



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 03:10 AM UTC

PDB ID : 7SX4 / pdb_00007sx4
EMDB ID : EMD-25493
Title : Human NALCN-FAM155A-UNC79-UNC80 channelosome with CaM bound, conformation 2/2
Authors : Kschonsak, M.; Chua, H.C.; Weidling, C.; Chakouri, N.; Noland, C.L.; Schott, K.; Chang, T.; Tam, C.; Patel, N.; Arthur, C.P.; Leitner, A.; Ben-Johny, M.; Ciferri, C.; Pless, S.A.; Payandeh, J.
Deposited on : 2021-11-22
Resolution : 3.50 Å(reported)

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

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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

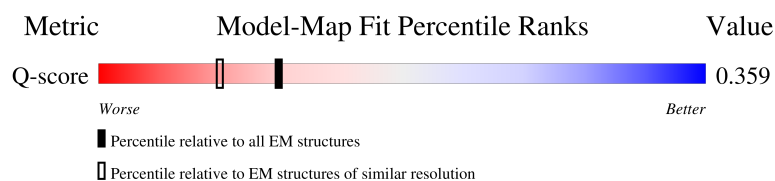
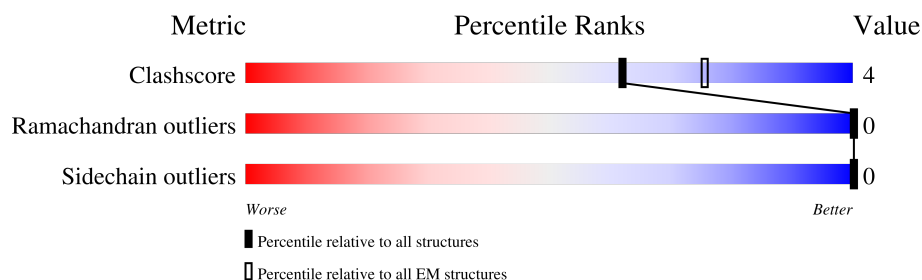
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	2042	
2	B	483	
3	C	149	

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Mol	Chain	Length	Quality of chain
4	D	2561	26%49%6%45%
5	E	3283	16%43%6%52%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 37505 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, Enhanced green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1383	11319	7463	1864	1902	90	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1739	GLY	-	linker	UNP Q8IZF0
A	1740	GLY	-	linker	UNP Q8IZF0
A	1741	SER	-	linker	UNP Q8IZF0
A	1742	LEU	-	linker	UNP Q8IZF0
A	1743	VAL	-	linker	UNP Q8IZF0
A	1744	PRO	-	linker	UNP Q8IZF0
A	1745	ARG	-	linker	UNP Q8IZF0
A	1746	GLY	-	linker	UNP Q8IZF0
A	1747	SER	-	linker	UNP Q8IZF0
A	1748	SER	-	linker	UNP Q8IZF0
A	1749	GLY	-	linker	UNP Q8IZF0
A	1750	GLU	-	linker	UNP Q8IZF0
A	1751	ASN	-	linker	UNP Q8IZF0
A	1752	LEU	-	linker	UNP Q8IZF0
A	1753	TYR	-	linker	UNP Q8IZF0
A	1754	PHE	-	linker	UNP Q8IZF0
A	1755	GLN	-	linker	UNP Q8IZF0
A	1756	GLY	-	linker	UNP Q8IZF0
A	1757	SER	-	linker	UNP Q8IZF0
A	1758	SER	-	linker	UNP Q8IZF0
A	1759	GLY	-	linker	UNP Q8IZF0
A	1966	LYS	ALA	conflict	UNP A0A7G8ZY66
A	2001	GLY	-	expression tag	UNP A0A7G8ZY66
A	2002	ASP	-	expression tag	UNP A0A7G8ZY66
A	2003	TYR	-	expression tag	UNP A0A7G8ZY66
A	2004	LYS	-	expression tag	UNP A0A7G8ZY66
A	2005	ASP	-	expression tag	UNP A0A7G8ZY66

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2006	ASP	-	expression tag	UNP A0A7G8ZY66
A	2007	ASP	-	expression tag	UNP A0A7G8ZY66
A	2008	ASP	-	expression tag	UNP A0A7G8ZY66
A	2009	LYS	-	expression tag	UNP A0A7G8ZY66
A	2010	GLY	-	expression tag	UNP A0A7G8ZY66
A	2011	SER	-	expression tag	UNP A0A7G8ZY66
A	2012	GLY	-	expression tag	UNP A0A7G8ZY66
A	2013	SER	-	expression tag	UNP A0A7G8ZY66
A	2014	ALA	-	expression tag	UNP A0A7G8ZY66
A	2015	TRP	-	expression tag	UNP A0A7G8ZY66
A	2016	SER	-	expression tag	UNP A0A7G8ZY66
A	2017	HIS	-	expression tag	UNP A0A7G8ZY66
A	2018	PRO	-	expression tag	UNP A0A7G8ZY66
A	2019	GLN	-	expression tag	UNP A0A7G8ZY66
A	2020	PHE	-	expression tag	UNP A0A7G8ZY66
A	2021	GLU	-	expression tag	UNP A0A7G8ZY66
A	2022	LYS	-	expression tag	UNP A0A7G8ZY66
A	2023	GLY	-	expression tag	UNP A0A7G8ZY66
A	2024	GLY	-	expression tag	UNP A0A7G8ZY66
A	2025	GLY	-	expression tag	UNP A0A7G8ZY66
A	2026	SER	-	expression tag	UNP A0A7G8ZY66
A	2027	GLY	-	expression tag	UNP A0A7G8ZY66
A	2028	GLY	-	expression tag	UNP A0A7G8ZY66
A	2029	GLY	-	expression tag	UNP A0A7G8ZY66
A	2030	SER	-	expression tag	UNP A0A7G8ZY66
A	2031	GLY	-	expression tag	UNP A0A7G8ZY66
A	2032	GLY	-	expression tag	UNP A0A7G8ZY66
A	2033	SER	-	expression tag	UNP A0A7G8ZY66
A	2034	ALA	-	expression tag	UNP A0A7G8ZY66
A	2035	TRP	-	expression tag	UNP A0A7G8ZY66
A	2036	SER	-	expression tag	UNP A0A7G8ZY66
A	2037	HIS	-	expression tag	UNP A0A7G8ZY66
A	2038	PRO	-	expression tag	UNP A0A7G8ZY66
A	2039	GLN	-	expression tag	UNP A0A7G8ZY66
A	2040	PHE	-	expression tag	UNP A0A7G8ZY66
A	2041	GLU	-	expression tag	UNP A0A7G8ZY66
A	2042	LYS	-	expression tag	UNP A0A7G8ZY66

- Molecule 2 is a protein called Transmembrane protein FAM155A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	151	Total	C	N	O	S	
			1241	792	191	243	15	
							0	0

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
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 a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	114	Total	C	N	O	S	0	0
			926	579	149	189	9		

- Molecule 4 is a protein called UNC79,Protein unc-79 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1406	Total	C	N	O	S	0	0
			11012	7152	1830	1936	94		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2636	GLY	-	expression tag	UNP Q9P2D8
D	2637	GLY	-	expression tag	UNP Q9P2D8
D	2638	SER	-	expression tag	UNP Q9P2D8
D	2639	GLY	-	expression tag	UNP Q9P2D8
D	2640	GLY	-	expression tag	UNP Q9P2D8
D	2641	SER	-	expression tag	UNP Q9P2D8
D	2642	ASP	-	expression tag	UNP Q9P2D8
D	2643	TYR	-	expression tag	UNP Q9P2D8
D	2644	LYS	-	expression tag	UNP Q9P2D8
D	2645	ASP	-	expression tag	UNP Q9P2D8
D	2646	ASP	-	expression tag	UNP Q9P2D8
D	2647	ASP	-	expression tag	UNP Q9P2D8
D	2648	ASP	-	expression tag	UNP Q9P2D8
D	2649	LYS	-	expression tag	UNP Q9P2D8
D	2650	GLY	-	expression tag	UNP Q9P2D8
D	2651	ASN	-	expression tag	UNP Q9P2D8
D	2652	SER	-	expression tag	UNP Q9P2D8
D	2653	ASP	-	expression tag	UNP Q9P2D8
D	2654	TYR	-	expression tag	UNP Q9P2D8
D	2655	LYS	-	expression tag	UNP Q9P2D8
D	2656	ASP	-	expression tag	UNP Q9P2D8
D	2657	ASP	-	expression tag	UNP Q9P2D8
D	2658	ASP	-	expression tag	UNP Q9P2D8
D	2659	ASP	-	expression tag	UNP Q9P2D8
D	2660	LYS	-	expression tag	UNP Q9P2D8

- Molecule 5 is a protein called Protein unc-80 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1587	Total	C	N	O	S	0	0
			12799	8306	2171	2232	90		

There are 25 discrepancies between the modelled and reference sequences:

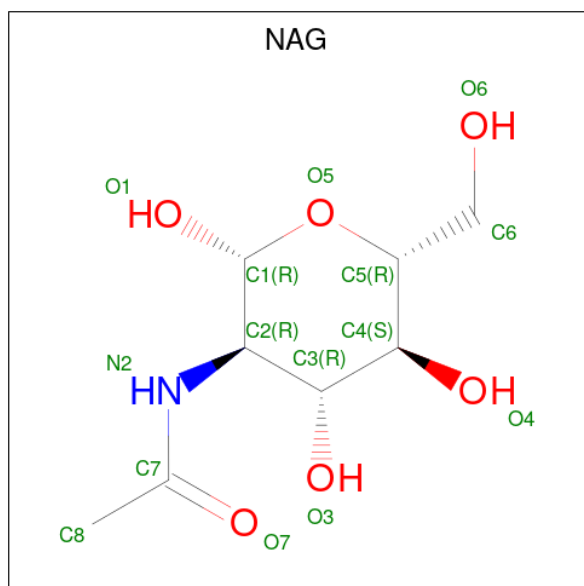
Chain	Residue	Modelled	Actual	Comment	Reference
E	3259	GLY	-	expression tag	UNP Q8N2C7
E	3260	GLY	-	expression tag	UNP Q8N2C7
E	3261	SER	-	expression tag	UNP Q8N2C7
E	3262	GLY	-	expression tag	UNP Q8N2C7
E	3263	GLY	-	expression tag	UNP Q8N2C7
E	3264	SER	-	expression tag	UNP Q8N2C7
E	3265	ASP	-	expression tag	UNP Q8N2C7
E	3266	TYR	-	expression tag	UNP Q8N2C7

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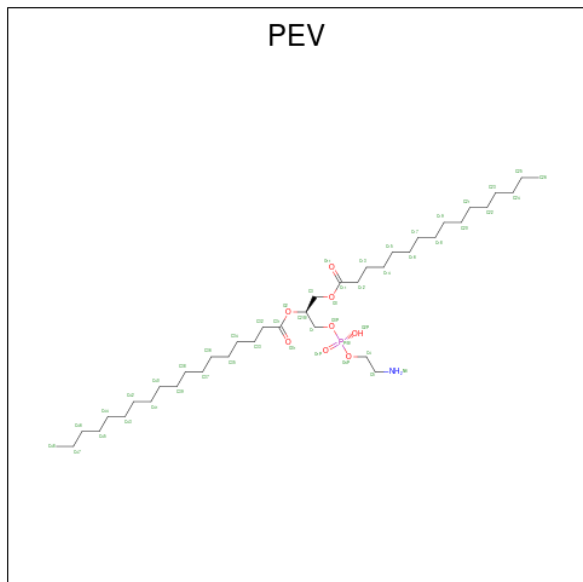
Chain	Residue	Modelled	Actual	Comment	Reference
E	3267	LYS	-	expression tag	UNP Q8N2C7
E	3268	ASP	-	expression tag	UNP Q8N2C7
E	3269	ASP	-	expression tag	UNP Q8N2C7
E	3270	ASP	-	expression tag	UNP Q8N2C7
E	3271	ASP	-	expression tag	UNP Q8N2C7
E	3272	LYS	-	expression tag	UNP Q8N2C7
E	3273	GLY	-	expression tag	UNP Q8N2C7
E	3274	ASN	-	expression tag	UNP Q8N2C7
E	3275	SER	-	expression tag	UNP Q8N2C7
E	3276	ASP	-	expression tag	UNP Q8N2C7
E	3277	TYR	-	expression tag	UNP Q8N2C7
E	3278	LYS	-	expression tag	UNP Q8N2C7
E	3279	ASP	-	expression tag	UNP Q8N2C7
E	3280	ASP	-	expression tag	UNP Q8N2C7
E	3281	ASP	-	expression tag	UNP Q8N2C7
E	3282	ASP	-	expression tag	UNP Q8N2C7
E	3283	LYS	-	expression tag	UNP Q8N2C7

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



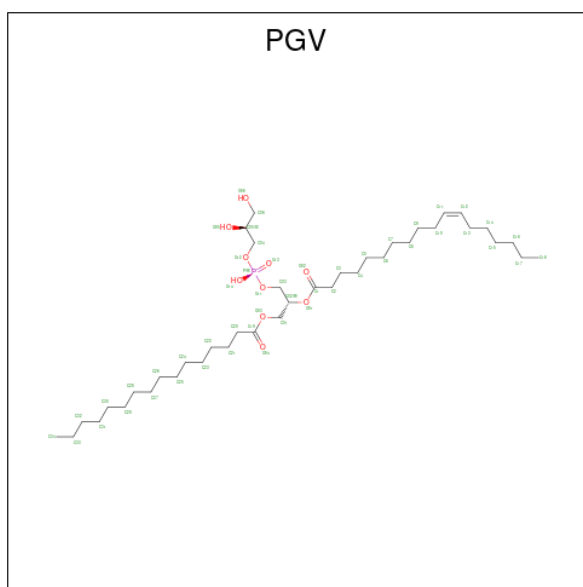
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C₃₉H₇₈NO₈P).



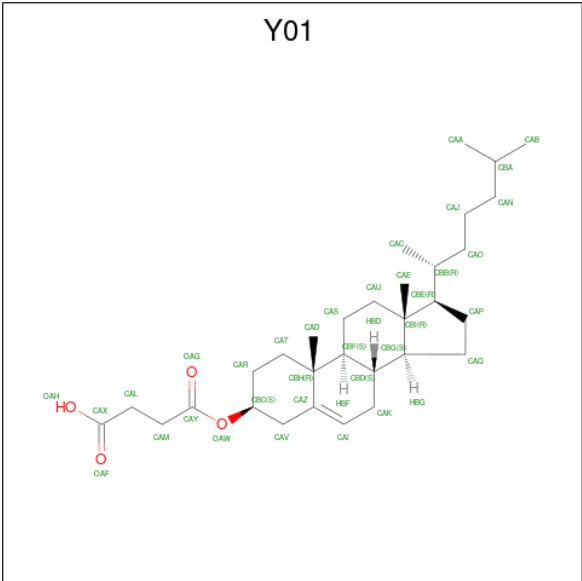
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	35	25	1	8	1	0

- Molecule 8 is (1R)-2-[[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 9 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).

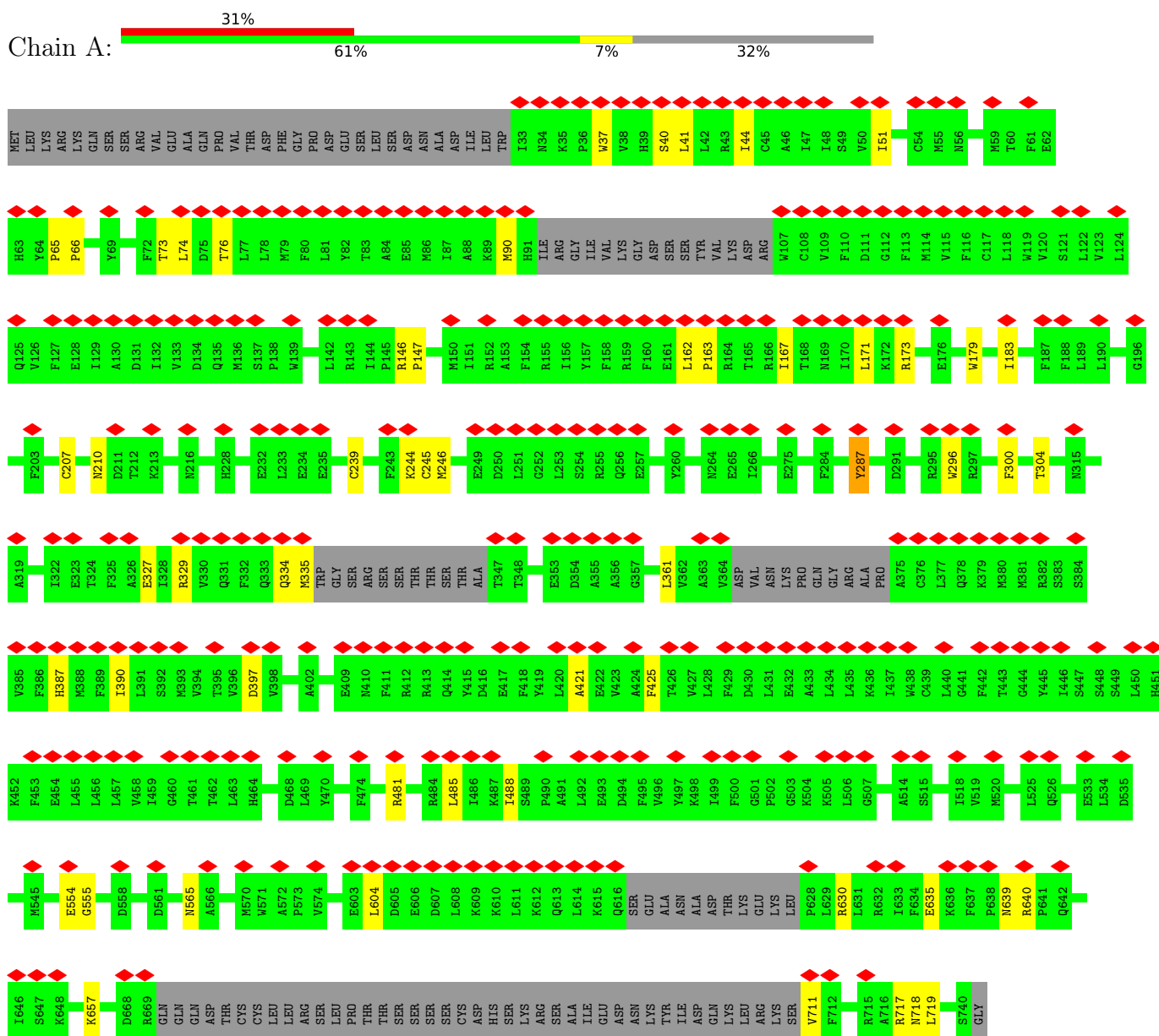


Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			35	31	4	
9	A	1	Total	C	O	0
			35	31	4	
9	A	1	Total	C	O	0
			35	31	4	

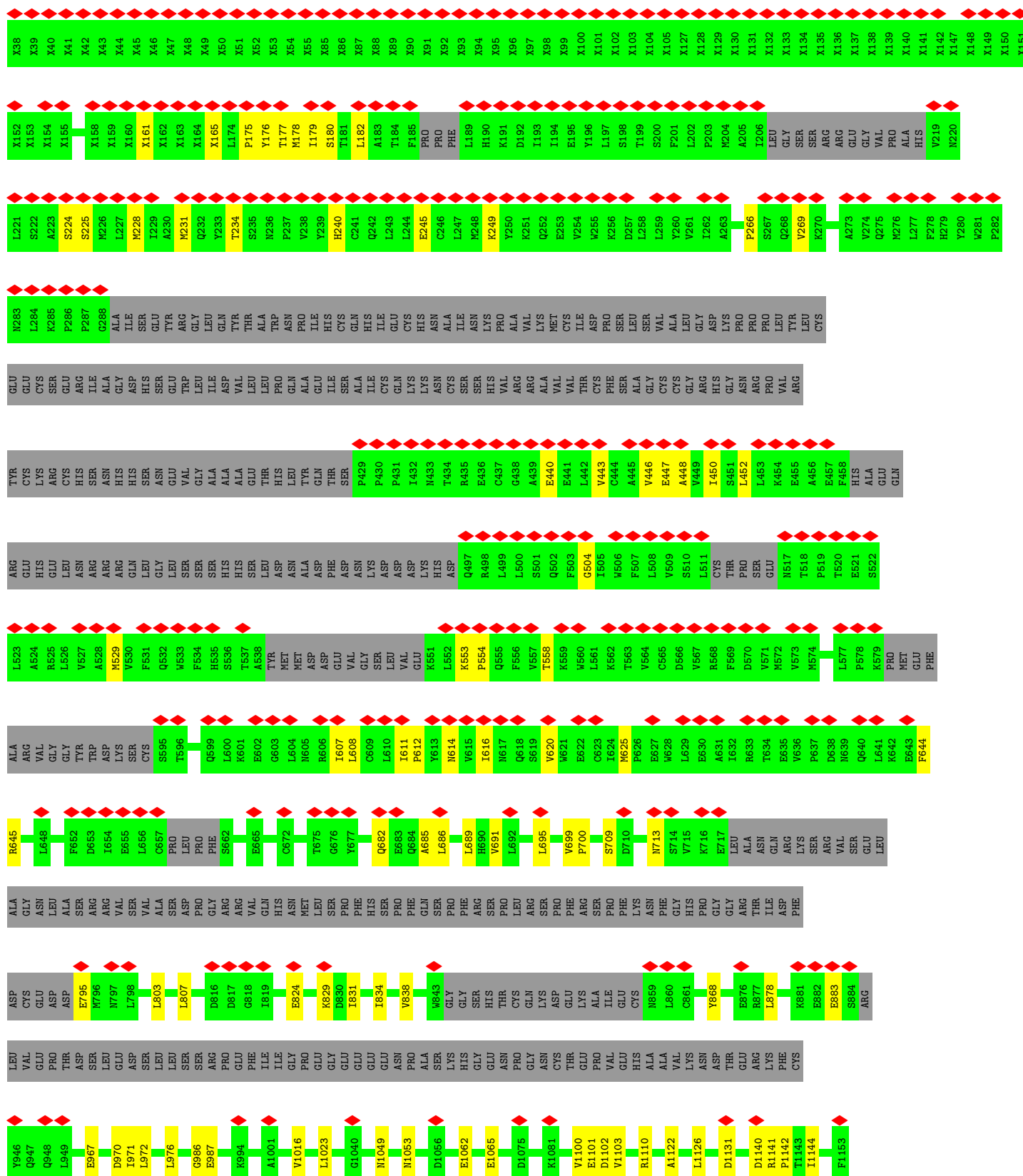
3 Residue-property plots

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

- Molecule 1: Sodium leak channel non-selective protein,Enhanced green fluorescent protein















[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56037	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; selected micrographs with a CTF fit of 10.0 Å or better	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	64.009	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	43.384	Depositor
Minimum map value	-32.628	Depositor
Average map value	-0.044	Depositor
Map value standard deviation	2.276	Depositor
Recommended contour level	8	Depositor
Map size (Å)	469.28, 469.28, 469.28	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1732, 1.1732, 1.1732	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.11	0/11587	0.29	0/15684
2	B	0.11	0/1271	0.27	0/1720
3	C	0.10	0/932	0.32	0/1240
4	D	0.11	0/10866	0.29	0/14708
5	E	0.13	0/13083	0.32	0/17737
All	All	0.12	0/37739	0.30	0/51089

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11319	0	11559	90	0
2	B	1241	0	1134	9	0
3	C	926	0	892	4	0
4	D	11012	0	10986	104	0
5	E	12799	0	13059	128	0
6	A	28	0	26	0	0
7	A	35	0	43	0	0
8	A	40	0	51	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	105	0	147	3	0
All	All	37505	0	37897	321	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 4.

The worst 5 of 321 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)
5:E:2419:THR:HG23	5:E:2539:GLU:HG3	1.57	0.83
9:A:2107:Y01:HAC1	9:A:2107:Y01:HAE2	1.65	0.78
5:E:2419:THR:HG23	5:E:2539:GLU:CG	2.14	0.78
4:D:1397:MET:SD	5:E:1876:GLN:NE2	2.60	0.74
2:B:349:ASP:OD1	2:B:350:GLU:N	2.20	0.74

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	1366/2042 (67%)	1335 (98%)	31 (2%)	0	100	100
2	B	143/483 (30%)	141 (99%)	2 (1%)	0	100	100
3	C	102/149 (68%)	100 (98%)	2 (2%)	0	100	100
4	D	1278/2561 (50%)	1252 (98%)	26 (2%)	0	100	100
5	E	1531/3283 (47%)	1493 (98%)	38 (2%)	0	100	100
All	All	4420/8518 (52%)	4321 (98%)	99 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1248/1822 (68%)	1248 (100%)	0	100	100
2	B	142/417 (34%)	142 (100%)	0	100	100
3	C	102/127 (80%)	102 (100%)	0	100	100
4	D	1200/2219 (54%)	1200 (100%)	0	100	100
5	E	1421/2873 (50%)	1421 (100%)	0	100	100
All	All	4113/7458 (55%)	4113 (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. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	2393	HIS
5	E	2498	ASN
5	E	1267	GLN
5	E	2856	GLN
5	E	2119	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.64	3 (20%)	15,22,24	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TYS	A	287	1	-	4/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	TYS	O1-S	4.28	1.63	1.45
1	A	287	TYS	OH-CZ	-3.36	1.37	1.42
1	A	287	TYS	OH-S	-2.37	1.53	1.58

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	287	TYS	CZ-OH-S-O1
1	A	287	TYS	CA-CB-CG-CD2
1	A	287	TYS	CA-CB-CG-CD1
1	A	287	TYS	CZ-OH-S-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	287	TYS	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 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
6	NAG	A	2101	-	14,14,15	0.20	0	17,19,21	0.42	0
7	PEV	A	2103	-	34,34,48	1.23	3 (8%)	37,39,53	1.12	2 (5%)
9	Y01	A	2105	-	38,38,38	1.35	5 (13%)	57,57,57	1.94	9 (15%)
9	Y01	A	2106	-	38,38,38	1.21	3 (7%)	57,57,57	1.92	11 (19%)
8	PGV	A	2104	-	39,39,50	1.08	5 (12%)	42,44,56	1.13	2 (4%)
6	NAG	A	2102	1	14,14,15	0.24	0	17,19,21	0.42	0
9	Y01	A	2107	-	38,38,38	1.28	4 (10%)	57,57,57	1.97	13 (22%)

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
6	NAG	A	2101	-	-	1/6/23/26	0/1/1/1
7	PEV	A	2103	-	-	15/38/38/52	-
9	Y01	A	2105	-	-	9/19/77/77	0/4/4/4
9	Y01	A	2106	-	-	4/19/77/77	0/4/4/4
8	PGV	A	2104	-	-	16/41/41/55	-
6	NAG	A	2102	1	-	0/6/23/26	0/1/1/1
9	Y01	A	2107	-	-	10/19/77/77	0/4/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2105	Y01	CAK-CAI	-4.52	1.41	1.50
9	A	2107	Y01	CAK-CAI	-4.51	1.41	1.50
9	A	2106	Y01	CAK-CAI	-4.36	1.41	1.50
7	A	2103	PEV	O3-C11	3.10	1.42	1.33

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2103	PEV	O2-C31	2.99	1.42	1.34

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2106	Y01	CAV-CAZ-CBH	7.68	126.25	116.42
9	A	2105	Y01	CAV-CAZ-CBH	7.61	126.17	116.42
9	A	2107	Y01	CAV-CAZ-CBH	7.45	125.96	116.42
9	A	2106	Y01	OAW-CAY-CAM	5.28	122.90	111.48
9	A	2107	Y01	OAW-CAY-OAG	-5.26	111.40	123.70

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

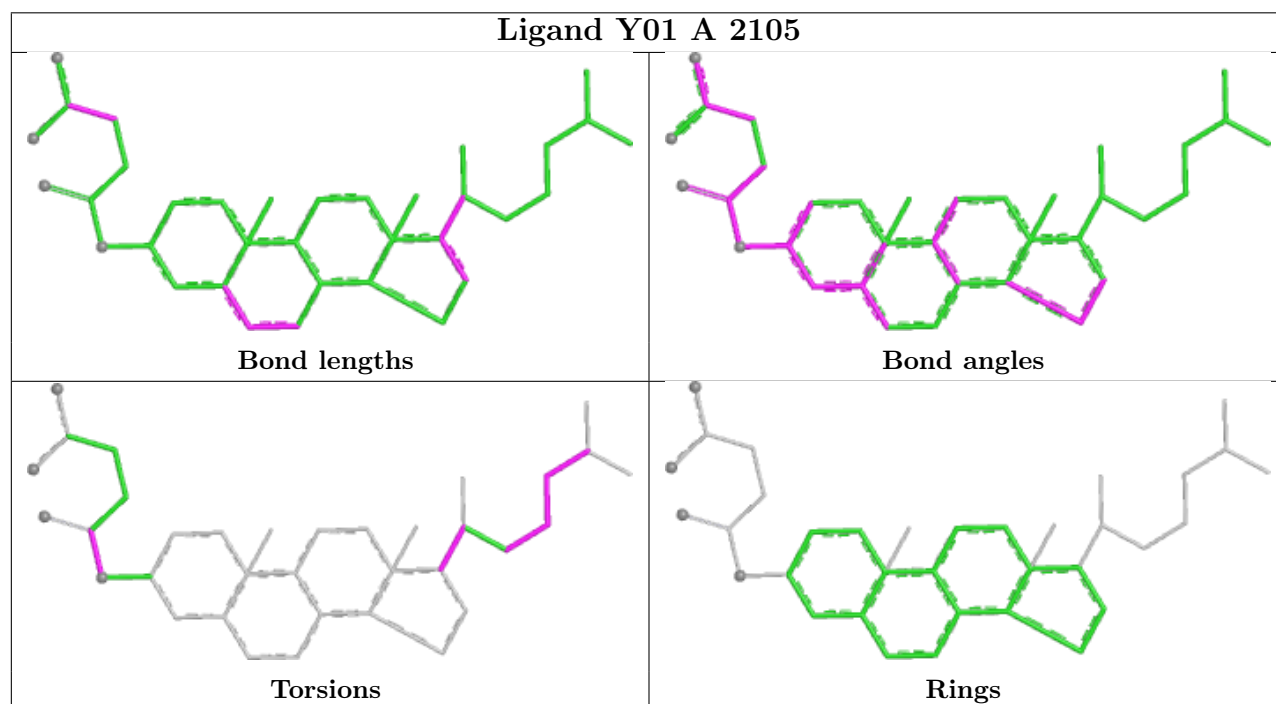
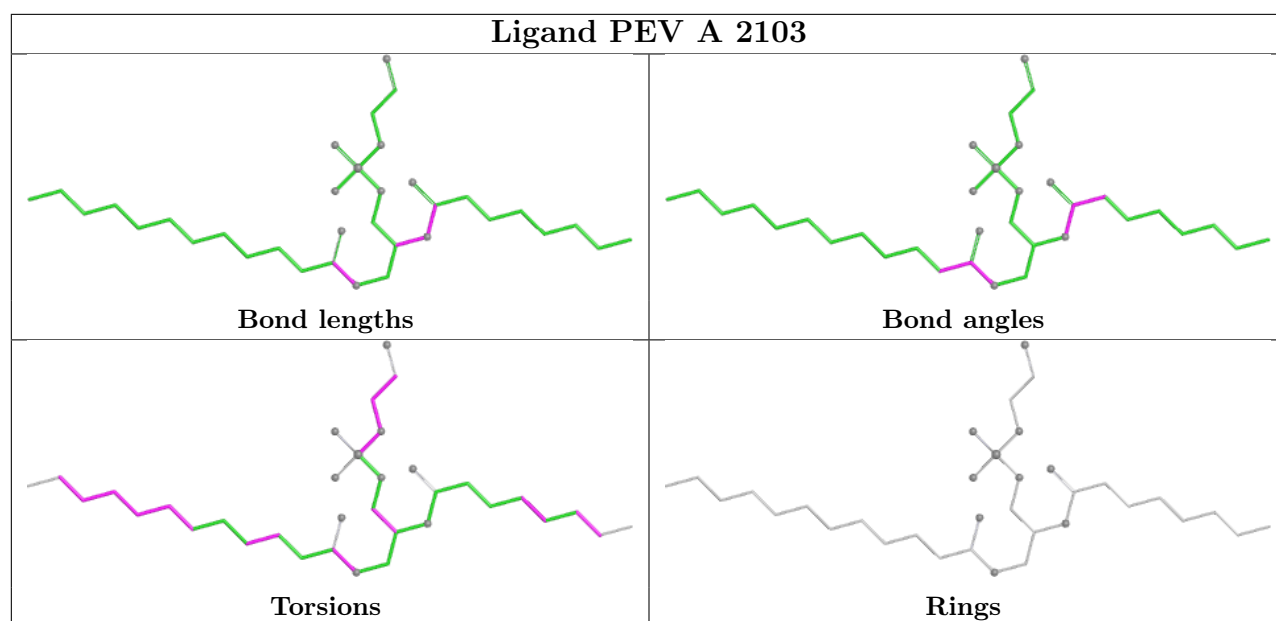
Mol	Chain	Res	Type	Atoms
7	A	2103	PEV	C5-C4-O4P-P
7	A	2103	PEV	O4P-C4-C5-N6
8	A	2104	PGV	C2-C1-O01-C02
9	A	2107	Y01	OAG-CAY-OAW-CBC
9	A	2107	Y01	CAM-CAY-OAW-CBC

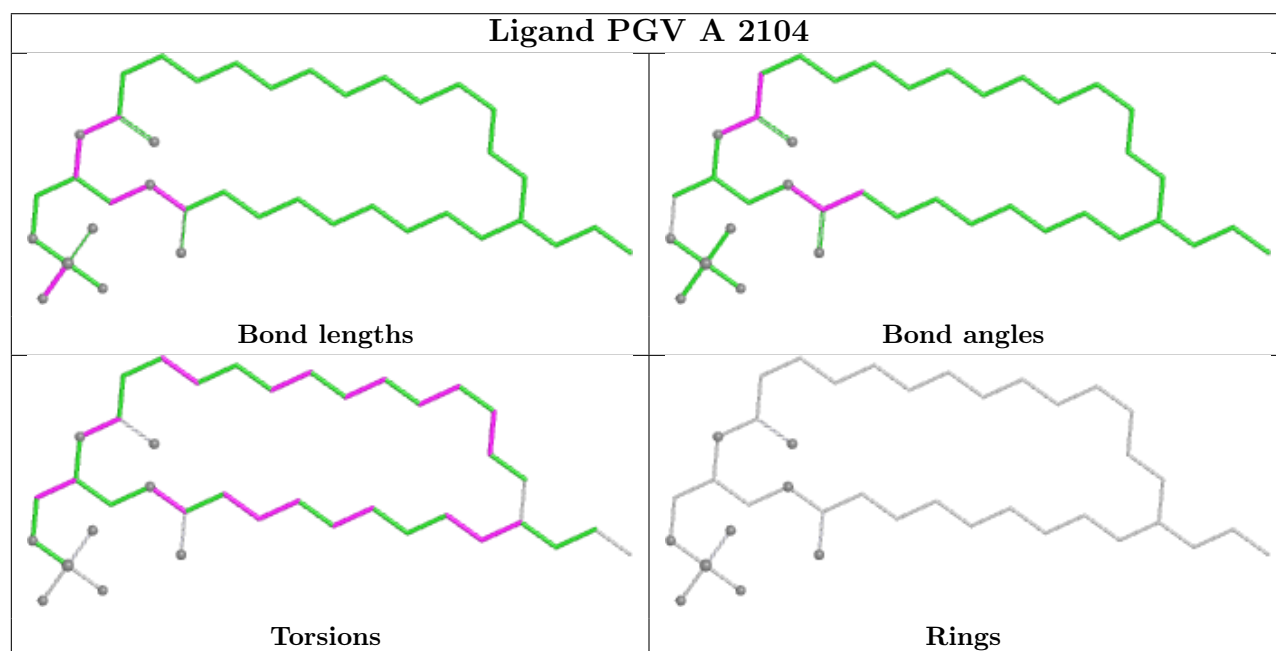
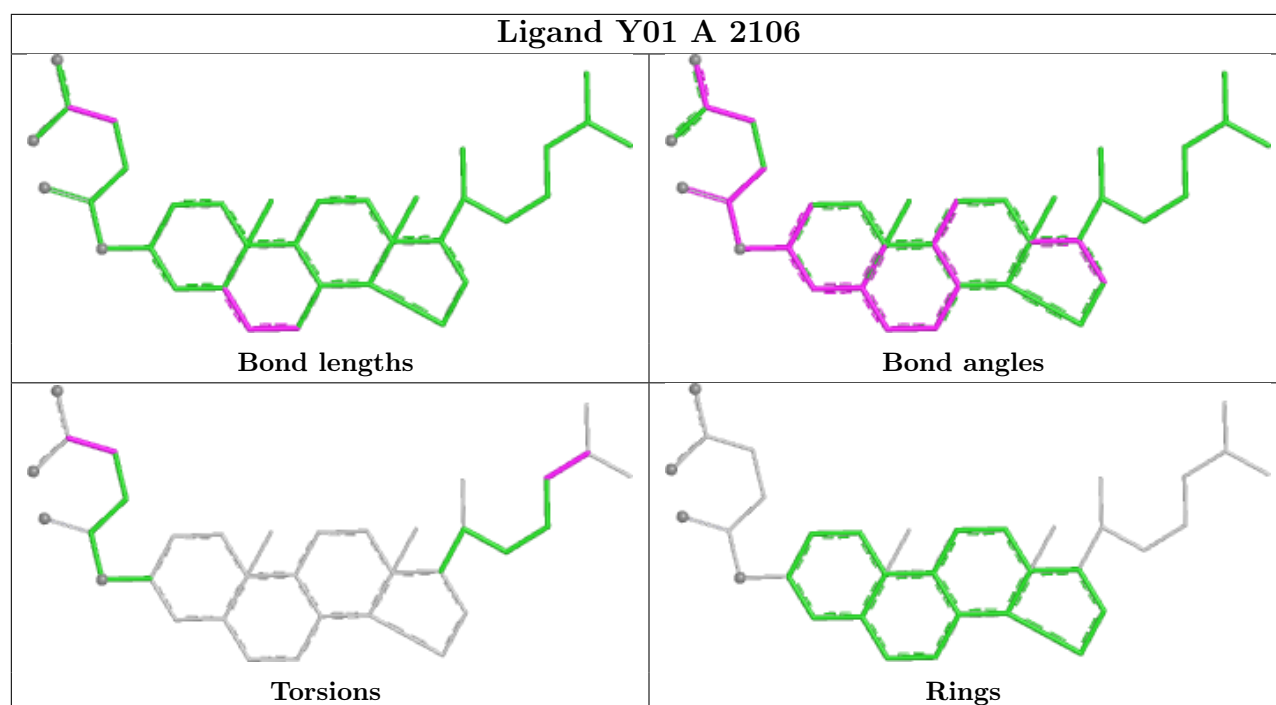
There are no ring outliers.

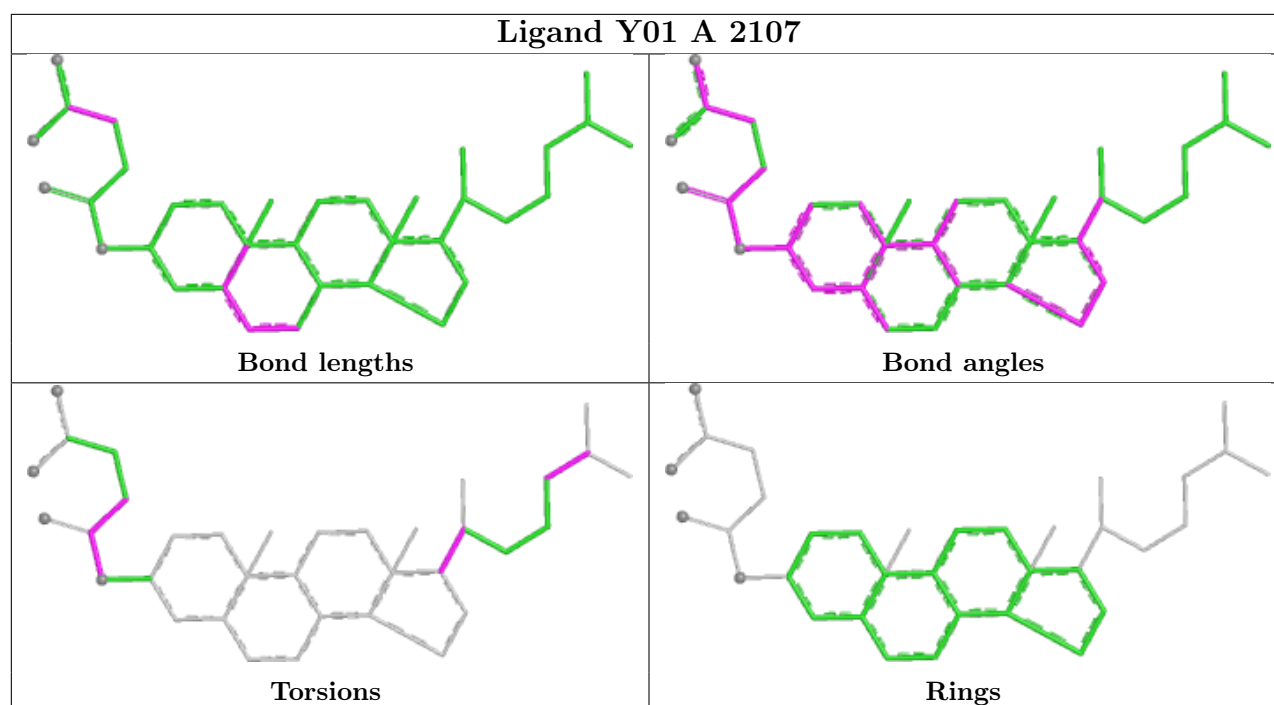
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2106	Y01	1	0
9	A	2107	Y01	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	105:UNK	C	127:UNK	N	15.52
1	D	55:UNK	C	85:UNK	N	11.89
1	D	165:UNK	C	174:LEU	N	11.70
1	D	142:UNK	C	147:UNK	N	10.07

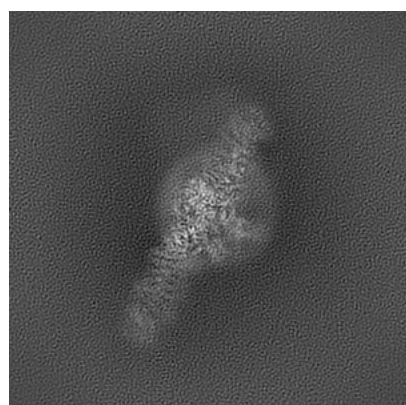
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25493. These allow visual inspection of the internal detail of the map and identification of artifacts.

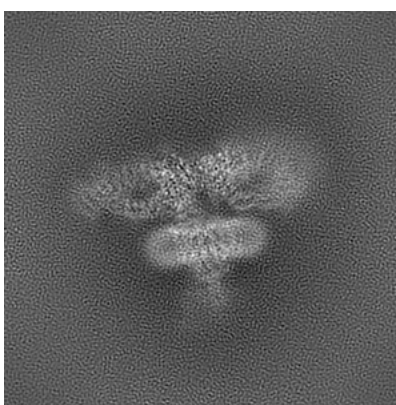
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

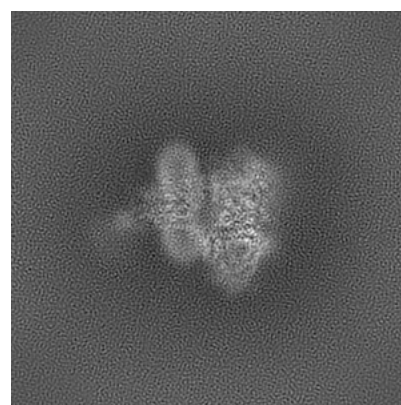
6.1.1 Primary map



X



Y

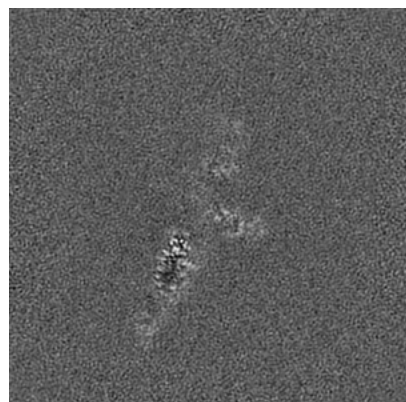


Z

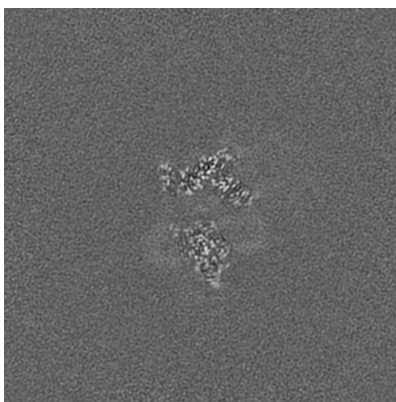
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

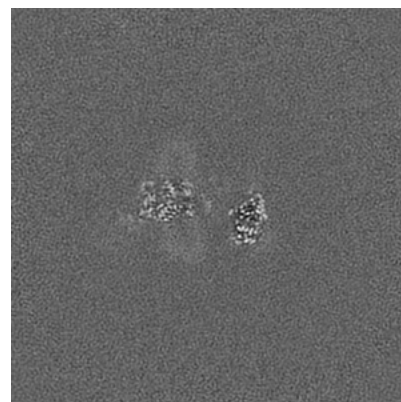
6.2.1 Primary map



X Index: 200



Y Index: 200

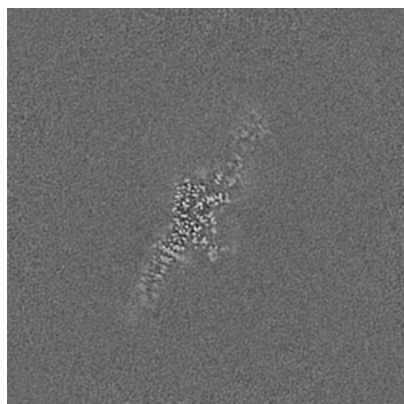


Z Index: 200

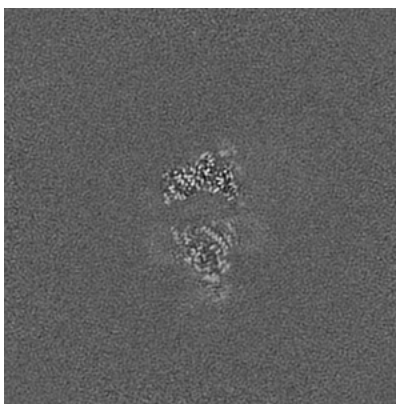
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

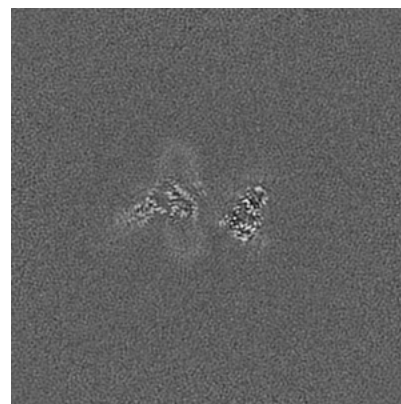
6.3.1 Primary map



X Index: 237



Y Index: 193

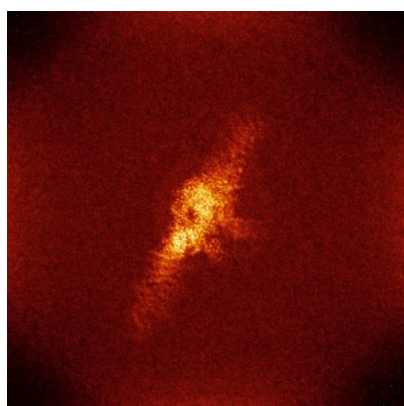


Z Index: 208

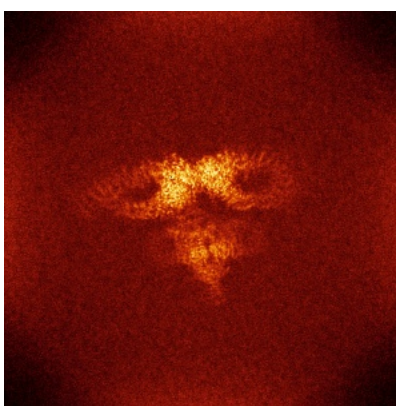
The images above show the largest variance slices of the map in three orthogonal directions.

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

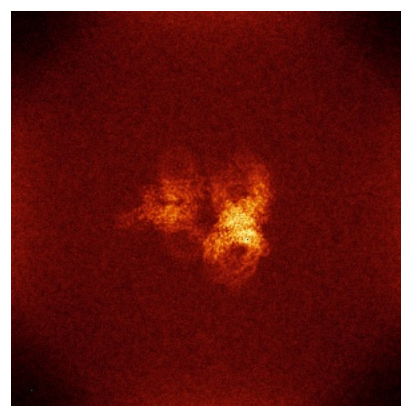
6.4.1 Primary map



X



Y

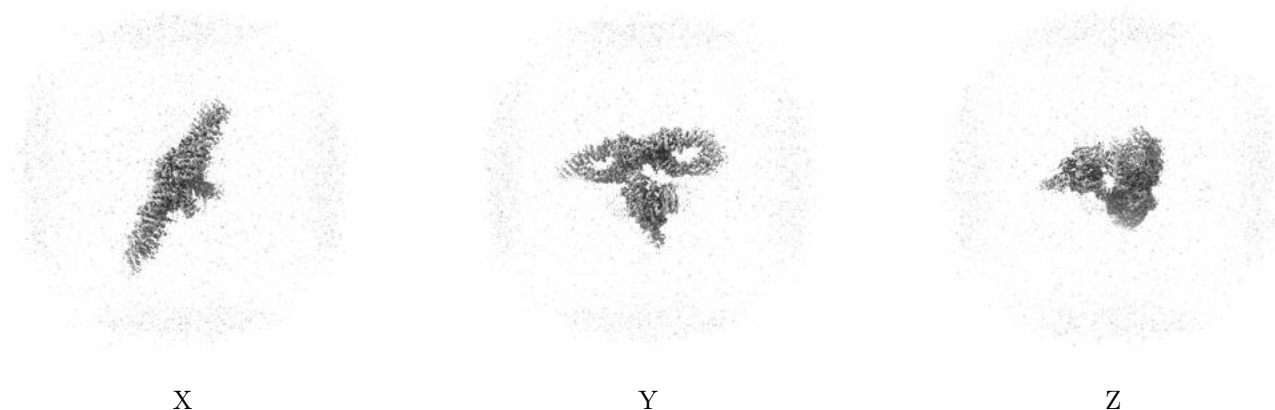


Z

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

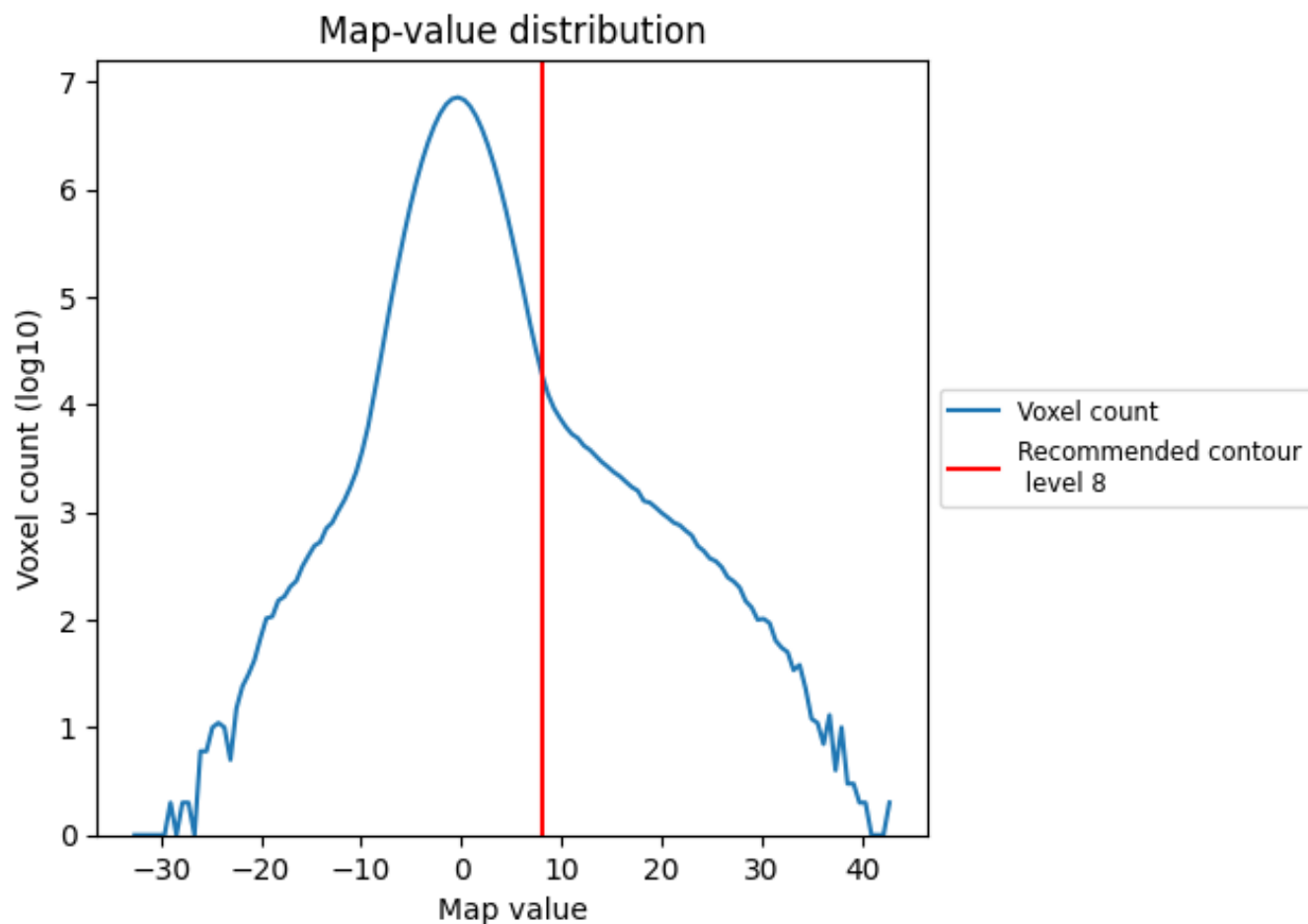
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

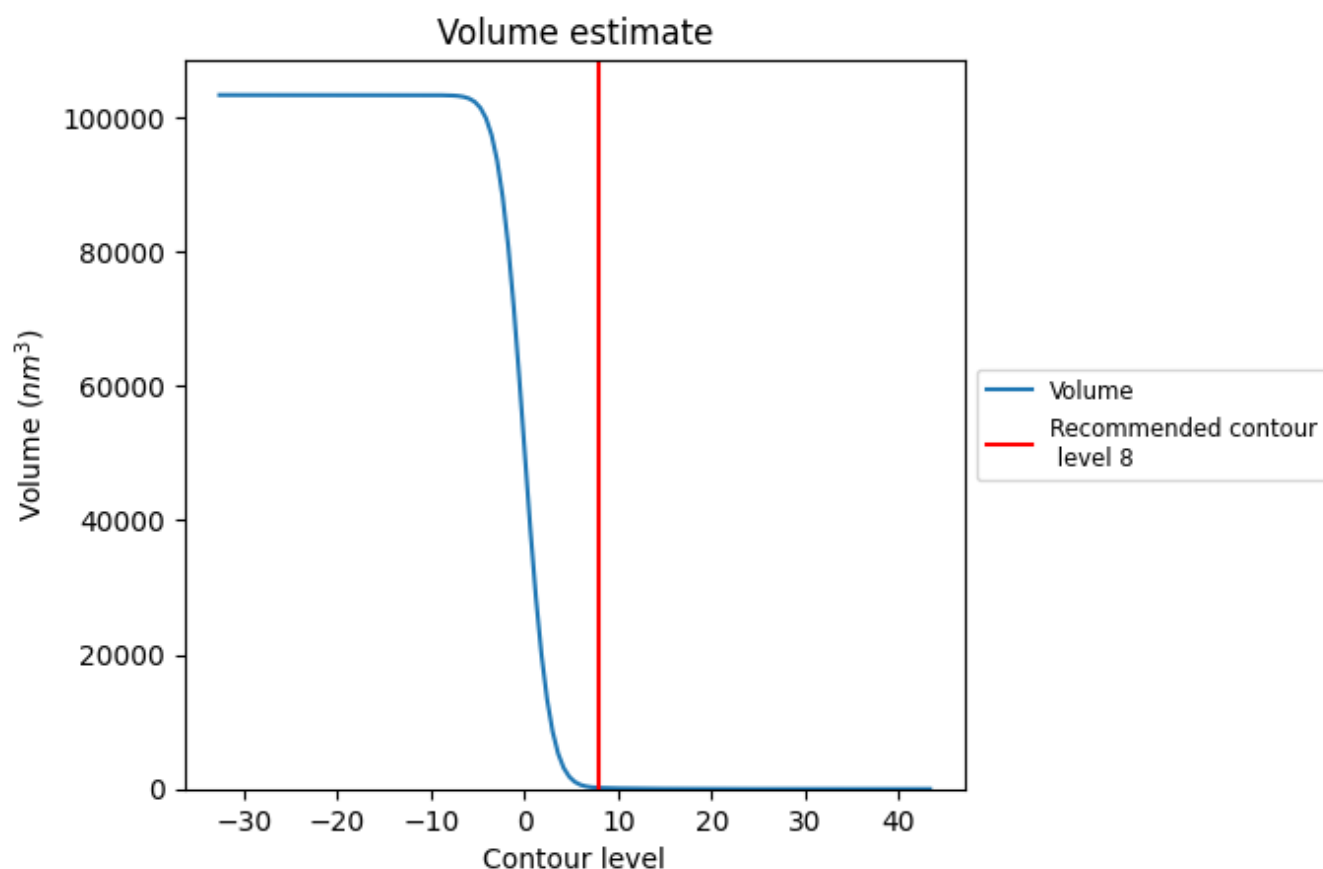
This section contains the results of statistical analysis of the map.

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.

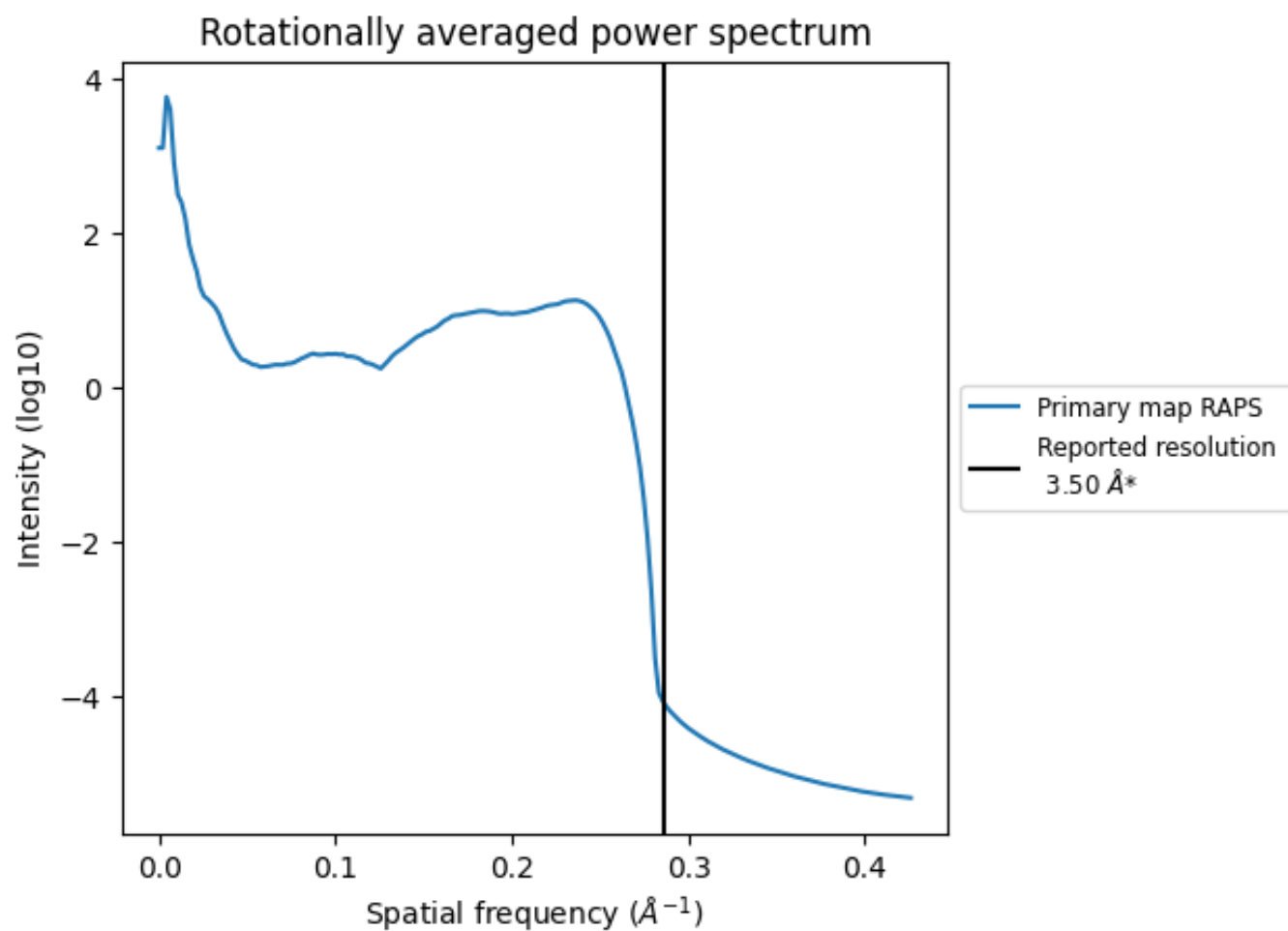
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm^3 ; this corresponds to an approximate mass of 157 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 0.286 Å⁻¹

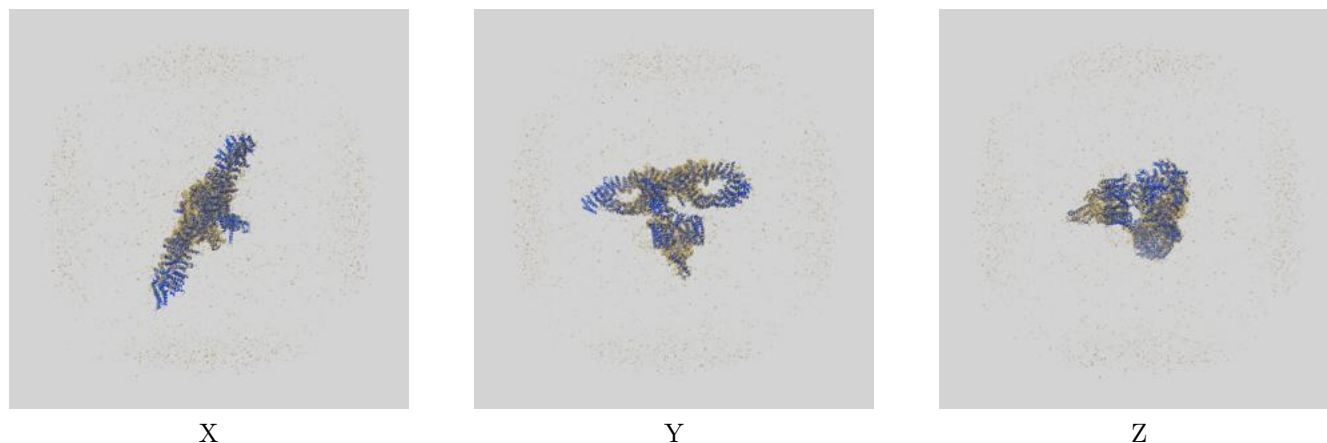
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

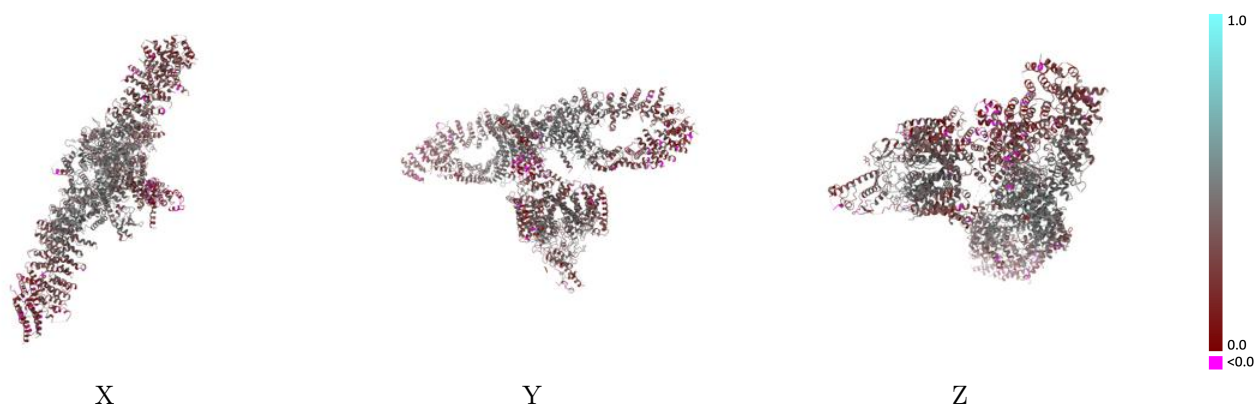
This section contains information regarding the fit between EMDB map EMD-25493 and PDB model 7SX4. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



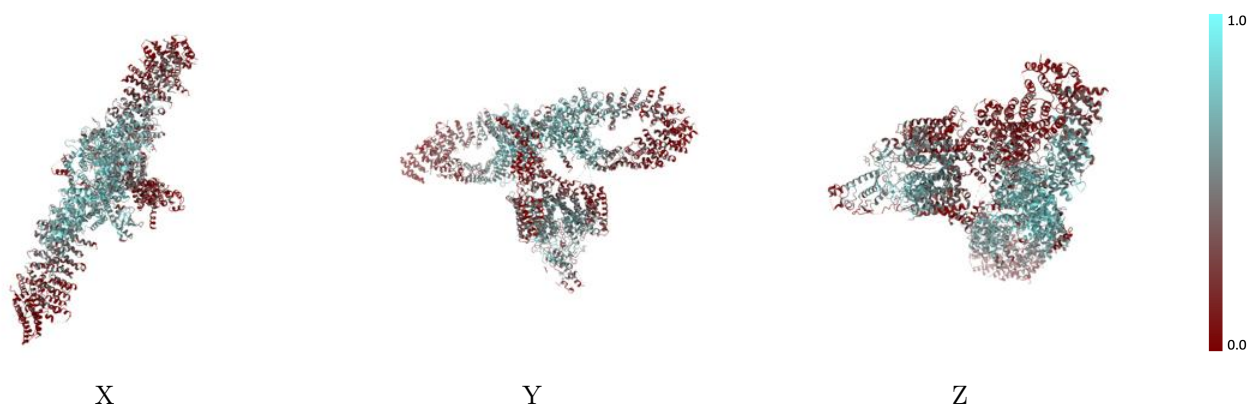
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



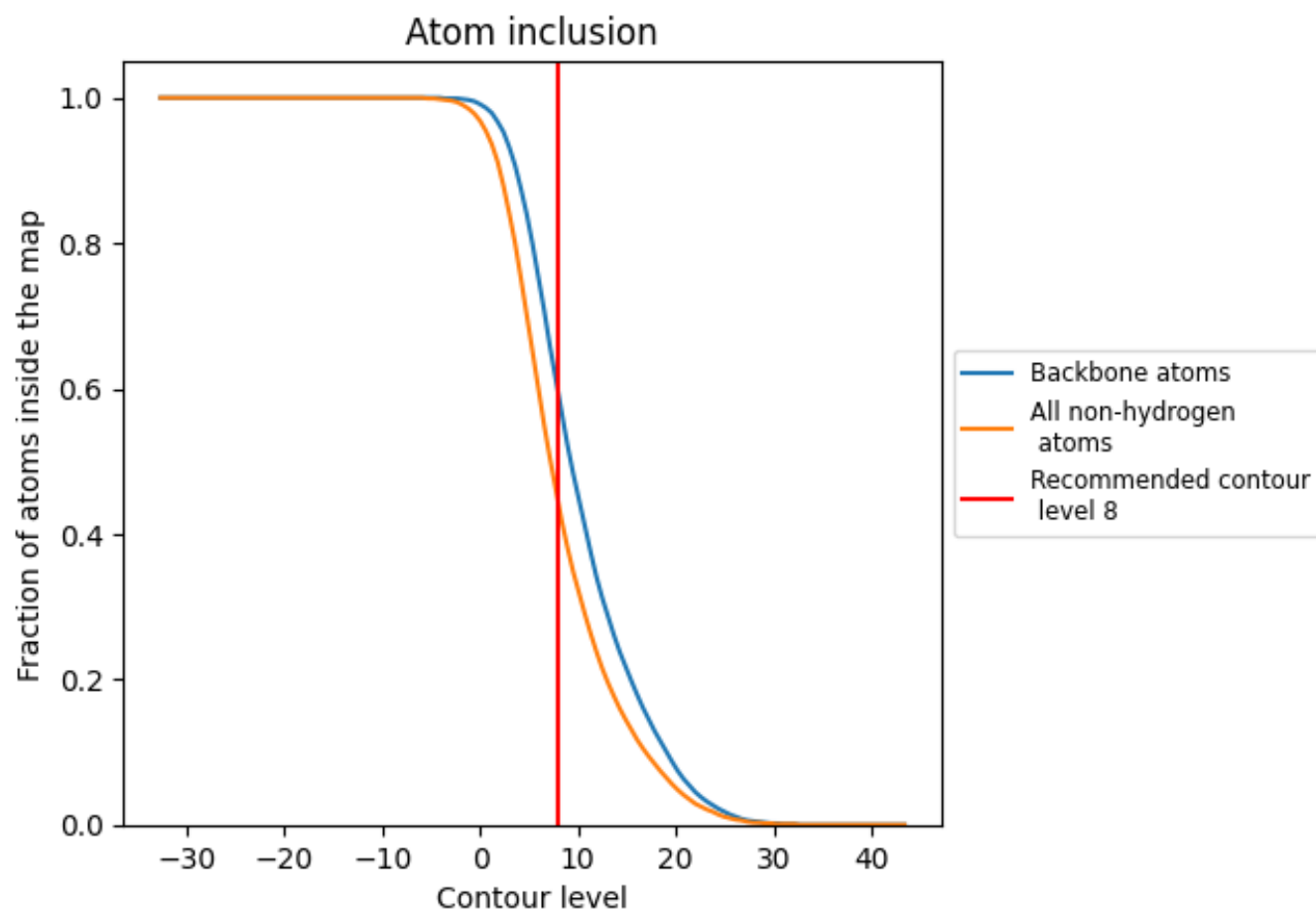
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 44% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4430	0.3590
A	0.4180	0.3610
B	0.4070	0.3200
C	0.0700	0.1780
D	0.4350	0.3480
E	0.5020	0.3850

