Full wwPDB EM Validation Report

Apr 11, 2023 – 02:05 pm BST

PDB ID	:	7ZGO
EMDB ID	:	EMD-14709
Title	:	Cryo-EM structure of human NKCC1 (TM domain)
Authors	:	Nissen, P.; Fenton, R.; Neumann, C.; Lindtoft Rosenbaek, L.; Kock Flygaard, R.; Habeck, M.; Lykkegaard Karlsen, J.; Wang, Y.; Lindorff-Larsen, K.; Gad, H.; Hartmann, R.; Lyons, J.
Deposited on	:	2022-04-04
Resolution	:	2.55 Å(reported)
Based on initial model	:	6NPL

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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

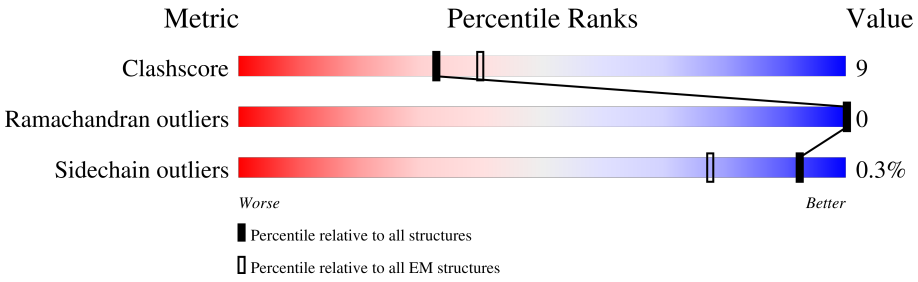
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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	1216	5% 32% 7% 61%
1	B	1216	5% 32% 7% 61%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7754 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 Solute carrier family 12 member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	470	Total 3574	C 2372	N 554	O 626	S 22	0	0
1	B	470	Total 3574	C 2372	N 554	O 626	S 22	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P55011
A	-2	PRO	-	expression tag	UNP P55011
A	-1	ALA	-	expression tag	UNP P55011
A	0	ALA	-	expression tag	UNP P55011
A	1	ALA	-	expression tag	UNP P55011
B	-3	GLY	-	expression tag	UNP P55011
B	-2	PRO	-	expression tag	UNP P55011
B	-1	ALA	-	expression tag	UNP P55011
B	0	ALA	-	expression tag	UNP P55011
B	1	ALA	-	expression tag	UNP P55011

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Na 1	0
2	B	1	Total 1	Na 1	0

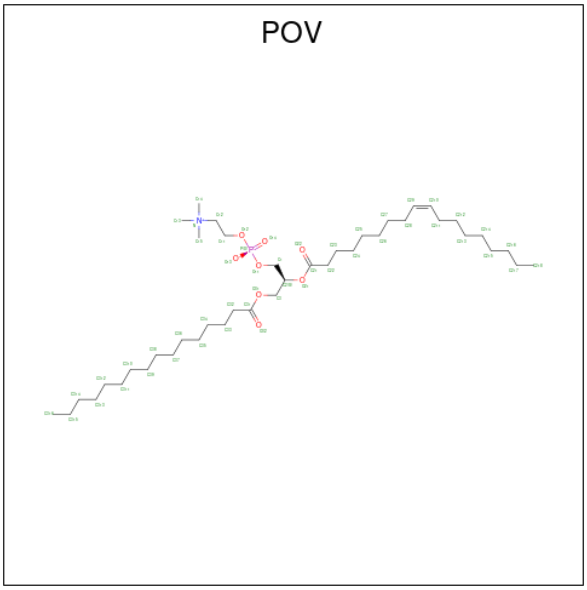
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total K 1 1	0
3	B	1	Total K 1 1	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Cl 2 2	0
4	B	2	Total Cl 2 2	0

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O P 52 42 1 8 1	0
5	A	1	Total C N O P 52 42 1 8 1	0
5	A	1	Total C N O P 52 42 1 8 1	0
5	A	1	Total C N O P 52 42 1 8 1	0

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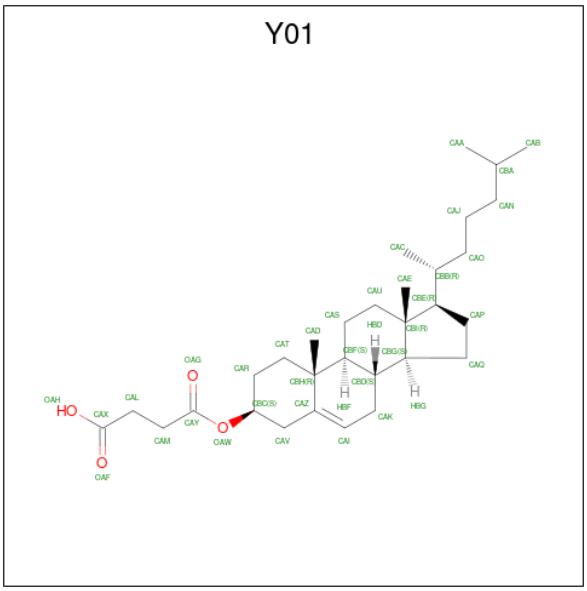
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



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	
6	B	1	Total	C	O	0
			35	31	4	
6	B	1	Total	C	O	0
			35	31	4	
6	B	1	Total	C	O	0
			35	31	4	

- Molecule 7 is water.

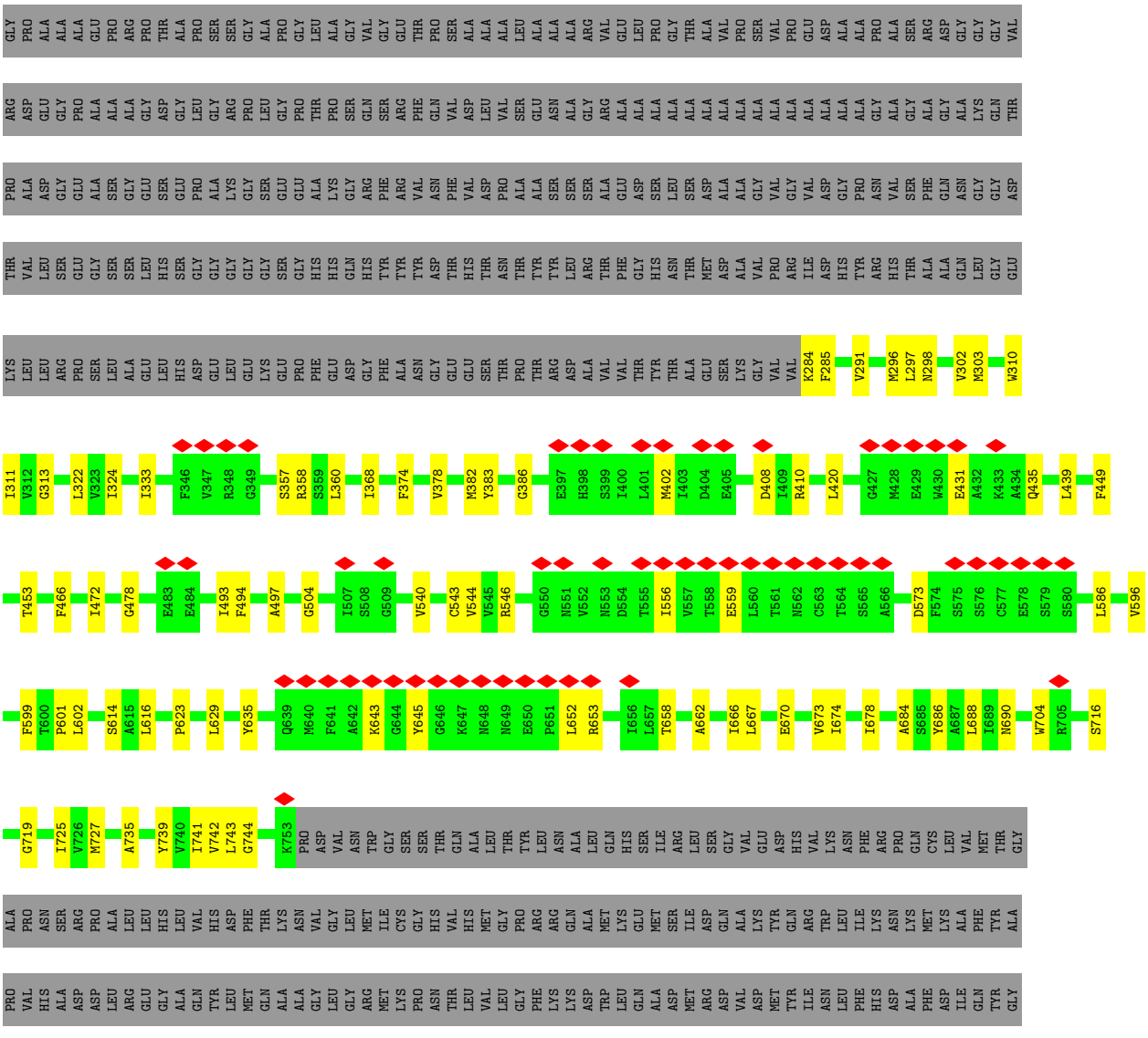
Mol	Chain	Residues	Atoms	AltConf
7	A	12	Total O 12 12	0
7	B	12	Total O 12 12	0

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.

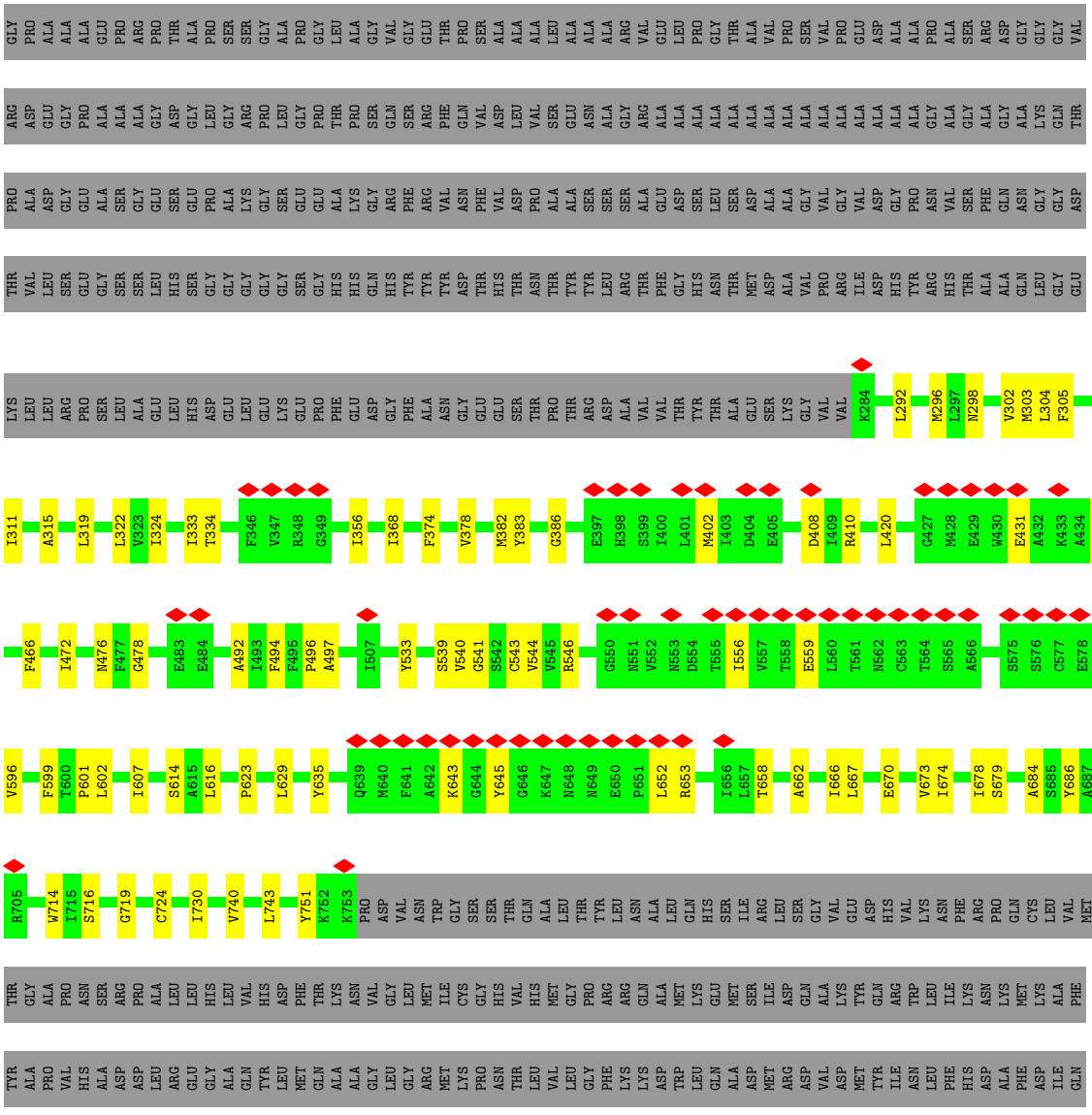
- Molecule 1: Solute carrier family 12 member 2

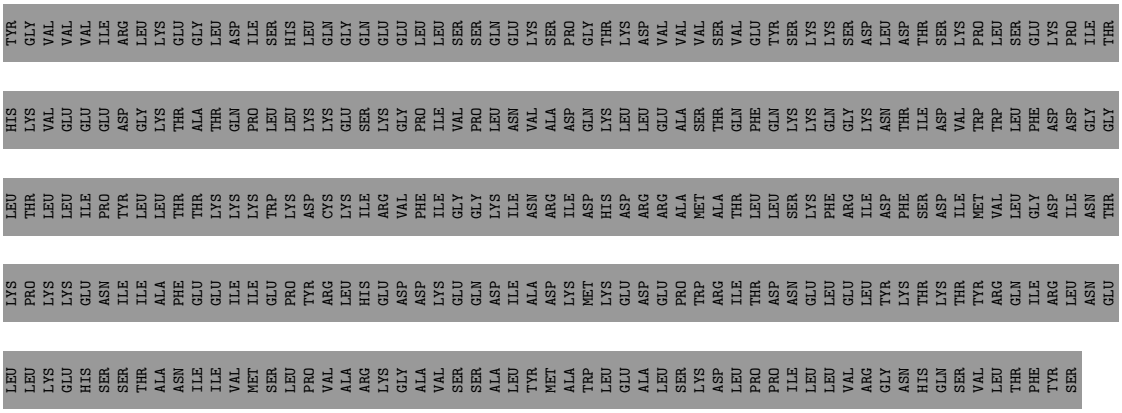
Chain A: 



• Molecule 1: Solute carrier family 12 member 2

Chain B:




TYR GLY VAL VAL VAL ILE ARG LEU LYS GLU GLY LEU ASP ILE SER HIS LEU GLN GLY GLN GLU GLU LEU LEU SER SER GLN GLU LYS SER PRO GLY THR LYS ASP VAL VAL SER VAL GLU TYR SER LYS LYS SER ASP LEU ASP THR SER LYS PRO LEU SER GLU LYS PRO ILE THR
HIS LYS VAL GLU GLU GLU ASP GLY LYS THR ALA THR GLN PRO LEU LEU LYS LYS GLU SER LYS GLY PRO ILE VAL PRO LEU ASN VAL ALA ASP GLN LYS LEU LEU GLU ALA SER THR GLN PHE GLN LYS LYS GLN GLY LYS VAL ASP ASP GLY GLY
LEU THR LEU LEU ILE PRO TYR LEU LEU THR THR LYS LYS TRP LYS ASP CYS LYS ILE ARG VAL PHE ILE GLY GLY LYS ILE ASN ARG ILE ASP HIS ASP ARG ARG ALA MET ALA THR LEU LEU SER LYS PHE ARG ILE ASP PHE SER ASP ILE MET VAL LEU GLY ASP ILE ASN THR
LYS PRO LYS LYS GLU ASN ILE ILE ALA PHE GLU GLU ILE ILE GLU PRO TYR ARG LEU HIS GLU ASP ASP LYS GLU GLN ASP ILE ALA ASP LYS MET LYS GLU ASP GLU PRO TRP ARG ILE THR ASP ASN GLU LEU GLU LEU TYR LYS THR LYS THR TYR ARG GLN ILE ARG LEU ASN GLU
LEU LEU LYS GLU HIS SER SER THR ALA ASN ILE ILE VAL MET SER LEU PRO VAL ALA ARG LYS GLY ALA VAL SER SER ALA LEU TYR MET ALA TRP LEU GLU ALA LEU SER LYS ASP LEU PRO PRO ILE LEU LEU VAL ARG GLY ASN HIS GLN SER VAL LEU THR PHE TYR SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	258791	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/Å^2$)	40.12, 30.78, 60.438	Depositor
Minimum defocus (nm)	600, 500	Depositor
Maximum defocus (nm)	1600, 2400	Depositor
Magnification	165000, 130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.201	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	243.36002, 243.36002, 243.36002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, K, CL, Y01, POV

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	0.27	0/3657	0.44	1/4976 (0.0%)
1	B	0.27	0/3657	0.44	0/4976
All	All	0.27	0/7314	0.44	1/9952 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	573	ASP	CB-CG-OD2	5.18	122.96	118.30

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	3574	0	3678	59	0
1	B	3574	0	3678	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	2	0
4	B	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	208	0	328	19	0
5	B	156	0	246	16	0
6	A	105	0	147	8	0
6	B	105	0	147	7	0
7	A	12	0	0	1	0
7	B	12	0	0	0	0
All	All	7754	0	8224	148	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 9.

All (148) 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:B:476:ASN:HA	1:B:546:ARG:NH2	2.00	0.77
1:B:623:PRO:HG3	1:B:658:THR:HG21	1.70	0.72
1:B:304:LEU:HB2	1:B:533:TYR:HE1	1.56	0.70
1:A:478:GLY:O	1:A:546:ARG:NH2	2.24	0.69
1:A:322:LEU:HD21	6:A:1309:Y01:HAU1	1.74	0.69
1:A:623:PRO:HG3	1:A:658:THR:HG21	1.76	0.68
1:B:322:LEU:HD21	6:B:1308:Y01:HAU1	1.77	0.67
1:A:313:GLY:O	1:A:546:ARG:NH1	2.28	0.66
1:A:744:GLY:HA2	5:B:1306:POV:H27	1.78	0.65
1:A:310:TRP:CZ3	1:A:493:ILE:HD13	2.33	0.62
1:B:714:TRP:HE1	5:B:1307:POV:H2	1.65	0.61
1:A:357:SER:OG	1:A:358:ARG:NH1	2.34	0.60
1:A:303:MET:HB2	1:A:497:ALA:HB2	1.83	0.60
1:B:315:ALA:HB1	1:B:319:LEU:HB3	1.84	0.59
1:A:556:ILE:HD11	1:A:559:GLU:HA	1.84	0.59
1:B:368:ILE:HG12	1:B:688:LEU:HB3	1.83	0.58
1:B:556:ILE:HD11	1:B:559:GLU:HA	1.85	0.58
1:B:688:LEU:HD13	5:B:1306:POV:H21G	1.85	0.58
1:B:305:PHE:HB3	1:B:607:ILE:HG12	1.84	0.58
1:B:478:GLY:O	1:B:546:ARG:NH2	2.36	0.58
1:A:431:GLU:OE2	7:A:1401:HOH:O	2.17	0.58
1:B:302:VAL:HG21	1:B:386:GLY:HA3	1.86	0.57
1:A:310:TRP:CH2	1:A:493:ILE:CD1	2.89	0.55
1:A:599:PHE:HD2	1:A:602:LEU:HB2	1.73	0.54
5:B:1305:POV:H31F	5:B:1307:POV:H218	1.89	0.54
1:B:645:TYR:HD2	1:B:652:LEU:HD12	1.72	0.53
5:A:1308:POV:H215	5:B:1306:POV:H21C	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ASN:ND2	1:B:541:GLY:O	2.33	0.52
1:B:497:ALA:HA	4:B:1304:CL:CL	2.47	0.52
1:A:333:ILE:HG21	1:A:719:GLY:HA3	1.92	0.52
1:A:497:ALA:HA	4:A:1303:CL:CL	2.47	0.52
1:A:725:ILE:HD11	5:A:1306:POV:H217	1.92	0.52
5:A:1307:POV:H32A	5:A:1307:POV:H23A	1.92	0.52
5:A:1308:POV:H314	1:B:743:LEU:HD22	1.92	0.52
1:A:739:TYR:HD1	5:A:1308:POV:H31B	1.74	0.51
1:B:476:ASN:HA	1:B:546:ARG:HH21	1.74	0.51
1:B:466:PHE:HB2	1:B:472:ILE:HD11	1.91	0.51
5:B:1305:POV:H31E	5:B:1305:POV:H216	1.93	0.51
1:B:333:ILE:HG21	1:B:719:GLY:HA3	1.93	0.50
1:A:310:TRP:CZ3	1:A:493:ILE:CD1	2.94	0.50
1:A:410:ARG:NE	1:A:667:LEU:O	2.44	0.50
1:B:714:TRP:HB3	5:B:1307:POV:H37A	1.92	0.50
1:A:688:LEU:HG	5:A:1305:POV:H21H	1.93	0.49
1:B:311:ILE:HD13	1:B:494:PHE:HB2	1.94	0.49
1:B:599:PHE:HD2	1:B:602:LEU:HB2	1.76	0.49
1:B:724:CYS:HB2	5:B:1306:POV:H213	1.95	0.49
1:A:310:TRP:CH2	1:A:493:ILE:HD13	2.47	0.49
6:B:1310:Y01:HAJ1	6:B:1310:Y01:HAC3	1.64	0.49
1:A:311:ILE:HD13	1:A:494:PHE:HB2	1.94	0.49
1:A:743:LEU:HD23	5:B:1306:POV:H29	1.95	0.49
6:A:1310:Y01:HAO2	6:A:1310:Y01:HAP1	1.50	0.49
1:B:382:MET:SD	1:B:678:ILE:HG13	2.53	0.49
1:A:599:PHE:CE2	1:A:601:PRO:HG2	2.48	0.48
1:A:466:PHE:HB2	1:A:472:ILE:HD11	1.95	0.48
1:B:670:GLU:HB2	1:B:673:VAL:HG22	1.94	0.48
1:B:292:LEU:HG	1:B:296:MET:HE2	1.96	0.48
6:A:1309:Y01:HAC2	6:A:1309:Y01:HAJ2	1.66	0.48
1:A:291:VAL:HG13	1:A:504:GLY:HA3	1.96	0.48
1:A:546:ARG:HA	1:A:586:LEU:HB2	1.95	0.47
5:A:1306:POV:H21E	1:B:740:VAL:HG21	1.97	0.47
5:A:1306:POV:H39A	5:A:1306:POV:H36A	1.48	0.47
5:A:1308:POV:H23A	5:A:1308:POV:H26A	1.73	0.47
1:A:741:ILE:HG12	5:B:1306:POV:H310	1.97	0.47
1:A:629:LEU:HD21	1:A:635:TYR:HD2	1.80	0.46
1:B:684:ALA:O	1:B:688:LEU:HD23	2.15	0.46
5:B:1306:POV:C31	5:B:1307:POV:H29	2.44	0.46
1:B:643:LYS:HE3	1:B:645:TYR:HE1	1.80	0.46
1:A:360:LEU:HD21	1:A:704:TRP:CE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:SER:HB2	6:B:1309:Y01:HAP2	1.97	0.46
5:B:1307:POV:C31	5:B:1307:POV:H25A	2.46	0.46
1:A:449:PHE:O	1:A:453:THR:HG23	2.16	0.46
5:A:1305:POV:H32	5:A:1305:POV:H35A	1.62	0.46
5:A:1307:POV:H311	5:A:1307:POV:H38A	1.86	0.45
1:B:688:LEU:HA	5:B:1306:POV:H21G	1.98	0.45
1:A:543:CYS:SG	1:A:544:VAL:HG23	2.56	0.45
1:B:431:GLU:O	1:B:435:GLN:HG2	2.17	0.45
1:A:670:GLU:HB2	1:A:673:VAL:HG22	1.97	0.45
1:B:543:CYS:SG	1:B:544:VAL:HG23	2.56	0.45
1:A:368:ILE:HG12	1:A:688:LEU:HB3	1.97	0.45
1:A:420:LEU:HD22	1:A:616:LEU:HD13	1.98	0.45
1:A:690:ASN:HB3	1:A:716:SER:O	2.17	0.45
1:B:599:PHE:CE2	1:B:601:PRO:HG2	2.51	0.45
1:A:296:MET:HE3	1:A:439:LEU:HD21	1.98	0.45
1:B:303:MET:HB2	1:B:497:ALA:HB2	1.99	0.45
1:B:492:ALA:HB2	1:B:730:ILE:HG12	1.99	0.45
5:A:1306:POV:H31C	5:A:1306:POV:H315	1.90	0.45
1:B:662:ALA:O	1:B:666:ILE:HG13	2.17	0.45
1:B:356:ILE:HD13	1:B:368:ILE:HG21	1.99	0.44
1:B:674:ILE:O	1:B:678:ILE:HG12	2.17	0.44
5:A:1305:POV:H210	1:B:743:LEU:HD23	1.99	0.44
6:A:1310:Y01:HAC2	6:A:1310:Y01:HAJ2	1.61	0.44
1:A:645:TYR:HD2	1:A:652:LEU:HB2	1.83	0.44
5:A:1306:POV:H21J	5:A:1306:POV:H213	2.00	0.44
1:A:302:VAL:HG21	1:A:386:GLY:HA3	1.98	0.44
5:A:1305:POV:H15A	1:B:751:TYR:HB3	2.00	0.44
1:B:449:PHE:O	1:B:453:THR:HG23	2.17	0.44
6:B:1310:Y01:HAE2	6:B:1310:Y01:HBB	1.77	0.44
1:A:643:LYS:HB3	1:A:653:ARG:HD2	1.99	0.44
1:B:368:ILE:CG1	1:B:688:LEU:HB3	2.48	0.44
1:B:690:ASN:HB3	1:B:716:SER:O	2.17	0.44
1:A:725:ILE:HD11	5:A:1306:POV:H215	2.00	0.43
5:A:1306:POV:H13A	5:A:1306:POV:H11	1.85	0.43
1:B:476:ASN:CA	1:B:546:ARG:NH2	2.76	0.43
1:A:383:TYR:CE2	1:A:614:SER:HB3	2.54	0.43
1:A:431:GLU:O	1:A:435:GLN:HG2	2.19	0.43
1:B:420:LEU:HD22	1:B:616:LEU:HD13	2.00	0.43
5:B:1307:POV:H216	5:B:1307:POV:H31B	2.01	0.43
1:A:674:ILE:O	1:A:678:ILE:HG12	2.18	0.43
1:B:410:ARG:NH1	1:B:667:LEU:O	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:LEU:HD22	5:A:1308:POV:H214	2.01	0.42
6:A:1310:Y01:HBB	6:A:1310:Y01:HAE2	1.67	0.42
1:B:580:SER:HB2	1:B:581:PRO:HD2	2.01	0.42
1:B:383:TYR:CE2	1:B:614:SER:HB3	2.55	0.42
1:A:684:ALA:HB2	1:A:727:MET:HE1	2.00	0.42
1:B:540:VAL:HG22	1:B:586:LEU:HD21	2.00	0.42
5:A:1305:POV:H311	5:A:1305:POV:H38	1.75	0.42
6:A:1311:Y01:HAE2	6:A:1311:Y01:HBB	1.74	0.42
1:A:688:LEU:HD21	1:A:742:VAL:HG11	2.01	0.42
1:A:402:MET:HB2	1:A:408:ASP:OD1	2.20	0.42
1:B:374:PHE:O	1:B:378:VAL:HG22	2.20	0.42
1:B:402:MET:HB2	1:B:408:ASP:OD1	2.20	0.42
1:B:629:LEU:HD21	1:B:635:TYR:HD2	1.84	0.42
6:B:1309:Y01:HAE2	6:B:1309:Y01:HBB	1.74	0.42
6:A:1311:Y01:HAO1	6:A:1311:Y01:HAP1	1.76	0.41
6:A:1311:Y01:HAR1	6:A:1311:Y01:HAL2	2.02	0.41
1:B:453:THR:HG22	1:B:596:VAL:HG11	2.01	0.41
5:B:1305:POV:H14B	5:B:1305:POV:H11A	1.80	0.41
1:A:540:VAL:HG22	1:A:586:LEU:HD21	2.02	0.41
1:A:453:THR:HG22	1:A:596:VAL:HG11	2.02	0.41
1:B:496:PRO:HD3	1:B:679:SER:OG	2.19	0.41
1:A:431:GLU:OE2	1:A:435:GLN:NE2	2.53	0.41
1:A:662:ALA:O	1:A:666:ILE:HG13	2.20	0.41
1:B:629:LEU:HD21	1:B:635:TYR:CD2	2.56	0.41
1:A:284:LYS:HB3	1:A:285:PHE:H	1.62	0.41
1:A:374:PHE:O	1:A:378:VAL:HG22	2.21	0.41
1:A:686:TYR:OH	4:A:1304:CL:CL	2.65	0.41
1:B:431:GLU:OE2	1:B:435:GLN:NE2	2.54	0.41
5:B:1305:POV:H31E	5:B:1305:POV:H311	1.83	0.41
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.83	0.41
1:B:643:LYS:HB3	1:B:653:ARG:HD2	2.03	0.41
1:B:324:ILE:HG12	1:B:494:PHE:CZ	2.56	0.40
1:A:324:ILE:HG12	1:A:494:PHE:CZ	2.56	0.40
6:B:1308:Y01:HAC2	6:B:1308:Y01:HAJ2	1.71	0.40
1:A:382:MET:SD	1:A:678:ILE:HG13	2.61	0.40
1:A:735:ALA:O	1:A:739:TYR:HD2	2.04	0.40
1:B:334:THR:HG21	1:B:686:TYR:CD1	2.57	0.40
1:A:629:LEU:HD21	1:A:635:TYR:CD2	2.56	0.40
6:B:1309:Y01:HAC3	6:B:1309:Y01:HAJ1	1.80	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	468/1216 (38%)	453 (97%)	15 (3%)	0	100	100
1	B	468/1216 (38%)	451 (96%)	17 (4%)	0	100	100
All	All	936/2432 (38%)	904 (97%)	32 (3%)	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	381/983 (39%)	380 (100%)	1 (0%)	92	96
1	B	381/983 (39%)	380 (100%)	1 (0%)	92	96
All	All	762/1966 (39%)	760 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	B	298	ASN

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
5	POV	A	1308	-	51,51,51	1.06	3 (5%)	57,59,59	1.16	3 (5%)
6	Y01	A	1310	-	38,38,38	0.67	1 (2%)	57,57,57	1.54	11 (19%)
5	POV	B	1307	-	51,51,51	1.09	3 (5%)	57,59,59	1.10	3 (5%)
6	Y01	A	1309	-	38,38,38	0.64	1 (2%)	57,57,57	1.45	9 (15%)
6	Y01	B	1309	-	38,38,38	0.66	1 (2%)	57,57,57	1.52	10 (17%)
6	Y01	A	1311	-	38,38,38	0.67	1 (2%)	57,57,57	1.50	8 (14%)
5	POV	A	1307	-	51,51,51	1.08	3 (5%)	57,59,59	1.10	3 (5%)
5	POV	A	1306	-	51,51,51	1.08	3 (5%)	57,59,59	1.13	3 (5%)
6	Y01	B	1308	-	38,38,38	0.64	1 (2%)	57,57,57	1.44	9 (15%)
5	POV	A	1305	-	51,51,51	1.08	3 (5%)	57,59,59	1.16	3 (5%)
5	POV	B	1306	-	51,51,51	1.06	3 (5%)	57,59,59	1.17	3 (5%)
5	POV	B	1305	-	51,51,51	1.08	3 (5%)	57,59,59	1.13	3 (5%)
6	Y01	B	1310	-	38,38,38	0.67	1 (2%)	57,57,57	1.48	8 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	A	1308	-	-	20/55/55/55	-
6	Y01	A	1310	-	-	17/19/77/77	0/4/4/4
5	POV	B	1307	-	-	26/55/55/55	-
6	Y01	A	1309	-	-	6/19/77/77	0/4/4/4
6	Y01	B	1309	-	-	9/19/77/77	0/4/4/4
6	Y01	A	1311	-	-	11/19/77/77	0/4/4/4
5	POV	A	1307	-	-	30/55/55/55	-
5	POV	A	1306	-	-	31/55/55/55	-
6	Y01	B	1308	-	-	5/19/77/77	0/4/4/4
5	POV	A	1305	-	-	20/55/55/55	-
5	POV	B	1306	-	-	19/55/55/55	-
5	POV	B	1305	-	-	17/55/55/55	-
6	Y01	B	1310	-	-	9/19/77/77	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1307	POV	O31-C31	2.81	1.41	1.33
5	B	1305	POV	O31-C31	2.80	1.41	1.33
5	B	1306	POV	O31-C31	2.79	1.41	1.33
5	A	1305	POV	O31-C31	2.78	1.41	1.33
5	A	1307	POV	O31-C31	2.78	1.41	1.33
5	A	1308	POV	O31-C31	2.76	1.41	1.33
5	A	1306	POV	O31-C31	2.75	1.41	1.33
5	A	1306	POV	O21-C21	2.72	1.42	1.34
5	B	1307	POV	O21-C21	2.69	1.41	1.34
5	B	1305	POV	O21-C21	2.69	1.41	1.34
5	A	1307	POV	O21-C21	2.68	1.41	1.34
5	A	1305	POV	O21-C21	2.64	1.41	1.34
5	A	1308	POV	O21-C21	2.62	1.41	1.34
5	B	1306	POV	O21-C21	2.57	1.41	1.34
6	A	1310	Y01	CBH-CBF	-2.37	1.52	1.56
5	B	1306	POV	O21-C2	-2.37	1.40	1.46
5	A	1305	POV	O21-C2	-2.36	1.40	1.46
6	B	1310	Y01	CBH-CBF	-2.35	1.52	1.56
5	B	1307	POV	O21-C2	-2.33	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1311	Y01	CBH-CBF	-2.31	1.52	1.56
5	A	1308	POV	O21-C2	-2.31	1.40	1.46
5	A	1307	POV	O21-C2	-2.29	1.40	1.46
5	B	1305	POV	O21-C2	-2.29	1.40	1.46
6	B	1309	Y01	CBH-CBF	-2.27	1.52	1.56
5	A	1306	POV	O21-C2	-2.25	1.41	1.46
6	A	1309	Y01	CBH-CBF	-2.14	1.52	1.56
6	B	1308	Y01	CBH-CBF	-2.06	1.52	1.56

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1310	Y01	CBI-CBE-CBB	-4.83	111.92	119.49
5	A	1305	POV	O21-C21-C22	4.45	121.09	111.50
6	A	1311	Y01	CBI-CBE-CBB	-4.29	112.76	119.49
5	B	1306	POV	O21-C21-C22	4.14	120.43	111.50
6	B	1310	Y01	OAW-CAY-CAM	4.13	120.39	111.50
5	A	1308	POV	O21-C21-C22	4.10	120.34	111.50
6	B	1309	Y01	CBI-CBE-CBB	-4.07	113.12	119.49
6	B	1310	Y01	CBI-CBE-CBB	-4.04	113.16	119.49
5	A	1306	POV	O21-C21-C22	4.00	120.12	111.50
6	A	1311	Y01	OAW-CAY-CAM	4.00	120.11	111.50
5	B	1305	POV	O21-C21-C22	3.97	120.05	111.50
6	A	1310	Y01	OAW-CAY-CAM	3.88	119.87	111.50
5	B	1307	POV	O21-C21-C22	3.84	119.77	111.50
6	A	1309	Y01	OAW-CAY-CAM	3.83	119.75	111.50
5	A	1307	POV	O21-C21-C22	3.80	119.68	111.50
6	B	1308	Y01	OAW-CAY-CAM	3.78	119.65	111.50
6	B	1309	Y01	OAW-CAY-CAM	3.71	119.50	111.50
5	A	1305	POV	C37-C36-C35	3.47	132.02	114.42
5	A	1306	POV	C37-C36-C35	3.42	131.80	114.42
5	B	1305	POV	C37-C36-C35	3.35	131.46	114.42
5	B	1307	POV	C37-C36-C35	3.34	131.38	114.42
5	A	1308	POV	C37-C36-C35	3.34	131.36	114.42
5	B	1306	POV	C37-C36-C35	3.25	130.93	114.42
5	A	1307	POV	C37-C36-C35	3.24	130.87	114.42
6	A	1309	Y01	CBI-CBE-CBB	-3.19	114.48	119.49
6	A	1311	Y01	CBI-CBG-CBD	-3.09	109.80	114.38
6	B	1310	Y01	CBI-CBG-CBD	-3.02	109.91	114.38
6	B	1308	Y01	CBI-CBE-CBB	-2.82	115.08	119.49
6	B	1309	Y01	CAV-CAZ-CBH	2.79	120.13	116.42
6	A	1309	Y01	CBI-CBG-CBD	-2.73	110.33	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1310	Y01	CBI-CBG-CBD	-2.73	110.34	114.38
5	B	1306	POV	O31-C31-C32	2.67	120.28	111.91
6	A	1310	Y01	CAQ-CBG-CBI	-2.66	100.64	103.84
6	B	1309	Y01	CAQ-CBG-CBI	-2.65	100.65	103.84
6	B	1308	Y01	CBI-CBG-CBD	-2.64	110.47	114.38
5	A	1308	POV	O31-C31-C32	2.63	120.17	111.91
6	B	1308	Y01	CAK-CBD-CBG	-2.63	107.10	110.91
6	B	1309	Y01	CAD-CBH-CBF	-2.62	108.55	111.68
6	B	1310	Y01	CAS-CBF-CBH	-2.61	109.64	113.08
5	B	1307	POV	O31-C31-C32	2.57	119.96	111.91
6	A	1310	Y01	CAD-CBH-CBF	-2.56	108.63	111.68
6	A	1310	Y01	CAV-CAZ-CBH	2.54	119.80	116.42
5	A	1306	POV	O31-C31-C32	2.54	119.87	111.91
6	A	1311	Y01	CAS-CBF-CBH	-2.52	109.76	113.08
5	B	1305	POV	O31-C31-C32	2.49	119.72	111.91
6	A	1311	Y01	CAD-CBH-CBF	-2.48	108.72	111.68
6	B	1309	Y01	CAV-CAZ-CAI	-2.48	117.03	120.61
5	A	1307	POV	O31-C31-C32	2.47	119.66	111.91
6	B	1310	Y01	CAD-CBH-CBF	-2.46	108.74	111.68
6	A	1309	Y01	CAK-CBD-CBG	-2.46	107.34	110.91
5	A	1305	POV	O31-C31-C32	2.42	119.49	111.91
6	B	1309	Y01	CAK-CBD-CBG	-2.41	107.42	110.91
6	B	1309	Y01	CBI-CBG-CBD	-2.35	110.89	114.38
6	A	1310	Y01	CAS-CAU-CBI	-2.35	108.76	112.78
6	A	1309	Y01	CAQ-CBG-CBD	-2.34	115.22	119.08
6	B	1308	Y01	CAQ-CBG-CBD	-2.31	115.28	119.08
6	B	1310	Y01	CAS-CAU-CBI	-2.30	108.84	112.78
6	A	1311	Y01	CAQ-CBG-CBI	-2.30	101.08	103.84
6	A	1309	Y01	CAD-CBH-CBF	-2.29	108.95	111.68
6	B	1310	Y01	CAQ-CBG-CBI	-2.29	101.09	103.84
6	B	1308	Y01	CAD-CBH-CBF	-2.26	108.99	111.68
6	B	1308	Y01	CBF-CBH-CAZ	2.23	113.15	109.65
6	A	1311	Y01	CAS-CAU-CBI	-2.21	108.99	112.78
6	B	1308	Y01	CAM-CAL-CAX	-2.18	108.91	113.60
6	B	1308	Y01	CAQ-CBG-CBI	-2.18	101.22	103.84
6	B	1309	Y01	CAS-CAU-CBI	-2.17	109.05	112.78
6	A	1310	Y01	CAV-CAZ-CAI	-2.14	117.52	120.61
6	A	1309	Y01	CBF-CBH-CAZ	2.13	113.00	109.65
6	A	1310	Y01	CAS-CBF-CBH	-2.11	110.30	113.08
6	A	1309	Y01	CAQ-CBG-CBI	-2.10	101.32	103.84
6	A	1311	Y01	CAJ-CAO-CBB	-2.09	109.02	115.03
6	B	1309	Y01	CAQ-CBG-CBD	-2.08	115.66	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1310	Y01	CAC-CBB-CBE	-2.06	109.77	112.92
6	A	1310	Y01	CAM-CAL-CAX	-2.05	109.18	113.60
6	B	1310	Y01	CBF-CBH-CAZ	2.05	112.87	109.65
6	A	1309	Y01	CAM-CAL-CAX	-2.02	109.26	113.60

There are no chirality outliers.

All (220) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1305	POV	O12-C11-C12-N
5	A	1305	POV	C22-C21-O21-C2
5	A	1305	POV	O22-C21-O21-C2
5	A	1306	POV	C1-O11-P-O13
5	A	1306	POV	C1-O11-P-O14
5	A	1306	POV	O12-C11-C12-N
5	A	1307	POV	O21-C2-C3-O31
5	A	1308	POV	C1-O11-P-O13
5	A	1308	POV	C1-O11-P-O14
5	B	1305	POV	O21-C2-C3-O31
5	B	1305	POV	O12-C11-C12-N
5	B	1305	POV	C22-C21-O21-C2
6	A	1309	Y01	CAM-CAY-OAW-CBC
6	A	1311	Y01	CAR-CBC-OAW-CAY
6	B	1310	Y01	OAG-CAY-OAW-CBC
6	B	1310	Y01	CAM-CAY-OAW-CBC
5	A	1306	POV	O32-C31-O31-C3
5	A	1306	POV	C32-C31-O31-C3
5	B	1305	POV	O22-C21-O21-C2
6	A	1309	Y01	OAG-CAY-OAW-CBC
6	B	1308	Y01	OAG-CAY-OAW-CBC
6	A	1310	Y01	CAC-CBB-CBE-CBI
6	A	1310	Y01	CAO-CBB-CBE-CBI
6	B	1308	Y01	CAM-CAY-OAW-CBC
6	B	1309	Y01	CAC-CBB-CBE-CBI
6	A	1310	Y01	CAJ-CAO-CBB-CBE
5	A	1306	POV	C22-C21-O21-C2
6	A	1311	Y01	CAM-CAY-OAW-CBC
6	A	1310	Y01	CAJ-CAO-CBB-CAC
5	A	1307	POV	C32-C31-O31-C3
5	A	1307	POV	C31-C32-C33-C34
6	A	1311	Y01	OAG-CAY-OAW-CBC
6	A	1310	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
5	A	1305	POV	C21-C22-C23-C24
5	B	1306	POV	C31-C32-C33-C34
5	B	1307	POV	C31-C32-C33-C34
5	A	1306	POV	O22-C21-O21-C2
5	A	1307	POV	O32-C31-O31-C3
6	A	1310	Y01	CAM-CAY-OAW-CBC
6	B	1310	Y01	CAN-CAJ-CAO-CBB
5	A	1306	POV	C1-O11-P-O12
5	A	1306	POV	C11-O12-P-O11
5	A	1308	POV	C1-O11-P-O12
5	B	1306	POV	C11-O12-P-O11
5	B	1307	POV	C1-O11-P-O12
5	B	1307	POV	C11-O12-P-O11
6	A	1310	Y01	OAG-CAY-OAW-CBC
6	B	1309	Y01	CAO-CBB-CBE-CBI
5	B	1307	POV	C26-C27-C28-C29
6	A	1310	Y01	CAX-CAL-CAM-CAY
6	B	1309	Y01	CAX-CAL-CAM-CAY
5	A	1306	POV	C214-C215-C216-C217
5	B	1307	POV	C22-C23-C24-C25
5	A	1305	POV	C22-C23-C24-C25
5	A	1307	POV	C214-C215-C216-C217
5	B	1306	POV	C23-C24-C25-C26
5	B	1306	POV	C24-C25-C26-C27
5	A	1305	POV	C33-C34-C35-C36
5	B	1306	POV	C213-C214-C215-C216
5	A	1308	POV	C37-C38-C39-C310
6	A	1310	Y01	CAC-CBB-CBE-CAP
5	A	1308	POV	C31-C32-C33-C34
5	A	1305	POV	C37-C38-C39-C310
5	B	1306	POV	C33-C34-C35-C36
5	B	1307	POV	C24-C25-C26-C27
5	B	1305	POV	C31-C32-C33-C34
6	B	1309	Y01	CAN-CAJ-CAO-CBB
5	A	1306	POV	C213-C214-C215-C216
5	A	1305	POV	C311-C310-C39-C38
5	A	1306	POV	C33-C34-C35-C36
5	A	1307	POV	C312-C313-C314-C315
6	A	1310	Y01	CAO-CAJ-CAN-CBA
5	B	1307	POV	C212-C213-C214-C215
5	B	1307	POV	C210-C211-C212-C213
5	A	1307	POV	C311-C310-C39-C38

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Mol	Chain	Res	Type	Atoms
5	B	1305	POV	C211-C212-C213-C214
5	B	1306	POV	C2-C1-O11-P
5	B	1306	POV	C211-C212-C213-C214
5	A	1308	POV	C21-C22-C23-C24
5	B	1305	POV	C33-C34-C35-C36
6	B	1308	Y01	CAN-CAJ-CAO-CBB
5	A	1307	POV	C26-C27-C28-C29
5	B	1307	POV	C23-C24-C25-C26
5	A	1305	POV	C26-C27-C28-C29
5	A	1308	POV	C26-C27-C28-C29
6	B	1310	Y01	CAX-CAL-CAM-CAY
5	B	1307	POV	C22-C21-O21-C2
5	A	1307	POV	O11-C1-C2-C3
5	B	1307	POV	O11-C1-C2-C3
6	A	1310	Y01	CAO-CBB-CBE-CAP
5	B	1306	POV	C26-C27-C28-C29
6	B	1309	Y01	CAC-CBB-CBE-CAP
5	A	1307	POV	C1-C2-C3-O31
5	A	1307	POV	C36-C37-C38-C39
5	B	1305	POV	C1-C2-C3-O31
5	A	1305	POV	C32-C33-C34-C35
5	A	1306	POV	C21-C22-C23-C24
5	A	1307	POV	C21-C22-C23-C24
6	A	1311	Y01	CAC-CBB-CBE-CBI
5	A	1306	POV	C311-C310-C39-C38
5	A	1308	POV	C312-C313-C314-C315
5	A	1306	POV	C312-C313-C314-C315
5	A	1306	POV	C313-C314-C315-C316
5	A	1306	POV	C31-C32-C33-C34
6	B	1310	Y01	CAC-CBB-CBE-CBI
5	A	1305	POV	C212-C213-C214-C215
5	A	1307	POV	C311-C312-C313-C314
5	A	1306	POV	C310-C311-C312-C313
5	B	1307	POV	C214-C215-C216-C217
5	B	1306	POV	C212-C213-C214-C215
5	B	1307	POV	C1-C2-C3-O31
5	B	1307	POV	O22-C21-O21-C2
6	B	1310	Y01	CAV-CBC-OAW-CAY
5	A	1306	POV	C215-C216-C217-C218
5	A	1307	POV	O11-C1-C2-O21
5	B	1306	POV	C25-C26-C27-C28
5	A	1308	POV	C210-C211-C212-C213

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Mol	Chain	Res	Type	Atoms
5	B	1307	POV	O21-C2-C3-O31
5	A	1306	POV	C36-C37-C38-C39
5	A	1306	POV	C22-C23-C24-C25
5	A	1307	POV	C22-C21-O21-C2
5	A	1307	POV	C33-C34-C35-C36
6	B	1309	Y01	CAO-CBB-CBE-CAP
6	A	1311	Y01	CAO-CBB-CBE-CBI
5	A	1307	POV	C24-C25-C26-C27
5	A	1307	POV	C37-C38-C39-C310
5	B	1307	POV	O11-C1-C2-O21
5	A	1307	POV	O22-C21-O21-C2
5	B	1305	POV	C32-C33-C34-C35
5	A	1306	POV	C32-C33-C34-C35
5	A	1306	POV	C2-C1-O11-P
5	A	1306	POV	C11-O12-P-O14
5	B	1306	POV	C11-O12-P-O13
5	B	1307	POV	C1-O11-P-O13
5	B	1307	POV	C11-O12-P-O13
5	A	1305	POV	O11-C1-C2-C3
5	A	1308	POV	C23-C24-C25-C26
5	A	1308	POV	C36-C37-C38-C39
5	B	1307	POV	C211-C212-C213-C214
5	A	1305	POV	O11-C1-C2-O21
5	A	1307	POV	C215-C216-C217-C218
5	A	1305	POV	C213-C214-C215-C216
6	B	1310	Y01	CAR-CBC-OAW-CAY
5	A	1306	POV	C23-C24-C25-C26
5	A	1307	POV	O12-C11-C12-N
5	A	1308	POV	O12-C11-C12-N
5	B	1306	POV	O12-C11-C12-N
5	B	1307	POV	O12-C11-C12-N
5	A	1306	POV	C26-C27-C28-C29
5	A	1308	POV	C39-C310-C311-C312
5	A	1305	POV	C23-C24-C25-C26
5	A	1306	POV	C35-C36-C37-C38
6	B	1310	Y01	CAO-CBB-CBE-CBI
6	A	1311	Y01	CAO-CAJ-CAN-CBA
5	A	1306	POV	C27-C28-C29-C210
6	A	1311	Y01	CAC-CBB-CBE-CAP
5	A	1305	POV	C11-O12-P-O11
5	A	1307	POV	C11-O12-P-O11
5	B	1305	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
5	A	1308	POV	C22-C21-O21-C2
6	A	1310	Y01	CAJ-CAN-CBA-CAA
5	A	1308	POV	O22-C21-O21-C2
5	A	1306	POV	C24-C25-C26-C27
6	A	1310	Y01	CAJ-CAN-CBA-CAB
5	A	1307	POV	O21-C21-C22-C23
5	B	1305	POV	C23-C24-C25-C26
5	A	1308	POV	C24-C25-C26-C27
5	A	1307	POV	C310-C311-C312-C313
5	B	1305	POV	C37-C38-C39-C310
5	A	1307	POV	C2-C1-O11-P
6	A	1309	Y01	CAM-CAL-CAX-OAH
5	A	1306	POV	C210-C211-C212-C213
5	B	1306	POV	C210-C211-C212-C213
5	A	1308	POV	O31-C31-C32-C33
6	A	1309	Y01	CAM-CAL-CAX-OAF
6	A	1310	Y01	CAM-CAL-CAX-OAF
6	B	1309	Y01	CAM-CAL-CAX-OAF
5	A	1306	POV	C3-C2-O21-C21
5	A	1305	POV	C29-C210-C211-C212
5	A	1307	POV	C34-C35-C36-C37
5	B	1306	POV	C1-O11-P-O12
6	A	1309	Y01	CAN-CAJ-CAO-CBB
5	B	1306	POV	O31-C31-C32-C33
6	A	1311	Y01	CAM-CAL-CAX-OAF
6	A	1311	Y01	CAM-CAL-CAX-OAH
6	A	1310	Y01	CAM-CAL-CAX-OAH
6	B	1309	Y01	CAM-CAL-CAX-OAH
5	A	1307	POV	C29-C210-C211-C212
5	B	1305	POV	O11-C1-C2-O21
6	A	1310	Y01	CAL-CAM-CAY-OAW
5	A	1305	POV	O31-C31-C32-C33
5	A	1308	POV	O21-C21-C22-C23
5	B	1307	POV	O21-C21-C22-C23
6	B	1308	Y01	CAM-CAL-CAX-OAF
5	B	1307	POV	C29-C210-C211-C212
5	B	1305	POV	O21-C21-C22-C23
6	A	1309	Y01	CAC-CBB-CBE-CBI
5	B	1307	POV	C32-C33-C34-C35
5	B	1306	POV	C310-C311-C312-C313
5	B	1305	POV	C27-C28-C29-C210
6	B	1308	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
6	B	1310	Y01	CAC-CBB-CBE-CAP
5	A	1305	POV	C27-C28-C29-C210
5	A	1308	POV	C29-C210-C211-C212
5	B	1306	POV	C29-C210-C211-C212
6	A	1311	Y01	CAN-CAJ-CAO-CBB
5	A	1305	POV	O32-C31-C32-C33
5	B	1306	POV	C311-C312-C313-C314
5	B	1307	POV	O22-C21-C22-C23
5	A	1308	POV	O22-C21-C22-C23
5	A	1307	POV	C27-C28-C29-C210
6	A	1310	Y01	CAL-CAM-CAY-OAG
5	A	1307	POV	C22-C23-C24-C25
5	B	1305	POV	O22-C21-C22-C23
5	B	1305	POV	C29-C210-C211-C212
5	A	1307	POV	C12-C11-O12-P
5	B	1307	POV	C215-C216-C217-C218
5	B	1307	POV	O31-C31-C32-C33
6	A	1311	Y01	CAO-CBB-CBE-CAP
6	B	1309	Y01	CAO-CAJ-CAN-CBA

There are no ring outliers.

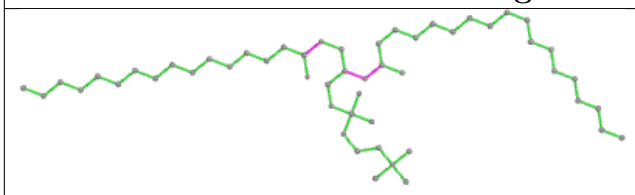
13 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1308	POV	5	0
6	A	1310	Y01	3	0
5	B	1307	POV	6	0
6	A	1309	Y01	2	0
6	B	1309	Y01	3	0
6	A	1311	Y01	3	0
5	A	1307	POV	2	0
5	A	1306	POV	7	0
6	B	1308	Y01	2	0
5	A	1305	POV	5	0
5	B	1306	POV	8	0
5	B	1305	POV	4	0
6	B	1310	Y01	2	0

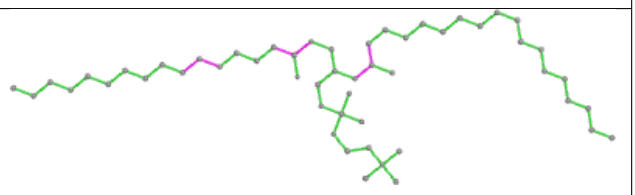
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

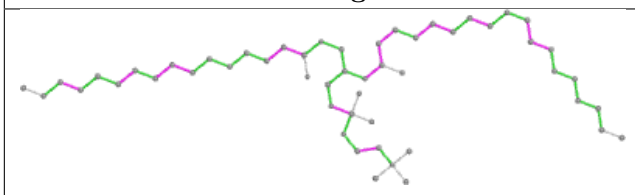
Ligand POV A 1308



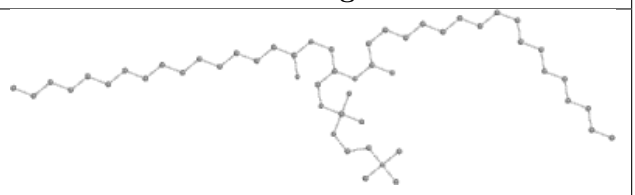
Bond lengths



Bond angles

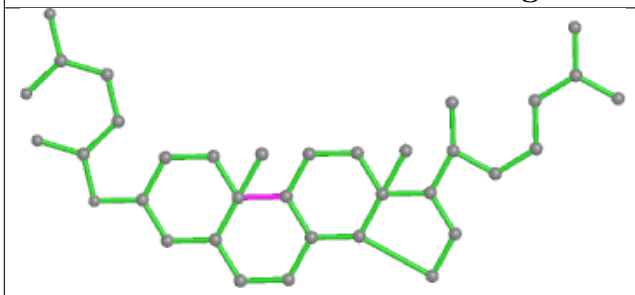


Torsions

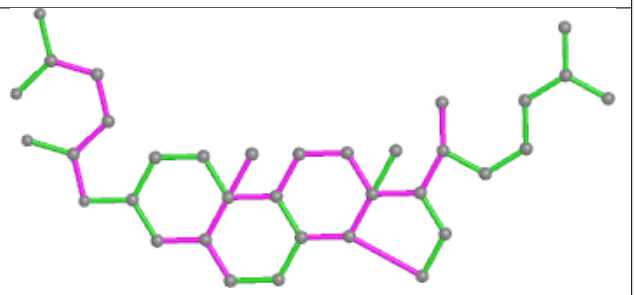


Rings

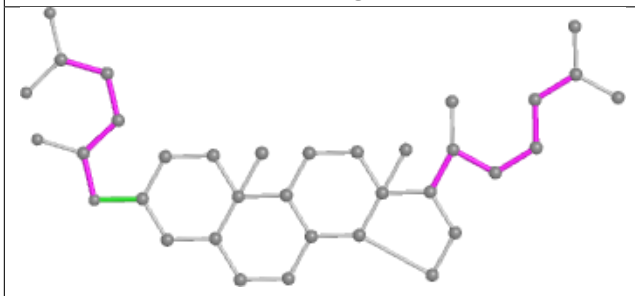
Ligand Y01 A 1310



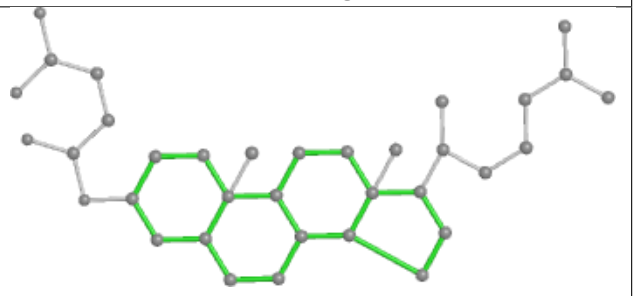
Bond lengths



Bond angles

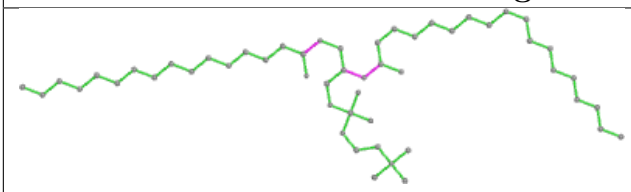


Torsions

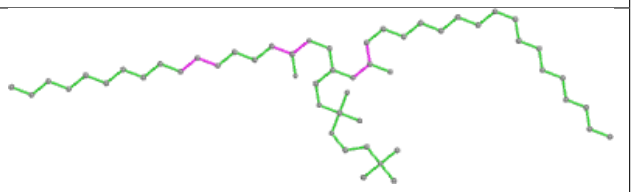


Rings

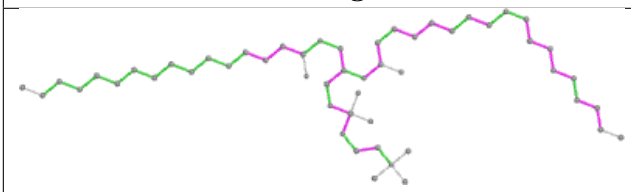
Ligand POV B 1307



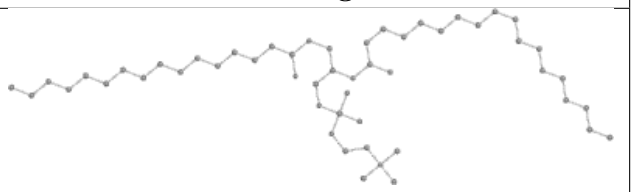
Bond lengths



Bond angles

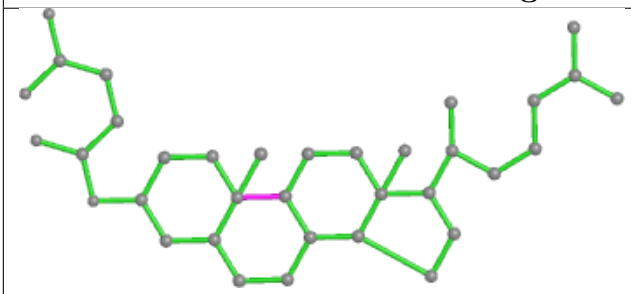


Torsions

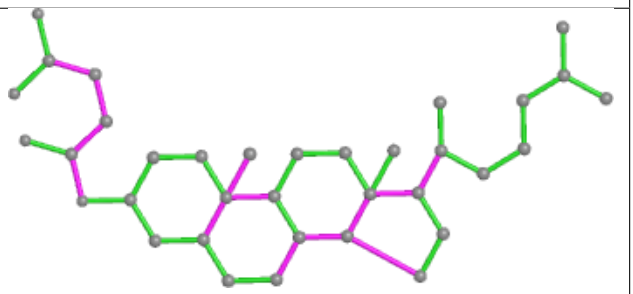


Rings

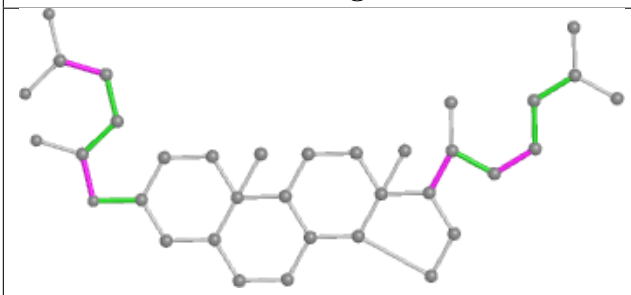
Ligand Y01 A 1309



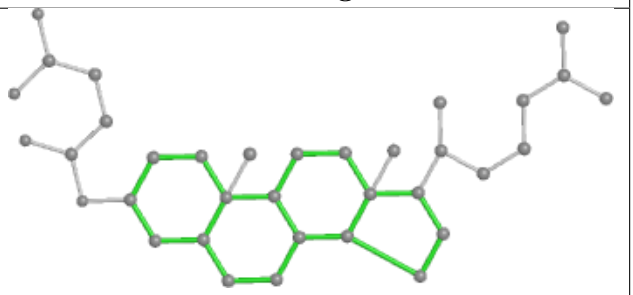
Bond lengths



Bond angles

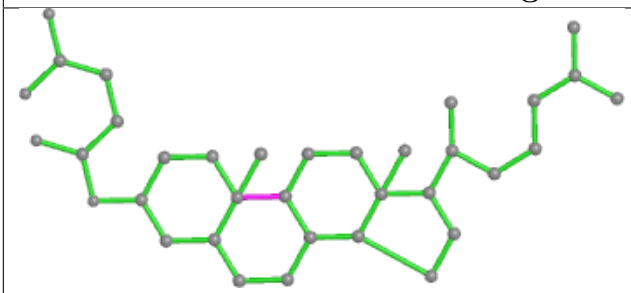


Torsions

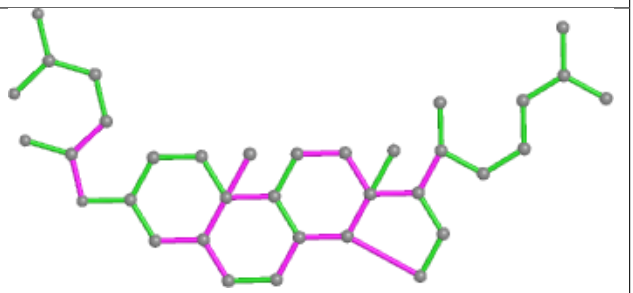


Rings

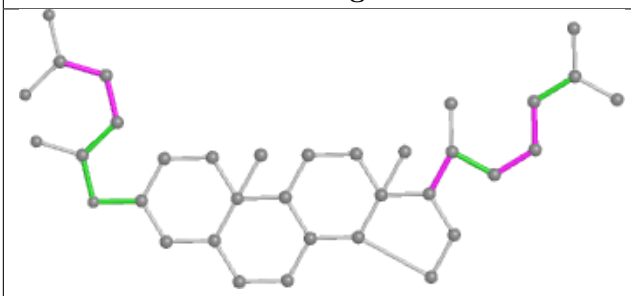
Ligand Y01 B 1309



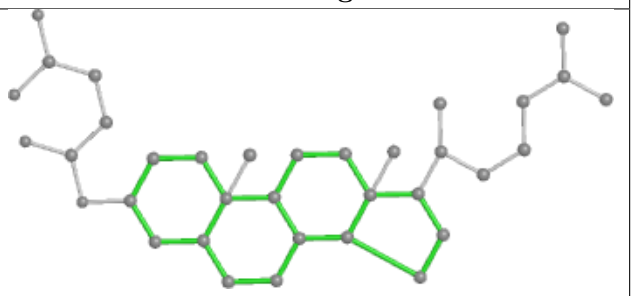
Bond lengths



Bond angles

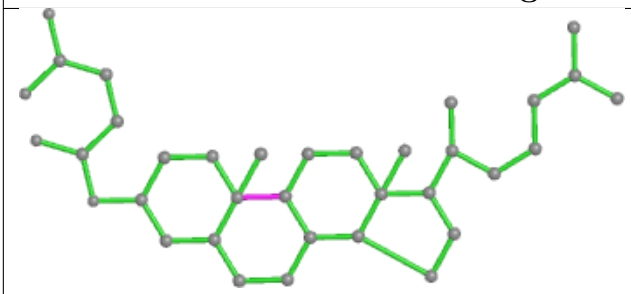


Torsions

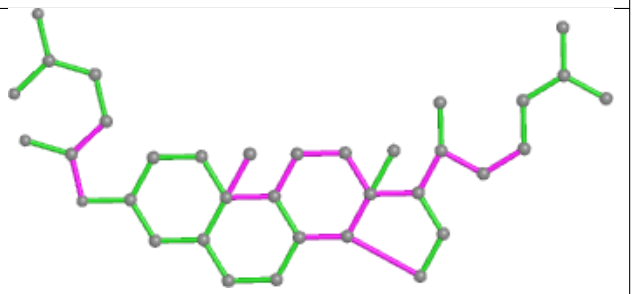


Rings

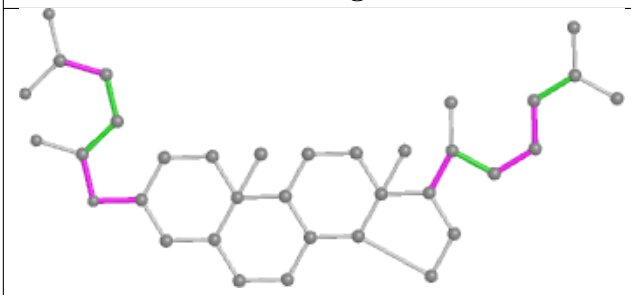
Ligand Y01 A 1311



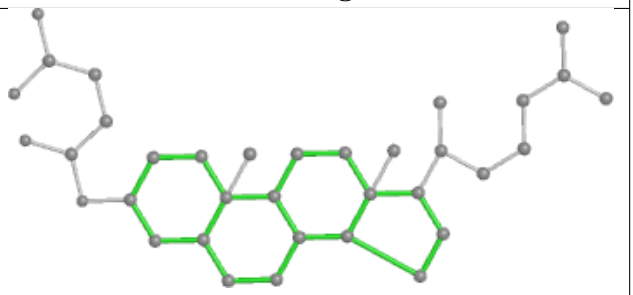
Bond lengths



Bond angles

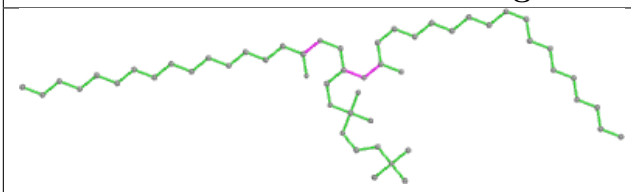


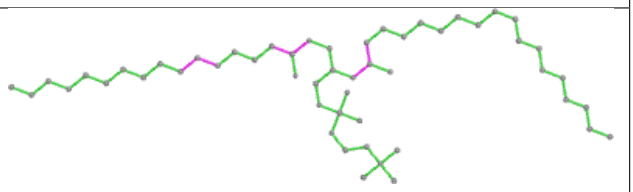
Torsions

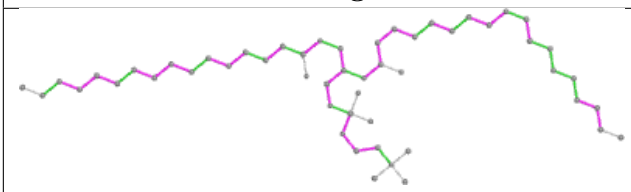


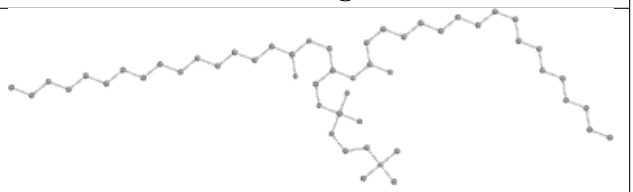
Rings

Ligand POV A 1307

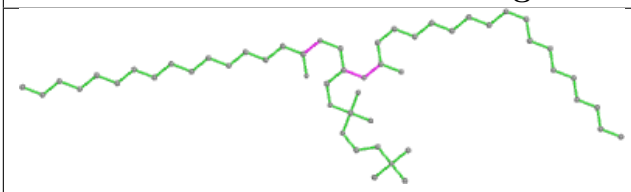

Bond lengths

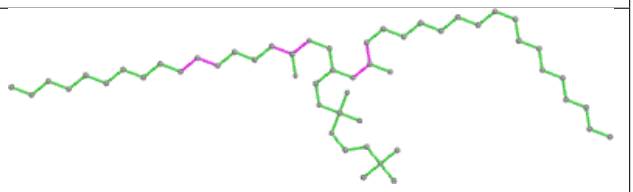

Bond angles

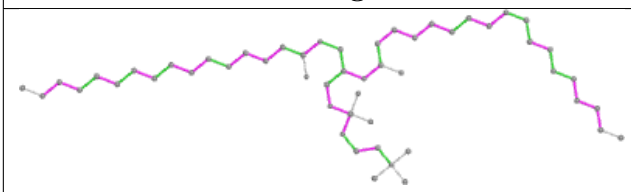

Torsions

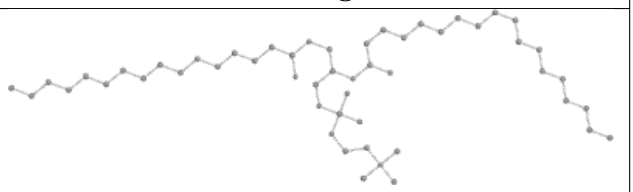

Rings

Ligand POV A 1306

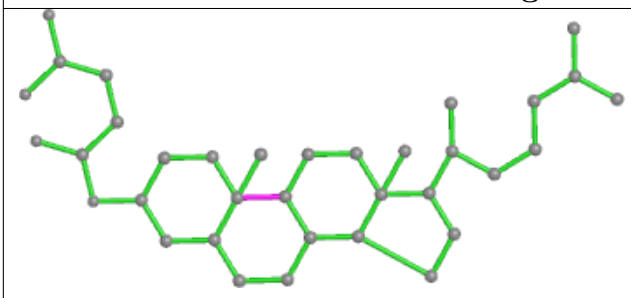

Bond lengths

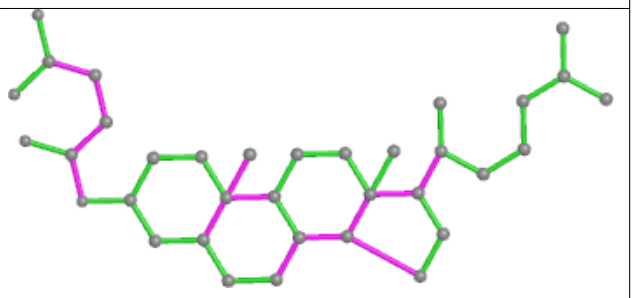

Bond angles

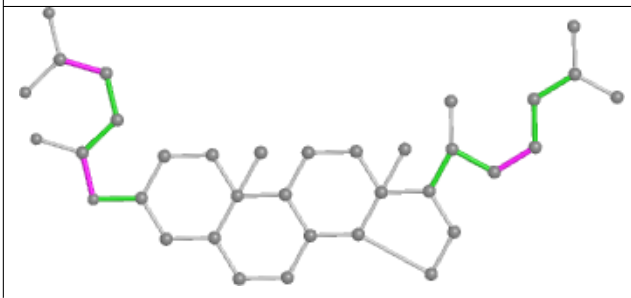

Torsions

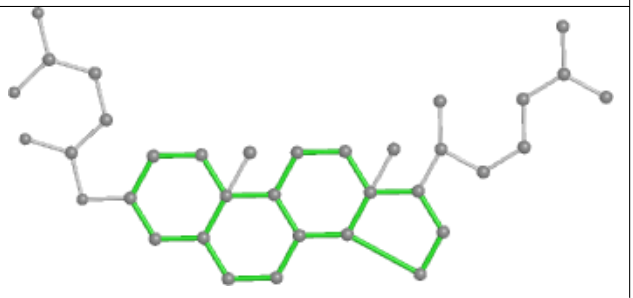

Rings

Ligand Y01 B 1308

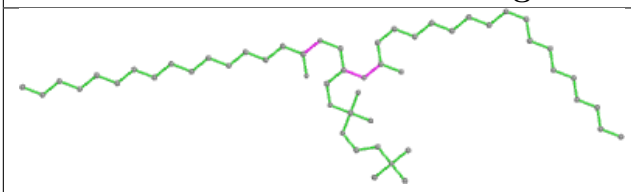

Bond lengths


Bond angles

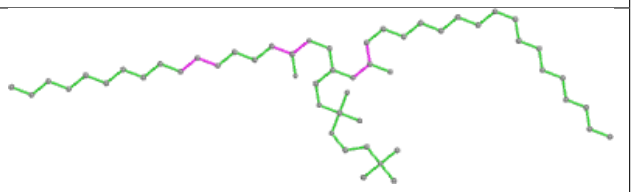

Torsions


Rings

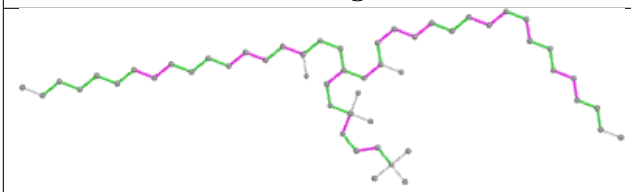
Ligand POV A 1305



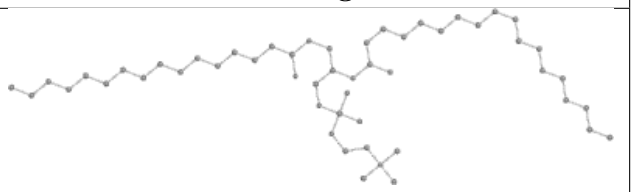
Bond lengths



Bond angles

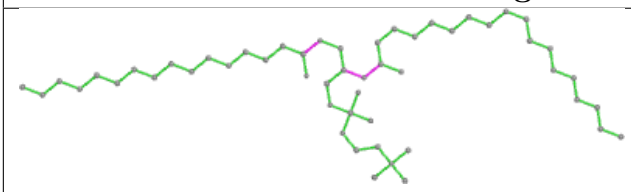


Torsions

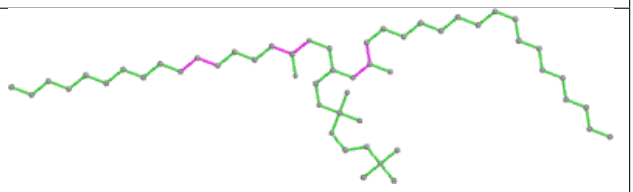


Rings

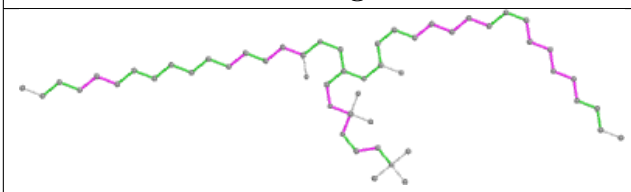
Ligand POV B 1306



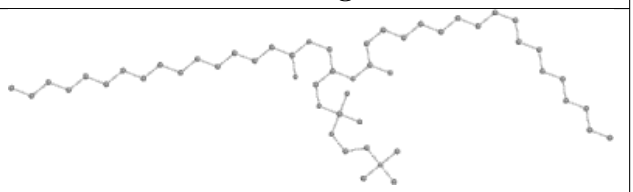
Bond lengths



Bond angles

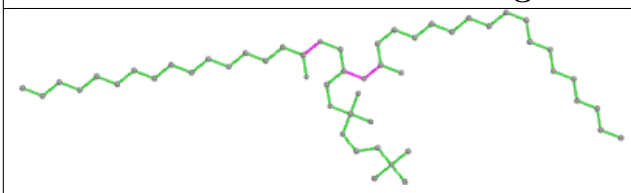


Torsions

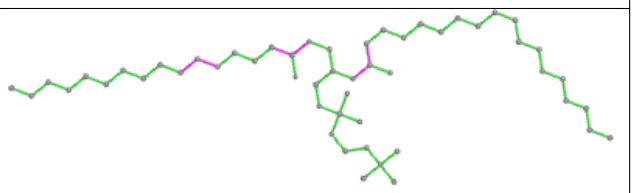


Rings

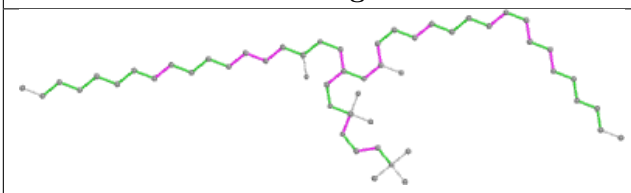
Ligand POV B 1305



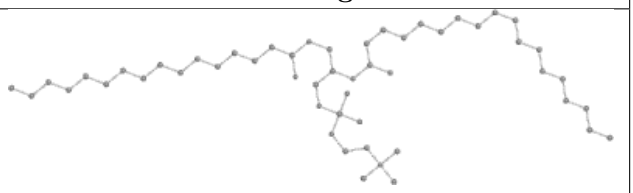
Bond lengths



Bond angles

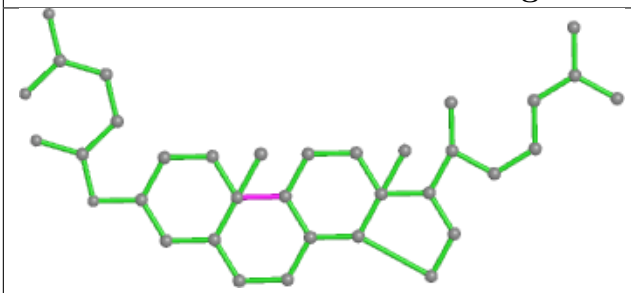


Torsions

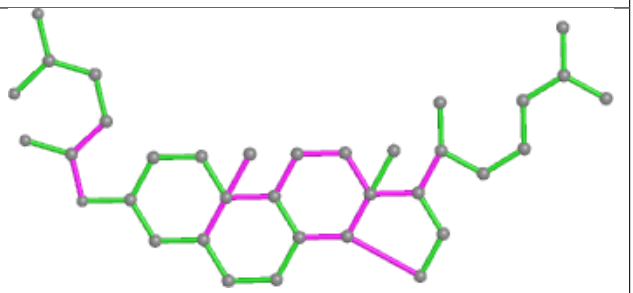


Rings

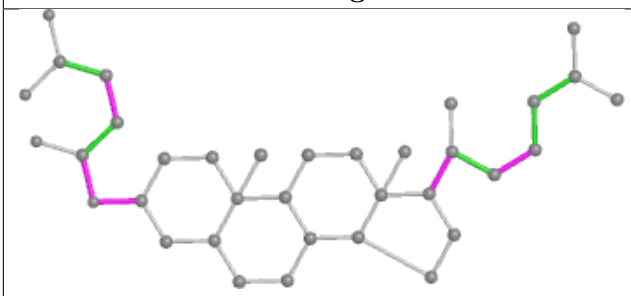
Ligand Y01 B 1310



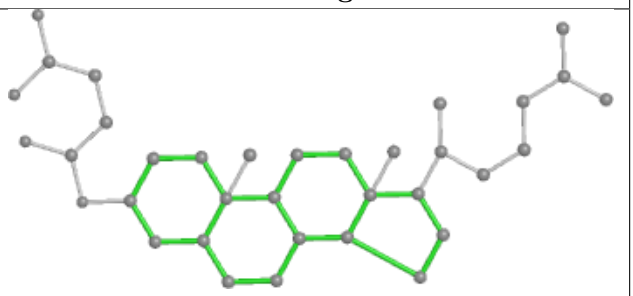
Bond lengths



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.

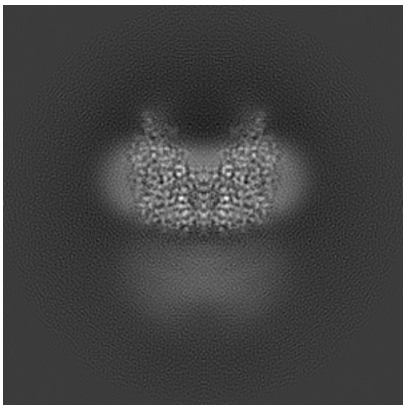
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14709. These allow visual inspection of the internal detail of the map and identification of artifacts.

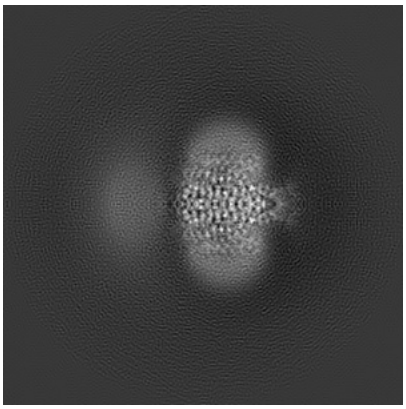
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

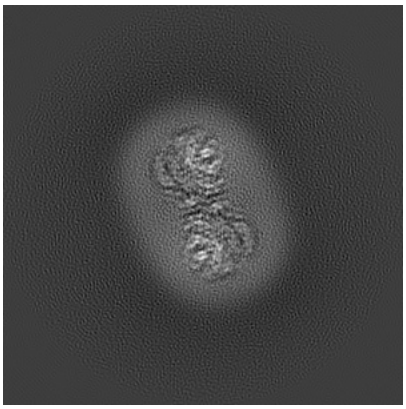
6.1.1 Primary map



X

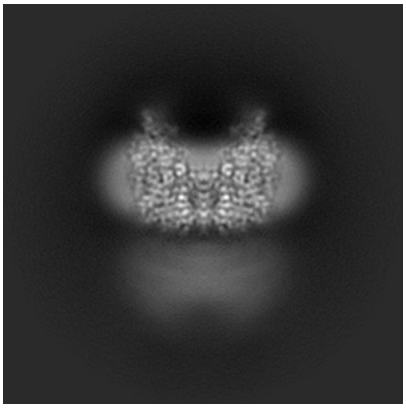


Y

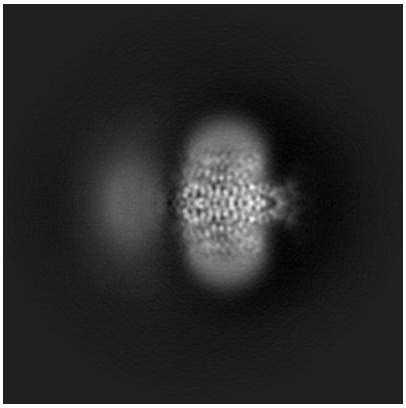


Z

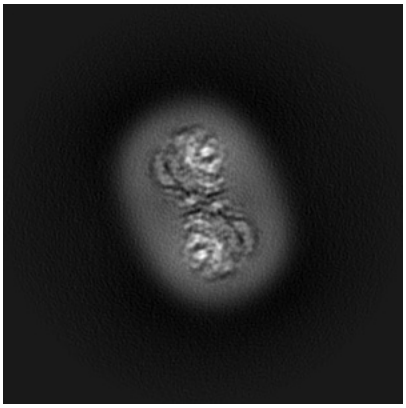
6.1.2 Raw map



X



Y

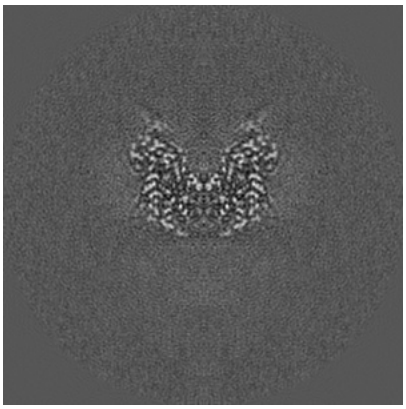


Z

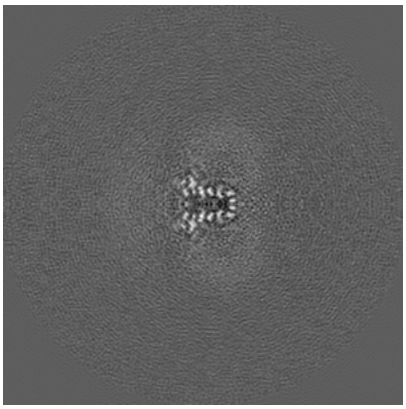
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

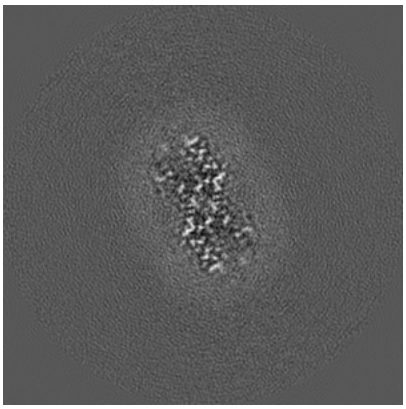
6.2.1 Primary map



X Index: 120

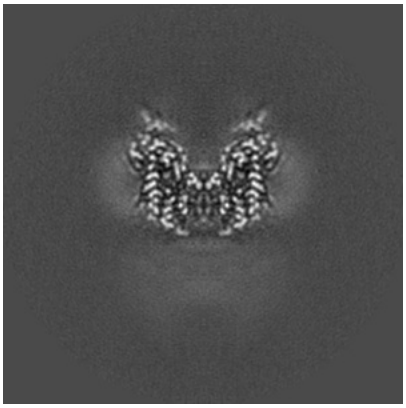


Y Index: 120

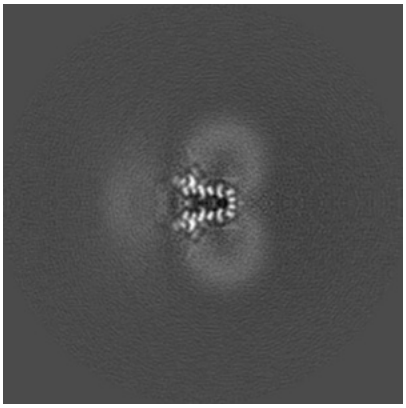


Z Index: 120

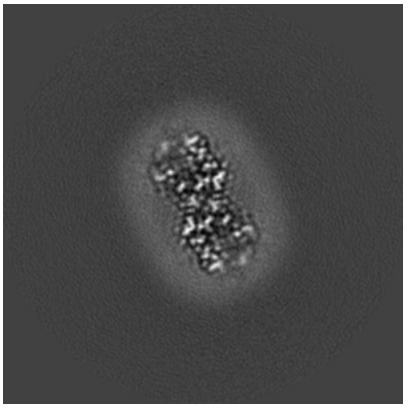
6.2.2 Raw map



X Index: 120



Y Index: 120

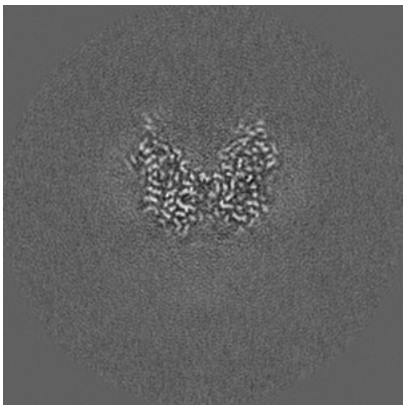


Z Index: 120

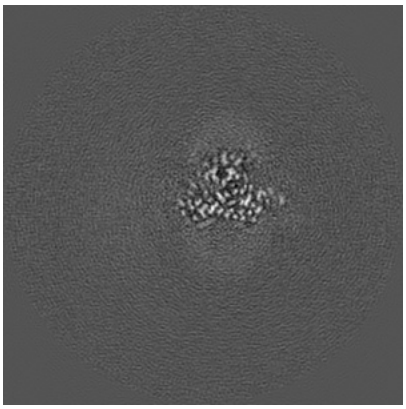
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

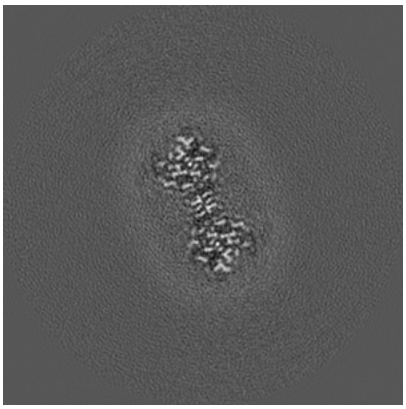
6.3.1 Primary map



X Index: 118

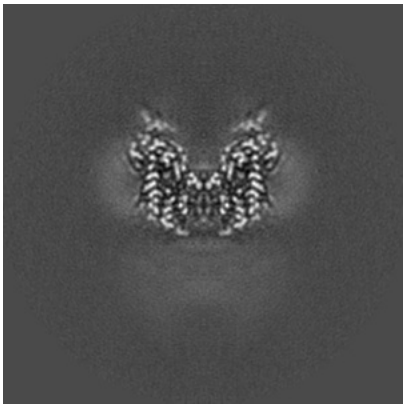


Y Index: 98

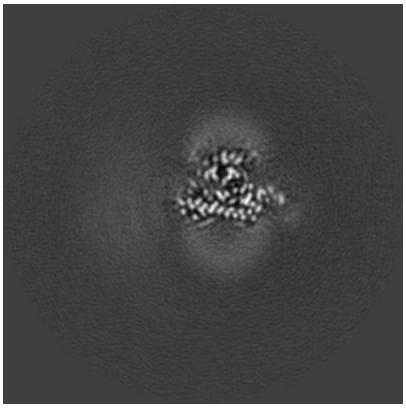


Z Index: 135

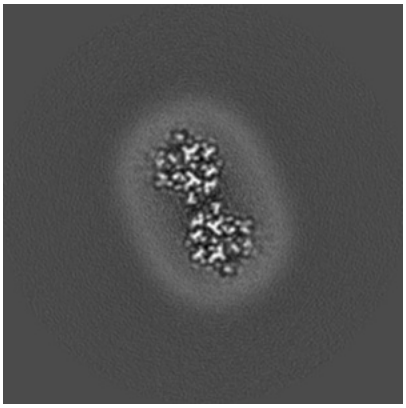
6.3.2 Raw map



X Index: 120



Y Index: 98

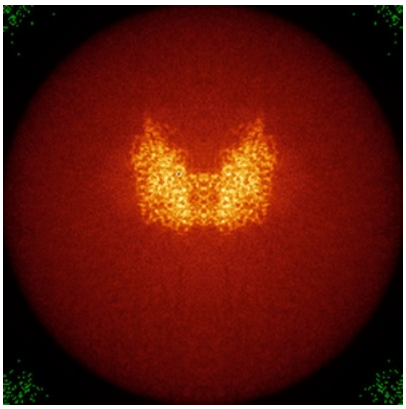


Z Index: 128

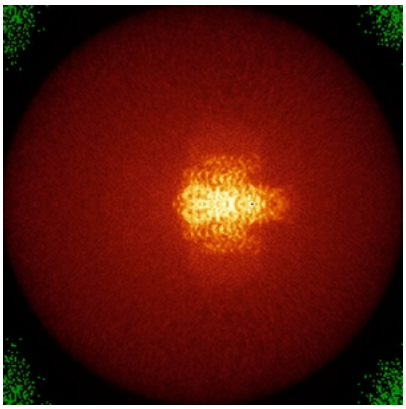
The images above show the largest variance slices of the map in three orthogonal directions.

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

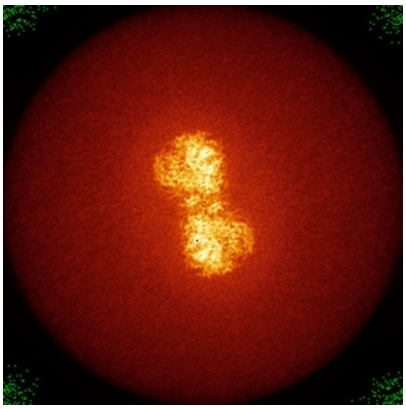
6.4.1 Primary map



X

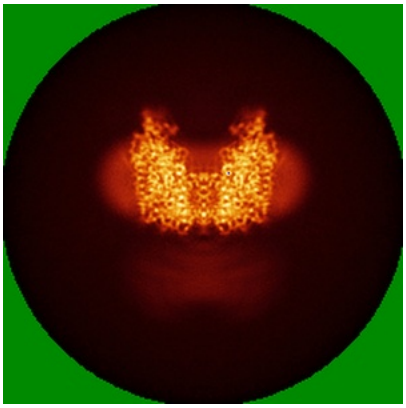


Y

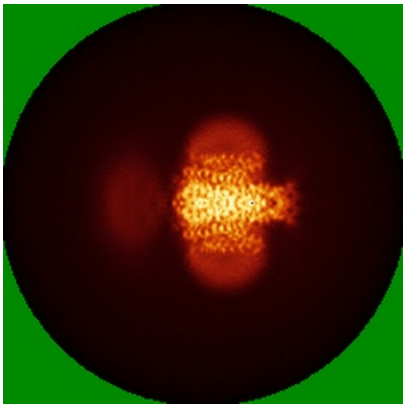


Z

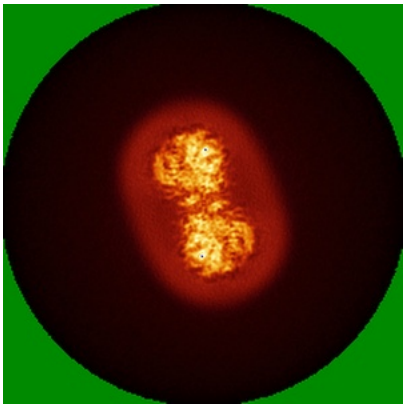
6.4.2 Raw map



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.

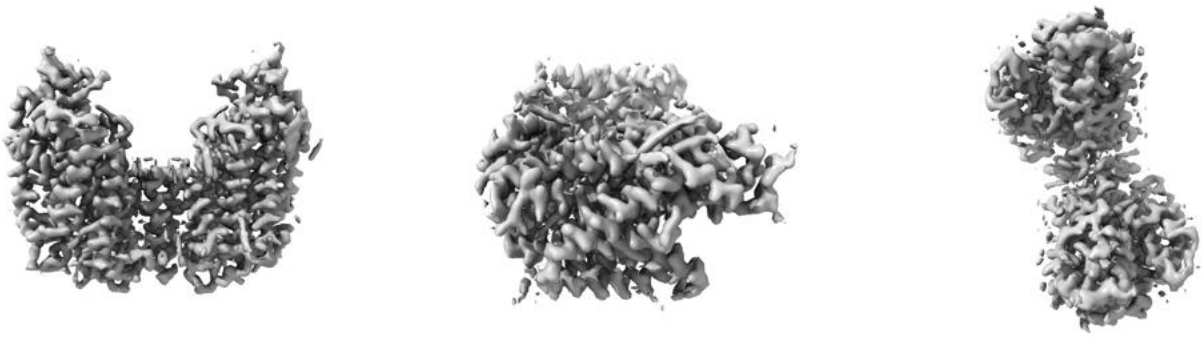
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

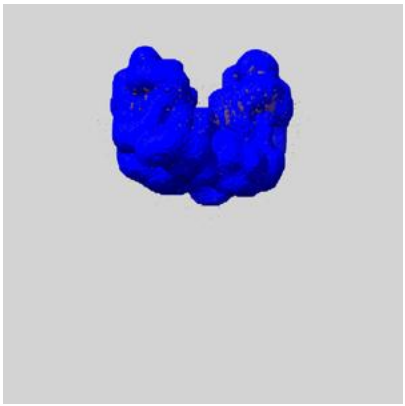
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

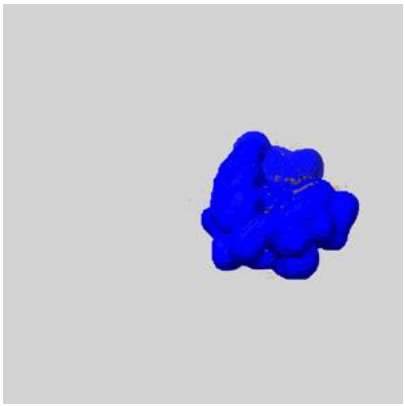
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

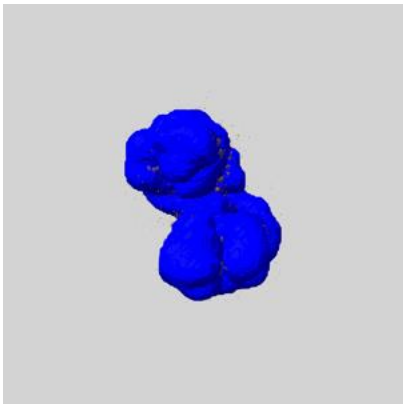
6.6.1 emd_14709_msk_1.map (i)



X



Y

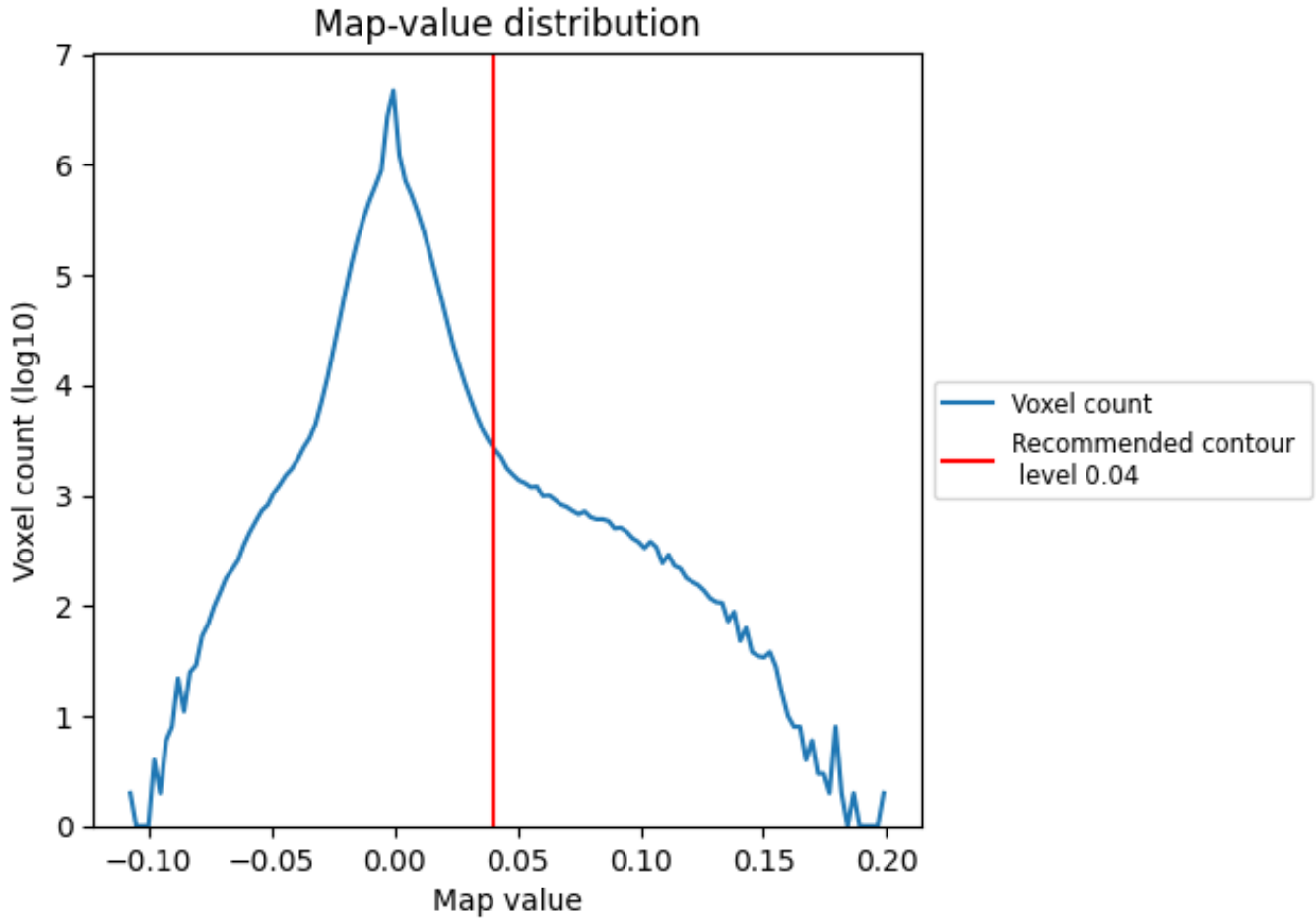


Z

7 Map analysis

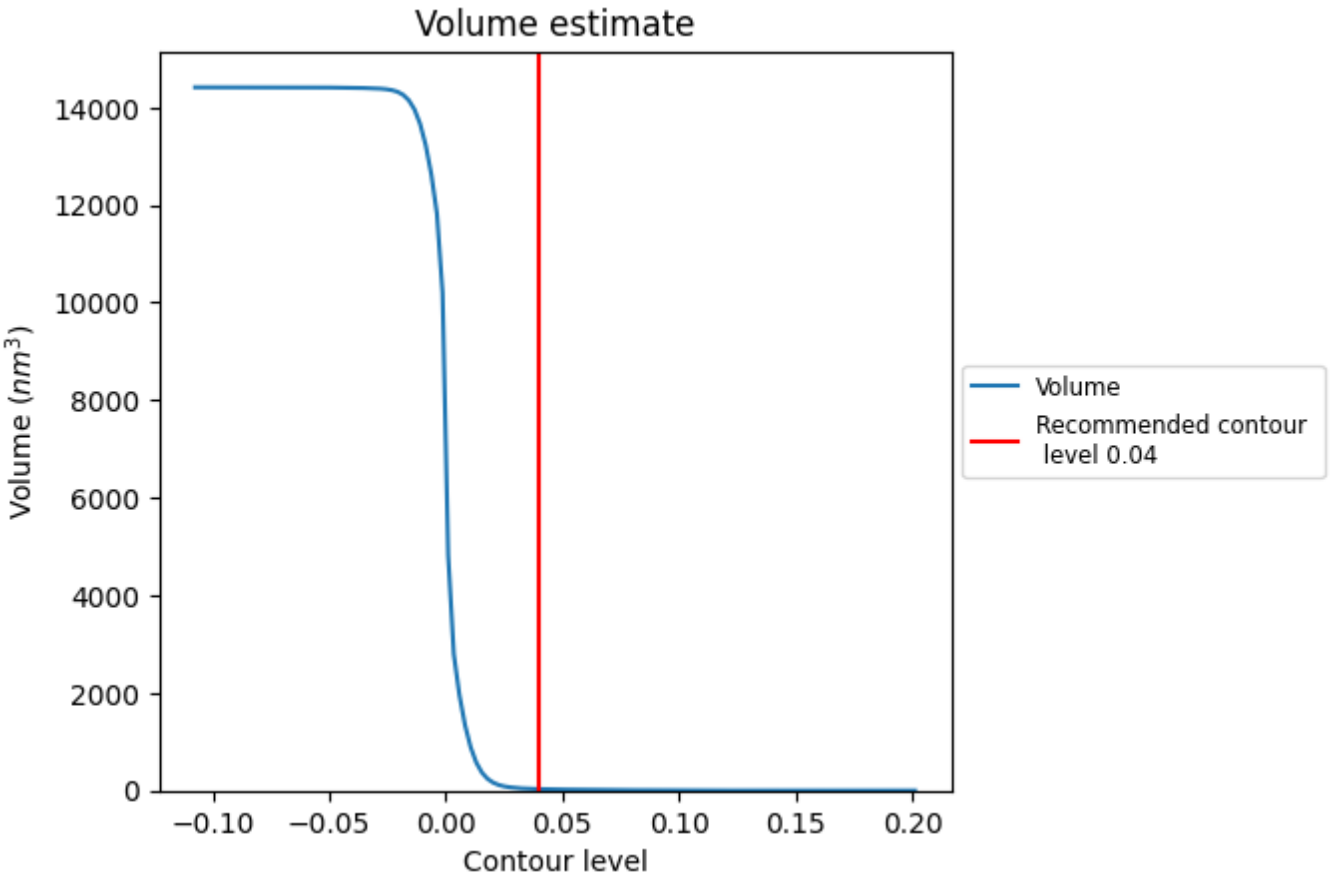
This section contains the results of statistical analysis of the map.

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.

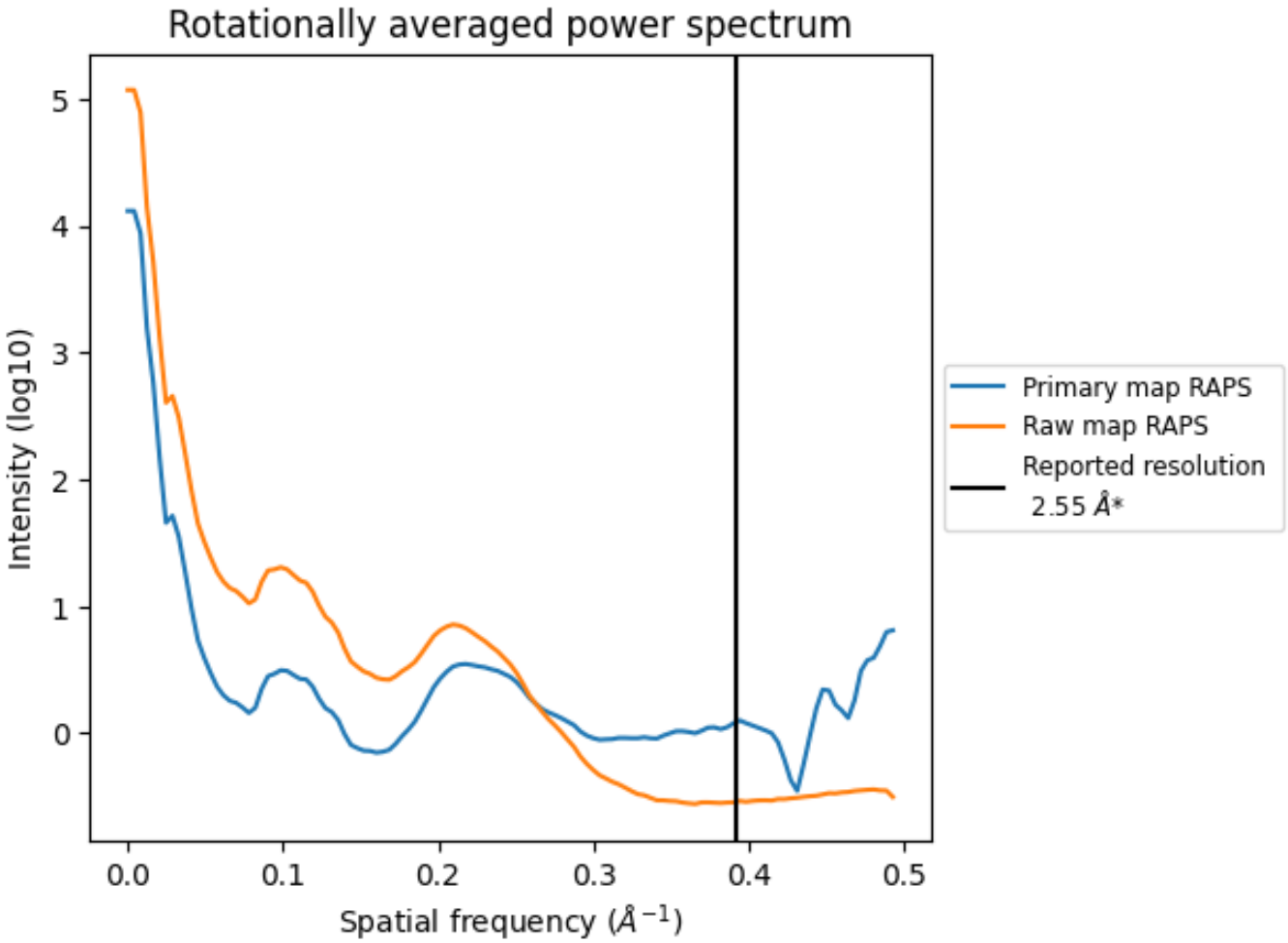
7.2 Volume estimate



The volume at the recommended contour level is 30 nm^3; this corresponds to an approximate mass of 27 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)

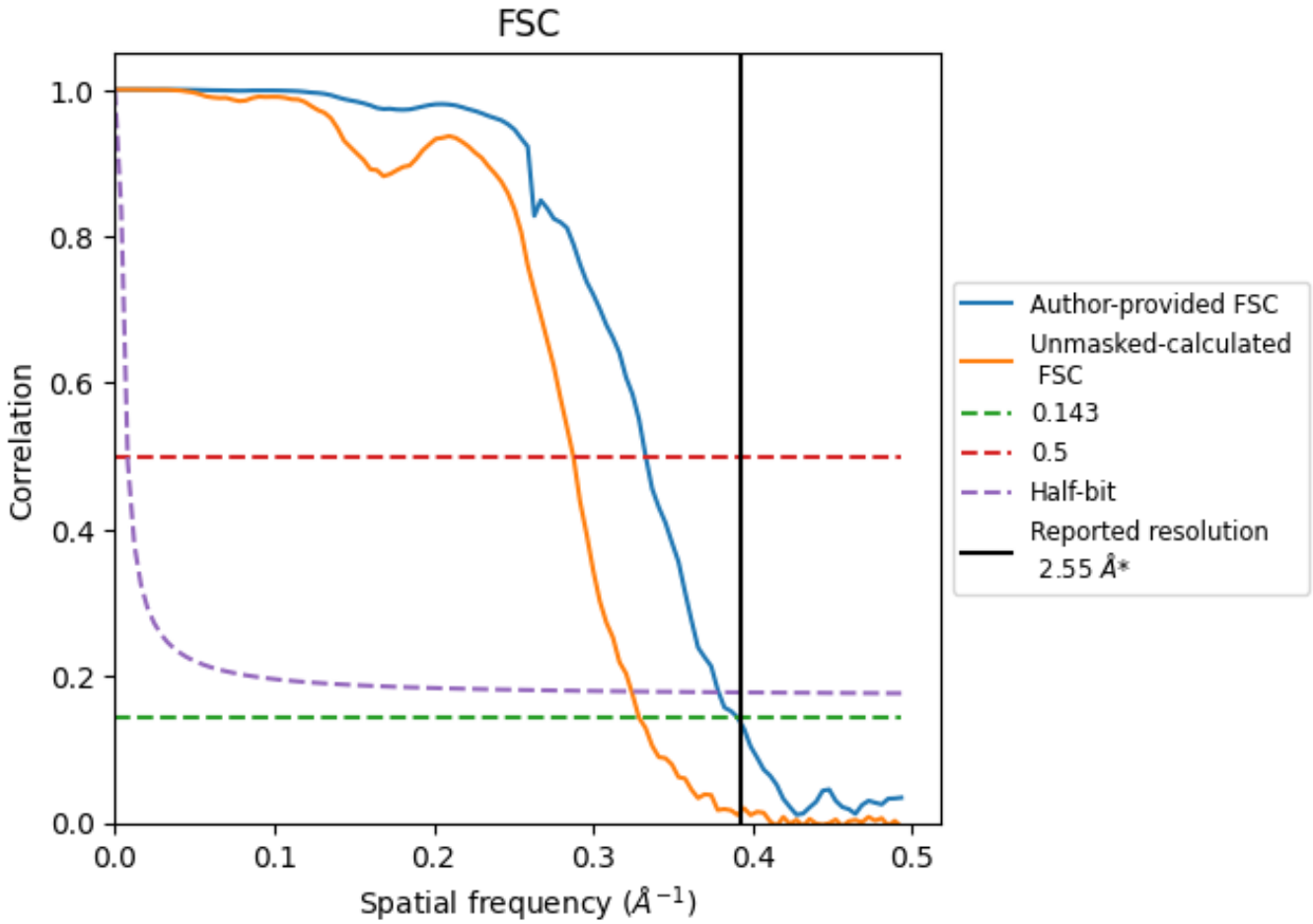


*Reported resolution corresponds to spatial frequency of 0.392 Å^{-1}

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 0.392 Å^{-1}

8.2 Resolution estimates (i)

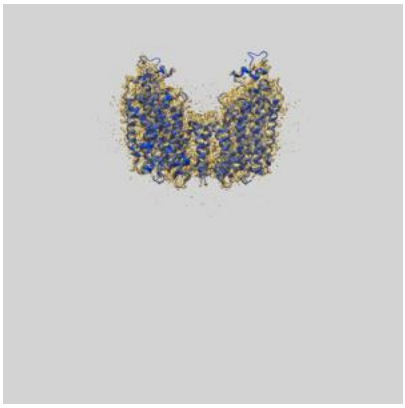
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.56	3.00	2.64
Unmasked-calculated*	3.04	3.48	3.09

*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 3.04 differs from the reported value 2.55 by more than 10 %

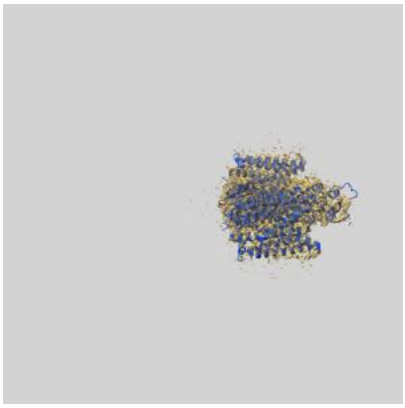
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14709 and PDB model 7ZGO. Per-residue inclusion information can be found in section 3 on page 7.

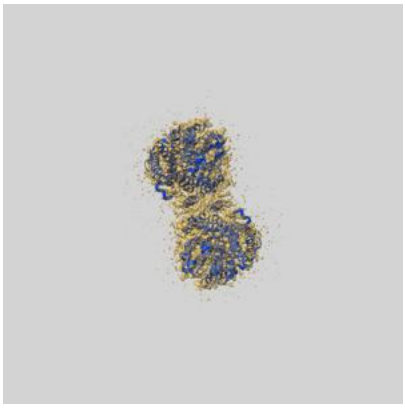
9.1 Map-model overlay



X



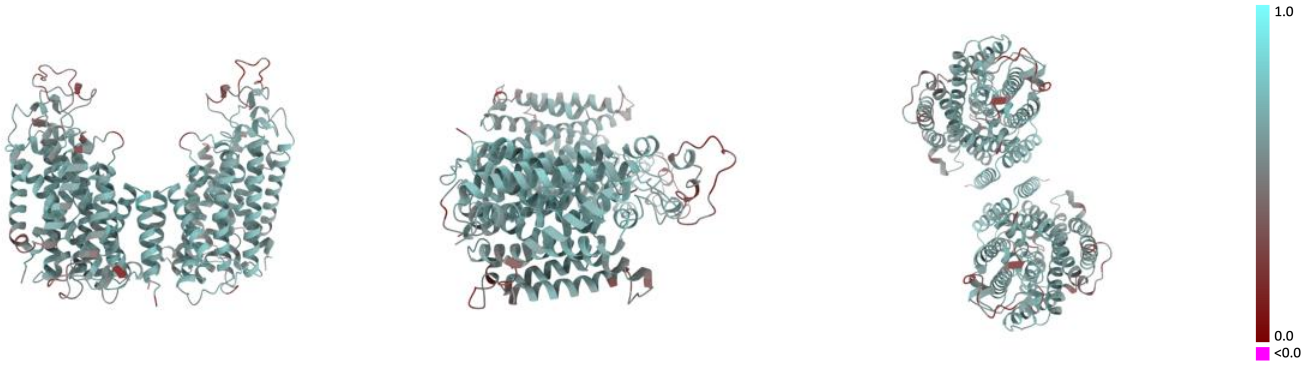
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

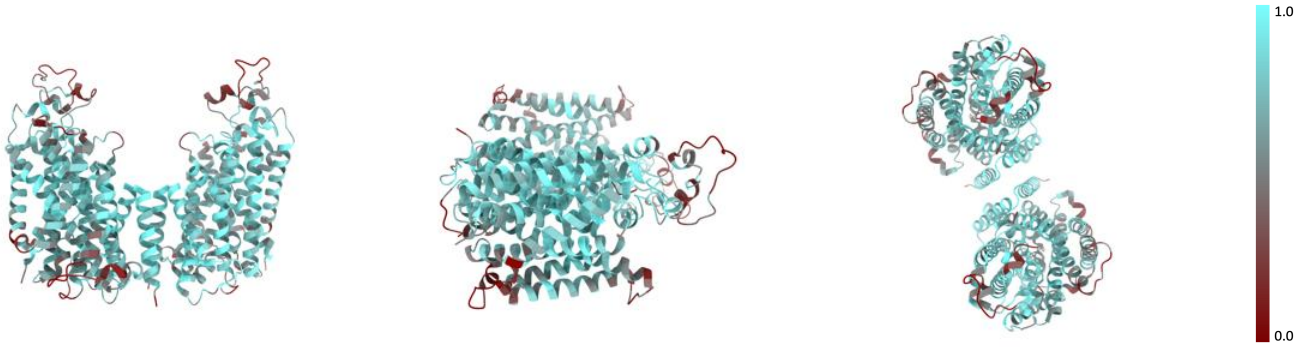
9.2 Q-score mapped to coordinate model (i)



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.

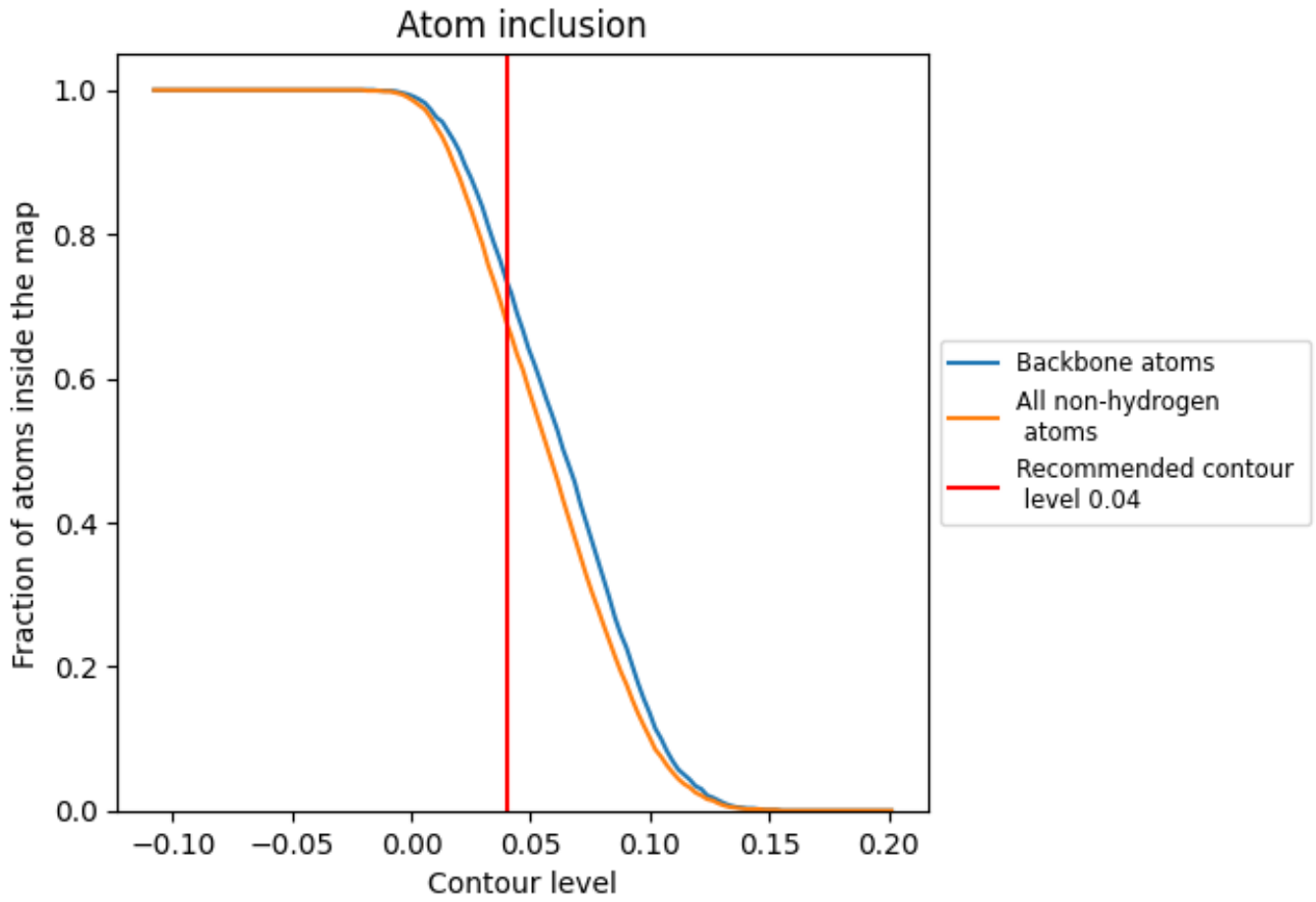
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6770	0.5760
A	0.6760	0.5750
B	0.6790	0.5780