



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 11:48 AM UTC

PDB ID : 9C0E / pdb_00009c0e
EMDB ID : EMD-45081
Title : Phosphorylated human NKCC1_K289NA492E in complex with furosemide
Authors : Zhao, Y.X.; Cao, E.H.
Deposited on : 2024-05-25
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

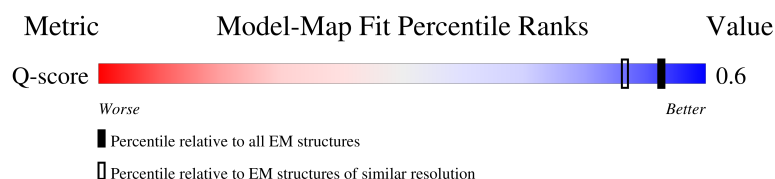
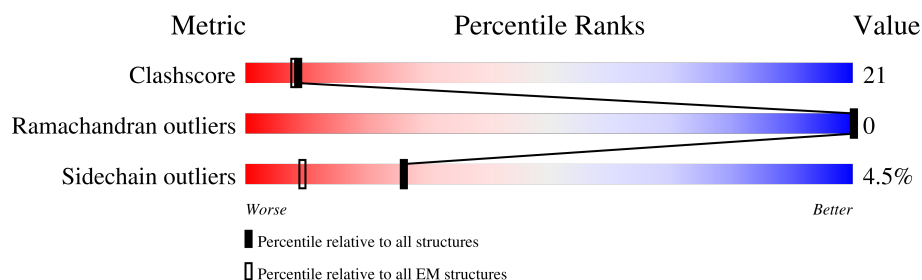
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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 $\leq 5\%$. 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	1212	
1	B	1212	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13584 atoms, of which 46 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

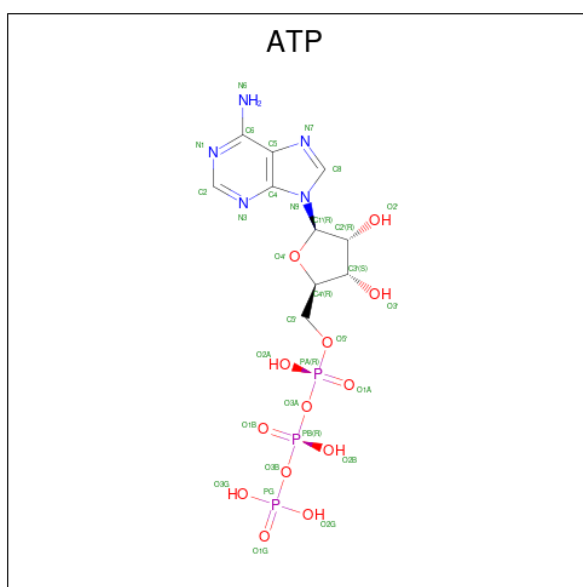
- Molecule 1 is a protein called Solute carrier family 12 member 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	909	Total	C	N	O	P	S	0	0
			6716	4373	1138	1164	3	38		
1	B	909	Total	C	N	O	P	S	0	0
			6710	4370	1138	1162	3	37		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	ASN	LYS	engineered mutation	UNP P55011
A	492	GLU	ALA	engineered mutation	UNP P55011
B	289	ASN	LYS	engineered mutation	UNP P55011
B	492	GLU	ALA	engineered mutation	UNP P55011

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



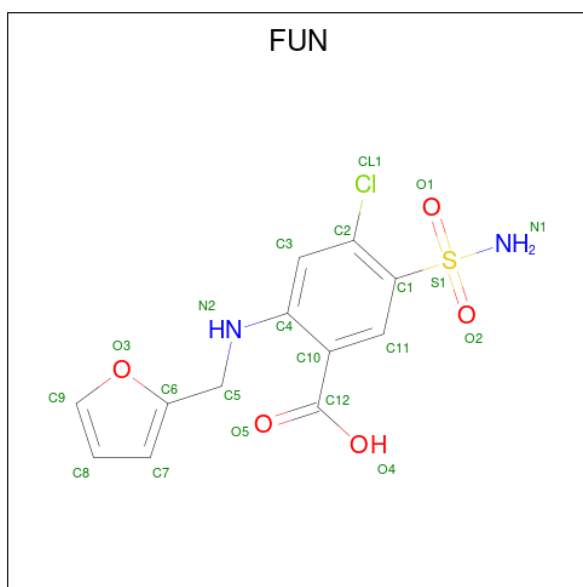
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf	
2	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 3 is 5-(AMINOSULFONYL)-4-CHLORO-2-[(2-FURYL METHYL)AMINO]BENZ OIC ACID (CCD ID: FUN) (formula: C₁₂H₁₁ClN₂O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
3	A	1	Total	C	Cl	H	N	O	S	0
			32	12	1	11	2	5	1	
3	B	1	Total	C	Cl	H	N	O	S	0
			32	12	1	11	2	5	1	

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Cl	0
			1	1	

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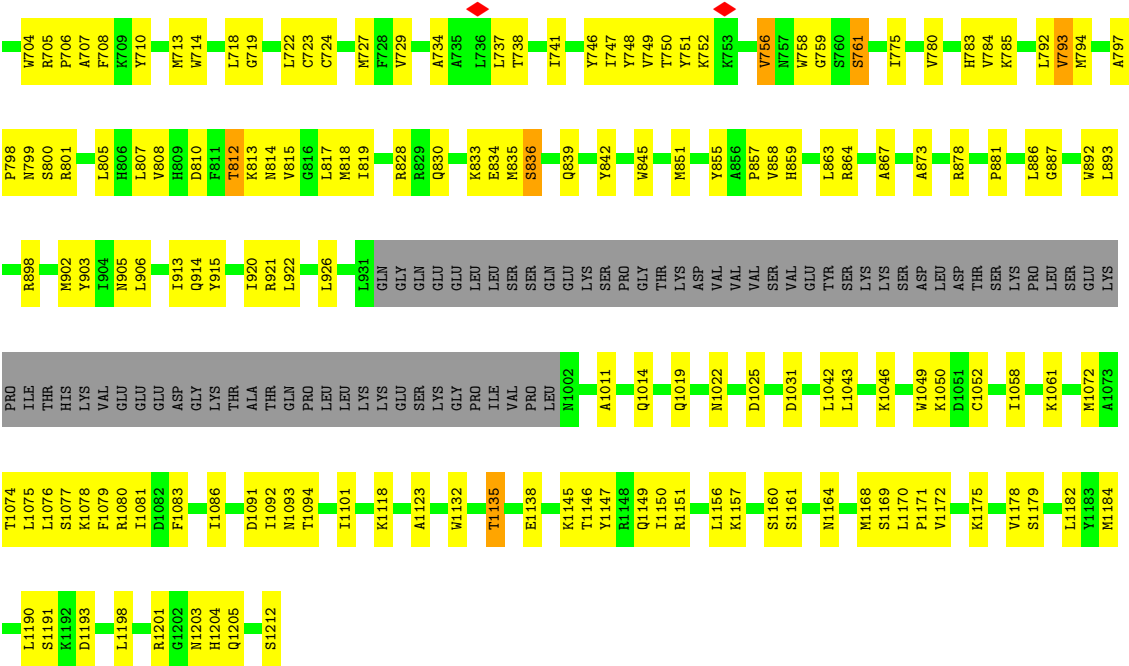
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Cl	0
			1	1	

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

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8051818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.046	Depositor
Minimum map value	-0.434	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	297.216, 297.216, 297.216	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8256, 0.8256, 0.8256	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: FUN, ATP, K, TPO, MG, CL, NA

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	0/6837	0.24	0/9299
1	B	0.11	0/6831	0.23	0/9292
All	All	0.12	0/13668	0.24	0/18591

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	6716	0	6499	291	0
1	B	6710	0	6489	301	0
2	A	31	12	12	3	0
2	B	31	12	12	2	0
3	A	21	11	10	0	0
3	B	21	11	10	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	13538	46	13032	563	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 21.

All (563) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:HD11	1:A:688:LEU:HD12	1.36	1.03
1:B:368:ILE:HD11	1:B:688:LEU:HD12	1.44	0.98
1:B:407:ASN:O	1:B:411:ILE:HD12	1.65	0.94
1:A:368:ILE:CD1	1:A:688:LEU:HD12	2.03	0.89
1:B:363:GLU:HA	1:B:749:VAL:HG11	1.57	0.87
1:A:363:GLU:HA	1:A:749:VAL:HG11	1.54	0.87
1:A:867:ALA:HB3	1:A:906:LEU:HD11	1.56	0.87
1:B:1072:MET:HA	1:B:1072:MET:HE2	1.57	0.86
1:A:303:MET:HE2	1:A:307:ARG:HB3	1.58	0.85
1:A:1072:MET:HE2	1:A:1072:MET:HA	1.58	0.84
1:B:333:ILE:HG21	1:B:719:GLY:HA3	1.59	0.83
1:B:1156:LEU:HD11	1:B:1168:MET:HE2	1.60	0.83
1:B:1091:ASP:O	1:B:1151:ARG:NH1	2.11	0.82
1:B:356:ILE:HD11	1:B:689:ILE:HG13	1.60	0.82
1:B:867:ALA:HB3	1:B:906:LEU:HD11	1.60	0.81
1:B:887:GLY:O	1:B:903:TYR:OH	1.98	0.81
1:B:350:GLY:O	1:B:508:SER:OG	1.97	0.81
1:A:1156:LEU:HD11	1:A:1168:MET:HE2	1.61	0.81
1:A:1076:LEU:HD21	1:A:1086:ILE:HD11	1.63	0.79
1:A:887:GLY:O	1:A:903:TYR:OH	2.00	0.79
1:B:584:TYR:HB2	1:B:589:ASN:HB2	1.64	0.79
1:A:861:ASP:N	1:A:865:GLU:OE2	2.15	0.79
1:B:328:THR:OG1	1:B:530:THR:OG1	2.01	0.78
1:B:391:VAL:HG11	1:B:412:ILE:HG21	1.66	0.78
1:A:860:ALA:HB1	1:A:865:GLU:HG3	1.65	0.78
1:A:297:LEU:HD13	1:A:613:SER:HB2	1.64	0.78
1:B:1079:PHE:HB3	1:B:1081:ILE:CD1	2.13	0.77
1:A:812:THR:HG21	1:A:818:MET:HB2	1.67	0.77
1:A:1148:ARG:NH2	1:B:217:TPO:O1P	2.18	0.76
1:A:333:ILE:HG21	1:A:719:GLY:HA3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HD11	1:A:689:ILE:HG13	1.66	0.76
1:A:1022:ASN:O	1:A:1023:THR:OG1	2.04	0.76
1:A:368:ILE:HD11	1:A:688:LEU:CD1	2.15	0.75
1:A:328:THR:HG1	1:A:530:THR:HG1	1.27	0.75
1:B:1076:LEU:HD21	1:B:1086:ILE:HD11	1.67	0.75
1:B:433:LYS:O	1:B:436:ILE:HG22	1.87	0.74
1:A:705:ARG:NH1	1:B:1079:PHE:O	2.19	0.74
1:A:873:ALA:HB3	1:B:873:ALA:HB3	1.69	0.74
1:B:734:ALA:O	1:B:738:THR:HG23	1.86	0.74
1:B:437:VAL:O	1:B:440:VAL:HG12	1.87	0.74
1:B:867:ALA:CB	1:B:906:LEU:HD11	2.18	0.74
1:B:921:ARG:NH1	1:B:1191:SER:O	2.20	0.74
1:B:1156:LEU:HD11	1:B:1168:MET:CE	2.18	0.74
1:A:546:ARG:HA	1:A:586:LEU:HB3	1.69	0.73
1:A:363:GLU:HG3	1:A:749:VAL:HG12	1.70	0.72
1:A:410:ARG:NH1	1:A:667:LEU:O	2.22	0.72
1:A:391:VAL:HG11	1:A:412:ILE:HG21	1.71	0.72
1:A:1203:ASN:HD22	1:A:1205:GLN:HG2	1.54	0.72
1:A:867:ALA:CB	1:A:906:LEU:HD11	2.19	0.72
1:B:363:GLU:HG3	1:B:749:VAL:HG12	1.72	0.72
1:A:1091:ASP:O	1:A:1151:ARG:NH1	2.23	0.72
1:B:339:SER:HB2	1:B:519:PRO:HB3	1.70	0.72
1:B:1170:LEU:HD12	1:B:1171:PRO:HD2	1.72	0.71
1:A:343:THR:HB	1:A:707:ALA:HB3	1.72	0.71
1:B:449:PHE:O	1:B:453:THR:HG22	1.91	0.71
1:A:805:LEU:CD2	1:A:851:MET:HE2	2.21	0.70
1:A:1079:PHE:O	1:B:705:ARG:NH1	2.23	0.70
1:B:1094:THR:OG1	1:B:1151:ARG:NH1	2.23	0.70
1:B:513:ASP:OD1	1:B:516:SER:OG	2.09	0.70
1:A:584:TYR:HB2	1:A:589:ASN:HB2	1.73	0.70
1:A:697:SER:HB3	1:A:713:MET:HE2	1.73	0.70
1:B:572:PHE:O	1:B:575:SER:OG	2.10	0.70
1:A:801:ARG:HG2	1:A:926:LEU:HB3	1.74	0.70
1:B:1072:MET:HG3	1:B:1086:ILE:HD13	1.74	0.70
1:B:812:THR:HG21	1:B:818:MET:HB2	1.72	0.70
1:A:328:THR:OG1	1:A:530:THR:OG1	2.00	0.69
1:A:449:PHE:O	1:A:453:THR:HG22	1.92	0.69
1:B:810:ASP:O	1:B:1046:LYS:HE2	1.93	0.69
1:A:459:SER:O	1:A:462:PRO:HD2	1.93	0.69
1:A:697:SER:HB3	1:A:713:MET:CE	2.23	0.69
1:A:507:ILE:HG22	1:A:507:ILE:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1070:ARG:O	1:A:1074:THR:HG23	1.92	0.68
1:A:363:GLU:HA	1:A:749:VAL:CG1	2.24	0.68
1:A:1025:ASP:OD2	1:A:1160:SER:OG	2.09	0.68
1:A:242:SER:OG	1:A:245:GLU:HG3	1.94	0.68
1:B:797:ALA:O	1:B:800:SER:OG	2.11	0.68
1:A:708:PHE:CZ	1:A:710:TYR:HB2	2.29	0.68
1:B:1203:ASN:HD22	1:B:1205:GLN:HG2	1.58	0.68
1:B:351:GLY:HA3	1:B:506:ASN:HA	1.75	0.67
1:B:368:ILE:HD11	1:B:688:LEU:CD1	2.23	0.67
1:A:862:ASP:OD1	1:A:865:GLU:HG2	1.94	0.67
1:A:282:VAL:HG13	1:A:283:VAL:HG13	1.76	0.66
1:B:311:ILE:HD13	1:B:490:VAL:HG13	1.77	0.66
1:B:1145:LYS:O	1:B:1149:GLN:HG2	1.96	0.66
1:A:510:ASP:OD2	1:A:624:LYS:NZ	2.27	0.66
1:B:343:THR:HB	1:B:707:ALA:HB3	1.75	0.66
1:A:339:SER:OG	1:A:519:PRO:HB3	1.95	0.66
1:A:1156:LEU:HD11	1:A:1168:MET:CE	2.25	0.66
1:B:374:PHE:O	1:B:378:VAL:HG23	1.95	0.66
1:A:797:ALA:O	1:A:800:SER:OG	2.12	0.66
1:A:345:GLY:HA3	1:B:1212:SER:HB3	1.77	0.65
1:B:353:TYR:OH	1:B:632:ASP:OD2	2.11	0.65
1:A:364:PHE:O	1:A:368:ILE:HG12	1.97	0.65
1:B:507:ILE:HG22	1:B:507:ILE:O	1.96	0.65
1:B:708:PHE:CZ	1:B:710:TYR:HB2	2.32	0.65
1:B:363:GLU:HA	1:B:749:VAL:CG1	2.27	0.64
1:B:697:SER:HB3	1:B:713:MET:CE	2.26	0.64
1:A:1145:LYS:O	1:A:1149:GLN:HG2	1.97	0.64
1:A:502:LEU:O	1:A:506:ASN:ND2	2.30	0.64
1:A:445:ALA:HA	1:A:602:LEU:CD1	2.27	0.64
1:A:735:ALA:O	1:A:738:THR:HG22	1.97	0.64
1:B:510:ASP:OD2	1:B:624:LYS:NZ	2.30	0.64
1:B:686:TYR:O	1:B:690:ASN:ND2	2.29	0.64
1:B:516:SER:O	1:B:520:LYS:HD2	1.98	0.63
1:A:520:LYS:HG2	1:A:521:GLY:N	2.12	0.63
1:A:785:LYS:NZ	1:B:759:GLY:O	2.31	0.63
1:A:1072:MET:HG3	1:A:1086:ILE:HD13	1.80	0.63
1:B:308:LEU:HD23	1:B:536:ILE:HG22	1.79	0.63
1:B:724:CYS:HA	1:B:727:MET:HE3	1.80	0.63
1:A:860:ALA:HB1	1:A:865:GLU:CG	2.28	0.63
1:A:305:PHE:HB2	1:A:607:ILE:HG12	1.80	0.63
1:B:696:ALA:HA	1:B:761:SER:OG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:794:MET:HB3	2:B:1301:ATP:H8	1.64	0.62
1:A:724:CYS:HA	1:A:727:MET:HE3	1.81	0.62
1:B:385:VAL:HG21	1:B:671:LEU:CD2	2.30	0.62
1:B:305:PHE:HB2	1:B:607:ILE:HG12	1.81	0.62
1:B:697:SER:HB3	1:B:713:MET:HE2	1.82	0.62
1:A:673:VAL:O	1:A:676:PRO:HD2	2.00	0.62
1:B:805:LEU:CD2	1:B:851:MET:HE2	2.29	0.62
1:A:516:SER:O	1:A:520:LYS:HD2	1.99	0.62
1:A:519:PRO:O	1:A:523:LEU:HD23	2.00	0.62
1:B:783:HIS:ND1	1:B:785:LYS:HG2	2.15	0.62
1:B:513:ASP:OD1	1:B:513:ASP:O	2.19	0.61
1:B:1076:LEU:HD11	1:B:1083:PHE:CE1	2.36	0.61
1:B:387:PHE:O	1:B:391:VAL:HG12	2.01	0.61
1:B:218:MET:HB3	1:B:246:LEU:HD21	1.83	0.60
1:B:291:VAL:HG13	1:B:504:GLY:HA3	1.83	0.60
1:A:387:PHE:O	1:A:391:VAL:HG12	2.01	0.60
1:B:1178:VAL:HG13	1:B:1182:LEU:HD23	1.83	0.60
1:B:368:ILE:CD1	1:B:688:LEU:HD12	2.23	0.60
1:B:459:SER:O	1:B:462:PRO:HD2	2.02	0.60
1:B:1135:THR:O	1:B:1138:GLU:HG2	2.01	0.60
1:B:238:LEU:O	1:B:239:LEU:HD23	2.01	0.60
1:B:341:ILE:HG12	1:B:693:VAL:HG22	1.84	0.60
1:A:205:THR:OG1	1:A:207:THR:HG23	2.02	0.59
1:A:1135:THR:O	1:A:1138:GLU:HG2	2.02	0.59
1:B:920:ILE:HG13	1:B:1198:LEU:HG	1.85	0.59
1:A:1076:LEU:HD11	1:A:1083:PHE:CE1	2.37	0.59
1:B:448:ASP:OD1	1:B:602:LEU:HB3	2.03	0.59
1:B:385:VAL:HG21	1:B:671:LEU:HD21	1.84	0.59
1:B:342:ALA:O	1:B:515:GLN:HG2	2.02	0.59
1:B:1022:ASN:CB	1:B:1164:ASN:HB2	2.33	0.59
1:A:855:TYR:CD2	1:A:857:PRO:HD3	2.37	0.58
1:B:478:GLY:O	1:B:546:ARG:NH2	2.34	0.58
1:A:794:MET:HB3	2:A:1301:ATP:H8	1.68	0.58
1:B:855:TYR:CD2	1:B:857:PRO:HD3	2.38	0.58
1:A:285:PHE:HE2	1:A:428:MET:HG2	1.68	0.58
1:B:1025:ASP:OD2	1:B:1160:SER:OG	2.13	0.58
1:A:713:MET:HG3	1:A:714:TRP:N	2.19	0.58
1:B:351:GLY:CA	1:B:506:ASN:HA	2.32	0.58
1:A:871:MET:HB3	1:A:913:ILE:CD1	2.34	0.58
1:A:718:LEU:HD11	1:A:722:LEU:HD11	1.85	0.58
1:A:1072:MET:O	1:A:1076:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:MET:HG3	1:B:714:TRP:N	2.18	0.58
1:A:308:LEU:HD23	1:A:536:ILE:HG22	1.85	0.58
1:B:320:SER:O	1:B:323:VAL:HG22	2.04	0.58
1:B:230:TPO:HG23	1:B:232:ALA:O	2.04	0.58
1:B:440:VAL:HG13	1:B:441:ILE:HD12	1.86	0.58
1:A:640:MET:HG3	1:A:653:ARG:HH11	1.68	0.58
1:A:341:ILE:HG12	1:A:693:VAL:HG22	1.87	0.57
1:B:1170:LEU:HB3	1:B:1201:ARG:HB2	1.86	0.57
1:B:308:LEU:HD23	1:B:536:ILE:CG2	2.34	0.57
1:B:356:ILE:HD12	1:B:368:ILE:HG21	1.85	0.57
1:B:801:ARG:NH1	2:B:1301:ATP:O3G	2.36	0.57
1:A:319:LEU:HD12	1:A:487:PHE:CD1	2.39	0.57
1:A:1080:ARG:HG2	1:B:707:ALA:HB2	1.86	0.57
1:B:756:VAL:HG21	1:B:758:TRP:CZ2	2.40	0.57
1:A:374:PHE:O	1:A:378:VAL:HG23	2.03	0.57
1:B:520:LYS:HG2	1:B:521:GLY:N	2.19	0.57
1:A:1101:ILE:HD13	1:A:1147:TYR:CE1	2.40	0.57
1:A:308:LEU:HD23	1:A:536:ILE:CG2	2.35	0.57
1:A:927:ASP:HB2	2:A:1301:ATP:O3G	2.05	0.57
1:B:347:VAL:HG22	1:B:514:PRO:HG2	1.86	0.57
1:B:1168:MET:HG3	1:B:1169:SER:N	2.20	0.56
1:A:368:ILE:N	1:A:368:ILE:HD13	2.18	0.56
1:A:390:THR:HG22	1:A:608:PHE:HE1	1.70	0.56
1:A:480:ASP:OD2	1:A:482:ARG:HG3	2.05	0.56
1:A:1072:MET:HE1	1:A:1075:LEU:HD23	1.87	0.56
1:A:285:PHE:CE2	1:A:428:MET:HG2	2.40	0.56
1:A:864:ARG:HA	1:A:906:LEU:HD13	1.86	0.56
1:B:450:VAL:O	1:B:453:THR:HG23	2.06	0.56
1:B:519:PRO:O	1:B:523:LEU:HD23	2.06	0.56
1:B:648:ASN:O	1:B:650:GLU:HG2	2.06	0.56
1:B:794:MET:HE2	1:B:867:ALA:HB2	1.87	0.56
1:A:597:SER:OG	1:A:603:ILE:HG13	2.06	0.56
1:A:599:PHE:HE1	1:A:601:PRO:HB2	1.71	0.56
1:A:449:PHE:HB2	1:A:603:ILE:HD11	1.88	0.55
1:B:680:ASN:HB3	1:B:738:THR:HG21	1.88	0.55
1:A:342:ALA:O	1:A:515:GLN:HG2	2.05	0.55
1:A:686:TYR:O	1:A:690:ASN:ND2	2.38	0.55
1:A:1211:TYR:OH	1:B:230:TPO:O3P	2.19	0.55
1:B:391:VAL:CG1	1:B:412:ILE:HG21	2.35	0.55
1:B:482:ARG:NH2	1:B:587:MET:HG3	2.21	0.55
1:B:623:PRO:HG2	1:B:655:TYR:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:PHE:CZ	1:A:502:LEU:HD12	2.42	0.55
1:A:656:ILE:O	1:A:660:LEU:HD23	2.06	0.55
1:B:737:LEU:O	1:B:741:ILE:HG13	2.06	0.55
1:A:1175:LYS:HG2	1:B:249:GLU:HG2	1.89	0.54
1:B:376:ASN:O	1:B:380:VAL:HG23	2.07	0.54
1:B:830:GLN:O	1:B:834:GLU:HG3	2.06	0.54
1:A:1132:TRP:O	1:A:1179:SER:OG	2.25	0.54
1:B:887:GLY:HA3	1:B:926:LEU:HD12	1.90	0.54
1:A:622:ALA:HB3	1:A:623:PRO:HD3	1.90	0.54
1:A:794:MET:HE1	1:A:870:LEU:HD12	1.90	0.54
1:B:622:ALA:HB3	1:B:623:PRO:HD3	1.89	0.54
1:A:1074:THR:O	1:A:1078:LYS:HG3	2.07	0.54
1:B:835:MET:HG2	1:B:857:PRO:HB2	1.90	0.54
1:A:351:GLY:H	1:A:506:ASN:HA	1.72	0.54
1:A:839:GLN:HG2	1:A:857:PRO:HG3	1.88	0.54
1:B:1072:MET:HE1	1:B:1075:LEU:HD23	1.89	0.54
1:A:351:GLY:HA3	1:A:506:ASN:HA	1.90	0.54
1:A:476:ASN:HA	1:A:546:ARG:NH1	2.23	0.54
1:A:548:ALA:HA	1:A:574:PHE:CB	2.37	0.54
1:B:819:ILE:HD12	1:B:881:PRO:HG3	1.90	0.54
1:A:524:LEU:O	1:A:528:ILE:HG13	2.07	0.54
1:B:892:TRP:CE3	1:B:1184:MET:HG2	2.43	0.54
1:B:372:PHE:CZ	1:B:502:LEU:HD12	2.43	0.53
1:B:718:LEU:HD11	1:B:722:LEU:HD11	1.90	0.53
1:B:1072:MET:O	1:B:1076:LEU:HG	2.08	0.53
1:A:376:ASN:O	1:A:380:VAL:HG23	2.08	0.53
1:B:718:LEU:HD12	1:B:722:LEU:HG	1.90	0.53
1:A:417:VAL:HG13	1:A:659:PHE:CE1	2.44	0.53
1:A:445:ALA:HA	1:A:602:LEU:HD12	1.89	0.53
1:A:448:ASP:OD1	1:A:602:LEU:HB3	2.09	0.53
1:A:892:TRP:CE3	1:A:1184:MET:HG2	2.43	0.53
1:A:920:ILE:HG13	1:A:1198:LEU:HG	1.89	0.53
1:A:450:VAL:O	1:A:453:THR:HG23	2.08	0.53
1:B:442:LEU:CD1	1:B:610:ALA:HB2	2.38	0.53
1:A:382:MET:HE1	1:A:678:ILE:HB	1.91	0.53
1:A:385:VAL:HG21	1:A:671:LEU:CD2	2.39	0.53
1:B:546:ARG:HA	1:B:586:LEU:HB3	1.88	0.53
1:B:794:MET:CE	1:B:867:ALA:HB2	2.39	0.53
1:A:480:ASP:HB3	1:A:546:ARG:NH2	2.23	0.53
1:A:1080:ARG:NH1	1:B:344:ASN:OD1	2.42	0.53
1:B:1083:PHE:CE2	1:B:1086:ILE:HG13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:THR:OG1	1:B:206:ASN:N	2.40	0.53
1:B:368:ILE:HD13	1:B:368:ILE:N	2.24	0.53
1:B:748:TYR:CZ	1:B:752:LYS:HD2	2.44	0.53
1:B:898:ARG:HB3	1:B:898:ARG:CZ	2.38	0.53
1:A:1113:LEU:CD1	1:A:1126:MET:HG2	2.39	0.53
1:A:222:PRO:HA	1:B:1031:ASP:HB2	1.91	0.52
1:A:448:ASP:OD2	1:A:448:ASP:C	2.52	0.52
1:A:599:PHE:CD1	1:A:601:PRO:HD2	2.45	0.52
1:B:218:MET:HB3	1:B:246:LEU:CD2	2.39	0.52
1:B:1079:PHE:HB3	1:B:1081:ILE:HD12	1.89	0.52
1:B:390:THR:HG22	1:B:608:PHE:HE1	1.74	0.52
1:B:460:LYS:HD3	1:B:465:PHE:HD2	1.74	0.52
1:B:656:ILE:O	1:B:660:LEU:HD23	2.08	0.52
1:A:480:ASP:HB3	1:A:546:ARG:CZ	2.40	0.52
1:A:746:TYR:O	1:A:750:THR:HG22	2.09	0.52
1:A:1145:LYS:HE3	1:B:217:TPO:O1P	2.10	0.52
1:B:668:ILE:HG22	1:B:670:GLU:H	1.74	0.52
1:A:1157:LYS:O	1:A:1161:SER:HB3	2.10	0.52
1:B:448:ASP:OD2	1:B:448:ASP:C	2.52	0.52
1:A:599:PHE:HD1	1:A:602:LEU:H	1.57	0.52
1:A:828:ARG:HB3	1:A:828:ARG:NH1	2.25	0.52
1:A:1175:LYS:CG	1:B:249:GLU:HG2	2.40	0.52
1:A:898:ARG:HB3	1:A:898:ARG:CZ	2.39	0.52
1:B:417:VAL:HG13	1:B:659:PHE:CE1	2.45	0.52
1:B:1132:TRP:O	1:B:1179:SER:OG	2.26	0.52
1:A:1031:ASP:OD1	1:B:227:TYR:OH	2.21	0.52
1:B:333:ILE:HG22	1:B:690:ASN:OD1	2.10	0.52
1:B:839:GLN:HG2	1:B:857:PRO:HG3	1.91	0.52
1:A:284:LYS:HB3	1:A:512:ALA:HA	1.92	0.52
1:B:746:TYR:O	1:B:750:THR:HG22	2.10	0.52
1:A:218:MET:HB3	1:A:246:LEU:CD2	2.39	0.51
1:A:737:LEU:O	1:A:741:ILE:HG13	2.10	0.51
1:B:549:THR:H	1:B:574:PHE:HA	1.75	0.51
1:B:1157:LYS:O	1:B:1161:SER:HB3	2.10	0.51
1:A:420:LEU:HD22	1:A:616:LEU:HG	1.91	0.51
1:A:623:PRO:HG2	1:A:655:TYR:CD1	2.45	0.51
1:B:1076:LEU:HD12	1:B:1077:SER:N	2.25	0.51
1:A:668:ILE:HG22	1:A:670:GLU:H	1.74	0.51
1:A:860:ALA:HB1	1:A:865:GLU:CD	2.35	0.51
1:A:783:HIS:ND1	1:A:785:LYS:HG2	2.25	0.51
1:A:886:LEU:HD23	1:A:903:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:THR:HG22	1:A:1024:ILE:N	2.25	0.51
1:B:525:ALA:O	1:B:529:THR:HG23	2.10	0.51
1:A:1031:ASP:HB2	1:B:222:PRO:HA	1.92	0.51
1:B:305:PHE:HB2	1:B:607:ILE:CG1	2.41	0.51
1:B:382:MET:HE1	1:B:678:ILE:HB	1.93	0.51
1:B:311:ILE:CD1	1:B:490:VAL:HG13	2.40	0.51
1:A:305:PHE:HB2	1:A:607:ILE:CG1	2.40	0.51
1:B:489:SER:O	1:B:493:ILE:HD13	2.11	0.51
1:B:585:GLY:H	1:B:589:ASN:HB2	1.76	0.51
1:B:808:VAL:O	1:B:812:THR:HB	2.11	0.51
1:B:449:PHE:HB2	1:B:603:ILE:HD11	1.93	0.51
1:B:460:LYS:HD3	1:B:465:PHE:CD2	2.47	0.51
1:B:813:LYS:O	1:B:814:ASN:HB2	2.11	0.51
1:A:314:GLN:HA	1:A:587:MET:HE1	1.93	0.50
1:B:828:ARG:HG2	1:B:859:HIS:NE2	2.26	0.50
1:A:417:VAL:HG13	1:A:659:PHE:HE1	1.77	0.50
1:B:748:TYR:OH	1:B:752:LYS:HD2	2.12	0.50
1:A:525:ALA:O	1:A:529:THR:HG23	2.11	0.50
1:A:1083:PHE:CE2	1:A:1086:ILE:HG13	2.46	0.50
1:A:1076:LEU:HD12	1:A:1077:SER:N	2.27	0.49
1:A:1203:ASN:O	1:A:1204:HIS:HB2	2.12	0.49
1:B:347:VAL:HG23	1:B:347:VAL:O	2.12	0.49
1:B:817:LEU:HD21	1:B:819:ILE:HD11	1.94	0.49
1:A:437:VAL:O	1:A:441:ILE:HD13	2.12	0.49
1:A:747:ILE:HA	1:A:750:THR:HG22	1.95	0.49
1:A:282:VAL:CG1	1:A:283:VAL:HG13	2.42	0.49
1:A:864:ARG:CZ	1:A:905:ASN:HB3	2.42	0.49
1:B:322:LEU:HD23	1:B:487:PHE:CZ	2.48	0.49
1:B:1203:ASN:O	1:B:1204:HIS:HB2	2.12	0.49
1:A:1188:GLU:O	1:A:1192:LYS:HB3	2.11	0.49
1:B:652:LEU:O	1:B:656:ILE:HG12	2.13	0.49
1:A:718:LEU:HD12	1:A:722:LEU:HG	1.94	0.49
1:B:303:MET:HE2	1:B:307:ARG:HB3	1.93	0.49
1:B:718:LEU:O	1:B:722:LEU:HG	2.12	0.49
1:A:295:CYS:O	1:A:299:ILE:HD12	2.12	0.49
1:A:813:LYS:O	1:A:814:ASN:HB2	2.11	0.49
1:A:303:MET:HE2	1:A:307:ARG:CB	2.38	0.49
1:A:442:LEU:CD1	1:A:610:ALA:HB2	2.43	0.48
1:A:718:LEU:O	1:A:722:LEU:HG	2.13	0.48
1:B:697:SER:HB3	1:B:713:MET:HE3	1.95	0.48
1:B:1074:THR:O	1:B:1078:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:GLY:CA	1:B:1212:SER:HB3	2.43	0.48
1:A:544:VAL:HG12	1:A:586:LEU:HB2	1.95	0.48
1:B:417:VAL:HG13	1:B:659:PHE:HE1	1.79	0.48
1:A:648:ASN:O	1:A:650:GLU:HG2	2.13	0.48
1:B:218:MET:HE3	1:B:218:MET:HB2	1.73	0.48
1:B:1050:LYS:HA	1:B:1050:LYS:HD3	1.64	0.48
1:A:249:GLU:HG2	1:B:1175:LYS:HG3	1.95	0.48
1:A:476:ASN:ND2	1:A:541:GLY:O	2.41	0.48
1:B:1168:MET:HE3	1:B:1190:LEU:HD11	1.94	0.48
1:A:1043:LEU:O	1:A:1049:TRP:HB2	2.14	0.48
1:A:1072:MET:CE	1:A:1075:LEU:HD23	2.44	0.48
1:B:886:LEU:N	1:B:886:LEU:HD23	2.28	0.48
1:A:303:MET:HB2	1:A:303:MET:HE3	1.78	0.48
1:A:313:GLY:C	1:A:587:MET:HE2	2.39	0.48
1:A:463:LYS:CG	1:A:584:TYR:HE1	2.27	0.48
1:A:507:ILE:O	1:A:507:ILE:CG2	2.61	0.48
1:B:314:GLN:HA	1:B:587:MET:HE1	1.96	0.48
1:A:704:TRP:CE2	1:A:706:PRO:HG3	2.49	0.48
1:B:420:LEU:HD22	1:B:616:LEU:HG	1.96	0.48
1:B:913:ILE:HG23	1:B:915:TYR:CD1	2.49	0.48
1:A:702:PRO:HB3	1:B:1042:LEU:HD21	1.96	0.47
1:A:1087:MET:HE3	1:A:1087:MET:HB2	1.77	0.47
1:A:1168:MET:HG3	1:A:1169:SER:N	2.28	0.47
1:B:1072:MET:HE2	1:B:1072:MET:CA	2.36	0.47
1:B:592:VAL:O	1:B:596:VAL:HG23	2.14	0.47
1:B:652:LEU:HD23	1:B:652:LEU:N	2.29	0.47
1:A:323:VAL:HG23	1:A:487:PHE:CE1	2.50	0.47
1:A:386:GLY:O	1:A:389:GLU:HG2	2.15	0.47
1:A:817:LEU:HD21	1:A:819:ILE:HD11	1.96	0.47
1:A:1011:ALA:O	1:A:1014:GLN:HG2	2.15	0.47
1:B:428:MET:HE2	1:B:428:MET:HB2	1.84	0.47
1:B:864:ARG:CZ	1:B:905:ASN:HB3	2.44	0.47
1:B:1076:LEU:HD12	1:B:1076:LEU:C	2.39	0.47
1:A:592:VAL:O	1:A:596:VAL:HG23	2.15	0.47
1:A:794:MET:HB3	2:A:1301:ATP:C8	2.48	0.47
1:B:688:LEU:HD23	1:B:688:LEU:HA	1.71	0.47
1:B:780:VAL:O	1:B:878:ARG:NE	2.48	0.47
1:B:798:PRO:HG2	1:B:842:TYR:HB3	1.96	0.47
1:B:747:ILE:HA	1:B:750:THR:HG22	1.96	0.47
1:A:227:TYR:OH	1:B:1031:ASP:OD1	2.21	0.46
1:A:366:GLY:HA2	1:A:629:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ARG:HA	1:B:586:LEU:CB	2.45	0.46
1:A:333:ILE:HG22	1:A:690:ASN:OD1	2.16	0.46
1:A:1031:ASP:OD2	1:B:240:ARG:NE	2.43	0.46
1:A:910:ALA:O	1:A:915:TYR:HB2	2.16	0.46
1:A:287:TRP:CE2	1:A:288:ILE:HG13	2.51	0.46
1:A:291:VAL:HG13	1:A:504:GLY:HA3	1.96	0.46
1:B:863:LEU:H	1:B:902:MET:HE1	1.81	0.46
1:A:353:TYR:OH	1:A:632:ASP:OD2	2.12	0.46
1:A:584:TYR:CB	1:A:589:ASN:HB2	2.42	0.46
1:B:207:THR:O	1:B:208:TYR:HB3	2.15	0.46
1:B:381:ALA:HB2	1:B:662:ALA:HA	1.98	0.46
1:B:421:LEU:HD22	1:B:421:LEU:O	2.15	0.46
1:A:436:ILE:O	1:A:440:VAL:HG12	2.16	0.46
1:A:325:MET:O	1:A:329:VAL:HG23	2.16	0.46
1:A:421:LEU:O	1:A:421:LEU:HD22	2.16	0.46
1:A:391:VAL:CG1	1:A:412:ILE:HG21	2.43	0.46
1:A:549:THR:HA	1:A:582:CYS:HB2	1.98	0.46
1:B:284:LYS:HB3	1:B:512:ALA:HA	1.98	0.45
1:A:486:THR:OG1	1:A:487:PHE:N	2.48	0.45
1:A:747:ILE:HA	1:A:750:THR:CG2	2.46	0.45
1:A:805:LEU:HD21	1:A:851:MET:HE2	1.97	0.45
1:A:886:LEU:HD21	1:A:906:LEU:HD23	1.98	0.45
1:B:388:ALA:HA	1:B:391:VAL:CG1	2.46	0.45
1:B:1092:ILE:HG22	1:B:1093:ASN:N	2.31	0.45
1:A:793:VAL:CG2	1:A:808:VAL:HG11	2.46	0.45
1:A:212:TPO:OG1	1:B:1061:LYS:HD2	2.15	0.45
1:A:380:VAL:HG22	1:A:618:SER:HB2	1.98	0.45
1:A:686:TYR:OH	5:A:1304:CL:CL	2.65	0.45
1:B:704:TRP:HA	1:B:704:TRP:CE3	2.51	0.45
1:A:1032:ASP:HB2	1:A:1202:GLY:H	1.82	0.45
1:A:353:TYR:CE1	1:A:629:LEU:HD12	2.51	0.45
1:A:240:ARG:HE	1:B:1031:ASP:CG	2.24	0.45
1:B:863:LEU:N	1:B:902:MET:HE1	2.32	0.45
1:A:240:ARG:O	1:A:240:ARG:HG3	2.14	0.45
1:A:468:TYR:O	1:A:469:LYS:HD3	2.16	0.45
1:B:833:LYS:HA	1:B:836:SER:OG	2.16	0.45
1:A:344:ASN:OD1	1:B:1080:ARG:NH2	2.49	0.45
1:A:351:GLY:N	1:A:506:ASN:HA	2.31	0.45
1:A:704:TRP:HA	1:A:704:TRP:CE3	2.52	0.45
1:B:793:VAL:HG11	1:B:818:MET:HE3	1.99	0.45
1:A:348:ARG:O	1:A:509:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:THR:O	1:A:1150:ILE:HG13	2.16	0.45
1:B:390:THR:HG22	1:B:608:PHE:CE1	2.51	0.45
1:B:1151:ARG:HG2	1:B:1151:ARG:HH11	1.81	0.45
1:B:482:ARG:HG2	1:B:482:ARG:HH11	1.82	0.44
1:B:704:TRP:HA	1:B:704:TRP:HE3	1.82	0.44
1:A:704:TRP:HA	1:A:704:TRP:HE3	1.83	0.44
1:A:780:VAL:O	1:A:878:ARG:NE	2.50	0.44
1:A:1076:LEU:HD12	1:A:1076:LEU:C	2.42	0.44
1:B:341:ILE:HG21	1:B:355:LEU:HB3	2.00	0.44
1:B:678:ILE:O	1:B:682:PHE:HD1	2.01	0.44
1:B:320:SER:O	1:B:324:ILE:HG13	2.18	0.44
1:B:464:GLY:HA2	1:B:545:VAL:HG22	1.99	0.44
1:B:704:TRP:CE2	1:B:706:PRO:HG3	2.52	0.44
1:B:1092:ILE:HG22	1:B:1093:ASN:H	1.82	0.44
1:A:351:GLY:CA	1:A:506:ASN:HA	2.47	0.44
1:A:448:ASP:OD2	1:A:597:SER:HB2	2.17	0.44
1:A:662:ALA:O	1:A:666:ILE:HD12	2.18	0.44
1:B:312:VAL:CG2	1:B:537:ALA:HB1	2.48	0.44
1:B:442:LEU:HD12	1:B:610:ALA:HB2	1.98	0.44
1:B:486:THR:HG23	1:B:489:SER:H	1.83	0.44
1:A:284:LYS:HB3	1:A:512:ALA:CA	2.47	0.44
1:A:805:LEU:HG	1:A:851:MET:CE	2.47	0.44
1:B:341:ILE:CG2	1:B:355:LEU:HB3	2.47	0.44
1:B:482:ARG:CZ	1:B:587:MET:HG3	2.48	0.44
1:B:681:PHE:CE1	1:B:738:THR:HG22	2.51	0.44
1:B:864:ARG:HA	1:B:906:LEU:HD13	1.99	0.44
1:B:1146:THR:O	1:B:1150:ILE:HG13	2.17	0.44
1:A:331:THR:HG21	1:A:498:ALA:O	2.18	0.44
1:A:659:PHE:CD2	1:A:660:LEU:HD22	2.53	0.44
1:A:697:SER:HB3	1:A:713:MET:HE3	2.00	0.44
1:B:285:PHE:CE2	1:B:428:MET:HG2	2.53	0.44
1:A:1172:VAL:CG2	1:A:1201:ARG:HG2	2.47	0.44
1:B:640:MET:HE3	1:B:640:MET:HB2	1.81	0.44
1:A:1043:LEU:HD23	1:A:1043:LEU:HA	1.85	0.44
1:B:297:LEU:HD13	1:B:613:SER:HB2	2.00	0.44
1:B:514:PRO:O	1:B:515:GLN:HB2	2.18	0.44
1:B:718:LEU:HD12	1:B:718:LEU:O	2.18	0.44
1:B:747:ILE:HA	1:B:750:THR:CG2	2.48	0.44
1:A:480:ASP:OD2	1:A:480:ASP:C	2.60	0.43
1:A:1031:ASP:CG	1:B:240:ARG:HE	2.25	0.43
1:B:339:SER:CB	1:B:519:PRO:HB3	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1118:LYS:CB	1:B:1123:ALA:HB2	2.48	0.43
1:A:819:ILE:HD12	1:A:881:PRO:HG3	2.01	0.43
1:A:860:ALA:HB1	1:A:865:GLU:OE2	2.18	0.43
1:B:482:ARG:HG2	1:B:482:ARG:NH1	2.32	0.43
1:B:548:ALA:HA	1:B:574:PHE:CB	2.47	0.43
1:B:800:SER:H	1:B:800:SER:HG	1.56	0.43
1:B:437:VAL:O	1:B:441:ILE:HD13	2.18	0.43
1:A:678:ILE:O	1:A:682:PHE:HD1	2.02	0.43
1:A:688:LEU:HA	1:A:688:LEU:HD23	1.56	0.43
1:A:1072:MET:HE2	1:A:1072:MET:CA	2.36	0.43
1:B:886:LEU:HD12	1:B:903:TYR:CE1	2.53	0.43
1:B:892:TRP:CD2	1:B:1184:MET:HG2	2.53	0.43
1:A:864:ARG:H	1:A:902:MET:HE3	1.84	0.43
1:B:285:PHE:HE2	1:B:428:MET:HG2	1.83	0.43
1:A:794:MET:HG2	1:A:884:LEU:HD11	2.01	0.43
1:B:1172:VAL:CG2	1:B:1201:ARG:HG2	2.49	0.43
1:A:415:ILE:O	1:A:419:ILE:HG12	2.19	0.43
1:A:597:SER:CB	1:A:603:ILE:HG13	2.49	0.43
1:B:351:GLY:HA2	1:B:505:ALA:O	2.18	0.43
1:A:390:THR:HG22	1:A:608:PHE:CE1	2.52	0.43
1:A:892:TRP:CD2	1:A:1184:MET:HG2	2.54	0.43
1:B:415:ILE:O	1:B:419:ILE:HG12	2.19	0.43
1:B:593:MET:HE3	1:B:593:MET:HB3	1.88	0.43
1:B:705:ARG:N	1:B:706:PRO:HD3	2.34	0.43
1:B:893:LEU:HD23	1:B:893:LEU:HA	1.87	0.43
1:A:593:MET:HE3	1:A:593:MET:HB3	1.93	0.43
1:A:805:LEU:HD23	1:A:851:MET:HE2	1.98	0.43
1:B:1092:ILE:O	1:B:1093:ASN:HB2	2.19	0.43
1:A:888:PHE:CD2	1:A:921:ARG:HD2	2.54	0.43
1:B:322:LEU:HD23	1:B:487:PHE:HZ	1.83	0.43
1:B:686:TYR:OH	5:B:1304:CL:CL	2.59	0.43
1:B:851:MET:HE3	1:B:851:MET:HB3	1.91	0.43
1:A:388:ALA:HA	1:A:391:VAL:CG1	2.48	0.42
1:B:303:MET:O	1:B:303:MET:HG3	2.18	0.42
1:A:381:ALA:HB2	1:A:662:ALA:HA	2.00	0.42
1:A:1170:LEU:HD23	1:A:1201:ARG:HB3	2.01	0.42
1:B:366:GLY:HA2	1:B:629:LEU:CD1	2.48	0.42
1:B:442:LEU:HD11	1:B:610:ALA:HB2	2.00	0.42
1:B:687:ALA:HB2	1:B:723:CYS:HB2	2.01	0.42
1:A:871:MET:HB3	1:A:913:ILE:HD13	2.01	0.42
1:B:623:PRO:HG2	1:B:655:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ASN:HB3	1:A:715:ILE:HG12	2.02	0.42
1:A:1032:ASP:O	1:A:1204:HIS:HA	2.18	0.42
1:A:1097:LYS:O	1:A:1101:ILE:HG13	2.19	0.42
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.90	0.42
1:A:657:LEU:O	1:A:661:ILE:HG13	2.18	0.42
1:B:1022:ASN:O	1:B:1052:CYS:HA	2.19	0.42
1:B:1043:LEU:O	1:B:1049:TRP:HB2	2.20	0.42
1:A:341:ILE:HG22	1:A:355:LEU:HD22	2.02	0.42
1:A:480:ASP:OD2	1:A:480:ASP:O	2.37	0.42
1:A:1170:LEU:HB3	1:A:1201:ARG:HB2	2.01	0.42
1:B:577:CYS:HB3	1:B:582:CYS:HB3	1.96	0.42
1:A:473:PHE:HD1	1:A:542:SER:HG	1.67	0.42
1:A:683:LEU:HD13	1:A:727:MET:CA	2.49	0.42
1:A:1151:ARG:HH11	1:A:1151:ARG:HG2	1.84	0.42
1:B:288:ILE:HG22	1:B:289:ASN:N	2.35	0.42
1:B:641:PHE:CD1	1:B:653:ARG:HB3	2.55	0.42
1:B:921:ARG:O	1:B:922:LEU:HD12	2.20	0.42
1:B:799:ASN:HB3	1:B:845:TRP:CZ2	2.55	0.42
1:A:1107:ILE:O	1:A:1110:PRO:HD2	2.20	0.42
1:B:507:ILE:O	1:B:511:LEU:HG	2.20	0.42
1:B:683:LEU:HD13	1:B:727:MET:CA	2.50	0.42
1:B:807:LEU:HD23	1:B:807:LEU:HA	1.86	0.42
1:A:366:GLY:HA2	1:A:629:LEU:HD11	2.02	0.41
1:A:431:GLU:O	1:A:435:GLN:HG2	2.19	0.41
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.72	0.41
1:A:852:LYS:HG2	1:B:775:ILE:HG21	2.02	0.41
1:B:353:TYR:CE1	1:B:629:LEU:HD12	2.55	0.41
1:A:442:LEU:HD11	1:A:610:ALA:HB2	2.02	0.41
1:A:817:LEU:HD22	1:A:879:MET:O	2.20	0.41
1:A:1075:LEU:HD13	1:B:224:ILE:HA	2.02	0.41
1:B:906:LEU:HD12	1:B:906:LEU:HA	1.90	0.41
1:B:1058:ILE:HD13	1:B:1072:MET:HB2	2.02	0.41
1:B:347:VAL:CG2	1:B:514:PRO:HG2	2.50	0.41
1:A:1019:GLN:O	1:A:1020:GLY:C	2.61	0.41
1:B:460:LYS:H	1:B:460:LYS:HG2	1.65	0.41
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.83	0.41
1:A:680:ASN:OD1	1:A:727:MET:HB2	2.20	0.41
1:A:1129:ASP:OD1	1:A:1129:ASP:N	2.51	0.41
1:A:1148:ARG:HH22	1:B:217:TPO:P	2.44	0.41
1:B:366:GLY:HA2	1:B:629:LEU:HD11	2.02	0.41
1:B:388:ALA:HA	1:B:391:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ALA:O	1:B:438:LEU:HD13	2.20	0.41
1:B:864:ARG:H	1:B:902:MET:HE3	1.86	0.41
1:B:347:VAL:O	1:B:347:VAL:CG2	2.69	0.41
1:B:645:TYR:CD1	1:B:652:LEU:HG	2.55	0.41
1:B:681:PHE:HE1	1:B:738:THR:HG22	1.86	0.41
1:A:249:GLU:HG2	1:B:1175:LYS:CG	2.51	0.41
1:A:341:ILE:HG12	1:A:693:VAL:CG2	2.50	0.41
1:A:482:ARG:HB2	1:A:587:MET:SD	2.61	0.41
1:B:599:PHE:CD1	1:B:601:PRO:HD2	2.56	0.41
1:A:385:VAL:HG21	1:A:671:LEU:HD21	2.02	0.41
1:B:229:HIS:ND1	1:B:229:HIS:C	2.79	0.41
1:B:353:TYR:CZ	1:B:629:LEU:HA	2.56	0.41
1:B:414:ALA:O	1:B:418:VAL:HG23	2.21	0.41
1:B:518:ILE:N	1:B:519:PRO:HD2	2.36	0.41
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.76	0.41
1:B:659:PHE:CD2	1:B:660:LEU:HD22	2.56	0.41
1:A:489:SER:O	1:A:493:ILE:HD13	2.21	0.40
1:B:207:THR:C	1:B:209:TYR:H	2.29	0.40
1:B:792:LEU:O	1:B:792:LEU:HG	2.20	0.40
1:A:347:VAL:CG2	1:A:508:SER:HB2	2.52	0.40
1:A:428:MET:HE2	1:A:428:MET:HB2	1.75	0.40
1:A:460:LYS:HE2	1:A:595:MET:O	2.21	0.40
1:A:832:MET:HE2	1:B:914:GLN:HG3	2.03	0.40
1:A:1069:ARG:HH11	1:A:1069:ARG:HG2	1.86	0.40
1:B:1019:GLN:HG3	1:B:1049:TRP:CE3	2.56	0.40
1:B:1083:PHE:CD2	1:B:1086:ILE:HG13	2.57	0.40
1:A:341:ILE:HG21	1:A:355:LEU:HB3	2.02	0.40
1:A:480:ASP:HB3	1:A:546:ARG:NE	2.36	0.40
1:A:817:LEU:HG	1:A:818:MET:N	2.36	0.40
1:B:1101:ILE:HD13	1:B:1147:TYR:CE1	2.56	0.40
1:A:437:VAL:O	1:A:440:VAL:CG1	2.69	0.40
1:A:450:VAL:HA	1:A:453:THR:CG2	2.52	0.40
1:A:705:ARG:N	1:A:706:PRO:HD3	2.37	0.40
1:A:807:LEU:HD23	1:A:807:LEU:HA	1.90	0.40
1:B:864:ARG:H	1:B:902:MET:CE	2.35	0.40
1:B:1011:ALA:O	1:B:1014:GLN:HG2	2.21	0.40
1:A:785:LYS:HB2	1:A:785:LYS:HE2	1.73	0.40
1:A:864:ARG:HB2	1:A:902:MET:HE3	2.03	0.40
1:B:364:PHE:O	1:B:368:ILE:HG12	2.21	0.40
1:B:450:VAL:HA	1:B:453:THR:CG2	2.52	0.40
1:B:514:PRO:C	1:B:516:SER:H	2.29	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	900/1212 (74%)	854 (95%)	46 (5%)	0	100	100
1	B	900/1212 (74%)	866 (96%)	34 (4%)	0	100	100
All	All	1800/2424 (74%)	1720 (96%)	80 (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	644/981 (66%)	613 (95%)	31 (5%)	23	50
1	B	642/981 (65%)	615 (96%)	27 (4%)	26	55
All	All	1286/1962 (66%)	1228 (96%)	58 (4%)	26	52

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	THR
1	A	205	THR
1	A	207	THR
1	A	224	ILE
1	A	229	HIS

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Mol	Chain	Res	Type
1	A	302	VAL
1	A	323	VAL
1	A	328	THR
1	A	392	VAL
1	A	417	VAL
1	A	421	LEU
1	A	436	ILE
1	A	453	THR
1	A	474	ASN
1	A	490	VAL
1	A	536	ILE
1	A	540	VAL
1	A	592	VAL
1	A	671	LEU
1	A	692	SER
1	A	697	SER
1	A	716	SER
1	A	728	PHE
1	A	729	VAL
1	A	765	LEU
1	A	784	VAL
1	A	793	VAL
1	A	815	VAL
1	A	858	VAL
1	A	1045	THR
1	A	1191	SER
1	B	205	THR
1	B	229	HIS
1	B	303	MET
1	B	328	THR
1	B	343	THR
1	B	392	VAL
1	B	417	VAL
1	B	421	LEU
1	B	453	THR
1	B	536	ILE
1	B	540	VAL
1	B	592	VAL
1	B	671	LEU
1	B	692	SER
1	B	697	SER
1	B	729	VAL

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Mol	Chain	Res	Type
1	B	751	TYR
1	B	756	VAL
1	B	761	SER
1	B	784	VAL
1	B	793	VAL
1	B	812	THR
1	B	815	VAL
1	B	836	SER
1	B	858	VAL
1	B	1135	THR
1	B	1193	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	506	ASN
1	A	849	ASN
1	A	1203	ASN
1	B	407	ASN
1	B	849	ASN
1	B	914	GLN
1	B	1093	ASN
1	B	1114	HIS
1	B	1203	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	TPO	B	230	1	8,10,11	1.09	0	10,14,16	2.13	1 (10%)
1	TPO	A	212	1	8,10,11	1.10	0	10,14,16	2.17	1 (10%)
1	TPO	B	212	1	8,10,11	0.70	0	10,14,16	1.04	1 (10%)
1	TPO	A	217	1	8,10,11	1.08	0	10,14,16	2.10	1 (10%)
1	TPO	A	230	1	8,10,11	1.12	0	10,14,16	2.14	1 (10%)
1	TPO	B	217	1	8,10,11	1.09	0	10,14,16	2.09	1 (10%)

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
1	TPO	B	230	1	-	4/9/11/13	-
1	TPO	A	212	1	-	1/9/11/13	-
1	TPO	B	212	1	-	0/9/11/13	-
1	TPO	A	217	1	-	3/9/11/13	-
1	TPO	A	230	1	-	4/9/11/13	-
1	TPO	B	217	1	-	2/9/11/13	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	TPO	P-OG1-CB	-6.21	106.44	123.33
1	A	230	TPO	P-OG1-CB	-6.11	106.73	123.33
1	B	230	TPO	P-OG1-CB	-6.10	106.77	123.33
1	A	217	TPO	P-OG1-CB	-6.01	107.01	123.33
1	B	217	TPO	P-OG1-CB	-5.95	107.16	123.33
1	B	212	TPO	O-C-CA	-2.56	118.19	124.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	217	TPO	N-CA-CB-OG1
1	A	217	TPO	O-C-CA-CB
1	A	230	TPO	N-CA-CB-CG2
1	A	230	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
1	A	230	TPO	C-CA-CB-CG2
1	A	230	TPO	O-C-CA-CB
1	B	217	TPO	N-CA-CB-OG1
1	B	217	TPO	O-C-CA-CB
1	B	230	TPO	N-CA-CB-CG2
1	B	230	TPO	N-CA-CB-OG1
1	B	230	TPO	C-CA-CB-CG2
1	B	230	TPO	O-C-CA-CB
1	A	217	TPO	CB-OG1-P-O3P
1	A	212	TPO	C-CA-CB-CG2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	230	TPO	2	0
1	A	212	TPO	1	0
1	B	217	TPO	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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$
2	ATP	B	1301	7	32,33,33	1.54	4 (12%)	48,52,52	1.77	9 (18%)
3	FUN	A	1302	4	22,22,22	1.94	5 (22%)	32,32,32	1.79	5 (15%)
2	ATP	A	1301	7	32,33,33	1.52	4 (12%)	48,52,52	1.77	9 (18%)
3	FUN	B	1302	4	22,22,22	1.93	5 (22%)	32,32,32	1.79	5 (15%)

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
2	ATP	B	1301	7	-	1/22/38/38	0/3/3/3
3	FUN	A	1302	4	-	0/15/15/15	0/2/2/2
2	ATP	A	1301	7	-	4/22/38/38	0/3/3/3
3	FUN	B	1302	4	-	0/15/15/15	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	FUN	S1-N1	5.40	1.70	1.60
3	B	1302	FUN	S1-N1	5.39	1.70	1.60
2	B	1301	ATP	C6-N6	4.10	1.44	1.34
2	A	1301	ATP	C6-N6	4.09	1.44	1.34
3	A	1302	FUN	O3-C6	-3.71	1.26	1.36
3	B	1302	FUN	O3-C6	-3.69	1.26	1.36
2	B	1301	ATP	PG-O1G	3.44	1.61	1.50
3	A	1302	FUN	C2-CL1	3.29	1.81	1.73
3	B	1302	FUN	C2-CL1	3.27	1.81	1.73
2	A	1301	ATP	PA-O1A	2.99	1.61	1.50
2	B	1301	ATP	PA-O1A	2.97	1.61	1.50
2	A	1301	ATP	PB-O1B	2.94	1.61	1.50
3	B	1302	FUN	C4-N2	2.94	1.45	1.37
3	A	1302	FUN	C4-N2	2.93	1.45	1.37
2	A	1301	ATP	C5-N7	-2.42	1.34	1.39
2	B	1301	ATP	C5-N7	-2.37	1.34	1.39
3	A	1302	FUN	C1-S1	-2.20	1.75	1.77
3	B	1302	FUN	C1-S1	-2.12	1.75	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	FUN	O2-S1-O1	-6.16	109.32	118.80
3	B	1302	FUN	O2-S1-O1	-6.16	109.33	118.80
2	A	1301	ATP	C5-C4-N3	-5.34	119.36	126.72
2	B	1301	ATP	C5-C4-N3	-5.31	119.40	126.72
2	B	1301	ATP	N3-C2-N1	-5.18	120.74	128.58
2	A	1301	ATP	N3-C2-N1	-5.16	120.77	128.58
2	A	1301	ATP	C2-N3-C4	3.60	120.62	111.83
2	B	1301	ATP	C2-N3-C4	3.59	120.59	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	ATP	N9-C8-N7	-3.47	109.01	113.94
2	B	1301	ATP	N3-C4-N9	3.42	132.98	127.17
2	B	1301	ATP	N9-C8-N7	-3.41	109.11	113.94
2	A	1301	ATP	N3-C4-N9	3.40	132.95	127.17
3	B	1302	FUN	C2-C1-S1	-2.99	119.88	123.47
3	A	1302	FUN	C2-C1-S1	-2.94	119.95	123.47
2	A	1301	ATP	C3'-C2'-C1'	2.64	106.46	101.46
2	B	1301	ATP	C3'-C2'-C1'	2.61	106.39	101.46
2	A	1301	ATP	C5-N7-C8	2.55	107.46	103.45
2	A	1301	ATP	C4-C5-N7	-2.50	107.72	110.58
2	B	1301	ATP	C5-N7-C8	2.50	107.39	103.45
2	B	1301	ATP	C4-C5-N7	-2.48	107.75	110.58
3	A	1302	FUN	O3-C6-C5	2.32	125.44	117.50
3	B	1302	FUN	O3-C6-C5	2.32	125.43	117.50
2	B	1301	ATP	C4-N9-C8	2.29	108.14	105.74
2	A	1301	ATP	C4-N9-C8	2.27	108.12	105.74
3	B	1302	FUN	C5-C6-C7	-2.19	125.60	133.07
3	A	1302	FUN	C5-C6-C7	-2.18	125.63	133.07
3	A	1302	FUN	C9-O3-C6	2.13	110.46	106.22
3	B	1302	FUN	C9-O3-C6	2.10	110.40	106.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ATP	C5'-O5'-PA-O3A
2	B	1301	ATP	O4'-C4'-C5'-O5'
2	A	1301	ATP	C5'-O5'-PA-O1A
2	A	1301	ATP	O4'-C4'-C5'-O5'
2	A	1301	ATP	O4'-C1'-N9-C8

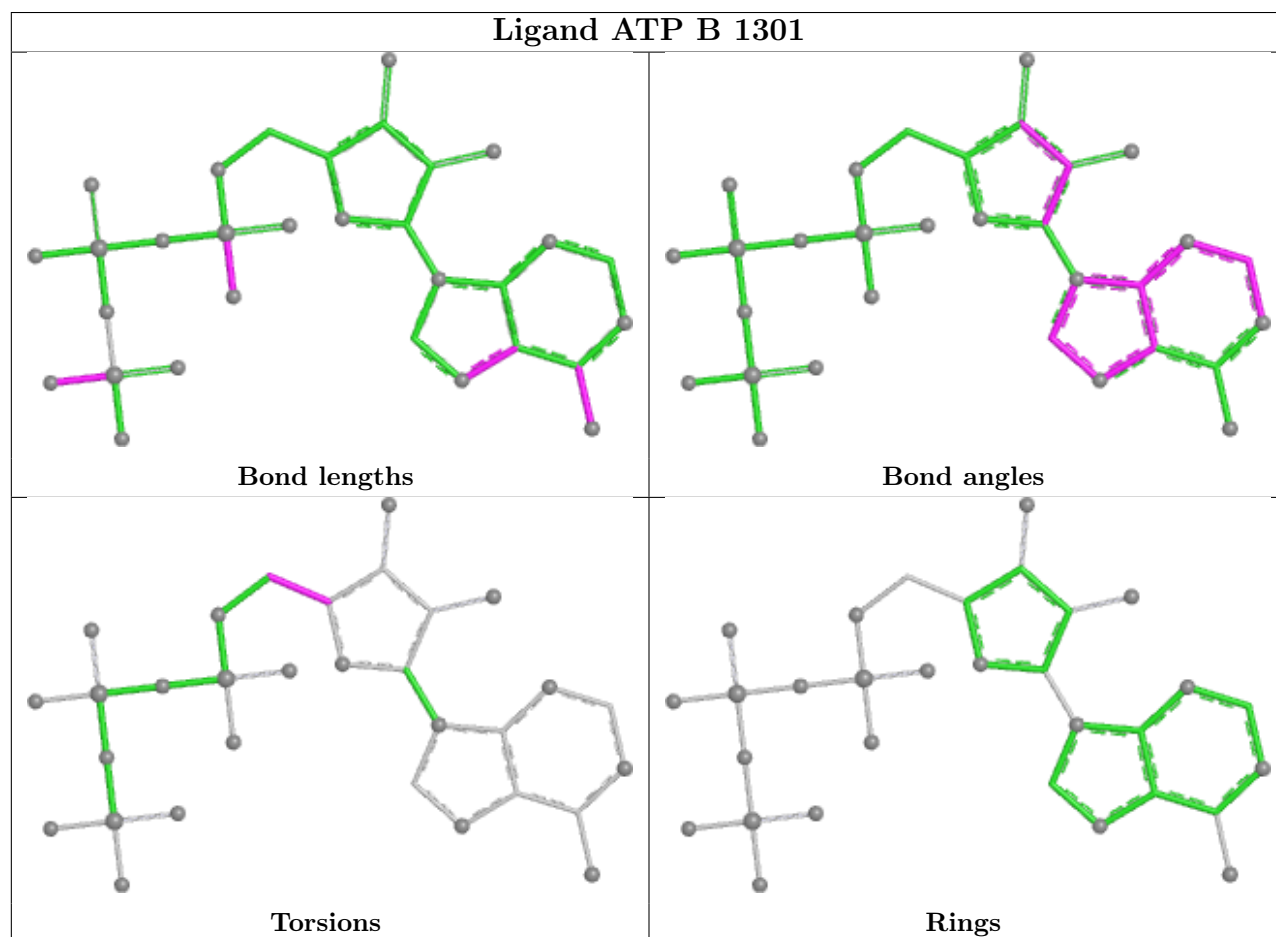
There are no ring outliers.

2 monomers are involved in 5 short contacts:

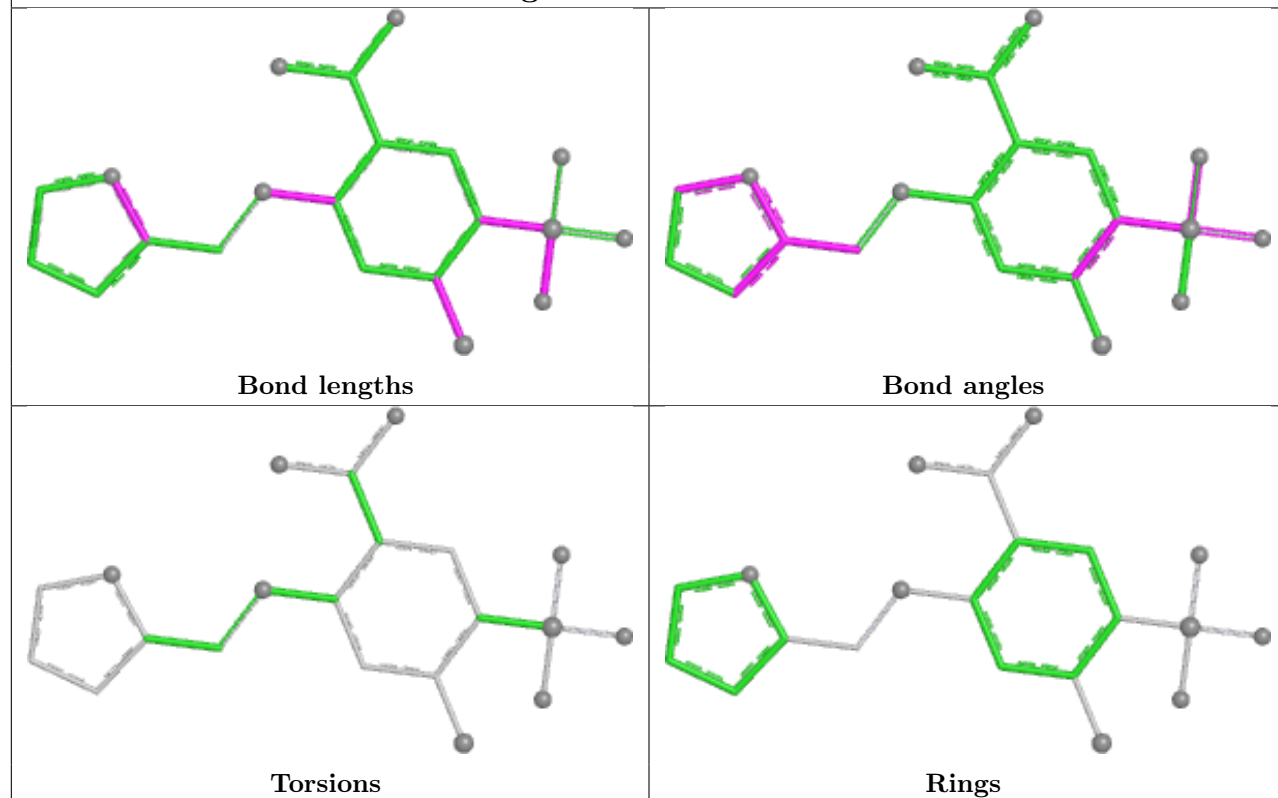
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	ATP	2	0
2	A	1301	ATP	3	0

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

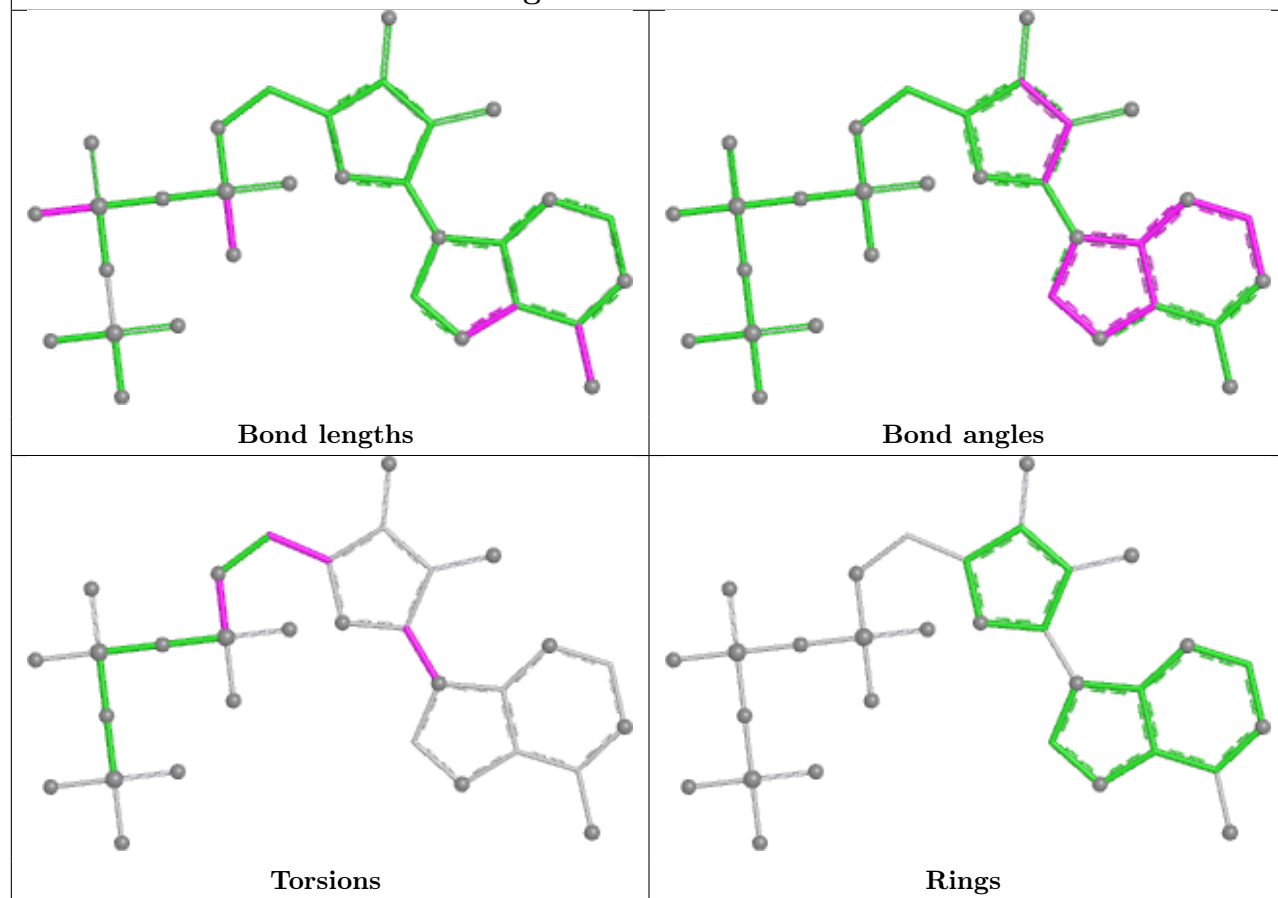
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

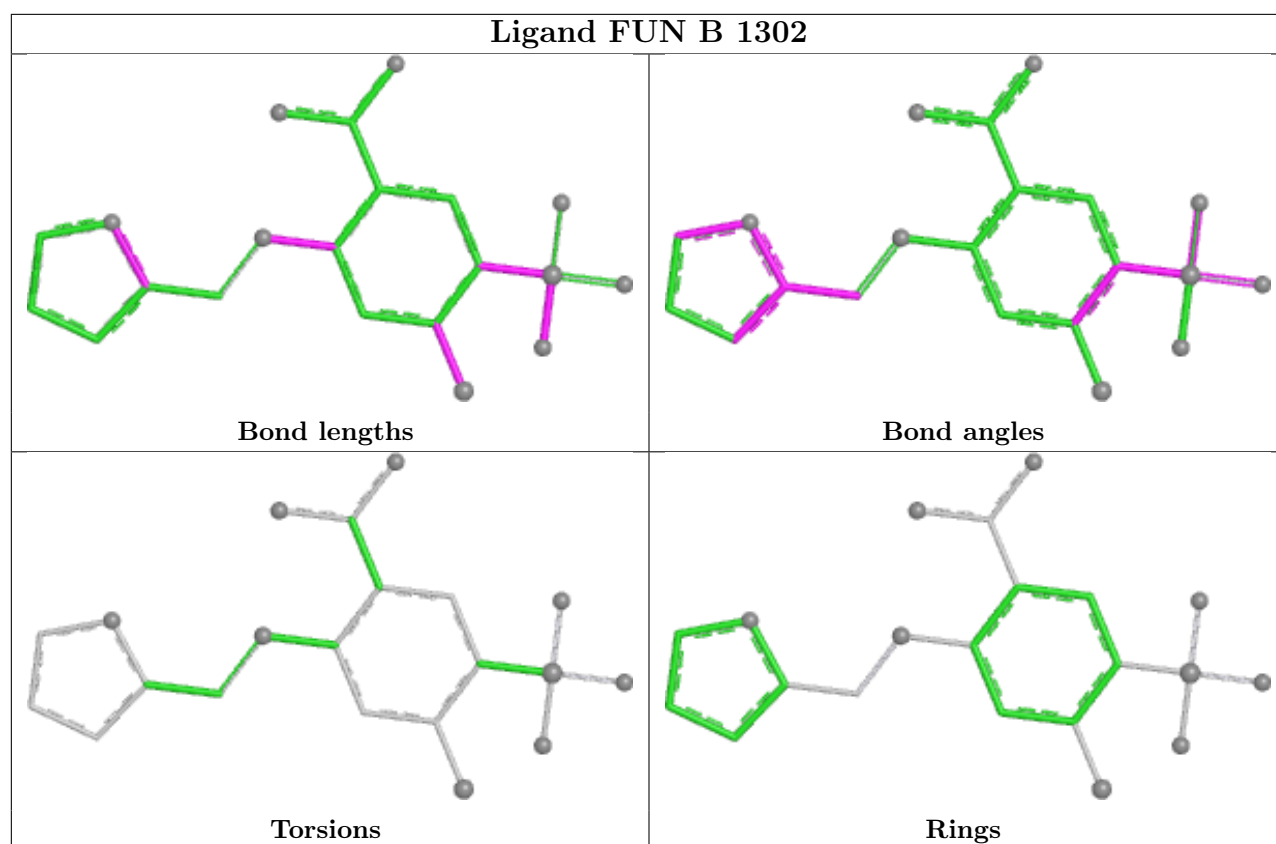


Ligand FUN A 1302



Ligand ATP A 1301





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.

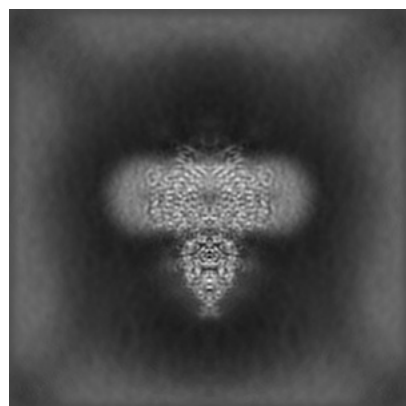
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45081. These allow visual inspection of the internal detail of the map and identification of artifacts.

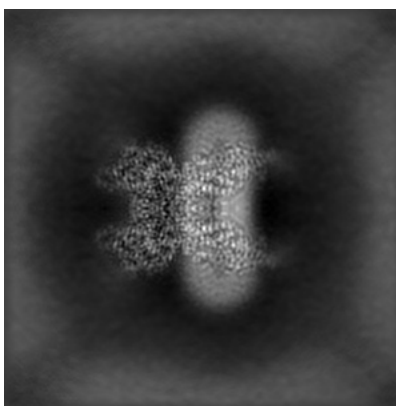
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

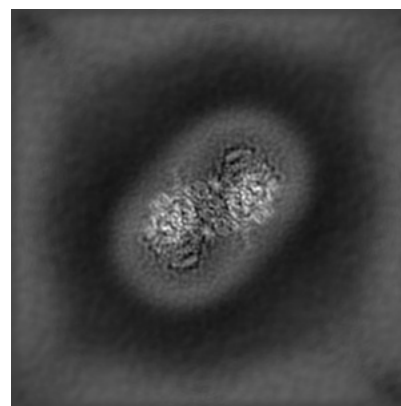
6.1.1 Primary map



X

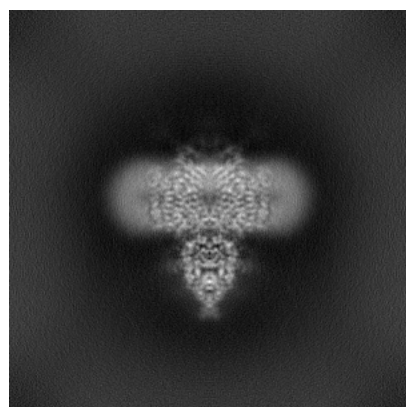


Y

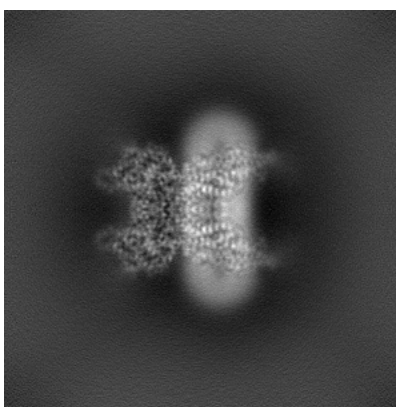


Z

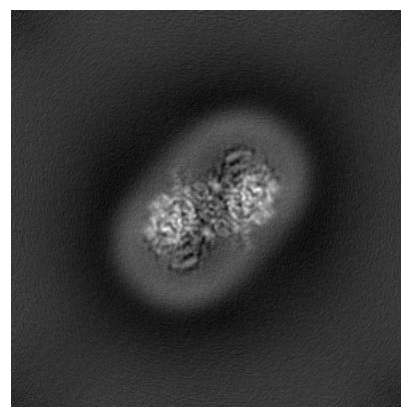
6.1.2 Raw map



X



Y

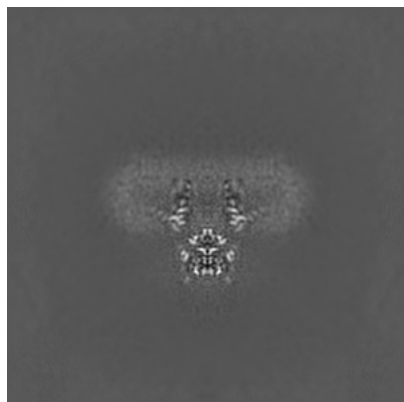


Z

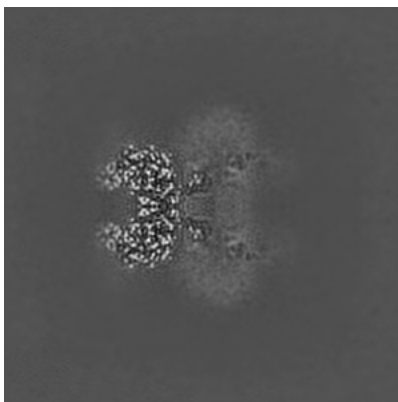
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

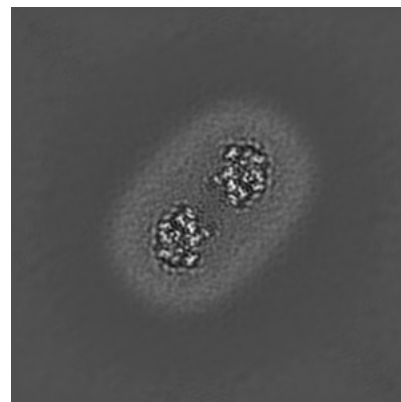
6.2.1 Primary map



X Index: 180

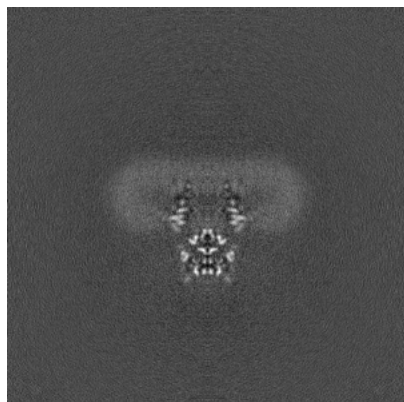


Y Index: 180

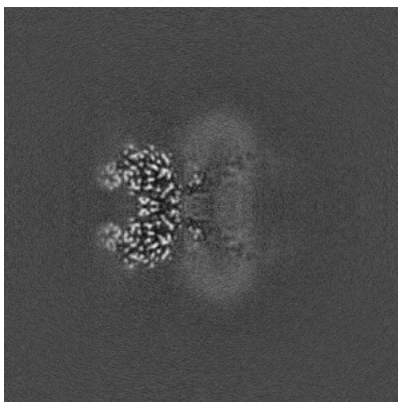


Z Index: 180

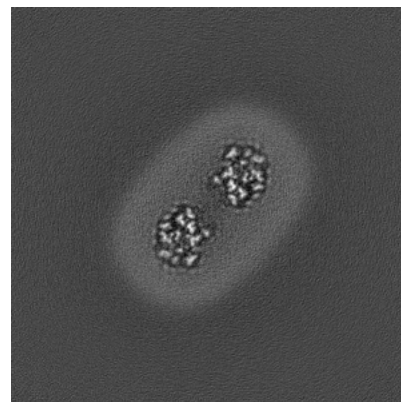
6.2.2 Raw map



X Index: 180



Y Index: 180

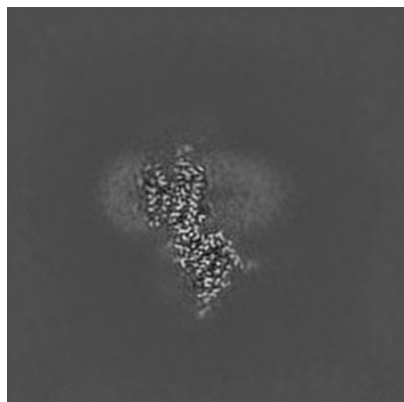


Z Index: 180

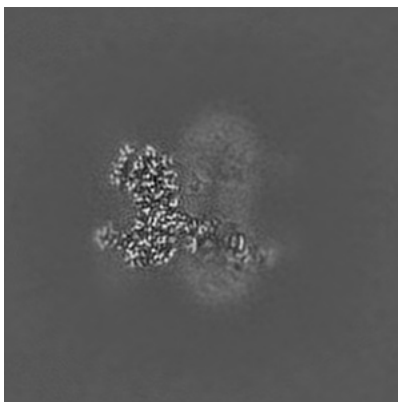
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

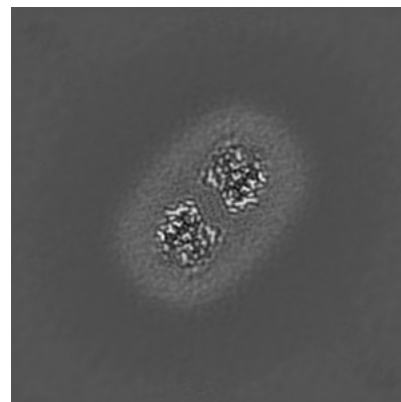
6.3.1 Primary map



X Index: 150

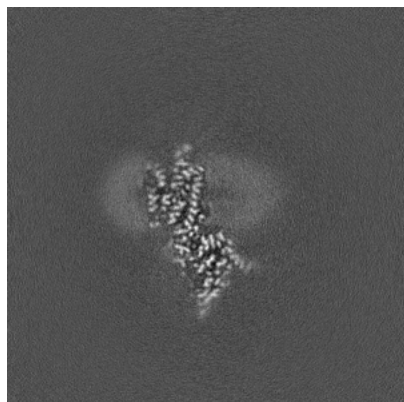


Y Index: 175

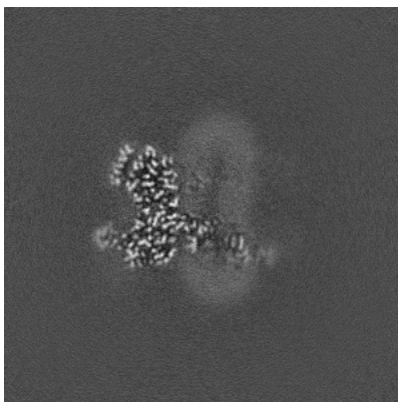


Z Index: 171

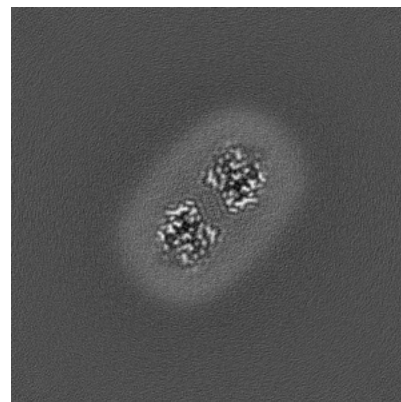
6.3.2 Raw map



X Index: 149



Y Index: 175

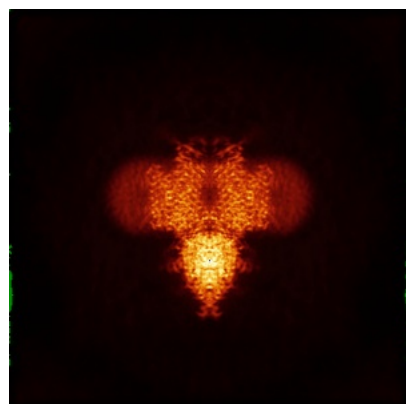


Z Index: 171

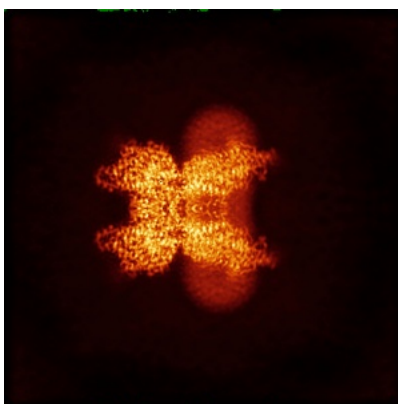
The images above show the largest variance slices of the map in three orthogonal directions.

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

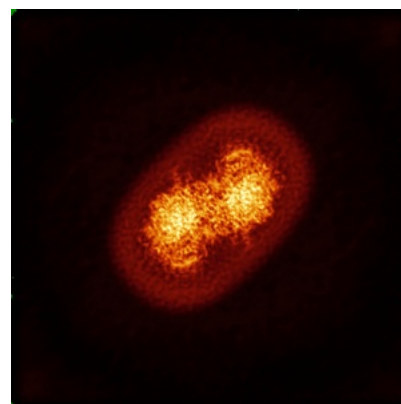
6.4.1 Primary map



X

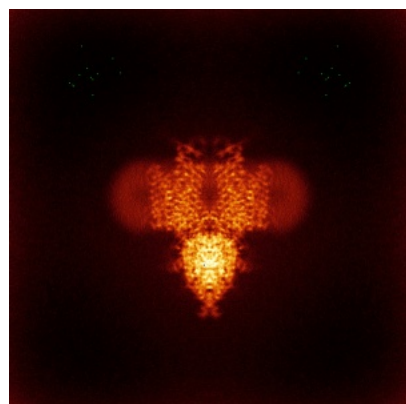


Y

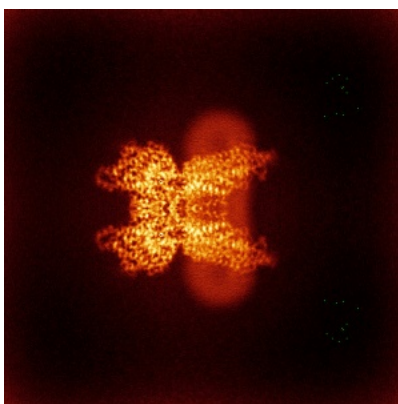


Z

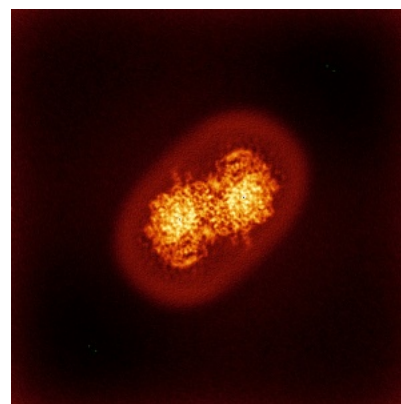
6.4.2 Raw map



X



Y

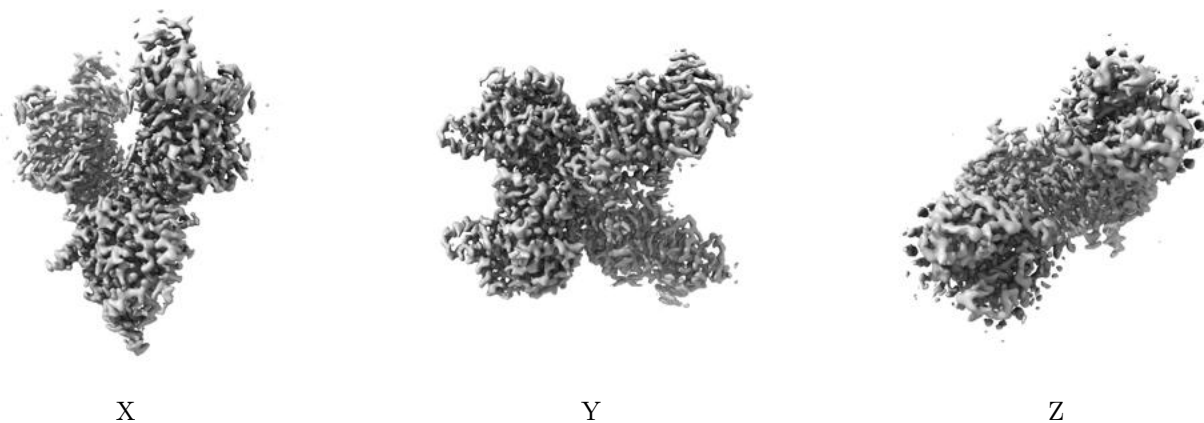


Z

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.

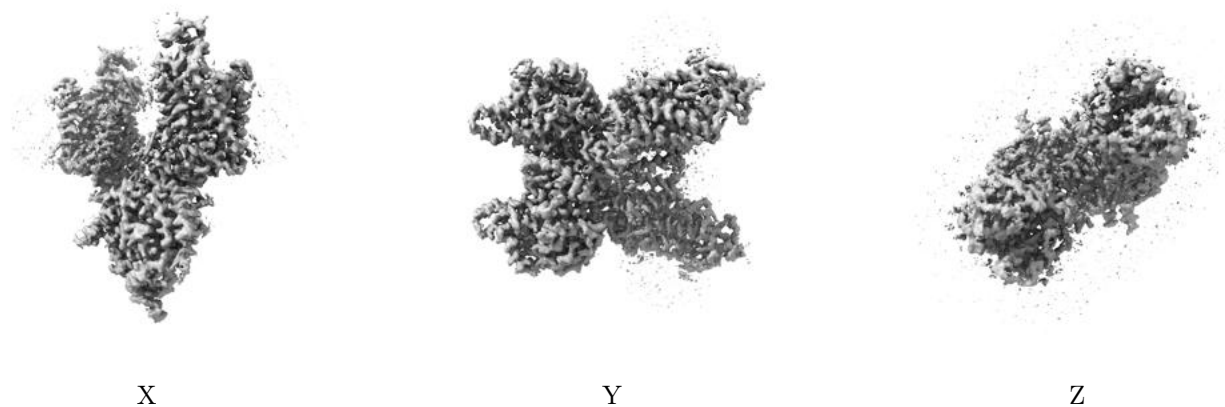
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

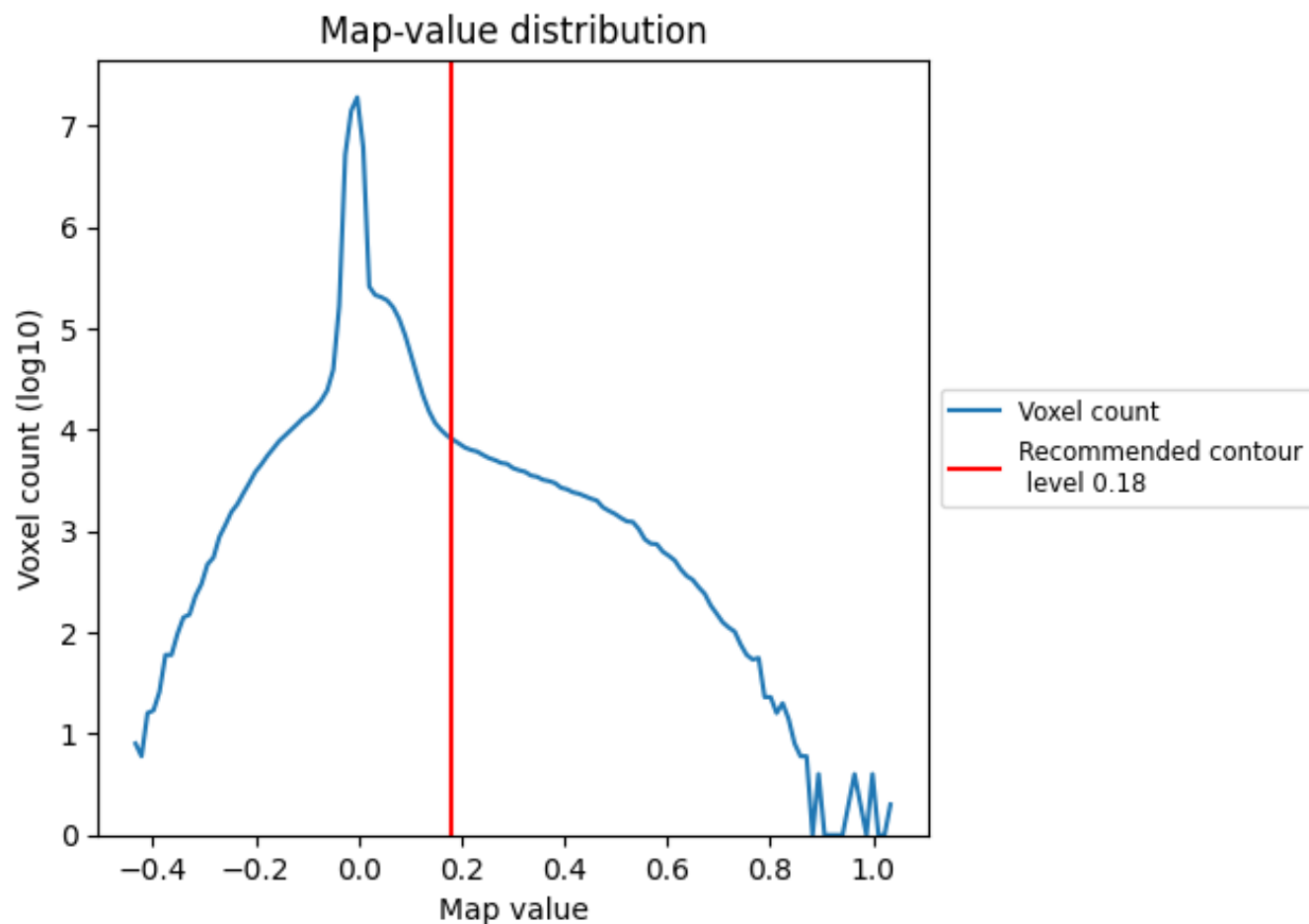
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

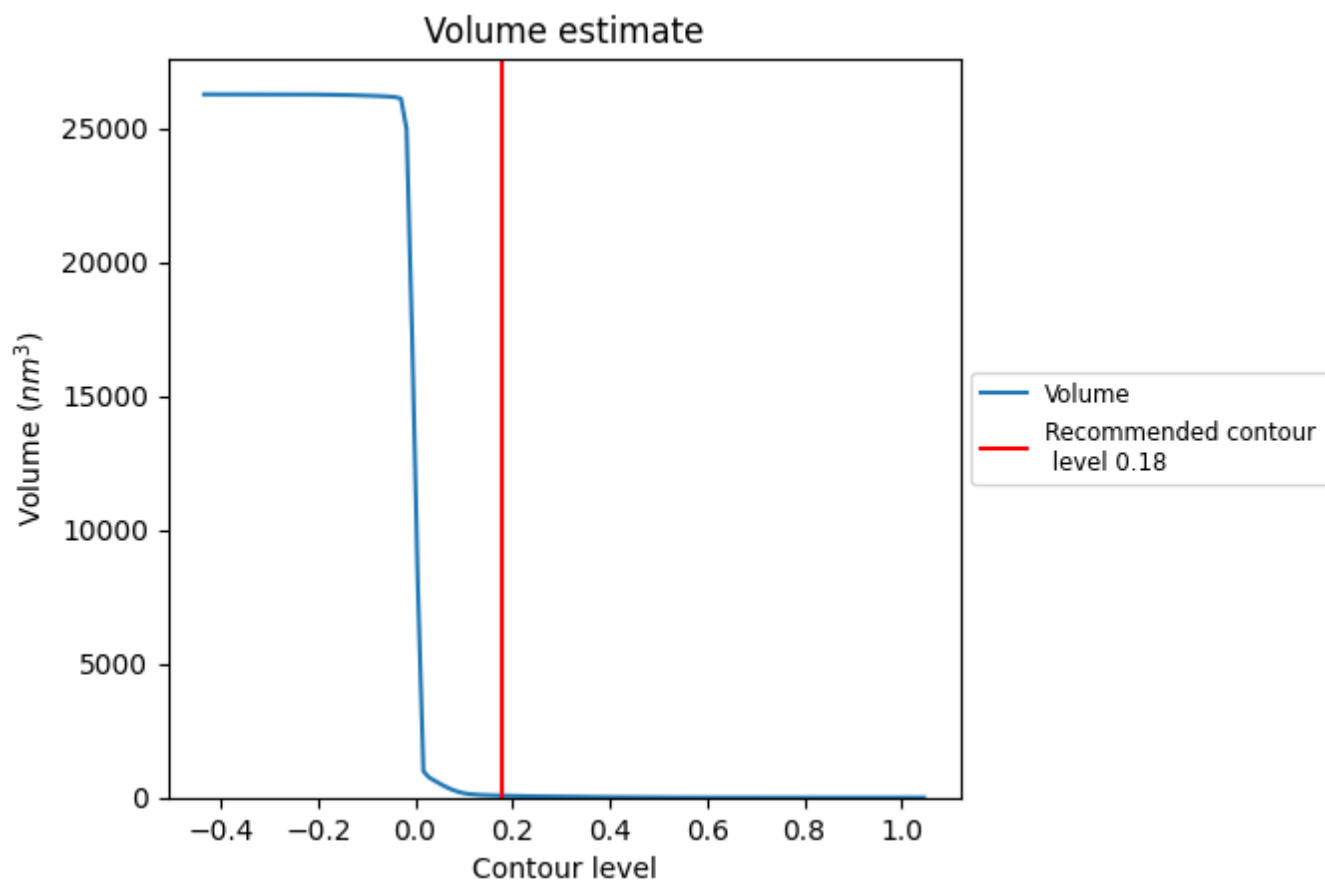
This section contains the results of statistical analysis of the map.

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.

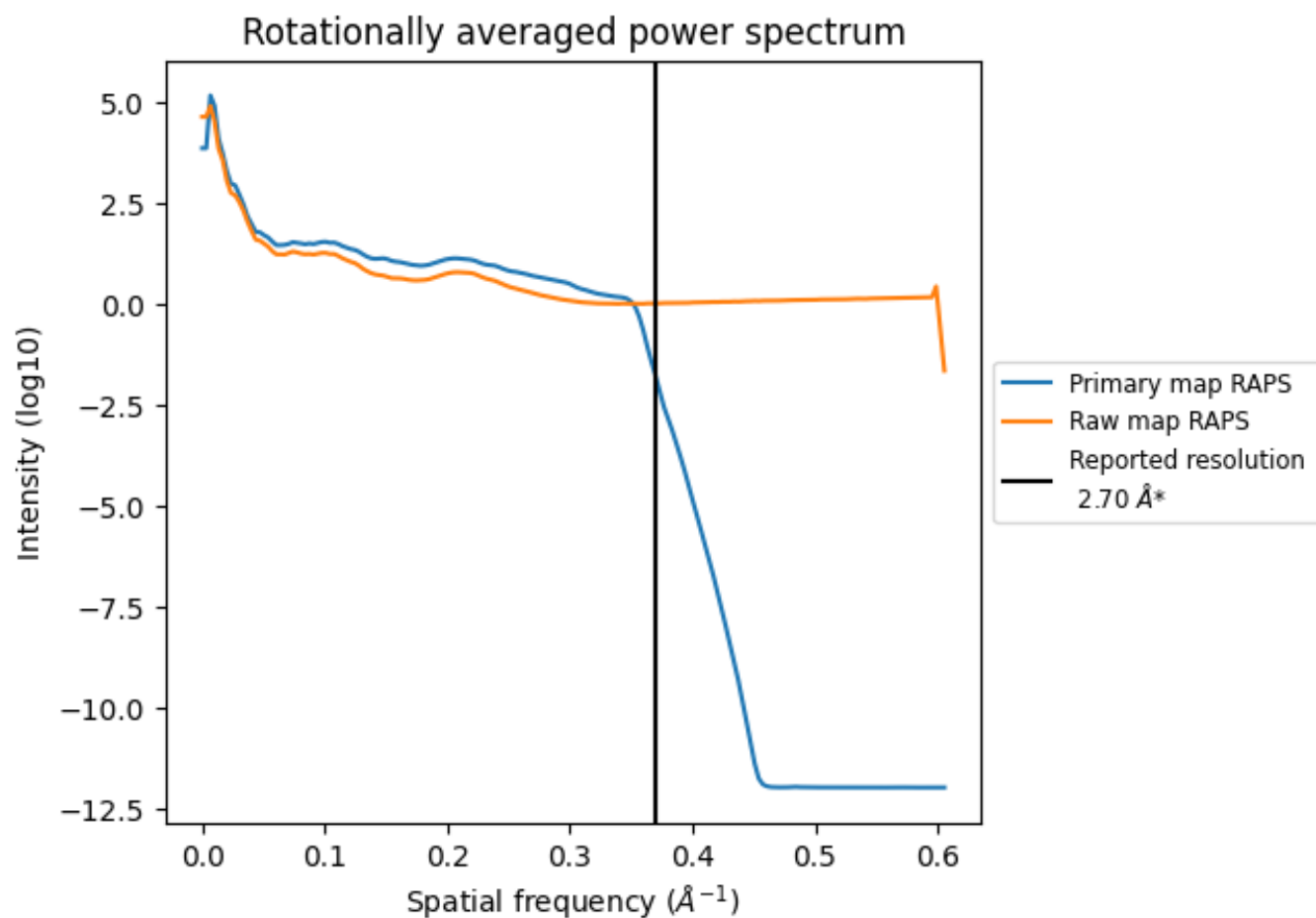
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm^3 ; this corresponds to an approximate mass of 63 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 ⓘ

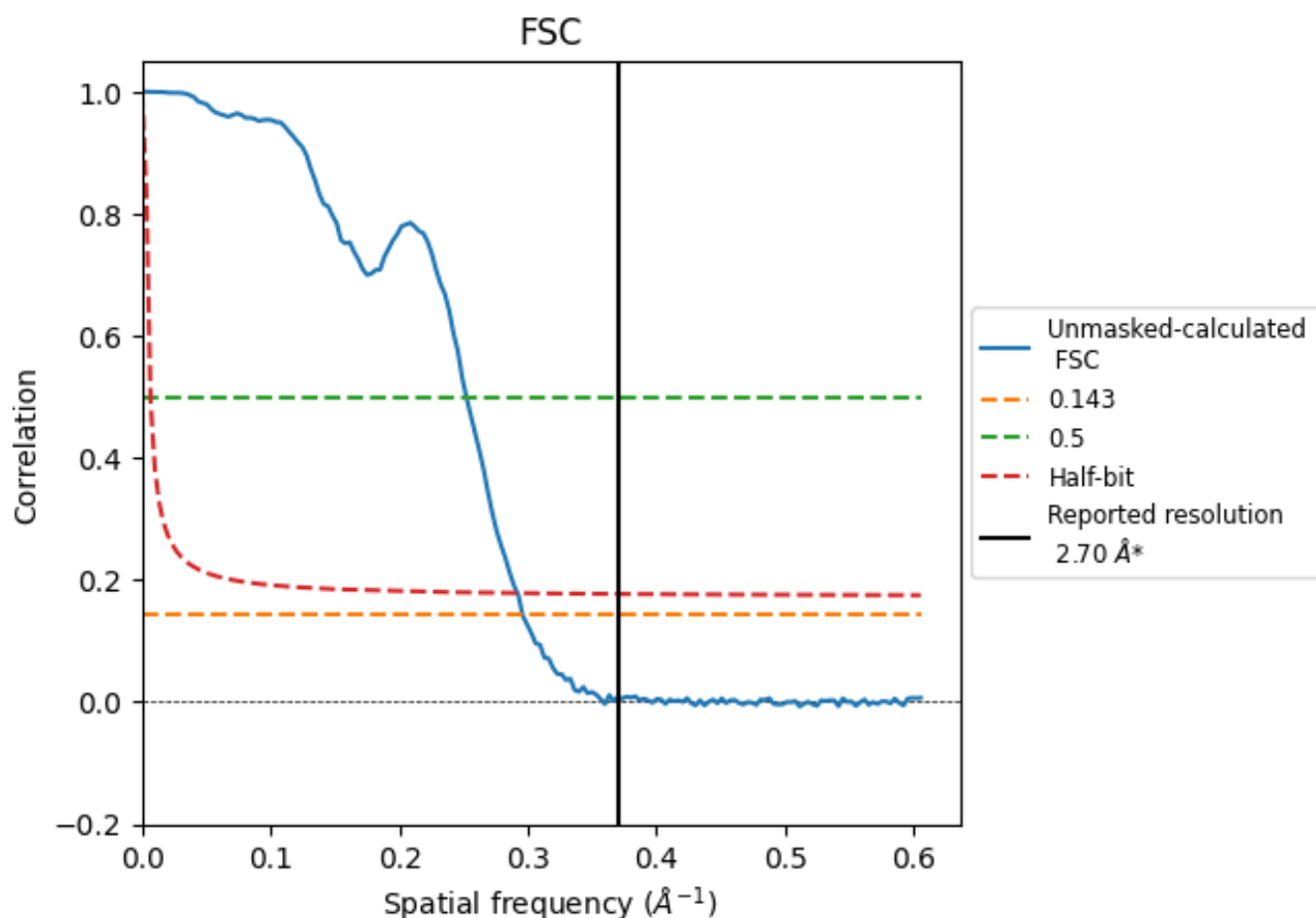


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

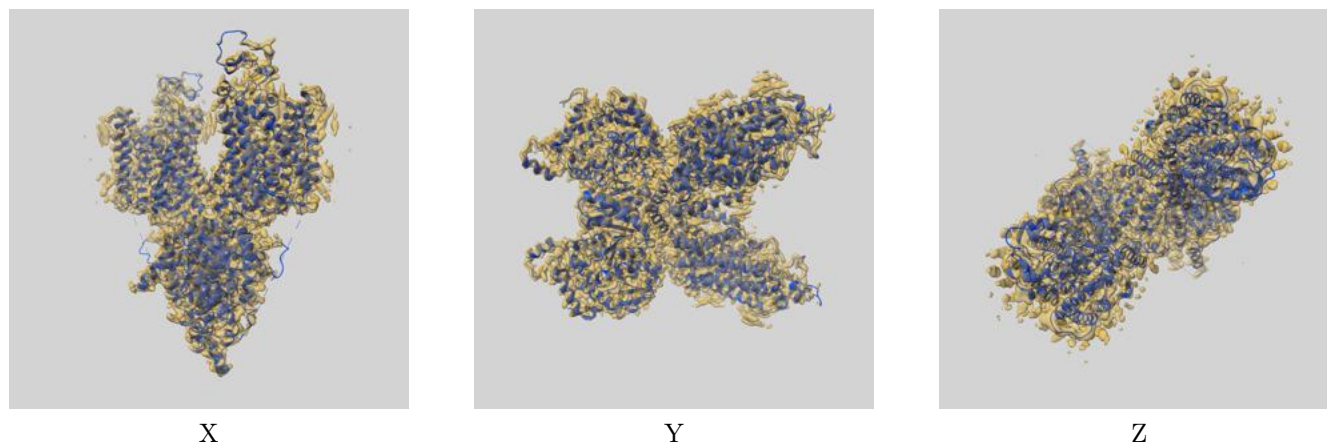
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.97	3.43

*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 3.38 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

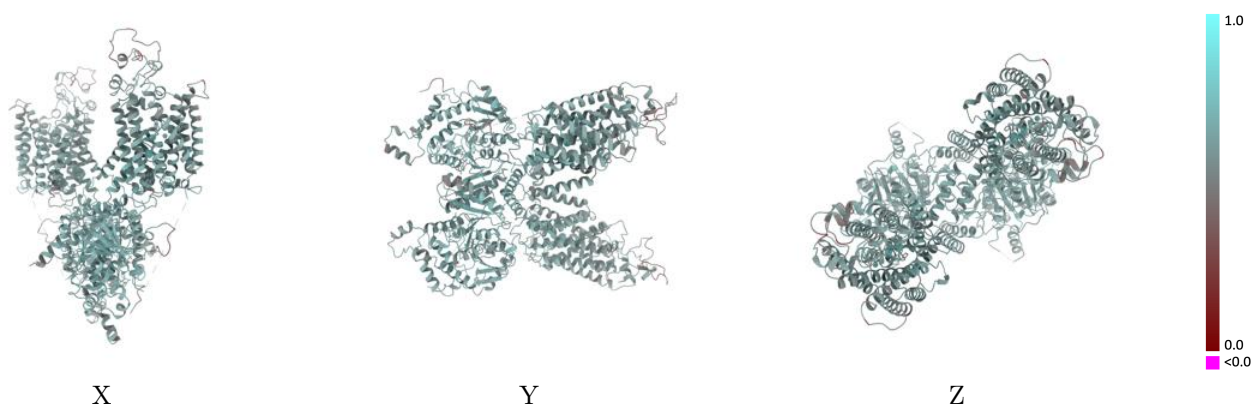
This section contains information regarding the fit between EMDB map EMD-45081 and PDB model 9C0E. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



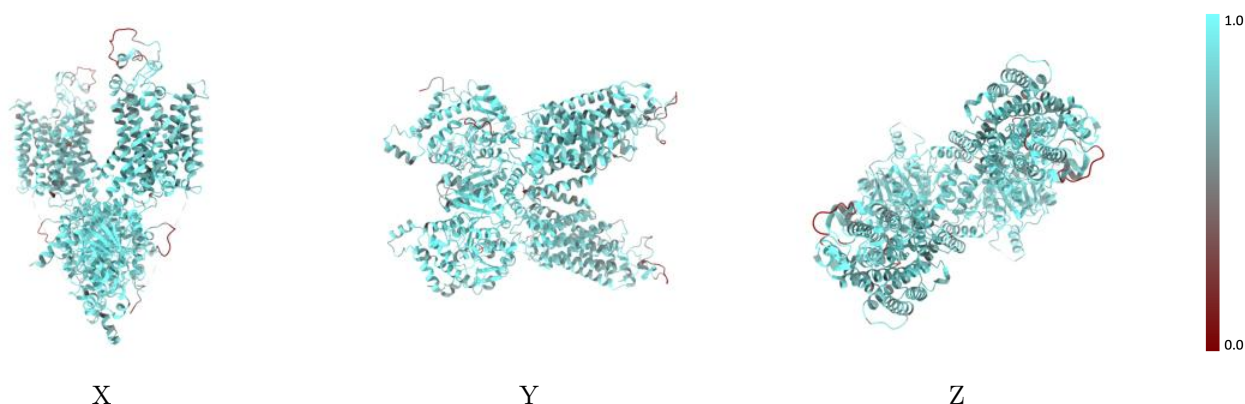
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



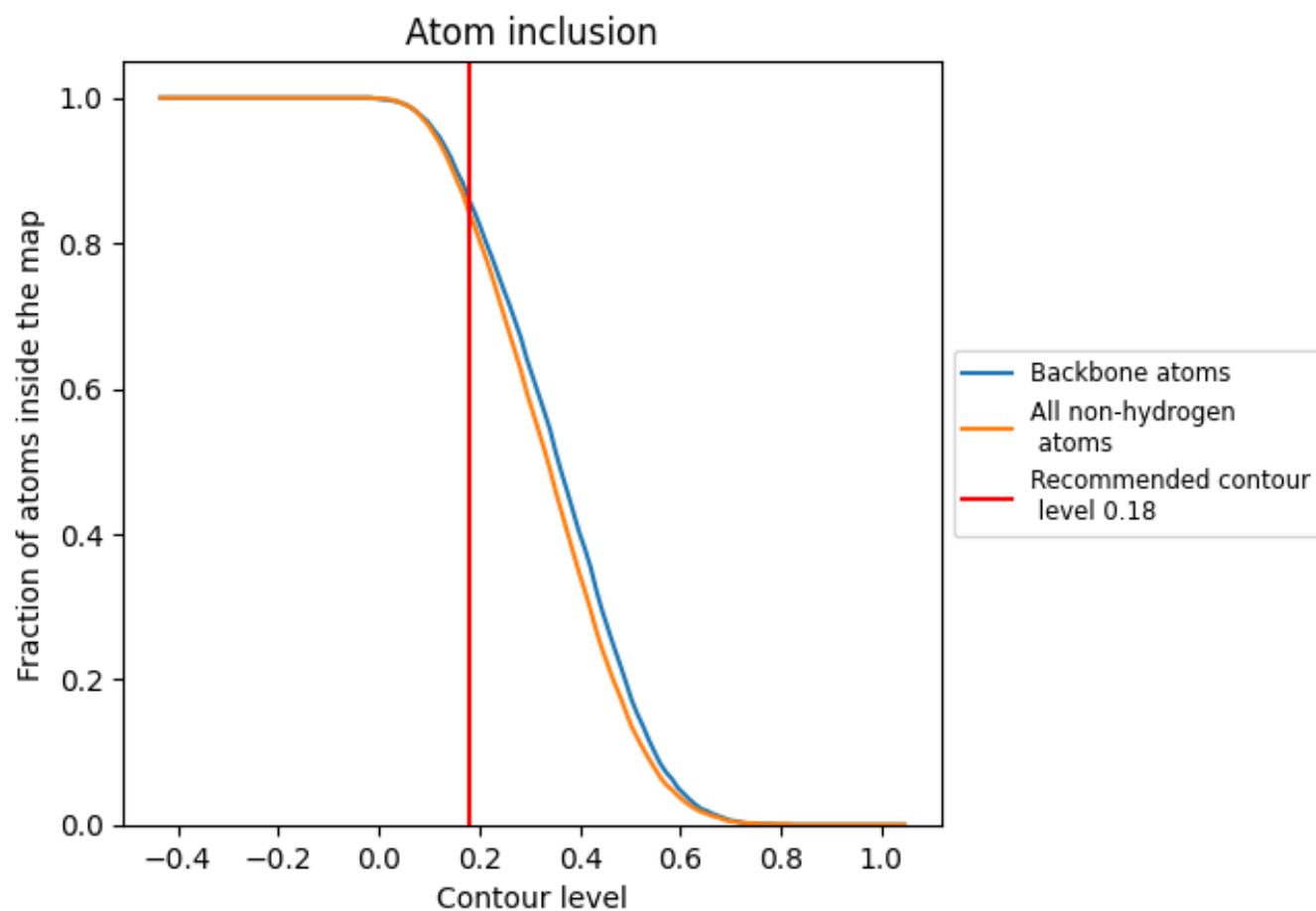
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.8410	0.6000
A	0.8430	0.6010
B	0.8430	0.6000

