wwPDB EM Validation Summary Report (i)

Nov 15, 2022 – 10:47 AM EST

PDB ID	:	6XIW
EMDB ID	:	EMD-22203
Title	:	Cryo-EM structure of the sodium leak channel NALCN-FAM155A complex
Authors	:	Kschonsak, M.; Chua, H.C.; Noland, C.L.; Weidling, C.; Clairfeuille, T.; Bahlke, O.O.; Ameen, A.O.; Li, Z.R.; Arthur, C.P.; Ciferri, C.; Pless, S.A.; Payandeh, J.
Deposited on	:	2020-06-22
Resolution	:	2.80 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

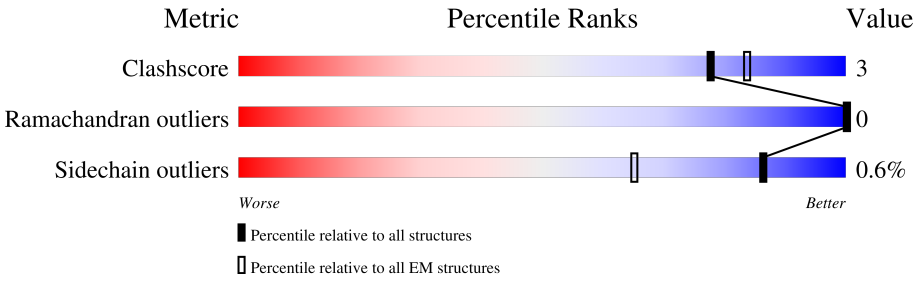
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1794	64% 6% 30%
2	B	483	28% 70%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11819 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 leak channel non-selective protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1256	10244	6771	1661	1730	82	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1739	GLY	-	expression tag	UNP Q8IZF0
A	1740	GLY	-	expression tag	UNP Q8IZF0
A	1741	GLY	-	expression tag	UNP Q8IZF0
A	1742	SER	-	expression tag	UNP Q8IZF0
A	1743	GLY	-	expression tag	UNP Q8IZF0
A	1744	GLY	-	expression tag	UNP Q8IZF0
A	1745	TRP	-	expression tag	UNP Q8IZF0
A	1746	SER	-	expression tag	UNP Q8IZF0
A	1747	HIS	-	expression tag	UNP Q8IZF0
A	1748	PRO	-	expression tag	UNP Q8IZF0
A	1749	GLN	-	expression tag	UNP Q8IZF0
A	1750	PHE	-	expression tag	UNP Q8IZF0
A	1751	GLU	-	expression tag	UNP Q8IZF0
A	1752	LYS	-	expression tag	UNP Q8IZF0
A	1753	GLY	-	expression tag	UNP Q8IZF0
A	1754	GLY	-	expression tag	UNP Q8IZF0
A	1755	GLY	-	expression tag	UNP Q8IZF0
A	1756	SER	-	expression tag	UNP Q8IZF0
A	1757	GLY	-	expression tag	UNP Q8IZF0
A	1758	GLY	-	expression tag	UNP Q8IZF0
A	1759	GLY	-	expression tag	UNP Q8IZF0
A	1760	SER	-	expression tag	UNP Q8IZF0
A	1761	GLY	-	expression tag	UNP Q8IZF0
A	1762	GLY	-	expression tag	UNP Q8IZF0
A	1763	SER	-	expression tag	UNP Q8IZF0
A	1764	ALA	-	expression tag	UNP Q8IZF0
A	1765	TRP	-	expression tag	UNP Q8IZF0
A	1766	SER	-	expression tag	UNP Q8IZF0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1767	HIS	-	expression tag	UNP Q8IZF0
A	1768	PRO	-	expression tag	UNP Q8IZF0
A	1769	GLN	-	expression tag	UNP Q8IZF0
A	1770	PHE	-	expression tag	UNP Q8IZF0
A	1771	GLU	-	expression tag	UNP Q8IZF0
A	1772	LYS	-	expression tag	UNP Q8IZF0
A	1773	GLY	-	expression tag	UNP Q8IZF0
A	1774	SER	-	expression tag	UNP Q8IZF0
A	1775	GLY	-	expression tag	UNP Q8IZF0
A	1776	ASP	-	expression tag	UNP Q8IZF0
A	1777	TYR	-	expression tag	UNP Q8IZF0
A	1778	LYS	-	expression tag	UNP Q8IZF0
A	1779	ASP	-	expression tag	UNP Q8IZF0
A	1780	ASP	-	expression tag	UNP Q8IZF0
A	1781	ASP	-	expression tag	UNP Q8IZF0
A	1782	ASP	-	expression tag	UNP Q8IZF0
A	1783	LYS	-	expression tag	UNP Q8IZF0
A	1784	GLY	-	expression tag	UNP Q8IZF0
A	1785	ASN	-	expression tag	UNP Q8IZF0
A	1786	SER	-	expression tag	UNP Q8IZF0
A	1787	ASP	-	expression tag	UNP Q8IZF0
A	1788	TYR	-	expression tag	UNP Q8IZF0
A	1789	LYS	-	expression tag	UNP Q8IZF0
A	1790	ASP	-	expression tag	UNP Q8IZF0
A	1791	ASP	-	expression tag	UNP Q8IZF0
A	1792	ASP	-	expression tag	UNP Q8IZF0
A	1793	ASP	-	expression tag	UNP Q8IZF0
A	1794	LYS	-	expression tag	UNP Q8IZF0

- Molecule 2 is a protein called Transmembrane protein FAM155A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			1193	764	184	231	14		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	459	GLY	-	expression tag	UNP B1AL88
B	460	GLY	-	expression tag	UNP B1AL88
B	461	SER	-	expression tag	UNP B1AL88
B	462	GLY	-	expression tag	UNP B1AL88

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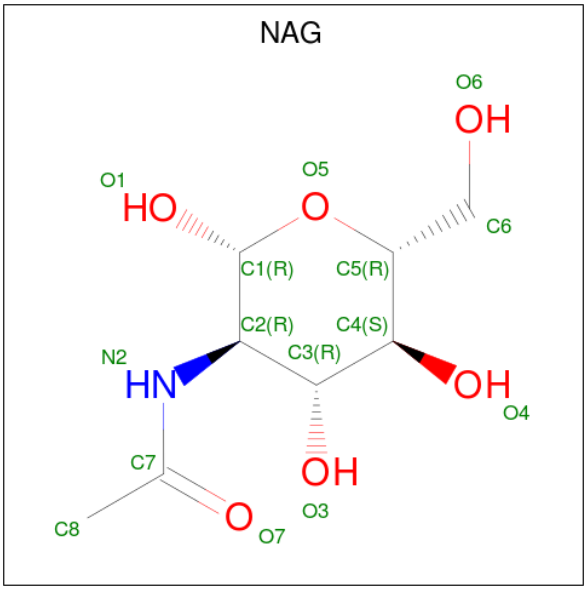
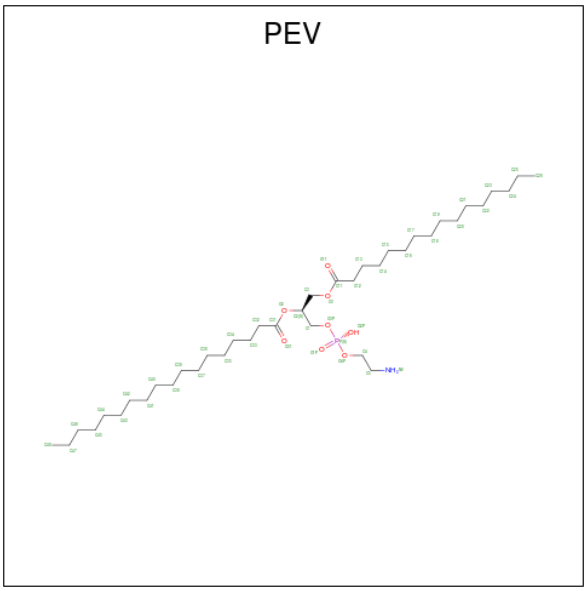
Chain	Residue	Modelled	Actual	Comment	Reference
B	463	GLY	-	expression tag	UNP B1AL88
B	464	SER	-	expression tag	UNP B1AL88
B	465	ASP	-	expression tag	UNP B1AL88
B	466	TYR	-	expression tag	UNP B1AL88
B	467	LYS	-	expression tag	UNP B1AL88
B	468	ASP	-	expression tag	UNP B1AL88
B	469	ASP	-	expression tag	UNP B1AL88
B	470	ASP	-	expression tag	UNP B1AL88
B	471	ASP	-	expression tag	UNP B1AL88
B	472	LYS	-	expression tag	UNP B1AL88
B	473	GLY	-	expression tag	UNP B1AL88
B	474	ASN	-	expression tag	UNP B1AL88
B	475	SER	-	expression tag	UNP B1AL88
B	476	ASP	-	expression tag	UNP B1AL88
B	477	TYR	-	expression tag	UNP B1AL88
B	478	LYS	-	expression tag	UNP B1AL88
B	479	ASP	-	expression tag	UNP B1AL88
B	480	ASP	-	expression tag	UNP B1AL88
B	481	ASP	-	expression tag	UNP B1AL88
B	482	ASP	-	expression tag	UNP B1AL88
B	483	LYS	-	expression tag	UNP B1AL88

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



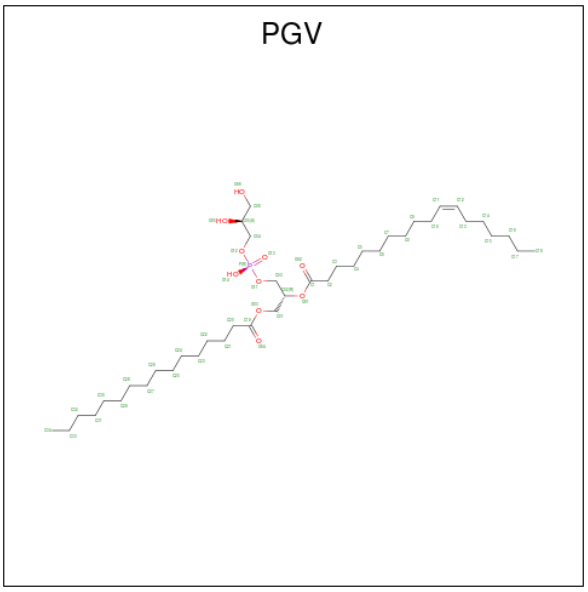
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			28	16	2	10	
3	A	1	Total	C	N	O	0
			28	16	2	10	

- Molecule 4 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: $C_{39}H_{78}NO_8P$).



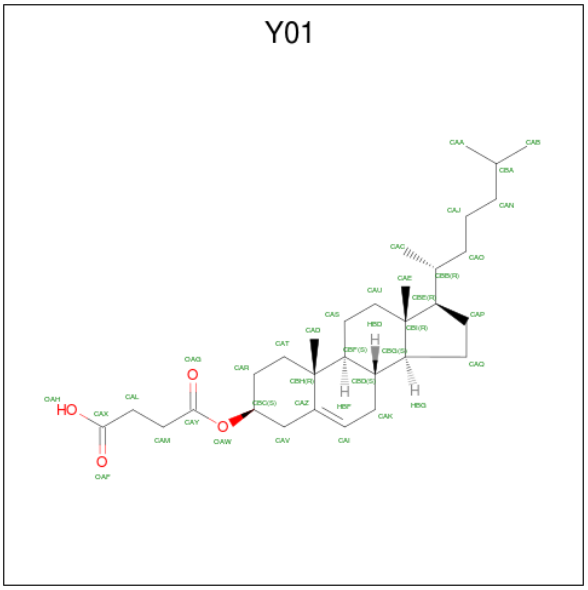
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			182	132	5	40	5	
4	A	1	Total	C	N	O	P	0
			182	132	5	40	5	
4	A	1	Total	C	N	O	P	0
			182	132	5	40	5	
4	A	1	Total	C	N	O	P	0
			182	132	5	40	5	
4	A	1	Total	C	N	O	P	0
			182	132	5	40	5	

- Molecule 5 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			74	56	16	2	
5	A	1	Total	C	O	P	0
			74	56	16	2	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			93	83	10	
6	A	1	Total	C	O	0
			93	83	10	

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Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 93	C 83	O 10	0

- Molecule 7 is water.

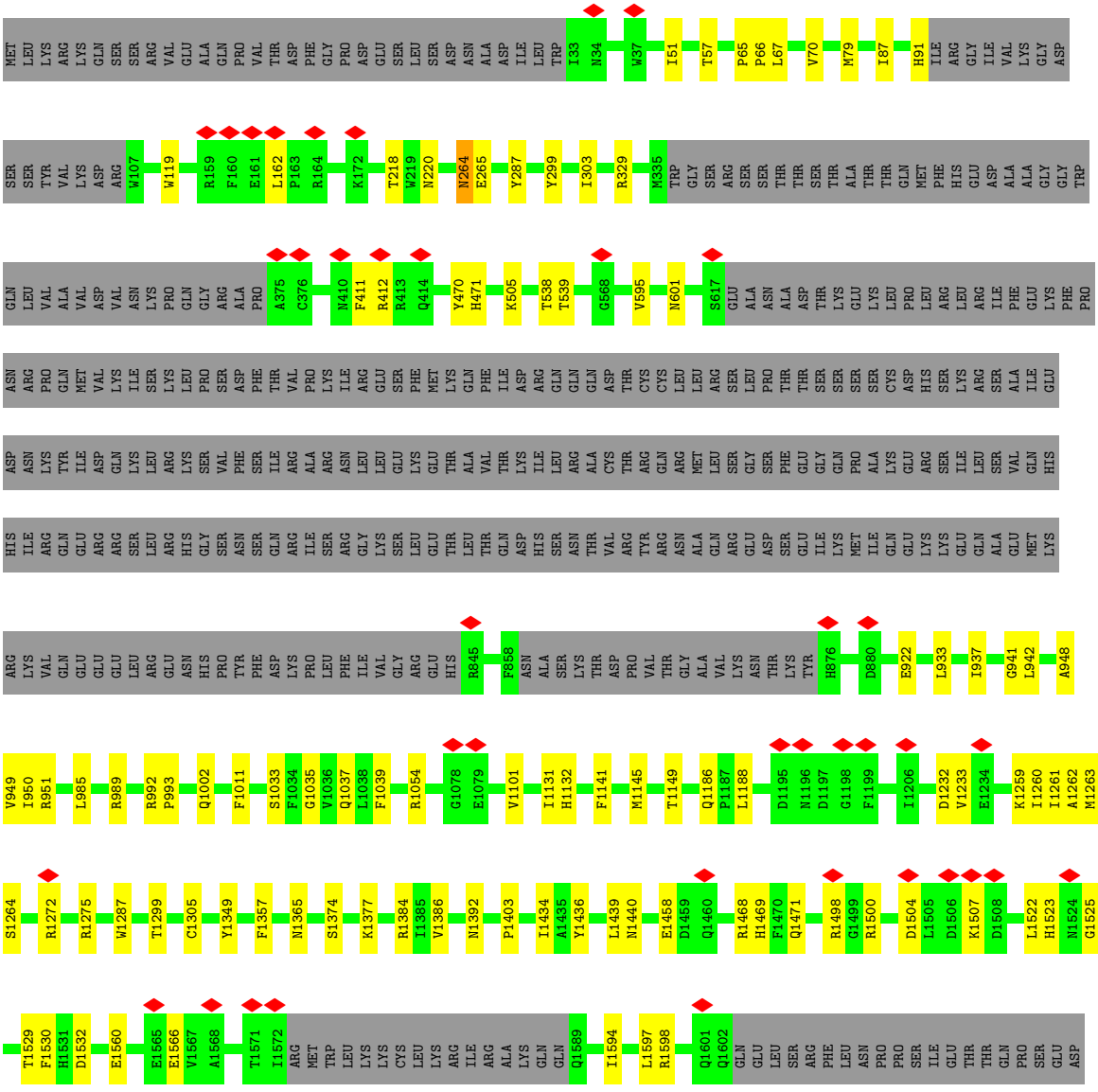
Mol	Chain	Residues	Atoms		AltConf
7	A	4	Total 4	O 4	0
7	B	1	Total 1	O 1	0

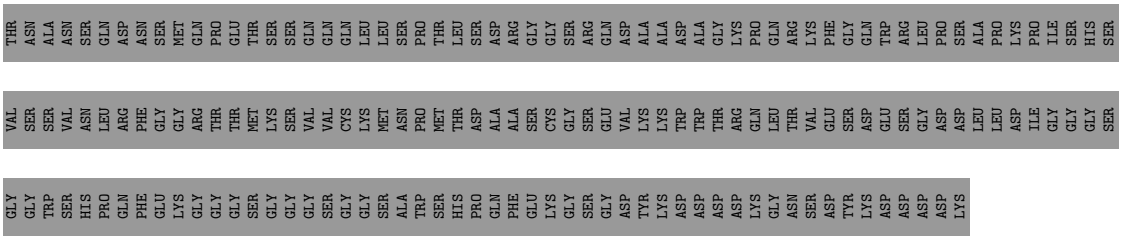
3 Residue-property plots (i)

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: Sodium leak channel non-selective protein

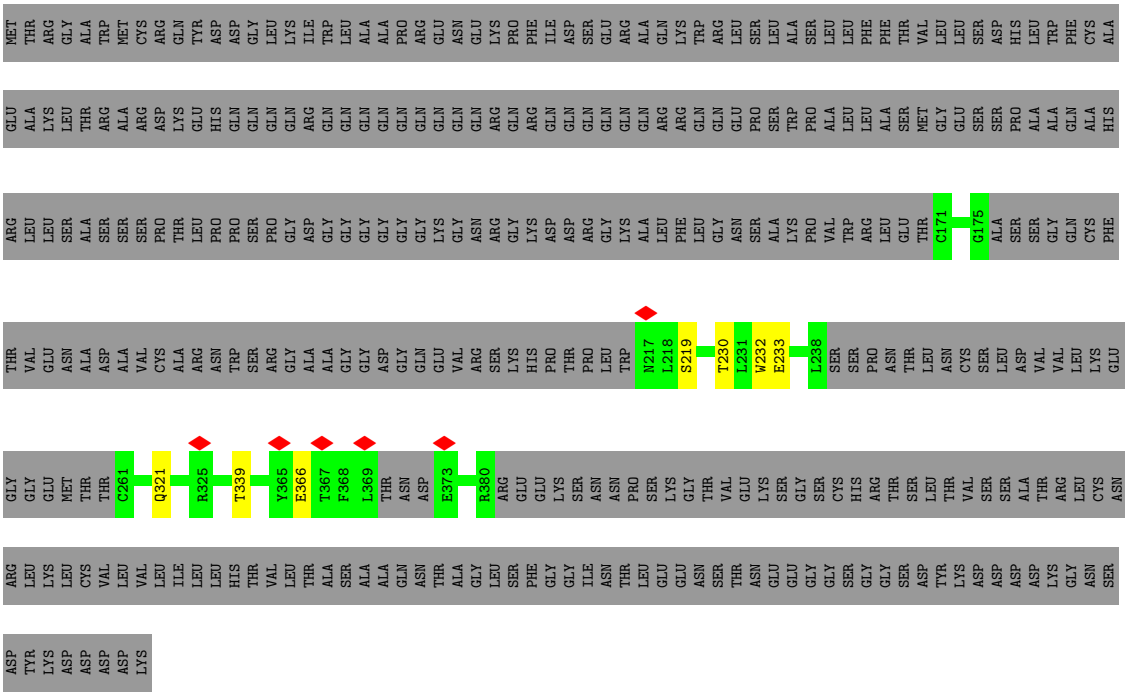
Chain A:





• Molecule 2: Transmembrane protein FAM155A

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	365512	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.967	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.929	Depositor
Minimum map value	-0.613	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	296.64, 296.64, 296.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82400006, 0.82400006, 0.82400006	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, TYS, PEV, NAG, PGV

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	0.26	0/10490	0.40	0/14220
2	B	0.26	0/1224	0.40	0/1655
All	All	0.26	0/11714	0.40	0/15875

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10244	0	10422	62	0
2	B	1193	0	1091	5	0
3	A	28	0	26	0	0
4	A	182	0	229	4	0
5	A	74	0	96	2	0
6	A	93	0	125	7	0
7	A	4	0	0	0	0
7	B	1	0	0	0	0
All	All	11819	0	11989	69	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 3.

The worst 5 of 69 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:1594:ILE:HD13	1:A:1597:LEU:HD12	1.66	0.77
1:A:933:LEU:O	1:A:937:ILE:HG12	1.94	0.68
2:B:219:SER:HA	2:B:230:THR:HG21	1.74	0.68
6:A:1811:Y01:HAE2	6:A:1811:Y01:HAC1	1.79	0.63
1:A:942:LEU:H	1:A:942:LEU:HD23	1.64	0.62

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	1243/1794 (69%)	1198 (96%)	45 (4%)	0	100	100
2	B	136/483 (28%)	128 (94%)	8 (6%)	0	100	100
All	All	1379/2277 (61%)	1326 (96%)	53 (4%)	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	1131/1606 (70%)	1124 (99%)	7 (1%)	86	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	136/417 (33%)	136 (100%)	0	100 100
All	All	1267/2023 (63%)	1260 (99%)	7 (1%)	86 96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1145	MET
1	A	1357	PHE
1	A	1566	GLU
1	A	1439	LEU
1	A	329	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	TYS	A	287	1	15,16,17	1.50	1 (6%)	18,22,24	1.17	2 (11%)

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
1	TYS	A	287	1	-	4/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	TYS	OH-S	4.94	1.65	1.58

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	TYS	OH-CZ-CE2	2.09	122.75	118.64
1	A	287	TYS	O3-S-OH	2.04	110.74	105.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	287	TYS	CE1-CZ-OH-S
1	A	287	TYS	CE2-CZ-OH-S
1	A	287	TYS	CA-CB-CG-CD2
1	A	287	TYS	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\|>2$
4	PEV	A	1803	-	36,36,48	1.00	4 (11%)	39,41,53	1.14	2 (5%)
6	Y01	A	1810	-	38,38,38	0.76	0	57,57,57	1.52	8 (14%)
3	NAG	A	1802	1	14,14,15	0.20	0	17,19,21	0.41	0
4	PEV	A	1805	-	33,33,48	1.04	4 (12%)	36,38,53	1.13	2 (5%)
6	Y01	A	1811	-	34,34,38	0.61	1 (2%)	52,52,57	1.35	6 (11%)
4	PEV	A	1807	-	30,30,48	1.09	4 (13%)	33,35,53	1.20	2 (6%)
4	PEV	A	1804	-	39,39,48	0.97	4 (10%)	42,44,53	1.12	2 (4%)
3	NAG	A	1801	-	14,14,15	0.19	0	17,19,21	0.43	0
6	Y01	A	1812	-	30,30,38	0.85	1 (3%)	46,46,57	1.38	7 (15%)
5	PGV	A	1808	-	30,30,50	1.18	2 (6%)	32,35,56	1.18	2 (6%)
4	PEV	A	1806	-	39,39,48	0.97	4 (10%)	42,44,53	1.14	2 (4%)
5	PGV	A	1809	-	42,42,50	1.22	3 (7%)	46,47,56	1.14	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
4	PEV	A	1803	-	-	19/40/40/52	-
6	Y01	A	1810	-	-	11/19/77/77	0/4/4/4
3	NAG	A	1802	1	-	2/6/23/26	0/1/1/1
4	PEV	A	1805	-	-	15/37/37/52	-
6	Y01	A	1811	-	-	2/14/72/77	0/4/4/4
4	PEV	A	1807	-	-	12/34/34/52	-
4	PEV	A	1804	-	-	18/43/43/52	-
3	NAG	A	1801	-	-	1/6/23/26	0/1/1/1
6	Y01	A	1812	-	-	2/9/63/77	0/4/4/4
5	PGV	A	1808	-	-	14/33/33/55	-
4	PEV	A	1806	-	-	19/43/43/52	-
5	PGV	A	1809	-	-	18/44/44/55	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1809	PGV	O03-C19	3.43	1.43	1.33
5	A	1808	PGV	O01-C02	-3.03	1.41	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1808	PGV	O01-C1	2.96	1.42	1.34
5	A	1809	PGV	O01-C1	2.92	1.42	1.34
4	A	1803	PEV	O2-C2	-2.55	1.40	1.46

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1810	Y01	CBI-CBE-CBB	-5.15	111.42	119.49
6	A	1811	Y01	CBI-CBE-CBB	-4.15	112.98	119.49
4	A	1807	PEV	O2-C31-C32	4.12	120.37	111.50
6	A	1812	Y01	CAS-CAU-CBI	-4.07	107.17	113.37
4	A	1806	PEV	O2-C31-C32	4.03	120.19	111.50

There are no chirality outliers.

5 of 133 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1803	PEV	C4-O4P-P-O1P
4	A	1803	PEV	O4P-C4-C5-N6
4	A	1804	PEV	C1-O3P-P-O2P
4	A	1805	PEV	C32-C31-O2-C2
4	A	1805	PEV	O31-C31-O2-C2

There are no ring outliers.

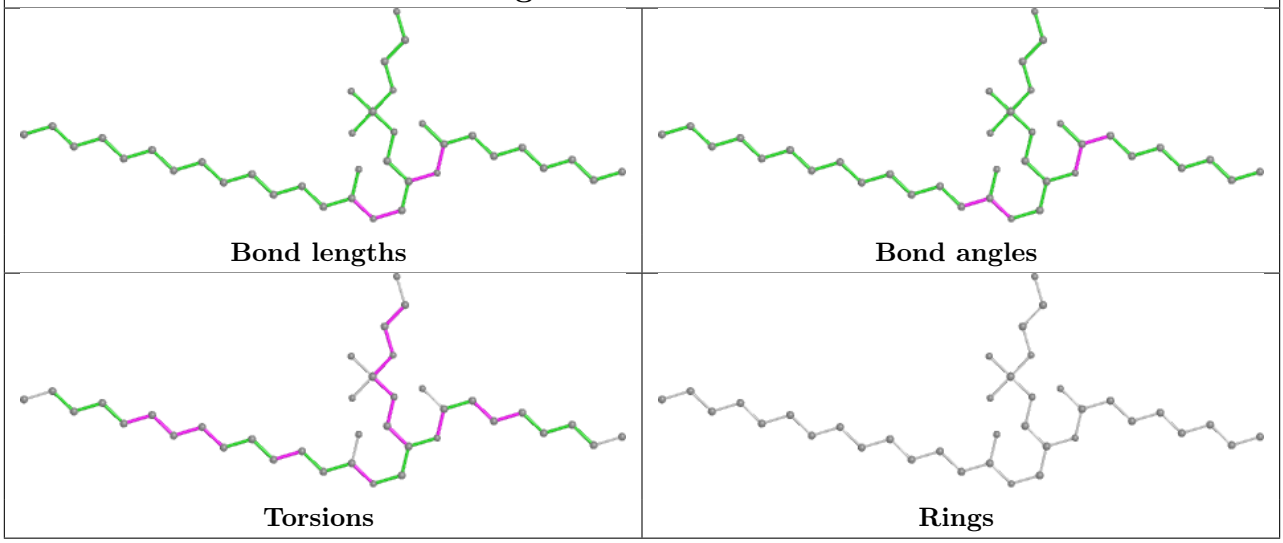
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1803	PEV	1	0
6	A	1810	Y01	3	0
4	A	1805	PEV	1	0
6	A	1811	Y01	4	0
4	A	1807	PEV	1	0
5	A	1808	PGV	1	0
4	A	1806	PEV	1	0
5	A	1809	PGV	1	0

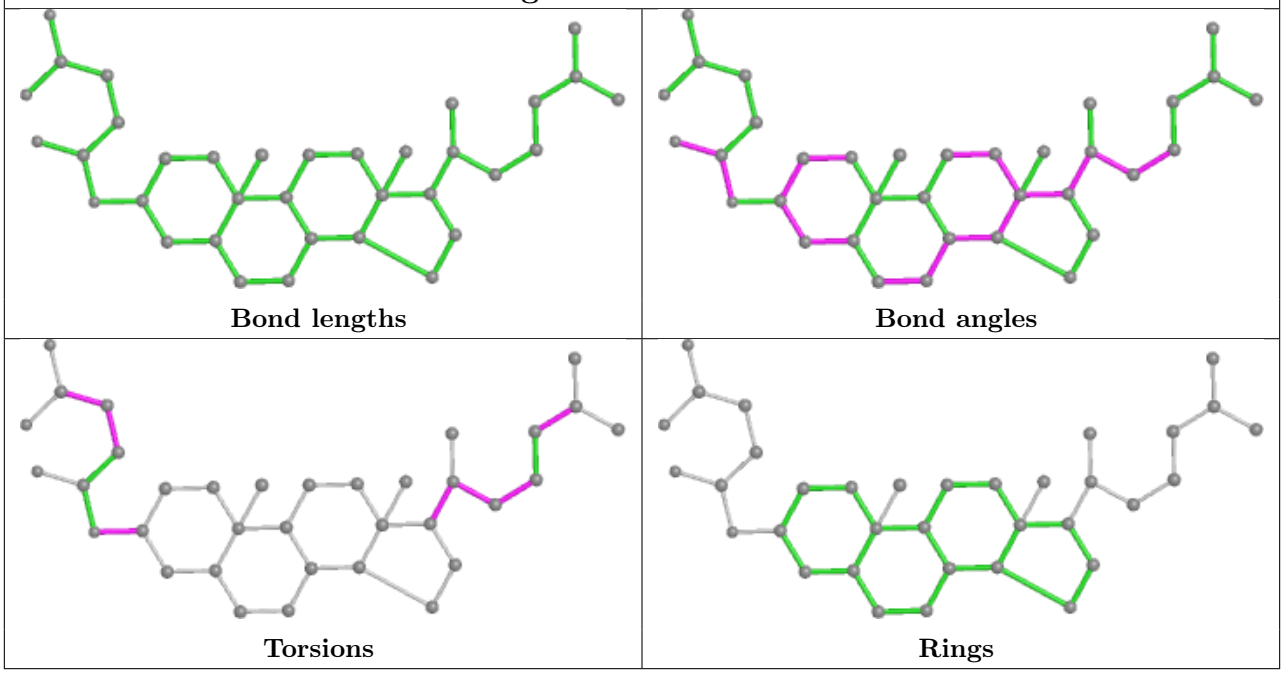
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

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

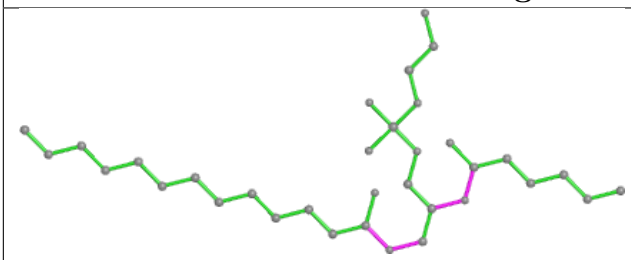
Ligand PEV A 1803



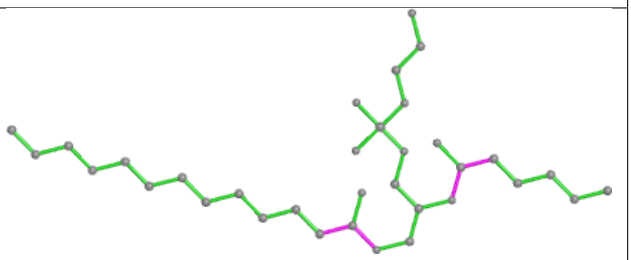
Ligand Y01 A 1810



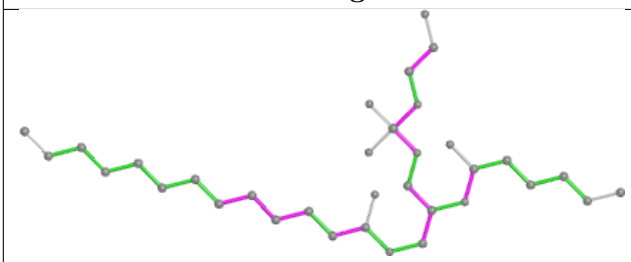
Ligand PEV A 1805



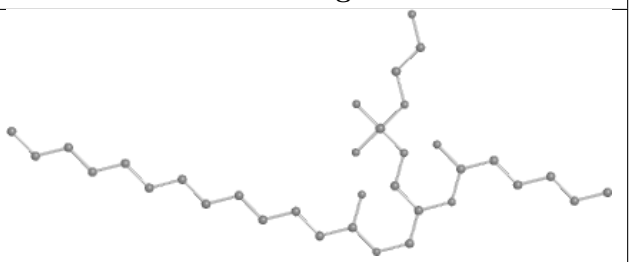
Bond lengths



Bond angles

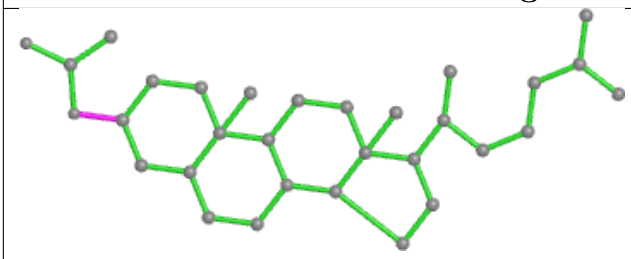


Torsions

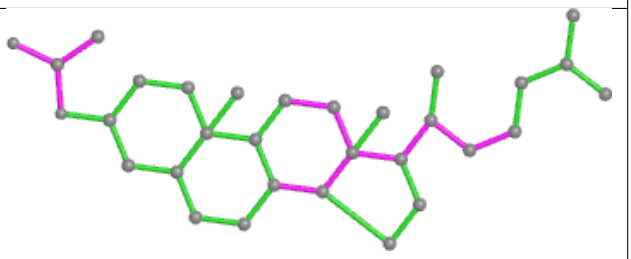


Rings

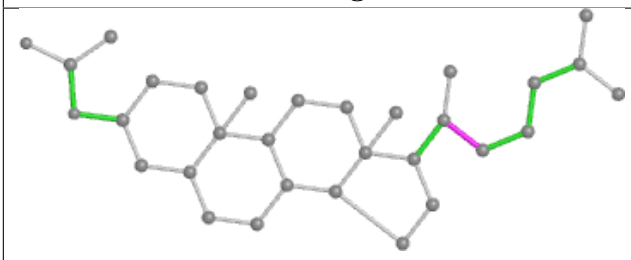
Ligand Y01 A 1811



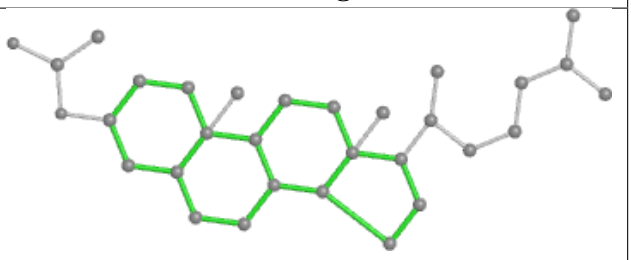
Bond lengths



Bond angles

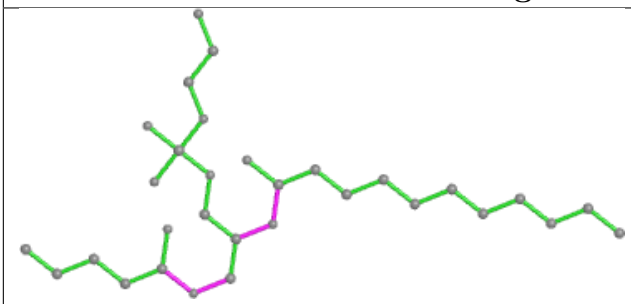


Torsions

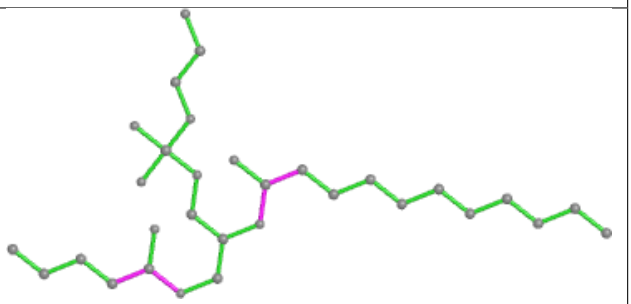


Rings

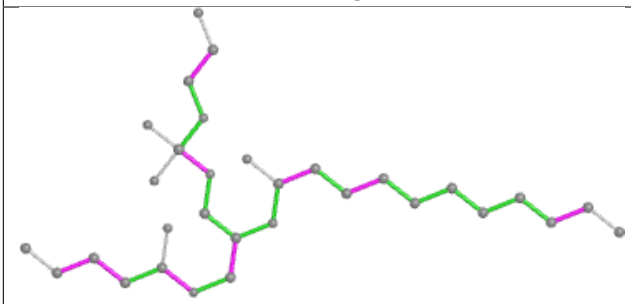
Ligand PEV A 1807



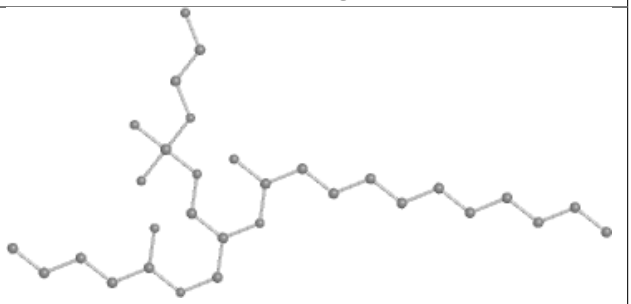
Bond lengths



Bond angles

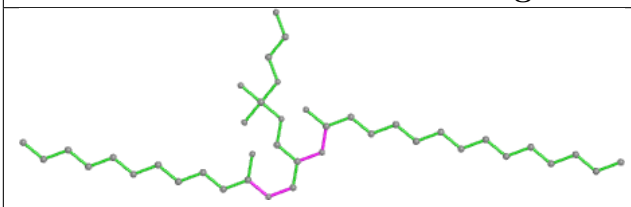


Torsions

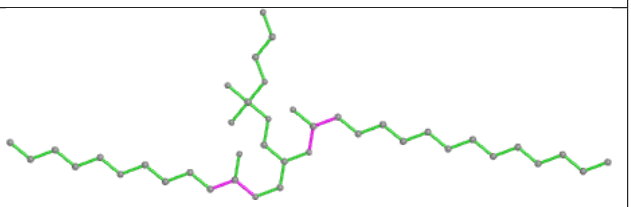


Rings

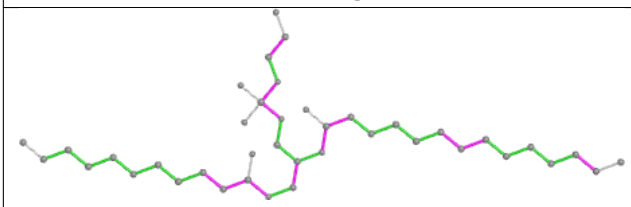
Ligand PEV A 1804



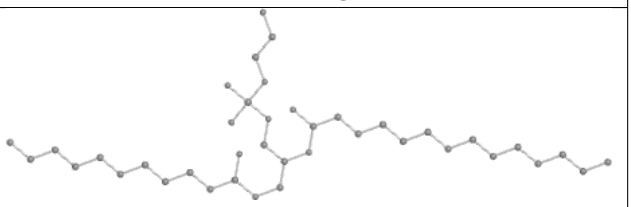
Bond lengths



Bond angles

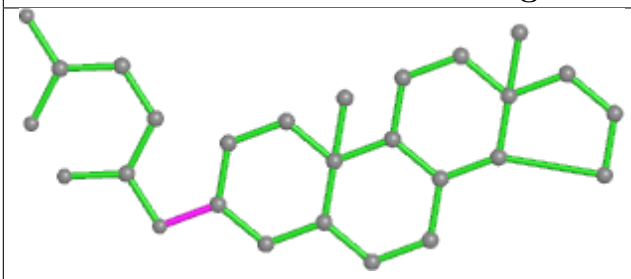


Torsions

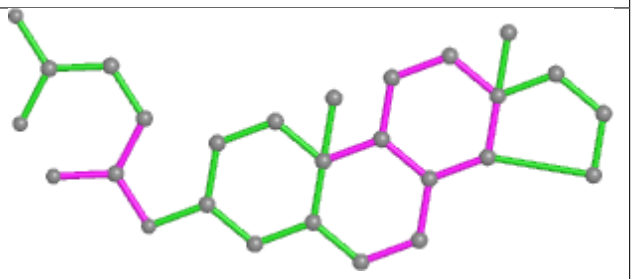


Rings

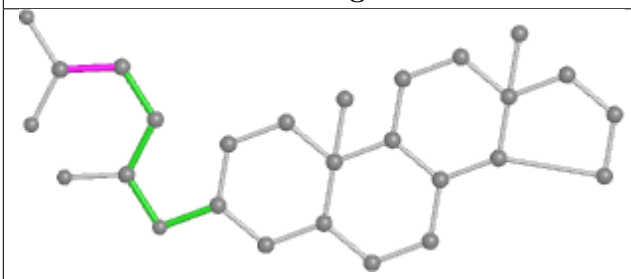
Ligand Y01 A 1812



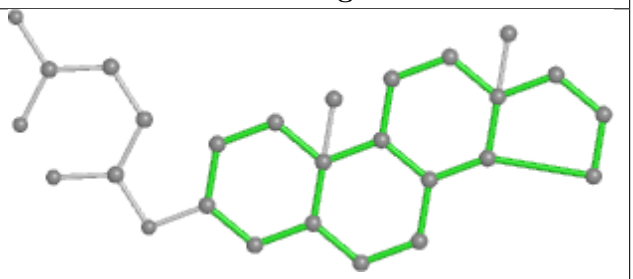
Bond lengths



Bond angles

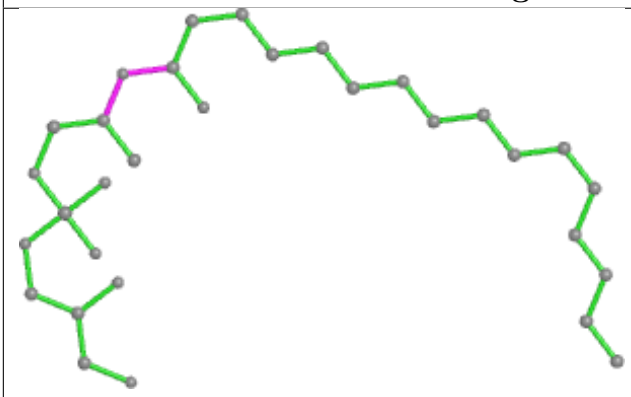


Torsions

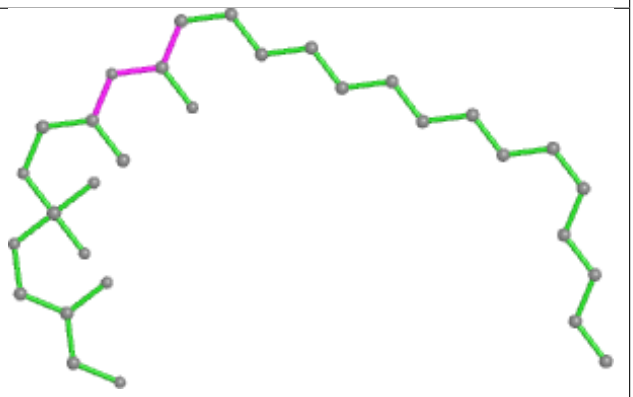


Rings

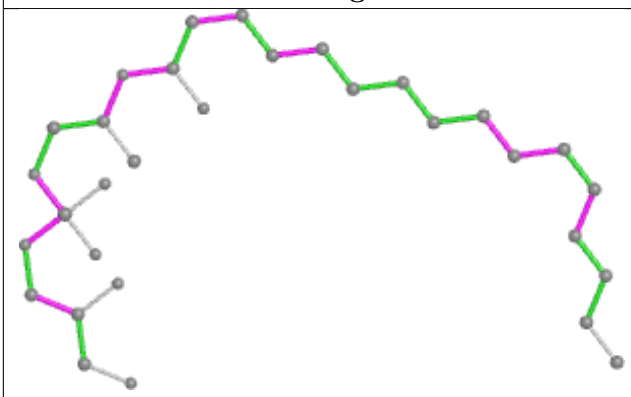
Ligand PGV A 1808



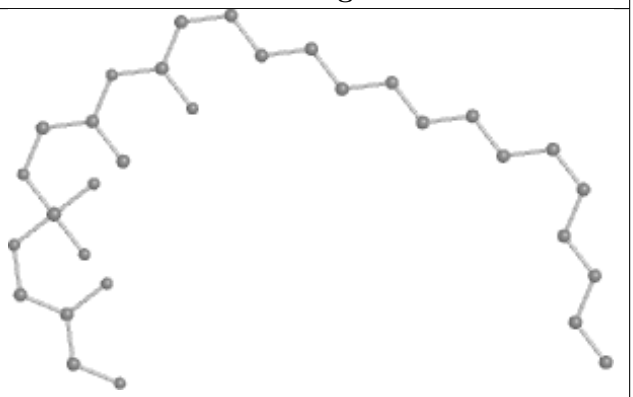
Bond lengths



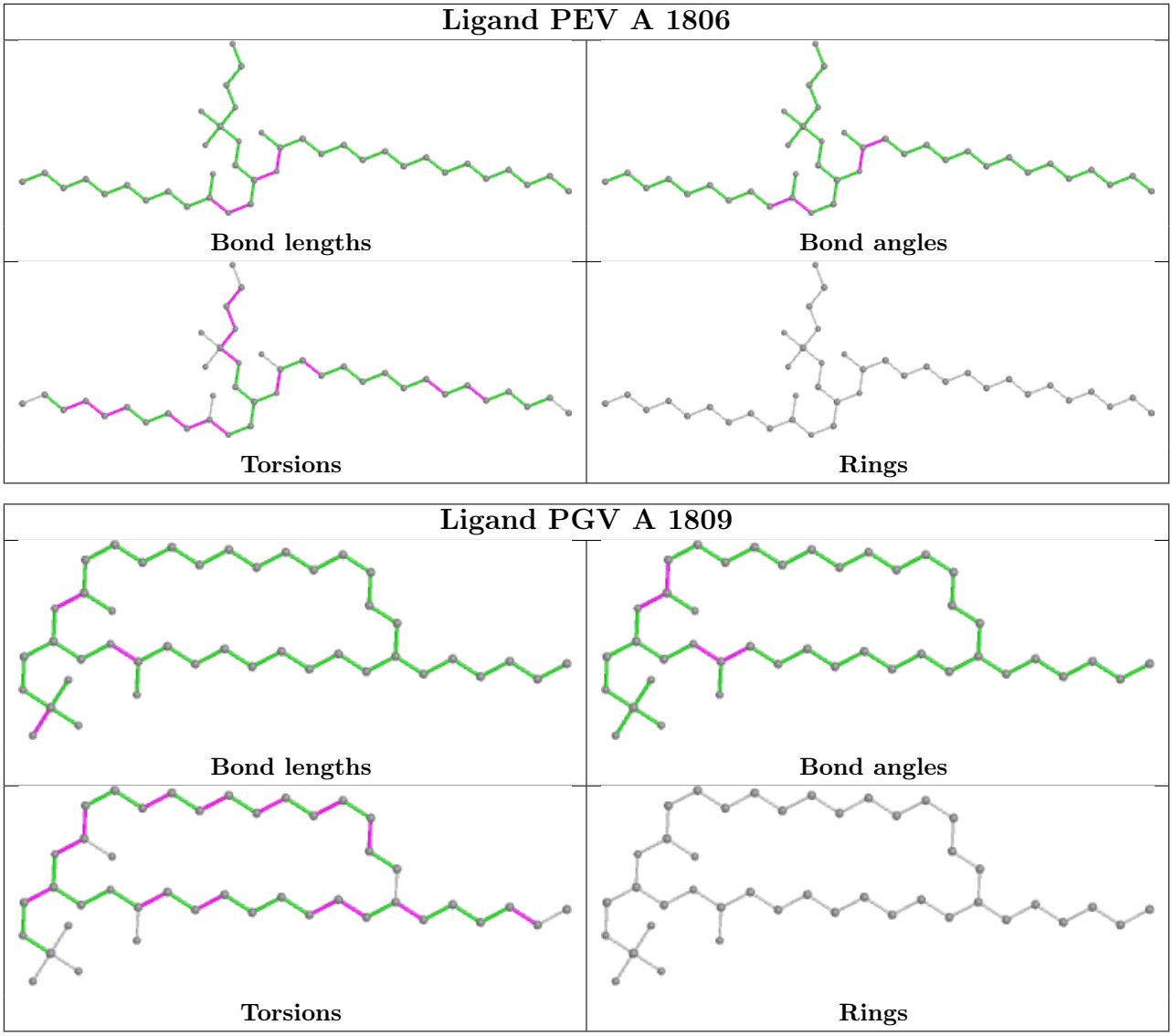
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

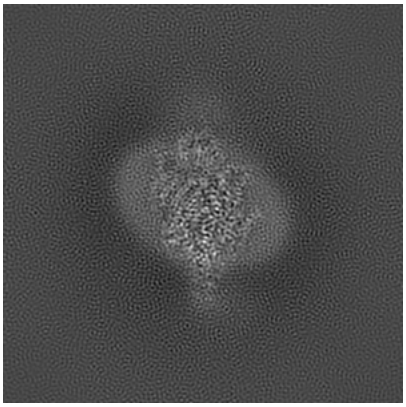
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22203. These allow visual inspection of the internal detail of the map and identification of artifacts.

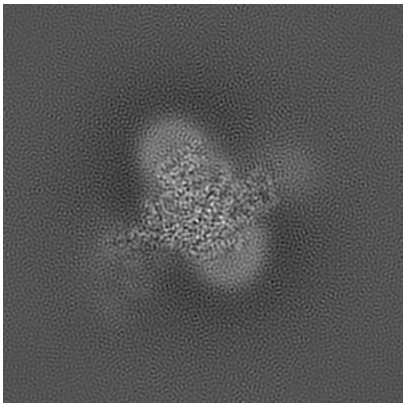
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

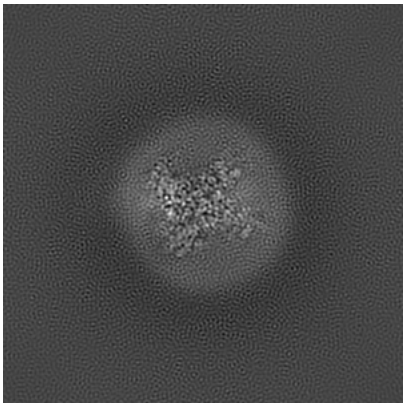
6.1.1 Primary map



X



Y

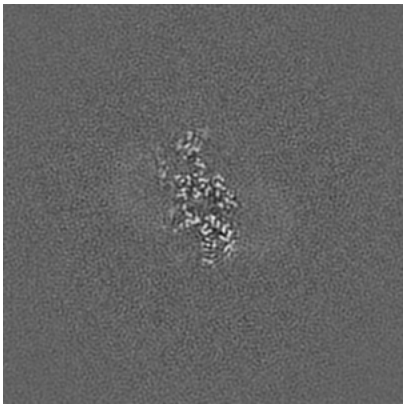


Z

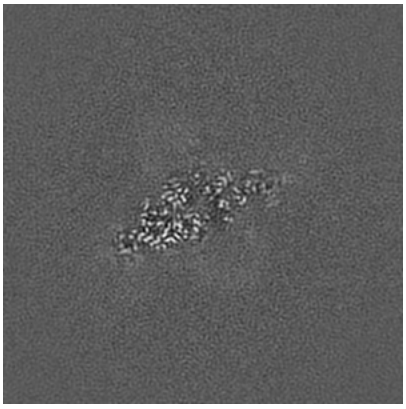
The images above show the map projected in three orthogonal directions.

6.2 Central slices

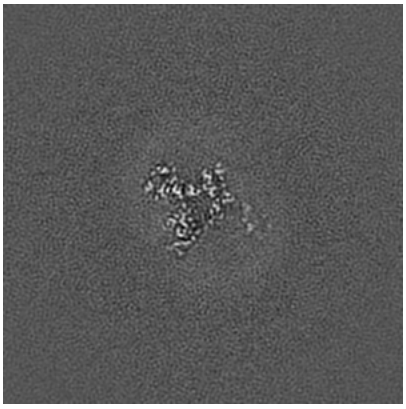
6.2.1 Primary map



X Index: 180



Y Index: 180

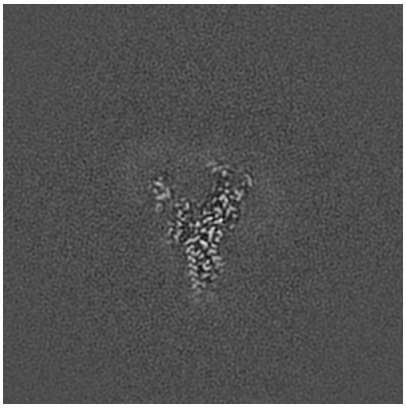


Z Index: 180

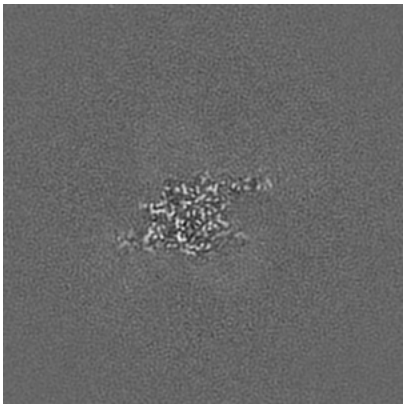
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

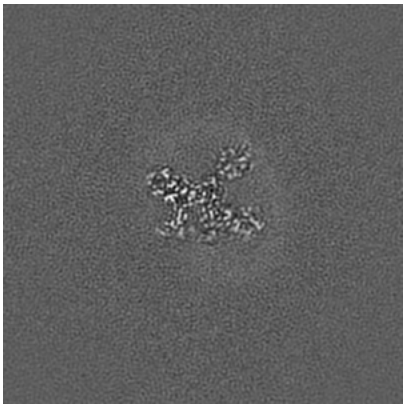
6.3.1 Primary map



X Index: 151



Y Index: 189

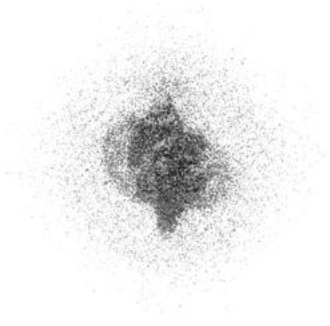


Z Index: 166

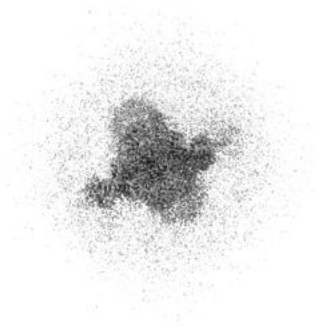
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

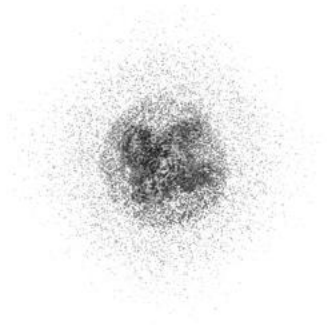
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

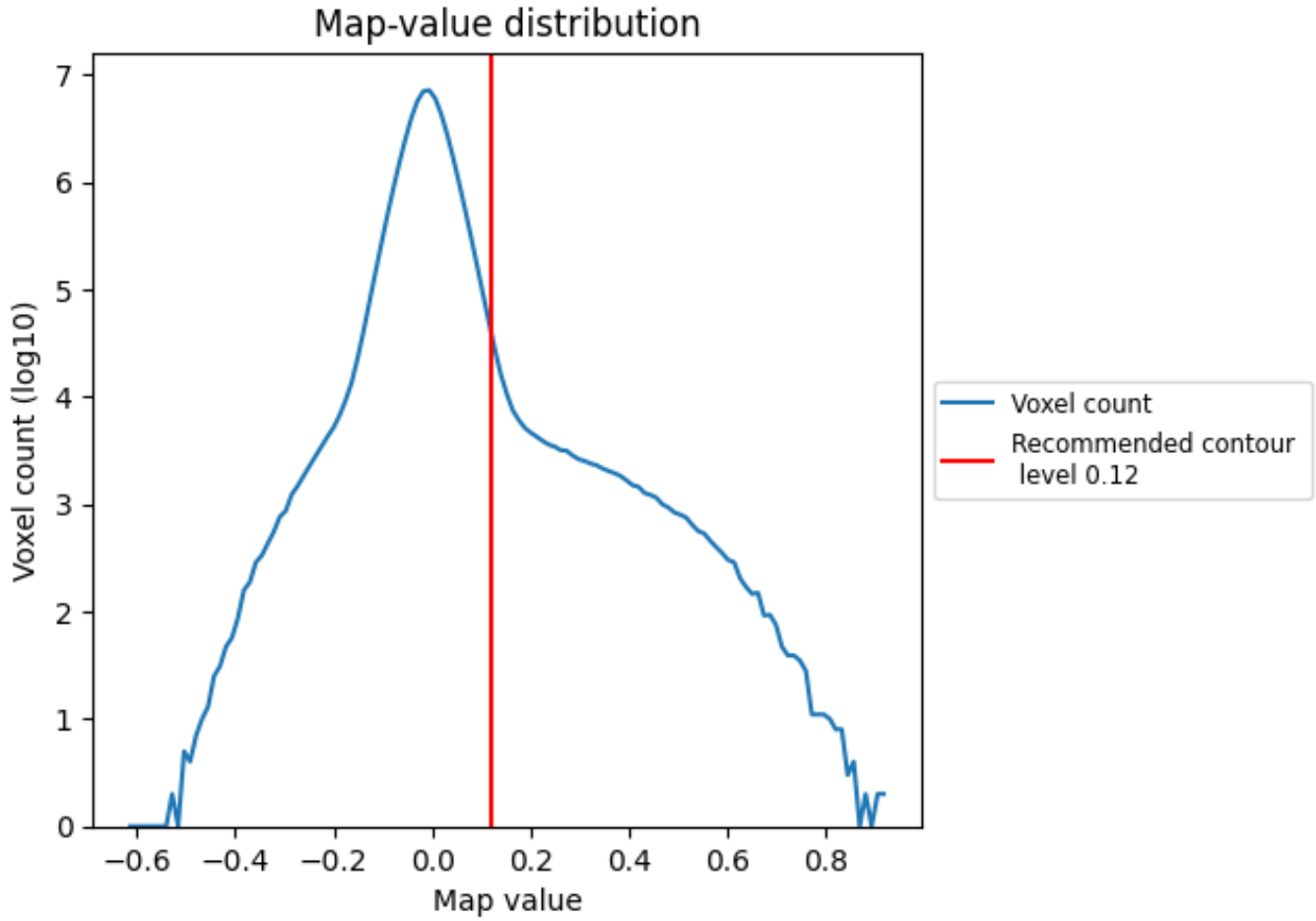
6.5 Mask visualisation (i)

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

7 Map analysis

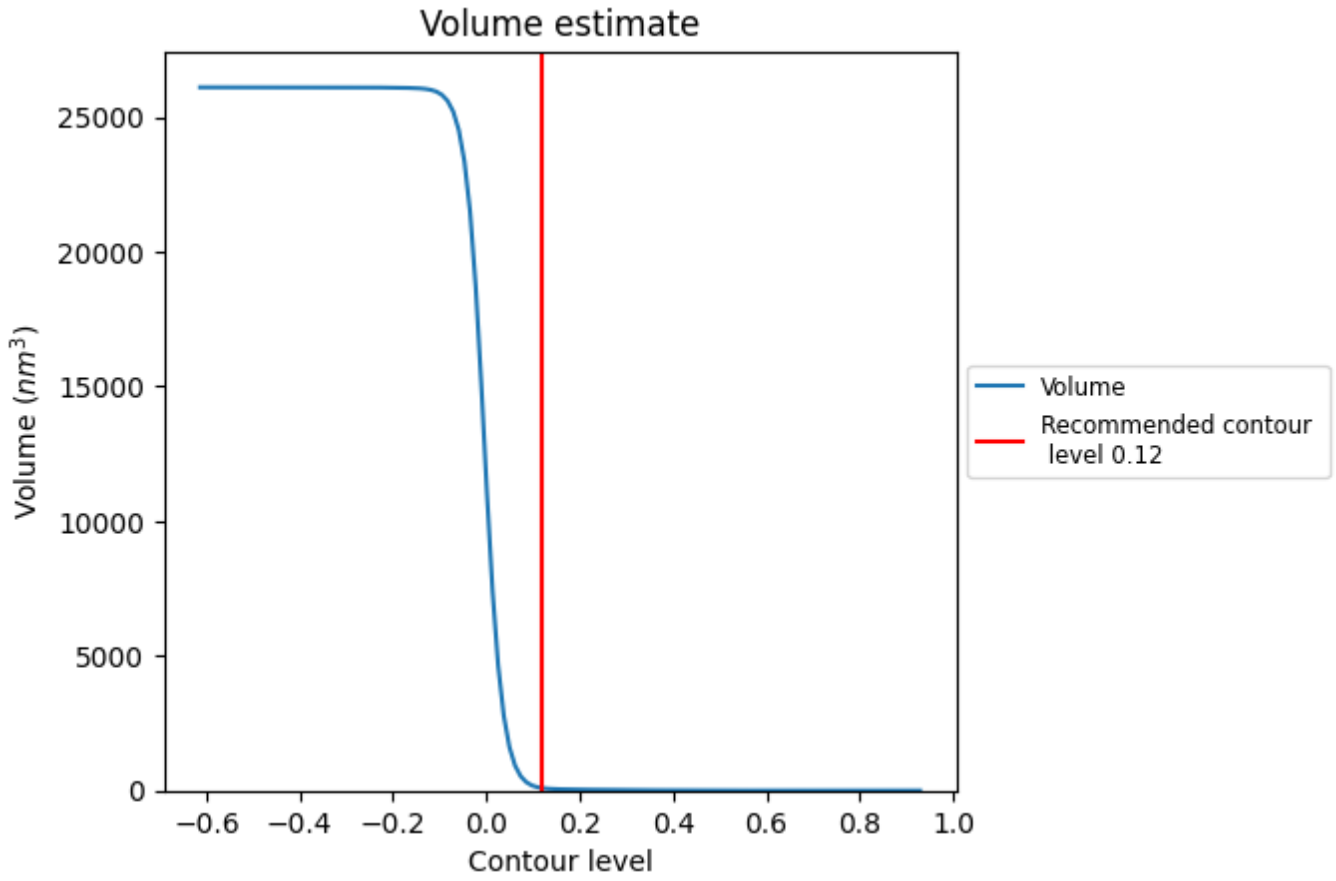
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

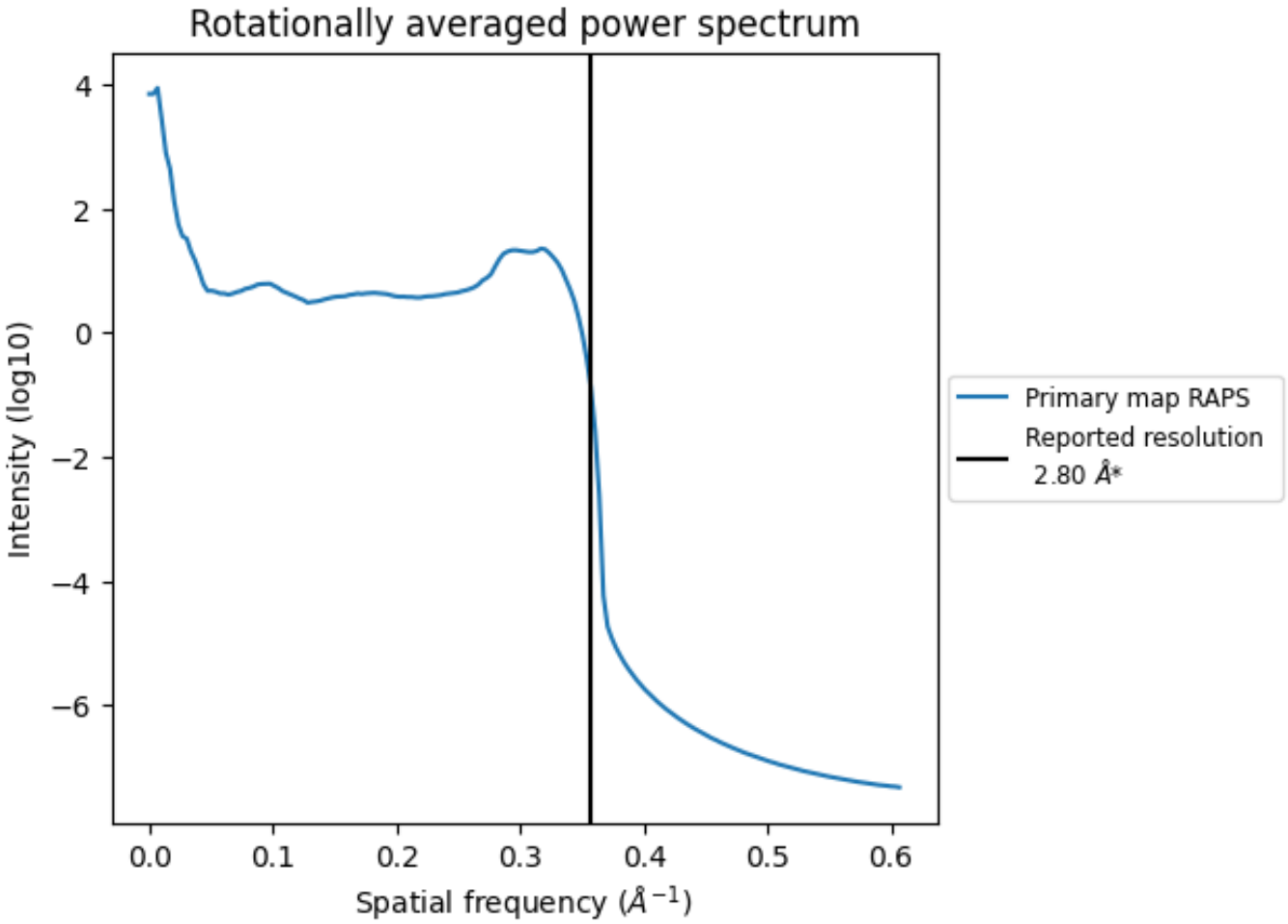
7.2 Volume estimate (i)



The volume at the recommended contour level is 93 nm^3; this corresponds to an approximate mass of 84 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

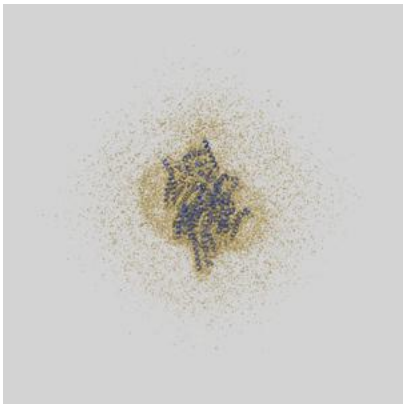
8 Fourier-Shell correlation (i)

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

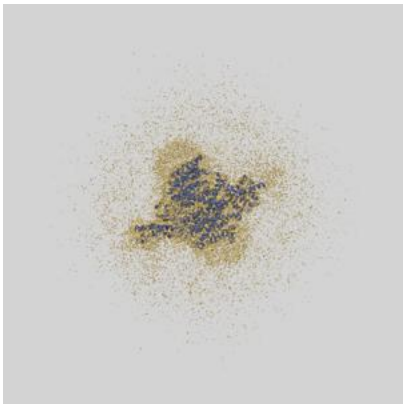
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22203 and PDB model 6XIW. Per-residue inclusion information can be found in section 3 on page 9.

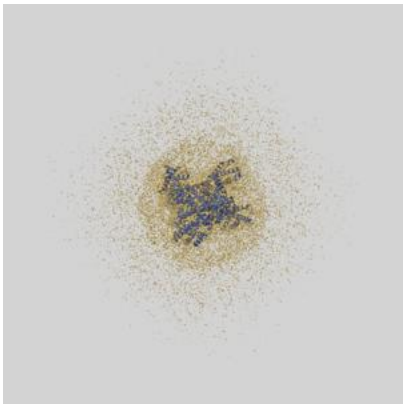
9.1 Map-model overlay



X



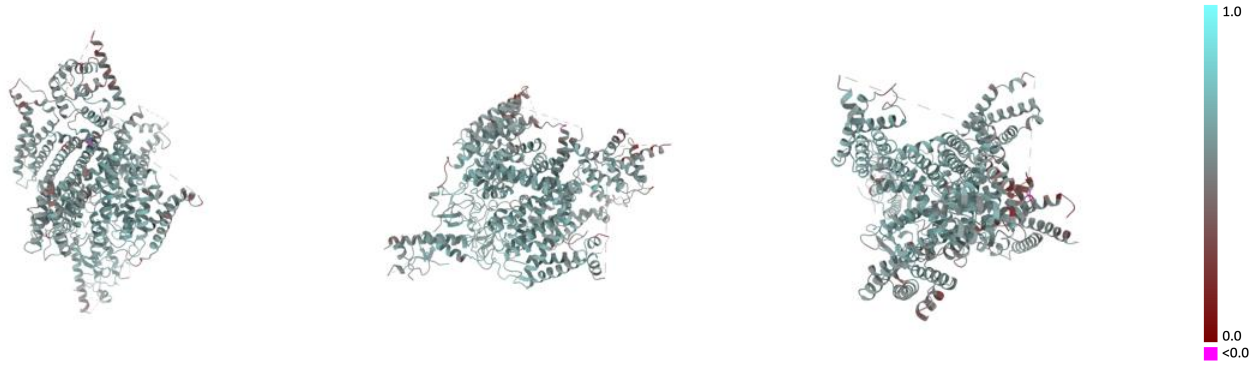
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

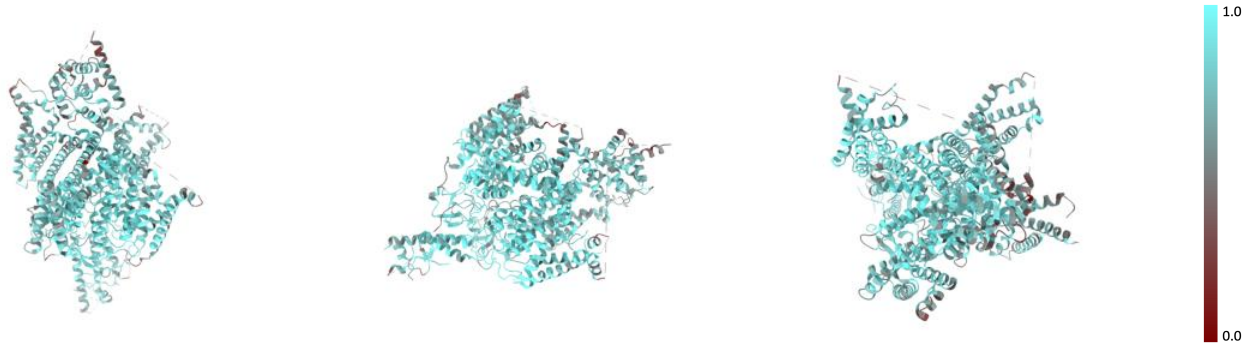
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

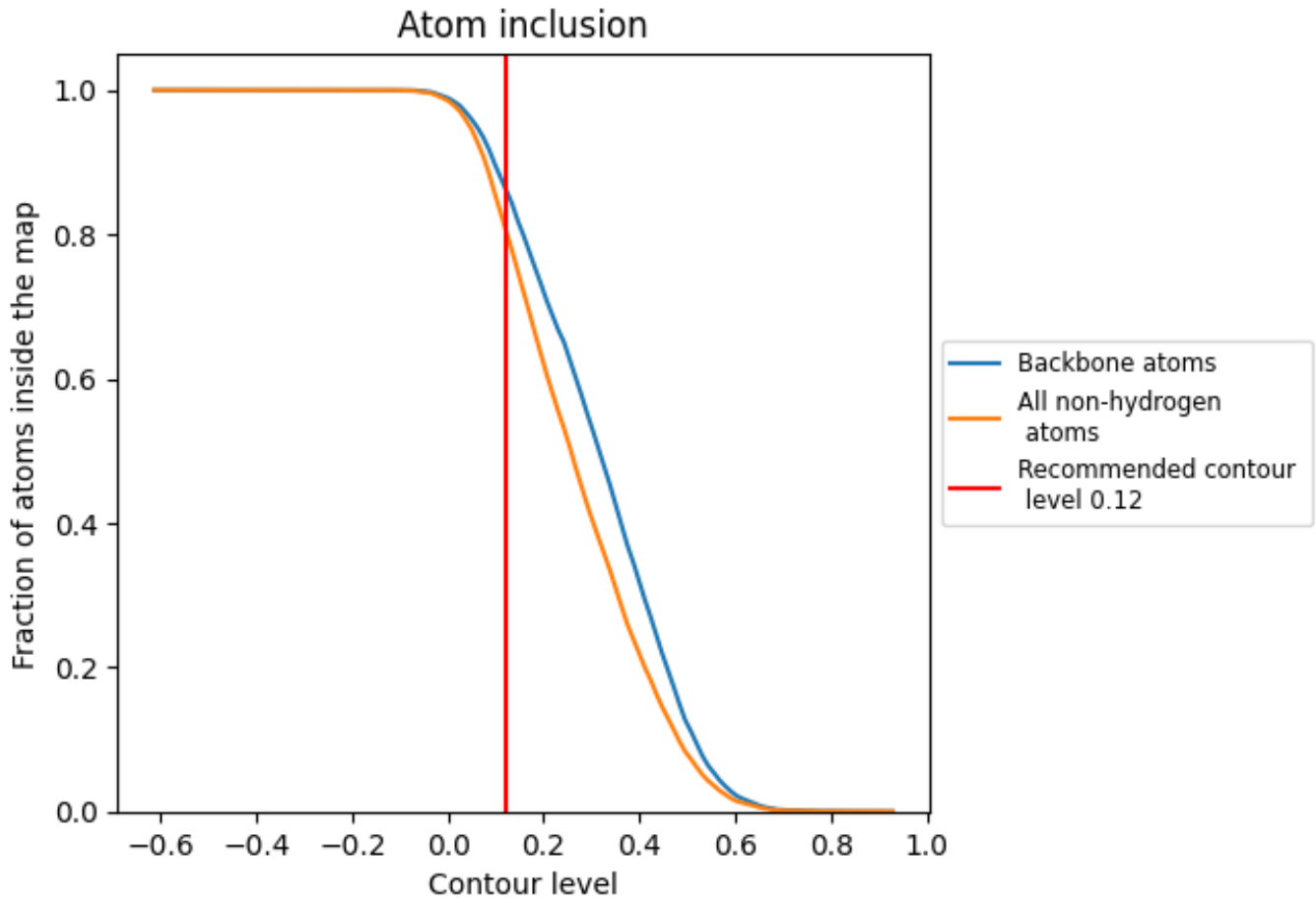
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 86% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8074	0.5720
A	0.8073	0.5720
B	0.8145	0.5730