Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:18 AM UTC

PDB ID	:	9AYK / pdb_00009ayk
EMDB ID	:	EMD-43994
Title	:	Cryo-EM structure of human Cav3.2 with ML218
Authors	:	Fan, X.; Huang, J.; Yan, N.
Deposited on	:	2024-03-08
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

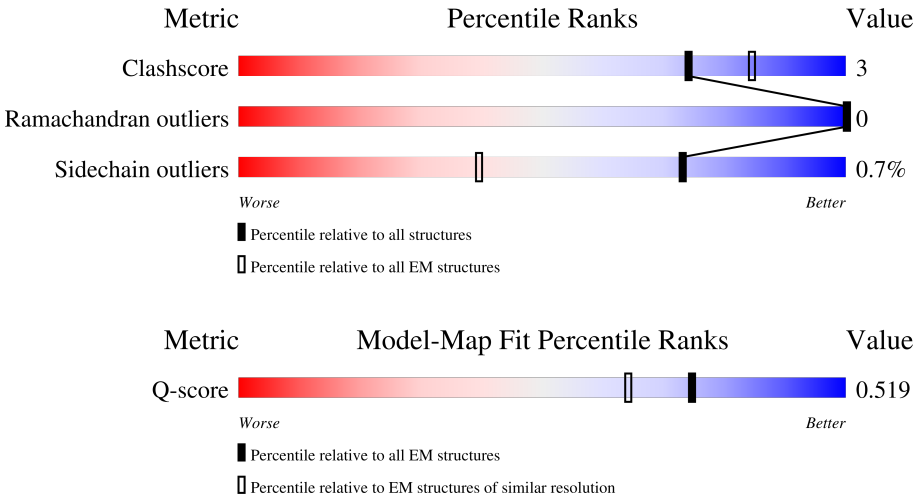
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2116	46% · 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8851 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 Voltage-dependent T-type calcium channel subunit alpha-1H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1056	8473	5565	1402	1436	70	0	0

There are 43 discrepancies between the modelled and reference sequences:

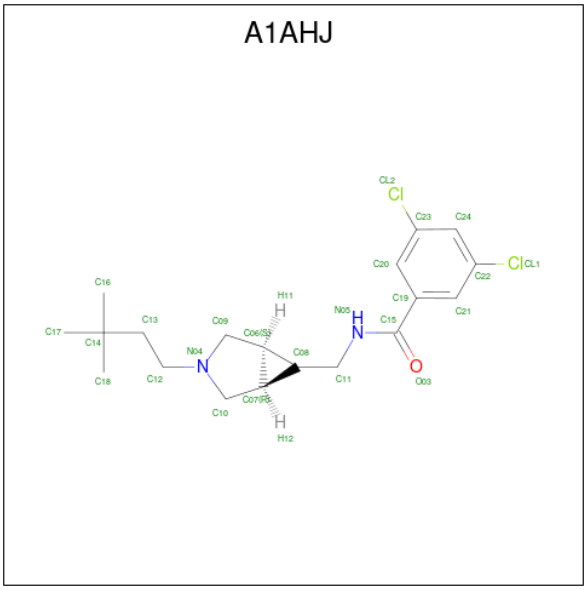
Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP O95180
A	-41	ALA	-	expression tag	UNP O95180
A	-40	SER	-	expression tag	UNP O95180
A	-39	TRP	-	expression tag	UNP O95180
A	-38	SER	-	expression tag	UNP O95180
A	-37	HIS	-	expression tag	UNP O95180
A	-36	PRO	-	expression tag	UNP O95180
A	-35	GLN	-	expression tag	UNP O95180
A	-34	PHE	-	expression tag	UNP O95180
A	-33	GLU	-	expression tag	UNP O95180
A	-32	LYS	-	expression tag	UNP O95180
A	-31	GLY	-	expression tag	UNP O95180
A	-30	GLY	-	expression tag	UNP O95180
A	-29	GLY	-	expression tag	UNP O95180
A	-28	ALA	-	expression tag	UNP O95180
A	-27	ARG	-	expression tag	UNP O95180
A	-26	GLY	-	expression tag	UNP O95180
A	-25	GLY	-	expression tag	UNP O95180
A	-24	SER	-	expression tag	UNP O95180
A	-23	GLY	-	expression tag	UNP O95180
A	-22	GLY	-	expression tag	UNP O95180
A	-21	GLY	-	expression tag	UNP O95180
A	-20	SER	-	expression tag	UNP O95180
A	-19	TRP	-	expression tag	UNP O95180
A	-18	SER	-	expression tag	UNP O95180
A	-17	HIS	-	expression tag	UNP O95180
A	-16	PRO	-	expression tag	UNP O95180
A	-15	GLN	-	expression tag	UNP O95180

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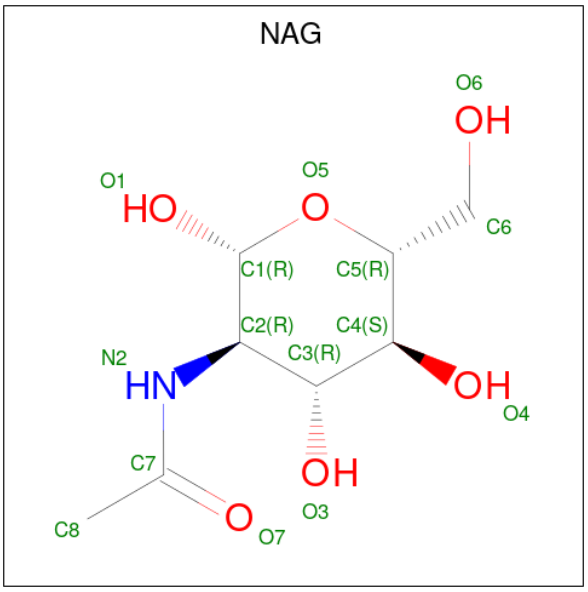
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP O95180
A	-13	GLU	-	expression tag	UNP O95180
A	-12	LYS	-	expression tag	UNP O95180
A	-11	GLY	-	expression tag	UNP O95180
A	-10	PHE	-	expression tag	UNP O95180
A	-9	ASP	-	expression tag	UNP O95180
A	-8	TYR	-	expression tag	UNP O95180
A	-7	LYS	-	expression tag	UNP O95180
A	-6	ASP	-	expression tag	UNP O95180
A	-5	ASP	-	expression tag	UNP O95180
A	-4	ASP	-	expression tag	UNP O95180
A	-3	ASP	-	expression tag	UNP O95180
A	-2	LYS	-	expression tag	UNP O95180
A	-1	GLY	-	expression tag	UNP O95180
A	0	THR	-	expression tag	UNP O95180

- Molecule 2 is 3,5-dichloro-N-{[(1R,5S,6r)-3-(3,3-dimethylbutyl)-3-azabicyclo[3.1.0]hexan-6-yl]methyl}benzamide (CCD ID: A1AHJ) (formula: $C_{19}H_{26}Cl_2N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Cl	N	O	0
			24	19	2	2	1	

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

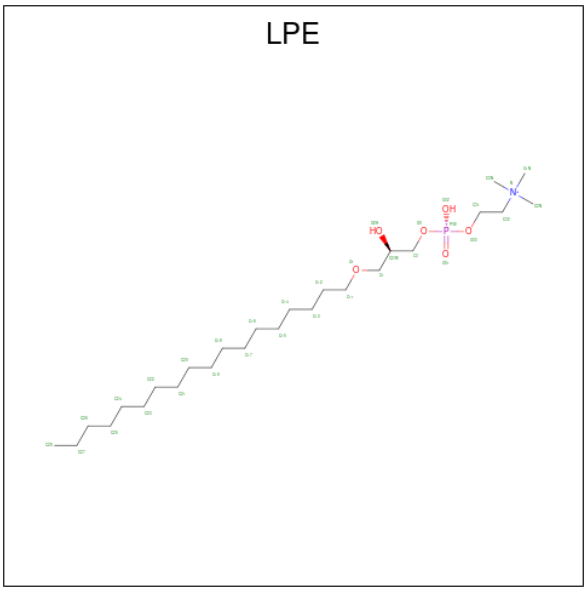


Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

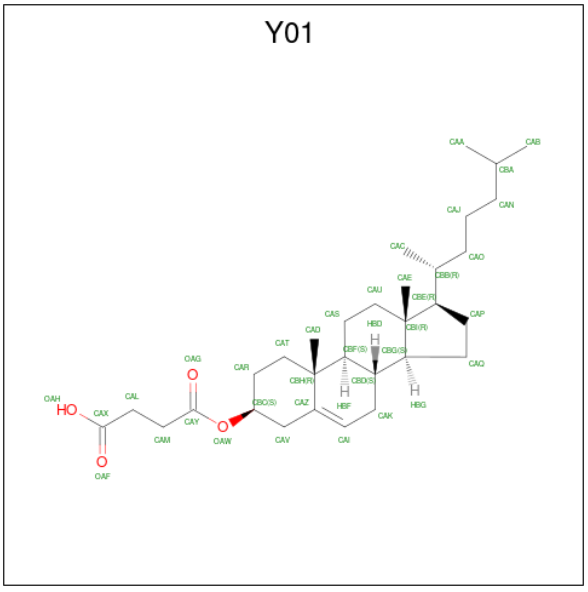
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0

- Molecule 5 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: $C_{26}H_{57}NO_6P$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	19	1	6	1	

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



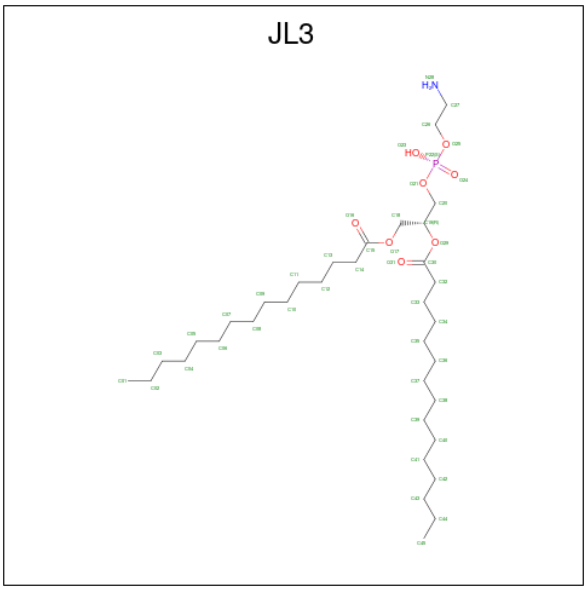
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	
6	A	1	Total	C	O	0
			35	31	4	

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

- Molecule 7 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-pentadecanoyloxy-propyl] pentadecanoate (CCD ID: JL3) (formula: $C_{35}H_{70}NO_8P$).



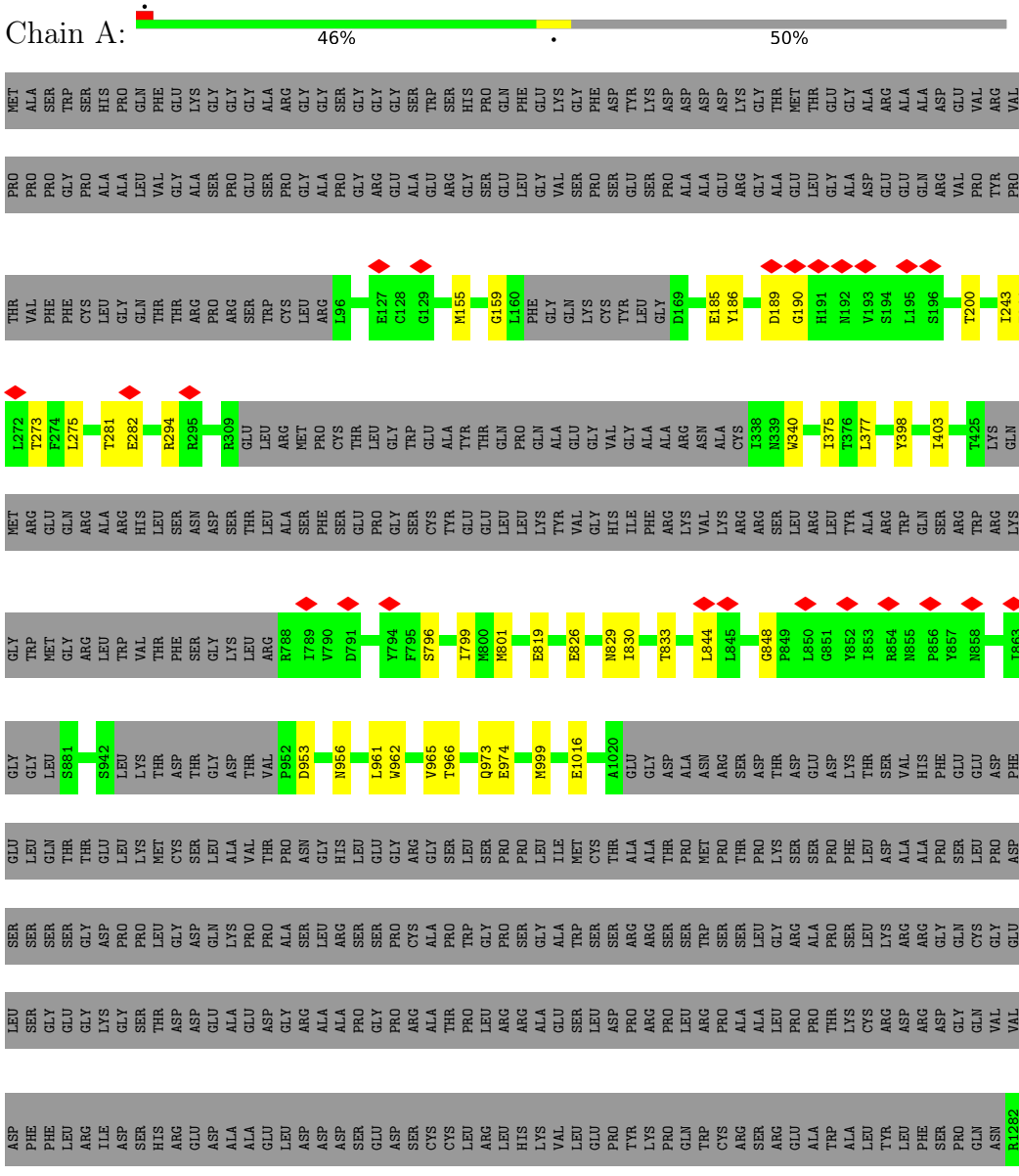
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total 45	C 35	N 1	O 8	P 1	0
7	A	1	Total 42	C 32	N 1	O 8	P 1	0
7	A	1	Total 36	C 26	N 1	O 8	P 1	0
7	A	1	Total 35	C 25	N 1	O 8	P 1	0

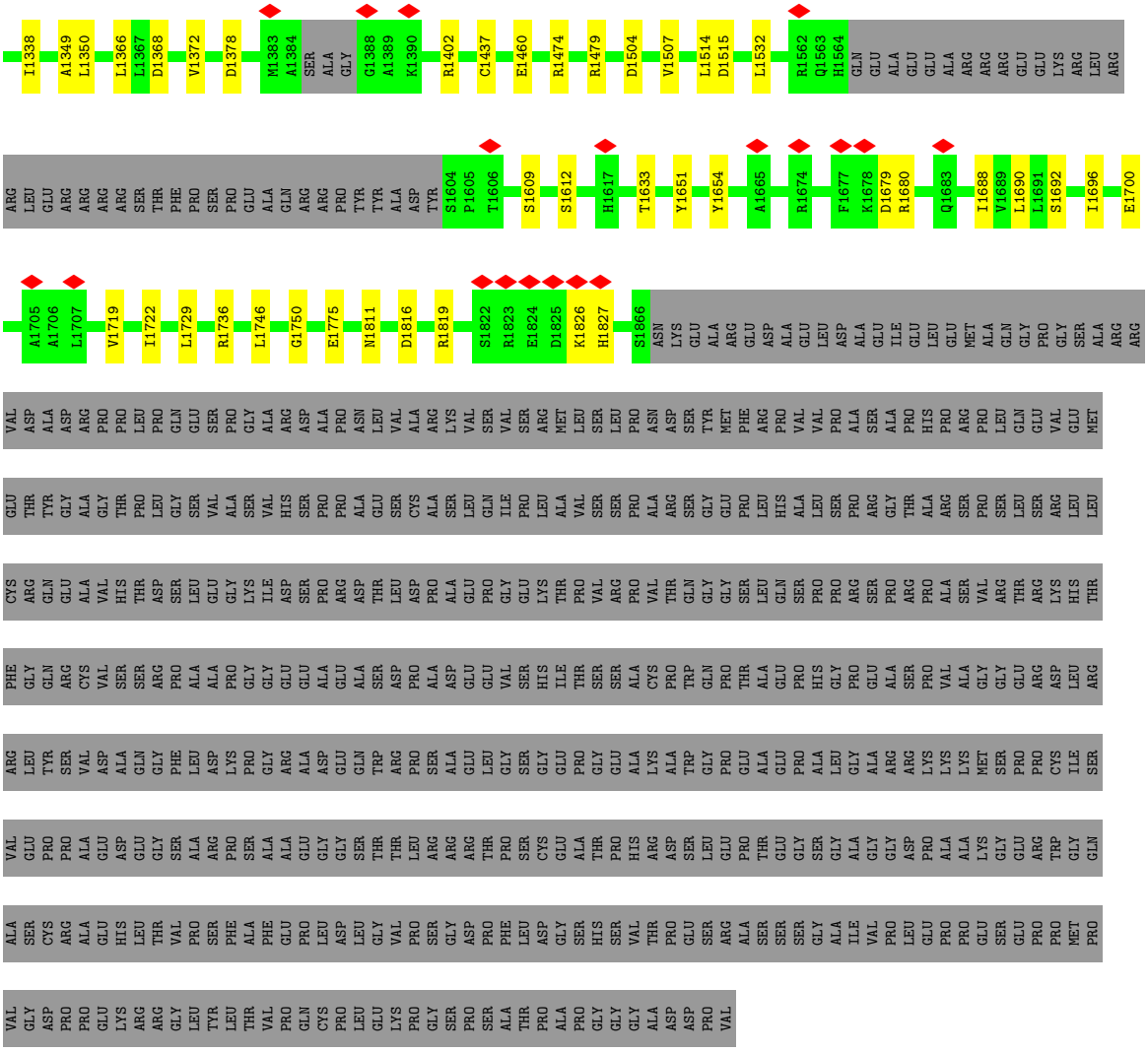
3 Residue-property plots (i)

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: Voltage-dependent T-type calcium channel subunit alpha-1H

Chain A:




I1338 A1349 L1350 L1366 L1367 D1368 V1372 D1378 M1383 A1384 SER ALA GLY G1388 A1389 K1390 R1402 C1437 E1460 R1474 R1479 D1504 V1507 L1514 D1515 L1532 R1562 Q1563 H1564 GLN GLU ALA GLU GLU ALA ARG ARG ARG GLU GLU LYS ARG LEU ARG
ARG LEU GLU ARG ARG ARG SER THR PHE PRO SER PRO GLU ALA GLN ARG ARG PRO TYR TYR ALA ASP TYR S1604 P1605 T1606 S1609 S1612 H1617 T1633 Y1651 Y1654 A1665 R1674 F1677 K1678 D1679 R1680 Q1683 I1688 V1689 L1690 L1691 S1692 I1696 E1700
A1705 A1706 L1707 V1719 I1722 L1729 R1736 L1746 G1750 E1775 N1811 D1816 R1819 S1822 R1823 E1824 D1825 K1826 H1827 S1866 ASN LYS GLU ALA ARG GLU ASP ALA GLU LEU ASP ALA GLU ILE GLU LEU MET ALA GLN GLY PRO GLY SER ALA ARG ARG
VAL ASP ALA ASP ARG PRO PRO LEU PRO GLN GLU SER PRO GLY ALA ARG ASP ALA PRO ASN LEU VAL ALA ARG LYS VAL SER VAL SER ARG MET LEU SER LEU PRO ASN ASP SER TYR MET PHE ARG PRO VAL VAL PRO ALA SER ALA PRO HIS PRO ARG PRO LEU GLN GLU VAL GLU MET
GLU THR TYR GLY ALA GLY THR PRO LEU GLY SER VAL ALA SER VAL HIS SER PRO PRO ALA SER LEU GLN ILE PRO LEU ALA VAL SER SER PRO ALA ARG SER GLY GLU PRO LEU HIS ALA LEU SER PRO ARG GLY THR ALA ARG SER PRO SER LEU SER ARG LEU LEU
CYS ARG GLN GLU ALA VAL HIS THR ASP SER LEU GLU GLY LYS ILE ASP SER PRO ARG ASP THR LEU ASP PRO ALA GLU PRO GLY GLU LYS THR PRO VAL ARG PRO VAL THR GLN GLY GLY SER LEU GLN SER PRO PRO ARG SER PRO ARG PRO ALA SER VAL ARG THR ARG LYS HIS THR
PHE GLY GLN ARG CYS VAL SER SER ARG PRO ALA ALA ALA PRO GLY GLY GLU GLU ALA GLU ALA SER ASP PRO ALA ASP GLU GLU VAL SER HIS ILE THR SER SER ALA CYS PRO TRP GLN PRO THR ALA GLU PRO HIS GLY PRO GLU ALA SER PRO ARG PRO VAL ALA ALA GLY GLY GLU ARG ASP LEU ARG
ARG LEU TYR SER VAL ASP ALA GLN GLY PHE LEU ASP LYS PRO GLY ARG ALA ASP GLU GLN TRP ARG PRO SER ALA GLU LEU GLY SER GLY GLU PRO GLY GLU ALA LYS ALA TRP GLY PRO GLU ALA GLU PRO ALA LEU GLY ALA ARG ARG LYS LYS LYS MET SER PRO PRO CYS ILE SER
VAL GLU PRO PRO ALA GLU ASP GLU GLY SER ALA ARG PRO SER ALA GLU GLY GLY SER THR THR LEU ARG ARG ARG THR PRO SER CYS GLU ALA THR PRO HIS ARG ASP SER LEU GLU PRO THR GLU GLY SER GLY ALA GLY GLY ASP PRO ALA ALA LYS GLY GLU GLY ARG TRP GLY GLN
ALA SER CYS ARG ALA GLU HIS LEU THR VAL PRO SER PHE ALA PHE GLU PRO LEU ASP LEU GLY VAL PRO SER GLY ASP PRO PHE LEU ASP GLY SER HIS SER VAL THR PRO GLU SER ARG ALA SER SER SER GLY ALA ILE VAL PRO LEU GLU PRO PRO GLU SER GLU PRO PRO MET PRO
VAL GLY ASP PRO PRO GLU LYS ARG ARG GLY LEU TYR LEU THR VAL PRO GLN CYS PRO LEU GLU LYS PRO GLY SER PRO SER ALA THR PRO ALA PRO GLY GLY GLY ALA ASP ASP PRO VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126670	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.433	Depositor
Minimum map value	-2.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	265.216, 265.216, 265.216	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.036, 1.036, 1.036	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, LPE, Y01, A1AHJ, CA, JL3

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	0.10	0/8662	0.24	0/11741

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	8473	0	8661	55	0
2	A	24	0	0	0	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
5	A	27	0	39	0	0
6	A	140	0	196	1	0
7	A	158	0	0	0	0
All	All	8851	0	8922	56	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.

All (56) 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:1514:LEU:HD21	1:A:1532:LEU:HD12	1.71	0.71
1:A:294:ARG:NE	1:A:294:ARG:O	2.27	0.68
1:A:273:THR:HG22	1:A:273:THR:O	2.00	0.61
1:A:1775:GLU:N	1:A:1775:GLU:OE1	2.33	0.60
1:A:282:GLU:N	1:A:282:GLU:OE1	2.39	0.56
1:A:819:GLU:N	1:A:819:GLU:OE2	2.36	0.55
1:A:1654:TYR:CD1	1:A:1696:ILE:HD11	2.44	0.53
1:A:801:MET:HA	1:A:801:MET:HE2	1.92	0.52
1:A:1016:GLU:C	1:A:1016:GLU:OE2	2.53	0.52
1:A:377:LEU:CD2	1:A:403:ILE:HD12	2.39	0.52
6:A:2413:Y01:HAC1	6:A:2413:Y01:HAU2	1.92	0.51
1:A:244:PHE:O	1:A:398:TYR:OH	2.26	0.50
1:A:1504:ASP:OD1	1:A:1811:ASN:ND2	2.44	0.50
1:A:1514:LEU:CD2	1:A:1532:LEU:HD12	2.41	0.48
1:A:1688:ILE:O	1:A:1692:SER:N	2.37	0.48
1:A:1826:LYS:O	1:A:1827:HIS:ND1	2.46	0.48
1:A:155:MET:O	1:A:159:GLY:N	2.41	0.48
1:A:281:THR:OG1	1:A:282:GLU:OE1	2.29	0.47
1:A:829:ASN:O	1:A:833:THR:HG22	2.15	0.47
1:A:243:ILE:HA	1:A:1722:ILE:HD11	1.95	0.47
1:A:1775:GLU:O	1:A:1819:ARG:NH2	2.47	0.46
1:A:185:GLU:OE2	1:A:186:TYR:N	2.48	0.46
1:A:1378:ASP:OD2	1:A:1402:ARG:NE	2.48	0.46
1:A:830:ILE:HD13	1:A:872:ILE:HD13	1.97	0.46
1:A:965:VAL:HG21	1:A:1532:LEU:HD21	1.99	0.45
1:A:974:GLU:HG2	1:A:1507:VAL:HG23	1.99	0.45
1:A:1654:TYR:OH	1:A:1700:GLU:OE2	2.29	0.45
1:A:1816:ASP:O	1:A:1819:ARG:NH1	2.42	0.44
1:A:245:GLY:O	1:A:249:VAL:HG23	2.18	0.44
1:A:185:GLU:CD	1:A:185:GLU:C	2.86	0.44
1:A:1474:ARG:HG2	1:A:1474:ARG:HH11	1.82	0.44
1:A:1746:LEU:O	1:A:1750:GLY:N	2.44	0.44
1:A:844:LEU:O	1:A:848:GLY:N	2.50	0.43
1:A:973:GLN:HG2	1:A:999:MET:HE1	1.99	0.43
1:A:1378:ASP:OD1	1:A:1378:ASP:C	2.62	0.43
1:A:953:ASP:O	1:A:956:ASN:ND2	2.43	0.43
1:A:1366:LEU:HD12	1:A:1366:LEU:O	2.19	0.43
1:A:1349:ALA:C	1:A:1350:LEU:HD12	2.43	0.43
1:A:1654:TYR:CE1	1:A:1696:ILE:HD11	2.54	0.43
1:A:1690:LEU:C	1:A:1690:LEU:HD23	2.44	0.43
1:A:1729:LEU:HD23	1:A:1736:ARG:HD3	2.00	0.42
1:A:1368:ASP:O	1:A:1372:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:LEU:O	1:A:965:VAL:HG23	2.20	0.42
1:A:1679:ASP:OD1	1:A:1680:ARG:N	2.52	0.42
1:A:833:THR:HG21	1:A:872:ILE:HD11	2.02	0.41
1:A:189:ASP:OD1	1:A:190:GLY:N	2.53	0.41
1:A:962:TRP:O	1:A:966:THR:OG1	2.36	0.41
1:A:200:THR:HG22	1:A:200:THR:O	2.20	0.41
1:A:826:GLU:HA	1:A:826:GLU:OE2	2.20	0.41
1:A:275:LEU:HD11	1:A:340:TRP:CE3	2.56	0.41
1:A:1334:ILE:O	1:A:1338:ILE:HG13	2.21	0.41
1:A:1609:SER:O	1:A:1612:SER:OG	2.37	0.40
1:A:1651:TYR:N	1:A:1651:TYR:CD1	2.88	0.40
1:A:377:LEU:HD23	1:A:403:ILE:HD12	2.03	0.40
1:A:1515:ASP:OD1	1:A:1515:ASP:N	2.54	0.40
1:A:1460:GLU:OE1	1:A:1479:ARG:NH2	2.54	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	1038/2116 (49%)	1022 (98%)	16 (2%)	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	939/1793 (52%)	932 (99%)	7 (1%)	76 86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	375	ILE
1	A	796	SER
1	A	799	ILE
1	A	1290	VAL
1	A	1437	CYS
1	A	1633	THR
1	A	1719	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	829	ASN
1	A	973	GLN
1	A	1288	GLN
1	A	1332	ASN
1	A	1521	GLN
1	A	1559	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	Y01	A	2412	-	38,38,38	0.45	0	57,57,57	0.51	0
6	Y01	A	2408	-	38,38,38	0.45	0	57,57,57	0.60	0
7	JL3	A	2410	-	35,35,44	0.60	0	38,40,49	0.63	1 (2%)
6	Y01	A	2413	-	38,38,38	0.44	0	57,57,57	0.48	0
7	JL3	A	2409	-	41,41,44	0.56	0	44,46,49	0.55	1 (2%)
3	NAG	A	2402	-	14,14,15	0.27	0	17,19,21	0.64	0
7	JL3	A	2407	-	44,44,44	0.55	0	47,49,49	0.52	1 (2%)
3	NAG	A	2403	-	14,14,15	0.28	0	17,19,21	0.53	0
6	Y01	A	2406	-	38,38,38	0.47	0	57,57,57	0.62	0
7	JL3	A	2411	-	34,34,44	0.61	0	37,39,49	0.61	1 (2%)
2	A1AHJ	A	2401	-	25,26,26	6.63	13 (52%)	32,39,39	1.72	7 (21%)
5	LPE	A	2405	-	26,26,33	0.26	0	30,32,39	0.36	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
6	Y01	A	2412	-	-	5/19/77/77	0/4/4/4
6	Y01	A	2408	-	-	6/19/77/77	0/4/4/4
7	JL3	A	2410	-	-	18/39/39/48	-
6	Y01	A	2413	-	-	4/19/77/77	0/4/4/4
7	JL3	A	2409	-	-	17/45/45/48	-
3	NAG	A	2402	-	-	0/6/23/26	0/1/1/1
7	JL3	A	2407	-	-	20/48/48/48	-
3	NAG	A	2403	-	-	0/6/23/26	0/1/1/1
6	Y01	A	2406	-	-	2/19/77/77	0/4/4/4
7	JL3	A	2411	-	-	15/38/38/48	-
2	A1AHJ	A	2401	-	-	4/15/32/32	0/3/3/3
5	LPE	A	2405	-	-	2/27/27/34	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	A1AHJ	C09-C06	-14.88	1.34	1.52
2	A	2401	A1AHJ	C12-N04	-13.82	1.16	1.47
2	A	2401	A1AHJ	C10-N04	-10.26	1.31	1.47
2	A	2401	A1AHJ	C21-C22	9.52	1.53	1.38
2	A	2401	A1AHJ	C21-C19	9.18	1.53	1.39
2	A	2401	A1AHJ	C20-C19	8.96	1.52	1.39
2	A	2401	A1AHJ	C24-C22	8.79	1.52	1.38
2	A	2401	A1AHJ	C20-C23	8.49	1.52	1.38
2	A	2401	A1AHJ	C24-C23	8.23	1.51	1.38
2	A	2401	A1AHJ	C09-N04	7.13	1.57	1.47
2	A	2401	A1AHJ	C15-N05	5.66	1.46	1.33
2	A	2401	A1AHJ	C10-C07	3.30	1.57	1.52
2	A	2401	A1AHJ	O03-C15	-2.33	1.17	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2401	A1AHJ	C10-C07-C06	-3.91	105.01	107.79
2	A	2401	A1AHJ	C12-N04-C09	-3.56	104.92	113.18
2	A	2401	A1AHJ	C21-C22-CL1	3.31	123.32	119.17
2	A	2401	A1AHJ	C12-C13-C14	-2.96	110.48	115.48
2	A	2401	A1AHJ	C09-N04-C10	2.95	108.41	104.12
2	A	2401	A1AHJ	C24-C22-CL1	-2.64	115.85	119.17
7	A	2410	JL3	O23-P22-O24	2.53	124.20	112.44
2	A	2401	A1AHJ	C23-C24-C22	2.52	120.46	117.43
7	A	2411	JL3	O23-P22-O24	2.46	123.87	112.44
7	A	2407	JL3	O23-P22-O24	2.44	123.78	112.44
7	A	2409	JL3	O23-P22-O24	2.40	123.59	112.44

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2405	LPE	O1-C1-C2-C3
7	A	2407	JL3	C26-O25-P22-O21
7	A	2407	JL3	C26-O25-P22-O24
7	A	2407	JL3	O31-C30-O29-C19
7	A	2407	JL3	C32-C30-O29-C19
7	A	2409	JL3	C20-O21-P22-O24
7	A	2409	JL3	C20-O21-P22-O25
7	A	2409	JL3	C26-O25-P22-O21

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Mol	Chain	Res	Type	Atoms
7	A	2409	JL3	O17-C18-C19-O29
7	A	2409	JL3	O25-C26-C27-N28
7	A	2409	JL3	C32-C30-O29-C19
7	A	2410	JL3	C26-O25-P22-O21
7	A	2410	JL3	C26-O25-P22-O23
7	A	2410	JL3	O25-C26-C27-N28
7	A	2411	JL3	C26-O25-P22-O24
7	A	2411	JL3	O25-C26-C27-N28
6	A	2408	Y01	CAV-CBC-OAW-CAY
6	A	2412	Y01	CAV-CBC-OAW-CAY
7	A	2411	JL3	O16-C15-O17-C18
7	A	2409	JL3	O31-C30-O29-C19
7	A	2411	JL3	O31-C30-O29-C19
7	A	2407	JL3	C14-C15-O17-C18
7	A	2411	JL3	C14-C15-O17-C18
7	A	2411	JL3	C32-C30-O29-C19
7	A	2407	JL3	O16-C15-O17-C18
5	A	2405	LPE	O1-C1-C2-O2H
7	A	2410	JL3	O29-C19-C20-O21
7	A	2410	JL3	C14-C15-O17-C18
6	A	2408	Y01	CAN-CAJ-CAO-CBB
7	A	2410	JL3	O16-C15-O17-C18
6	A	2408	Y01	CAJ-CAN-CBA-CAA
6	A	2408	Y01	CAJ-CAN-CBA-CAB
6	A	2408	Y01	CAM-CAY-OAW-CBC
7	A	2410	JL3	C32-C30-O29-C19
7	A	2410	JL3	C35-C36-C37-C38
7	A	2411	JL3	C33-C34-C35-C36
7	A	2407	JL3	C37-C38-C39-C40
2	A	2401	A1AHJ	O03-C15-C19-C21
7	A	2410	JL3	O31-C30-O29-C19
7	A	2407	JL3	C08-C09-C10-C11
2	A	2401	A1AHJ	O03-C15-C19-C20
7	A	2407	JL3	C09-C10-C11-C12
7	A	2407	JL3	C39-C40-C41-C42
7	A	2407	JL3	C40-C41-C42-C43
7	A	2407	JL3	C33-C34-C35-C36
6	A	2408	Y01	OAG-CAY-OAW-CBC
7	A	2410	JL3	O17-C18-C19-C20
7	A	2409	JL3	C33-C34-C35-C36
6	A	2412	Y01	CAO-CAJ-CAN-CBA
6	A	2406	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
7	A	2409	JL3	C03-C04-C05-C06
6	A	2406	Y01	CAO-CAJ-CAN-CBA
7	A	2410	JL3	C10-C11-C12-C13
7	A	2410	JL3	C18-C19-C20-O21
7	A	2411	JL3	C18-C19-C20-O21
2	A	2401	A1AHJ	N05-C15-C19-C20
7	A	2409	JL3	O17-C18-C19-C20
2	A	2401	A1AHJ	N05-C15-C19-C21
7	A	2410	JL3	O17-C18-C19-O29
7	A	2407	JL3	C11-C12-C13-C14
7	A	2407	JL3	C35-C36-C37-C38
7	A	2410	JL3	C36-C37-C38-C39
7	A	2411	JL3	O29-C19-C20-O21
7	A	2411	JL3	C27-C26-O25-P22
6	A	2412	Y01	CAM-CAY-OAW-CBC
7	A	2407	JL3	C26-O25-P22-O23
7	A	2409	JL3	C20-O21-P22-O23
7	A	2409	JL3	C26-O25-P22-O24
7	A	2410	JL3	C34-C35-C36-C37
7	A	2407	JL3	C19-C20-O21-P22
7	A	2411	JL3	C18-C19-O29-C30
7	A	2407	JL3	C04-C05-C06-C07
7	A	2411	JL3	C11-C12-C13-C14
6	A	2413	Y01	CAM-CAL-CAX-OAH
6	A	2412	Y01	CAR-CBC-OAW-CAY
7	A	2410	JL3	C05-C06-C07-C08
7	A	2409	JL3	C09-C10-C11-C12
6	A	2413	Y01	CAJ-CAO-CBB-CBE
6	A	2413	Y01	CAM-CAL-CAX-OAF
7	A	2409	JL3	C10-C11-C12-C13
7	A	2407	JL3	C42-C43-C44-C45
7	A	2407	JL3	C02-C03-C04-C05
7	A	2411	JL3	C08-C09-C10-C11
7	A	2409	JL3	C35-C36-C37-C38
7	A	2409	JL3	C04-C05-C06-C07
7	A	2411	JL3	C13-C14-C15-O17
7	A	2410	JL3	C06-C07-C08-C09
6	A	2412	Y01	OAG-CAY-OAW-CBC
6	A	2413	Y01	CAJ-CAO-CBB-CAC
7	A	2410	JL3	C32-C33-C34-C35
7	A	2411	JL3	C13-C14-C15-O16
7	A	2409	JL3	C13-C14-C15-O17

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Mol	Chain	Res	Type	Atoms
7	A	2407	JL3	O29-C30-C32-C33

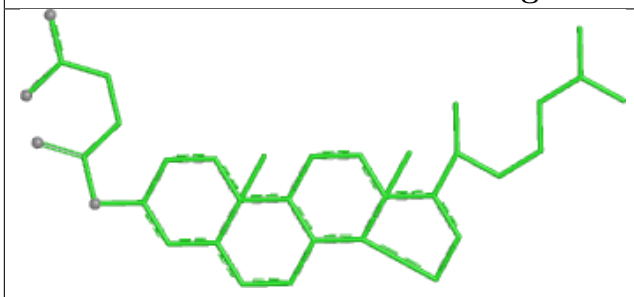
There are no ring outliers.

1 monomer is involved in 1 short contact:

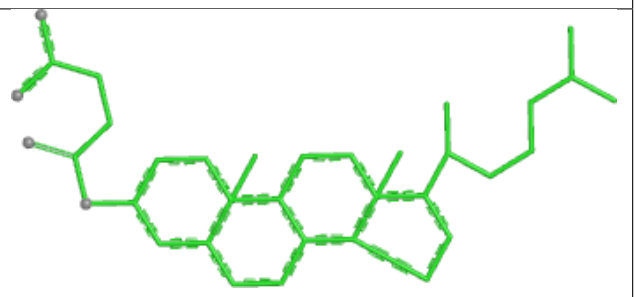
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2413	Y01	1	0

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.

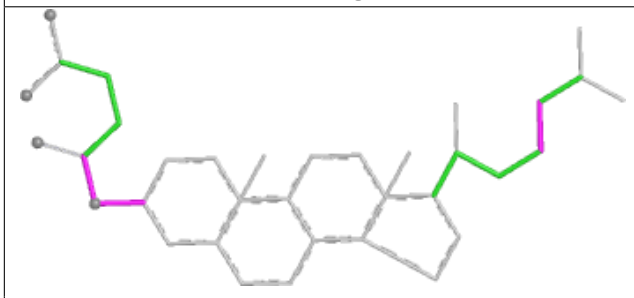
Ligand Y01 A 2412



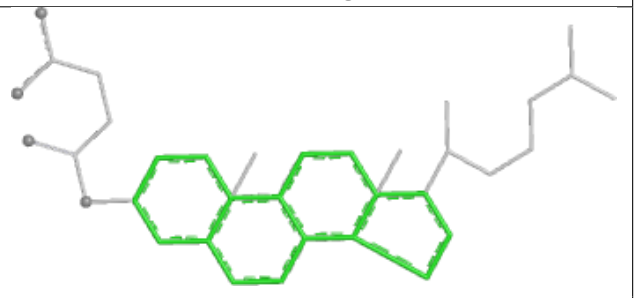
Bond lengths



Bond angles

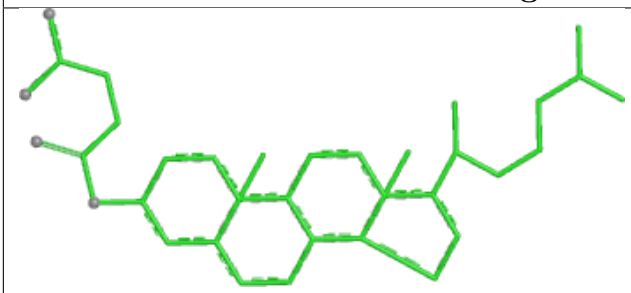


Torsions

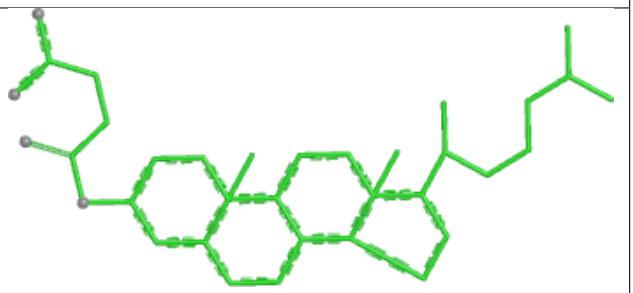


Rings

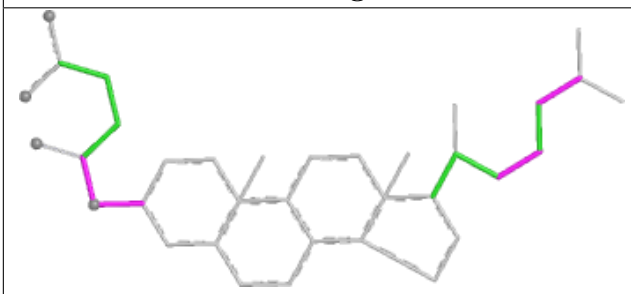
Ligand Y01 A 2408



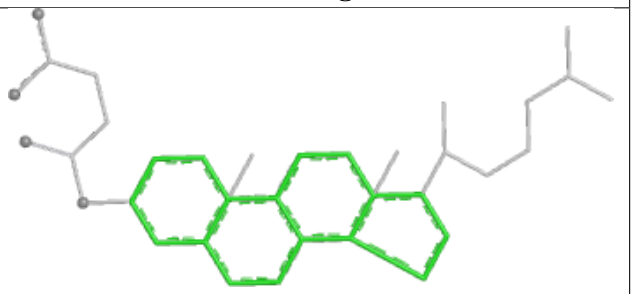
Bond lengths



Bond angles

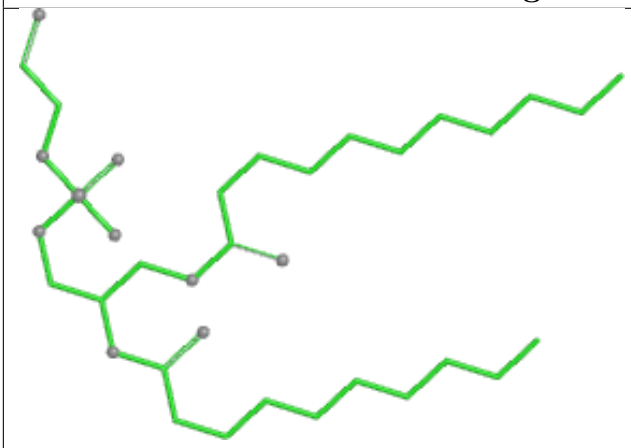


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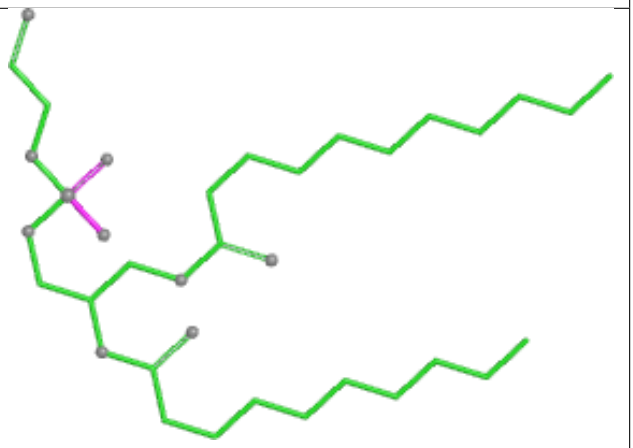


Rings

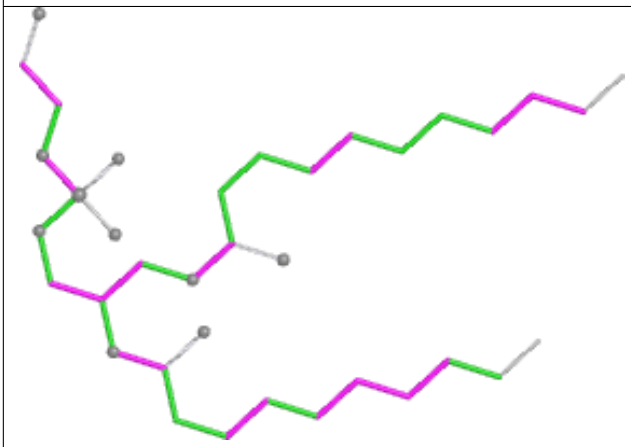
Ligand JL3 A 2410



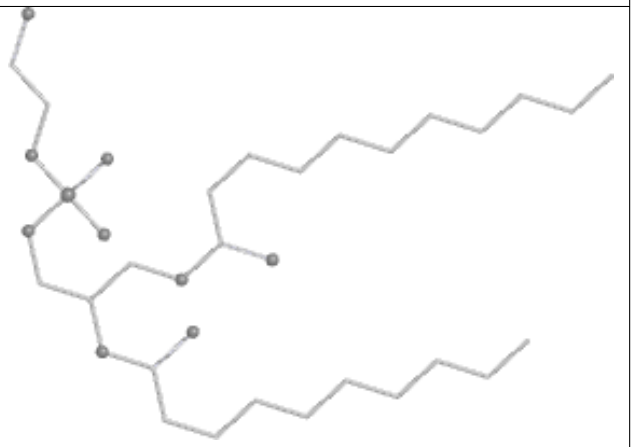
Bond lengths



Bond angles

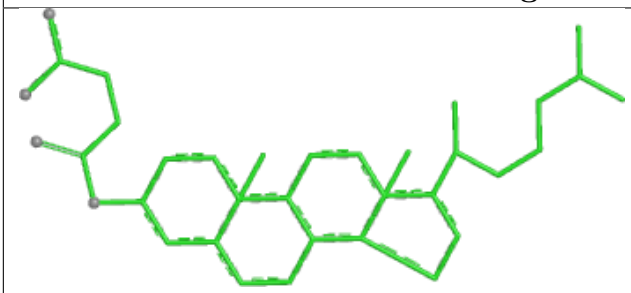


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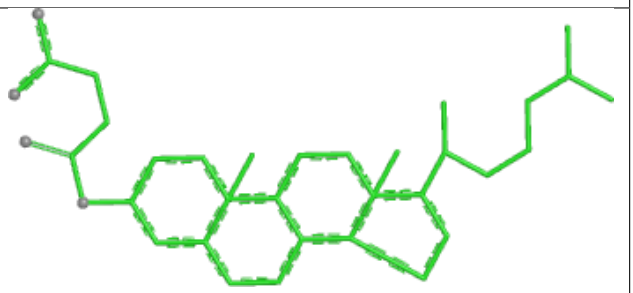


Rings

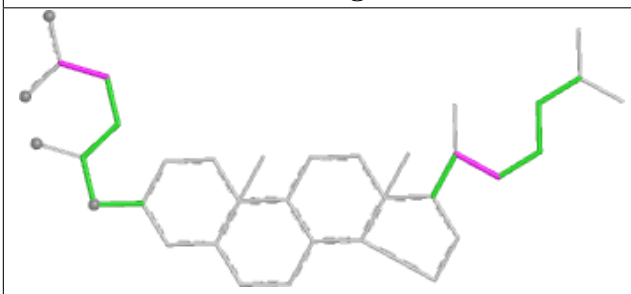
Ligand Y01 A 2413



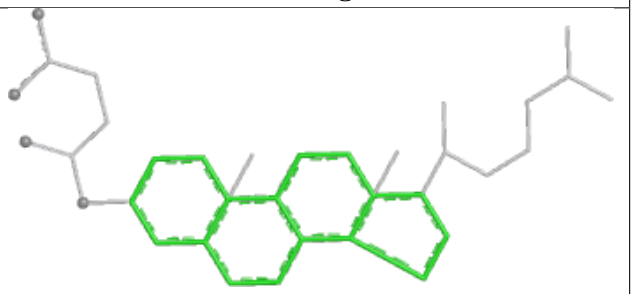
Bond lengths



Bond angles

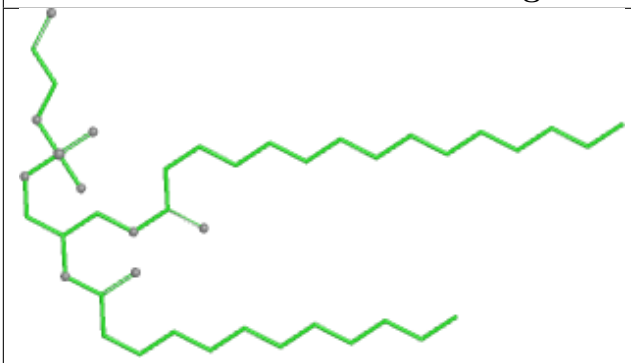


Torsions

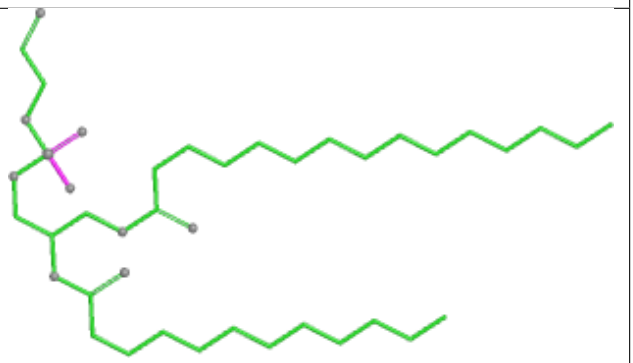


Rings

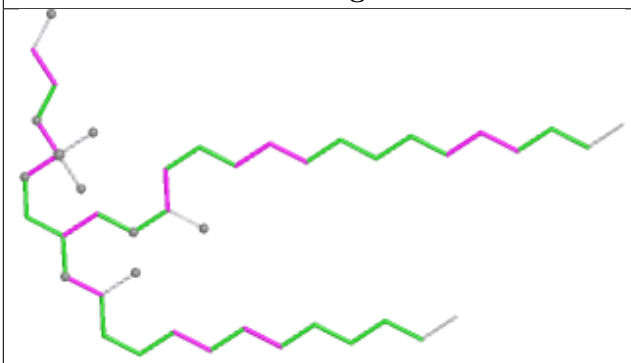
Ligand JL3 A 2409



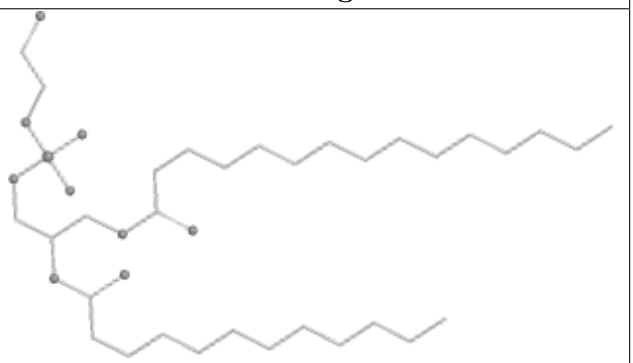
Bond lengths



Bond angles

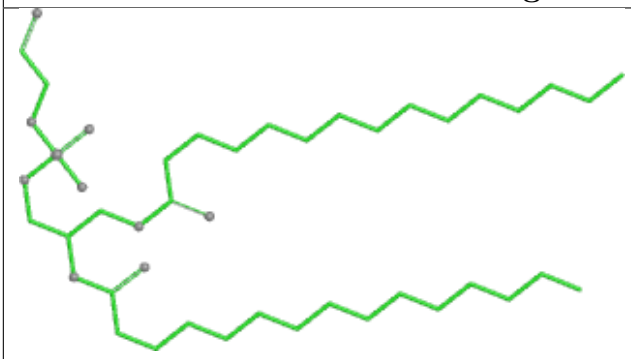


Torsions

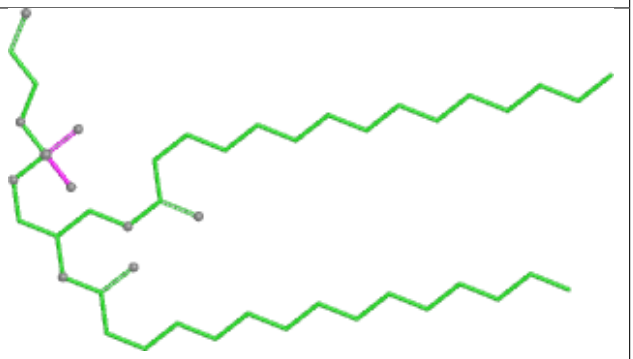


Rings

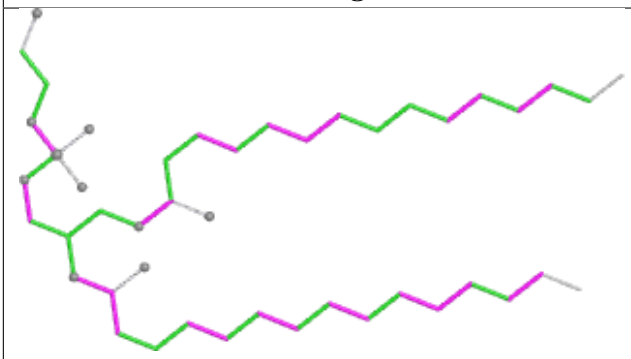
Ligand JL3 A 2407



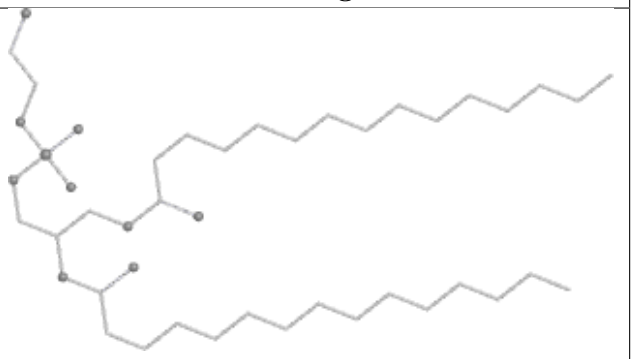
Bond lengths



Bond angles

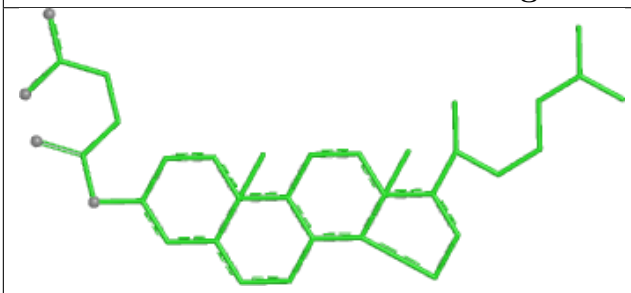


Torsions

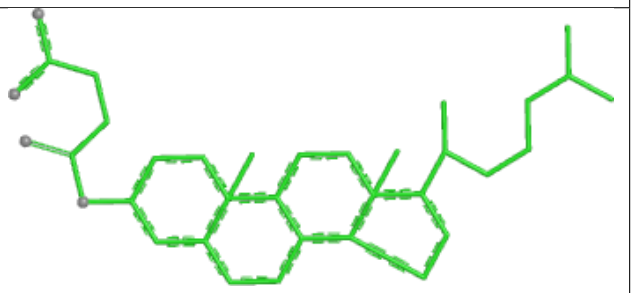


Rings

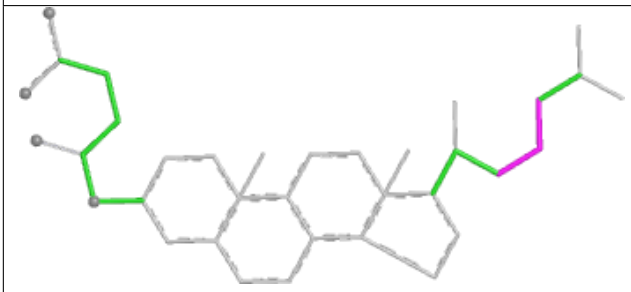
Ligand Y01 A 2406



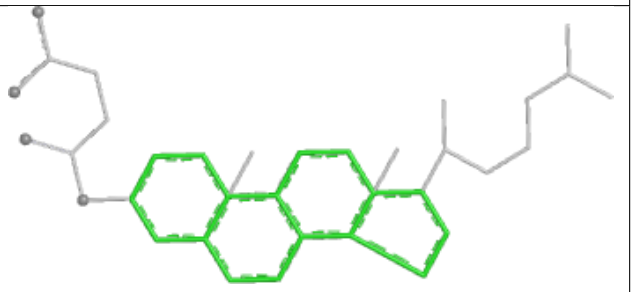
Bond lengths



Bond angles

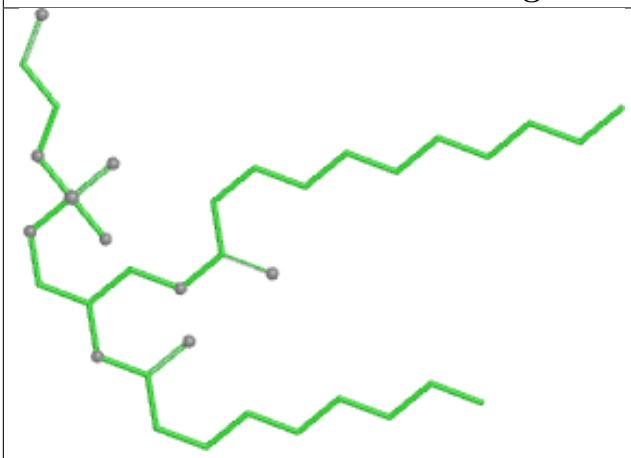


Torsions

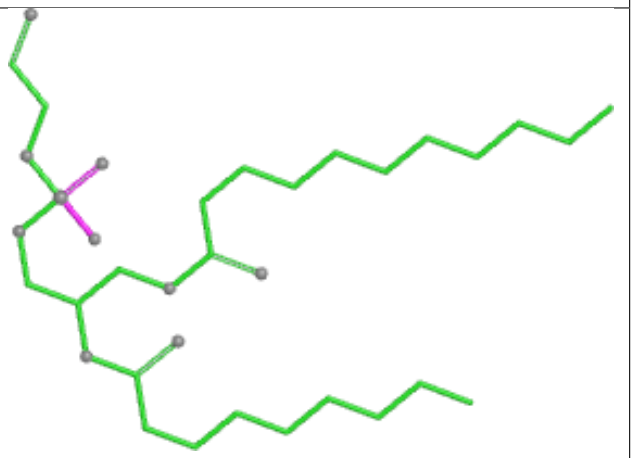


Rings

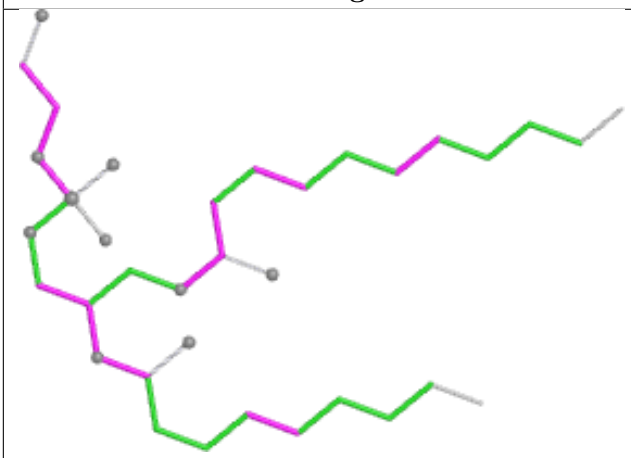
Ligand JL3 A 2411



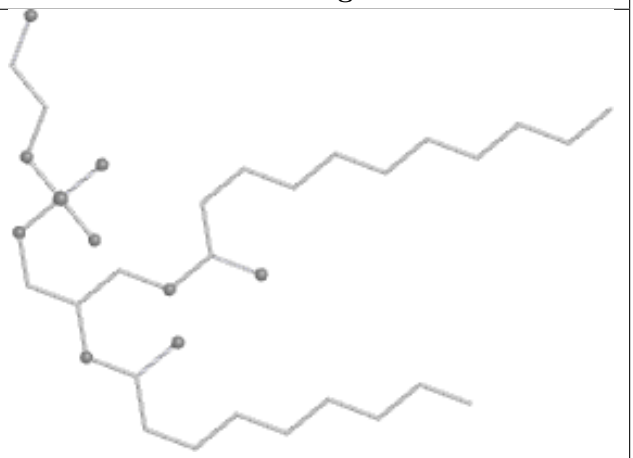
Bond lengths



Bond angles

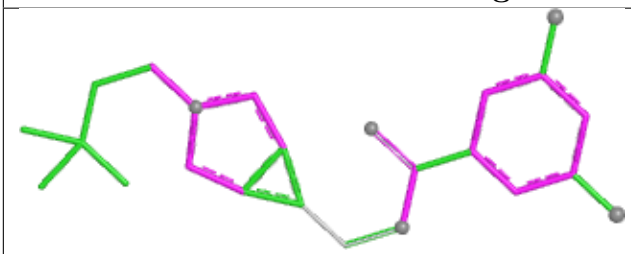


Torsions

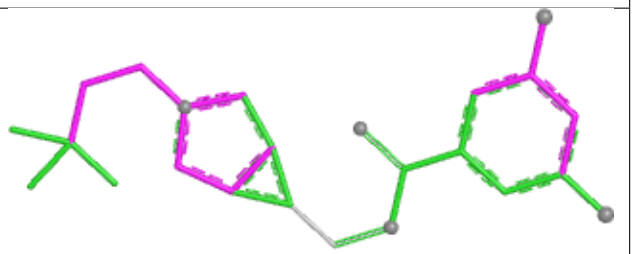


Rings

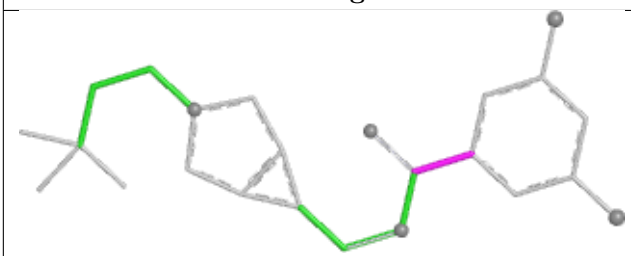
Ligand A1AHJ A 2401



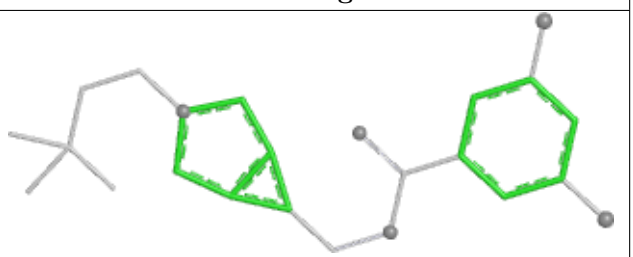
Bond lengths



Bond angles

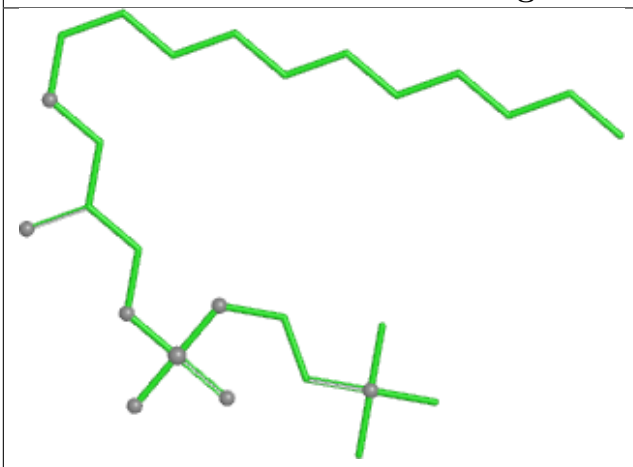


Torsions

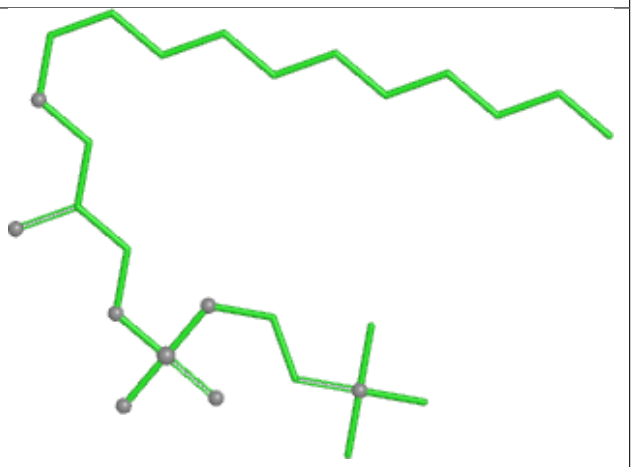


Rings

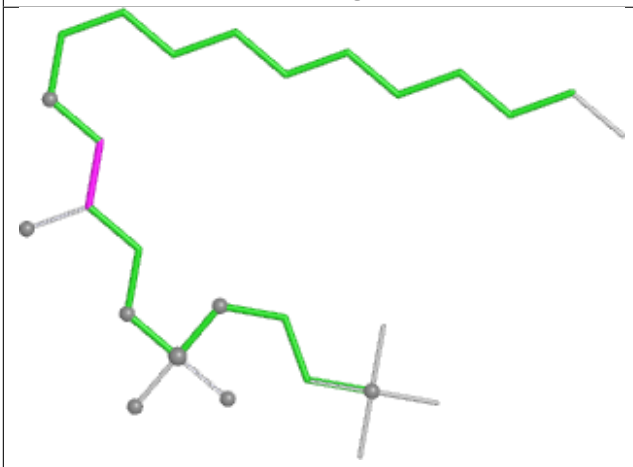
Ligand LPE A 2405



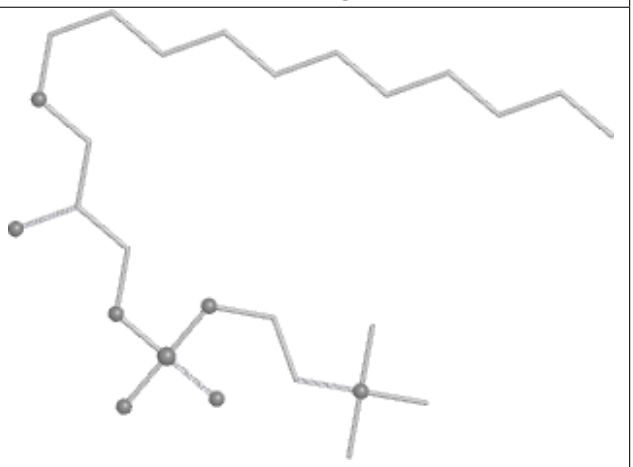
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

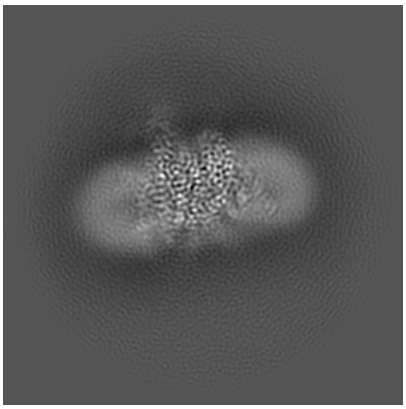
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43994. These allow visual inspection of the internal detail of the map and identification of artifacts.

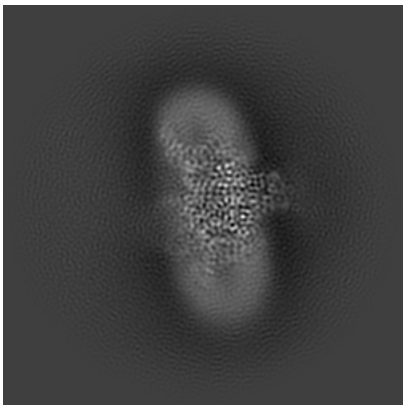
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

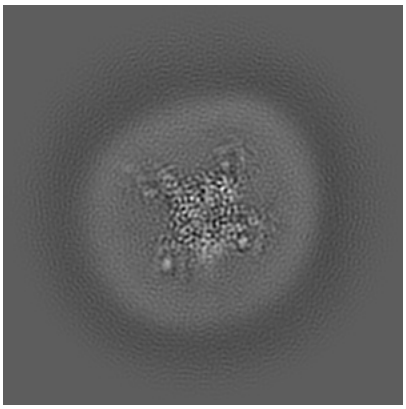
6.1.1 Primary map



X

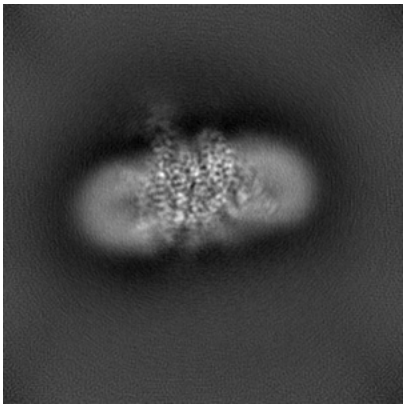


Y

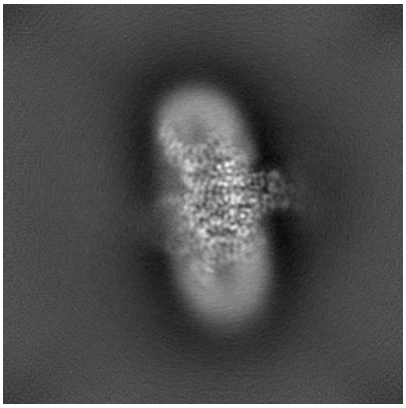


Z

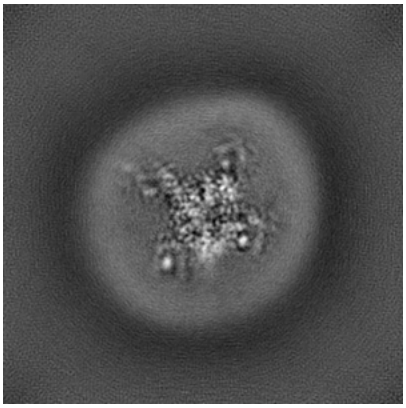
6.1.2 Raw map



X



Y

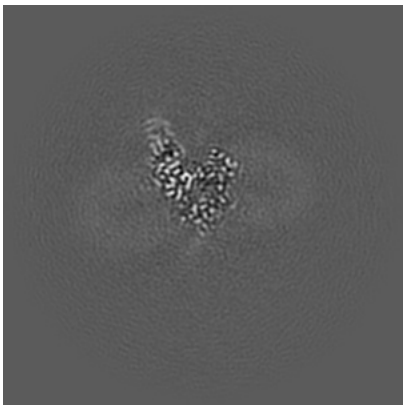


Z

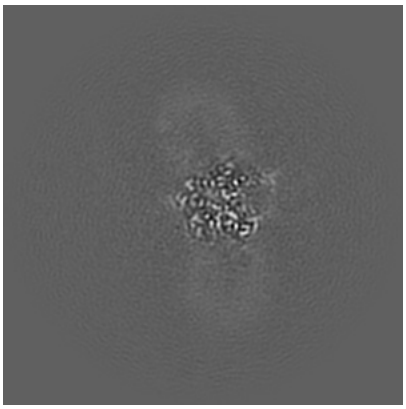
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

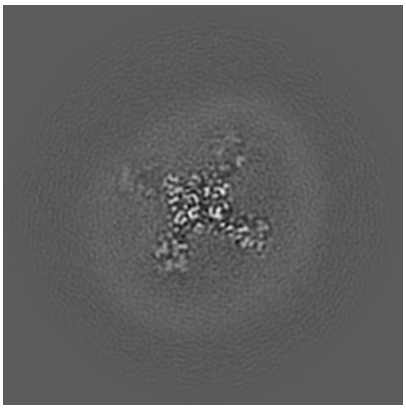
6.2.1 Primary map



X Index: 128

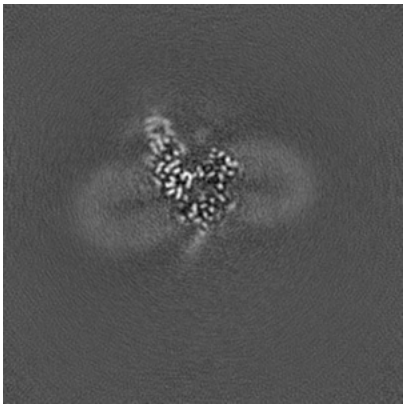


Y Index: 128

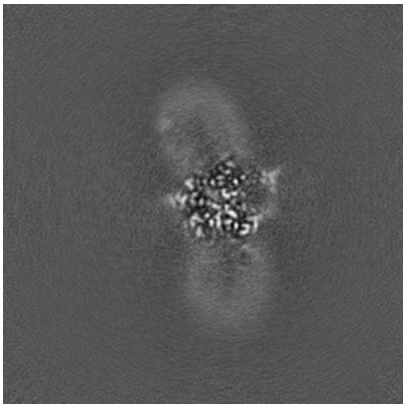


Z Index: 128

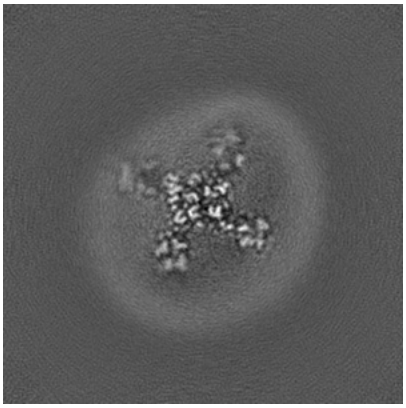
6.2.2 Raw map



X Index: 128



Y Index: 128

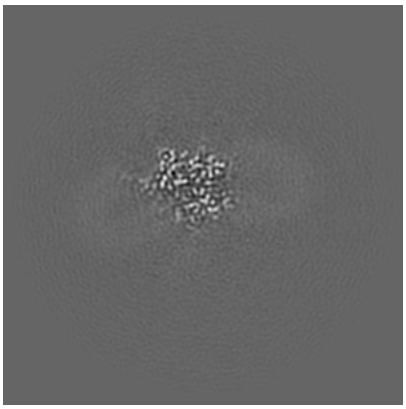


Z Index: 128

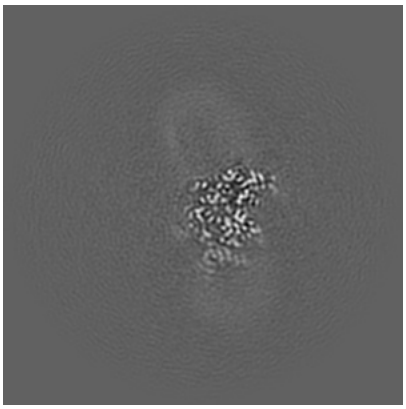
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

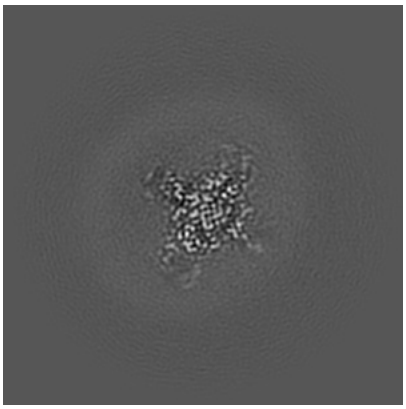
6.3.1 Primary map



X Index: 120

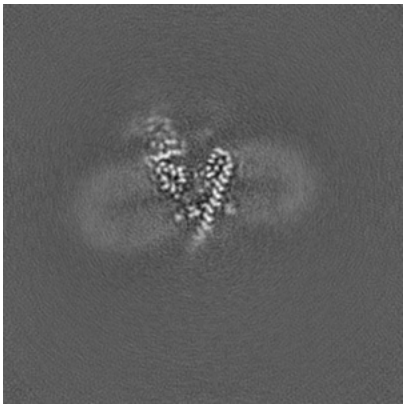


Y Index: 136

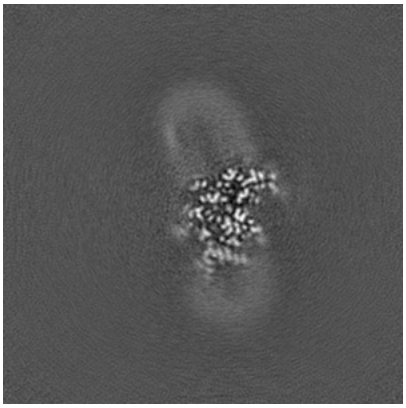


Z Index: 146

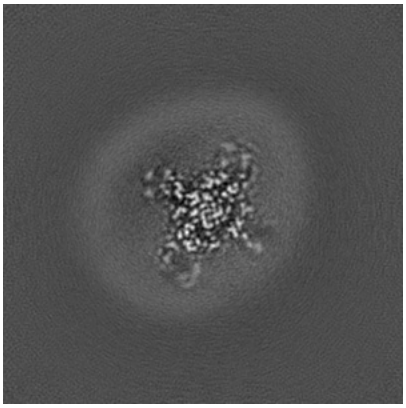
6.3.2 Raw map



X Index: 130



Y Index: 136

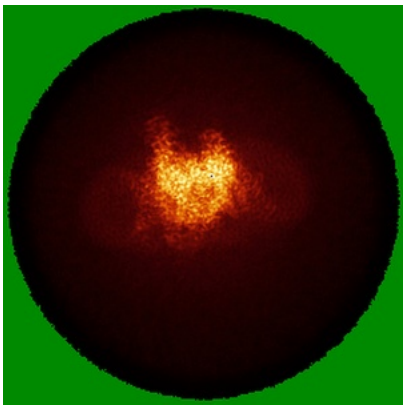


Z Index: 146

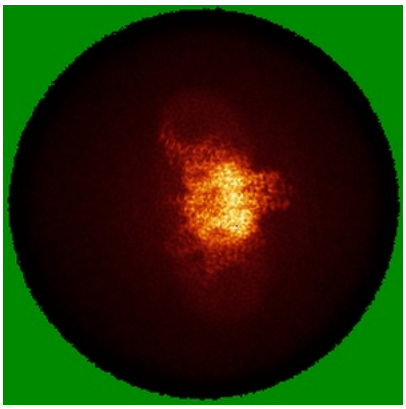
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

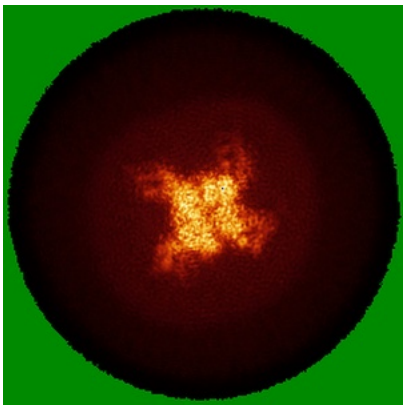
6.4.1 Primary map



X

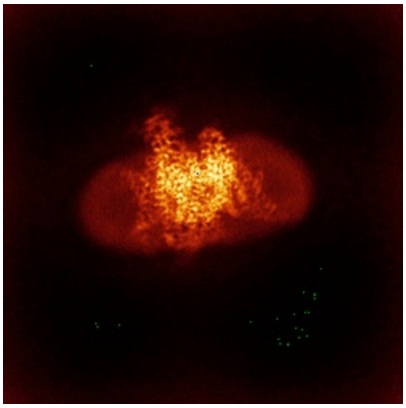


Y

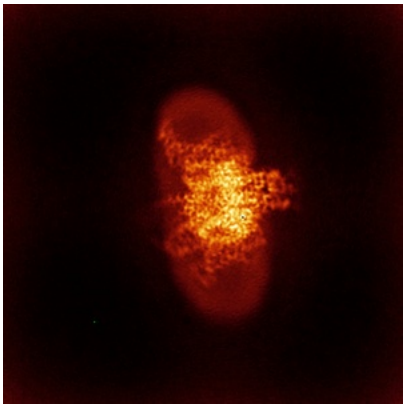


Z

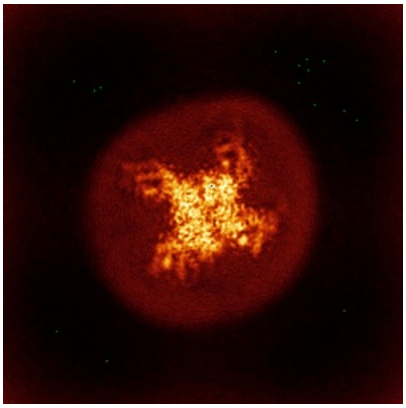
6.4.2 Raw map



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

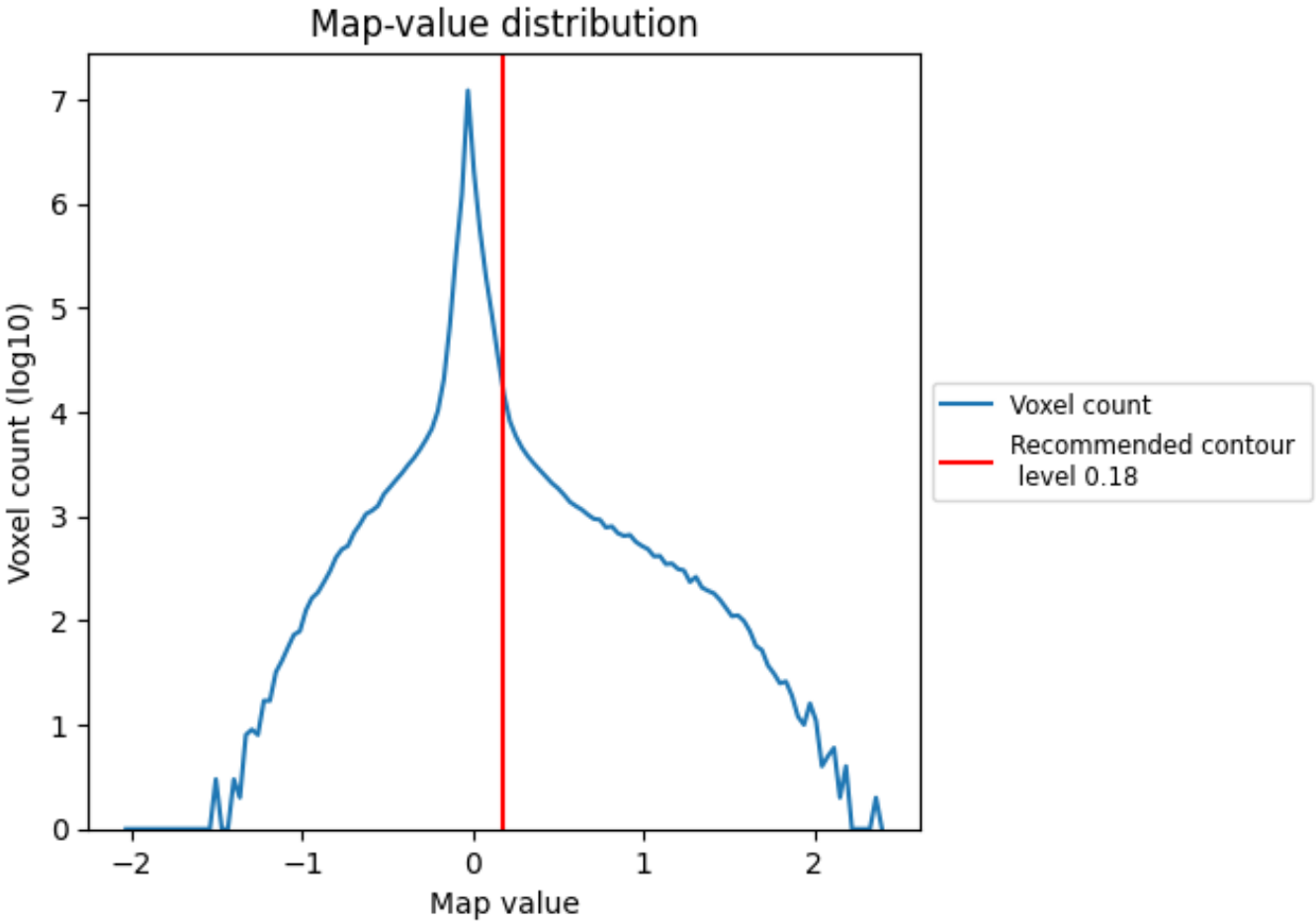
6.6 Mask visualisation (i)

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

7 Map analysis

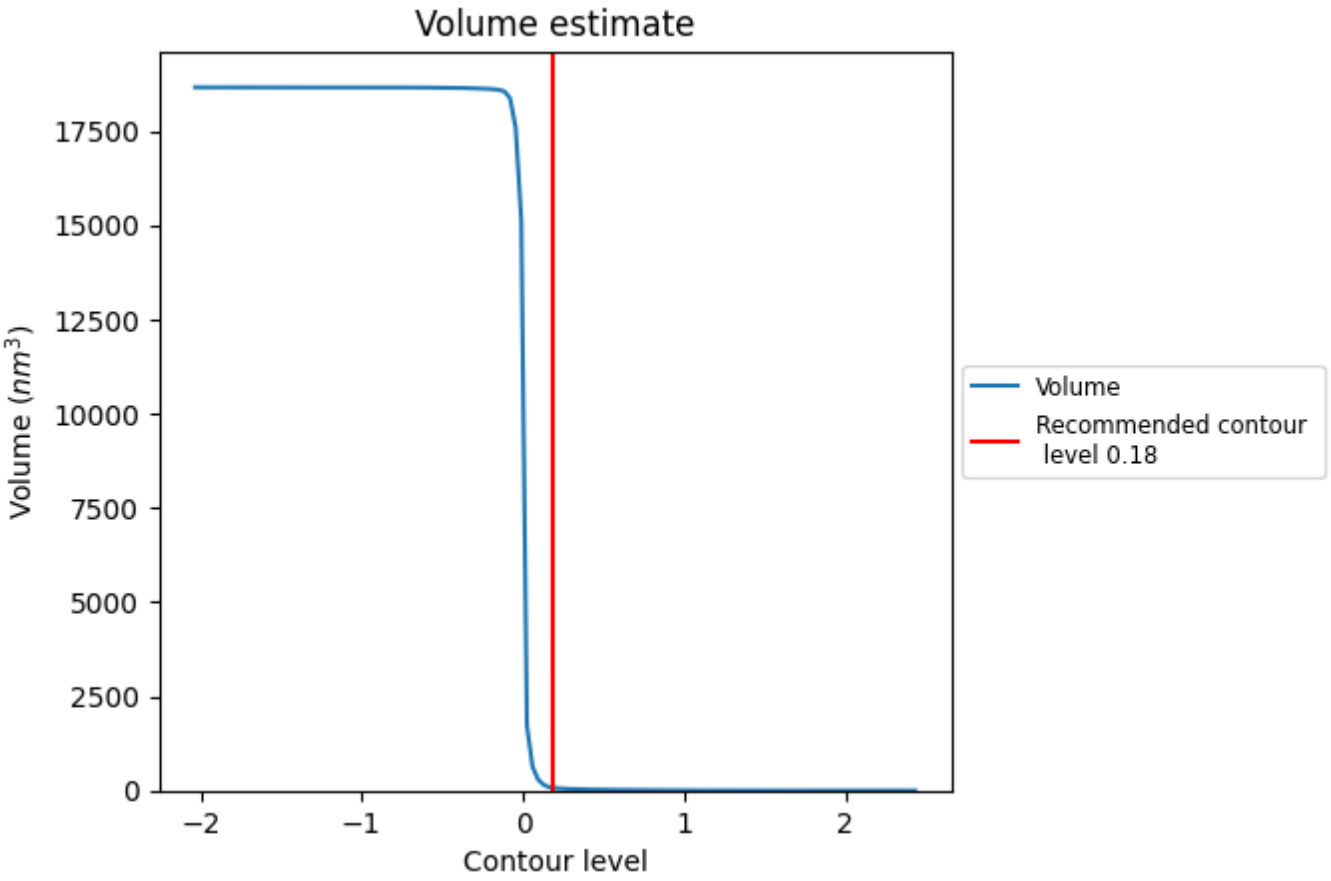
This section contains the results of statistical analysis of the map.

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.

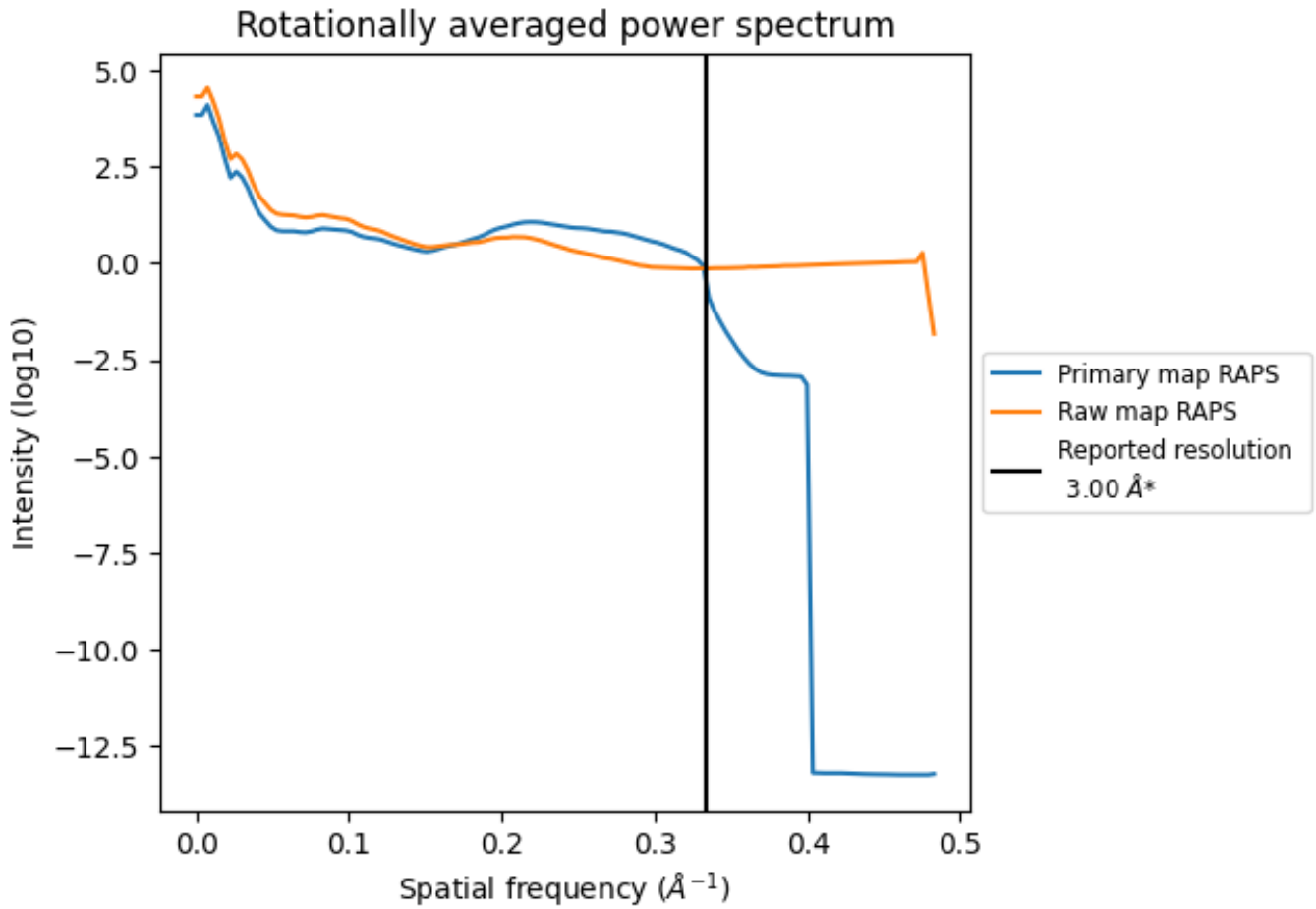
7.2 Volume estimate (i)



The volume at the recommended contour level is 79 nm^3; this corresponds to an approximate mass of 71 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)

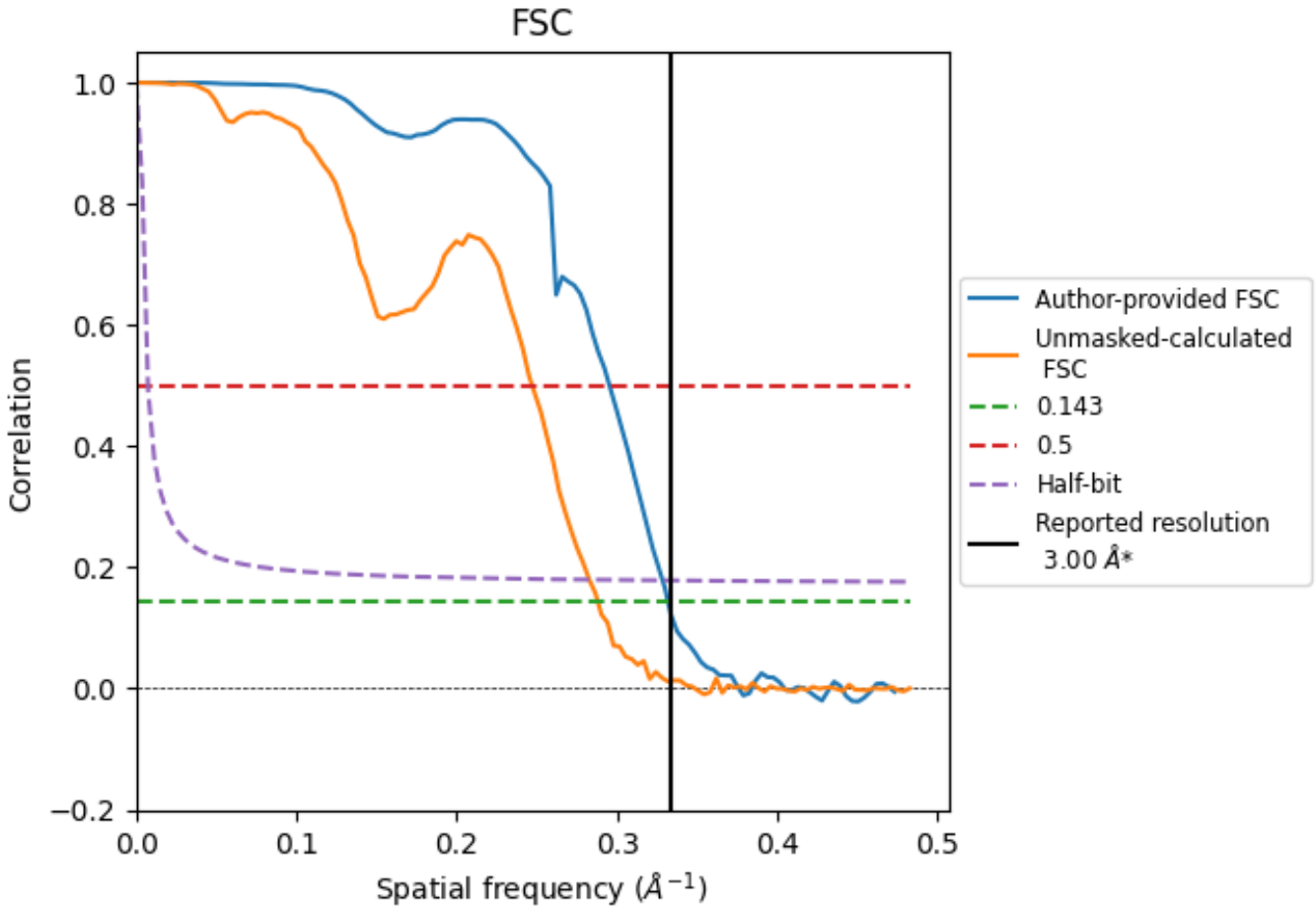


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

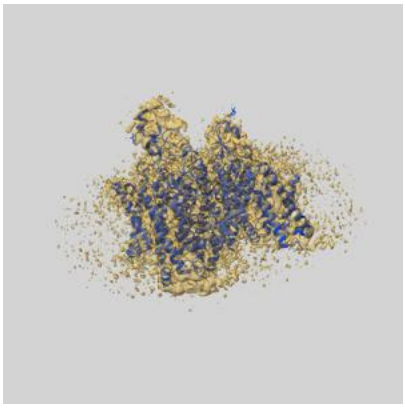
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.39	3.04
Unmasked-calculated*	3.47	4.05	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 3.0 by more than 10 %

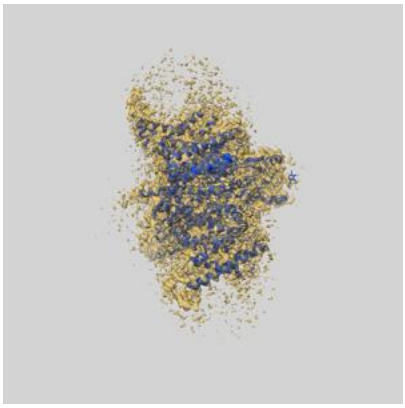
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43994 and PDB model 9AYK. Per-residue inclusion information can be found in section 3 on page 8.

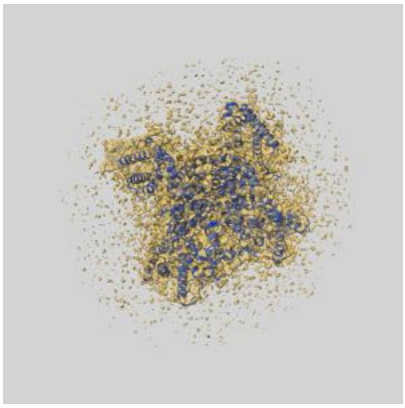
9.1 Map-model overlay



X



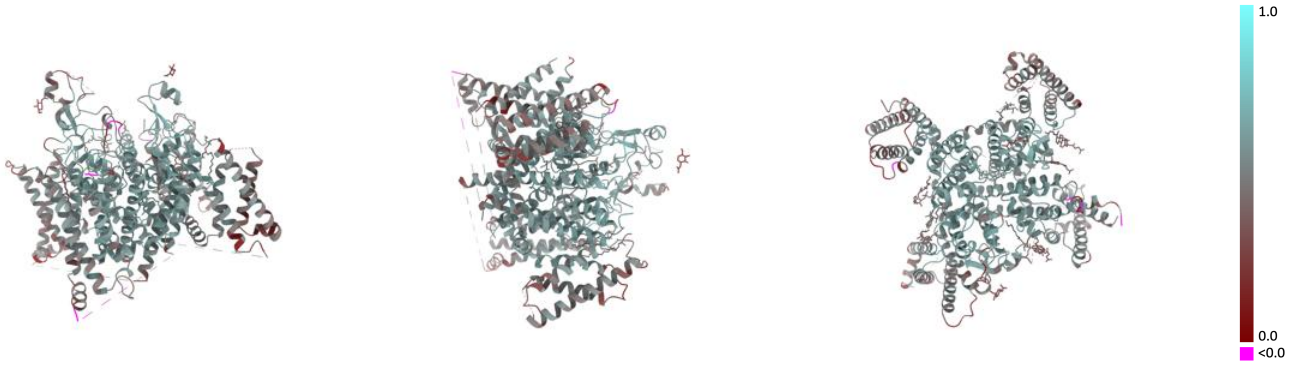
Y



Z

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

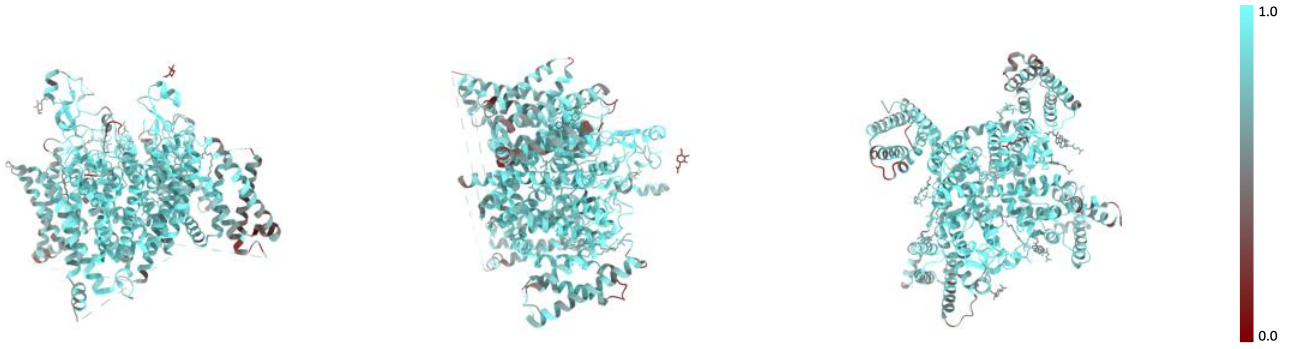
9.2 Q-score mapped to coordinate model (i)



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.

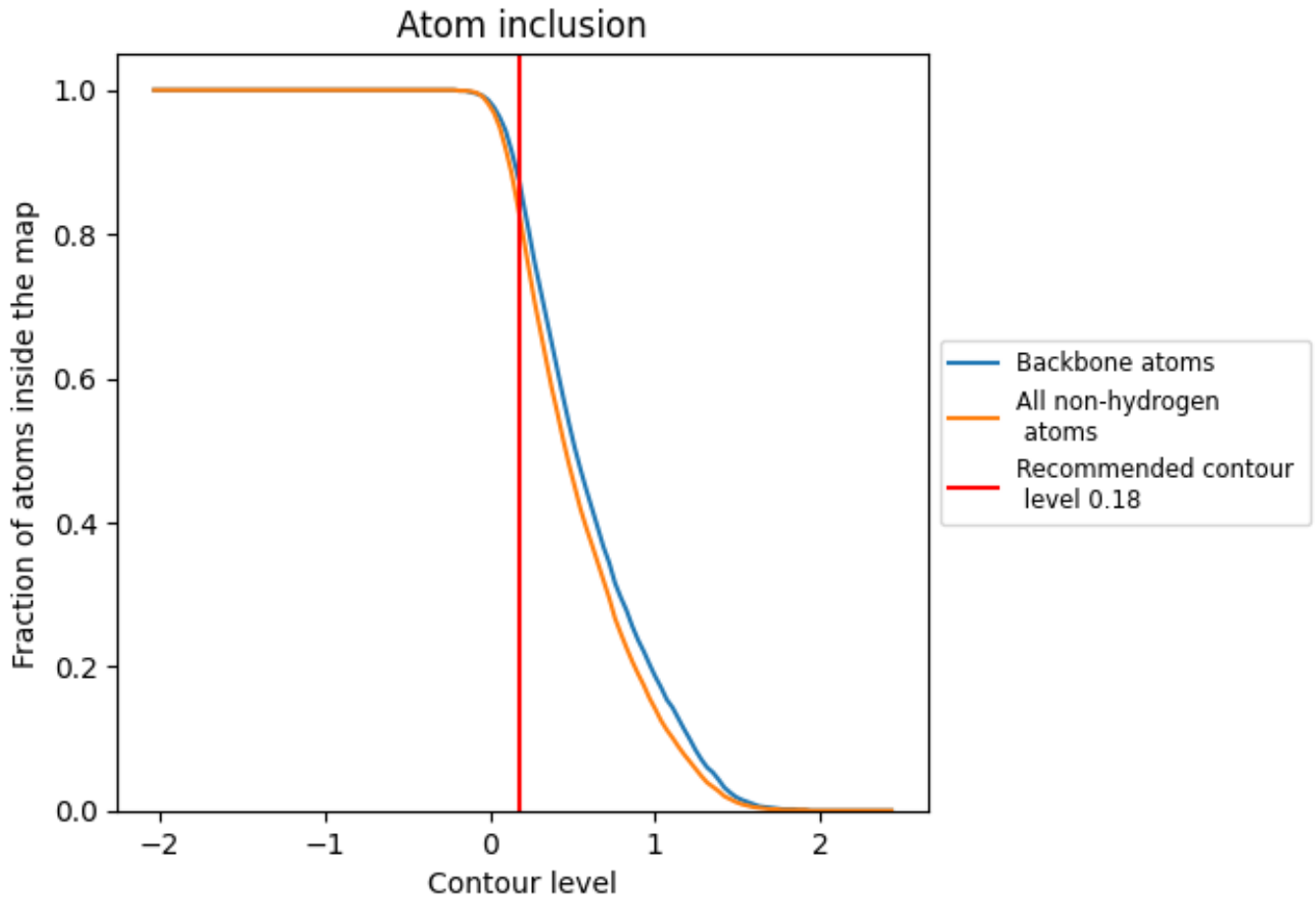
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.18).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8260	0.5190
A	0.8260	0.5190