



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 10:54 AM EDT

PDB ID : 7M5Y / pdb_00007m5y
EMDB ID : EMD-23685
Title : human ATP13A2 in the outward-facing E2 state bound to spermine and magnesium fluoride
Authors : Lee, K.P.K.
Deposited on : 2021-03-25
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

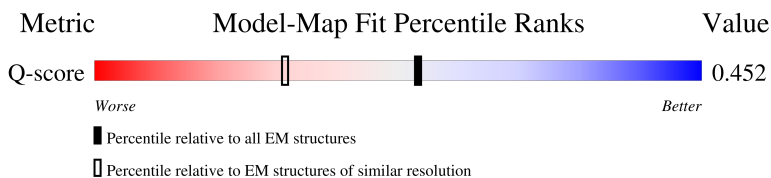
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	1189	 74% 10% 16%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 16158 atoms, of which 8245 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 Polyamine-transporting ATPase 13A2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1000	Total	C	H	N	O	S	0	0
			14990	4818	7534	1262	1326	50		

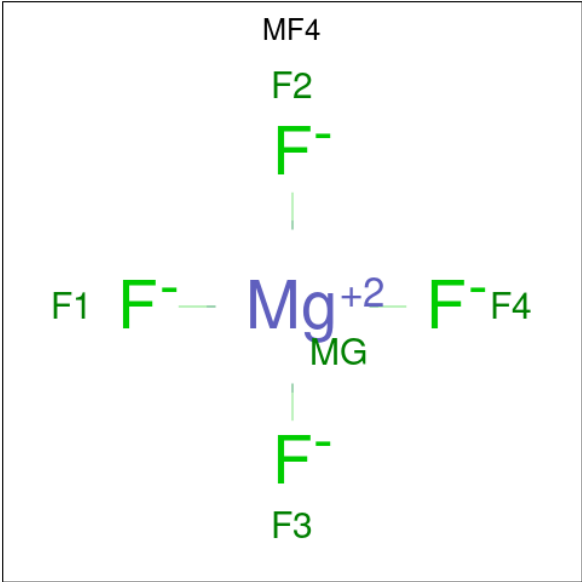
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1181	SER	-	expression tag	UNP Q9NQ11
A	1182	ASN	-	expression tag	UNP Q9NQ11
A	1183	SER	-	expression tag	UNP Q9NQ11
A	1184	LEU	-	expression tag	UNP Q9NQ11
A	1185	GLU	-	expression tag	UNP Q9NQ11
A	1186	VAL	-	expression tag	UNP Q9NQ11
A	1187	LEU	-	expression tag	UNP Q9NQ11
A	1188	PHE	-	expression tag	UNP Q9NQ11
A	1189	GLN	-	expression tag	UNP Q9NQ11

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

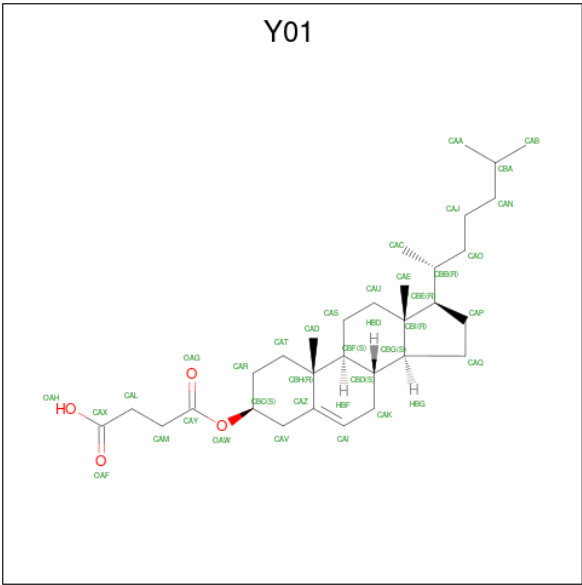
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	

- Molecule 3 is TETRAFLUOROMAGNESATE(2-) (CCD ID: MF4) (formula: F₄Mg) (labeled as "Ligand of Interest" by depositor).



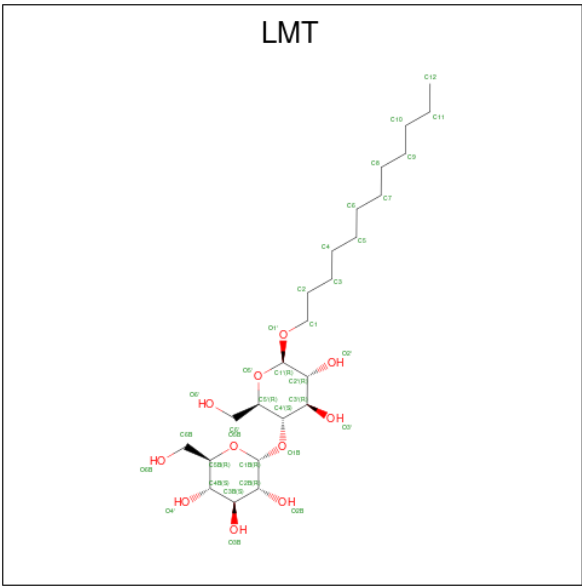
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	F	Mg	0
			5	4	1	

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



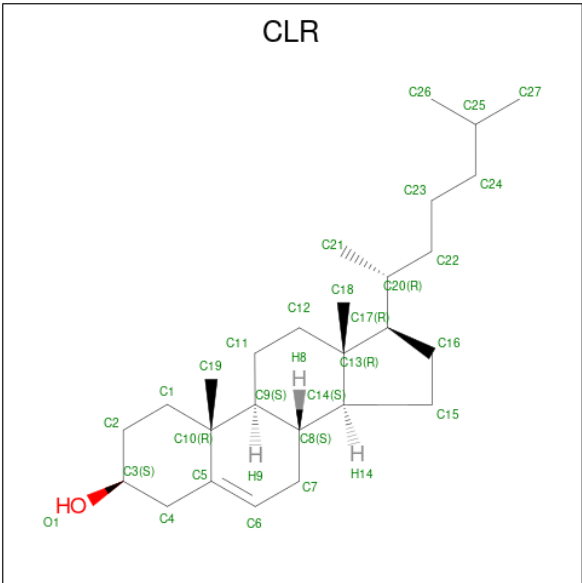
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			84	31	49	4	
4	A	1	Total	C	H	O	0
			84	31	49	4	
4	A	1	Total	C	H	O	0
			84	31	49	4	

- Molecule 5 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	O	0
			74	24	39	11	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



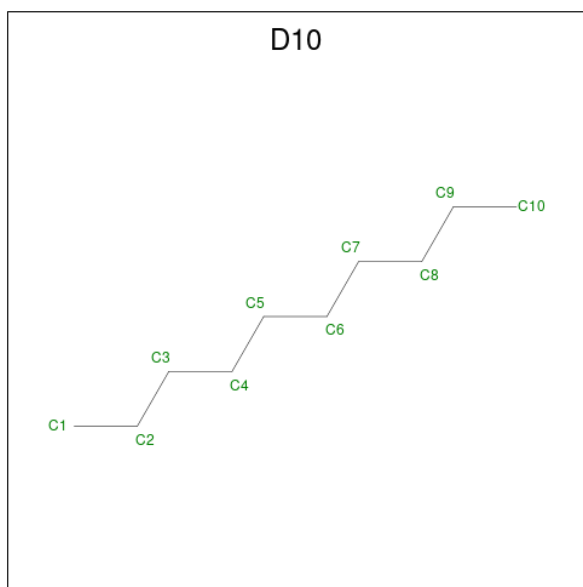
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	H	O	0
			74	27	46	1	
6	A	1	Total	C	H	O	0
			74	27	46	1	

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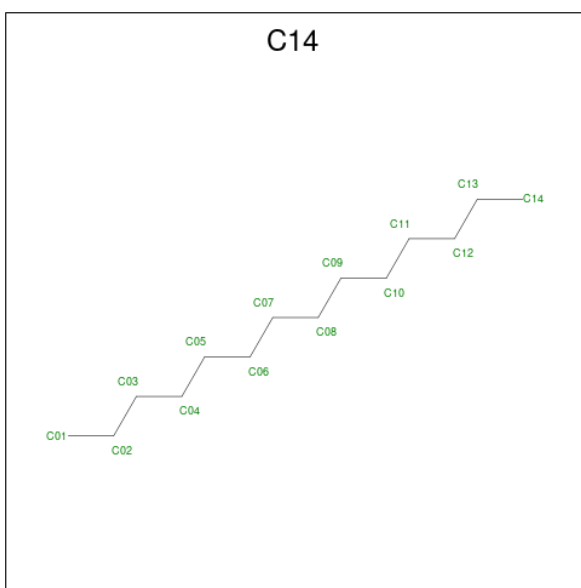
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	H	O	0
			74	27	46	1	
6	A	1	Total	C	H	O	0
			74	27	46	1	

- Molecule 7 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



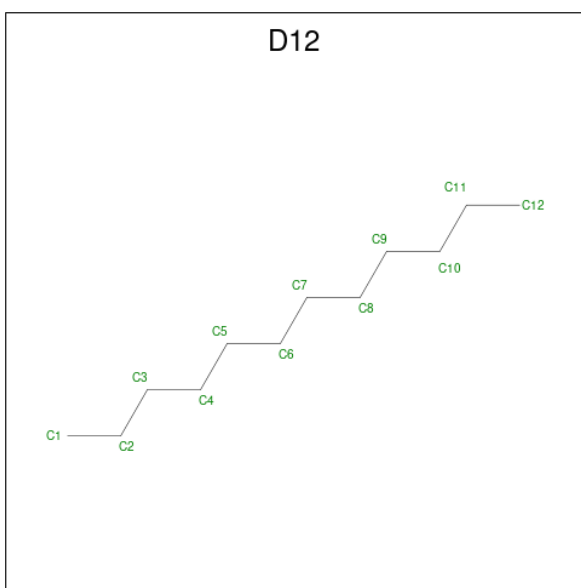
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	H	0
			32	10	22	
7	A	1	Total	C	H	0
			32	10	22	
7	A	1	Total	C	H	0
			32	10	22	
7	A	1	Total	C	H	0
			32	10	22	
7	A	1	Total	C	H	0
			32	10	22	
7	A	1	Total	C	H	0
			32	10	22	
7	A	1	Total	C	H	0
			32	10	22	
7	A	1	Total	C	H	0
			32	10	22	

- Molecule 8 is TETRADECANE (CCD ID: C14) (formula: $C_{14}H_{30}$).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	H	0
			44	14	30	

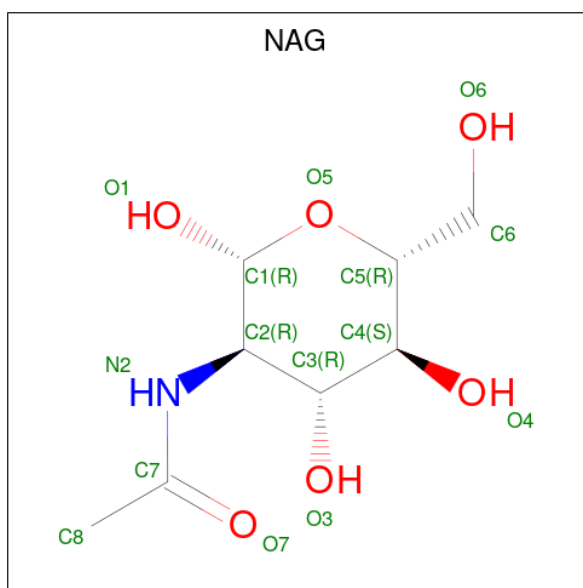
- Molecule 9 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	H	0
			38	12	26	

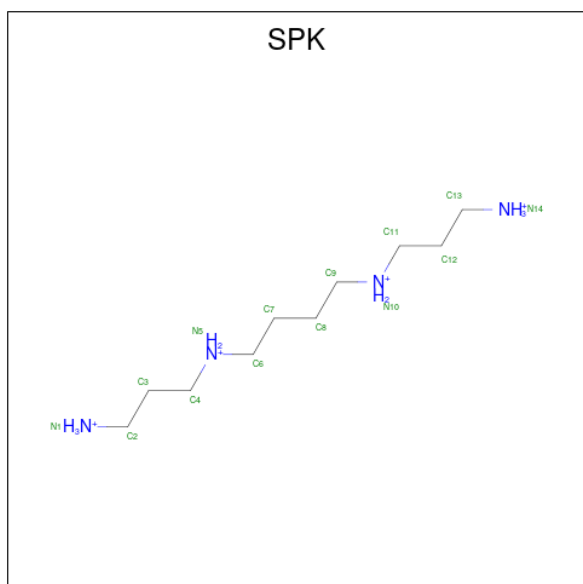
- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



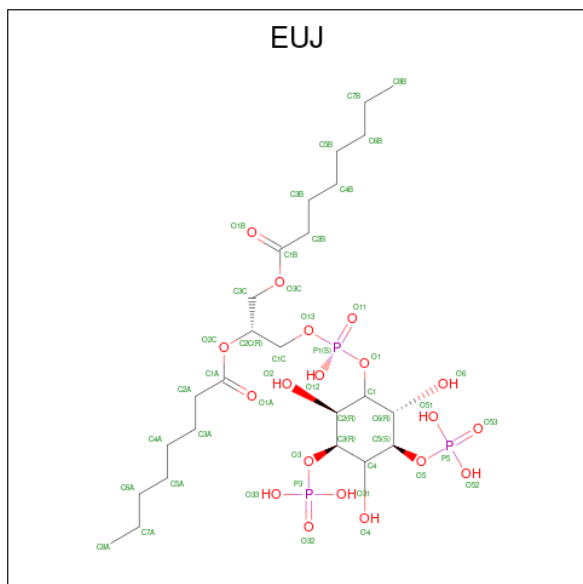
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

- Molecule 11 is SPERMINE (FULLY PROTONATED FORM) (CCD ID: SPK) (formula: C₁₀H₃₀N₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	H	N	0
			44	10	30	4	

- Molecule 12 is (2R)-3-{{[(S)-hydroxy{[(1S,2R,3R,4S,5S,6R)-2,4,6-trihydroxy-3,5-bis(phosphonoxy)cyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dioctanoate (CCD ID: EUJ) (formula: C₂₅H₄₉O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	H	O	P	0
			91	25	44	19	3	

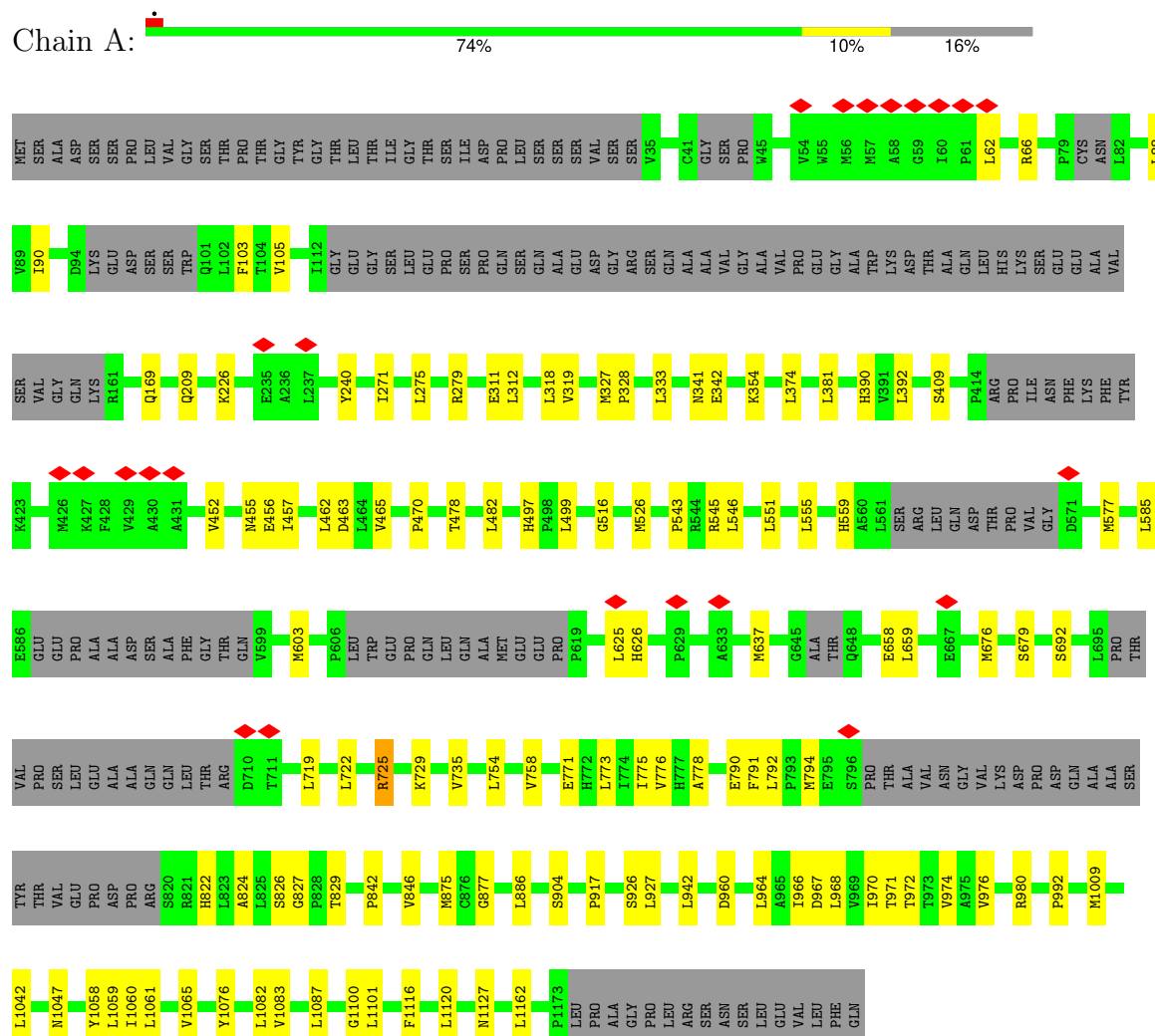
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	8	Total	O	0
			8	8	

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: Polyamine-transporting ATPase 13A2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	285797	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 ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.810	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EUJ, LMT, MF4, NAG, Y01, D12, D10, CLR, C14, MG, SPK

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	0.23	0/7604	0.56	1/10375 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	725	ARG	CB-CG-CD	5.36	123.64	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	926	SER	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7456	7534	7549	73	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	105	147	147	2	0
5	A	35	39	46	1	0
6	A	112	184	184	2	0
7	A	90	198	198	0	0
8	A	14	30	30	0	0
9	A	12	26	26	0	0
10	A	14	13	13	0	0
11	A	14	30	30	1	0
12	A	47	44	0	0	0
13	A	8	0	0	1	0
All	All	7913	8245	8223	75	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 (75) 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:A:775:ILE:HD13	1:A:824:ALA:HB3	1.56	0.85
1:A:240:TYR:OH	1:A:470:PRO:O	2.02	0.78
1:A:478:THR:HG22	1:A:499:LEU:HD11	1.65	0.77
1:A:967:ASP:O	1:A:971:THR:OG1	2.06	0.72
6:A:1207:CLR:H183	6:A:1207:CLR:H212	1.74	0.69
1:A:226:LYS:O	1:A:279:ARG:NH1	2.26	0.68
1:A:758:VAL:HG21	1:A:794:MET:HE1	1.76	0.68
1:A:462:LEU:O	1:A:465:VAL:HG12	1.95	0.66
1:A:875:MET:SD	1:A:877:GLY:N	2.69	0.65
1:A:886:LEU:HD13	1:A:904:SER:OG	1.98	0.64
1:A:980:ARG:NH1	4:A:1205:Y01:OAH	2.30	0.64
6:A:1220:CLR:H212	6:A:1220:CLR:H183	1.80	0.64
1:A:625:LEU:HD23	1:A:626:HIS:ND1	2.13	0.63
1:A:754:LEU:HD21	1:A:775:ILE:HD12	1.80	0.63
1:A:62:LEU:O	1:A:66:ARG:N	2.35	0.60
1:A:516:GLY:O	1:A:729:LYS:NZ	2.29	0.60
1:A:846:VAL:HG21	1:A:1162:LEU:HB3	1.84	0.59
1:A:463:ASP:OD2	13:A:1301:HOH:O	2.17	0.58
1:A:966:ILE:HD12	1:A:1058:TYR:CE2	2.40	0.57
1:A:319:VAL:HG13	1:A:390:HIS:ND1	2.20	0.56
1:A:342:GLU:OE2	1:A:354:LYS:NZ	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LEU:O	1:A:555:LEU:HD23	2.08	0.53
1:A:842:PRO:O	1:A:846:VAL:HG23	2.09	0.53
1:A:497:HIS:ND1	5:A:1204:LMT:O3B	2.42	0.53
1:A:90:ILE:HD12	1:A:103:PHE:O	2.09	0.53
1:A:545:ARG:O	1:A:546:LEU:HD12	2.09	0.52
1:A:790:GLU:OE1	1:A:792:LEU:HD21	2.10	0.51
1:A:976:VAL:HG11	4:A:1205:Y01:HAD1	1.92	0.51
1:A:585:LEU:HD12	1:A:603:MET:HE1	1.92	0.50
1:A:327:MET:HE3	1:A:328:PRO:HD2	1.93	0.50
1:A:452:VAL:HG23	1:A:457:ILE:HG13	1.93	0.49
1:A:927:LEU:HD23	1:A:992:PRO:HG2	1.95	0.49
1:A:1076:TYR:HA	1:A:1082:LEU:HD11	1.94	0.49
1:A:658:GLU:HG2	1:A:659:LEU:HD22	1.96	0.48
1:A:209:GLN:NE2	1:A:311:GLU:O	2.47	0.48
1:A:846:VAL:HG21	1:A:1162:LEU:CB	2.44	0.47
1:A:778:ALA:CB	1:A:829:THR:HG23	2.45	0.47
1:A:826:SER:OG	1:A:827:GLY:N	2.48	0.47
1:A:390:HIS:HE1	1:A:392:LEU:HD21	1.80	0.46
1:A:455:ASN:OD1	1:A:456:GLU:N	2.46	0.46
1:A:970:ILE:O	1:A:974:VAL:HG22	2.15	0.46
1:A:526:MET:HE2	1:A:725:ARG:HH12	1.80	0.45
1:A:526:MET:HE2	1:A:725:ARG:NH1	2.32	0.45
1:A:972:THR:O	1:A:976:VAL:HG12	2.16	0.45
1:A:692:SER:OG	1:A:719:LEU:HD21	2.16	0.45
1:A:771:GLU:OE1	1:A:822:HIS:NE2	2.48	0.45
1:A:776:VAL:HG12	1:A:791:PHE:HD1	1.82	0.45
1:A:543:PRO:O	1:A:546:LEU:HD13	2.17	0.44
1:A:942:LEU:HB3	1:A:1009:MET:HE2	1.99	0.44
1:A:758:VAL:HG23	1:A:773:LEU:HD21	1.98	0.44
1:A:559:HIS:C	1:A:637:MET:HE1	2.42	0.44
1:A:970:ILE:HD12	1:A:1059:LEU:HD21	1.99	0.44
1:A:1083:VAL:O	1:A:1087:LEU:HD23	2.17	0.44
1:A:271:ILE:O	1:A:275:LEU:HD23	2.18	0.43
1:A:964:LEU:HG	1:A:968:LEU:HD12	2.01	0.43
1:A:312:LEU:HD22	1:A:318:LEU:HD11	2.01	0.43
1:A:390:HIS:CE1	1:A:392:LEU:HD21	2.53	0.42
1:A:88:LEU:HD12	1:A:105:VAL:O	2.18	0.42
1:A:478:THR:O	1:A:482:LEU:HD13	2.19	0.42
1:A:875:MET:HE1	1:A:886:LEU:HG	2.02	0.42
1:A:1042:LEU:HD22	1:A:1047:ASN:HD22	1.85	0.42
1:A:169:GLN:O	1:A:409:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:MET:O	1:A:679:SER:OG	2.32	0.41
1:A:692:SER:HB3	1:A:719:LEU:HD11	2.00	0.41
1:A:735:VAL:HG13	1:A:917:PRO:HG3	2.03	0.41
1:A:1100:GLY:O	1:A:1101:LEU:HD22	2.19	0.41
1:A:341:ASN:HB2	1:A:381:LEU:HD21	2.03	0.41
1:A:577:MET:HE2	1:A:722:LEU:HD22	2.01	0.41
1:A:960:ASP:OD1	11:A:1223:SPK:N10	2.52	0.41
1:A:1061:LEU:O	1:A:1065:VAL:HG22	2.20	0.41
1:A:778:ALA:HB3	1:A:829:THR:HG23	2.04	0.40
1:A:1116:PHE:CE2	1:A:1120:LEU:HD11	2.55	0.40
1:A:311:GLU:N	1:A:311:GLU:OE1	2.54	0.40
1:A:1060:ILE:HG21	1:A:1127:ASN:OD1	2.20	0.40
1:A:333:LEU:HG	1:A:374:LEU:HD23	2.03	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	976/1189 (82%)	926 (95%)	50 (5%)	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	794/1011 (78%)	794 (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. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	897	GLN
1	A	1041	ASN
1	A	1047	ASN
1	A	1110	ASN
1	A	1169	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MF4	A	1202	1	0,4,4	-	-	-		
7	D10	A	1210	-	9,9,9	0.30	0	8,8,8	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	D10	A	1209	-	9,9,9	0.28	0	8,8,8	0.57	0
9	D12	A	1216	-	11,11,11	0.27	0	10,10,10	0.66	0
7	D10	A	1211	-	9,9,9	0.28	0	8,8,8	0.59	0
12	EUJ	A	1224	-	47,47,47	0.61	0	62,65,65	1.12	7 (11%)
7	D10	A	1213	-	9,9,9	0.25	0	8,8,8	0.59	0
4	Y01	A	1205	-	38,38,38	1.24	3 (7%)	57,57,57	1.83	10 (17%)
6	CLR	A	1221	-	31,31,31	0.68	0	48,48,48	1.27	5 (10%)
6	CLR	A	1220	-	31,31,31	0.63	0	48,48,48	1.43	8 (16%)
4	Y01	A	1203	-	38,38,38	1.25	2 (5%)	57,57,57	1.92	11 (19%)
6	CLR	A	1207	-	31,31,31	0.44	0	48,48,48	0.73	0
10	NAG	A	1222	1	14,14,15	2.28	3 (21%)	17,19,21	1.63	5 (29%)
8	C14	A	1215	-	13,13,13	0.30	0	12,12,12	0.72	0
7	D10	A	1212	-	9,9,9	0.32	0	8,8,8	0.49	0
6	CLR	A	1206	-	31,31,31	0.66	1 (3%)	48,48,48	1.31	6 (12%)
7	D10	A	1218	-	9,9,9	0.28	0	8,8,8	0.61	0
4	Y01	A	1208	-	38,38,38	1.29	3 (7%)	57,57,57	2.09	13 (22%)
5	LMT	A	1204	-	36,36,36	1.04	3 (8%)	47,47,47	1.59	11 (23%)
7	D10	A	1217	-	9,9,9	0.27	0	8,8,8	0.59	0
7	D10	A	1214	-	9,9,9	0.34	0	8,8,8	0.55	0
7	D10	A	1219	-	9,9,9	0.25	0	8,8,8	0.53	0
11	SPK	A	1223	-	13,13,13	0.79	0	12,12,12	1.81	4 (33%)

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	D10	A	1210	-	-	4/7/7/7	-
7	D10	A	1209	-	-	2/7/7/7	-
9	D12	A	1216	-	-	4/9/9/9	-
7	D10	A	1211	-	-	0/7/7/7	-
12	EUJ	A	1224	-	-	19/44/68/68	0/1/1/1
7	D10	A	1213	-	-	0/7/7/7	-
4	Y01	A	1205	-	-	6/19/77/77	0/4/4/4
6	CLR	A	1221	-	-	1/10/68/68	0/4/4/4
6	CLR	A	1220	-	-	3/10/68/68	0/4/4/4
4	Y01	A	1203	-	-	6/19/77/77	0/4/4/4
6	CLR	A	1207	-	-	4/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	1222	1	-	1/6/23/26	0/1/1/1
8	C14	A	1215	-	-	3/11/11/11	-
7	D10	A	1212	-	-	3/7/7/7	-
6	CLR	A	1206	-	-	6/10/68/68	0/4/4/4
7	D10	A	1218	-	-	1/7/7/7	-
4	Y01	A	1208	-	-	6/19/77/77	0/4/4/4
5	LMT	A	1204	-	-	9/21/61/61	0/2/2/2
7	D10	A	1217	-	-	2/7/7/7	-
7	D10	A	1214	-	-	2/7/7/7	-
7	D10	A	1219	-	-	2/7/7/7	-
11	SPK	A	1223	-	-	1/11/11/11	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1222	NAG	C1-C2	6.99	1.61	1.52
4	A	1203	Y01	CAK-CAI	-4.45	1.41	1.50
4	A	1208	Y01	CAK-CAI	-4.37	1.41	1.50
4	A	1205	Y01	CAK-CAI	-4.23	1.41	1.50
4	A	1208	Y01	CAI-CAZ	2.90	1.39	1.33
4	A	1205	Y01	CAI-CAZ	2.90	1.39	1.33
4	A	1203	Y01	CAI-CAZ	2.82	1.38	1.33
6	A	1206	CLR	C16-C17	2.70	1.59	1.54
10	A	1222	NAG	C3-C2	2.61	1.58	1.52
4	A	1208	Y01	CAL-CAX	2.36	1.56	1.50
4	A	1205	Y01	CBH-CAZ	-2.29	1.48	1.52
5	A	1204	LMT	O3'-C3'	-2.23	1.37	1.43
5	A	1204	LMT	O2B-C2B	-2.12	1.37	1.43
5	A	1204	LMT	O4'-C4B	-2.09	1.37	1.43
10	A	1222	NAG	C7-N2	2.05	1.41	1.34

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1208	Y01	CAV-CAZ-CBH	7.40	125.89	116.42
4	A	1205	Y01	CAV-CAZ-CBH	7.21	125.65	116.42
4	A	1203	Y01	CAV-CAZ-CBH	7.19	125.63	116.42
4	A	1208	Y01	OAW-CAY-CAM	5.62	123.64	111.48
4	A	1208	Y01	OAW-CAY-OAG	-5.24	111.45	123.70
4	A	1205	Y01	OAW-CAY-CAM	5.12	122.55	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1203	Y01	OAW-CAY-CAM	4.98	122.27	111.48
4	A	1203	Y01	OAW-CAY-OAG	-4.78	112.54	123.70
4	A	1208	Y01	CAV-CAZ-CAI	-4.57	114.38	120.57
4	A	1205	Y01	OAW-CAY-OAG	-4.42	113.37	123.70
4	A	1203	Y01	CAV-CAZ-CAI	-4.28	114.77	120.57
6	A	1220	CLR	C1-C10-C9	4.20	114.30	108.74
6	A	1206	CLR	C16-C17-C13	-4.09	99.03	103.84
5	A	1204	LMT	O1'-C1'-C2'	-4.02	102.17	108.27
4	A	1205	Y01	CAV-CAZ-CAI	-3.89	115.29	120.57
4	A	1208	Y01	CBF-CBD-CBG	3.89	114.17	109.09
12	A	1224	EUJ	C4-C3-C2	3.75	116.06	110.86
12	A	1224	EUJ	O3-C3-C4	-3.75	100.80	108.73
5	A	1204	LMT	C4B-C3B-C2B	-3.24	105.14	110.83
4	A	1208	Y01	CAS-CBF-CBH	3.21	117.04	113.08
5	A	1204	LMT	C6B-C5B-C4B	-3.19	105.18	113.02
6	A	1221	CLR	C10-C9-C8	-3.16	108.10	112.71
10	A	1222	NAG	O3-C3-C2	-3.11	102.94	109.40
5	A	1204	LMT	C3'-C4'-C5'	-3.10	104.05	110.93
6	A	1220	CLR	C3-C4-C5	2.99	116.82	112.05
12	A	1224	EUJ	C5-C6-C1	2.98	115.16	109.11
6	A	1220	CLR	C10-C9-C8	-2.98	108.36	112.71
4	A	1208	Y01	CBH-CBF-CBD	-2.97	108.37	112.71
6	A	1206	CLR	C1-C10-C9	2.92	112.60	108.74
6	A	1221	CLR	C11-C9-C8	2.87	115.78	111.78
6	A	1221	CLR	C15-C14-C13	2.84	107.19	103.84
6	A	1206	CLR	C16-C17-C20	2.82	116.44	112.18
11	A	1223	SPK	C8-C9-N10	-2.81	104.54	112.07
6	A	1220	CLR	C15-C14-C13	2.79	107.12	103.84
6	A	1221	CLR	C17-C13-C14	2.73	103.24	100.10
6	A	1206	CLR	C14-C8-C9	2.73	112.65	109.09
6	A	1220	CLR	C9-C10-C5	-2.69	105.71	109.65
11	A	1223	SPK	C7-C6-N5	-2.69	104.85	112.07
10	A	1222	NAG	C2-N2-C7	-2.69	119.30	122.90
4	A	1205	Y01	CBH-CAZ-CAI	-2.66	119.05	122.93
5	A	1204	LMT	C1'-C2'-C3'	-2.61	104.53	110.01
11	A	1223	SPK	C12-C11-N10	-2.60	105.08	112.07
4	A	1203	Y01	CAD-CBH-CBF	2.57	114.55	111.66
6	A	1221	CLR	C3-C4-C5	2.57	116.15	112.05
4	A	1205	Y01	OAW-CBC-CAV	-2.55	102.79	108.04
5	A	1204	LMT	C6'-C5'-C4'	-2.54	106.25	113.38
5	A	1204	LMT	O3'-C3'-C2'	-2.52	104.44	110.38
4	A	1208	Y01	OAW-CBC-CAV	-2.49	102.91	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1208	Y01	CAK-CBD-CBF	-2.48	106.85	109.72
5	A	1204	LMT	O4'-C4B-C3B	-2.43	104.66	110.38
4	A	1203	Y01	OAW-CBC-CAV	-2.42	103.06	108.04
4	A	1203	Y01	OAW-CBC-CAR	2.40	114.05	108.37
4	A	1208	Y01	CAP-CBE-CBI	-2.38	101.04	103.84
4	A	1203	Y01	CAS-CBF-CBH	2.36	115.99	113.08
5	A	1204	LMT	O5'-C1'-O1'	-2.34	104.53	110.04
4	A	1208	Y01	CAD-CBH-CBF	2.33	114.27	111.66
4	A	1208	Y01	OAF-CAX-CAL	-2.31	115.77	123.09
6	A	1206	CLR	C10-C9-C8	-2.30	109.36	112.71
12	A	1224	EUJ	O2C-C1A-C2A	2.29	116.44	111.48
4	A	1203	Y01	CBH-CAZ-CAI	-2.28	119.60	122.93
4	A	1205	Y01	CAD-CBH-CBF	2.25	114.19	111.66
4	A	1205	Y01	OAW-CBC-CAR	2.23	113.65	108.37
11	A	1223	SPK	C7-C8-C9	-2.21	103.36	113.56
4	A	1208	Y01	CBH-CAZ-CAI	-2.20	119.71	122.93
6	A	1206	CLR	C17-C13-C14	2.20	102.62	100.10
12	A	1224	EUJ	C3-C2-C1	2.17	113.52	109.11
5	A	1204	LMT	C1'-O5'-C5'	2.17	117.96	113.72
6	A	1220	CLR	C11-C9-C10	2.17	115.76	113.08
4	A	1203	Y01	OAF-CAX-CAL	-2.17	116.21	123.09
4	A	1205	Y01	CAP-CBE-CBI	-2.17	101.29	103.84
6	A	1220	CLR	C1-C2-C3	2.16	113.35	110.48
12	A	1224	EUJ	C6-C5-C4	2.15	113.85	110.86
6	A	1220	CLR	C11-C12-C13	-2.14	109.13	112.74
4	A	1203	Y01	CAP-CAQ-CBG	-2.13	100.97	105.14
10	A	1222	NAG	O4-C4-C3	-2.11	105.41	110.38
12	A	1224	EUJ	C5-C4-C3	2.09	113.35	109.11
5	A	1204	LMT	O3B-C3B-C2B	-2.08	105.48	110.38
10	A	1222	NAG	C6-C5-C4	-2.07	107.94	113.02
10	A	1222	NAG	O5-C5-C4	2.03	115.77	110.83
4	A	1205	Y01	CBD-CAK-CAI	2.01	115.54	112.76

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1208	Y01	CAM-CAY-OAW-CBC
12	A	1224	EUJ	C1-O1-P1-O13
12	A	1224	EUJ	C1C-O13-P1-O11
5	A	1204	LMT	O5B-C1B-O1B-C4'
4	A	1208	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
5	A	1204	LMT	C2B-C1B-O1B-C4'
12	A	1224	EUJ	O1A-C1A-O2C-C2C
5	A	1204	LMT	O5'-C5'-C6'-O6'
12	A	1224	EUJ	C2A-C1A-O2C-C2C
6	A	1207	CLR	C13-C17-C20-C21
4	A	1205	Y01	CAJ-CAO-CBB-CBE
6	A	1220	CLR	C17-C20-C22-C23
4	A	1205	Y01	CAJ-CAO-CBB-CAC
12	A	1224	EUJ	C2B-C1B-O3C-C3C
5	A	1204	LMT	C4'-C5'-C6'-O6'
6	A	1220	CLR	C21-C20-C22-C23
6	A	1206	CLR	C13-C17-C20-C22
12	A	1224	EUJ	O1B-C1B-O3C-C3C
4	A	1203	Y01	CAX-CAL-CAM-CAY
6	A	1207	CLR	C16-C17-C20-C22
6	A	1220	CLR	C22-C23-C24-C25
6	A	1206	CLR	C13-C17-C20-C21
4	A	1205	Y01	CAJ-CAN-CBA-CAB
4	A	1208	Y01	CAJ-CAN-CBA-CAB
7	A	1219	D10	C5-C6-C7-C8
12	A	1224	EUJ	C3A-C4A-C5A-C6A
4	A	1203	Y01	CAM-CAY-OAW-CBC
4	A	1203	Y01	OAG-CAY-OAW-CBC
7	A	1218	D10	C3-C4-C5-C6
10	A	1222	NAG	O5-C5-C6-O6
8	A	1215	C14	C05-C06-C07-C08
6	A	1221	CLR	C20-C22-C23-C24
7	A	1212	D10	C5-C6-C7-C8
6	A	1206	CLR	C16-C17-C20-C21
6	A	1207	CLR	C16-C17-C20-C21
12	A	1224	EUJ	C1A-C2A-C3A-C4A
7	A	1217	D10	C5-C6-C7-C8
12	A	1224	EUJ	C4A-C5A-C6A-C7A
6	A	1206	CLR	C22-C23-C24-C25
7	A	1209	D10	C7-C8-C9-C10
4	A	1208	Y01	CAJ-CAN-CBA-CAA
6	A	1206	CLR	C16-C17-C20-C22
6	A	1206	CLR	C20-C22-C23-C24
4	A	1205	Y01	CAJ-CAN-CBA-CAA
11	A	1223	SPK	N1-C2-C3-C4
12	A	1224	EUJ	O13-C1C-C2C-C3C
9	A	1216	D12	C11-C10-C9-C8

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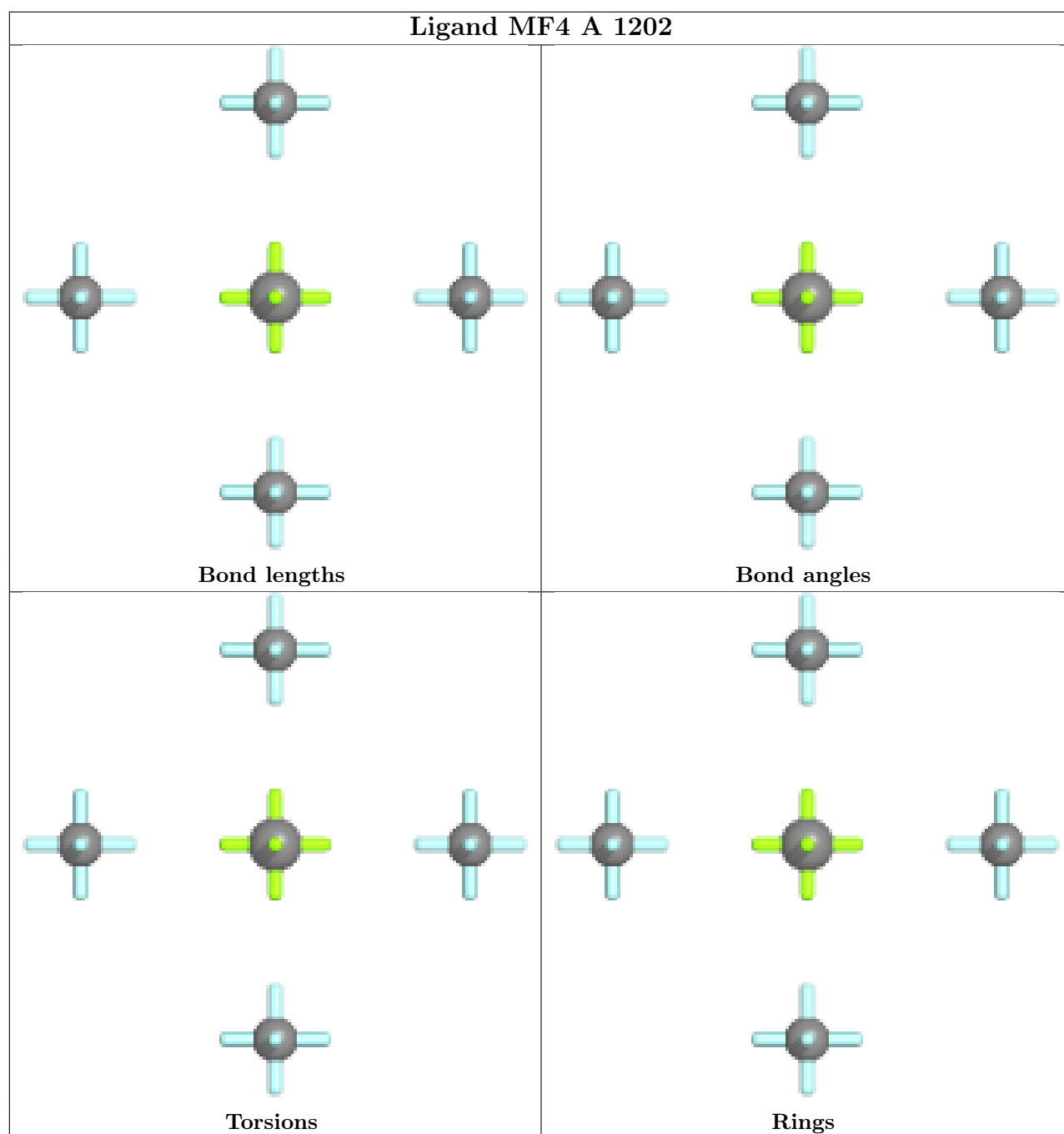
Mol	Chain	Res	Type	Atoms
12	A	1224	EUJ	C1-O1-P1-O11
6	A	1207	CLR	C13-C17-C20-C22
9	A	1216	D12	C9-C10-C11-C12
7	A	1219	D10	C7-C8-C9-C10
4	A	1205	Y01	CAR-CBC-OAW-CAY
12	A	1224	EUJ	O13-C1C-C2C-O2C
7	A	1210	D10	C4-C5-C6-C7
7	A	1209	D10	C5-C6-C7-C8
12	A	1224	EUJ	C2B-C3B-C4B-C5B
8	A	1215	C14	C01-C02-C03-C04
5	A	1204	LMT	C5-C6-C7-C8
12	A	1224	EUJ	C4-C5-O5-P5
5	A	1204	LMT	C2-C1-O1'-C1'
7	A	1214	D10	C4-C5-C6-C7
7	A	1217	D10	C4-C5-C6-C7
12	A	1224	EUJ	C2C-C1C-O13-P1
12	A	1224	EUJ	C2-C3-O3-P3
4	A	1205	Y01	CAV-CBC-OAW-CAY
4	A	1203	Y01	CAM-CAL-CAX-OAF
7	A	1212	D10	C4-C5-C6-C7
5	A	1204	LMT	C11-C10-C9-C8
12	A	1224	EUJ	C5-O5-P5-O53
5	A	1204	LMT	C3-C4-C5-C6
7	A	1210	D10	C1-C2-C3-C4
9	A	1216	D12	C4-C5-C6-C7
4	A	1203	Y01	CAM-CAL-CAX-OAH
4	A	1208	Y01	CAJ-CAO-CBB-CBE
5	A	1204	LMT	C1-C2-C3-C4
4	A	1208	Y01	CAJ-CAO-CBB-CAC
7	A	1210	D10	C3-C4-C5-C6
12	A	1224	EUJ	C1-O1-P1-O12
7	A	1212	D10	C1-C2-C3-C4
9	A	1216	D12	C6-C7-C8-C9
7	A	1214	D10	C5-C6-C7-C8
8	A	1215	C14	C04-C05-C06-C07
7	A	1210	D10	C5-C6-C7-C8
12	A	1224	EUJ	O2C-C1A-C2A-C3A
4	A	1203	Y01	CAJ-CAO-CBB-CBE

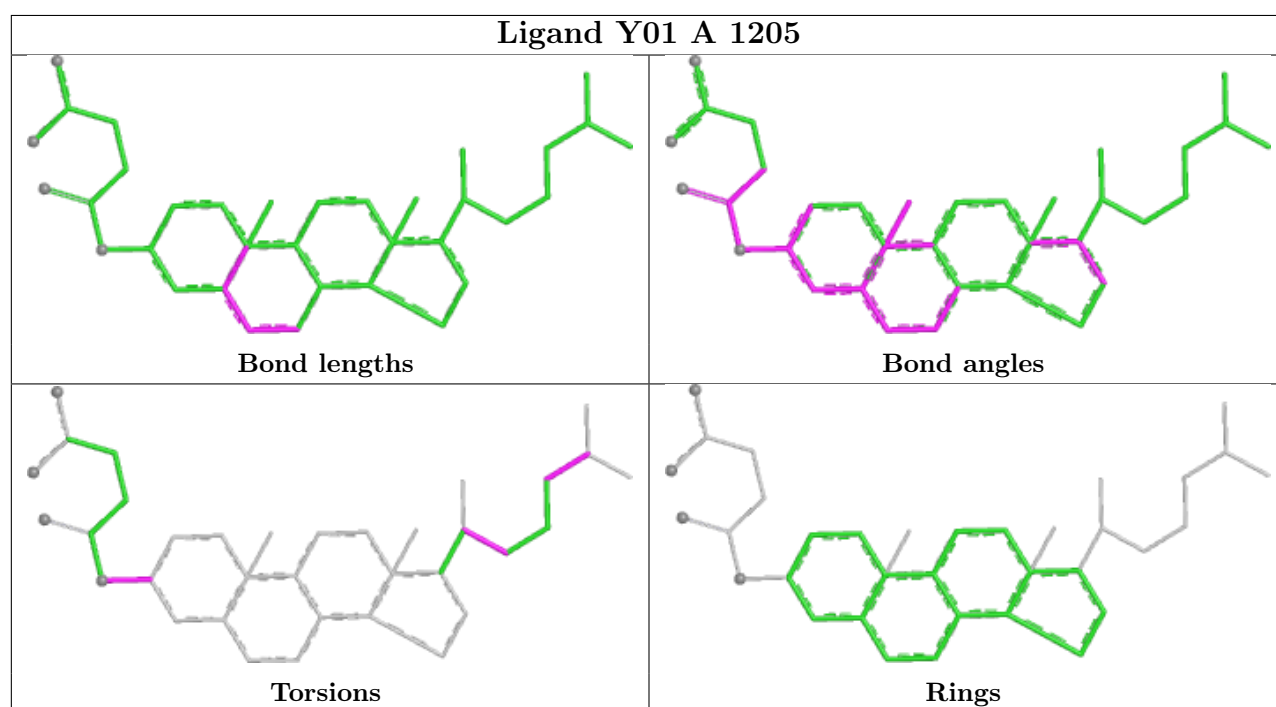
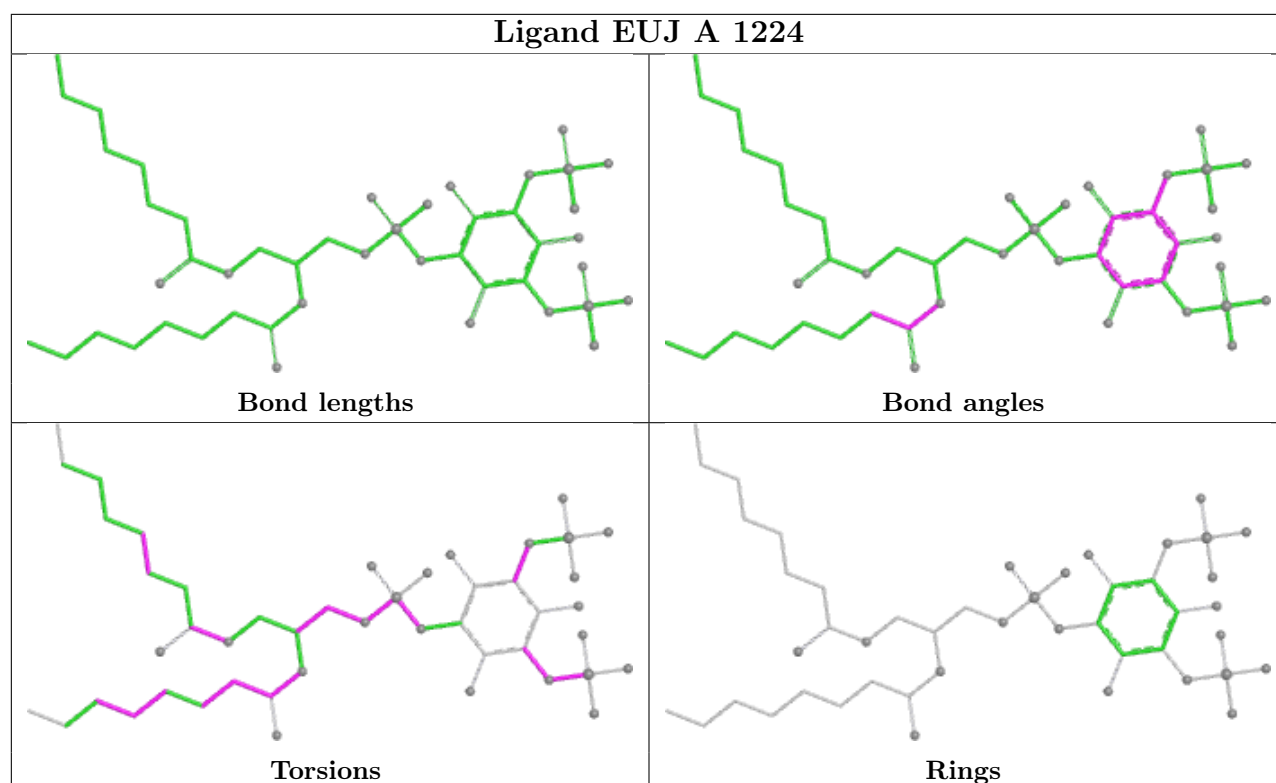
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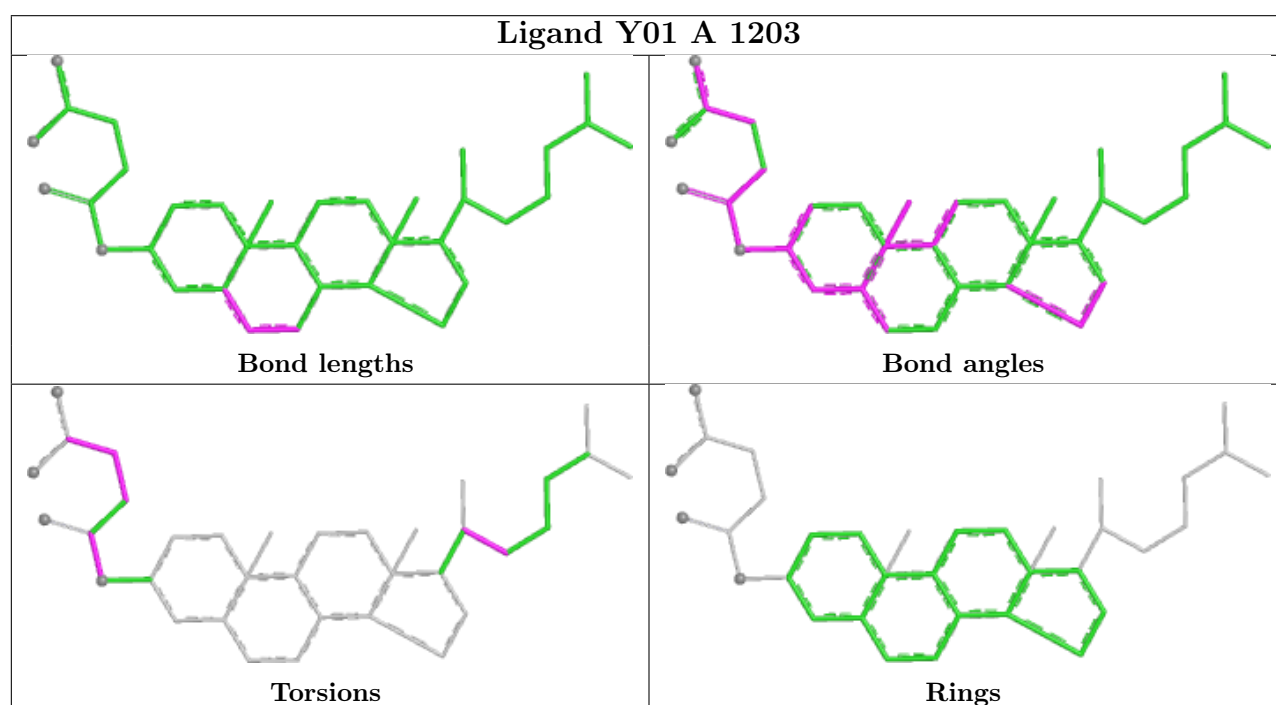
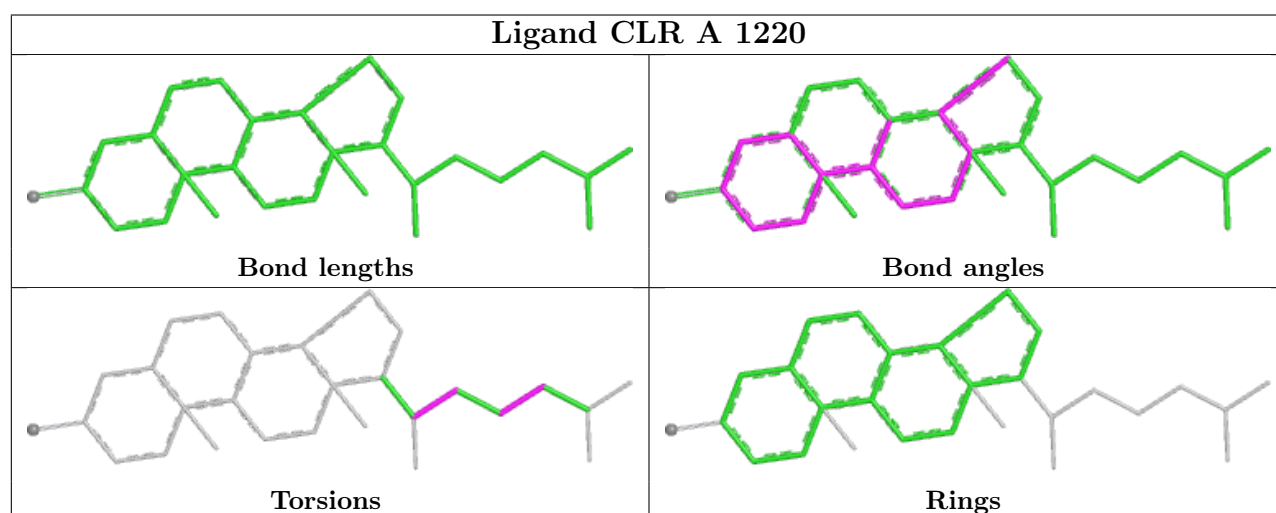
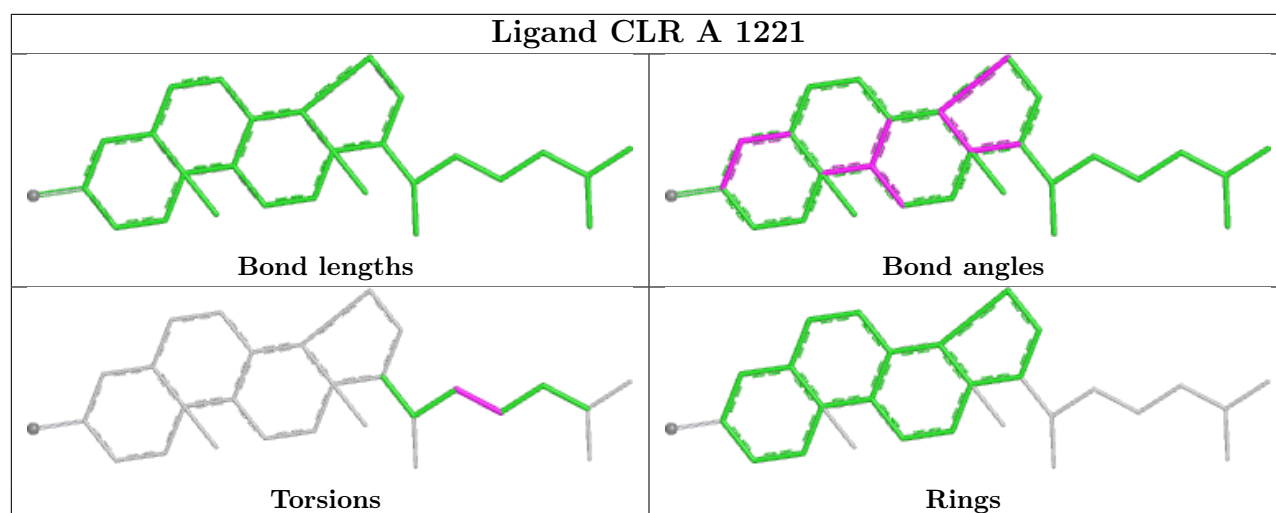
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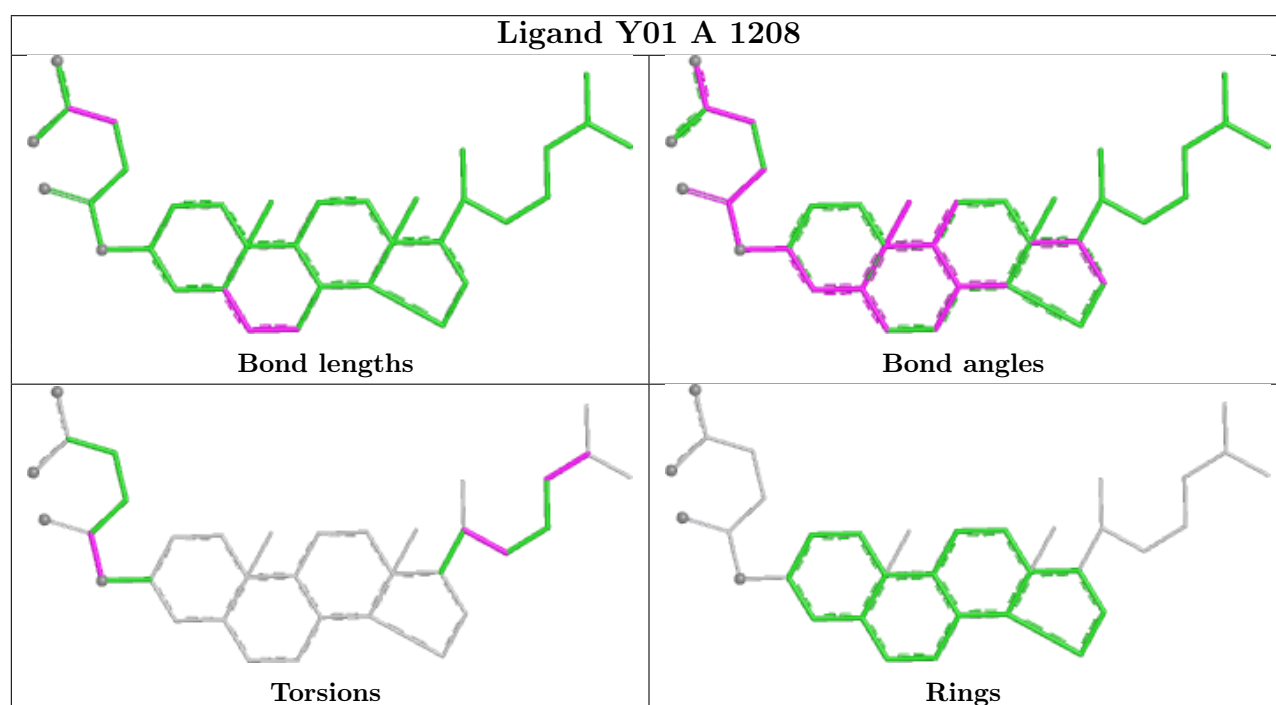
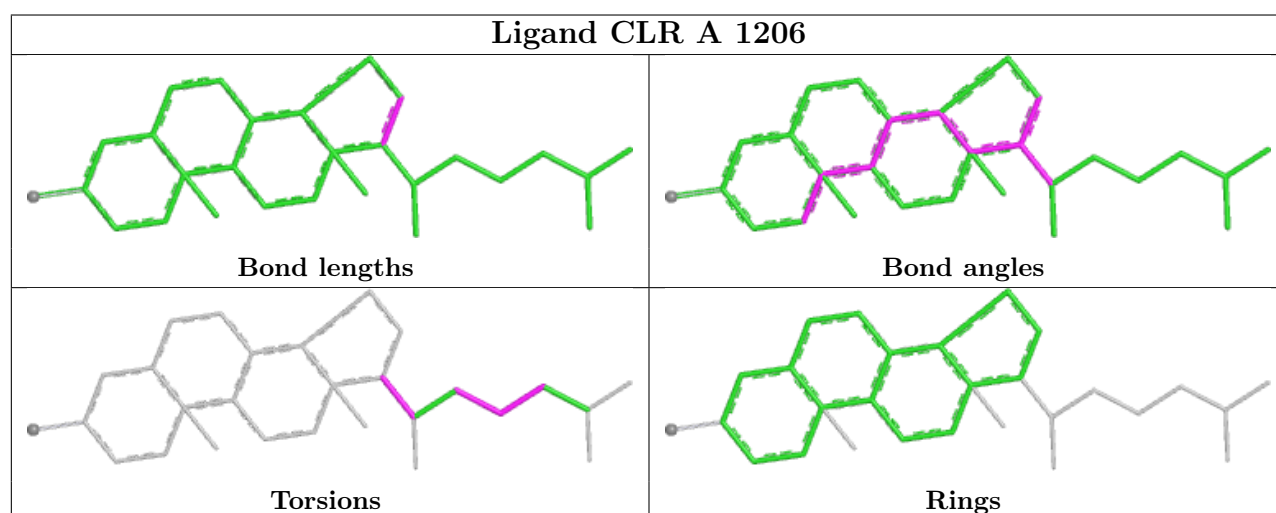
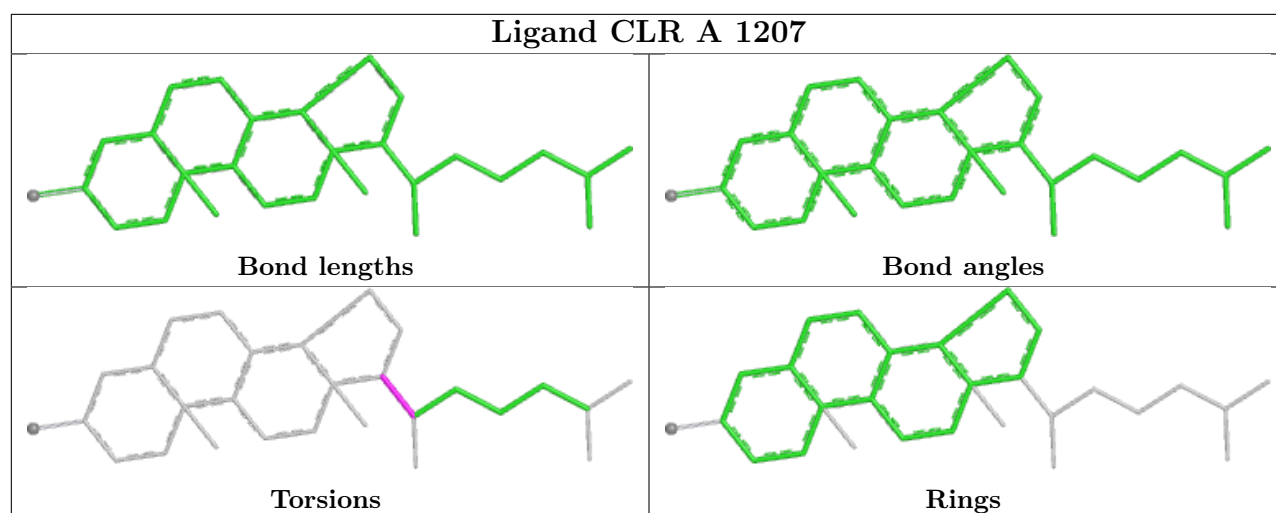
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1205	Y01	2	0
6	A	1220	CLR	1	0
6	A	1207	CLR	1	0
5	A	1204	LMT	1	0
11	A	1223	SPK	1	0

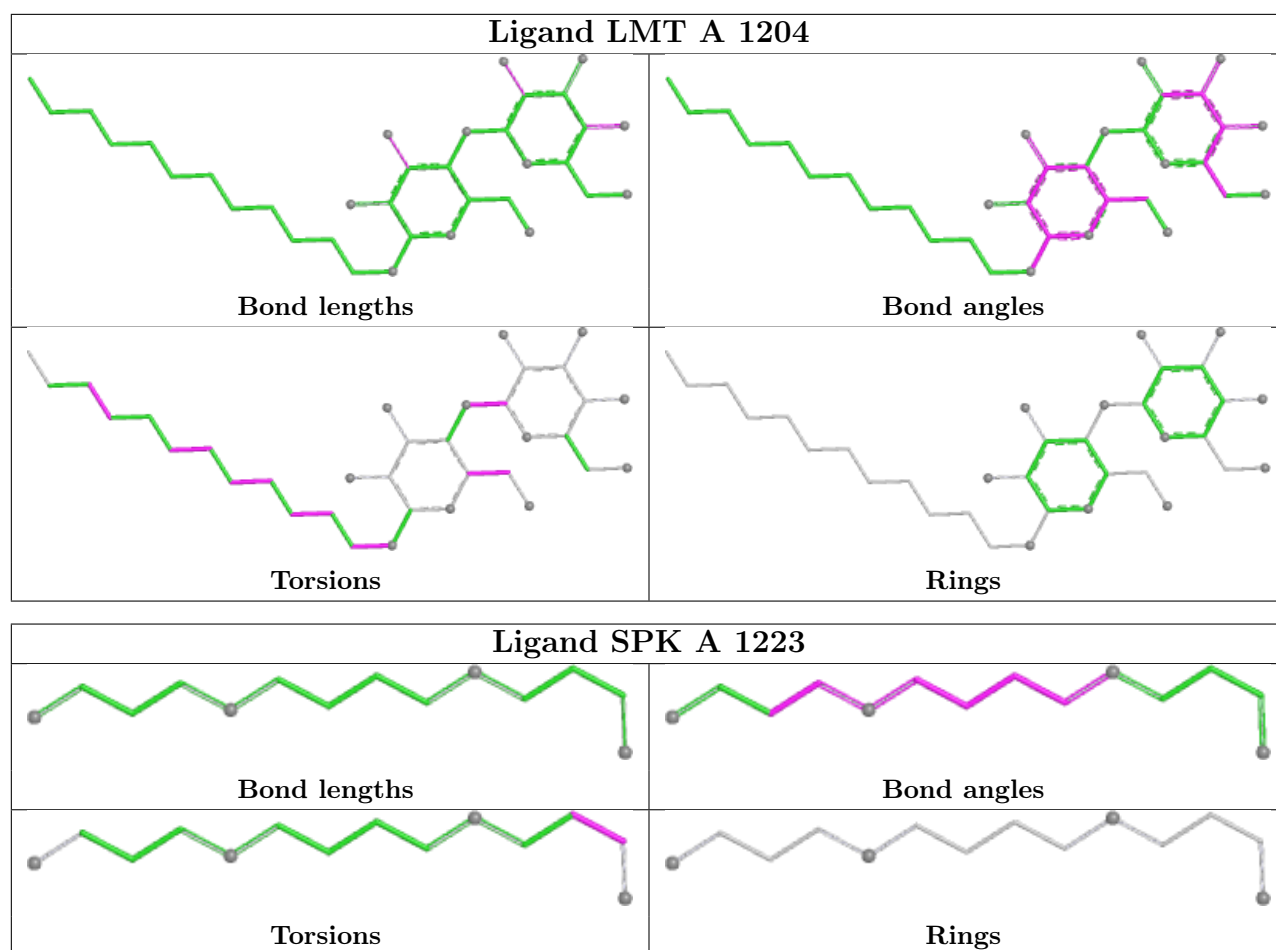
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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.

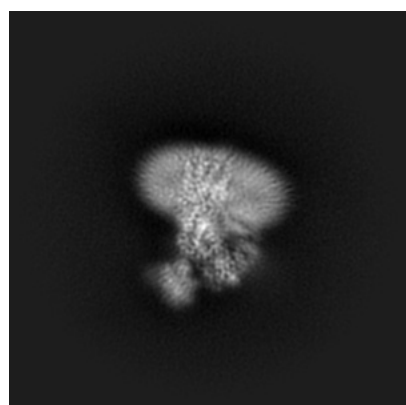
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23685. These allow visual inspection of the internal detail of the map and identification of artifacts.

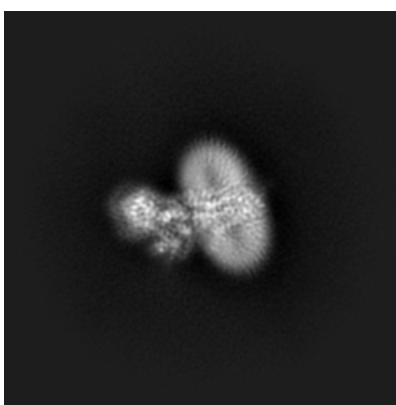
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

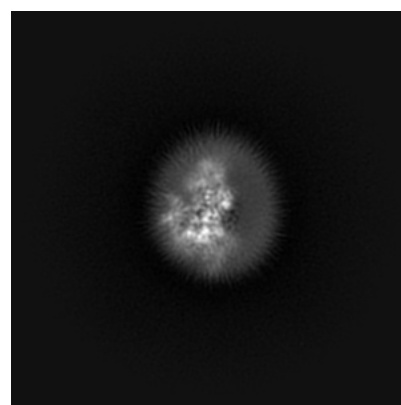
6.1.1 Primary map



X



Y

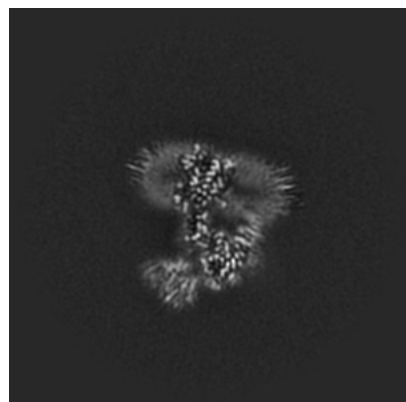


Z

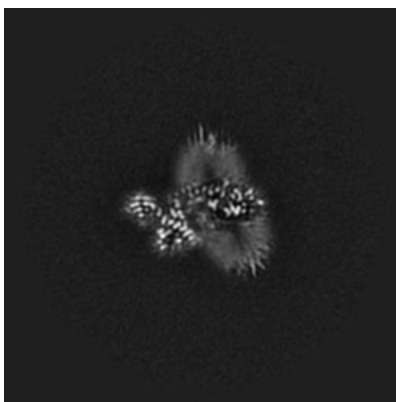
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

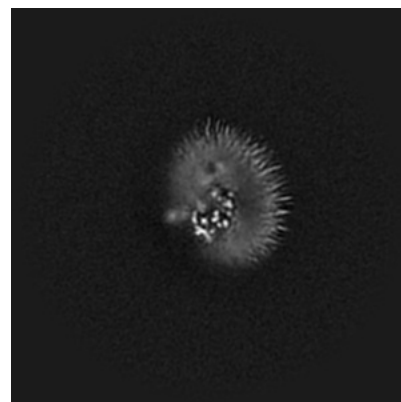
6.2.1 Primary map



X Index: 192



Y Index: 192

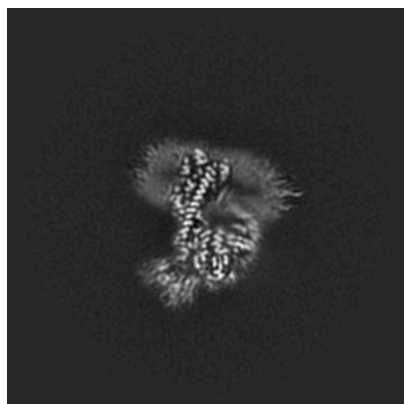


Z Index: 192

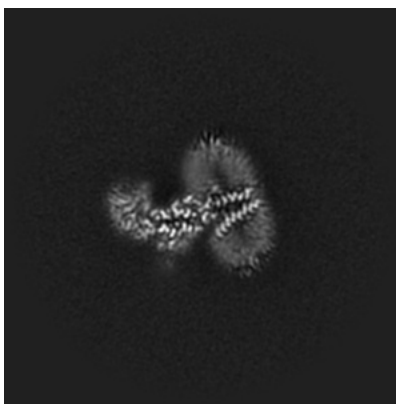
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

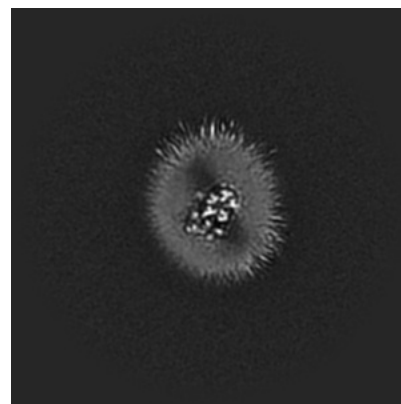
6.3.1 Primary map



X Index: 188



Y Index: 170



Z Index: 212

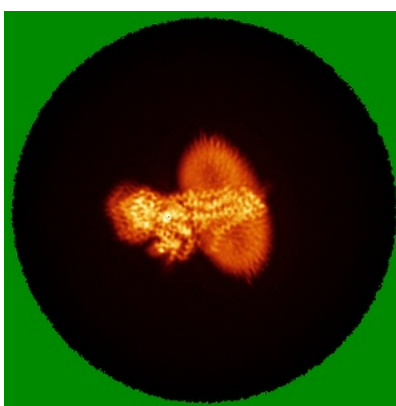
The images above show the largest variance slices of the map in three orthogonal directions.

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

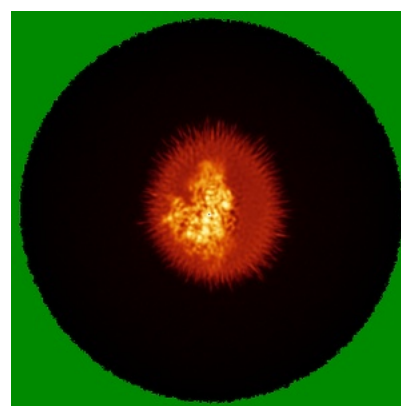
6.4.1 Primary map



X



Y

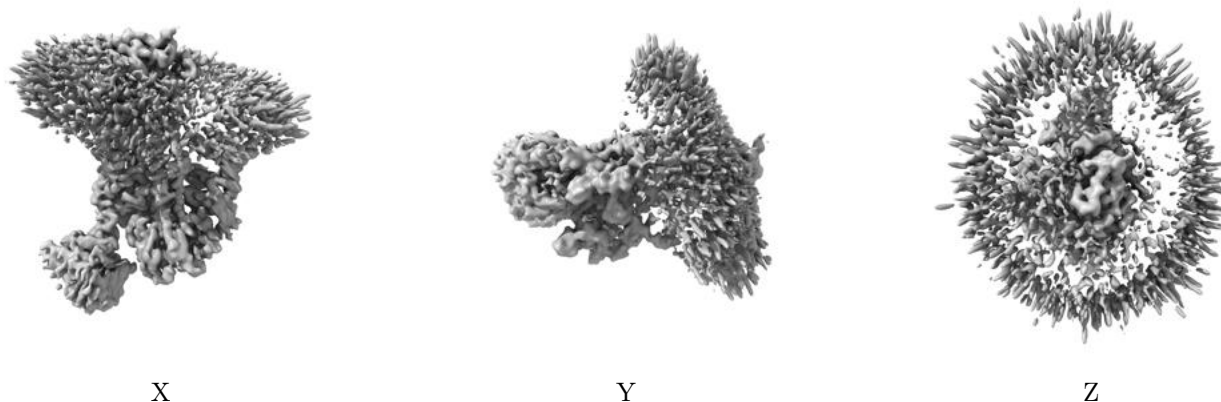


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

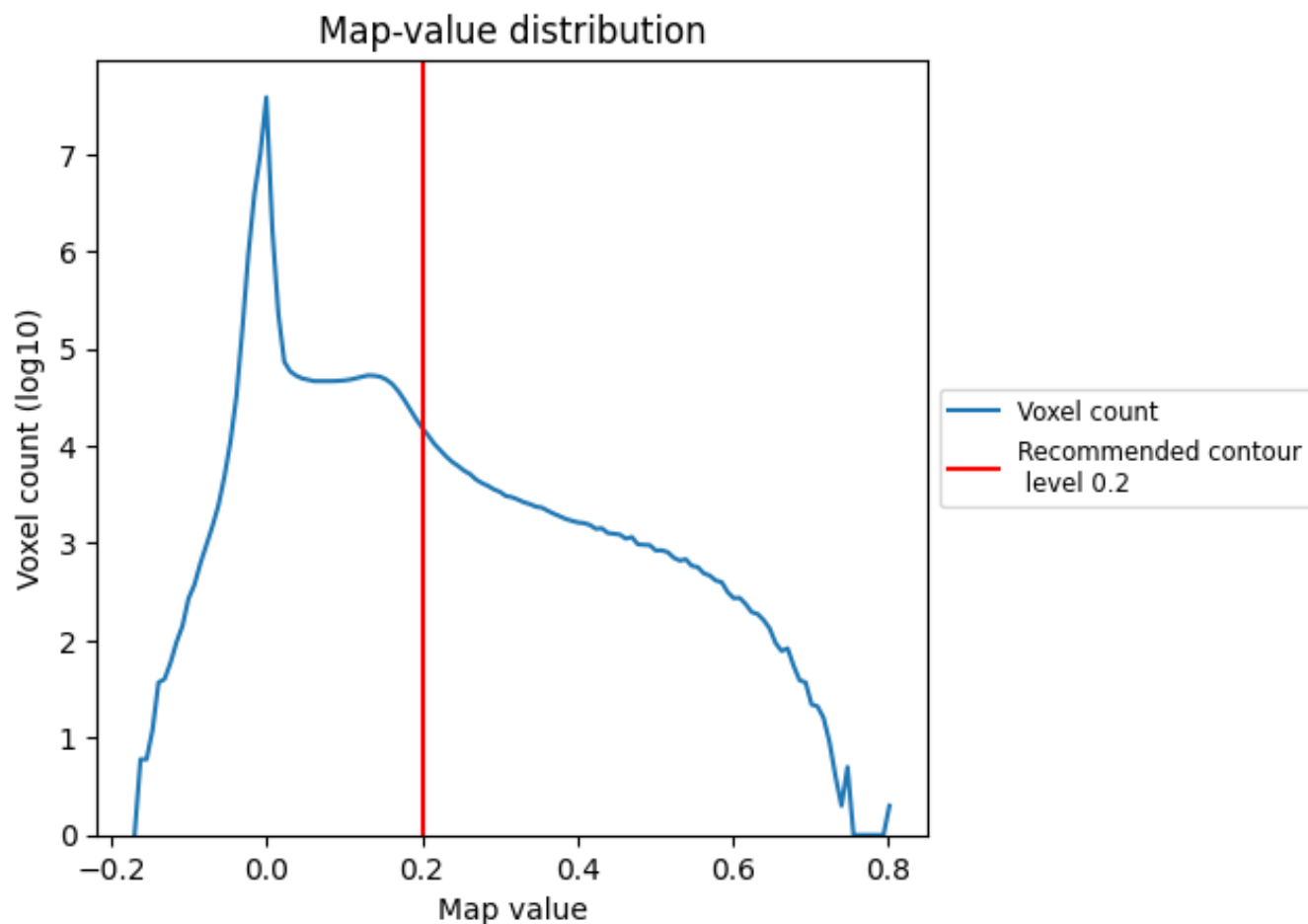
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

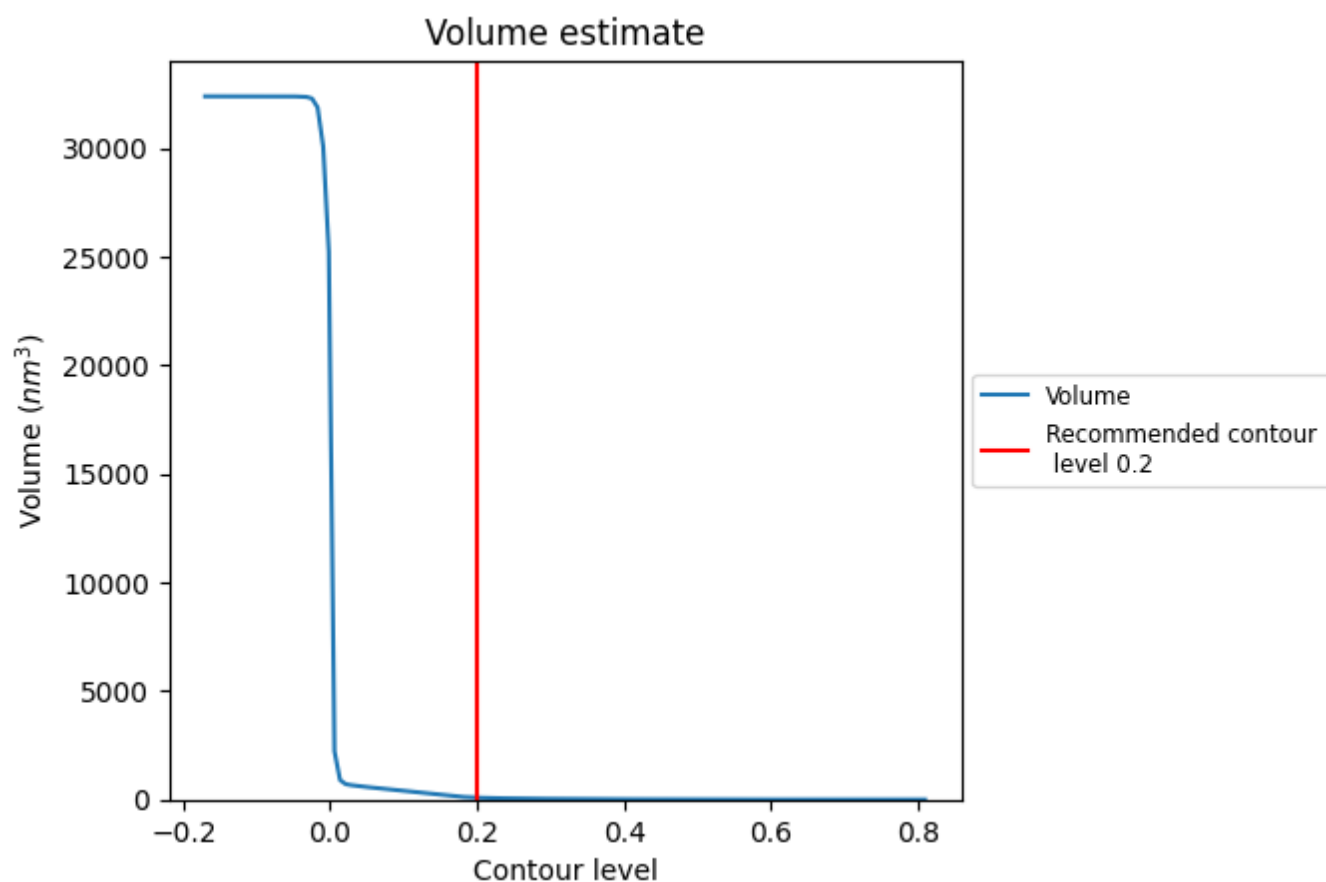
This section contains the results of statistical analysis of the map.

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.

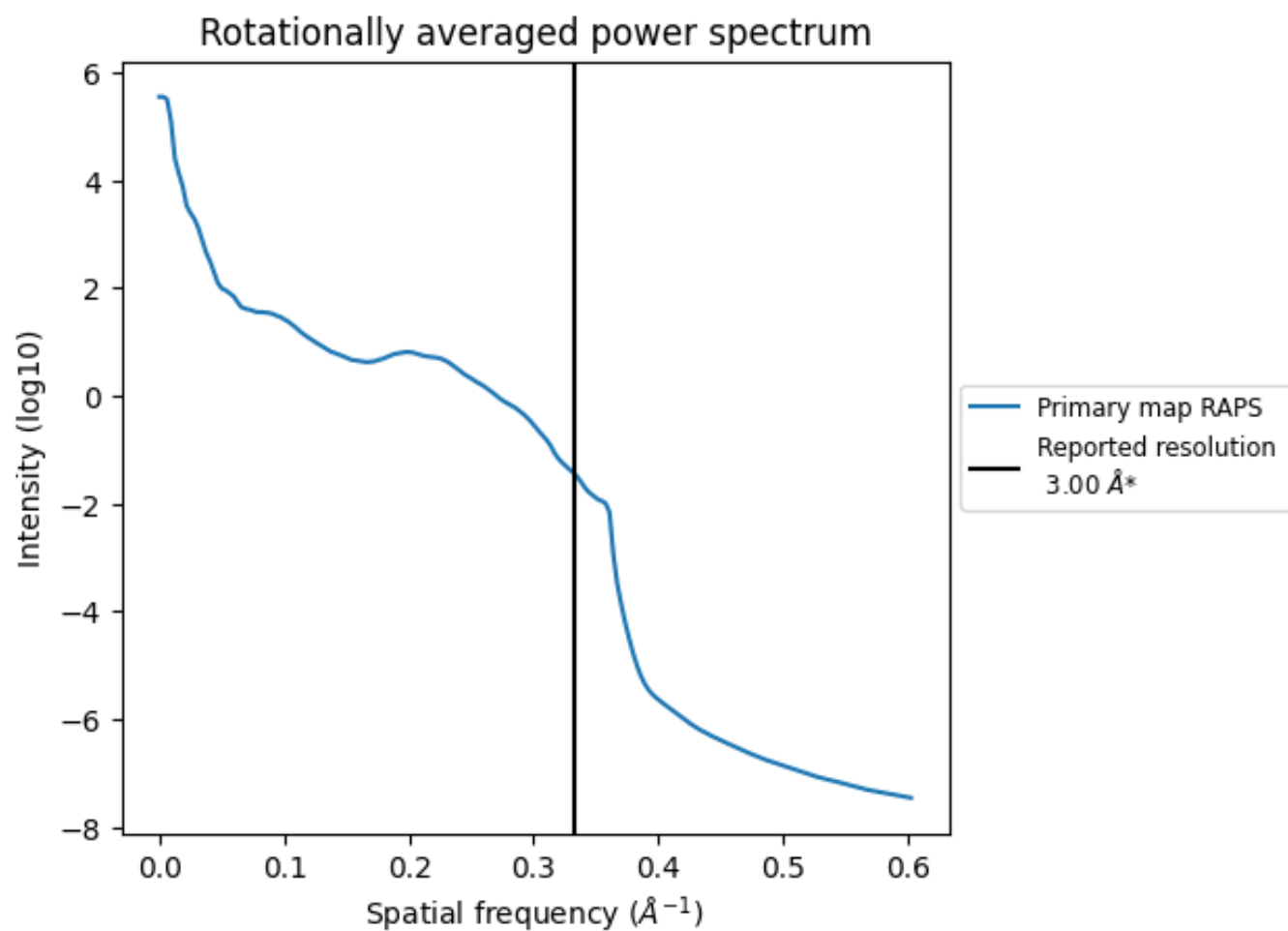
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88 nm^3 ; this corresponds to an approximate mass of 80 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 0.333 Å⁻¹

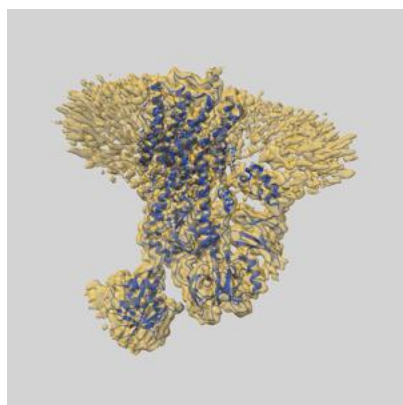
8 Fourier-Shell correlation

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

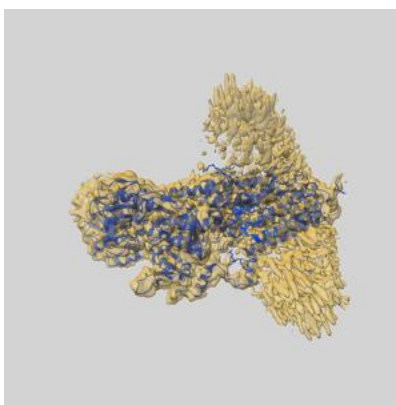
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23685 and PDB model 7M5Y. Per-residue inclusion information can be found in section 3 on page 10.

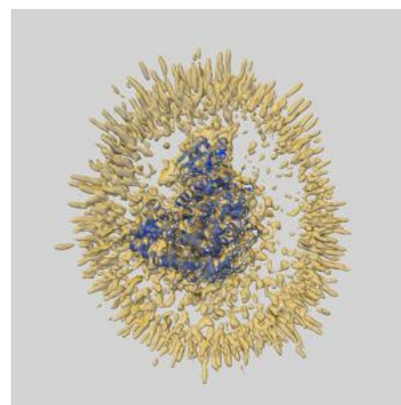
9.1 Map-model overlay [i](#)



X



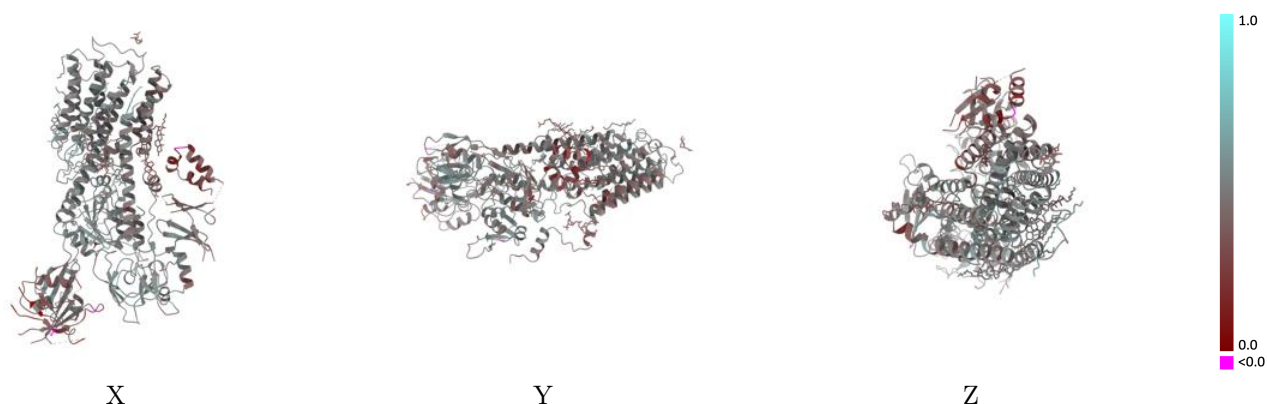
Y



Z

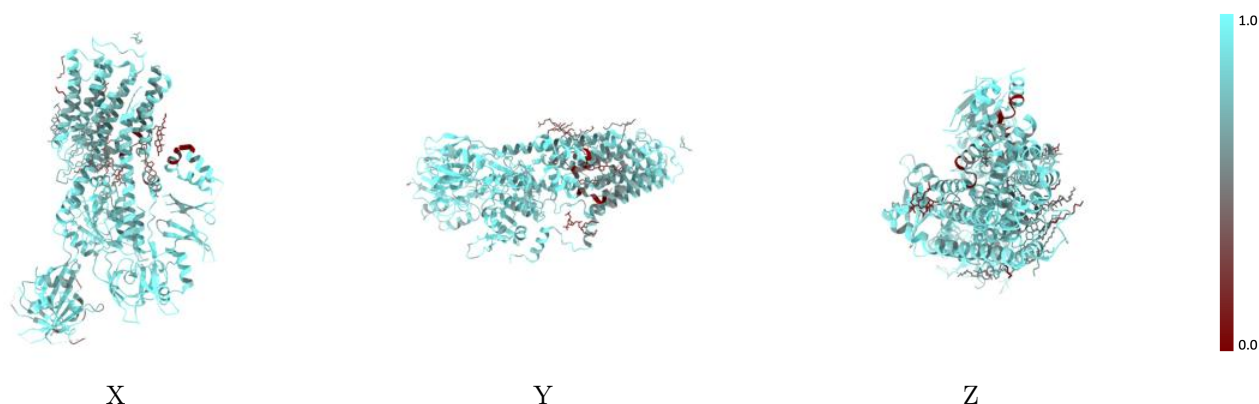
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



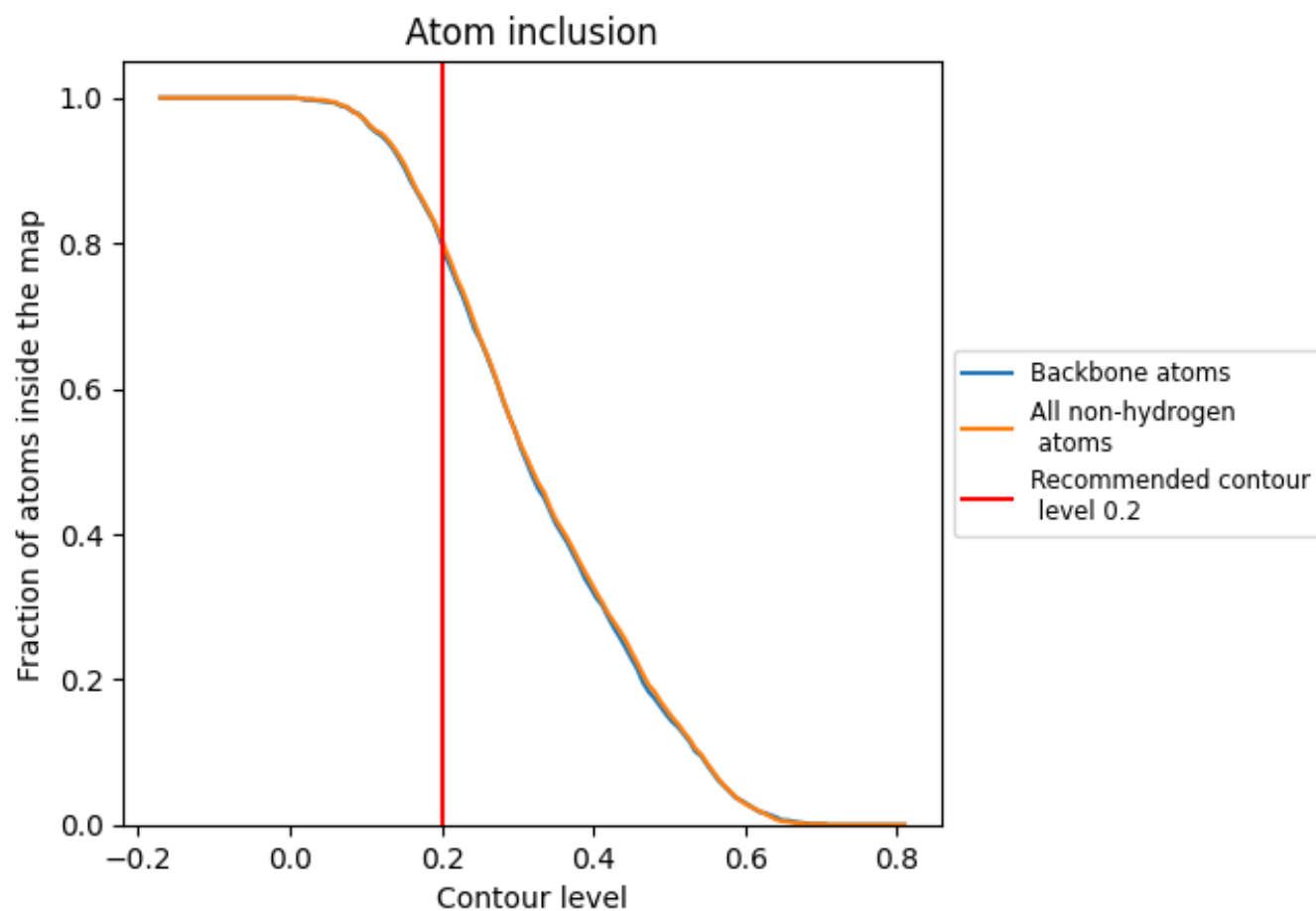
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 81% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8060	0.4520
A	0.8130	0.4520

