



Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 09:27 am BST

PDB ID : 7Z6H / pdb_00007z6h
EMDB ID : EMD-14527
Title : Structure of DNA-bound human RAD17-RFC clamp loader and 9-1-1 checkpoint clamp
Authors : Day, M.; Oliver, A.W.; Pearl, L.H.
Deposited on : 2022-03-11
Resolution : 3.59 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

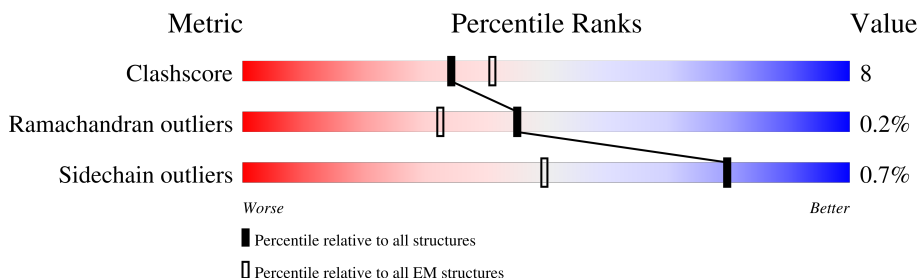
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.59 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	405	
2	B	1021	
2	K	1021	
3	C	280	
4	D	363	
5	E	356	
6	F	354	
7	G	360	

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Mol	Chain	Length	Quality of chain
8	X	77	<div><div><div></div><div></div><div></div></div><div>19%9%71%</div></div>
8	Y	77	<div><div><div></div><div></div><div></div></div><div>10%87%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20629 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 Cell cycle checkpoint control protein RAD9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	247	Total	C	N	O	S	0	0
			1911	1222	333	340	16		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	THR	-	expression tag	UNP Q99638
A	393	SER	-	expression tag	UNP Q99638
A	394	ALA	-	expression tag	UNP Q99638
A	395	GLY	-	expression tag	UNP Q99638
A	396	SER	-	expression tag	UNP Q99638
A	397	ARG	-	expression tag	UNP Q99638
A	398	HIS	-	expression tag	UNP Q99638
A	399	HIS	-	expression tag	UNP Q99638
A	400	HIS	-	expression tag	UNP Q99638
A	401	HIS	-	expression tag	UNP Q99638
A	402	HIS	-	expression tag	UNP Q99638
A	403	HIS	-	expression tag	UNP Q99638
A	404	HIS	-	expression tag	UNP Q99638
A	405	HIS	-	expression tag	UNP Q99638

- Molecule 2 is a protein called Cell cycle checkpoint protein RAD1,Cell cycle checkpoint protein RAD17.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	260	Total	C	N	O	S	0	0
			2049	1301	337	393	18		
2	K	439	Total	C	N	O	S	0	0
			3518	2249	606	646	17		

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	283	GLY	-	linker	UNP O60671
B	284	ARG	-	linker	UNP O60671
B	285	GLY	-	linker	UNP O60671
B	286	SER	-	linker	UNP O60671
B	287	MET	-	linker	UNP O60671
B	288	SER	-	linker	UNP O60671
B	289	ALA	-	linker	UNP O60671
B	290	TRP	-	linker	UNP O60671
B	291	SER	-	linker	UNP O60671
B	292	HIS	-	linker	UNP O60671
B	293	PRO	-	linker	UNP O60671
B	294	GLN	-	linker	UNP O60671
B	295	PHE	-	linker	UNP O60671
B	296	GLU	-	linker	UNP O60671
B	297	LYS	-	linker	UNP O60671
B	298	GLY	-	linker	UNP O60671
B	299	SER	-	linker	UNP O60671
B	300	ALA	-	linker	UNP O60671
B	301	GLY	-	linker	UNP O60671
B	302	SER	-	linker	UNP O60671
B	303	ALA	-	linker	UNP O60671
B	304	ALA	-	linker	UNP O60671
B	305	GLY	-	linker	UNP O60671
B	306	SER	-	linker	UNP O60671
B	307	GLY	-	linker	UNP O60671
B	308	ALA	-	linker	UNP O60671
B	309	GLY	-	linker	UNP O60671
B	310	TRP	-	linker	UNP O60671
B	311	SER	-	linker	UNP O60671
B	312	HIS	-	linker	UNP O60671
B	313	PRO	-	linker	UNP O60671
B	314	GLN	-	linker	UNP O60671
B	315	PHE	-	linker	UNP O60671
B	316	GLU	-	linker	UNP O60671
B	317	LYS	-	linker	UNP O60671
B	318	LEU	-	linker	UNP O60671
B	319	GLU	-	linker	UNP O60671
B	320	VAL	-	linker	UNP O60671
B	321	LEU	-	linker	UNP O60671
B	322	PHE	-	linker	UNP O60671
B	323	GLN	-	linker	UNP O60671
B	324	GLY	-	linker	UNP O60671
B	325	PRO	-	linker	UNP O60671

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Chain	Residue	Modelled	Actual	Comment	Reference
B	326	GLY	-	linker	UNP O60671
B	327	HIS	-	linker	UNP O60671
B	1009	LEU	-	expression tag	UNP O75943
B	1010	GLU	-	expression tag	UNP O75943
B	1011	GLY	-	expression tag	UNP O75943
B	1012	ALA	-	expression tag	UNP O75943
B	1013	SER	-	expression tag	UNP O75943
B	1014	HIS	-	expression tag	UNP O75943
B	1015	HIS	-	expression tag	UNP O75943
B	1016	HIS	-	expression tag	UNP O75943
B	1017	HIS	-	expression tag	UNP O75943
B	1018	HIS	-	expression tag	UNP O75943
B	1019	HIS	-	expression tag	UNP O75943
B	1020	HIS	-	expression tag	UNP O75943
B	1021	HIS	-	expression tag	UNP O75943
K	-44	GLY	-	linker	UNP O60671
K	-43	ARG	-	linker	UNP O60671
K	-42	GLY	-	linker	UNP O60671
K	-41	SER	-	linker	UNP O60671
K	-40	MET	-	linker	UNP O60671
K	-39	SER	-	linker	UNP O60671
K	-38	ALA	-	linker	UNP O60671
K	-37	TRP	-	linker	UNP O60671
K	-36	SER	-	linker	UNP O60671
K	-35	HIS	-	linker	UNP O60671
K	-34	PRO	-	linker	UNP O60671
K	-33	GLN	-	linker	UNP O60671
K	-32	PHE	-	linker	UNP O60671
K	-31	GLU	-	linker	UNP O60671
K	-30	LYS	-	linker	UNP O60671
K	-29	GLY	-	linker	UNP O60671
K	-28	SER	-	linker	UNP O60671
K	-27	ALA	-	linker	UNP O60671
K	-26	GLY	-	linker	UNP O60671
K	-25	SER	-	linker	UNP O60671
K	-24	ALA	-	linker	UNP O60671
K	-23	ALA	-	linker	UNP O60671
K	-22	GLY	-	linker	UNP O60671
K	-21	SER	-	linker	UNP O60671
K	-20	GLY	-	linker	UNP O60671
K	-19	ALA	-	linker	UNP O60671
K	-18	GLY	-	linker	UNP O60671

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-17	TRP	-	linker	UNP O60671
K	-16	SER	-	linker	UNP O60671
K	-15	HIS	-	linker	UNP O60671
K	-14	PRO	-	linker	UNP O60671
K	-13	GLN	-	linker	UNP O60671
K	-12	PHE	-	linker	UNP O60671
K	-11	GLU	-	linker	UNP O60671
K	-10	LYS	-	linker	UNP O60671
K	-9	LEU	-	linker	UNP O60671
K	-8	GLU	-	linker	UNP O60671
K	-7	VAL	-	linker	UNP O60671
K	-6	LEU	-	linker	UNP O60671
K	-5	PHE	-	linker	UNP O60671
K	-4	GLN	-	linker	UNP O60671
K	-3	GLY	-	linker	UNP O60671
K	-2	PRO	-	linker	UNP O60671
K	-1	GLY	-	linker	UNP O60671
K	0	HIS	-	linker	UNP O60671
K	682	LEU	-	expression tag	UNP O75943
K	683	GLU	-	expression tag	UNP O75943
K	684	GLY	-	expression tag	UNP O75943
K	685	ALA	-	expression tag	UNP O75943
K	686	SER	-	expression tag	UNP O75943
K	687	HIS	-	expression tag	UNP O75943
K	688	HIS	-	expression tag	UNP O75943
K	689	HIS	-	expression tag	UNP O75943
K	690	HIS	-	expression tag	UNP O75943
K	691	HIS	-	expression tag	UNP O75943
K	692	HIS	-	expression tag	UNP O75943
K	693	HIS	-	expression tag	UNP O75943
K	694	HIS	-	expression tag	UNP O75943

- Molecule 3 is a protein called Checkpoint protein HUS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	273	Total	C	N	O	S	0	0
			2171	1380	371	404	16		

- Molecule 4 is a protein called Replication factor C subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	324	Total	C	N	O	S	0	0
			2499	1577	428	483	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	363	SER	CYS	conflict	UNP P35249

- Molecule 5 is a protein called Replication factor C subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	338	Total	C	N	O	S	0	0
			2671	1681	480	487	23		

- Molecule 6 is a protein called Replication factor C subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	315	Total	C	N	O	S	0	0
			2480	1574	431	457	18		

- Molecule 7 is a protein called Replication factor C subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	317	Total	C	N	O	S	0	0
			2523	1606	434	470	13		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	MET	-	initiating methionine	UNP P40937
G	-18	GLY	-	expression tag	UNP P40937
G	-17	SER	-	expression tag	UNP P40937
G	-16	HIS	-	expression tag	UNP P40937
G	-15	HIS	-	expression tag	UNP P40937
G	-14	HIS	-	expression tag	UNP P40937
G	-13	HIS	-	expression tag	UNP P40937
G	-12	HIS	-	expression tag	UNP P40937
G	-11	HIS	-	expression tag	UNP P40937
G	-10	SER	-	expression tag	UNP P40937
G	-9	ALA	-	expression tag	UNP P40937
G	-8	ALA	-	expression tag	UNP P40937
G	-7	LEU	-	expression tag	UNP P40937

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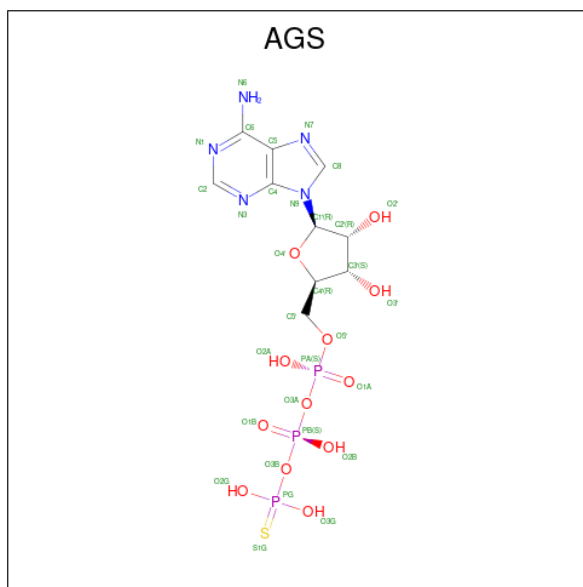
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLU	-	expression tag	UNP P40937
G	-5	VAL	-	expression tag	UNP P40937
G	-4	LEU	-	expression tag	UNP P40937
G	-3	PHE	-	expression tag	UNP P40937
G	-2	GLN	-	expression tag	UNP P40937
G	-1	GLY	-	expression tag	UNP P40937
G	0	PRO	-	expression tag	UNP P40937
G	1	GLY	-	expression tag	UNP P40937

- Molecule 8 is a DNA chain called Hairpin DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	22	Total	C	N	O	P	0	0
			454	216	84	132	22		
8	Y	10	Total	C	N	O	P	0	0
			198	97	32	60	9		

- Molecule 9 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
9	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
9	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
9	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

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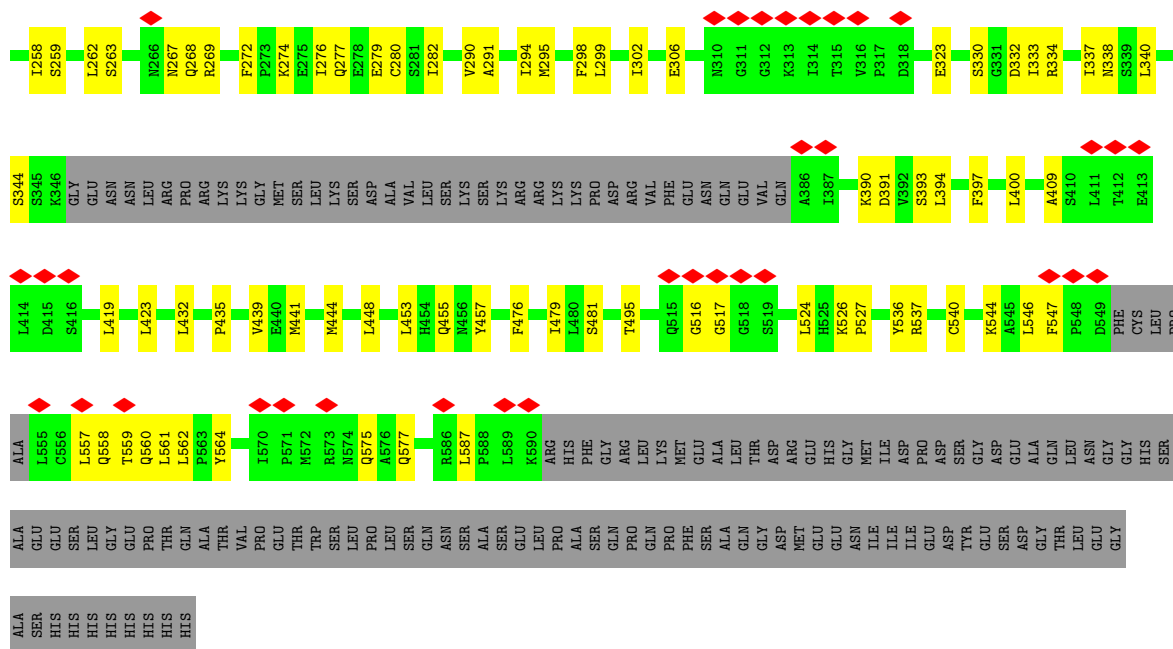
Mol	Chain	Residues	Atoms						AltConf
9	G	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	K	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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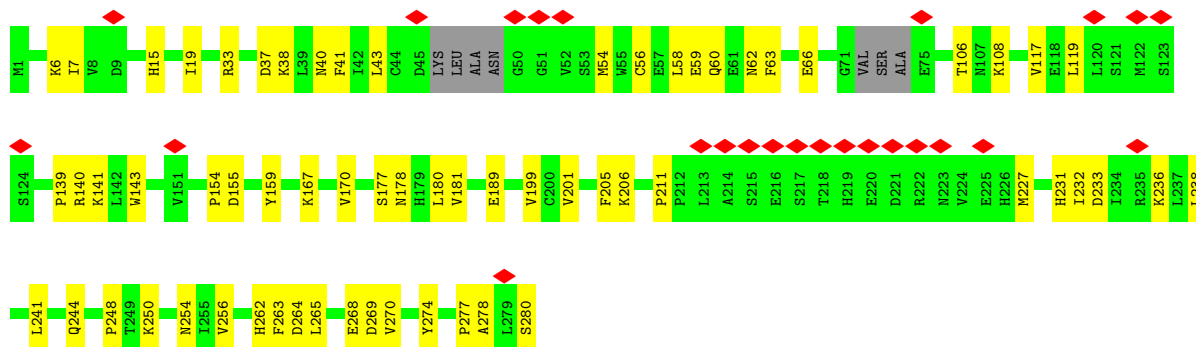
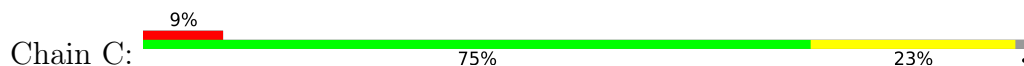
- Molecule 2: Cell cycle checkpoint protein RAD1,Cell cycle checkpoint protein RAD17

Chain K:

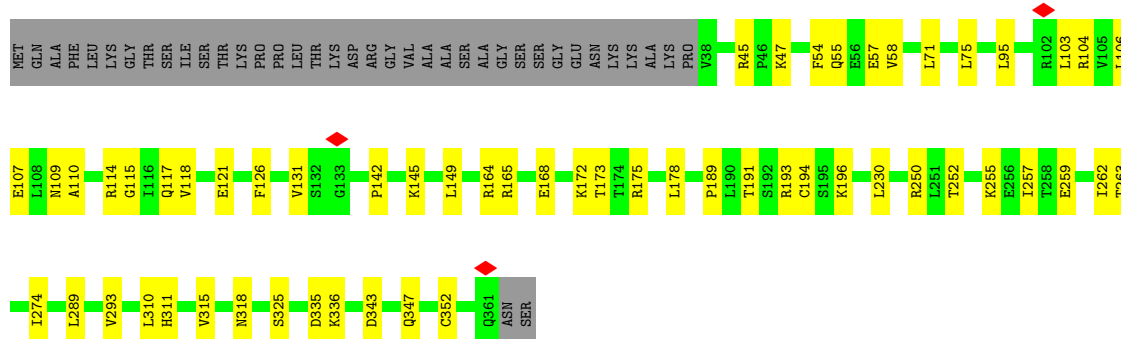
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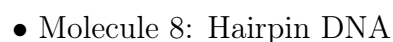
• Molecule 3: Checkpoint protein HUS1

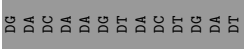
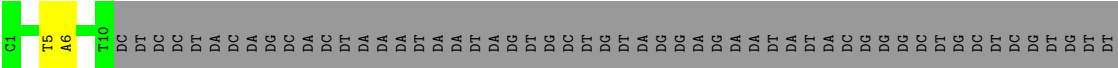


• Molecule 4: Replication factor C subunit 4



• Molecule 5: Replication factor C subunit 3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150626	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34.9	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.084	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	254.56, 254.56, 254.56	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS

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	0.11	0/1943	0.34	0/2614
2	B	0.13	0/2087	0.35	0/2823
2	K	0.11	0/3588	0.31	0/4842
3	C	0.12	0/2208	0.36	0/2985
4	D	0.12	0/2530	0.30	0/3413
5	E	0.12	0/2714	0.32	0/3661
6	F	0.16	0/2519	0.39	1/3400 (0.0%)
7	G	0.13	0/2566	0.35	1/3471 (0.0%)
8	X	0.16	0/508	0.33	0/780
8	Y	0.20	0/220	0.39	0/337
All	All	0.13	0/20883	0.34	2/28326 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	77	PRO	CA-N-CD	-11.19	96.33	112.00
7	G	21	PRO	N-CA-CB	7.20	110.80	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1911	0	1951	20	0
2	B	2049	0	2030	34	0
2	K	3518	0	3564	68	0
3	C	2171	0	2219	41	0
4	D	2499	0	2574	37	0
5	E	2671	0	2746	51	0
6	F	2480	0	2544	37	0
7	G	2523	0	2579	57	0
8	X	454	0	250	6	0
8	Y	198	0	116	1	0
9	D	31	0	12	1	0
9	E	31	0	12	1	0
9	F	31	0	12	1	0
9	G	31	0	10	0	0
9	K	31	0	12	3	0
All	All	20629	0	20631	324	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 8.

All (324) 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)
3:C:263:PHE:HB2	3:C:274:TYR:HB2	1.54	0.90
2:B:185:LYS:HB3	2:B:186:PRO:HD3	1.55	0.88
2:K:476:PHE:HA	2:K:479:ILE:HD12	1.56	0.86
1:A:57:PHE:HD1	1:A:58:PHE:H	1.22	0.86
2:K:276:ILE:O	2:K:280:CYS:HB2	1.83	0.79
2:B:158:LEU:HD21	2:B:163:LEU:HD11	1.65	0.77
2:B:205:LYS:HA	2:B:210:MET:HG3	1.68	0.75
3:C:244:GLN:NE2	3:C:274:TYR:OH	2.18	0.74
2:B:16:SER:OG	2:B:112:TYR:O	2.05	0.74
2:B:57:LYS:NZ	7:G:84:GLY:O	2.20	0.74
6:F:111:ARG:HA	6:F:116:VAL:HG21	1.69	0.73
1:A:144:MET:HE1	1:A:206:GLN:HB3	1.68	0.73
3:C:54:MET:HE1	3:C:274:TYR:CD1	2.25	0.71
2:K:559:THR:OG1	2:K:560:GLN:NE2	2.23	0.71
7:G:101:ILE:HG23	7:G:105:ILE:HD12	1.71	0.71
2:B:159:GLN:HB2	2:B:209:LEU:HD23	1.74	0.70
2:K:231:GLN:HE21	2:K:235:ASP:HB2	1.57	0.70
2:B:83:ARG:H	2:B:138:GLU:HB3	1.58	0.69
3:C:54:MET:HE2	3:C:54:MET:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:109:ASN:HB3	5:E:150:ARG:HG2	1.75	0.69
3:C:62:ASN:ND2	3:C:269:ASP:OD2	2.28	0.67
7:G:266:ILE:HD12	7:G:326:ILE:HD11	1.77	0.67
7:G:108:PHE:O	7:G:111:THR:OG1	2.12	0.67
3:C:236:LYS:HZ1	3:C:277:PRO:HD2	1.60	0.66
3:C:262:HIS:NE2	3:C:264:ASP:OD1	2.29	0.66
5:E:303:CYS:HB2	5:E:308:LYS:HD3	1.78	0.65
2:K:211:MET:HE2	2:K:211:MET:H	1.62	0.65
4:D:191:THR:O	7:G:215:ARG:NH2	2.31	0.64
5:E:30:VAL:HG12	5:E:35:PHE:HZ	1.62	0.64
6:F:162:SER:O	6:F:166:ARG:NH1	2.30	0.64
3:C:248:PRO:HG2	3:C:265:LEU:HD22	1.80	0.64
2:B:185:LYS:HB3	2:B:186:PRO:CD	2.28	0.64
4:D:252:THR:HG21	4:D:257:ILE:HG22	1.80	0.63
2:B:160:SER:OG	2:B:164:ARG:NH1	2.32	0.63
2:K:274:LYS:HD2	2:K:274:LYS:O	1.98	0.63
2:B:176:VAL:HG21	2:B:222:ARG:HD3	1.79	0.63
6:F:118:ASN:O	6:F:122:MET:HG2	1.99	0.63
5:E:285:CYS:HA	2:K:536:TYR:HE1	1.65	0.62
6:F:203:MET:HE1	6:F:218:LEU:HD13	1.81	0.62
4:D:289:LEU:HD11	4:D:352:CYS:HB3	1.81	0.62
5:E:100:ALA:HB1	5:E:103:SER:HB2	1.82	0.62
2:K:444:MET:HE2	2:K:448:LEU:HB3	1.82	0.62
5:E:7:LYS:NZ	5:E:203:GLU:OE1	2.33	0.61
6:F:159:GLU:OE1	6:F:184:ARG:NH1	2.33	0.61
3:C:38:LYS:HG2	3:C:59:GLU:HA	1.82	0.61
4:D:104:ARG:HH12	4:D:131:VAL:HG13	1.65	0.61
4:D:318:ASN:O	4:D:318:ASN:ND2	2.31	0.61
3:C:43:LEU:HB3	3:C:54:MET:HB3	1.83	0.61
3:C:41:PHE:HB2	3:C:56:CYS:HB3	1.83	0.60
2:K:272:PHE:HA	2:K:276:ILE:HD11	1.81	0.60
5:E:60:TYR:OH	5:E:129:PHE:O	2.18	0.60
4:D:71:LEU:O	4:D:175:ARG:NH1	2.36	0.59
4:D:164:ARG:HD2	4:D:189:PRO:HB2	1.85	0.59
6:F:144:ASP:N	6:F:144:ASP:OD1	2.35	0.59
2:K:299:LEU:HD22	2:K:340:LEU:HD22	1.83	0.58
2:K:143:LYS:NZ	9:K:701:AGS:O1B	2.35	0.58
2:K:558:GLN:HA	2:K:562:LEU:HB2	1.86	0.58
4:D:95:LEU:HD22	4:D:142:PRO:HG3	1.86	0.57
6:F:239:THR:HA	6:F:254:VAL:HG11	1.85	0.57
6:F:82:LYS:NZ	6:F:171:CYS:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:193:ILE:HD11	2:K:231:GLN:HG2	1.85	0.57
2:K:344:SER:O	2:K:344:SER:OG	2.23	0.57
3:C:106:THR:HG21	3:C:108:LYS:HE3	1.87	0.57
2:B:154:ASN:HB2	2:B:245:THR:HG23	1.86	0.57
6:F:256:ASP:OD1	6:F:257:GLU:N	2.38	0.57
3:C:6:LYS:HD2	3:C:7:ILE:N	2.20	0.57
6:F:266:MET:HE3	6:F:341:LEU:HD11	1.87	0.57
3:C:38:LYS:HE2	3:C:59:GLU:HG2	1.86	0.56
2:K:132:ILE:HB	2:K:282:ILE:HG12	1.86	0.56
5:E:13:LEU:HD22	5:E:23:ALA:HB1	1.87	0.56
8:X:68:DA:H2''	8:X:69:DA:H5''	1.86	0.56
3:C:15:HIS:HB3	3:C:63:PHE:HE2	1.70	0.56
3:C:33:ARG:HB3	3:C:40:ASN:HB2	1.87	0.56
3:C:154:PRO:HB3	3:C:254:ASN:HB3	1.87	0.56
4:D:54:PHE:HD1	4:D:55:GLN:H	1.51	0.56
4:D:106:LEU:HD13	4:D:126:PHE:HD2	1.70	0.56
2:K:540:CYS:SG	2:K:558:GLN:NE2	2.69	0.56
2:B:272:CYS:SG	7:G:111:THR:HG22	2.45	0.56
2:K:439:VAL:HG11	2:K:495:THR:HG21	1.86	0.56
2:B:132:CYS:HB3	3:C:201:VAL:HG22	1.87	0.56
7:G:295:SER:OG	7:G:296:SER:N	2.37	0.55
5:E:26:LEU:HD22	5:E:55:ILE:HD11	1.88	0.55
6:F:140:LEU:HD13	6:F:146:MET:HE1	1.89	0.55
6:F:342:ALA:HB1	7:G:299:ILE:HG23	1.89	0.55
1:A:30:GLU:HG2	1:A:72:ARG:HD3	1.89	0.55
4:D:145:LYS:NZ	4:D:173:THR:OG1	2.40	0.55
6:F:189:ARG:NH2	2:K:391:ASP:OD1	2.39	0.55
6:F:267:ILE:O	6:F:271:VAL:HG23	2.07	0.54
2:K:557:LEU:HB3	2:K:561:LEU:HD23	1.87	0.54
2:B:18:VAL:HG12	2:B:74:LYS:HB3	1.89	0.54
7:G:145:PHE:O	7:G:145:PHE:HD1	1.91	0.54
3:C:19:ILE:HD11	3:C:270:VAL:HG21	1.89	0.54
9:D:401:AGS:O3G	9:D:401:AGS:O2B	2.26	0.54
5:E:328:ALA:O	5:E:332:LEU:HD12	2.08	0.54
2:K:557:LEU:O	2:K:562:LEU:N	2.39	0.54
2:B:156:ILE:HG22	2:B:243:ILE:HB	1.89	0.53
4:D:106:LEU:HD13	4:D:126:PHE:CD2	2.43	0.53
5:E:262:ILE:HD11	5:E:336:VAL:HG13	1.88	0.53
7:G:179:PRO:HB3	7:G:206:VAL:HG11	1.90	0.53
3:C:189:GLU:HA	3:C:205:PHE:O	2.07	0.53
6:F:94:LEU:HD12	6:F:98:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:111:GLU:O	2:K:115:THR:HG22	2.08	0.53
4:D:259:GLU:O	4:D:263:THR:HG23	2.08	0.53
2:B:24:VAL:HG22	2:B:108:LEU:HD22	1.90	0.53
3:C:181:VAL:HG22	3:C:231:HIS:HB3	1.90	0.53
4:D:196:LYS:HE2	7:G:215:ARG:HH12	1.74	0.53
6:F:44:PRO:HG2	6:F:84:THR:HG21	1.91	0.53
5:E:288:PRO:HA	5:E:291:ILE:HD12	1.91	0.53
9:E:401:AGS:O1B	9:E:401:AGS:O3G	2.27	0.53
7:G:212:ASP:N	7:G:212:ASP:OD1	2.39	0.52
2:K:330:SER:O	2:K:330:SER:OG	2.28	0.52
2:K:481:SER:O	2:K:481:SER:OG	2.27	0.52
4:D:107:GLU:OE2	4:D:109:ASN:ND2	2.38	0.52
4:D:336:LYS:HE3	7:G:314:VAL:HG21	1.91	0.52
7:G:96:ARG:HH11	7:G:130:MET:HG2	1.74	0.52
2:K:262:LEU:HB2	2:K:393:SER:HB2	1.91	0.52
3:C:6:LYS:HB3	3:C:66:GLU:HB2	1.92	0.52
5:E:238:TYR:HB2	5:E:239:PRO:HD3	1.90	0.52
5:E:137:VAL:HG12	5:E:165:CYS:HB3	1.91	0.52
5:E:262:ILE:HG13	5:E:340:MET:HE3	1.92	0.52
2:K:419:LEU:HB3	2:K:423:LEU:HB2	1.92	0.52
4:D:57:GLU:HG2	4:D:58:VAL:N	2.25	0.52
2:K:394:LEU:HD22	2:K:441:MET:HE2	1.92	0.52
3:C:167:LYS:HA	3:C:241:LEU:HD23	1.91	0.52
4:D:274:ILE:HD11	4:D:310:LEU:HD12	1.92	0.51
2:B:170:LEU:HD11	2:B:177:LEU:HD11	1.91	0.51
3:C:155:ASP:HB2	3:C:256:VAL:HA	1.93	0.51
6:F:158:MET:SD	6:F:184:ARG:HD2	2.51	0.51
7:G:107:SER:O	7:G:111:THR:HG23	2.11	0.51
2:K:230:ASN:HD22	2:K:230:ASN:C	2.18	0.51
5:E:259:ALA:O	5:E:262:ILE:HG22	2.10	0.51
5:E:95:VAL:HG13	5:E:97:PRO:HD3	1.93	0.51
9:K:701:AGS:O2B	9:K:701:AGS:O3G	2.29	0.51
7:G:96:ARG:NH1	7:G:130:MET:HG2	2.26	0.51
7:G:102:ARG:O	7:G:106:LEU:HB2	2.11	0.51
7:G:308:ILE:HD13	7:G:311:ARG:HH21	1.76	0.51
3:C:232:ILE:HG22	3:C:278:ALA:HA	1.93	0.50
3:C:140:ARG:HA	3:C:143:TRP:CD1	2.45	0.50
7:G:258:ASP:OD1	7:G:259:PHE:N	2.34	0.50
2:K:298:PHE:O	2:K:302:ILE:HG13	2.11	0.50
6:F:142:GLU:N	6:F:142:GLU:OE1	2.44	0.50
8:X:51:DC:H2"	8:X:52:DG:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:142:GLU:CD	7:G:140:ARG:HH22	2.20	0.50
2:K:121:VAL:HG21	2:K:156:ILE:HD11	1.94	0.50
2:B:27:LEU:HD23	2:B:93:LEU:HD11	1.94	0.50
3:C:233:ASP:HB2	3:C:280:SER:HB2	1.94	0.50
4:D:230:LEU:HD12	4:D:262:ILE:HD12	1.92	0.50
6:F:333:SER:OG	7:G:309:GLU:OE2	2.28	0.50
2:K:269:ARG:HE	8:X:56:DT:H73	1.76	0.50
2:B:155:LYS:HG3	2:B:244:ARG:HG3	1.94	0.50
8:Y:5:DT:H2''	8:Y:6:DA:C8	2.46	0.49
2:K:134:LEU:HD11	2:K:258:ILE:HD11	1.93	0.49
5:E:56:LEU:HD21	5:E:131:VAL:HG21	1.93	0.49
7:G:167:SER:O	7:G:167:SER:OG	2.29	0.49
1:A:50:CYS:HB3	1:A:259:HIS:CD2	2.47	0.49
1:A:152:LEU:HD22	1:A:236:LEU:HD12	1.95	0.49
2:B:15:TYR:O	2:B:17:LEU:N	2.45	0.49
2:K:526:LYS:HG2	2:K:527:PRO:HD2	1.94	0.49
7:G:146:THR:HG22	7:G:146:THR:O	2.12	0.49
4:D:45:ARG:O	4:D:47:LYS:NZ	2.46	0.49
2:B:122:PHE:HD2	2:B:131:VAL:HG22	1.76	0.48
2:B:167:PHE:HD2	2:B:232:THR:HG22	1.78	0.48
4:D:149:LEU:HD21	4:D:178:LEU:HG	1.94	0.48
6:F:107:ALA:H	7:G:140:ARG:HD2	1.77	0.48
4:D:103:LEU:HD23	4:D:103:LEU:H	1.78	0.48
2:K:244:ARG:NH2	2:K:279:GLU:OE1	2.46	0.48
5:E:275:ARG:HH22	2:K:455:GLN:HA	1.78	0.48
6:F:259:HIS:CE1	6:F:298:ASN:HD22	2.31	0.48
6:F:282:LEU:HD11	6:F:337:MET:HB3	1.94	0.48
2:K:291:ALA:HB3	2:K:294:ILE:HD12	1.96	0.48
2:K:544:LYS:HZ3	2:K:557:LEU:HB2	1.78	0.48
7:G:259:PHE:HE1	7:G:326:ILE:HG22	1.78	0.48
7:G:130:MET:HE3	7:G:135:GLN:HG2	1.95	0.48
6:F:123:PHE:O	6:F:136:LYS:NZ	2.47	0.47
7:G:262:ALA:O	7:G:266:ILE:HG13	2.14	0.47
1:A:37:SER:OG	1:A:39:ARG:NH1	2.46	0.47
5:E:80:LYS:HE2	5:E:80:LYS:HB3	1.76	0.47
6:F:280:LYS:NZ	6:F:284:HIS:HB2	2.29	0.47
1:A:183:GLU:OE2	2:K:205:LYS:NZ	2.47	0.47
2:B:120:MET:HE1	2:B:133:LYS:HB3	1.96	0.47
4:D:347:GLN:NE2	5:E:316:ALA:HB1	2.30	0.47
1:A:152:LEU:HD23	1:A:222:PHE:HZ	1.80	0.47
5:E:17:ASP:OD1	5:E:17:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:300:LEU:HD22	5:E:308:LYS:HG3	1.97	0.47
7:G:111:THR:OG1	7:G:120:LYS:HE2	2.15	0.47
7:G:139:ARG:HD3	7:G:168:ARG:HH12	1.80	0.47
3:C:59:GLU:OE1	3:C:62:ASN:ND2	2.47	0.47
5:E:26:LEU:O	5:E:30:VAL:HG13	2.15	0.47
5:E:284:HIS:CE1	2:K:587:LEU:HB3	2.49	0.47
2:K:397:PHE:HD1	2:K:524:LEU:HD12	1.79	0.47
2:B:22:ASP:OD1	2:B:71:GLN:NE2	2.40	0.47
3:C:58:LEU:HD12	3:C:59:GLU:N	2.30	0.47
2:B:229:LYS:HE3	2:B:229:LYS:HB2	1.61	0.46
5:E:186:ALA:HB1	5:E:221:ARG:HB2	1.96	0.46
2:K:234:ARG:NH1	8:X:67:DC:O4'	2.48	0.46
1:A:254:SER:C	1:A:255:LEU:HD23	2.40	0.46
2:B:20:SER:HB2	2:B:72:GLU:HB3	1.97	0.46
7:G:45:GLN:HE22	7:G:76:GLN:HE22	1.62	0.46
1:A:74:LYS:HD3	1:A:129:CYS:HB3	1.96	0.46
7:G:189:VAL:HG11	7:G:217:LEU:HD21	1.97	0.46
3:C:170:VAL:HG12	3:C:238:LEU:HD13	1.98	0.46
4:D:165:ARG:HG2	7:G:91:ASN:HB3	1.97	0.46
7:G:250:ILE:O	7:G:254:MET:HG3	2.15	0.46
2:K:453:LEU:O	2:K:457:TYR:HB3	2.15	0.46
2:K:259:SER:OG	9:K:701:AGS:S1G	2.67	0.46
2:K:516:GLY:HA2	2:K:517:GLY:HA2	1.61	0.46
2:K:333:ILE:O	2:K:337:ILE:HG12	2.16	0.46
7:G:22:TRP:CE3	7:G:221:GLN:HB2	2.51	0.46
6:F:300:PHE:CE1	6:F:317:ILE:HD12	2.51	0.46
7:G:196:ASP:OD1	7:G:196:ASP:N	2.43	0.46
1:A:83:VAL:O	1:A:87:LEU:HB2	2.15	0.45
2:B:17:LEU:HA	2:B:74:LYS:O	2.17	0.45
3:C:189:GLU:HG2	3:C:206:LYS:HG2	1.97	0.45
4:D:325:SER:HA	7:G:327:ALA:HB1	1.98	0.45
1:A:78:LYS:HG3	2:K:167:PRO:HG3	1.99	0.45
2:K:211:MET:HE2	2:K:211:MET:N	2.30	0.45
5:E:30:VAL:HG12	5:E:35:PHE:CZ	2.49	0.45
7:G:164:ALA:O	7:G:168:ARG:NH1	2.50	0.45
2:B:231:SER:OG	2:B:255:TYR:OH	2.20	0.45
4:D:289:LEU:O	4:D:293:VAL:HG23	2.17	0.45
2:B:46:LYS:HE2	2:B:46:LYS:HB3	1.58	0.45
6:F:347:LYS:HA	6:F:347:LYS:HD3	1.73	0.45
7:G:138:LEU:HD23	7:G:165:LEU:HD21	1.97	0.45
1:A:78:LYS:HD3	1:A:78:LYS:HA	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:130:MET:HE1	7:G:138:LEU:HD22	1.99	0.45
7:G:204:ALA:HB1	7:G:236:TYR:HE1	1.82	0.45
2:K:95:TYR:OH	2:K:306:GLU:OE2	2.28	0.44
8:X:67:DC:H2"	8:X:68:DA:C8	2.51	0.44
4:D:343:ASP:OD2	5:E:293:LYS:NZ	2.47	0.44
5:E:111:MET:O	5:E:115:VAL:HG23	2.16	0.44
5:E:321:ARG:HD2	2:K:479:ILE:HD11	1.99	0.44
5:E:345:LYS:HE2	5:E:345:LYS:HB2	1.61	0.44
3:C:180:LEU:HD23	3:C:181:VAL:N	2.31	0.44
6:F:107:ALA:HB3	7:G:140:ARG:HD2	1.99	0.44
2:K:140:GLY:HA3	2:K:332:ASP:OD2	2.18	0.44
1:A:193:MET:HB3	1:A:193:MET:HE3	1.80	0.44
3:C:117:VAL:HG12	3:C:119:LEU:HD22	2.00	0.44
5:E:228:LEU:HD22	2:K:564:TYR:CE1	2.53	0.44
2:K:231:GLN:NE2	2:K:235:ASP:HB2	2.29	0.44
2:K:334:ARG:O	2:K:338:ASN:ND2	2.45	0.44
1:A:96:LYS:HB2	1:A:113:HIS:HB2	1.98	0.44
6:F:256:ASP:CG	6:F:257:GLU:H	2.25	0.44
7:G:270:LYS:HB3	7:G:270:LYS:HE2	1.83	0.44
2:K:546:LEU:HD21	2:K:577:GLN:NE2	2.33	0.44
6:F:313:LYS:O	6:F:317:ILE:HG12	2.18	0.44
7:G:144:LYS:HA	7:G:144:LYS:HD2	1.89	0.44
2:K:547:PHE:HB3	2:K:561:LEU:HD21	2.00	0.44
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.82	0.43
2:K:290:VAL:HG23	2:K:295:MET:HE2	1.99	0.43
5:E:27:ARG:HA	5:E:30:VAL:HG22	2.00	0.43
5:E:149:ARG:HB2	5:E:175:ILE:HG13	1.99	0.43
4:D:252:THR:O	4:D:255:LYS:NZ	2.42	0.43
5:E:74:ILE:HD11	5:E:107:VAL:HG22	2.01	0.43
5:E:105:ARG:O	5:E:109:GLN:HG3	2.18	0.43
5:E:254:TYR:HD2	5:E:281:LEU:HD12	1.83	0.43
2:K:263:SER:OG	2:K:393:SER:HB3	2.18	0.43
2:K:537:ARG:NH2	8:X:58:DC:O3'	2.51	0.43
1:A:24:GLY:HA3	1:A:40:THR:OG1	2.19	0.43
3:C:54:MET:HE1	3:C:274:TYR:CE1	2.52	0.43
3:C:177:SER:OG	3:C:178:ASN:N	2.51	0.43
4:D:250:ARG:NH2	5:E:34:ASP:OD2	2.51	0.43
6:F:107:ALA:H	7:G:140:ARG:CD	2.32	0.43
7:G:30:THR:HG23	7:G:32:ASN:H	1.83	0.43
2:K:575:GLN:O	2:K:575:GLN:NE2	2.52	0.43
6:F:43:ARG:NH2	9:F:401:AGS:O1A	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:CYS:SG	1:A:259:HIS:NE2	2.92	0.43
4:D:311:HIS:O	4:D:315:VAL:HG23	2.19	0.43
3:C:139:PRO:HB2	3:C:141:LYS:HD2	2.01	0.42
2:K:267:ASN:OD1	2:K:268:GLN:N	2.52	0.42
3:C:37:ASP:O	3:C:60:GLN:HB3	2.19	0.42
4:D:117:GLN:NE2	4:D:121:GLU:HG3	2.35	0.42
5:E:13:LEU:N	5:E:54:CYS:SG	2.92	0.42
2:B:84:ILE:HD13	2:B:89:LEU:HD22	2.00	0.42
5:E:4:TRP:HA	5:E:224:ARG:HG3	2.01	0.42
6:F:300:PHE:HE1	6:F:317:ILE:HD12	1.83	0.42
7:G:136:ASN:OD1	7:G:139:ARG:NH2	2.46	0.42
4:D:168:GLU:OE2	4:D:193:ARG:NH1	2.53	0.42
2:K:544:LYS:NZ	2:K:557:LEU:HB2	2.34	0.42
5:E:170:LYS:H	5:E:170:LYS:HG2	1.68	0.42
5:E:285:CYS:HA	2:K:536:TYR:CE1	2.50	0.42
6:F:148:ASP:OD1	6:F:148:ASP:N	2.53	0.42
6:F:217:GLY:HA3	6:F:246:ILE:O	2.20	0.42
7:G:292:ASP:OD1	7:G:292:ASP:C	2.63	0.42
5:E:108:ILE:O	5:E:112:LEU:HB2	2.19	0.42
2:K:272:PHE:HB3	2:K:277:GLN:HE21	1.85	0.42
4:D:110:ALA:HA	4:D:114:ARG:HH21	1.85	0.41
5:E:287:PRO:HG2	5:E:290:ILE:HG12	2.01	0.41
5:E:295:LEU:HD23	5:E:295:LEU:HA	1.83	0.41
7:G:246:ASP:O	7:G:250:ILE:HG13	2.20	0.41
2:B:88:VAL:HG11	3:C:199:VAL:HG21	2.02	0.41
3:C:250:LYS:O	3:C:250:LYS:HD3	2.20	0.41
5:E:76:THR:HB	5:E:77:PRO:HD2	2.01	0.41
5:E:90:ASN:OD1	5:E:90:ASN:N	2.53	0.41
7:G:55:HIS:CG	7:G:142:ILE:HD11	2.55	0.41
2:K:435:PRO:O	2:K:439:VAL:HG23	2.21	0.41
2:B:167:PHE:CD2	2:B:232:THR:HG22	2.55	0.41
7:G:107:SER:HA	7:G:110:SER:HB2	2.02	0.41
4:D:115:GLY:H	4:D:118:VAL:CG1	2.33	0.41
5:E:41:TYR:HA	5:E:165:CYS:O	2.20	0.41
7:G:162:ILE:HG23	7:G:165:LEU:H	1.86	0.41
7:G:294:PRO:O	7:G:296:SER:N	2.53	0.41
2:K:323:GLU:H	2:K:323:GLU:CD	2.28	0.41
2:K:540:CYS:O	2:K:544:LYS:HG2	2.20	0.41
2:B:30:ILE:HD11	2:B:265:CYS:HB2	2.03	0.41
5:E:134:LEU:HB2	5:E:163:LEU:HD23	2.01	0.41
6:F:132:LYS:HA	6:F:132:LYS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:40:ILE:HG21	7:G:174:PHE:HE1	1.85	0.41
1:A:144:MET:SD	1:A:145:LEU:N	2.93	0.41
7:G:141:VAL:HG13	7:G:145:PHE:CZ	2.55	0.41
2:K:390:LYS:HE2	2:K:390:LYS:HB3	1.84	0.41
2:K:409:ALA:HB2	2:K:432:LEU:HD11	2.02	0.41
2:B:165:GLU:H	2:B:165:GLU:HG3	1.70	0.40
4:D:75:LEU:HD12	4:D:194:CYS:HB2	2.04	0.40
6:F:305:THR:O	6:F:305:THR:OG1	2.31	0.40
7:G:304:LYS:HA	7:G:304:LYS:HD2	1.80	0.40
3:C:159:TYR:HD1	3:C:211:PRO:HD3	1.86	0.40
5:E:309:GLY:O	5:E:313:GLN:HG3	2.22	0.40
7:G:31:LEU:HD12	7:G:31:LEU:HA	1.86	0.40
1:A:147:ALA:HB2	1:A:204:PHE:CD2	2.57	0.40
3:C:268:GLU:HB2	3:C:269:ASP:H	1.71	0.40
4:D:252:THR:HB	4:D:255:LYS:HG2	2.03	0.40
5:E:49:LYS:HB3	5:E:49:LYS:HE3	1.88	0.40
7:G:333:ARG:HD2	7:G:333:ARG:HA	1.81	0.40
2:K:557:LEU:HA	2:K:561:LEU:HB3	2.03	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	237/405 (58%)	217 (92%)	19 (8%)	1 (0%)	30	63
2	B	258/1021 (25%)	237 (92%)	19 (7%)	2 (1%)	16	51
2	K	427/1021 (42%)	401 (94%)	26 (6%)	0	100	100
3	C	267/280 (95%)	255 (96%)	12 (4%)	0	100	100
4	D	320/363 (88%)	305 (95%)	15 (5%)	0	100	100
5	E	334/356 (94%)	305 (91%)	28 (8%)	1 (0%)	37	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	311/354 (88%)	290 (93%)	21 (7%)	0	100	100
7	G	315/360 (88%)	297 (94%)	17 (5%)	1 (0%)	37	67
All	All	2469/4160 (59%)	2307 (93%)	157 (6%)	5 (0%)	45	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	16	SER
2	B	185	LYS
7	G	21	PRO
5	E	91	TYR
1	A	62	GLN

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	209/346 (60%)	206 (99%)	3 (1%)	62	79
2	B	234/908 (26%)	232 (99%)	2 (1%)	75	87
2	K	394/908 (43%)	393 (100%)	1 (0%)	91	96
3	C	252/257 (98%)	251 (100%)	1 (0%)	89	95
4	D	278/309 (90%)	276 (99%)	2 (1%)	81	90
5	E	297/316 (94%)	295 (99%)	2 (1%)	81	90
6	F	271/296 (92%)	268 (99%)	3 (1%)	70	83
7	G	283/318 (89%)	281 (99%)	2 (1%)	81	90
All	All	2218/3658 (61%)	2202 (99%)	16 (1%)	80	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	57	PHE

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Mol	Chain	Res	Type
1	A	235	ASN
2	B	158	LEU
2	B	264	ILE
3	C	227	MET
4	D	172	LYS
4	D	335	ASP
5	E	17	ASP
5	E	171	VAL
6	F	127	LYS
6	F	202	LEU
6	F	267	ILE
7	G	107	SER
7	G	281	LEU
2	K	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
2	B	200	HIS
2	B	214	HIS
3	C	244	GLN
3	C	254	ASN
4	D	347	GLN
5	E	222	ASN
5	E	302	ASN
6	F	172	ASN
6	F	259	HIS
6	F	298	ASN
7	G	45	GLN
7	G	49	ASN
7	G	91	ASN
7	G	218	ASN
2	K	125	GLN
2	K	207	ASN
2	K	231	GLN
2	K	240	HIS
2	K	560	GLN
2	K	575	GLN

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 ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	AGS	G	401	7	26,33,33	0.72	1 (3%)	26,52,52	1.05	2 (7%)
9	AGS	D	401	4	26,33,33	0.71	1 (3%)	26,52,52	1.02	2 (7%)
9	AGS	F	401	6	26,33,33	0.69	0	26,52,52	1.10	2 (7%)
9	AGS	E	401	5	26,33,33	0.71	1 (3%)	26,52,52	1.11	2 (7%)
9	AGS	K	701	2	26,33,33	0.67	0	26,52,52	1.01	2 (7%)

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
9	AGS	G	401	7	-	6/17/38/38	0/3/3/3
9	AGS	D	401	4	-	6/17/38/38	0/3/3/3
9	AGS	F	401	6	-	4/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	AGS	E	401	5	-	5/17/38/38	0/3/3/3
9	AGS	K	701	2	-	4/17/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	401	AGS	PG-S1G	2.17	1.95	1.90
9	E	401	AGS	PG-S1G	2.11	1.95	1.90
9	D	401	AGS	PG-S1G	2.07	1.95	1.90

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	401	AGS	PA-O3A-PB	-4.26	118.22	132.83
9	D	401	AGS	PA-O3A-PB	-3.68	120.19	132.83
9	G	401	AGS	PA-O3A-PB	-3.68	120.21	132.83
9	F	401	AGS	PA-O3A-PB	-3.61	120.43	132.83
9	K	701	AGS	PA-O3A-PB	-3.41	121.14	132.83
9	G	401	AGS	C5-C6-N6	2.28	123.81	120.35
9	K	701	AGS	C5-C6-N6	2.26	123.78	120.35
9	F	401	AGS	C5-C6-N6	2.25	123.77	120.35
9	E	401	AGS	C5-C6-N6	2.24	123.75	120.35
9	D	401	AGS	C5-C6-N6	2.24	123.75	120.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	401	AGS	PB-O3B-PG-O2G
9	D	401	AGS	PB-O3B-PG-O3G
9	E	401	AGS	PB-O3B-PG-O2G
9	E	401	AGS	PB-O3B-PG-O3G
9	E	401	AGS	C5'-O5'-PA-O1A
9	E	401	AGS	C5'-O5'-PA-O2A
9	F	401	AGS	C5'-O5'-PA-O2A
9	F	401	AGS	C5'-O5'-PA-O3A
9	F	401	AGS	O4'-C4'-C5'-O5'
9	G	401	AGS	PB-O3B-PG-O3G
9	G	401	AGS	C5'-O5'-PA-O1A
9	G	401	AGS	C5'-O5'-PA-O2A
9	K	701	AGS	C3'-C4'-C5'-O5'

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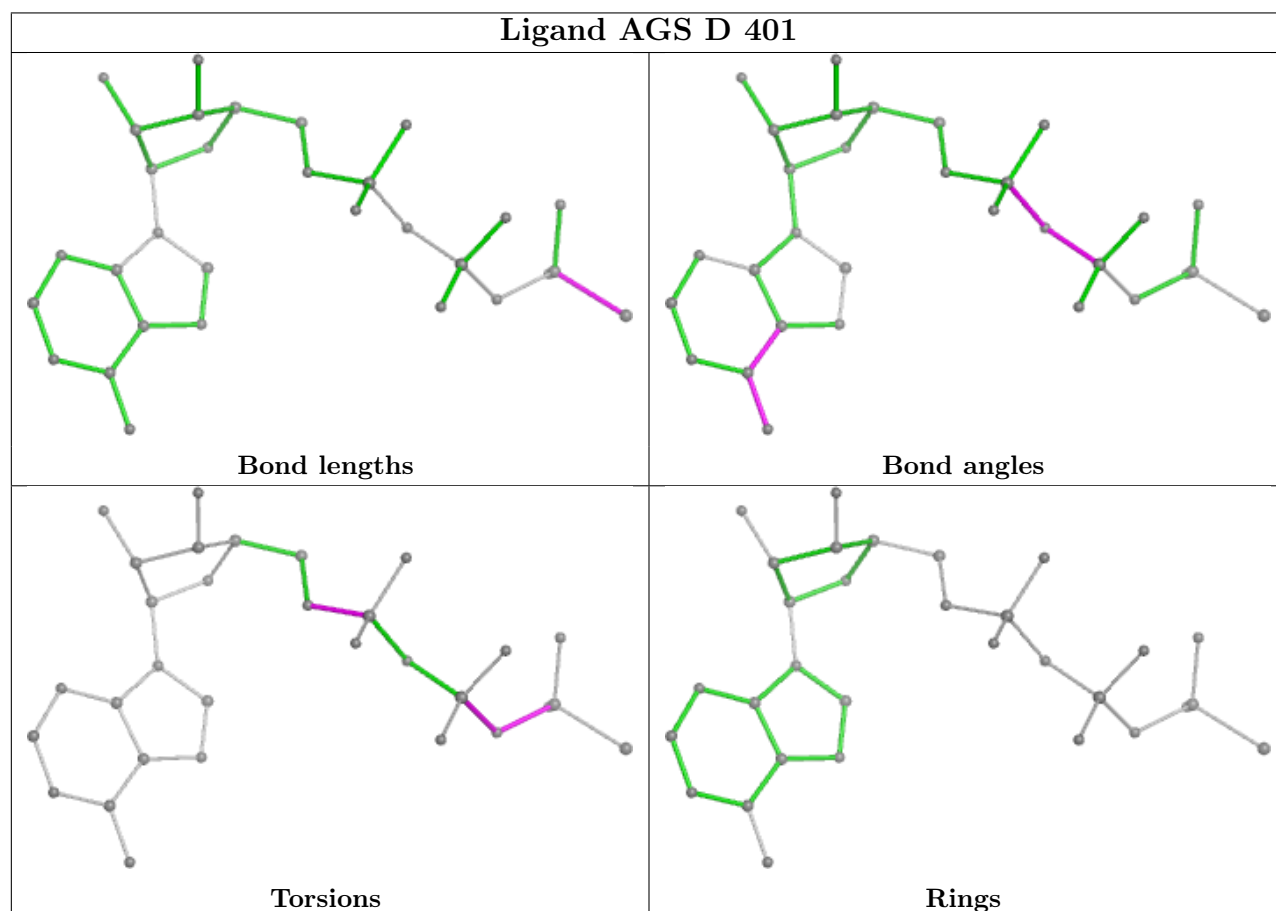
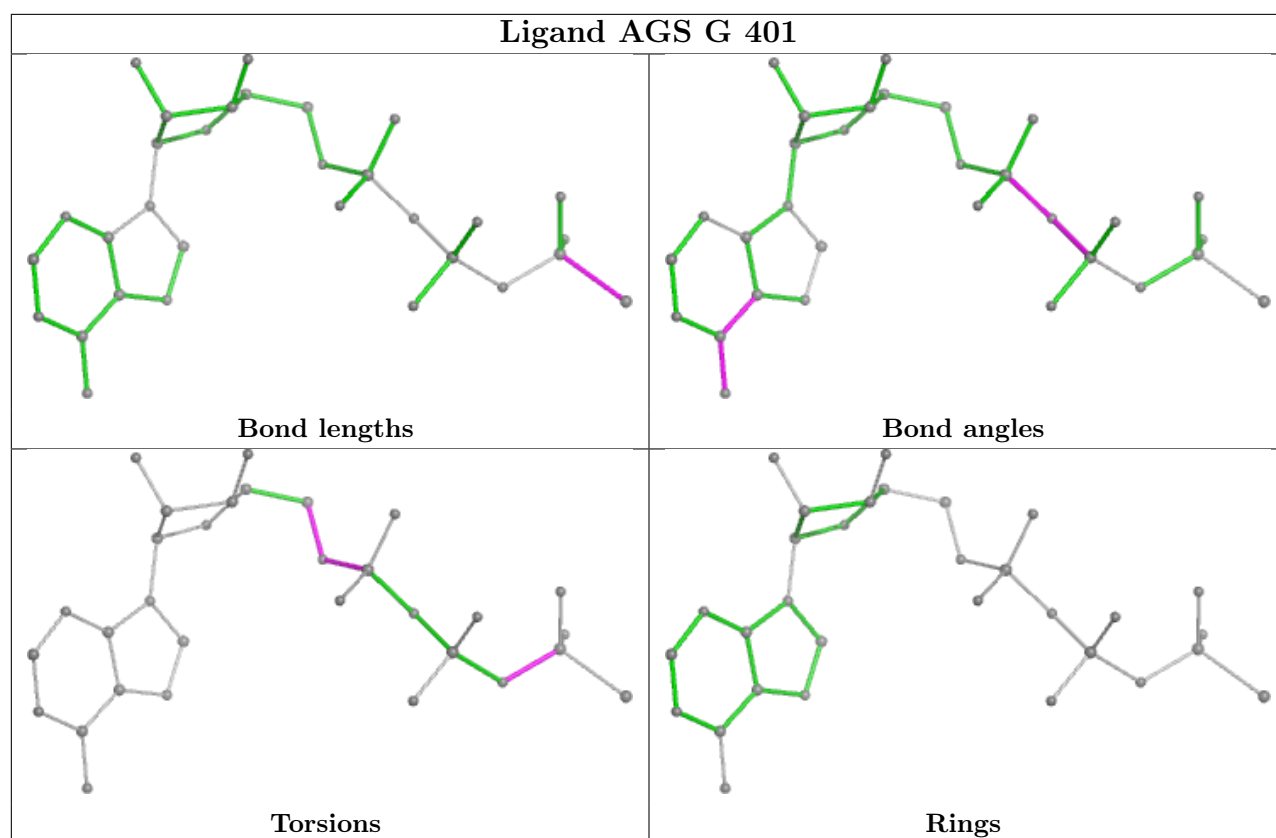
Mol	Chain	Res	Type	Atoms
9	F	401	AGS	C3'-C4'-C5'-O5'
9	K	701	AGS	O4'-C4'-C5'-O5'
9	D	401	AGS	PG-O3B-PB-O1B
9	K	701	AGS	PA-O3A-PB-O3B
9	G	401	AGS	C4'-C5'-O5'-PA
9	G	401	AGS	PB-O3B-PG-O2G
9	D	401	AGS	PG-O3B-PB-O2B
9	D	401	AGS	C5'-O5'-PA-O3A
9	E	401	AGS	C5'-O5'-PA-O3A
9	G	401	AGS	C5'-O5'-PA-O3A
9	D	401	AGS	C5'-O5'-PA-O1A
9	K	701	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

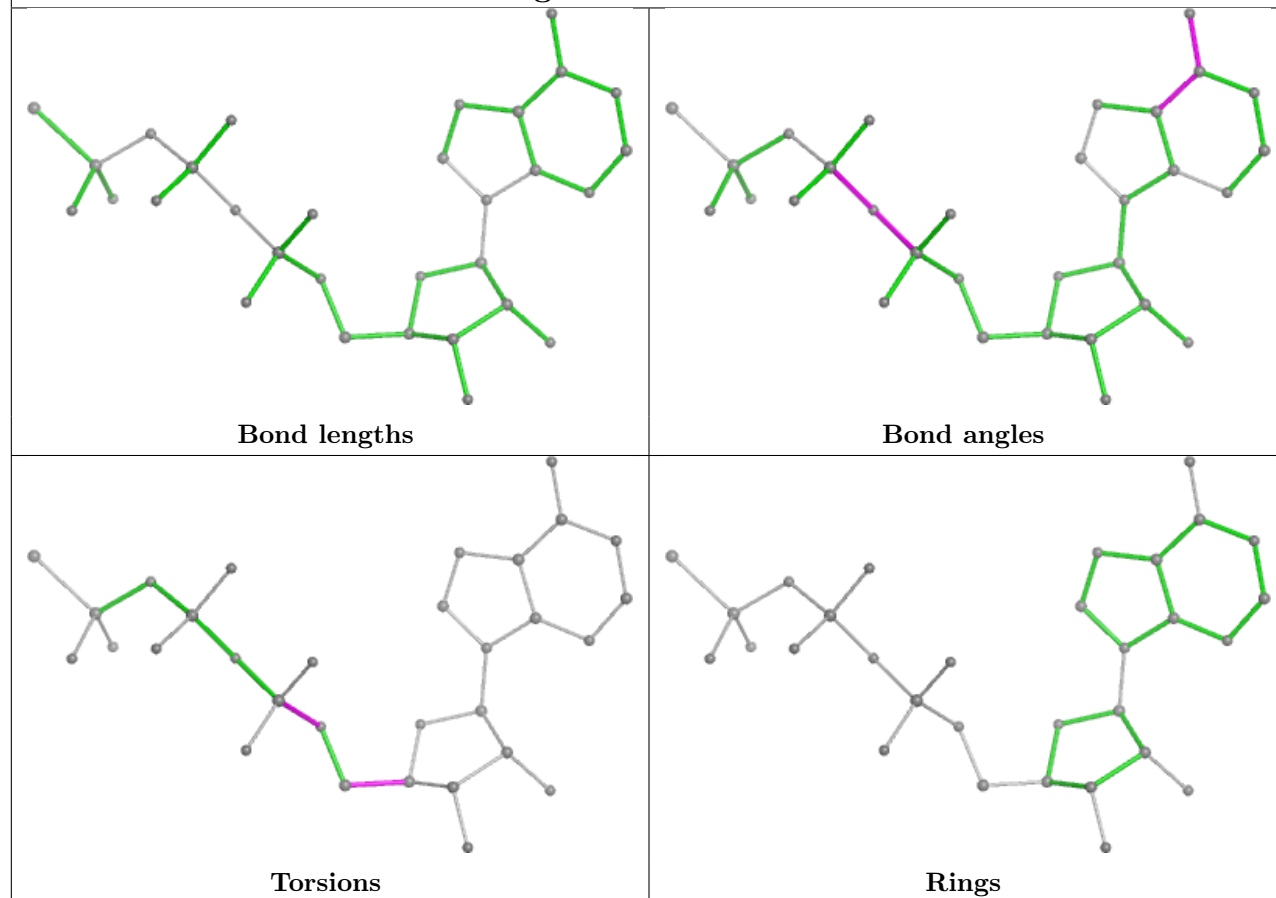
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	401	AGS	1	0
9	F	401	AGS	1	0
9	E	401	AGS	1	0
9	K	701	AGS	3	0

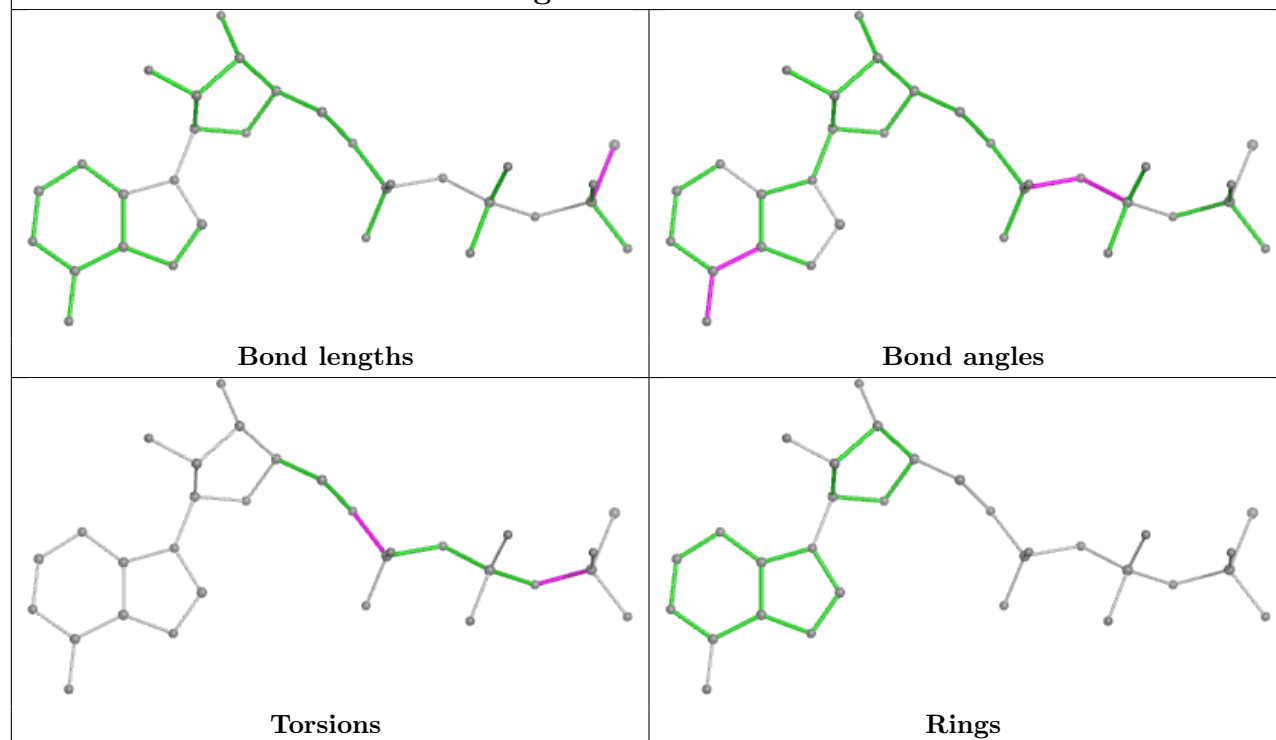
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

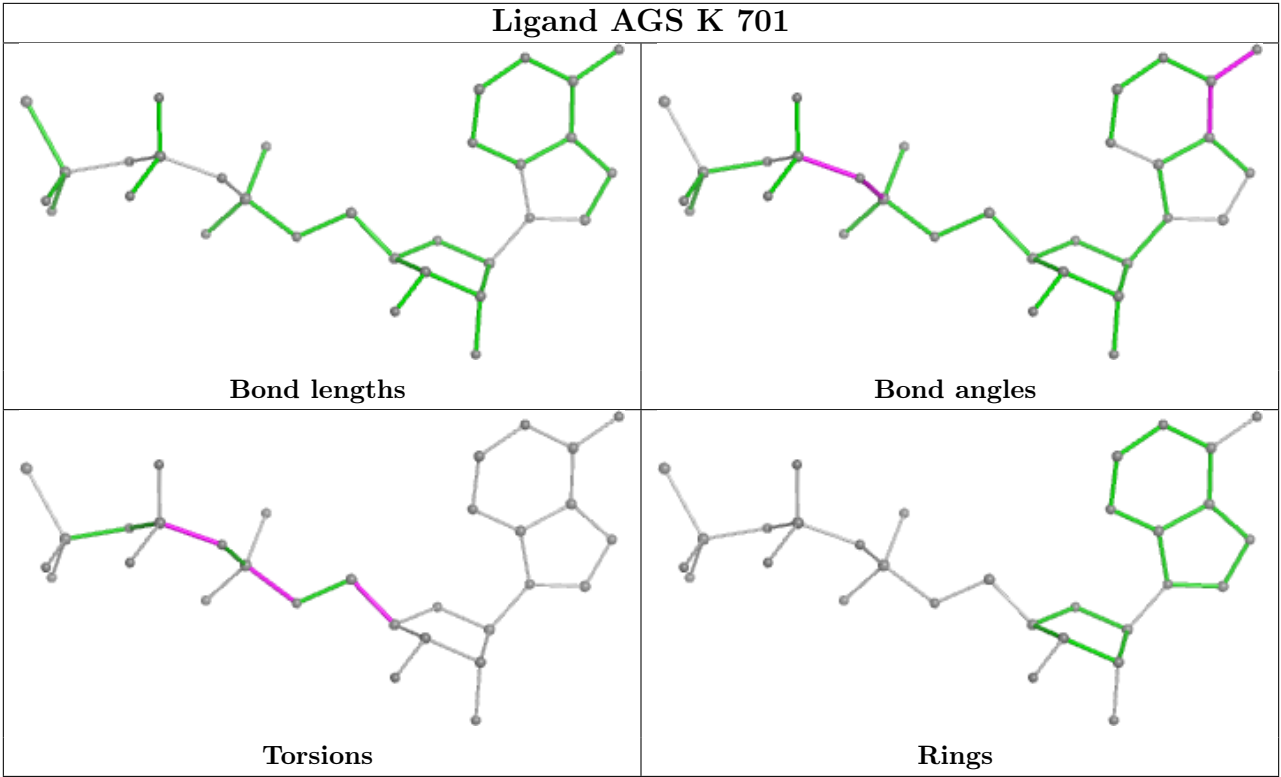


Ligand AGS F 401



Ligand AGS E 401





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	K	2
6	F	1
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	545:ALA	C	546:LEU	N	4.21
1	F	255:CYS	C	256:ASP	N	3.26
1	K	547:PHE	C	548:PRO	N	3.17
1	D	201:PRO	C	202:LEU	N	3.08

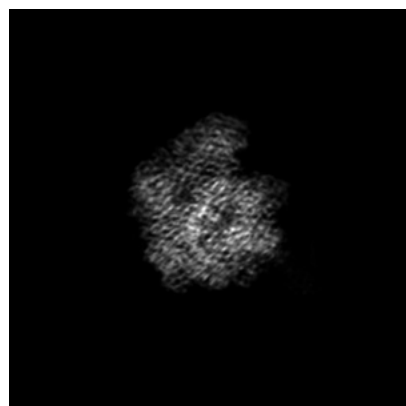
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14527. These allow visual inspection of the internal detail of the map and identification of artifacts.

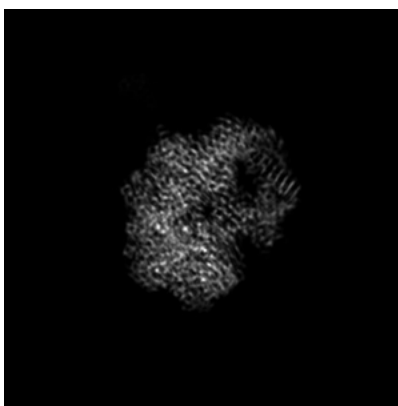
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

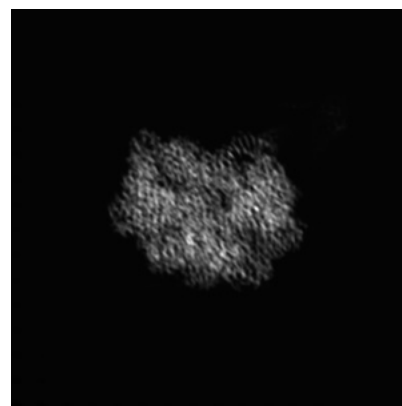
6.1.1 Primary map



X

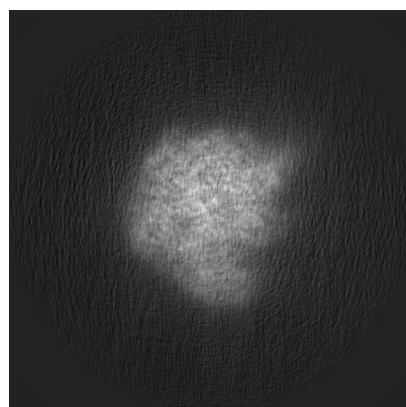


Y

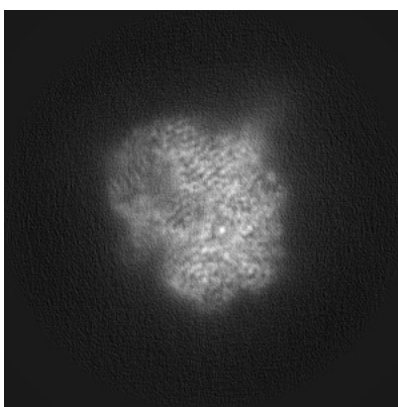


Z

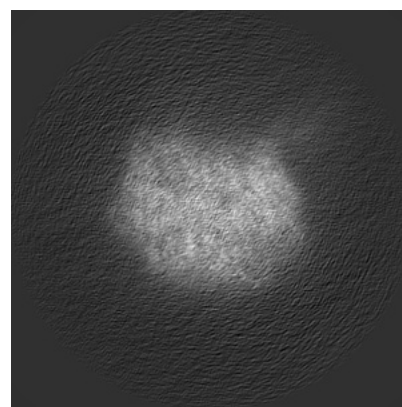
6.1.2 Raw map



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: 148

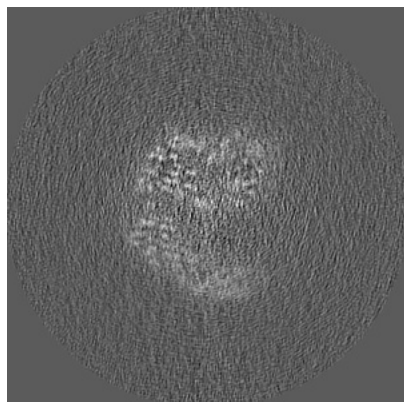


Y Index: 148

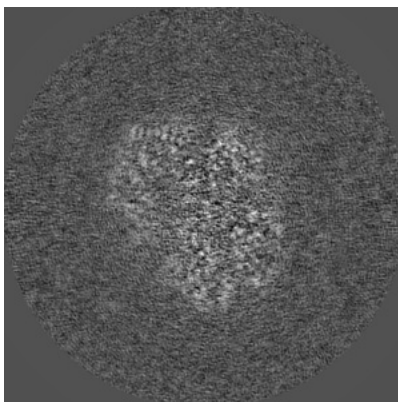


Z Index: 148

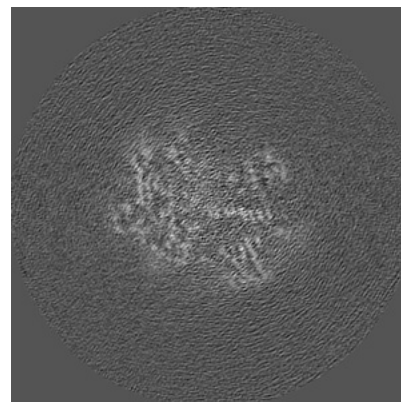
6.2.2 Raw map



X Index: 148



Y Index: 148

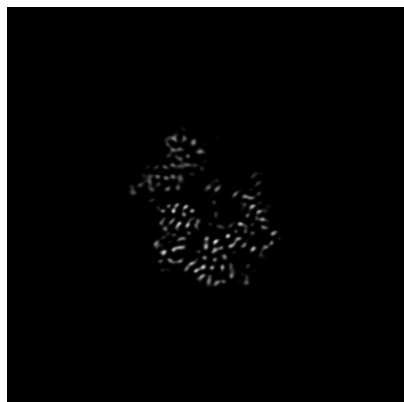


Z Index: 148

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

6.3 Largest variance slices [i](#)

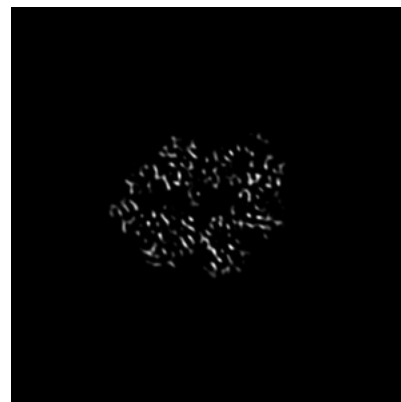
6.3.1 Primary map



X Index: 131

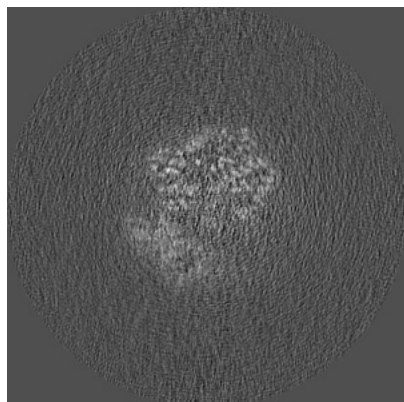


Y Index: 153

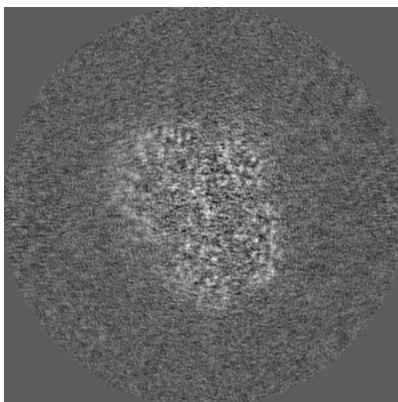


Z Index: 133

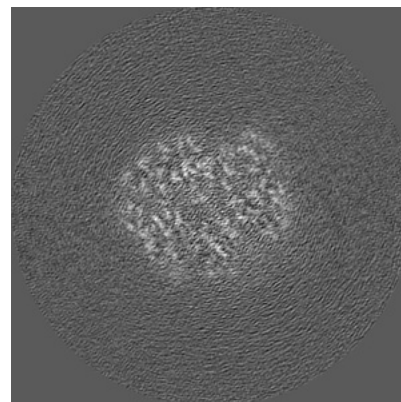
6.3.2 Raw map



X Index: 133



Y Index: 145



Z Index: 166

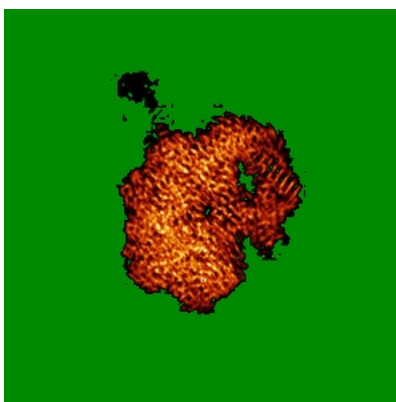
The images above show the largest variance slices of the map in three orthogonal directions.

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

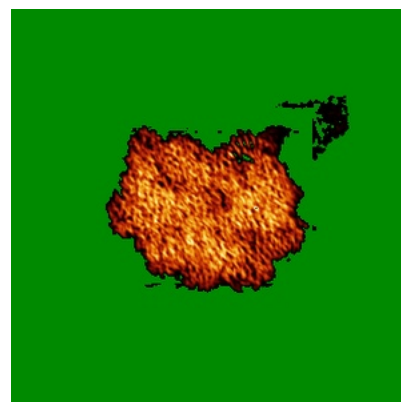
6.4.1 Primary map



X

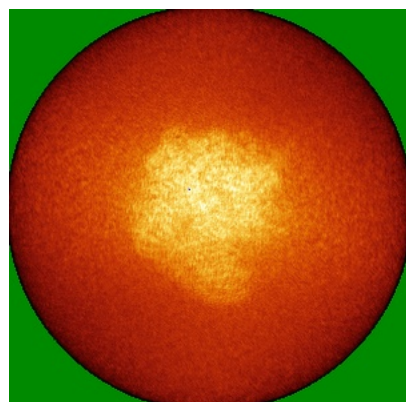


Y

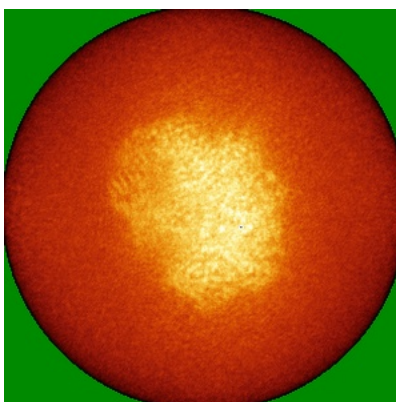


Z

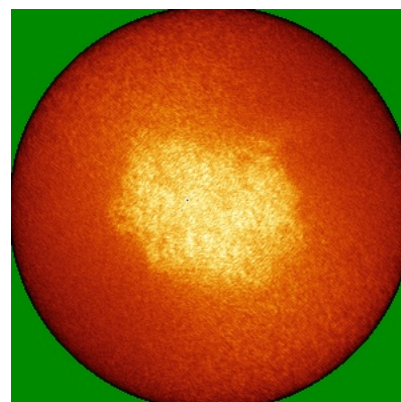
6.4.2 Raw map



X



Y

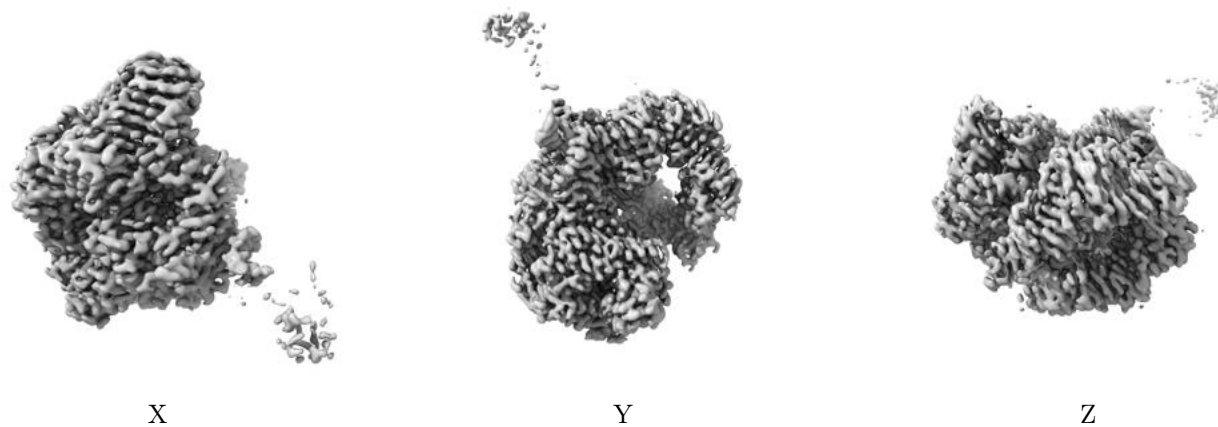


Z

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.

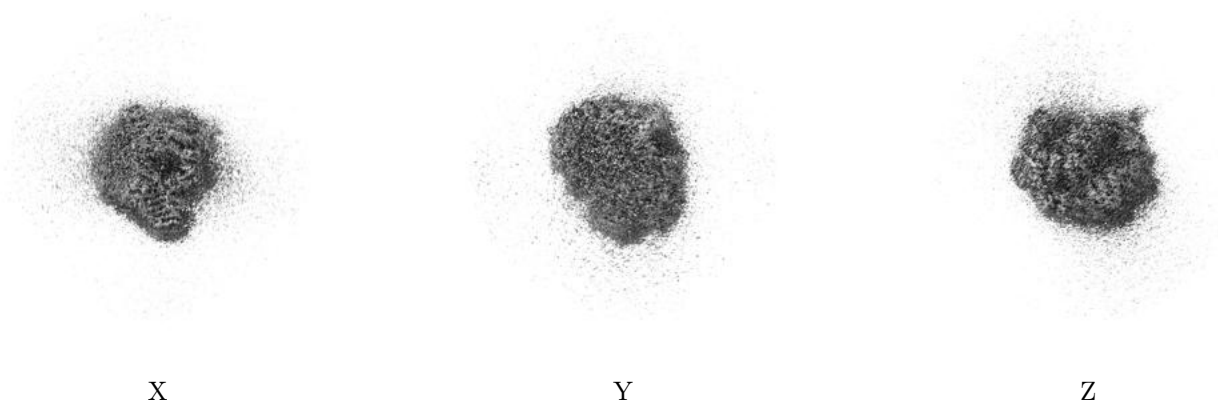
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

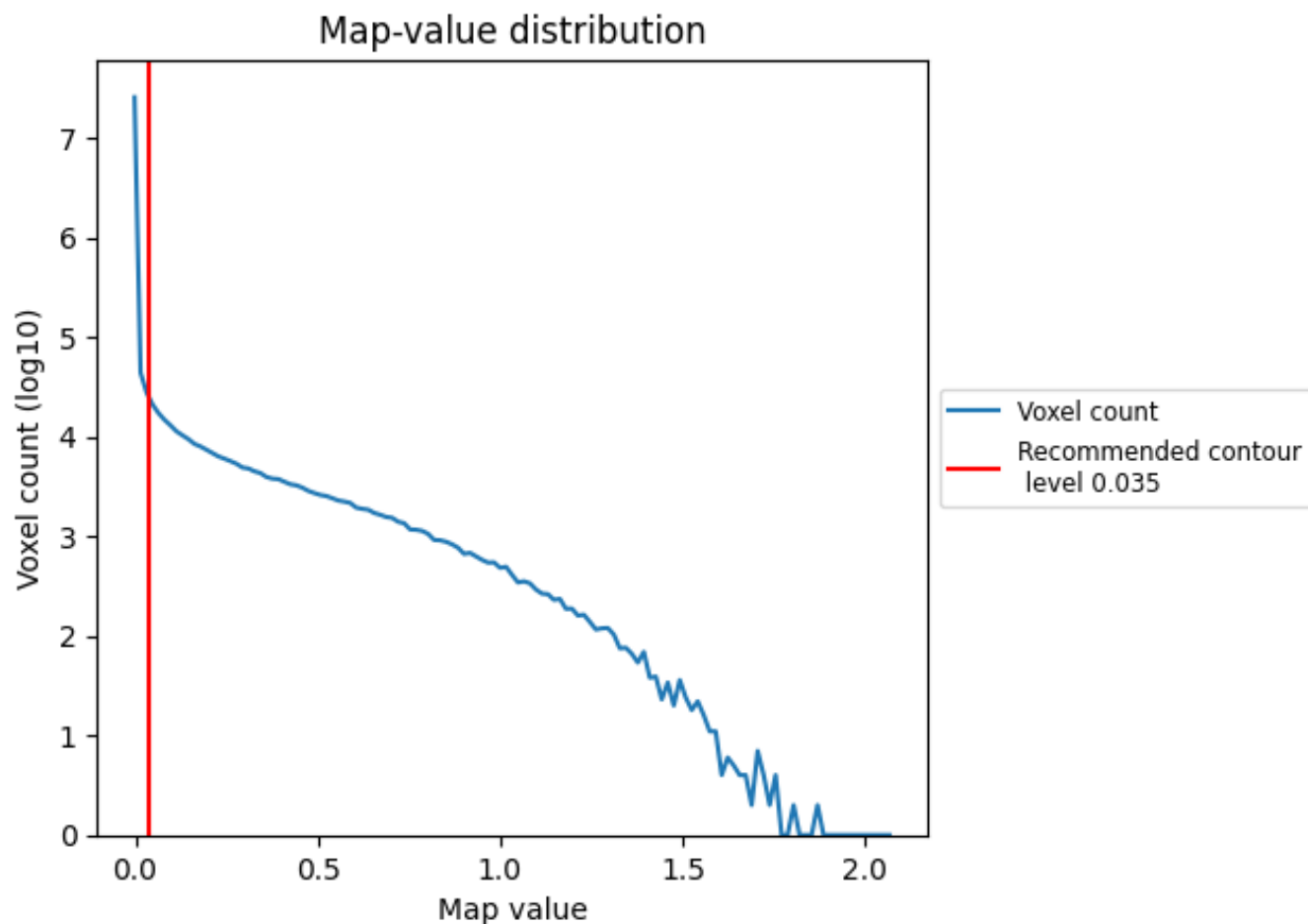
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

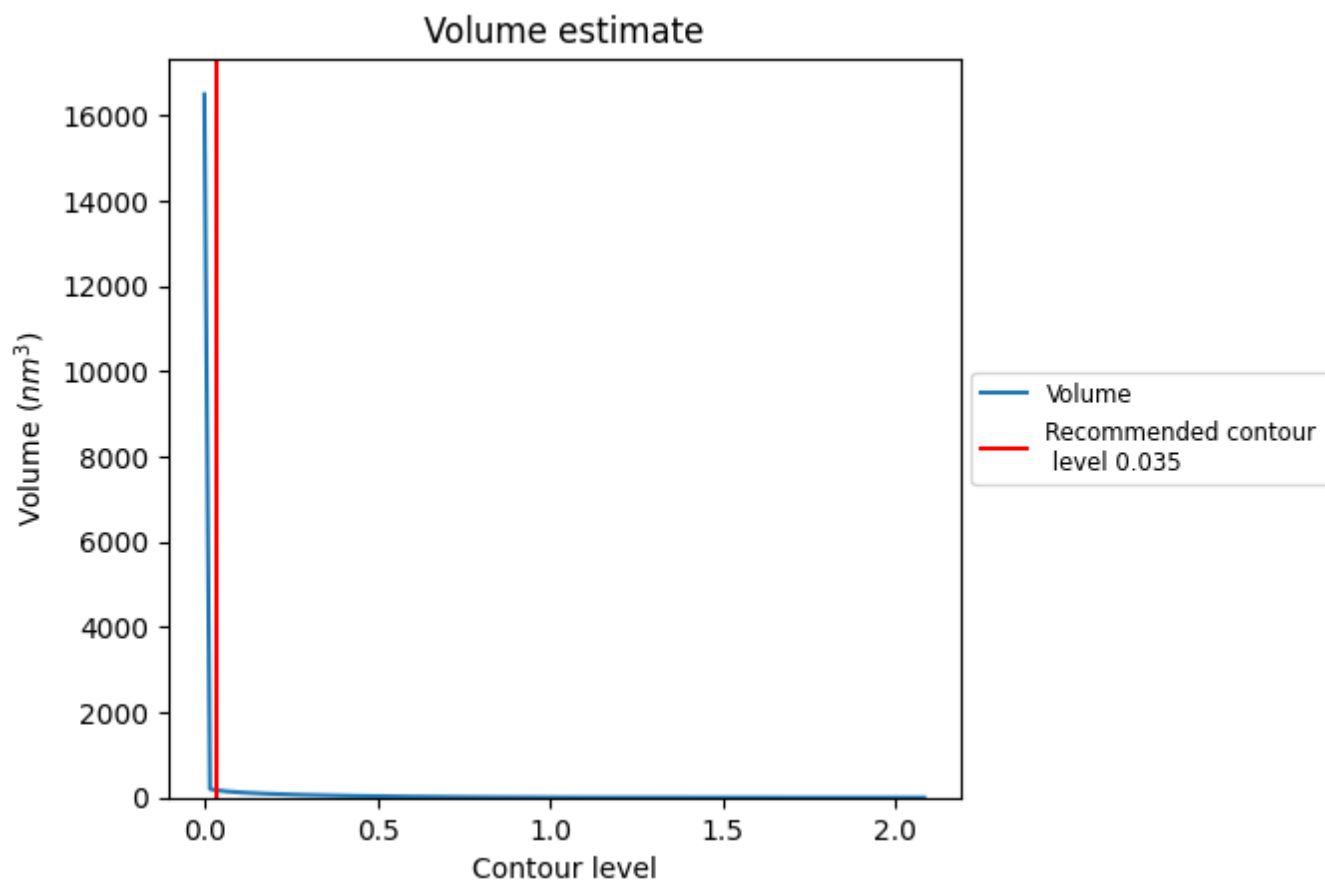
This section contains the results of statistical analysis of the map.

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.

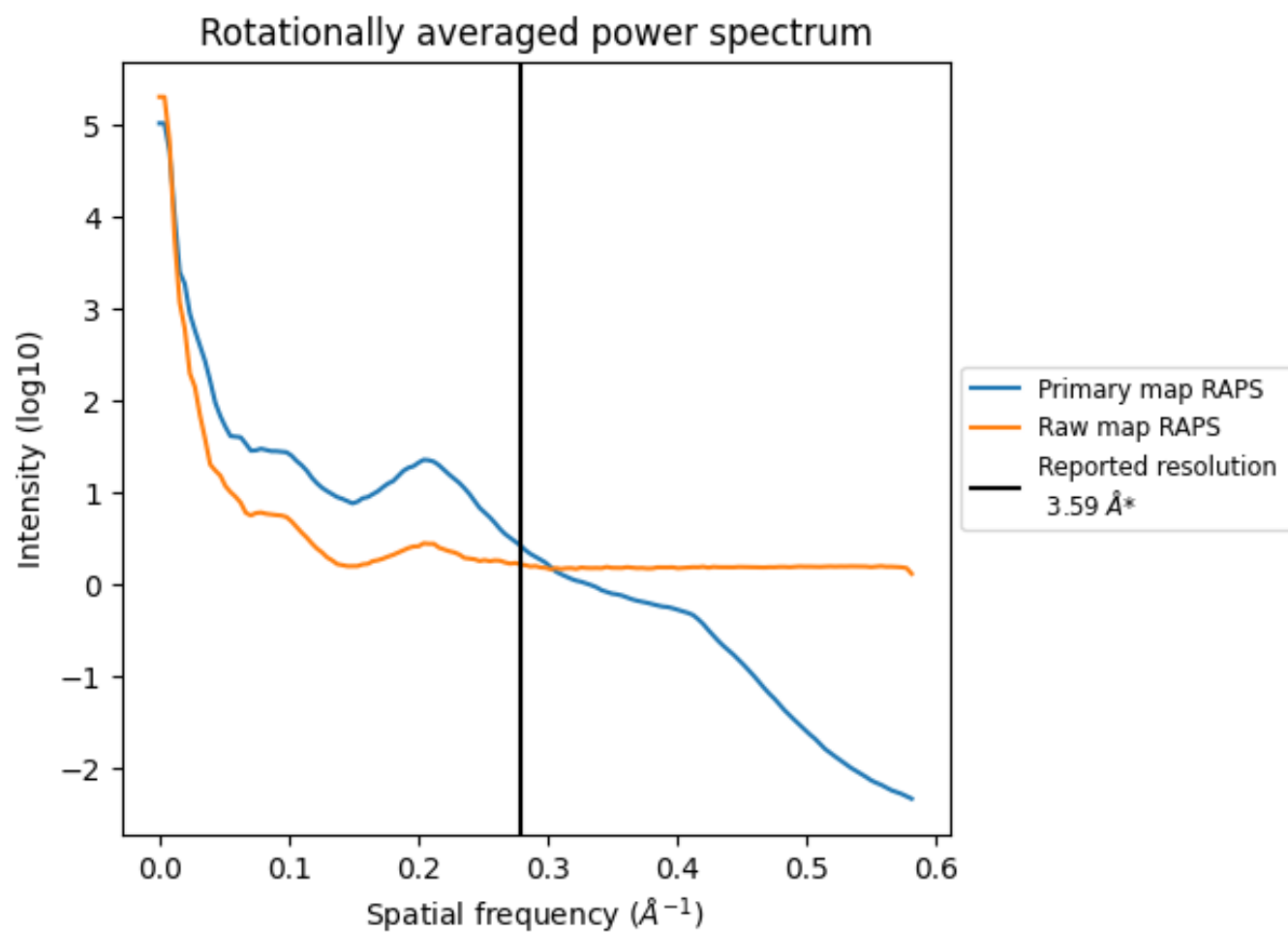
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 171 nm^3 ; this corresponds to an approximate mass of 154 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

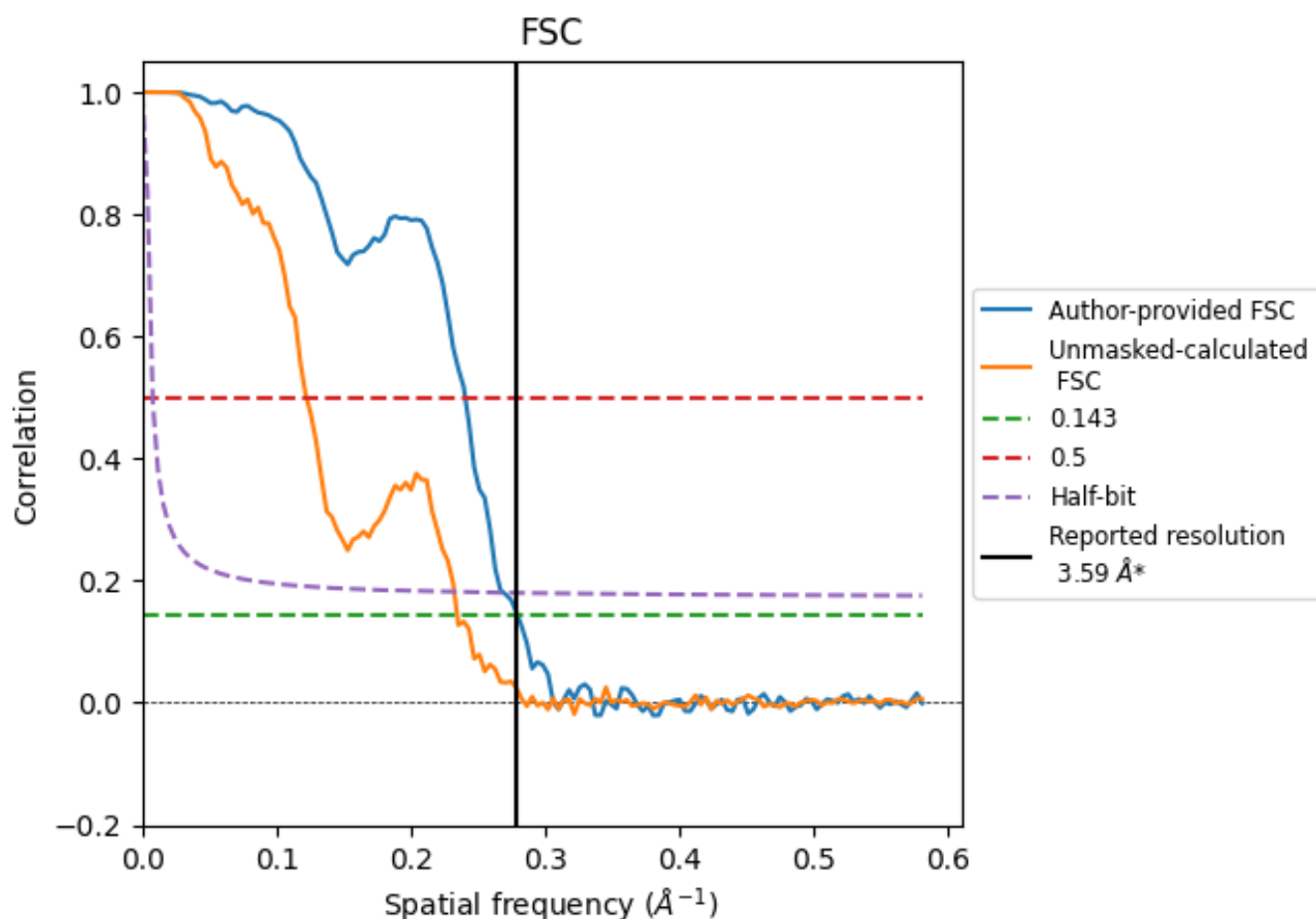


*Reported resolution corresponds to spatial frequency of 0.279 \AA^{-1}

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 0.279 \AA^{-1}

8.2 Resolution estimates [i](#)

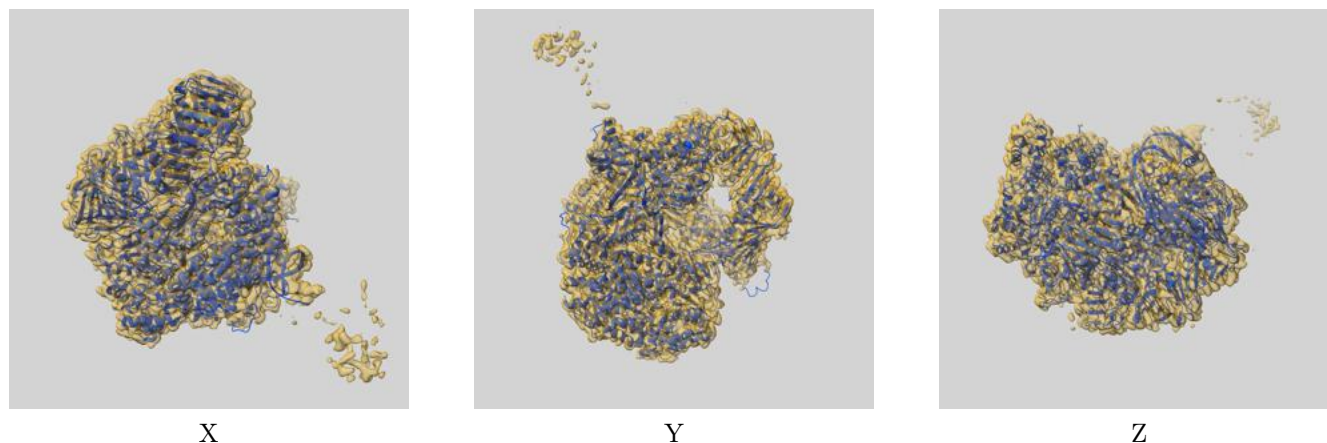
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	3.57	4.15	3.71
Unmasked-calculated*	4.26	8.17	4.30

*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 4.26 differs from the reported value 3.59 by more than 10 %

9 Map-model fit [i](#)

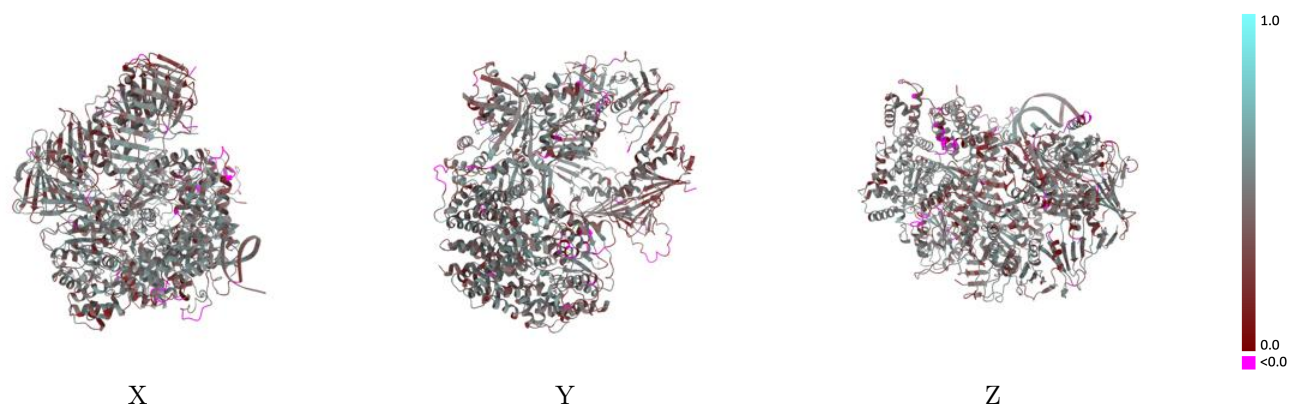
This section contains information regarding the fit between EMDB map EMD-14527 and PDB model 7Z6H. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



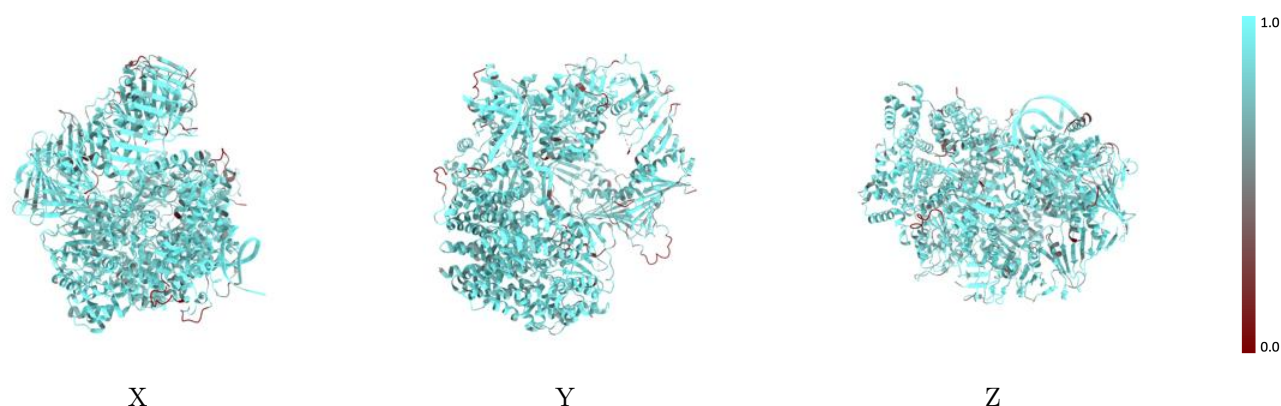
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



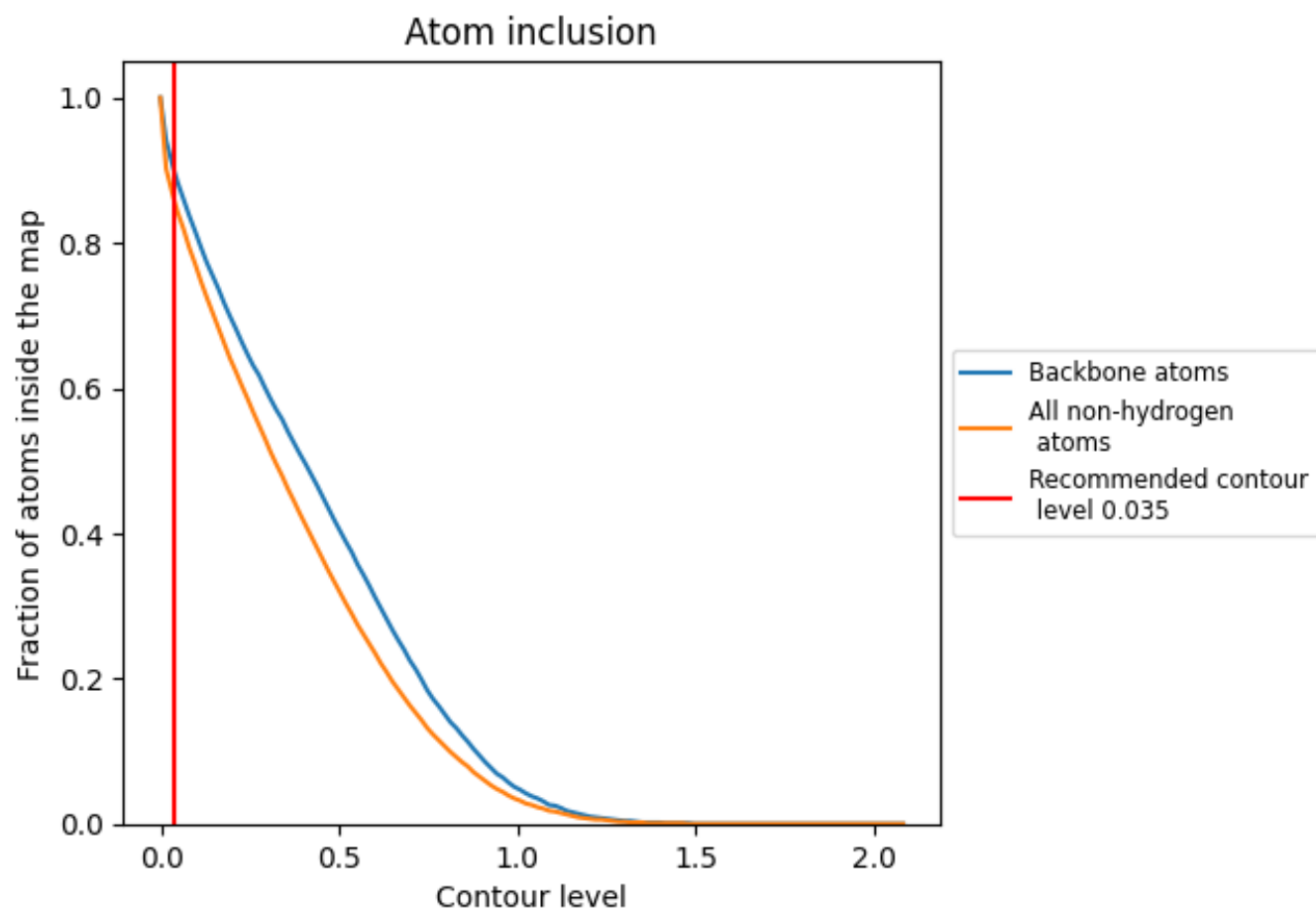
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8620	<div><div></div></div> 0.4180
A	<div><div></div></div> 0.8530	<div><div></div></div> 0.4230
B	<div><div></div></div> 0.8670	<div><div></div></div> 0.4240
C	<div><div></div></div> 0.7650	<div><div></div></div> 0.3150
D	<div><div></div></div> 0.8970	<div><div></div></div> 0.4620
E	<div><div></div></div> 0.8920	<div><div></div></div> 0.4270
F	<div><div></div></div> 0.8990	<div><div></div></div> 0.4400
G	<div><div></div></div> 0.9050	<div><div></div></div> 0.4540
K	<div><div></div></div> 0.8090	<div><div></div></div> 0.3850
X	<div><div></div></div> 0.9140	<div><div></div></div> 0.4690
Y	<div><div></div></div> 0.9040	<div><div></div></div> 0.4250

1.0

0.0

<0.0