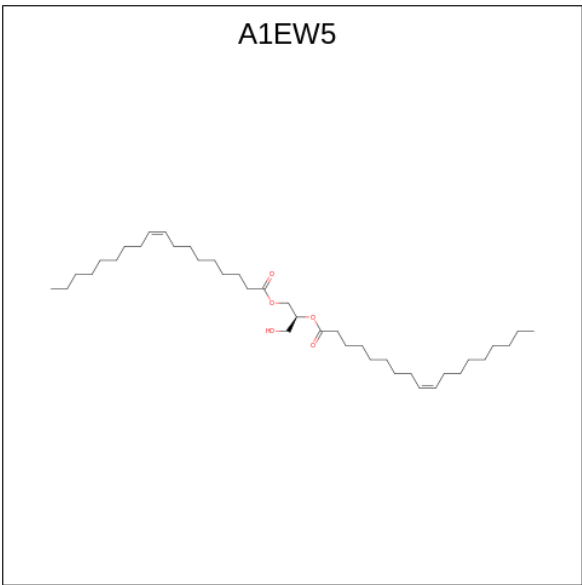
- Molecule 5 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of

Interest" by depositor).



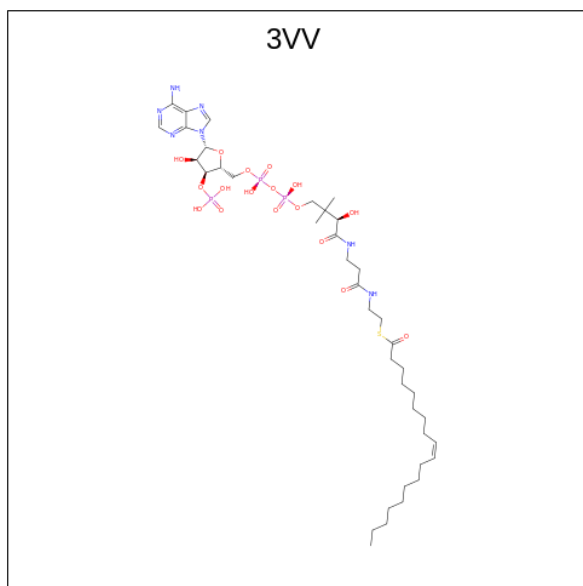
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	O	P	0
			44	35	8	1	
5	A	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 6 is [(2 {S})-2-[({Z})-octadec-9-enoyl]oxy-3-oxidanyl-propyl] ({Z})-octadec-9-enoate (CCD ID: A1EW5) (formula: C₃₉H₇₂O₅).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			44	39	5	
6	A	1	Total	C	O	0
			44	39	5	
6	A	1	Total	C	O	0
			44	39	5	
6	A	1	Total	C	O	0
			44	39	5	

- Molecule 7 is S-{(3R,5R,9R)-1-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)tetrahydrofuran-2-yl]-3,5,9-trihydroxy-8,8-dimethyl-3,5-dioxido-10,14-dioxo-2,4,6-trioxa-11,15-diaza-3lambda 5 ,5lambda 5 -diphosphaheptadecan-17-yl} (9Z)-octadec-9-enethioate (non-preferred name) (CCD ID: 3VV) (formula: C₃₉H₆₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	N	O	P	S	0
			67	39	7	17	3	1	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	B	2	Total	O	0
			2	2	
8	A	4	Total	O	0
			4	4	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67838	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.340	Depositor
Minimum map value	-0.866	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	266.4, 266.4, 266.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	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: OLA, COA, LPP, A1LVF, A1EW5, 3VV

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	0.65	0/3580	1.00	0/4870
1	B	0.66	0/3572	1.01	0/4859
All	All	0.66	0/7152	1.00	0/9729

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	3466	0	3527	12	0
1	B	3462	0	3521	16	0
2	A	100	0	165	1	0
2	B	80	0	132	6	0
3	B	48	0	32	3	0
4	B	63	0	0	0	0
5	A	44	0	67	2	0
5	B	44	0	67	1	0
6	A	132	0	0	0	0
6	B	44	0	0	0	0
7	A	67	0	64	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	4	0	0	0	0
8	B	2	0	0	0	0
All	All	7556	0	7575	32	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 2.

All (32) 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:417:MET:HG3	3:B:605:COA:H141	1.80	0.64
1:B:337:VAL:HG21	2:B:602:OLA:H10	1.83	0.60
1:B:394:LYS:HB2	1:B:408:MET:HB3	1.86	0.57
3:B:605:COA:H51A	3:B:605:COA:O4A	2.04	0.56
1:A:342:HIS:HB3	1:A:345:LYS:HB2	1.93	0.50
1:B:372:CYS:HA	1:B:376:LEU:HD12	1.95	0.49
1:B:109:PRO:O	1:A:419:ARG:NH2	2.46	0.48
1:B:112:PRO:O	1:B:115:ARG:NH2	2.45	0.48
1:B:232:ASP:N	1:B:232:ASP:OD1	2.47	0.48
3:B:605:COA:H132	3:B:605:COA:O5A	2.13	0.47
1:A:505:VAL:HG22	2:A:602:OLA:H51	1.96	0.47
1:A:394:LYS:HB2	1:A:408:MET:HB2	1.97	0.46
1:B:179:PHE:O	1:B:182:CYS:HB2	2.16	0.46
1:B:169:SER:OG	1:B:170:SER:N	2.49	0.46
1:A:196:GLU:OE1	1:A:263:ARG:NH1	2.44	0.45
1:A:355:VAL:HG13	1:A:502:PRO:HB2	1.98	0.45
1:A:404:ASP:OD1	1:A:407:ARG:NH1	2.50	0.44
1:A:197:LYS:HA	1:A:197:LYS:HD3	1.82	0.44
1:A:364:TYR:O	1:A:368:CYS:HB2	2.16	0.44
5:A:607:LPP:H312	5:A:607:LPP:H341	1.83	0.44
1:B:462:ALA:HA	2:B:604:OLA:H31	2.00	0.44
5:A:607:LPP:HC7	5:A:607:LPP:H121	1.77	0.44
1:B:236:LEU:HD11	2:B:603:OLA:H82	1.99	0.43
1:A:460:LEU:HB3	1:A:463:PHE:HB3	2.01	0.42
1:B:251:LYS:NZ	1:B:288:PHE:O	2.46	0.42
1:B:424:PRO:HB3	5:B:607:LPP:HC62	2.02	0.42
1:A:375:HIS:ND1	1:A:393:TYR:OH	2.50	0.41
1:B:122:LEU:HD23	1:B:127:ILE:HG12	2.01	0.41
1:B:503:MET:HE3	2:B:604:OLA:H122	2.01	0.41
2:B:603:OLA:H82	2:B:603:OLA:H111	1.88	0.41
1:B:465:GLY:HA3	2:B:604:OLA:C7	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:CYS:HA	1:A:376:LEU:HD12	2.02	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	420/528 (80%)	408 (97%)	12 (3%)	0	100	100
1	B	420/528 (80%)	409 (97%)	11 (3%)	0	100	100
All	All	840/1056 (80%)	817 (97%)	23 (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	378/457 (83%)	372 (98%)	6 (2%)	58	79
1	B	377/457 (82%)	372 (99%)	5 (1%)	65	84
All	All	755/914 (83%)	744 (98%)	11 (2%)	60	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	98	ARG
1	B	107	TYR
1	B	243	LEU
1	B	276	VAL
1	B	334	ASN
1	A	98	ARG
1	A	106	THR
1	A	107	TYR
1	A	175	ASP
1	A	236	LEU
1	A	498	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	147	ASN
1	B	201	GLN
1	B	297	GLN
1	B	379	ASN
1	B	501	GLN
1	A	339	ASN
1	A	362	ASN
1	A	379	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](#)

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	$\# Z > 2$
5	LPP	B	607	-	43,43,43	0.34	0	47,48,48	0.69	1 (2%)
2	OLA	B	603	-	19,19,19	0.48	0	19,19,19	0.77	0
7	3VV	A	606	-	61,69,69	0.56	0	72,95,95	1.08	7 (9%)
6	A1EW5	B	608	-	43,43,43	1.23	3 (6%)	45,45,45	1.40	5 (11%)
6	A1EW5	A	608	-	43,43,43	1.22	3 (6%)	45,45,45	1.43	6 (13%)
2	OLA	A	603	-	19,19,19	0.46	0	19,19,19	1.02	1 (5%)
2	OLA	B	601	-	19,19,19	0.50	0	19,19,19	0.82	0
2	OLA	A	604	-	19,19,19	0.50	0	19,19,19	0.79	0
2	OLA	A	602	-	19,19,19	0.52	0	19,19,19	1.08	1 (5%)
4	A1LVF	B	606	-	62,62,62	1.28	5 (8%)	65,65,65	1.44	8 (12%)
5	LPP	A	607	-	43,43,43	0.42	0	47,48,48	1.12	2 (4%)
6	A1EW5	A	610	-	43,43,43	1.21	4 (9%)	45,45,45	1.52	5 (11%)
2	OLA	A	601	-	19,19,19	0.50	0	19,19,19	0.85	1 (5%)
2	OLA	B	602	-	19,19,19	0.49	0	19,19,19	0.70	0
3	COA	B	605	-	41,50,50	0.61	0	52,75,75	0.76	1 (1%)
2	OLA	B	604	-	19,19,19	0.57	0	19,19,19	0.52	0
2	OLA	A	605	-	19,19,19	0.50	0	19,19,19	0.75	0
6	A1EW5	A	609	-	43,43,43	1.21	3 (6%)	45,45,45	1.29	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LPP	B	607	-	-	11/45/45/45	-
2	OLA	B	603	-	-	3/17/17/17	-
7	3VV	A	606	-	-	19/64/84/84	0/3/3/3
6	A1EW5	B	608	-	-	24/45/45/45	-
6	A1EW5	A	608	-	-	29/45/45/45	-
2	OLA	A	603	-	-	3/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLA	B	601	-	-	7/17/17/17	-
2	OLA	A	604	-	-	5/17/17/17	-
2	OLA	A	602	-	-	7/17/17/17	-
4	A1LVF	B	606	-	-	32/65/65/65	-
5	LPP	A	607	-	-	9/45/45/45	-
6	A1EW5	A	610	-	-	20/45/45/45	-
2	OLA	A	601	-	-	7/17/17/17	-
2	OLA	B	602	-	-	3/17/17/17	-
3	COA	B	605	-	-	10/44/64/64	0/3/3/3
2	OLA	B	604	-	-	7/17/17/17	-
2	OLA	A	605	-	-	5/17/17/17	-
6	A1EW5	A	609	-	-	27/45/45/45	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	608	A1EW5	O25-C26	3.97	1.45	1.34
6	A	608	A1EW5	O25-C26	3.79	1.45	1.34
6	A	609	A1EW5	O25-C26	3.76	1.44	1.34
4	B	606	A1LVF	O02-C59	3.70	1.44	1.33
6	A	610	A1EW5	O25-C26	3.59	1.44	1.34
6	A	608	A1EW5	O20-C18	3.50	1.43	1.33
6	A	609	A1EW5	O20-C18	3.49	1.43	1.33
6	B	608	A1EW5	O20-C18	3.45	1.43	1.33
6	A	610	A1EW5	O20-C18	3.43	1.43	1.33
4	B	606	A1LVF	O03-C60	3.25	1.42	1.33
4	B	606	A1LVF	O01-C58	2.95	1.42	1.34
4	B	606	A1LVF	C45-C60	2.60	1.58	1.50
6	A	608	A1EW5	C28-C26	2.18	1.57	1.50
6	A	610	A1EW5	O25-C22	-2.17	1.41	1.46
6	A	610	A1EW5	C28-C26	2.15	1.57	1.50
4	B	606	A1LVF	C44-C59	2.08	1.56	1.50
6	B	608	A1EW5	C28-C26	2.08	1.56	1.50
6	A	609	A1EW5	C28-C26	2.03	1.56	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	610	A1EW5	O25-C26-C28	5.47	123.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	607	LPP	O9-C11-C12	4.89	122.04	111.50
6	B	608	A1EW5	C11-C10-C09	4.64	160.36	124.73
6	A	610	A1EW5	C11-C10-C09	4.62	160.20	124.73
6	B	608	A1EW5	C08-C09-C10	4.62	160.19	124.73
6	A	610	A1EW5	C08-C09-C10	4.61	160.10	124.73
6	A	608	A1EW5	C08-C09-C10	4.53	159.46	124.73
6	A	608	A1EW5	C11-C10-C09	4.41	158.56	124.73
6	A	609	A1EW5	C08-C09-C10	4.07	155.95	124.73
6	A	609	A1EW5	C11-C10-C09	4.06	155.92	124.73
4	B	606	A1LVF	C37-C47-C46	3.87	154.45	124.73
4	B	606	A1LVF	C13-C24-C36	3.86	130.60	113.79
6	A	608	A1EW5	O25-C26-C28	3.70	119.48	111.50
4	B	606	A1LVF	O03-C60-C45	3.65	123.36	111.91
6	A	609	A1EW5	O25-C26-C28	3.62	119.31	111.50
4	B	606	A1LVF	C41-C53-C51	3.58	152.19	124.73
6	B	608	A1EW5	C22-O25-C26	3.56	126.56	117.79
4	B	606	A1LVF	O02-C59-C44	3.31	122.30	111.91
4	B	606	A1LVF	O01-C58-C43	3.26	118.54	111.50
7	A	606	3VV	P42-O41-P38	3.26	144.01	132.83
7	A	606	3VV	C49-N58-C67	-3.04	121.31	126.64
6	A	608	A1EW5	O20-C18-C17	2.81	120.71	111.91
6	A	610	A1EW5	O20-C18-C17	2.76	120.56	111.91
7	A	606	3VV	C34-C33-C31	2.74	113.57	108.82
6	A	609	A1EW5	O20-C18-C17	2.69	120.34	111.91
6	A	608	A1EW5	C22-O25-C26	2.62	124.25	117.79
7	A	606	3VV	C50-C52-C47	-2.59	98.63	103.22
6	B	608	A1EW5	O25-C26-C28	2.47	116.83	111.50
2	A	603	OLA	C3-C2-C1	-2.47	108.25	114.47
3	B	605	COA	C5A-C6A-N6A	2.47	124.10	120.35
7	A	606	3VV	C34-C33-C36	-2.37	104.36	108.23
5	B	607	LPP	O9-C7-C6	2.36	116.94	108.40
7	A	606	3VV	C31-C29-N28	2.32	121.20	116.58
4	B	606	A1LVF	O02-C59-O05	-2.31	117.77	123.59
6	A	610	A1EW5	O25-C26-O27	-2.22	118.33	123.70
5	A	607	LPP	O9-C11-O10	-2.22	118.34	123.70
6	B	608	A1EW5	O20-C18-C17	2.20	118.83	111.91
2	A	602	OLA	C12-C11-C10	-2.16	100.07	112.43
6	A	608	A1EW5	O25-C22-C21	2.14	116.13	108.40
7	A	606	3VV	C61-C62-N63	2.06	123.49	120.35
2	A	601	OLA	C3-C2-C1	-2.05	109.31	114.47
4	B	606	A1LVF	O03-C60-O06	-2.00	118.54	123.59

There are no chirality outliers.

All (228) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	605	COA	CCP-O6A-P2A-O3A
3	B	605	COA	CBP-CCP-O6A-P2A
3	B	605	COA	CAP-CBP-CCP-O6A
4	B	606	A1LVF	C43-C58-O01-C55
4	B	606	A1LVF	C44-C59-O02-C56
4	B	606	A1LVF	O05-C59-O02-C56
4	B	606	A1LVF	C45-C60-O03-C57
4	B	606	A1LVF	O06-C60-O03-C57
5	A	607	LPP	O10-C11-O9-C7
5	A	607	LPP	C12-C11-O9-C7
5	A	607	LPP	O28-C29-O27-C8
5	A	607	LPP	C30-C29-O27-C8
6	A	608	A1EW5	C21-C22-O25-C26
6	A	608	A1EW5	C28-C26-O25-C22
6	A	609	A1EW5	C21-C22-C23-O24
6	A	609	A1EW5	O25-C22-C23-O24
6	A	610	A1EW5	C28-C26-O25-C22
6	A	610	A1EW5	O27-C26-O25-C22
7	A	606	3VV	S20-C21-C22-N23
7	A	606	3VV	C17-C18-S20-C21
7	A	606	3VV	O19-C18-S20-C21
7	A	606	3VV	N28-C29-C31-C33
7	A	606	3VV	O30-C29-C31-C33
7	A	606	3VV	C31-C33-C36-O37
7	A	606	3VV	C34-C33-C36-O37
5	B	607	LPP	O28-C29-O27-C8
5	B	607	LPP	C30-C29-O27-C8
6	A	608	A1EW5	O19-C18-O20-C21
6	A	609	A1EW5	O19-C18-O20-C21
4	B	606	A1LVF	O04-C58-O01-C55
6	A	608	A1EW5	C17-C18-O20-C21
6	A	609	A1EW5	C17-C18-O20-C21
6	A	610	A1EW5	C17-C18-O20-C21
6	A	608	A1EW5	O27-C26-O25-C22
4	B	606	A1LVF	C12-C09-C21-C32
4	B	606	A1LVF	C20-C18-C28-C40
4	B	606	A1LVF	C17-C19-C29-C41
6	A	610	A1EW5	O19-C18-O20-C21
6	A	609	A1EW5	C15-C16-C17-C18
6	B	608	A1EW5	C26-C28-C29-C30
6	A	609	A1EW5	C28-C26-O25-C22
6	B	608	A1EW5	C17-C18-O20-C21

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Mol	Chain	Res	Type	Atoms
6	A	609	A1EW5	O27-C26-O25-C22
6	A	609	A1EW5	C03-C04-C05-C06
7	A	606	3VV	C35-C33-C36-O37
6	A	609	A1EW5	C31-C32-C33-C34
6	A	610	A1EW5	C31-C32-C33-C34
6	A	608	A1EW5	C13-C14-C15-C16
2	A	601	OLA	C3-C4-C5-C6
4	B	606	A1LVF	C21-C09-C12-C23
5	B	607	LPP	C13-C14-C15-C16
4	B	606	A1LVF	C09-C21-C32-C44
4	B	606	A1LVF	C10-C22-C33-C45
6	A	609	A1EW5	C12-C13-C14-C15
4	B	606	A1LVF	C19-C29-C41-C53
6	A	610	A1EW5	C05-C06-C07-C08
6	B	608	A1EW5	C02-C03-C04-C05
4	B	606	A1LVF	C07-C11-C31-C43
2	A	601	OLA	C11-C12-C13-C14
2	A	605	OLA	C4-C5-C6-C7
6	B	608	A1EW5	O19-C18-O20-C21
6	A	608	A1EW5	C15-C16-C17-C18
4	B	606	A1LVF	C09-C12-C23-C35
2	B	601	OLA	C10-C11-C12-C13
6	B	608	A1EW5	C06-C07-C08-C09
6	A	608	A1EW5	C10-C11-C12-C13
6	A	610	A1EW5	C37-C38-C39-C40
6	A	609	A1EW5	C37-C38-C39-C40
6	A	609	A1EW5	C26-C28-C29-C30
6	A	608	A1EW5	C11-C12-C13-C14
6	A	610	A1EW5	C07-C08-C09-C10
6	A	609	A1EW5	C14-C15-C16-C17
2	A	605	OLA	C10-C11-C12-C13
6	B	608	A1EW5	C36-C37-C38-C39
6	A	610	A1EW5	C10-C11-C12-C13
6	B	608	A1EW5	C03-C04-C05-C06
6	A	609	A1EW5	C04-C05-C06-C07
6	A	609	A1EW5	C11-C12-C13-C14
6	B	608	A1EW5	C13-C14-C15-C16
4	B	606	A1LVF	C12-C23-C35-C51
6	A	610	A1EW5	C36-C37-C38-C39
4	B	606	A1LVF	C21-C32-C44-C59
6	A	610	A1EW5	C40-C41-C42-C43
6	A	609	A1EW5	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
4	B	606	A1LVF	C27-C17-C19-C29
5	A	607	LPP	C34-C35-C36-C37
2	A	602	OLA	C11-C10-C9-C8
6	A	608	A1EW5	C37-C38-C39-C40
6	A	609	A1EW5	C01-C02-C03-C04
2	B	601	OLA	C1-C2-C3-C4
2	A	605	OLA	C1-C2-C3-C4
6	A	610	A1EW5	C01-C02-C03-C04
3	B	605	COA	O9P-C9P-CAP-OAP
2	A	601	OLA	C6-C7-C8-C9
4	B	606	A1LVF	C20-C30-C42-C54
6	B	608	A1EW5	C32-C33-C34-C35
2	B	604	OLA	C4-C5-C6-C7
3	B	605	COA	CDP-CBP-CCP-O6A
3	B	605	COA	CEP-CBP-CCP-O6A
2	A	604	OLA	C15-C16-C17-C18
6	A	608	A1EW5	C04-C05-C06-C07
6	A	610	A1EW5	C14-C15-C16-C17
4	B	606	A1LVF	C17-C27-C39-C49
2	B	601	OLA	C6-C7-C8-C9
6	A	608	A1EW5	C06-C07-C08-C09
6	A	610	A1EW5	C38-C39-C40-C41
5	B	607	LPP	O9-C11-C12-C13
6	A	609	A1EW5	O25-C26-C28-C29
4	B	606	A1LVF	C11-C31-C43-C58
2	A	604	OLA	C13-C14-C15-C16
5	B	607	LPP	C6-C7-C8-O27
6	A	609	A1EW5	C38-C39-C40-C41
3	B	605	COA	N8P-C9P-CAP-CBP
2	B	604	OLA	C5-C6-C7-C8
6	A	610	A1EW5	C30-C31-C32-C33
6	A	610	A1EW5	C12-C13-C14-C15
2	A	601	OLA	C5-C6-C7-C8
6	A	609	A1EW5	C07-C08-C09-C10
3	B	605	COA	P1A-O3A-P2A-O6A
4	B	606	A1LVF	C07-C08-C16-C34
2	A	604	OLA	C5-C6-C7-C8
7	A	606	3VV	O45-C46-C47-O48
7	A	606	3VV	N28-C29-C31-O32
4	B	606	A1LVF	C28-C18-C20-C30
2	B	603	OLA	C3-C4-C5-C6
6	B	608	A1EW5	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
6	A	610	A1EW5	C03-C04-C05-C06
6	B	608	A1EW5	C11-C12-C13-C14
6	A	610	A1EW5	C39-C40-C41-C42
6	B	608	A1EW5	C15-C16-C17-C18
4	B	606	A1LVF	C18-C20-C30-C42
2	A	605	OLA	C15-C16-C17-C18
6	A	608	A1EW5	C41-C42-C43-C44
2	A	603	OLA	C2-C3-C4-C5
3	B	605	COA	CCP-O6A-P2A-O4A
6	B	608	A1EW5	C12-C13-C14-C15
6	A	610	A1EW5	C28-C29-C30-C31
4	B	606	A1LVF	C26-C38-C48-C61
5	A	607	LPP	C11-C12-C13-C14
2	A	602	OLA	C13-C14-C15-C16
2	A	602	OLA	C3-C4-C5-C6
2	B	601	OLA	C5-C6-C7-C8
6	A	608	A1EW5	C01-C02-C03-C04
6	A	609	A1EW5	C21-C22-O25-C26
6	A	608	A1EW5	C02-C03-C04-C05
5	B	607	LPP	C16-C17-C18-C19
6	B	608	A1EW5	C33-C34-C35-C36
4	B	606	A1LVF	O01-C55-C57-O03
5	B	607	LPP	O9-C7-C8-O27
2	A	604	OLA	C12-C13-C14-C15
2	A	601	OLA	C4-C5-C6-C7
2	A	605	OLA	C12-C13-C14-C15
6	B	608	A1EW5	C37-C38-C39-C40
2	A	601	OLA	C10-C11-C12-C13
6	A	608	A1EW5	C09-C10-C11-C12
7	A	606	3VV	C05-C06-C07-C08
6	A	608	A1EW5	C28-C29-C30-C31
3	B	605	COA	O9P-C9P-CAP-CBP
2	B	604	OLA	O1-C1-C2-C3
6	A	608	A1EW5	O20-C21-C22-O25
6	A	609	A1EW5	O20-C21-C22-O25
2	B	604	OLA	C7-C8-C9-C10
6	A	609	A1EW5	C09-C10-C11-C12
7	A	606	3VV	C09-C10-C11-C12
2	B	601	OLA	O2-C1-C2-C3
2	B	601	OLA	O1-C1-C2-C3
2	B	602	OLA	C2-C3-C4-C5
4	B	606	A1LVF	C08-C16-C34-C46

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Mol	Chain	Res	Type	Atoms
4	B	606	A1LVF	C28-C40-C50-C63
6	B	608	A1EW5	C21-C22-O25-C26
6	B	608	A1EW5	O27-C26-O25-C22
6	B	608	A1EW5	C09-C10-C11-C12
6	A	608	A1EW5	C33-C34-C35-C36
2	B	604	OLA	O2-C1-C2-C3
2	B	602	OLA	C1-C2-C3-C4
6	A	608	A1EW5	C14-C15-C16-C17
6	B	608	A1EW5	C28-C26-O25-C22
6	B	608	A1EW5	C05-C06-C07-C08
5	A	607	LPP	C14-C15-C16-C17
2	B	602	OLA	C7-C8-C9-C10
2	B	604	OLA	C9-C10-C11-C12
4	B	606	A1LVF	C25-C37-C47-C46
7	A	606	3VV	C16-C17-C18-O19
7	A	606	3VV	C16-C17-C18-S20
5	B	607	LPP	O10-C11-C12-C13
2	A	601	OLA	C7-C8-C9-C10
6	B	608	A1EW5	C28-C29-C30-C31
6	B	608	A1EW5	O25-C22-C23-O24
2	A	603	OLA	O1-C1-C2-C3
6	A	608	A1EW5	C03-C04-C05-C06
6	B	608	A1EW5	C35-C36-C37-C38
6	A	608	A1EW5	C07-C08-C09-C10
6	B	608	A1EW5	C29-C30-C31-C32
5	B	607	LPP	C12-C13-C14-C15
6	A	608	A1EW5	O25-C26-C28-C29
6	A	608	A1EW5	C16-C17-C18-O20
2	B	601	OLA	C9-C10-C11-C12
2	A	602	OLA	O2-C1-C2-C3
6	A	609	A1EW5	O27-C26-C28-C29
2	A	602	OLA	C12-C13-C14-C15
7	A	606	3VV	C12-C13-C14-C15
2	B	604	OLA	C12-C13-C14-C15
7	A	606	3VV	C07-C08-C09-C10
5	B	607	LPP	C7-C8-O27-C29
2	B	603	OLA	O2-C1-C2-C3
2	A	603	OLA	O2-C1-C2-C3
7	A	606	3VV	C50-C52-O53-P54
6	A	608	A1EW5	C35-C36-C37-C38
6	A	610	A1EW5	C04-C05-C06-C07
2	A	604	OLA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
7	A	606	3VV	O45-C46-C47-C52
7	A	606	3VV	C33-C36-O37-P38
6	A	609	A1EW5	C35-C36-C37-C38
2	A	602	OLA	C4-C5-C6-C7
6	A	608	A1EW5	O20-C21-C22-C23
6	A	608	A1EW5	O27-C26-C28-C29
5	B	607	LPP	C30-C31-C32-C33
6	A	608	A1EW5	C16-C17-C18-O19
6	A	608	A1EW5	C05-C06-C07-C08
2	B	603	OLA	O1-C1-C2-C3
2	A	602	OLA	O1-C1-C2-C3
6	A	609	A1EW5	C40-C41-C42-C43
4	B	606	A1LVF	C23-C35-C51-C53
4	B	606	A1LVF	C33-C45-C60-O03
5	A	607	LPP	O9-C11-C12-C13
4	B	606	A1LVF	C16-C34-C46-C47
5	A	607	LPP	O10-C11-C12-C13
6	A	609	A1EW5	C16-C17-C18-O20

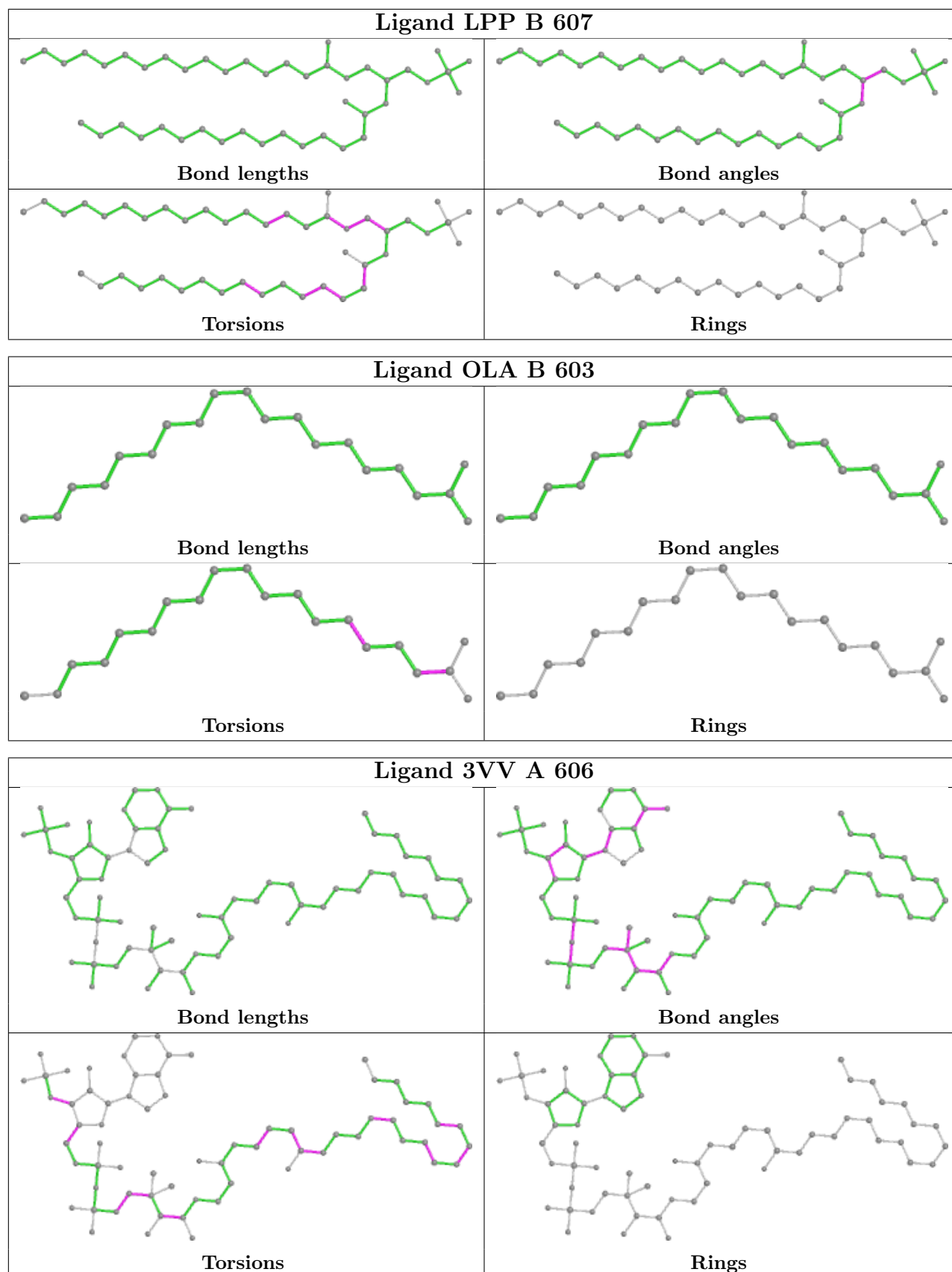
There are no ring outliers.

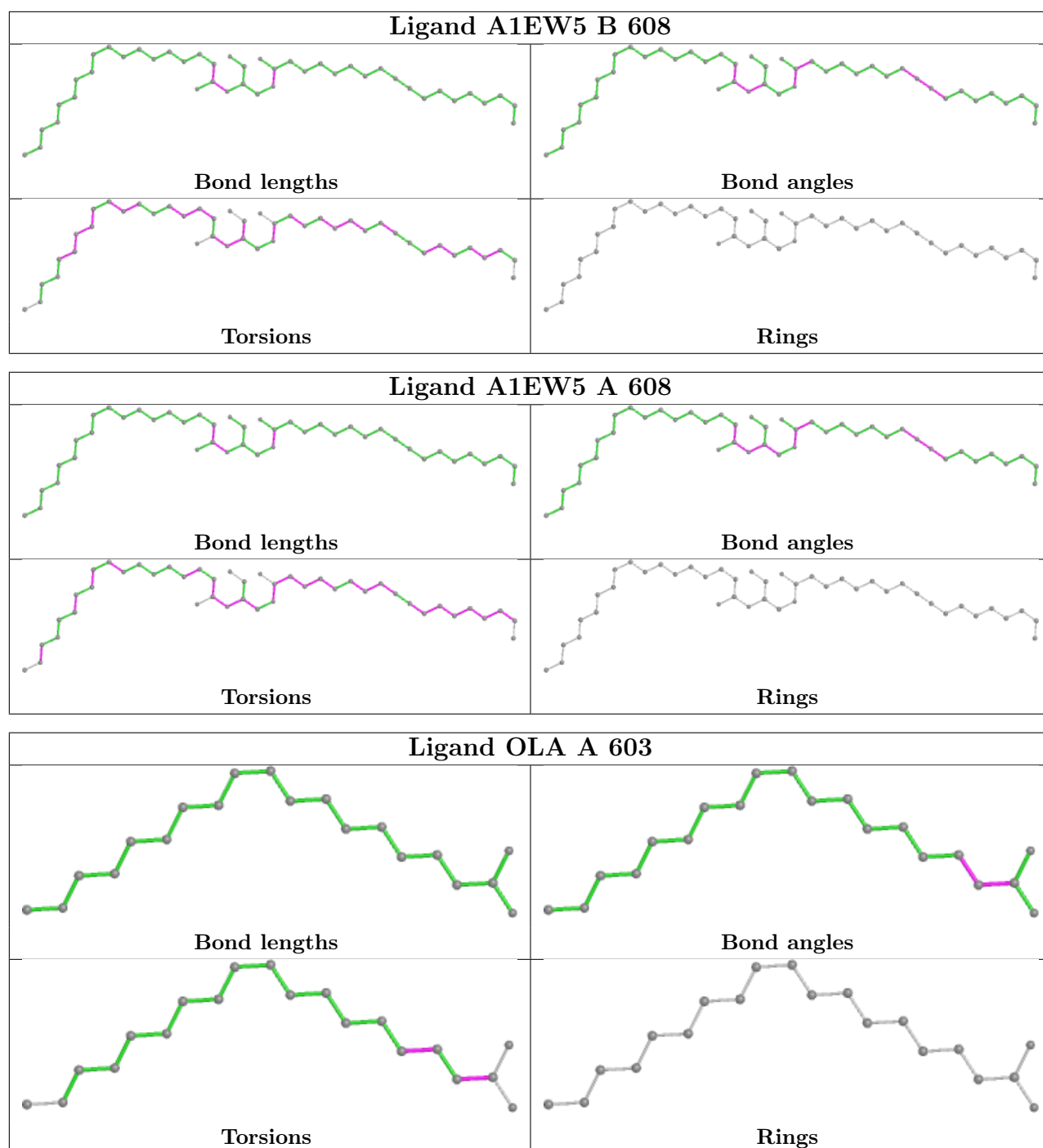
7 monomers are involved in 13 short contacts:

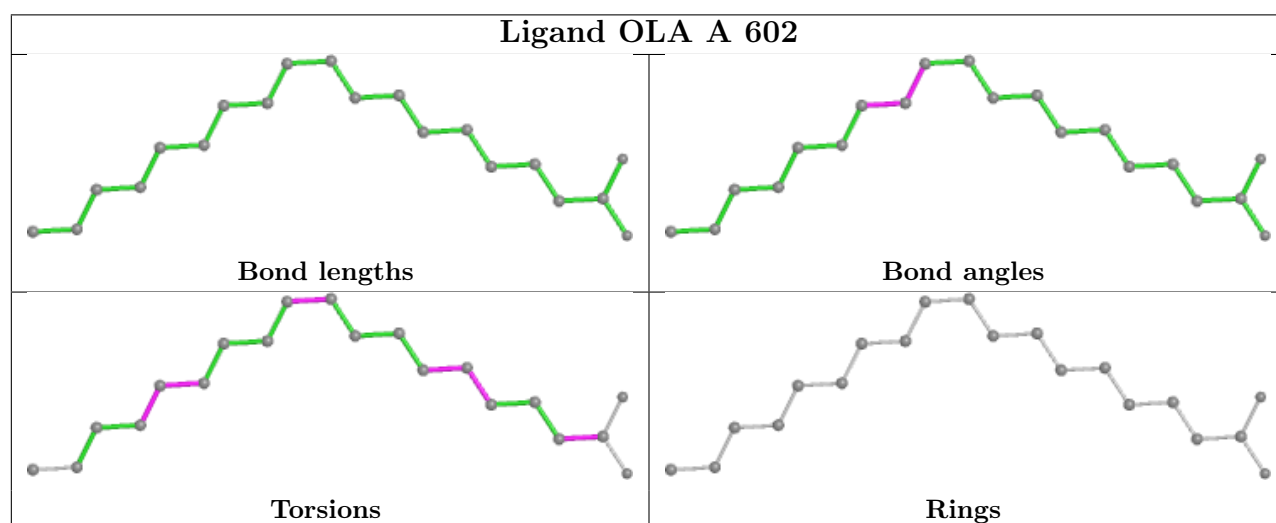
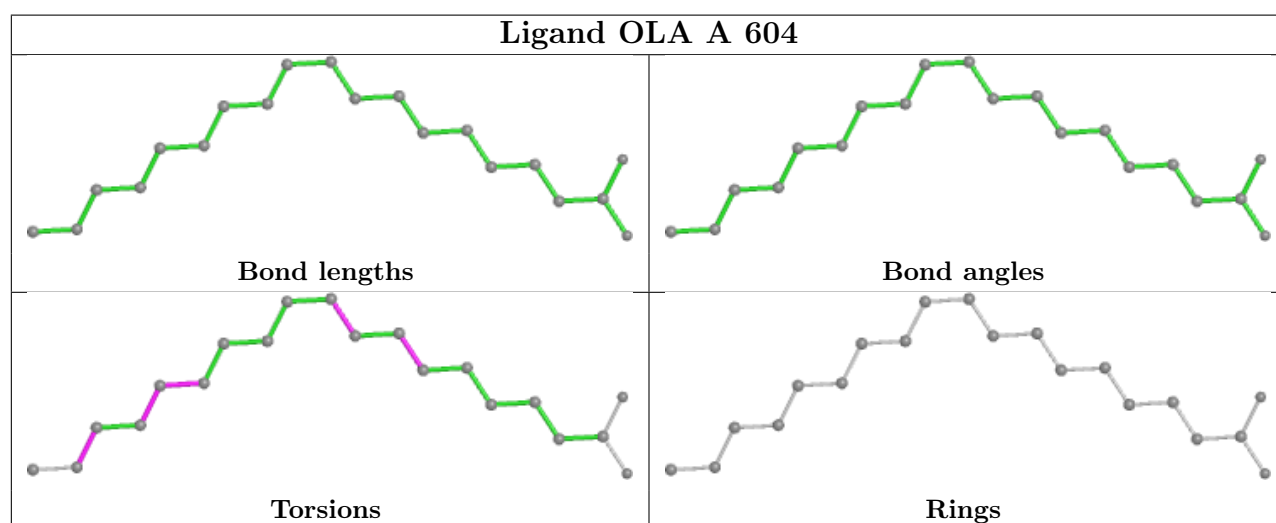
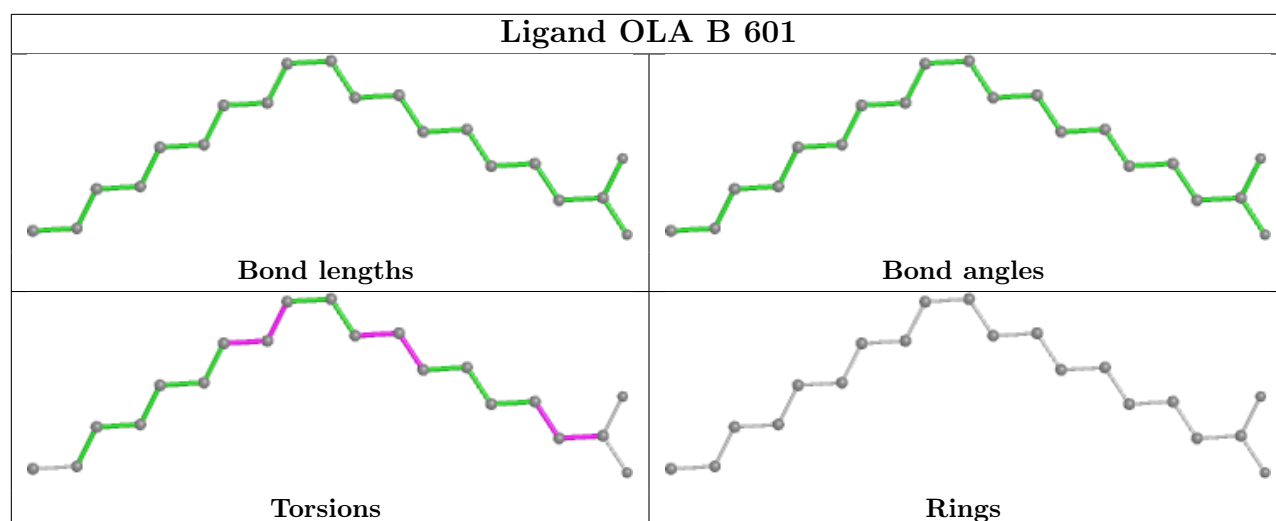
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	607	LPP	1	0
2	B	603	OLA	2	0
2	A	602	OLA	1	0
5	A	607	LPP	2	0
2	B	602	OLA	1	0
3	B	605	COA	3	0
2	B	604	OLA	3	0

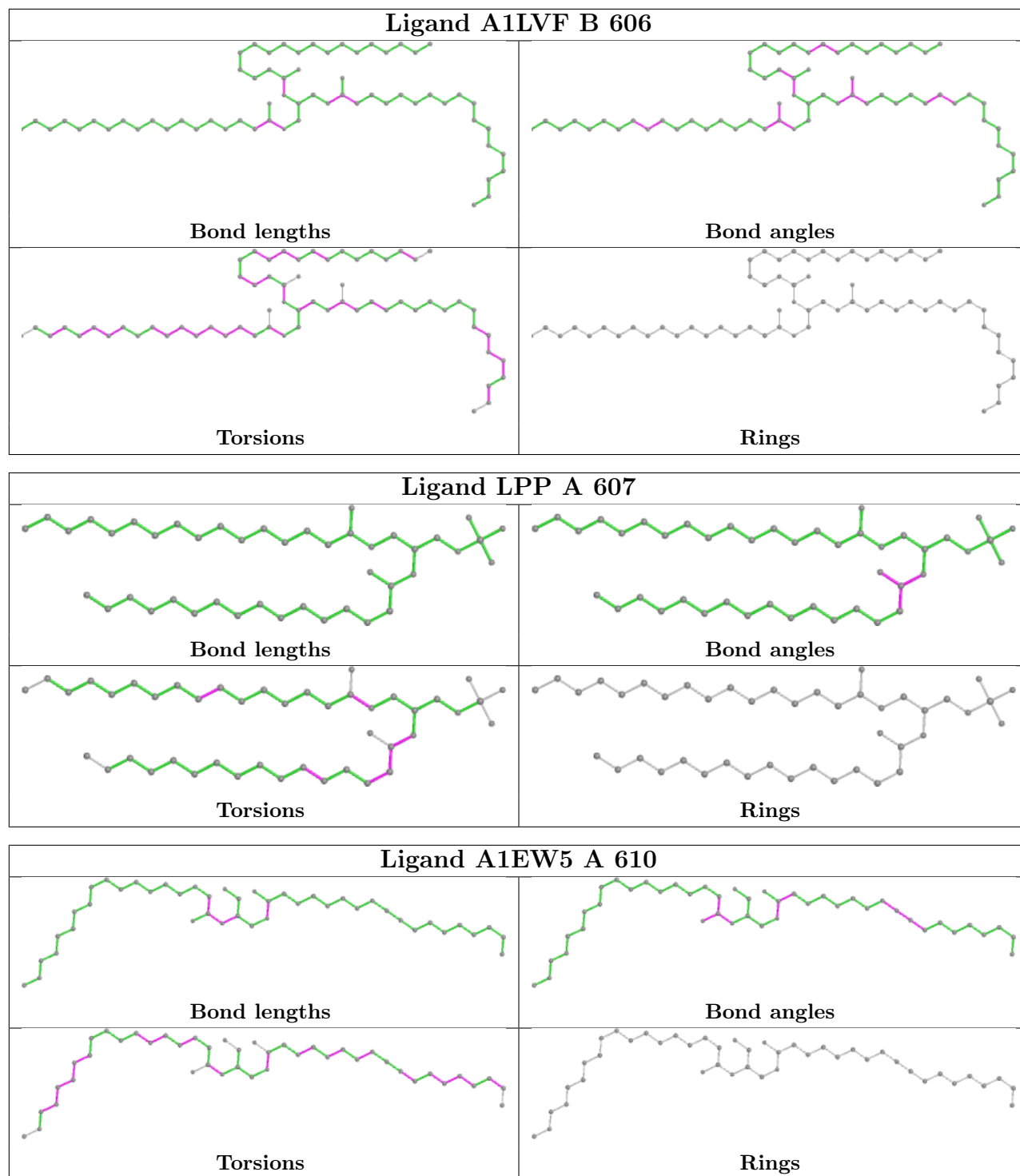
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

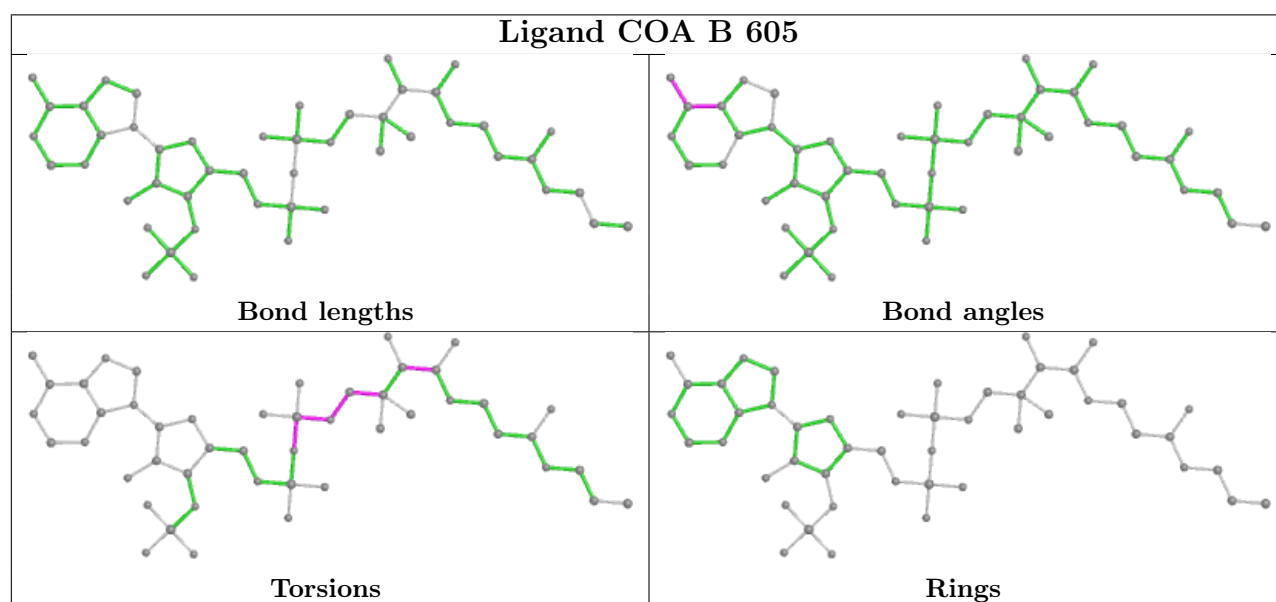
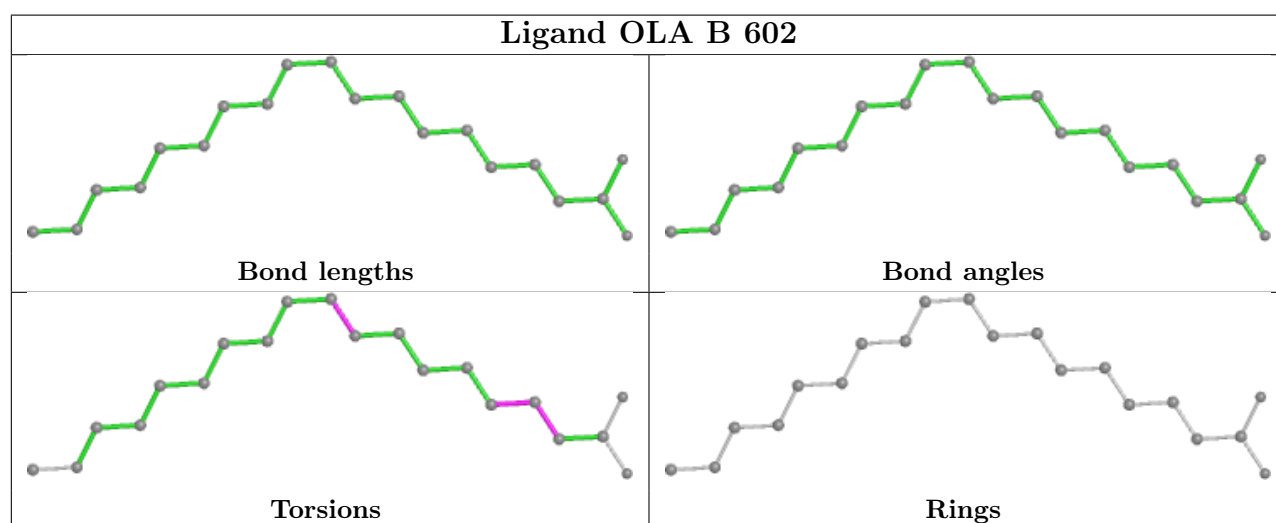
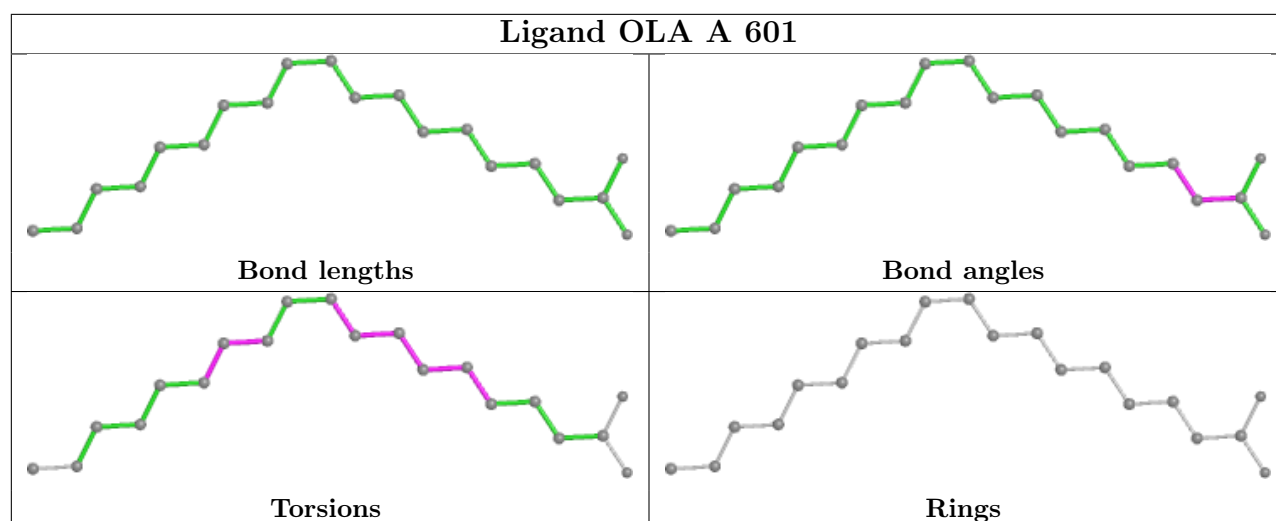
equivalents in the CSD to analyse the geometry.

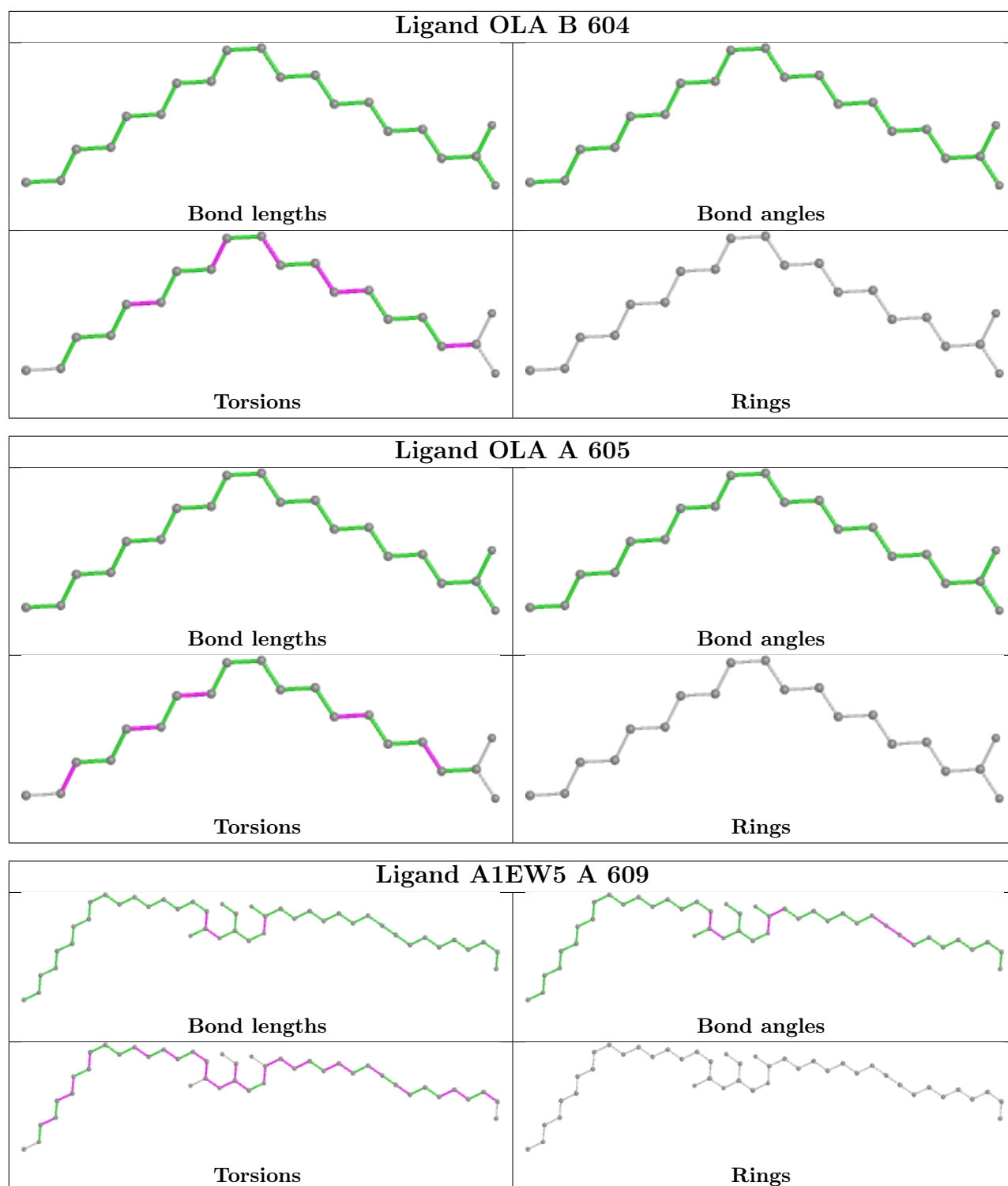












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

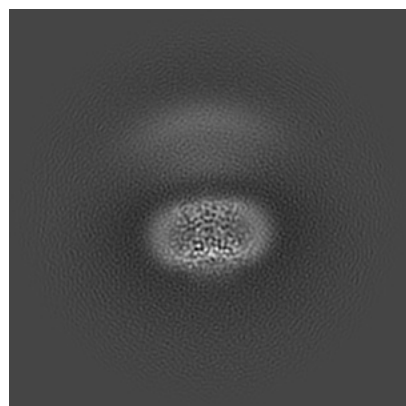
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65126. These allow visual inspection of the internal detail of the map and identification of artifacts.

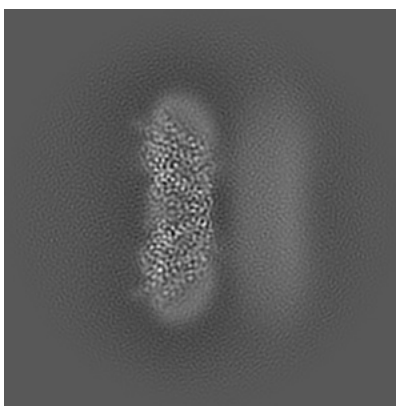
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

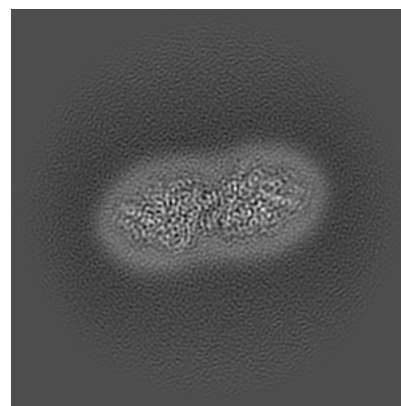
6.1.1 Primary map



X

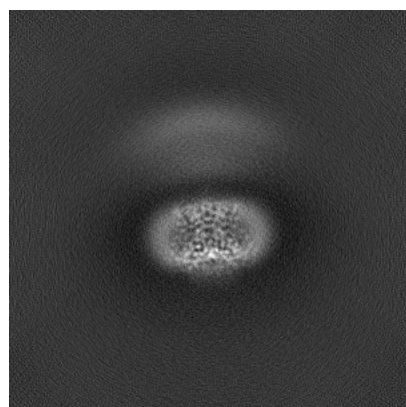


Y

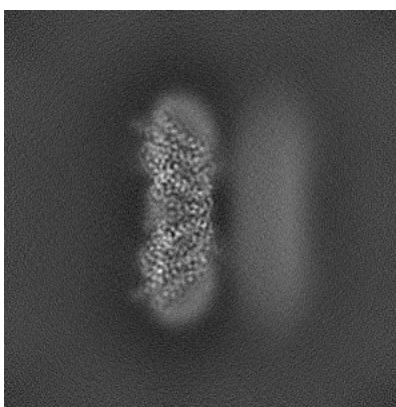


Z

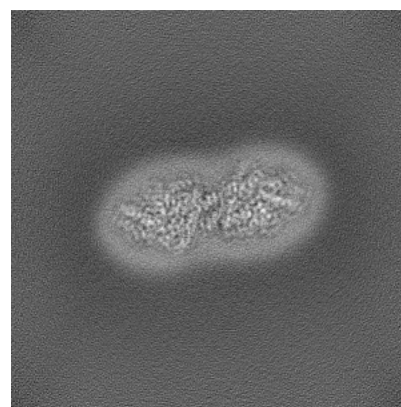
6.1.2 Raw map



X



Y

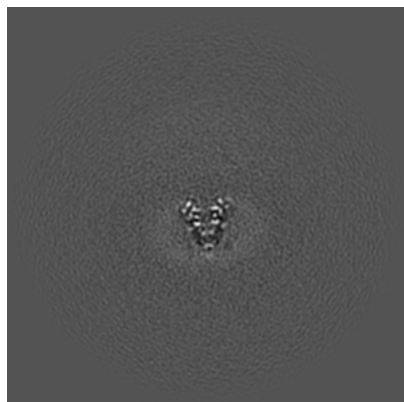


Z

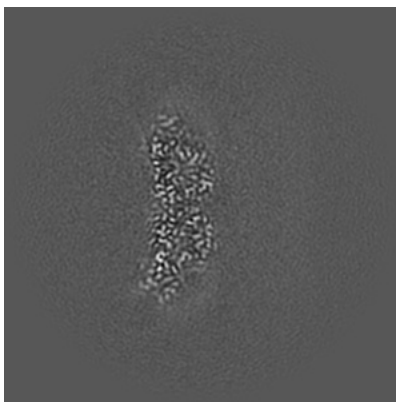
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

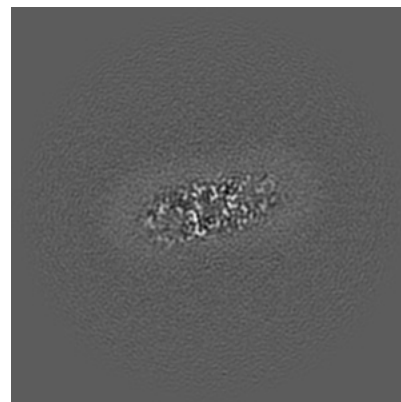
6.2.1 Primary map



X Index: 180

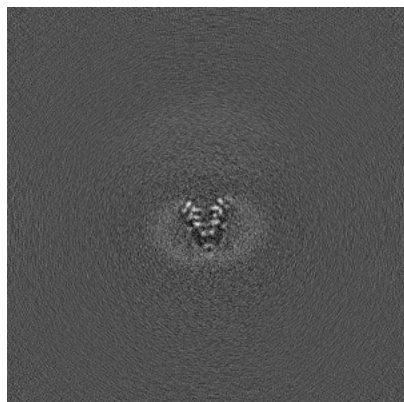


Y Index: 180

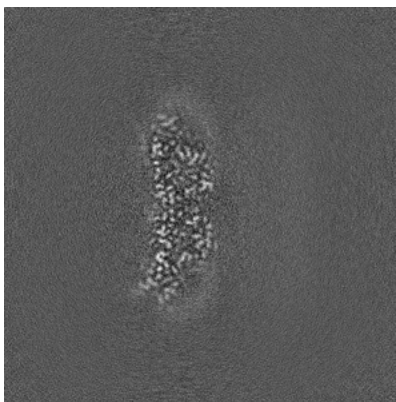


Z Index: 180

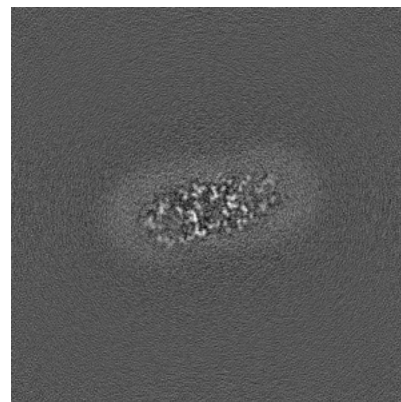
6.2.2 Raw map



X Index: 180



Y Index: 180

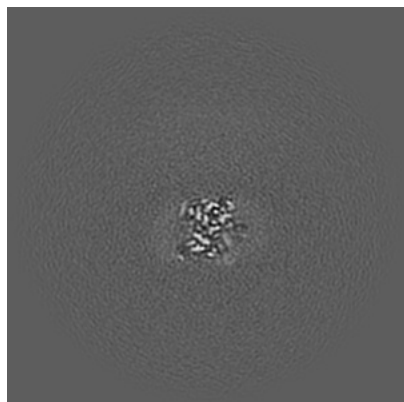


Z Index: 180

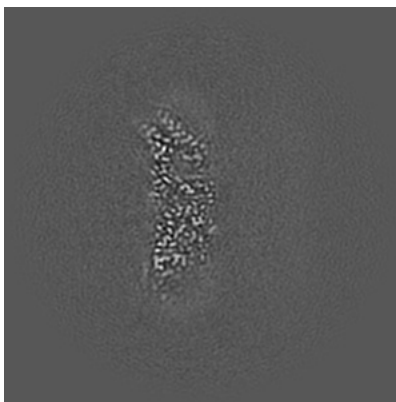
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

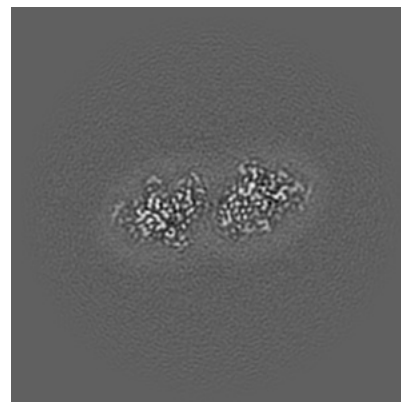
6.3.1 Primary map



X Index: 196

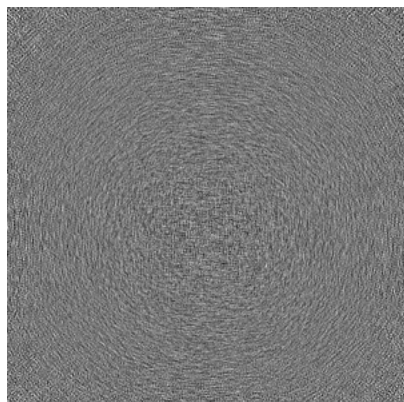


Y Index: 185

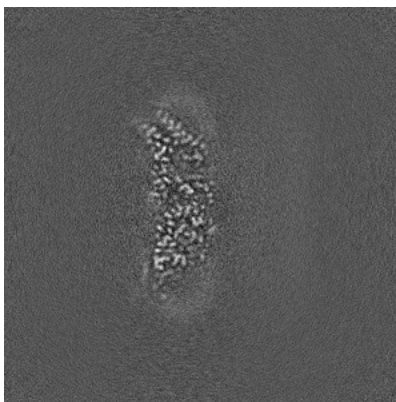


Z Index: 141

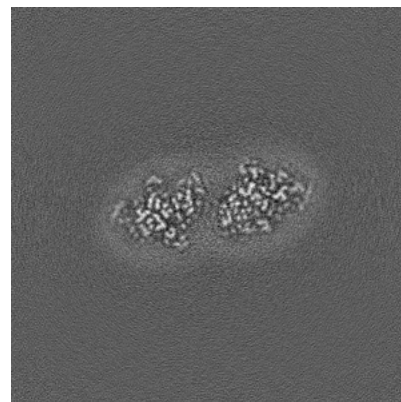
6.3.2 Raw map



X Index: 0



Y Index: 185

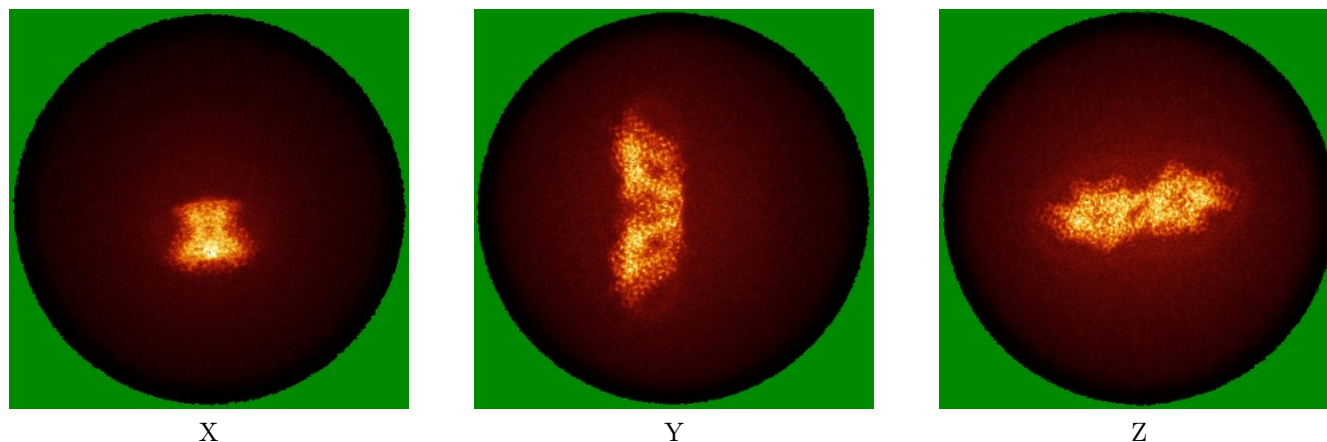


Z Index: 141

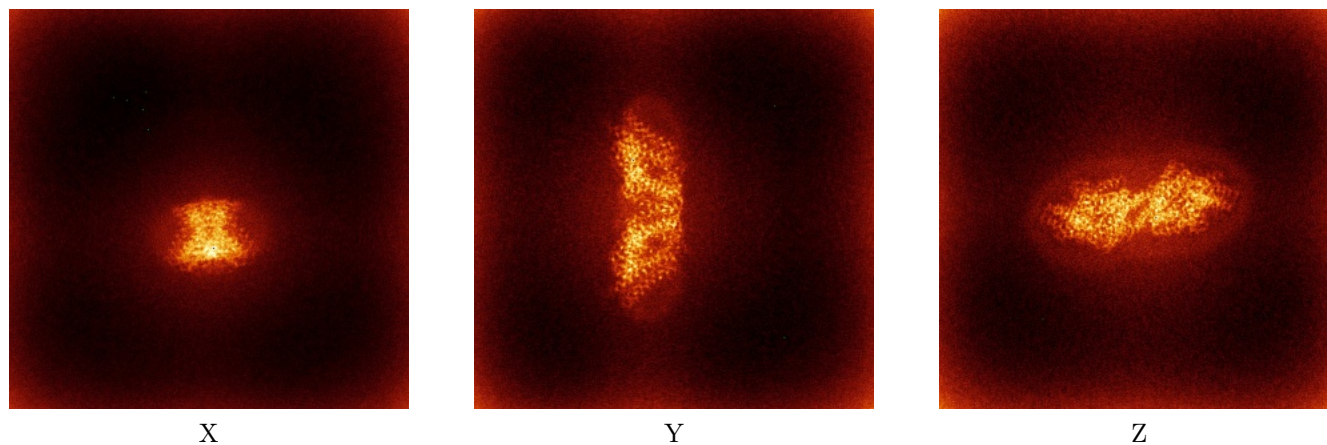
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



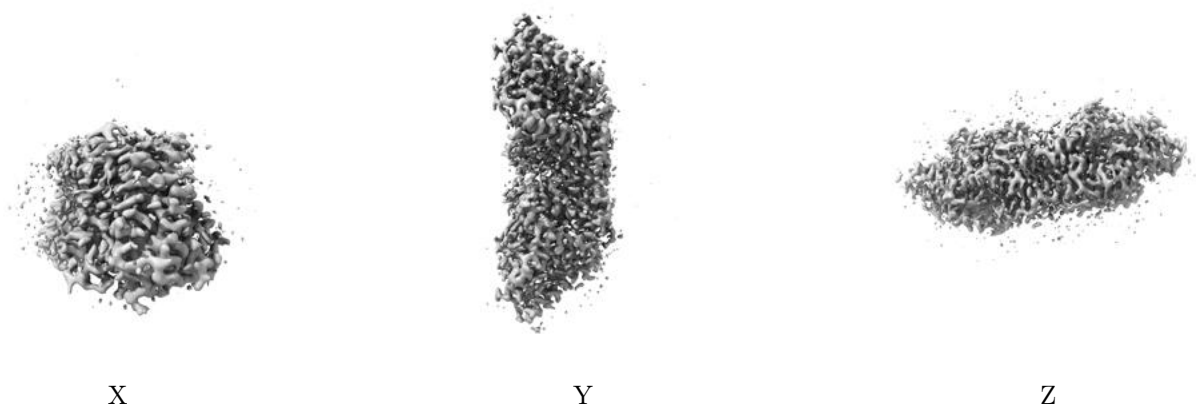
6.4.2 Raw map



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

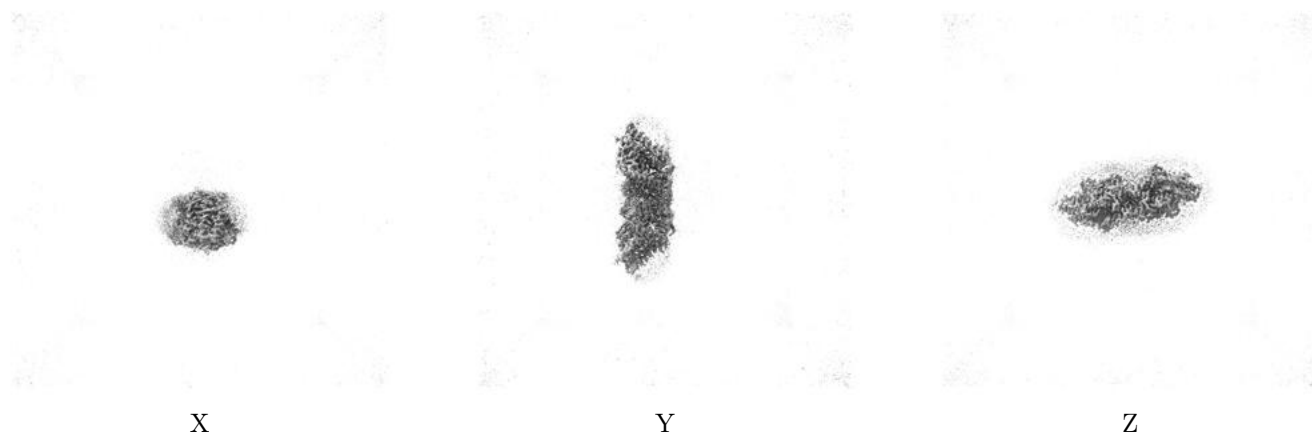
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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



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.

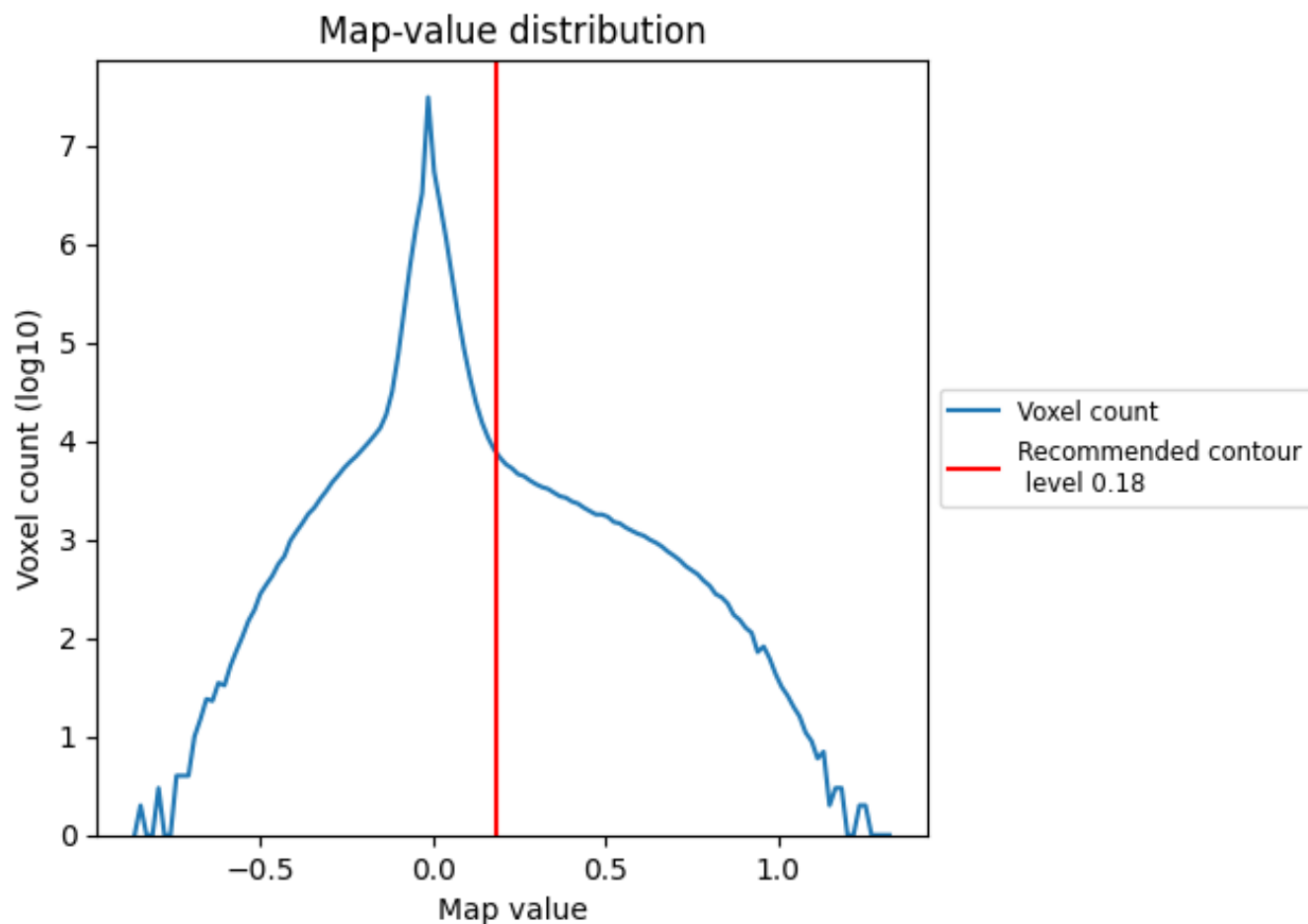
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

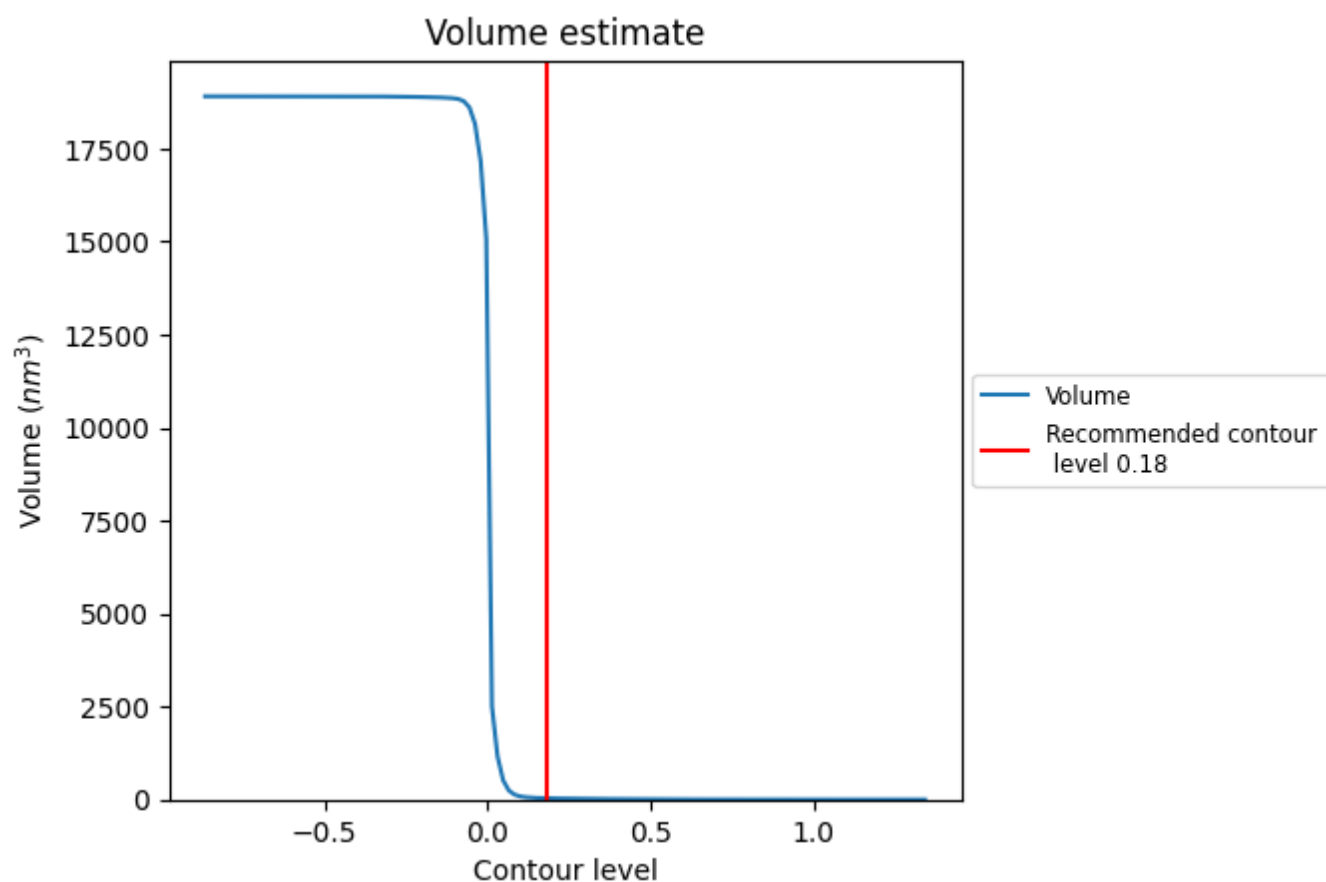
This section contains the results of statistical analysis of the map.

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.

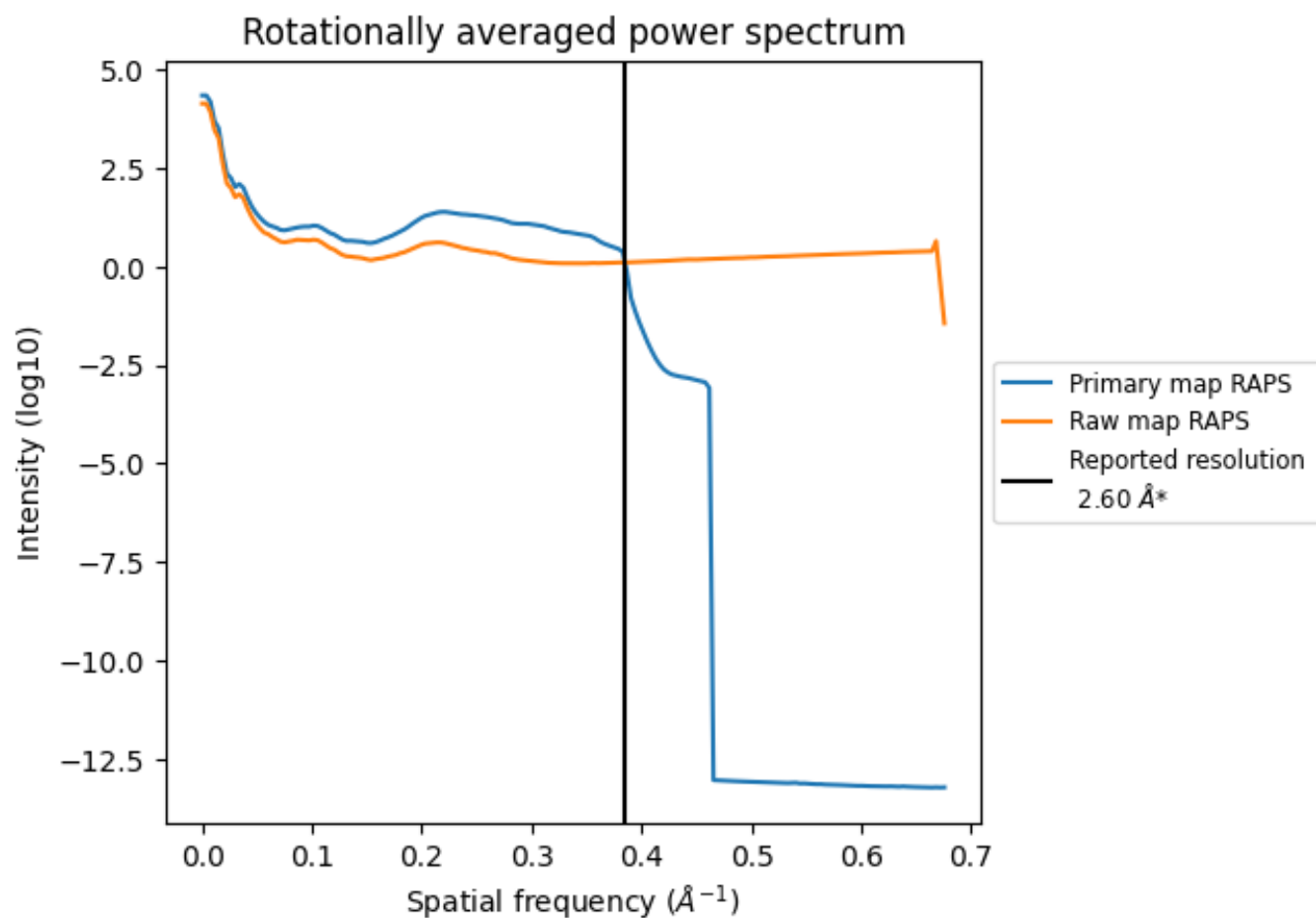
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 35 nm^3 ; this corresponds to an approximate mass of 32 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 ⓘ

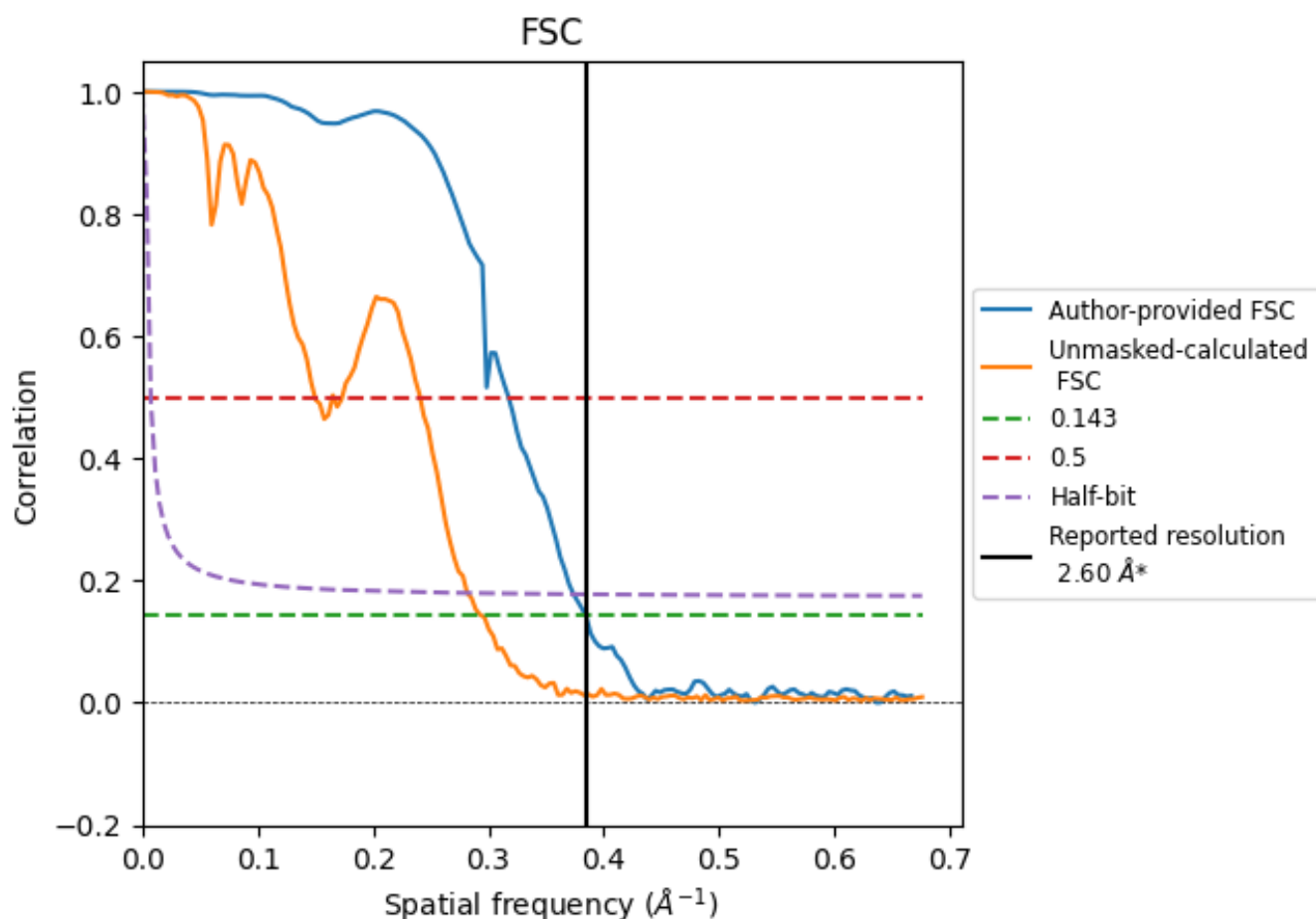


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

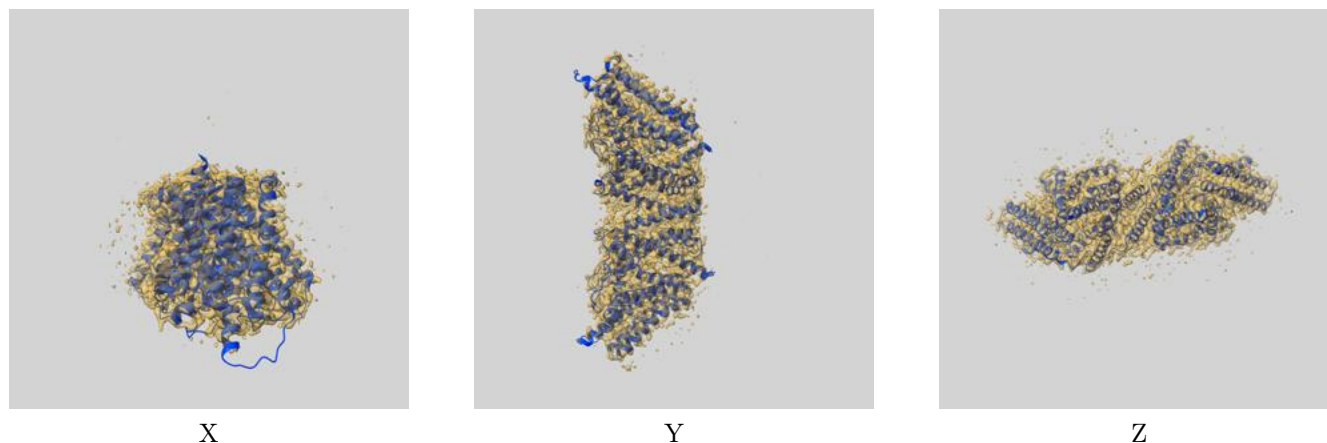
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.15	2.68
Unmasked-calculated*	3.41	6.68	3.55

*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 3.41 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

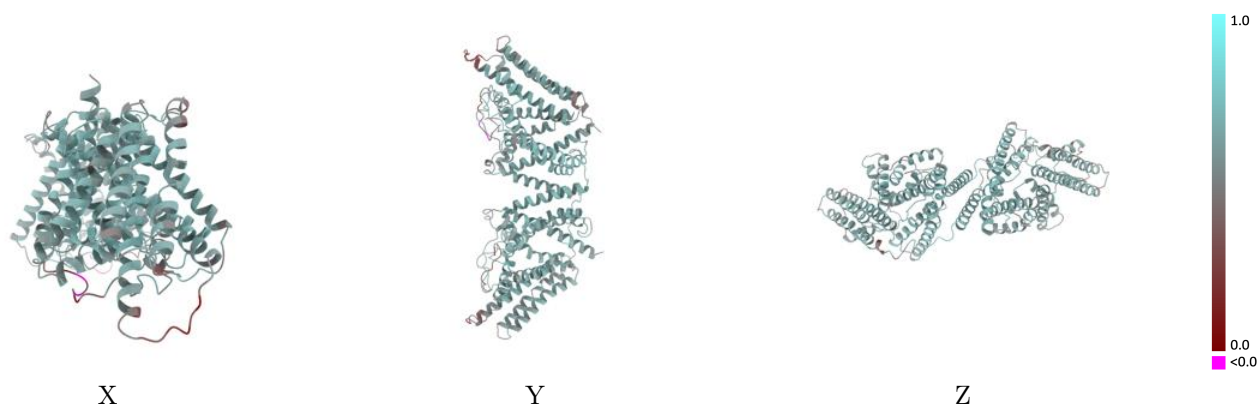
This section contains information regarding the fit between EMDB map EMD-65126 and PDB model 9VJX. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



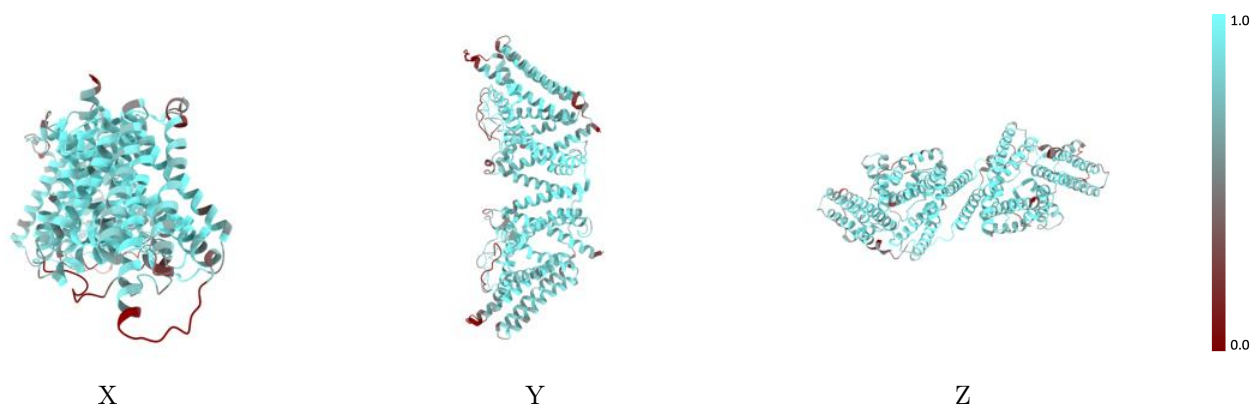
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



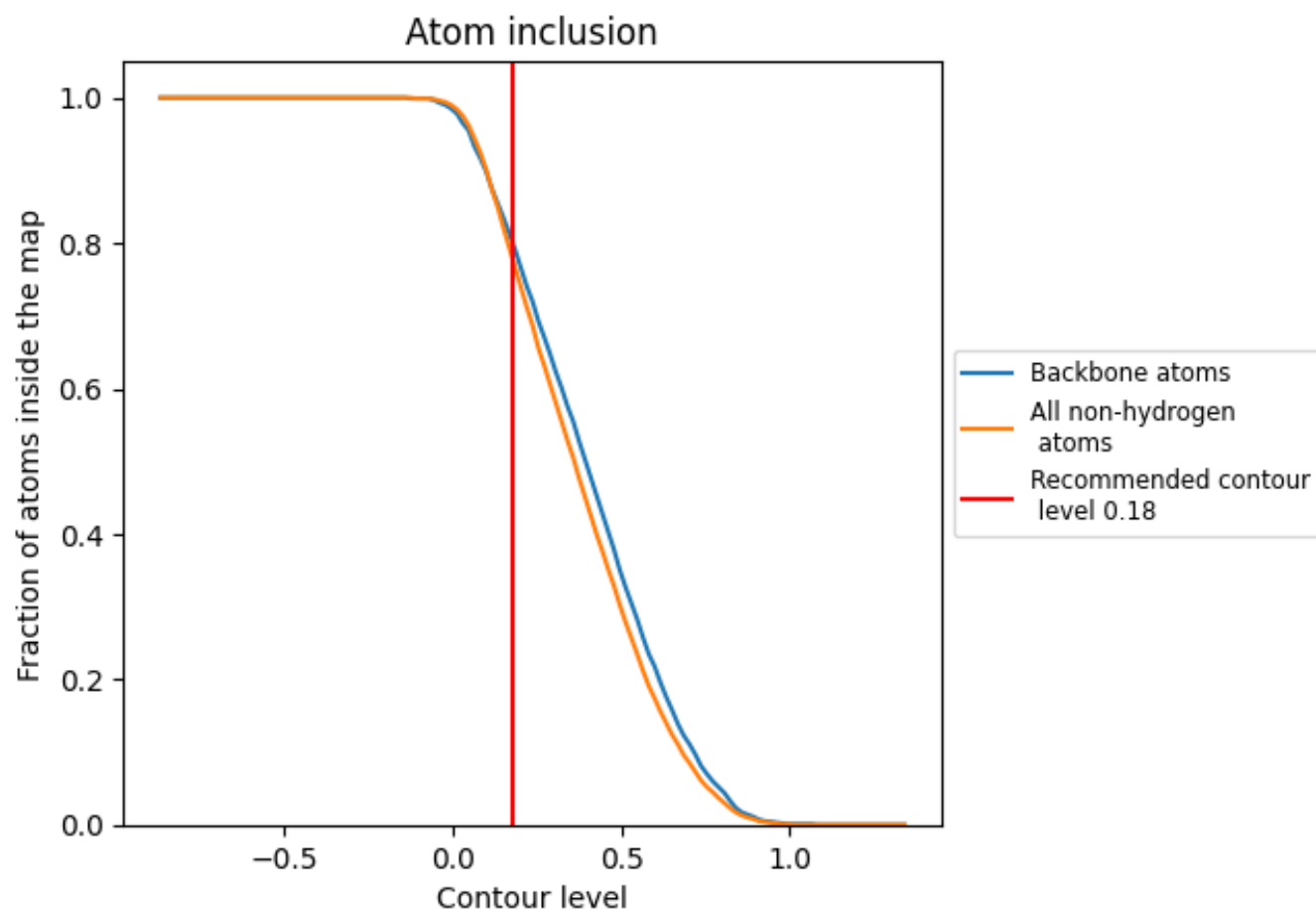
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7750	<div></div> 0.5910
A	<div></div> 0.7690	<div></div> 0.5910
B	<div></div> 0.7890	<div></div> 0.5910

