



## Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 10:39 AM EST

PDB ID : 9CZK  
EMDB ID : EMD-46419  
Title : Ca<sup>2+</sup> free hSlo1 + beta2N-beta4 channel in nanodisc.  
Authors : Agarwal, S.; Nimigean, C.  
Deposited on : 2024-08-05  
Resolution : 3.50 Å (reported)  
Based on initial model : 6v35

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.41.4

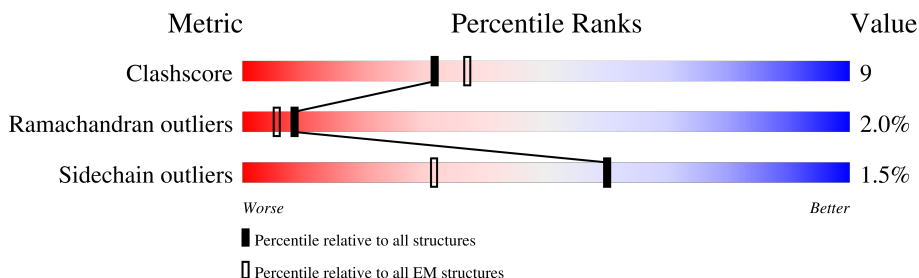
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1056	
1	B	1056	
1	C	1056	
1	D	1056	
2	E	239	
2	F	239	
2	G	239	
2	H	239	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	POV	G	301	-	-	X	-
5	CLR	A	1104	-	-	X	-
5	CLR	B	1102	-	-	X	-
5	CLR	C	1101	-	-	X	-
5	CLR	D	1101	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 69751 atoms, of which 34676 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 Isoform 5 of Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	887	Total	C	H	N	O	S	0	0
			14145	4598	7073	1148	1278	48		
1	B	887	Total	C	H	N	O	S	0	0
			14145	4598	7073	1148	1278	48		
1	C	887	Total	C	H	N	O	S	0	0
			14145	4598	7073	1148	1278	48		
1	D	887	Total	C	H	N	O	S	0	0
			14145	4598	7073	1148	1278	48		

- Molecule 2 is a protein called Large-conductance Ca<sup>2+</sup>-activated K<sup>+</sup> channel beta2 subunit, Calcium-activated potassium channel subunit beta-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	212	Total	C	H	N	O	S	0	0
			3231	1043	1596	277	302	13		
2	F	212	Total	C	H	N	O	S	0	0
			3231	1043	1596	277	302	13		
2	G	212	Total	C	H	N	O	S	0	0
			3231	1043	1596	277	302	13		
2	H	212	Total	C	H	N	O	S	0	0
			3231	1043	1596	277	302	13		

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

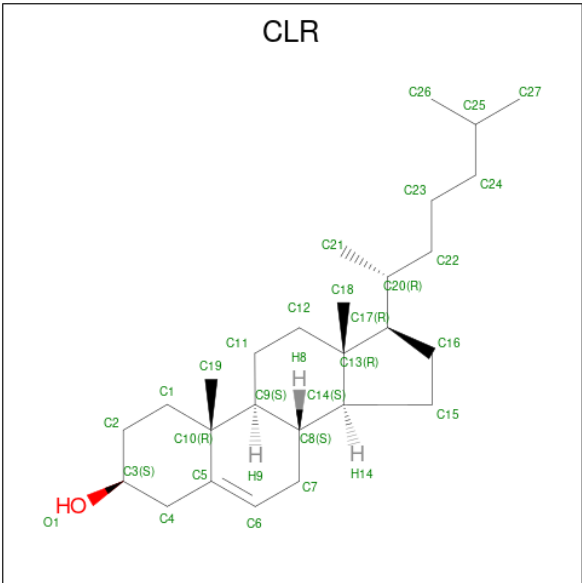
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	K	0
			2	2	

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			34	25	8	1	
4	B	1	Total	C	O	P	0
			31	22	8	1	
4	F	1	Total	C	O	P	0
			34	25	8	1	
4	G	1	Total	C	O	P	0
			34	25	8	1	

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O) (labeled as "Ligand of Interest" by depositor).

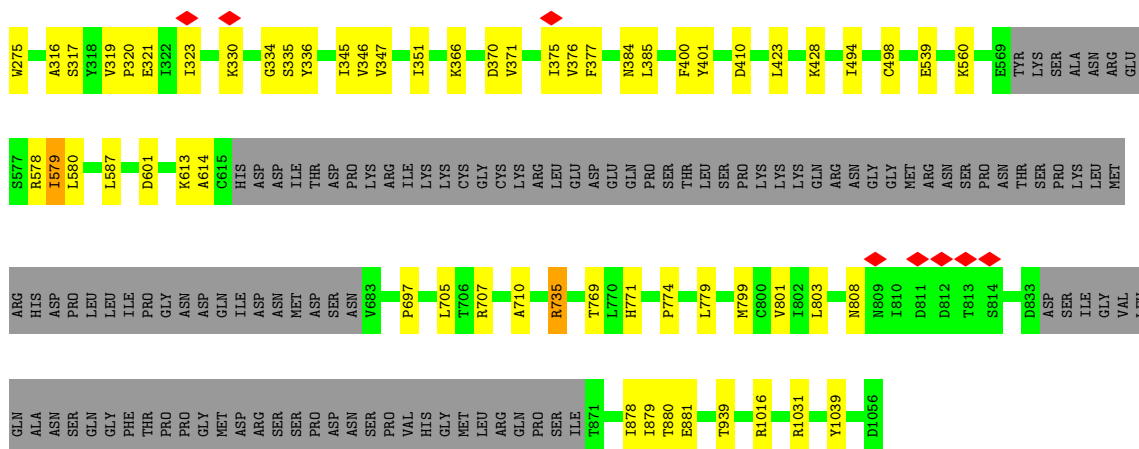


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 28	C 27	O 1	0
5	B	1	Total 28	C 27	O 1	0
5	C	1	Total 28	C 27	O 1	0
5	D	1	Total 28	C 27	O 1	0

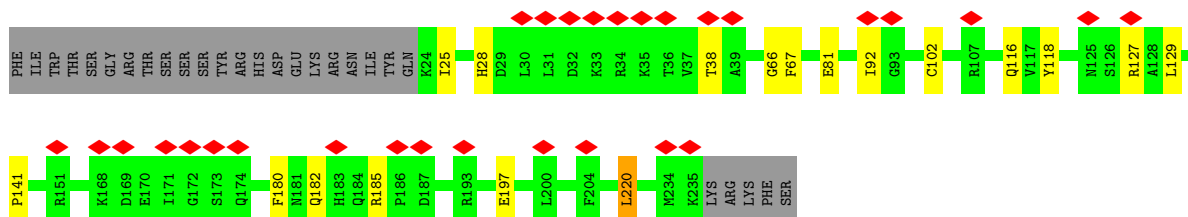
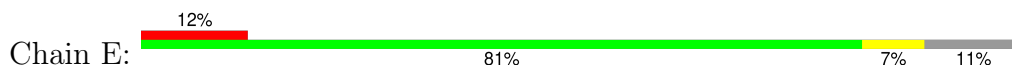




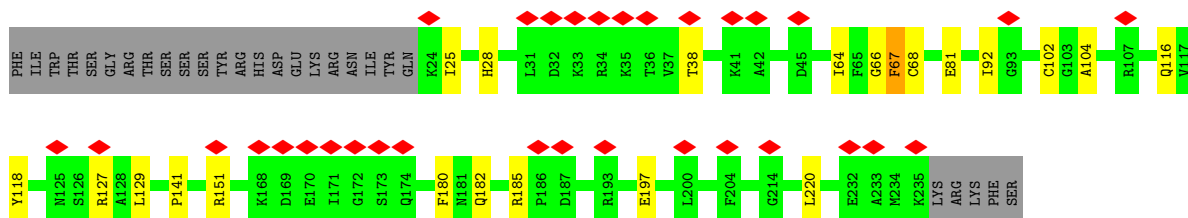
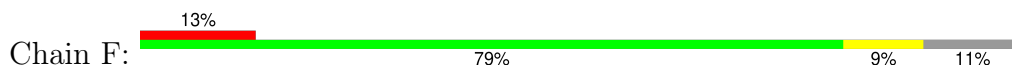




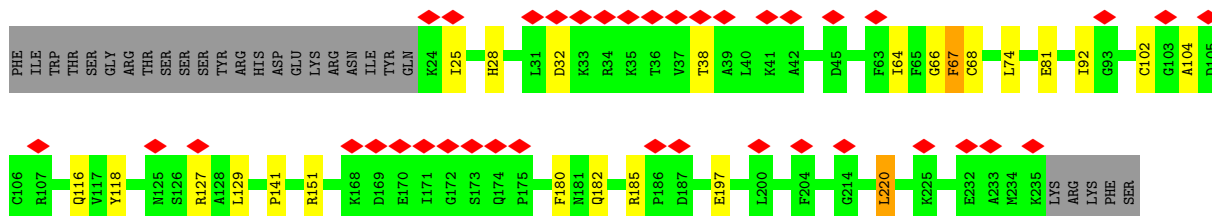
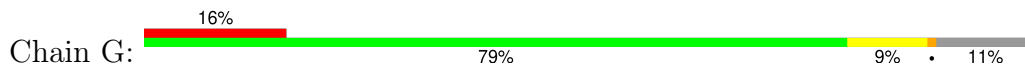
- Molecule 2: Large-conductance  $\text{Ca}^{2+}$ -activated  $\text{K}^{+}$  channel beta2 subunit, Calcium-activated potassium channel subunit beta-4



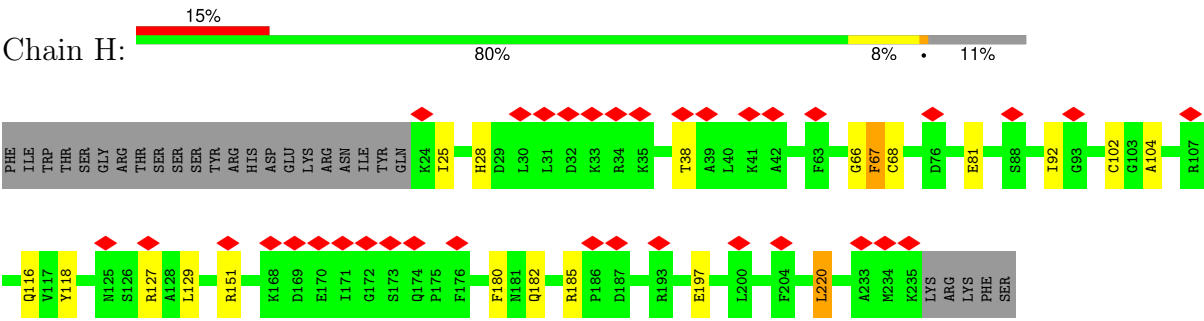
- Molecule 2: Large-conductance  $\text{Ca}^{2+}$ -activated  $\text{K}^{+}$  channel beta2 subunit, Calcium-activated potassium channel subunit beta-4



- Molecule 2: Large-conductance  $\text{Ca}^{2+}$ -activated  $\text{K}^{+}$  channel beta2 subunit, Calcium-activated potassium channel subunit beta-4



- Molecule 2: Large-conductance Ca2+-activated K+ channel beta2 subunit,Calcium-activated potassium channel subunit beta-4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	58904	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47.08	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0167	Depositor
Map size ( $\text{\AA}$ )	324.6, 324.6, 324.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.082, 1.082, 1.082	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.64	0/7237	0.91	0/9824
1	B	0.64	0/7237	0.91	0/9824
1	C	0.64	0/7237	0.91	0/9824
1	D	0.64	0/7237	0.91	0/9824
2	E	0.66	0/1671	0.87	0/2276
2	F	0.67	0/1671	0.87	0/2276
2	G	0.66	0/1671	0.87	0/2276
2	H	0.67	0/1671	0.87	0/2276
All	All	0.64	0/35632	0.90	0/48400

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7072	7073	7068	121	0
1	B	7072	7073	7068	112	0
1	C	7072	7073	7068	120	0
1	D	7072	7073	7068	127	0
2	E	1635	1596	1570	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1635	1596	1570	33	0
2	G	1635	1596	1570	43	0
2	H	1635	1596	1570	22	0
3	A	2	0	0	0	0
4	A	34	0	37	7	0
4	B	31	0	33	2	0
4	F	34	0	37	20	0
4	G	34	0	37	22	0
5	A	28	0	46	27	0
5	B	28	0	46	30	0
5	C	28	0	46	30	0
5	D	28	0	46	34	0
All	All	35075	34676	34880	596	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 (596) 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:C:41:LEU:HD23	2:G:220:LEU:CD2	1.38	1.50
1:D:41:LEU:HD23	2:H:220:LEU:CD2	1.52	1.40
2:G:68:CYS:CB	4:G:301:POV:H23	1.67	1.24
1:C:41:LEU:CD2	2:G:220:LEU:HD22	1.67	1.22
1:A:41:LEU:HB3	2:E:220:LEU:HD21	1.23	1.20
1:A:259:SER:HB3	5:A:1104:CLR:C19	1.73	1.19
2:F:68:CYS:CB	4:F:301:POV:H23	1.78	1.14
1:B:259:SER:CB	5:B:1102:CLR:C19	2.26	1.14
1:A:259:SER:CB	5:A:1104:CLR:C19	2.25	1.13
2:F:67:PHE:HE1	4:F:301:POV:H28	1.04	1.12
2:G:68:CYS:HB2	4:G:301:POV:H23	1.19	1.12
2:F:68:CYS:HB2	4:F:301:POV:H23	1.31	1.11
2:G:67:PHE:HE1	4:G:301:POV:H28	1.09	1.11
1:A:41:LEU:HD23	2:E:220:LEU:CD2	1.81	1.10
1:B:259:SER:HB3	5:B:1102:CLR:C19	1.83	1.09
1:C:259:SER:CB	5:C:1101:CLR:C19	2.31	1.09
1:B:259:SER:HB3	5:B:1102:CLR:H191	1.34	1.08
1:D:41:LEU:HD23	2:H:220:LEU:HD22	1.13	1.06
1:C:259:SER:HB3	5:C:1101:CLR:C19	1.87	1.05
1:A:41:LEU:HB3	2:E:220:LEU:CD2	1.86	1.04
1:A:41:LEU:HD23	2:E:220:LEU:HD22	1.33	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:67:PHE:HE1	4:G:301:POV:C28	1.72	1.03
2:F:67:PHE:HE1	4:F:301:POV:C28	1.72	1.02
1:C:41:LEU:CD2	2:G:220:LEU:CD2	2.32	1.02
1:A:259:SER:HB3	5:A:1104:CLR:H191	1.41	1.01
1:C:114:VAL:HG21	1:C:117:VAL:CG2	1.92	1.00
1:A:114:VAL:HG21	1:A:117:VAL:CG2	1.92	1.00
1:B:114:VAL:HG21	1:B:117:VAL:CG2	1.91	0.99
1:D:114:VAL:HG21	1:D:117:VAL:CG2	1.92	0.99
2:F:67:PHE:CE1	4:F:301:POV:H28	1.96	0.99
1:D:41:LEU:CD2	2:H:220:LEU:HD22	1.92	0.98
2:G:67:PHE:CE1	4:G:301:POV:H28	1.99	0.97
1:D:319:VAL:CG1	1:D:320:PRO:HD3	1.95	0.97
1:D:114:VAL:HG21	1:D:117:VAL:HG21	1.47	0.97
1:B:319:VAL:CG1	1:B:320:PRO:HD3	1.95	0.96
1:C:114:VAL:HG21	1:C:117:VAL:HG21	1.47	0.96
1:C:319:VAL:CG1	1:C:320:PRO:HD3	1.95	0.96
1:A:319:VAL:CG1	1:A:320:PRO:HD3	1.95	0.96
2:G:64:ILE:HG12	4:G:301:POV:H29	1.49	0.95
1:C:259:SER:HB3	5:C:1101:CLR:H191	1.44	0.95
1:D:259:SER:CB	5:D:1101:CLR:C19	2.46	0.94
1:B:114:VAL:HG21	1:B:117:VAL:HG21	1.47	0.94
1:A:114:VAL:HG21	1:A:117:VAL:HG21	1.47	0.94
1:B:114:VAL:HG23	1:B:117:VAL:HB	1.48	0.94
1:A:114:VAL:HG23	1:A:117:VAL:HB	1.48	0.93
1:A:259:SER:CB	5:A:1104:CLR:H192	1.98	0.91
1:C:114:VAL:HG23	1:C:117:VAL:HB	1.48	0.91
1:D:41:LEU:HD23	2:H:220:LEU:HD23	1.50	0.91
1:D:319:VAL:HG12	1:D:320:PRO:HD3	1.53	0.91
1:C:319:VAL:HG12	1:C:320:PRO:HD3	1.53	0.91
1:A:266:PHE:CZ	5:A:1104:CLR:H72	2.05	0.91
1:D:114:VAL:HG23	1:D:117:VAL:HB	1.48	0.91
1:D:41:LEU:CD2	2:H:220:LEU:CD2	2.45	0.91
1:D:705:LEU:HD13	1:D:710:ALA:HB2	1.53	0.90
1:C:705:LEU:HD13	1:C:710:ALA:HB2	1.53	0.90
1:A:319:VAL:HG12	1:A:320:PRO:HD3	1.53	0.90
1:D:259:SER:HB3	5:D:1101:CLR:C19	2.02	0.90
1:B:319:VAL:HG12	1:B:320:PRO:HD3	1.53	0.90
1:B:705:LEU:HD13	1:B:710:ALA:HB2	1.53	0.89
1:A:41:LEU:CD2	2:E:220:LEU:HD22	2.01	0.89
1:A:705:LEU:HD13	1:A:710:ALA:HB2	1.53	0.88
2:E:185:ARG:HH22	2:F:104:ALA:HB3	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:SER:OG	5:B:1102:CLR:H192	1.72	0.88
1:D:259:SER:HB3	5:D:1101:CLR:H191	1.56	0.87
1:D:114:VAL:CG2	1:D:117:VAL:CG2	2.54	0.86
1:B:203:TRP:HH2	5:B:1102:CLR:H112	1.41	0.86
1:D:41:LEU:HB3	2:H:220:LEU:HD21	1.58	0.86
1:A:114:VAL:CG2	1:A:117:VAL:CG2	2.54	0.85
1:B:114:VAL:CG2	1:B:117:VAL:CG2	2.54	0.85
2:G:185:ARG:HD3	2:H:102:CYS:O	1.75	0.85
1:B:336:TYR:HB2	1:B:401:TYR:CE2	2.12	0.85
1:C:114:VAL:CG2	1:C:117:VAL:CG2	2.54	0.85
1:C:259:SER:CB	5:C:1101:CLR:H192	2.05	0.85
1:C:37:LEU:O	1:C:41:LEU:HD13	1.77	0.85
1:A:336:TYR:HB2	1:A:401:TYR:CE2	2.12	0.85
1:D:203:TRP:HH2	5:D:1101:CLR:H112	1.39	0.85
1:B:37:LEU:O	1:B:41:LEU:HD13	1.77	0.84
1:C:336:TYR:HB2	1:C:401:TYR:CE2	2.12	0.84
1:D:37:LEU:O	1:D:41:LEU:HD13	1.77	0.84
1:B:259:SER:CB	5:B:1102:CLR:H192	2.06	0.84
4:A:1103:POV:H28	2:H:67:PHE:HE1	1.42	0.84
1:A:37:LEU:O	1:A:41:LEU:HD13	1.77	0.83
1:D:336:TYR:HB2	1:D:401:TYR:CE2	2.12	0.83
1:A:259:SER:HB3	5:A:1104:CLR:H192	1.52	0.83
1:A:266:PHE:CE1	5:A:1104:CLR:H72	2.14	0.83
1:D:879:ILE:HD12	1:D:879:ILE:O	1.79	0.83
1:C:879:ILE:HD12	1:C:879:ILE:O	1.79	0.82
1:D:705:LEU:CD1	1:D:710:ALA:HB2	2.10	0.82
1:C:705:LEU:CD1	1:C:710:ALA:HB2	2.10	0.81
1:A:705:LEU:CD1	1:A:710:ALA:HB2	2.10	0.81
1:C:259:SER:OG	5:C:1101:CLR:H192	1.80	0.81
1:B:879:ILE:HD12	1:B:879:ILE:O	1.79	0.81
1:B:705:LEU:CD1	1:B:710:ALA:HB2	2.10	0.80
2:G:67:PHE:CE1	4:G:301:POV:C28	2.60	0.80
1:D:203:TRP:CH2	5:D:1101:CLR:H11	2.15	0.80
1:A:879:ILE:HD12	1:A:879:ILE:O	1.79	0.80
2:F:67:PHE:CE1	4:F:301:POV:C28	2.60	0.79
1:A:41:LEU:HD23	2:E:220:LEU:HD23	1.63	0.79
2:E:185:ARG:HD3	2:F:102:CYS:O	1.83	0.79
1:A:144:PHE:CE1	1:A:149:THR:HG21	2.19	0.78
1:B:144:PHE:CE1	1:B:149:THR:HG21	2.18	0.78
1:A:266:PHE:CZ	5:A:1104:CLR:C7	2.65	0.78
1:B:144:PHE:HE1	1:B:149:THR:HG21	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LEU:HD21	1:A:587:LEU:HD13	1.65	0.78
1:D:144:PHE:CE1	1:D:149:THR:HG21	2.19	0.78
1:B:580:LEU:HD21	1:B:587:LEU:HD13	1.65	0.78
1:C:144:PHE:CE1	1:C:149:THR:HG21	2.19	0.78
1:D:580:LEU:HD21	1:D:587:LEU:HD13	1.65	0.77
1:A:144:PHE:HE1	1:A:149:THR:HG21	1.49	0.77
1:C:144:PHE:HE1	1:C:149:THR:HG21	1.49	0.77
1:B:104:MET:HG2	1:B:111:THR:OG1	1.85	0.77
1:C:580:LEU:HD21	1:C:587:LEU:HD13	1.65	0.77
1:D:104:MET:HG2	1:D:111:THR:OG1	1.85	0.77
1:B:259:SER:OG	5:B:1102:CLR:C19	2.29	0.77
2:F:64:ILE:HG12	4:F:301:POV:H29	1.66	0.77
2:G:68:CYS:CA	4:G:301:POV:H23	2.15	0.77
2:G:68:CYS:HA	4:G:301:POV:C23	2.15	0.77
2:G:68:CYS:CB	4:G:301:POV:C23	2.58	0.77
1:C:104:MET:HG2	1:C:111:THR:OG1	1.85	0.77
1:A:41:LEU:CD2	2:E:220:LEU:CD2	2.61	0.77
1:D:144:PHE:HE1	1:D:149:THR:HG21	1.49	0.77
1:A:104:MET:HG2	1:A:111:THR:OG1	1.85	0.76
1:C:203:TRP:HH2	5:C:1101:CLR:H112	1.50	0.75
1:A:114:VAL:HG23	1:A:117:VAL:CB	2.17	0.75
1:A:259:SER:OG	5:A:1104:CLR:H192	1.86	0.75
1:A:336:TYR:HA	1:A:401:TYR:OH	1.87	0.75
1:C:114:VAL:HG23	1:C:117:VAL:CB	2.17	0.74
1:C:336:TYR:HA	1:C:401:TYR:OH	1.87	0.74
1:D:336:TYR:HA	1:D:401:TYR:OH	1.87	0.74
1:B:336:TYR:HA	1:B:401:TYR:OH	1.87	0.74
2:G:68:CYS:SG	4:G:301:POV:C22	2.75	0.74
1:B:114:VAL:HG23	1:B:117:VAL:CB	2.17	0.74
1:C:259:SER:CB	5:C:1101:CLR:H191	2.11	0.74
1:D:114:VAL:HG23	1:D:117:VAL:CB	2.17	0.73
1:A:319:VAL:HG13	1:A:320:PRO:HD3	1.71	0.73
1:B:319:VAL:HG13	1:B:320:PRO:HD3	1.71	0.73
1:D:259:SER:OG	5:D:1101:CLR:H192	1.89	0.73
1:B:259:SER:CB	5:B:1102:CLR:H191	2.02	0.73
1:D:801:VAL:HG13	1:D:879:ILE:HD11	1.72	0.72
1:A:801:VAL:HG13	1:A:879:ILE:HD11	1.72	0.72
2:G:68:CYS:CA	4:G:301:POV:C23	2.68	0.72
1:C:41:LEU:HD23	2:G:220:LEU:HD22	0.74	0.72
1:B:801:VAL:HG13	1:B:879:ILE:HD11	1.72	0.71
1:C:801:VAL:HG13	1:C:879:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:68:CYS:HA	4:F:301:POV:C23	2.20	0.71
2:F:68:CYS:CA	4:F:301:POV:H23	2.21	0.71
1:C:266:PHE:CZ	5:C:1101:CLR:H72	2.24	0.71
1:D:319:VAL:HG13	1:D:320:PRO:HD3	1.71	0.70
1:D:259:SER:CB	5:D:1101:CLR:H192	2.21	0.70
1:C:319:VAL:HG13	1:C:320:PRO:HD3	1.71	0.70
1:B:345:ILE:O	1:B:376:VAL:CG2	2.40	0.69
1:D:203:TRP:CH2	5:D:1101:CLR:H112	2.24	0.69
1:B:579:ILE:HG21	1:B:939:THR:HG21	1.75	0.69
1:C:345:ILE:O	1:C:376:VAL:CG2	2.40	0.69
2:F:118:TYR:CZ	2:F:127:ARG:NH1	2.61	0.69
2:E:118:TYR:CZ	2:E:127:ARG:NH1	2.61	0.69
2:F:185:ARG:HD3	2:G:102:CYS:O	1.93	0.69
1:A:579:ILE:HG21	1:A:939:THR:HG21	1.75	0.69
1:D:494:ILE:HG23	1:D:879:ILE:CD1	2.23	0.69
1:A:345:ILE:O	1:A:376:VAL:CG2	2.40	0.69
1:B:266:PHE:CZ	5:B:1102:CLR:H72	2.28	0.68
1:D:345:ILE:O	1:D:376:VAL:CG2	2.40	0.68
1:A:494:ILE:HG23	1:A:879:ILE:CD1	2.23	0.68
2:G:118:TYR:CZ	2:G:127:ARG:NH1	2.61	0.68
2:H:118:TYR:CZ	2:H:127:ARG:NH1	2.61	0.68
1:B:494:ILE:HG23	1:B:879:ILE:CD1	2.23	0.68
1:D:203:TRP:CH2	5:D:1101:CLR:C1	2.76	0.68
1:C:579:ILE:HG21	1:C:939:THR:HG21	1.75	0.68
1:D:579:ILE:HG21	1:D:939:THR:HG21	1.75	0.68
1:B:336:TYR:HB2	1:B:401:TYR:CZ	2.29	0.68
1:C:494:ILE:HG23	1:C:879:ILE:CD1	2.23	0.68
1:D:336:TYR:HB2	1:D:401:TYR:CZ	2.29	0.67
1:C:336:TYR:HB2	1:C:401:TYR:CZ	2.29	0.67
1:D:203:TRP:CZ3	5:D:1101:CLR:H11	2.30	0.67
1:C:203:TRP:CH2	5:C:1101:CLR:H11	2.29	0.67
1:A:260:GLY:O	1:A:266:PHE:HD1	1.78	0.67
1:A:336:TYR:HB2	1:A:401:TYR:CZ	2.29	0.67
1:D:203:TRP:CZ3	5:D:1101:CLR:C1	2.78	0.67
1:D:266:PHE:CZ	5:D:1101:CLR:H72	2.30	0.67
1:D:260:GLY:O	1:D:266:PHE:HD1	1.78	0.66
1:D:114:VAL:HG21	1:D:117:VAL:HG23	1.77	0.66
1:B:260:GLY:O	1:B:266:PHE:HD1	1.78	0.66
1:A:114:VAL:HG21	1:A:117:VAL:HG23	1.77	0.66
1:C:114:VAL:HG21	1:C:117:VAL:HG23	1.77	0.65
1:C:260:GLY:O	1:C:266:PHE:HD1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1102:CLR:H272	5:B:1102:CLR:H222	1.78	0.65
1:B:580:LEU:HD21	1:B:587:LEU:CD1	2.27	0.65
1:A:879:ILE:O	1:A:879:ILE:CD1	2.45	0.65
1:C:41:LEU:HB3	2:G:220:LEU:HD21	1.77	0.65
1:C:259:SER:OG	5:C:1101:CLR:C19	2.40	0.65
1:B:114:VAL:HG21	1:B:117:VAL:HG23	1.77	0.65
5:D:1101:CLR:C22	5:D:1101:CLR:H272	2.26	0.65
1:C:580:LEU:HD21	1:C:587:LEU:CD1	2.27	0.65
1:D:366:LYS:CE	2:G:32:ASP:CB	2.75	0.65
1:B:879:ILE:O	1:B:879:ILE:CD1	2.45	0.65
5:C:1101:CLR:H272	5:C:1101:CLR:H222	1.78	0.65
1:D:366:LYS:NZ	2:G:32:ASP:CB	2.59	0.64
1:D:259:SER:CB	5:D:1101:CLR:H191	2.21	0.64
5:D:1101:CLR:H272	5:D:1101:CLR:H222	1.78	0.64
1:A:580:LEU:HD21	1:A:587:LEU:CD1	2.27	0.64
5:A:1104:CLR:H222	5:A:1104:CLR:H272	1.78	0.64
1:D:203:TRP:HH2	5:D:1101:CLR:H11	1.61	0.64
5:B:1102:CLR:H272	5:B:1102:CLR:H211	1.79	0.64
1:C:259:SER:HB3	5:C:1101:CLR:H192	1.68	0.64
2:F:68:CYS:SG	4:F:301:POV:C22	2.85	0.64
5:B:1102:CLR:H272	5:B:1102:CLR:C22	2.26	0.64
5:C:1101:CLR:H272	5:C:1101:CLR:C22	2.27	0.64
5:C:1101:CLR:H272	5:C:1101:CLR:H211	1.80	0.64
4:A:1103:POV:H23	2:H:68:CYS:HB2	1.80	0.64
1:D:145:TYR:HA	1:D:149:THR:OG1	1.98	0.63
1:C:879:ILE:O	1:C:879:ILE:CD1	2.45	0.63
1:D:580:LEU:HD21	1:D:587:LEU:CD1	2.27	0.63
1:A:145:TYR:HA	1:A:149:THR:OG1	1.98	0.63
1:D:879:ILE:O	1:D:879:ILE:CD1	2.45	0.63
2:F:68:CYS:CA	4:F:301:POV:C23	2.76	0.63
5:A:1104:CLR:H272	5:A:1104:CLR:H211	1.80	0.63
5:A:1104:CLR:H272	5:A:1104:CLR:C22	2.27	0.63
2:G:68:CYS:SG	4:G:301:POV:H23	2.38	0.63
1:D:366:LYS:HE2	2:G:32:ASP:CB	2.28	0.62
1:A:316:ALA:O	1:A:319:VAL:HG12	1.99	0.62
1:B:145:TYR:HA	1:B:149:THR:OG1	1.98	0.62
1:A:580:LEU:CD2	1:A:587:LEU:HD13	2.29	0.62
5:D:1101:CLR:H272	5:D:1101:CLR:H211	1.80	0.62
1:A:41:LEU:CB	2:E:220:LEU:CD2	2.69	0.62
1:B:316:ALA:O	1:B:319:VAL:HG12	1.99	0.62
1:D:316:ALA:O	1:D:319:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ILE:HG23	1:A:879:ILE:HD11	1.82	0.62
1:B:203:TRP:CH2	5:B:1102:CLR:H11	2.34	0.62
1:C:494:ILE:HG23	1:C:879:ILE:HD11	1.82	0.62
1:B:579:ILE:HG23	1:B:579:ILE:O	2.00	0.62
5:B:1102:CLR:C16	5:B:1102:CLR:H232	2.29	0.62
1:C:145:TYR:HA	1:C:149:THR:OG1	1.98	0.62
1:D:580:LEU:CD2	1:D:587:LEU:HD13	2.29	0.62
1:B:203:TRP:CH2	5:B:1102:CLR:H112	2.28	0.62
1:D:260:GLY:O	1:D:266:PHE:CD1	2.53	0.62
1:B:260:GLY:O	1:B:266:PHE:CD1	2.53	0.62
1:C:316:ALA:O	1:C:319:VAL:HG12	1.99	0.62
1:C:579:ILE:HG23	1:C:579:ILE:O	2.00	0.62
1:C:580:LEU:CD2	1:C:587:LEU:HD13	2.29	0.62
1:B:114:VAL:CG2	1:B:117:VAL:HG23	2.30	0.61
1:B:494:ILE:HG23	1:B:879:ILE:HD11	1.82	0.61
1:A:579:ILE:O	1:A:579:ILE:HG23	2.00	0.61
1:D:494:ILE:HG23	1:D:879:ILE:HD11	1.82	0.61
5:C:1101:CLR:C16	5:C:1101:CLR:H232	2.29	0.61
1:D:22:TRP:HE1	5:D:1101:CLR:H6	1.65	0.61
1:D:579:ILE:HG23	1:D:579:ILE:O	2.00	0.61
1:B:580:LEU:CD2	1:B:587:LEU:HD13	2.29	0.61
1:C:260:GLY:O	1:C:266:PHE:CD1	2.53	0.61
1:A:114:VAL:CG2	1:A:117:VAL:HG23	2.31	0.61
1:A:275:TRP:CD2	4:A:1103:POV:H27	2.36	0.61
1:A:260:GLY:O	1:A:266:PHE:CD1	2.53	0.61
5:D:1101:CLR:C16	5:D:1101:CLR:H232	2.29	0.61
1:D:259:SER:OG	5:D:1101:CLR:C19	2.48	0.61
1:C:266:PHE:CE1	5:C:1101:CLR:H72	2.35	0.60
5:A:1104:CLR:C16	5:A:1104:CLR:H232	2.30	0.60
1:A:697:PRO:HB3	1:A:771:HIS:CD2	2.37	0.60
1:C:114:VAL:CG2	1:C:117:VAL:HG23	2.30	0.60
1:D:114:VAL:CG2	1:D:117:VAL:HG23	2.31	0.60
1:D:345:ILE:O	1:D:376:VAL:HG22	2.01	0.60
1:D:697:PRO:HB3	1:D:771:HIS:CD2	2.37	0.60
1:A:879:ILE:O	1:A:879:ILE:CG1	2.49	0.60
1:C:114:VAL:CG2	1:C:117:VAL:HG21	2.26	0.60
1:C:697:PRO:HB3	1:C:771:HIS:CD2	2.37	0.60
1:B:879:ILE:O	1:B:879:ILE:CG1	2.50	0.60
1:A:259:SER:CB	5:A:1104:CLR:H193	2.29	0.60
1:A:345:ILE:O	1:A:376:VAL:HG22	2.01	0.59
1:B:697:PRO:HB3	1:B:771:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PHE:CE1	5:B:1102:CLR:H72	2.37	0.59
1:D:879:ILE:O	1:D:879:ILE:CG1	2.50	0.59
1:B:345:ILE:O	1:B:376:VAL:HG22	2.01	0.59
1:C:345:ILE:O	1:C:376:VAL:HG22	2.01	0.59
1:C:879:ILE:O	1:C:879:ILE:CG1	2.50	0.59
1:A:203:TRP:HH2	5:A:1104:CLR:H112	1.67	0.59
2:F:68:CYS:CB	4:F:301:POV:C23	2.69	0.59
4:A:1103:POV:H23	2:H:68:CYS:CB	2.33	0.59
2:F:68:CYS:SG	4:F:301:POV:H23	2.42	0.59
5:B:1102:CLR:H272	5:B:1102:CLR:C21	2.33	0.58
1:C:203:TRP:CH2	5:C:1101:CLR:H112	2.37	0.58
1:C:351:ILE:HD11	1:C:400:PHE:HE2	1.68	0.58
2:G:67:PHE:CE1	4:G:301:POV:H28A	2.36	0.58
5:D:1101:CLR:H272	5:D:1101:CLR:C21	2.34	0.58
1:A:351:ILE:HD11	1:A:400:PHE:HE2	1.68	0.57
5:A:1104:CLR:H272	5:A:1104:CLR:C21	2.34	0.57
1:B:259:SER:HB3	5:B:1102:CLR:H192	1.73	0.57
1:D:114:VAL:CG2	1:D:117:VAL:HG21	2.26	0.57
5:C:1101:CLR:H272	5:C:1101:CLR:C21	2.34	0.57
1:B:351:ILE:HD11	1:B:400:PHE:HE2	1.68	0.57
2:G:68:CYS:SG	4:G:301:POV:H22	2.45	0.57
1:A:259:SER:OG	5:A:1104:CLR:C19	2.46	0.57
1:C:203:TRP:CH2	5:C:1101:CLR:C1	2.88	0.56
1:D:351:ILE:HD11	1:D:400:PHE:HE2	1.68	0.56
2:F:92:ILE:HD11	2:F:116:GLN:OE1	2.05	0.56
1:C:266:PHE:CZ	5:C:1101:CLR:C7	2.87	0.56
1:C:330:LYS:O	1:C:330:LYS:HG2	2.06	0.56
1:D:330:LYS:HG2	1:D:330:LYS:O	2.06	0.56
2:E:92:ILE:HD11	2:E:116:GLN:OE1	2.05	0.56
2:G:92:ILE:HD11	2:G:116:GLN:OE1	2.05	0.56
1:D:347:VAL:CG1	1:D:377:PHE:CE1	2.88	0.56
2:H:92:ILE:HD11	2:H:116:GLN:OE1	2.05	0.56
1:A:580:LEU:CD2	1:A:587:LEU:CD1	2.84	0.56
1:B:347:VAL:CG1	1:B:377:PHE:CE1	2.89	0.56
1:A:347:VAL:CG1	1:A:377:PHE:CE1	2.89	0.55
1:C:580:LEU:CD2	1:C:587:LEU:CD1	2.84	0.55
1:D:580:LEU:CD2	1:D:587:LEU:CD1	2.84	0.55
2:F:67:PHE:CE1	4:F:301:POV:H28A	2.40	0.55
1:A:330:LYS:O	1:A:330:LYS:HG2	2.06	0.55
1:C:347:VAL:CG1	1:C:377:PHE:CE1	2.89	0.55
1:B:203:TRP:CZ3	5:B:1102:CLR:C1	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:LEU:CD2	1:B:587:LEU:CD1	2.84	0.55
1:B:266:PHE:CZ	5:B:1102:CLR:C7	2.89	0.55
1:C:104:MET:CG	1:C:111:THR:OG1	2.55	0.55
1:A:22:TRP:HE1	5:A:1104:CLR:H6	1.71	0.55
1:C:705:LEU:HD12	1:C:779:LEU:HD13	1.90	0.54
1:B:203:TRP:CZ3	5:B:1102:CLR:H11	2.43	0.54
1:D:705:LEU:HD12	1:D:779:LEU:HD13	1.90	0.54
1:A:705:LEU:HD12	1:A:779:LEU:HD13	1.90	0.54
5:C:1101:CLR:C16	5:C:1101:CLR:C23	2.86	0.54
1:C:347:VAL:HG11	1:C:377:PHE:CE1	2.43	0.54
1:A:104:MET:SD	1:A:111:THR:OG1	2.65	0.54
1:D:104:MET:CG	1:D:111:THR:OG1	2.55	0.54
1:D:347:VAL:HG11	1:D:377:PHE:CE1	2.43	0.54
1:B:330:LYS:O	1:B:330:LYS:HG2	2.06	0.54
1:B:705:LEU:HD12	1:B:779:LEU:HD13	1.90	0.54
1:C:22:TRP:HE1	5:C:1101:CLR:H6	1.72	0.54
1:C:203:TRP:CZ3	5:C:1101:CLR:C1	2.91	0.53
1:B:347:VAL:HG11	1:B:377:PHE:CE1	2.43	0.53
1:A:347:VAL:HG11	1:A:377:PHE:CE1	2.43	0.53
1:D:95:THR:HG22	1:D:95:THR:O	2.09	0.53
2:G:64:ILE:HG12	4:G:301:POV:C29	2.30	0.53
1:A:498:CYS:SG	1:A:799:MET:HG2	2.49	0.53
1:A:95:THR:HG22	1:A:95:THR:O	2.09	0.53
1:A:319:VAL:HG13	1:A:320:PRO:CD	2.39	0.53
1:B:498:CYS:SG	1:B:799:MET:HG2	2.49	0.53
1:B:319:VAL:HG13	1:B:320:PRO:CD	2.39	0.53
1:D:319:VAL:HG13	1:D:320:PRO:CD	2.39	0.53
1:D:498:CYS:SG	1:D:799:MET:HG2	2.49	0.53
4:A:1103:POV:H28	2:H:67:PHE:CE1	2.33	0.53
1:C:203:TRP:HH2	5:C:1101:CLR:H11	1.72	0.52
1:D:106:SER:HB2	1:D:116:VAL:HG23	1.90	0.52
1:D:317:SER:O	1:D:320:PRO:HD2	2.09	0.52
1:A:106:SER:HB2	1:A:116:VAL:HG23	1.90	0.52
1:C:319:VAL:HG13	1:C:320:PRO:CD	2.39	0.52
1:C:498:CYS:SG	1:C:799:MET:HG2	2.49	0.52
1:C:95:THR:HG22	1:C:95:THR:O	2.09	0.52
1:C:317:SER:O	1:C:320:PRO:HD2	2.10	0.52
1:C:375:ILE:O	1:C:376:VAL:HG13	2.10	0.52
2:G:68:CYS:HA	4:G:301:POV:H23A	1.91	0.52
1:A:104:MET:CG	1:A:111:THR:OG1	2.55	0.52
1:C:106:SER:HB2	1:C:116:VAL:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:ILE:O	1:D:376:VAL:HG13	2.10	0.52
1:B:106:SER:HB2	1:B:116:VAL:HG23	1.90	0.52
1:B:203:TRP:CH2	5:B:1102:CLR:C1	2.92	0.52
1:B:375:ILE:O	1:B:376:VAL:HG13	2.10	0.52
2:G:68:CYS:SG	4:G:301:POV:H22A	2.49	0.52
1:D:203:TRP:HH2	5:D:1101:CLR:C1	2.20	0.51
1:A:114:VAL:CG2	1:A:117:VAL:HG21	2.26	0.51
1:B:95:THR:O	1:B:95:THR:HG22	2.09	0.51
1:A:317:SER:O	1:A:320:PRO:HD2	2.09	0.51
1:B:114:VAL:HG23	1:B:117:VAL:CG2	2.37	0.51
1:B:317:SER:O	1:B:320:PRO:HD2	2.09	0.51
1:D:203:TRP:HZ3	5:D:1101:CLR:C1	2.23	0.51
1:C:203:TRP:CZ3	5:C:1101:CLR:H11	2.45	0.51
2:E:141:PRO:O	2:F:151:ARG:NH2	2.44	0.51
1:D:104:MET:SD	1:D:111:THR:OG1	2.65	0.51
1:A:114:VAL:HG23	1:A:114:VAL:O	2.10	0.51
1:D:22:TRP:NE1	5:D:1101:CLR:C6	2.73	0.51
1:B:104:MET:CG	1:B:111:THR:OG1	2.55	0.51
1:C:114:VAL:HG23	1:C:114:VAL:O	2.10	0.51
1:D:22:TRP:NE1	5:D:1101:CLR:H6	2.26	0.51
1:A:375:ILE:O	1:A:376:VAL:HG13	2.10	0.51
1:C:104:MET:SD	1:C:111:THR:OG1	2.66	0.51
1:D:114:VAL:HG23	1:D:114:VAL:O	2.10	0.51
2:G:92:ILE:HD11	2:G:116:GLN:CD	2.32	0.51
5:A:1104:CLR:C16	5:A:1104:CLR:C23	2.86	0.51
2:F:92:ILE:HD11	2:F:116:GLN:CD	2.32	0.51
2:H:92:ILE:HD11	2:H:116:GLN:CD	2.32	0.51
1:A:203:TRP:CH2	5:A:1104:CLR:H11	2.46	0.50
1:A:494:ILE:HG23	1:A:879:ILE:HD13	1.92	0.50
2:E:92:ILE:HD11	2:E:116:GLN:CD	2.32	0.50
1:B:494:ILE:HG23	1:B:879:ILE:HD13	1.92	0.50
1:D:114:VAL:CG2	1:D:117:VAL:CB	2.85	0.50
2:G:68:CYS:SG	4:G:301:POV:C23	2.99	0.50
1:B:114:VAL:HG23	1:B:114:VAL:O	2.10	0.50
5:C:1101:CLR:H232	5:C:1101:CLR:H161	1.94	0.50
1:D:259:SER:HB3	5:D:1101:CLR:H192	1.85	0.50
2:F:220:LEU:HD23	2:F:220:LEU:O	2.12	0.50
1:A:319:VAL:CG1	1:A:320:PRO:CD	2.82	0.49
1:C:114:VAL:CG2	1:C:117:VAL:CB	2.85	0.49
5:D:1101:CLR:H232	5:D:1101:CLR:H161	1.94	0.49
2:E:102:CYS:O	2:H:185:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:ILE:CG2	1:D:879:ILE:HD11	2.42	0.49
1:B:259:SER:CB	5:B:1102:CLR:H193	2.35	0.49
1:B:104:MET:SD	1:B:111:THR:OG1	2.65	0.49
1:A:494:ILE:CG2	1:A:879:ILE:HD11	2.42	0.49
1:C:494:ILE:CG2	1:C:879:ILE:HD11	2.42	0.49
5:B:1102:CLR:H183	5:B:1102:CLR:H20	1.68	0.49
1:C:375:ILE:O	1:C:376:VAL:CG1	2.61	0.49
1:D:336:TYR:CA	1:D:401:TYR:OH	2.61	0.49
1:C:41:LEU:HD23	2:G:220:LEU:HD21	1.69	0.48
1:B:375:ILE:O	1:B:376:VAL:CG1	2.61	0.48
5:B:1102:CLR:H232	5:B:1102:CLR:H161	1.94	0.48
1:D:319:VAL:CG1	1:D:320:PRO:CD	2.82	0.48
2:G:68:CYS:HA	4:G:301:POV:H22A	1.94	0.48
1:A:114:VAL:HG23	1:A:117:VAL:CG2	2.37	0.48
1:B:37:LEU:O	1:B:41:LEU:CD1	2.57	0.48
1:B:494:ILE:CG2	1:B:879:ILE:HD11	2.42	0.48
1:D:494:ILE:HG23	1:D:879:ILE:HD13	1.92	0.48
1:D:266:PHE:CZ	5:D:1101:CLR:C7	2.97	0.48
1:A:144:PHE:HE1	1:A:149:THR:CG2	2.25	0.48
1:B:44:ARG:HH21	1:B:44:ARG:HG3	1.78	0.48
1:D:266:PHE:CE1	5:D:1101:CLR:H72	2.49	0.48
5:A:1104:CLR:H232	5:A:1104:CLR:H161	1.94	0.48
1:D:375:ILE:O	1:D:376:VAL:CG1	2.61	0.48
1:D:22:TRP:HE1	5:D:1101:CLR:C6	2.26	0.48
2:F:185:ARG:HH22	2:G:104:ALA:HB3	1.79	0.48
2:G:68:CYS:HA	4:G:301:POV:C22	2.43	0.48
1:A:375:ILE:O	1:A:376:VAL:CG1	2.61	0.48
1:A:259:SER:CB	5:A:1104:CLR:H191	2.14	0.48
1:A:37:LEU:O	1:A:41:LEU:CD1	2.57	0.47
1:A:539:GLU:OE1	1:A:539:GLU:HA	2.15	0.47
1:B:114:VAL:CG2	1:B:117:VAL:HG21	2.26	0.47
1:B:539:GLU:OE1	1:B:539:GLU:HA	2.14	0.47
1:B:705:LEU:HD12	1:B:705:LEU:C	2.35	0.47
1:C:539:GLU:HA	1:C:539:GLU:OE1	2.15	0.47
1:D:705:LEU:HD12	1:D:705:LEU:C	2.35	0.47
1:A:705:LEU:HD12	1:A:705:LEU:C	2.35	0.47
2:E:185:ARG:NH2	2:F:104:ALA:HB3	2.17	0.47
5:A:1104:CLR:H183	5:A:1104:CLR:H20	1.68	0.47
1:B:579:ILE:CG2	1:B:939:THR:HG21	2.44	0.47
1:D:144:PHE:CE2	2:G:74:LEU:HD13	2.49	0.47
1:A:44:ARG:HH21	1:A:44:ARG:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ARG:HH21	1:C:44:ARG:HG3	1.78	0.47
1:B:323:ILE:HD12	1:B:323:ILE:H	1.80	0.47
1:C:494:ILE:HG23	1:C:879:ILE:HD13	1.92	0.47
1:A:346:VAL:HA	1:A:376:VAL:HG23	1.97	0.47
1:C:705:LEU:HD12	1:C:705:LEU:C	2.35	0.47
5:C:1101:CLR:H183	5:C:1101:CLR:H20	1.68	0.47
1:D:539:GLU:OE1	1:D:539:GLU:HA	2.15	0.47
5:B:1102:CLR:H221	5:B:1102:CLR:H162	1.58	0.47
1:B:319:VAL:CG1	1:B:320:PRO:CD	2.82	0.46
1:C:323:ILE:HD12	1:C:323:ILE:H	1.80	0.46
1:A:705:LEU:HD11	1:A:710:ALA:HB2	1.96	0.46
1:D:44:ARG:HH21	1:D:44:ARG:HG3	1.78	0.46
1:D:375:ILE:O	1:D:375:ILE:HG22	2.15	0.46
1:A:375:ILE:O	1:A:375:ILE:HG22	2.15	0.46
2:G:141:PRO:O	2:H:151:ARG:NH2	2.45	0.46
1:C:142:GLN:C	1:C:142:GLN:NE2	2.69	0.46
2:F:68:CYS:HA	4:F:301:POV:H23A	1.97	0.46
2:G:185:ARG:HH22	2:H:104:ALA:HB3	1.79	0.46
1:A:336:TYR:CA	1:A:401:TYR:OH	2.60	0.46
1:C:336:TYR:CA	1:C:401:TYR:OH	2.60	0.46
2:F:68:CYS:SG	4:F:301:POV:H22	2.56	0.46
1:B:142:GLN:NE2	1:B:142:GLN:C	2.69	0.46
1:B:346:VAL:HA	1:B:376:VAL:HG23	1.97	0.46
1:D:41:LEU:HB3	2:H:220:LEU:CD2	2.39	0.46
1:A:735:ARG:NH2	1:A:769:THR:O	2.49	0.46
1:D:142:GLN:NE2	1:D:142:GLN:C	2.69	0.46
1:D:323:ILE:HD12	1:D:323:ILE:H	1.80	0.46
1:B:375:ILE:O	1:B:375:ILE:HG22	2.15	0.46
1:B:705:LEU:HD11	1:B:710:ALA:HB2	1.96	0.46
1:C:261:ASP:OD1	1:C:268:ASN:HB3	2.16	0.46
1:D:735:ARG:NH2	1:D:769:THR:O	2.49	0.45
1:A:142:GLN:C	1:A:142:GLN:NE2	2.69	0.45
5:A:1104:CLR:H221	5:A:1104:CLR:H162	1.58	0.45
1:C:375:ILE:O	1:C:375:ILE:HG22	2.15	0.45
1:A:323:ILE:HD12	1:A:323:ILE:H	1.80	0.45
1:A:878:ILE:HG22	1:A:880:THR:HG23	1.99	0.45
1:B:144:PHE:HE1	1:B:149:THR:CG2	2.25	0.45
1:B:203:TRP:HZ3	5:B:1102:CLR:C1	2.30	0.45
1:C:346:VAL:HA	1:C:376:VAL:HG23	1.97	0.45
1:C:579:ILE:CG2	1:C:939:THR:HG21	2.44	0.45
1:C:735:ARG:NH2	1:C:769:THR:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:TRP:CD2	4:G:301:POV:H27	2.51	0.45
1:D:878:ILE:HG22	1:D:880:THR:HG23	1.99	0.45
1:B:336:TYR:CA	1:B:401:TYR:OH	2.61	0.45
1:C:319:VAL:CG1	1:C:320:PRO:CD	2.82	0.45
1:D:346:VAL:HA	1:D:376:VAL:HG23	1.97	0.45
2:F:68:CYS:SG	4:F:301:POV:H22A	2.56	0.45
1:B:261:ASP:OD1	1:B:268:ASN:HB3	2.16	0.45
1:B:735:ARG:NH2	1:B:769:THR:O	2.49	0.45
5:D:1101:CLR:C16	5:D:1101:CLR:C23	2.86	0.45
1:A:261:ASP:OD1	1:A:268:ASN:HB3	2.16	0.45
1:C:275:TRP:CD2	4:F:301:POV:H27	2.52	0.45
1:D:261:ASP:OD1	1:D:268:ASN:HB3	2.16	0.45
1:D:579:ILE:CG2	1:D:939:THR:HG21	2.44	0.45
5:D:1101:CLR:H162	5:D:1101:CLR:H221	1.58	0.45
1:D:347:VAL:HG11	1:D:377:PHE:HE1	1.81	0.45
2:F:68:CYS:SG	4:F:301:POV:C23	3.05	0.45
1:C:144:PHE:HE1	1:C:149:THR:CG2	2.25	0.45
1:C:336:TYR:O	1:C:336:TYR:CG	2.70	0.45
1:C:878:ILE:HG22	1:C:880:THR:HG23	1.99	0.45
1:A:275:TRP:CZ2	4:A:1103:POV:H28A	2.52	0.44
1:B:336:TYR:O	1:B:336:TYR:CG	2.70	0.44
1:D:336:TYR:O	1:D:336:TYR:CG	2.70	0.44
1:A:336:TYR:O	1:A:336:TYR:CD2	2.71	0.44
1:A:1016:ARG:O	1:A:1031:ARG:HB3	2.18	0.44
1:C:336:TYR:O	1:C:336:TYR:CD2	2.71	0.44
1:C:1016:ARG:O	1:C:1031:ARG:HB3	2.18	0.44
1:B:319:VAL:N	1:B:320:PRO:CD	2.81	0.44
1:A:697:PRO:HB3	1:A:771:HIS:NE2	2.33	0.44
1:B:878:ILE:HG22	1:B:880:THR:HG23	1.99	0.44
1:C:347:VAL:HG11	1:C:377:PHE:HE1	1.81	0.44
1:D:697:PRO:HB3	1:D:771:HIS:NE2	2.33	0.44
1:A:347:VAL:CG1	1:A:377:PHE:HE1	2.31	0.44
1:B:336:TYR:O	1:B:336:TYR:CD2	2.71	0.44
1:B:697:PRO:HB3	1:B:771:HIS:NE2	2.33	0.44
1:C:319:VAL:N	1:C:320:PRO:CD	2.81	0.44
1:C:705:LEU:HD11	1:C:710:ALA:HB2	1.96	0.44
1:D:203:TRP:CH2	5:D:1101:CLR:H12	2.50	0.44
2:F:81:GLU:N	2:F:81:GLU:OE1	2.51	0.44
2:G:81:GLU:N	2:G:81:GLU:OE1	2.51	0.44
1:D:336:TYR:O	1:D:336:TYR:CD2	2.71	0.44
1:A:336:TYR:O	1:A:336:TYR:CG	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1016:ARG:O	1:B:1031:ARG:HB3	2.18	0.44
1:C:347:VAL:CG1	1:C:377:PHE:HE1	2.31	0.44
1:C:697:PRO:HB3	1:C:771:HIS:NE2	2.33	0.44
1:A:145:TYR:O	1:A:147:ASP:O	2.36	0.43
1:D:203:TRP:HZ3	5:D:1101:CLR:H21	1.83	0.43
2:E:81:GLU:N	2:E:81:GLU:OE1	2.51	0.43
2:H:81:GLU:OE1	2:H:81:GLU:N	2.51	0.43
1:D:1016:ARG:O	1:D:1031:ARG:HB3	2.17	0.43
1:C:145:TYR:O	1:C:147:ASP:O	2.36	0.43
1:D:144:PHE:HE1	1:D:149:THR:CG2	2.25	0.43
1:D:319:VAL:N	1:D:320:PRO:CD	2.81	0.43
1:D:347:VAL:CG1	1:D:377:PHE:HE1	2.31	0.43
1:B:879:ILE:O	1:B:879:ILE:HG13	2.19	0.43
1:D:145:TYR:O	1:D:147:ASP:O	2.36	0.43
2:H:180:PHE:CE2	2:H:182:GLN:HG2	2.54	0.43
1:A:347:VAL:HG11	1:A:377:PHE:HE1	1.81	0.43
1:B:145:TYR:O	1:B:147:ASP:O	2.36	0.43
2:E:180:PHE:CE2	2:E:182:GLN:HG2	2.54	0.43
1:C:879:ILE:O	1:C:879:ILE:HG13	2.19	0.43
2:F:180:PHE:CE2	2:F:182:GLN:HG2	2.54	0.43
2:F:118:TYR:CE1	2:F:129:LEU:CD1	3.02	0.43
2:H:118:TYR:CE1	2:H:129:LEU:CD1	3.02	0.43
1:B:96:SER:HA	1:B:99:ASP:HB3	2.01	0.43
2:G:180:PHE:CE2	2:G:182:GLN:HG2	2.54	0.43
1:A:203:TRP:HH2	5:A:1104:CLR:H11	1.83	0.42
1:B:347:VAL:CG1	1:B:377:PHE:HE1	2.31	0.42
1:A:22:TRP:HE1	5:A:1104:CLR:C6	2.31	0.42
1:A:351:ILE:O	1:A:351:ILE:HG13	2.20	0.42
1:A:319:VAL:N	1:A:320:PRO:CD	2.81	0.42
1:C:351:ILE:HG13	1:C:351:ILE:O	2.19	0.42
2:G:118:TYR:CE1	2:G:129:LEU:CD1	3.02	0.42
1:A:266:PHE:CZ	5:A:1104:CLR:H71	2.53	0.42
1:A:579:ILE:CG2	1:A:939:THR:HG21	2.44	0.42
4:A:1103:POV:C28	2:H:67:PHE:HE1	2.24	0.42
1:A:96:SER:HA	1:A:99:ASP:HB3	2.01	0.42
1:C:96:SER:HA	1:C:99:ASP:HB3	2.01	0.42
1:D:375:ILE:C	1:D:376:VAL:HG13	2.40	0.42
1:C:375:ILE:C	1:C:376:VAL:HG13	2.40	0.42
1:D:96:SER:HA	1:D:99:ASP:HB3	2.01	0.42
2:E:118:TYR:CE1	2:E:129:LEU:CD1	3.02	0.42
1:B:347:VAL:HG11	1:B:377:PHE:HE1	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ILE:C	1:A:376:VAL:HG13	2.40	0.42
1:C:203:TRP:HH2	5:C:1101:CLR:C1	2.29	0.42
1:D:351:ILE:HG13	1:D:351:ILE:O	2.20	0.42
1:A:879:ILE:O	1:A:879:ILE:HG13	2.19	0.41
1:A:98:LYS:HE2	1:A:98:LYS:HA	2.03	0.41
1:B:22:TRP:HE1	5:B:1102:CLR:H6	1.85	0.41
5:C:1101:CLR:H162	5:C:1101:CLR:H221	1.58	0.41
1:D:580:LEU:HD12	1:D:580:LEU:HA	1.88	0.41
1:B:375:ILE:C	1:B:376:VAL:HG13	2.40	0.41
1:B:705:LEU:O	1:B:779:LEU:HD12	2.21	0.41
1:C:104:MET:CG	1:C:111:THR:HG1	2.29	0.41
1:D:705:LEU:HD11	1:D:710:ALA:HB2	1.96	0.41
1:B:275:TRP:HB3	4:B:1101:POV:H32	2.03	0.41
5:B:1102:CLR:C16	5:B:1102:CLR:C23	2.86	0.41
1:A:41:LEU:CG	2:E:220:LEU:CD2	2.99	0.41
1:B:275:TRP:CE2	4:B:1101:POV:H25A	2.55	0.41
1:D:879:ILE:O	1:D:879:ILE:HG13	2.19	0.41
2:F:141:PRO:O	2:G:151:ARG:NH2	2.48	0.41
1:B:98:LYS:HE2	1:B:98:LYS:HA	2.03	0.41
1:B:351:ILE:O	1:B:351:ILE:HG13	2.19	0.41
1:D:37:LEU:O	1:D:41:LEU:CD1	2.57	0.41
1:B:455:ARG:HA	1:B:481:ASP:OD1	2.21	0.41
1:C:98:LYS:HE2	1:C:98:LYS:HA	2.03	0.41
1:D:705:LEU:O	1:D:779:LEU:HD12	2.21	0.41
1:A:705:LEU:CD1	1:A:779:LEU:HD13	2.51	0.41
1:B:203:TRP:HH2	5:B:1102:CLR:H11	1.82	0.41
1:C:705:LEU:O	1:C:779:LEU:HD12	2.21	0.41
1:A:579:ILE:HD12	1:A:579:ILE:HA	1.94	0.41
1:A:705:LEU:O	1:A:779:LEU:HD12	2.21	0.41
1:C:37:LEU:O	1:C:41:LEU:CD1	2.57	0.41
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.94	0.41
1:C:803:LEU:HA	1:C:881:GLU:OE2	2.21	0.41
1:D:98:LYS:HE2	1:D:98:LYS:HA	2.03	0.41
1:A:803:LEU:HA	1:A:881:GLU:OE2	2.21	0.40
1:B:803:LEU:HA	1:B:881:GLU:OE2	2.21	0.40
1:C:22:TRP:NE1	5:C:1101:CLR:C6	2.84	0.40
1:A:799:MET:SD	1:A:879:ILE:HG23	2.62	0.40
1:C:705:LEU:CD1	1:C:779:LEU:HD13	2.51	0.40
1:D:803:LEU:HA	1:D:881:GLU:OE2	2.21	0.40
2:F:68:CYS:HA	4:F:301:POV:H22A	2.02	0.40
1:A:330:LYS:O	1:A:330:LYS:CG	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:MET:SD	1:C:879:ILE:HG23	2.62	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	877/1056 (83%)	811 (92%)	49 (6%)	17 (2%)	6	34
1	B	877/1056 (83%)	811 (92%)	50 (6%)	16 (2%)	7	35
1	C	877/1056 (83%)	811 (92%)	50 (6%)	16 (2%)	7	35
1	D	877/1056 (83%)	811 (92%)	50 (6%)	16 (2%)	7	35
2	E	210/239 (88%)	190 (90%)	15 (7%)	5 (2%)	5	30
2	F	210/239 (88%)	190 (90%)	15 (7%)	5 (2%)	5	30
2	G	210/239 (88%)	190 (90%)	15 (7%)	5 (2%)	5	30
2	H	210/239 (88%)	190 (90%)	15 (7%)	5 (2%)	5	30
All	All	4348/5180 (84%)	4004 (92%)	259 (6%)	85 (2%)	8	33

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	385	LEU
1	B	108	GLN
1	B	385	LEU
1	C	108	GLN
1	C	385	LEU
1	D	108	GLN
1	D	385	LEU
1	A	114	VAL

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Mol	Chain	Res	Type
1	A	148	PHE
1	A	172	ASN
1	A	614	ALA
1	B	114	VAL
1	B	148	PHE
1	B	172	ASN
1	B	614	ALA
1	C	114	VAL
1	C	148	PHE
1	C	172	ASN
1	C	614	ALA
1	D	114	VAL
1	D	148	PHE
1	D	172	ASN
1	D	614	ALA
2	E	66	GLY
2	F	66	GLY
2	G	66	GLY
2	H	66	GLY
1	A	613	LYS
1	A	808	ASN
1	A	1039	TYR
1	B	613	LYS
1	B	808	ASN
1	B	1039	TYR
1	C	613	LYS
1	C	808	ASN
1	C	1039	TYR
1	D	613	LYS
1	D	808	ASN
1	D	1039	TYR
2	E	25	ILE
2	E	28	HIS
2	E	197	GLU
2	F	25	ILE
2	F	28	HIS
2	F	197	GLU
2	G	25	ILE
2	G	28	HIS
2	G	197	GLU
2	H	25	ILE
2	H	28	HIS

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Mol	Chain	Res	Type
2	H	197	GLU
1	A	578	ARG
1	A	601	ASP
1	B	601	ASP
1	C	601	ASP
1	D	601	ASP
2	E	38	THR
2	F	38	THR
2	G	38	THR
2	H	38	THR
1	A	335	SER
1	A	370	ASP
1	A	774	PRO
1	B	335	SER
1	B	370	ASP
1	B	774	PRO
1	C	335	SER
1	C	370	ASP
1	C	774	PRO
1	D	335	SER
1	D	370	ASP
1	D	774	PRO
1	A	579	ILE
1	B	579	ILE
1	C	579	ILE
1	D	579	ILE
1	A	334	GLY
1	B	334	GLY
1	C	334	GLY
1	D	334	GLY
1	C	371	VAL
1	A	371	VAL
1	B	371	VAL
1	D	371	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	781/928 (84%)	768 (98%)	13 (2%)	56	75
1	B	781/928 (84%)	768 (98%)	13 (2%)	56	75
1	C	781/928 (84%)	768 (98%)	13 (2%)	56	75
1	D	781/928 (84%)	768 (98%)	13 (2%)	56	75
2	E	178/218 (82%)	176 (99%)	2 (1%)	70	83
2	F	178/218 (82%)	177 (99%)	1 (1%)	84	91
2	G	178/218 (82%)	176 (99%)	2 (1%)	70	83
2	H	178/218 (82%)	176 (99%)	2 (1%)	70	83
All	All	3836/4584 (84%)	3777 (98%)	59 (2%)	60	77

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	145	TYR
1	A	158	VAL
1	A	210	ARG
1	A	321	GLU
1	A	384	ASN
1	A	410	ASP
1	A	423	LEU
1	A	428	LYS
1	A	560	LYS
1	A	578	ARG
1	A	707	ARG
1	A	735	ARG
1	B	142	GLN
1	B	145	TYR
1	B	158	VAL
1	B	210	ARG
1	B	321	GLU
1	B	384	ASN
1	B	410	ASP
1	B	423	LEU
1	B	428	LYS
1	B	560	LYS
1	B	578	ARG
1	B	707	ARG
1	B	735	ARG
1	C	142	GLN

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Mol	Chain	Res	Type
1	C	145	TYR
1	C	158	VAL
1	C	210	ARG
1	C	321	GLU
1	C	384	ASN
1	C	410	ASP
1	C	423	LEU
1	C	428	LYS
1	C	560	LYS
1	C	578	ARG
1	C	707	ARG
1	C	735	ARG
1	D	142	GLN
1	D	145	TYR
1	D	158	VAL
1	D	210	ARG
1	D	321	GLU
1	D	384	ASN
1	D	410	ASP
1	D	423	LEU
1	D	428	LYS
1	D	560	LYS
1	D	578	ARG
1	D	707	ARG
1	D	735	ARG
2	E	67	PHE
2	E	220	LEU
2	F	67	PHE
2	G	67	PHE
2	G	220	LEU
2	H	67	PHE
2	H	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	379	HIS
1	A	451	HIS
1	A	749	HIS
1	B	142	GLN
1	B	379	HIS

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Mol	Chain	Res	Type
1	B	451	HIS
1	B	749	HIS
1	C	142	GLN
1	C	379	HIS
1	C	451	HIS
1	C	749	HIS
1	D	142	GLN
1	D	379	HIS
1	D	451	HIS
1	D	749	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
4	POV	B	1101	-	30,30,51	1.18	2 (6%)	33,35,59	1.25	3 (9%)
4	POV	F	301	-	33,33,51	0.65	1 (3%)	36,38,59	0.56	0
4	POV	G	301	-	33,33,51	0.65	1 (3%)	36,38,59	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CLR	D	1101	-	31,31,31	0.85	2 (6%)	48,48,48	1.57	8 (16%)
5	CLR	B	1102	-	31,31,31	0.85	2 (6%)	48,48,48	1.57	8 (16%)
5	CLR	A	1104	-	31,31,31	0.85	2 (6%)	48,48,48	1.57	8 (16%)
5	CLR	C	1101	-	31,31,31	0.85	2 (6%)	48,48,48	1.57	8 (16%)
4	POV	A	1103	-	33,33,51	0.65	1 (3%)	36,38,59	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	B	1101	-	-	15/34/34/55	-
4	POV	F	301	-	-	7/37/37/55	-
4	POV	G	301	-	-	7/37/37/55	-
5	CLR	D	1101	-	-	6/10/68/68	0/4/4/4
5	CLR	B	1102	-	-	6/10/68/68	0/4/4/4
5	CLR	A	1104	-	-	6/10/68/68	0/4/4/4
5	CLR	C	1101	-	-	6/10/68/68	0/4/4/4
4	POV	A	1103	-	-	7/37/37/55	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	POV	O31-C31	4.26	1.45	1.33
4	B	1101	POV	O21-C21	4.09	1.45	1.34
5	B	1102	CLR	C10-C9	-2.20	1.52	1.56
5	D	1101	CLR	C10-C9	-2.18	1.52	1.56
4	G	301	POV	P-O12	2.18	1.66	1.58
4	A	1103	POV	P-O12	2.17	1.66	1.58
5	C	1101	CLR	C10-C9	-2.17	1.52	1.56
4	F	301	POV	P-O12	2.16	1.66	1.58
5	A	1104	CLR	C10-C9	-2.16	1.52	1.56
5	A	1104	CLR	C13-C14	-2.12	1.51	1.55
5	D	1101	CLR	C13-C14	-2.11	1.51	1.55
5	C	1101	CLR	C13-C14	-2.10	1.51	1.55
5	B	1102	CLR	C13-C14	-2.10	1.51	1.55

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1102	CLR	C13-C17-C20	-4.76	112.14	119.50
5	D	1101	CLR	C13-C17-C20	-4.74	112.18	119.50
5	A	1104	CLR	C13-C17-C20	-4.73	112.20	119.50
5	C	1101	CLR	C13-C17-C20	-4.73	112.20	119.50
5	B	1102	CLR	C13-C14-C8	-4.16	108.51	114.41
5	D	1101	CLR	C13-C14-C8	-4.15	108.52	114.41
5	A	1104	CLR	C13-C14-C8	-4.14	108.53	114.41
5	C	1101	CLR	C13-C14-C8	-4.13	108.56	114.41
4	B	1101	POV	O21-C21-C22	4.04	120.23	111.48
5	C	1101	CLR	C17-C13-C14	3.40	104.00	100.10
5	D	1101	CLR	C17-C13-C14	3.37	103.96	100.10
5	A	1104	CLR	C17-C13-C14	3.36	103.96	100.10
5	B	1102	CLR	C17-C13-C14	3.36	103.95	100.10
4	B	1101	POV	O31-C31-C32	2.77	120.29	111.83
5	A	1104	CLR	C4-C5-C10	2.72	119.90	116.42
5	D	1101	CLR	C4-C5-C10	2.71	119.89	116.42
5	C	1101	CLR	C4-C5-C10	2.71	119.89	116.42
5	B	1102	CLR	C4-C5-C10	2.69	119.87	116.42
5	A	1104	CLR	C11-C12-C13	-2.66	108.25	112.74
5	C	1101	CLR	C11-C12-C13	-2.66	108.25	112.74
5	D	1101	CLR	C11-C12-C13	-2.66	108.25	112.74
5	B	1102	CLR	C11-C12-C13	-2.63	108.31	112.74
4	B	1101	POV	C2-O21-C21	-2.58	111.62	117.80
5	B	1102	CLR	C7-C6-C5	-2.28	121.17	125.02
5	C	1101	CLR	C7-C6-C5	-2.27	121.18	125.02
5	A	1104	CLR	C7-C6-C5	-2.27	121.19	125.02
5	D	1101	CLR	C7-C6-C5	-2.24	121.25	125.02
5	C	1101	CLR	C10-C9-C8	-2.20	109.50	112.71
5	B	1102	CLR	C10-C9-C8	-2.14	109.58	112.71
5	A	1104	CLR	C10-C9-C8	-2.14	109.58	112.71
5	D	1101	CLR	C10-C9-C8	-2.12	109.61	112.71
5	D	1101	CLR	C10-C5-C6	-2.11	119.85	122.93
5	C	1101	CLR	C10-C5-C6	-2.08	119.89	122.93
5	A	1104	CLR	C10-C5-C6	-2.06	119.92	122.93
5	B	1102	CLR	C10-C5-C6	-2.05	119.93	122.93

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1101	POV	C11-O12-P-O13
4	B	1101	POV	C22-C21-O21-C2
5	A	1104	CLR	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
5	B	1102	CLR	C13-C17-C20-C21
5	C	1101	CLR	C13-C17-C20-C21
5	D	1101	CLR	C13-C17-C20-C21
4	B	1101	POV	O22-C21-O21-C2
5	A	1104	CLR	C16-C17-C20-C21
5	B	1102	CLR	C16-C17-C20-C21
5	C	1101	CLR	C16-C17-C20-C21
5	D	1101	CLR	C16-C17-C20-C21
5	A	1104	CLR	C13-C17-C20-C22
5	B	1102	CLR	C13-C17-C20-C22
5	C	1101	CLR	C13-C17-C20-C22
5	D	1101	CLR	C13-C17-C20-C22
5	A	1104	CLR	C16-C17-C20-C22
5	B	1102	CLR	C16-C17-C20-C22
5	C	1101	CLR	C16-C17-C20-C22
5	D	1101	CLR	C16-C17-C20-C22
4	B	1101	POV	C32-C31-O31-C3
4	B	1101	POV	C32-C33-C34-C35
4	B	1101	POV	O32-C31-O31-C3
4	B	1101	POV	C22-C23-C24-C25
4	G	301	POV	C22-C23-C24-C25
4	A	1103	POV	C22-C23-C24-C25
4	F	301	POV	C22-C23-C24-C25
5	A	1104	CLR	C23-C24-C25-C26
5	B	1102	CLR	C23-C24-C25-C26
5	C	1101	CLR	C23-C24-C25-C26
5	D	1101	CLR	C23-C24-C25-C26
4	B	1101	POV	C31-C32-C33-C34
4	B	1101	POV	C35-C36-C37-C38
4	B	1101	POV	C25-C26-C27-C28
4	B	1101	POV	O21-C2-C3-O31
5	A	1104	CLR	C23-C24-C25-C27
5	B	1102	CLR	C23-C24-C25-C27
5	C	1101	CLR	C23-C24-C25-C27
5	D	1101	CLR	C23-C24-C25-C27
4	B	1101	POV	C24-C25-C26-C27
4	A	1103	POV	O11-C1-C2-O21
4	F	301	POV	O11-C1-C2-O21
4	G	301	POV	O11-C1-C2-O21
4	B	1101	POV	C1-C2-C3-O31
4	B	1101	POV	C33-C34-C35-C36
4	B	1101	POV	C34-C35-C36-C37

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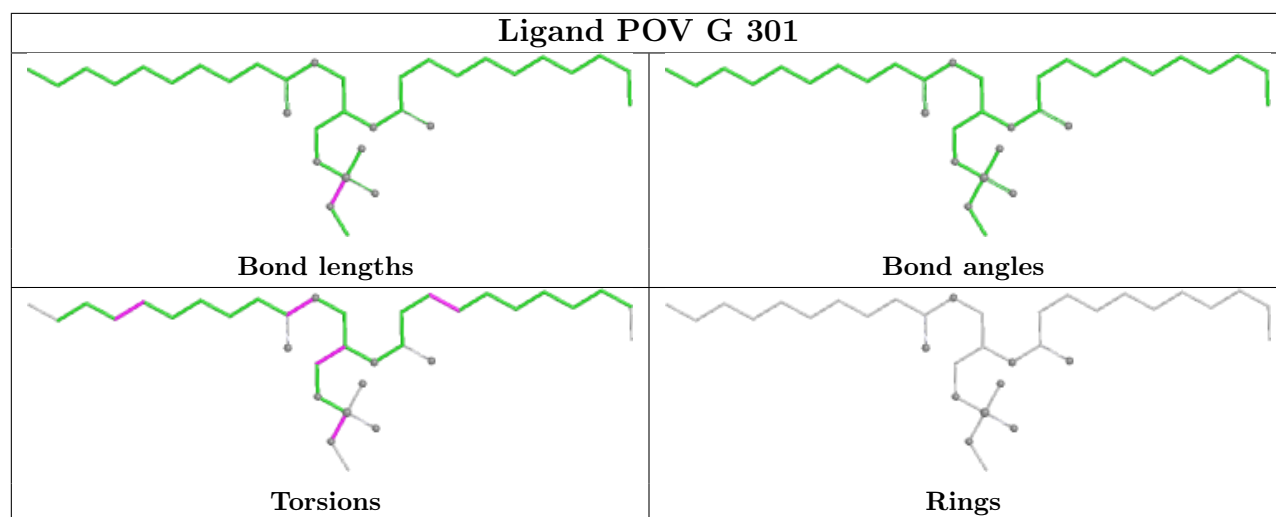
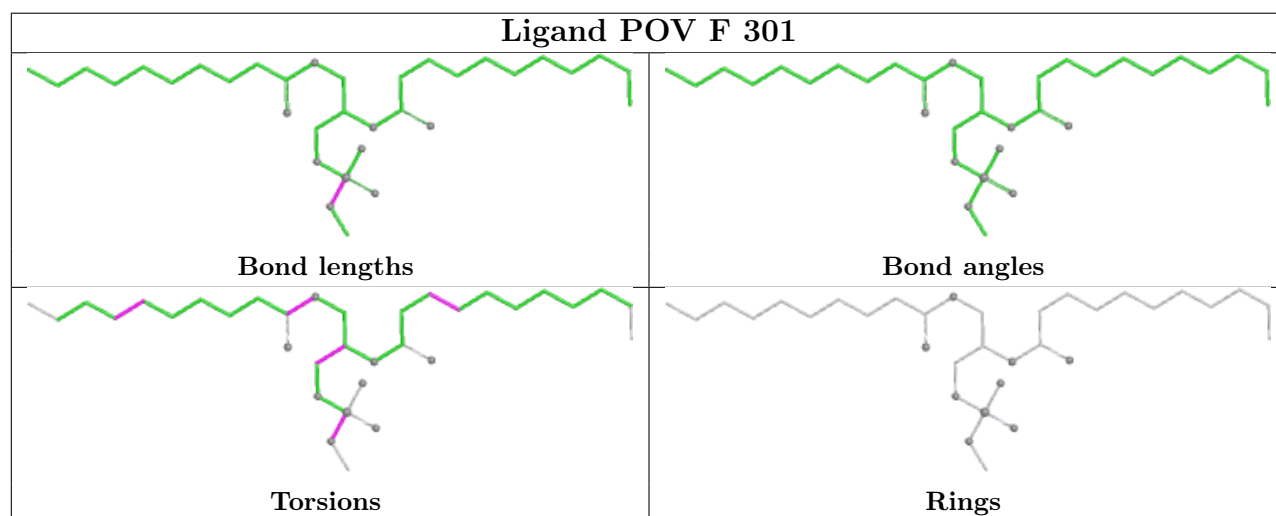
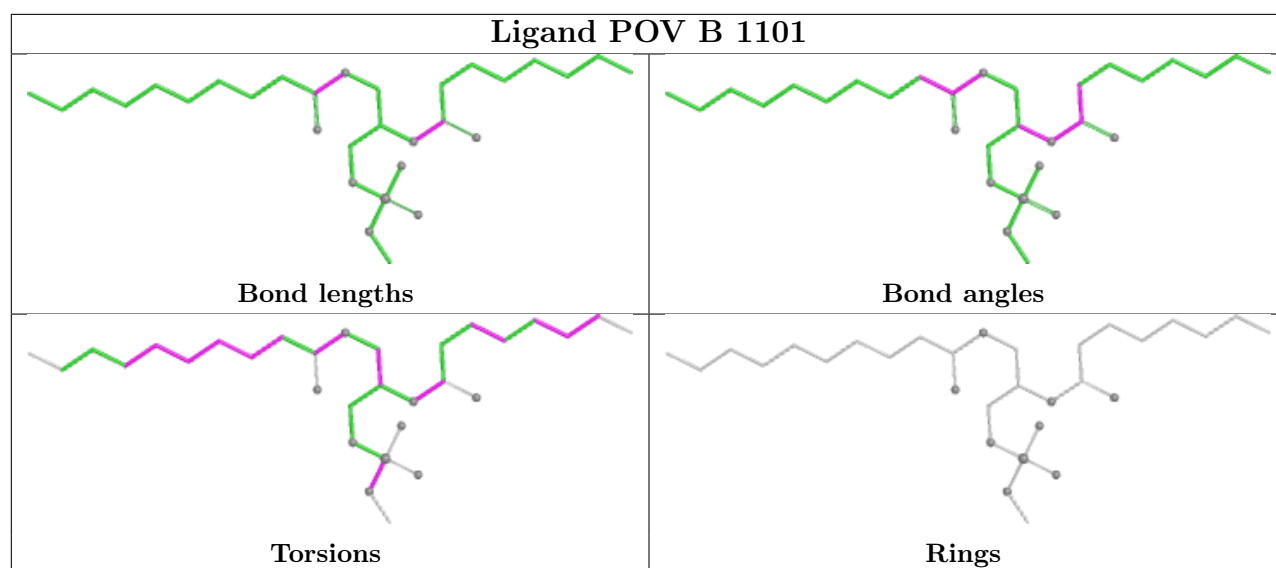
Mol	Chain	Res	Type	Atoms
4	A	1103	POV	C11-O12-P-O13
4	F	301	POV	C11-O12-P-O13
4	G	301	POV	C11-O12-P-O13
4	A	1103	POV	C35-C36-C37-C38
4	F	301	POV	C35-C36-C37-C38
4	G	301	POV	C35-C36-C37-C38
4	A	1103	POV	C32-C31-O31-C3
4	F	301	POV	C32-C31-O31-C3
4	G	301	POV	C32-C31-O31-C3
4	A	1103	POV	O32-C31-O31-C3
4	F	301	POV	O32-C31-O31-C3
4	G	301	POV	O32-C31-O31-C3
4	A	1103	POV	O11-C1-C2-C3
4	F	301	POV	O11-C1-C2-C3
4	G	301	POV	O11-C1-C2-C3

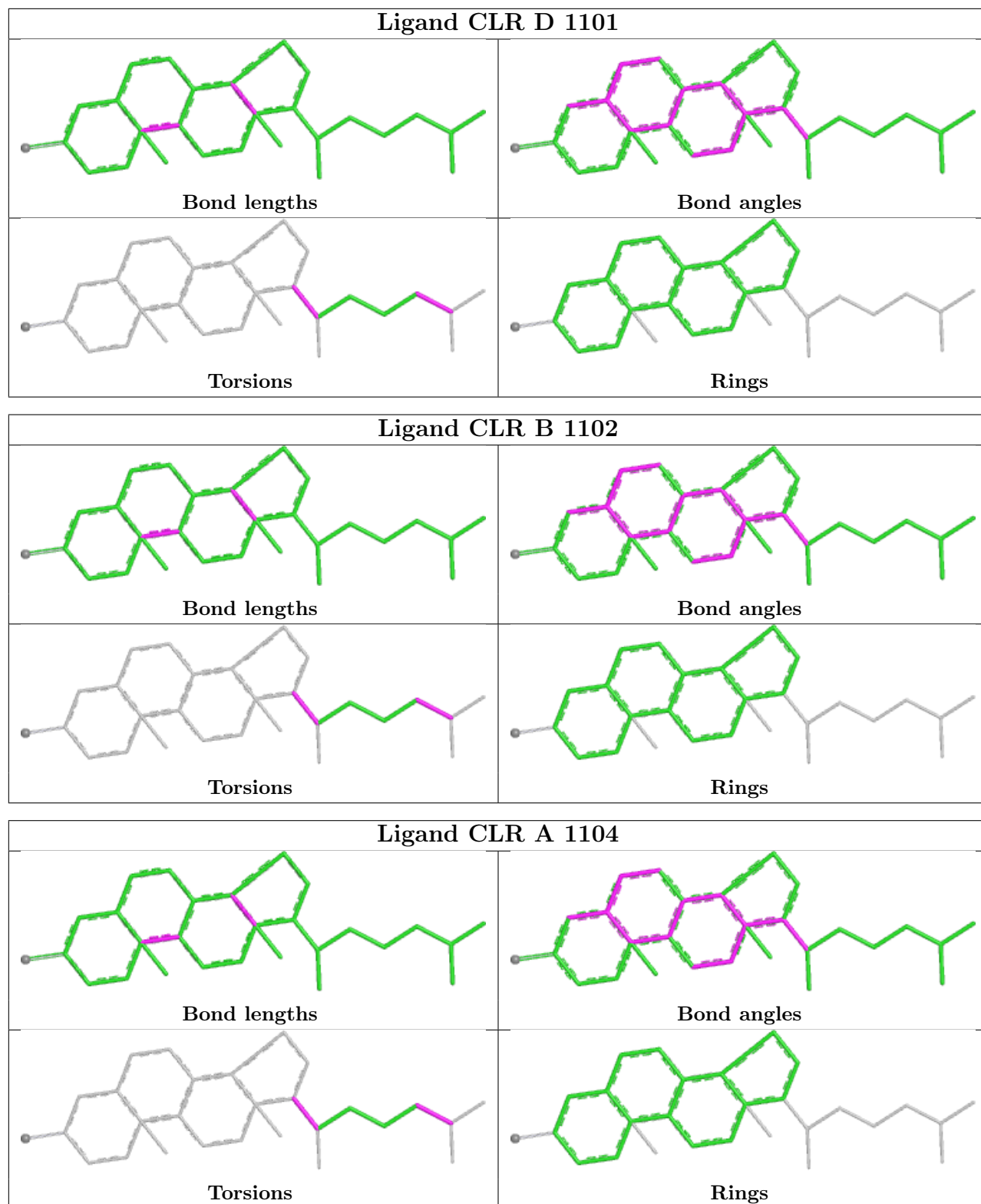
There are no ring outliers.

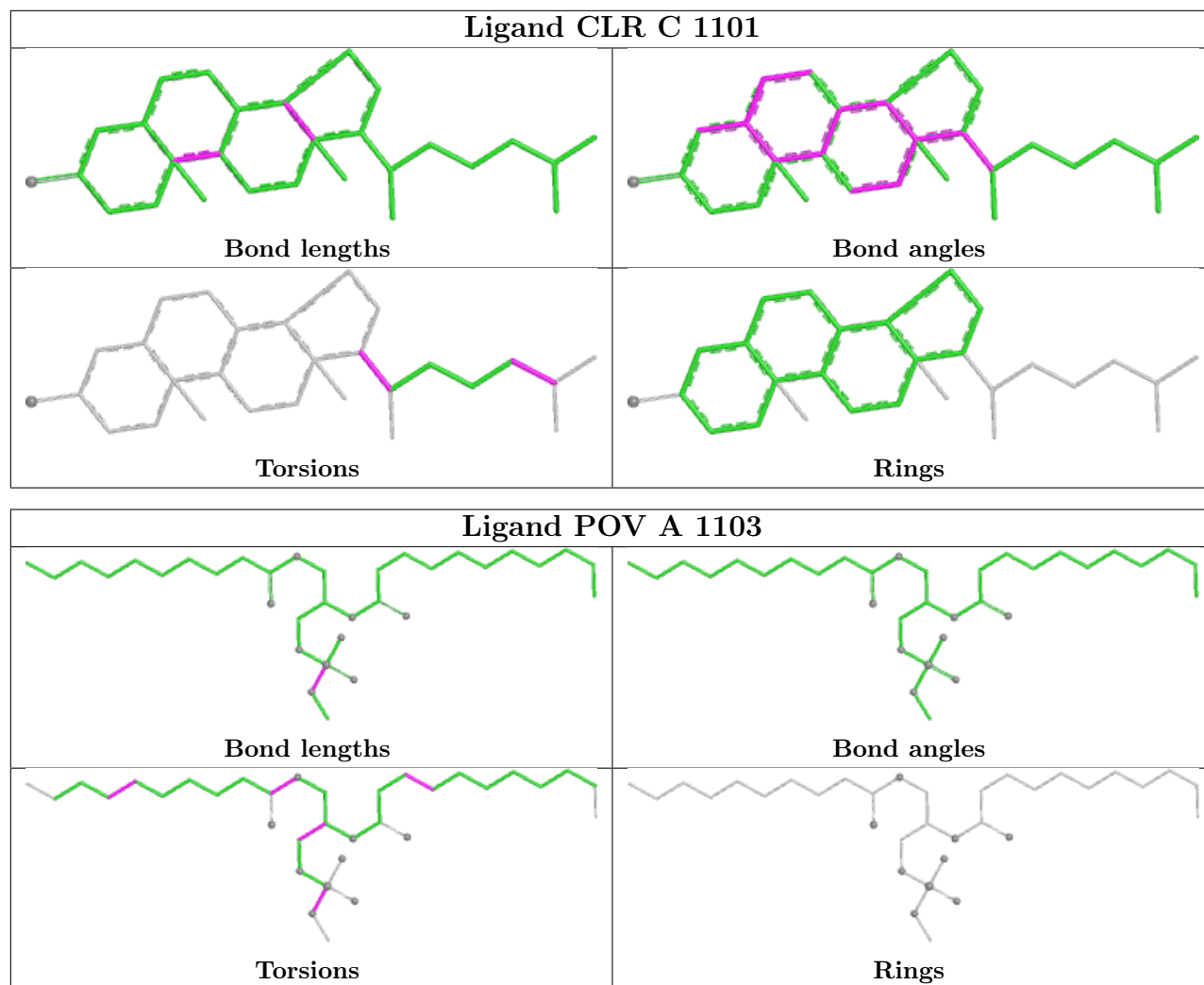
8 monomers are involved in 172 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1101	POV	2	0
4	F	301	POV	20	0
4	G	301	POV	22	0
5	D	1101	CLR	34	0
5	B	1102	CLR	30	0
5	A	1104	CLR	27	0
5	C	1101	CLR	30	0
4	A	1103	POV	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



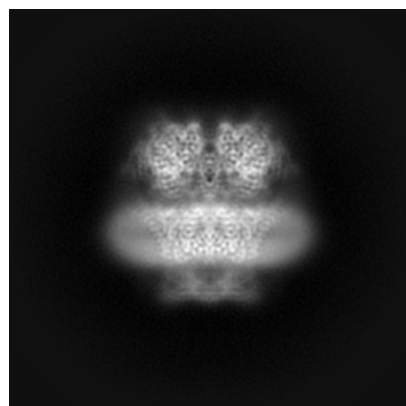
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46419. These allow visual inspection of the internal detail of the map and identification of artifacts.

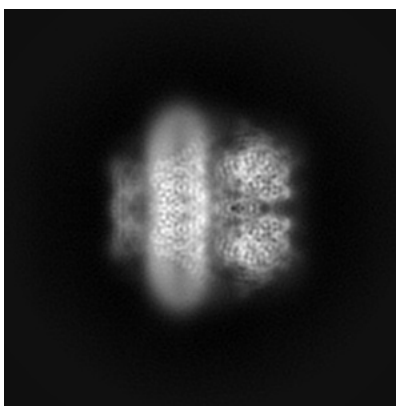
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

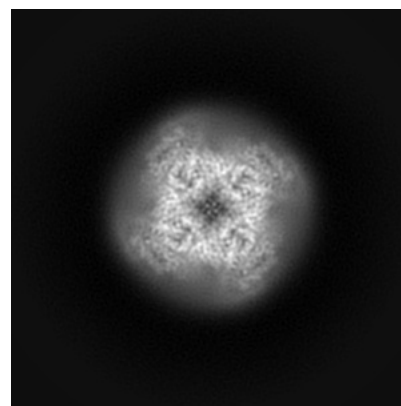
#### 6.1.1 Primary map



X

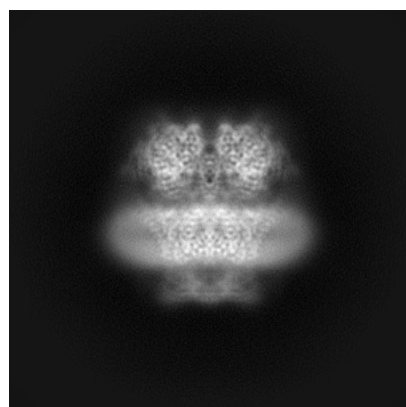


Y

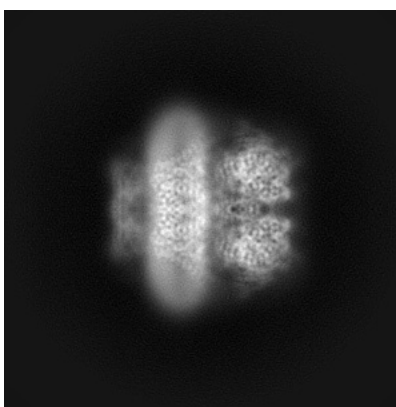


Z

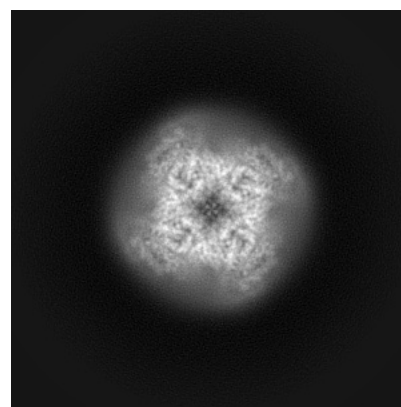
#### 6.1.2 Raw map



X



Y

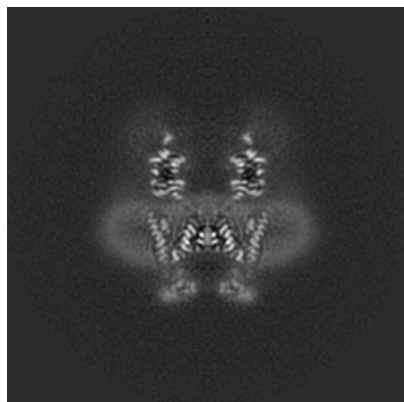


Z

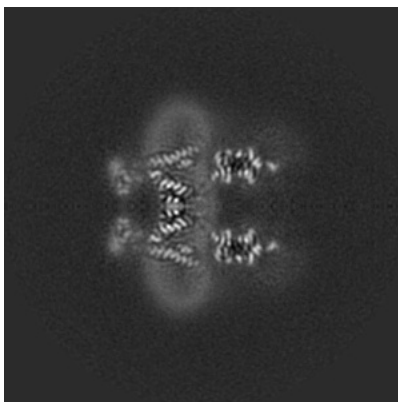
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

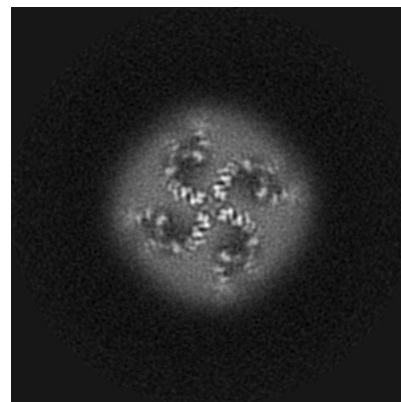
### 6.2.1 Primary map



X Index: 150

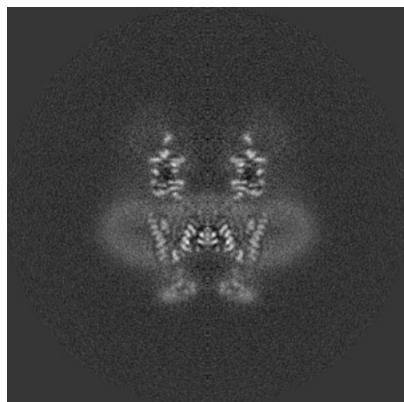


Y Index: 150

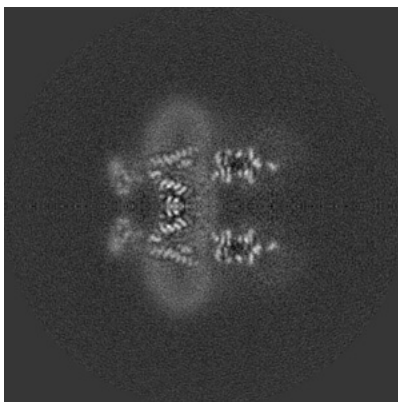


Z Index: 150

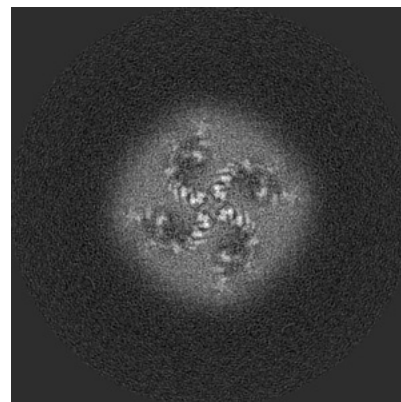
### 6.2.2 Raw map



X Index: 150



Y Index: 150

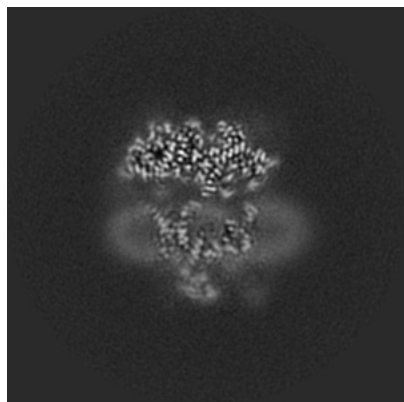


Z Index: 150

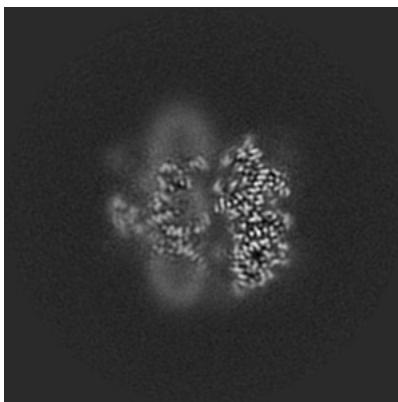
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

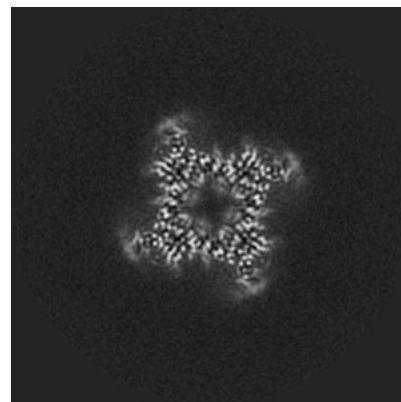
### 6.3.1 Primary map



X Index: 176

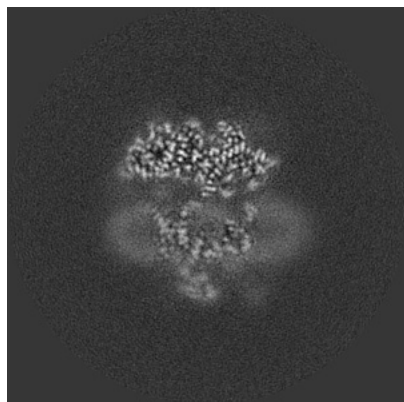


Y Index: 124

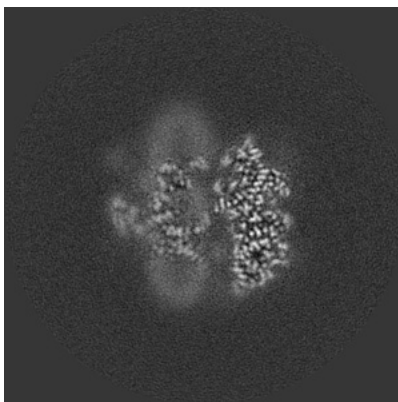


Z Index: 179

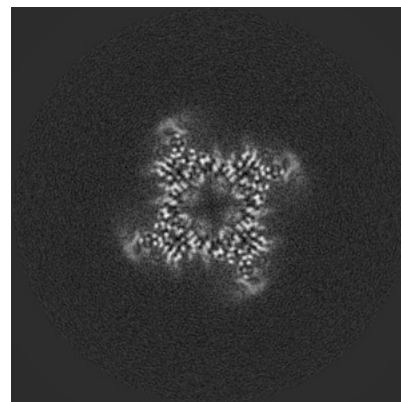
### 6.3.2 Raw map



X Index: 176



Y Index: 124

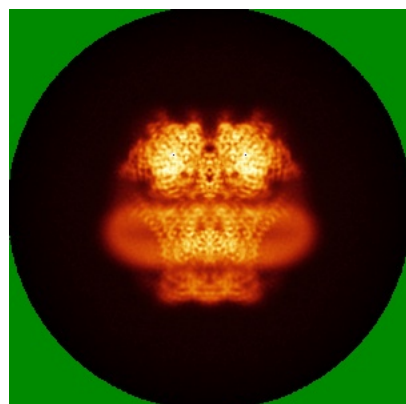


Z Index: 179

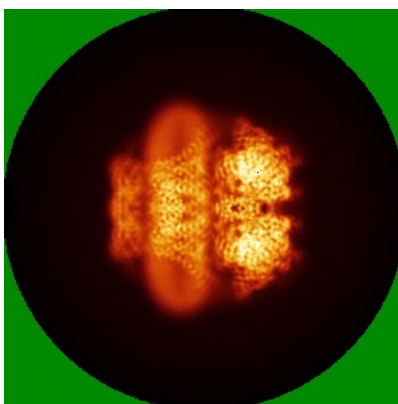
The images above show the largest variance slices of the map in three orthogonal directions.

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

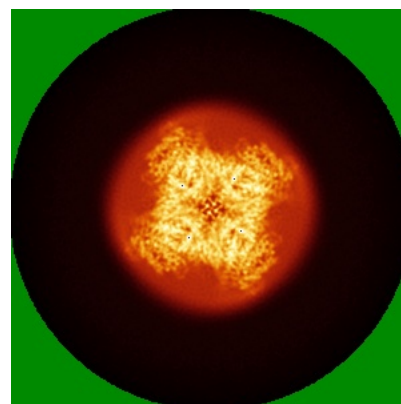
### 6.4.1 Primary map



X

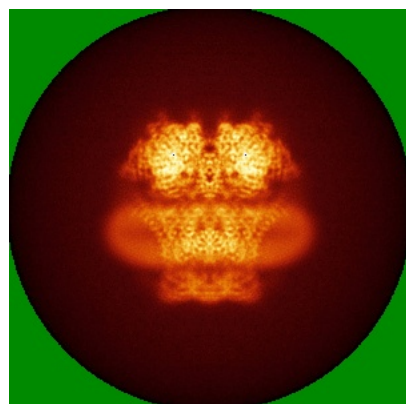


Y

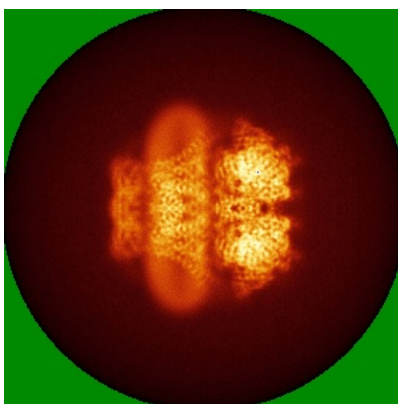


Z

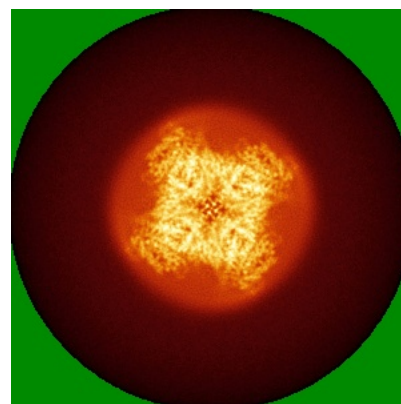
### 6.4.2 Raw map



X



Y



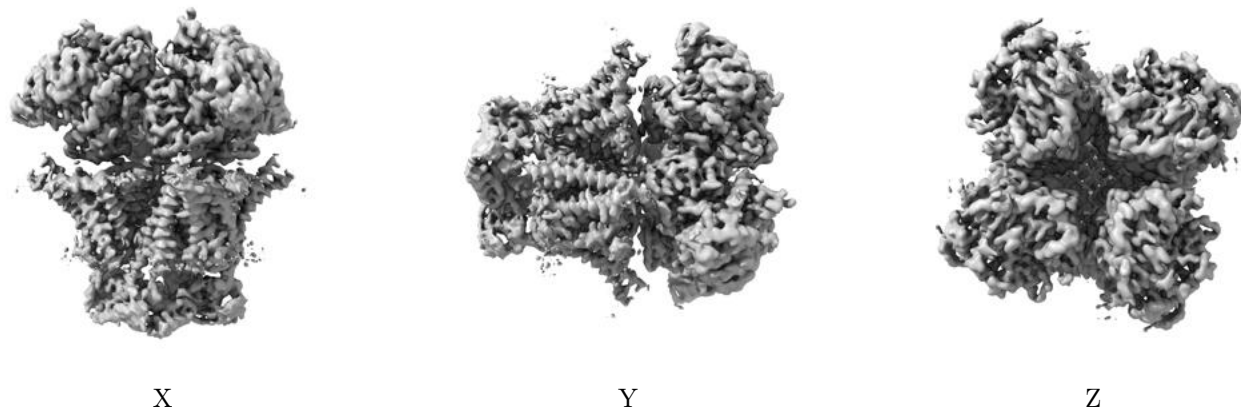
Z

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.



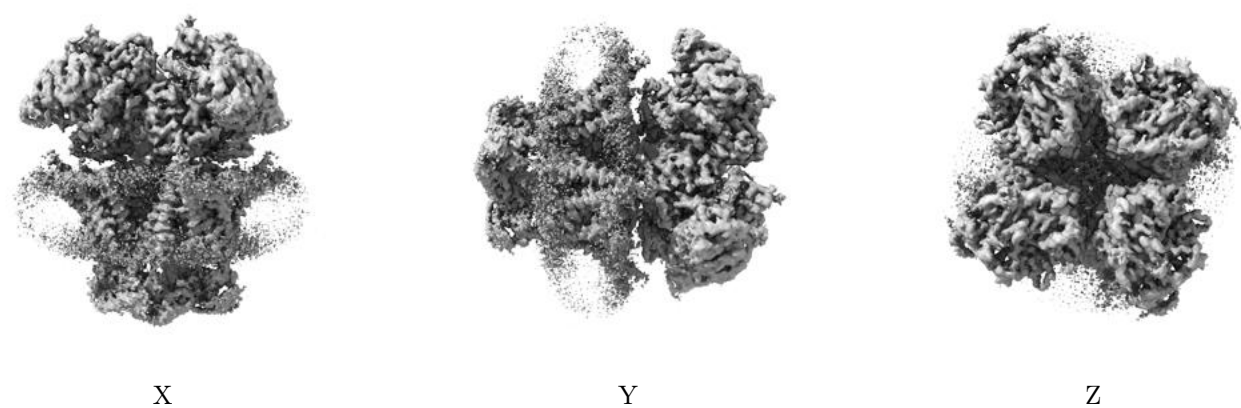
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0167. 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



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.

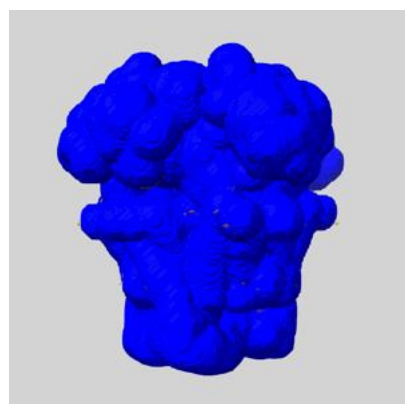
## 6.6 Mask visualisation [i](#)

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

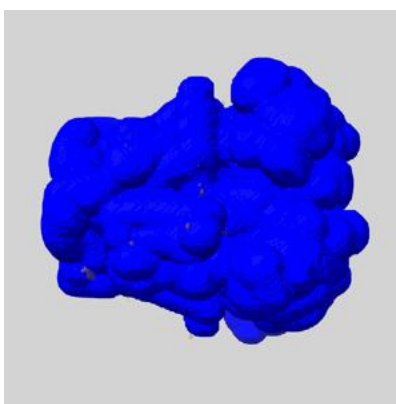
A mask typically either:

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

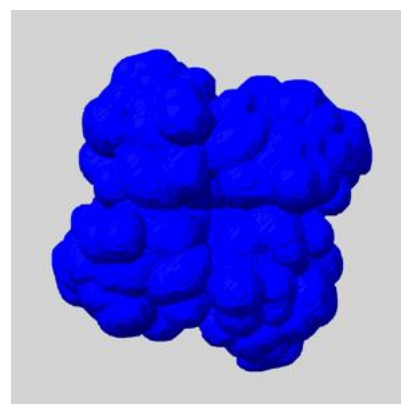
### 6.6.1 emd\_46419\_msk\_1.map [i](#)



X



Y

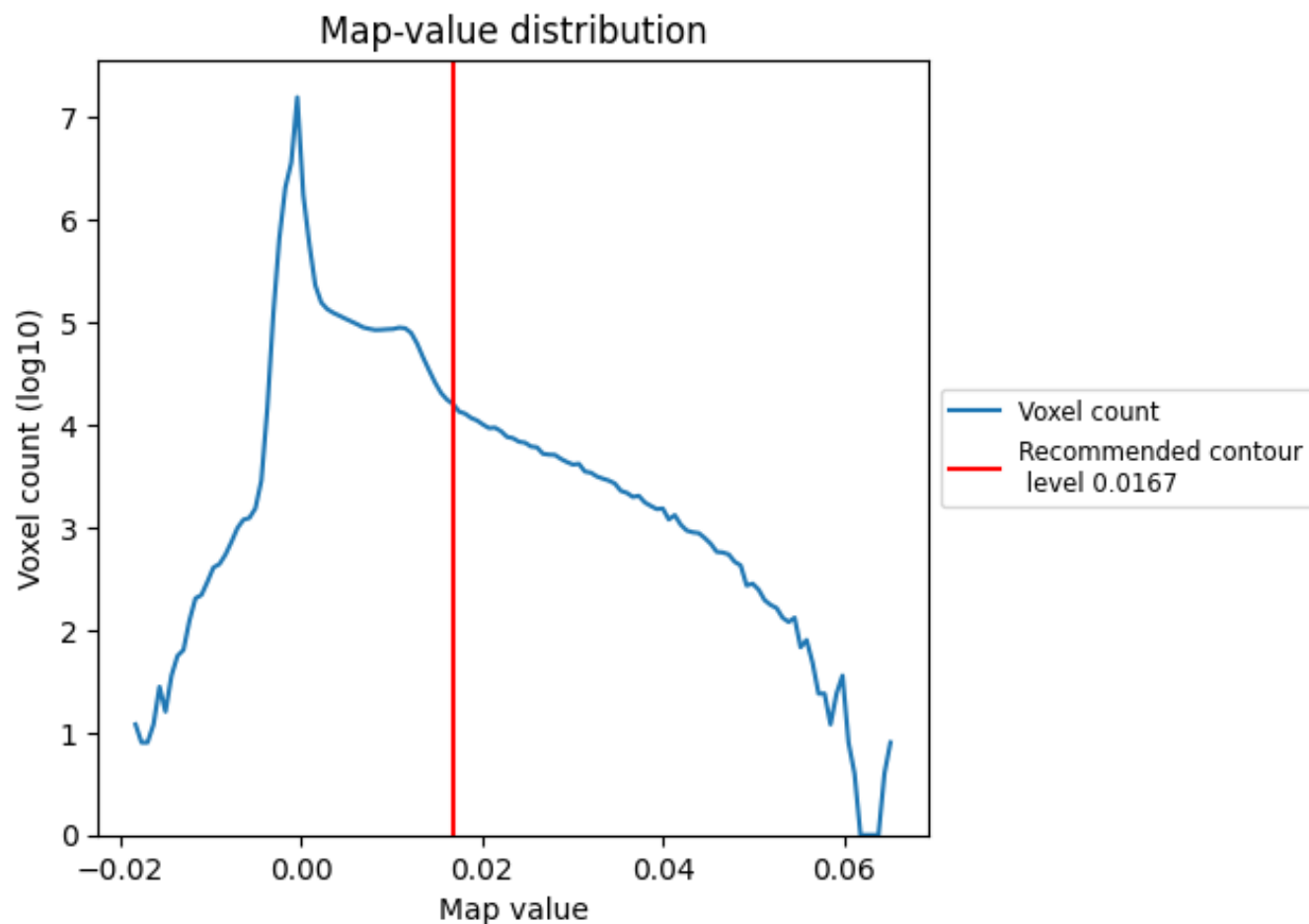


Z

## 7 Map analysis [i](#)

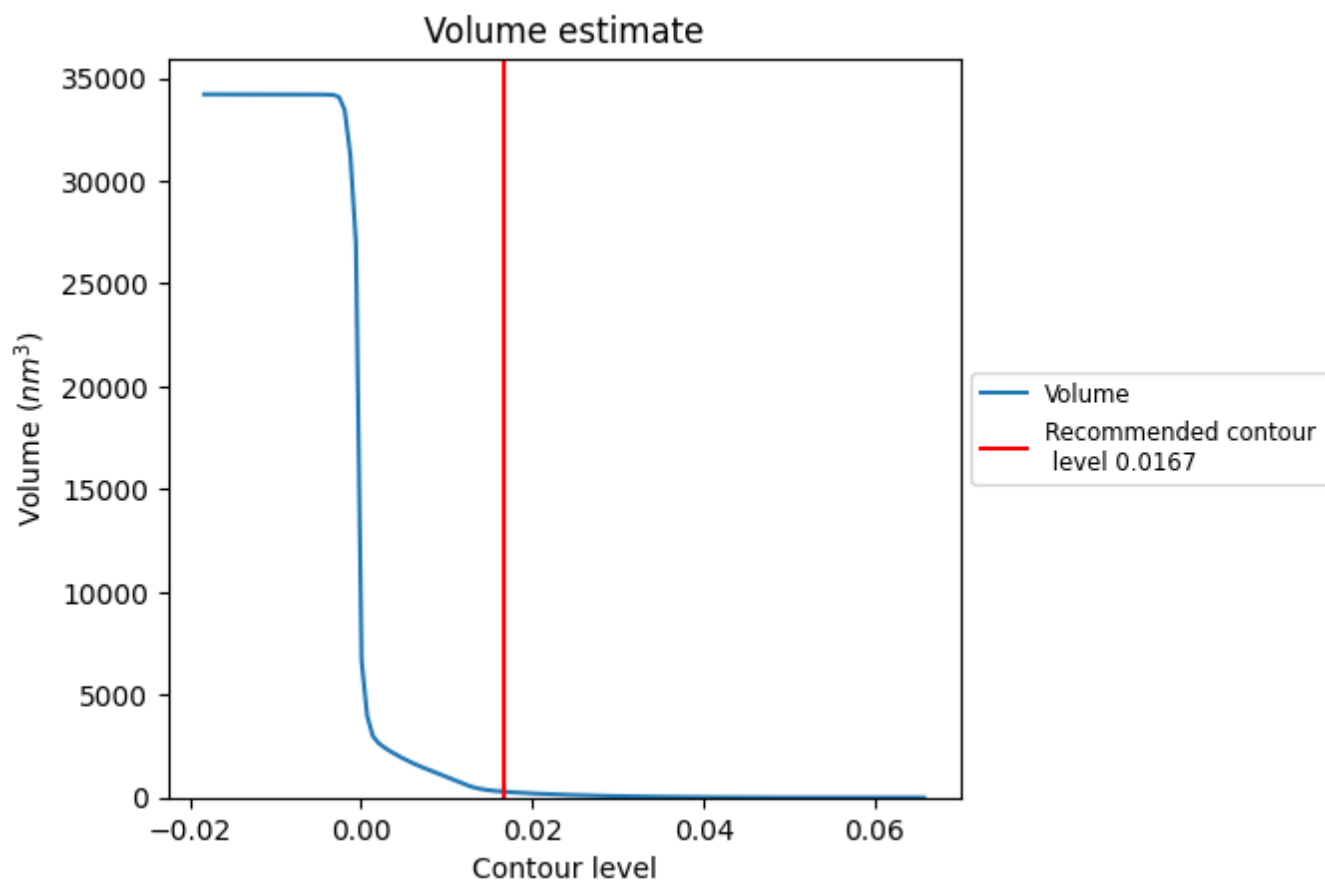
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

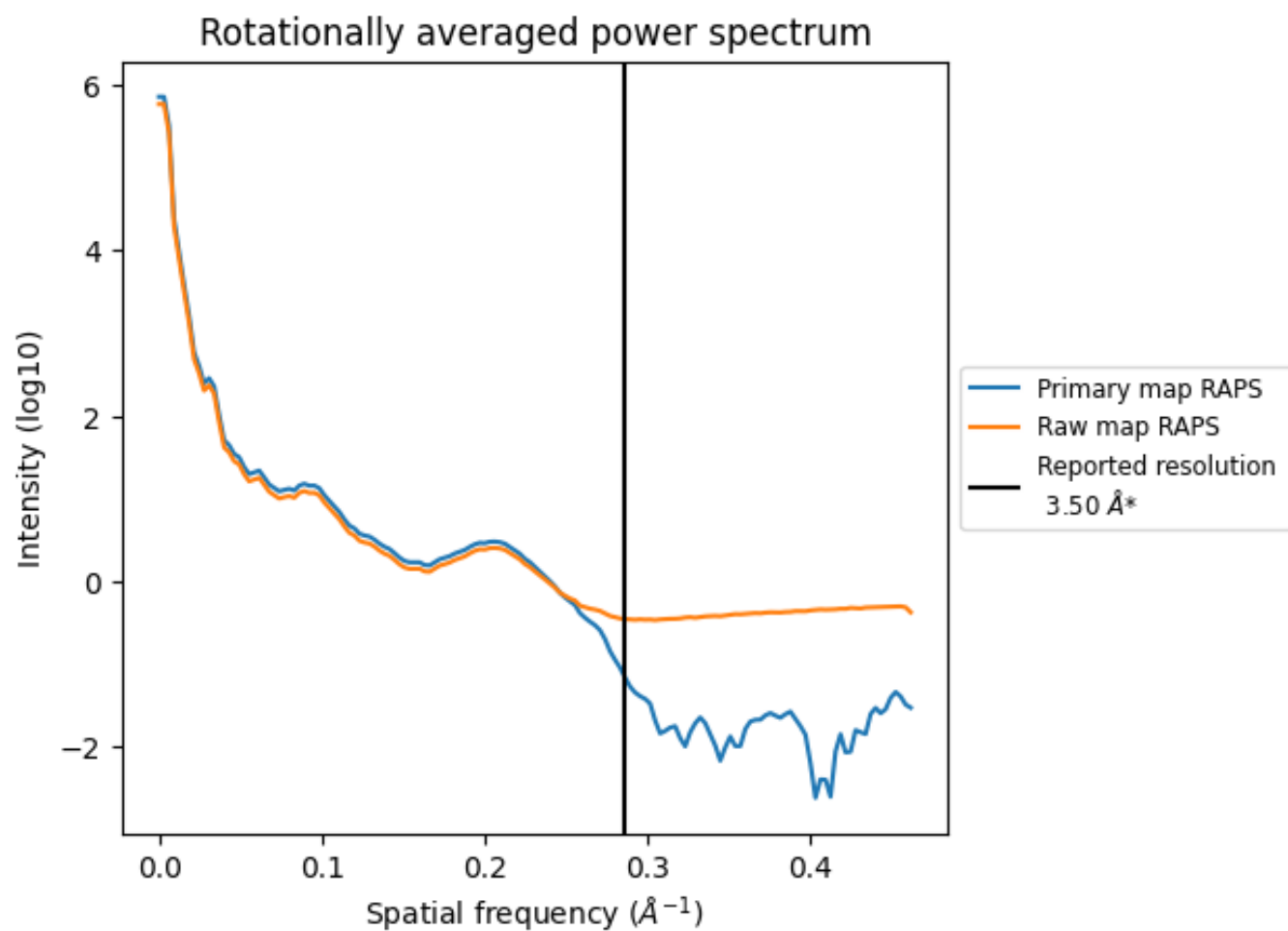


The volume at the recommended contour level is 285 nm<sup>3</sup>; this corresponds to an approximate mass of 257 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

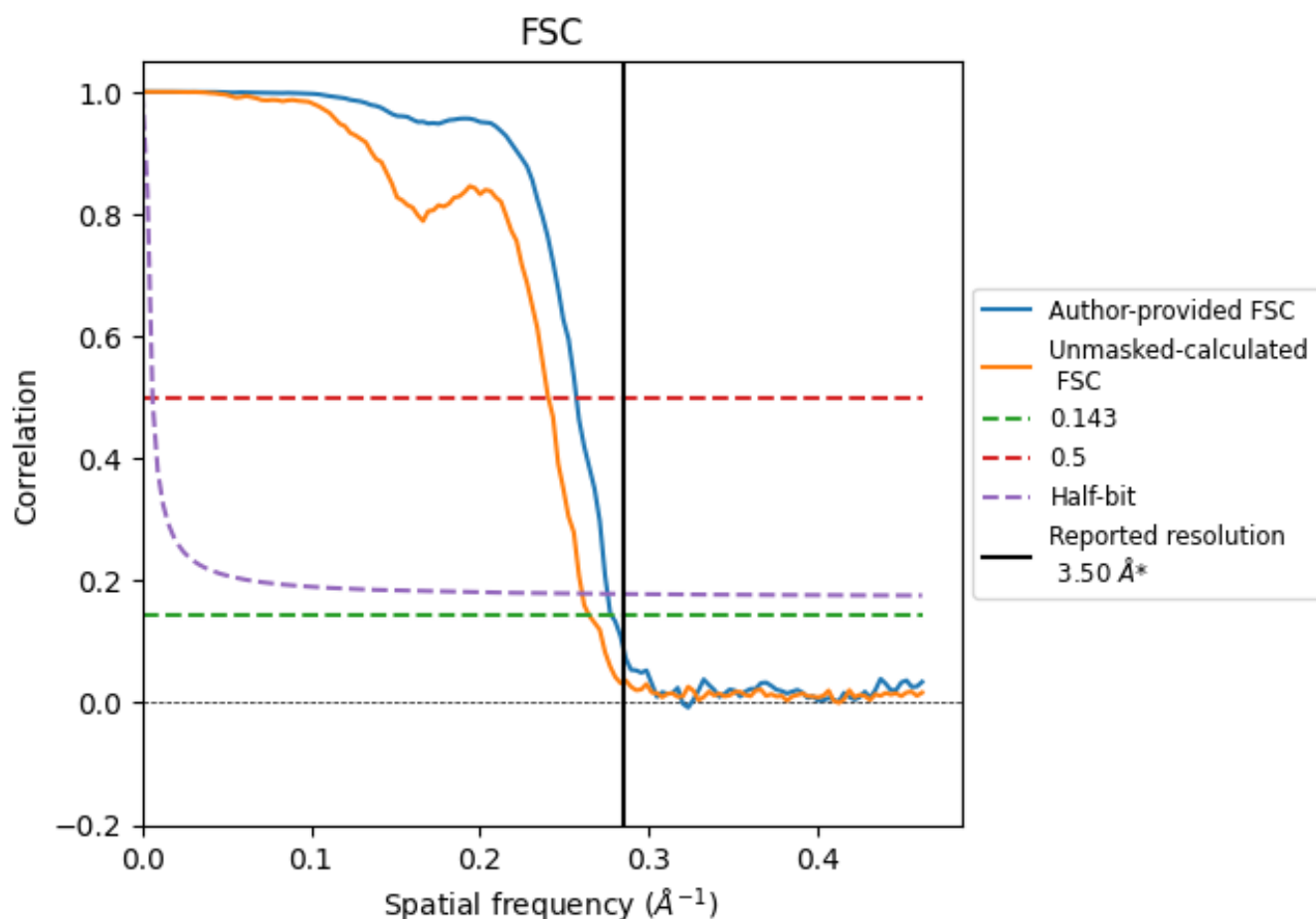


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.286 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

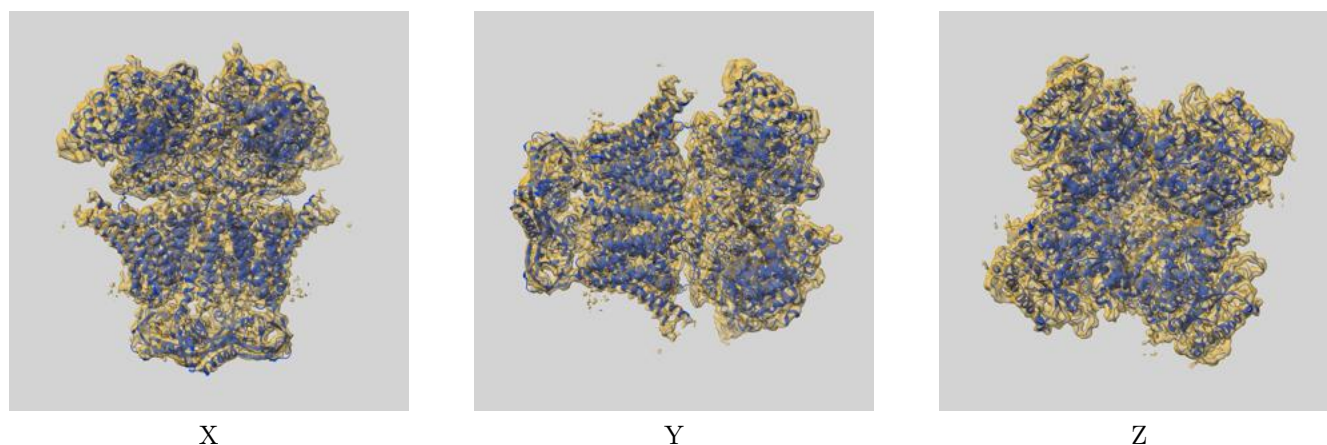
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.60	3.89	3.63
Unmasked-calculated*	3.78	4.16	3.84

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

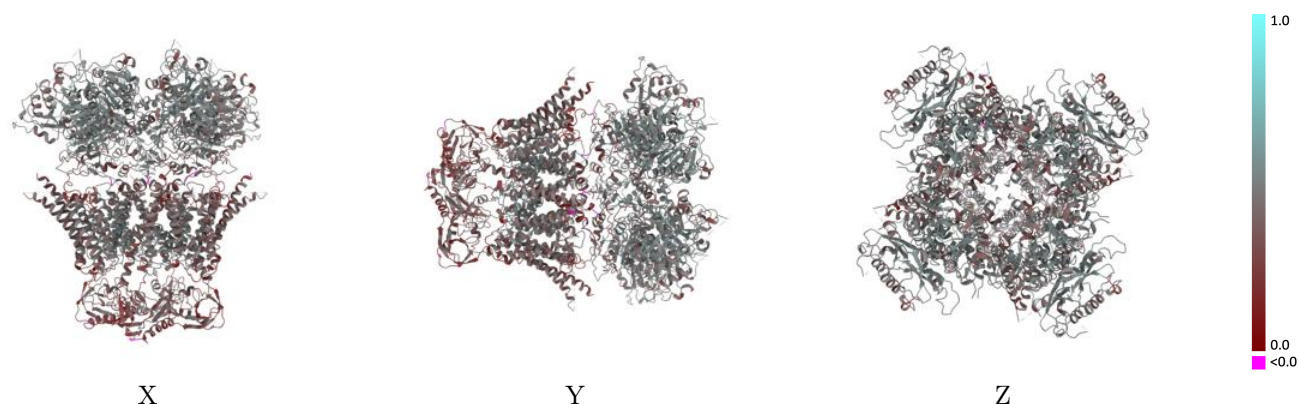
This section contains information regarding the fit between EMDB map EMD-46419 and PDB model 9CZK. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



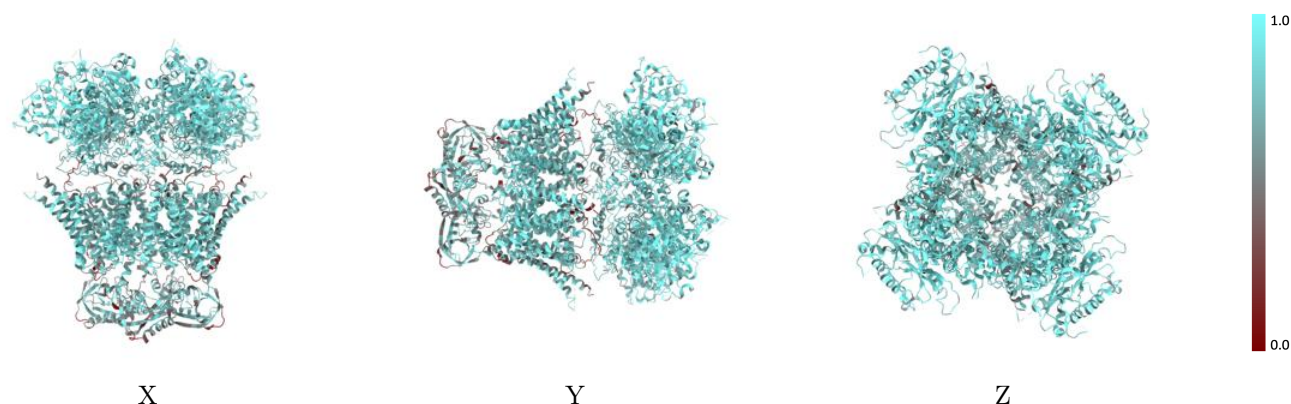
The images above show the 3D surface view of the map at the recommended contour level 0.0167 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



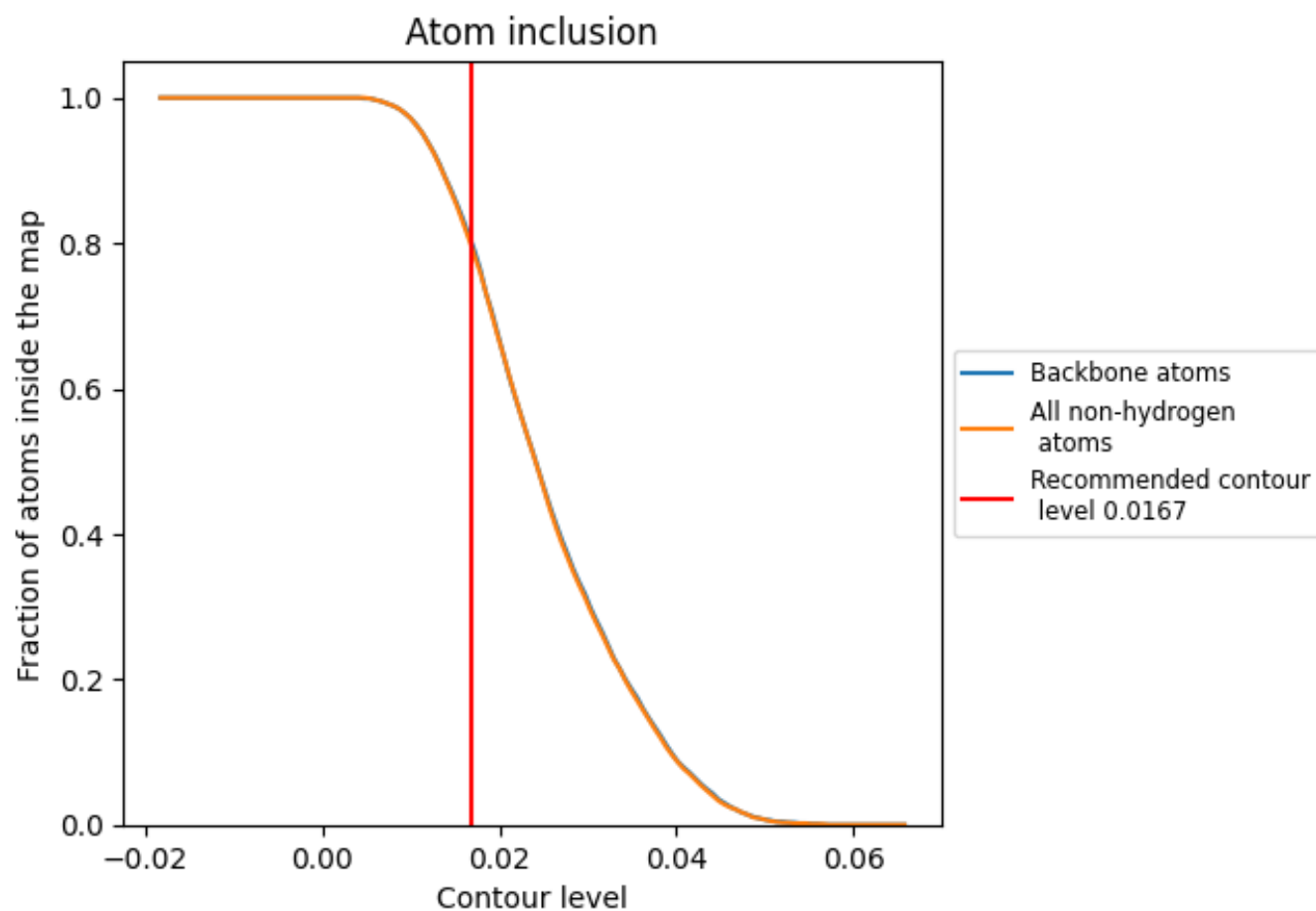
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0167).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.0167) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8000	<div><div></div></div> 0.4310
A	<div><div></div></div> 0.8360	<div><div></div></div> 0.4560
B	<div><div></div></div> 0.8350	<div><div></div></div> 0.4550
C	<div><div></div></div> 0.8350	<div><div></div></div> 0.4560
D	<div><div></div></div> 0.8350	<div><div></div></div> 0.4540
E	<div><div></div></div> 0.6600	<div><div></div></div> 0.3440
F	<div><div></div></div> 0.6400	<div><div></div></div> 0.3310
G	<div><div></div></div> 0.6270	<div><div></div></div> 0.3220
H	<div><div></div></div> 0.6280	<div><div></div></div> 0.3120

1.0

0.0

<0.0