



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:34 AM UTC

PDB ID : 7TJ8 / pdb_00007tj8
EMDB ID : EMD-25919
Title : Cryo-EM structure of the human Nax channel in complex with beta3 solved in nanodiscs
Authors : Noland, C.L.; Kschonsak, M.; Ciferri, C.; Payandeh, J.
Deposited on : 2022-01-14
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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) : 2.49

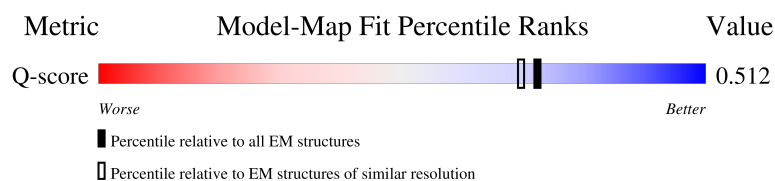
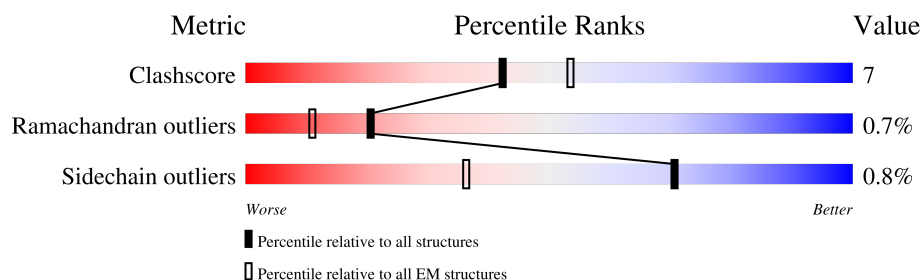
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1737	
2	B	215	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	POV	A	2402	-	X	-	-
4	POV	A	2403	-	X	-	-
4	POV	A	2408	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10551 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 Sodium channel protein type 7 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1080	Total	C	N	O	S	0	0
			8805	5898	1373	1456	78		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-54	MET	-	expression tag	UNP Q01118
A	-53	TRP	-	expression tag	UNP Q01118
A	-52	SER	-	expression tag	UNP Q01118
A	-51	HIS	-	expression tag	UNP Q01118
A	-50	PRO	-	expression tag	UNP Q01118
A	-49	GLN	-	expression tag	UNP Q01118
A	-48	PHE	-	expression tag	UNP Q01118
A	-47	GLU	-	expression tag	UNP Q01118
A	-46	LYS	-	expression tag	UNP Q01118
A	-45	GLY	-	expression tag	UNP Q01118
A	-44	GLY	-	expression tag	UNP Q01118
A	-43	GLY	-	expression tag	UNP Q01118
A	-42	SER	-	expression tag	UNP Q01118
A	-41	GLY	-	expression tag	UNP Q01118
A	-40	GLY	-	expression tag	UNP Q01118
A	-39	GLY	-	expression tag	UNP Q01118
A	-38	SER	-	expression tag	UNP Q01118
A	-37	GLY	-	expression tag	UNP Q01118
A	-36	GLY	-	expression tag	UNP Q01118
A	-35	SER	-	expression tag	UNP Q01118
A	-34	ALA	-	expression tag	UNP Q01118
A	-33	TRP	-	expression tag	UNP Q01118
A	-32	SER	-	expression tag	UNP Q01118
A	-31	HIS	-	expression tag	UNP Q01118
A	-30	PRO	-	expression tag	UNP Q01118
A	-29	GLN	-	expression tag	UNP Q01118
A	-28	PHE	-	expression tag	UNP Q01118
A	-27	GLU	-	expression tag	UNP Q01118

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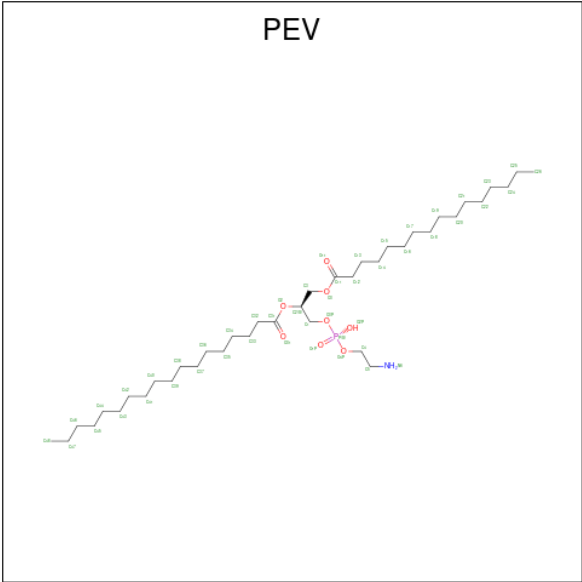
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	LYS	-	expression tag	UNP Q01118
A	-25	PHE	-	expression tag	UNP Q01118
A	-24	PHE	-	expression tag	UNP Q01118
A	-23	SER	-	expression tag	UNP Q01118
A	-22	PHE	-	expression tag	UNP Q01118
A	-21	PHE	-	expression tag	UNP Q01118
A	-20	ASP	-	expression tag	UNP Q01118
A	-19	TYR	-	expression tag	UNP Q01118
A	-18	LYS	-	expression tag	UNP Q01118
A	-17	ASP	-	expression tag	UNP Q01118
A	-16	ASP	-	expression tag	UNP Q01118
A	-15	ASP	-	expression tag	UNP Q01118
A	-14	ASP	-	expression tag	UNP Q01118
A	-13	LYS	-	expression tag	UNP Q01118
A	-12	GLY	-	expression tag	UNP Q01118
A	-11	GLY	-	expression tag	UNP Q01118
A	-10	SER	-	expression tag	UNP Q01118
A	-9	GLY	-	expression tag	UNP Q01118
A	-8	GLY	-	expression tag	UNP Q01118
A	-7	ASP	-	expression tag	UNP Q01118
A	-6	TYR	-	expression tag	UNP Q01118
A	-5	LYS	-	expression tag	UNP Q01118
A	-4	ASP	-	expression tag	UNP Q01118
A	-3	ASP	-	expression tag	UNP Q01118
A	-2	ASP	-	expression tag	UNP Q01118
A	-1	ASP	-	expression tag	UNP Q01118
A	0	LYS	-	expression tag	UNP Q01118

- Molecule 2 is a protein called Sodium channel subunit beta-3.

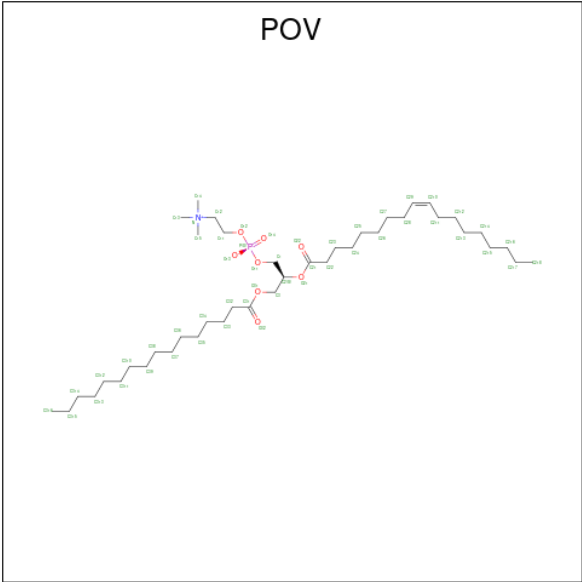
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1322	846	217	249	10		

- Molecule 3 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C₃₉H₇₈NO₈P).



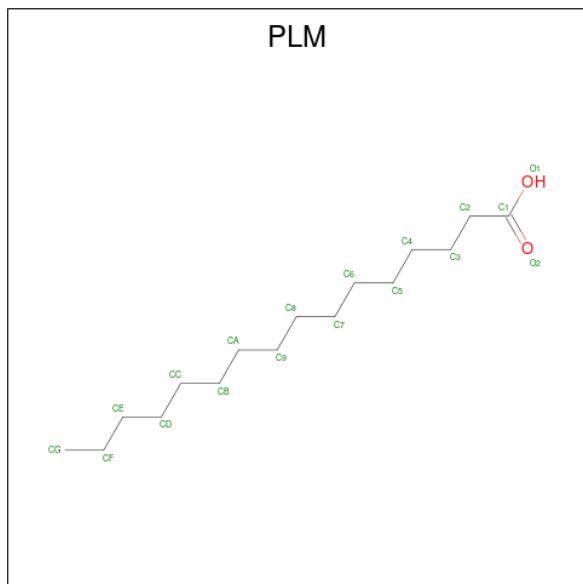
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
3	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
3	A	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 42 37 5	0
4	A	1	Total C 16 16	0
4	A	1	Total C O P 26 19 6 1	0

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



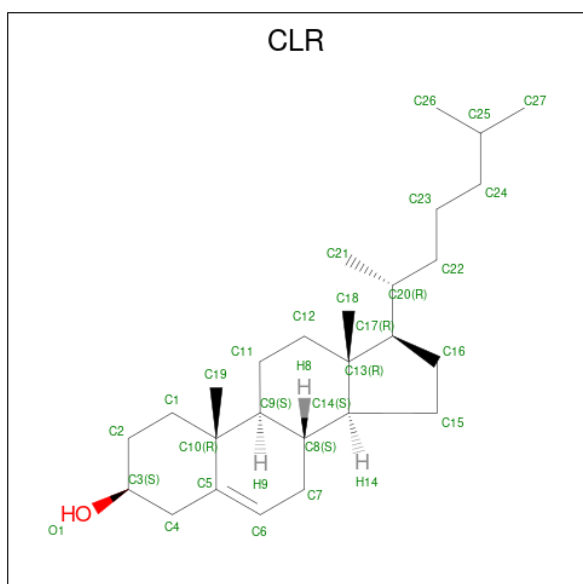
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 18 16 2	0
5	A	1	Total C O 18 16 2	0
5	A	1	Total C 10 10	0
5	A	1	Total C O 18 16 2	0
5	A	1	Total C 16 16	0
5	A	1	Total C O 15 13 2	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			28	27	1	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1238338	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 ($e^-/\text{\AA}^2$)	0.972	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.272	Depositor
Minimum map value	-0.610	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.161	Depositor
Map size (Å)	305.63998, 305.63998, 305.63998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.849, 0.849, 0.849	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, PEV, NAG, POV, PLM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/9040	0.43	0/12249
2	B	0.38	0/1350	0.87	9/1829 (0.5%)
All	All	0.21	0/10390	0.51	9/14078 (0.1%)

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
2	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	72	PHE	N-CA-C	11.40	130.06	111.37
2	B	66	PRO	CB-CA-C	-9.10	96.54	111.56
2	B	64	TYR	N-CA-C	8.14	121.18	111.33
2	B	63	PHE	CA-C-N	6.42	129.17	120.38
2	B	63	PHE	C-N-CA	6.42	129.17	120.38
2	B	84	VAL	O-C-N	-5.54	115.75	122.06
2	B	74	ILE	N-CA-CB	5.53	120.35	111.23
2	B	71	ASP	N-CA-C	5.47	119.22	112.54
2	B	63	PHE	N-CA-C	5.21	118.49	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	84	VAL	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	8805	0	9012	81	0
2	B	1322	0	1306	55	0
3	A	147	0	231	3	0
4	A	84	0	130	0	0
5	A	95	0	165	1	0
6	A	28	0	26	3	0
6	B	42	0	39	7	0
7	A	28	0	46	9	0
All	All	10551	0	10955	143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (143) 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)
2:B:95:ASN:ND2	6:B:302:NAG:C1	2.09	1.16
2:B:109:ASN:HD22	6:B:303:NAG:C1	1.65	1.10
2:B:109:ASN:ND2	6:B:303:NAG:C1	2.17	1.07
2:B:74:ILE:HG23	2:B:88:PHE:CE2	2.00	0.96
2:B:84:VAL:CG1	2:B:89:GLN:HB3	1.96	0.94
2:B:74:ILE:HG23	2:B:88:PHE:HE2	1.42	0.84
1:A:1252:ALA:O	1:A:1256:ILE:HG12	1.79	0.82
2:B:84:VAL:HG12	2:B:89:GLN:HB3	1.61	0.82
2:B:95:ASN:HD21	6:B:302:NAG:C1	1.93	0.80
2:B:66:PRO:HD2	2:B:66:PRO:O	1.82	0.79
2:B:64:TYR:O	2:B:65:ARG:HG3	1.85	0.77
2:B:95:ASN:O	2:B:95:ASN:OD1	2.04	0.75
7:A:2415:CLR:H263	7:A:2415:CLR:H222	1.67	0.74
2:B:84:VAL:HG11	2:B:89:GLN:HB3	1.70	0.72
2:B:69:GLY:O	2:B:72:PHE:HD1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:PRO:O	2:B:66:PRO:CD	2.39	0.71
2:B:72:PHE:O	2:B:73:LEU:HD12	1.90	0.70
2:B:95:ASN:CG	6:B:302:NAG:C1	2.65	0.69
1:A:1334:THR:HG22	1:A:1334:THR:O	1.90	0.69
2:B:69:GLY:O	2:B:72:PHE:CD1	2.46	0.68
2:B:74:ILE:HG23	2:B:88:PHE:CD2	2.31	0.66
1:A:1253:PHE:O	1:A:1257:VAL:HG23	1.98	0.63
2:B:74:ILE:CG2	2:B:88:PHE:HE2	2.12	0.63
1:A:556:ILE:HG22	1:A:556:ILE:O	1.99	0.62
1:A:1384:ILE:HG23	7:A:2415:CLR:H20	1.82	0.61
2:B:47:SER:O	2:B:124:ARG:NH2	2.34	0.61
2:B:85:GLU:HG2	2:B:85:GLU:O	2.00	0.60
2:B:74:ILE:CG2	2:B:88:PHE:CE2	2.82	0.60
1:A:322:CYS:SG	6:A:2412:NAG:H82	2.43	0.59
1:A:142:LYS:O	1:A:142:LYS:HG2	2.02	0.58
2:B:64:TYR:HB3	2:B:70:LYS:O	2.03	0.58
1:A:1331:LEU:HB2	1:A:1332:PRO:CD	2.34	0.57
2:B:74:ILE:HD13	2:B:88:PHE:CE2	2.39	0.57
1:A:108:ARG:O	1:A:111:THR:HG22	2.05	0.56
1:A:131:ASP:OD1	1:A:209:ARG:NH2	2.36	0.56
2:B:111:THR:O	2:B:145:VAL:HG11	2.06	0.56
1:A:148:GLU:OE1	1:A:195:ARG:NH2	2.33	0.56
1:A:144:ARG:N	1:A:145:PRO:HD2	2.21	0.56
2:B:66:PRO:CD	2:B:70:LYS:HA	2.35	0.55
2:B:42:LYS:HB2	6:B:302:NAG:H82	1.87	0.55
2:B:63:PHE:CD1	2:B:71:ASP:O	2.59	0.55
2:B:170:THR:O	2:B:170:THR:HG22	2.06	0.55
1:A:1334:THR:O	1:A:1334:THR:CG2	2.55	0.54
1:A:1330:CYS:O	1:A:1334:THR:N	2.37	0.54
5:A:2406:PLM:HG3	3:A:2413:PEV:H391	1.90	0.54
1:A:1384:ILE:CG2	7:A:2415:CLR:H222	2.38	0.53
7:A:2415:CLR:H121	7:A:2415:CLR:H212	1.91	0.53
2:B:64:TYR:CG	2:B:72:PHE:HB2	2.43	0.52
1:A:1445:ASN:OD1	1:A:1446:SER:N	2.42	0.52
1:A:947:SER:O	1:A:1033:ARG:NH1	2.43	0.52
1:A:509:LEU:HA	1:A:512:ILE:HG22	1.91	0.51
1:A:557:ILE:O	1:A:559:MET:N	2.44	0.51
1:A:138:THR:HG22	1:A:140:LEU:H	1.76	0.51
1:A:1335:VAL:HG12	1:A:1335:VAL:O	2.11	0.51
1:A:557:ILE:O	1:A:557:ILE:HG22	2.11	0.51
1:A:1030:LYS:O	1:A:1033:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:ILE:HD11	3:A:2401:PEV:H411	1.93	0.50
1:A:1183:LEU:HB3	1:A:1184:PRO:HD3	1.94	0.49
2:B:145:VAL:O	2:B:145:VAL:HG13	2.11	0.49
2:B:65:ARG:O	2:B:65:ARG:CG	2.61	0.49
1:A:542:LEU:C	1:A:542:LEU:HD23	2.37	0.49
2:B:138:THR:OG1	6:B:301:NAG:O7	2.29	0.49
1:A:1326:ILE:O	1:A:1330:CYS:SG	2.55	0.49
1:A:1330:CYS:O	1:A:1331:LEU:HG	2.13	0.48
1:A:1384:ILE:HG23	7:A:2415:CLR:C22	2.43	0.48
2:B:65:ARG:O	2:B:65:ARG:HD2	2.13	0.48
1:A:947:SER:HB2	1:A:1033:ARG:HH11	1.79	0.48
2:B:41:MET:SD	2:B:42:LYS:N	2.87	0.48
2:B:64:TYR:CB	2:B:70:LYS:O	2.62	0.48
1:A:1271:ASP:OD1	1:A:1272:THR:N	2.48	0.47
1:A:556:ILE:O	1:A:556:ILE:CG2	2.62	0.47
7:A:2415:CLR:H212	7:A:2415:CLR:H183	1.95	0.47
2:B:103:VAL:HG23	2:B:103:VAL:O	2.13	0.47
2:B:66:PRO:CG	2:B:70:LYS:HA	2.45	0.47
1:A:513:ILE:O	1:A:517:LEU:HD13	2.15	0.47
1:A:542:LEU:HD23	1:A:542:LEU:O	2.15	0.47
2:B:33:THR:C	2:B:143:LEU:HD12	2.39	0.47
2:B:65:ARG:N	2:B:66:PRO:HD3	2.29	0.47
1:A:349:LEU:HD21	1:A:358:LEU:HD23	1.98	0.46
1:A:1429:GLN:HA	1:A:1432:ILE:HG12	1.96	0.46
1:A:1384:ILE:HG23	7:A:2415:CLR:C20	2.45	0.46
7:A:2415:CLR:H263	7:A:2415:CLR:C22	2.39	0.46
1:A:144:ARG:N	1:A:145:PRO:CD	2.78	0.46
1:A:1488:VAL:O	1:A:1492:ILE:HG12	2.16	0.46
1:A:371:MET:HE3	1:A:374:PHE:HB2	1.96	0.46
1:A:545:ILE:HD11	1:A:602:ARG:HH21	1.80	0.46
1:A:573:ASP:OD1	1:A:605:LYS:NZ	2.42	0.45
1:A:1331:LEU:HD12	1:A:1332:PRO:N	2.32	0.45
1:A:1332:PRO:HB2	1:A:1336:GLY:HA3	1.99	0.45
1:A:933:ASN:C	1:A:933:ASN:OD1	2.59	0.45
1:A:1096:PHE:CE2	1:A:1116:MET:HE2	2.52	0.45
1:A:1287:ASN:O	1:A:1291:VAL:HG23	2.16	0.45
1:A:1268:MET:HE1	1:A:1350:LEU:HB2	1.97	0.44
2:B:65:ARG:CB	2:B:117:LEU:O	2.65	0.44
1:A:111:THR:HG23	1:A:112:ILE:N	2.33	0.44
1:A:568:GLY:O	1:A:571:ILE:HG12	2.17	0.44
1:A:683:ARG:HE	1:A:688:GLU:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:TYR:C	2:B:181:TYR:CD1	2.96	0.44
1:A:1016:ILE:O	1:A:1019:THR:OG1	2.26	0.44
2:B:102:ASP:OD1	2:B:103:VAL:N	2.51	0.44
1:A:193:ILE:O	1:A:197:SER:HB3	2.18	0.43
1:A:1330:CYS:HB2	1:A:1334:THR:OG1	2.18	0.43
1:A:1021:GLU:OE2	1:A:1021:GLU:N	2.50	0.43
1:A:1331:LEU:HD13	1:A:1332:PRO:HD2	2.00	0.43
1:A:264:LYS:HB2	1:A:324:LYS:HG3	2.00	0.43
1:A:1089:ASP:OD1	1:A:1089:ASP:C	2.61	0.43
1:A:344:PHE:CD2	3:A:2413:PEV:H452	2.53	0.43
2:B:64:TYR:HD2	2:B:66:PRO:HG3	1.84	0.43
1:A:1240:LEU:HD12	1:A:1240:LEU:O	2.18	0.43
1:A:997:SER:O	1:A:1002:ARG:NH2	2.51	0.42
2:B:66:PRO:HD3	2:B:70:LYS:HA	2.00	0.42
1:A:1330:CYS:O	1:A:1334:THR:HA	2.19	0.42
1:A:309:ASN:OD1	6:A:2412:NAG:H2	2.19	0.42
7:A:2415:CLR:H232	7:A:2415:CLR:H17	1.82	0.42
2:B:129:GLU:HA	2:B:129:GLU:OE2	2.18	0.42
1:A:552:MET:HG2	1:A:564:TYR:OH	2.20	0.42
1:A:1436:TRP:HZ3	1:A:1440:LEU:HD22	1.83	0.42
2:B:66:PRO:HD2	2:B:70:LYS:HG2	2.00	0.42
2:B:74:ILE:CD1	2:B:88:PHE:CE2	3.03	0.42
2:B:64:TYR:CD2	2:B:66:PRO:HG3	2.55	0.42
1:A:246:PHE:CZ	1:A:250:ILE:HD11	2.55	0.42
1:A:384:TYR:HD2	1:A:385:MET:HE2	1.84	0.42
1:A:1429:GLN:HB2	1:A:1434:ALA:HB3	2.01	0.41
2:B:127:GLU:HG3	2:B:127:GLU:O	2.20	0.41
2:B:65:ARG:HG2	2:B:118:TYR:HE1	1.84	0.41
1:A:217:ILE:HB	1:A:218:PRO:CD	2.50	0.41
1:A:1053:LYS:HD2	1:A:1199:HIS:CE1	2.55	0.41
2:B:153:PHE:O	2:B:156:VAL:HG12	2.20	0.41
2:B:84:VAL:HG12	2:B:89:GLN:OE1	2.20	0.41
1:A:141:PRO:O	1:A:142:LYS:HB3	2.20	0.41
1:A:973:MET:HA	1:A:976:THR:HG22	2.03	0.41
1:A:1023:LEU:HD13	1:A:1023:LEU:HA	1.92	0.41
1:A:1308:PHE:O	1:A:1308:PHE:CD2	2.73	0.41
1:A:124:ILE:HG21	1:A:158:GLU:OE2	2.20	0.41
6:A:2414:NAG:O3	6:A:2414:NAG:H82	2.21	0.41
1:A:553:ILE:HG22	1:A:553:ILE:O	2.21	0.41
1:A:708:PHE:O	1:A:712:VAL:HG23	2.21	0.40
1:A:1331:LEU:CB	1:A:1332:PRO:CD	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLY:O	1:A:689:TRP:N	2.54	0.40
1:A:706:ILE:HB	1:A:707:PRO:HD3	2.03	0.40
2:B:84:VAL:CG1	2:B:89:GLN:OE1	2.69	0.40
2:B:99:ASP:OD2	2:B:101:GLN:HB2	2.21	0.40
1:A:107:ILE:HG13	1:A:108:ARG:H	1.86	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	1066/1737 (61%)	1006 (94%)	56 (5%)	4 (0%)	30	62
2	B	160/215 (74%)	139 (87%)	17 (11%)	4 (2%)	4	27
All	All	1226/1952 (63%)	1145 (93%)	73 (6%)	8 (1%)	20	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1331	LEU
2	B	66	PRO
1	A	505	PRO
2	B	87	PRO
1	A	1328	GLY
2	B	74	ILE
2	B	86	SER
1	A	556	ILE

5.3.2 Protein sidechains ⓘ

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	974/1561 (62%)	967 (99%)	7 (1%)	76	83
2	B	150/195 (77%)	148 (99%)	2 (1%)	61	78
All	All	1124/1756 (64%)	1115 (99%)	9 (1%)	70	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	140	LEU
1	A	538	ASN
1	A	542	LEU
1	A	594	LEU
1	A	601	LEU
1	A	1023	LEU
2	B	73	LEU
2	B	101	GLN

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

Mol	Chain	Res	Type
1	A	232	HIS
1	A	560	HIS
1	A	702	GLN
1	A	1199	HIS
1	A	1287	ASN
1	A	1346	GLN
2	B	95	ASN
2	B	109	ASN

5.3.3 RNA ⓘ

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	PLM	A	2411	-	14,14,17	1.04	1 (7%)	14,14,17	0.96	2 (14%)
6	NAG	A	2412	-	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
5	PLM	A	2409	-	17,17,17	0.93	1 (5%)	17,17,17	0.74	2 (11%)
3	PEV	A	2401	-	48,48,48	2.24	12 (25%)	51,53,53	1.29	3 (5%)
4	POV	A	2408	-	25,25,51	3.21	18 (72%)	28,28,59	0.83	1 (3%)
3	PEV	A	2413	-	48,48,48	2.23	11 (22%)	51,53,53	1.04	2 (3%)
3	PEV	A	2405	-	48,48,48	2.24	11 (22%)	51,53,53	1.11	2 (3%)
5	PLM	A	2407	-	9,9,17	0.39	0	8,8,17	0.17	0
6	NAG	B	301	2	14,14,15	0.48	0	17,19,21	0.79	1 (5%)
4	POV	A	2403	-	15,15,51	2.74	13 (86%)	14,14,59	0.68	0
6	NAG	B	303	-	14,14,15	0.26	0	17,19,21	0.59	0
7	CLR	A	2415	-	31,31,31	0.77	0	48,48,48	1.23	4 (8%)
5	PLM	A	2406	-	17,17,17	0.93	1 (5%)	17,17,17	0.74	2 (11%)
5	PLM	A	2410	-	15,15,17	0.49	0	14,14,17	0.17	0
6	NAG	A	2414	1	14,14,15	0.51	0	17,19,21	0.73	0
6	NAG	B	302	-	14,14,15	0.39	0	17,19,21	2.06	2 (11%)
5	PLM	A	2404	-	17,17,17	0.94	1 (5%)	17,17,17	0.74	2 (11%)
4	POV	A	2402	-	41,41,51	2.88	32 (78%)	43,43,59	0.92	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PLM	A	2411	-	-	11/12/12/15	-
6	NAG	A	2412	-	-	0/6/23/26	0/1/1/1
5	PLM	A	2409	-	-	3/15/15/15	-
3	PEV	A	2401	-	-	26/52/52/52	-
4	POV	A	2408	-	-	12/24/24/55	-
3	PEV	A	2413	-	-	28/52/52/52	-
3	PEV	A	2405	-	-	24/52/52/52	-
5	PLM	A	2407	-	-	1/7/7/15	-
6	NAG	B	301	2	-	3/6/23/26	0/1/1/1
4	POV	A	2403	-	-	6/13/13/55	-
6	NAG	B	303	-	-	3/6/23/26	0/1/1/1
7	CLR	A	2415	-	-	1/10/68/68	0/4/4/4
5	PLM	A	2406	-	-	7/15/15/15	-
5	PLM	A	2410	-	-	8/13/13/15	-
6	NAG	A	2414	1	-	3/6/23/26	0/1/1/1
6	NAG	B	302	-	-	0/6/23/26	0/1/1/1
5	PLM	A	2404	-	-	3/15/15/15	-
4	POV	A	2402	-	-	21/43/43/55	-

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2408	POV	P-O14	8.09	1.75	1.50
4	A	2402	POV	O31-C31	6.11	1.51	1.33
4	A	2408	POV	O31-C31	6.07	1.51	1.33
4	A	2402	POV	O21-C21	5.91	1.51	1.34
4	A	2403	POV	C29-C210	5.80	1.64	1.31
4	A	2408	POV	P-O11	5.23	1.76	1.60
3	A	2413	PEV	O2-C2	-4.96	1.34	1.46
4	A	2408	POV	C32-C31	4.96	1.65	1.50
4	A	2402	POV	C32-C31	4.93	1.65	1.50
3	A	2401	PEV	O2-C2	-4.92	1.35	1.46
3	A	2405	PEV	O3-C11	4.89	1.47	1.33
3	A	2401	PEV	O2-C31	4.86	1.48	1.34
3	A	2413	PEV	O3-C11	4.82	1.47	1.33
3	A	2405	PEV	O2-C2	-4.78	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2405	PEV	O2-C31	4.74	1.47	1.34
3	A	2401	PEV	O3-C11	4.69	1.47	1.33
4	A	2402	POV	C22-C21	4.68	1.64	1.50
3	A	2413	PEV	O2-C31	4.67	1.47	1.34
4	A	2402	POV	C1-C2	4.21	1.61	1.51
3	A	2401	PEV	C12-C11	3.61	1.61	1.50
3	A	2405	PEV	C12-C11	3.58	1.61	1.50
3	A	2413	PEV	P-O3P	3.57	1.73	1.59
3	A	2405	PEV	P-O3P	3.57	1.73	1.59
3	A	2413	PEV	P-O4P	3.57	1.73	1.59
3	A	2405	PEV	P-O4P	3.57	1.73	1.59
3	A	2401	PEV	P-O3P	3.57	1.73	1.59
4	A	2402	POV	C3-C2	3.56	1.61	1.50
3	A	2401	PEV	C32-C31	3.56	1.61	1.50
3	A	2401	PEV	P-O4P	3.56	1.73	1.59
4	A	2402	POV	C23-C22	3.50	1.65	1.52
3	A	2413	PEV	C12-C11	3.48	1.60	1.50
3	A	2405	PEV	C32-C31	3.46	1.60	1.50
3	A	2413	PEV	C32-C31	3.43	1.60	1.50
4	A	2408	POV	C33-C32	3.32	1.64	1.52
4	A	2402	POV	C33-C32	3.31	1.64	1.52
4	A	2402	POV	C27-C28	3.04	1.65	1.52
5	A	2404	PLM	C2-C1	3.00	1.57	1.50
5	A	2411	PLM	C2-C1	2.99	1.57	1.50
5	A	2409	PLM	C2-C1	2.93	1.57	1.50
5	A	2406	PLM	C2-C1	2.92	1.57	1.50
4	A	2403	POV	C212-C211	2.91	1.64	1.52
4	A	2403	POV	C27-C28	2.88	1.64	1.52
4	A	2402	POV	C212-C211	2.67	1.63	1.52
3	A	2401	PEV	C5-C4	2.67	1.60	1.49
3	A	2413	PEV	C5-C4	2.66	1.60	1.49
3	A	2405	PEV	C5-C4	2.65	1.60	1.49
4	A	2402	POV	C24-C23	2.65	1.65	1.51
4	A	2402	POV	O31-C3	2.63	1.51	1.45
4	A	2403	POV	C28-C29	2.60	1.64	1.50
4	A	2408	POV	C2-C3	2.58	1.61	1.51
4	A	2402	POV	C36-C35	2.57	1.64	1.51
4	A	2408	POV	C38-C37	2.57	1.64	1.51
4	A	2402	POV	C27-C26	2.57	1.64	1.51
4	A	2402	POV	C38-C37	2.56	1.64	1.51
4	A	2408	POV	C36-C35	2.56	1.64	1.51
4	A	2402	POV	C25-C24	2.56	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2402	POV	C26-C25	2.55	1.64	1.51
4	A	2408	POV	C39-C310	2.54	1.64	1.51
4	A	2408	POV	C39-C38	2.53	1.64	1.51
4	A	2402	POV	C39-C310	2.53	1.64	1.51
4	A	2403	POV	C213-C212	2.52	1.64	1.51
4	A	2402	POV	C39-C38	2.52	1.64	1.51
4	A	2403	POV	C211-C210	2.51	1.63	1.50
4	A	2408	POV	C35-C34	2.49	1.64	1.51
4	A	2408	POV	C2-C1	2.49	1.61	1.51
4	A	2402	POV	C35-C34	2.49	1.64	1.51
4	A	2408	POV	C34-C33	2.48	1.64	1.51
4	A	2403	POV	C214-C213	2.47	1.64	1.51
4	A	2402	POV	C214-C213	2.47	1.64	1.51
4	A	2402	POV	C34-C33	2.45	1.64	1.51
4	A	2402	POV	C215-C214	2.44	1.63	1.51
4	A	2403	POV	C27-C26	2.43	1.63	1.51
4	A	2402	POV	C311-C310	2.42	1.63	1.51
3	A	2405	PEV	C13-C12	2.42	1.61	1.52
4	A	2402	POV	C37-C36	2.41	1.63	1.51
4	A	2408	POV	C37-C36	2.41	1.63	1.51
4	A	2408	POV	C311-C310	2.41	1.63	1.51
4	A	2403	POV	C25-C24	2.40	1.63	1.51
4	A	2408	POV	C313-C312	2.40	1.63	1.51
3	A	2401	PEV	C13-C12	2.39	1.60	1.52
4	A	2402	POV	C313-C312	2.38	1.63	1.51
3	A	2413	PEV	C13-C12	2.38	1.60	1.52
4	A	2403	POV	C26-C25	2.37	1.63	1.51
4	A	2408	POV	C312-C311	2.36	1.63	1.51
3	A	2401	PEV	P-O1P	2.35	1.59	1.50
3	A	2413	PEV	P-O1P	2.35	1.58	1.50
4	A	2402	POV	C312-C311	2.34	1.63	1.51
3	A	2405	PEV	P-O1P	2.33	1.58	1.50
4	A	2402	POV	C216-C215	2.32	1.63	1.51
4	A	2402	POV	C213-C212	2.32	1.63	1.51
4	A	2408	POV	C314-C313	2.31	1.63	1.51
3	A	2405	PEV	C33-C32	2.31	1.60	1.52
4	A	2403	POV	C24-C23	2.30	1.63	1.51
4	A	2402	POV	C314-C313	2.30	1.63	1.51
4	A	2402	POV	C211-C210	2.28	1.62	1.50
3	A	2413	PEV	C33-C32	2.26	1.60	1.52
3	A	2401	PEV	C33-C32	2.26	1.60	1.52
4	A	2402	POV	C28-C29	2.16	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2403	POV	C216-C215	2.06	1.65	1.50
4	A	2403	POV	C215-C214	2.06	1.64	1.51
3	A	2401	PEV	C35-C36	2.06	1.62	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	302	NAG	O5-C1-C2	-7.46	99.74	111.29
3	A	2401	PEV	O2-C31-C32	5.82	124.08	111.48
3	A	2413	PEV	O2-C31-C32	3.99	120.11	111.48
4	A	2402	POV	O21-C21-C22	3.82	119.75	111.48
7	A	2415	CLR	C13-C17-C20	-3.80	113.63	119.50
3	A	2405	PEV	O2-C31-C32	3.52	119.09	111.48
3	A	2405	PEV	O3-C11-C12	3.25	121.75	111.83
6	A	2412	NAG	C1-C2-N2	3.25	115.56	110.43
7	A	2415	CLR	C17-C13-C14	2.92	103.45	100.10
7	A	2415	CLR	C13-C14-C8	-2.81	110.42	114.41
7	A	2415	CLR	C11-C12-C13	-2.77	108.07	112.74
4	A	2408	POV	O31-C31-C32	2.74	120.19	111.83
5	A	2411	PLM	O2-C1-C2	-2.71	114.51	123.09
6	B	302	NAG	C1-C2-N2	2.68	114.65	110.43
3	A	2401	PEV	O3-C11-C12	2.51	119.49	111.83
4	A	2402	POV	O31-C31-C32	2.46	119.32	111.83
3	A	2401	PEV	O2-C31-O31	-2.44	118.00	123.70
3	A	2413	PEV	O3-C11-C12	2.28	118.80	111.83
6	B	301	NAG	C1-O5-C5	2.20	115.13	112.19
5	A	2409	PLM	O1-C1-O2	2.15	128.85	123.33
5	A	2404	PLM	O1-C1-O2	2.14	128.82	123.33
5	A	2406	PLM	O1-C1-O2	2.13	128.82	123.33
5	A	2411	PLM	O1-C1-O2	2.13	128.80	123.33
5	A	2406	PLM	O2-C1-C2	-2.05	116.58	123.09
5	A	2404	PLM	O2-C1-C2	-2.04	116.62	123.09
5	A	2409	PLM	O2-C1-C2	-2.04	116.62	123.09

There are no chirality outliers.

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2401	PEV	C32-C31-O2-C2
3	A	2401	PEV	O31-C31-O2-C2
3	A	2401	PEV	O4P-C4-C5-N6
3	A	2405	PEV	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
3	A	2405	PEV	C4-O4P-P-O1P
3	A	2405	PEV	C4-O4P-P-O2P
3	A	2405	PEV	O4P-C4-C5-N6
3	A	2413	PEV	C32-C31-O2-C2
3	A	2413	PEV	C1-O3P-P-O2P
3	A	2413	PEV	C1-O3P-P-O4P
3	A	2413	PEV	C4-O4P-P-O3P
3	A	2413	PEV	C4-O4P-P-O1P
3	A	2413	PEV	C4-O4P-P-O2P
4	A	2402	POV	O11-C1-C2-C3
4	A	2402	POV	O11-C1-C2-O21
4	A	2402	POV	C22-C21-O21-C2
6	B	301	NAG	C1-C2-N2-C7
3	A	2405	PEV	O11-C11-O3-C3
3	A	2405	PEV	C12-C11-O3-C3
3	A	2401	PEV	O11-C11-O3-C3
3	A	2413	PEV	O31-C31-O2-C2
3	A	2401	PEV	C12-C11-O3-C3
4	A	2402	POV	O22-C21-O21-C2
6	B	301	NAG	O5-C5-C6-O6
4	A	2408	POV	C32-C31-O31-C3
3	A	2401	PEV	C34-C35-C36-C37
4	A	2408	POV	O32-C31-O31-C3
3	A	2413	PEV	C43-C44-C45-C46
6	A	2414	NAG	C8-C7-N2-C2
6	A	2414	NAG	O7-C7-N2-C2
6	B	303	NAG	C8-C7-N2-C2
6	B	303	NAG	O7-C7-N2-C2
4	A	2408	POV	C31-C32-C33-C34
5	A	2411	PLM	C1-C2-C3-C4
3	A	2413	PEV	C31-C32-C33-C34
4	A	2402	POV	C31-C32-C33-C34
6	B	301	NAG	C4-C5-C6-O6
4	A	2408	POV	C1-C2-C3-O31
3	A	2413	PEV	C14-C15-C16-C17
3	A	2401	PEV	C16-C17-C18-C19
3	A	2405	PEV	C20-C21-C22-C23
4	A	2403	POV	C211-C210-C29-C28
3	A	2405	PEV	C12-C13-C14-C15
4	A	2408	POV	C37-C38-C39-C310
3	A	2401	PEV	C15-C16-C17-C18
4	A	2403	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	A	2405	PEV	C38-C39-C40-C41
3	A	2413	PEV	C16-C17-C18-C19
4	A	2403	POV	C24-C25-C26-C27
5	A	2410	PLM	C7-C8-C9-CA
5	A	2411	PLM	C6-C7-C8-C9
4	A	2402	POV	C214-C215-C216-C217
3	A	2401	PEV	C37-C38-C39-C40
4	A	2402	POV	C24-C25-C26-C27
5	A	2410	PLM	C9-CA-CB-CC
3	A	2413	PEV	C12-C13-C14-C15
3	A	2401	PEV	C18-C19-C20-C21
3	A	2401	PEV	C22-C23-C24-C25
3	A	2401	PEV	C20-C21-C22-C23
3	A	2405	PEV	C43-C44-C45-C46
4	A	2402	POV	C212-C213-C214-C215
4	A	2402	POV	C213-C214-C215-C216
3	A	2405	PEV	C40-C41-C42-C43
5	A	2411	PLM	C7-C8-C9-CA
3	A	2405	PEV	C13-C14-C15-C16
3	A	2413	PEV	C20-C21-C22-C23
3	A	2405	PEV	C33-C34-C35-C36
3	A	2405	PEV	C32-C33-C34-C35
3	A	2401	PEV	C17-C18-C19-C20
3	A	2401	PEV	C32-C33-C34-C35
4	A	2408	POV	C35-C36-C37-C38
3	A	2413	PEV	C35-C36-C37-C38
5	A	2410	PLM	CB-CC-CD-CE
3	A	2401	PEV	C39-C40-C41-C42
6	B	303	NAG	O5-C5-C6-O6
3	A	2413	PEV	C38-C39-C40-C41
3	A	2413	PEV	C40-C41-C42-C43
3	A	2413	PEV	O3P-C1-C2-C3
5	A	2411	PLM	C3-C4-C5-C6
3	A	2401	PEV	C13-C14-C15-C16
4	A	2402	POV	C32-C31-O31-C3
5	A	2411	PLM	C5-C6-C7-C8
3	A	2405	PEV	C18-C19-C20-C21
3	A	2405	PEV	C35-C36-C37-C38
4	A	2408	POV	C33-C34-C35-C36
3	A	2405	PEV	C45-C46-C47-C48
4	A	2402	POV	O32-C31-O31-C3
3	A	2405	PEV	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	A	2408	POV	C313-C314-C315-C316
4	A	2408	POV	C32-C33-C34-C35
5	A	2411	PLM	C8-C9-CA-CB
5	A	2406	PLM	C8-C9-CA-CB
3	A	2405	PEV	C41-C42-C43-C44
3	A	2413	PEV	C45-C46-C47-C48
3	A	2401	PEV	O3P-C1-C2-C3
3	A	2401	PEV	C14-C15-C16-C17
4	A	2402	POV	C33-C34-C35-C36
3	A	2413	PEV	C39-C40-C41-C42
5	A	2410	PLM	C1-C2-C3-C4
3	A	2401	PEV	C35-C36-C37-C38
3	A	2413	PEV	C23-C24-C25-C26
3	A	2413	PEV	C19-C20-C21-C22
5	A	2410	PLM	CD-CE-CF-CG
3	A	2401	PEV	O3P-C1-C2-O2
3	A	2413	PEV	C44-C45-C46-C47
5	A	2410	PLM	C2-C3-C4-C5
4	A	2402	POV	C215-C216-C217-C218
4	A	2402	POV	C210-C211-C212-C213
3	A	2413	PEV	O3P-C1-C2-O2
3	A	2413	PEV	C21-C22-C23-C24
3	A	2405	PEV	C5-C4-O4P-P
3	A	2401	PEV	O2-C2-C3-O3
5	A	2410	PLM	CC-CD-CE-CF
5	A	2411	PLM	CA-CB-CC-CD
4	A	2408	POV	O11-C1-C2-C3
3	A	2413	PEV	C15-C16-C17-C18
5	A	2411	PLM	C2-C3-C4-C5
3	A	2401	PEV	C19-C20-C21-C22
3	A	2401	PEV	C1-C2-C3-O3
3	A	2405	PEV	C1-C2-O2-C31
3	A	2413	PEV	C3-C2-O2-C31
4	A	2402	POV	C3-C2-O21-C21
3	A	2413	PEV	C13-C14-C15-C16
4	A	2403	POV	C213-C214-C215-C216
4	A	2403	POV	C210-C211-C212-C213
3	A	2401	PEV	C42-C43-C44-C45
3	A	2401	PEV	C41-C42-C43-C44
5	A	2406	PLM	C7-C8-C9-CA
3	A	2401	PEV	C40-C41-C42-C43
5	A	2407	PLM	C9-CA-CB-CC

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Mol	Chain	Res	Type	Atoms
4	A	2403	POV	C25-C26-C27-C28
4	A	2402	POV	C35-C36-C37-C38
4	A	2402	POV	C23-C24-C25-C26
4	A	2408	POV	C39-C310-C311-C312
7	A	2415	CLR	C22-C23-C24-C25
5	A	2406	PLM	C9-CA-CB-CC
4	A	2402	POV	C26-C27-C28-C29
5	A	2409	PLM	C3-C4-C5-C6
3	A	2405	PEV	O3P-C1-C2-C3
5	A	2406	PLM	O1-C1-C2-C3
5	A	2411	PLM	C4-C5-C6-C7
5	A	2404	PLM	O2-C1-C2-C3
5	A	2409	PLM	O1-C1-C2-C3
3	A	2405	PEV	O3P-C1-C2-O2
5	A	2406	PLM	O2-C1-C2-C3
5	A	2410	PLM	C8-C9-CA-CB
3	A	2405	PEV	C36-C37-C38-C39
3	A	2413	PEV	O2-C2-C3-O3
4	A	2402	POV	C22-C23-C24-C25
5	A	2409	PLM	O2-C1-C2-C3
5	A	2404	PLM	O1-C1-C2-C3
6	A	2414	NAG	O5-C5-C6-O6
4	A	2408	POV	C311-C310-C39-C38
4	A	2402	POV	O31-C31-C32-C33
5	A	2404	PLM	C5-C6-C7-C8
5	A	2406	PLM	C3-C4-C5-C6
5	A	2411	PLM	O2-C1-C2-C3
5	A	2406	PLM	C2-C3-C4-C5
5	A	2411	PLM	O1-C1-C2-C3
4	A	2402	POV	O32-C31-C32-C33

There are no ring outliers.

9 monomers are involved in 22 short contacts:

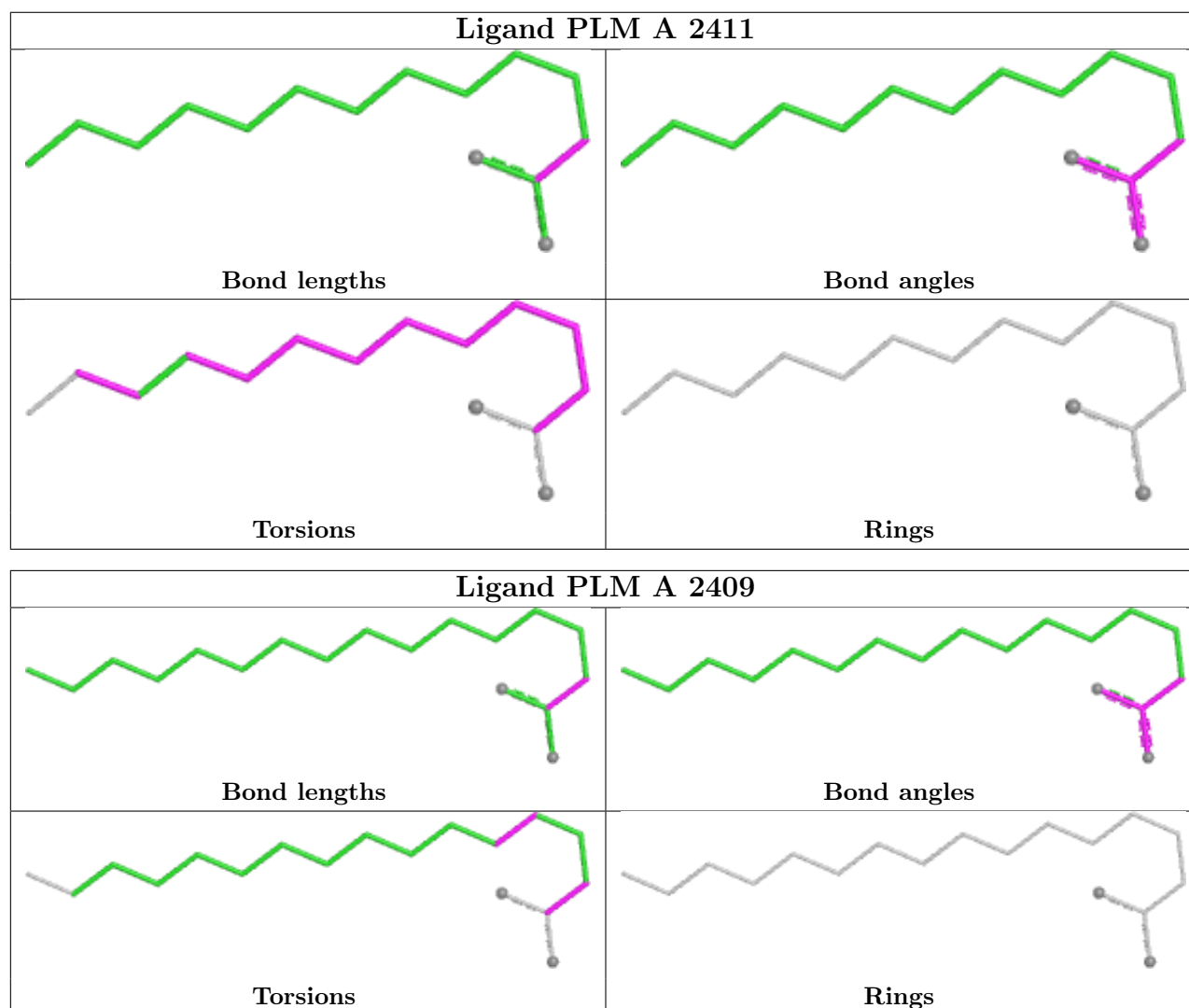
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2412	NAG	2	0
3	A	2401	PEV	1	0
3	A	2413	PEV	2	0
6	B	301	NAG	1	0
6	B	303	NAG	2	0
7	A	2415	CLR	9	0
5	A	2406	PLM	1	0

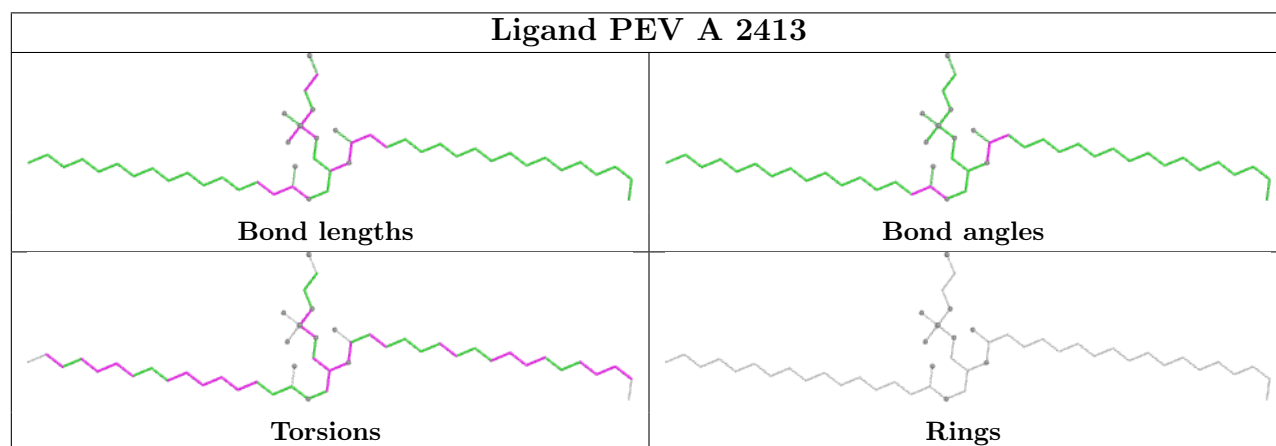
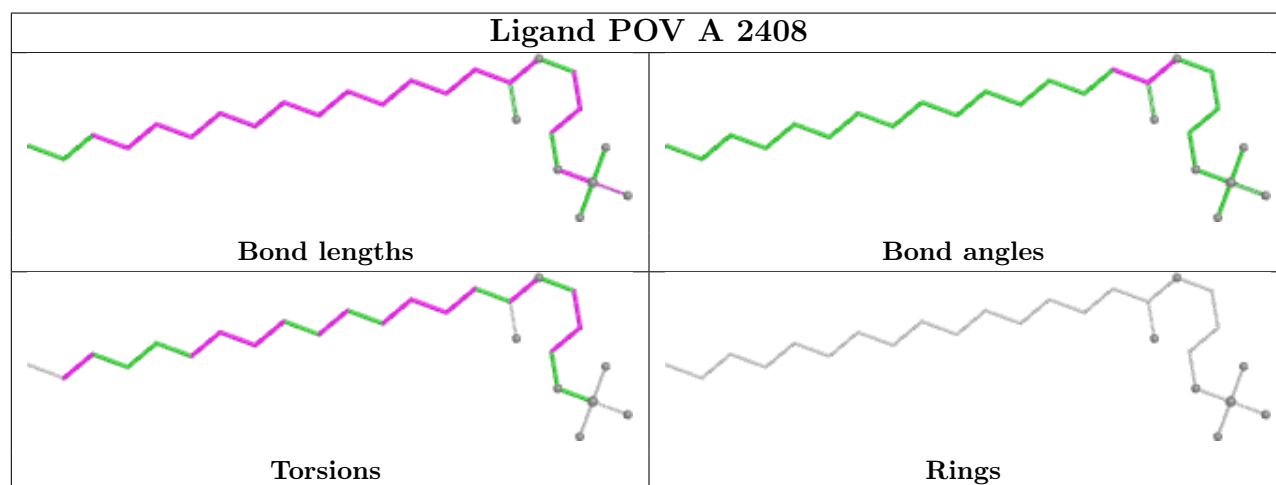
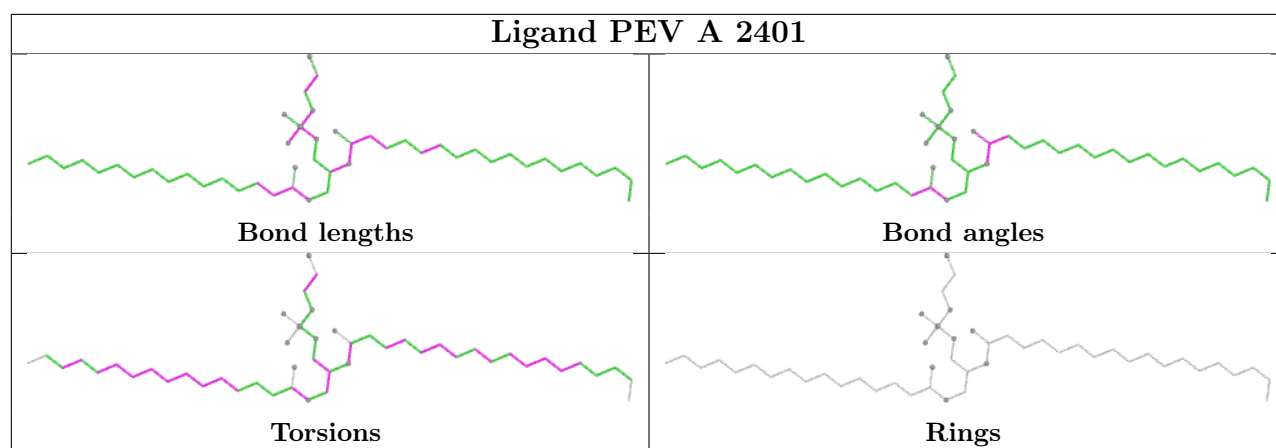
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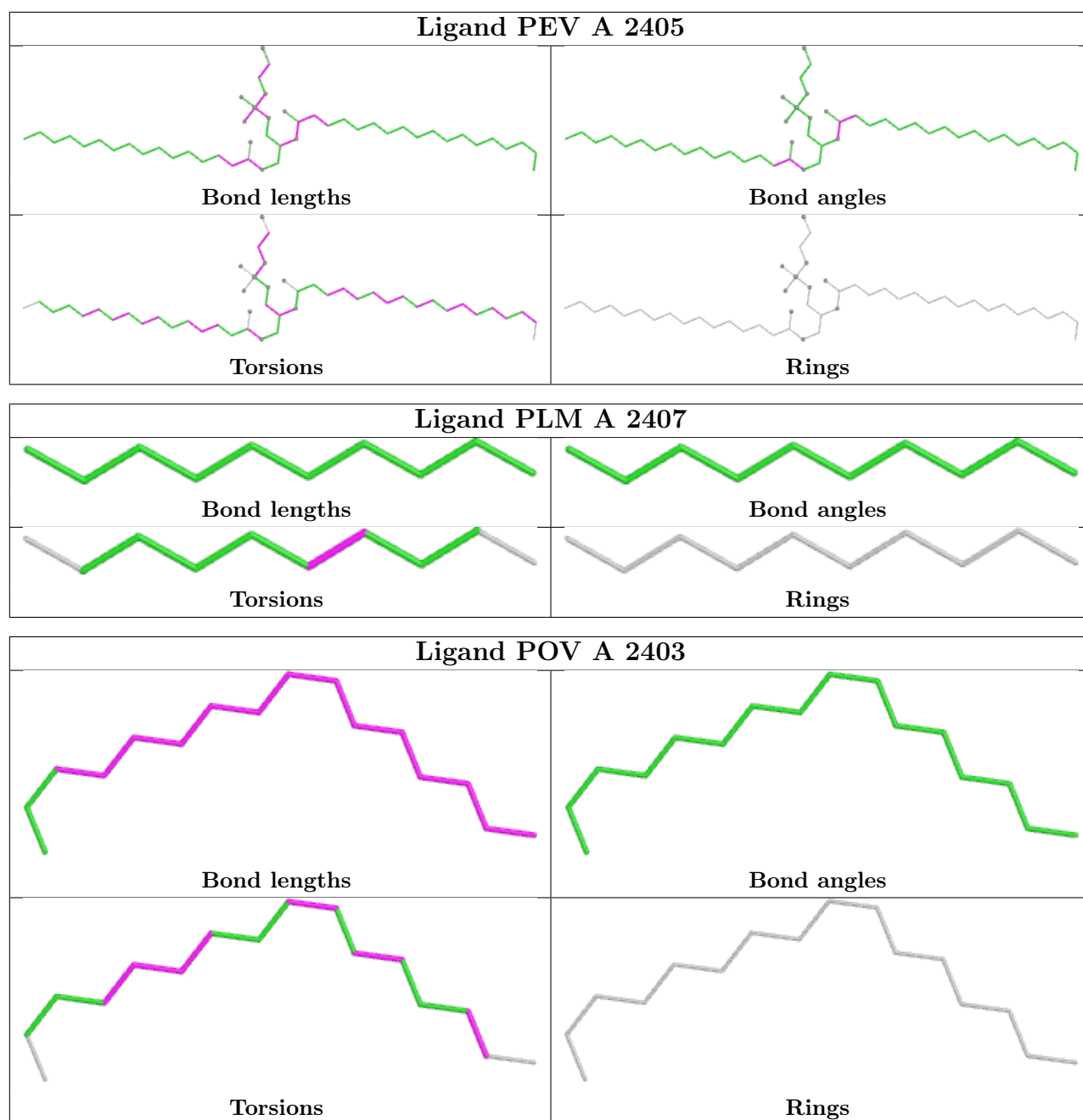
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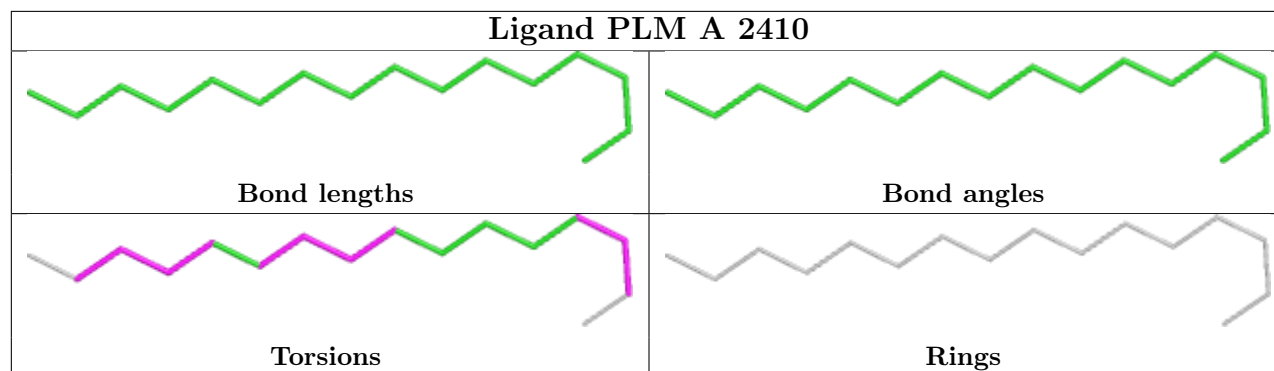
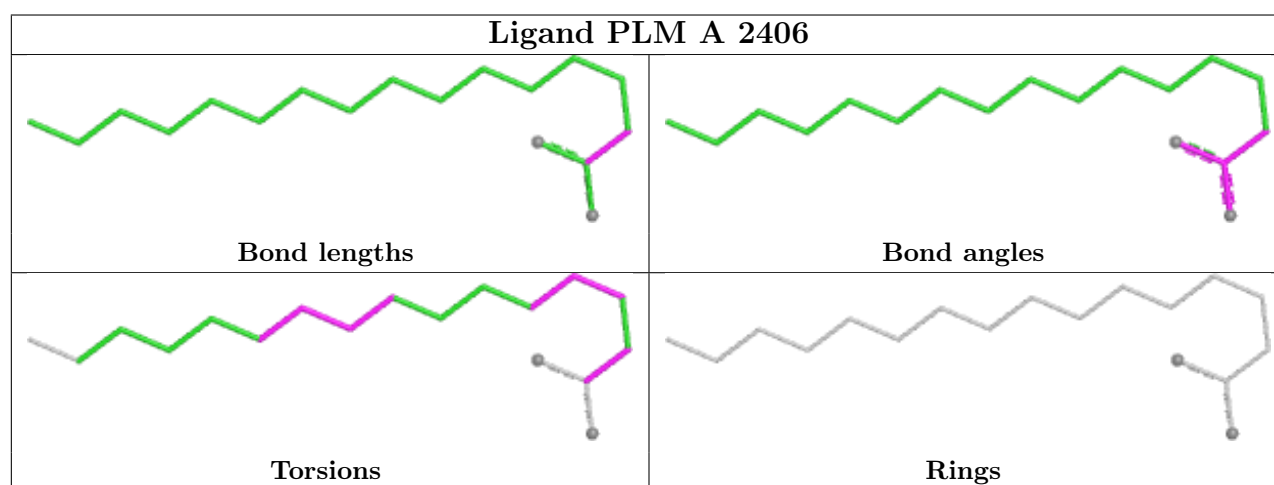
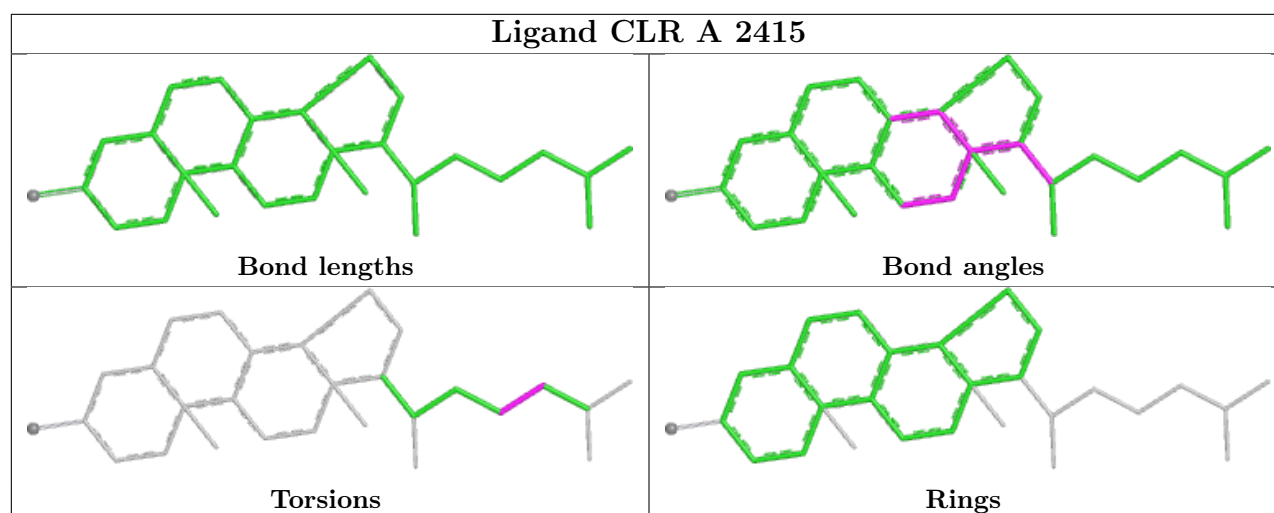
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2414	NAG	1	0
6	B	302	NAG	4	0

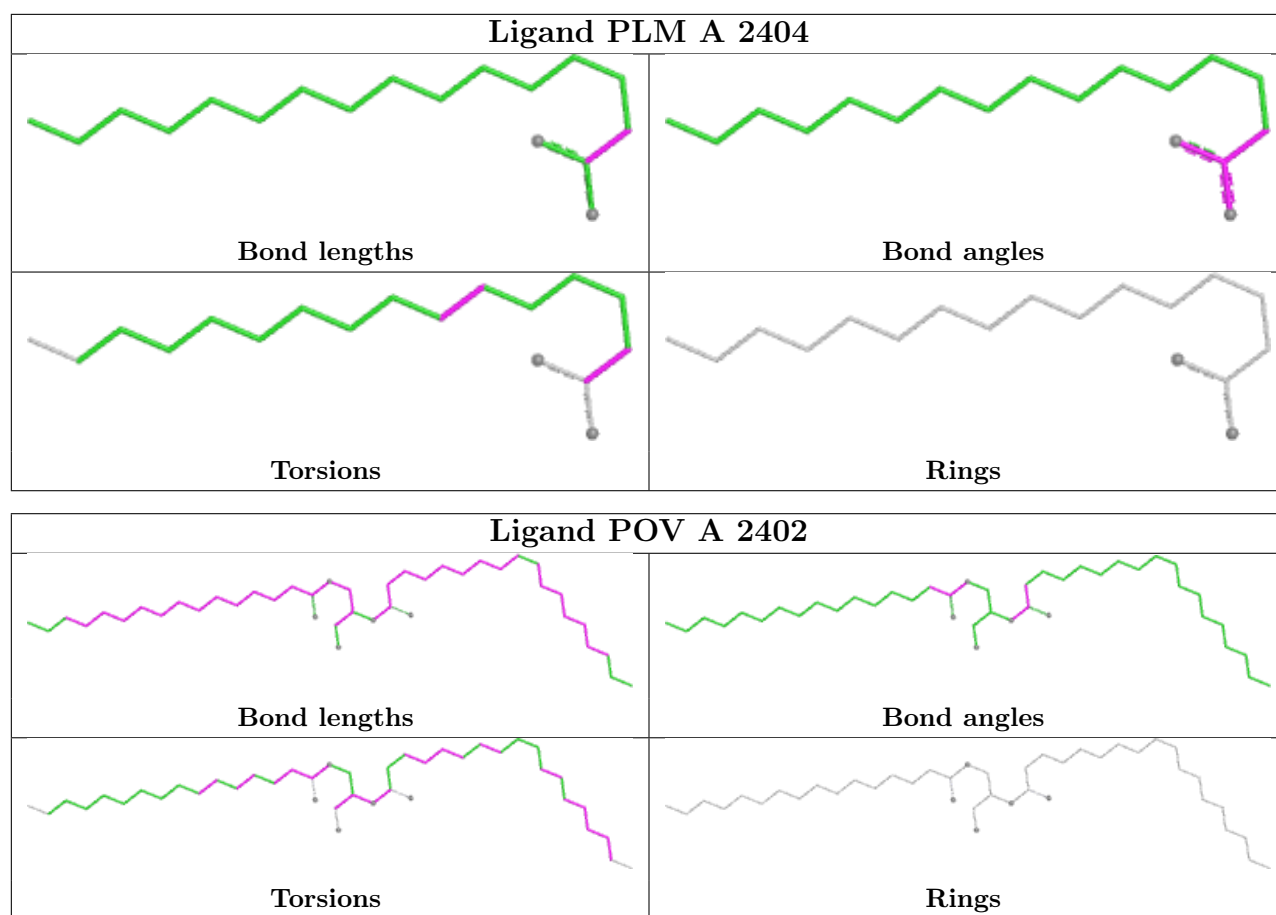
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

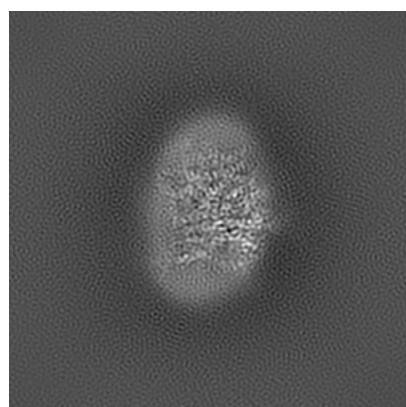
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25919. These allow visual inspection of the internal detail of the map and identification of artifacts.

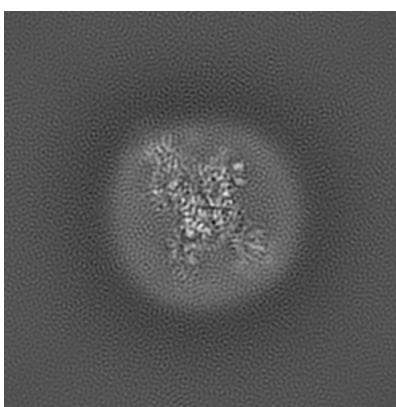
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

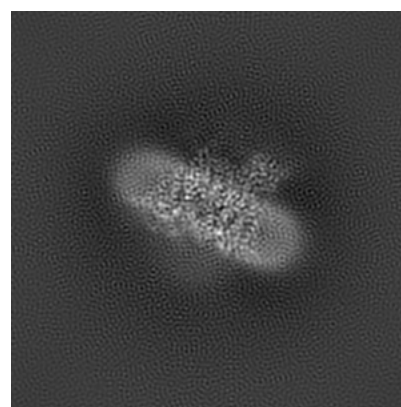
6.1.1 Primary map



X



Y

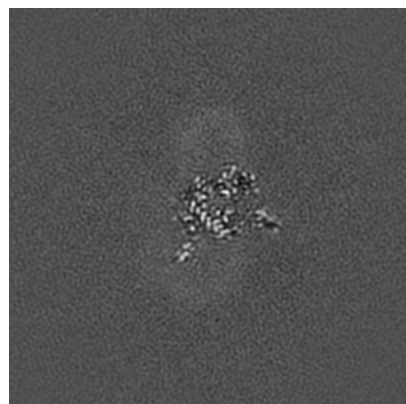


Z

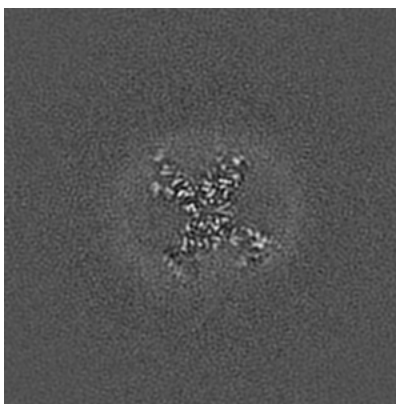
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

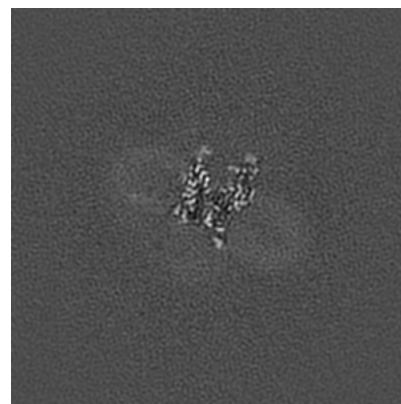
6.2.1 Primary map



X Index: 180



Y Index: 180

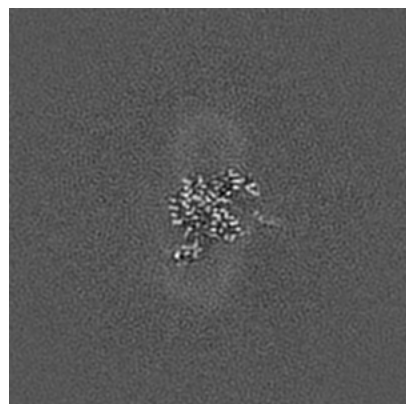


Z Index: 180

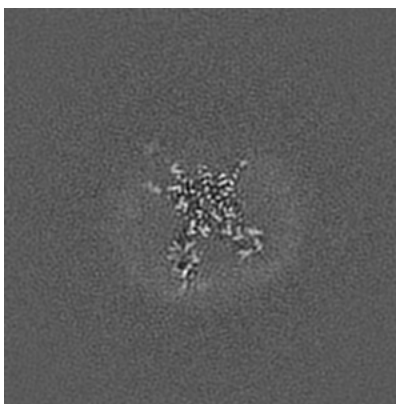
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

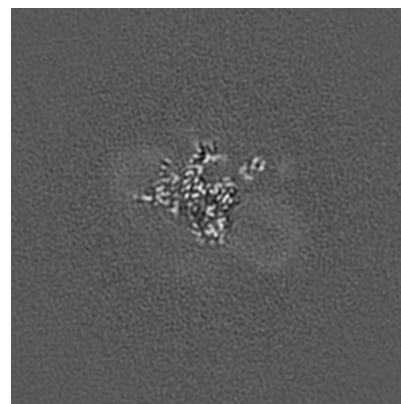
6.3.1 Primary map



X Index: 186



Y Index: 191

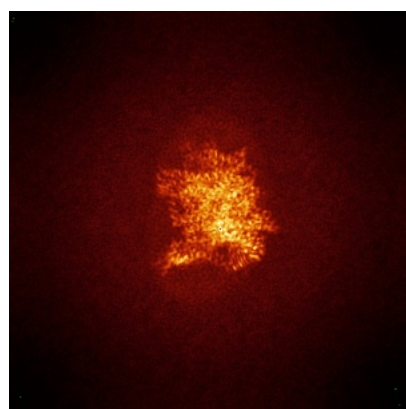


Z Index: 170

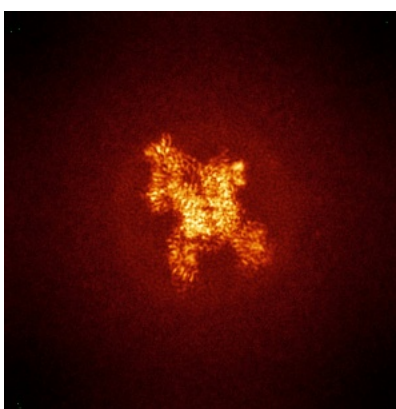
The images above show the largest variance slices of the map in three orthogonal directions.

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

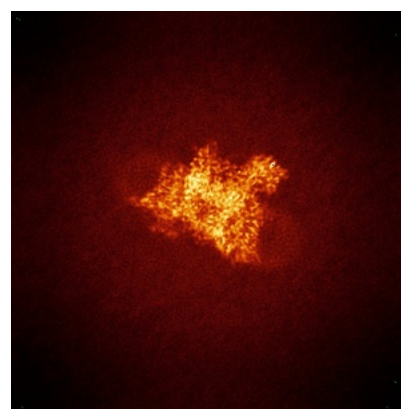
6.4.1 Primary map



X



Y

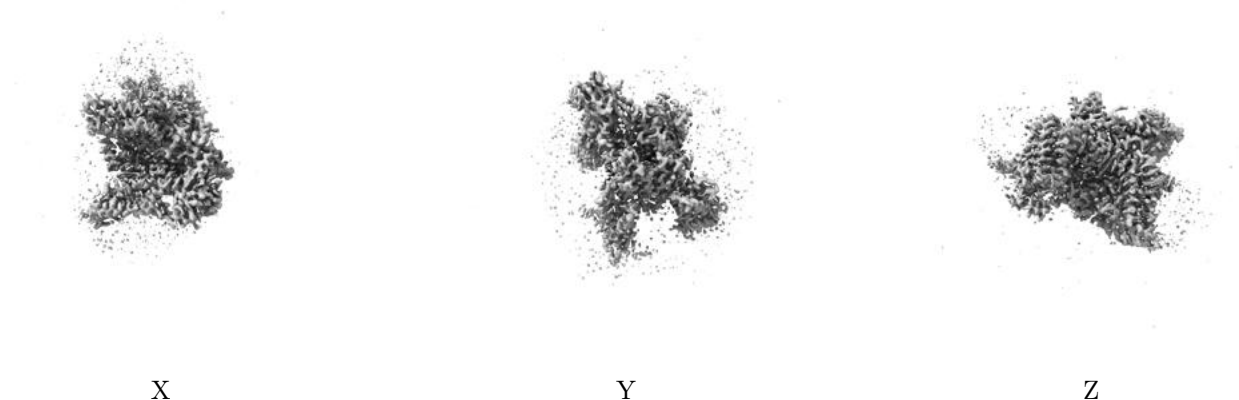


Z

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 0.161. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

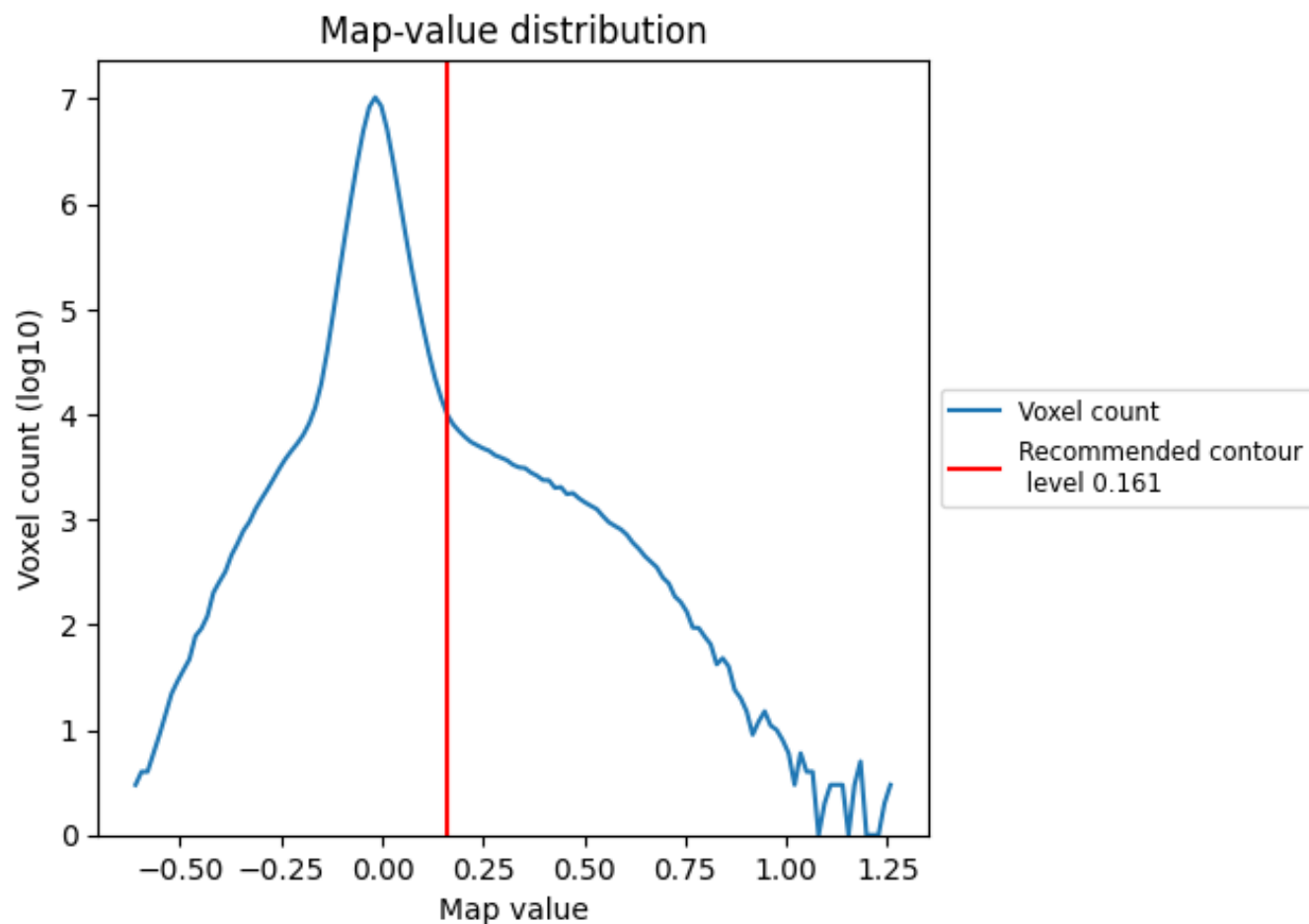
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

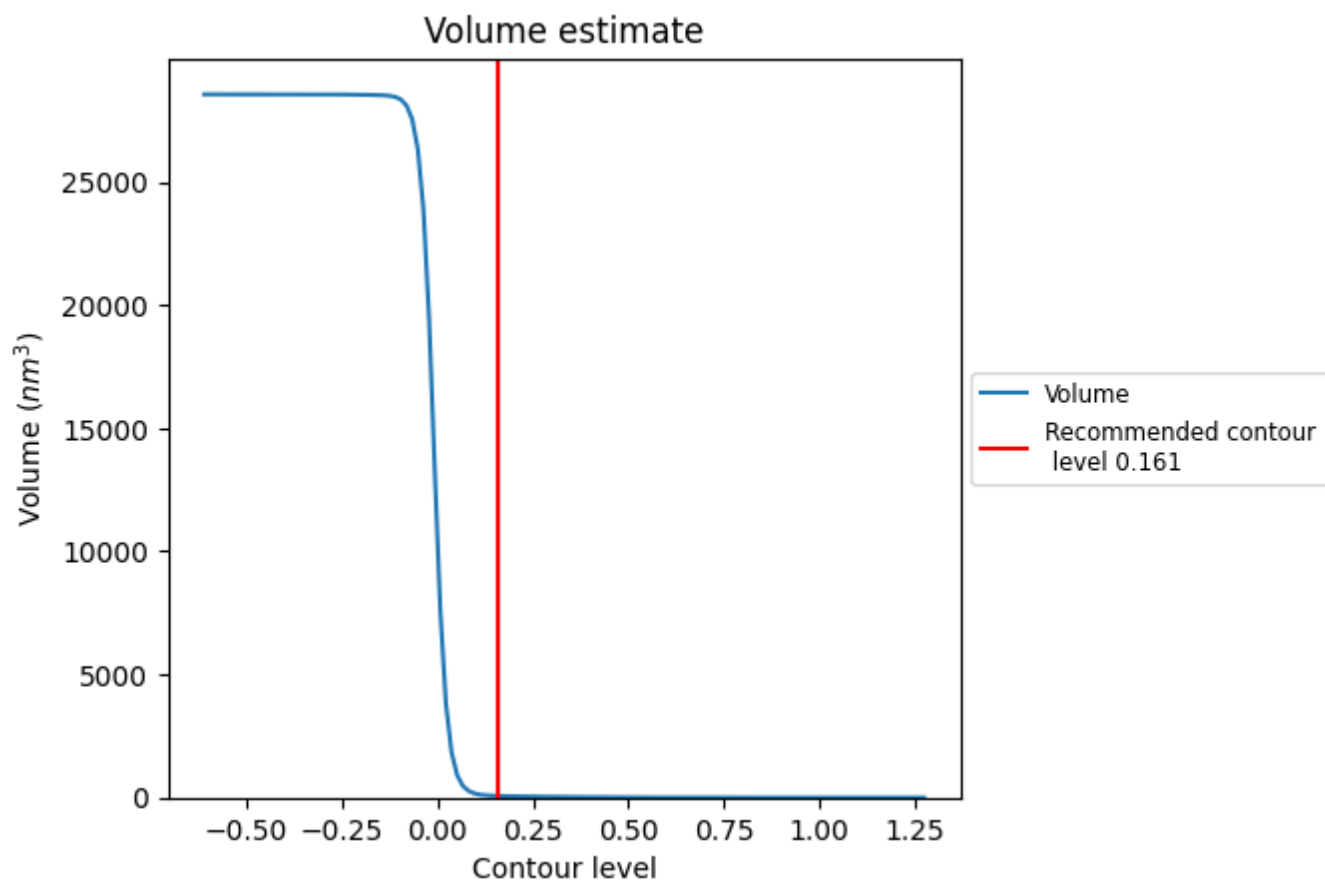
This section contains the results of statistical analysis of the map.

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.

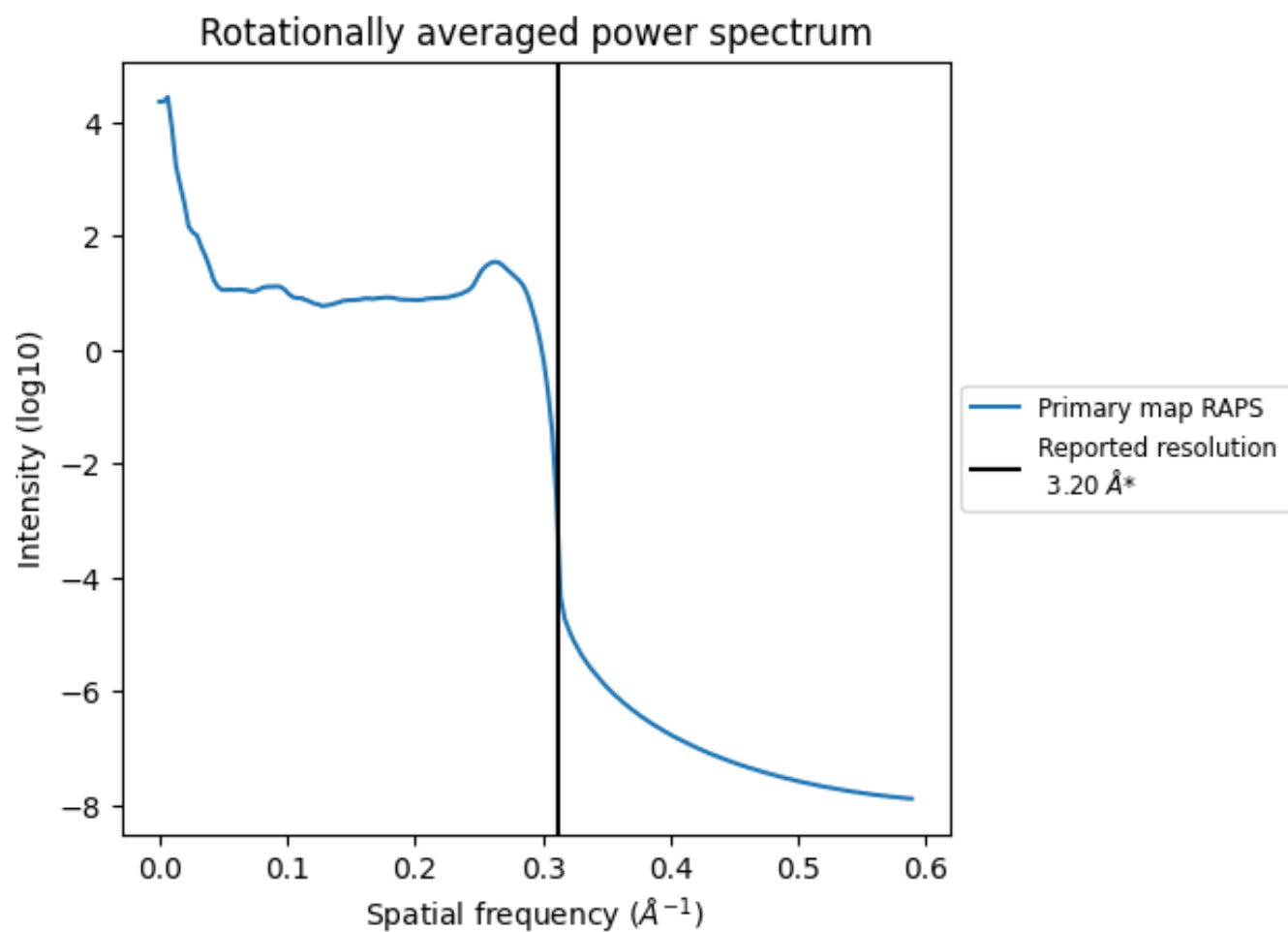
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm^3 ; this corresponds to an approximate mass of 58 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 0.312 Å⁻¹

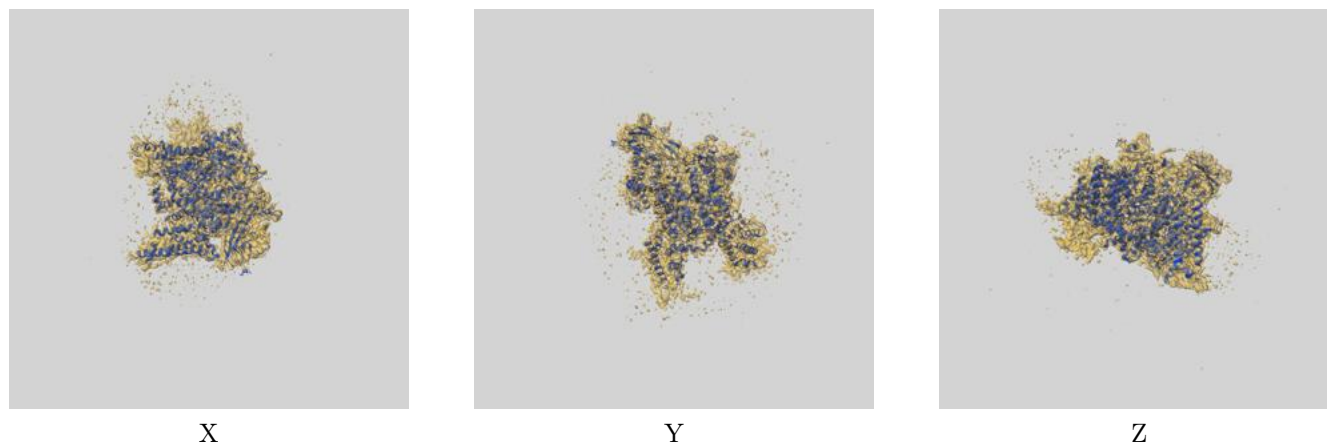
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

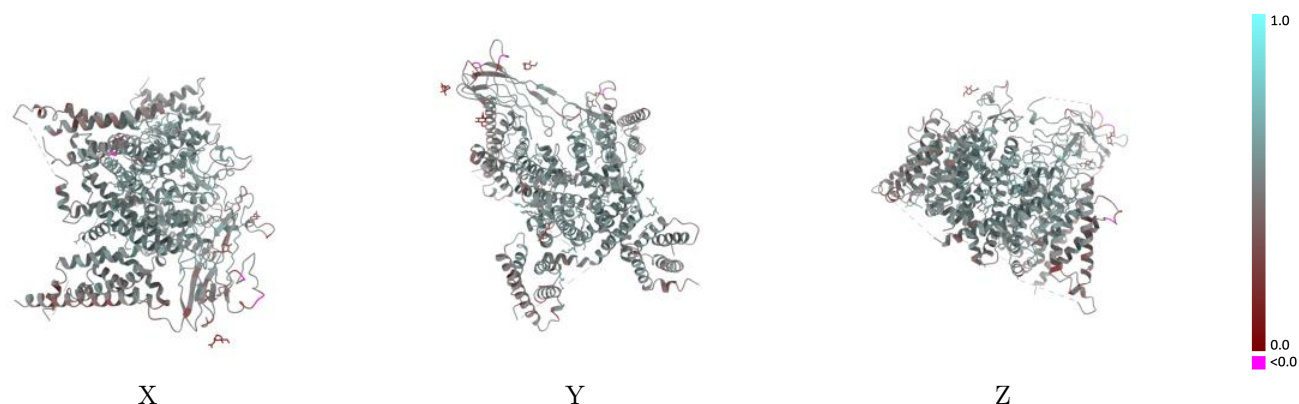
This section contains information regarding the fit between EMDB map EMD-25919 and PDB model 7TJ8. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



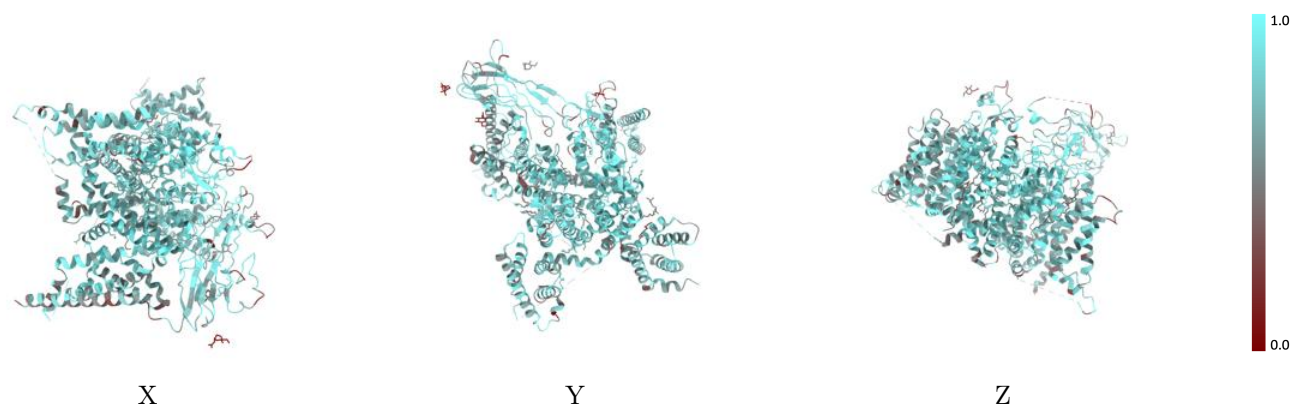
The images above show the 3D surface view of the map at the recommended contour level 0.161 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



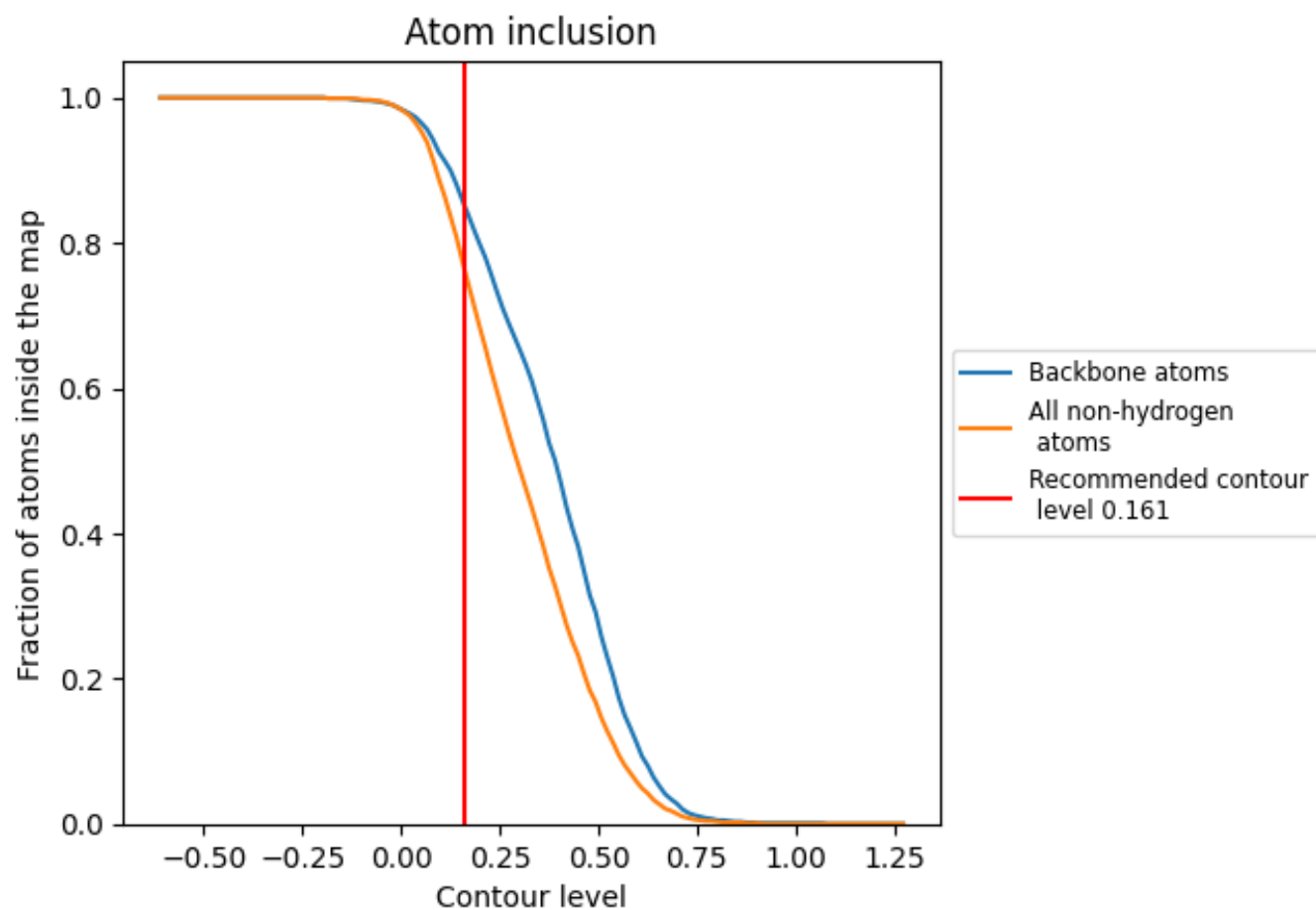
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.161).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 76% 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 (0.161) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7630	0.5120
A	0.7750	0.5210
B	0.6810	0.4510

