



Full wwPDB EM Validation Report ⓘ

Oct 15, 2025 – 05:06 PM JST

PDB ID : 8YY4 / pdb_00008yy4
EMDB ID : EMD-39666
Title : Kinesin-14 with AlF3 bound to 13 PF Microtubule
Authors : Shibata, S.; Imasaki, T.; Shigematsu, H.; Hagio, H.; Endow, S.A.; Nitta, R.
Deposited on : 2024-04-03
Resolution : 4.02 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

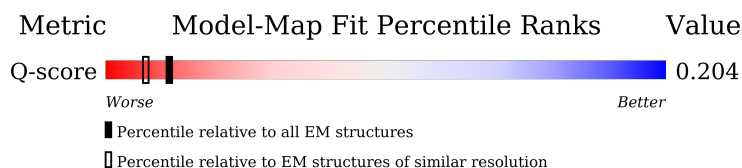
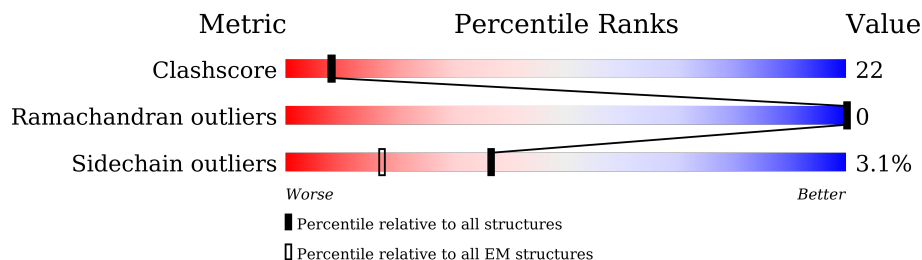
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.02 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	6727 (3.52 - 4.52)

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
5	GDP	B	501	-	-	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		

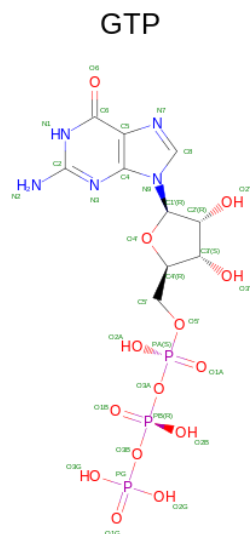
- Molecule 3 is a protein called Protein claret segregational.

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:

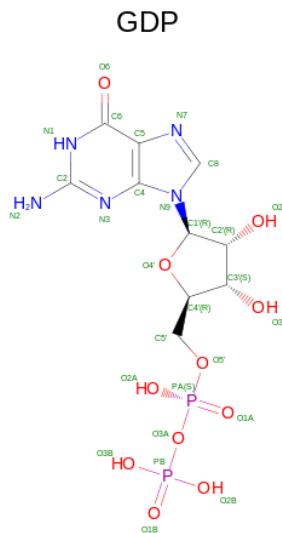
Chain	Residue	Modelled	Actual	Comment	Reference
C	292	MET	GLU	engineered mutation	UNP P20480
C	485	LYS	TYR	engineered mutation	UNP P20480
C	697	ASN	SER	engineered mutation	UNP P20480
D	292	MET	GLU	engineered mutation	UNP P20480
D	485	LYS	TYR	engineered mutation	UNP P20480
D	697	ASN	SER	engineered mutation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

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



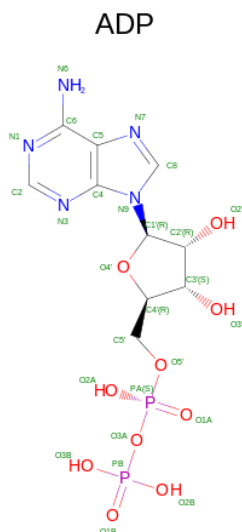
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- 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	C	N	O	P	0
			28	10	5	11	2	

- 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).

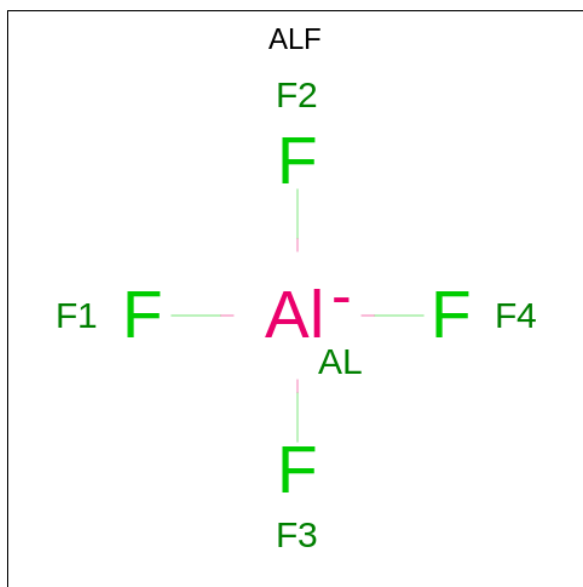


Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total 27	C 10	N 5	O 10	P 2	0
6	D	1	Total 27	C 10	N 5	O 10	P 2	0

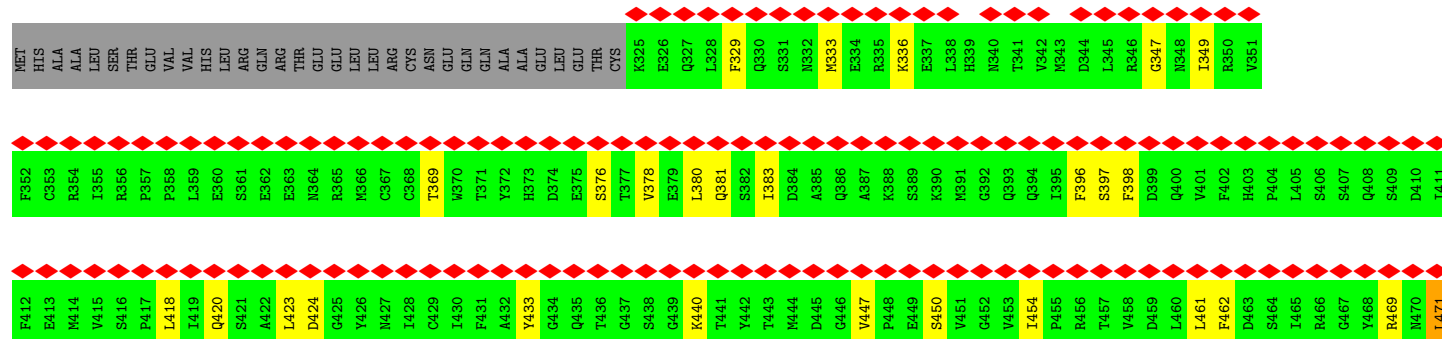
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- 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



D652	C653	F654	Q655	E656	S657	V658	K659	S660	L661	R662	F663	A664	A665	S666	V667	N668	S669	CYS	LYS	THR	LYS	ALA	ARG	ASN	ARG	TYR	LEU	ASN	ASN	SER	VAL	ALA	ASN	SER	SER	THR	GLN	SER	ASN	ASN	SER	GLY	ASN	PHE	ASP	LYS														
G472	W473	E474	Y475	E476	I477	K478	A479	T480	F481	L482	E483	I484	K485	N486	E487	V488	L489	Y490	D491	L492	L493	S494	N495	E496	Q497	K498	D499	M500	E501	I502	R503	M504	A505	K506	N507	N508	K509	N510	D511	I512	Y513	V514	S515	N516	I517	T518	E519	E520	T521	V522	L523	D524	P525	N526	H527	L528	R529	H530	I531	
M532	H533	T534	A535	K536	M537	N538	R539	A540	T541	A542	S543	T544	A545	G546	H547	E548	R549	S550	S551	R552	S553	H554	A555	V556	T557	K558	L559	E560	L561	T562	G563	R564	H565	A566	E567	K568	G569	E570	N571	S572	V573	G574	S575	T576	N577	L578	V579	D580	L581	A582	G583	S584	E585	S586	P587	LYS	THR	SER	THR	
ARG	MET	THR	GLU	THR	LYS	ASN	T599	M600	R601	S602	L603	S604	E605	L606	T607	M608	V609	L610	L611	A612	L613	L614	L615	K616	Q617	D618	H619	I620	P621	Y622	M623	A624	S625	K626	L627	T628	H629	L630	L631	M632	P633	S634	L635	G636	G637	H638	S639	K640	T641	L642	M643	F644	I645	M646	V647	S648	P649	F650	Q651	

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-27.6964°, rise=9.37998 Å, axial sym=C1	Depositor
Number of segments used	28547	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	0.011	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0005	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/3429	0.39	0/4656
2	B	0.26	0/3431	0.42	0/4652
3	C	0.15	0/2882	0.30	0/3882
3	D	0.12	0/2695	0.25	0/3636
All	All	0.21	0/12437	0.35	0/16826

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	3352	0	3268	192	0
2	B	3356	0	3241	206	0
3	C	2836	0	2826	104	0
3	D	2650	0	2623	39	0
4	A	32	0	12	2	0
5	B	28	0	12	10	0
6	C	27	0	12	4	0
6	D	27	0	12	0	0
7	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
8	C	5	0	0	1	0
All	All	12315	0	12006	525	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 22.

All (525) 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:221:ARG:NH1	2:B:323:MET:SD	2.43	0.90
1:A:311:LYS:HD3	1:A:342:GLN:HB3	1.55	0.88
2:B:99:ASN:HA	2:B:142:GLY:H	1.42	0.84
2:B:323:MET:SD	2:B:323:MET:N	2.47	0.83
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.46	0.80
3:D:461:LEU:HD11	3:D:561:LEU:HD21	1.65	0.78
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.18	0.76
2:B:240:LEU:HD12	2:B:249:ASP:HB2	1.65	0.76
2:B:178:THR:HB	2:B:181:GLU:HB3	1.67	0.76
2:B:334:GLN:O	2:B:338:SER:OG	2.02	0.76
3:C:349:ILE:HG21	3:C:643:MET:HG2	1.68	0.75
3:C:595:GLU:HA	3:C:598:ASN:ND2	2.03	0.73
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.53	0.73
3:C:373:HIS:NE2	3:C:379:GLU:OE1	2.18	0.73
3:C:439:GLY:N	6:C:901:ADP:O1B	2.20	0.73
1:A:288:VAL:O	1:A:292:THR:OG1	2.06	0.72
6:C:901:ADP:O3B	8:C:903:ALF:F3	1.98	0.72
2:B:3:GLU:HG3	2:B:49:VAL:HA	1.72	0.71
2:B:287:PRO:HA	2:B:329:GLN:HE22	1.55	0.71
2:B:314:ALA:HA	2:B:350:LYS:HB2	1.73	0.71
2:B:156:ARG:NH2	2:B:195:ASN:O	2.24	0.70
2:B:261:PRO:O	2:B:264:HIS:ND1	2.14	0.70
1:A:265:ILE:HG23	1:A:432:TYR:HE1	1.55	0.70
1:A:68:VAL:HG22	1:A:93:ILE:HB	1.74	0.69
2:B:164:MET:HE1	2:B:166:THR:HG22	1.75	0.69
2:B:133:PHE:H	2:B:164:MET:HA	1.57	0.69
2:B:244:GLY:O	2:B:247:ASN:ND2	2.26	0.69
2:B:375:GLN:HB2	2:B:419:VAL:HG13	1.75	0.68
2:B:346:PRO:HG2	2:B:347:ASN:ND2	2.08	0.68
3:C:587:PRO:O	3:C:591:THR:OG1	2.12	0.68
2:B:48:SER:O	2:B:62:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HD13	1:A:354:GLY:HA3	1.76	0.68
3:C:498:LYS:HB2	3:C:500:MET:HE2	1.76	0.67
1:A:221:ARG:HH22	2:B:323:MET:HE1	1.59	0.67
2:B:406:MET:SD	2:B:407:GLU:N	2.68	0.67
2:B:20:PHE:CZ	2:B:24:ILE:HD11	2.29	0.67
3:D:397:SER:O	3:D:668:ASN:ND2	2.27	0.67
2:B:145:SER:OG	2:B:188:SER:OG	2.08	0.66
3:D:454:ILE:HG12	3:D:578:LEU:HD13	1.77	0.66
2:B:223:GLY:O	2:B:226:ASN:ND2	2.29	0.66
2:B:342:VAL:HG22	2:B:345:ILE:H	1.59	0.66
3:C:369:THR:H	3:C:382:SER:HA	1.60	0.66
1:A:179:THR:HG21	2:B:246:LEU:HD11	1.78	0.66
2:B:192:LEU:O	2:B:196:THR:N	2.21	0.66
1:A:69:ASP:HB3	1:A:75:ILE:HD11	1.77	0.66
3:D:420:GLN:HA	3:D:423:LEU:HD12	1.78	0.66
1:A:175:PRO:O	1:A:394:LYS:NZ	2.27	0.65
1:A:274:PRO:HG3	1:A:371:VAL:HG11	1.78	0.65
1:A:386:GLU:N	1:A:386:GLU:OE1	2.29	0.65
2:B:67:ASP:OD1	2:B:68:LEU:N	2.28	0.65
1:A:50:ASN:O	1:A:64:ARG:NH1	2.29	0.65
1:A:356:ASN:OD1	1:A:358:GLN:N	2.27	0.65
2:B:272:PRO:HA	2:B:292:GLN:NE2	2.12	0.64
2:B:273:LEU:HG	2:B:298:ASN:HD21	1.61	0.64
2:B:309:ARG:HG3	2:B:426:GLN:HG3	1.78	0.64
1:A:345:ASP:N	1:A:345:ASP:OD1	2.30	0.64
3:C:353:CYS:HA	3:C:645:ILE:HB	1.80	0.64
1:A:288:VAL:HG11	1:A:323:VAL:HG13	1.79	0.64
2:B:272:PRO:HD2	2:B:361:LEU:HD21	1.80	0.64
3:C:615:GLN:OE1	3:C:617:GLN:NE2	2.31	0.64
2:B:213:ARG:HH12	2:B:297:LYS:HG2	1.63	0.63
3:C:360:GLU:O	3:C:364:ASN:ND2	2.32	0.63
2:B:51:TYR:HB3	2:B:59:TYR:HB3	1.78	0.63
2:B:209:ASP:O	2:B:213:ARG:HG2	1.99	0.63
2:B:372:THR:O	2:B:375:GLN:NE2	2.27	0.63
3:C:420:GLN:OE1	3:C:468:TYR:OH	2.15	0.63
2:B:269:GLY:O	2:B:367:PHE:N	2.31	0.63
1:A:205:ASP:OD1	1:A:206:ASN:N	2.31	0.63
1:A:213:CYS:HA	1:A:217:LEU:HB3	1.80	0.63
1:A:173:PRO:HG2	1:A:391:LEU:HD11	1.79	0.63
3:C:437:GLY:HA2	6:C:901:ADP:H5'2	1.81	0.63
1:A:229:ARG:HD2	1:A:363:VAL:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:CYS:HA	2:B:215:LEU:HB2	1.78	0.63
2:B:139:LEU:O	2:B:184:ASN:ND2	2.33	0.62
2:B:149:THR:O	2:B:191:GLN:NE2	2.32	0.62
1:A:245:ASP:HA	1:A:249:ASN:HD21	1.65	0.62
2:B:238:THR:HG21	2:B:318:ARG:HE	1.63	0.62
3:C:640:LYS:HE3	3:C:675:ALA:HB2	1.81	0.62
1:A:119:LEU:HD23	1:A:122:ILE:HD11	1.81	0.62
3:C:351:VAL:HA	3:C:643:MET:HB2	1.82	0.61
3:C:368:CYS:HB3	3:C:651:GLN:HB2	1.82	0.61
3:C:569:GLN:HG3	3:C:682:ASN:HB2	1.82	0.61
3:D:333:MET:HG3	3:D:336:LYS:HE3	1.82	0.61
1:A:206:ASN:O	1:A:209:ILE:HG22	2.01	0.61
3:C:564:ARG:HG3	3:C:571:ILE:HG12	1.82	0.60
3:C:336:LYS:O	3:C:340:ASN:ND2	2.32	0.60
3:D:469:ARG:NH1	3:D:474:GLU:OE1	2.35	0.60
1:A:4:CYS:SG	1:A:5:ILE:N	2.74	0.60
3:C:595:GLU:HA	3:C:598:ASN:HD21	1.65	0.60
3:C:348:ASN:HD22	3:C:672:MET:HB2	1.67	0.60
1:A:224:TYR:CD2	4:A:501:GTP:C6	2.89	0.60
3:C:504:MET:HA	3:C:512:ILE:HA	1.83	0.60
1:A:415:GLU:HA	1:A:418:PHE:HD2	1.67	0.60
1:A:139:HIS:CG	1:A:150:THR:HG21	2.36	0.59
1:A:60:LYS:NZ	1:A:61:HIS:O	2.34	0.59
1:A:53:PHE:HB3	1:A:61:HIS:HB3	1.84	0.59
2:B:333:VAL:HA	2:B:336:LYS:HG2	1.85	0.59
2:B:235:GLY:HA3	2:B:366:THR:HG21	1.85	0.59
3:C:659:LYS:HA	3:C:662:ARG:HD2	1.84	0.59
1:A:413:MET:HE1	1:A:417:GLU:HG2	1.85	0.59
3:C:357:PRO:HA	3:C:404:PRO:HB3	1.85	0.58
2:B:170:VAL:HG11	2:B:377:LEU:HD21	1.86	0.58
3:C:386:GLN:OE1	3:C:390:LYS:NZ	2.29	0.58
3:D:491:ASP:HB2	3:D:500:MET:HE1	1.84	0.58
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.38	0.58
1:A:19:ALA:O	1:A:22:GLU:HG2	2.03	0.58
1:A:74:VAL:HA	1:A:77:GLU:CD	2.29	0.58
2:B:4:ILE:O	2:B:62:ARG:NH1	2.30	0.58
3:D:555:ALA:HB3	3:D:580:ASP:HB3	1.84	0.58
1:A:217:LEU:HG	1:A:219:ILE:HG12	1.84	0.58
1:A:353:VAL:HG22	1:A:355:ILE:H	1.69	0.58
1:A:259:LEU:HD21	1:A:316:CYS:HB2	1.85	0.58
1:A:414:GLU:HG2	1:A:416:GLY:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:MET:SD	2:B:196:THR:OG1	2.58	0.57
3:C:597:LYS:HD3	3:C:597:LYS:N	2.19	0.57
3:D:369:THR:HB	3:D:381:GLN:HB3	1.84	0.57
2:B:8:GLN:HG3	2:B:65:LEU:HD23	1.86	0.57
2:B:140:GLY:HA3	5:B:501:GDP:H4'	1.85	0.57
1:A:398:MET:HE1	2:B:346:PRO:HD2	1.85	0.57
3:C:350:ARG:HH22	3:C:640:LYS:HB3	1.68	0.57
3:C:481:PHE:HB2	3:C:493:LEU:HG	1.86	0.57
1:A:9:VAL:HG21	1:A:149:PHE:HD2	1.70	0.57
2:B:130:LEU:HB2	2:B:162:ARG:HD2	1.86	0.57
1:A:139:HIS:ND1	1:A:146:GLY:O	2.37	0.57
2:B:197:ASP:O	2:B:264:HIS:HB2	2.04	0.57
3:C:349:ILE:HG12	3:C:641:THR:HB	1.87	0.57
3:D:447:VAL:HG23	3:D:450:SER:H	1.70	0.56
2:B:189:VAL:HA	2:B:192:LEU:HB2	1.86	0.56
2:B:117:LEU:HA	2:B:120:VAL:HG12	1.88	0.56
2:B:272:PRO:HA	2:B:292:GLN:HE22	1.68	0.56
3:C:348:ASN:HB2	3:C:671:LYS:HA	1.87	0.56
3:C:631:LEU:HB3	3:C:634:SER:HB2	1.87	0.56
1:A:155:GLU:OE2	1:A:156:ARG:NE	2.38	0.56
2:B:8:GLN:HB2	2:B:65:LEU:HA	1.87	0.56
2:B:153:SER:HB3	2:B:191:GLN:HE21	1.71	0.56
3:C:491:ASP:HB2	3:C:500:MET:HE3	1.86	0.56
1:A:35:GLN:OE1	1:A:35:GLN:N	2.39	0.56
1:A:60:LYS:HZ2	1:A:61:HIS:C	2.13	0.56
1:A:221:ARG:HD3	2:B:322:SER:HB2	1.87	0.56
2:B:167:PHE:HA	2:B:200:TYR:HD2	1.71	0.56
3:C:503:ARG:HH22	3:C:506:LYS:HG2	1.71	0.56
3:C:577:ASN:ND2	3:C:634:SER:OG	2.39	0.56
1:A:265:ILE:HD12	1:A:432:TYR:CE1	2.41	0.55
3:D:556:VAL:HG13	3:D:579:VAL:HG22	1.88	0.55
1:A:34:GLY:O	1:A:61:HIS:N	2.35	0.55
2:B:3:GLU:HA	2:B:49:VAL:HG23	1.88	0.55
2:B:72:THR:O	2:B:75:SER:OG	2.22	0.55
3:C:408:GLN:NE2	3:C:451:VAL:O	2.40	0.55
1:A:221:ARG:NH2	2:B:323:MET:HE1	2.21	0.55
2:B:143:THR:O	2:B:147:MET:HG3	2.06	0.55
1:A:88:HIS:HB3	1:A:91:GLN:HE22	1.72	0.55
1:A:170:SER:OG	1:A:171:ILE:N	2.40	0.55
2:B:72:THR:OG1	2:B:73:MET:SD	2.64	0.55
2:B:153:SER:HB3	2:B:191:GLN:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:435:GLN:O	3:C:440:LYS:NZ	2.40	0.54
2:B:165:ASN:HA	2:B:198:GLU:HG3	1.89	0.54
3:C:597:LYS:O	3:C:601:ARG:HG2	2.08	0.54
2:B:16:ILE:HG22	2:B:226:ASN:HB2	1.90	0.54
3:C:371:THR:HG23	3:C:379:GLU:HB3	1.90	0.54
2:B:249:ASP:OD1	2:B:252:LYS:HG2	2.08	0.54
2:B:346:PRO:HG2	2:B:347:ASN:HD21	1.73	0.54
1:A:111:GLY:C	1:A:113:GLU:H	2.15	0.54
2:B:47:ILE:HG12	2:B:51:TYR:HB2	1.90	0.54
1:A:200:CYS:HA	1:A:266:HIS:HB2	1.89	0.54
1:A:317:LEU:HB3	1:A:319:TYR:CE1	2.38	0.54
2:B:268:PRO:HG2	2:B:300:MET:HG3	1.90	0.54
3:C:502:ILE:HD13	3:C:630:LEU:HD13	1.90	0.53
1:A:118:VAL:O	1:A:122:ILE:HG23	2.09	0.53
2:B:36:TYR:HB2	2:B:59:TYR:HE2	1.73	0.53
1:A:217:LEU:HD11	1:A:367:ASP:HB2	1.89	0.53
1:A:409:VAL:HG23	3:C:601:ARG:HH22	1.74	0.53
3:C:440:LYS:O	3:C:443:THR:OG1	2.24	0.53
3:C:557:THR:HB	3:C:578:LEU:HB2	1.89	0.53
3:D:599:ILE:HG22	3:D:601:ARG:H	1.73	0.53
1:A:3:GLU:HG2	1:A:51:THR:HA	1.91	0.53
1:A:172:TYR:HB2	1:A:203:MET:HE3	1.89	0.53
3:C:432:ALA:HA	3:C:644:PHE:HB2	1.91	0.53
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.37	0.53
3:D:336:LYS:HD3	3:D:424:ASP:CG	2.33	0.53
1:A:27:GLU:OE2	1:A:243:ARG:NE	2.42	0.53
1:A:212:ILE:HG13	1:A:302:MET:HE1	1.89	0.53
1:A:324:VAL:HG21	1:A:326:LYS:HE2	1.90	0.53
2:B:314:ALA:HB3	2:B:368:ILE:HB	1.90	0.53
2:B:141:GLY:HA3	5:B:501:GDP:O3A	2.07	0.53
1:A:195:LEU:HD11	1:A:264:ARG:HB3	1.91	0.53
3:C:552:ARG:HB2	3:C:599:ILE:HD11	1.91	0.53
3:D:502:ILE:HB	3:D:629:HIS:HD2	1.74	0.53
2:B:12:CYS:SG	5:B:501:GDP:C4	3.02	0.52
3:D:559:LEU:HB2	3:D:576:ILE:HB	1.90	0.52
2:B:118:ASP:OD1	2:B:119:VAL:N	2.41	0.52
1:A:99:ALA:O	1:A:105:ARG:HD3	2.09	0.52
1:A:298:PRO:O	1:A:301:GLN:NE2	2.36	0.52
1:A:101:ASN:HD22	1:A:144:GLY:N	2.07	0.52
2:B:147:MET:SD	2:B:148:GLY:N	2.83	0.52
2:B:330:MET:HA	2:B:333:VAL:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:380:LEU:HD22	3:D:661:LEU:HD12	1.90	0.52
1:A:222:PRO:HD2	2:B:324:LYS:NZ	2.25	0.52
2:B:16:ILE:HG22	2:B:226:ASN:CB	2.40	0.52
2:B:170:VAL:HG11	2:B:377:LEU:HD11	1.92	0.52
1:A:154:MET:HE2	1:A:194:THR:HG23	1.92	0.51
3:C:615:GLN:O	3:C:616:LYS:HG3	2.10	0.51
1:A:70:LEU:HB3	1:A:97:GLU:O	2.10	0.51
1:A:323:VAL:HB	1:A:355:ILE:HD11	1.93	0.51
3:C:554:HIS:CE1	3:C:582:ALA:H	2.29	0.51
3:C:372:TYR:HE2	3:C:403:HIS:HA	1.75	0.51
1:A:80:THR:HA	1:A:84:ARG:HH21	1.74	0.51
1:A:188:ILE:HG23	1:A:189:LEU:HD23	1.92	0.51
1:A:175:PRO:HB3	1:A:390:ARG:CZ	2.40	0.51
2:B:12:CYS:HB2	5:B:501:GDP:C8	2.45	0.51
2:B:318:ARG:HH11	2:B:358:PRO:HG3	1.76	0.51
1:A:213:CYS:SG	1:A:222:PRO:HG3	2.51	0.51
1:A:212:ILE:HD11	1:A:300:ASN:HA	1.92	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.50
2:B:217:LEU:HA	2:B:276:ARG:HH21	1.74	0.50
2:B:46:ARG:NH1	2:B:46:ARG:O	2.44	0.50
2:B:49:VAL:O	2:B:62:ARG:NH1	2.19	0.50
2:B:46:ARG:NH2	2:B:241:ARG:HA	2.26	0.50
2:B:91:VAL:HB	2:B:116:VAL:HG12	1.94	0.50
1:A:74:VAL:O	1:A:77:GLU:HG2	2.10	0.50
2:B:25:SER:OG	2:B:30:ILE:O	2.29	0.50
2:B:338:SER:HA	2:B:341:PHE:HB3	1.94	0.50
2:B:299:MET:HE2	2:B:301:ALA:H	1.77	0.50
1:A:185:TYR:O	1:A:189:LEU:HG	2.10	0.50
1:A:322:ASP:N	1:A:322:ASP:OD1	2.42	0.50
2:B:69:GLU:N	2:B:69:GLU:OE1	2.45	0.50
2:B:107:THR:O	2:B:110:ALA:N	2.33	0.50
2:B:150:LEU:O	2:B:153:SER:OG	2.26	0.50
1:A:69:ASP:OD1	1:A:70:LEU:N	2.45	0.50
2:B:100:ASN:OD1	2:B:103:LYS:N	2.37	0.50
2:B:188:SER:O	2:B:192:LEU:HD23	2.12	0.50
3:C:340:ASN:HA	3:C:343:MET:HE2	1.93	0.50
1:A:209:ILE:HD11	1:A:230:LEU:HD13	1.93	0.50
3:D:504:MET:HA	3:D:512:ILE:HD12	1.94	0.50
1:A:335:ILE:HA	1:A:338:LYS:HG2	1.93	0.49
2:B:317:PHE:H	2:B:365:VAL:HG23	1.76	0.49
1:A:327:ASP:OD1	1:A:328:VAL:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:GLY:H	5:B:501:GDP:PA	2.35	0.49
3:C:504:MET:HG3	3:C:509:LYS:HD2	1.95	0.49
2:B:171:PRO:O	2:B:380:ARG:NH2	2.46	0.49
3:C:633:PRO:HA	3:C:637:GLY:HA3	1.94	0.49
1:A:24:TYR:HA	1:A:27:GLU:HG2	1.94	0.49
1:A:172:TYR:HE2	1:A:390:ARG:HH22	1.61	0.49
2:B:187:LEU:HD11	2:B:408:PHE:CZ	2.47	0.49
2:B:427:ASP:OD1	2:B:428:ALA:N	2.45	0.49
3:D:396:PHE:HD1	3:D:665:ALA:HB2	1.78	0.49
3:C:579:VAL:HG21	3:C:631:LEU:HD11	1.94	0.49
3:D:552:ARG:NH2	3:D:585:GLU:O	2.43	0.49
1:A:387:ALA:HA	1:A:390:ARG:HG2	1.95	0.49
3:C:590:SER:O	3:C:591:THR:HG23	2.12	0.49
3:C:454:ILE:HG12	3:C:578:LEU:HD13	1.95	0.49
1:A:20:CYS:SG	1:A:235:VAL:HG21	2.53	0.49
1:A:431:ASP:HA	1:A:434:GLU:HG2	1.95	0.49
2:B:11:GLN:NE2	5:B:501:GDP:O3A	2.45	0.49
2:B:73:MET:SD	2:B:73:MET:N	2.86	0.49
2:B:179:VAL:HG22	2:B:180:VAL:HG22	1.95	0.49
2:B:181:GLU:HG2	2:B:182:PRO:HD3	1.95	0.49
3:D:349:ILE:HG23	3:D:643:MET:HE1	1.95	0.49
2:B:20:PHE:CE1	2:B:24:ILE:HD11	2.48	0.49
3:C:438:SER:HB2	3:C:646:ASN:HB3	1.94	0.49
2:B:311:LEU:HD12	2:B:342:VAL:HG11	1.95	0.48
3:D:556:VAL:HG22	3:D:579:VAL:HG13	1.96	0.48
1:A:35:GLN:HB3	1:A:59:GLY:O	2.13	0.48
1:A:113:GLU:N	1:A:113:GLU:OE1	2.46	0.48
1:A:139:HIS:NE2	1:A:170:SER:HB2	2.28	0.48
2:B:265:PHE:HB2	2:B:422:TYR:OH	2.13	0.48
3:C:605:GLU:HG3	3:C:625:SER:HB3	1.95	0.48
1:A:33:ASP:HB2	1:A:35:GLN:HE22	1.79	0.48
1:A:245:ASP:OD1	1:A:245:ASP:N	2.44	0.48
1:A:317:LEU:O	1:A:354:GLY:N	2.36	0.48
3:C:552:ARG:HE	3:C:595:GLU:CD	2.21	0.48
1:A:66:VAL:HG22	1:A:68:VAL:HG23	1.96	0.48
2:B:205:GLU:HA	2:B:208:TYR:HB2	1.96	0.48
3:C:565:HIS:O	3:C:569:GLN:N	2.46	0.48
2:B:226:ASN:HD22	2:B:227:HIS:N	2.12	0.48
2:B:287:PRO:HA	2:B:329:GLN:NE2	2.25	0.48
3:C:461:LEU:O	3:C:465:ILE:HG12	2.13	0.48
2:B:291:GLN:HA	2:B:294:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD21	1:A:418:PHE:CE1	2.49	0.47
1:A:246:GLY:H	1:A:249:ASN:ND2	2.12	0.47
1:A:121:ARG:HA	1:A:121:ARG:HH11	1.78	0.47
3:C:559:LEU:HB2	3:C:576:ILE:HB	1.96	0.47
3:D:329:PHE:HB3	3:D:471:LEU:HD13	1.95	0.47
2:B:52:ASN:HD21	2:B:62:ARG:HE	1.62	0.47
2:B:154:LYS:O	2:B:157:GLU:HG2	2.15	0.47
2:B:245:GLN:NE2	2:B:355:ASP:OD2	2.42	0.47
3:D:347:GLY:O	3:D:349:ILE:N	2.45	0.47
2:B:176:SER:OG	2:B:181:GLU:OE2	2.25	0.47
2:B:193:VAL:HG21	2:B:418:LEU:HD21	1.95	0.47
1:A:367:ASP:OD1	1:A:368:LEU:N	2.47	0.47
2:B:6:HIS:CD2	2:B:8:GLN:HE21	2.32	0.47
1:A:154:MET:HE1	1:A:197:HIS:HB2	1.97	0.47
1:A:211:ASP:HB3	1:A:215:ARG:NH2	2.29	0.47
1:A:288:VAL:HG21	1:A:327:ASP:CG	2.40	0.47
2:B:238:THR:HA	2:B:241:ARG:HG2	1.97	0.47
2:B:323:MET:H	2:B:323:MET:CE	2.26	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.47
1:A:234:ILE:HD13	1:A:270:ALA:HB1	1.97	0.47
2:B:30:ILE:HG13	2:B:51:TYR:CE2	2.50	0.47
3:C:458:VAL:HG21	3:C:529:ARG:HH22	1.80	0.47
1:A:34:GLY:HA3	1:A:60:LYS:HD2	1.97	0.47
2:B:31:ASP:HB2	2:B:37:HIS:HD2	1.79	0.47
2:B:132:GLY:HA3	2:B:163:ILE:O	2.14	0.47
1:A:66:VAL:HA	1:A:91:GLN:HB3	1.98	0.46
1:A:169:PHE:CE1	1:A:202:PHE:HD2	2.33	0.46
2:B:203:ASP:HB3	2:B:205:GLU:OE1	2.15	0.46
1:A:240:ALA:O	1:A:244:PHE:N	2.47	0.46
2:B:20:PHE:HA	2:B:230:SER:HB2	1.96	0.46
2:B:285:THR:HG23	2:B:287:PRO:HD2	1.97	0.46
2:B:94:GLN:N	2:B:108:GLU:OE2	2.42	0.46
2:B:317:PHE:HB3	2:B:321:MET:HE2	1.97	0.46
1:A:25:CYS:HA	1:A:30:ILE:HB	1.98	0.46
1:A:318:LEU:O	1:A:375:VAL:HA	2.15	0.46
1:A:417:GLU:HA	1:A:420:GLU:HB2	1.96	0.46
2:B:217:LEU:HA	2:B:276:ARG:NH2	2.31	0.46
1:A:4:CYS:HB2	1:A:133:GLN:HB2	1.98	0.46
1:A:225:THR:HB	1:A:229:ARG:HH21	1.81	0.46
2:B:35:THR:HA	2:B:57:GLY:O	2.15	0.46
2:B:178:THR:HG22	2:B:180:VAL:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:GLY:HA3	2:B:373:ALA:HB2	1.98	0.46
3:C:357:PRO:HD2	6:C:901:ADP:N6	2.30	0.46
3:C:542:ALA:C	3:C:549:ARG:HD3	2.40	0.46
3:C:573:VAL:HB	3:C:678:ASN:HD21	1.80	0.46
1:A:35:GLN:HA	1:A:61:HIS:CE1	2.51	0.46
2:B:161:ASP:OD2	2:B:162:ARG:NH1	2.49	0.46
3:C:408:GLN:C	3:C:456:ARG:HH12	2.22	0.46
3:D:433:TYR:HB3	3:D:645:ILE:HD13	1.98	0.46
2:B:348:ASN:OD1	2:B:348:ASN:N	2.39	0.46
1:A:222:PRO:HD2	2:B:324:LYS:HE2	1.98	0.46
3:D:418:LEU:HD11	3:D:642:LEU:HD13	1.97	0.46
3:C:435:GLN:OE1	3:C:435:GLN:N	2.49	0.45
1:A:164:LYS:HA	1:A:164:LYS:HD3	1.75	0.45
1:A:388:TRP:CD1	1:A:432:TYR:HE2	2.34	0.45
2:B:334:GLN:OE1	2:B:335:ASN:ND2	2.49	0.45
1:A:3:GLU:HB2	1:A:129:CYS:SG	2.55	0.45
3:C:350:ARG:NH2	3:C:640:LYS:HB3	2.30	0.45
1:A:91:GLN:HG3	1:A:121:ARG:NH2	2.30	0.45
2:B:2:ARG:H	2:B:129:CYS:HB3	1.81	0.45
2:B:11:GLN:CD	2:B:11:GLN:H	2.25	0.45
2:B:89:ASN:O	2:B:91:VAL:HG23	2.16	0.45
2:B:237:THR:OG1	2:B:241:ARG:NH1	2.50	0.45
2:B:165:ASN:OD1	2:B:165:ASN:N	2.48	0.45
2:B:375:GLN:H	2:B:375:GLN:CD	2.22	0.45
1:A:334:THR:O	1:A:337:THR:OG1	2.24	0.45
2:B:135:LEU:O	2:B:137:HIS:HD2	1.99	0.45
1:A:378:LEU:HD13	1:A:378:LEU:HA	1.83	0.45
1:A:401:LYS:HA	1:A:401:LYS:HD3	1.70	0.45
2:B:321:MET:SD	2:B:321:MET:N	2.89	0.45
2:B:343:GLU:OE1	2:B:343:GLU:N	2.31	0.45
3:C:388:LYS:HE3	3:C:388:LYS:HB3	1.76	0.45
3:C:562:ILE:HG22	3:C:573:VAL:HG22	1.98	0.45
1:A:132:LEU:HB3	1:A:164:LYS:HE2	1.99	0.45
2:B:180:VAL:HG12	2:B:183:TYR:HB2	1.99	0.45
2:B:232:THR:O	2:B:236:VAL:HG23	2.17	0.45
3:C:443:THR:OG1	3:C:444:MET:SD	2.75	0.45
3:D:629:HIS:HA	3:D:632:MET:HE2	1.99	0.45
1:A:166:LYS:N	1:A:199:ASP:OD2	2.50	0.45
2:B:299:MET:HE1	2:B:303:CYS:O	2.17	0.45
1:A:70:LEU:HA	1:A:95:GLY:HA3	1.99	0.45
1:A:142:GLY:HA2	1:A:186:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:THR:HA	2:B:83:GLN:HE22	1.81	0.45
2:B:290:THR:O	2:B:293:VAL:HG12	2.17	0.45
1:A:181:VAL:HB	2:B:350:LYS:HE2	1.98	0.44
1:A:246:GLY:H	1:A:249:ASN:HD21	1.65	0.44
3:C:354:ARG:HG3	3:C:402:PHE:HB2	1.99	0.44
1:A:268:PRO:HB3	1:A:380:ASN:HB2	1.99	0.44
2:B:86:ARG:HD3	2:B:86:ARG:HA	1.65	0.44
2:B:309:ARG:HE	2:B:341:PHE:H	1.64	0.44
3:D:378:VAL:HG12	3:D:398:PHE:HE2	1.83	0.44
1:A:69:ASP:CG	1:A:71:GLU:H	2.25	0.44
1:A:246:GLY:H	1:A:249:ASN:CG	2.25	0.44
3:C:356:ARG:HG2	3:C:438:SER:O	2.17	0.44
3:C:362:GLU:HB2	3:C:650:PHE:CZ	2.52	0.44
3:C:485:LYS:HZ1	3:C:552:ARG:HG3	1.82	0.44
1:A:19:ALA:HA	1:A:22:GLU:CD	2.42	0.44
1:A:21:TRP:CE3	1:A:24:TYR:HD2	2.35	0.44
1:A:360:PRO:HG3	1:A:374:ALA:HB3	2.00	0.44
3:C:356:ARG:NH1	3:C:359:LEU:HG	2.32	0.44
3:C:463:ASP:O	3:C:466:ARG:HG2	2.18	0.44
1:A:214:ARG:O	1:A:218:ASP:HA	2.17	0.44
1:A:422:ARG:HH12	1:A:426:ALA:HB2	1.81	0.44
2:B:228:LEU:HD22	2:B:300:MET:HE1	2.00	0.44
3:C:422:ALA:HB2	3:C:428:ILE:HG13	2.00	0.44
3:D:474:GLU:N	3:D:564:ARG:O	2.44	0.44
1:A:54:SER:HB2	1:A:62:VAL:HG13	1.99	0.44
1:A:411:GLU:HA	3:C:597:LYS:HZ1	1.83	0.44
2:B:178:THR:N	2:B:181:GLU:OE1	2.49	0.44
1:A:9:VAL:HG13	1:A:139:HIS:HB3	1.99	0.44
1:A:288:VAL:HG13	1:A:373:ARG:NH1	2.33	0.44
1:A:398:MET:CE	2:B:346:PRO:HD2	2.48	0.44
2:B:382:SER:O	2:B:386:THR:HG22	2.18	0.44
3:C:361:SER:HA	3:C:364:ASN:HD21	1.82	0.44
3:C:408:GLN:HB3	3:C:456:ARG:NH1	2.33	0.44
1:A:222:PRO:HD2	2:B:324:LYS:CE	2.48	0.43
1:A:186:ASN:O	1:A:190:THR:HG22	2.17	0.43
1:A:407:TRP:CZ2	2:B:255:VAL:HA	2.52	0.43
2:B:262:ARG:NH2	2:B:417:ASP:OD2	2.51	0.43
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.99	0.43
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.86	0.43
2:B:323:MET:O	2:B:326:VAL:HG22	2.19	0.43
3:C:503:ARG:HG2	3:C:504:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ALA:HB1	2:B:144:GLY:HA2	2.00	0.43
2:B:271:ALA:HB3	2:B:365:VAL:HG12	1.99	0.43
2:B:77:ARG:HH12	2:B:92:PHE:HE2	1.65	0.43
3:C:670:CYS:SG	3:C:671:LYS:N	2.92	0.43
1:A:399:TYR:OH	1:A:402:ARG:NH2	2.52	0.43
2:B:146:GLY:O	2:B:149:THR:OG1	2.31	0.43
3:C:473:TRP:HB3	3:C:475:TYR:HE1	1.84	0.43
1:A:381:THR:HG23	1:A:383:ALA:H	1.83	0.43
3:C:416:SER:HB2	3:C:417:PRO:HD3	1.99	0.43
1:A:121:ARG:HH12	1:A:124:LYS:HD2	1.84	0.43
1:A:221:ARG:HA	1:A:221:ARG:HD2	1.84	0.43
1:A:422:ARG:NH2	1:A:423:GLU:HA	2.34	0.43
2:B:404:ASP:O	2:B:407:GLU:HG2	2.19	0.43
1:A:98:ASP:OD1	1:A:99:ALA:N	2.51	0.42
1:A:181:VAL:H	2:B:350:LYS:HZ1	1.66	0.42
1:A:328:VAL:O	1:A:332:ILE:HG22	2.19	0.42
2:B:172:SER:HA	2:B:203:ASP:OD1	2.19	0.42
2:B:211:CYS:SG	2:B:220:PRO:HB3	2.59	0.42
2:B:286:VAL:HB	2:B:363:MET:HE3	2.00	0.42
3:C:444:MET:HE3	3:C:580:ASP:HB3	2.00	0.42
1:A:101:ASN:HD22	1:A:144:GLY:H	1.66	0.42
1:A:119:LEU:HD11	1:A:156:ARG:HG2	2.01	0.42
2:B:244:GLY:N	2:B:247:ASN:OD1	2.52	0.42
1:A:125:LEU:HD13	1:A:125:LEU:HA	1.81	0.42
2:B:45:ASP:OD2	2:B:46:ARG:HG2	2.18	0.42
2:B:167:PHE:CE2	2:B:233:MET:HG2	2.54	0.42
3:C:442:TYR:O	3:C:446:GLY:HA2	2.19	0.42
3:D:383:ILE:H	3:D:651:GLN:HE22	1.67	0.42
3:D:481:PHE:HD1	3:D:493:LEU:HD11	1.84	0.42
2:B:215:LEU:HB3	2:B:217:LEU:HD23	2.00	0.42
1:A:156:ARG:HD3	1:A:156:ARG:HA	1.81	0.42
2:B:203:ASP:HB3	2:B:205:GLU:CD	2.44	0.42
2:B:296:ALA:O	2:B:299:MET:HG2	2.19	0.42
3:C:429:CYS:HA	3:C:577:ASN:HB2	2.01	0.42
3:C:486:ASN:O	3:C:486:ASN:ND2	2.52	0.42
3:D:663:PHE:O	3:D:666:SER:OG	2.24	0.42
1:A:91:GLN:HG3	1:A:121:ARG:HH21	1.85	0.42
1:A:139:HIS:CE1	1:A:170:SER:HB2	2.54	0.42
1:A:222:PRO:HG2	2:B:324:LYS:HZ1	1.84	0.42
1:A:311:LYS:HD2	1:A:343:PHE:O	2.20	0.42
2:B:105:HIS:CE1	2:B:150:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:THR:N	5:B:501:GDP:O3B	2.46	0.42
2:B:308:GLY:HA2	2:B:426:GLN:NE2	2.35	0.42
3:C:391:MET:SD	3:C:658:VAL:HG11	2.59	0.42
3:C:503:ARG:C	3:C:512:ILE:HG23	2.45	0.42
3:C:562:ILE:O	3:C:564:ARG:NH1	2.53	0.42
3:D:440:LYS:HE3	3:D:440:LYS:HB2	1.89	0.42
2:B:12:CYS:SG	5:B:501:GDP:N3	2.93	0.42
2:B:142:GLY:HA2	2:B:184:ASN:OD1	2.19	0.42
2:B:262:ARG:O	2:B:264:HIS:N	2.53	0.42
3:D:376:SER:HB2	3:D:398:PHE:O	2.20	0.42
3:D:502:ILE:HB	3:D:629:HIS:CD2	2.52	0.42
1:A:120:ASP:O	1:A:123:ARG:HG2	2.20	0.42
1:A:145:THR:HG22	4:A:501:GTP:O2B	2.20	0.42
1:A:270:ALA:HA	1:A:378:LEU:HD13	2.00	0.42
1:A:388:TRP:HD1	1:A:432:TYR:HE2	1.68	0.42
2:B:6:HIS:CG	2:B:21:TRP:HZ2	2.38	0.42
2:B:244:GLY:H	2:B:247:ASN:HD21	1.68	0.42
3:C:480:THR:HB	3:C:517:ILE:HG12	2.02	0.42
3:C:482:LEU:HD21	3:C:489:LEU:HD23	2.02	0.42
3:C:573:VAL:HB	3:C:678:ASN:ND2	2.35	0.42
1:A:75:ILE:HG23	1:A:92:LEU:HD22	2.01	0.42
1:A:332:ILE:HG12	1:A:351:PHE:HB2	2.01	0.42
2:B:251:ARG:O	2:B:255:VAL:HG22	2.20	0.42
3:C:465:ILE:HD12	3:C:475:TYR:HB2	2.02	0.42
1:A:227:LEU:O	1:A:231:ILE:HG12	2.20	0.42
1:A:252:LEU:O	1:A:255:PHE:HB2	2.20	0.42
1:A:195:LEU:HD12	1:A:266:HIS:NE2	2.35	0.41
3:C:645:ILE:HG22	3:C:647:VAL:HG23	2.01	0.41
1:A:139:HIS:ND1	1:A:140:SER:O	2.53	0.41
1:A:234:ILE:O	1:A:238:ILE:HG13	2.19	0.41
1:A:246:GLY:HA2	1:A:357:TYR:CD1	2.55	0.41
2:B:240:LEU:HB2	2:B:249:ASP:HA	2.02	0.41
2:B:363:MET:HE2	2:B:363:MET:HB2	1.76	0.41
1:A:76:ASP:O	1:A:80:THR:HG23	2.20	0.41
1:A:319:TYR:HB2	1:A:355:ILE:HA	2.02	0.41
1:A:337:THR:O	1:A:339:ARG:NH2	2.53	0.41
2:B:72:THR:O	2:B:76:VAL:HG23	2.19	0.41
2:B:309:ARG:NH1	2:B:343:GLU:OE1	2.53	0.41
1:A:116:ASP:OD1	1:A:116:ASP:N	2.54	0.41
1:A:196:GLU:OE1	1:A:196:GLU:N	2.38	0.41
1:A:246:GLY:N	1:A:249:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:HG3	1:A:300:ASN:HB2	2.01	0.41
3:C:379:GLU:HB2	3:C:395:ILE:HB	2.02	0.41
3:C:608:ASN:O	3:C:611:LEU:HG	2.21	0.41
3:D:543:SER:N	3:D:550:SER:HB3	2.34	0.41
1:A:175:PRO:HB3	1:A:390:ARG:NE	2.36	0.41
2:B:12:CYS:HB2	5:B:501:GDP:N9	2.35	0.41
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.81	0.41
1:A:402:ARG:O	1:A:405:VAL:HG22	2.21	0.41
2:B:385:PHE:CD1	2:B:412:GLU:HG3	2.55	0.41
3:C:458:VAL:HG11	3:C:529:ARG:HH12	1.86	0.41
1:A:90:GLU:HG3	1:A:121:ARG:CZ	2.51	0.41
3:C:366:MET:HG3	3:C:651:GLN:HB3	2.02	0.41
3:C:465:ILE:HD13	3:C:465:ILE:HA	1.87	0.41
2:B:118:ASP:OD1	2:B:118:ASP:N	2.53	0.41
2:B:374:ILE:HB	2:B:422:TYR:CE2	2.56	0.41
1:A:10:GLY:O	1:A:14:VAL:HG12	2.21	0.41
1:A:75:ILE:HA	1:A:78:VAL:HG22	2.02	0.41
1:A:141:PHE:HB2	1:A:173:PRO:HD3	2.03	0.41
2:B:13:GLY:O	2:B:16:ILE:HG12	2.21	0.41
2:B:179:VAL:HG13	2:B:180:VAL:HG23	2.03	0.41
2:B:226:ASN:HD22	2:B:227:HIS:H	1.68	0.41
3:C:435:GLN:HE22	3:C:648:SER:H	1.69	0.41
3:C:511:ASP:N	3:C:511:ASP:OD1	2.53	0.41
3:D:665:ALA:HA	3:D:668:ASN:ND2	2.36	0.41
1:A:290:GLU:OE2	1:A:291:ILE:HG23	2.21	0.41
1:A:330:ALA:O	1:A:334:THR:HG23	2.22	0.41
2:B:299:MET:SD	2:B:305:PRO:HD3	2.61	0.41
3:C:621:PRO:HB2	3:C:624:ASN:ND2	2.36	0.41
2:B:279:GLN:HA	2:B:282:ARG:NH1	2.36	0.40
3:C:441:THR:O	3:C:446:GLY:N	2.37	0.40
3:D:462:PHE:HZ	3:D:522:VAL:HG12	1.86	0.40
3:D:565:HIS:CD2	3:D:568:LYS:HB3	2.56	0.40
2:B:91:VAL:HG11	2:B:115:SER:O	2.21	0.40
2:B:211:CYS:O	2:B:217:LEU:HB2	2.21	0.40
2:B:226:ASN:HB3	5:B:501:GDP:HN1	1.85	0.40
2:B:106:TYR:HA	2:B:110:ALA:HB2	2.04	0.40
2:B:154:LYS:HA	2:B:154:LYS:HD3	1.95	0.40
2:B:217:LEU:HD13	2:B:276:ARG:NH2	2.37	0.40
3:D:333:MET:O	3:D:336:LYS:HG3	2.21	0.40
1:A:407:TRP:CZ2	2:B:255:VAL:HG12	2.56	0.40
2:B:73:MET:HE2	2:B:73:MET:HB2	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:GLU:CG	2:B:182:PRO:HD3	2.51	0.40
3:C:428:ILE:O	3:C:577:ASN:N	2.53	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	424/451 (94%)	393 (93%)	31 (7%)	0	100	100
2	B	426/444 (96%)	386 (91%)	40 (9%)	0	100	100
3	C	351/409 (86%)	332 (95%)	19 (5%)	0	100	100
3	D	330/409 (81%)	321 (97%)	9 (3%)	0	100	100
All	All	1531/1713 (89%)	1432 (94%)	99 (6%)	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	360/379 (95%)	342 (95%)	18 (5%)	20	44
2	B	366/379 (97%)	345 (94%)	21 (6%)	17	41
3	C	324/370 (88%)	322 (99%)	2 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	301/370 (81%)	300 (100%)	1 (0%)	91	92
All	All	1351/1498 (90%)	1309 (97%)	42 (3%)	37	56

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	26	LEU
1	A	62	VAL
1	A	66	VAL
1	A	70	LEU
1	A	77	GLU
1	A	88	HIS
1	A	94	THR
1	A	114	ILE
1	A	125	LEU
1	A	137	VAL
1	A	145	THR
1	A	177	VAL
1	A	260	VAL
1	A	286	LEU
1	A	320	ARG
1	A	345	ASP
1	A	353	VAL
2	B	44	LEU
2	B	45	ASP
2	B	60	VAL
2	B	152	ILE
2	B	163	ILE
2	B	166	THR
2	B	179	VAL
2	B	180	VAL
2	B	208	TYR
2	B	226	ASN
2	B	228	LEU
2	B	252	LYS
2	B	274	THR
2	B	322	SER
2	B	325	GLU
2	B	328	GLU
2	B	348	ASN
2	B	351	THR

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Mol	Chain	Res	Type
2	B	353	VAL
2	B	394	PHE
2	B	418	LEU
3	C	395	ILE
3	C	591	THR
3	D	471	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	133	GLN
1	A	192	HIS
2	B	8	GLN
2	B	83	GLN
2	B	131	GLN
2	B	191	GLN
2	B	226	ASN
2	B	298	ASN
3	C	332	ASN
3	C	348	ASN
3	C	364	ASN
3	C	470	ASN
3	C	554	HIS
3	C	577	ASN
3	D	394	GLN
3	D	495	ASN
3	D	629	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
6	ADP	C	901	8	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
4	GTP	A	501	-	26,34,34	1.16	3 (11%)	32,54,54	1.93	8 (25%)
8	ALF	C	903	6	0,4,4	-	-	-	-	-
5	GDP	B	501	-	24,30,30	1.08	2 (8%)	30,47,47	1.83	8 (26%)
6	ADP	D	802	7	24,29,29	0.97	1 (4%)	29,45,45	1.49	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	B	501	-	-	5/12/32/32	0/3/3/3
6	ADP	C	901	8	-	4/12/32/32	0/3/3/3
4	GTP	A	501	-	-	7/18/38/38	0/3/3/3
6	ADP	D	802	7	-	3/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GTP	C5-C6	-3.14	1.41	1.47
4	A	501	GTP	C2-N3	2.69	1.39	1.33
5	B	501	GDP	C6-N1	-2.56	1.34	1.37
6	D	802	ADP	C5-C4	2.51	1.47	1.40
4	A	501	GTP	C5-C4	-2.40	1.36	1.43
6	C	901	ADP	C5-C4	2.39	1.47	1.40
5	B	501	GDP	C2'-C1'	-2.05	1.50	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C3'-C2'-C1'	6.23	110.35	100.98
4	A	501	GTP	C2-N1-C6	-5.12	115.67	125.10
4	A	501	GTP	C5-C6-N1	4.83	122.48	113.95
4	A	501	GTP	C8-N7-C5	4.09	110.78	102.99
6	C	901	ADP	C3'-C2'-C1'	3.85	106.78	100.98
4	A	501	GTP	PB-O3B-PG	-3.67	120.22	132.83
6	D	802	ADP	C3'-C2'-C1'	3.59	106.38	100.98
6	D	802	ADP	PA-O3A-PB	-3.47	120.91	132.83
4	A	501	GTP	PA-O3A-PB	-3.30	121.51	132.83
6	D	802	ADP	N3-C2-N1	-3.22	123.64	128.68
6	C	901	ADP	N3-C2-N1	-3.05	123.90	128.68
6	C	901	ADP	C4-C5-N7	-3.01	106.27	109.40
6	C	901	ADP	PA-O3A-PB	-2.95	122.70	132.83
5	B	501	GDP	O6-C6-C5	-2.91	118.69	124.37
5	B	501	GDP	C5-C6-N1	2.88	119.04	113.95
5	B	501	GDP	PA-O3A-PB	-2.85	123.03	132.83
6	D	802	ADP	C4-C5-N7	-2.66	106.63	109.40
5	B	501	GDP	O4'-C1'-C2'	-2.57	103.18	106.93
4	A	501	GTP	O6-C6-C5	-2.55	119.39	124.37
4	A	501	GTP	C2'-C3'-C4'	2.25	107.01	102.64
5	B	501	GDP	C8-N7-C5	2.25	107.27	102.99
5	B	501	GDP	C2-N1-C6	-2.16	121.12	125.10
4	A	501	GTP	O6-C6-N1	-2.13	118.14	120.65
5	B	501	GDP	O3B-PB-O3A	2.01	111.38	104.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

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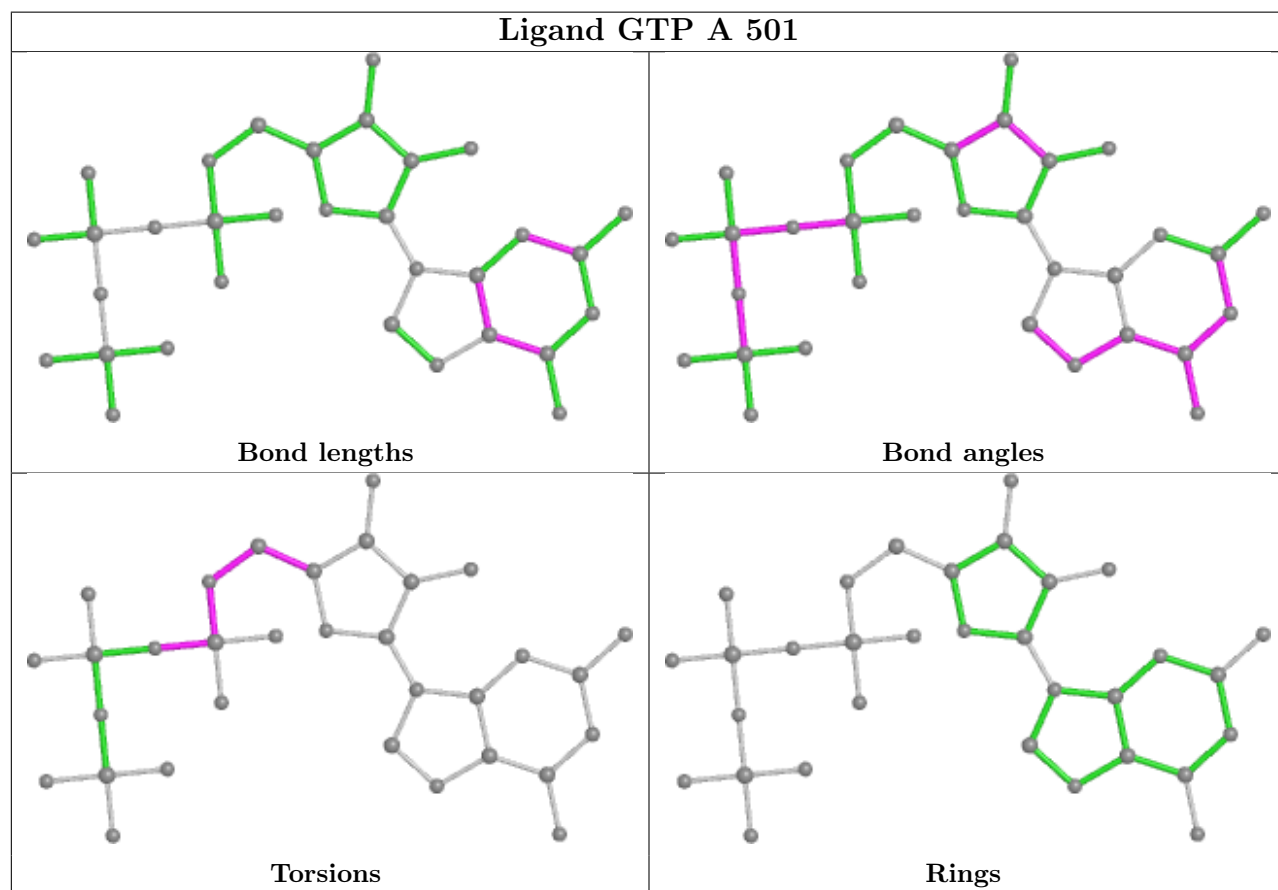
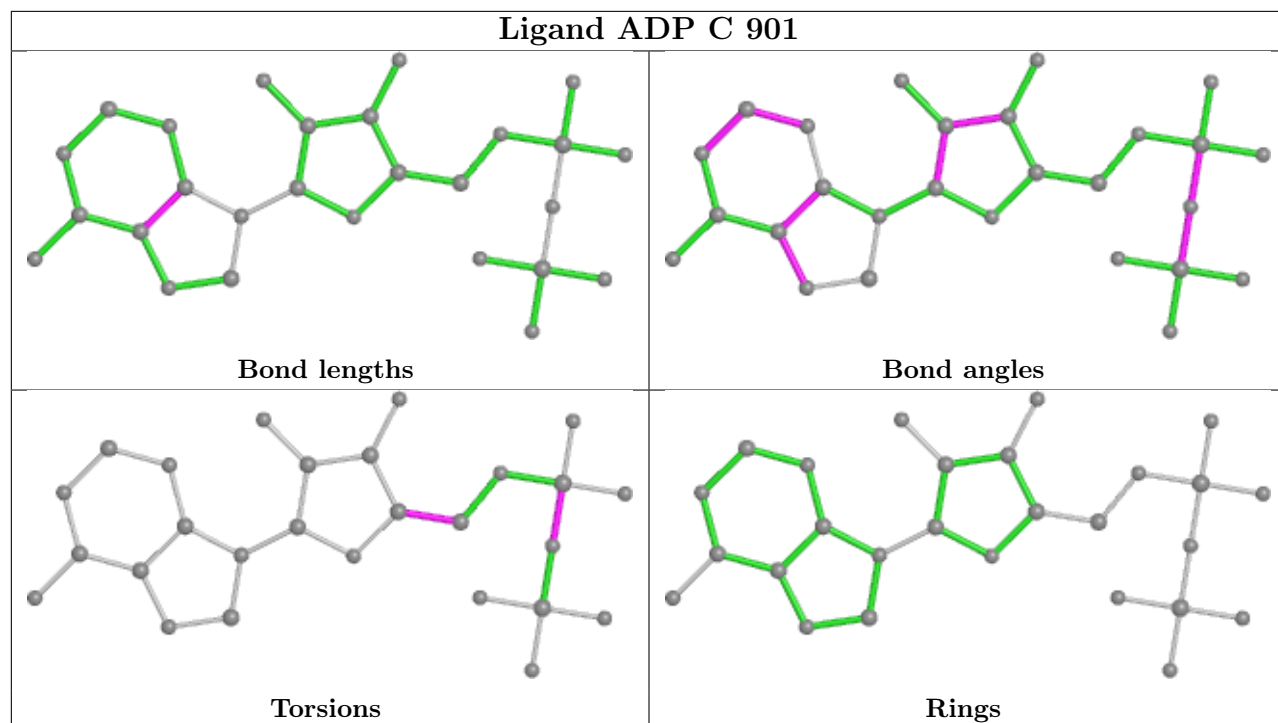
Mol	Chain	Res	Type	Atoms
6	D	802	ADP	C5'-O5'-PA-O1A
4	A	501	GTP	PB-O3A-PA-O1A
6	C	901	ADP	PB-O3A-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O3A
6	D	802	ADP	C5'-O5'-PA-O2A

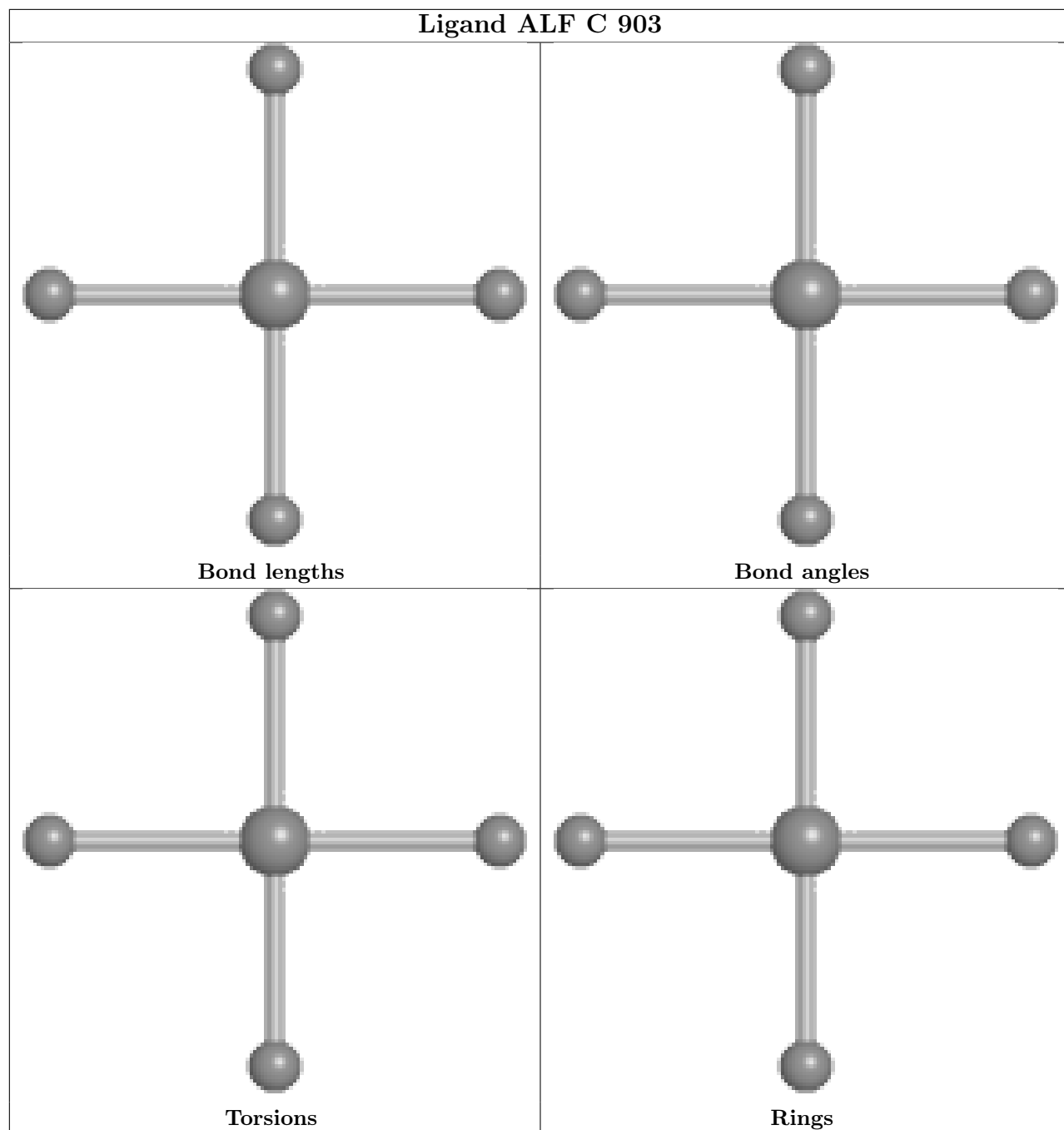
There are no ring outliers.

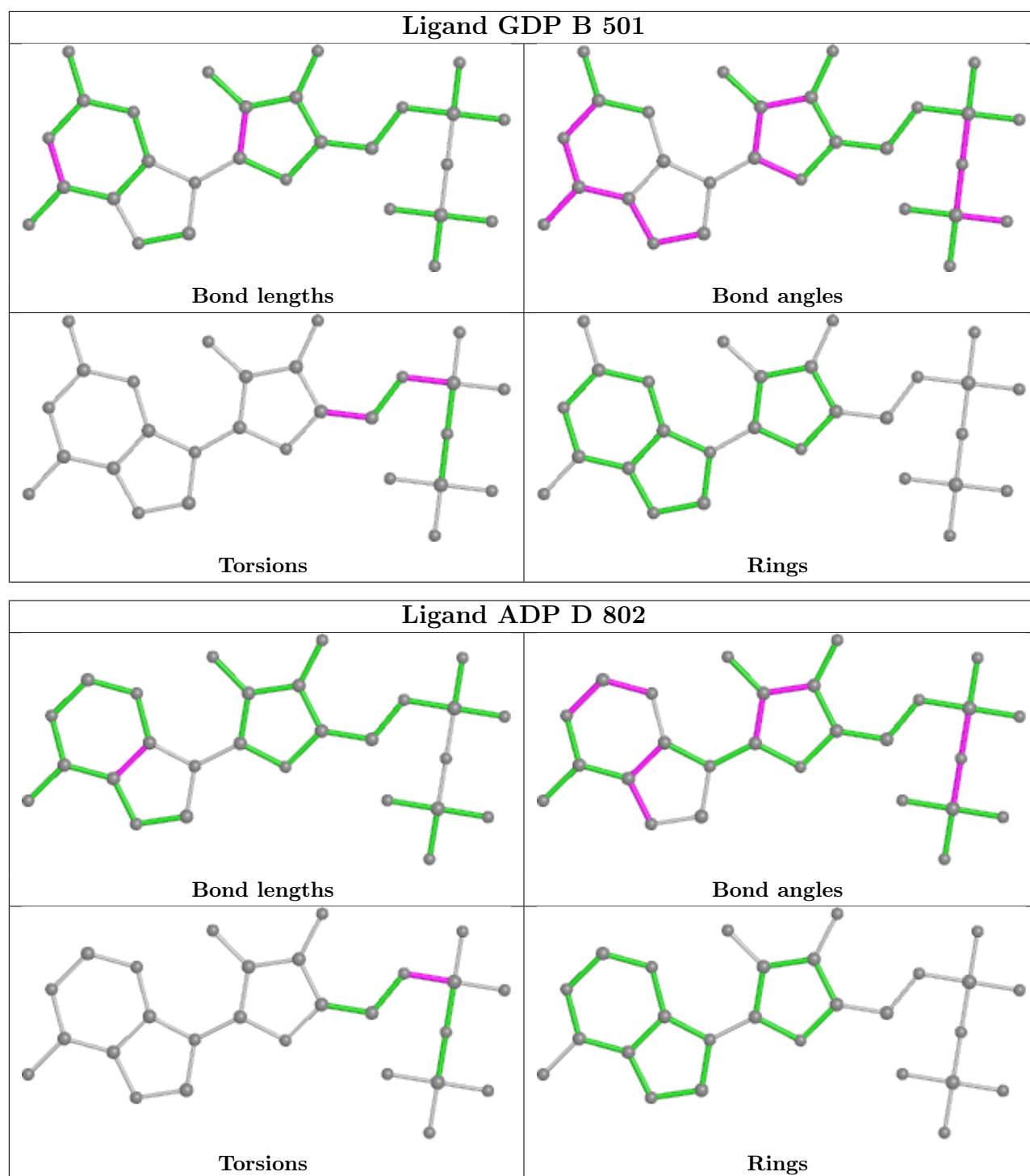
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	901	ADP	4	0
4	A	501	GTP	2	0
8	C	903	ALF	1	0
5	B	501	GDP	10	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

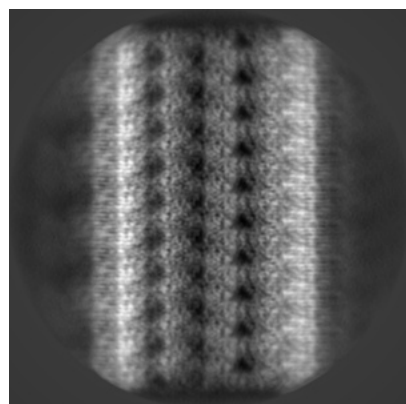
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39666. These allow visual inspection of the internal detail of the map and identification of artifacts.

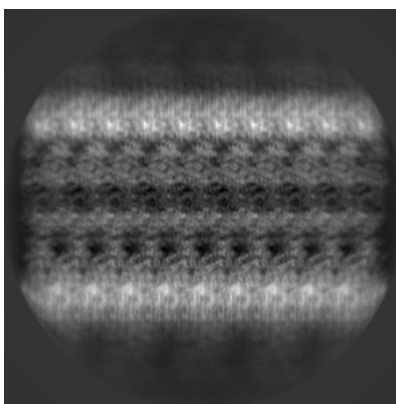
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

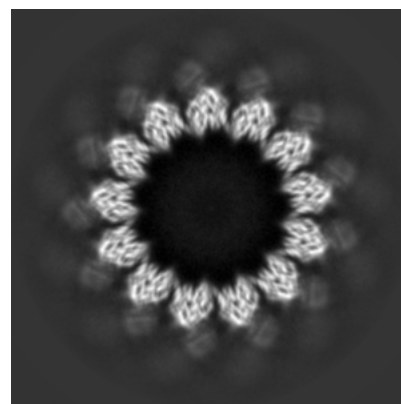
6.1.1 Primary map



X

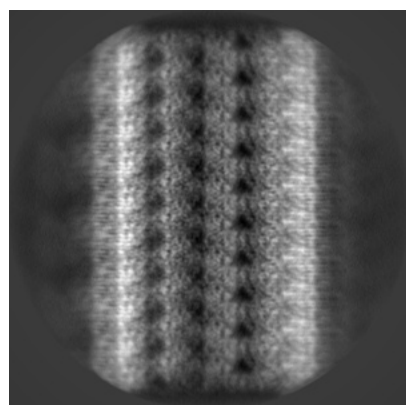


Y

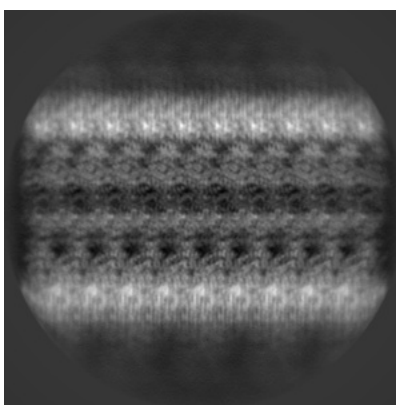


Z

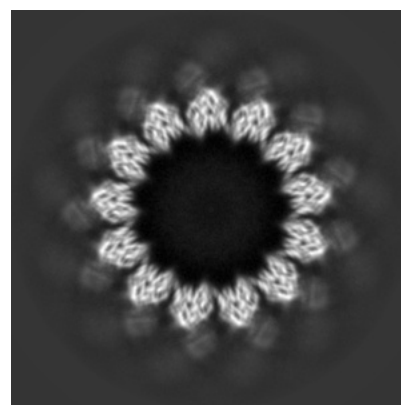
6.1.2 Raw map



X



Y

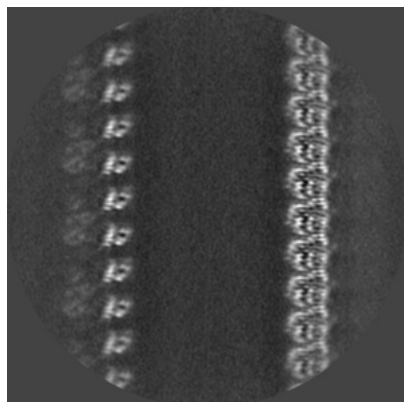


Z

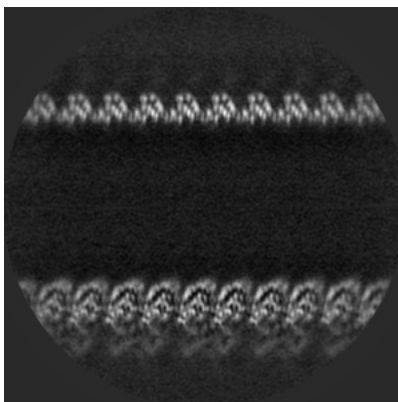
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

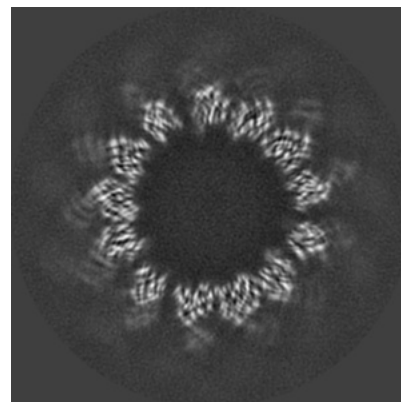
6.2.1 Primary map



X Index: 300

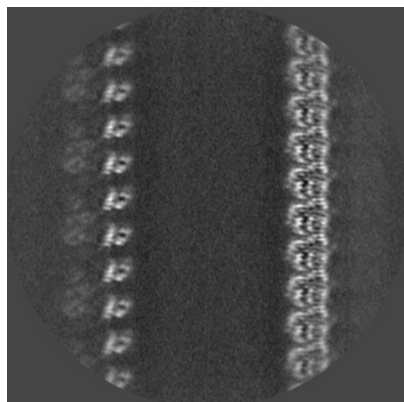


Y Index: 300

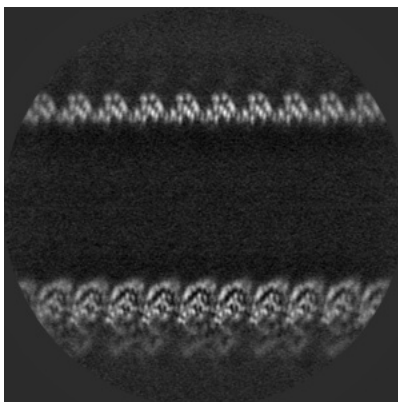


Z Index: 300

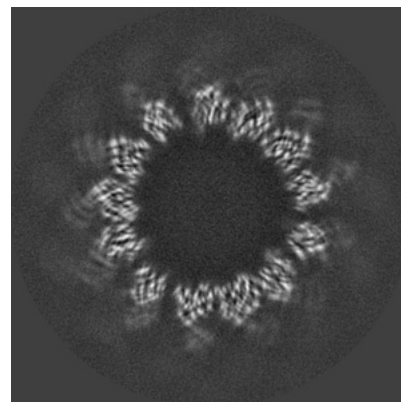
6.2.2 Raw map



X Index: 300



Y Index: 300

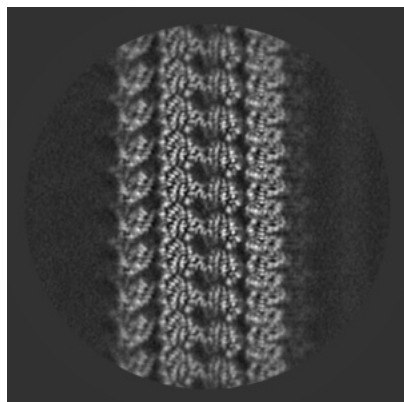


Z Index: 300

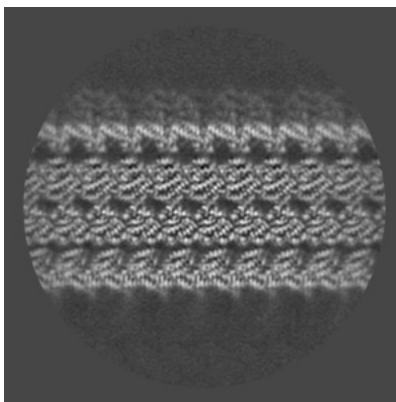
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

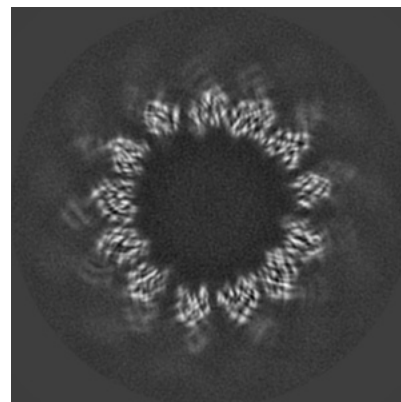
6.3.1 Primary map



X Index: 426

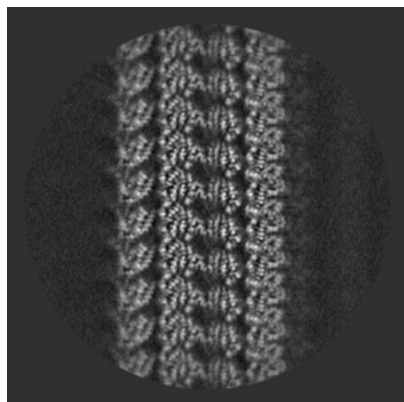


Y Index: 169

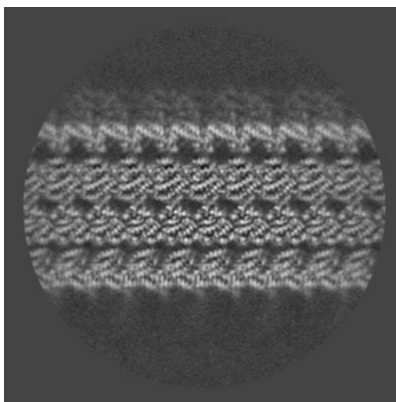


Z Index: 292

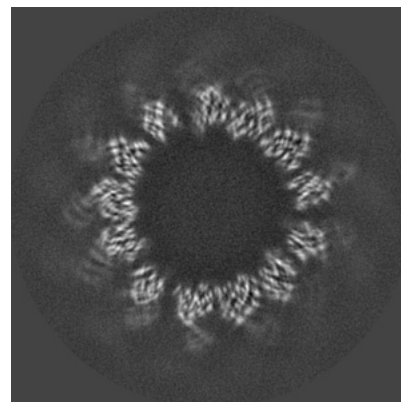
6.3.2 Raw map



X Index: 425



Y Index: 169

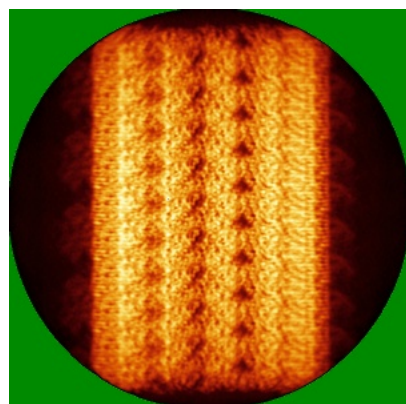


Z Index: 298

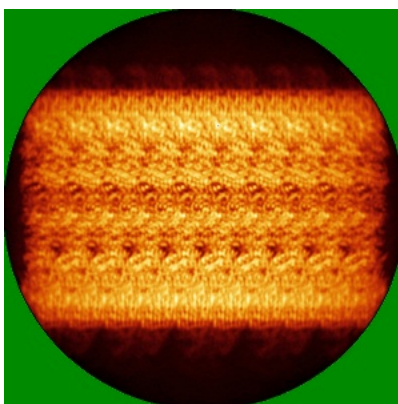
The images above show the largest variance slices of the map in three orthogonal directions.

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

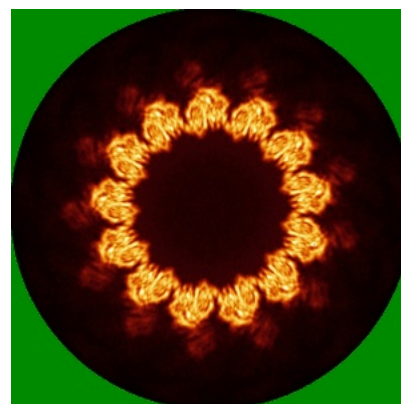
6.4.1 Primary map



X

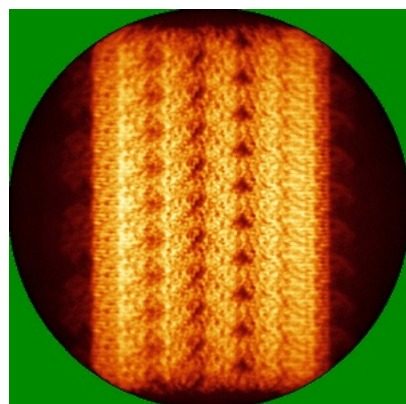


Y

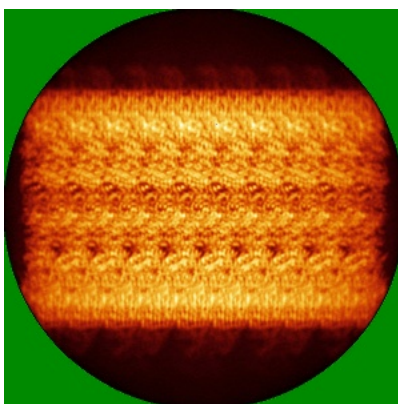


Z

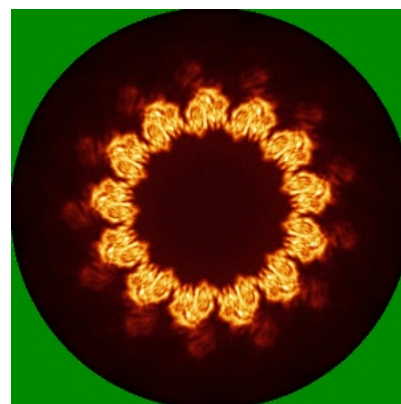
6.4.2 Raw map



X



Y

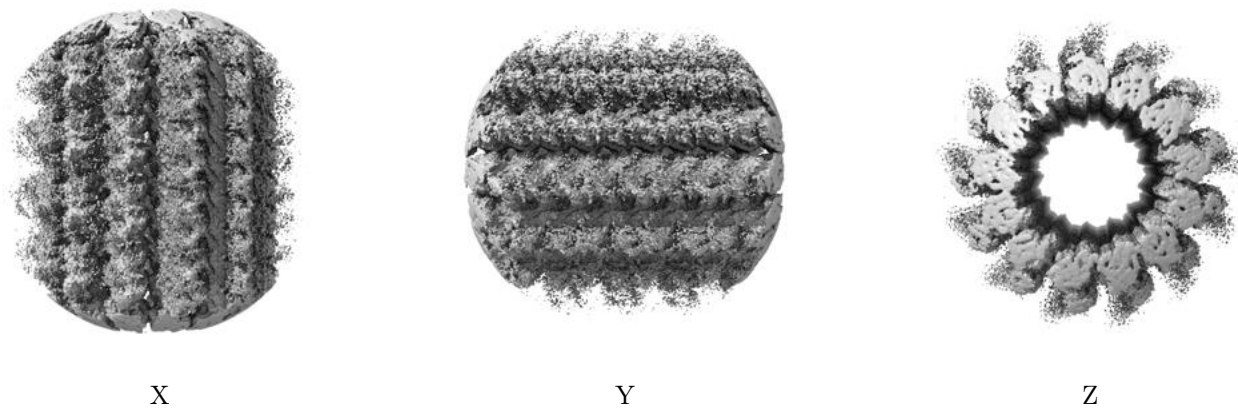


Z

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.

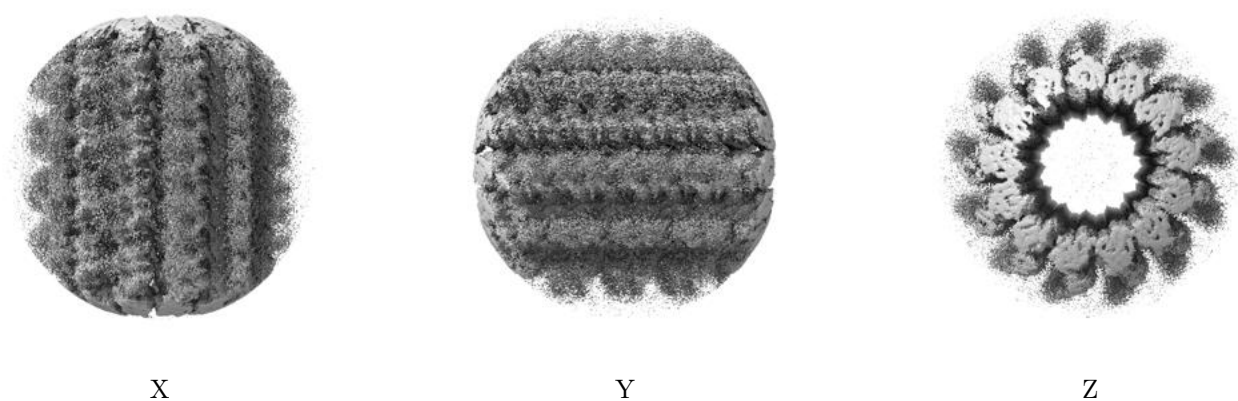
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0005. 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.

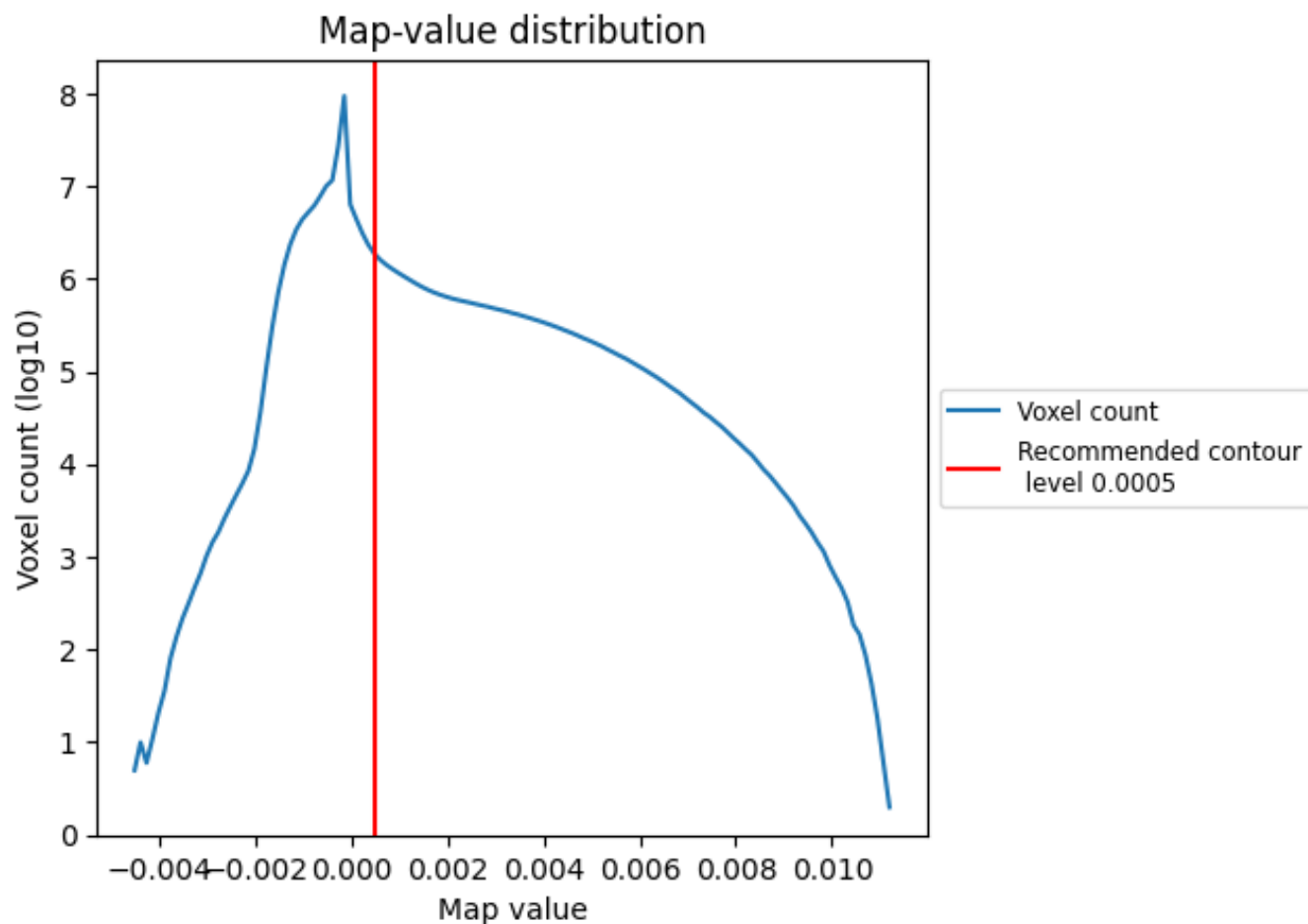
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

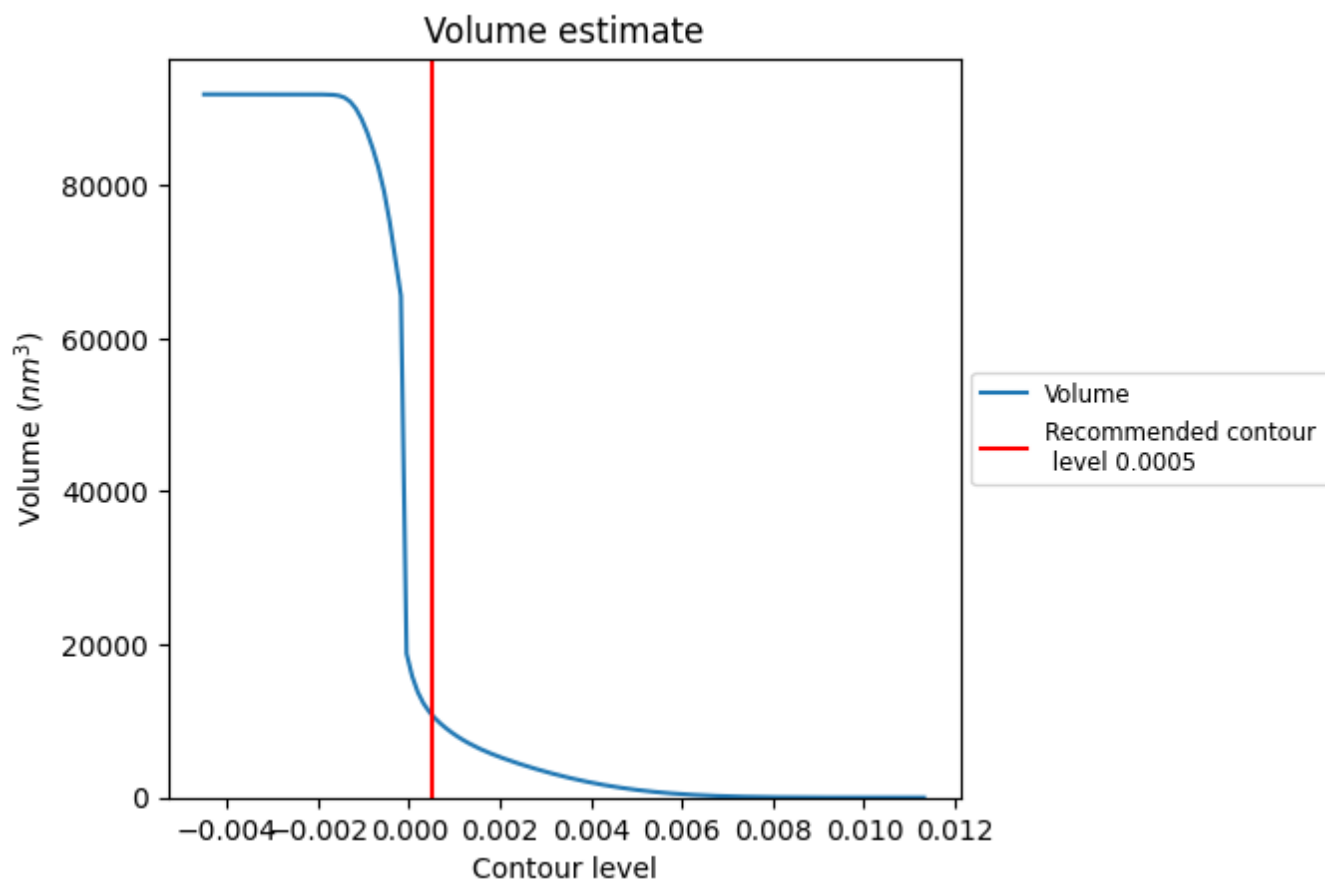
This section contains the results of statistical analysis of the map.

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.

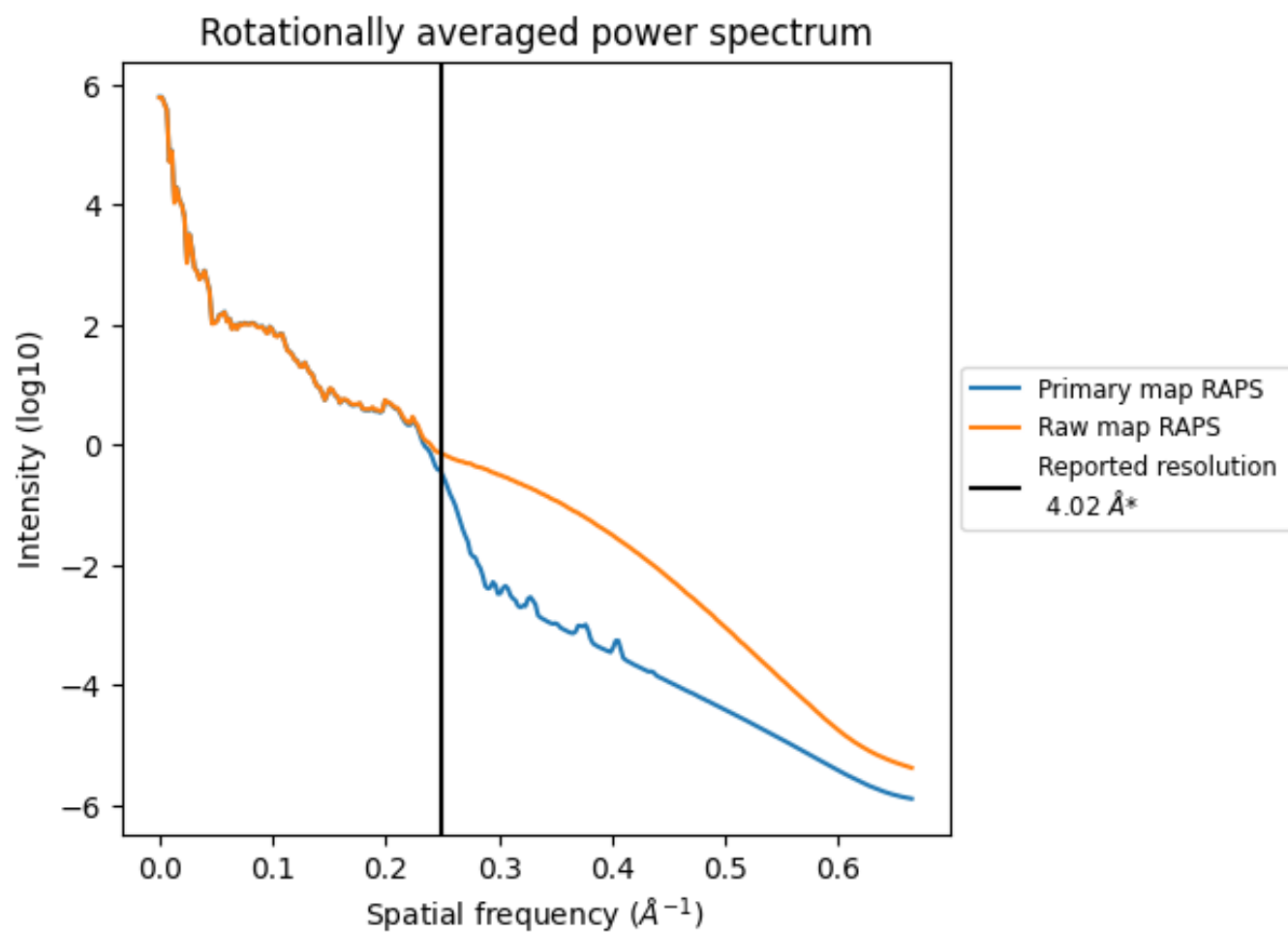
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10864 nm^3 ; this corresponds to an approximate mass of 9813 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](#)

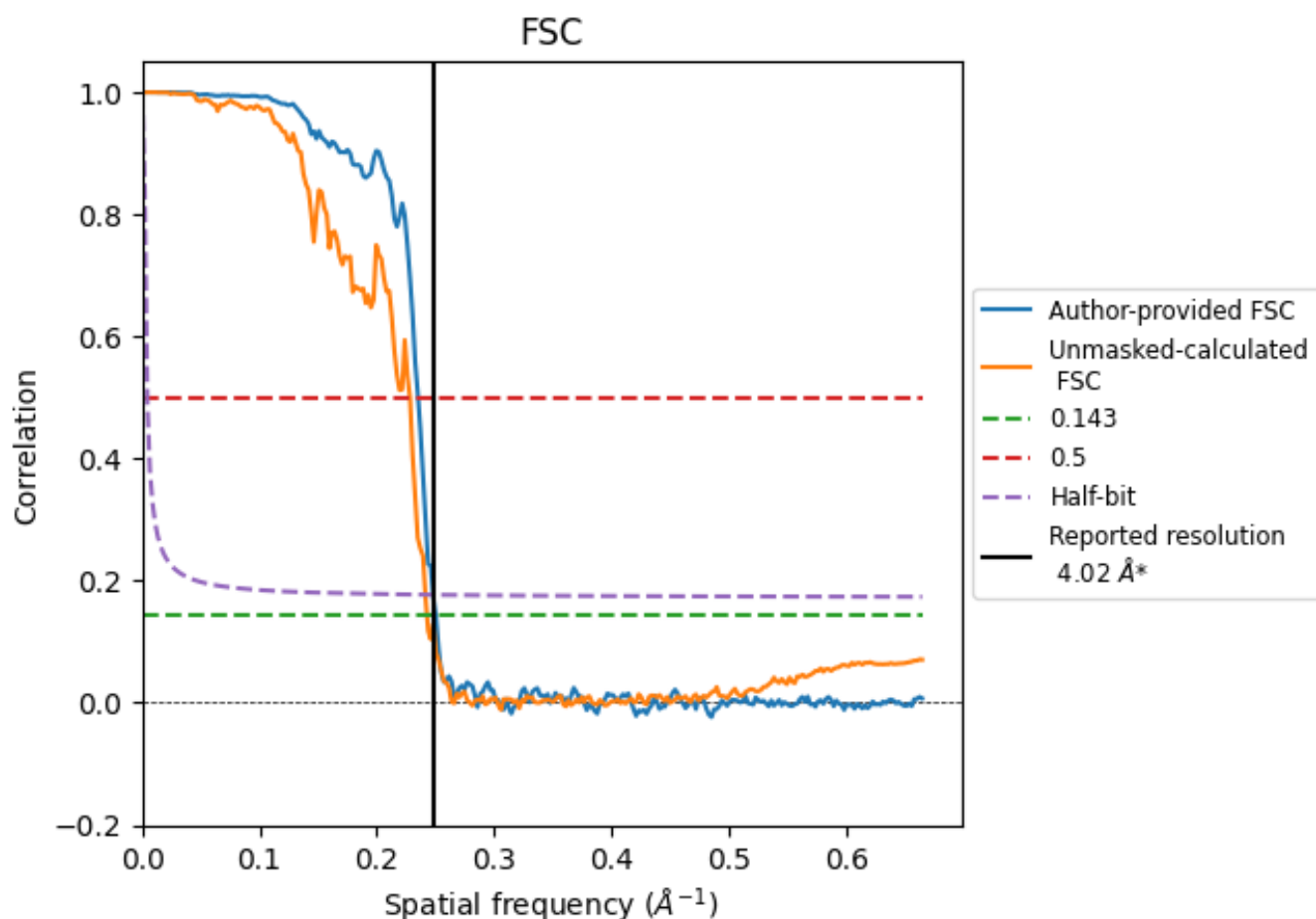


*Reported resolution corresponds to spatial frequency of 0.249 \AA^{-1}

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 0.249 \AA^{-1}

8.2 Resolution estimates [i](#)

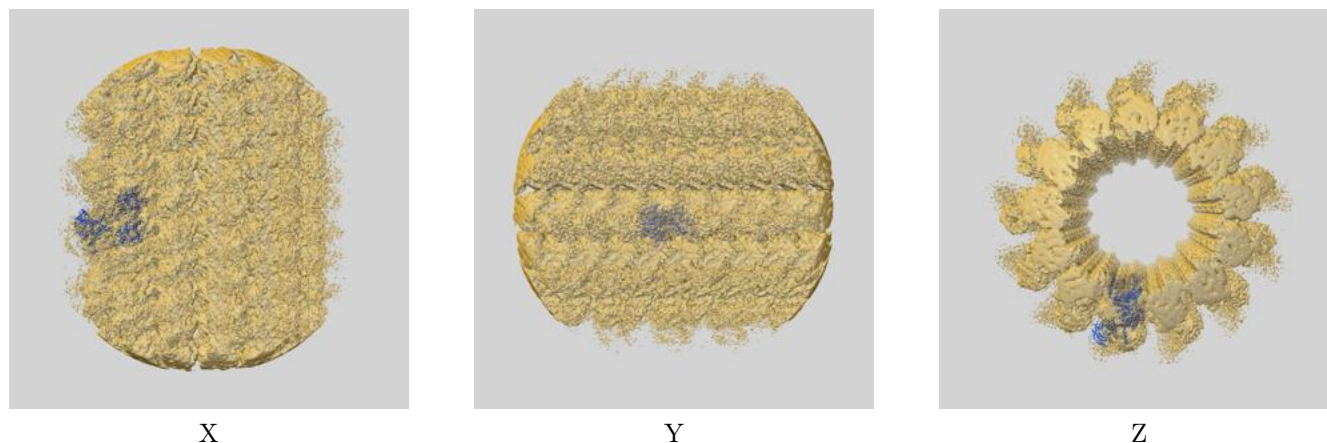
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.02	-	-
Author-provided FSC curve	4.00	4.25	4.03
Unmasked-calculated*	4.12	4.38	4.14

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

9 Map-model fit [i](#)

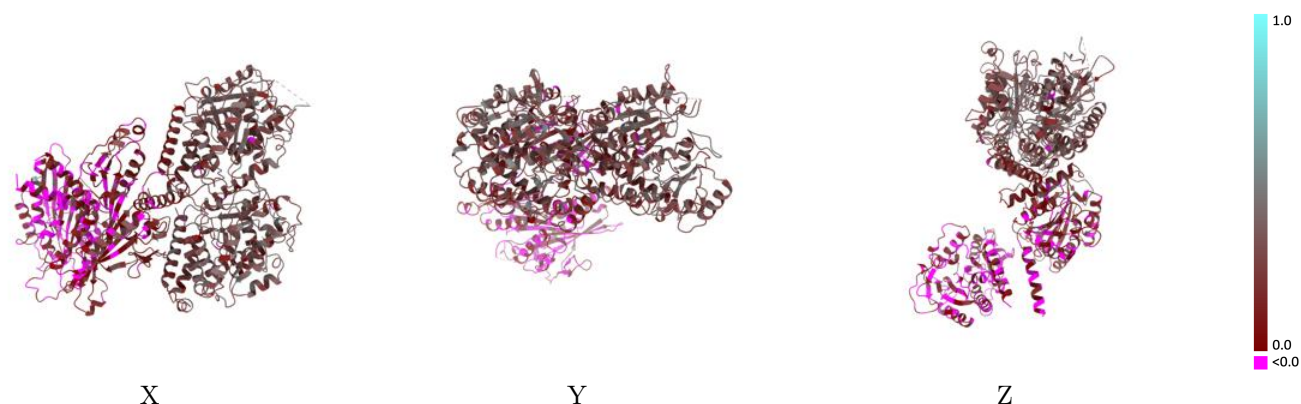
This section contains information regarding the fit between EMDB map EMD-39666 and PDB model 8YY4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



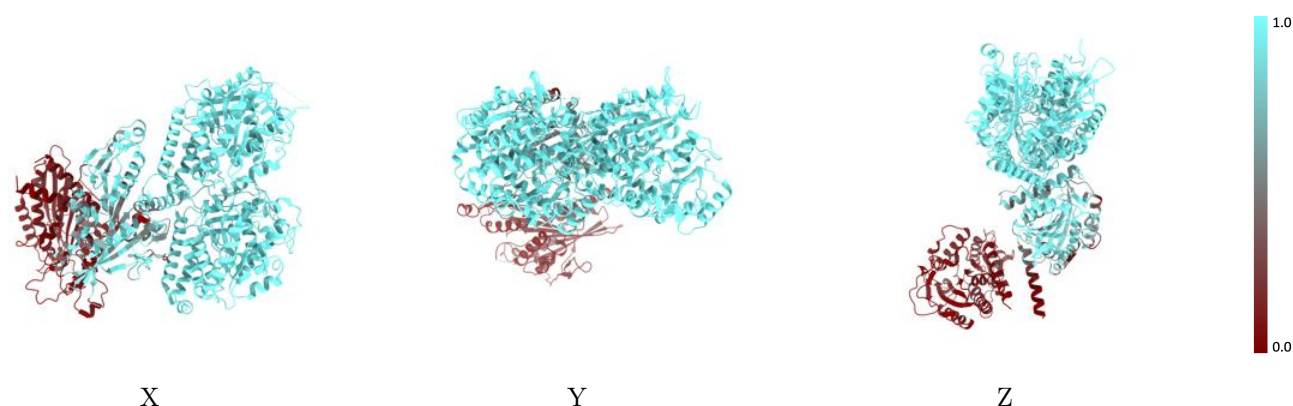
The images above show the 3D surface view of the map at the recommended contour level 0.0005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



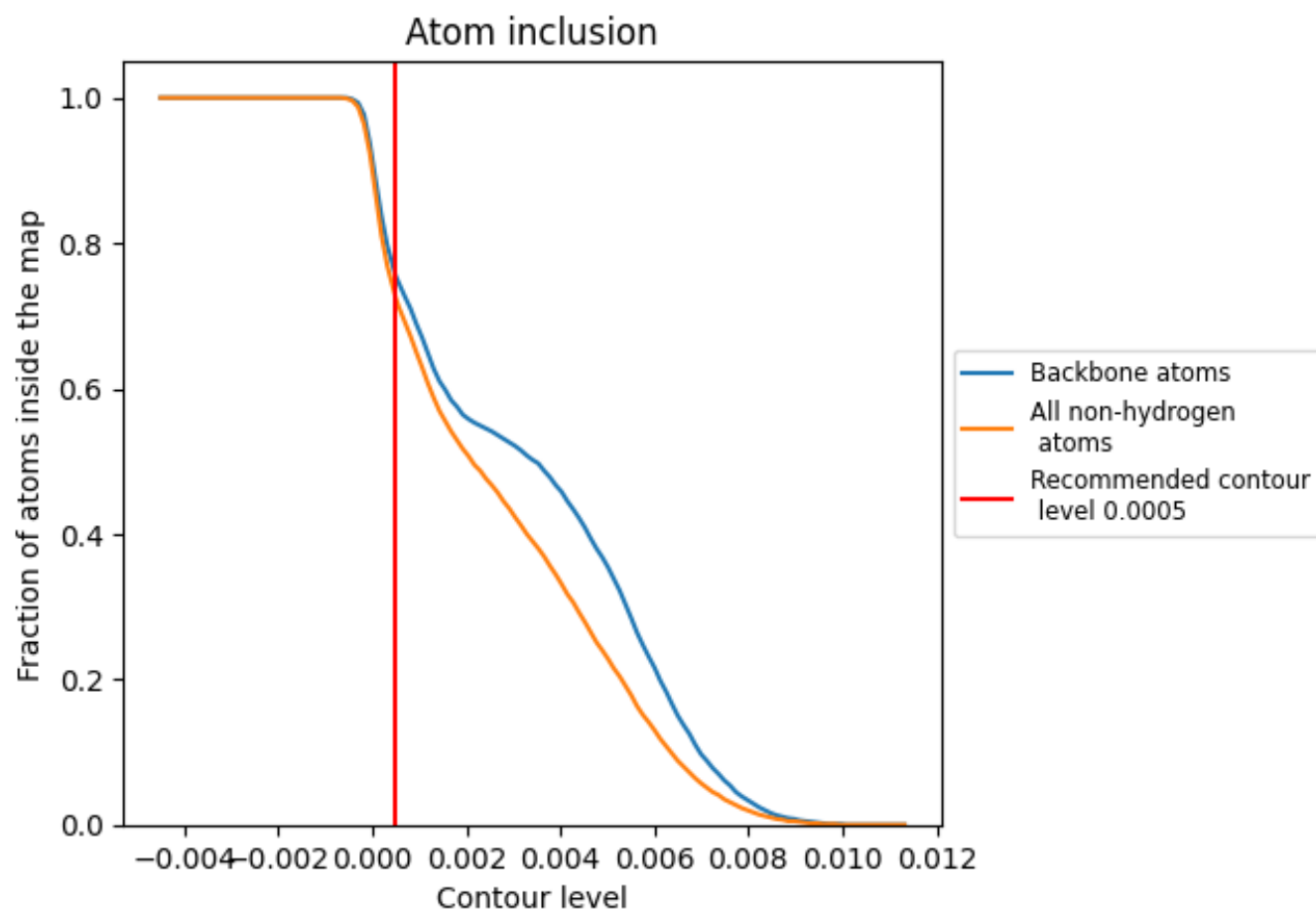
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.0005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7250	<div></div> 0.2040
A	<div></div> 0.9910	<div></div> 0.3120
B	<div></div> 0.9930	<div></div> 0.3110
C	<div></div> 0.7480	<div></div> 0.1240
D	<div></div> 0.0290	<div></div> 0.0200

