Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 10:47 PM EDT

PDB ID	:	9AYJ
EMDB ID	:	EMD-43993
Title	:	Cryo-EM structure of human Cav3.2 with TTA-P2
Authors	:	Fan, X.; Huang, J.; Yan, N.
Deposited on	:	2024-03-07
Resolution	:	3.20 Å(reported)

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

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

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

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

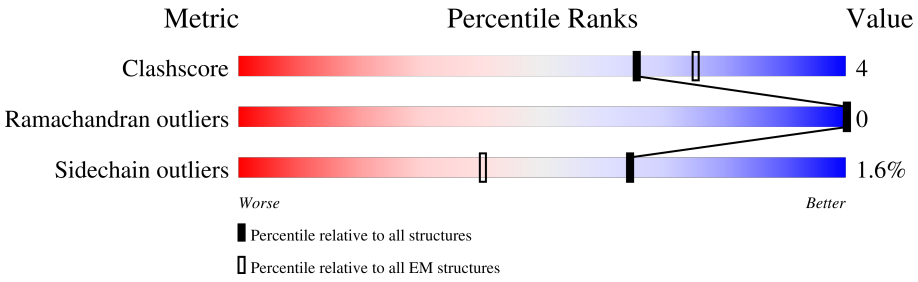
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	2116	45% 5% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8855 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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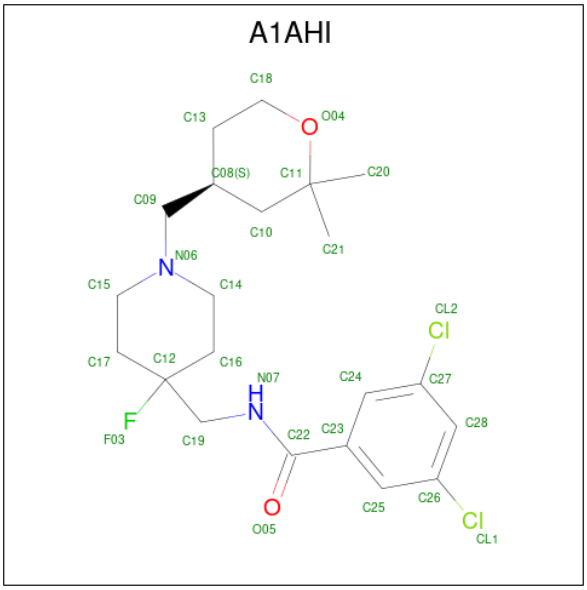
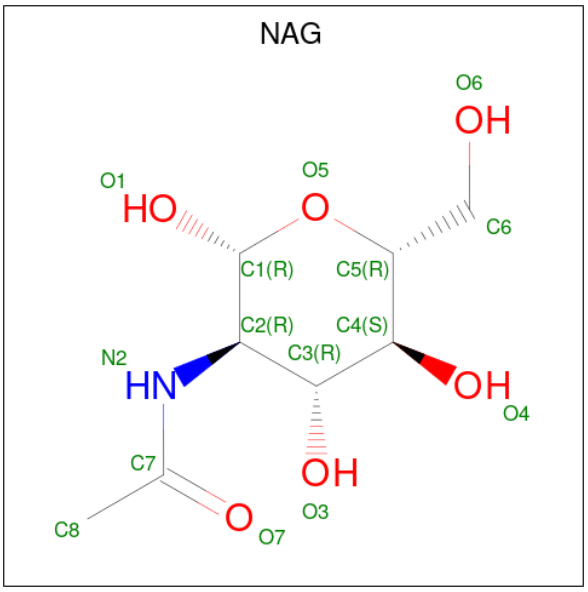
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP O95180
A	-13	GLU	-	expression tag	UNP O95180
A	-12	LYS	-	expression tag	UNP O95180
A	-11	GLY	-	expression tag	UNP O95180
A	-10	PHE	-	expression tag	UNP O95180
A	-9	ASP	-	expression tag	UNP O95180
A	-8	TYR	-	expression tag	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-[(1-{[(4S)-2,2-dimethyloxan-4-yl]methyl}-4-fluoropiperidin-4-yl)methyl]benzamide (three-letter code: A1AHI) (formula: $C_{21}H_{29}Cl_2FN_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	Cl	F	N	O	0
			28	21	2	1	2	2	

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

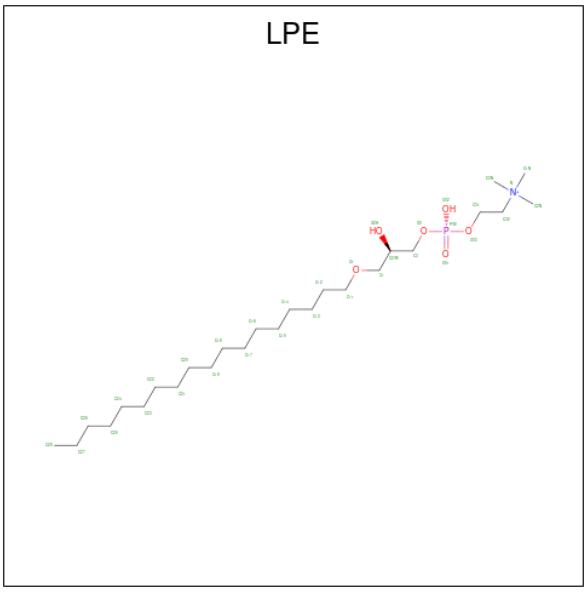


Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

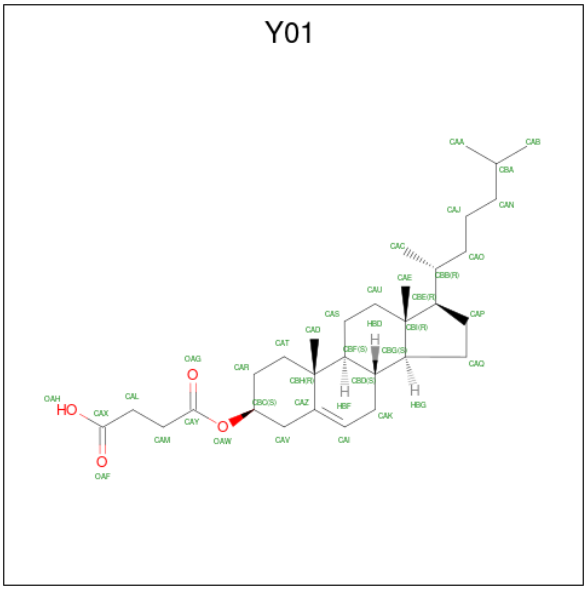
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0

- Molecule 5 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: 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 (three-letter code: 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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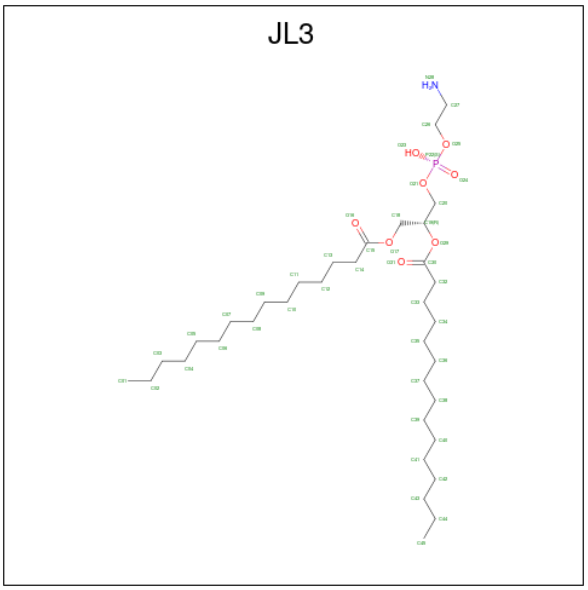
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 35	C 31	O 4	0

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



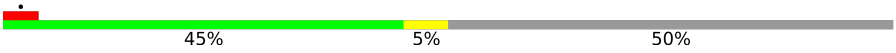
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total 45	C 35	N 1	O 8	P 1	0
7	A	1	Total 42	C 32	N 1	O 8	P 1	0
7	A	1	Total 36	C 26	N 1	O 8	P 1	0
7	A	1	Total 35	C 25	N 1	O 8	P 1	0

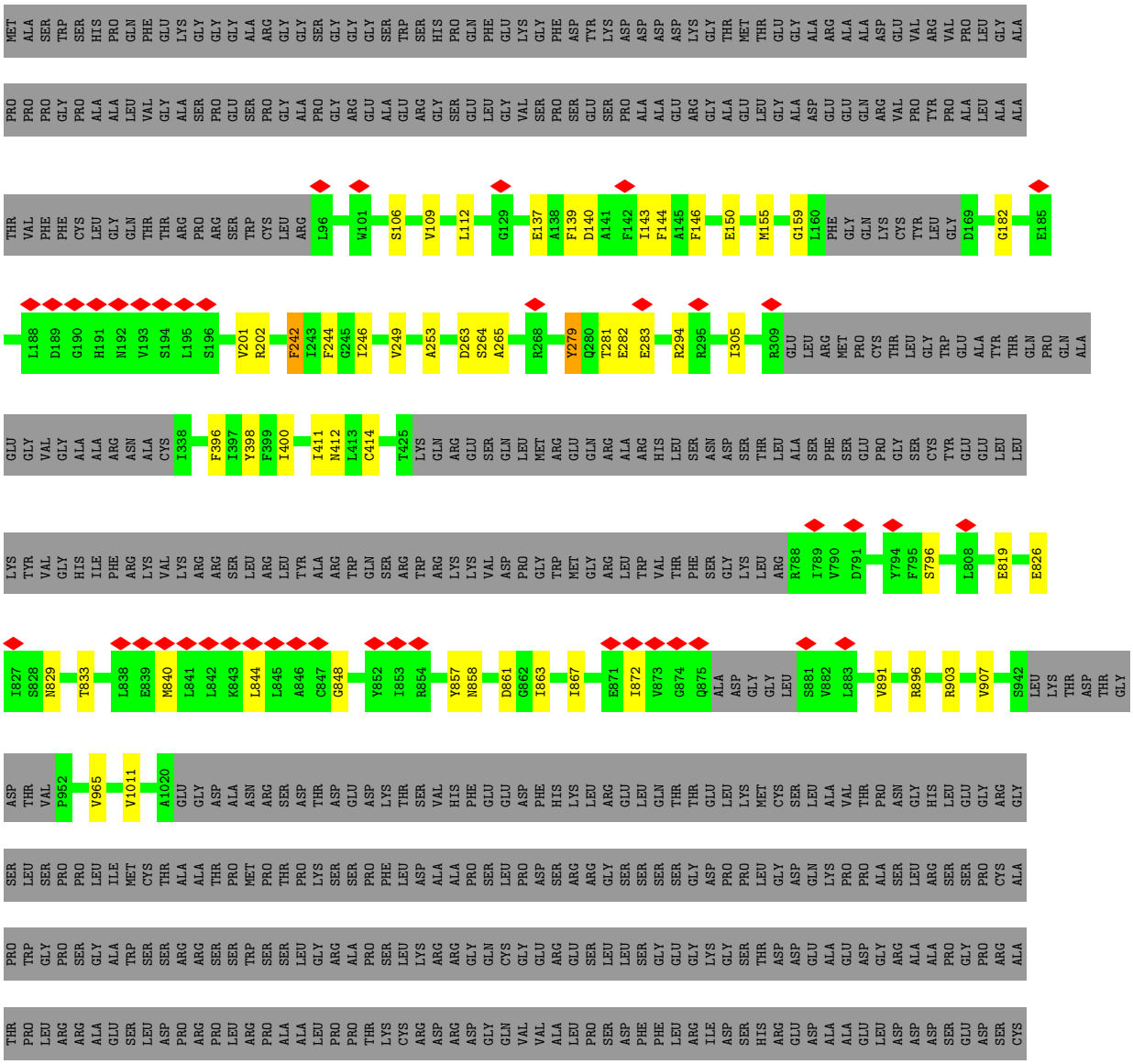
3 Residue-property plots (i)

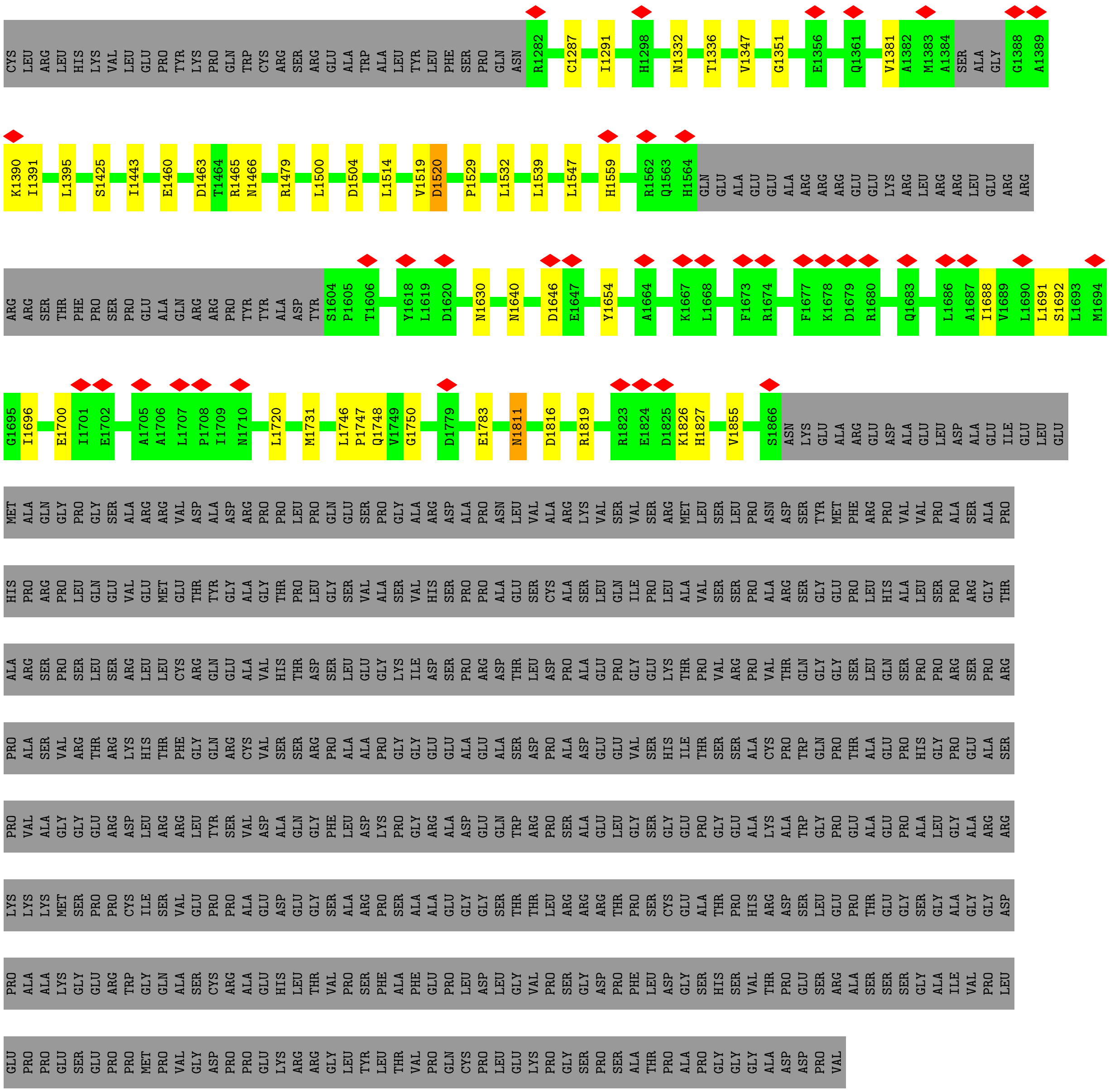
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113396	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	1.827	Depositor
Minimum map value	-1.388	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.041	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: Y01, CA, NAG, A1AHI, LPE, 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	0.25	0/8662	0.46	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	69	0
2	A	28	0	0	0	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
5	A	27	0	39	1	0
6	A	140	0	196	2	0
7	A	158	0	0	0	0
All	All	8855	0	8922	72	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.

All (72) 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:891:VAL:HG21	1:A:1443:ILE:HD11	1.50	0.93
1:A:294:ARG:NE	1:A:294:ARG:O	2.15	0.79
1:A:112:LEU:HD22	1:A:143:ILE:HD11	1.65	0.78
1:A:1816:ASP:O	1:A:1819:ARG:NH1	2.25	0.69
1:A:1514:LEU:HD21	1:A:1532:LEU:HD12	1.76	0.66
1:A:819:GLU:N	1:A:819:GLU:OE1	2.28	0.66
1:A:1460:GLU:OE1	1:A:1479:ARG:NH2	2.29	0.65
1:A:1654:TYR:HE1	1:A:1696:ILE:HD11	1.61	0.64
1:A:1332:ASN:O	1:A:1336:THR:OG1	2.18	0.61
1:A:1519:VAL:HG12	1:A:1520:ASP:OD2	2.02	0.60
1:A:279:TYR:CE1	1:A:305:ILE:HG23	2.38	0.58
1:A:1504:ASP:OD2	1:A:1811:ASN:ND2	2.37	0.57
1:A:1654:TYR:CE1	1:A:1696:ILE:HD11	2.42	0.54
1:A:109:VAL:HG13	1:A:143:ILE:HD12	1.91	0.53
1:A:1783:GLU:N	1:A:1816:ASP:OD1	2.43	0.51
1:A:1748:GLN:OE1	1:A:1748:GLN:O	2.29	0.51
1:A:1826:LYS:O	1:A:1827:HIS:ND1	2.44	0.51
1:A:1347:VAL:O	1:A:1351:GLY:N	2.38	0.50
1:A:112:LEU:HD22	1:A:143:ILE:CD1	2.37	0.49
1:A:1654:TYR:OH	1:A:1700:GLU:OE2	2.27	0.49
1:A:281:THR:HG22	1:A:282:GLU:OE1	2.13	0.48
1:A:833:THR:HG21	1:A:872:ILE:HD11	1.94	0.48
1:A:112:LEU:HD21	1:A:139:PHE:CE1	2.48	0.48
6:A:2413:Y01:HAC1	6:A:2413:Y01:HAU2	1.94	0.48
1:A:1381:VAL:HG12	1:A:1395:LEU:HD13	1.96	0.47
1:A:155:MET:O	1:A:159:GLY:N	2.43	0.47
1:A:412:ASN:HD22	1:A:1855:VAL:HG21	1.79	0.47
1:A:244:PHE:O	1:A:398:TYR:OH	2.30	0.47
1:A:1688:ILE:O	1:A:1692:SER:N	2.37	0.47
1:A:1691:LEU:HD21	1:A:1720:LEU:HG	1.96	0.47
1:A:826:GLU:HA	1:A:826:GLU:OE2	2.14	0.46
1:A:112:LEU:HD21	1:A:139:PHE:HE1	1.80	0.46
1:A:1463:ASP:OD2	1:A:1465:ARG:NH2	2.48	0.46
1:A:903:ARG:O	1:A:907:VAL:HG23	2.16	0.46
1:A:1691:LEU:HD11	1:A:1720:LEU:CD2	2.46	0.46
1:A:263:ASP:OD1	1:A:265:ALA:N	2.49	0.46
1:A:858:ASN:OD1	1:A:896:ARG:NH2	2.49	0.46
1:A:150:GLU:C	1:A:150:GLU:OE1	2.54	0.45
1:A:282:GLU:OE1	1:A:282:GLU:N	2.49	0.45
1:A:1529:PRO:O	1:A:1532:LEU:HD13	2.16	0.45
1:A:242:PHE:CE1	1:A:246:ILE:HD11	2.52	0.45
1:A:1514:LEU:CD2	1:A:1532:LEU:HD12	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:OD1	1:A:140:ASP:C	2.55	0.44
1:A:829:ASN:O	1:A:833:THR:HG22	2.18	0.44
1:A:1011:VAL:HG22	1:A:1547:LEU:HD22	1.98	0.44
1:A:140:ASP:OD2	1:A:202:ARG:NH1	2.51	0.44
1:A:249:VAL:O	1:A:253:ALA:HB2	2.18	0.44
1:A:1381:VAL:HG13	1:A:1391:ILE:HD12	1.99	0.43
1:A:396:PHE:HD1	1:A:400:ILE:HD12	1.82	0.43
1:A:965:VAL:HG21	1:A:1532:LEU:HD21	2.01	0.43
1:A:1466:ASN:OD1	1:A:1466:ASN:C	2.57	0.43
1:A:1466:ASN:OD1	1:A:1466:ASN:O	2.37	0.43
1:A:201:VAL:O	1:A:201:VAL:HG22	2.19	0.43
1:A:1731:MET:SD	1:A:1731:MET:N	2.92	0.42
1:A:1746:LEU:O	1:A:1750:GLY:N	2.46	0.42
1:A:1691:LEU:HD21	1:A:1720:LEU:CD2	2.50	0.42
1:A:1287:CYS:O	1:A:1291:ILE:HG23	2.20	0.42
1:A:1520:ASP:OD2	1:A:1520:ASP:N	2.53	0.42
1:A:840:MET:SD	1:A:844:LEU:HD12	2.60	0.41
1:A:857:TYR:HB2	1:A:896:ARG:NH2	2.35	0.41
5:A:2405:LPE:H2N2	5:A:2405:LPE:O33	2.20	0.41
1:A:844:LEU:O	1:A:848:GLY:N	2.47	0.41
1:A:411:ILE:HG22	1:A:411:ILE:O	2.20	0.41
1:A:1500:LEU:O	1:A:1539:LEU:HD21	2.19	0.41
1:A:1746:LEU:N	1:A:1747:PRO:HD2	2.35	0.41
6:A:2412:Y01:HAR2	6:A:2412:Y01:OAG	2.21	0.41
1:A:1390:LYS:O	1:A:1390:LYS:HG2	2.20	0.41
1:A:863:ILE:O	1:A:867:ILE:HG13	2.21	0.41
1:A:1691:LEU:HD11	1:A:1720:LEU:HD21	2.03	0.41
1:A:283:GLU:OE2	1:A:283:GLU:N	2.38	0.40
1:A:144:PHE:HE1	1:A:182:GLY:HA3	1.87	0.40
1:A:861:ASP:OD2	1:A:896:ARG:NH1	2.51	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%)	1021 (98%)	17 (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%)	924 (98%)	15 (2%)	62 84

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	137	GLU
1	A	146	PHE
1	A	242	PHE
1	A	264	SER
1	A	279	TYR
1	A	414	CYS
1	A	796	SER
1	A	1425	SER
1	A	1520	ASP
1	A	1559	HIS
1	A	1630	ASN
1	A	1640	ASN
1	A	1646	ASP
1	A	1811	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	391	HIS

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Mol	Chain	Res	Type
1	A	1357	HIS
1	A	1748	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	2408	-	38,38,38	0.45	0	57,57,57	0.78	2 (3%)
2	A1AHI	A	2401	-	28,30,30	2.82	8 (28%)	40,44,44	1.95	9 (22%)
6	Y01	A	2413	-	38,38,38	0.43	0	57,57,57	0.49	0
7	JL3	A	2407	-	44,44,44	0.54	0	47,49,49	0.53	1 (2%)
7	JL3	A	2410	-	35,35,44	0.60	0	38,40,49	0.61	1 (2%)
5	LPE	A	2405	-	26,26,33	0.27	0	30,32,39	0.40	0
6	Y01	A	2406	-	38,38,38	0.48	0	57,57,57	0.67	0
7	JL3	A	2411	-	34,34,44	0.60	0	37,39,49	0.60	1 (2%)
3	NAG	A	2402	-	14,14,15	0.26	0	17,19,21	0.63	0
7	JL3	A	2409	-	41,41,44	0.56	0	44,46,49	0.53	1 (2%)

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	0.55	0
3	NAG	A	2403	-	14,14,15	0.27	0	17,19,21	0.53	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	2408	-	-	8/19/77/77	0/4/4/4
2	A1AHI	A	2401	-	-	5/13/38/38	1/3/3/3
6	Y01	A	2413	-	-	8/19/77/77	0/4/4/4
7	JL3	A	2407	-	-	21/48/48/48	-
7	JL3	A	2410	-	-	20/39/39/48	-
5	LPE	A	2405	-	-	9/27/27/34	-
6	Y01	A	2406	-	-	3/19/77/77	0/4/4/4
7	JL3	A	2411	-	-	17/38/38/48	-
3	NAG	A	2402	-	-	0/6/23/26	0/1/1/1
7	JL3	A	2409	-	-	18/45/45/48	-
6	Y01	A	2412	-	-	6/19/77/77	0/4/4/4
3	NAG	A	2403	-	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2401	A1AHI	C09-N06	-8.51	1.31	1.47
2	A	2401	A1AHI	C14-N06	-5.66	1.31	1.46
2	A	2401	A1AHI	C15-N06	-5.56	1.31	1.46
2	A	2401	A1AHI	O04-C11	-5.56	1.41	1.45
2	A	2401	A1AHI	C22-N07	4.08	1.42	1.33
2	A	2401	A1AHI	O05-C22	-3.61	1.16	1.23
2	A	2401	A1AHI	O04-C18	-2.98	1.39	1.44
2	A	2401	A1AHI	F03-C12	-2.42	1.34	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2401	A1AHI	C12-C19-N07	-5.96	105.67	114.02
2	A	2401	A1AHI	C14-C16-C12	-4.84	108.56	112.38
2	A	2401	A1AHI	C08-C09-N06	-3.81	109.28	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2401	A1AHI	C14-N06-C15	3.37	116.41	108.83
2	A	2401	A1AHI	C23-C22-N07	2.92	123.37	117.09
2	A	2401	A1AHI	C16-C12-C17	-2.81	108.71	110.75
2	A	2401	A1AHI	C15-C17-C12	-2.74	110.22	112.38
2	A	2401	A1AHI	C16-C14-N06	2.60	113.80	111.23
6	A	2408	Y01	CAQ-CBG-CBI	2.51	106.86	103.84
7	A	2410	JL3	O23-P22-O24	2.42	124.23	112.24
2	A	2401	A1AHI	O05-C22-N07	-2.41	117.80	122.61
7	A	2407	JL3	O23-P22-O24	2.36	123.90	112.24
7	A	2411	JL3	O23-P22-O24	2.33	123.76	112.24
7	A	2409	JL3	O23-P22-O24	2.28	123.49	112.24
6	A	2408	Y01	CAU-CBI-CBG	-2.08	104.05	107.27

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2401	A1AHI	C10-C08-C09-N06
2	A	2401	A1AHI	C13-C08-C09-N06
2	A	2401	A1AHI	C17-C12-C19-N07
2	A	2401	A1AHI	C16-C12-C19-N07
5	A	2405	LPE	C1-C2-C3-O3
6	A	2408	Y01	CAV-CBC-OAW-CAY
6	A	2412	Y01	CAV-CBC-OAW-CAY
7	A	2407	JL3	C26-O25-P22-O24
7	A	2407	JL3	C32-C30-O29-C19
7	A	2409	JL3	C20-O21-P22-O24
7	A	2409	JL3	O25-C26-C27-N28
7	A	2409	JL3	C32-C30-O29-C19
7	A	2410	JL3	C26-O25-P22-O24
7	A	2411	JL3	C26-O25-P22-O24
7	A	2411	JL3	O25-C26-C27-N28
7	A	2411	JL3	O31-C30-O29-C19
7	A	2411	JL3	C32-C30-O29-C19
7	A	2411	JL3	O16-C15-O17-C18
7	A	2407	JL3	O31-C30-O29-C19
7	A	2409	JL3	O31-C30-O29-C19
7	A	2411	JL3	C14-C15-O17-C18
7	A	2407	JL3	C14-C15-O17-C18
5	A	2405	LPE	O2H-C2-C3-O3
7	A	2407	JL3	O16-C15-O17-C18
7	A	2410	JL3	C32-C30-O29-C19

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Mol	Chain	Res	Type	Atoms
7	A	2410	JL3	O31-C30-O29-C19
7	A	2410	JL3	O29-C19-C20-O21
7	A	2409	JL3	O17-C18-C19-O29
6	A	2408	Y01	CAN-CAJ-CAO-CBB
6	A	2413	Y01	CAM-CAY-OAW-CBC
6	A	2412	Y01	CAO-CAJ-CAN-CBA
7	A	2407	JL3	C26-O25-P22-O21
7	A	2409	JL3	C20-O21-P22-O25
7	A	2409	JL3	C26-O25-P22-O21
7	A	2410	JL3	C20-O21-P22-O25
7	A	2410	JL3	C26-O25-P22-O21
6	A	2408	Y01	CAM-CAY-OAW-CBC
6	A	2408	Y01	CAJ-CAN-CBA-CAA
7	A	2407	JL3	C08-C09-C10-C11
7	A	2407	JL3	C39-C40-C41-C42
5	A	2405	LPE	O1-C1-C2-O2H
6	A	2413	Y01	OAG-CAY-OAW-CBC
7	A	2407	JL3	C33-C34-C35-C36
6	A	2408	Y01	CAJ-CAN-CBA-CAB
7	A	2409	JL3	C33-C34-C35-C36
7	A	2409	JL3	C03-C04-C05-C06
7	A	2411	JL3	C33-C34-C35-C36
6	A	2408	Y01	OAG-CAY-OAW-CBC
7	A	2407	JL3	C37-C38-C39-C40
5	A	2405	LPE	O1-C1-C2-C3
7	A	2410	JL3	C33-C34-C35-C36
6	A	2412	Y01	CAM-CAY-OAW-CBC
6	A	2412	Y01	OAG-CAY-OAW-CBC
7	A	2411	JL3	C18-C19-C20-O21
7	A	2410	JL3	C14-C15-O17-C18
6	A	2406	Y01	CAN-CAJ-CAO-CBB
7	A	2407	JL3	C09-C10-C11-C12
7	A	2407	JL3	C11-C12-C13-C14
6	A	2406	Y01	CAO-CAJ-CAN-CBA
2	A	2401	A1AHI	C08-C09-N06-C15
7	A	2410	JL3	C18-C19-C20-O21
7	A	2409	JL3	C35-C36-C37-C38
6	A	2413	Y01	CAX-CAL-CAM-CAY
7	A	2409	JL3	O17-C18-C19-C20
7	A	2410	JL3	O17-C18-C19-C20
7	A	2411	JL3	C26-O25-P22-O21
7	A	2407	JL3	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
7	A	2410	JL3	O16-C15-O17-C18
7	A	2409	JL3	C09-C10-C11-C12
6	A	2413	Y01	CAJ-CAO-CBB-CBE
7	A	2411	JL3	C18-C19-O29-C30
7	A	2407	JL3	C19-C20-O21-P22
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	C20-O21-P22-O23
7	A	2410	JL3	C26-O25-P22-O23
7	A	2411	JL3	C27-C26-O25-P22
7	A	2411	JL3	O29-C19-C20-O21
7	A	2407	JL3	C40-C41-C42-C43
7	A	2409	JL3	C04-C05-C06-C07
6	A	2412	Y01	CAN-CAJ-CAO-CBB
7	A	2410	JL3	O17-C18-C19-O29
7	A	2407	JL3	C04-C05-C06-C07
5	A	2405	LPE	C12-C11-O1-C1
7	A	2410	JL3	C37-C38-C39-C40
7	A	2411	JL3	C06-C07-C08-C09
5	A	2405	LPE	C2-C1-O1-C11
6	A	2408	Y01	CAO-CAJ-CAN-CBA
7	A	2409	JL3	C19-C20-O21-P22
7	A	2407	JL3	C07-C08-C09-C10
6	A	2413	Y01	CAJ-CAO-CBB-CAC
7	A	2410	JL3	C36-C37-C38-C39
7	A	2409	JL3	C10-C11-C12-C13
6	A	2413	Y01	CAM-CAL-CAX-OAF
5	A	2405	LPE	C12-C13-C14-C15
6	A	2413	Y01	CAM-CAL-CAX-OAH
7	A	2410	JL3	C10-C11-C12-C13
7	A	2407	JL3	C01-C02-C03-C04
6	A	2412	Y01	CAR-CBC-OAW-CAY
7	A	2407	JL3	O29-C30-C32-C33
7	A	2410	JL3	C35-C36-C37-C38
5	A	2405	LPE	C16-C17-C18-C19
7	A	2410	JL3	C05-C06-C07-C08
7	A	2411	JL3	C13-C14-C15-O17
6	A	2408	Y01	CAL-CAM-CAY-OAW
6	A	2406	Y01	CAM-CAY-OAW-CBC
5	A	2405	LPE	O1-C11-C12-C13
7	A	2407	JL3	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
7	A	2411	JL3	C08-C09-C10-C11
7	A	2411	JL3	C13-C14-C15-O16
7	A	2409	JL3	C32-C33-C34-C35
6	A	2413	Y01	CAN-CAJ-CAO-CBB
7	A	2411	JL3	C10-C11-C12-C13
7	A	2410	JL3	C06-C07-C08-C09

All (1) ring outliers are listed below:

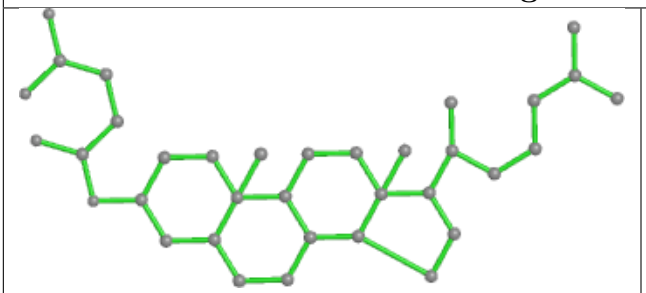
Mol	Chain	Res	Type	Atoms
2	A	2401	A1AHI	C12-C14-C15-C16-C17-N06

3 monomers are involved in 3 short contacts:

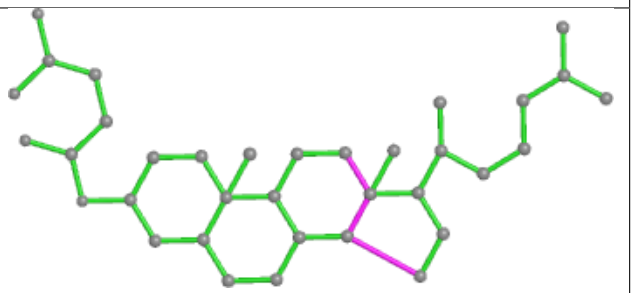
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2413	Y01	1	0
5	A	2405	LPE	1	0
6	A	2412	Y01	1	0

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.

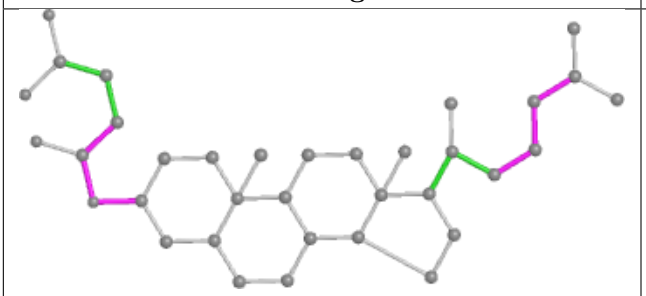
Ligand Y01 A 2408



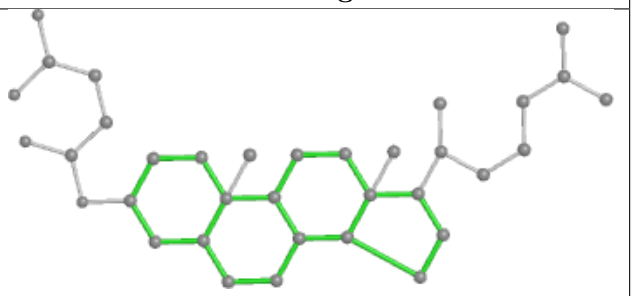
Bond lengths



Bond angles

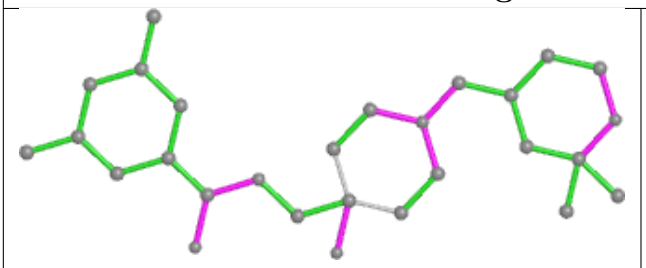


Torsions

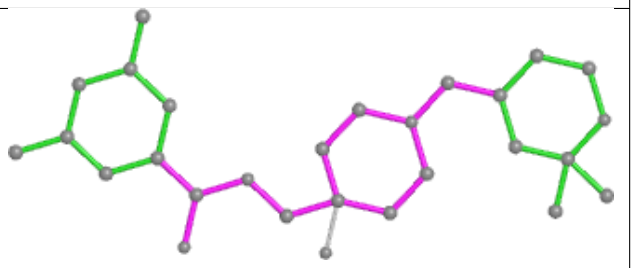


Rings

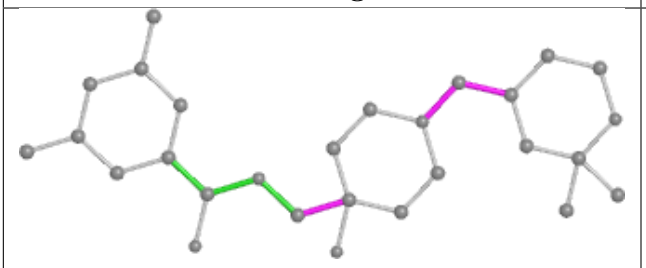
Ligand A1AHI A 2401



Bond lengths



Bond angles



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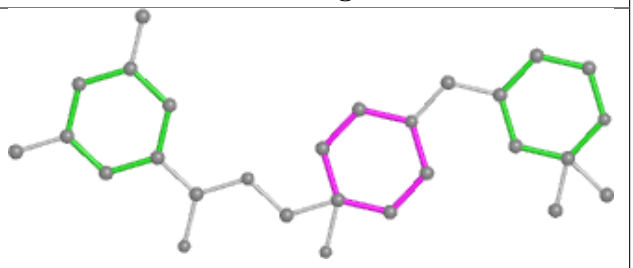
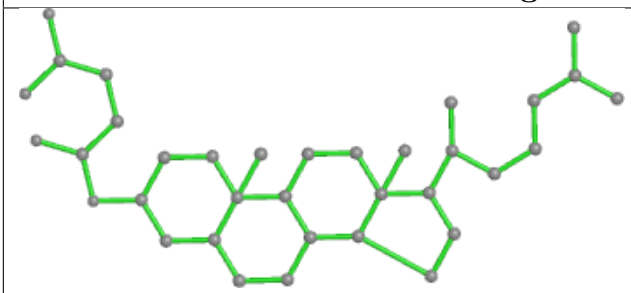
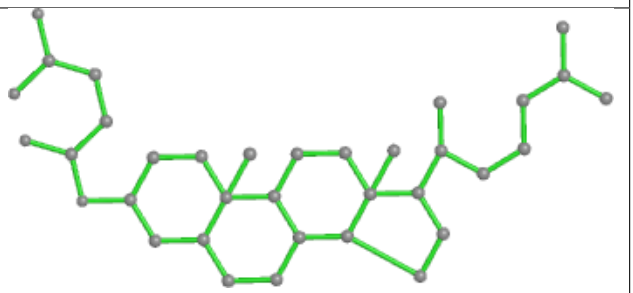


Rings

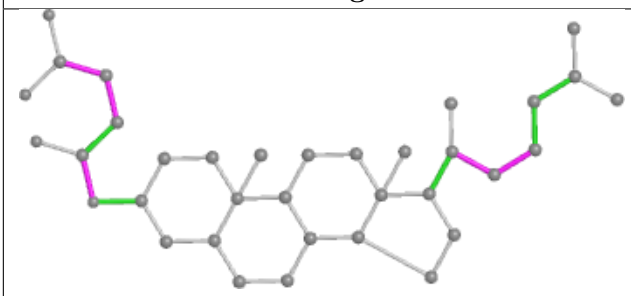
Ligand Y01 A 2413



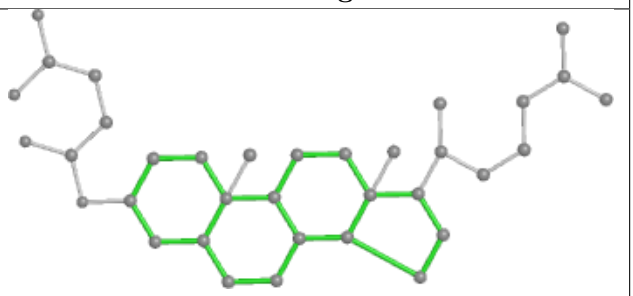
Bond lengths



Bond angles

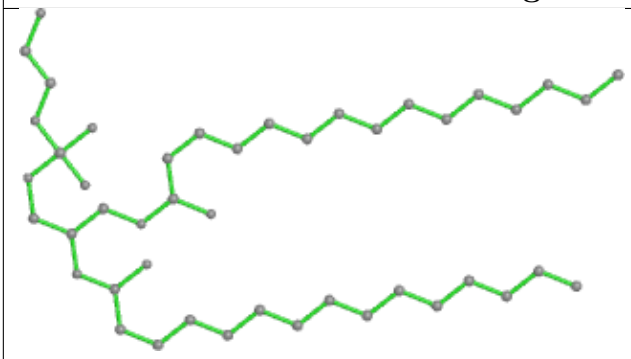


Torsions

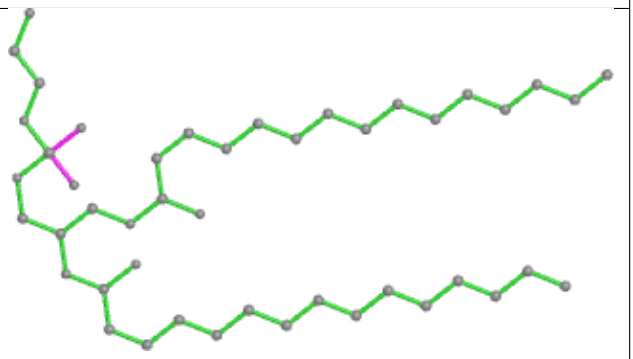


Rings

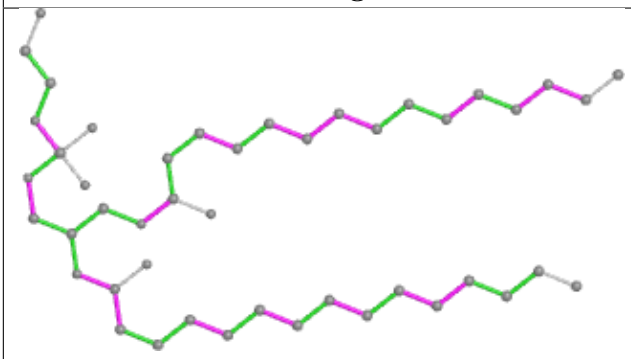
Ligand JL3 A 2407



Bond lengths



Bond angles



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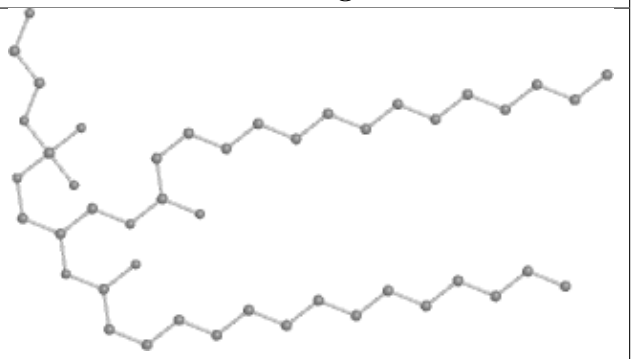
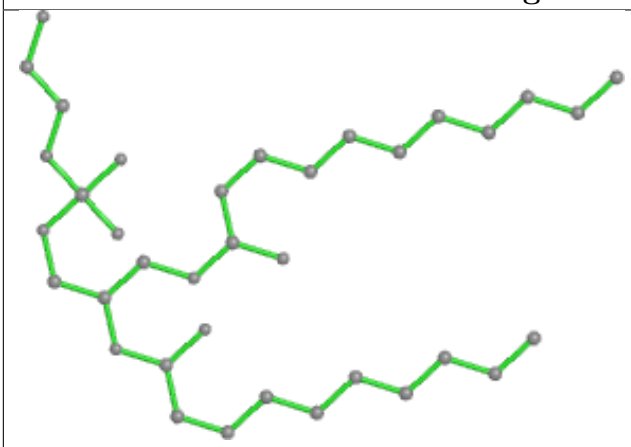
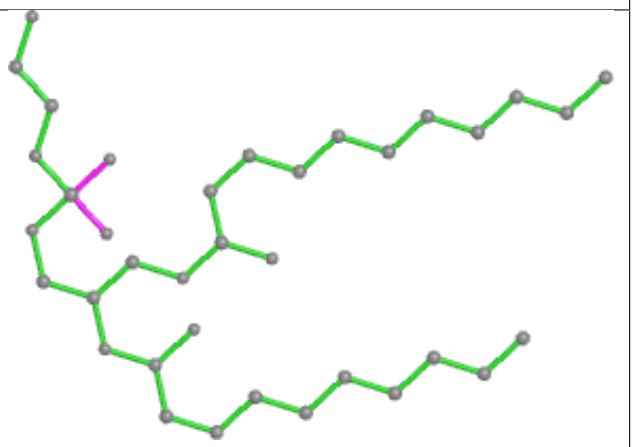


Rings

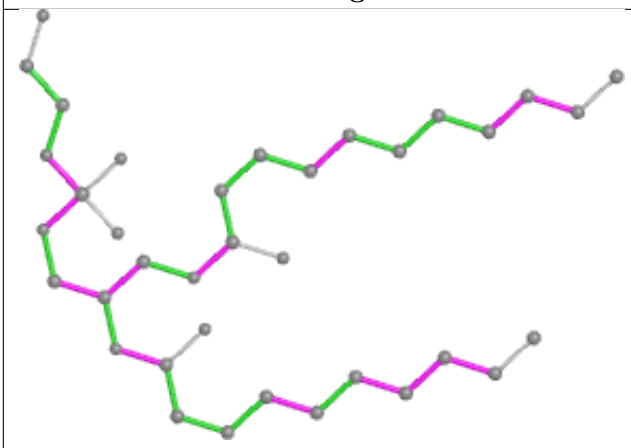
Ligand JL3 A 2410



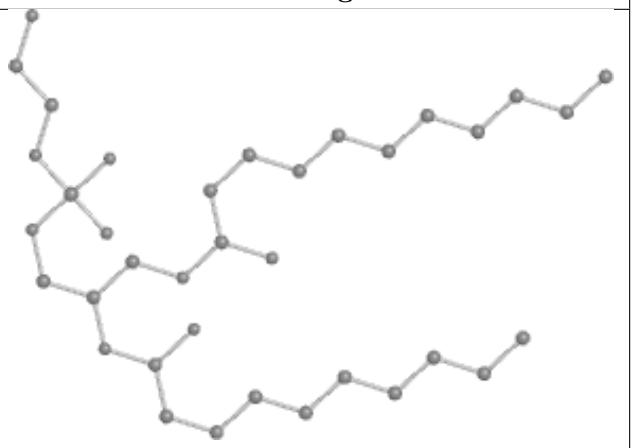
Bond lengths



Bond angles

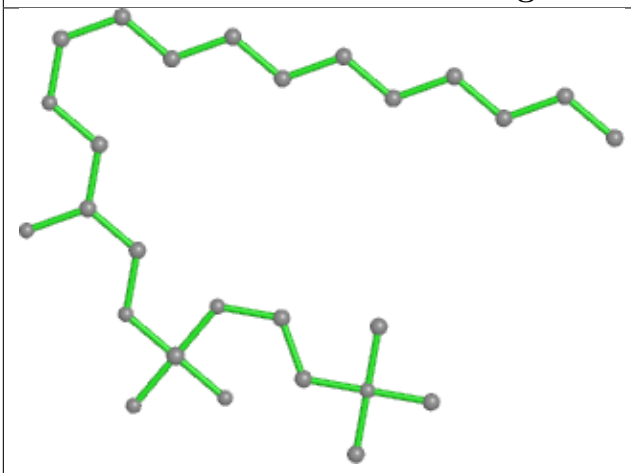


Torsions

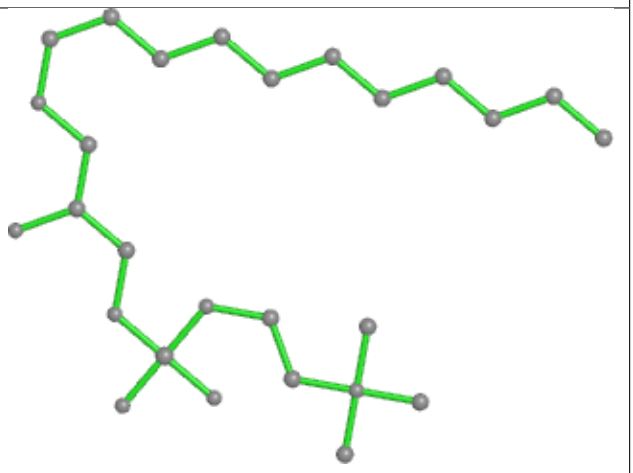


Rings

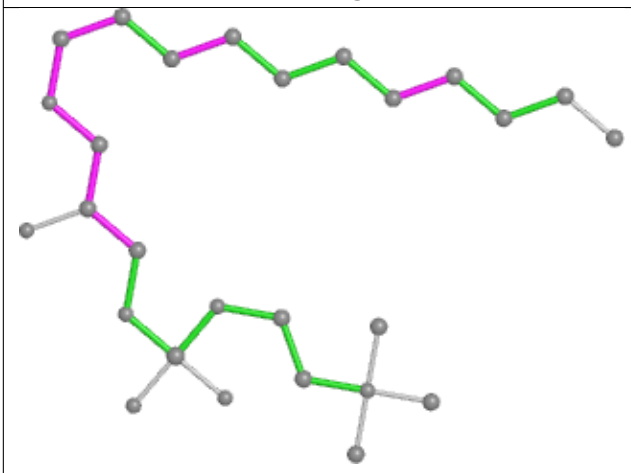
Ligand LPE A 2405



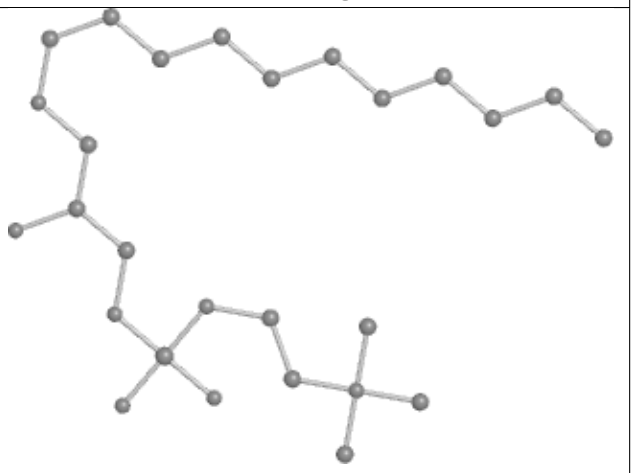
Bond lengths



Bond angles

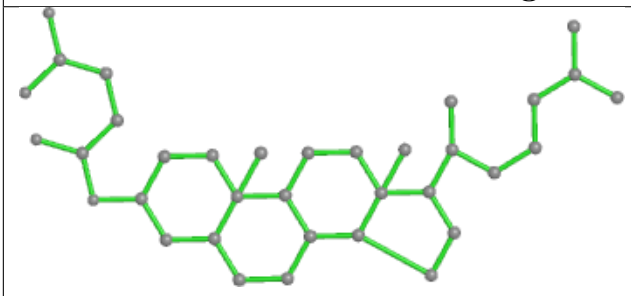


Torsions

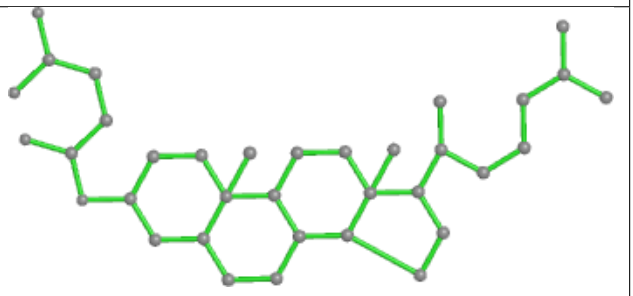


Rings

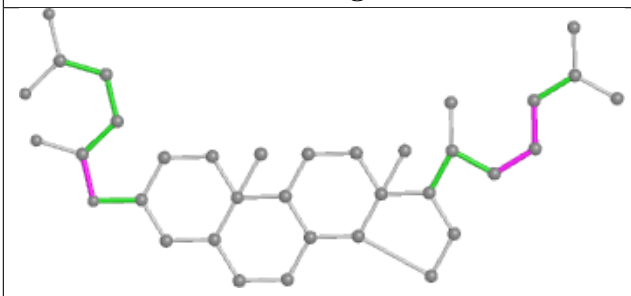
Ligand Y01 A 2406



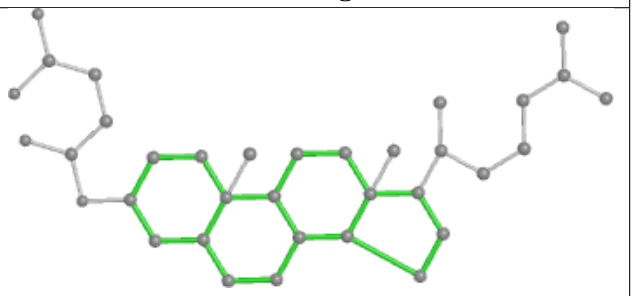
Bond lengths



Bond angles

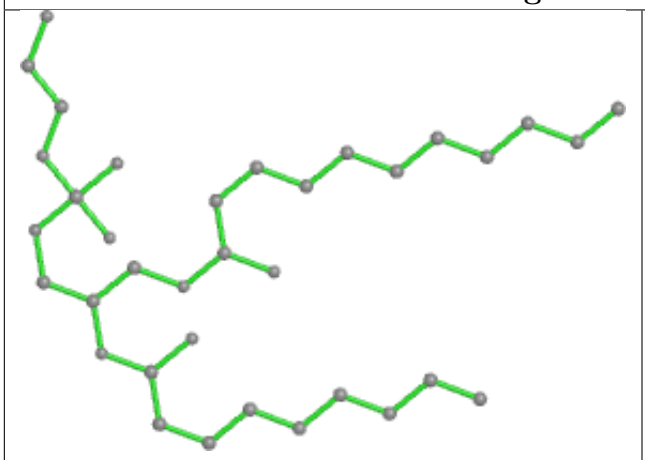


Torsions

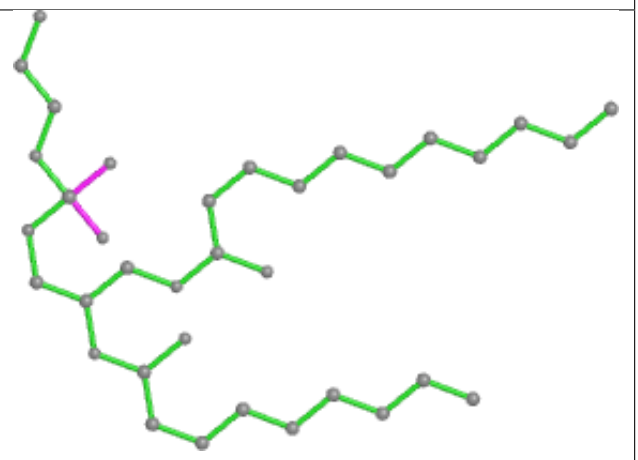


Rings

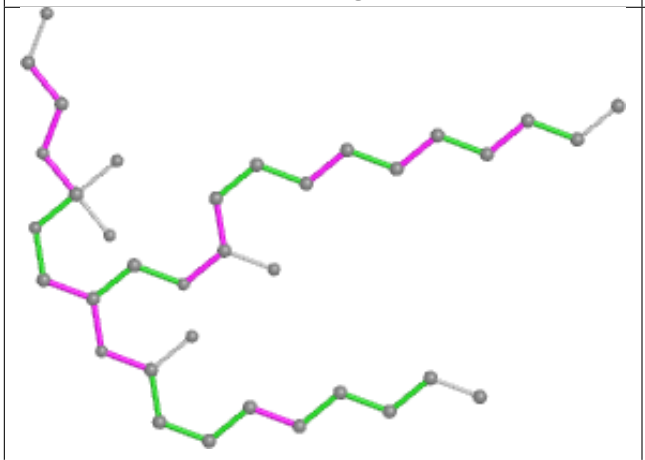
Ligand JL3 A 2411



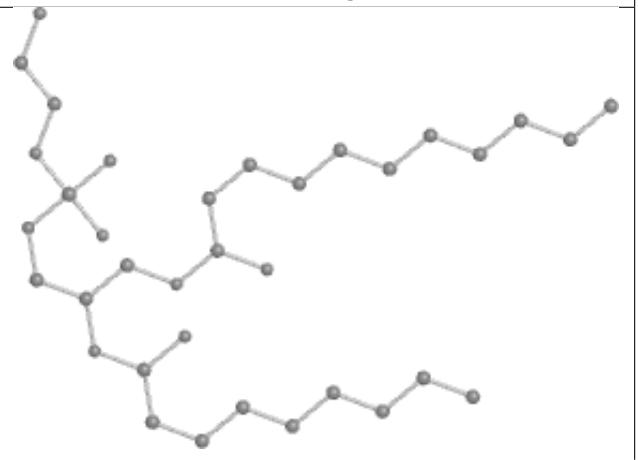
Bond lengths



Bond angles

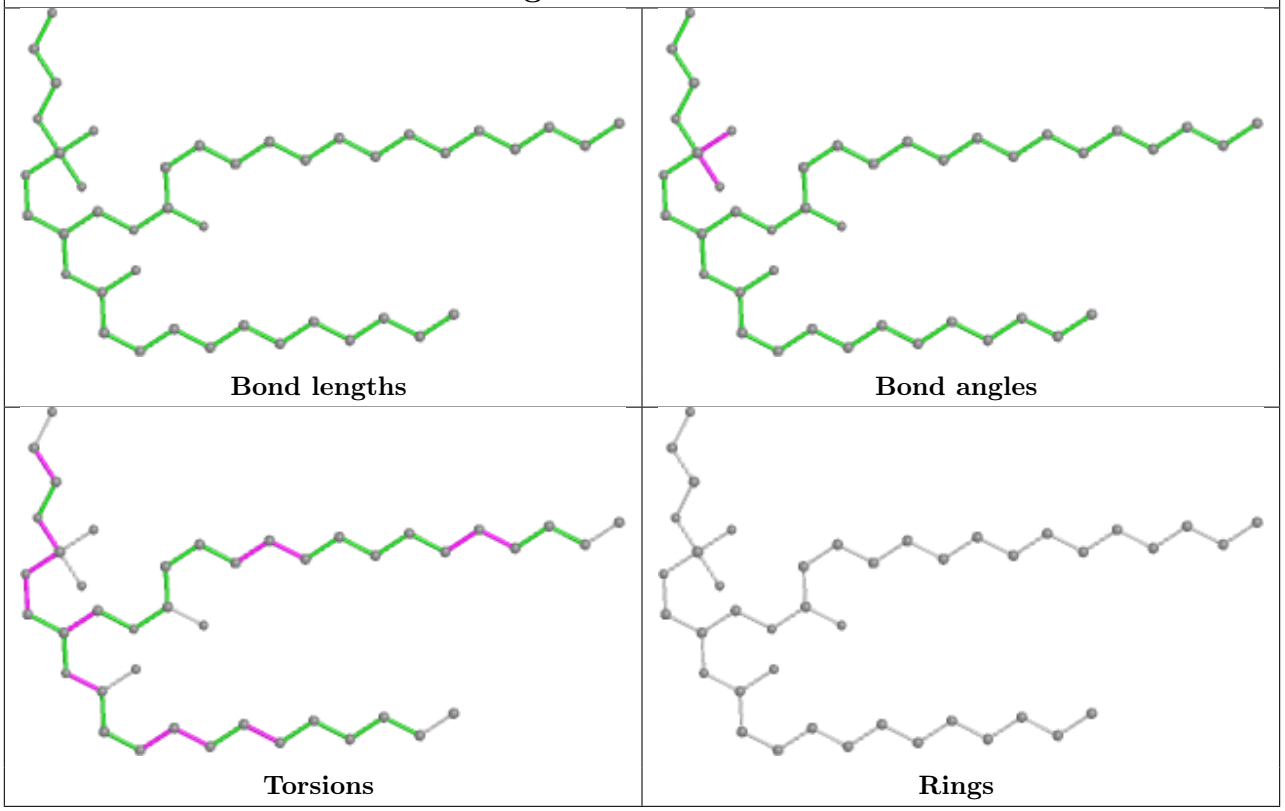


Torsions

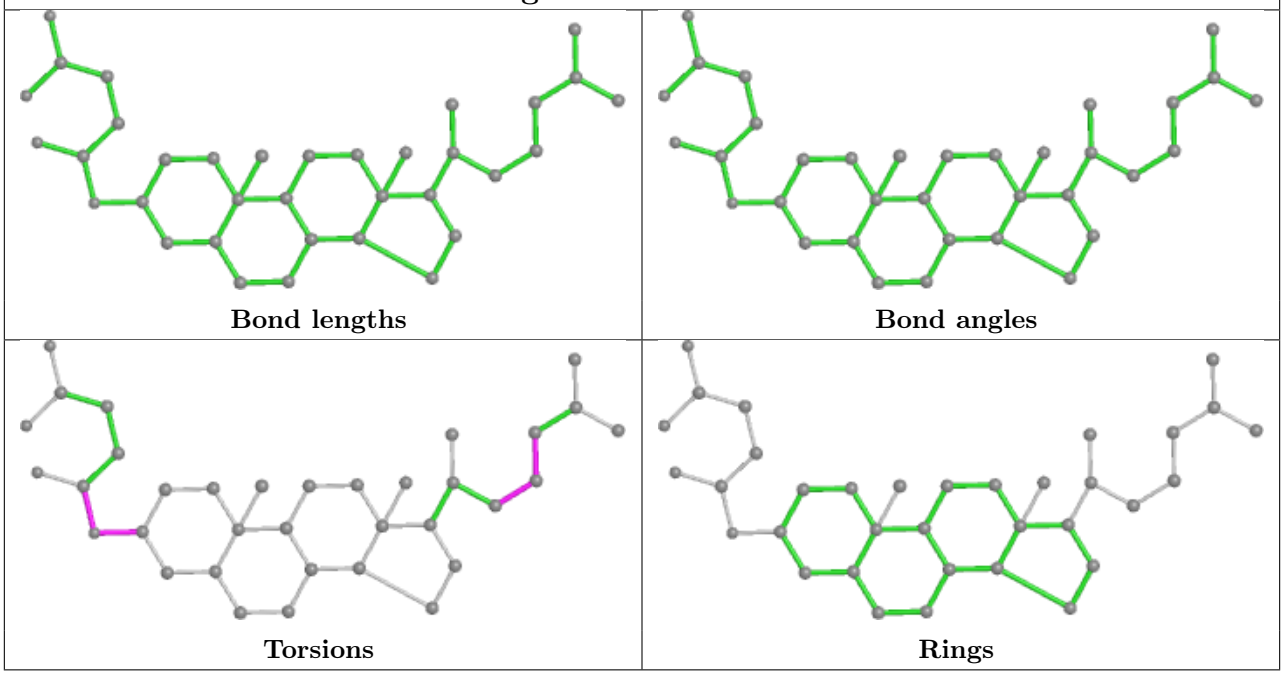


Rings

Ligand JL3 A 2409



Ligand Y01 A 2412



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.

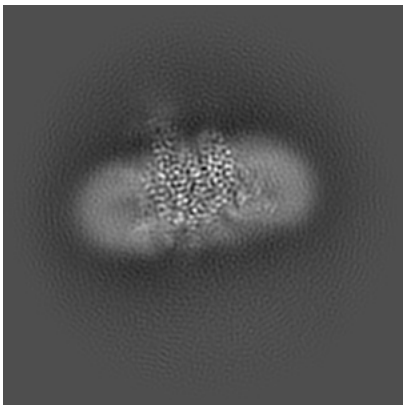
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43993. These allow visual inspection of the internal detail of the map and identification of artifacts.

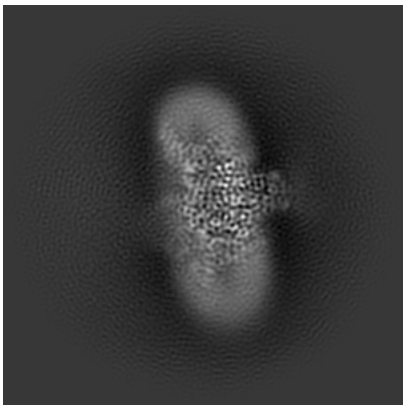
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

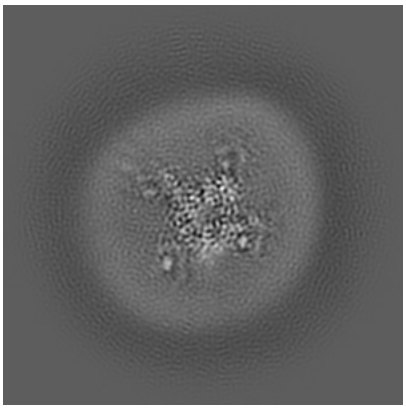
6.1.1 Primary map



X

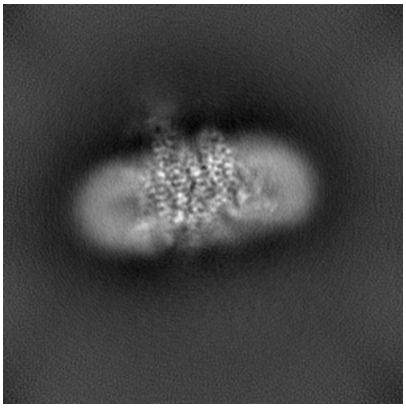


Y

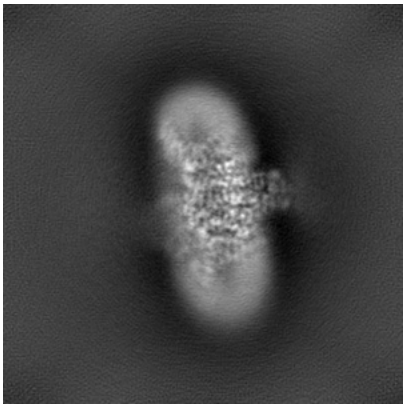


Z

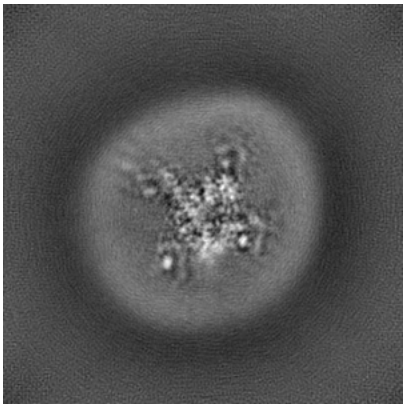
6.1.2 Raw map



X



Y

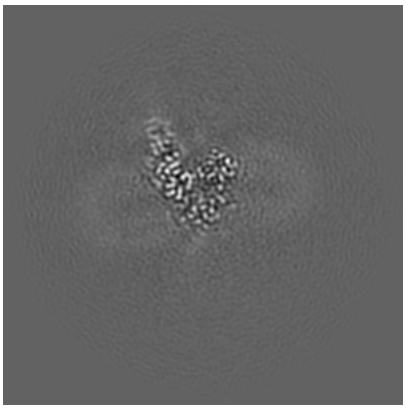


Z

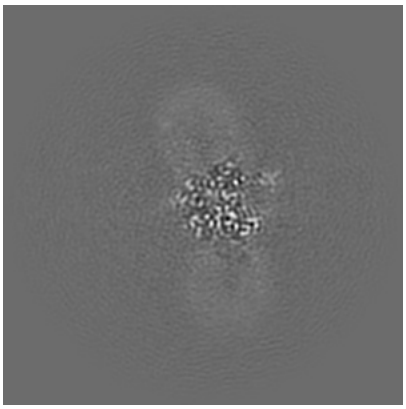
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

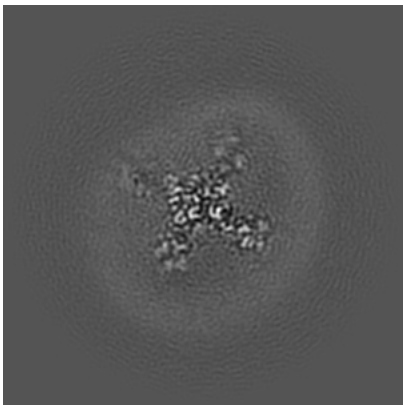
6.2.1 Primary map



X Index: 128

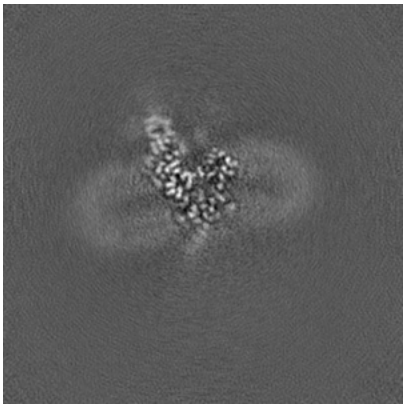


Y Index: 128

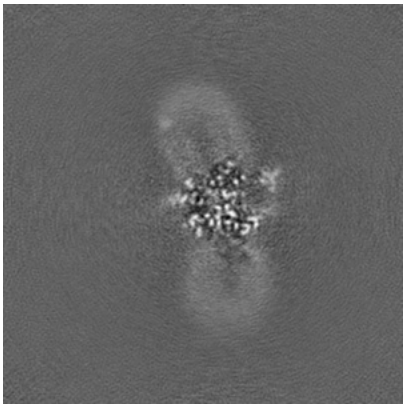


Z Index: 128

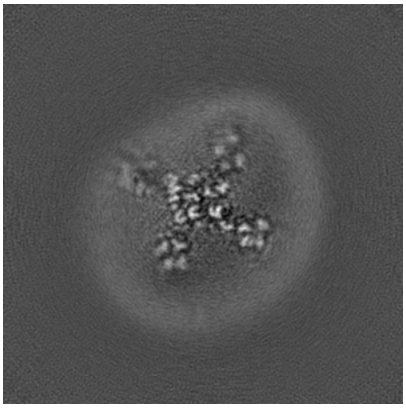
6.2.2 Raw map



X Index: 128



Y Index: 128

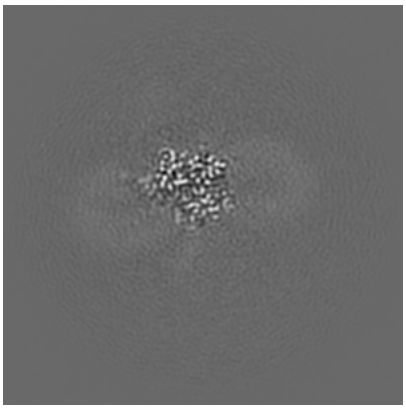


Z Index: 128

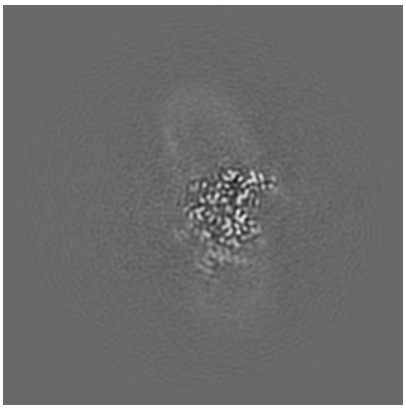
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

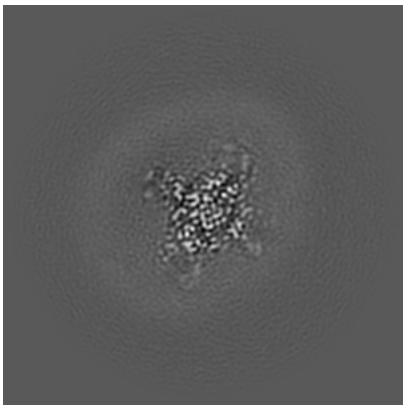
6.3.1 Primary map



X Index: 120

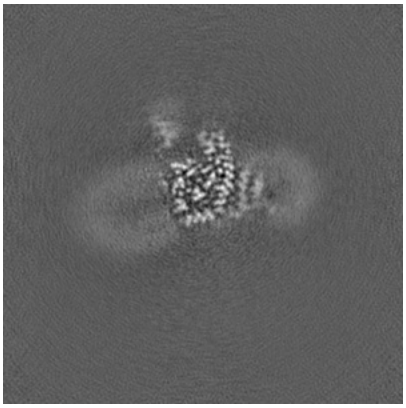


Y Index: 136

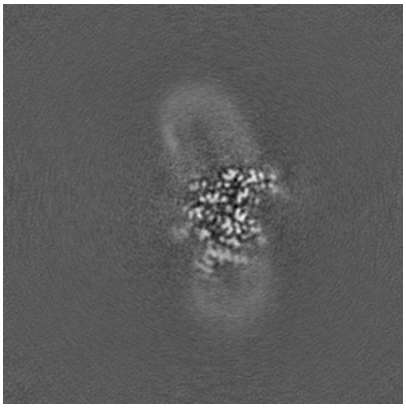


Z Index: 146

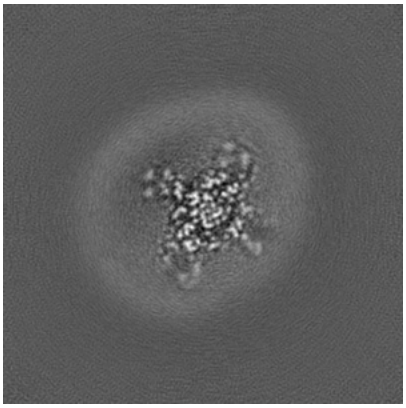
6.3.2 Raw map



X Index: 141



Y Index: 136

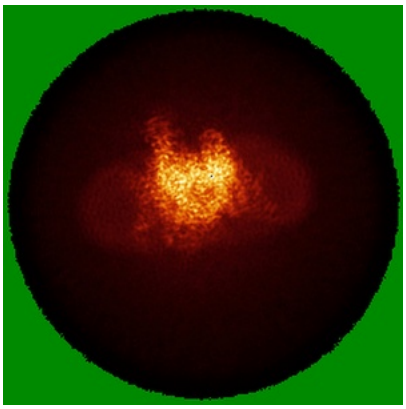


Z Index: 146

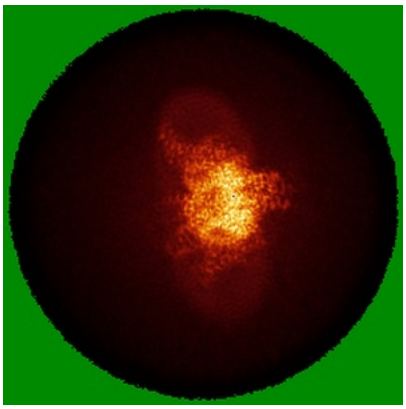
The images above show the largest variance slices of the map in three orthogonal directions.

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

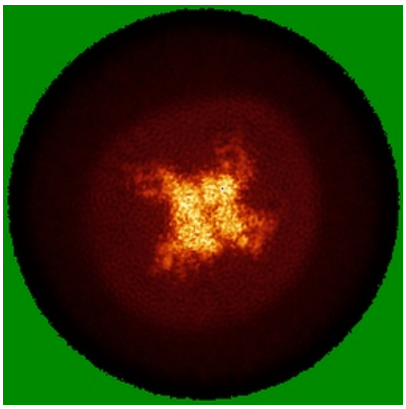
6.4.1 Primary map



X

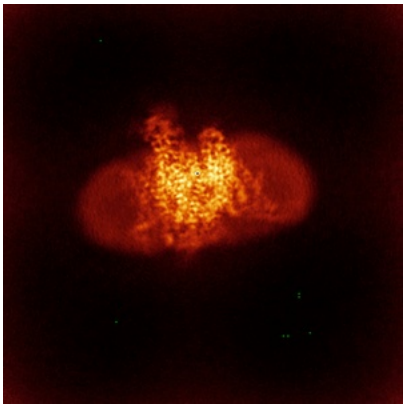


Y

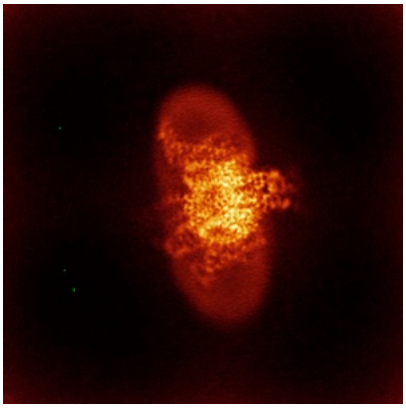


Z

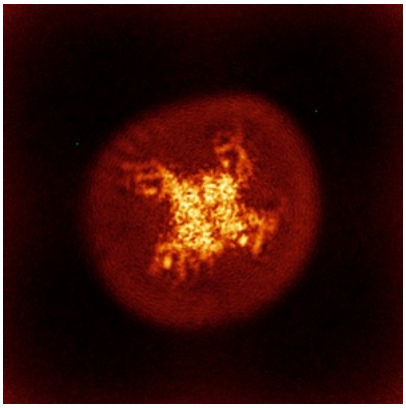
6.4.2 Raw map



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.

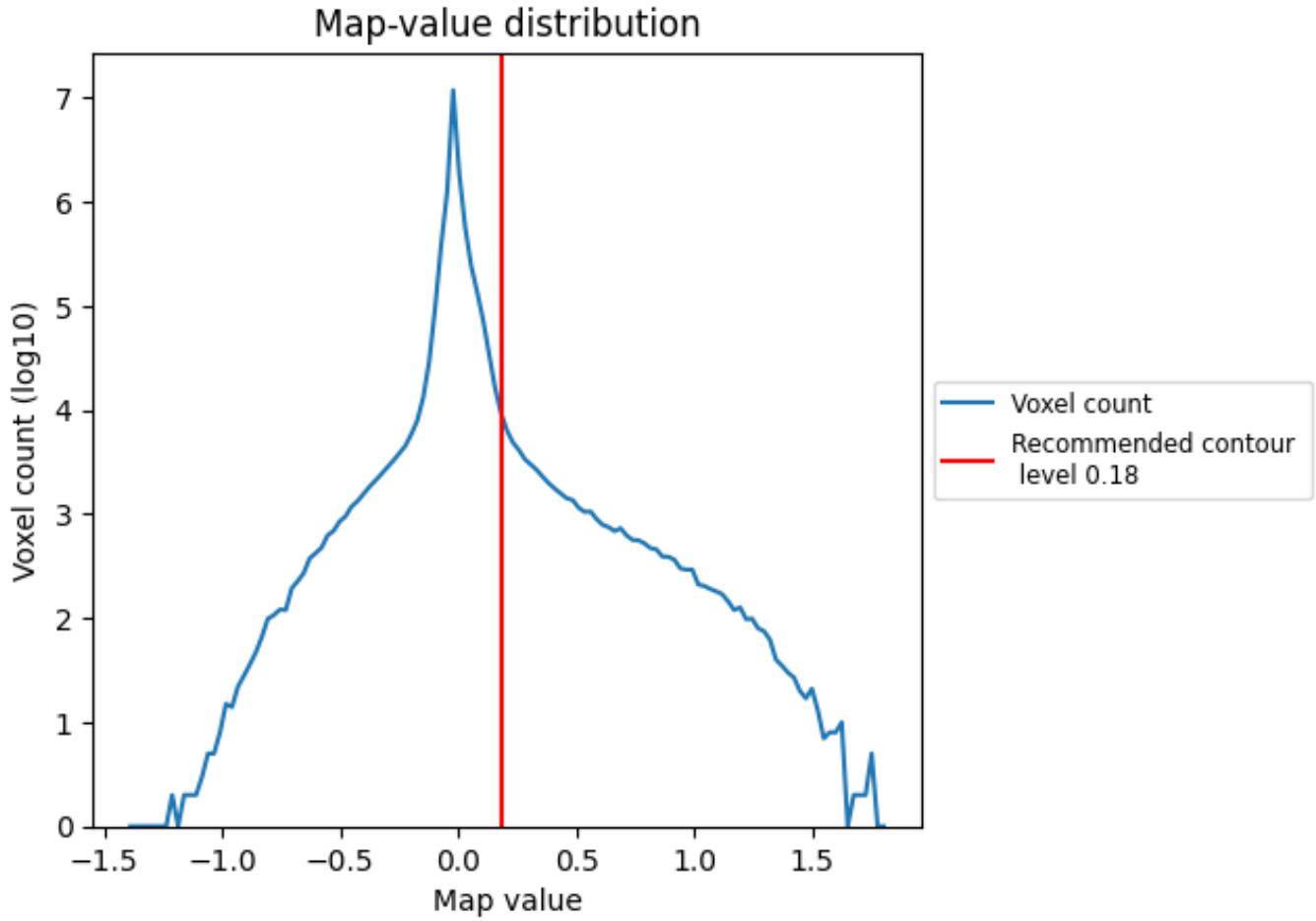
6.6 Mask visualisation (i)

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

7 Map analysis

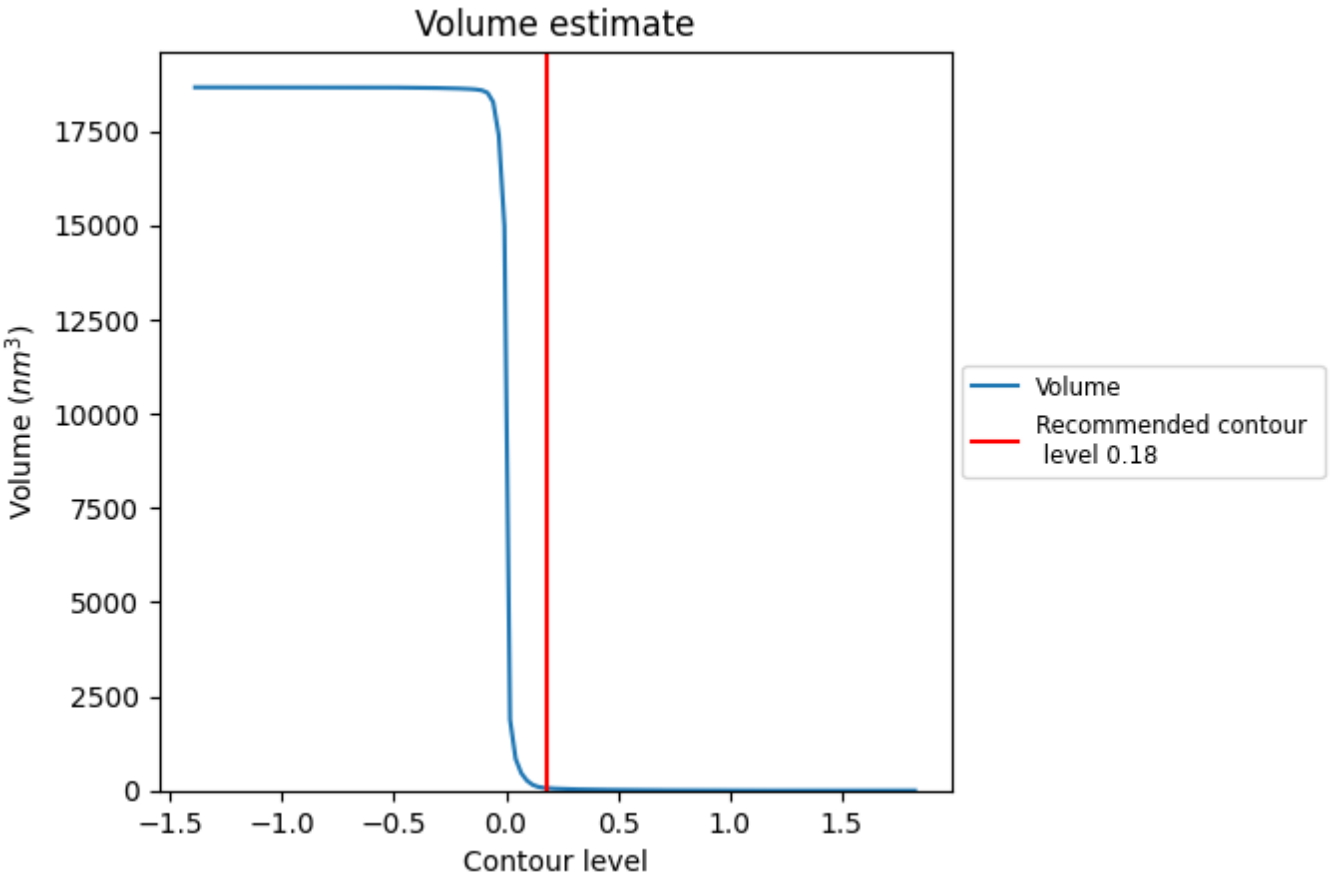
This section contains the results of statistical analysis of the map.

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.

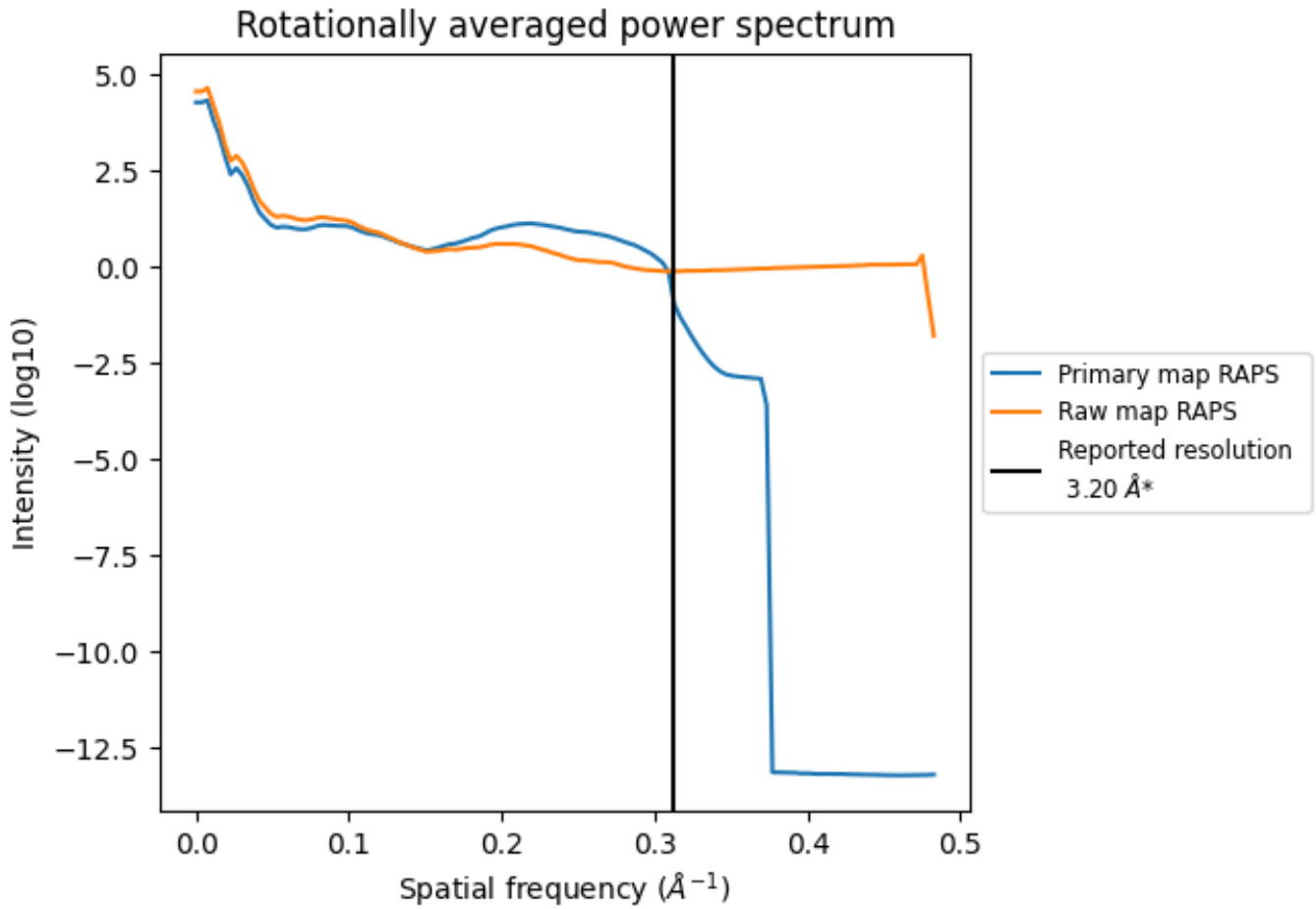
7.2 Volume estimate



The volume at the recommended contour level is 67 nm^3; this corresponds to an approximate mass of 60 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)

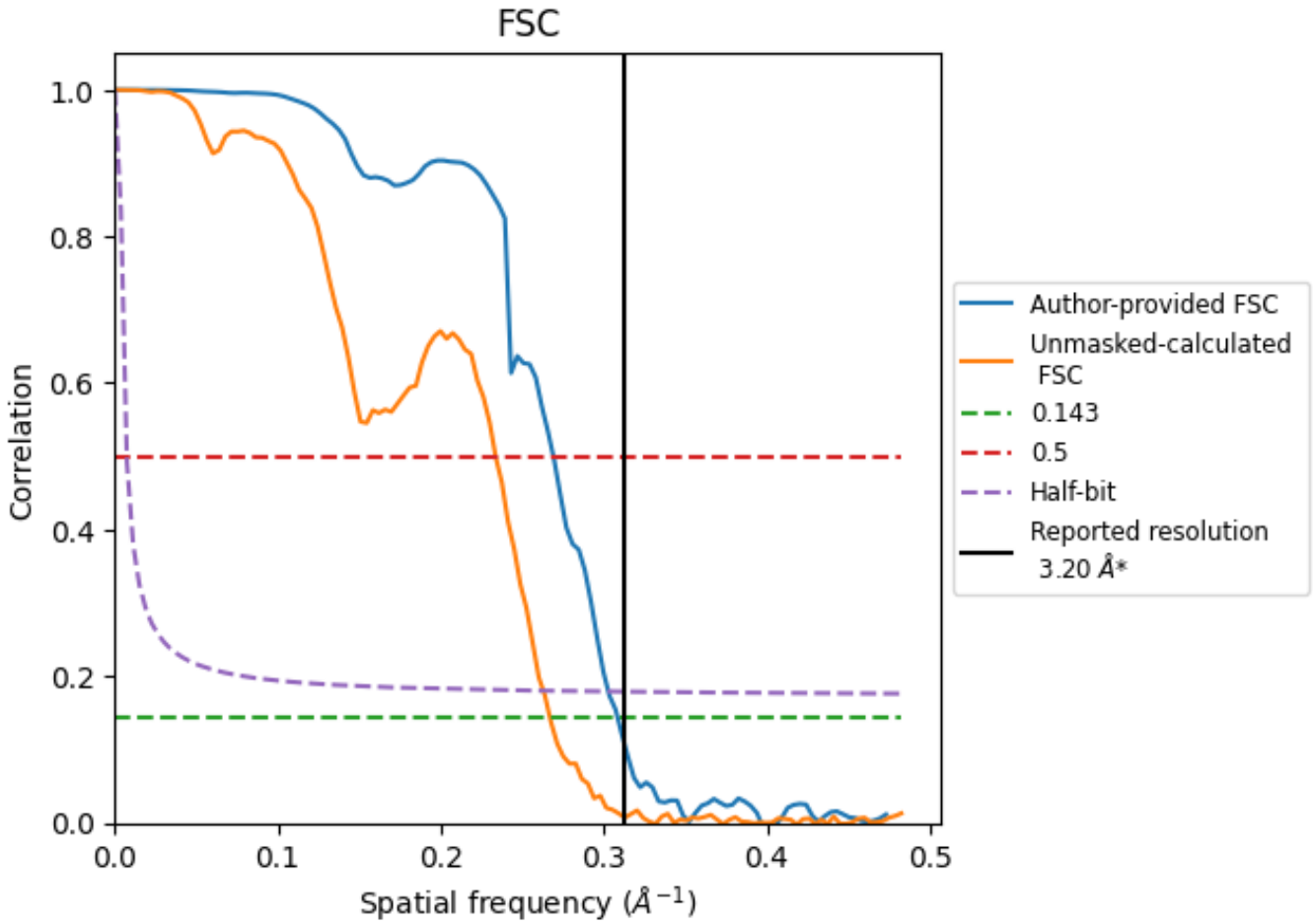


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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 0.312 $Å^{-1}$

8.2 Resolution estimates (i)

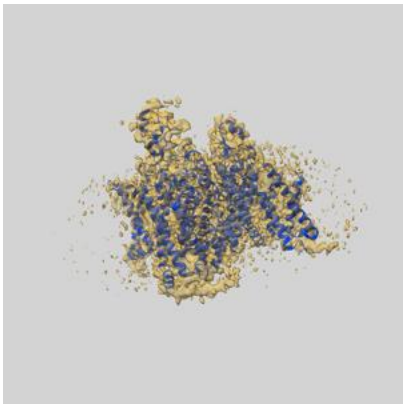
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.24	3.72	3.30
Unmasked-calculated*	3.74	4.28	3.80

*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 3.74 differs from the reported value 3.2 by more than 10 %

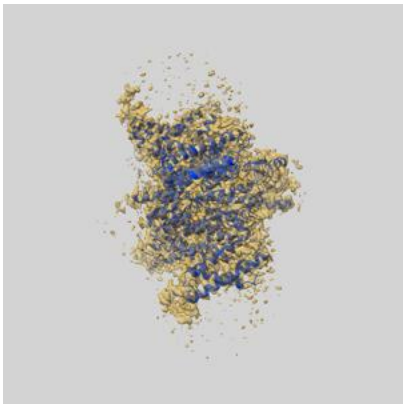
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43993 and PDB model 9AYJ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay



X

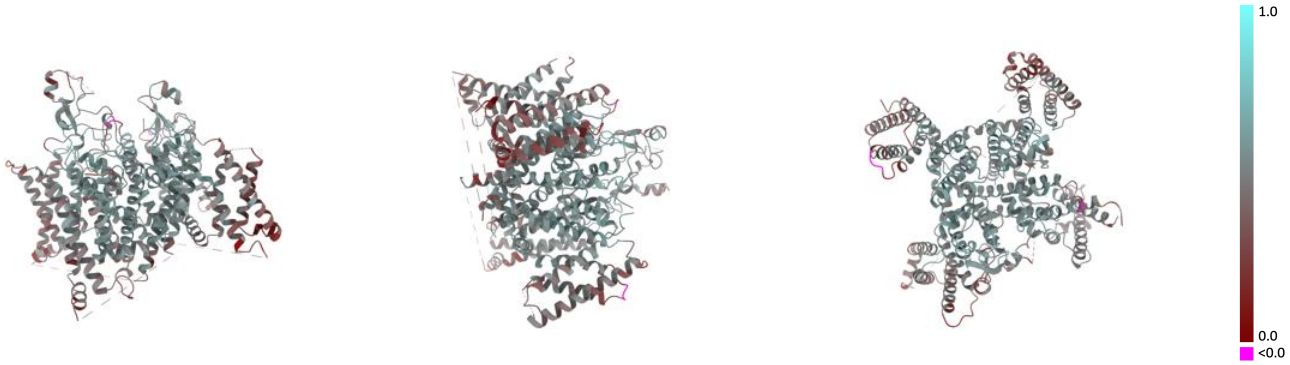


Y

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.

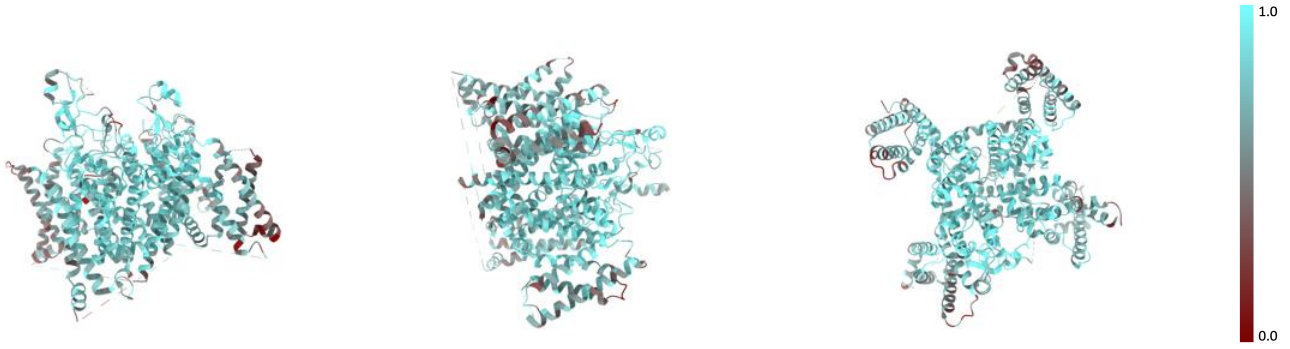
9.2 Q-score mapped to coordinate model (i)



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.

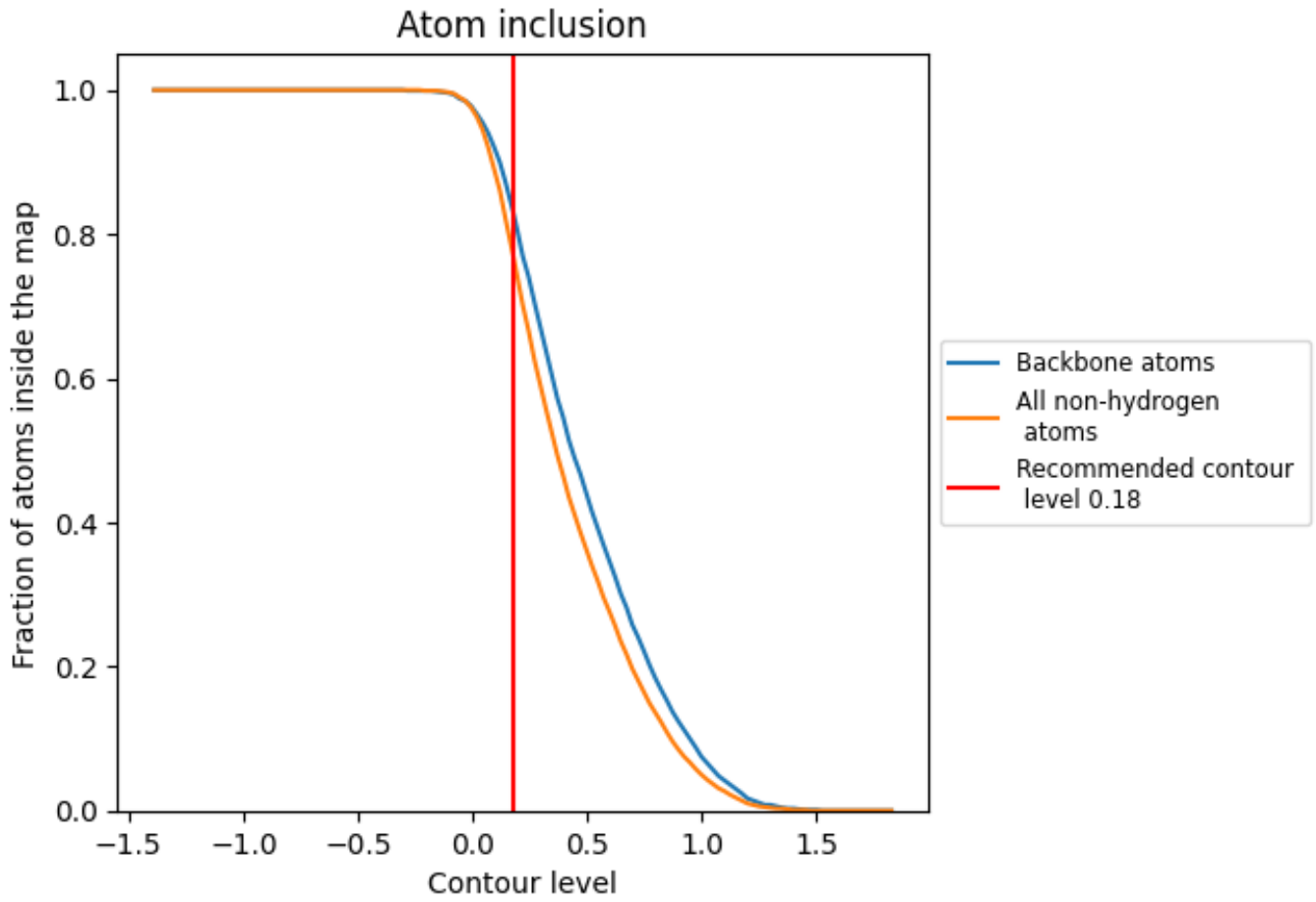
9.3 Atom inclusion mapped to coordinate model (i)



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, 83% of all backbone atoms, 77% 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	0.7660	0.4840
A	0.7660	0.4840