Full wwPDB EM Validation Report

May 18, 2025 – 05:33 PM EDT

PDB ID	:	8DDT / pdb_00008ddt
EMDB ID	:	EMD-27341
Title	:	cryo-EM structure of TRPM3 ion channel in the presence of PIP2, state2
Authors	:	Zhao, C.; MacKinnon, R.
Deposited on	:	2022-06-18
Resolution	:	3.10 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:

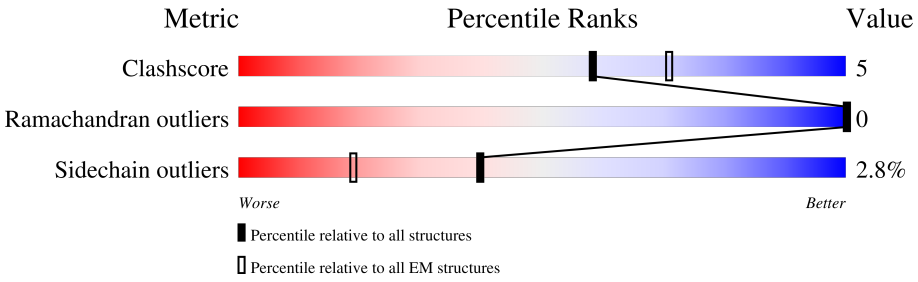
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1371	9% 62% 9% 29%
1	B	1371	9% 62% 8% 29%
1	C	1371	9% 62% 8% 29%
1	D	1371	9% 63% 8% 29%
2	E	17	47% 94% 6%
2	F	17	47% 94% 6%
2	G	17	47% 94% 6%
2	H	17	47% 94% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32229 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.

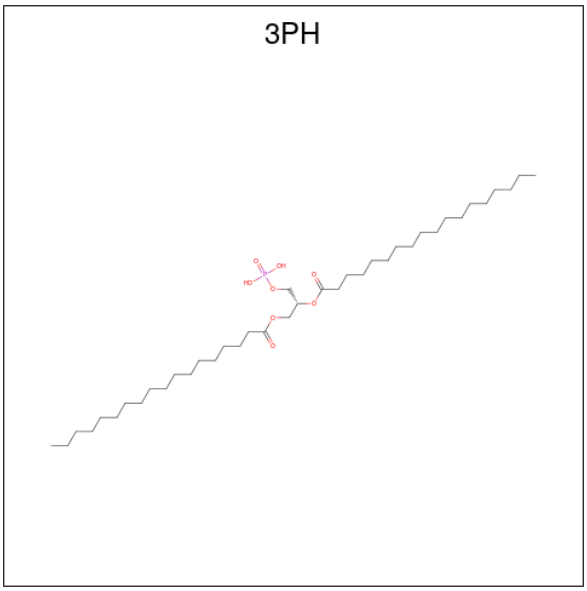
- Molecule 1 is a protein called Transient receptor potential cation channel, subfamily M, member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		
1	B	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		
1	C	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		
1	D	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		

- Molecule 2 is a protein called Unidentified segment at the N-terminus of TRPM3.

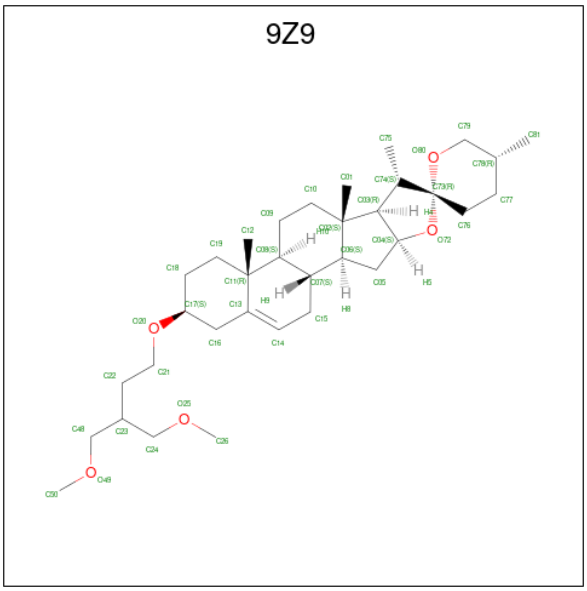
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	17	Total	C	N	O	0	0
			85	51	17	17		
2	F	17	Total	C	N	O	0	0
			85	51	17	17		
2	G	17	Total	C	N	O	0	0
			85	51	17	17		
2	H	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 3 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



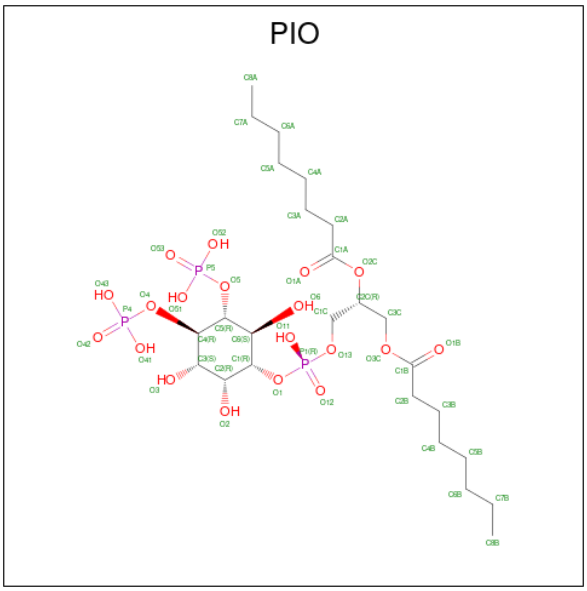
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			45	36	8	1	
3	B	1	Total	C	O	P	0
			45	36	8	1	
3	C	1	Total	C	O	P	0
			45	36	8	1	
3	D	1	Total	C	O	P	0
			45	36	8	1	

- Molecule 4 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: $C_{34}H_{56}O_5$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 39 34 5	0
4	B	1	Total C O 39 34 5	0
4	C	1	Total C O 39 34 5	0
4	D	1	Total C O 39 34 5	0

- Molecule 5 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: $C_{25}H_{49}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O P 47 25 19 3	0
5	B	1	Total C O P 47 25 19 3	0
5	C	1	Total C O P 47 25 19 3	0
5	D	1	Total C O P 47 25 19 3	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

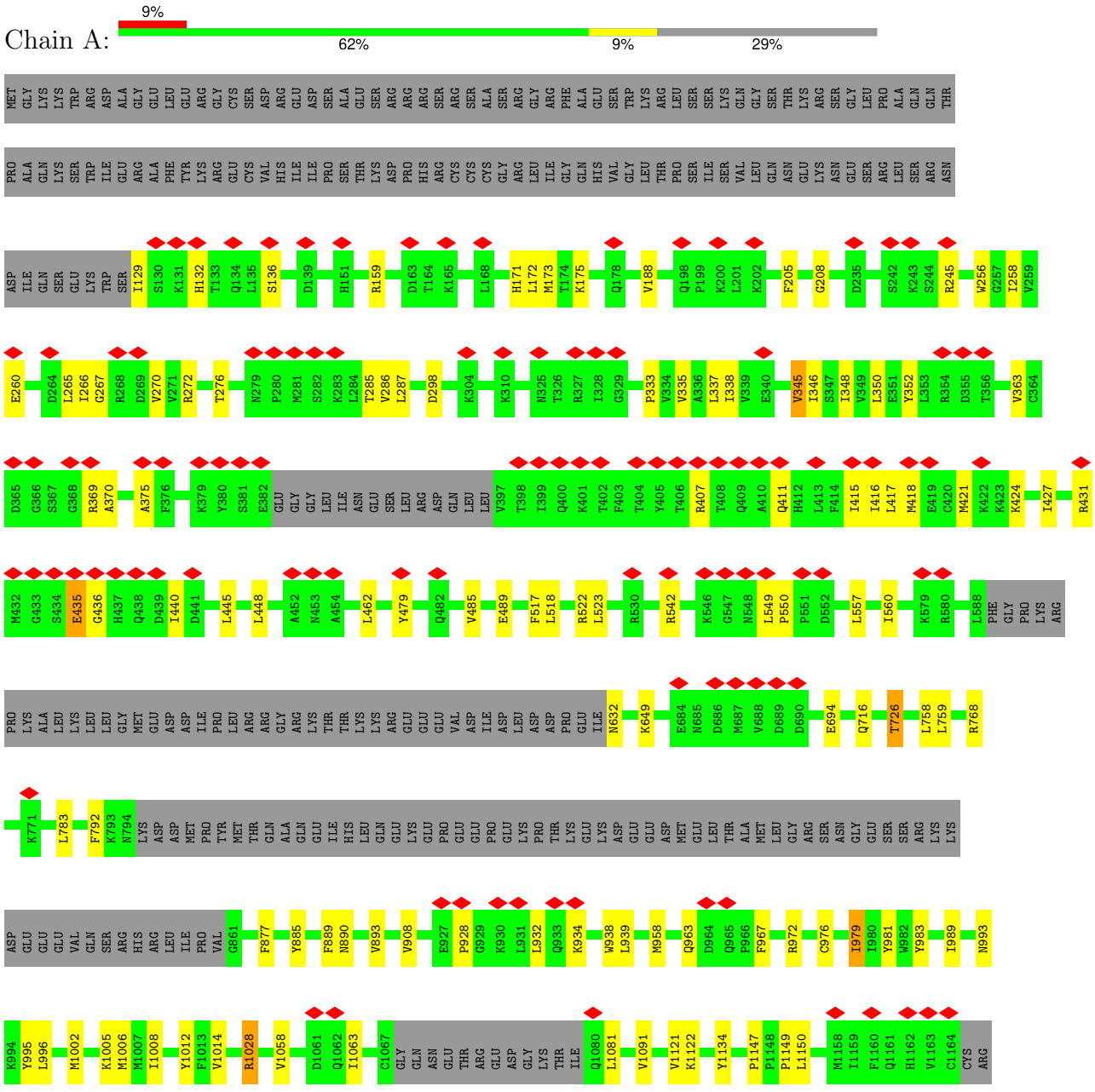
Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total Na 1 1	0

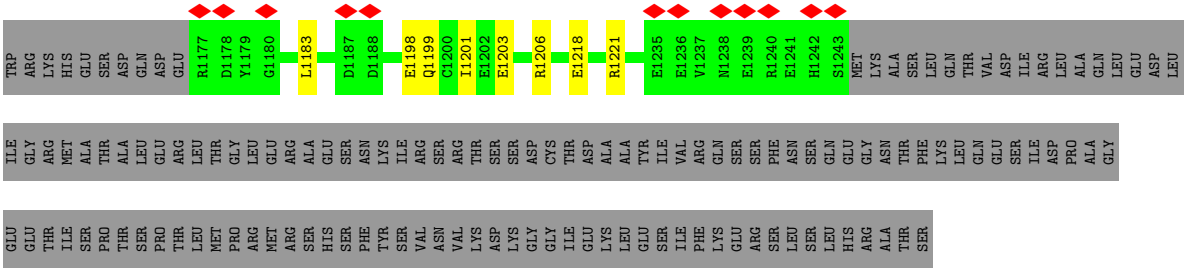
3 Residue-property plots (i)

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: Transient receptor potential cation channel, subfamily M, member 3

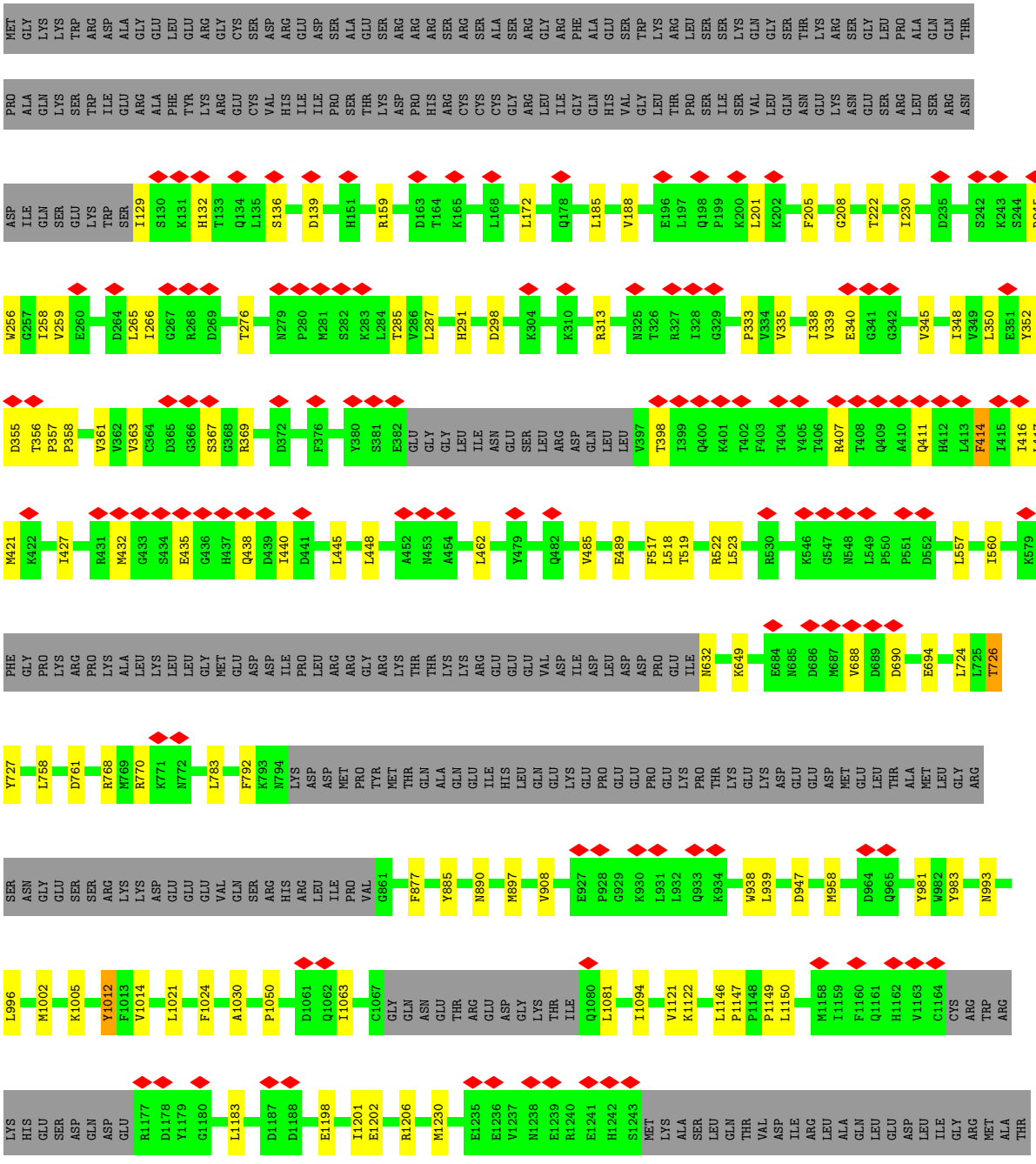
Chain A:

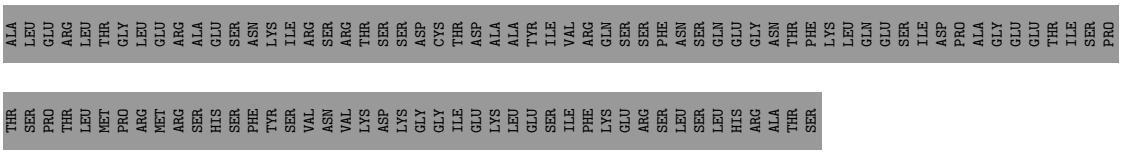




• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

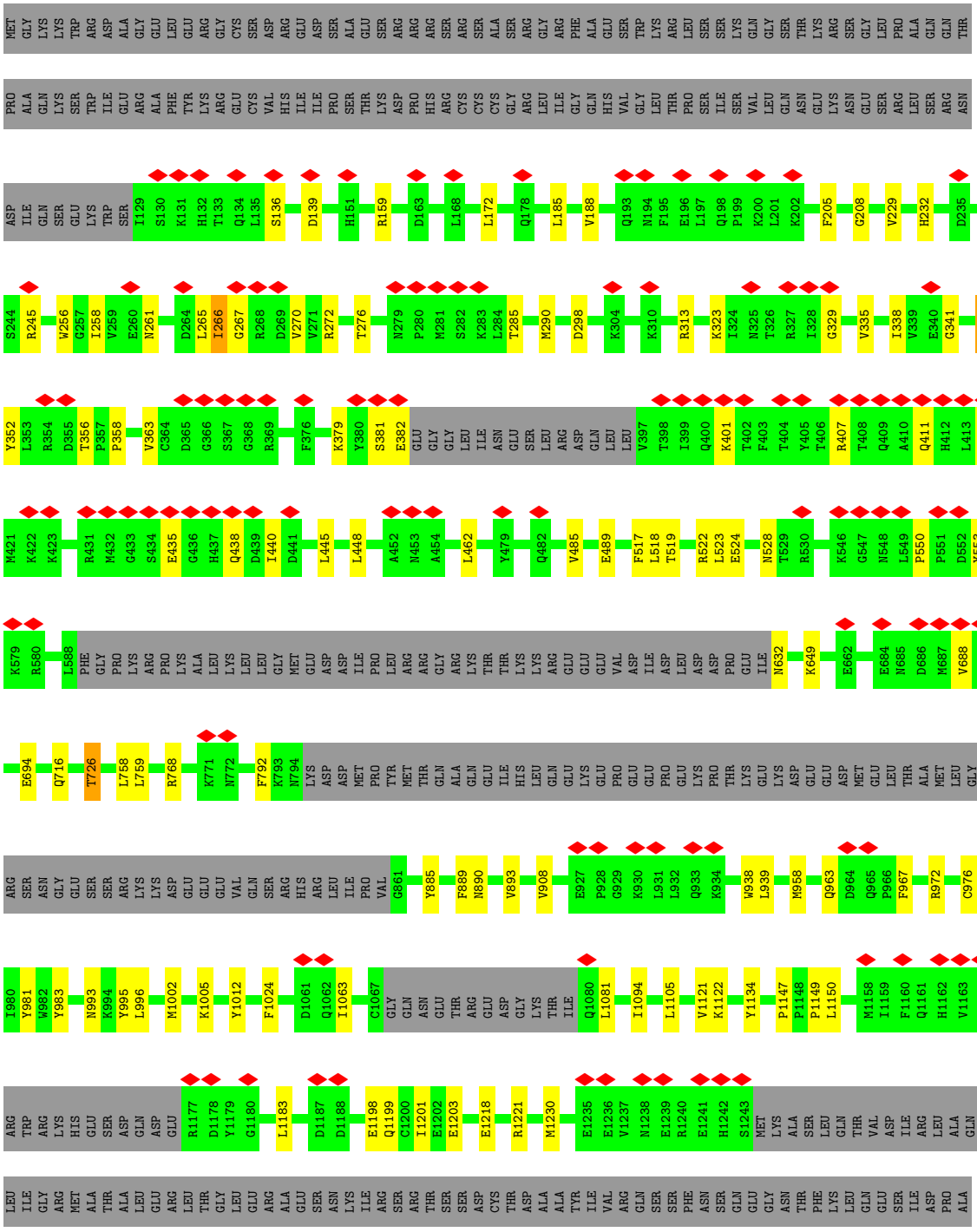
Chain B:





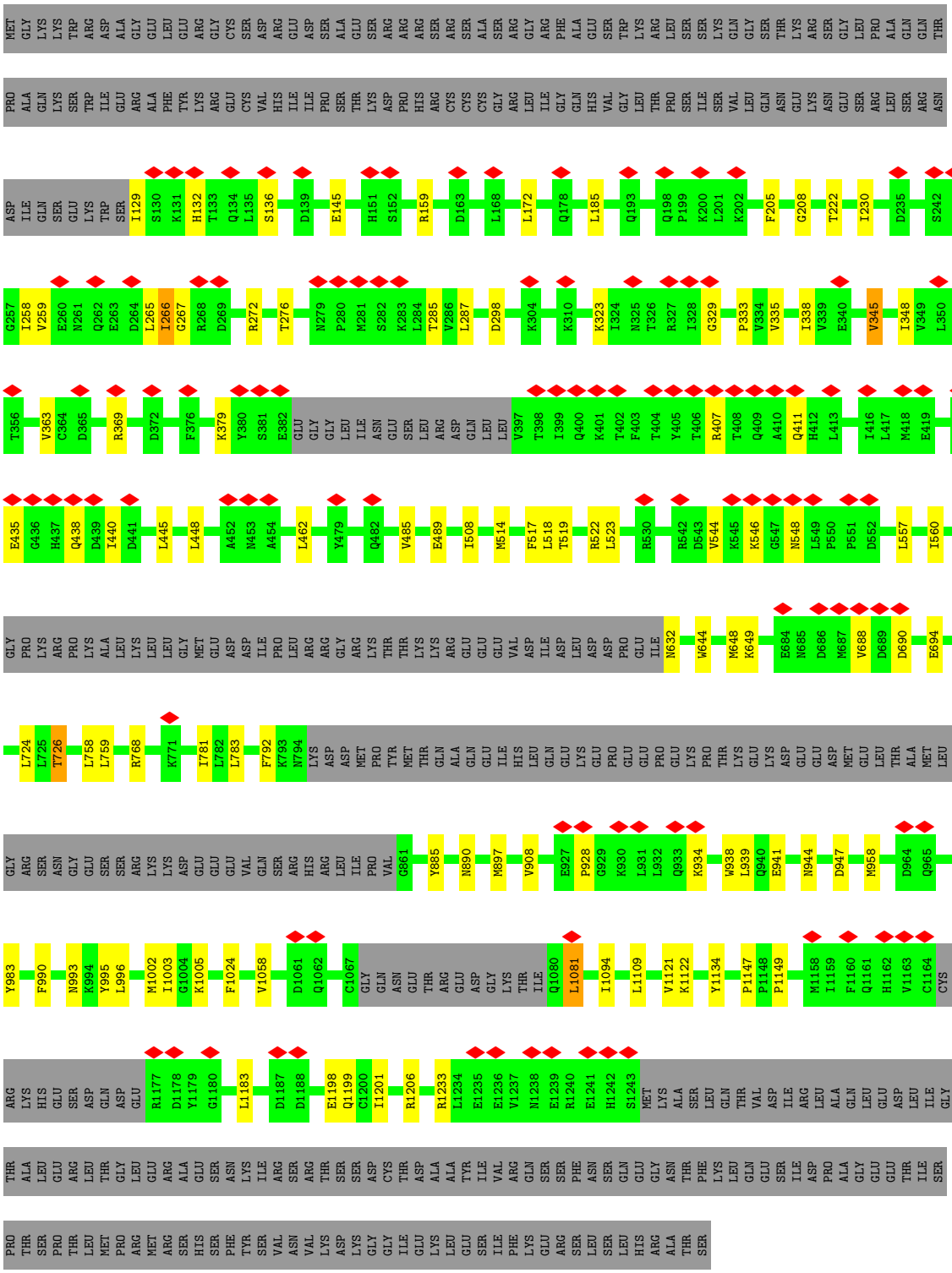
• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

Chain C:



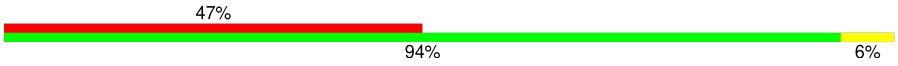
• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

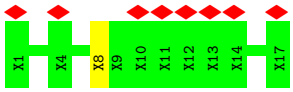
Chain D:



• Molecule 2: Unidentified segment at the N-terminus of TRPM3

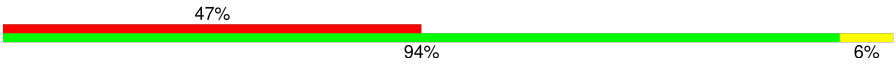
Chain E:

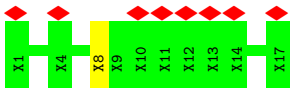




• Molecule 2: Unidentified segment at the N-terminus of TRPM3

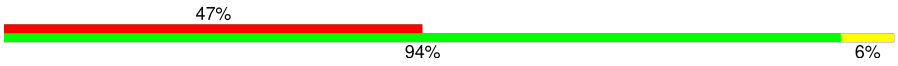
Chain F:

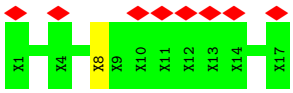




• Molecule 2: Unidentified segment at the N-terminus of TRPM3

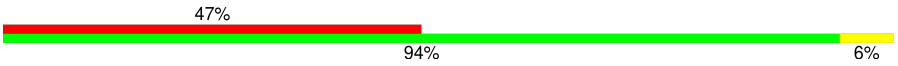
Chain G:

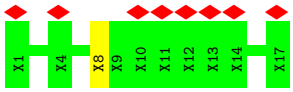




• Molecule 2: Unidentified segment at the N-terminus of TRPM3

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	93174	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 ($e^-/Å^2$)	51.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.333	Depositor
Minimum map value	-2.392	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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, 3PH, PIO, 9Z9

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	0.12	0/8023	0.29	0/10848
1	B	0.12	0/8023	0.28	0/10848
1	C	0.12	0/8023	0.28	0/10848
1	D	0.12	0/8023	0.28	0/10848
All	All	0.12	0/32092	0.28	0/43392

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	7841	0	7955	60	0
1	B	7841	0	7955	58	0
1	C	7841	0	7955	64	0
1	D	7841	0	7955	59	0
2	E	85	0	23	1	0
2	F	85	0	23	1	0
2	G	85	0	23	1	0
2	H	85	0	23	1	0
3	A	45	0	66	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	66	1	0
3	C	45	0	66	1	0
3	D	45	0	66	0	0
4	A	39	0	0	14	0
4	B	39	0	0	15	0
4	C	39	0	0	15	0
4	D	39	0	0	14	0
5	A	47	0	44	1	0
5	B	47	0	44	0	0
5	C	47	0	44	0	0
5	D	47	0	44	1	0
6	B	1	0	0	0	0
All	All	32229	0	32352	291	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 5.

All (291) 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)
4:C:1402:9Z9:C73	4:C:1402:9Z9:C74	1.81	1.58
4:A:1402:9Z9:C06	4:A:1402:9Z9:C07	1.83	1.57
4:D:1402:9Z9:C74	4:D:1402:9Z9:C73	1.81	1.56
4:C:1402:9Z9:C06	4:C:1402:9Z9:C07	1.84	1.55
4:B:1402:9Z9:C73	4:B:1402:9Z9:C74	1.81	1.54
4:B:1402:9Z9:C07	4:B:1402:9Z9:C06	1.84	1.53
4:A:1402:9Z9:C73	4:A:1402:9Z9:C74	1.81	1.52
4:D:1402:9Z9:C06	4:D:1402:9Z9:C07	1.84	1.51
4:C:1402:9Z9:C74	4:C:1402:9Z9:C75	1.90	1.50
4:A:1402:9Z9:C74	4:A:1402:9Z9:C75	1.90	1.47
4:D:1402:9Z9:C74	4:D:1402:9Z9:C75	1.90	1.47
4:B:1402:9Z9:C74	4:B:1402:9Z9:C75	1.90	1.47
4:A:1402:9Z9:C75	4:A:1402:9Z9:C03	2.32	1.06
4:B:1402:9Z9:C75	4:B:1402:9Z9:C03	2.34	1.05
4:D:1402:9Z9:C75	4:D:1402:9Z9:C03	2.34	1.05
4:D:1402:9Z9:C06	4:D:1402:9Z9:C02	1.78	1.03
4:C:1402:9Z9:C75	4:C:1402:9Z9:C03	2.34	1.03
4:A:1402:9Z9:C06	4:A:1402:9Z9:C02	1.78	1.00
4:C:1402:9Z9:C06	4:C:1402:9Z9:C02	1.78	0.95
4:B:1402:9Z9:C06	4:B:1402:9Z9:C02	1.78	0.94
4:B:1402:9Z9:C74	4:B:1402:9Z9:O80	2.15	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1402:9Z9:C74	4:D:1402:9Z9:O80	2.14	0.93
4:C:1402:9Z9:C74	4:C:1402:9Z9:O80	2.15	0.93
4:A:1402:9Z9:C74	4:A:1402:9Z9:O80	2.15	0.93
4:D:1402:9Z9:C07	4:D:1402:9Z9:C05	2.51	0.82
4:B:1402:9Z9:C07	4:B:1402:9Z9:C05	2.51	0.81
4:A:1402:9Z9:C06	4:A:1402:9Z9:C15	2.59	0.81
4:A:1402:9Z9:C07	4:A:1402:9Z9:C05	2.49	0.79
4:C:1402:9Z9:C06	4:C:1402:9Z9:C15	2.61	0.79
4:D:1402:9Z9:C06	4:D:1402:9Z9:C15	2.61	0.78
4:C:1402:9Z9:C07	4:C:1402:9Z9:C05	2.51	0.78
4:B:1402:9Z9:C06	4:B:1402:9Z9:C15	2.61	0.77
4:A:1402:9Z9:C06	4:A:1402:9Z9:C10	2.63	0.77
4:B:1402:9Z9:C06	4:B:1402:9Z9:C10	2.64	0.76
4:D:1402:9Z9:C06	4:D:1402:9Z9:C10	2.64	0.75
4:C:1402:9Z9:C06	4:C:1402:9Z9:C10	2.64	0.75
4:D:1402:9Z9:C06	4:D:1402:9Z9:C08	2.69	0.71
4:C:1402:9Z9:C06	4:C:1402:9Z9:C08	2.69	0.70
4:A:1402:9Z9:C06	4:A:1402:9Z9:C08	2.68	0.70
4:B:1402:9Z9:C06	4:B:1402:9Z9:C08	2.69	0.70
1:B:340:GLU:HG3	1:B:369:ARG:HB2	1.72	0.69
4:B:1402:9Z9:C75	4:B:1402:9Z9:O80	2.41	0.69
4:C:1402:9Z9:C75	4:C:1402:9Z9:O80	2.41	0.68
4:D:1402:9Z9:C75	4:D:1402:9Z9:O80	2.41	0.68
4:A:1402:9Z9:C75	4:A:1402:9Z9:O80	2.42	0.67
4:B:1402:9Z9:C06	4:B:1402:9Z9:C01	2.72	0.67
1:C:981:TYR:HB2	3:C:1401:3PH:H3C2	1.76	0.67
4:C:1402:9Z9:C06	4:C:1402:9Z9:C01	2.72	0.67
4:D:1402:9Z9:C06	4:D:1402:9Z9:C01	2.72	0.66
4:A:1402:9Z9:C06	4:A:1402:9Z9:C01	2.73	0.64
1:D:716:GLN:NE2	1:D:1199:GLN:OE1	2.34	0.61
1:D:508:ILE:HD11	1:D:514:MET:HE2	1.83	0.61
1:A:716:GLN:NE2	1:A:1199:GLN:OE1	2.34	0.60
1:B:353:LEU:HD11	1:B:427:ILE:HD11	1.84	0.59
1:C:1005:LYS:HD2	1:C:1121:VAL:HG13	1.84	0.59
1:B:1005:LYS:HD2	1:B:1121:VAL:HG13	1.85	0.58
1:B:489:GLU:OE2	1:B:522:ARG:NH1	2.37	0.58
1:D:890:ASN:ND2	1:D:983:TYR:OH	2.35	0.57
1:B:350:LEU:HD22	1:B:416:ILE:HG13	1.86	0.57
1:A:1206:ARG:HE	1:D:245:ARG:HD3	1.70	0.56
1:C:489:GLU:OE2	1:C:522:ARG:NH1	2.38	0.56
1:B:890:ASN:ND2	1:B:983:TYR:OH	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLU:HB2	1:B:367:SER:HB3	1.86	0.56
1:C:335:VAL:HB	1:C:448:LEU:HD21	1.88	0.56
1:D:489:GLU:OE2	1:D:522:ARG:NH1	2.39	0.56
1:B:335:VAL:HB	1:B:448:LEU:HD21	1.88	0.56
1:A:1005:LYS:HD2	1:A:1121:VAL:HG13	1.87	0.55
1:B:445:LEU:HA	1:B:448:LEU:HD12	1.89	0.55
1:C:445:LEU:HA	1:C:448:LEU:HD12	1.89	0.55
1:B:688:VAL:HG23	1:B:690:ASP:H	1.72	0.55
1:A:335:VAL:HB	1:A:448:LEU:HD21	1.89	0.55
1:A:424:LYS:HA	1:A:427:ILE:HD13	1.89	0.55
1:D:267:GLY:HA3	1:D:272:ARG:HD3	1.89	0.55
1:A:1002:MET:HG2	1:A:1121:VAL:HG12	1.88	0.54
1:C:1002:MET:HE2	1:C:1122:LYS:HA	1.89	0.54
1:C:726:THR:HG23	1:C:758:LEU:HD21	1.89	0.54
1:D:335:VAL:HB	1:D:448:LEU:HD21	1.88	0.54
1:D:445:LEU:HA	1:D:448:LEU:HD12	1.90	0.54
1:B:1202:GLU:OE2	1:B:1206:ARG:NH2	2.41	0.54
1:D:1005:LYS:HD2	1:D:1121:VAL:HG13	1.88	0.54
1:B:726:THR:HG23	1:B:758:LEU:HD21	1.89	0.54
1:B:1002:MET:HE2	1:B:1122:LYS:HA	1.88	0.53
1:B:398:THR:HA	1:B:414:PHE:HE2	1.72	0.53
1:A:726:THR:HG23	1:A:758:LEU:HD21	1.88	0.53
4:A:1402:9Z9:C07	4:A:1402:9Z9:C02	2.86	0.53
1:A:350:LEU:HD22	1:A:416:ILE:HG23	1.90	0.52
1:A:445:LEU:HA	1:A:448:LEU:HD12	1.91	0.52
1:C:550:PRO:HG2	1:C:553:TYR:HB2	1.90	0.52
1:D:726:THR:HG23	1:D:758:LEU:HD21	1.90	0.52
1:C:208:GLY:HA3	1:C:440:ILE:HB	1.90	0.52
1:B:245:ARG:NE	1:C:1203:GLU:OE2	2.40	0.52
1:C:347:SER:HA	1:C:416:ILE:HD11	1.91	0.51
1:C:768:ARG:NH2	1:C:792:PHE:O	2.43	0.51
1:D:1002:MET:HG2	1:D:1121:VAL:HG12	1.92	0.51
1:D:208:GLY:HA3	1:D:440:ILE:HB	1.92	0.51
1:B:208:GLY:HA3	1:B:440:ILE:HB	1.92	0.51
1:A:208:GLY:HA3	1:A:440:ILE:HB	1.91	0.51
1:A:981:TYR:HB2	3:A:1401:3PH:H3C1	1.93	0.51
1:A:489:GLU:OE2	1:A:522:ARG:NH1	2.44	0.50
1:B:338:ILE:HB	1:B:363:VAL:HG12	1.93	0.50
1:C:205:PHE:HA	1:C:440:ILE:HG13	1.92	0.50
1:D:768:ARG:NH2	1:D:792:PHE:O	2.43	0.50
1:A:768:ARG:NH2	1:A:792:PHE:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LEU:HA	1:B:560:ILE:HD12	1.93	0.50
1:C:557:LEU:HA	1:C:560:ILE:HD12	1.93	0.50
1:C:267:GLY:HA3	1:C:272:ARG:HD3	1.93	0.50
1:D:159:ARG:NH2	1:D:298:ASP:OD2	2.43	0.50
1:D:205:PHE:HA	1:D:440:ILE:HG13	1.94	0.50
1:A:890:ASN:ND2	1:A:983:TYR:OH	2.43	0.50
1:A:171:HIS:HD2	1:A:175:LYS:HD3	1.76	0.50
1:C:1002:MET:HG2	1:C:1121:VAL:HG12	1.94	0.50
1:D:1002:MET:HE2	1:D:1122:LYS:HA	1.93	0.50
1:A:205:PHE:HA	1:A:440:ILE:HG13	1.94	0.49
1:C:407:ARG:HB2	1:C:411:GLN:HB3	1.94	0.49
1:A:159:ARG:NH2	1:A:298:ASP:OD2	2.45	0.49
1:B:1002:MET:HG2	1:B:1121:VAL:HG12	1.95	0.49
1:C:245:ARG:HD3	1:D:1206:ARG:HD2	1.93	0.49
4:C:1402:9Z9:C07	4:C:1402:9Z9:C02	2.89	0.49
1:A:557:LEU:HA	1:A:560:ILE:HD12	1.94	0.49
1:C:338:ILE:HB	1:C:363:VAL:HG12	1.94	0.49
1:B:768:ARG:NH2	1:B:792:PHE:O	2.46	0.49
1:D:557:LEU:HA	1:D:560:ILE:HD12	1.95	0.49
1:B:205:PHE:HA	1:B:440:ILE:HG13	1.94	0.48
1:A:1006:MET:HG3	1:D:1109:LEU:HD13	1.95	0.48
4:B:1402:9Z9:C06	4:B:1402:9Z9:C09	2.92	0.48
1:C:890:ASN:ND2	1:C:983:TYR:OH	2.43	0.48
1:D:323:LYS:NZ	1:D:329:GLY:O	2.41	0.48
1:A:267:GLY:HA3	1:A:272:ARG:HD3	1.94	0.48
4:B:1402:9Z9:C07	4:B:1402:9Z9:C02	2.89	0.48
1:C:238:LYS:HG2	1:C:290:MET:HG3	1.95	0.48
4:A:1402:9Z9:C06	4:A:1402:9Z9:C09	2.92	0.48
1:D:519:THR:HG22	1:D:522:ARG:HB2	1.96	0.48
1:B:222:THR:HB	1:B:230:ILE:HD12	1.96	0.48
1:B:345:VAL:HA	1:B:348:ILE:HG12	1.96	0.48
1:D:644:TRP:NE1	1:D:648:MET:SD	2.87	0.47
1:B:761:ASP:OD1	1:B:770:ARG:NH2	2.48	0.47
1:C:341:GLY:HA3	1:C:345:VAL:HG21	1.97	0.47
1:C:716:GLN:NE2	1:C:1199:GLN:OE1	2.47	0.47
1:A:1002:MET:HE2	1:A:1122:LYS:HA	1.96	0.47
1:C:159:ARG:NH2	1:C:298:ASP:OD2	2.43	0.47
1:B:159:ARG:NH2	1:B:298:ASP:OD2	2.44	0.47
1:A:136:SER:O	2:E:8:UNK:N	2.48	0.47
1:A:976:CYS:O	1:A:979:ILE:HG22	2.14	0.47
1:B:356:THR:HB	1:B:357:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1402:9Z9:C06	4:C:1402:9Z9:C09	2.92	0.47
1:D:435:GLU:O	1:D:438:GLN:NE2	2.48	0.47
4:D:1402:9Z9:C06	4:D:1402:9Z9:C09	2.92	0.47
1:A:928:PRO:HD2	1:A:934:LYS:HG2	1.96	0.47
1:B:313:ARG:NH2	1:B:355:ASP:OD2	2.45	0.47
1:C:519:THR:HG22	1:C:522:ARG:HB2	1.96	0.47
1:D:256:TRP:HB3	1:D:298:ASP:HB3	1.97	0.47
1:B:947:ASP:OD1	1:B:981:TYR:OH	2.32	0.47
1:A:435:GLU:OE1	1:A:436:GLY:N	2.46	0.46
1:B:519:THR:HG22	1:B:522:ARG:HB2	1.96	0.46
1:C:136:SER:O	2:G:8:UNK:N	2.48	0.46
1:C:245:ARG:HD3	1:D:1206:ARG:HH11	1.80	0.46
4:D:1402:9Z9:C07	4:D:1402:9Z9:C02	2.89	0.46
1:A:1203:GLU:OE2	1:D:245:ARG:NH1	2.49	0.46
1:A:1081:LEU:HD23	1:A:1081:LEU:H	1.81	0.46
1:C:976:CYS:O	1:C:979:ILE:HG22	2.15	0.46
1:D:947:ASP:OD1	1:D:981:TYR:OH	2.25	0.46
1:B:136:SER:O	2:F:8:UNK:N	2.48	0.46
1:A:129:ILE:HD12	1:A:132:HIS:HB2	1.97	0.46
1:A:1147:PRO:HB2	1:A:1149:PRO:HD2	1.98	0.46
1:A:1198:GLU:HA	1:A:1201:ILE:HG22	1.97	0.46
1:C:256:TRP:HB3	1:C:298:ASP:HB3	1.96	0.46
1:C:401:LYS:HD2	1:C:414:PHE:HD1	1.81	0.46
1:A:375:ALA:O	1:A:431:ARG:NH2	2.48	0.46
1:A:489:GLU:HG2	1:A:517:PHE:HD1	1.81	0.46
1:C:323:LYS:NZ	1:C:329:GLY:O	2.39	0.46
1:B:649:LYS:NZ	1:B:694:GLU:OE1	2.42	0.45
1:D:136:SER:O	2:H:8:UNK:N	2.48	0.45
1:D:1198:GLU:HA	1:D:1201:ILE:HG22	1.97	0.45
1:A:407:ARG:HB2	1:A:411:GLN:HB3	1.97	0.45
1:D:345:VAL:HA	1:D:348:ILE:HG12	1.99	0.45
1:A:649:LYS:NZ	1:A:694:GLU:OE1	2.43	0.45
1:A:989:ILE:HG22	5:A:1403:PIO:H5B	1.98	0.45
1:C:313:ARG:HA	1:C:313:ARG:HD2	1.78	0.45
1:C:1024:PHE:HD1	1:C:1094:ILE:HG22	1.81	0.45
1:B:414:PHE:HD1	1:B:414:PHE:HA	1.67	0.45
1:C:1081:LEU:HD23	1:C:1081:LEU:H	1.82	0.45
1:D:941:GLU:OE1	1:D:944:ASN:ND2	2.50	0.45
1:A:549:LEU:HD12	1:A:550:PRO:HD2	1.98	0.45
1:B:407:ARG:HB2	1:B:411:GLN:HB3	1.98	0.45
1:B:1030:ALA:O	1:C:972:ARG:NH1	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:VAL:HA	1:C:232:HIS:HD2	1.82	0.45
1:C:1198:GLU:HA	1:C:1201:ILE:HG22	2.00	0.44
1:D:129:ILE:HD12	1:D:132:HIS:HB2	1.99	0.44
1:B:435:GLU:O	1:B:438:GLN:NE2	2.50	0.44
1:B:1230:MET:HE3	1:C:1230:MET:HE1	1.99	0.44
1:D:548:ASN:OD1	1:D:548:ASN:N	2.49	0.44
1:A:270:VAL:HG13	1:A:272:ARG:HD3	1.99	0.44
1:B:1081:LEU:HD23	1:B:1081:LEU:H	1.82	0.44
1:D:338:ILE:HB	1:D:363:VAL:HG12	1.99	0.44
1:A:333:PRO:HB2	1:A:448:LEU:HD22	1.99	0.44
1:C:270:VAL:HG13	1:C:272:ARG:HD3	2.00	0.44
1:C:435:GLU:O	1:C:438:GLN:NE2	2.50	0.44
1:C:938:TRP:HE3	1:C:939:LEU:HD12	1.83	0.44
1:B:1147:PRO:HB2	1:B:1149:PRO:HD2	1.99	0.44
1:C:553:TYR:OH	1:C:559:ASP:OD2	2.33	0.44
1:C:1147:PRO:HB2	1:C:1149:PRO:HD2	1.99	0.44
1:B:1024:PHE:HD1	1:B:1094:ILE:HG22	1.83	0.43
1:C:489:GLU:HG2	1:C:517:PHE:HD1	1.83	0.43
1:A:518:LEU:HD11	1:A:523:LEU:HD13	1.99	0.43
1:D:222:THR:HB	1:D:230:ILE:HD12	2.00	0.43
1:D:369:ARG:HD3	1:D:369:ARG:HA	1.90	0.43
1:D:407:ARG:HB2	1:D:411:GLN:HB3	1.99	0.43
1:D:938:TRP:HE3	1:D:939:LEU:HD12	1.83	0.43
1:B:1198:GLU:HA	1:B:1201:ILE:HG22	2.00	0.43
1:D:1147:PRO:HB2	1:D:1149:PRO:HD2	2.00	0.43
1:C:356:THR:O	1:C:358:PRO:HD3	2.19	0.43
1:D:649:LYS:NZ	1:D:694:GLU:OE1	2.43	0.43
1:D:885:TYR:HE1	1:D:908:VAL:HG13	1.84	0.43
1:A:258:ILE:HG22	1:A:285:THR:HG22	2.01	0.43
1:B:356:THR:O	1:B:358:PRO:HD3	2.17	0.43
1:B:489:GLU:HG2	1:B:517:PHE:HD1	1.84	0.43
1:D:518:LEU:HD11	1:D:523:LEU:HD13	2.00	0.43
1:A:963:GLN:HB2	1:A:967:PHE:HB2	2.01	0.43
1:B:258:ILE:HG22	1:B:285:THR:HG22	2.00	0.43
1:B:1146:LEU:HA	1:B:1147:PRO:HD3	1.91	0.43
1:C:258:ILE:HG22	1:C:285:THR:HG22	1.99	0.43
1:C:649:LYS:NZ	1:C:694:GLU:OE1	2.42	0.43
1:C:963:GLN:HB2	1:C:967:PHE:HB2	2.01	0.43
1:A:338:ILE:HB	1:A:363:VAL:HG12	2.00	0.43
1:D:489:GLU:HG2	1:D:517:PHE:HD1	1.83	0.43
1:A:256:TRP:HB3	1:A:298:ASP:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:993:ASN:HB3	1:C:996:LEU:HB2	2.01	0.43
1:C:518:LEU:HD11	1:C:523:LEU:HD13	2.01	0.42
1:D:990:PHE:HE1	5:D:1403:PIO:H6B	1.84	0.42
1:A:993:ASN:ND2	1:A:995:TYR:H	2.18	0.42
1:B:518:LEU:HD11	1:B:523:LEU:HD13	2.00	0.42
1:D:258:ILE:HG22	1:D:285:THR:HG22	2.00	0.42
1:B:129:ILE:HD12	1:B:132:HIS:HB2	2.02	0.42
1:B:333:PRO:HB2	1:B:448:LEU:HD22	2.02	0.42
1:D:546:LYS:HE3	1:D:546:LYS:HB2	1.87	0.42
1:D:993:ASN:HB3	1:D:996:LEU:HB2	2.00	0.42
1:C:893:VAL:O	1:C:972:ARG:NH2	2.52	0.42
1:A:415:ILE:O	1:A:418:MET:HG3	2.20	0.42
1:A:938:TRP:HE3	1:A:939:LEU:HD12	1.84	0.42
1:A:1028:ARG:HD2	1:A:1063:ILE:HD13	2.01	0.42
3:B:1401:3PH:H3C1	3:B:1401:3PH:H3F1	1.80	0.42
1:D:688:VAL:HG23	1:D:690:ASP:H	1.85	0.42
1:A:889:PHE:CG	1:A:979:ILE:HD13	2.55	0.42
1:B:256:TRP:HB3	1:B:298:ASP:HB3	2.01	0.42
1:B:885:TYR:HE1	1:B:908:VAL:HG13	1.84	0.42
1:C:885:TYR:HE1	1:C:908:VAL:HG13	1.84	0.42
1:C:889:PHE:CG	1:C:979:ILE:HD13	2.55	0.42
1:A:205:PHE:HE1	1:A:337:LEU:HD21	1.84	0.42
4:B:1402:9Z9:C05	4:B:1402:9Z9:C01	2.87	0.42
1:C:379:LYS:HE3	1:C:379:LYS:HB3	1.87	0.42
1:D:333:PRO:HB2	1:D:448:LEU:HD22	2.01	0.42
1:A:893:VAL:O	1:A:972:ARG:NH2	2.53	0.42
1:B:938:TRP:HE3	1:B:939:LEU:HD12	1.85	0.42
1:D:759:LEU:HD21	1:D:1134:TYR:HD1	1.85	0.42
1:A:885:TYR:HE1	1:A:908:VAL:HG13	1.84	0.41
1:C:759:LEU:HD21	1:C:1134:TYR:HD1	1.85	0.41
1:D:1024:PHE:HD1	1:D:1094:ILE:HG22	1.85	0.41
1:A:993:ASN:HB3	1:A:996:LEU:HB2	2.01	0.41
1:C:688:VAL:HG23	1:C:690:ASP:H	1.85	0.41
4:C:1402:9Z9:C05	4:C:1402:9Z9:C01	2.87	0.41
1:C:266:ILE:H	1:C:266:ILE:HG12	1.71	0.41
1:A:173:MET:HE3	1:A:173:MET:HB2	1.94	0.41
1:C:1218:GLU:OE2	1:C:1221:ARG:NH2	2.39	0.41
1:C:139:ASP:OD1	1:C:139:ASP:N	2.54	0.41
1:D:259:VAL:HG12	1:D:287:LEU:HD13	2.03	0.41
1:D:928:PRO:HD2	1:D:934:LYS:HG2	2.03	0.41
1:A:369:ARG:HD3	1:A:369:ARG:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ASP:OD1	1:B:139:ASP:N	2.53	0.41
1:B:724:LEU:HD12	1:B:727:TYR:HE1	1.85	0.41
1:B:1021:LEU:HG	1:B:1050:PRO:HB2	2.02	0.41
1:D:379:LYS:HB3	1:D:379:LYS:HE3	1.89	0.41
1:B:259:VAL:HG12	1:B:287:LEU:HD13	2.03	0.41
1:B:345:VAL:HG23	1:B:348:ILE:HD11	2.02	0.41
1:A:260:GLU:HG2	1:A:286:VAL:HG23	2.03	0.40
1:B:201:LEU:HA	1:B:432:MET:HE1	2.02	0.40
1:B:993:ASN:HB3	1:B:996:LEU:HB2	2.02	0.40
1:C:993:ASN:ND2	1:C:995:TYR:H	2.18	0.40
1:C:1105:LEU:HD21	1:D:1003:ILE:HG23	2.02	0.40
1:D:1233:ARG:HA	1:D:1233:ARG:HD2	1.93	0.40
1:A:1218:GLU:OE2	1:A:1221:ARG:NH2	2.39	0.40
1:B:1012:TYR:HD1	1:B:1012:TYR:HA	1.79	0.40
1:A:346:ILE:HD11	1:A:370:ALA:HB1	2.03	0.40
1:A:759:LEU:HD21	1:A:1134:TYR:HD1	1.85	0.40
1:A:979:ILE:HD12	1:A:979:ILE:HA	1.82	0.40
1:C:313:ARG:HD3	1:C:352:TYR:HE1	1.85	0.40
1:C:381:SER:OG	1:C:382:GLU:N	2.55	0.40
1:D:1081:LEU:HD23	1:D:1081:LEU:H	1.86	0.40
1:C:524:GLU:O	1:C:528:ASN:ND2	2.42	0.40
1:D:266:ILE:H	1:D:266:ILE:HG12	1.72	0.40
1:A:345:VAL:HA	1:A:348:ILE:HG12	2.03	0.40
1:D:993:ASN:ND2	1:D:995:TYR:H	2.20	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	956/1371 (70%)	918 (96%)	38 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	956/1371 (70%)	925 (97%)	31 (3%)	0	100	100
1	C	956/1371 (70%)	926 (97%)	30 (3%)	0	100	100
1	D	956/1371 (70%)	923 (96%)	33 (4%)	0	100	100
All	All	3824/5484 (70%)	3692 (96%)	132 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	859/1219 (70%)	828 (96%)	31 (4%)	30	60
1	B	858/1219 (70%)	832 (97%)	26 (3%)	36	64
1	C	859/1219 (70%)	841 (98%)	18 (2%)	48	72
1	D	859/1219 (70%)	838 (98%)	21 (2%)	44	70
All	All	3435/4876 (70%)	3339 (97%)	96 (3%)	40	66

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	LEU
1	A	188	VAL
1	A	245	ARG
1	A	265	LEU
1	A	266	ILE
1	A	276	THR
1	A	287	LEU
1	A	345	VAL
1	A	352	TYR
1	A	417	LEU
1	A	421	MET
1	A	435	GLU
1	A	462	LEU

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Mol	Chain	Res	Type
1	A	479	TYR
1	A	485	VAL
1	A	542	ARG
1	A	632	ASN
1	A	726	THR
1	A	783	LEU
1	A	877	PHE
1	A	932	LEU
1	A	958	MET
1	A	979	ILE
1	A	1008	ILE
1	A	1012	TYR
1	A	1014	VAL
1	A	1028	ARG
1	A	1058	VAL
1	A	1091	VAL
1	A	1150	LEU
1	A	1183	LEU
1	B	172	LEU
1	B	185	LEU
1	B	188	VAL
1	B	265	LEU
1	B	266	ILE
1	B	276	THR
1	B	291	HIS
1	B	339	VAL
1	B	352	TYR
1	B	361	VAL
1	B	414	PHE
1	B	417	LEU
1	B	421	MET
1	B	462	LEU
1	B	485	VAL
1	B	632	ASN
1	B	726	THR
1	B	783	LEU
1	B	877	PHE
1	B	897	MET
1	B	958	MET
1	B	1012	TYR
1	B	1014	VAL
1	B	1063	ILE

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Mol	Chain	Res	Type
1	B	1150	LEU
1	B	1183	LEU
1	C	172	LEU
1	C	185	LEU
1	C	188	VAL
1	C	261	ASN
1	C	265	LEU
1	C	266	ILE
1	C	276	THR
1	C	345	VAL
1	C	351	GLU
1	C	462	LEU
1	C	485	VAL
1	C	632	ASN
1	C	726	THR
1	C	958	MET
1	C	1012	TYR
1	C	1063	ILE
1	C	1150	LEU
1	C	1183	LEU
1	D	145	GLU
1	D	172	LEU
1	D	185	LEU
1	D	265	LEU
1	D	266	ILE
1	D	276	THR
1	D	345	VAL
1	D	352	TYR
1	D	462	LEU
1	D	485	VAL
1	D	544	VAL
1	D	632	ASN
1	D	724	LEU
1	D	726	THR
1	D	781	ILE
1	D	783	LEU
1	D	897	MET
1	D	958	MET
1	D	1058	VAL
1	D	1081	LEU
1	D	1183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	HIS
1	A	314	GLN
1	A	318	HIS
1	A	411	GLN
1	A	632	ASN
1	A	633	HIS
1	A	697	HIS
1	A	719	GLN
1	A	739	GLN
1	A	890	ASN
1	A	940	GLN
1	A	965	GLN
1	A	978	ASN
1	A	993	ASN
1	A	1115	ASN
1	A	1126	ASN
1	A	1213	ASN
1	B	153	ASN
1	B	240	HIS
1	B	279	ASN
1	B	314	GLN
1	B	411	GLN
1	B	632	ASN
1	B	697	HIS
1	B	716	GLN
1	B	719	GLN
1	B	739	GLN
1	B	890	ASN
1	B	940	GLN
1	B	965	GLN
1	B	978	ASN
1	B	1115	ASN
1	B	1127	GLN
1	B	1213	ASN
1	B	1229	ASN
1	C	232	HIS
1	C	279	ASN
1	C	314	GLN
1	C	318	HIS
1	C	411	GLN
1	C	632	ASN
1	C	697	HIS

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Mol	Chain	Res	Type
1	C	719	GLN
1	C	739	GLN
1	C	890	ASN
1	C	965	GLN
1	C	978	ASN
1	C	993	ASN
1	C	1115	ASN
1	C	1127	GLN
1	C	1213	ASN
1	C	1229	ASN
1	D	275	GLN
1	D	279	ASN
1	D	293	HIS
1	D	314	GLN
1	D	318	HIS
1	D	378	HIS
1	D	411	GLN
1	D	539	HIS
1	D	632	ASN
1	D	651	GLN
1	D	697	HIS
1	D	719	GLN
1	D	739	GLN
1	D	890	ASN
1	D	944	ASN
1	D	965	GLN
1	D	978	ASN
1	D	1115	ASN
1	D	1126	ASN
1	D	1213	ASN
1	D	1229	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PIO	C	1403	-	47,47,47	1.20	6 (12%)	62,65,65	1.04	3 (4%)
5	PIO	A	1403	-	47,47,47	1.19	6 (12%)	62,65,65	1.03	2 (3%)
3	3PH	D	1401	-	44,44,47	1.17	3 (6%)	47,49,52	1.17	2 (4%)
4	9Z9	C	1402	-	44,44,44	9.36	24 (54%)	64,68,68	4.96	23 (35%)
4	9Z9	A	1402	-	44,44,44	9.34	22 (50%)	64,68,68	5.03	24 (37%)
5	PIO	B	1403	-	47,47,47	1.22	7 (14%)	62,65,65	1.07	2 (3%)
3	3PH	B	1401	-	44,44,47	1.16	3 (6%)	47,49,52	1.18	3 (6%)
5	PIO	D	1403	-	47,47,47	1.21	6 (12%)	62,65,65	1.05	4 (6%)
4	9Z9	B	1402	-	44,44,44	9.35	24 (54%)	64,68,68	4.97	22 (34%)
4	9Z9	D	1402	-	44,44,44	9.35	24 (54%)	64,68,68	4.97	23 (35%)
3	3PH	A	1401	-	44,44,47	1.17	3 (6%)	47,49,52	1.17	2 (4%)
3	3PH	C	1401	-	44,44,47	1.16	3 (6%)	47,49,52	1.18	3 (6%)

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	PIO	C	1403	-	-	17/44/68/68	0/1/1/1
5	PIO	A	1403	-	-	19/44/68/68	0/1/1/1
3	3PH	D	1401	-	-	26/46/46/49	-
4	9Z9	C	1402	-	-	1/12/100/100	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	9Z9	A	1402	-	-	3/12/100/100	0/6/6/6
5	PIO	B	1403	-	-	21/44/68/68	0/1/1/1
3	3PH	B	1401	-	-	28/46/46/49	-
5	PIO	D	1403	-	-	22/44/68/68	0/1/1/1
4	9Z9	B	1402	-	-	1/12/100/100	0/6/6/6
4	9Z9	D	1402	-	-	1/12/100/100	0/6/6/6
3	3PH	A	1401	-	-	19/46/46/49	-
3	3PH	C	1401	-	-	29/46/46/49	-

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1402	9Z9	C02-C03	-29.57	1.01	1.56
4	B	1402	9Z9	C02-C03	-29.55	1.01	1.56
4	C	1402	9Z9	C02-C03	-29.55	1.01	1.56
4	A	1402	9Z9	C02-C03	-29.49	1.01	1.56
4	A	1402	9Z9	C03-C74	-24.91	0.83	1.54
4	B	1402	9Z9	C03-C74	-24.85	0.84	1.54
4	D	1402	9Z9	C03-C74	-24.82	0.84	1.54
4	C	1402	9Z9	C03-C74	-24.81	0.84	1.54
4	A	1402	9Z9	C05-C06	-23.27	1.04	1.54
4	C	1402	9Z9	C05-C06	-23.18	1.04	1.54
4	B	1402	9Z9	C05-C06	-23.17	1.04	1.54
4	D	1402	9Z9	C05-C06	-23.16	1.04	1.54
4	A	1402	9Z9	O72-C73	-18.57	1.03	1.42
4	C	1402	9Z9	O72-C73	-18.52	1.03	1.42
4	B	1402	9Z9	O72-C73	-18.49	1.03	1.42
4	D	1402	9Z9	O72-C73	-18.47	1.03	1.42
4	A	1402	9Z9	C75-C74	17.97	1.90	1.53
4	C	1402	9Z9	C75-C74	17.87	1.90	1.53
4	B	1402	9Z9	C75-C74	17.84	1.90	1.53
4	D	1402	9Z9	C75-C74	17.81	1.90	1.53
4	D	1402	9Z9	C07-C06	16.37	1.84	1.53
4	B	1402	9Z9	C07-C06	16.32	1.84	1.53
4	C	1402	9Z9	C07-C06	16.32	1.84	1.53
4	A	1402	9Z9	C07-C06	15.99	1.83	1.53
4	A	1402	9Z9	C73-C74	14.23	1.81	1.53
4	C	1402	9Z9	C73-C74	14.16	1.81	1.53
4	B	1402	9Z9	C73-C74	14.15	1.81	1.53
4	D	1402	9Z9	C73-C74	14.15	1.81	1.53
4	B	1402	9Z9	C02-C06	12.90	1.78	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1402	9Z9	C02-C06	12.88	1.78	1.55
4	C	1402	9Z9	C02-C06	12.87	1.78	1.55
4	A	1402	9Z9	C02-C06	12.80	1.78	1.55
4	D	1402	9Z9	C10-C09	-12.19	1.29	1.53
4	C	1402	9Z9	C10-C09	-12.19	1.29	1.53
4	B	1402	9Z9	C10-C09	-12.14	1.29	1.53
4	A	1402	9Z9	C10-C09	-11.79	1.29	1.53
4	A	1402	9Z9	C15-C07	-10.15	1.36	1.53
4	C	1402	9Z9	C15-C07	-10.03	1.36	1.53
4	D	1402	9Z9	C15-C07	-10.02	1.36	1.53
4	B	1402	9Z9	C15-C07	-9.99	1.37	1.53
4	D	1402	9Z9	C10-C02	9.48	1.70	1.54
4	C	1402	9Z9	C10-C02	9.46	1.70	1.54
4	B	1402	9Z9	C10-C02	9.44	1.70	1.54
4	A	1402	9Z9	C10-C02	9.42	1.70	1.54
4	D	1402	9Z9	C03-C04	-5.73	1.43	1.54
4	B	1402	9Z9	C03-C04	-5.71	1.43	1.54
4	C	1402	9Z9	C03-C04	-5.71	1.43	1.54
4	A	1402	9Z9	C03-C04	-5.71	1.43	1.54
4	C	1402	9Z9	C14-C13	5.69	1.44	1.33
4	B	1402	9Z9	C14-C13	5.67	1.44	1.33
4	D	1402	9Z9	C14-C13	5.64	1.44	1.33
4	A	1402	9Z9	C14-C13	5.55	1.44	1.33
4	C	1402	9Z9	C09-C08	-4.72	1.46	1.53
4	B	1402	9Z9	C09-C08	-4.70	1.46	1.53
4	D	1402	9Z9	C09-C08	-4.69	1.46	1.53
4	A	1402	9Z9	C09-C08	-4.33	1.46	1.53
4	C	1402	9Z9	C15-C14	4.13	1.58	1.50
4	D	1402	9Z9	C15-C14	4.12	1.58	1.50
4	B	1402	9Z9	C15-C14	4.10	1.58	1.50
4	A	1402	9Z9	C19-C18	3.98	1.61	1.53
4	A	1402	9Z9	C15-C14	3.87	1.58	1.50
4	B	1402	9Z9	C19-C18	3.76	1.60	1.53
4	D	1402	9Z9	C19-C18	3.74	1.60	1.53
4	C	1402	9Z9	C19-C18	3.72	1.60	1.53
4	A	1402	9Z9	C11-C08	3.62	1.61	1.56
5	B	1403	PIO	P4-O4	3.56	1.65	1.59
5	D	1403	PIO	P4-O4	3.49	1.65	1.59
4	D	1402	9Z9	C01-C02	3.36	1.59	1.54
4	A	1402	9Z9	C01-C02	3.36	1.59	1.54
4	B	1402	9Z9	C01-C02	3.34	1.59	1.54
4	C	1402	9Z9	C01-C02	3.32	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1403	PIO	P5-O5	3.32	1.65	1.59
5	C	1403	PIO	P5-O5	3.31	1.65	1.59
4	C	1402	9Z9	C11-C08	3.27	1.61	1.56
5	D	1403	PIO	P5-O5	3.27	1.65	1.59
5	B	1403	PIO	P5-O5	3.27	1.65	1.59
4	B	1402	9Z9	C11-C08	3.24	1.61	1.56
5	C	1403	PIO	P4-O4	3.23	1.65	1.59
4	D	1402	9Z9	C11-C08	3.21	1.61	1.56
5	A	1403	PIO	P4-O4	3.19	1.65	1.59
3	D	1401	3PH	O31-C31	2.91	1.41	1.33
3	A	1401	3PH	O31-C31	2.90	1.41	1.33
3	C	1401	3PH	O31-C31	2.89	1.41	1.33
3	B	1401	3PH	O31-C31	2.89	1.41	1.33
4	C	1402	9Z9	C19-C11	-2.88	1.48	1.54
4	B	1402	9Z9	C19-C11	-2.87	1.49	1.54
3	A	1401	3PH	O21-C21	2.87	1.42	1.34
4	D	1402	9Z9	C19-C11	-2.86	1.49	1.54
3	D	1401	3PH	O21-C21	2.86	1.42	1.34
3	C	1401	3PH	O21-C21	2.82	1.42	1.34
4	B	1402	9Z9	C76-C73	2.81	1.56	1.51
4	A	1402	9Z9	C18-C17	2.80	1.58	1.51
4	D	1402	9Z9	C76-C73	2.79	1.56	1.51
3	B	1401	3PH	O21-C21	2.78	1.42	1.34
4	A	1402	9Z9	C19-C11	-2.74	1.49	1.54
4	C	1402	9Z9	C76-C73	2.74	1.56	1.51
4	B	1402	9Z9	C18-C17	2.73	1.58	1.51
4	D	1402	9Z9	C18-C17	2.72	1.58	1.51
4	C	1402	9Z9	C18-C17	2.72	1.58	1.51
4	C	1402	9Z9	C07-C08	-2.71	1.48	1.53
4	B	1402	9Z9	C07-C08	-2.70	1.48	1.53
4	D	1402	9Z9	C07-C08	-2.69	1.48	1.53
4	A	1402	9Z9	C07-C08	-2.65	1.48	1.53
3	B	1401	3PH	O21-C2	-2.63	1.40	1.46
5	D	1403	PIO	O2C-C1A	2.61	1.41	1.34
3	C	1401	3PH	O21-C2	-2.59	1.40	1.46
3	A	1401	3PH	O21-C2	-2.58	1.40	1.46
3	D	1401	3PH	O21-C2	-2.57	1.40	1.46
4	A	1402	9Z9	C76-C73	2.48	1.55	1.51
5	B	1403	PIO	O3C-C1B	2.44	1.40	1.33
5	C	1403	PIO	O3C-C1B	2.40	1.40	1.33
5	D	1403	PIO	O3C-C1B	2.38	1.40	1.33
5	C	1403	PIO	O2C-C1A	2.38	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1403	PIO	O2C-C2C	-2.35	1.41	1.46
5	B	1403	PIO	O2C-C1A	2.31	1.40	1.34
5	A	1403	PIO	O3C-C1B	2.30	1.40	1.33
5	A	1403	PIO	O2C-C1A	2.28	1.40	1.34
5	A	1403	PIO	O3C-C3C	-2.22	1.40	1.45
5	D	1403	PIO	O3C-C3C	-2.22	1.40	1.45
5	C	1403	PIO	O3C-C3C	-2.18	1.40	1.45
5	A	1403	PIO	O2C-C2C	-2.17	1.41	1.46
5	B	1403	PIO	O3C-C3C	-2.17	1.40	1.45
5	C	1403	PIO	O2C-C2C	-2.13	1.41	1.46
5	D	1403	PIO	O2C-C2C	-2.05	1.41	1.46
4	D	1402	9Z9	O20-C17	-2.04	1.38	1.43
4	B	1402	9Z9	C05-C04	2.04	1.57	1.52
4	C	1402	9Z9	O20-C17	-2.03	1.38	1.43
5	B	1403	PIO	P1-O1	2.03	1.65	1.59
4	C	1402	9Z9	C05-C04	2.03	1.57	1.52
4	B	1402	9Z9	O20-C17	-2.02	1.38	1.43
4	D	1402	9Z9	C05-C04	2.01	1.57	1.52

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1402	9Z9	C76-C73-C74	27.46	165.40	115.66
4	D	1402	9Z9	C76-C73-C74	27.46	165.40	115.66
4	C	1402	9Z9	C76-C73-C74	27.41	165.31	115.66
4	A	1402	9Z9	C76-C73-C74	27.05	164.65	115.66
4	A	1402	9Z9	O72-C73-C76	-18.66	70.65	108.54
4	B	1402	9Z9	O72-C73-C76	-18.61	70.74	108.54
4	D	1402	9Z9	O72-C73-C76	-18.60	70.77	108.54
4	C	1402	9Z9	O72-C73-C76	-18.58	70.80	108.54
4	A	1402	9Z9	O80-C73-O72	12.46	139.53	109.88
4	B	1402	9Z9	O80-C73-O72	11.58	137.43	109.88
4	C	1402	9Z9	O80-C73-O72	11.57	137.40	109.88
4	D	1402	9Z9	O80-C73-O72	11.56	137.39	109.88
4	B	1402	9Z9	O80-C73-C74	-8.32	82.45	107.26
4	D	1402	9Z9	O80-C73-C74	-8.32	82.46	107.26
4	C	1402	9Z9	O80-C73-C74	-8.32	82.46	107.26
4	A	1402	9Z9	O80-C73-C74	-8.18	82.88	107.26
4	A	1402	9Z9	C02-C06-C07	-6.96	104.53	114.41
4	A	1402	9Z9	C10-C02-C06	-6.13	98.08	107.25
4	D	1402	9Z9	C02-C06-C07	-6.08	105.78	114.41
4	B	1402	9Z9	C02-C06-C07	-6.04	105.84	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1402	9Z9	C02-C06-C07	-6.03	105.86	114.41
4	B	1402	9Z9	C10-C02-C06	-5.81	98.56	107.25
4	C	1402	9Z9	C10-C02-C06	-5.79	98.59	107.25
4	D	1402	9Z9	C10-C02-C06	-5.77	98.61	107.25
4	A	1402	9Z9	C07-C15-C14	-5.32	105.39	112.76
4	D	1402	9Z9	C07-C15-C14	-4.60	106.39	112.76
4	B	1402	9Z9	C07-C15-C14	-4.53	106.48	112.76
4	C	1402	9Z9	C07-C15-C14	-4.53	106.49	112.76
4	D	1402	9Z9	C06-C05-C04	-4.49	94.58	102.40
4	B	1402	9Z9	C06-C05-C04	-4.48	94.60	102.40
4	C	1402	9Z9	C06-C05-C04	-4.46	94.64	102.40
4	A	1402	9Z9	C06-C05-C04	-4.42	94.69	102.40
4	B	1402	9Z9	C09-C08-C11	-4.33	107.75	113.08
5	C	1403	PIO	O2C-C1A-C2A	4.30	120.78	111.48
4	D	1402	9Z9	C09-C08-C11	-4.27	107.81	113.08
5	B	1403	PIO	O2C-C1A-C2A	4.27	120.71	111.48
4	C	1402	9Z9	C09-C08-C11	-4.22	107.88	113.08
5	A	1403	PIO	O2C-C1A-C2A	4.06	120.26	111.48
3	D	1401	3PH	O21-C21-C22	4.03	120.20	111.48
3	C	1401	3PH	O21-C21-C22	4.03	120.19	111.48
3	B	1401	3PH	O21-C21-C22	4.02	120.19	111.48
3	A	1401	3PH	O21-C21-C22	3.89	119.91	111.48
4	A	1402	9Z9	C73-C74-C03	3.80	108.97	103.37
4	C	1402	9Z9	C73-C74-C03	3.78	108.93	103.37
4	B	1402	9Z9	C73-C74-C03	3.76	108.91	103.37
4	D	1402	9Z9	C73-C74-C03	3.76	108.91	103.37
4	C	1402	9Z9	C09-C10-C02	-3.67	106.55	112.74
4	B	1402	9Z9	C09-C10-C02	-3.67	106.55	112.74
4	A	1402	9Z9	C10-C09-C08	3.66	119.36	113.14
4	A	1402	9Z9	C01-C02-C03	3.66	119.53	111.58
4	D	1402	9Z9	C09-C10-C02	-3.64	106.60	112.74
4	A	1402	9Z9	C17-C16-C13	-3.50	106.29	111.45
4	A	1402	9Z9	O72-C04-C03	3.45	109.80	105.12
4	B	1402	9Z9	C01-C02-C03	3.39	118.95	111.58
4	D	1402	9Z9	C01-C02-C03	3.39	118.95	111.58
4	C	1402	9Z9	C01-C02-C03	3.39	118.95	111.58
4	A	1402	9Z9	C09-C08-C11	-3.34	108.97	113.08
4	C	1402	9Z9	O80-C79-C78	-3.26	107.98	112.17
4	A	1402	9Z9	C15-C14-C13	-3.25	119.53	125.02
4	A	1402	9Z9	C09-C10-C02	-3.24	107.27	112.74
4	A	1402	9Z9	C74-C03-C04	3.24	109.49	104.27
4	D	1402	9Z9	O80-C79-C78	-3.20	108.07	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1402	9Z9	O80-C79-C78	-3.16	108.12	112.17
5	D	1403	PIO	O2C-C1A-C2A	3.14	118.28	111.48
4	C	1402	9Z9	C15-C14-C13	-2.91	120.10	125.02
3	A	1401	3PH	O31-C31-C32	2.91	120.71	111.83
4	B	1402	9Z9	C15-C14-C13	-2.89	120.14	125.02
4	D	1402	9Z9	C15-C14-C13	-2.88	120.16	125.02
5	B	1403	PIO	O3C-C1B-C2B	2.85	120.52	111.83
4	D	1402	9Z9	C74-C03-C04	2.84	108.84	104.27
4	B	1402	9Z9	C74-C03-C04	2.83	108.83	104.27
4	C	1402	9Z9	C74-C03-C04	2.79	108.75	104.27
4	C	1402	9Z9	C10-C09-C08	2.74	117.79	113.14
3	B	1401	3PH	O31-C31-C32	2.74	120.19	111.83
5	C	1403	PIO	O3C-C1B-C2B	2.74	120.18	111.83
3	D	1401	3PH	O31-C31-C32	2.73	120.16	111.83
3	C	1401	3PH	O31-C31-C32	2.73	120.16	111.83
4	D	1402	9Z9	C10-C09-C08	2.70	117.73	113.14
5	A	1403	PIO	O3C-C1B-C2B	2.70	120.07	111.83
5	D	1403	PIO	C5-C6-C1	2.68	114.54	109.11
4	B	1402	9Z9	C10-C09-C08	2.68	117.69	113.14
5	D	1403	PIO	O3C-C1B-C2B	2.67	119.97	111.83
4	C	1402	9Z9	O72-C73-C74	-2.65	101.03	104.56
4	D	1402	9Z9	O72-C73-C74	-2.62	101.08	104.56
4	B	1402	9Z9	O72-C73-C74	-2.61	101.09	104.56
4	B	1402	9Z9	O72-C04-C03	2.57	108.60	105.12
4	C	1402	9Z9	O72-C04-C03	2.56	108.60	105.12
4	D	1402	9Z9	O72-C04-C03	2.56	108.59	105.12
4	A	1402	9Z9	C15-C07-C06	-2.52	107.37	110.93
4	D	1402	9Z9	C16-C13-C11	2.49	119.61	116.42
4	B	1402	9Z9	C16-C13-C11	2.49	119.61	116.42
4	C	1402	9Z9	C16-C13-C11	2.49	119.60	116.42
4	A	1402	9Z9	C02-C03-C04	2.42	106.81	104.20
4	B	1402	9Z9	C01-C02-C06	-2.35	107.42	111.68
4	D	1402	9Z9	C01-C02-C06	-2.34	107.42	111.68
4	C	1402	9Z9	C01-C02-C06	-2.31	107.48	111.68
4	B	1402	9Z9	C73-O72-C04	-2.29	101.80	108.14
4	D	1402	9Z9	C73-O72-C04	-2.29	101.81	108.14
4	C	1402	9Z9	C73-O72-C04	-2.29	101.82	108.14
4	A	1402	9Z9	C75-C74-C03	-2.20	110.10	114.50
4	D	1402	9Z9	C79-O80-C73	2.20	117.48	113.69
4	B	1402	9Z9	C79-O80-C73	2.19	117.47	113.69
4	C	1402	9Z9	C79-O80-C73	2.17	117.43	113.69
5	D	1403	PIO	C6-C1-C2	2.14	113.83	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1403	PIO	C5-C6-C1	2.07	113.31	109.11
3	B	1401	3PH	C2-O21-C21	-2.07	112.84	117.80
4	A	1402	9Z9	C01-C02-C06	-2.07	107.93	111.68
4	A	1402	9Z9	C16-C13-C11	2.05	119.05	116.42
4	A	1402	9Z9	C77-C78-C79	2.05	111.07	108.59
4	D	1402	9Z9	C15-C07-C06	-2.04	108.05	110.93
4	A	1402	9Z9	C11-C08-C07	-2.03	109.74	112.71
3	C	1401	3PH	C2-O21-C21	-2.02	112.95	117.80
4	C	1402	9Z9	C15-C07-C06	-2.00	108.10	110.93

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1401	3PH	C22-C21-O21-C2
3	A	1401	3PH	O32-C31-O31-C3
3	A	1401	3PH	C32-C31-O31-C3
3	B	1401	3PH	C1-O11-P-O14
3	B	1401	3PH	C22-C21-O21-C2
3	C	1401	3PH	C1-O11-P-O13
3	C	1401	3PH	C1-O11-P-O14
3	C	1401	3PH	C22-C21-O21-C2
3	D	1401	3PH	C1-O11-P-O13
3	D	1401	3PH	C1-O11-P-O14
3	D	1401	3PH	C22-C21-O21-C2
5	A	1403	PIO	C1-O1-P1-O12
5	A	1403	PIO	C1-O1-P1-O13
5	A	1403	PIO	C1C-O13-P1-O1
5	A	1403	PIO	C1C-O13-P1-O12
5	A	1403	PIO	C2A-C1A-O2C-C2C
5	B	1403	PIO	C3-C4-O4-P4
5	B	1403	PIO	C2A-C1A-O2C-C2C
5	C	1403	PIO	C2A-C1A-O2C-C2C
5	D	1403	PIO	C1-O1-P1-O13
5	D	1403	PIO	C1C-O13-P1-O1
5	D	1403	PIO	C1C-O13-P1-O11
5	D	1403	PIO	C1C-O13-P1-O12
5	D	1403	PIO	C3-C4-O4-P4
5	B	1403	PIO	O1B-C1B-O3C-C3C
3	A	1401	3PH	O22-C21-O21-C2
3	B	1401	3PH	O22-C21-O21-C2
3	C	1401	3PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	D	1401	3PH	O22-C21-O21-C2
5	A	1403	PIO	O1A-C1A-O2C-C2C
5	B	1403	PIO	O1A-C1A-O2C-C2C
5	C	1403	PIO	O1A-C1A-O2C-C2C
5	B	1403	PIO	C2B-C1B-O3C-C3C
5	A	1403	PIO	C2C-C1C-O13-P1
3	C	1401	3PH	C21-C22-C23-C24
3	D	1401	3PH	C21-C22-C23-C24
5	D	1403	PIO	C1B-C2B-C3B-C4B
3	B	1401	3PH	C21-C22-C23-C24
3	B	1401	3PH	C32-C31-O31-C3
3	D	1401	3PH	C32-C31-O31-C3
4	A	1402	9Z9	C23-C48-O49-C50
3	A	1401	3PH	C24-C25-C26-C27
5	C	1403	PIO	C4A-C5A-C6A-C7A
3	C	1401	3PH	C32-C31-O31-C3
3	B	1401	3PH	C2A-C2B-C2C-C2D
3	B	1401	3PH	O32-C31-O31-C3
5	D	1403	PIO	C4A-C5A-C6A-C7A
3	B	1401	3PH	C32-C33-C34-C35
3	C	1401	3PH	C32-C33-C34-C35
3	D	1401	3PH	C32-C33-C34-C35
5	A	1403	PIO	C1B-C2B-C3B-C4B
3	D	1401	3PH	O32-C31-O31-C3
3	B	1401	3PH	C3A-C3B-C3C-C3D
5	D	1403	PIO	C3B-C4B-C5B-C6B
3	A	1401	3PH	C22-C23-C24-C25
3	D	1401	3PH	C3A-C3B-C3C-C3D
3	D	1401	3PH	C23-C24-C25-C26
3	D	1401	3PH	C2A-C2B-C2C-C2D
3	C	1401	3PH	C2A-C2B-C2C-C2D
3	C	1401	3PH	C38-C39-C3A-C3B
4	A	1402	9Z9	O20-C21-C22-C23
5	D	1403	PIO	C1A-C2A-C3A-C4A
3	D	1401	3PH	C38-C39-C3A-C3B
3	C	1401	3PH	O32-C31-O31-C3
3	B	1401	3PH	C38-C39-C3A-C3B
3	B	1401	3PH	C35-C36-C37-C38
3	D	1401	3PH	C35-C36-C37-C38
3	D	1401	3PH	C29-C2A-C2B-C2C
3	C	1401	3PH	C29-C2A-C2B-C2C
3	B	1401	3PH	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
3	C	1401	3PH	C35-C36-C37-C38
3	C	1401	3PH	C3A-C3B-C3C-C3D
3	A	1401	3PH	C2B-C2C-C2D-C2E
3	C	1401	3PH	C33-C34-C35-C36
5	A	1403	PIO	C3B-C4B-C5B-C6B
3	D	1401	3PH	C33-C34-C35-C36
3	B	1401	3PH	C33-C34-C35-C36
3	C	1401	3PH	C23-C24-C25-C26
5	A	1403	PIO	C1C-C2C-C3C-O3C
3	B	1401	3PH	C24-C25-C26-C27
5	D	1403	PIO	C3A-C4A-C5A-C6A
5	B	1403	PIO	C1A-C2A-C3A-C4A
3	C	1401	3PH	C1-O11-P-O12
3	D	1401	3PH	C1-O11-P-O12
5	A	1403	PIO	C2B-C1B-O3C-C3C
5	A	1403	PIO	C1C-C2C-O2C-C1A
5	B	1403	PIO	C3C-C2C-O2C-C1A
5	C	1403	PIO	C3C-C2C-O2C-C1A
3	A	1401	3PH	C32-C33-C34-C35
3	C	1401	3PH	C24-C25-C26-C27
5	A	1403	PIO	C2B-C3B-C4B-C5B
4	B	1402	9Z9	C23-C48-O49-C50
4	C	1402	9Z9	C23-C48-O49-C50
4	D	1402	9Z9	C23-C48-O49-C50
5	D	1403	PIO	C2A-C3A-C4A-C5A
3	B	1401	3PH	C23-C24-C25-C26
5	B	1403	PIO	C2C-C1C-O13-P1
3	C	1401	3PH	C34-C35-C36-C37
3	A	1401	3PH	O11-C1-C2-C3
3	B	1401	3PH	C34-C35-C36-C37
3	D	1401	3PH	C34-C35-C36-C37
3	A	1401	3PH	C3A-C3B-C3C-C3D
3	B	1401	3PH	C1-C2-C3-O31
3	C	1401	3PH	C1-C2-C3-O31
3	D	1401	3PH	C1-C2-C3-O31
5	C	1403	PIO	C1C-C2C-C3C-O3C
3	C	1401	3PH	O11-C1-C2-O21
3	C	1401	3PH	O21-C2-C3-O31
3	D	1401	3PH	O21-C2-C3-O31
5	D	1403	PIO	C2B-C3B-C4B-C5B
3	B	1401	3PH	C3C-C3D-C3E-C3F
5	A	1403	PIO	O1B-C1B-O3C-C3C

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Mol	Chain	Res	Type	Atoms
3	D	1401	3PH	C3C-C3D-C3E-C3F
5	B	1403	PIO	C4A-C5A-C6A-C7A
3	B	1401	3PH	O11-C1-C2-C3
5	C	1403	PIO	O13-C1C-C2C-O2C
3	B	1401	3PH	C28-C29-C2A-C2B
3	B	1401	3PH	O21-C2-C3-O31
5	B	1403	PIO	O2C-C2C-C3C-O3C
3	D	1401	3PH	C28-C29-C2A-C2B
5	D	1403	PIO	C1-O1-P1-O12
3	C	1401	3PH	C28-C29-C2A-C2B
5	D	1403	PIO	C5B-C6B-C7B-C8B
3	C	1401	3PH	C3C-C3D-C3E-C3F
5	B	1403	PIO	C2B-C3B-C4B-C5B
3	A	1401	3PH	C2A-C2B-C2C-C2D
3	D	1401	3PH	C24-C25-C26-C27
3	C	1401	3PH	O11-C1-C2-C3
3	A	1401	3PH	C33-C34-C35-C36
5	C	1403	PIO	C5A-C6A-C7A-C8A
5	A	1403	PIO	C5-O5-P5-O53
3	A	1401	3PH	O11-C1-C2-O21
3	B	1401	3PH	O11-C1-C2-O21
3	D	1401	3PH	O11-C1-C2-O21
3	D	1401	3PH	C26-C27-C28-C29
5	A	1403	PIO	O2C-C2C-C3C-O3C
5	C	1403	PIO	O2C-C2C-C3C-O3C
5	C	1403	PIO	C3A-C4A-C5A-C6A
3	A	1401	3PH	C28-C29-C2A-C2B
5	A	1403	PIO	C1C-O13-P1-O11
5	C	1403	PIO	C2C-C1C-O13-P1
5	D	1403	PIO	C2C-C1C-O13-P1
3	A	1401	3PH	C3E-C3F-C3G-C3H
5	B	1403	PIO	C1B-C2B-C3B-C4B
3	B	1401	3PH	C1-O11-P-O12
3	D	1401	3PH	O11-C1-C2-C3
5	C	1403	PIO	O13-C1C-C2C-C3C
5	C	1403	PIO	O2C-C1A-C2A-C3A
5	B	1403	PIO	C1C-C2C-C3C-O3C
3	A	1401	3PH	C37-C38-C39-C3A
3	B	1401	3PH	C36-C37-C38-C39
3	B	1401	3PH	C26-C27-C28-C29
5	D	1403	PIO	C4-O4-P4-O41
3	A	1401	3PH	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	C	1401	3PH	C26-C27-C28-C29
5	D	1403	PIO	O13-C1C-C2C-C3C
3	D	1401	3PH	C36-C37-C38-C39
3	C	1401	3PH	C36-C37-C38-C39
5	D	1403	PIO	C1C-C2C-O2C-C1A
5	C	1403	PIO	C1B-C2B-C3B-C4B
3	C	1401	3PH	C39-C3A-C3B-C3C
5	B	1403	PIO	C3B-C4B-C5B-C6B
5	D	1403	PIO	O2C-C2C-C3C-O3C
5	B	1403	PIO	C4-O4-P4-O42
5	B	1403	PIO	C5-O5-P5-O53
5	D	1403	PIO	C4-O4-P4-O42
4	A	1402	9Z9	C23-C24-O25-C26
3	A	1401	3PH	C36-C37-C38-C39
3	B	1401	3PH	C1-O11-P-O13
5	C	1403	PIO	C4B-C5B-C6B-C7B
5	A	1403	PIO	C1-O1-P1-O11
5	C	1403	PIO	C1-O1-P1-O12
3	B	1401	3PH	C22-C23-C24-C25
5	B	1403	PIO	O3C-C1B-C2B-C3B
5	A	1403	PIO	C5-O5-P5-O52
5	B	1403	PIO	C5-O5-P5-O51
5	B	1403	PIO	C5-O5-P5-O52
5	D	1403	PIO	C4-O4-P4-O43
5	B	1403	PIO	C5B-C6B-C7B-C8B
5	C	1403	PIO	O3C-C1B-C2B-C3B
5	D	1403	PIO	C3C-C2C-O2C-C1A
3	C	1401	3PH	C22-C23-C24-C25
3	C	1401	3PH	C37-C38-C39-C3A
5	C	1403	PIO	O1B-C1B-C2B-C3B
5	B	1403	PIO	O1B-C1B-C2B-C3B
3	B	1401	3PH	C39-C3A-C3B-C3C
3	A	1401	3PH	C3C-C3D-C3E-C3F

There are no ring outliers.

9 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1403	PIO	1	0
4	C	1402	9Z9	15	0
4	A	1402	9Z9	14	0
3	B	1401	3PH	1	0

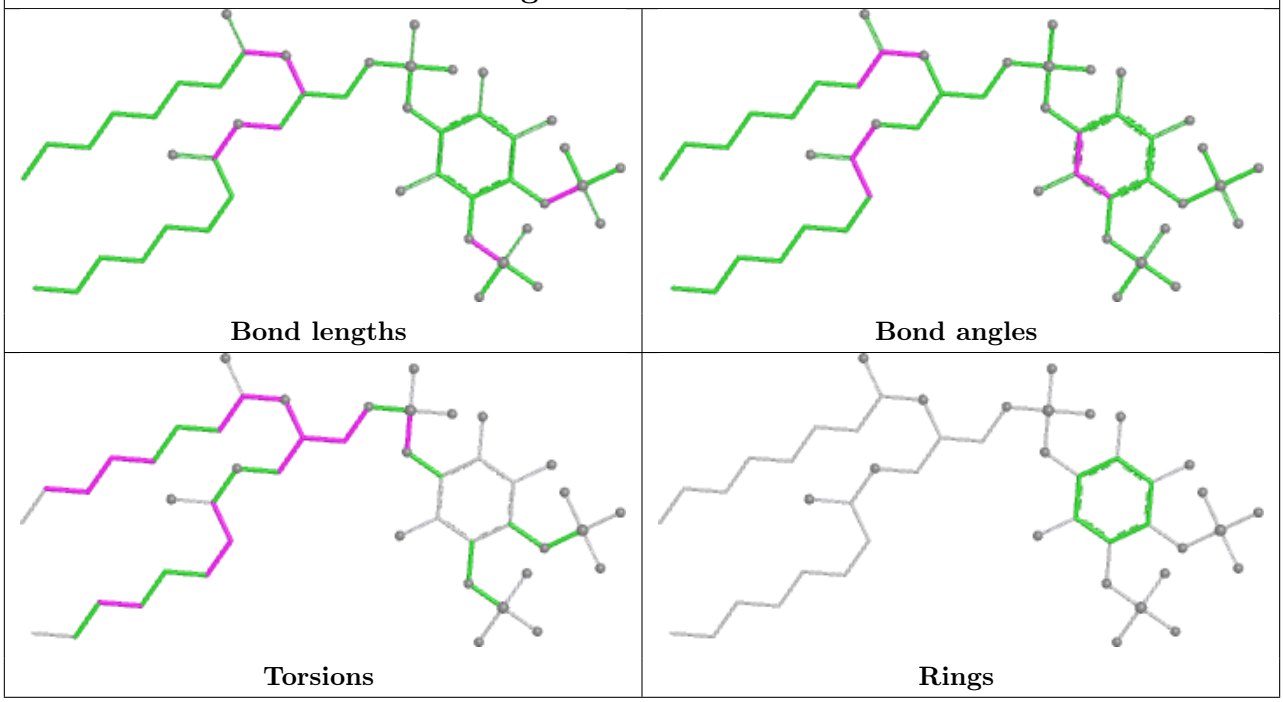
Continued on next page...

Continued from previous page...

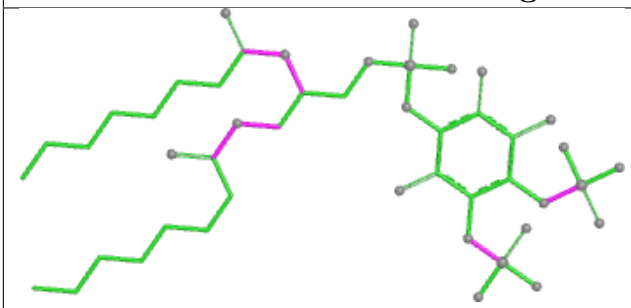
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1403	PIO	1	0
4	B	1402	9Z9	15	0
4	D	1402	9Z9	14	0
3	A	1401	3PH	1	0
3	C	1401	3PH	1	0

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.

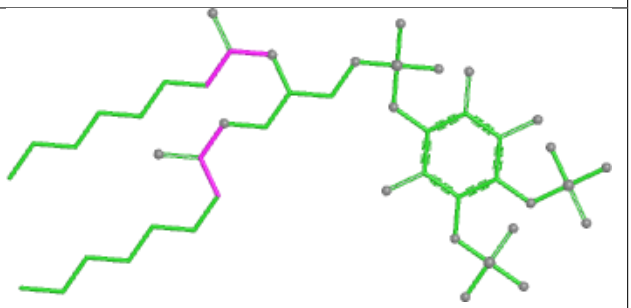
Ligand PIO C 1403



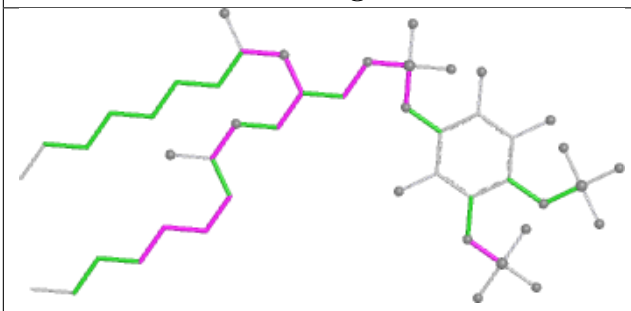
Ligand PIO A 1403



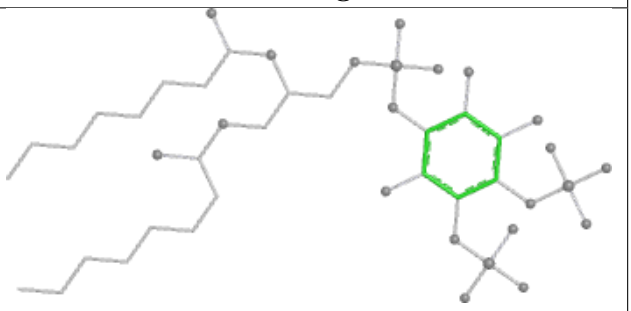
Bond lengths



Bond angles

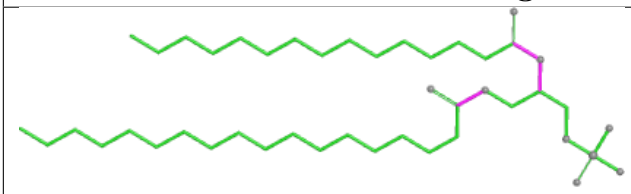


Torsions

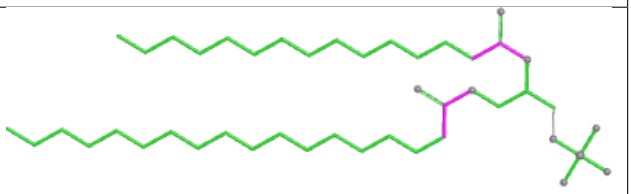


Rings

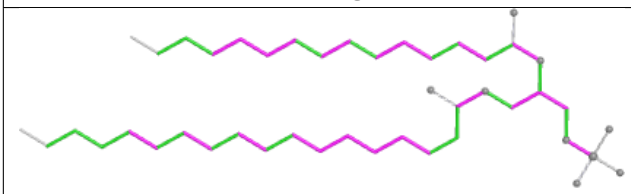
Ligand 3PH D 1401



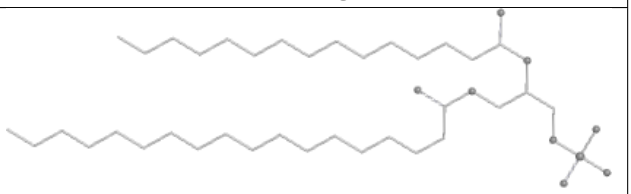
Bond lengths



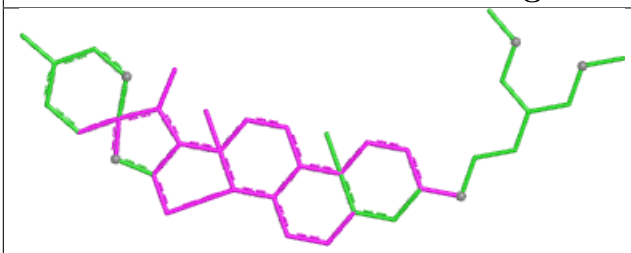
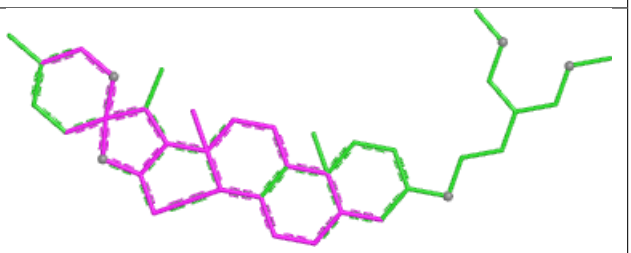
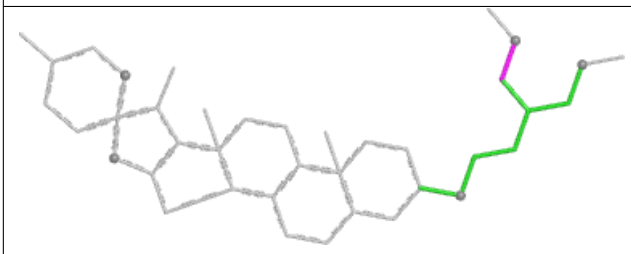
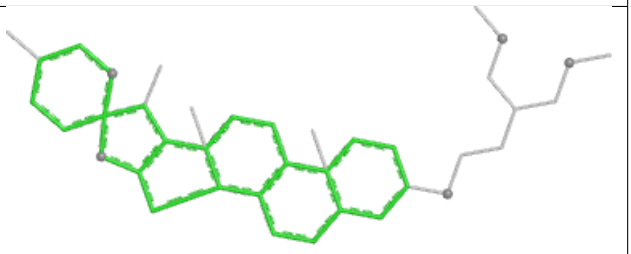
Bond angles

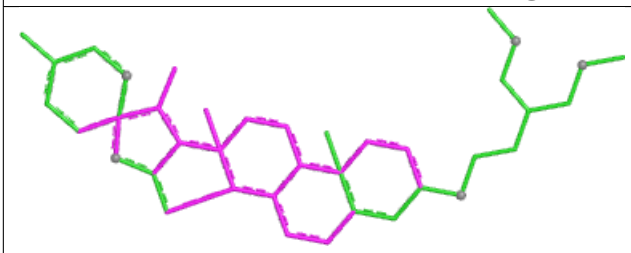
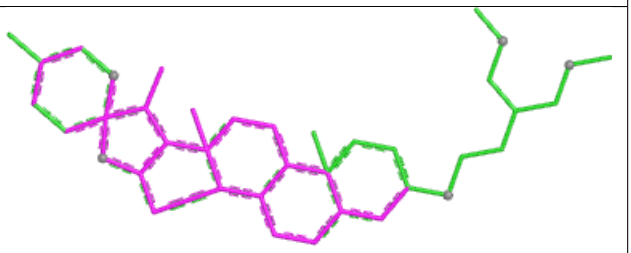
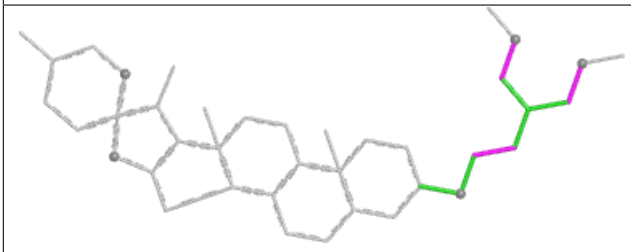
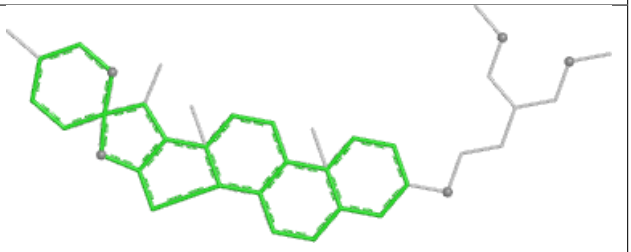


Torsions

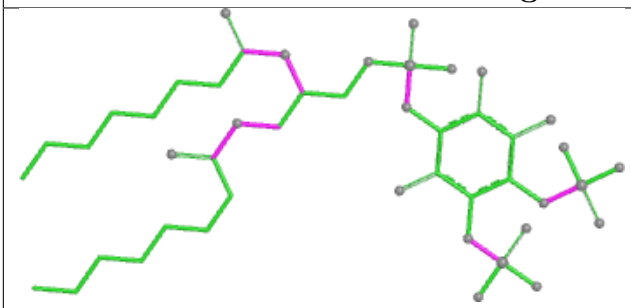


Rings

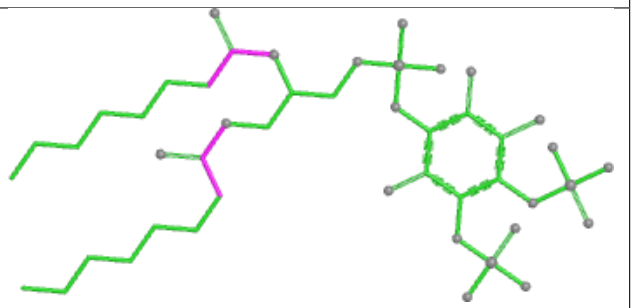
Ligand 9Z9 C 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 9Z9 A 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

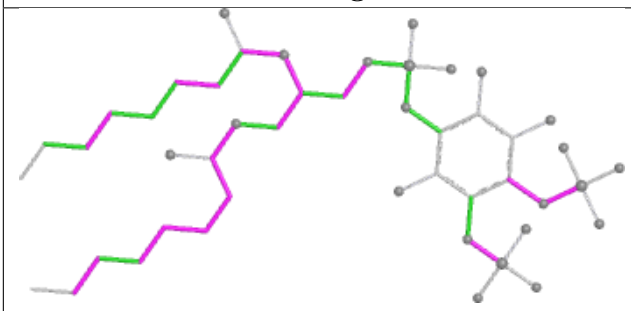
Ligand PIO B 1403



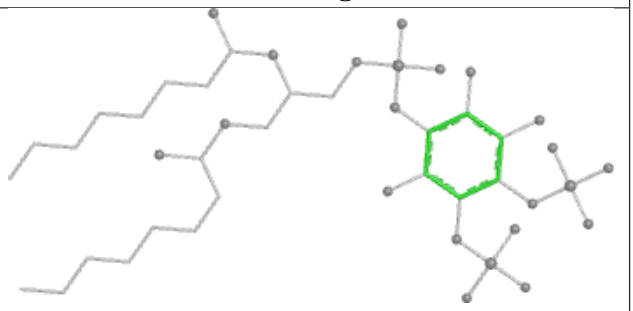
Bond lengths



Bond angles

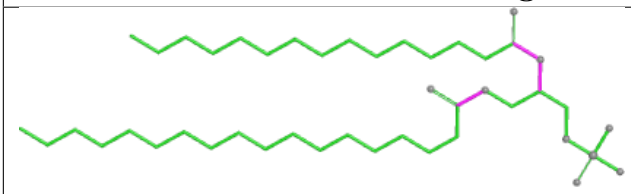


Torsions

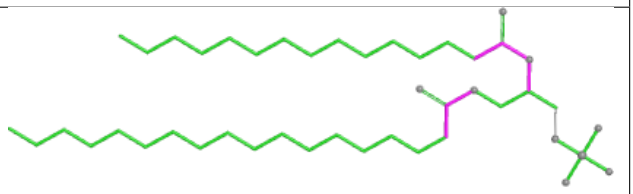


Rings

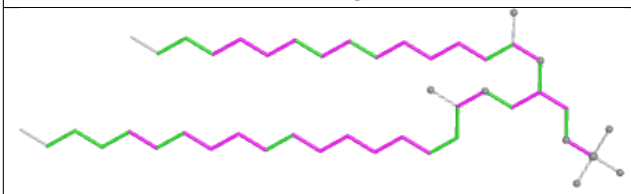
Ligand 3PH B 1401



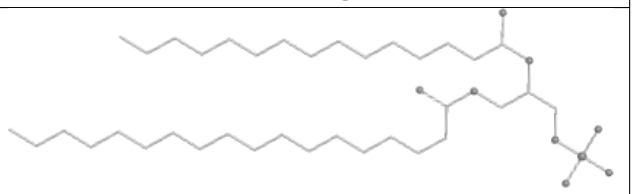
Bond lengths



Bond angles

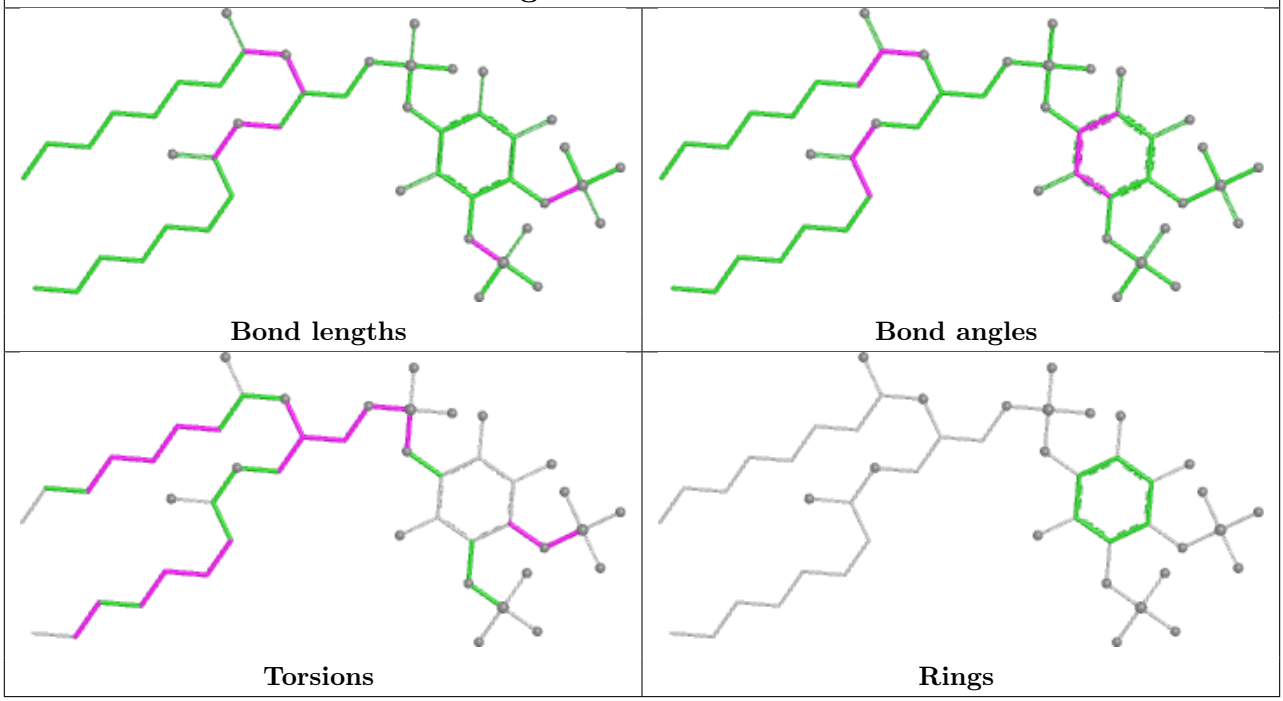


Torsions

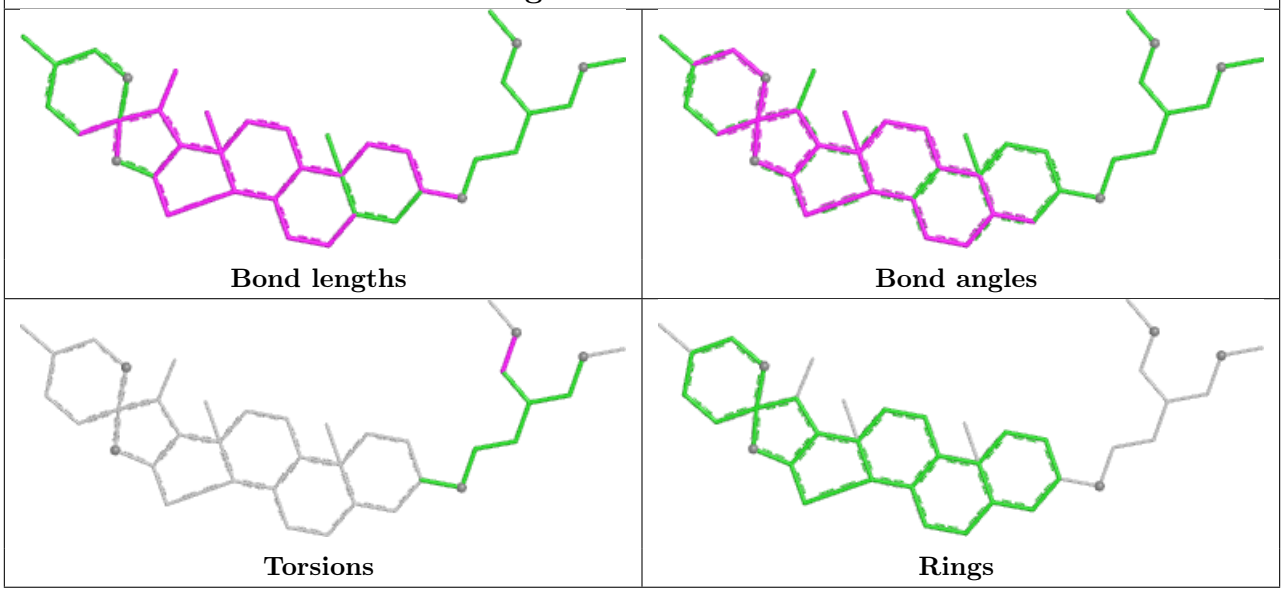


Rings

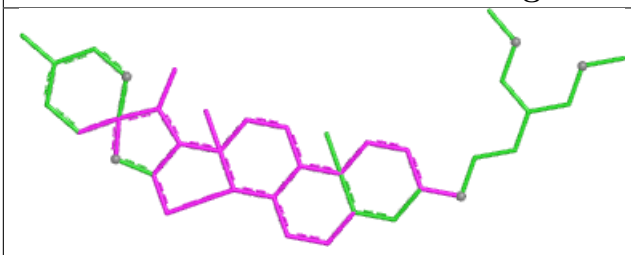
Ligand PIO D 1403



Ligand 9Z9 B 1402



Ligand 9Z9 D 1402



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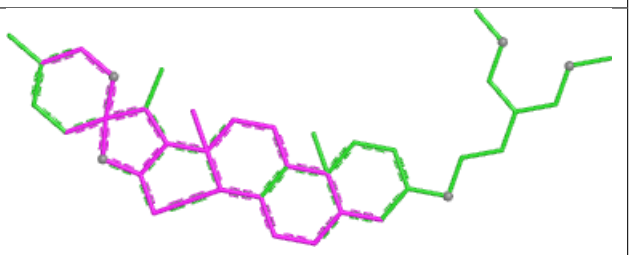
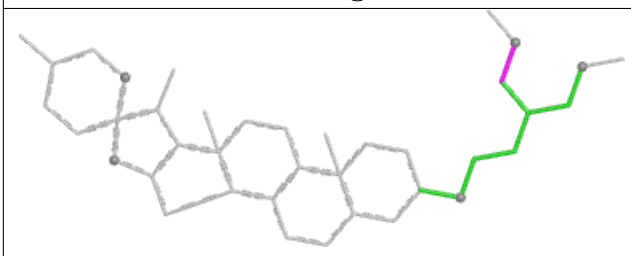
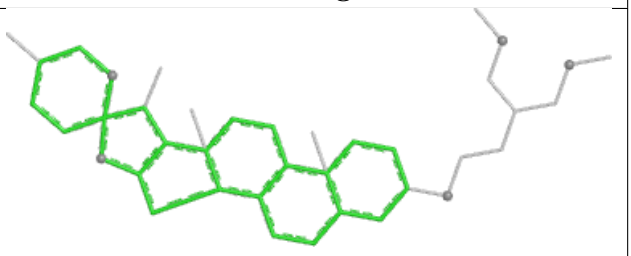


Bond angles

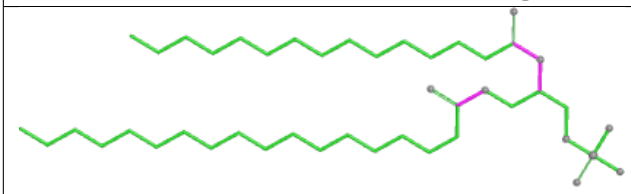


Torsions

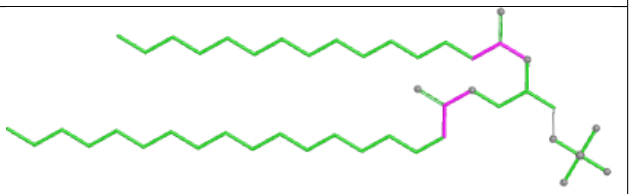


Rings

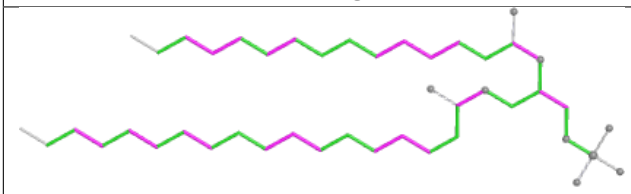
Ligand 3PH A 1401



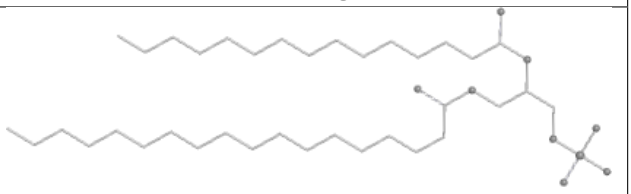
Bond lengths



Bond angles

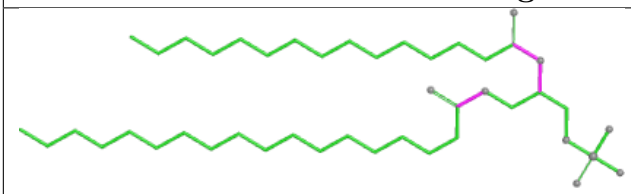


Torsions

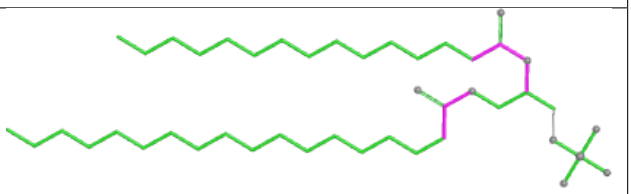


Rings

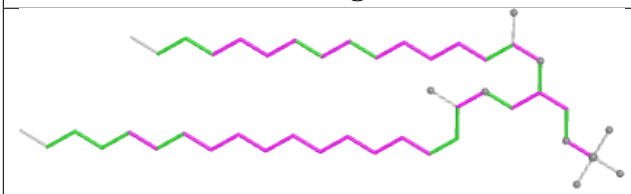
Ligand 3PH C 1401



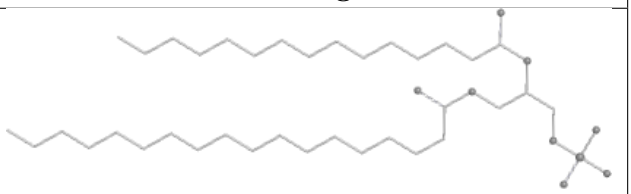
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

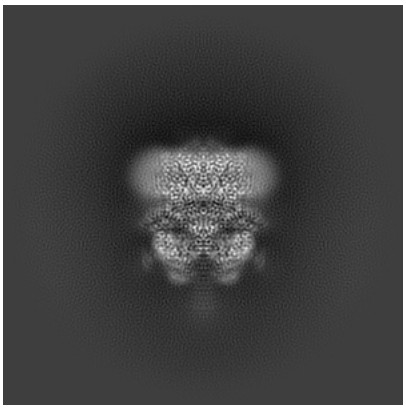
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27341. These allow visual inspection of the internal detail of the map and identification of artifacts.

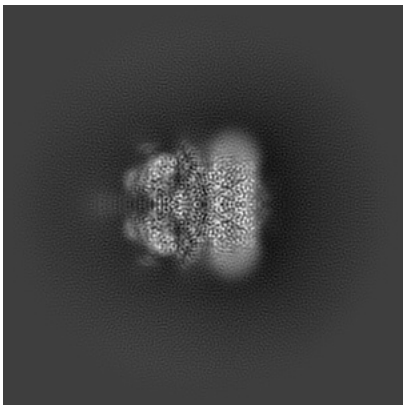
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

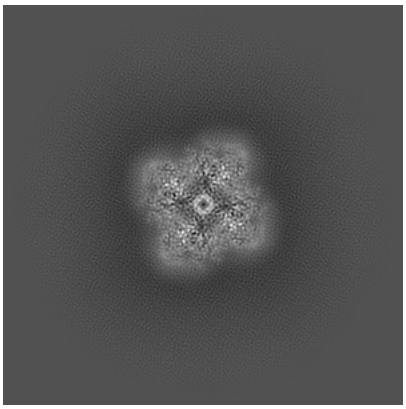
6.1.1 Primary map



X

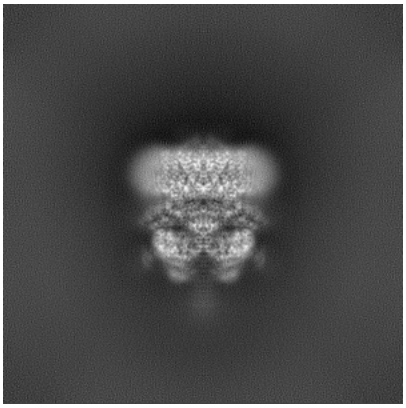


Y

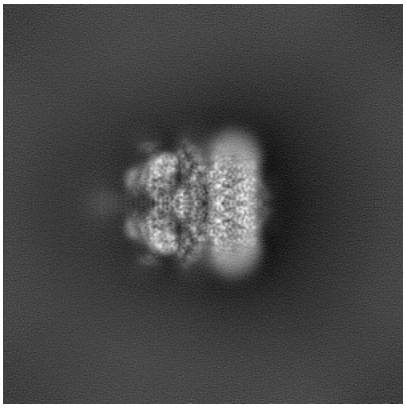


Z

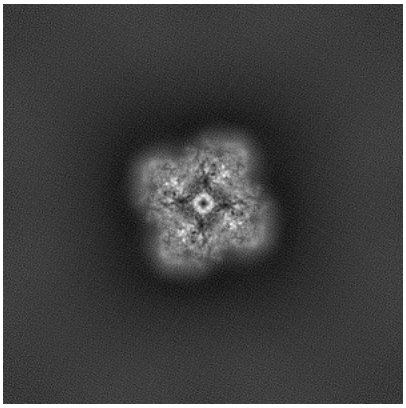
6.1.2 Raw map



X



Y

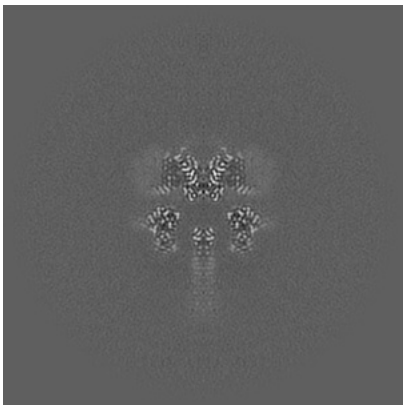


Z

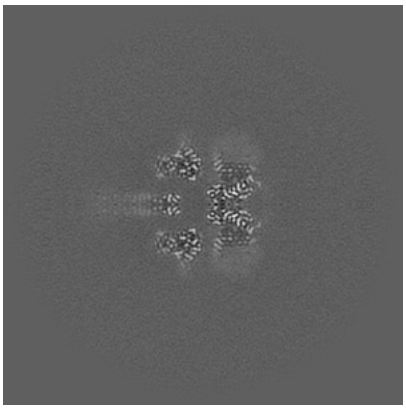
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

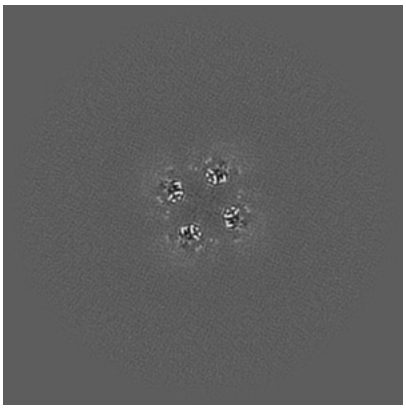
6.2.1 Primary map



X Index: 192

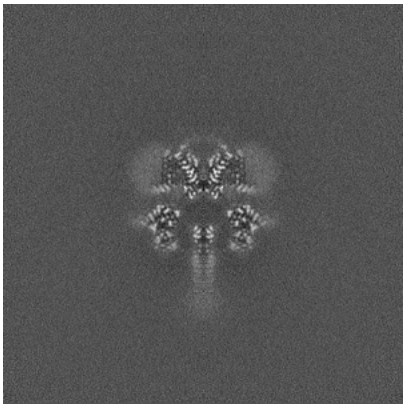


Y Index: 192

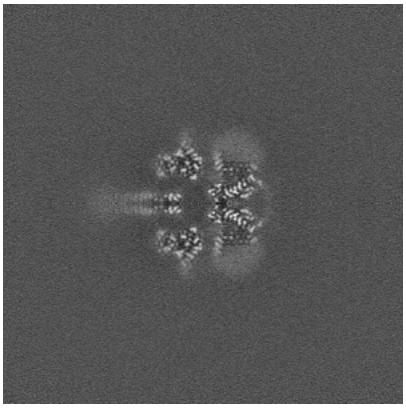


Z Index: 192

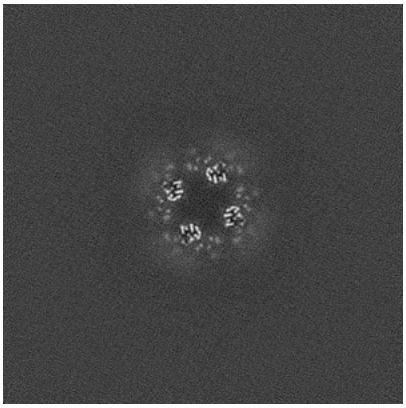
6.2.2 Raw map



X Index: 192



Y Index: 192

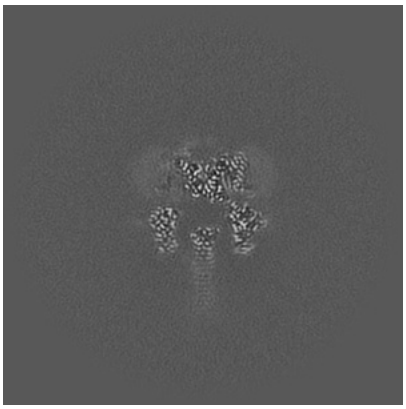


Z Index: 192

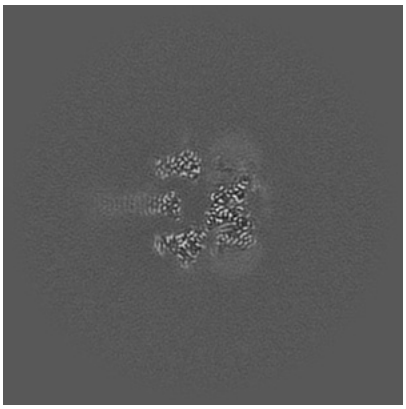
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

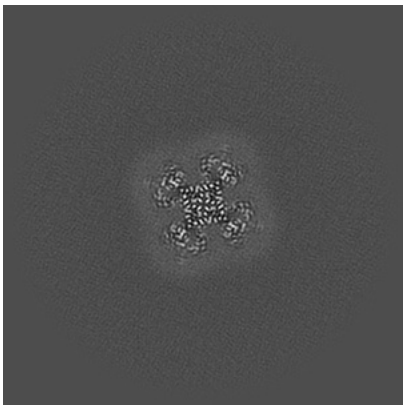
6.3.1 Primary map



X Index: 195

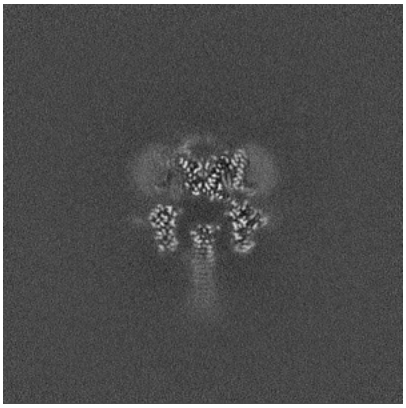


Y Index: 195

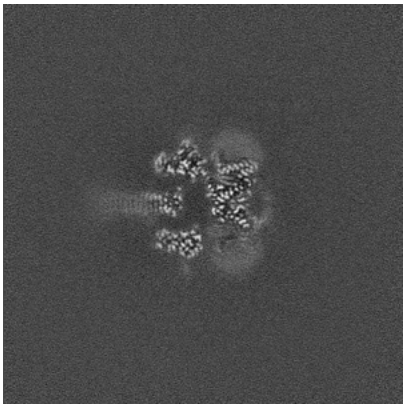


Z Index: 208

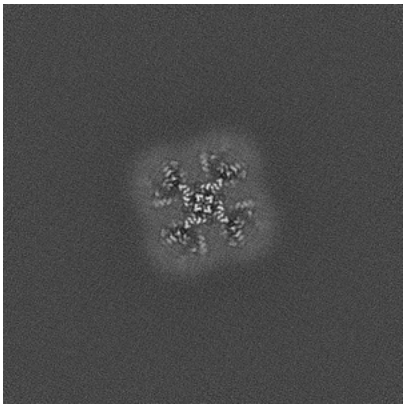
6.3.2 Raw map



X Index: 195



Y Index: 189

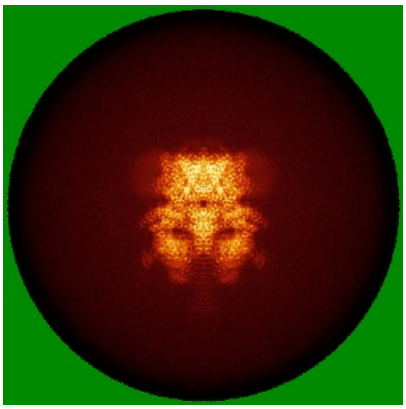


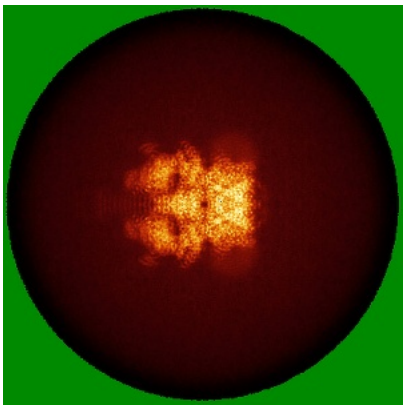
Z Index: 206

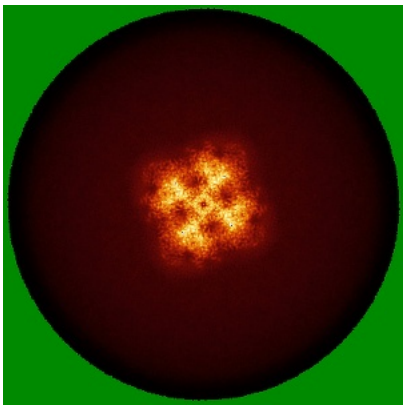
The images above show the largest variance slices of the map in three orthogonal directions.

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

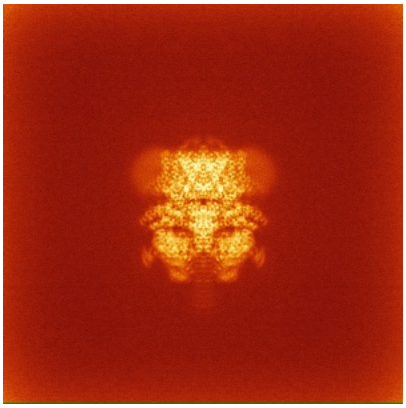
6.4.1 Primary map

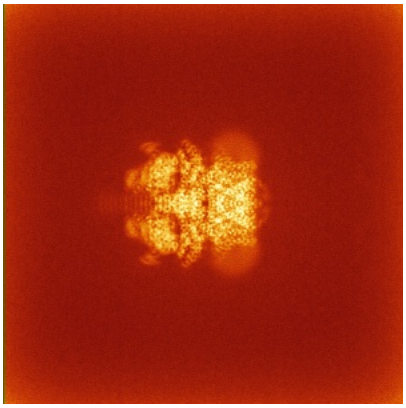

X

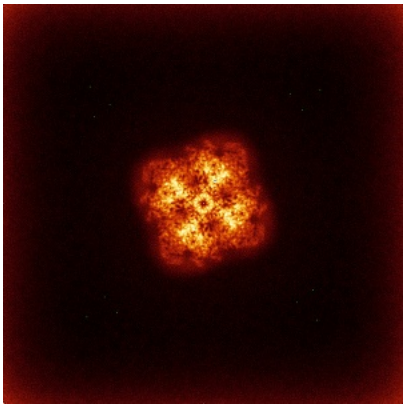

Y


Z

6.4.2 Raw map


X

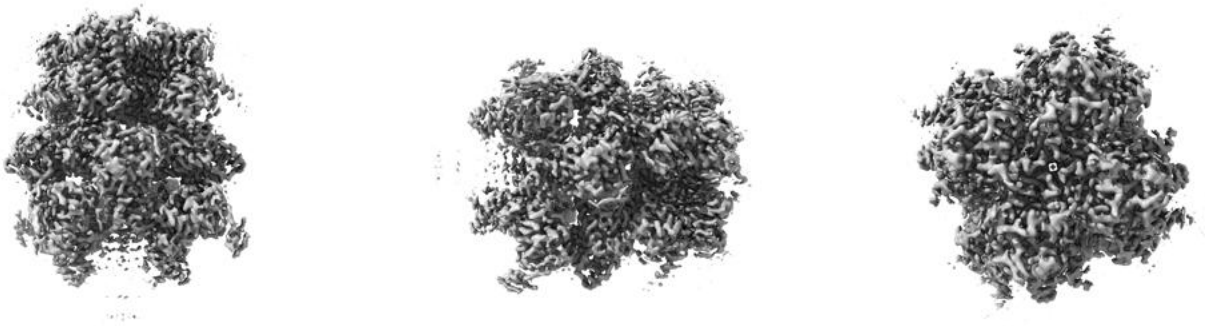

Y


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 0.6. 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.

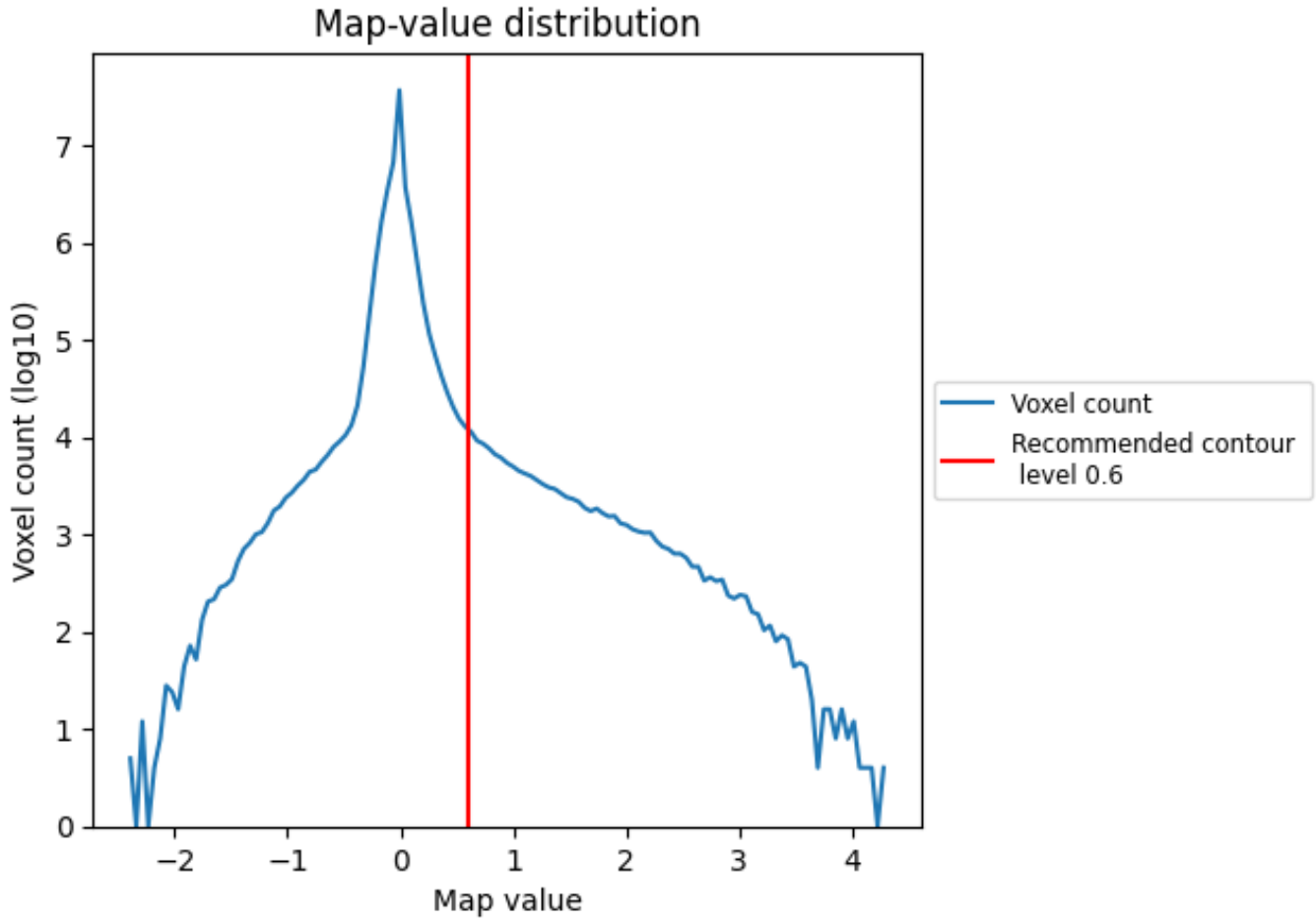
6.6 Mask visualisation (i)

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

7 Map analysis

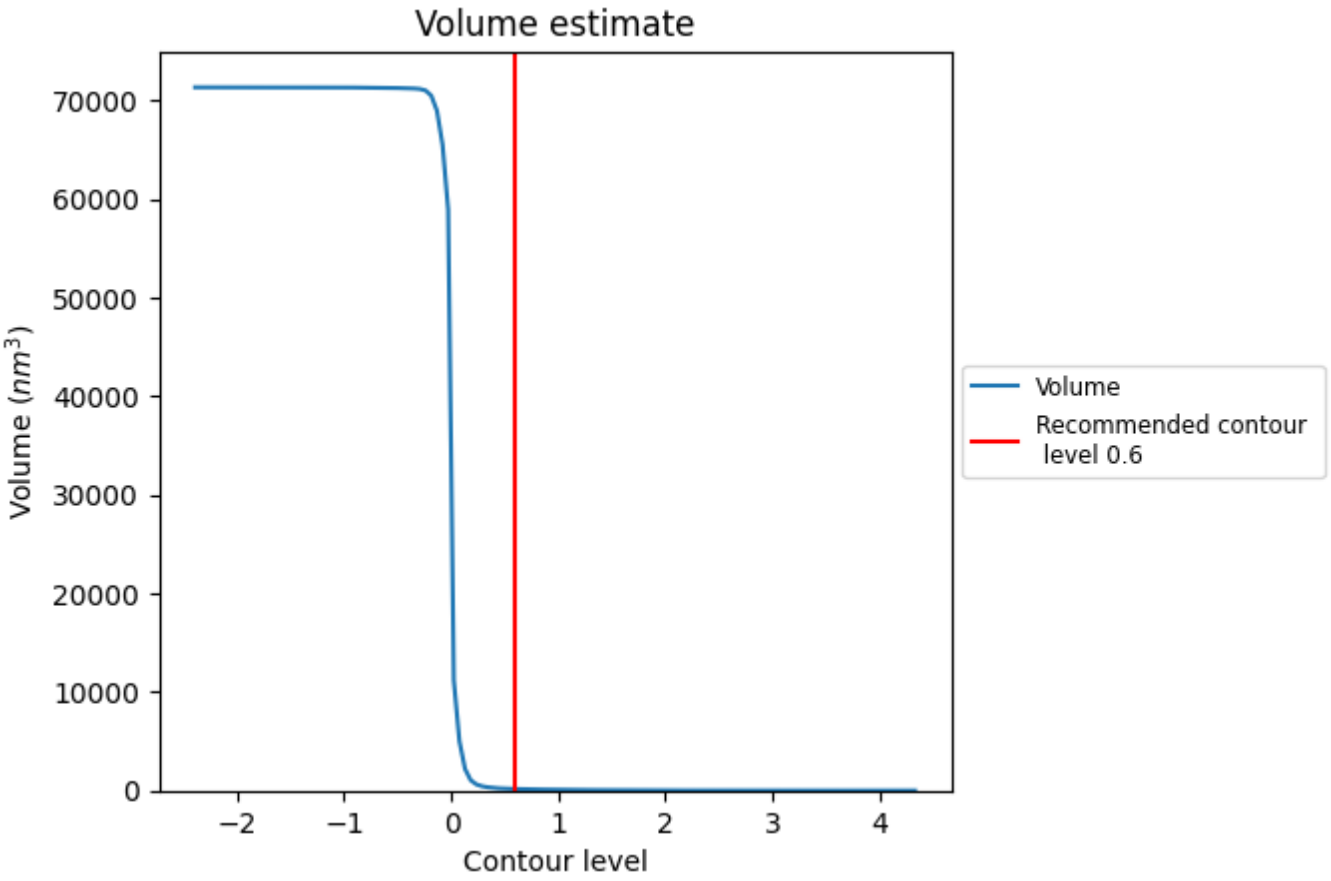
This section contains the results of statistical analysis of the map.

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.

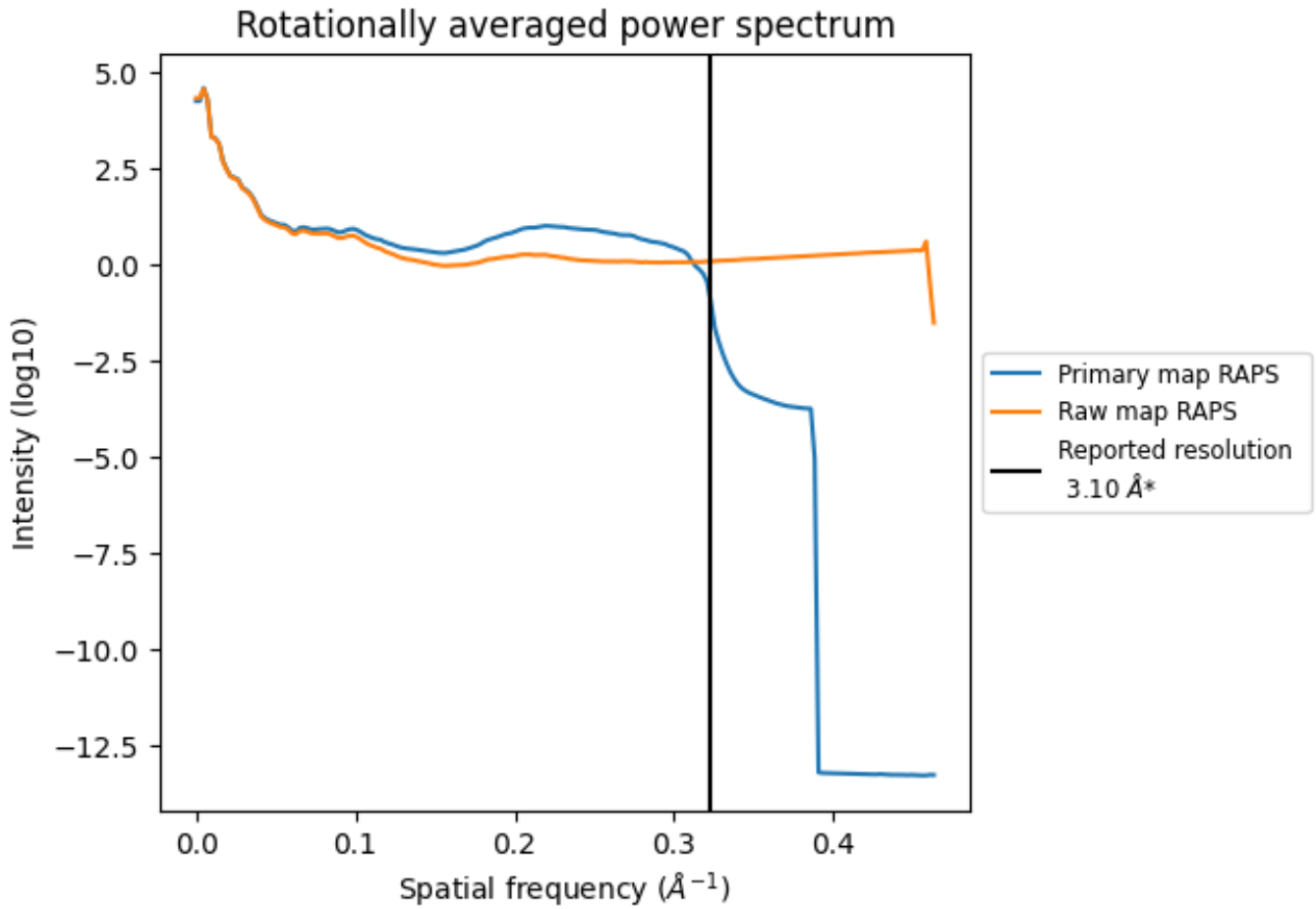
7.2 Volume estimate



The volume at the recommended contour level is 160 nm^3; this corresponds to an approximate mass of 145 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)

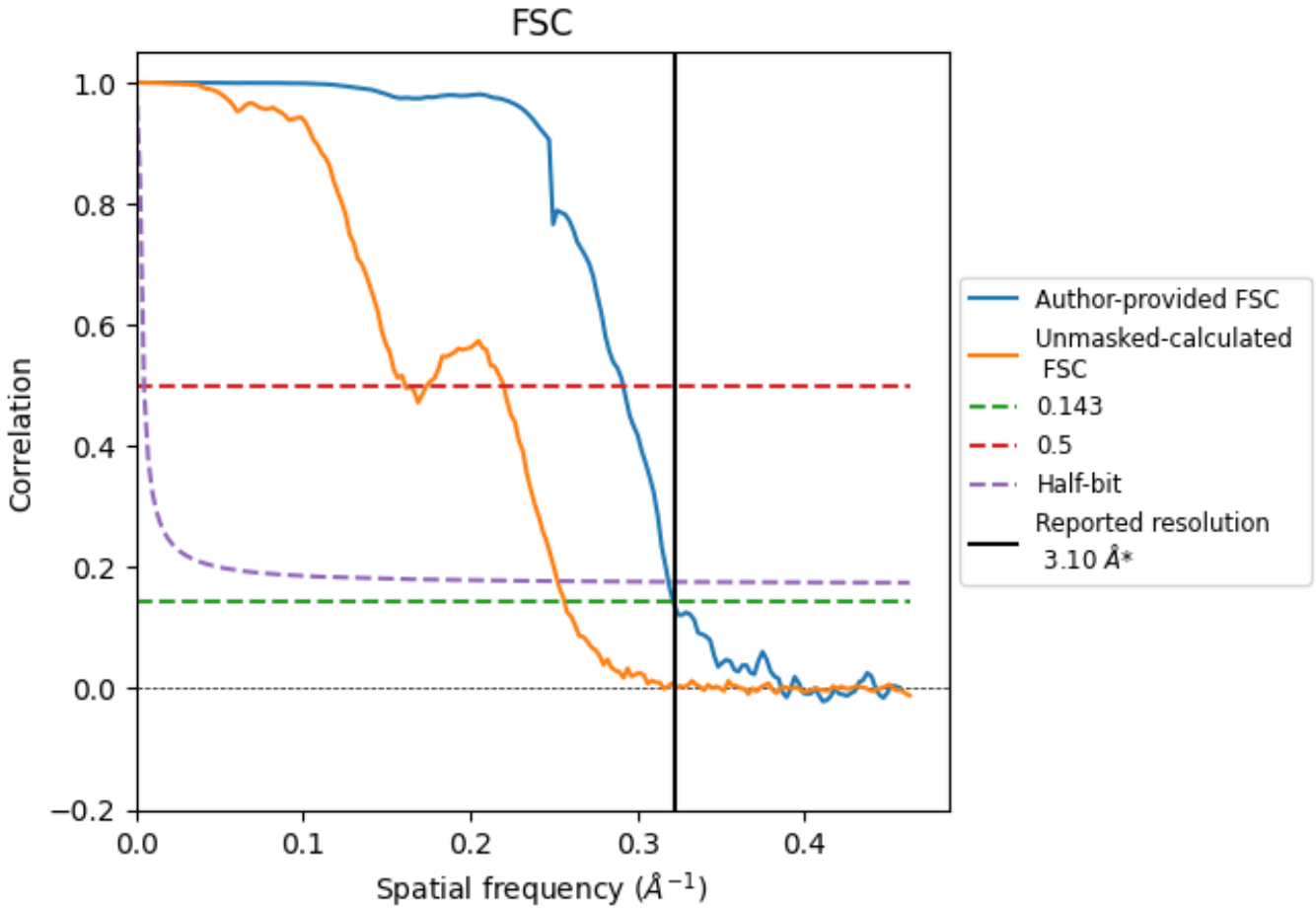


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

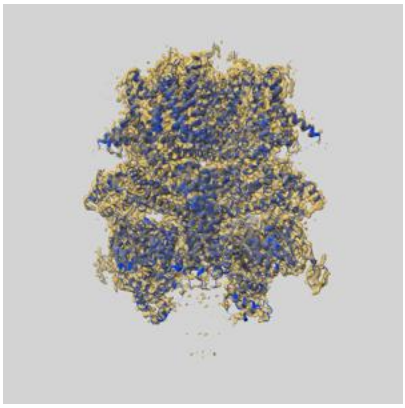
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.43	3.14
Unmasked-calculated*	3.90	6.21	3.96

*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 3.90 differs from the reported value 3.1 by more than 10 %

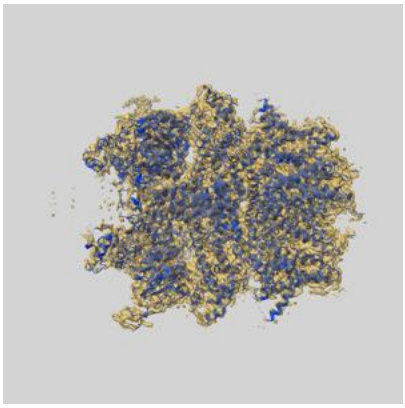
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27341 and PDB model 8DDT. Per-residue inclusion information can be found in section 3 on page 6.

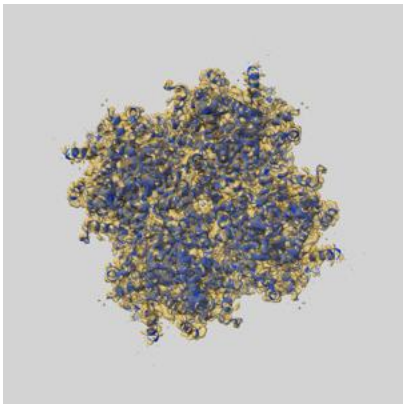
9.1 Map-model overlay



X



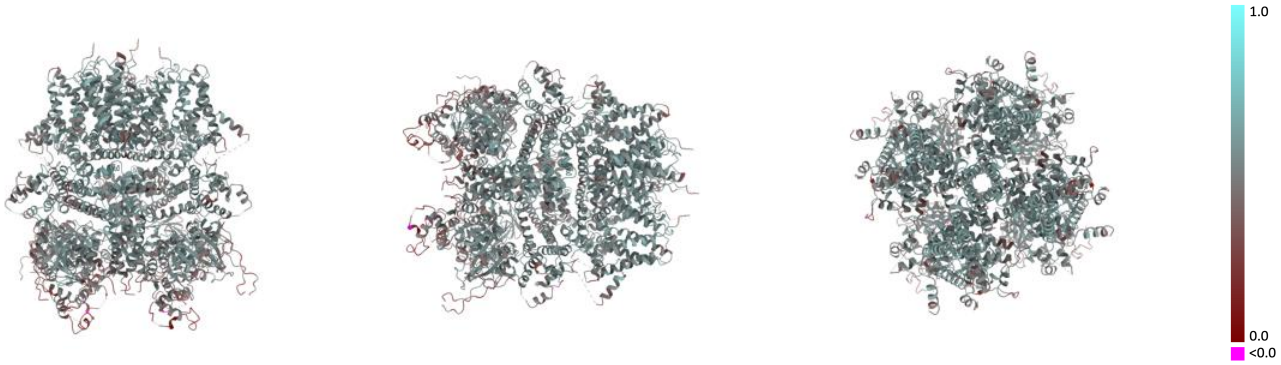
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

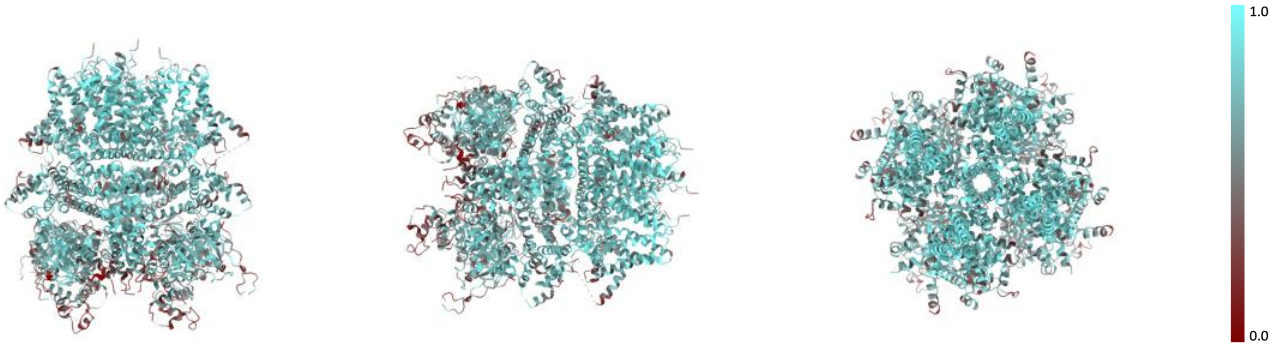
9.2 Q-score mapped to coordinate model (i)



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.

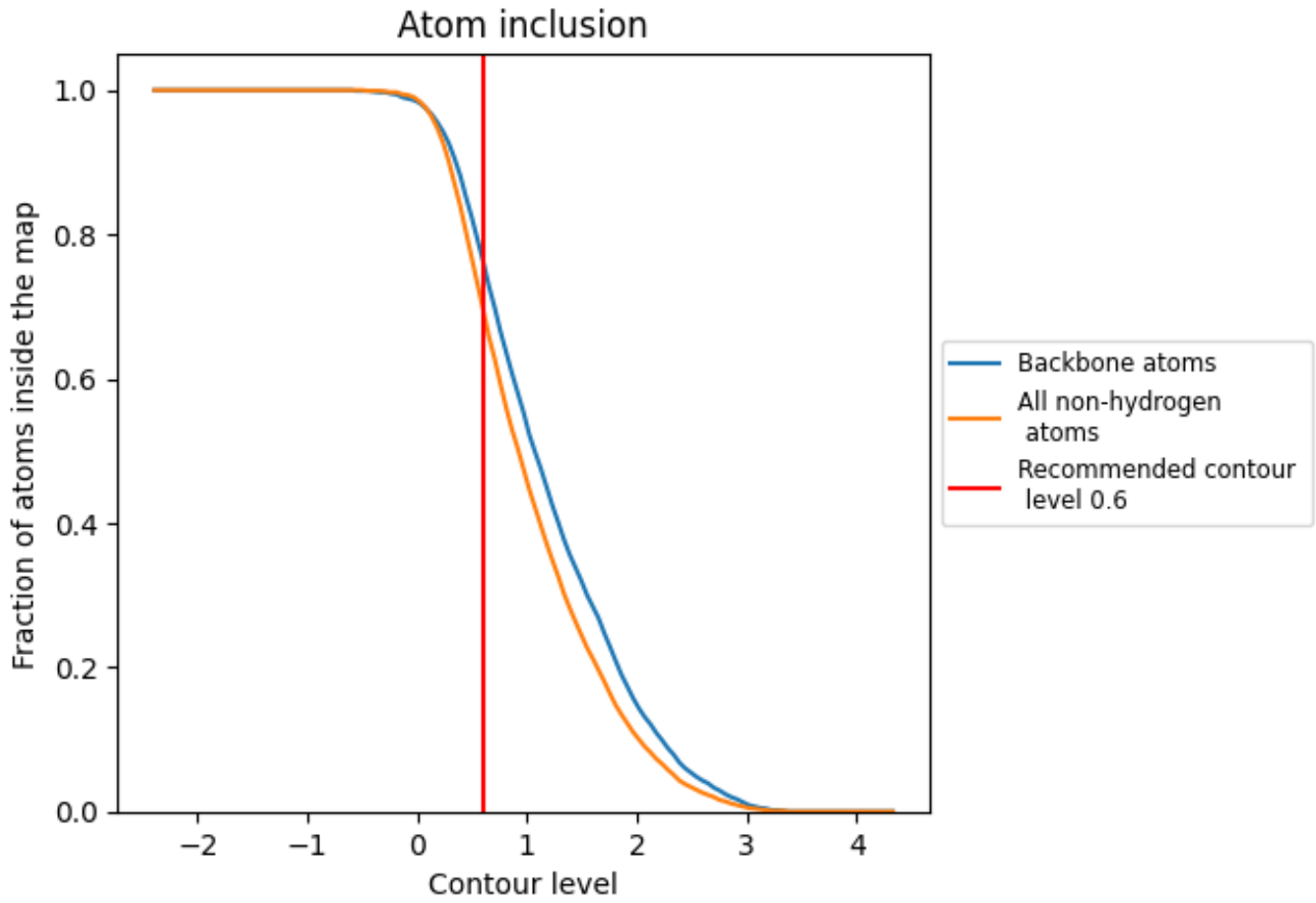
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6970	0.5070
A	0.6990	0.5080
B	0.6980	0.5090
C	0.7010	0.5080
D	0.7000	0.5110
E	0.4710	0.3600
F	0.4820	0.3550
G	0.4820	0.3660
H	0.4710	0.3590