



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 04:18 PM JST

PDB ID : 8YY5 / pdb_00008yy5
EMDB ID : EMD-39667
Title : Kinesin-14 with Alf3 bound to 14 PF Microtubule
Authors : Shibata, S.; Imasaki, T.; Shigematsu, H.; Endow, S.A.; Nitta, R.
Deposited on : 2024-04-03
Resolution : 3.99 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:

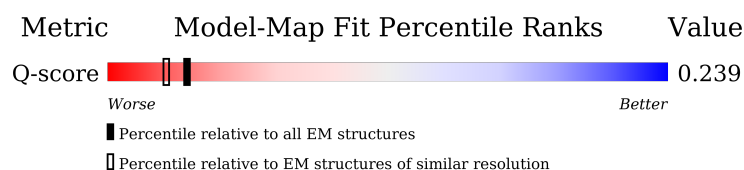
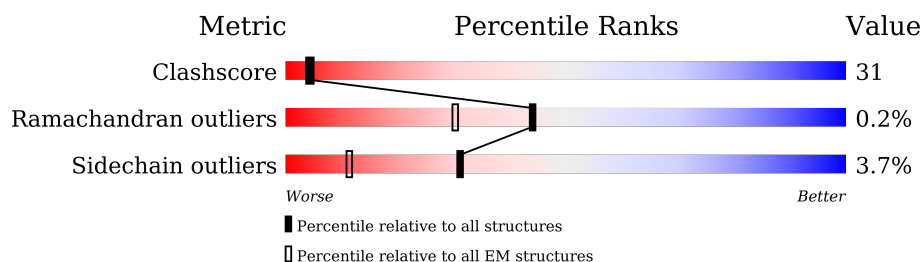
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.99 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	7463 (3.49 - 4.49)

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	451	
2	B	444	
3	C	409	
3	D	409	

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
8	ALF	C	903	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12315 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	428	Total	C	N	O	S	0	0
			3352	2127	571	633	21		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	428	Total	C	N	O	S	0	0
			3356	2111	575	646	24		

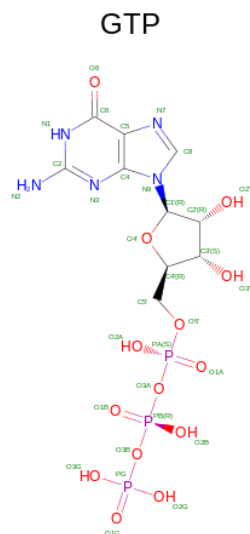
- Molecule 3 is a protein called Protein claret segregational.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	355	Total	C	N	O	S	0	0
			2836	1766	503	547	20		
3	D	334	Total	C	N	O	S	0	0
			2650	1655	465	513	17		

There are 6 discrepancies between the modelled and reference sequences:

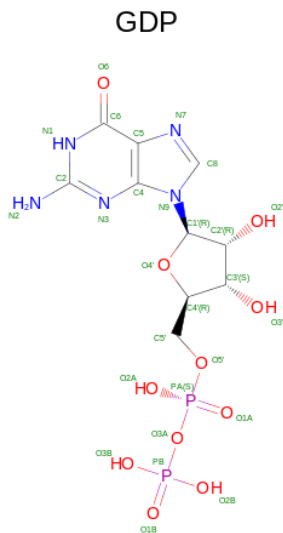
Chain	Residue	Modelled	Actual	Comment	Reference
C	292	MET	GLU	engineered mutation	UNP P20480
C	485	LYS	TYR	engineered mutation	UNP P20480
C	697	ASN	SER	engineered mutation	UNP P20480
D	292	MET	GLU	engineered mutation	UNP P20480
D	485	LYS	TYR	engineered mutation	UNP P20480
D	697	ASN	SER	engineered mutation	UNP P20480

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



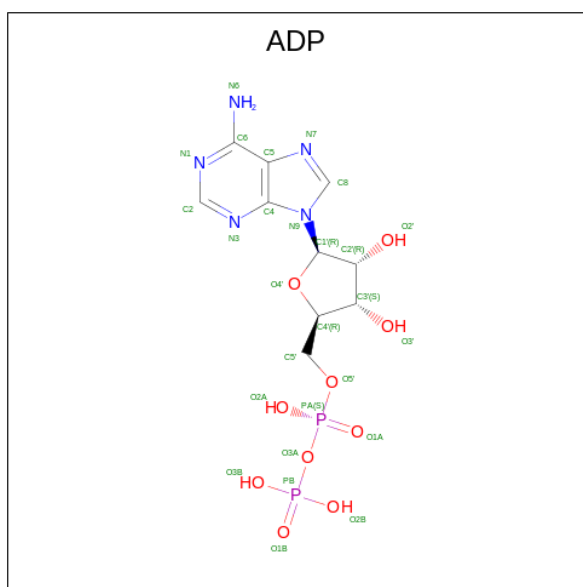
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total 28	C 10	N 5	O 11	P 2	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

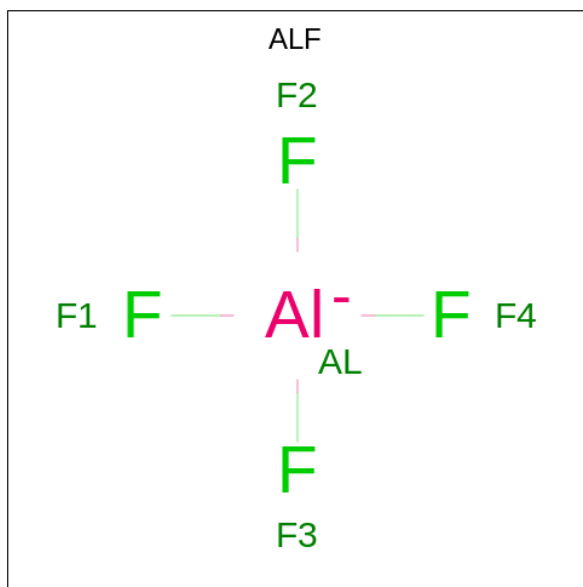


Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	P
			27	10	5	10	2
6	D	1	Total	C	N	O	P
			27	10	5	10	2

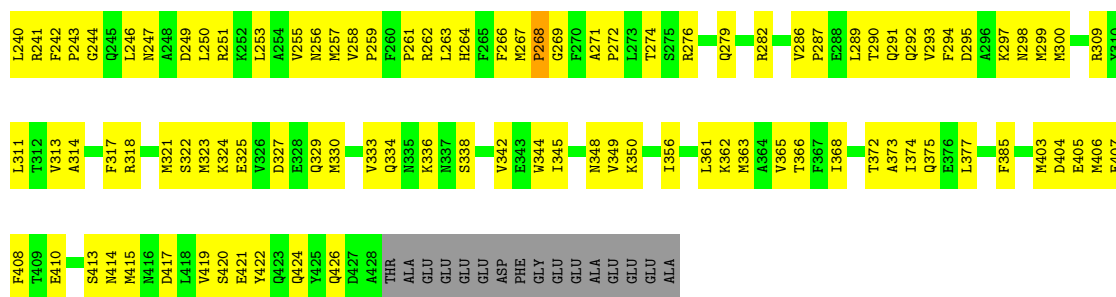
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total	Mg	0
			1	1	
7	D	1	Total	Mg	0
			1	1	

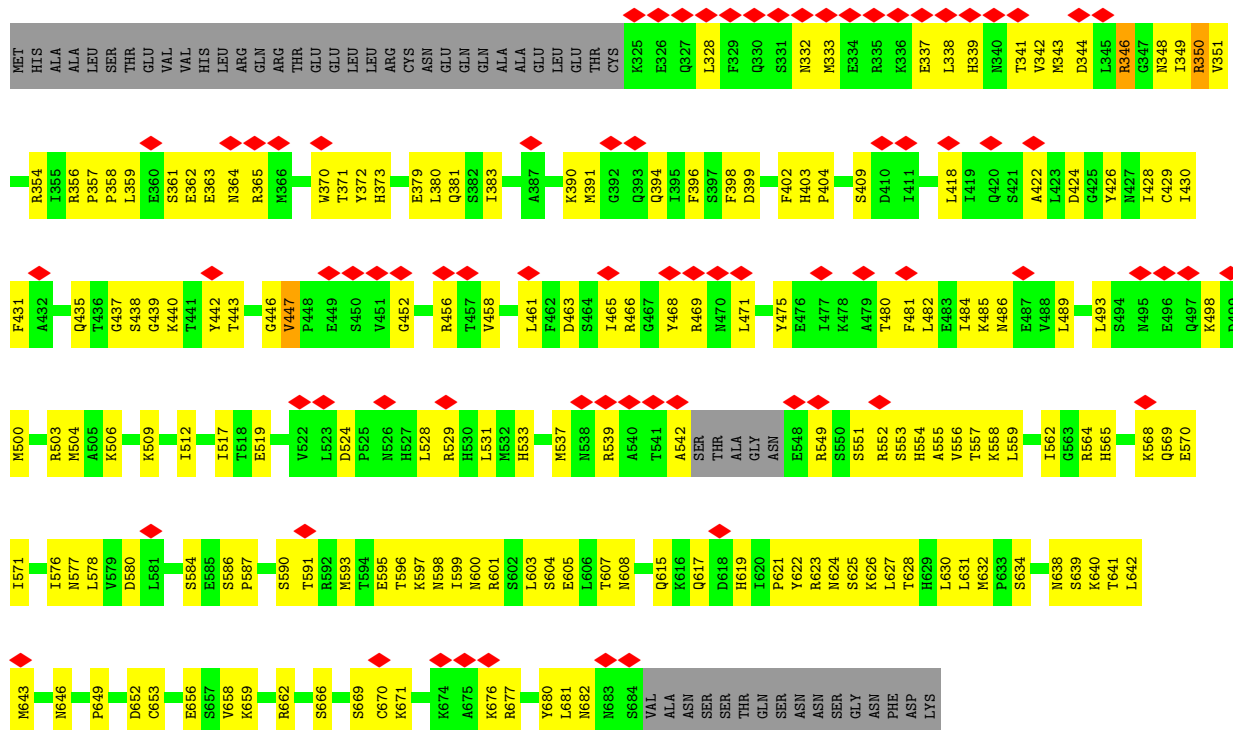
- Molecule 8 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



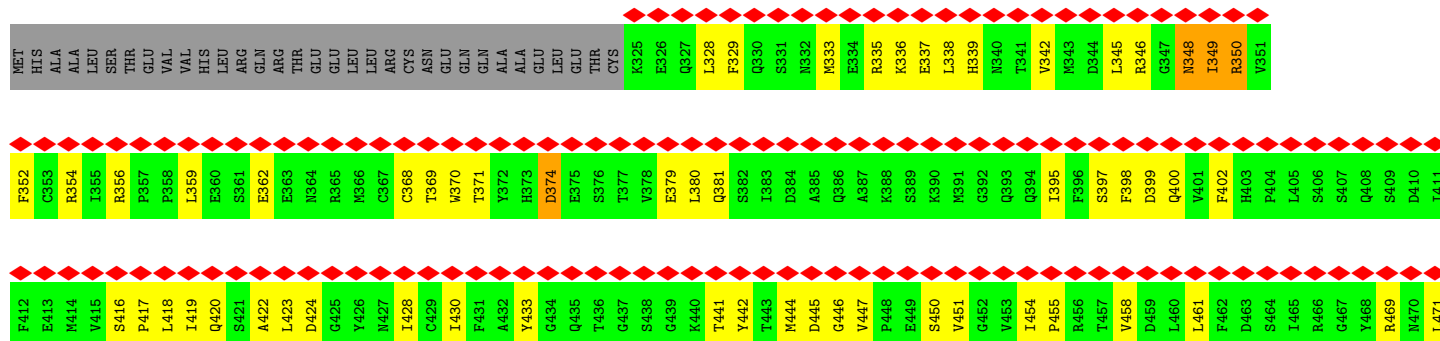
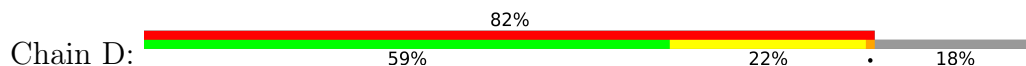
Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
8	C	1	5	1	4	0



• Molecule 3: Protein claret segregational



• Molecule 3: Protein claret segregational





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.7461°, rise=8.74441 Å, axial sym=C1	Depositor
Number of segments used	30975	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	451.19998, 451.19998, 451.19998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GDP, GTP, ADP, ALF

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	0.95	0/3429	1.15	2/4656 (0.0%)
2	B	0.48	0/3431	0.66	0/4652
3	C	0.29	0/2882	0.50	0/3882
3	D	0.27	0/2695	0.44	1/3636 (0.0%)
All	All	0.59	0/12437	0.76	3/16826 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
3	C	0	2
3	D	0	2
All	All	0	14

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	374	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	10	GLY	CA-C-O	-5.21	118.07	122.29
1	A	101	ASN	N-CA-C	-5.12	104.54	111.55

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	121	ARG	Sidechain
1	A	214	ARG	Sidechain
1	A	221	ARG	Sidechain
1	A	243	ARG	Sidechain
1	A	264	ARG	Sidechain
1	A	373	ARG	Sidechain
1	A	402	ARG	Sidechain
1	A	64	ARG	Sidechain
1	A	84	ARG	Sidechain
3	C	346	ARG	Sidechain
3	C	350	ARG	Sidechain
3	D	335	ARG	Sidechain
3	D	350	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3352	0	3268	281	0
2	B	3356	0	3241	298	0
3	C	2836	0	2824	305	0
3	D	2650	0	2622	63	0
4	A	32	0	12	1	0
5	B	28	0	12	2	0
6	C	27	0	12	5	0
6	D	27	0	12	1	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	5	0	0	3	0
All	All	12315	0	12003	759	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 31.

All (759) 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:410:GLY:C	3:C:597:LYS:HD2	1.37	1.50
2:B:417:ASP:HB2	3:C:623:ARG:NH2	1.34	1.43
2:B:410:GLU:HG2	3:C:504:MET:SD	1.61	1.40
1:A:412:GLY:C	3:C:587:PRO:HG2	1.49	1.36
1:A:410:GLY:O	3:C:597:LYS:CD	1.73	1.34
1:A:109:THR:HA	3:C:593:MET:CE	1.58	1.32
2:B:262:ARG:HD2	3:C:623:ARG:O	1.15	1.31
2:B:262:ARG:HD2	3:C:623:ARG:C	1.54	1.31
2:B:410:GLU:OE2	3:C:503:ARG:NH1	1.65	1.30
1:A:411:GLU:CA	3:C:597:LYS:HZ1	1.50	1.23
2:B:194:GLU:OE2	3:C:626:LYS:NZ	1.70	1.23
1:A:412:GLY:CA	3:C:587:PRO:HG2	1.68	1.22
1:A:412:GLY:O	3:C:587:PRO:HG2	1.37	1.21
1:A:109:THR:HG22	3:C:593:MET:SD	1.84	1.18
2:B:417:ASP:CB	3:C:623:ARG:NH2	2.08	1.17
1:A:409:VAL:CG2	3:C:600:ASN:HB3	1.78	1.14
1:A:410:GLY:O	3:C:597:LYS:HD2	0.98	1.14
1:A:411:GLU:HA	3:C:597:LYS:NZ	1.63	1.11
1:A:109:THR:HA	3:C:593:MET:HE1	1.19	1.11
1:A:409:VAL:HG23	3:C:600:ASN:HB3	1.33	1.09
1:A:412:GLY:HA2	3:C:587:PRO:CG	1.83	1.08
2:B:262:ARG:NH1	3:C:623:ARG:HB3	1.66	1.08
1:A:411:GLU:HA	3:C:597:LYS:HZ1	0.93	1.05
1:A:416:GLY:HA3	3:C:659:LYS:HD3	1.38	1.03
2:B:262:ARG:CD	3:C:623:ARG:O	2.06	1.02
2:B:410:GLU:OE2	3:C:503:ARG:HD2	1.61	1.00
2:B:417:ASP:HB2	3:C:623:ARG:HH22	1.23	0.99
2:B:410:GLU:CD	3:C:503:ARG:HD2	1.87	0.99
1:A:411:GLU:CA	3:C:597:LYS:NZ	2.20	0.99
1:A:412:GLY:O	3:C:587:PRO:CG	2.10	0.98
2:B:420:SER:OG	3:C:619:HIS:CD2	2.16	0.98
2:B:406:MET:CB	3:C:506:LYS:HD3	1.93	0.97
2:B:410:GLU:CG	3:C:504:MET:SD	2.53	0.96
1:A:108:TYR:O	3:C:593:MET:HE1	1.66	0.95
1:A:414:GLU:OE1	3:C:586:SER:OG	1.83	0.95
2:B:417:ASP:CB	3:C:623:ARG:HH21	1.74	0.95
2:B:262:ARG:NH1	3:C:623:ARG:CB	2.29	0.95
1:A:411:GLU:C	3:C:597:LYS:NZ	2.26	0.94
2:B:417:ASP:CG	3:C:623:ARG:HH21	1.74	0.94
2:B:417:ASP:OD1	3:C:619:HIS:NE2	2.00	0.94
2:B:262:ARG:CD	3:C:623:ARG:C	2.40	0.93
2:B:406:MET:HB3	3:C:506:LYS:HD3	1.49	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLY:CA	3:C:587:PRO:CG	2.43	0.92
2:B:417:ASP:HB2	3:C:623:ARG:HH21	1.26	0.92
2:B:413:SER:HB3	3:C:509:LYS:NZ	1.84	0.91
1:A:411:GLU:C	3:C:597:LYS:HZ1	1.79	0.91
1:A:410:GLY:C	3:C:597:LYS:CD	2.31	0.91
1:A:427:ALA:HB2	3:C:390:LYS:HZ1	1.34	0.90
1:A:416:GLY:HA3	3:C:659:LYS:CD	2.00	0.90
1:A:406:HIS:HB2	3:C:601:ARG:HH21	1.39	0.88
1:A:412:GLY:C	3:C:587:PRO:CG	2.43	0.87
1:A:135:PHE:HD2	1:A:166:LYS:HG2	1.41	0.86
1:A:427:ALA:HB2	3:C:390:LYS:NZ	1.91	0.84
1:A:318:LEU:HB2	1:A:376:CYS:HB3	1.59	0.84
1:A:409:VAL:HG23	3:C:600:ASN:CB	2.08	0.84
1:A:409:VAL:CB	3:C:600:ASN:HB3	2.06	0.83
1:A:416:GLY:HA3	3:C:659:LYS:CE	2.09	0.83
1:A:416:GLY:C	3:C:659:LYS:NZ	2.37	0.83
2:B:410:GLU:OE1	3:C:503:ARG:HD2	1.79	0.82
1:A:297:GLU:HG2	1:A:300:ASN:HB2	1.61	0.82
1:A:109:THR:HA	3:C:593:MET:HE3	1.59	0.81
2:B:417:ASP:OD1	3:C:619:HIS:CE1	2.33	0.81
1:A:53:PHE:HA	1:A:63:PRO:HA	1.60	0.81
2:B:181:GLU:HG2	2:B:182:PRO:HD3	1.63	0.81
2:B:410:GLU:HG2	3:C:504:MET:CE	2.10	0.80
1:A:49:PHE:HB2	1:A:53:PHE:HB2	1.61	0.80
1:A:416:GLY:CA	3:C:659:LYS:CE	2.60	0.80
1:A:410:GLY:HA2	3:C:597:LYS:HA	1.64	0.80
3:D:447:VAL:HG23	3:D:450:SER:H	1.47	0.80
1:A:412:GLY:HA2	3:C:587:PRO:HG3	1.64	0.80
2:B:406:MET:HE2	3:C:503:ARG:NE	1.96	0.80
3:C:351:VAL:HA	3:C:643:MET:HB2	1.63	0.79
1:A:416:GLY:C	3:C:659:LYS:HZ1	1.89	0.78
1:A:427:ALA:CB	3:C:390:LYS:NZ	2.46	0.78
1:A:5:ILE:HG22	1:A:64:ARG:HB3	1.66	0.78
1:A:213:CYS:HA	1:A:217:LEU:HB3	1.65	0.77
2:B:48:SER:O	2:B:62:ARG:NH2	2.17	0.77
2:B:178:THR:HB	2:B:181:GLU:HB3	1.64	0.77
3:C:349:ILE:HD11	3:C:643:MET:HG2	1.67	0.77
1:A:416:GLY:CA	3:C:659:LYS:HD3	2.15	0.77
1:A:109:THR:CG2	3:C:593:MET:SD	2.71	0.76
1:A:414:GLU:HB3	1:A:417:GLU:HG2	1.67	0.76
2:B:68:LEU:HD13	2:B:108:GLU:HB2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:MET:HE2	3:C:503:ARG:CZ	2.16	0.76
1:A:410:GLY:O	3:C:597:LYS:CE	2.35	0.75
2:B:262:ARG:CZ	3:C:623:ARG:HB2	2.17	0.75
2:B:424:GLN:HG2	3:C:617:GLN:OE1	1.87	0.75
2:B:262:ARG:HH11	3:C:623:ARG:HB3	1.50	0.74
1:A:414:GLU:OE1	3:C:656:GLU:OE2	2.06	0.74
3:C:504:MET:HA	3:C:512:ILE:HA	1.69	0.74
1:A:427:ALA:CB	3:C:390:LYS:HZ1	2.00	0.74
3:C:458:VAL:HG21	3:C:529:ARG:HH22	1.53	0.74
3:D:369:THR:HB	3:D:381:GLN:HB2	1.68	0.74
1:A:411:GLU:HA	3:C:597:LYS:CE	2.18	0.74
2:B:133:PHE:HB2	2:B:164:MET:HG3	1.69	0.74
1:A:180:ALA:HA	2:B:350:LYS:HZ3	1.52	0.74
2:B:410:GLU:OE1	3:C:503:ARG:HG3	1.89	0.73
2:B:262:ARG:HB2	3:C:624:ASN:HD21	1.53	0.73
2:B:410:GLU:OE2	3:C:503:ARG:CD	2.36	0.73
1:A:409:VAL:HB	3:C:600:ASN:HB3	1.69	0.73
3:C:446:GLY:CA	3:C:452:GLY:HA3	2.19	0.73
1:A:142:GLY:HA3	1:A:183:GLU:HG2	1.70	0.73
2:B:413:SER:HB3	3:C:509:LYS:HZ3	1.52	0.72
1:A:14:VAL:HG11	1:A:74:VAL:HB	1.69	0.72
2:B:420:SER:CB	3:C:619:HIS:CD2	2.73	0.72
2:B:3:GLU:HG3	2:B:49:VAL:HA	1.72	0.72
2:B:262:ARG:H	3:C:624:ASN:ND2	1.88	0.72
2:B:269:GLY:HA2	2:B:300:MET:HE2	1.72	0.71
1:A:109:THR:CA	3:C:593:MET:HE1	2.09	0.71
1:A:204:VAL:HG11	1:A:231:ILE:HD11	1.72	0.71
2:B:410:GLU:CD	3:C:503:ARG:CD	2.62	0.71
2:B:215:LEU:HB3	2:B:217:LEU:HD23	1.73	0.71
1:A:109:THR:CA	3:C:593:MET:CE	2.54	0.71
1:A:188:ILE:HG13	1:A:425:MET:HG2	1.73	0.71
3:C:469:ARG:HH12	3:C:475:TYR:H	1.36	0.71
3:C:539:ARG:NH1	3:C:553:SER:OG	2.22	0.71
2:B:240:LEU:HD12	2:B:249:ASP:HB2	1.73	0.70
1:A:7:ILE:HG22	1:A:66:VAL:HG13	1.73	0.70
1:A:238:ILE:HA	1:A:318:LEU:HG	1.74	0.70
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.74	0.70
1:A:87:PHE:HB3	1:A:92:LEU:HD21	1.74	0.70
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.72	0.70
3:C:371:THR:HB	3:C:381:GLN:HE22	1.56	0.70
2:B:211:CYS:HA	2:B:215:LEU:HB2	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:PRO:HA	2:B:329:GLN:HE22	1.56	0.69
1:A:416:GLY:HA3	3:C:659:LYS:NZ	2.08	0.69
2:B:262:ARG:HB2	3:C:624:ASN:ND2	2.06	0.69
1:A:344:VAL:HG23	1:A:347:CYS:H	1.58	0.69
3:C:557:THR:HB	3:C:578:LEU:HB2	1.73	0.69
1:A:412:GLY:O	3:C:587:PRO:CD	2.41	0.69
3:C:391:MET:HE3	3:C:394:GLN:HE22	1.58	0.69
1:A:414:GLU:CD	3:C:586:SER:OG	2.35	0.69
1:A:407:TRP:HE1	2:B:258:VAL:HG23	1.58	0.69
2:B:235:GLY:HA3	2:B:366:THR:HG21	1.75	0.69
2:B:417:ASP:OD2	3:C:623:ARG:NE	2.26	0.68
3:C:446:GLY:HA3	3:C:452:GLY:HA3	1.75	0.68
2:B:410:GLU:OE1	3:C:503:ARG:CD	2.40	0.68
1:A:217:LEU:HG	1:A:219:ILE:HG12	1.76	0.68
2:B:213:ARG:HD2	2:B:297:LYS:HE2	1.75	0.68
2:B:317:PHE:H	2:B:365:VAL:HG23	1.58	0.68
2:B:118:ASP:OD1	2:B:119:VAL:N	2.27	0.68
2:B:152:ILE:HD11	2:B:164:MET:HG2	1.76	0.68
1:A:75:ILE:HG23	1:A:92:LEU:HB3	1.76	0.67
1:A:119:LEU:HB3	1:A:123:ARG:HH21	1.60	0.67
3:C:435:GLN:NE2	3:C:584:SER:OG	2.27	0.67
1:A:406:HIS:O	3:C:601:ARG:NH2	2.25	0.67
1:A:409:VAL:HG21	3:C:604:SER:OG	1.94	0.67
3:C:469:ARG:HH12	3:C:475:TYR:N	1.92	0.67
1:A:416:GLY:HA3	3:C:659:LYS:HZ3	1.60	0.67
2:B:410:GLU:OE1	3:C:503:ARG:CG	2.43	0.67
2:B:286:VAL:HB	2:B:363:MET:HE3	1.77	0.67
3:C:396:PHE:HB3	3:C:398:PHE:HE1	1.60	0.67
1:A:414:GLU:OE2	3:C:656:GLU:OE1	2.13	0.66
2:B:424:GLN:HE21	3:C:617:GLN:CD	2.01	0.66
2:B:3:GLU:HA	2:B:49:VAL:HG23	1.78	0.66
2:B:314:ALA:HA	2:B:350:LYS:HB2	1.76	0.66
2:B:424:GLN:NE2	3:C:617:GLN:OE1	2.27	0.66
3:C:351:VAL:N	3:C:399:ASP:OD2	2.29	0.66
3:D:461:LEU:HD21	3:D:561:LEU:HD21	1.76	0.66
3:D:556:VAL:HG22	3:D:579:VAL:HG13	1.77	0.66
2:B:321:MET:SD	2:B:321:MET:N	2.69	0.66
2:B:406:MET:HB2	3:C:503:ARG:NH1	2.10	0.66
2:B:192:LEU:O	2:B:196:THR:N	2.29	0.66
2:B:413:SER:HB3	3:C:509:LYS:HZ1	1.61	0.66
2:B:421:GLU:OE2	3:C:619:HIS:ND1	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:446:GLY:HA3	3:C:452:GLY:CA	2.25	0.66
2:B:67:ASP:OD1	2:B:68:LEU:N	2.29	0.65
2:B:244:GLY:O	2:B:247:ASN:ND2	2.29	0.65
2:B:372:THR:O	2:B:375:GLN:NE2	2.27	0.65
3:C:424:ASP:OD2	3:C:677:ARG:NH1	2.30	0.65
1:A:135:PHE:CD2	1:A:166:LYS:HG2	2.29	0.64
2:B:262:ARG:NH1	3:C:623:ARG:HB2	2.12	0.64
3:C:344:ASP:HA	3:C:350:ARG:HD2	1.80	0.64
3:C:555:ALA:HB3	3:C:580:ASP:HB3	1.80	0.64
1:A:414:GLU:CB	3:C:586:SER:OG	2.46	0.64
1:A:141:PHE:HB2	1:A:173:PRO:HD3	1.80	0.64
2:B:209:ASP:OD1	2:B:213:ARG:NH2	2.30	0.64
2:B:204:ASN:OD1	2:B:205:GLU:N	2.31	0.64
2:B:405:GLU:OE2	3:C:506:LYS:NZ	2.31	0.64
2:B:424:GLN:CG	3:C:617:GLN:OE1	2.46	0.63
1:A:416:GLY:CA	3:C:659:LYS:NZ	2.61	0.63
2:B:4:ILE:O	2:B:62:ARG:NH1	2.28	0.63
2:B:2:ARG:H	2:B:129:CYS:HB3	1.61	0.63
3:C:370:TRP:HB3	3:C:380:LEU:HD23	1.79	0.63
1:A:321:GLY:HA2	1:A:359:PRO:HA	1.79	0.63
3:C:458:VAL:HG11	3:C:529:ARG:HH12	1.63	0.63
3:C:362:GLU:OE1	3:C:365:ARG:NH2	2.32	0.63
1:A:360:PRO:HG3	1:A:374:ALA:HB2	1.81	0.63
3:D:473:TRP:CD1	3:D:565:HIS:HD2	2.17	0.63
1:A:273:ALA:HB2	1:A:295:CYS:HB3	1.81	0.63
2:B:268:PRO:HG2	2:B:300:MET:HG3	1.81	0.63
2:B:72:THR:OG1	2:B:73:MET:SD	2.56	0.62
2:B:110:ALA:HA	2:B:150:LEU:CD2	2.30	0.62
2:B:417:ASP:CG	3:C:623:ARG:NH2	2.43	0.62
2:B:72:THR:O	2:B:75:SER:OG	2.16	0.62
2:B:406:MET:HE2	3:C:503:ARG:CD	2.29	0.62
1:A:98:ASP:O	1:A:105:ARG:NH2	2.33	0.61
3:D:552:ARG:NH2	3:D:585:GLU:O	2.33	0.61
3:D:359:LEU:HD11	6:D:802:ADP:H1'	1.81	0.61
1:A:406:HIS:CB	3:C:601:ARG:HH21	2.13	0.61
1:A:328:VAL:HG11	1:A:353:VAL:HG21	1.81	0.61
3:C:365:ARG:NH2	3:C:652:ASP:OD2	2.33	0.61
2:B:289:LEU:HD13	2:B:363:MET:HG3	1.82	0.61
1:A:415:GLU:HA	1:A:418:PHE:HD2	1.65	0.61
1:A:416:GLY:CA	3:C:659:LYS:CD	2.75	0.61
1:A:416:GLY:CA	3:C:659:LYS:HE2	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:GLU:OE2	3:C:619:HIS:CE1	2.54	0.61
2:B:155:ILE:HG22	2:B:164:MET:HE3	1.83	0.61
1:A:412:GLY:O	3:C:587:PRO:HD2	2.00	0.61
2:B:410:GLU:CD	3:C:503:ARG:CG	2.74	0.61
3:C:463:ASP:OD1	3:C:466:ARG:NH1	2.33	0.61
2:B:287:PRO:HA	2:B:329:GLN:NE2	2.16	0.60
3:C:595:GLU:O	3:C:599:ILE:HG12	2.01	0.60
1:A:75:ILE:HG21	1:A:94:THR:HG22	1.83	0.60
2:B:170:VAL:HG11	2:B:377:LEU:HD11	1.83	0.60
1:A:217:LEU:HD13	1:A:368:LEU:HD23	1.83	0.60
1:A:410:GLY:CA	3:C:597:LYS:HD2	2.26	0.60
2:B:237:THR:HG22	2:B:250:LEU:HD21	1.82	0.60
2:B:49:VAL:O	2:B:62:ARG:NH1	2.22	0.60
3:C:381:GLN:O	3:C:383:ILE:HG13	2.01	0.60
2:B:9:ALA:HB3	2:B:137:HIS:HB3	1.84	0.59
1:A:100:ALA:HB1	2:B:255:VAL:HG21	1.82	0.59
3:C:485:LYS:HZ1	3:C:552:ARG:HG3	1.66	0.59
2:B:406:MET:HA	3:C:506:LYS:NZ	2.17	0.59
2:B:52:ASN:OD1	2:B:62:ARG:NE	2.36	0.59
2:B:110:ALA:HA	2:B:150:LEU:HD21	1.83	0.59
2:B:289:LEU:HD21	2:B:365:VAL:HG12	1.83	0.59
2:B:309:ARG:HG3	2:B:426:GLN:HG3	1.82	0.59
1:A:70:LEU:HD23	1:A:99:ALA:HB2	1.85	0.59
1:A:181:VAL:H	2:B:350:LYS:HE2	1.68	0.59
1:A:410:GLY:O	3:C:597:LYS:CG	2.47	0.59
1:A:411:GLU:C	3:C:597:LYS:HZ2	2.10	0.59
2:B:272:PRO:HD2	2:B:361:LEU:HD21	1.85	0.59
2:B:51:TYR:HB3	2:B:59:TYR:HB3	1.84	0.59
1:A:30:ILE:HG12	1:A:36:MET:HB2	1.85	0.58
2:B:237:THR:OG1	2:B:241:ARG:NH1	2.35	0.58
3:C:503:ARG:HH22	3:C:506:LYS:HG2	1.67	0.58
1:A:14:VAL:HG23	1:A:67:PHE:HD1	1.68	0.58
2:B:189:VAL:HA	2:B:192:LEU:HB2	1.84	0.58
3:D:433:TYR:HB3	3:D:645:ILE:HD13	1.86	0.58
2:B:405:GLU:OE2	3:C:506:LYS:CE	2.52	0.58
2:B:421:GLU:OE2	3:C:621:PRO:HB3	2.04	0.58
3:C:396:PHE:HB3	3:C:398:PHE:CE1	2.38	0.58
3:C:642:LEU:O	3:C:643:MET:HE2	2.03	0.58
2:B:406:MET:SD	2:B:407:GLU:N	2.77	0.58
3:C:469:ARG:NH1	3:C:475:TYR:H	2.02	0.58
3:C:587:PRO:O	3:C:591:THR:CG2	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:631:LEU:HB2	3:C:634:SER:HB2	1.86	0.57
3:D:430:ILE:HG22	3:D:444:MET:HE1	1.85	0.57
2:B:17:GLY:O	2:B:21:TRP:HD1	1.87	0.57
2:B:132:GLY:HA2	2:B:162:ARG:HB3	1.86	0.57
2:B:197:ASP:O	2:B:264:HIS:HB2	2.03	0.57
2:B:405:GLU:CD	3:C:506:LYS:NZ	2.61	0.57
2:B:214:THR:OG1	2:B:297:LYS:NZ	2.38	0.57
3:C:446:GLY:CA	3:C:452:GLY:CA	2.82	0.57
1:A:107:HIS:CD2	1:A:152:LEU:HB2	2.39	0.57
2:B:20:PHE:CE2	2:B:24:ILE:HD11	2.40	0.57
3:C:439:GLY:N	6:C:901:ADP:O1B	2.37	0.57
2:B:3:GLU:N	2:B:129:CYS:O	2.37	0.57
1:A:121:ARG:HA	1:A:124:LYS:HE2	1.87	0.56
2:B:99:ASN:HA	2:B:142:GLY:H	1.69	0.56
2:B:262:ARG:CB	3:C:624:ASN:ND2	2.68	0.56
2:B:420:SER:OG	3:C:619:HIS:NE2	2.37	0.56
3:C:461:LEU:O	3:C:465:ILE:HG13	2.05	0.56
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.86	0.56
2:B:9:ALA:HB3	2:B:137:HIS:CB	2.36	0.56
2:B:66:VAL:HG11	2:B:147:MET:HE3	1.87	0.56
3:C:468:TYR:HA	3:C:471:LEU:HB2	1.88	0.56
1:A:210:TYR:CE1	1:A:227:LEU:HD21	2.41	0.56
3:C:485:LYS:NZ	3:C:552:ARG:HG3	2.21	0.56
1:A:409:VAL:HB	3:C:600:ASN:CB	2.36	0.56
2:B:213:ARG:HH11	2:B:297:LYS:HZ3	1.54	0.56
3:C:587:PRO:HG3	3:C:596:THR:HG21	1.89	0.55
3:D:349:ILE:HD13	3:D:641:THR:HB	1.87	0.55
2:B:140:GLY:HA3	5:B:501:GDP:H4'	1.86	0.55
3:C:528:LEU:HD12	3:C:531:LEU:HD11	1.89	0.55
1:A:5:ILE:HG12	1:A:132:LEU:HD11	1.86	0.55
1:A:412:GLY:N	3:C:597:LYS:HZ2	2.05	0.55
2:B:147:MET:SD	2:B:148:GLY:N	2.79	0.55
3:C:437:GLY:N	6:C:901:ADP:O3B	2.36	0.55
2:B:25:SER:OG	2:B:30:ILE:O	2.25	0.55
1:A:212:ILE:HG13	1:A:302:MET:HE1	1.89	0.55
2:B:290:THR:O	2:B:293:VAL:HG12	2.06	0.54
1:A:262:TYR:HB2	1:A:265:ILE:HB	1.89	0.54
2:B:153:SER:HB3	2:B:191:GLN:HE21	1.72	0.54
3:D:663:PHE:O	3:D:666:SER:OG	2.23	0.54
3:C:357:PRO:HA	3:C:404:PRO:HB3	1.90	0.54
2:B:404:ASP:HB3	2:B:406:MET:HG3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:622:TYR:CD2	3:C:632:MET:HG3	2.42	0.54
2:B:261:PRO:HG2	3:C:605:GLU:OE2	2.08	0.54
3:C:480:THR:HG22	3:C:519:GLU:HG2	1.89	0.54
3:D:354:ARG:HA	3:D:402:PHE:HB2	1.90	0.54
1:A:109:THR:HA	3:C:593:MET:SD	2.45	0.54
1:A:188:ILE:HG12	1:A:421:ALA:HB1	1.90	0.54
1:A:154:MET:HE1	1:A:197:HIS:HB2	1.90	0.54
2:B:73:MET:SD	2:B:73:MET:N	2.82	0.53
3:C:429:CYS:HA	3:C:577:ASN:HB2	1.89	0.53
3:C:542:ALA:C	3:C:549:ARG:HD3	2.33	0.53
2:B:420:SER:HB2	3:C:619:HIS:CD2	2.42	0.53
3:D:552:ARG:NH1	3:D:583:GLY:O	2.41	0.53
2:B:238:THR:HG21	2:B:318:ARG:HE	1.73	0.53
1:A:60:LYS:HE3	1:A:62:VAL:HB	1.90	0.53
3:C:431:PHE:HZ	3:C:631:LEU:HD22	1.73	0.53
3:D:420:GLN:HA	3:D:423:LEU:HD12	1.90	0.53
1:A:3:GLU:HB2	1:A:129:CYS:SG	2.48	0.53
2:B:406:MET:HA	3:C:506:LYS:HZ3	1.74	0.53
2:B:73:MET:HB3	2:B:77:ARG:NH1	2.24	0.53
2:B:405:GLU:CD	3:C:506:LYS:HZ1	2.17	0.53
1:A:136:LEU:HD11	1:A:167:LEU:HD23	1.90	0.53
1:A:272:TYR:HB3	1:A:275:VAL:HG13	1.90	0.53
1:A:321:GLY:HA2	1:A:359:PRO:CA	2.39	0.53
1:A:427:ALA:HB1	3:C:390:LYS:NZ	2.23	0.53
2:B:8:GLN:HE22	2:B:17:GLY:HA3	1.74	0.53
1:A:261:PRO:HG2	1:A:262:TYR:HD1	1.73	0.53
1:A:427:ALA:HB1	3:C:390:LYS:HZ3	1.73	0.53
2:B:68:LEU:HD23	2:B:112:LEU:HD22	1.92	0.53
2:B:36:TYR:HB2	2:B:59:TYR:HE2	1.73	0.52
3:C:440:LYS:O	3:C:443:THR:OG1	2.26	0.52
3:C:556:VAL:HG11	3:C:630:LEU:HD21	1.91	0.52
1:A:12:ALA:HB1	1:A:171:ILE:HD12	1.90	0.52
2:B:271:ALA:HB3	2:B:365:VAL:HG12	1.90	0.52
3:C:361:SER:HA	3:C:364:ASN:HD21	1.74	0.52
1:A:23:LEU:HD21	1:A:362:VAL:HA	1.90	0.52
1:A:297:GLU:HG3	1:A:299:ALA:H	1.75	0.52
2:B:362:LYS:HD3	2:B:363:MET:HB2	1.91	0.52
2:B:91:VAL:HB	2:B:116:VAL:HG12	1.92	0.52
3:C:359:LEU:O	3:C:363:GLU:HG3	2.10	0.52
1:A:137:VAL:HG22	1:A:139:HIS:CD2	2.44	0.52
1:A:414:GLU:CD	3:C:656:GLU:OE2	2.52	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.45	0.52
3:C:559:LEU:HB2	3:C:576:ILE:HB	1.91	0.52
2:B:410:GLU:OE2	3:C:503:ARG:CZ	2.51	0.52
3:C:539:ARG:HH12	3:C:553:SER:HG	1.58	0.52
1:A:343:PHE:HB3	1:A:348:PRO:HA	1.90	0.52
2:B:217:LEU:HA	2:B:276:ARG:HH21	1.75	0.52
2:B:149:THR:O	2:B:152:ILE:HG22	2.10	0.52
2:B:321:MET:HE3	2:B:363:MET:SD	2.50	0.52
3:D:352:PHE:HE2	3:D:642:LEU:HD11	1.75	0.52
1:A:268:PRO:HA	1:A:380:ASN:HA	1.91	0.51
1:A:395:PHE:HZ	1:A:418:PHE:HB3	1.75	0.51
2:B:158:GLU:HG3	2:B:159:TYR:CD2	2.44	0.51
1:A:7:ILE:HG13	1:A:137:VAL:HA	1.92	0.51
2:B:424:GLN:NE2	3:C:617:GLN:CD	2.66	0.51
3:C:597:LYS:O	3:C:601:ARG:HG2	2.10	0.51
1:A:121:ARG:HD2	1:A:124:LYS:HE2	1.92	0.51
2:B:149:THR:HG21	2:B:188:SER:HA	1.92	0.51
1:A:119:LEU:HD23	1:A:122:ILE:HD11	1.93	0.51
1:A:339:ARG:HE	1:A:339:ARG:HA	1.76	0.51
2:B:262:ARG:CZ	3:C:623:ARG:CB	2.80	0.51
2:B:244:GLY:H	2:B:247:ASN:HD21	1.57	0.51
2:B:330:MET:HA	2:B:333:VAL:HG22	1.92	0.51
3:C:373:HIS:NE2	3:C:379:GLU:OE1	2.28	0.51
3:C:564:ARG:HG3	3:C:571:ILE:HG12	1.93	0.51
3:C:600:ASN:HA	3:C:603:LEU:HG	1.92	0.51
2:B:20:PHE:HA	2:B:230:SER:HB2	1.91	0.51
3:C:332:ASN:OD1	3:C:333:MET:N	2.44	0.51
3:D:398:PHE:HZ	3:D:661:LEU:HD22	1.75	0.51
1:A:344:VAL:HG11	1:A:435:VAL:HG12	1.92	0.51
1:A:76:ASP:HA	1:A:79:ARG:HE	1.76	0.50
3:D:451:VAL:HB	3:D:455:PRO:HG2	1.94	0.50
1:A:3:GLU:HA	1:A:51:THR:HA	1.93	0.50
1:A:416:GLY:C	3:C:659:LYS:CE	2.83	0.50
2:B:185:ALA:O	2:B:189:VAL:HG22	2.11	0.50
2:B:406:MET:CE	3:C:503:ARG:CD	2.89	0.50
3:D:397:SER:OG	3:D:668:ASN:ND2	2.44	0.50
2:B:12:CYS:HB2	5:B:501:GDP:C8	2.45	0.50
3:C:354:ARG:HA	3:C:402:PHE:HB2	1.92	0.50
3:C:597:LYS:O	3:C:601:ARG:NH1	2.45	0.50
2:B:117:LEU:HA	2:B:120:VAL:HG12	1.93	0.50
3:C:565:HIS:O	3:C:569:GLN:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:666:SER:O	3:C:669:SER:OG	2.27	0.50
2:B:19:LYS:HA	2:B:22:GLU:OE1	2.12	0.50
3:C:615:GLN:OE1	3:C:617:GLN:NE2	2.44	0.50
1:A:14:VAL:HG23	1:A:67:PHE:CD1	2.47	0.50
1:A:112:LYS:HA	1:A:152:LEU:CD2	2.42	0.50
3:C:551:SER:OG	8:C:903:ALF:F2	2.15	0.50
1:A:360:PRO:HG3	1:A:374:ALA:CB	2.42	0.49
2:B:256:ASN:HB3	2:B:350:LYS:HE3	1.93	0.49
2:B:362:LYS:HE2	2:B:363:MET:HE2	1.94	0.49
3:C:346:ARG:HB2	3:D:345:LEU:HD21	1.93	0.49
2:B:9:ALA:HB1	2:B:144:GLY:HA2	1.94	0.49
2:B:324:LYS:O	2:B:327:ASP:N	2.45	0.49
1:A:79:ARG:HH12	1:A:94:THR:HG21	1.77	0.49
2:B:385:PHE:HZ	2:B:408:PHE:HB3	1.77	0.49
2:B:406:MET:CA	3:C:506:LYS:HD3	2.42	0.49
3:D:471:LEU:O	3:D:565:HIS:NE2	2.45	0.49
1:A:141:PHE:HD2	1:A:172:TYR:HA	1.78	0.49
2:B:97:ALA:HB3	2:B:143:THR:OG1	2.12	0.49
2:B:406:MET:CE	3:C:503:ARG:NE	2.72	0.49
2:B:410:GLU:HB3	3:C:504:MET:HE1	1.95	0.49
3:D:380:LEU:HD21	3:D:658:VAL:HG12	1.94	0.49
1:A:188:ILE:HD11	1:A:422:ARG:HA	1.93	0.49
2:B:267:MET:HE1	2:B:373:ALA:HB3	1.93	0.49
2:B:333:VAL:HA	2:B:336:LYS:HG2	1.95	0.49
3:C:350:ARG:HH22	3:C:640:LYS:HB3	1.77	0.49
2:B:217:LEU:HD13	2:B:276:ARG:NH2	2.27	0.49
2:B:261:PRO:O	2:B:264:HIS:ND1	2.24	0.49
3:C:569:GLN:HG3	3:C:682:ASN:HB2	1.95	0.49
3:D:336:LYS:HD3	3:D:424:ASP:CG	2.37	0.49
1:A:103:TYR:HE1	1:A:413:MET:HE3	1.77	0.49
1:A:210:TYR:HE1	1:A:227:LEU:HD21	1.78	0.49
3:C:638:ASN:HB2	3:C:676:LYS:H	1.78	0.49
2:B:262:ARG:HD3	3:C:624:ASN:ND2	2.28	0.49
1:A:431:ASP:O	1:A:435:VAL:HG23	2.13	0.49
2:B:73:MET:HE3	2:B:92:PHE:CB	2.43	0.49
2:B:415:MET:HE2	2:B:415:MET:N	2.28	0.49
1:A:325:PRO:HD3	1:A:355:ILE:HG12	1.94	0.48
2:B:334:GLN:O	2:B:338:SER:OG	2.15	0.48
2:B:272:PRO:HA	2:B:292:GLN:HE22	1.76	0.48
2:B:375:GLN:HB3	2:B:422:TYR:HB2	1.95	0.48
3:C:328:LEU:HD13	3:D:328:LEU:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:533:HIS:ND1	3:C:537:MET:HE1	2.28	0.48
1:A:23:LEU:HB2	1:A:232:SER:OG	2.13	0.48
2:B:6:HIS:CE1	2:B:21:TRP:HE1	2.31	0.48
3:C:339:HIS:HD2	3:D:338:LEU:CD2	2.26	0.48
3:C:517:ILE:HG23	3:C:519:GLU:HG3	1.95	0.48
3:C:601:ARG:HG2	3:C:601:ARG:HH11	1.78	0.48
3:C:652:ASP:OD1	3:C:653:CYS:N	2.46	0.48
1:A:246:GLY:HA3	1:A:356:ASN:HA	1.96	0.48
1:A:396:ASP:OD1	1:A:422:ARG:HG3	2.13	0.48
1:A:427:ALA:CB	3:C:390:LYS:HZ3	2.24	0.48
3:C:409:SER:OG	3:C:456:ARG:NH1	2.46	0.48
1:A:244:PHE:CD2	1:A:358:GLN:HG2	2.48	0.48
1:A:332:ILE:O	1:A:336:LYS:HG2	2.12	0.48
2:B:213:ARG:HH11	2:B:297:LYS:NZ	2.12	0.48
2:B:404:ASP:OD1	2:B:405:GLU:N	2.46	0.48
3:C:443:THR:HG21	3:C:646:ASN:HD21	1.79	0.48
3:C:658:VAL:O	3:C:662:ARG:HG3	2.14	0.48
2:B:375:GLN:OE1	2:B:375:GLN:N	2.32	0.48
1:A:224:TYR:HA	1:A:227:LEU:HD13	1.95	0.48
2:B:149:THR:HB	2:B:191:GLN:OE1	2.13	0.48
3:C:469:ARG:HH22	3:C:475:TYR:H	1.62	0.48
3:C:605:GLU:HG3	3:C:625:SER:HB3	1.94	0.48
3:D:380:LEU:HD22	3:D:661:LEU:HD12	1.96	0.48
1:A:402:ARG:NH1	3:C:607:THR:HG21	2.28	0.47
2:B:240:LEU:HD13	2:B:250:LEU:HD23	1.96	0.47
3:C:446:GLY:HA3	3:C:452:GLY:N	2.29	0.47
3:D:442:TYR:HA	3:D:446:GLY:H	1.78	0.47
1:A:217:LEU:HG	1:A:219:ILE:CG1	2.43	0.47
1:A:217:LEU:O	1:A:277:SER:HB3	2.14	0.47
1:A:406:HIS:HB2	3:C:601:ARG:NH2	2.20	0.47
2:B:52:ASN:CG	2:B:62:ARG:HE	2.22	0.47
2:B:95:SER:HB3	2:B:108:GLU:HG2	1.95	0.47
2:B:203:ASP:HB3	2:B:205:GLU:OE1	2.14	0.47
3:C:481:PHE:HB2	3:C:493:LEU:HG	1.96	0.47
3:D:348:ASN:O	3:D:349:ILE:C	2.57	0.47
1:A:317:LEU:HG	1:A:377:MET:HG2	1.97	0.47
2:B:213:ARG:NH1	2:B:214:THR:OG1	2.47	0.47
2:B:311:LEU:HD12	2:B:342:VAL:HG11	1.97	0.47
2:B:322:SER:HB3	2:B:325:GLU:CG	2.44	0.47
3:C:351:VAL:HG22	3:C:643:MET:HG3	1.96	0.47
1:A:238:ILE:HG23	1:A:255:PHE:CE2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ILE:HD13	2:B:251:ARG:HD2	1.96	0.47
3:C:372:TYR:HE2	3:C:403:HIS:HA	1.78	0.47
3:C:587:PRO:O	3:C:591:THR:HG23	2.14	0.47
1:A:21:TRP:CZ3	1:A:52:PHE:HB3	2.49	0.47
1:A:195:LEU:HD21	1:A:264:ARG:HE	1.80	0.47
1:A:414:GLU:OE2	3:C:656:GLU:CD	2.56	0.47
2:B:263:LEU:HD11	2:B:421:GLU:HB3	1.95	0.47
3:C:428:ILE:O	3:C:577:ASN:N	2.44	0.47
3:D:428:ILE:HD13	3:D:640:LYS:HB2	1.97	0.47
1:A:18:ASN:HA	1:A:87:PHE:HZ	1.80	0.47
1:A:68:VAL:HB	1:A:93:ILE:HB	1.97	0.47
1:A:402:ARG:HB3	1:A:405:VAL:HG21	1.96	0.47
2:B:91:VAL:CG1	2:B:116:VAL:HG12	2.44	0.47
2:B:197:ASP:OD1	2:B:197:ASP:N	2.45	0.47
3:C:622:TYR:O	3:C:628:THR:HG23	2.15	0.47
2:B:295:ASP:OD1	2:B:295:ASP:N	2.48	0.47
3:C:391:MET:HG3	3:C:394:GLN:OE1	2.14	0.47
1:A:9:VAL:HG11	1:A:150:THR:HG22	1.97	0.47
1:A:70:LEU:HD11	1:A:114:ILE:HG13	1.96	0.47
3:C:390:LYS:HD2	3:C:390:LYS:HA	1.62	0.47
3:C:465:ILE:O	3:C:469:ARG:HD2	2.15	0.47
3:C:533:HIS:CE1	3:C:537:MET:HE1	2.50	0.47
1:A:189:LEU:HD11	1:A:418:PHE:HE1	1.80	0.46
1:A:66:VAL:HA	1:A:91:GLN:HB3	1.97	0.46
1:A:344:VAL:HG12	1:A:436:GLY:HA2	1.98	0.46
2:B:317:PHE:HB3	2:B:321:MET:HE2	1.96	0.46
3:C:341:THR:O	3:C:342:VAL:C	2.58	0.46
3:C:431:PHE:CZ	3:C:631:LEU:HD22	2.49	0.46
3:D:441:THR:O	3:D:445:ASP:N	2.43	0.46
1:A:72:PRO:HB3	1:A:94:THR:HB	1.96	0.46
1:A:99:ALA:HA	1:A:105:ARG:HH21	1.81	0.46
1:A:102:ASN:HD21	1:A:407:TRP:HB3	1.80	0.46
1:A:394:LYS:O	1:A:397:LEU:HG	2.15	0.46
1:A:414:GLU:HB2	3:C:586:SER:OG	2.14	0.46
1:A:427:ALA:HB2	3:C:390:LYS:CE	2.44	0.46
2:B:50:TYR:OH	2:B:237:THR:OG1	2.33	0.46
3:C:430:ILE:HD12	3:C:578:LEU:HD23	1.96	0.46
1:A:158:SER:HA	1:A:162:GLY:HA2	1.98	0.46
2:B:118:ASP:HA	2:B:121:ARG:NE	2.29	0.46
3:C:590:SER:C	3:C:591:THR:HG23	2.40	0.46
6:C:901:ADP:O3B	8:C:903:ALF:F3	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:511:ASP:HA	3:D:633:PRO:HB3	1.98	0.46
1:A:295:CYS:HB2	1:A:377:MET:HB2	1.97	0.46
2:B:6:HIS:HD2	2:B:7:ILE:N	2.13	0.46
1:A:182:VAL:HG22	1:A:185:TYR:HB2	1.98	0.46
2:B:149:THR:HA	2:B:152:ILE:HG22	1.96	0.46
2:B:375:GLN:NE2	2:B:426:GLN:OE1	2.49	0.46
2:B:42:LEU:HD11	2:B:243:PRO:HG3	1.98	0.46
2:B:291:GLN:HA	2:B:294:PHE:CZ	2.51	0.46
2:B:417:ASP:OD2	3:C:623:ARG:CZ	2.64	0.46
1:A:74:VAL:O	1:A:77:GLU:HG2	2.15	0.46
2:B:279:GLN:HA	2:B:282:ARG:NH1	2.30	0.46
3:C:498:LYS:HB2	3:C:500:MET:HE3	1.98	0.46
1:A:4:CYS:HB2	1:A:133:GLN:HB2	1.98	0.46
1:A:238:ILE:HG23	1:A:255:PHE:HE2	1.81	0.46
2:B:44:LEU:HA	2:B:47:ILE:HB	1.97	0.46
2:B:65:LEU:HD11	2:B:85:PHE:CD2	2.51	0.46
3:D:504:MET:HB3	3:D:504:MET:HE3	1.85	0.46
3:D:599:ILE:HG22	3:D:601:ARG:H	1.81	0.46
2:B:118:ASP:HA	2:B:121:ARG:HE	1.81	0.45
3:C:358:PRO:HB2	3:C:363:GLU:OE2	2.17	0.45
3:C:480:THR:OG1	3:C:558:LYS:HB3	2.16	0.45
1:A:272:TYR:CE2	1:A:274:PRO:HG2	2.51	0.45
1:A:416:GLY:CA	3:C:659:LYS:HZ3	2.25	0.45
2:B:42:LEU:O	2:B:45:ASP:HB3	2.16	0.45
2:B:76:VAL:O	2:B:82:GLY:HA3	2.17	0.45
2:B:314:ALA:HB3	2:B:368:ILE:HB	1.98	0.45
2:B:417:ASP:OD2	3:C:623:ARG:NH2	2.50	0.45
3:D:336:LYS:HD2	3:D:337:GLU:N	2.31	0.45
3:D:339:HIS:NE2	3:D:417:PRO:HB3	2.31	0.45
1:A:318:LEU:HD13	1:A:318:LEU:HA	1.84	0.45
1:A:401:LYS:HB2	2:B:344:TRP:HZ2	1.81	0.45
2:B:47:ILE:HG12	2:B:51:TYR:HB2	1.98	0.45
2:B:327:ASP:O	2:B:330:MET:HG3	2.17	0.45
3:C:333:MET:O	3:C:337:GLU:HG2	2.15	0.45
3:D:555:ALA:HB3	3:D:580:ASP:HB3	1.97	0.45
3:D:543:SER:N	3:D:550:SER:HB3	2.31	0.45
1:A:6:SER:O	1:A:65:ALA:HA	2.17	0.45
3:D:329:PHE:HD2	3:D:471:LEU:HD13	1.81	0.45
1:A:371:VAL:HG12	1:A:373:ARG:H	1.82	0.45
2:B:73:MET:HB3	2:B:77:ARG:HH11	1.80	0.45
2:B:100:ASN:HB3	2:B:103:LYS:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:565:HIS:CG	3:C:568:LYS:HB3	2.52	0.45
1:A:21:TRP:HZ3	1:A:52:PHE:HB3	1.82	0.45
1:A:172:TYR:CE2	1:A:387:ALA:HB1	2.51	0.45
1:A:320:ARG:HH21	1:A:358:GLN:HG3	1.82	0.45
2:B:12:CYS:O	2:B:16:ILE:HG12	2.17	0.45
2:B:241:ARG:HG3	2:B:242:PHE:CD2	2.51	0.45
3:C:394:GLN:HE21	3:C:658:VAL:HG21	1.82	0.45
1:A:343:PHE:CB	1:A:348:PRO:HA	2.46	0.45
2:B:39:ASP:OD1	2:B:40:SER:N	2.50	0.45
3:D:333:MET:HG3	3:D:336:LYS:HE3	1.98	0.45
3:D:342:VAL:O	3:D:346:ARG:HG2	2.16	0.45
1:A:108:TYR:C	3:C:593:MET:HE1	2.40	0.45
1:A:135:PHE:H	1:A:166:LYS:HA	1.82	0.45
1:A:402:ARG:CB	3:C:608:ASN:OD1	2.65	0.45
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.32	0.45
3:D:454:ILE:HB	3:D:455:PRO:HD3	1.99	0.45
3:D:505:ALA:HA	3:D:513:TYR:CD1	2.51	0.45
3:D:556:VAL:HG13	3:D:579:VAL:HG22	1.98	0.45
2:B:262:ARG:O	2:B:264:HIS:N	2.50	0.45
2:B:293:VAL:HA	2:B:298:ASN:HD22	1.82	0.45
3:C:458:VAL:O	3:C:461:LEU:HG	2.17	0.45
3:C:475:TYR:HA	3:C:562:ILE:O	2.17	0.45
3:C:590:SER:O	3:C:591:THR:CG2	2.65	0.45
1:A:157:LEU:HD13	1:A:157:LEU:HA	1.75	0.44
1:A:248:LEU:HD23	1:A:353:VAL:O	2.16	0.44
1:A:260:VAL:HB	1:A:266:HIS:HA	1.98	0.44
3:C:482:LEU:HD21	3:C:489:LEU:HD12	1.99	0.44
1:A:199:ASP:O	1:A:260:VAL:HG11	2.17	0.44
2:B:286:VAL:CG1	2:B:287:PRO:HD3	2.48	0.44
2:B:406:MET:HB3	3:C:506:LYS:CD	2.33	0.44
1:A:246:GLY:H	1:A:249:ASN:HD21	1.65	0.44
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.98	0.44
2:B:274:THR:CB	2:B:282:ARG:HH21	2.30	0.44
2:B:421:GLU:CD	3:C:621:PRO:HB3	2.41	0.44
1:A:5:ILE:HG22	1:A:64:ARG:HD3	2.00	0.44
1:A:119:LEU:HD11	1:A:156:ARG:HG2	1.99	0.44
1:A:305:CYS:SG	1:A:384:ILE:HA	2.58	0.44
1:A:336:LYS:HD3	1:A:351:PHE:HB3	2.00	0.44
2:B:374:ILE:HB	2:B:422:TYR:CE2	2.53	0.44
3:D:356:ARG:NH2	3:D:362:GLU:OE1	2.50	0.44
3:D:416:SER:OG	3:D:417:PRO:HD3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:CYS:SG	1:A:351:PHE:HA	2.57	0.44
1:A:332:ILE:HG12	1:A:351:PHE:HB2	1.99	0.44
2:B:322:SER:HB3	2:B:325:GLU:HG3	1.98	0.44
1:A:5:ILE:HD11	1:A:135:PHE:CE1	2.52	0.44
1:A:221:ARG:HD2	1:A:221:ARG:HA	1.68	0.44
2:B:19:LYS:O	2:B:23:VAL:HG23	2.18	0.44
2:B:146:GLY:O	2:B:149:THR:OG1	2.31	0.44
2:B:317:PHE:N	2:B:365:VAL:HG23	2.29	0.44
1:A:55:GLU:HB2	1:A:61:HIS:CD2	2.52	0.44
1:A:177:VAL:HG11	2:B:327:ASP:CG	2.43	0.44
1:A:188:ILE:HD13	1:A:395:PHE:CD2	2.52	0.44
1:A:213:CYS:HA	1:A:217:LEU:CB	2.43	0.44
2:B:162:ARG:HE	2:B:162:ARG:HA	1.82	0.44
3:D:455:PRO:HA	3:D:458:VAL:HG12	1.98	0.44
1:A:109:THR:CB	3:C:593:MET:SD	3.06	0.44
1:A:145:THR:HG23	4:A:501:GTP:O1G	2.17	0.44
1:A:180:ALA:HA	2:B:350:LYS:NZ	2.29	0.44
2:B:287:PRO:O	2:B:291:GLN:HG2	2.17	0.44
2:B:406:MET:HB2	3:C:506:LYS:HD3	1.88	0.44
3:C:568:LYS:HG3	3:C:570:GLU:HB2	2.00	0.44
6:C:901:ADP:O3B	8:C:903:ALF:F2	2.26	0.44
3:D:422:ALA:HB2	3:D:428:ILE:HG13	2.00	0.44
1:A:158:SER:HA	1:A:162:GLY:CA	2.47	0.43
1:A:167:LEU:HD11	1:A:202:PHE:CZ	2.53	0.43
2:B:262:ARG:CG	3:C:624:ASN:ND2	2.81	0.43
3:C:485:LYS:HZ3	3:C:549:ARG:HG3	1.83	0.43
2:B:145:SER:O	2:B:149:THR:HG23	2.18	0.43
1:A:55:GLU:HA	1:A:61:HIS:HA	2.00	0.43
1:A:179:THR:HG21	2:B:246:LEU:HD11	1.99	0.43
1:A:316:CYS:HB3	1:A:378:LEU:HB2	2.00	0.43
3:C:426:TYR:CZ	3:C:677:ARG:HB3	2.54	0.43
1:A:53:PHE:HA	1:A:63:PRO:CA	2.40	0.43
1:A:335:ILE:HG23	1:A:341:ILE:HG13	2.00	0.43
1:A:414:GLU:CG	3:C:586:SER:OG	2.67	0.43
2:B:375:GLN:HB3	2:B:422:TYR:CB	2.47	0.43
2:B:403:MET:HE2	2:B:403:MET:HA	2.00	0.43
1:A:132:LEU:HD21	1:A:135:PHE:CE1	2.53	0.43
1:A:292:THR:HG22	1:A:335:ILE:HD12	2.00	0.43
2:B:67:ASP:HB3	2:B:73:MET:CE	2.49	0.43
2:B:262:ARG:CG	3:C:624:ASN:HD22	2.32	0.43
2:B:299:MET:HE3	2:B:299:MET:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:442:TYR:HD1	3:C:447:VAL:HB	1.83	0.43
1:A:204:VAL:HA	1:A:302:MET:HB3	2.01	0.43
1:A:243:ARG:HH21	1:A:244:PHE:HE2	1.66	0.43
3:D:368:CYS:HB2	3:D:370:TRP:NE1	2.34	0.43
1:A:24:TYR:HB3	1:A:53:PHE:HE1	1.84	0.43
1:A:109:THR:CA	3:C:593:MET:HE3	2.39	0.43
1:A:398:MET:SD	2:B:345:ILE:HD12	2.59	0.43
1:A:409:VAL:HB	3:C:600:ASN:CG	2.43	0.43
2:B:66:VAL:CG1	2:B:147:MET:HE3	2.48	0.43
3:C:627:LEU:O	3:C:631:LEU:HG	2.18	0.43
3:C:670:CYS:SG	3:C:671:LYS:N	2.92	0.43
1:A:5:ILE:HD11	1:A:135:PHE:HE1	1.82	0.43
1:A:29:GLY:O	1:A:37:PRO:HD2	2.19	0.43
1:A:321:GLY:HA3	1:A:373:ARG:HA	2.00	0.43
2:B:6:HIS:ND1	2:B:21:TRP:NE1	2.66	0.43
2:B:217:LEU:HA	2:B:276:ARG:NH2	2.34	0.43
2:B:415:MET:O	2:B:419:VAL:HG23	2.18	0.43
3:C:587:PRO:O	3:C:591:THR:HG21	2.19	0.43
1:A:154:MET:CE	1:A:194:THR:HA	2.48	0.43
2:B:5:VAL:HG12	2:B:62:ARG:CD	2.48	0.43
2:B:200:TYR:HA	2:B:266:PHE:O	2.19	0.43
3:C:338:LEU:HB2	3:D:338:LEU:HD23	2.00	0.43
3:C:458:VAL:CG1	3:C:529:ARG:HH12	2.30	0.43
1:A:406:HIS:C	3:C:601:ARG:NH2	2.77	0.43
1:A:416:GLY:C	3:C:659:LYS:HE2	2.43	0.43
2:B:49:VAL:C	2:B:62:ARG:HH12	2.18	0.43
2:B:73:MET:HE3	2:B:92:PHE:HB3	2.00	0.43
3:C:429:CYS:HB3	3:C:641:THR:HG23	2.00	0.43
3:C:437:GLY:HA2	6:C:901:ADP:H5'2	2.01	0.43
3:C:593:MET:O	3:C:597:LYS:HG2	2.19	0.43
3:D:552:ARG:HD3	3:D:552:ARG:HA	1.88	0.43
1:A:36:MET:HE3	1:A:36:MET:HB3	1.68	0.42
1:A:105:ARG:HD2	2:B:251:ARG:HH21	1.83	0.42
1:A:408:TYR:C	1:A:413:MET:HB2	2.45	0.42
3:C:570:GLU:OE1	3:C:680:TYR:N	2.51	0.42
3:D:469:ARG:NH1	3:D:474:GLU:OE1	2.52	0.42
3:D:474:GLU:O	3:D:563:GLY:HA2	2.19	0.42
3:D:526:ASN:OD1	3:D:529:ARG:NH1	2.49	0.42
1:A:237:SER:OG	1:A:376:CYS:HB2	2.19	0.42
2:B:274:THR:HB	2:B:282:ARG:HH21	1.85	0.42
3:D:352:PHE:CD1	3:D:400:GLN:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:578:LEU:HD12	3:D:578:LEU:O	2.19	0.42
2:B:118:ASP:OD1	2:B:119:VAL:HG23	2.19	0.42
2:B:342:VAL:HG22	2:B:345:ILE:H	1.83	0.42
2:B:350:LYS:HD3	2:B:350:LYS:HA	1.88	0.42
1:A:256:GLN:O	1:A:260:VAL:HG13	2.20	0.42
2:B:262:ARG:CG	3:C:623:ARG:O	2.65	0.42
2:B:356:ILE:HD13	2:B:356:ILE:HA	1.92	0.42
2:B:405:GLU:OE2	3:C:506:LYS:HE2	2.20	0.42
3:C:358:PRO:HG3	3:C:649:PRO:HG2	2.01	0.42
3:C:422:ALA:HB2	3:C:428:ILE:HG13	2.00	0.42
3:D:333:MET:HA	3:D:336:LYS:HE3	2.01	0.42
2:B:50:TYR:HH	2:B:237:THR:HG1	1.61	0.42
2:B:143:THR:O	2:B:147:MET:HG3	2.20	0.42
2:B:159:TYR:HB3	2:B:162:ARG:CG	2.50	0.42
2:B:313:VAL:HG23	2:B:349:VAL:HA	2.01	0.42
3:D:418:LEU:HD12	3:D:642:LEU:HD22	2.01	0.42
2:B:253:LEU:O	2:B:257:MET:HG2	2.20	0.42
2:B:262:ARG:HG3	3:C:624:ASN:HD22	1.85	0.42
3:C:350:ARG:HB2	3:C:642:LEU:CD2	2.49	0.42
1:A:53:PHE:HB3	1:A:61:HIS:HB3	2.00	0.42
1:A:267:PHE:HB2	1:A:432:TYR:OH	2.19	0.42
1:A:275:VAL:HA	1:A:368:LEU:HD22	2.00	0.42
1:A:402:ARG:HG3	3:C:608:ASN:OD1	2.20	0.42
3:C:639:SER:O	3:C:640:LYS:HD2	2.20	0.42
1:A:3:GLU:HG2	1:A:51:THR:HA	2.02	0.42
1:A:22:GLU:HA	1:A:83:TYR:OH	2.20	0.42
2:B:52:ASN:O	2:B:60:VAL:HG12	2.20	0.42
3:C:342:VAL:O	3:C:343:MET:C	2.62	0.42
3:C:484:ILE:HB	3:C:554:HIS:HB2	2.02	0.42
3:D:471:LEU:O	3:D:471:LEU:HD23	2.20	0.42
1:A:33:ASP:HB2	1:A:35:GLN:OE1	2.20	0.42
1:A:264:ARG:NH2	1:A:424:ASP:O	2.53	0.42
1:A:312:TYR:H	1:A:343:PHE:HA	1.85	0.42
2:B:67:ASP:HB3	2:B:73:MET:HE1	2.02	0.42
2:B:135:LEU:HB2	2:B:166:THR:HB	2.02	0.41
2:B:188:SER:O	2:B:192:LEU:HD23	2.19	0.41
3:C:356:ARG:HG2	3:C:438:SER:O	2.19	0.41
3:C:524:ASP:OD1	3:C:524:ASP:N	2.53	0.41
1:A:116:ASP:O	1:A:119:LEU:HB2	2.20	0.41
2:B:139:LEU:HG	2:B:168:SER:OG	2.20	0.41
3:D:350:ARG:HH12	3:D:418:LEU:HD21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PHE:CZ	1:A:378:LEU:HD13	2.56	0.41
2:B:259:PRO:HG3	2:B:311:LEU:HD21	2.01	0.41
3:C:379:GLU:HA	3:C:394:GLN:O	2.21	0.41
1:A:198:SER:HB3	1:A:266:HIS:CE1	2.56	0.41
3:D:379:GLU:HB3	3:D:395:ILE:HA	2.00	0.41
1:A:321:GLY:CA	1:A:359:PRO:HA	2.47	0.41
1:A:431:ASP:O	1:A:434:GLU:HG2	2.21	0.41
1:A:15:GLN:HB3	1:A:228:ASN:ND2	2.36	0.41
1:A:91:GLN:HG3	1:A:121:ARG:CZ	2.51	0.41
1:A:115:ILE:HG13	1:A:116:ASP:N	2.36	0.41
1:A:180:ALA:CA	2:B:350:LYS:HZ3	2.27	0.41
1:A:416:GLY:O	3:C:659:LYS:HE2	2.20	0.41
2:B:32:PRO:HG3	2:B:81:PHE:CE2	2.56	0.41
2:B:66:VAL:HG13	2:B:112:LEU:CD2	2.50	0.41
2:B:323:MET:SD	2:B:323:MET:N	2.94	0.41
2:B:348:ASN:OD1	2:B:348:ASN:O	2.38	0.41
3:C:681:LEU:H	3:C:681:LEU:HD23	1.86	0.41
1:A:247:ALA:HB3	1:A:355:ILE:HG23	2.03	0.41
1:A:313:MET:HG3	1:A:435:VAL:HG11	2.02	0.41
2:B:92:PHE:HA	2:B:112:LEU:HD21	2.02	0.41
2:B:261:PRO:CG	3:C:605:GLU:OE2	2.68	0.41
1:A:78:VAL:HB	1:A:87:PHE:HD2	1.86	0.41
1:A:139:HIS:CG	1:A:150:THR:HG21	2.55	0.41
1:A:185:TYR:HE1	1:A:398:MET:HB2	1.85	0.41
1:A:320:ARG:HD3	1:A:360:PRO:HB3	2.03	0.41
2:B:66:VAL:HG22	2:B:116:VAL:HG11	2.02	0.41
2:B:156:ARG:CZ	2:B:164:MET:HE2	2.51	0.41
2:B:413:SER:CB	3:C:509:LYS:HZ1	2.32	0.41
3:D:371:THR:HB	3:D:379:GLU:OE1	2.21	0.41
1:A:7:ILE:HD11	1:A:137:VAL:HB	2.02	0.41
1:A:9:VAL:CG1	1:A:150:THR:HG22	2.51	0.41
1:A:108:TYR:HB2	1:A:411:GLU:O	2.21	0.41
1:A:176:GLN:NE2	1:A:177:VAL:HB	2.35	0.41
2:B:7:ILE:HG21	2:B:151:LEU:CD2	2.50	0.41
2:B:32:PRO:O	2:B:83:GLN:NE2	2.54	0.41
1:A:313:MET:N	1:A:380:ASN:O	2.50	0.40
2:B:100:ASN:OD1	2:B:103:LYS:N	2.34	0.40
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.91	0.40
1:A:407:TRP:CE2	2:B:255:VAL:HA	2.56	0.40
1:A:414:GLU:OE2	3:C:656:GLU:OE2	2.39	0.40
2:B:205:GLU:HA	2:B:208:TYR:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ARG:NH1	2:B:297:LYS:HZ3	2.19	0.40
2:B:329:GLN:O	2:B:333:VAL:HG13	2.21	0.40
3:C:418:LEU:HD12	3:C:418:LEU:HA	1.92	0.40
3:C:485:LYS:HD2	3:C:486:ASN:H	1.85	0.40
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.56	0.40
2:B:121:ARG:O	2:B:125:GLU:OE1	2.40	0.40
2:B:133:PHE:HD2	2:B:164:MET:SD	2.44	0.40
2:B:152:ILE:HD12	2:B:152:ILE:HA	1.84	0.40
2:B:187:LEU:HD11	2:B:408:PHE:CZ	2.56	0.40
2:B:262:ARG:H	3:C:624:ASN:HD22	1.68	0.40
3:C:598:ASN:C	3:C:598:ASN:HD22	2.28	0.40
3:C:659:LYS:HA	3:C:662:ARG:HD2	2.04	0.40
3:D:419:ILE:HD12	3:D:576:ILE:HD13	2.04	0.40
2:B:8:GLN:HG3	2:B:65:LEU:CD2	2.51	0.40
2:B:149:THR:O	2:B:191:GLN:NE2	2.54	0.40
2:B:414:ASN:C	2:B:415:MET:HE2	2.46	0.40
3:D:532:MET:HE3	3:D:532:MET:HB3	2.00	0.40
1:A:5:ILE:HG22	1:A:64:ARG:CB	2.45	0.40
1:A:301:GLN:H	1:A:301:GLN:CD	2.29	0.40
3:D:352:PHE:CE1	3:D:399:ASP:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	424/451 (94%)	398 (94%)	25 (6%)	1 (0%)	43	75
2	B	426/444 (96%)	389 (91%)	35 (8%)	2 (0%)	24	60
3	C	351/409 (86%)	332 (95%)	19 (5%)	0	100	100
3	D	330/409 (81%)	323 (98%)	7 (2%)	0	100	100
All	All	1531/1713 (89%)	1442 (94%)	86 (6%)	3 (0%)	44	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASP
2	B	143	THR
2	B	268	PRO

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	360/379 (95%)	321 (89%)	39 (11%)	6	24
2	B	366/379 (97%)	360 (98%)	6 (2%)	55	70
3	C	324/370 (88%)	322 (99%)	2 (1%)	78	81
3	D	301/370 (81%)	298 (99%)	3 (1%)	68	76
All	All	1351/1498 (90%)	1301 (96%)	50 (4%)	31	52

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	23	LEU
1	A	25	CYS
1	A	26	LEU
1	A	36	MET
1	A	62	VAL
1	A	66	VAL
1	A	68	VAL
1	A	70	LEU
1	A	103	TYR
1	A	112	LYS
1	A	113	GLU
1	A	118	VAL
1	A	122	ILE
1	A	124	LYS
1	A	125	LEU
1	A	136	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	137	VAL
1	A	154	MET
1	A	157	LEU
1	A	200	CYS
1	A	221	ARG
1	A	229	ARG
1	A	259	LEU
1	A	260	VAL
1	A	269	LEU
1	A	286	LEU
1	A	290	GLU
1	A	318	LEU
1	A	319	TYR
1	A	339	ARG
1	A	349	THR
1	A	353	VAL
1	A	363	VAL
1	A	375	VAL
1	A	377	MET
1	A	413	MET
1	A	425	MET
1	A	434	GLU
2	B	45	ASP
2	B	145	SER
2	B	162	ARG
2	B	164	MET
2	B	166	THR
2	B	228	LEU
3	C	348	ASN
3	C	447	VAL
3	D	348	ASN
3	D	349	ILE
3	D	374	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	102	ASN
1	A	133	GLN
1	A	176	GLN
1	A	186	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	ASN
2	B	8	GLN
2	B	137	HIS
2	B	191	GLN
2	B	245	GLN
2	B	256	ASN
2	B	298	ASN
2	B	335	ASN
2	B	424	GLN
3	C	340	ASN
3	C	348	ASN
3	C	364	ASN
3	C	381	GLN
3	C	394	GLN
3	C	435	GLN
3	C	554	HIS
3	C	624	ASN
3	C	651	GLN
3	D	420	GLN
3	D	507	ASN
3	D	624	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GDP	B	501	-	28,30,30	0.48	0	44,47,47	0.45	0
6	ADP	D	802	7	27,29,29	1.36	4 (14%)	42,45,45	1.96	10 (23%)
8	ALF	C	903	6,3	0,4,4	-	-	-	-	-
6	ADP	C	901	8	27,29,29	1.35	4 (14%)	42,45,45	1.95	11 (26%)
4	GTP	A	501	-	30,34,34	0.53	0	46,54,54	0.52	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	GTP	A	501	-	-	1/22/38/38	0/3/3/3
5	GDP	B	501	-	-	2/16/32/32	0/3/3/3
6	ADP	D	802	7	-	4/16/32/32	0/3/3/3
6	ADP	C	901	8	-	5/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	802	ADP	C5-C4	4.52	1.47	1.39
6	C	901	ADP	C5-C4	4.50	1.47	1.39
6	C	901	ADP	C5-C6	2.71	1.48	1.41
6	D	802	ADP	C5-C6	2.71	1.48	1.41
6	D	802	ADP	C8-N7	2.45	1.36	1.31
6	C	901	ADP	C8-N7	2.42	1.36	1.31
6	D	802	ADP	C5-N7	-2.09	1.35	1.39
6	C	901	ADP	C5-N7	-2.06	1.35	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	802	ADP	C5-C4-N3	-6.23	118.62	126.75
6	C	901	ADP	C5-C4-N3	-5.95	118.99	126.75
6	D	802	ADP	N3-C4-N9	4.76	134.92	127.08
6	C	901	ADP	N3-C4-N9	4.64	134.73	127.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	802	ADP	C2-N3-C4	3.87	120.89	111.75
6	C	901	ADP	C2-N3-C4	3.86	120.86	111.75
6	D	802	ADP	PA-O3A-PB	-3.71	120.08	132.83
6	C	901	ADP	PA-O3A-PB	-3.40	121.16	132.83
6	D	802	ADP	C4-C5-N7	-3.39	106.49	110.62
6	C	901	ADP	C4-C5-N7	-3.31	106.58	110.62
6	C	901	ADP	N3-C2-N1	-3.24	123.53	128.60
6	D	802	ADP	N3-C2-N1	-3.14	123.69	128.60
6	C	901	ADP	C5-N7-C8	2.81	107.50	103.51
6	D	802	ADP	C5-N7-C8	2.80	107.48	103.51
6	C	901	ADP	C4-N9-C8	2.78	108.74	105.73
6	D	802	ADP	C4-N9-C8	2.43	108.36	105.73
6	C	901	ADP	C6-C5-N7	2.40	136.49	132.02
6	D	802	ADP	C3'-C2'-C1'	2.39	105.97	101.43
6	C	901	ADP	N9-C8-N7	-2.21	110.90	113.91
6	D	802	ADP	C6-C5-N7	2.19	136.10	132.02
6	C	901	ADP	C3'-C2'-C1'	2.01	105.25	101.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	901	ADP	O4'-C4'-C5'-O5'
6	D	802	ADP	C5'-O5'-PA-O1A
5	B	501	GDP	C3'-C4'-C5'-O5'
6	C	901	ADP	C3'-C4'-C5'-O5'
5	B	501	GDP	O4'-C4'-C5'-O5'
4	A	501	GTP	C4'-C5'-O5'-PA
6	C	901	ADP	C5'-O5'-PA-O3A
6	D	802	ADP	C5'-O5'-PA-O3A
6	D	802	ADP	C5'-O5'-PA-O2A
6	C	901	ADP	PB-O3A-PA-O1A
6	C	901	ADP	PB-O3A-PA-O2A
6	D	802	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 10 short contacts:

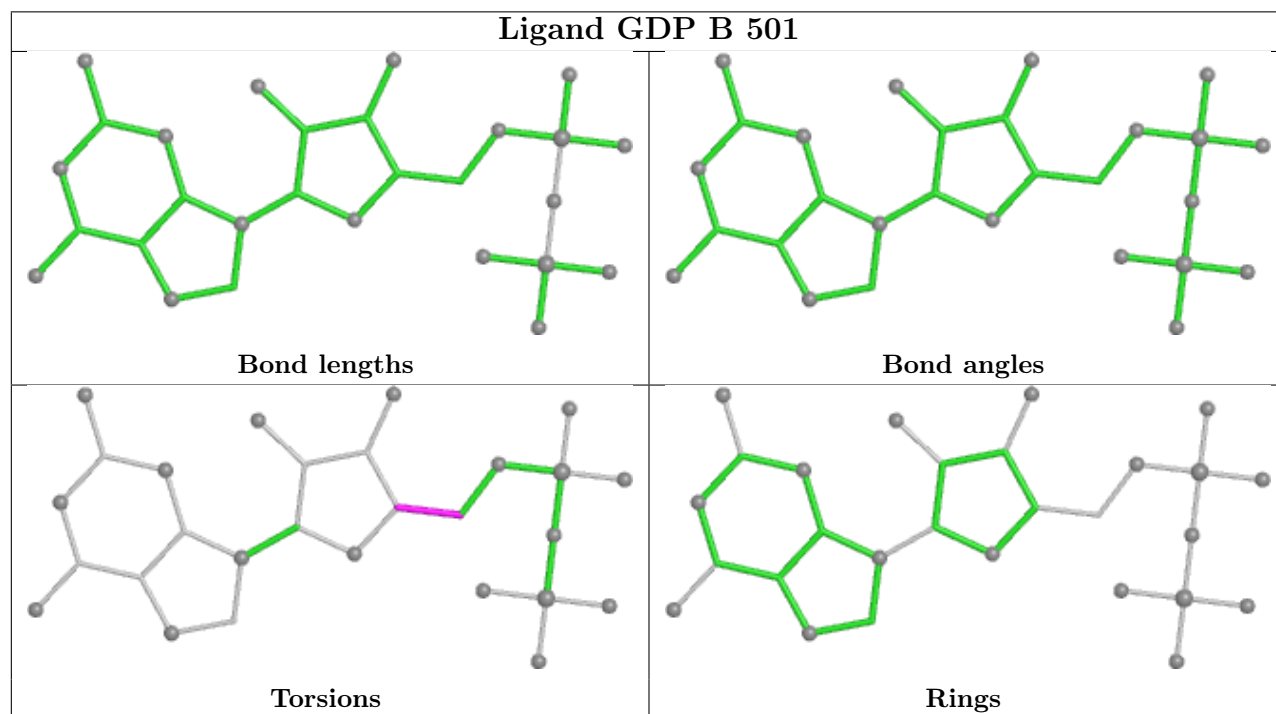
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	GDP	2	0
6	D	802	ADP	1	0

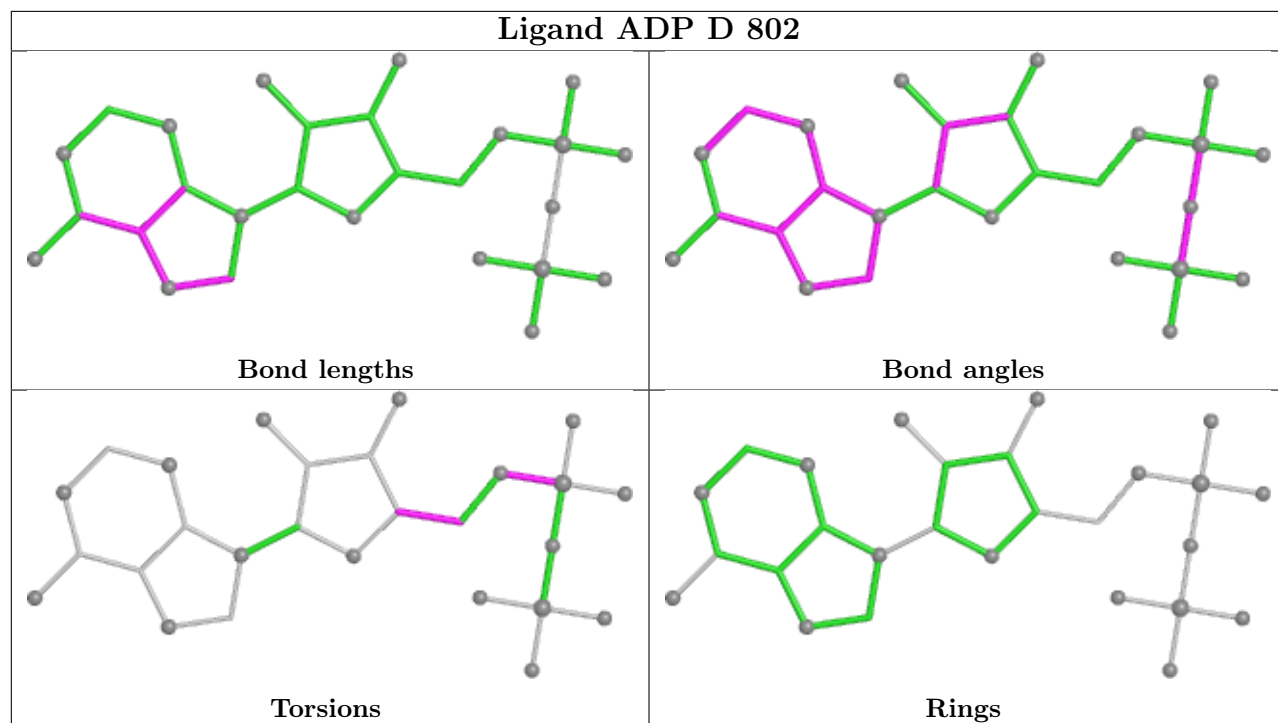
Continued on next page...

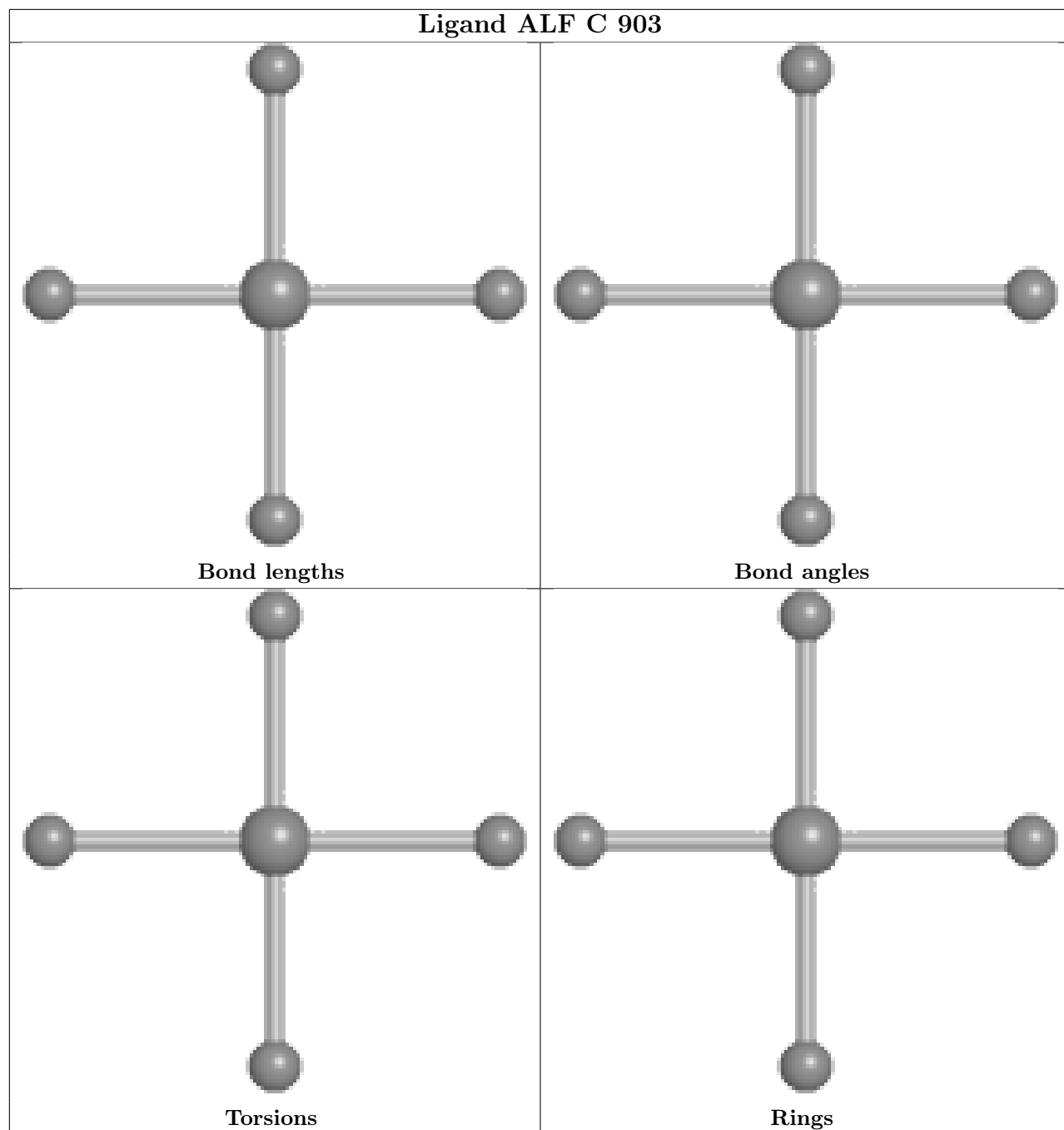
Continued from previous page...

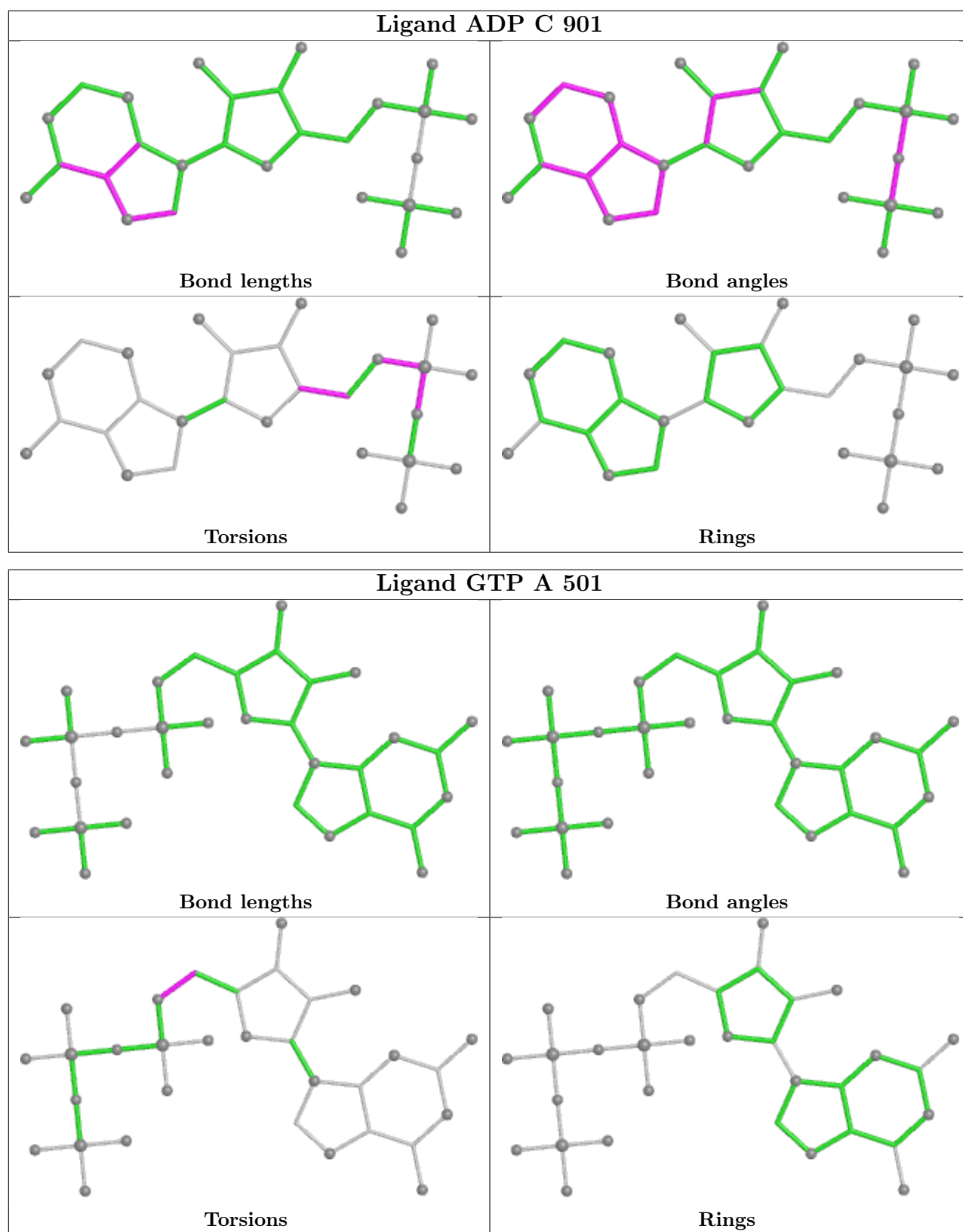
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	903	ALF	3	0
6	C	901	ADP	5	0
4	A	501	GTP	1	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

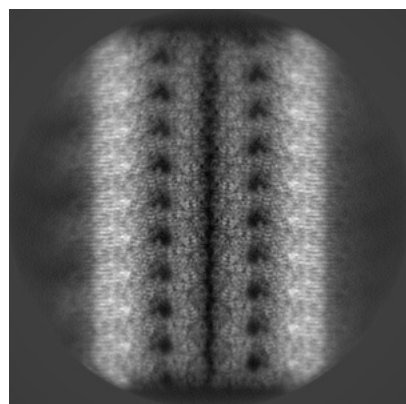
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39667. These allow visual inspection of the internal detail of the map and identification of artifacts.

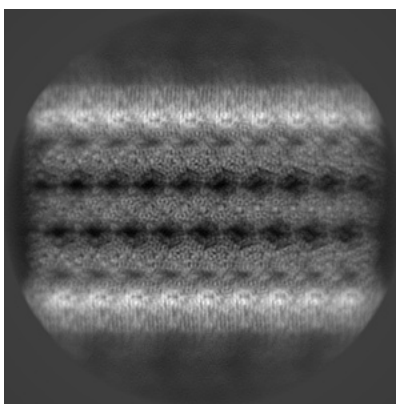
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

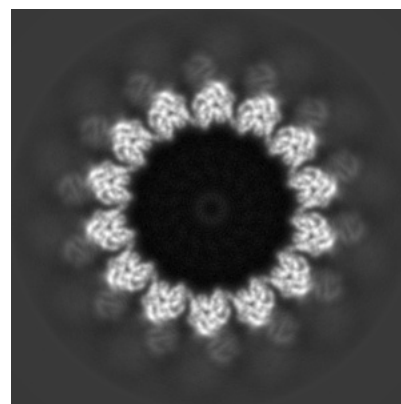
6.1.1 Primary map



X

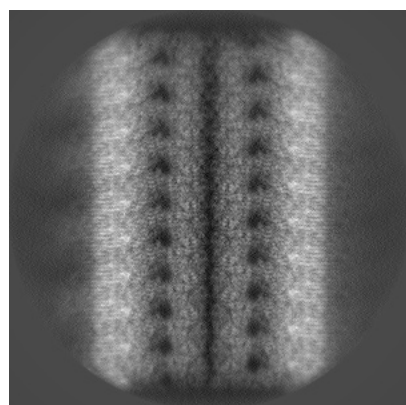


Y

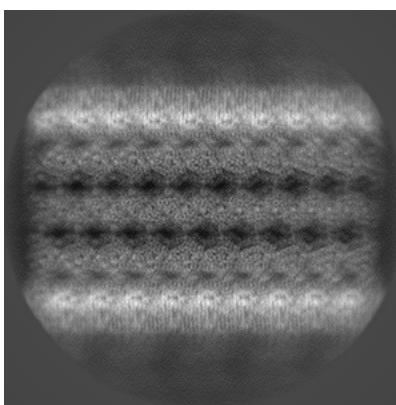


Z

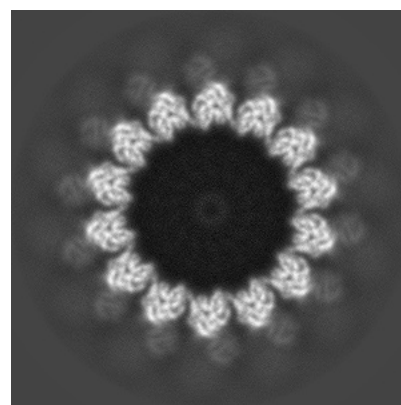
6.1.2 Raw map



X



Y

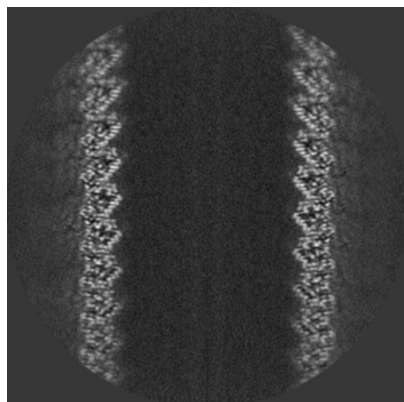


Z

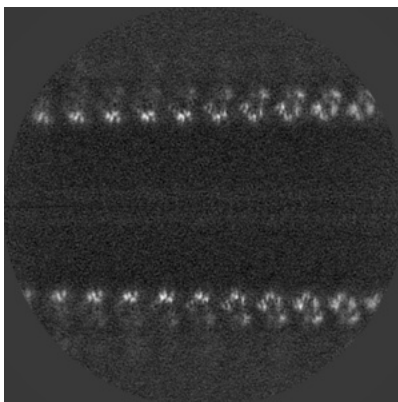
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

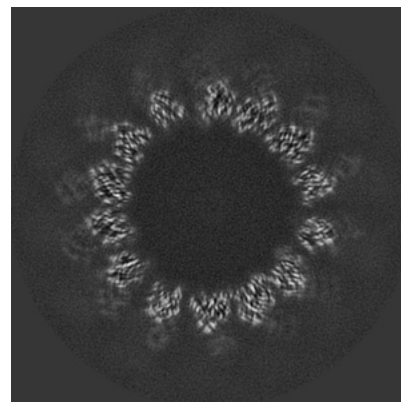
6.2.1 Primary map



X Index: 300

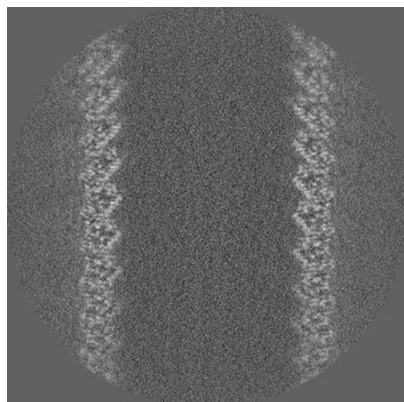


Y Index: 300

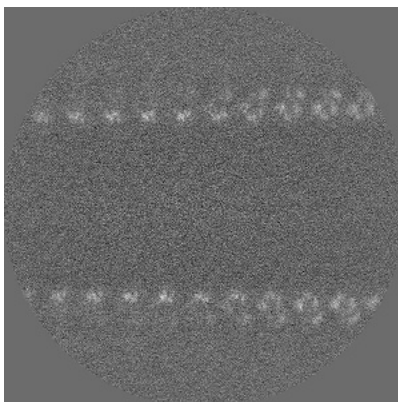


Z Index: 300

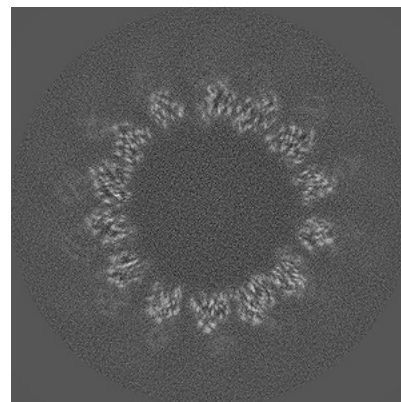
6.2.2 Raw map



X Index: 300



Y Index: 300

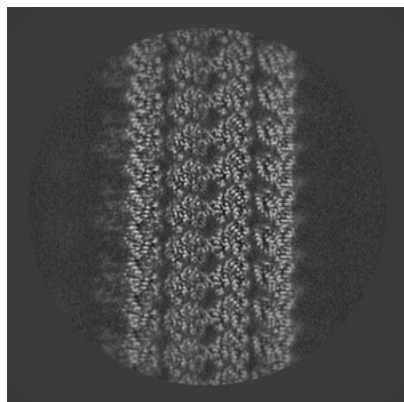


Z Index: 300

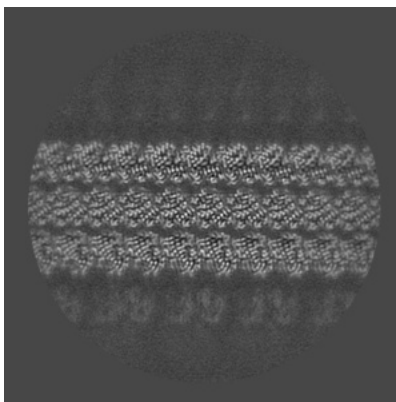
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

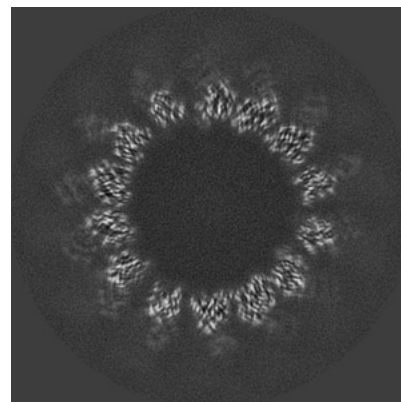
6.3.1 Primary map



X Index: 162

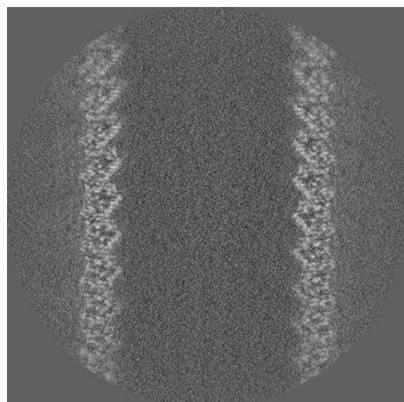


Y Index: 155

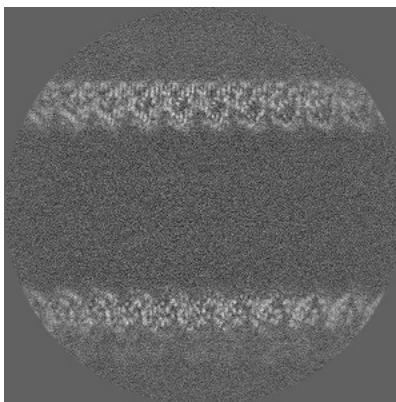


Z Index: 299

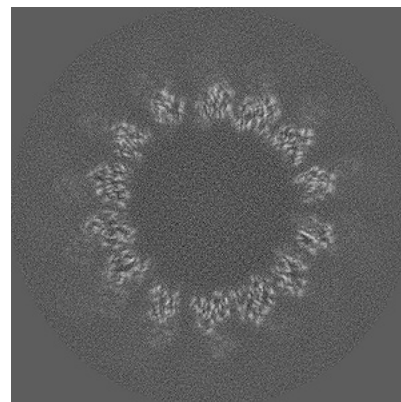
6.3.2 Raw map



X Index: 300



Y Index: 335

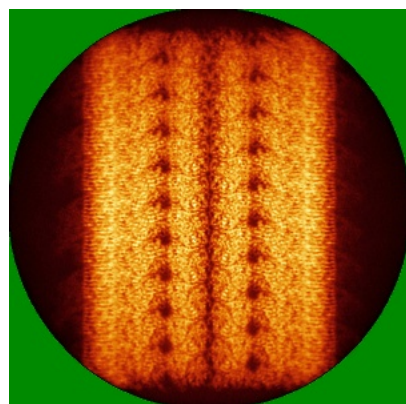


Z Index: 296

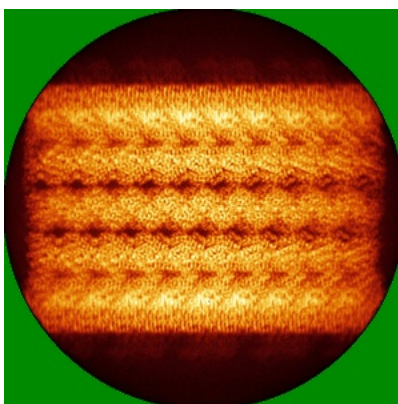
The images above show the largest variance slices of the map in three orthogonal directions.

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

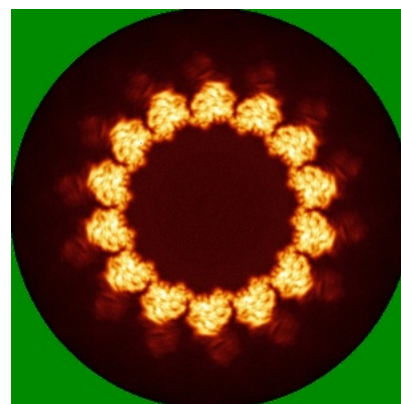
6.4.1 Primary map



X

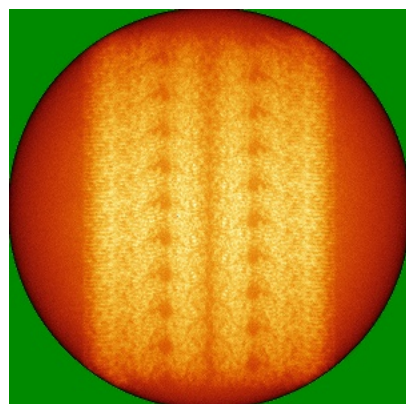


Y

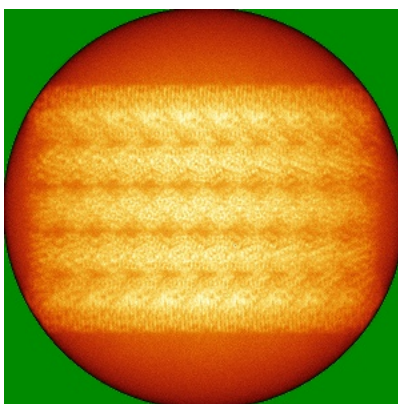


Z

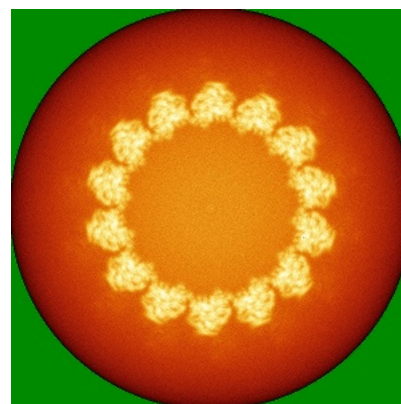
6.4.2 Raw map



X



Y

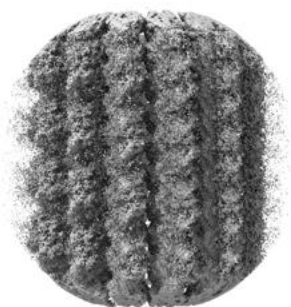


Z

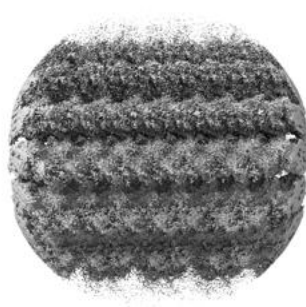
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

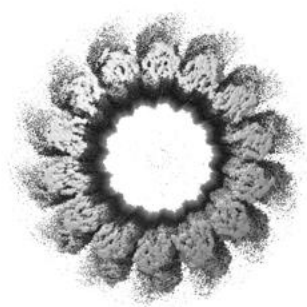
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

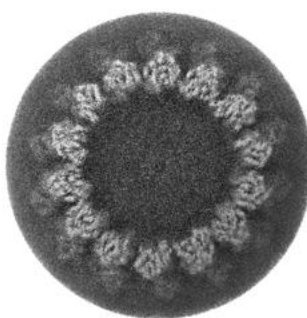
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

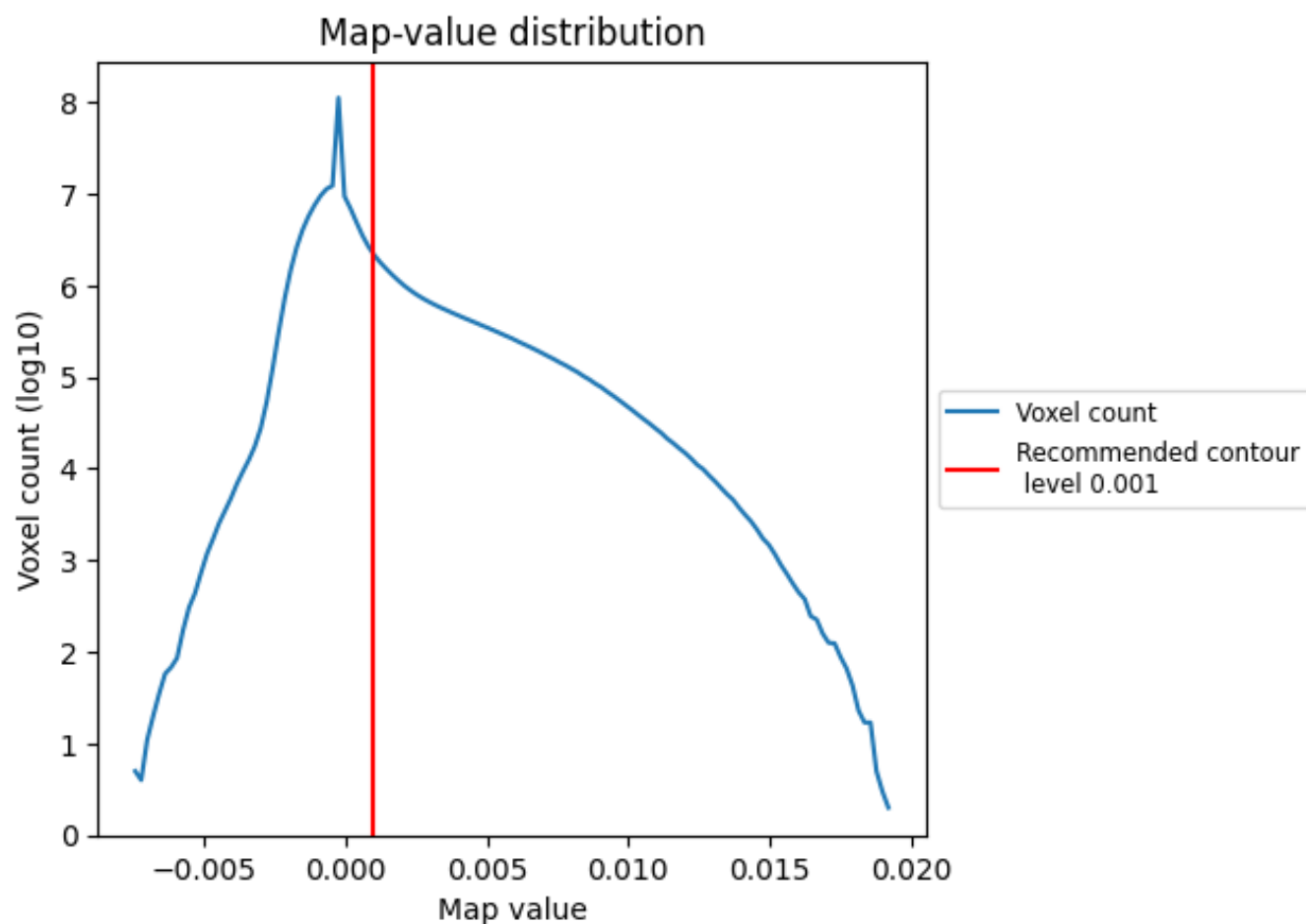
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

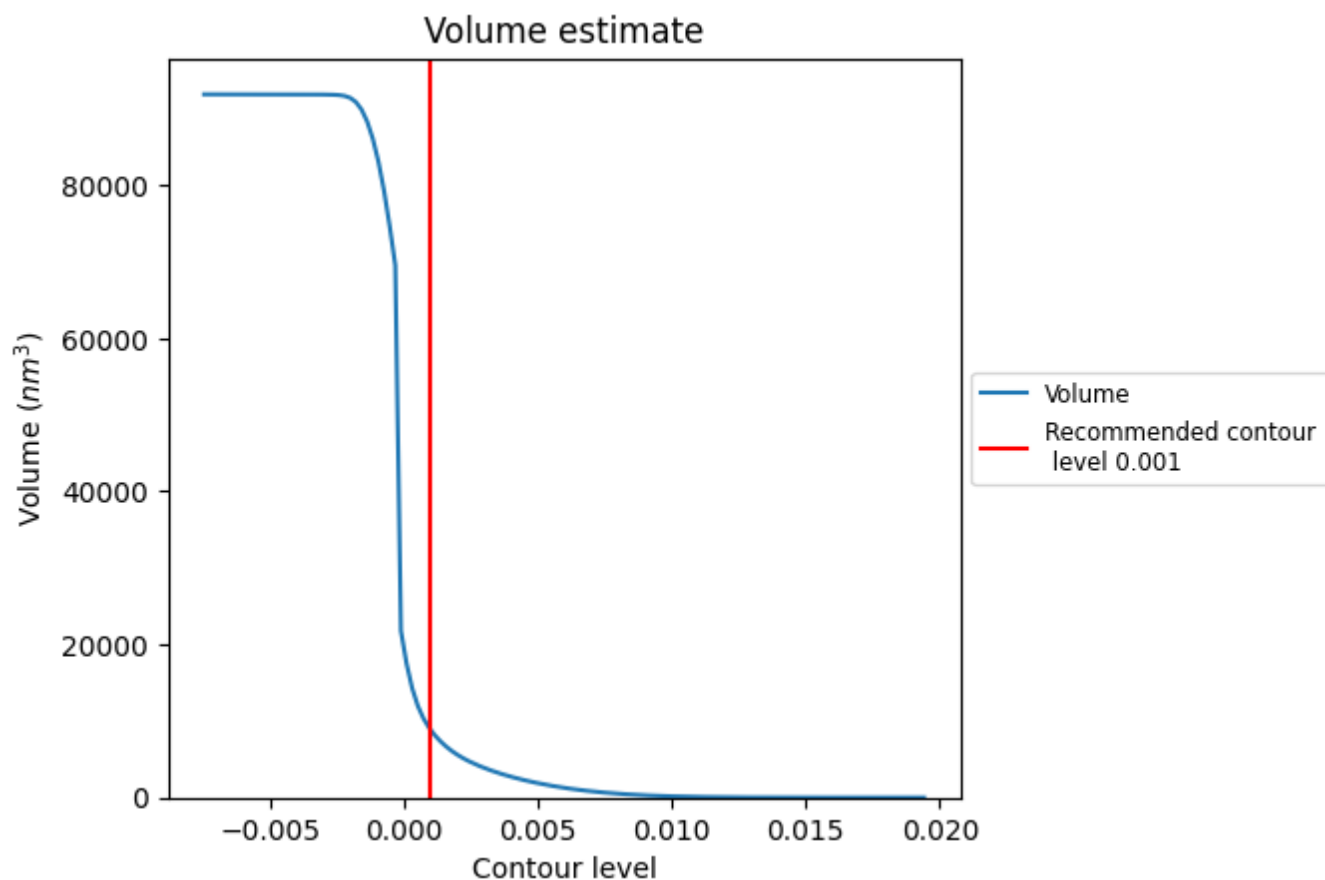
This section contains the results of statistical analysis of the map.

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.

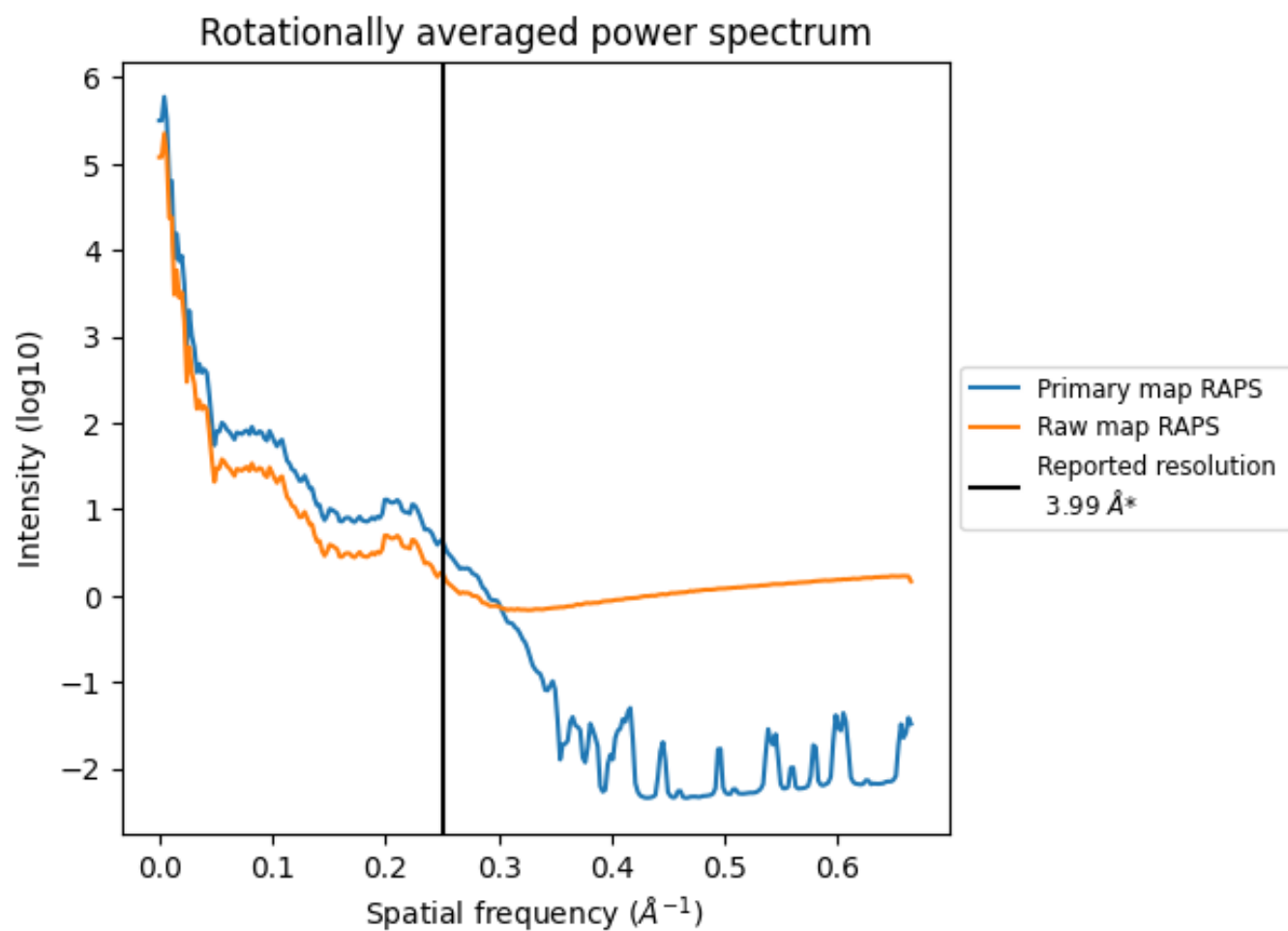
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8906 nm^3 ; this corresponds to an approximate mass of 8045 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

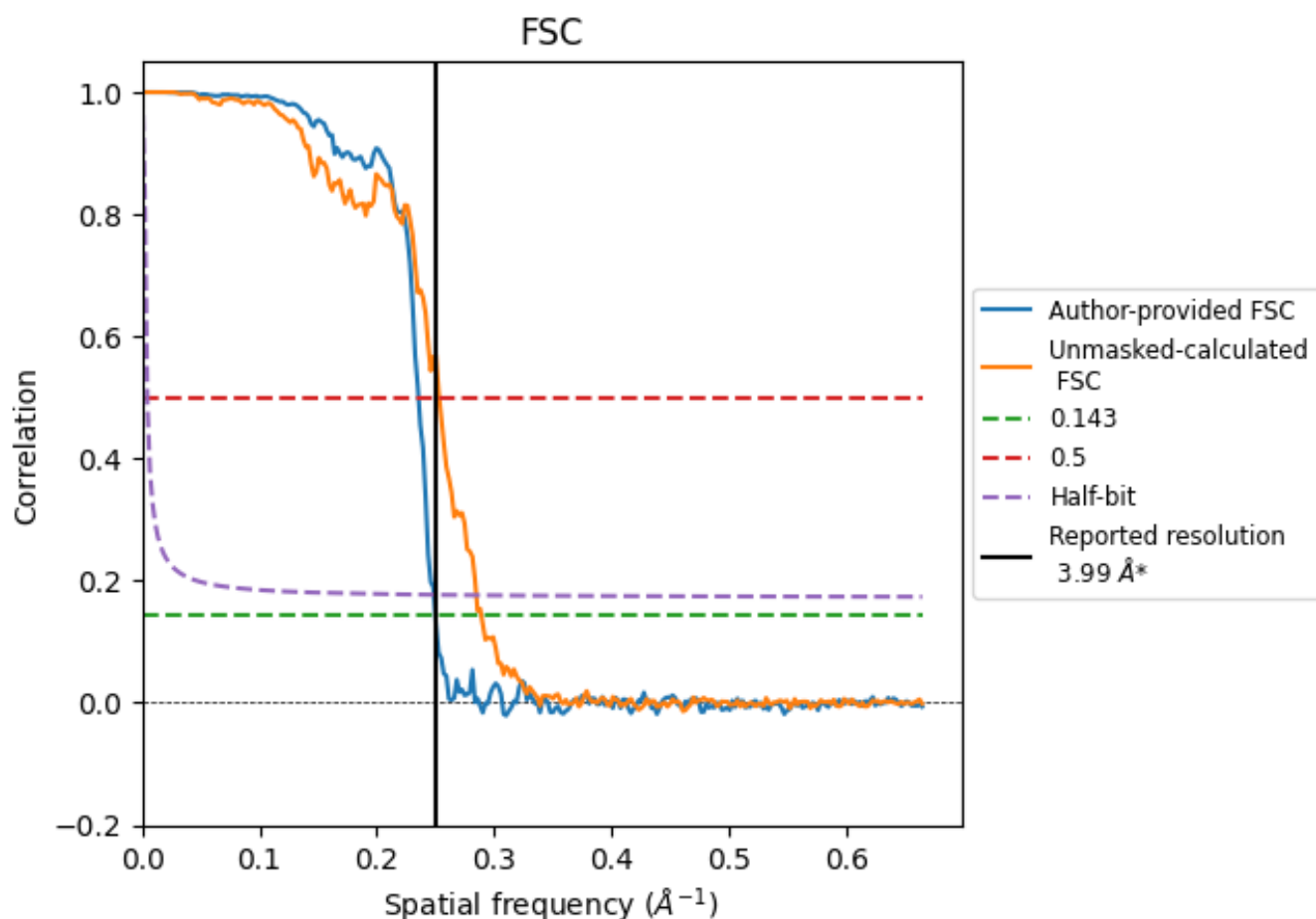


*Reported resolution corresponds to spatial frequency of $0.251 \text{ \AA}^{-1}$

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 0.251 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

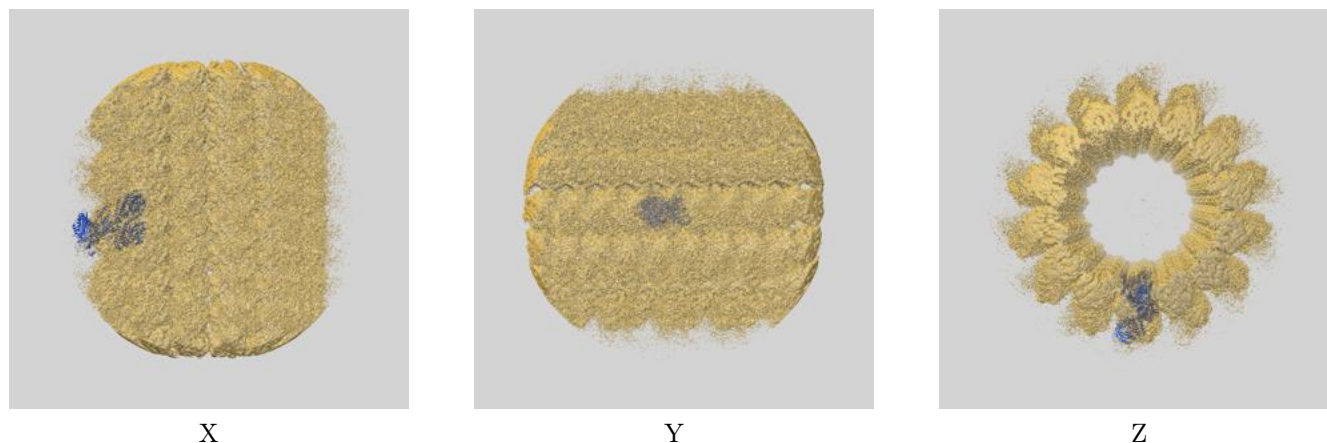
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	4.00	4.24	4.02
Unmasked-calculated*	3.46	3.95	3.51

*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 3.46 differs from the reported value 3.99 by more than 10 %

9 Map-model fit [i](#)

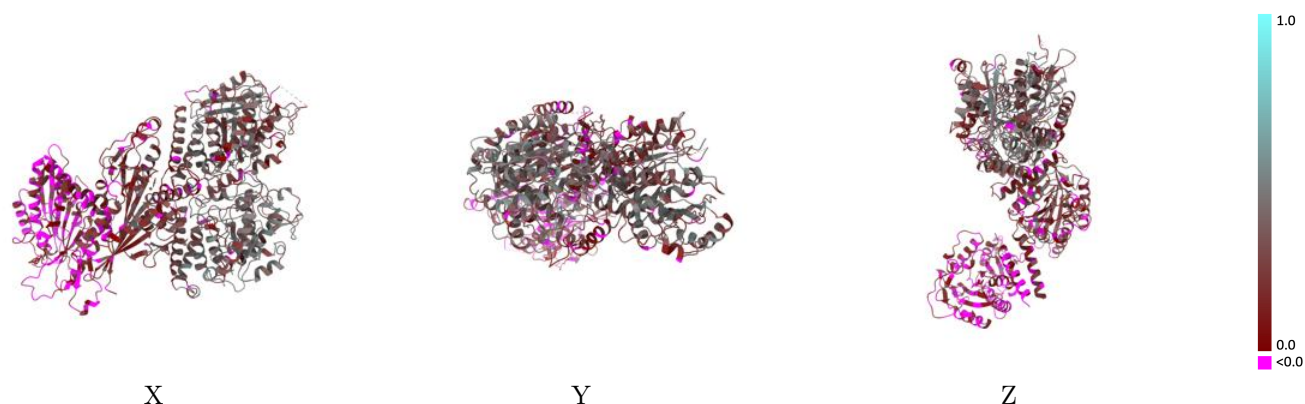
This section contains information regarding the fit between EMDB map EMD-39667 and PDB model 8YY5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



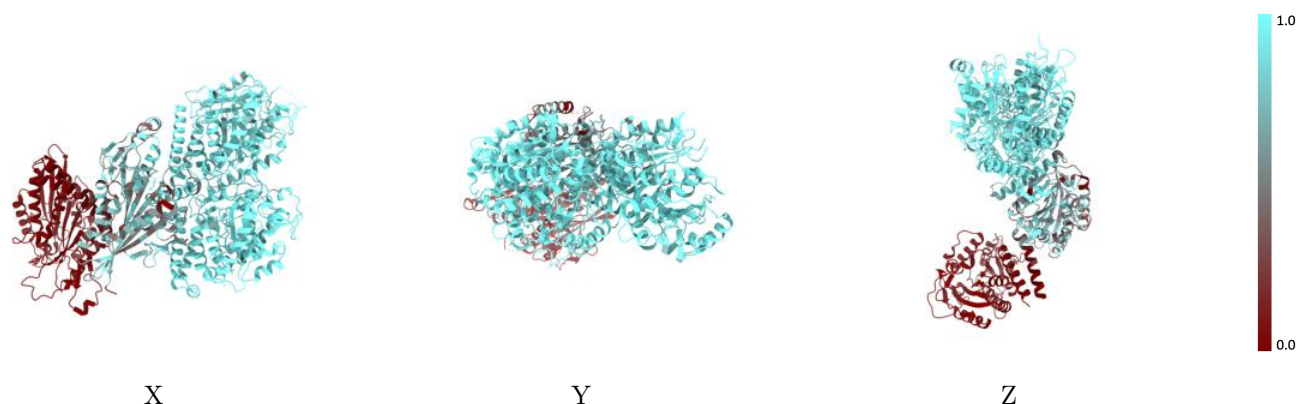
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



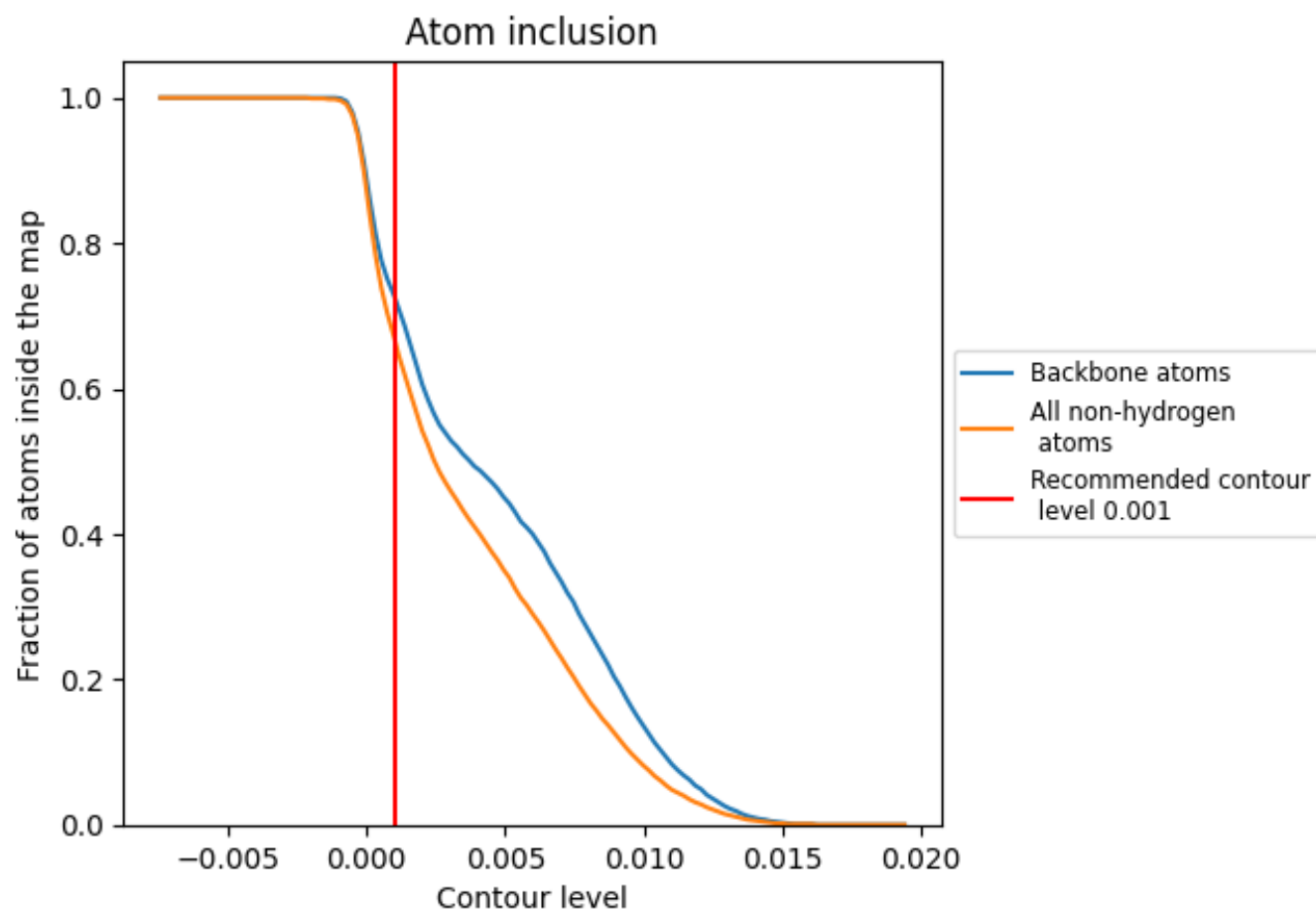
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.001).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 67% 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 (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6690	0.2390
A	0.9400	0.3230
B	0.9710	0.3770
C	0.6110	0.1920
D	0.0060	0.0080

