



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 10:01 PM UTC

PDB ID : 8DQX / pdb_00008dqx
EMDB ID : EMD-27663
Title : Open state of RFC:PCNA bound to a 3' ss/dsDNA junction
Authors : Schrecker, M.; Hite, R.K.
Deposited on : 2022-07-20
Resolution : 2.10 Å(reported)
Based on initial model : 1SXJ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

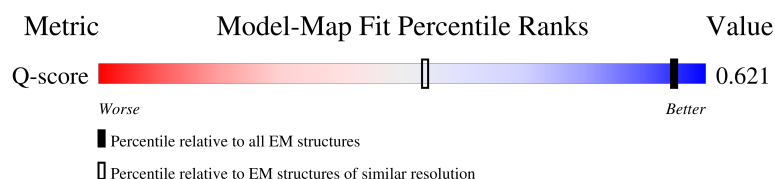
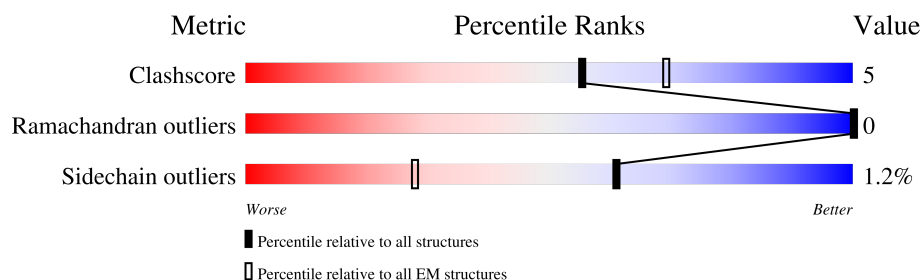
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	861	 50% 8% 42%
2	B	323	 90% 7% .
3	C	340	 83% 14% .
4	D	353	 88% 6% 6%

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Mol	Chain	Length	Quality of chain
5	E	354	92% 8%
6	F	259	85% 14%
6	G	259	85% 14%
6	H	259	85% 14%
7	I	6	83% 17%
8	J	10	60% 40%
9	K	10	90% 10%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 43240 atoms, of which 21210 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 Replication factor C subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	497	Total	C	H	N	O	S	0	0
			7919	2499	3982	691	729	18		

- Molecule 2 is a protein called Replication factor C subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	315	Total	C	H	N	O	S	0	0
			5039	1561	2564	441	460	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	330	Total	C	H	N	O	S	0	0
			5254	1643	2643	458	502	8		

- Molecule 4 is a protein called Replication factor C subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	332	Total	C	H	N	O	S	0	0
			5282	1659	2655	454	504	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	353	Total	C	H	N	O	S	0	0
			5685	1761	2902	484	520	18		

- Molecule 6 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	257	Total	C	H	N	O	S	0	0
			4046	1287	2032	318	399	10		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	256	Total	C	H	N	O	S	0	0
			4039	1284	2030	317	398	10		
6	H	258	Total	C	H	N	O	S	0	0
			4060	1293	2035	319	403	10		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP P15873
G	0	SER	-	expression tag	UNP P15873
H	0	SER	-	expression tag	UNP P15873

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	6	Total	C	H	N	O	P	0	0
			191	60	74	12	40	5		

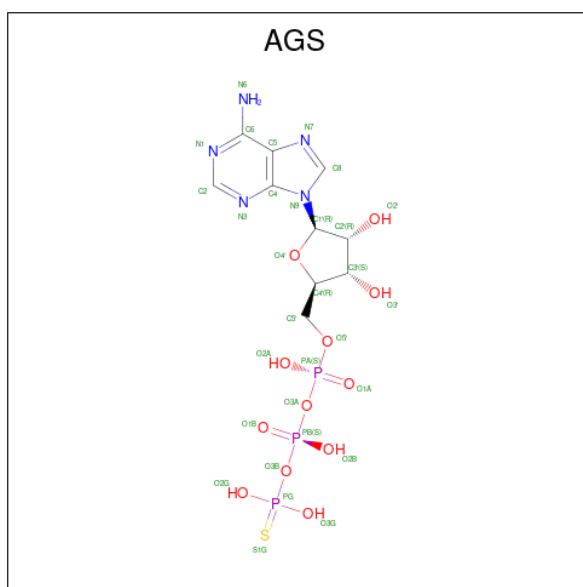
- Molecule 8 is a DNA chain called DNA (5'-D(P*TP*CP*CP*GP*AP*GP*CP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	10	Total	C	H	N	O	P	0	0
			318	97	112	41	58	10		

- Molecule 9 is a DNA chain called DNA (5'-D(P*TP*TP*TP*GP*CP*CP*CP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	10	Total	C	H	N	O	P	0	0
			318	97	114	35	62	10		

- Molecule 10 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

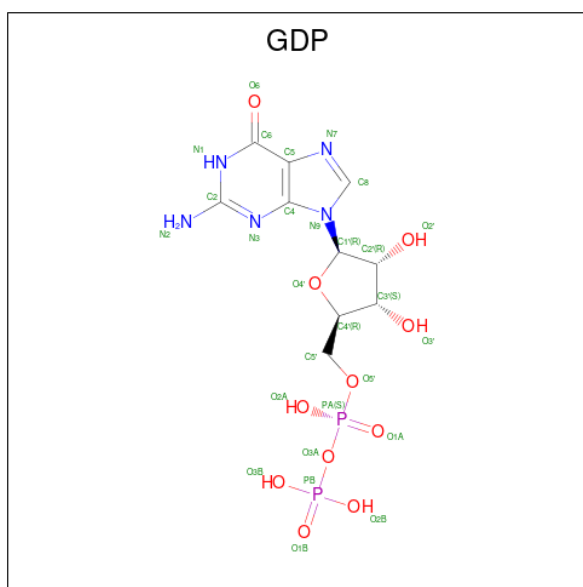


Mol	Chain	Residues	Atoms							AltConf
10	A	1	Total	C	H	N	O	P	S	0
			44	10	13	5	12	3	1	
10	B	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	
10	C	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	
10	D	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	
11	B	1	Total	Mg	0
			1	1	
11	C	1	Total	Mg	0
			1	1	
11	D	1	Total	Mg	0
			1	1	

- Molecule 12 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
12	E	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	126	Total 126	O 126	0
13	B	150	Total 150	O 150	0
13	C	156	Total 156	O 156	0
13	D	182	Total 182	O 182	0
13	E	170	Total 170	O 170	0
13	F	50	Total 50	O 50	0
13	G	8	Total 8	O 8	0
13	H	9	Total 9	O 9	0
13	I	12	Total 12	O 12	0
13	K	3	Total 3	O 3	0

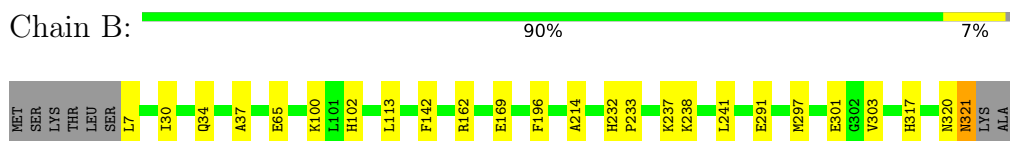
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Replication factor C subunit 1

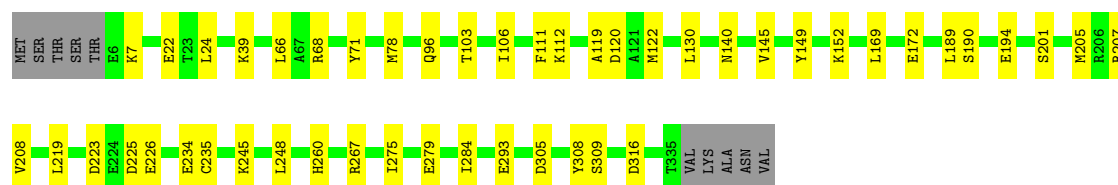


• Molecule 2: Replication factor C subunit 4



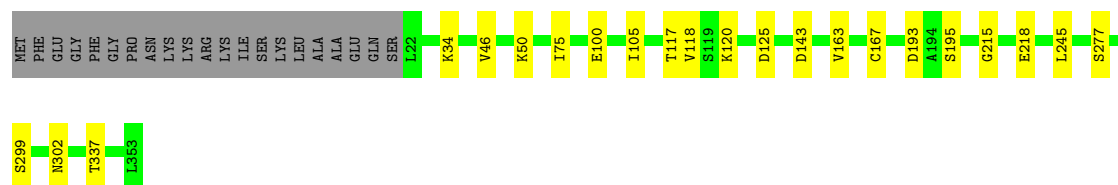
• Molecule 3: Replication factor C subunit 3

Chain C:  83% 14%



- Molecule 4: Replication factor C subunit 2

Chain D:  88% 6% 6%



- Molecule 5: Replication factor C subunit 5

Chain E:  92% 8%



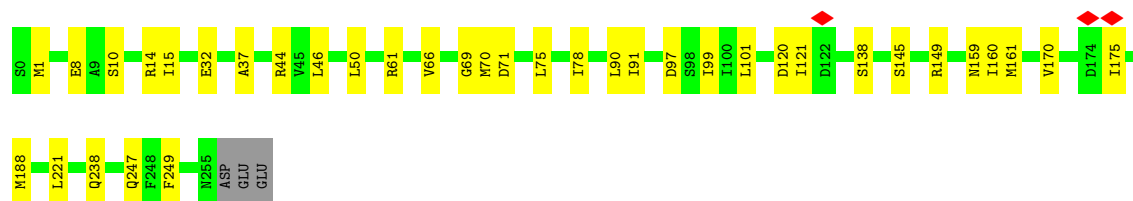
- Molecule 6: Proliferating cell nuclear antigen

Chain F:  85% 14%



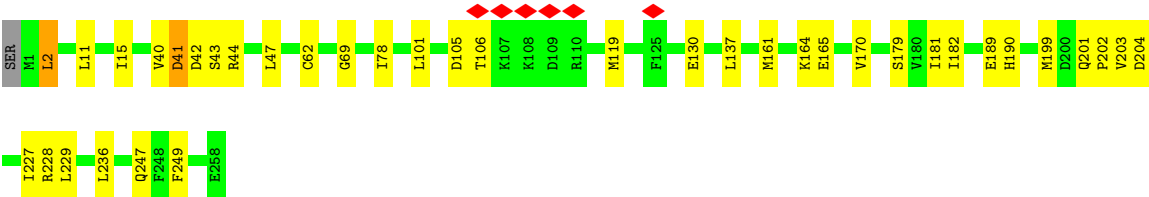
- Molecule 6: Proliferating cell nuclear antigen

Chain G:  85% 14%

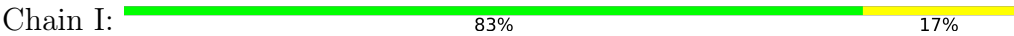


- Molecule 6: Proliferating cell nuclear antigen

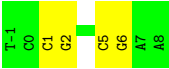
Chain H:  85% 14%



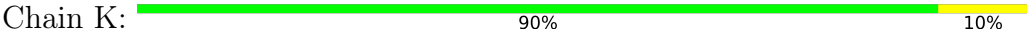
- Molecule 7: DNA (5'-D(*TP*TP*TP*TP*TP*T)-3')



- Molecule 8: DNA (5'-D(P*TP*CP*CP*GP*AP*GP*CP*GP*AP*A)-3')



- Molecule 9: DNA (5'-D(P*TP*TP*TP*GP*CP*CP*CP*GP*GP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	646330	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 ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.128	Depositor
Minimum map value	-0.658	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	317.184, 317.184, 317.184	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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, AGS, GDP

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	0.15	0/4016	0.34	0/5428
2	B	0.17	0/2510	0.35	0/3385
3	C	0.16	0/2651	0.34	0/3584
4	D	0.17	0/2672	0.35	0/3614
5	E	0.17	0/2823	0.33	0/3815
6	F	0.15	0/2044	0.33	0/2757
6	G	0.13	0/2039	0.30	0/2750
6	H	0.12	0/2055	0.27	0/2772
7	I	0.23	0/128	0.51	0/196
8	J	0.16	0/231	0.36	0/354
9	K	0.20	0/227	0.46	0/348
All	All	0.16	0/21396	0.33	0/29003

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	3937	3982	3981	48	0
2	B	2475	2564	2564	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2611	2643	2643	41	0
4	D	2627	2655	2655	17	0
5	E	2783	2902	2902	20	0
6	F	2014	2032	2032	30	0
6	G	2009	2030	2030	25	0
6	H	2025	2035	2037	25	0
7	I	117	74	74	1	0
8	J	206	112	112	3	0
9	K	204	114	114	1	0
10	A	31	13	12	1	0
10	B	31	14	11	0	0
10	C	31	14	11	0	0
10	D	31	14	12	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
12	E	28	12	11	0	0
13	A	126	0	0	7	0
13	B	150	0	0	5	0
13	C	156	0	0	5	0
13	D	182	0	0	4	0
13	E	170	0	0	13	0
13	F	50	0	0	6	0
13	G	8	0	0	0	0
13	H	9	0	0	0	0
13	I	12	0	0	1	0
13	K	3	0	0	0	0
All	All	22030	21210	21201	211	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 5.

All (211) 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)
2:B:214:ALA:O	3:C:39:LYS:NZ	1.98	0.96
5:E:142:GLU:OE2	13:E:501:HOH:O	1.88	0.91
1:A:635:GLU:OE1	13:A:1001:HOH:O	1.88	0.90
5:E:34:ARG:O	13:E:502:HOH:O	1.92	0.87
4:D:125:ASP:OD1	13:D:501:HOH:O	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:GLN:NE2	6:F:42:ASP:OD1	2.08	0.87
1:A:636:GLN:NE2	13:A:1002:HOH:O	2.06	0.86
1:A:544:GLU:OE2	2:B:162:ARG:NH1	2.09	0.86
6:G:8:GLU:N	6:G:8:GLU:OE1	2.11	0.84
3:C:207:ARG:NH1	13:C:501:HOH:O	2.09	0.83
5:E:15:ALA:O	13:E:503:HOH:O	1.96	0.83
2:B:100:LYS:NZ	6:G:120:ASP:OD1	2.11	0.83
1:A:633:SER:O	13:A:1002:HOH:O	1.97	0.83
2:B:102:HIS:O	13:B:501:HOH:O	1.98	0.82
1:A:584:ASP:OD1	13:A:1003:HOH:O	1.99	0.79
4:D:100:GLU:OE2	13:D:502:HOH:O	2.00	0.78
6:H:40:VAL:HG22	6:H:47:LEU:HD12	1.66	0.77
1:A:319:LYS:NZ	1:A:472:ASP:O	2.19	0.76
6:F:55:GLU:N	6:F:55:GLU:OE1	2.19	0.75
6:F:120:ASP:OD1	13:F:302:HOH:O	2.06	0.74
6:F:234:PRO:O	13:F:301:HOH:O	2.06	0.74
5:E:1:MET:N	13:E:507:HOH:O	2.20	0.73
2:B:196:PHE:O	13:B:502:HOH:O	2.06	0.73
2:B:291:GLU:OE2	13:B:503:HOH:O	2.09	0.70
1:A:697:ASP:OD1	13:A:1004:HOH:O	2.10	0.70
5:E:69:LYS:NZ	5:E:71:ASP:OD2	2.25	0.69
2:B:169:GLU:OE2	2:B:169:GLU:N	2.22	0.69
2:B:169:GLU:O	13:B:504:HOH:O	2.09	0.68
7:I:5:DT:OP2	13:I:101:HOH:O	2.11	0.68
5:E:330:GLU:OE1	13:E:504:HOH:O	2.10	0.68
3:C:305:ASP:OD1	13:C:502:HOH:O	2.11	0.68
6:G:90:LEU:HD22	6:G:101:LEU:HD22	1.77	0.67
6:G:70:MET:CE	6:G:75:LEU:HD22	2.24	0.67
5:E:182:LYS:NZ	13:E:510:HOH:O	2.24	0.66
1:A:483:ILE:HD12	1:A:487:LEU:HG	1.78	0.66
6:F:96:PRO:O	13:F:304:HOH:O	2.13	0.65
4:D:302:ASN:OD1	13:D:504:HOH:O	2.13	0.65
4:D:120:LYS:NZ	6:F:95:THR:O	2.30	0.65
3:C:103:THR:O	3:C:112:LYS:NZ	2.27	0.65
6:F:162:ILE:HB	6:F:203:VAL:HG22	1.79	0.65
6:F:103:PHE:O	13:F:305:HOH:O	2.14	0.65
6:H:236:LEU:HD11	6:H:247:GLN:HG2	1.78	0.65
3:C:267:ARG:NH1	3:C:316:ASP:OD2	2.30	0.64
3:C:260:HIS:ND1	13:C:503:HOH:O	2.26	0.63
4:D:193:ASP:OD1	4:D:195:SER:OG	2.17	0.62
1:A:717:PHE:HE1	1:A:725:ILE:HD13	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:46:VAL:HG12	4:D:50:LYS:HE2	1.83	0.60
1:A:483:ILE:HD11	1:A:507:ILE:HD11	1.82	0.60
3:C:245:LYS:HZ2	3:C:248:LEU:HD23	1.66	0.60
3:C:7:LYS:HE3	4:D:118:VAL:HG13	1.82	0.60
3:C:245:LYS:HE3	3:C:245:LYS:HA	1.85	0.59
6:G:69:GLY:HA3	6:G:121:ILE:HD12	1.85	0.58
6:H:199:MET:HE2	6:H:201:GLN:C	2.28	0.58
1:A:427:ASP:N	1:A:427:ASP:OD1	2.36	0.58
1:A:488:MET:HE3	1:A:488:MET:HA	1.86	0.58
3:C:245:LYS:NZ	3:C:248:LEU:HD23	2.17	0.58
6:H:130:GLU:N	6:H:130:GLU:OE1	2.37	0.58
6:F:188:MET:HE3	6:F:188:MET:HA	1.85	0.58
4:D:34:LYS:O	13:D:505:HOH:O	2.18	0.56
6:G:188:MET:HE3	6:G:188:MET:HA	1.87	0.56
2:B:303:VAL:O	2:B:303:VAL:HG12	2.06	0.56
1:A:627:VAL:HG21	1:A:647:LEU:HD12	1.86	0.56
3:C:140:ASN:ND2	13:C:505:HOH:O	2.34	0.56
3:C:245:LYS:HD2	3:C:284:ILE:HD13	1.88	0.56
3:C:189:LEU:HD23	3:C:194:GLU:OE1	2.06	0.56
6:H:42:ASP:OD1	6:H:43:SER:N	2.39	0.56
6:H:40:VAL:HG22	6:H:47:LEU:CD1	2.35	0.55
3:C:205:MET:HE3	13:C:616:HOH:O	2.04	0.55
1:A:478:PRO:HG3	1:A:514:ILE:HD11	1.88	0.55
1:A:338:ALA:HB2	1:A:345:VAL:HG13	1.89	0.55
5:E:112:LEU:HD23	5:E:113:LEU:N	2.23	0.54
6:H:164:LYS:NZ	6:H:165:GLU:OE1	2.27	0.54
3:C:24:LEU:HD11	3:C:66:LEU:HD23	1.89	0.54
1:A:565:SER:O	1:A:569:SER:OG	2.25	0.53
6:G:32:GLU:N	6:G:32:GLU:OE1	2.42	0.53
6:F:25:LEU:HD22	6:F:119:MET:HE1	1.88	0.53
5:E:253:PRO:O	13:E:506:HOH:O	2.19	0.53
3:C:7:LYS:HE3	4:D:118:VAL:HG22	1.90	0.53
6:H:41:ASP:OD1	6:H:44:ARG:N	2.42	0.52
1:A:515:ARG:NH2	10:A:901:AGS:S1G	2.82	0.52
6:F:128:ILE:HG23	6:F:128:ILE:O	2.10	0.52
1:A:672:GLN:OE1	13:A:1005:HOH:O	2.19	0.52
2:B:301:GLU:OE2	3:C:308:TYR:OH	2.28	0.52
6:G:175:ILE:O	6:G:175:ILE:HG22	2.09	0.52
3:C:22:GLU:O	3:C:68:ARG:NH1	2.43	0.51
3:C:106:ILE:HD11	6:F:45:VAL:C	2.36	0.51
6:G:78:ILE:CG2	6:G:101:LEU:HD12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:198:GLU:HA	6:F:198:GLU:OE1	2.09	0.51
5:E:47:THR:OG1	13:E:505:HOH:O	2.13	0.51
5:E:166:ARG:NH2	13:E:502:HOH:O	2.43	0.51
6:H:204:ASP:O	6:H:204:ASP:OD1	2.29	0.51
1:A:567:ILE:N	1:A:567:ILE:HD12	2.25	0.51
6:G:91:ILE:O	6:G:99:ILE:HD12	2.11	0.51
6:F:7:GLU:OE1	6:F:7:GLU:N	2.42	0.51
3:C:234:GLU:C	3:C:234:GLU:OE2	2.54	0.51
6:H:181:ILE:C	6:H:182:ILE:HD13	2.36	0.50
1:A:594:GLU:OE2	13:A:1006:HOH:O	2.19	0.50
5:E:225:ALA:HB2	5:E:254:ILE:HD13	1.94	0.50
6:G:61:ARG:HH11	6:G:61:ARG:HG2	1.77	0.50
6:F:71:ASP:OD2	6:F:73:THR:OG1	2.24	0.49
6:G:46:LEU:HD12	6:G:249:PHE:O	2.12	0.49
1:A:319:LYS:HE2	1:A:471:LEU:HD11	1.95	0.49
6:F:163:THR:OG1	6:F:166:THR:HG23	2.13	0.49
6:F:245:PHE:CD1	6:F:245:PHE:C	2.91	0.48
3:C:219:LEU:HD22	3:C:225:ASP:HB3	1.95	0.48
8:J:6:DG:H1	9:K:3:DT:H3	1.60	0.48
5:E:11:LYS:NZ	13:E:515:HOH:O	2.42	0.48
1:A:402:VAL:HG11	6:G:44:ARG:NH2	2.27	0.48
1:A:488:MET:O	1:A:492:ILE:HG13	2.13	0.48
6:H:41:ASP:OD2	6:H:43:SER:OG	2.31	0.48
5:E:317:ASN:ND2	13:E:513:HOH:O	2.30	0.48
6:F:179:SER:O	13:F:306:HOH:O	2.20	0.48
1:A:326:ASN:O	1:A:330:SER:OG	2.31	0.47
3:C:275:ILE:O	3:C:279:GLU:HG2	2.14	0.47
6:G:238:GLN:OE1	6:G:247:GLN:NE2	2.39	0.47
1:A:320:LEU:HD21	1:A:366:VAL:HG11	1.96	0.47
3:C:119:ALA:CB	3:C:145:VAL:HG13	2.45	0.47
6:G:1:MET:HE1	6:G:66:VAL:HG21	1.97	0.47
6:H:2:LEU:HD13	6:H:62:CYS:HB2	1.97	0.47
2:B:37:ALA:HB1	2:B:65:GLU:HG2	1.97	0.47
6:G:78:ILE:HG21	6:G:101:LEU:HD12	1.97	0.47
1:A:367:ALA:HB3	1:A:374:ILE:HD11	1.97	0.47
3:C:122:MET:HE1	3:C:130:LEU:HD11	1.97	0.47
3:C:201:SER:OG	3:C:208:VAL:HG22	2.15	0.46
8:J:1:DC:H2"	8:J:2:DG:C8	2.51	0.46
1:A:385:LYS:NZ	1:A:439:GLN:OE1	2.47	0.46
4:D:100:GLU:HG3	4:D:105:ILE:HG13	1.97	0.46
6:H:137:LEU:HD12	6:H:137:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:MET:O	1:A:318:MET:HE3	2.16	0.46
6:H:161:MET:HE1	6:H:170:VAL:HG23	1.98	0.45
2:B:113:LEU:HD12	2:B:142:PHE:CE2	2.52	0.45
3:C:234:GLU:OE2	3:C:235:CYS:N	2.49	0.45
3:C:245:LYS:HE3	3:C:245:LYS:CA	2.47	0.45
3:C:172:GLU:H	3:C:172:GLU:CD	2.24	0.45
6:G:145:SER:OG	6:G:149:ARG:NH1	2.49	0.45
3:C:223:ASP:N	3:C:223:ASP:OD1	2.50	0.45
2:B:7:LEU:HD13	3:C:111:PHE:CD1	2.52	0.44
6:F:19:PHE:CE1	6:F:72:LEU:HD11	2.52	0.44
6:H:199:MET:HE2	6:H:202:PRO:N	2.31	0.44
1:A:426:VAL:HG21	1:A:453:LEU:HD23	1.98	0.44
1:A:544:GLU:OE2	1:A:544:GLU:N	2.50	0.44
6:H:78:ILE:HG21	6:H:101:LEU:HD12	1.98	0.44
1:A:784:TYR:CZ	6:H:119:MET:HE1	2.52	0.44
2:B:232:HIS:N	2:B:233:PRO:CD	2.81	0.44
5:E:286:LEU:HD11	5:E:346:ILE:HD12	1.99	0.44
6:F:140:PRO:HG2	6:F:143:GLU:OE2	2.18	0.44
6:G:10:SER:O	6:G:14:ARG:HG3	2.18	0.44
6:H:11:LEU:O	6:H:15:ILE:HG13	2.17	0.44
1:A:338:ALA:HB1	1:A:342:GLY:HA2	2.00	0.44
8:J:5:DC:H2"	8:J:6:DG:C8	2.52	0.44
4:D:75:ILE:HD13	4:D:167:CYS:SG	2.57	0.44
5:E:335:GLY:O	13:E:508:HOH:O	2.21	0.44
6:F:7:GLU:N	6:F:7:GLU:CD	2.75	0.44
1:A:396:LEU:HD23	1:A:421:ILE:HD12	2.00	0.44
1:A:478:PRO:CG	1:A:514:ILE:HD11	2.47	0.43
1:A:681:ARG:O	1:A:685:GLU:HG3	2.18	0.43
1:A:546:ASN:OD1	2:B:162:ARG:NH2	2.51	0.43
3:C:7:LYS:NZ	4:D:117:THR:HG23	2.34	0.43
6:H:69:GLY:O	6:H:119:MET:N	2.51	0.43
1:A:298:TRP:HA	1:A:301:LYS:HG2	2.01	0.43
1:A:441:ALA:O	1:A:445:ARG:HG3	2.19	0.43
2:B:30:ILE:O	2:B:34:GLN:HG3	2.19	0.43
6:G:15:ILE:HA	6:G:221:LEU:HD11	2.01	0.43
4:D:337:THR:HB	5:E:329:ASP:OD2	2.18	0.43
5:E:106:ARG:NH2	5:E:149:ASP:OD2	2.51	0.43
6:H:228:ARG:C	6:H:229:LEU:HD22	2.44	0.43
6:F:164:LYS:O	6:F:166:THR:HG22	2.18	0.43
3:C:169:LEU:HD13	3:C:205:MET:CE	2.49	0.42
4:D:215:GLY:HA2	4:D:218:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:189:GLU:OE2	6:H:190:HIS:ND1	2.52	0.42
3:C:7:LYS:CE	4:D:118:VAL:HG22	2.49	0.42
5:E:208:ASN:ND2	13:E:518:HOH:O	2.44	0.42
1:A:372:TYR:CG	1:A:420:VAL:HG23	2.54	0.42
1:A:292:ARG:NH1	1:A:295:ASP:OD1	2.52	0.42
2:B:238:LYS:O	13:B:505:HOH:O	2.22	0.42
6:F:162:ILE:CD1	6:F:167:ILE:HG23	2.49	0.42
3:C:7:LYS:HE2	4:D:163:VAL:HG12	2.02	0.42
4:D:143:ASP:OD1	4:D:143:ASP:N	2.53	0.42
3:C:169:LEU:HD13	3:C:205:MET:HE3	2.01	0.42
6:G:37:ALA:HB3	6:G:50:LEU:HB3	2.02	0.42
6:H:236:LEU:HD13	6:H:249:PHE:CE2	2.54	0.42
6:F:42:ASP:OD1	6:F:42:ASP:C	2.63	0.41
1:A:372:TYR:CB	1:A:420:VAL:HG23	2.50	0.41
1:A:567:ILE:N	1:A:567:ILE:CD1	2.84	0.41
1:A:426:VAL:HG12	1:A:463:MET:HE1	2.03	0.41
6:F:36:ILE:HD12	6:F:125:PHE:HE2	1.86	0.41
1:A:544:GLU:O	1:A:544:GLU:CD	2.64	0.41
2:B:317:HIS:CD2	3:C:293:GLU:OE1	2.73	0.41
2:B:320:ASN:O	2:B:321:ASN:ND2	2.43	0.41
6:G:70:MET:HE1	6:G:75:LEU:HD22	2.00	0.41
3:C:96:GLN:CD	6:F:42:ASP:OD1	2.61	0.41
3:C:149:TYR:HB2	3:C:152:LYS:HD2	2.03	0.41
6:G:161:MET:HE1	6:G:170:VAL:HG21	2.02	0.41
6:H:227:ILE:HG22	6:H:229:LEU:HD21	2.02	0.41
3:C:190:SER:N	3:C:226:GLU:OE2	2.54	0.41
5:E:57:LEU:HD11	5:E:139:ILE:HD11	2.03	0.40
6:F:0:SER:O	6:F:61:ARG:NH1	2.48	0.40
1:A:541:LYS:HB3	1:A:541:LYS:HE2	1.98	0.40
2:B:102:HIS:ND1	6:G:97:ASP:OD1	2.44	0.40
2:B:237:LYS:NZ	2:B:241:LEU:HD11	2.35	0.40
3:C:71:TYR:CD1	3:C:78:MET:HE3	2.57	0.40
6:G:61:ARG:HG2	6:G:61:ARG:NH1	2.37	0.40
6:G:159:ASN:OD1	6:G:160:ILE:N	2.54	0.40
6:F:71:ASP:HB2	6:F:119:MET:CE	2.51	0.40
6:F:112:ALA:N	13:F:305:HOH:O	2.50	0.40
1:A:363:ALA:O	1:A:366:VAL:HG12	2.21	0.40
6:F:199:MET:O	6:F:199:MET:HG3	2.20	0.40
6:H:105:ASP:OD1	6:H:106:THR:N	2.52	0.40
1:A:514:ILE:O	1:A:517:VAL:HG12	2.21	0.40
1:A:630:LYS:NZ	2:B:297:MET:SD	2.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:78:ILE:HG21	6:H:101:LEU:CD1	2.51	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	495/861 (58%)	483 (98%)	12 (2%)	0	100	100
2	B	313/323 (97%)	304 (97%)	9 (3%)	0	100	100
3	C	328/340 (96%)	325 (99%)	3 (1%)	0	100	100
4	D	330/353 (94%)	327 (99%)	3 (1%)	0	100	100
5	E	351/354 (99%)	345 (98%)	6 (2%)	0	100	100
6	F	255/259 (98%)	247 (97%)	8 (3%)	0	100	100
6	G	254/259 (98%)	248 (98%)	6 (2%)	0	100	100
6	H	256/259 (99%)	252 (98%)	4 (2%)	0	100	100
All	All	2582/3008 (86%)	2531 (98%)	51 (2%)	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	432/742 (58%)	424 (98%)	8 (2%)	50	58
2	B	276/283 (98%)	275 (100%)	1 (0%)	84	89
3	C	286/296 (97%)	284 (99%)	2 (1%)	76	83
4	D	294/312 (94%)	291 (99%)	3 (1%)	68	76
5	E	322/324 (99%)	319 (99%)	3 (1%)	70	78
6	F	231/234 (99%)	226 (98%)	5 (2%)	45	53
6	G	231/234 (99%)	229 (99%)	2 (1%)	70	78
6	H	232/234 (99%)	228 (98%)	4 (2%)	53	62
All	All	2304/2659 (87%)	2276 (99%)	28 (1%)	61	72

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	SER
1	A	398	ASN
1	A	585	PHE
1	A	614	VAL
1	A	664	ILE
1	A	674	SER
1	A	729	ILE
1	A	783	ILE
2	B	321	ASN
3	C	120	ASP
3	C	309	SER
4	D	245	LEU
4	D	277	SER
4	D	299	SER
5	E	131	LEU
5	E	162	SER
5	E	352	CYS
6	F	22	CYS
6	F	64	HIS
6	F	157	SER
6	F	166	THR
6	F	193	THR
6	G	71	ASP
6	G	138	SER
6	H	2	LEU
6	H	41	ASP
6	H	179	SER

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Mol	Chain	Res	Type
6	H	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	GLN
1	A	474	GLN
1	A	562	GLN
1	A	659	HIS
2	B	60	HIS
2	B	95	HIS
2	B	148	ASN
3	C	77	ASN
3	C	171	GLN
3	C	264	ASN
3	C	317	GLN
4	D	35	ASN
4	D	338	ASN
4	D	345	ASN
5	E	19	ASN
5	E	86	ASN
5	E	118	GLN
5	E	141	ASN
5	E	264	HIS
6	F	132	GLN
6	F	247	GLN
6	G	94	ASN
6	G	190	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 9 ligands modelled in this entry, 4 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
10	AGS	C	402	11	32,33,33	3.37	16 (50%)	45,52,52	1.94	13 (28%)
10	AGS	B	402	11	32,33,33	3.40	17 (53%)	45,52,52	1.97	10 (22%)
12	GDP	E	401	-	29,30,30	3.39	15 (51%)	45,47,47	1.68	9 (20%)
10	AGS	D	402	11	32,33,33	3.35	17 (53%)	45,52,52	1.97	12 (26%)
10	AGS	A	901	11	32,33,33	3.41	17 (53%)	45,52,52	1.93	13 (28%)

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
10	AGS	C	402	11	-	1/21/38/38	0/3/3/3
10	AGS	B	402	11	-	2/21/38/38	0/3/3/3
12	GDP	E	401	-	-	2/16/32/32	0/3/3/3
10	AGS	D	402	11	-	2/21/38/38	0/3/3/3
10	AGS	A	901	11	-	3/21/38/38	0/3/3/3

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	402	AGS	C2'-C3'	-10.63	1.24	1.53
10	A	901	AGS	C2'-C3'	-10.62	1.24	1.53
10	D	402	AGS	C2'-C3'	-10.49	1.24	1.53
10	C	402	AGS	C2'-C3'	-10.47	1.25	1.53
12	E	401	GDP	C3'-C4'	-8.51	1.31	1.53
12	E	401	GDP	O4'-C4'	7.64	1.62	1.45
12	E	401	GDP	C4-N3	6.46	1.49	1.34
10	C	402	AGS	O4'-C4'	-6.12	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	402	AGS	O4'-C4'	-6.07	1.31	1.45
10	D	402	AGS	O4'-C4'	-5.97	1.31	1.45
10	A	901	AGS	O4'-C4'	-5.93	1.31	1.45
10	D	402	AGS	C3'-C4'	5.60	1.67	1.53
10	B	402	AGS	C3'-C4'	5.58	1.67	1.53
10	C	402	AGS	C3'-C4'	5.54	1.67	1.53
10	A	901	AGS	C3'-C4'	5.47	1.66	1.53
12	E	401	GDP	C2-N3	5.41	1.46	1.33
10	B	402	AGS	PB-O3B	5.20	1.65	1.59
10	A	901	AGS	PB-O3B	5.11	1.65	1.59
10	D	402	AGS	C6-N6	5.04	1.47	1.34
10	C	402	AGS	C6-N6	5.04	1.47	1.34
10	C	402	AGS	PB-O3B	5.01	1.64	1.59
10	B	402	AGS	C6-N6	5.01	1.47	1.34
10	A	901	AGS	C6-N6	4.99	1.47	1.34
10	D	402	AGS	PB-O3B	4.90	1.64	1.59
12	E	401	GDP	C2-N2	4.79	1.45	1.34
12	E	401	GDP	O4'-C1'	-4.72	1.31	1.42
10	B	402	AGS	C1'-N9	-4.69	1.33	1.46
10	A	901	AGS	C1'-N9	-4.61	1.33	1.46
12	E	401	GDP	PA-O3A	4.60	1.64	1.59
10	D	402	AGS	C1'-N9	-4.54	1.33	1.46
10	C	402	AGS	C1'-N9	-4.42	1.34	1.46
10	A	901	AGS	O4'-C1'	4.16	1.51	1.42
10	B	402	AGS	O4'-C1'	4.13	1.51	1.42
10	A	901	AGS	PG-O3G	4.13	1.68	1.54
10	C	402	AGS	PG-O3G	4.07	1.67	1.54
10	C	402	AGS	O4'-C1'	4.06	1.51	1.42
10	D	402	AGS	O4'-C1'	4.05	1.51	1.42
10	D	402	AGS	PG-O3G	4.01	1.67	1.54
10	B	402	AGS	PG-O3G	3.96	1.67	1.54
10	A	901	AGS	PG-O2G	3.65	1.66	1.54
10	B	402	AGS	PG-O2G	3.65	1.66	1.54
10	D	402	AGS	PG-O2G	3.56	1.66	1.54
10	C	402	AGS	PG-O2G	3.56	1.66	1.54
10	A	901	AGS	C5-C4	-3.42	1.33	1.39
10	D	402	AGS	C5-C4	-3.30	1.33	1.39
10	C	402	AGS	C5-C4	-3.26	1.33	1.39
10	B	402	AGS	C5-C4	-3.25	1.33	1.39
10	A	901	AGS	PB-O3A	3.19	1.62	1.59
10	C	402	AGS	PB-O3A	2.99	1.62	1.59
12	E	401	GDP	C5-N7	-2.99	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	402	AGS	C5-N7	-2.94	1.33	1.39
10	D	402	AGS	C5-N7	-2.86	1.33	1.39
10	B	402	AGS	PB-O3A	2.86	1.62	1.59
10	A	901	AGS	C5-N7	-2.82	1.33	1.39
10	B	402	AGS	C5-N7	-2.79	1.34	1.39
12	E	401	GDP	O2'-C2'	-2.76	1.36	1.43
12	E	401	GDP	O6-C6	-2.75	1.18	1.23
10	D	402	AGS	C8-N9	-2.74	1.32	1.37
10	B	402	AGS	C8-N9	-2.72	1.32	1.37
10	C	402	AGS	C8-N9	-2.69	1.33	1.37
12	E	401	GDP	C2-N1	2.66	1.44	1.37
12	E	401	GDP	O3'-C3'	2.65	1.49	1.43
10	D	402	AGS	PB-O3A	2.64	1.62	1.59
10	A	901	AGS	C8-N9	-2.60	1.33	1.37
12	E	401	GDP	C5-C6	2.54	1.53	1.44
10	D	402	AGS	O3'-C3'	2.54	1.49	1.43
10	C	402	AGS	O3'-C3'	2.53	1.49	1.43
10	A	901	AGS	C2'-C1'	2.52	1.61	1.53
10	C	402	AGS	C2'-C1'	2.52	1.61	1.53
10	D	402	AGS	C2'-C1'	2.52	1.61	1.53
10	A	901	AGS	O3'-C3'	2.52	1.49	1.43
10	A	901	AGS	O2'-C2'	2.50	1.49	1.43
10	C	402	AGS	O2'-C2'	2.48	1.49	1.43
10	B	402	AGS	O2'-C2'	2.47	1.49	1.43
12	E	401	GDP	C6-N1	2.40	1.43	1.38
10	B	402	AGS	C2'-C1'	2.38	1.61	1.53
10	B	402	AGS	O3'-C3'	2.38	1.48	1.43
10	D	402	AGS	O2'-C2'	2.34	1.48	1.43
10	A	901	AGS	PA-O5'	2.16	1.67	1.59
12	E	401	GDP	C4-N9	-2.12	1.32	1.38
10	B	402	AGS	PA-O5'	2.11	1.67	1.59
10	D	402	AGS	PA-O5'	2.07	1.67	1.59

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	402	AGS	N3-C2-N1	-5.61	120.09	128.58
10	C	402	AGS	C5-C4-N3	-5.56	119.06	126.72
10	A	901	AGS	N3-C2-N1	-5.53	120.21	128.58
10	D	402	AGS	N3-C2-N1	-5.51	120.25	128.58
10	B	402	AGS	C5-C4-N3	-5.41	119.26	126.72
10	D	402	AGS	C5-C4-N3	-5.41	119.27	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	901	AGS	C5-C4-N3	-5.38	119.31	126.72
10	C	402	AGS	N3-C2-N1	-5.37	120.45	128.58
12	E	401	GDP	C5-C4-N3	-4.99	120.45	128.39
12	E	401	GDP	C2-N3-C4	4.47	120.00	112.30
10	A	901	AGS	N9-C8-N7	-3.94	108.34	113.94
10	B	402	AGS	N9-C8-N7	-3.93	108.35	113.94
10	D	402	AGS	N9-C8-N7	-3.74	108.62	113.94
10	C	402	AGS	N9-C8-N7	-3.66	108.74	113.94
10	D	402	AGS	C2-N3-C4	3.59	120.60	111.83
10	C	402	AGS	C2-N3-C4	3.59	120.59	111.83
10	B	402	AGS	C2-N3-C4	3.56	120.52	111.83
10	A	901	AGS	C2-N3-C4	3.54	120.48	111.83
10	B	402	AGS	N3-C4-N9	3.46	133.05	127.17
12	E	401	GDP	N9-C8-N7	-3.44	107.03	113.40
10	C	402	AGS	N3-C4-N9	3.38	132.92	127.17
12	E	401	GDP	N9-C4-N3	3.26	132.47	125.95
10	D	402	AGS	N3-C4-N9	3.24	132.68	127.17
10	A	901	AGS	N3-C4-N9	3.22	132.65	127.17
10	B	402	AGS	C5-N7-C8	2.97	108.12	103.45
10	A	901	AGS	C4-N9-C1'	-2.92	119.79	126.63
10	A	901	AGS	C5-N7-C8	2.92	108.05	103.45
10	D	402	AGS	C5-N7-C8	2.91	108.03	103.45
12	E	401	GDP	C2-N1-C6	-2.91	119.83	125.11
10	D	402	AGS	C4-N9-C1'	-2.78	120.13	126.63
10	C	402	AGS	C5-N7-C8	2.77	107.81	103.45
12	E	401	GDP	C5-C6-N1	2.58	119.81	113.25
10	B	402	AGS	C4-N9-C1'	-2.52	120.73	126.63
10	A	901	AGS	C1'-N9-C8	2.49	132.62	127.09
10	A	901	AGS	PB-O3B-PG	-2.48	124.09	133.17
10	C	402	AGS	C4-N9-C1'	-2.44	120.93	126.63
10	D	402	AGS	C1'-N9-C8	2.39	132.41	127.09
12	E	401	GDP	C8-N7-C5	2.39	108.52	104.26
10	D	402	AGS	C4-C5-N7	-2.38	107.86	110.58
12	E	401	GDP	O6-C6-C5	-2.35	120.33	126.53
10	A	901	AGS	C6-C5-C4	2.32	120.34	117.18
10	C	402	AGS	C6-C5-C4	2.29	120.30	117.18
10	A	901	AGS	C4-C5-N7	-2.26	107.99	110.58
10	B	402	AGS	C6-C5-C4	2.26	120.26	117.18
10	D	402	AGS	C6-C5-C4	2.23	120.22	117.18
10	B	402	AGS	C4-C5-N7	-2.22	108.04	110.58
10	C	402	AGS	C4-C5-N7	-2.21	108.06	110.58
10	D	402	AGS	N6-C6-N1	-2.19	113.50	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	402	AGS	N6-C6-N1	-2.18	113.53	118.38
10	C	402	AGS	PB-O3B-PG	-2.09	125.54	133.17
10	D	402	AGS	C5-C4-N9	2.06	108.05	105.81
10	C	402	AGS	C1'-N9-C8	2.05	131.65	127.09
10	B	402	AGS	PB-O3B-PG	-2.05	125.66	133.17
10	A	901	AGS	N6-C6-N1	-2.05	113.82	118.38
10	A	901	AGS	C5-C4-N9	2.04	108.04	105.81
12	E	401	GDP	C1'-N9-C4	-2.04	120.47	126.49
10	C	402	AGS	C5-C4-N9	2.03	108.02	105.81

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	E	401	GDP	PA-O3A-PB-O3B
10	A	901	AGS	PA-O3A-PB-O1B
10	A	901	AGS	C5'-O5'-PA-O2A
10	B	402	AGS	PA-O3A-PB-O2B
10	D	402	AGS	PA-O3A-PB-O2B
12	E	401	GDP	PA-O3A-PB-O2B
10	C	402	AGS	PA-O3A-PB-O2B
10	A	901	AGS	PA-O3A-PB-O2B
10	B	402	AGS	PA-O3A-PB-O1B
10	D	402	AGS	PA-O3A-PB-O1B

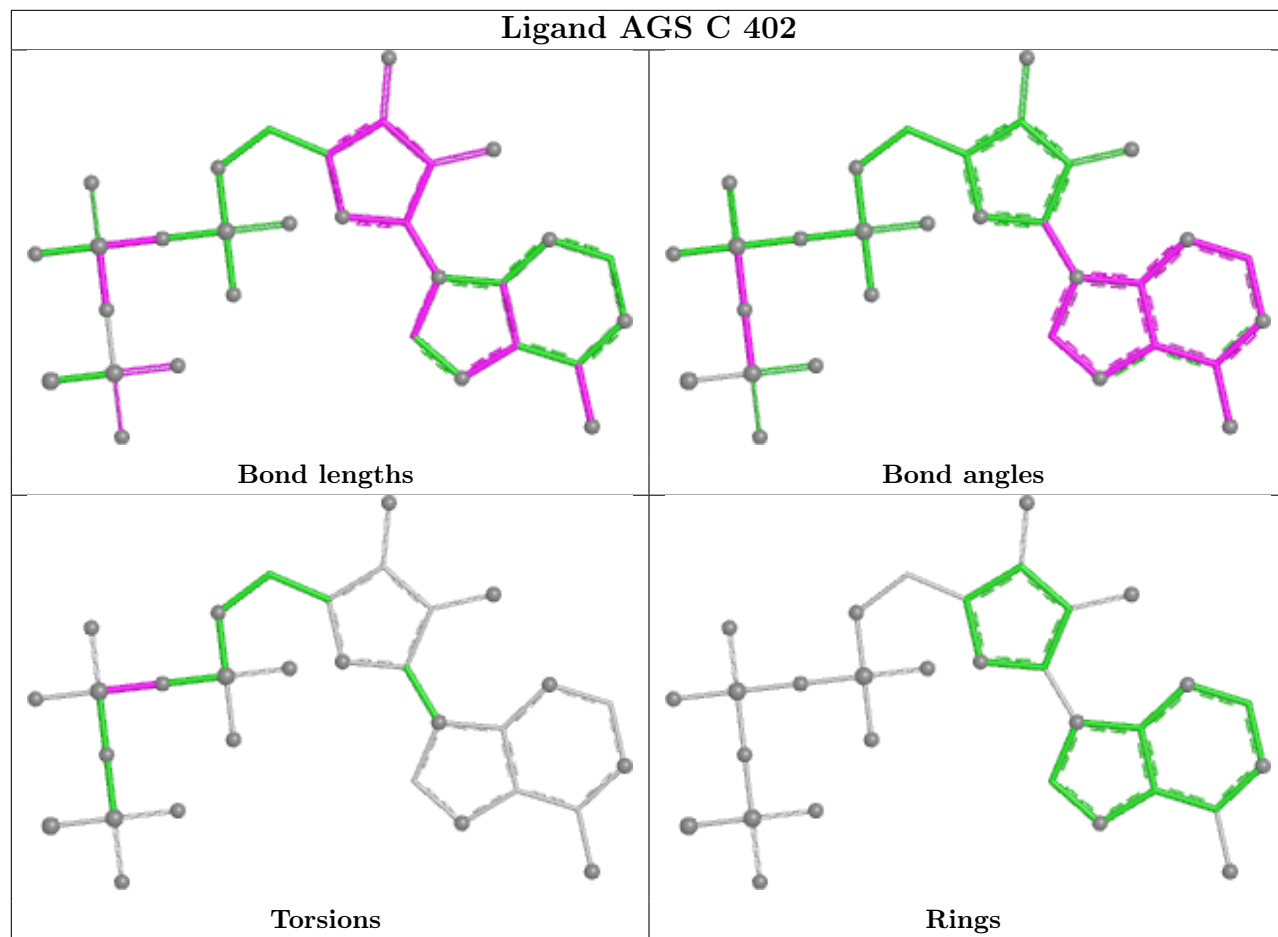
There are no ring outliers.

1 monomer is involved in 1 short contact:

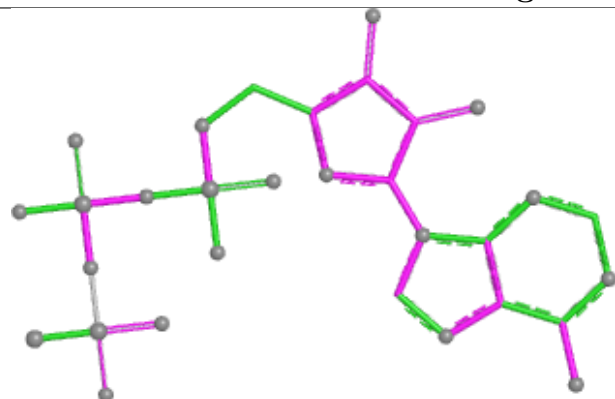
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	901	AGS	1	0

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

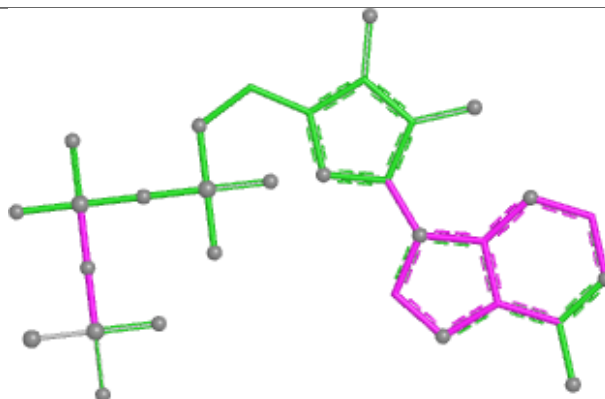
equivalents in the CSD to analyse the geometry.



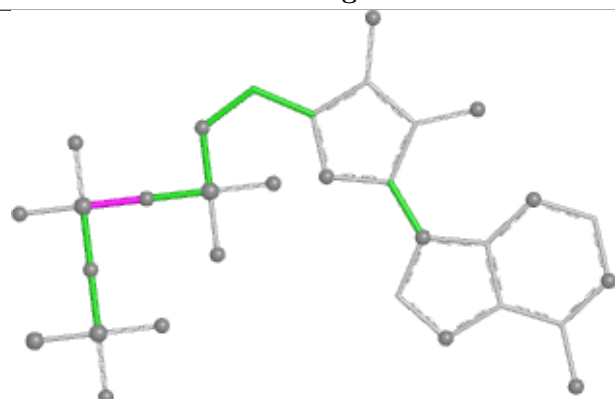
Ligand AGS B 402



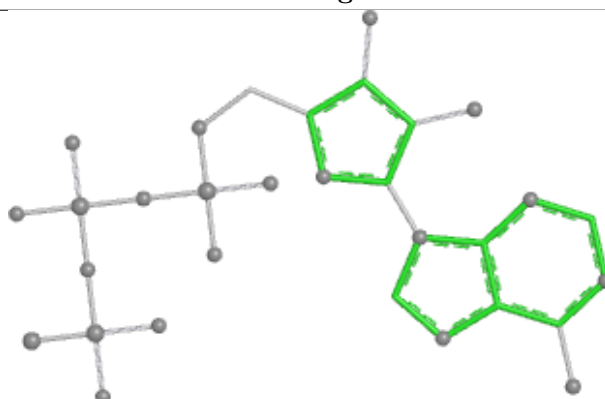
Bond lengths



Bond angles

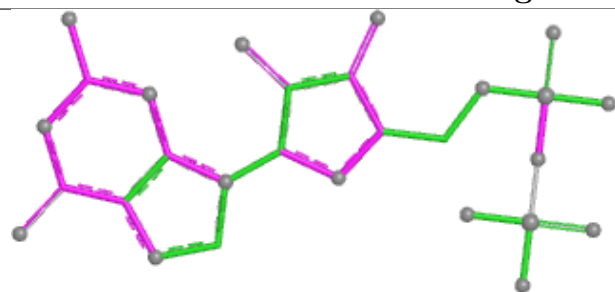


Torsions

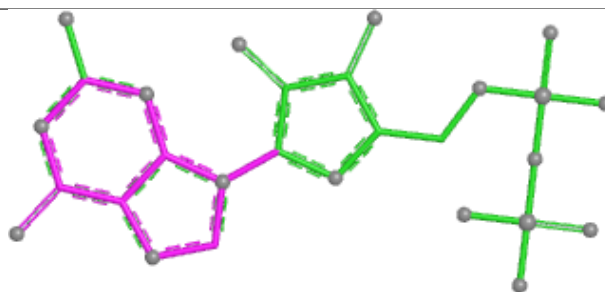


Rings

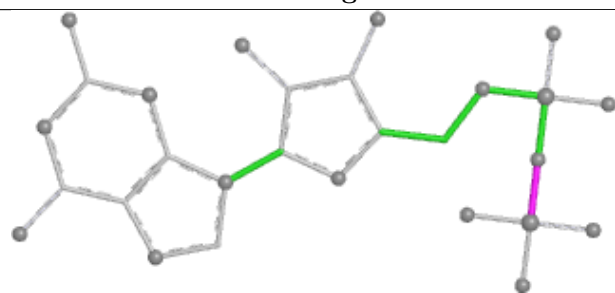
Ligand GDP E 401



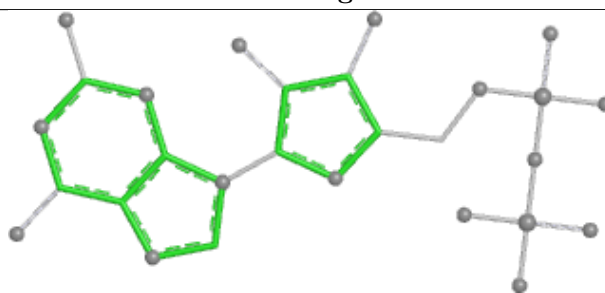
Bond lengths



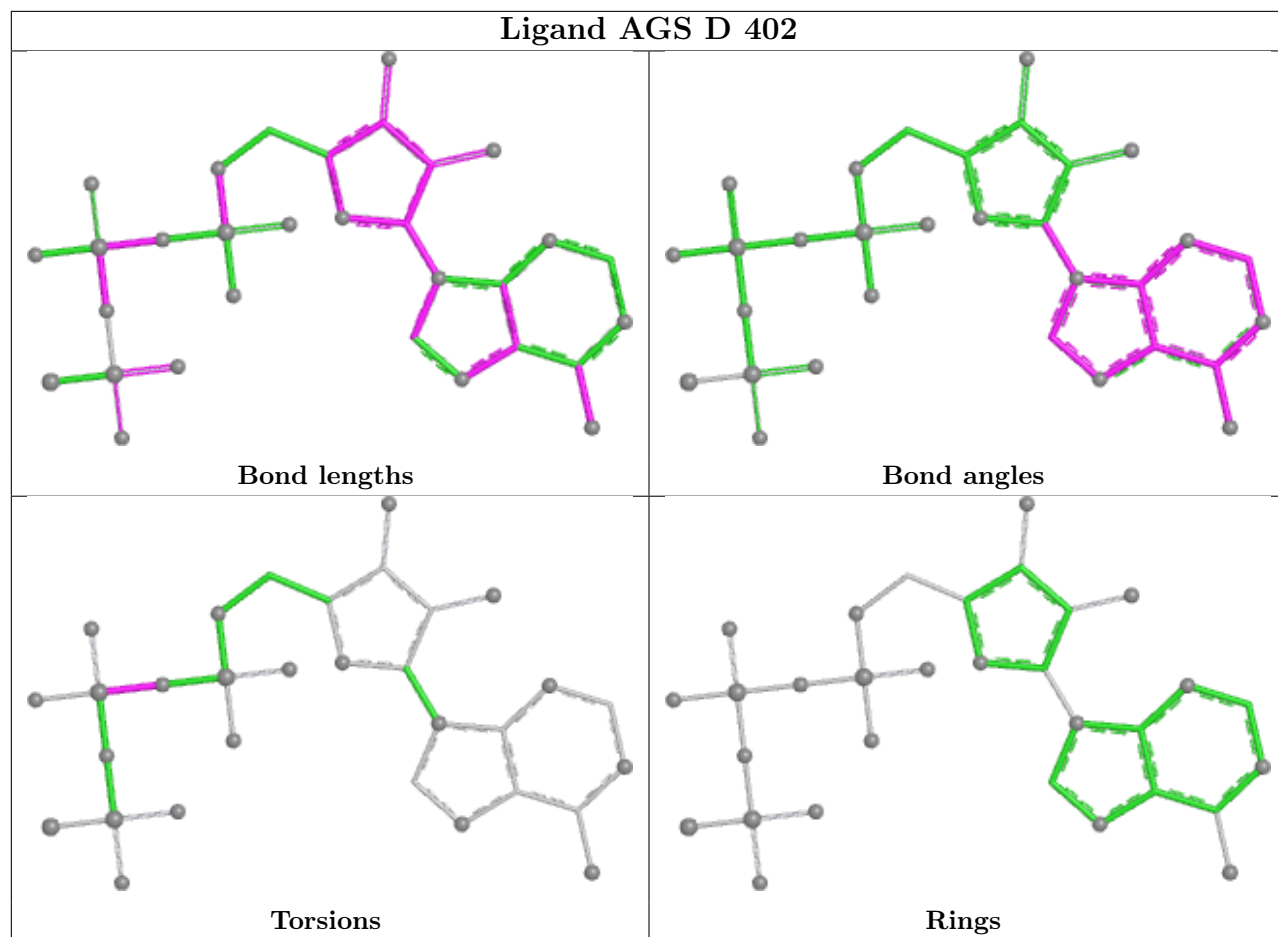
Bond angles

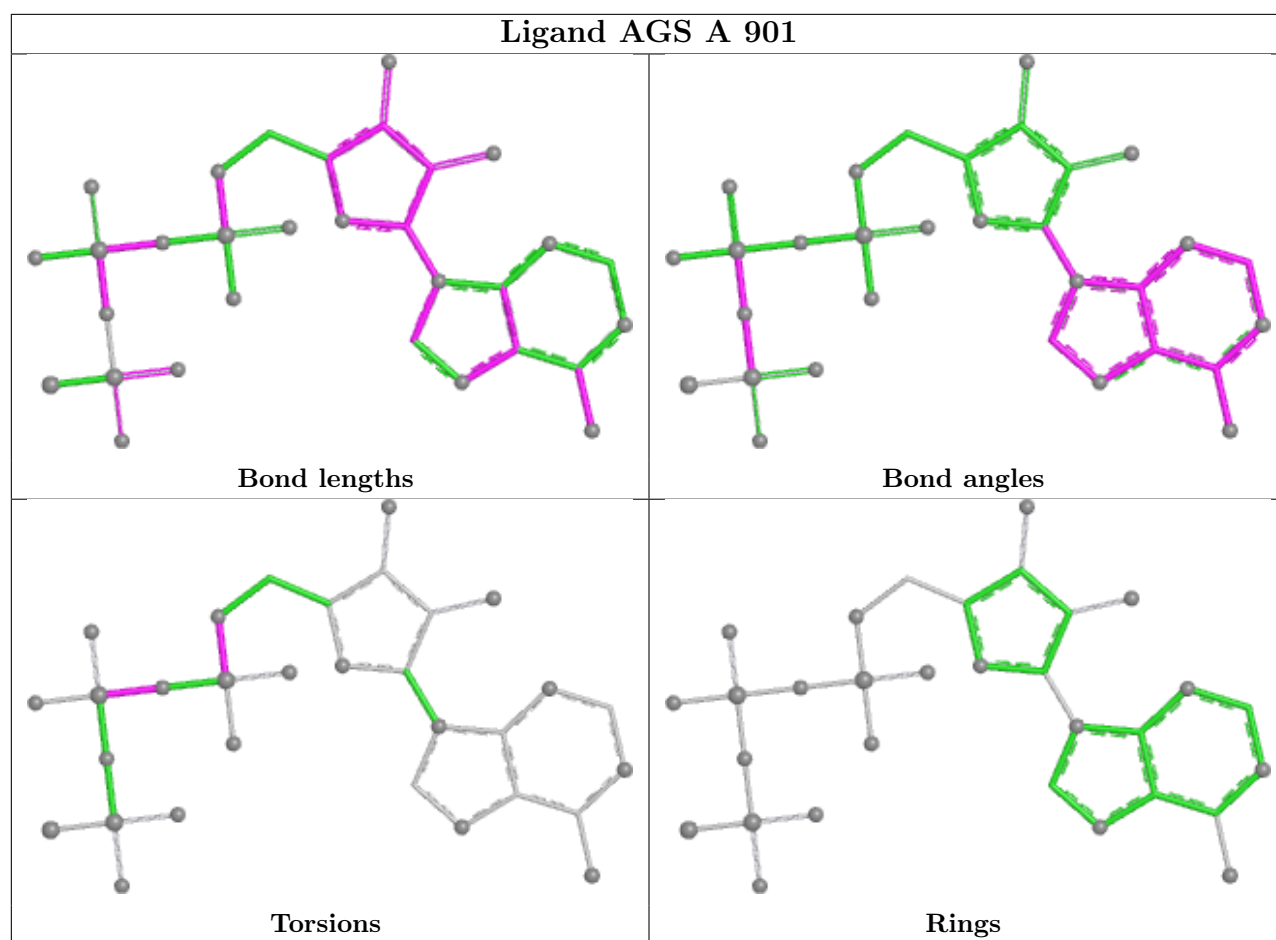


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

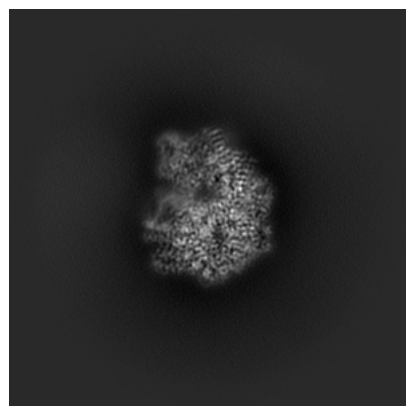
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27663. These allow visual inspection of the internal detail of the map and identification of artifacts.

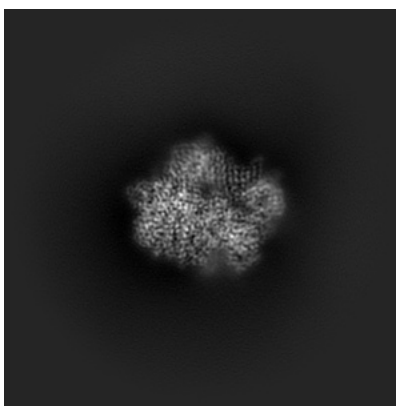
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

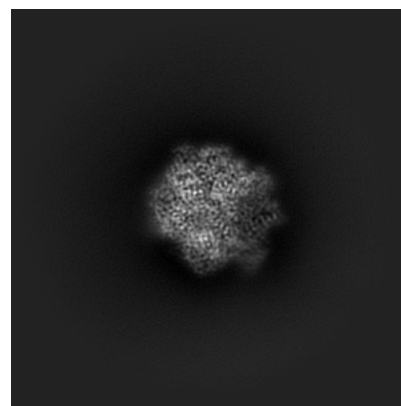
6.1.1 Primary map



X

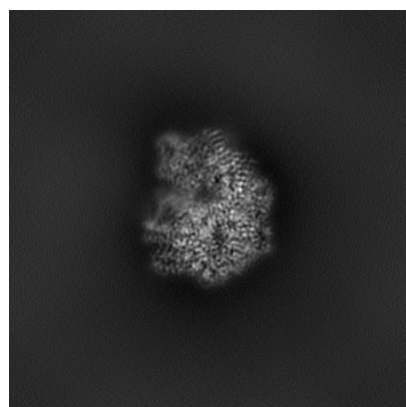


Y

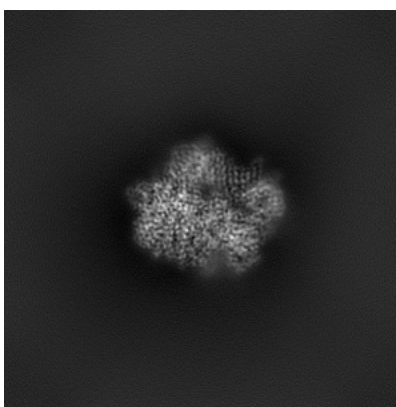


Z

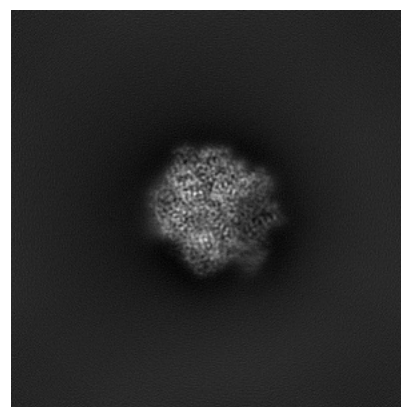
6.1.2 Raw map



X



Y

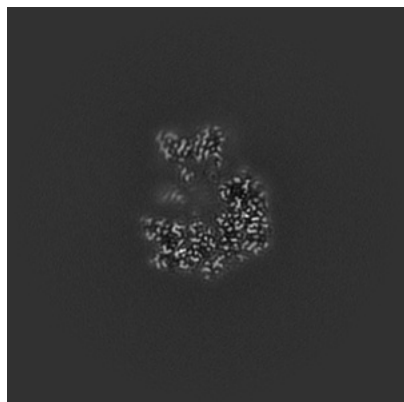


Z

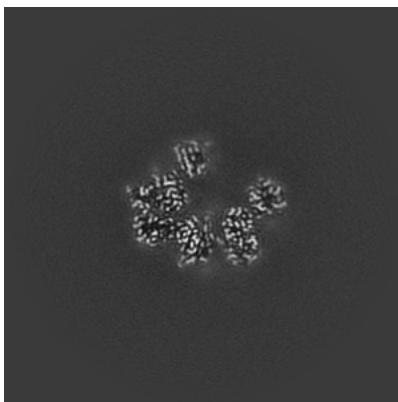
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

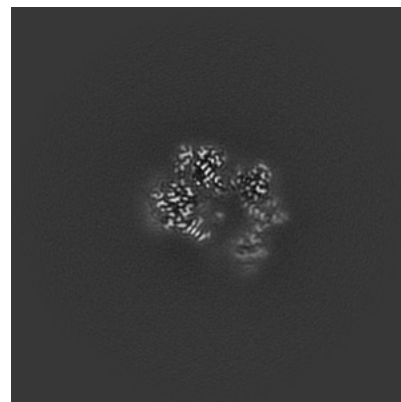
6.2.1 Primary map



X Index: 192

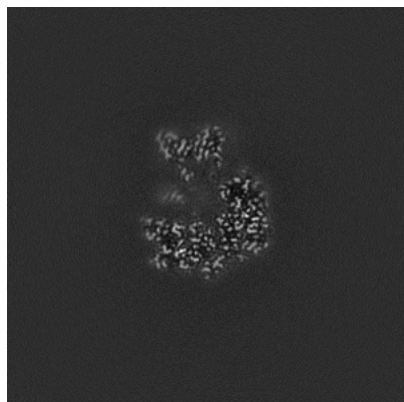


Y Index: 192

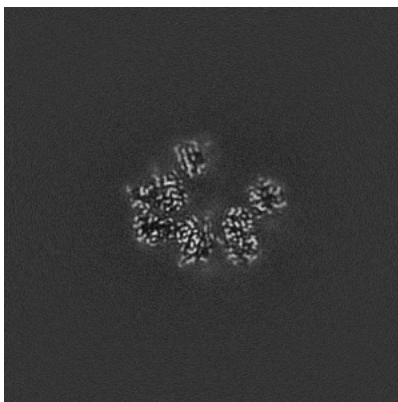


Z Index: 192

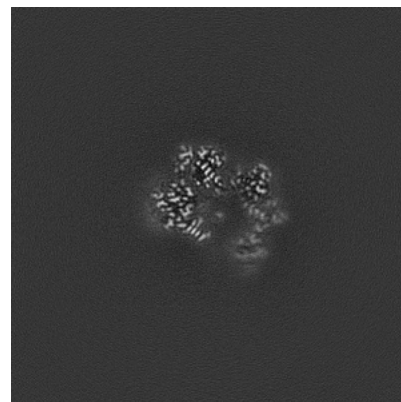
6.2.2 Raw map



X Index: 192



Y Index: 192

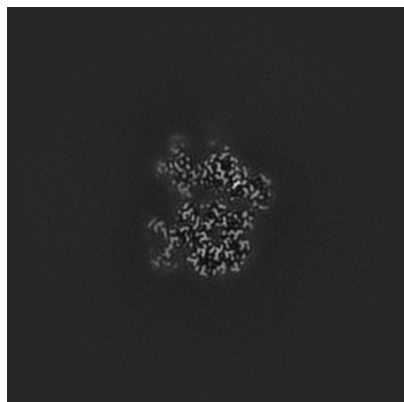


Z Index: 192

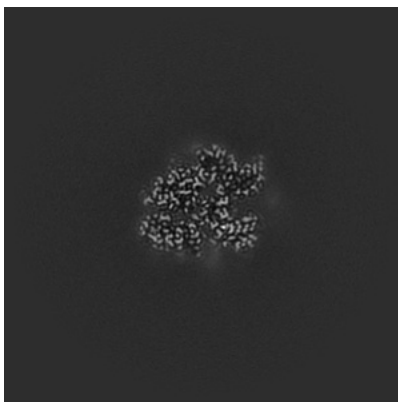
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

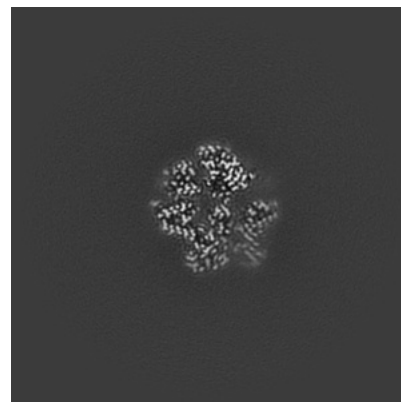
6.3.1 Primary map



X Index: 171

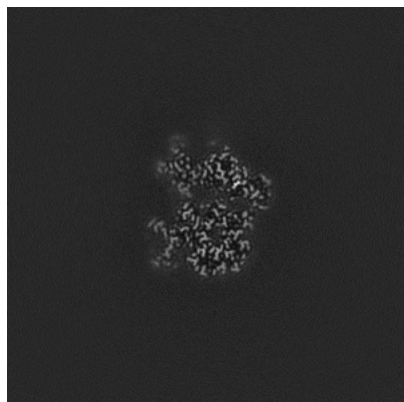


Y Index: 217

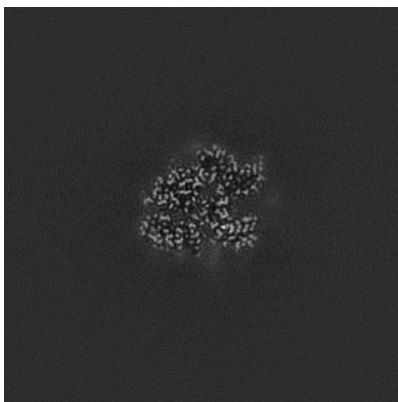


Z Index: 173

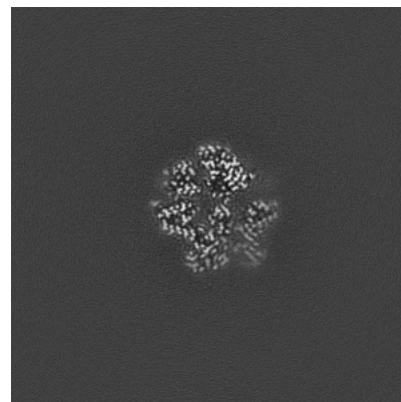
6.3.2 Raw map



X Index: 171



Y Index: 217

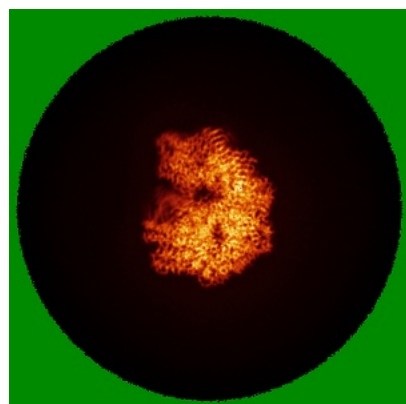


Z Index: 173

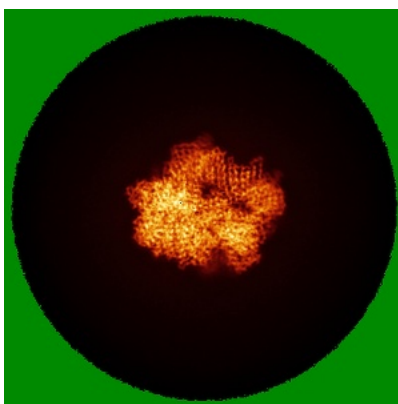
The images above show the largest variance slices of the map in three orthogonal directions.

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

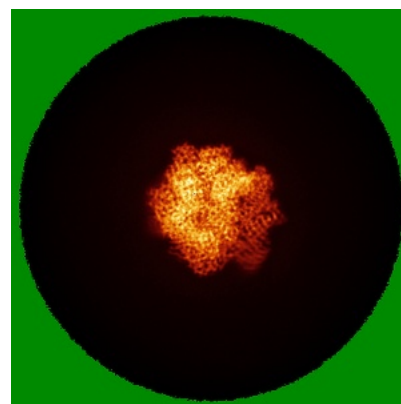
6.4.1 Primary map



X

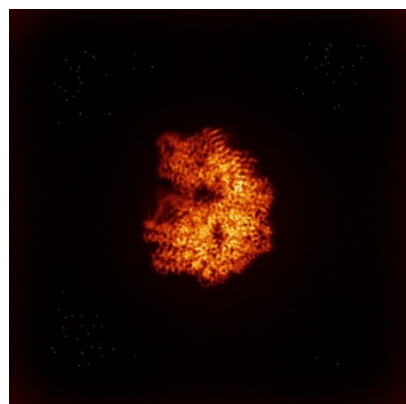


Y

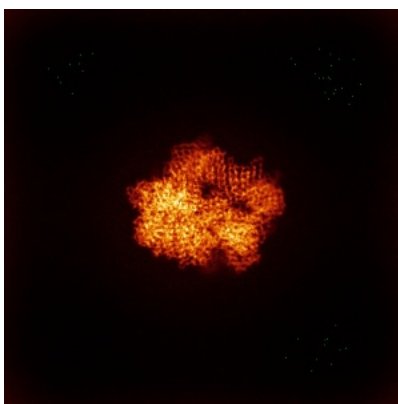


Z

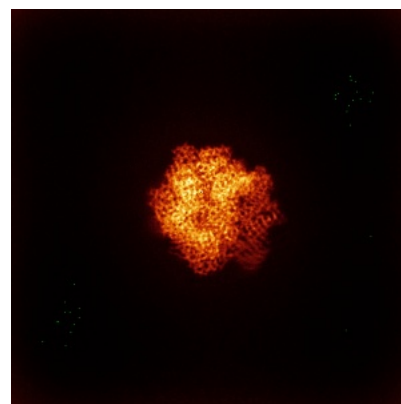
6.4.2 Raw map



X



Y

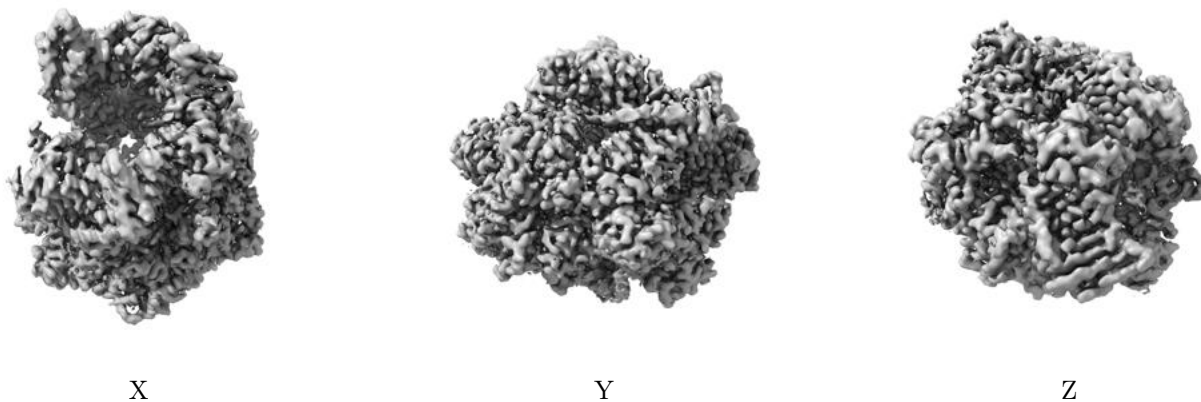


Z

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.

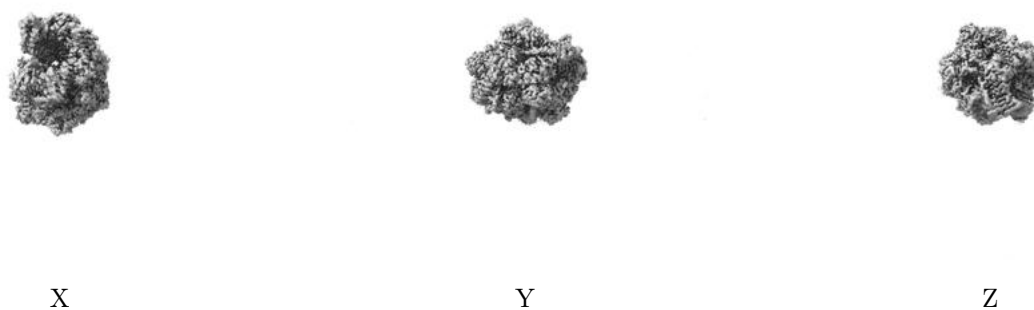
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

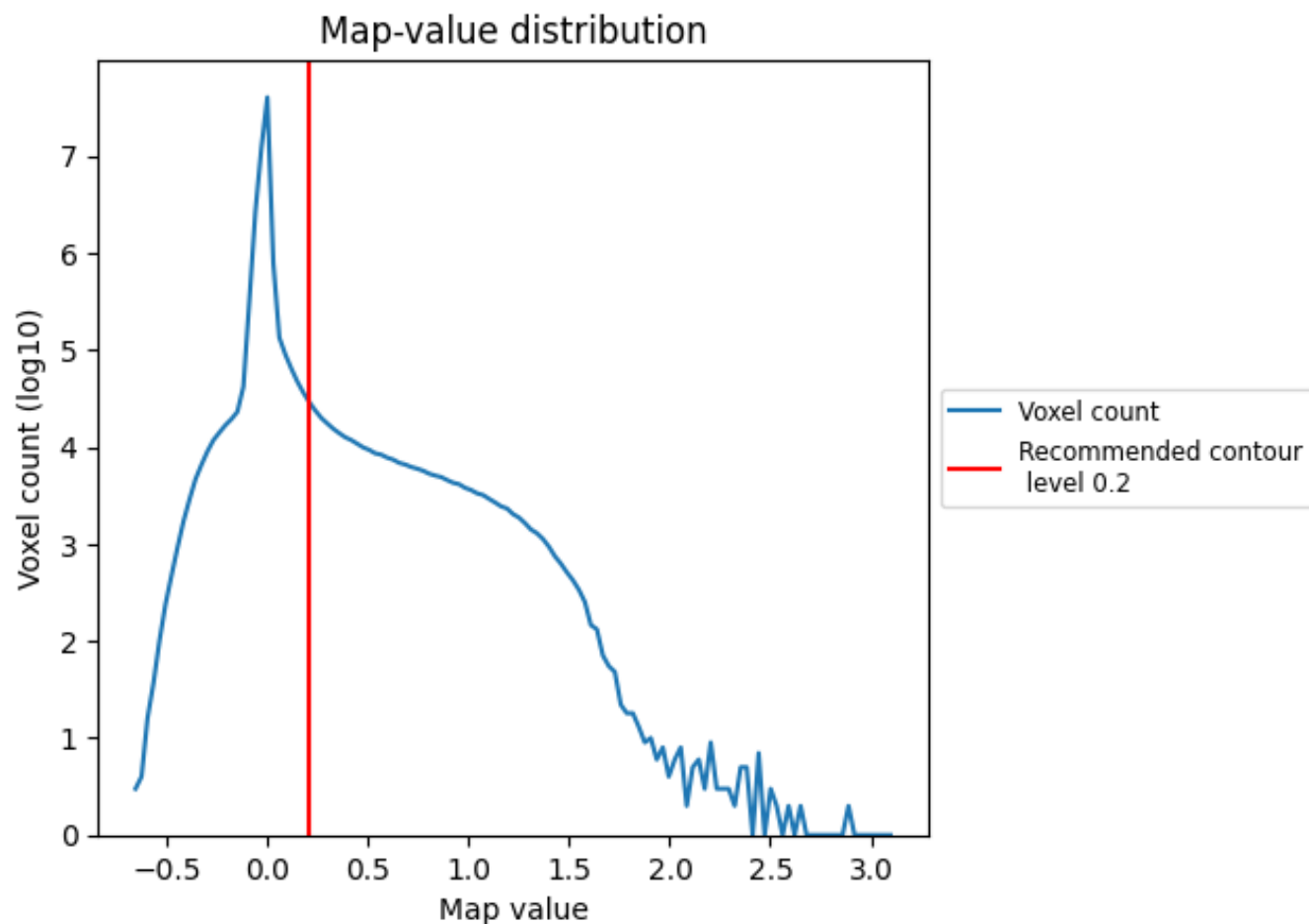
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

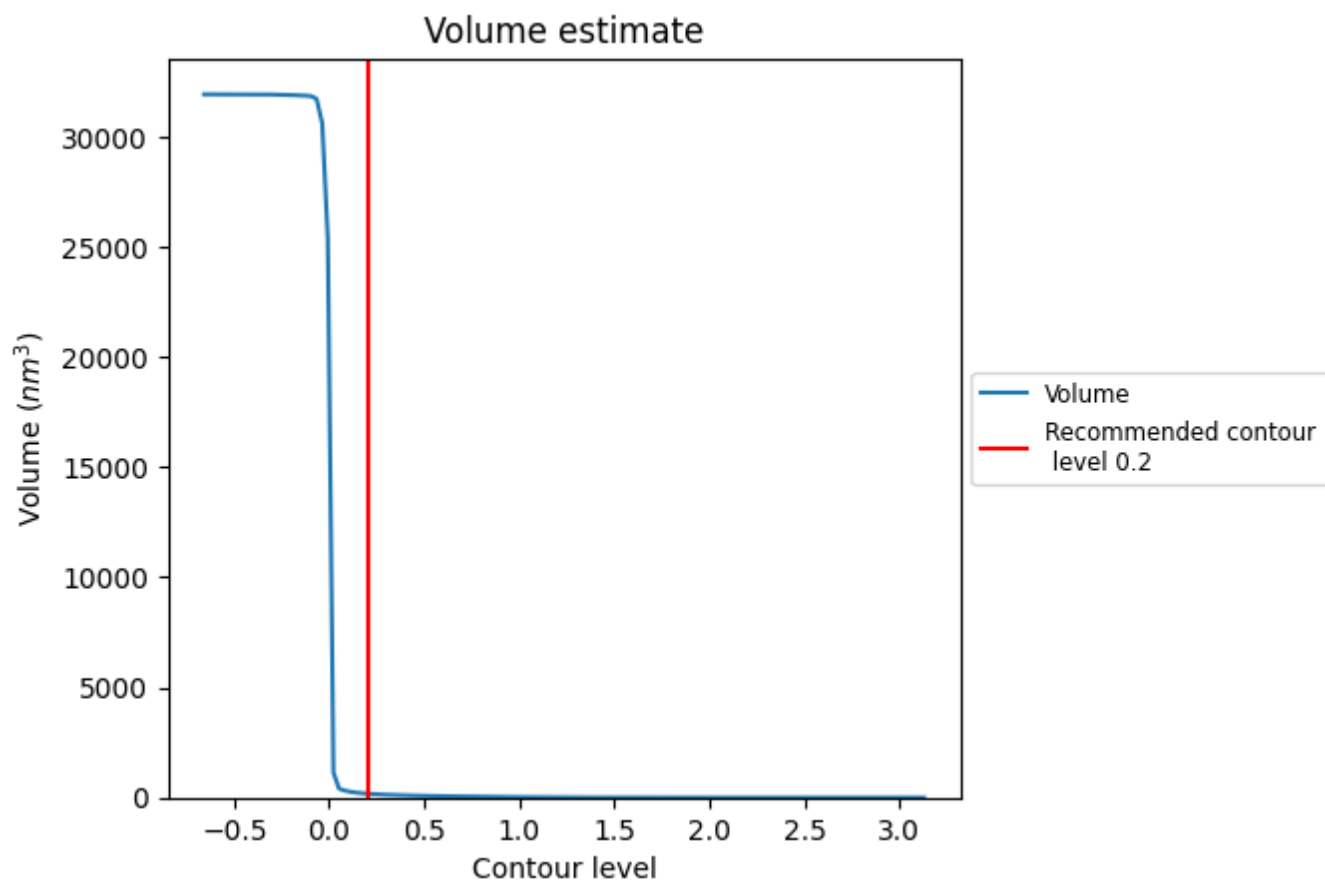
This section contains the results of statistical analysis of the map.

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.

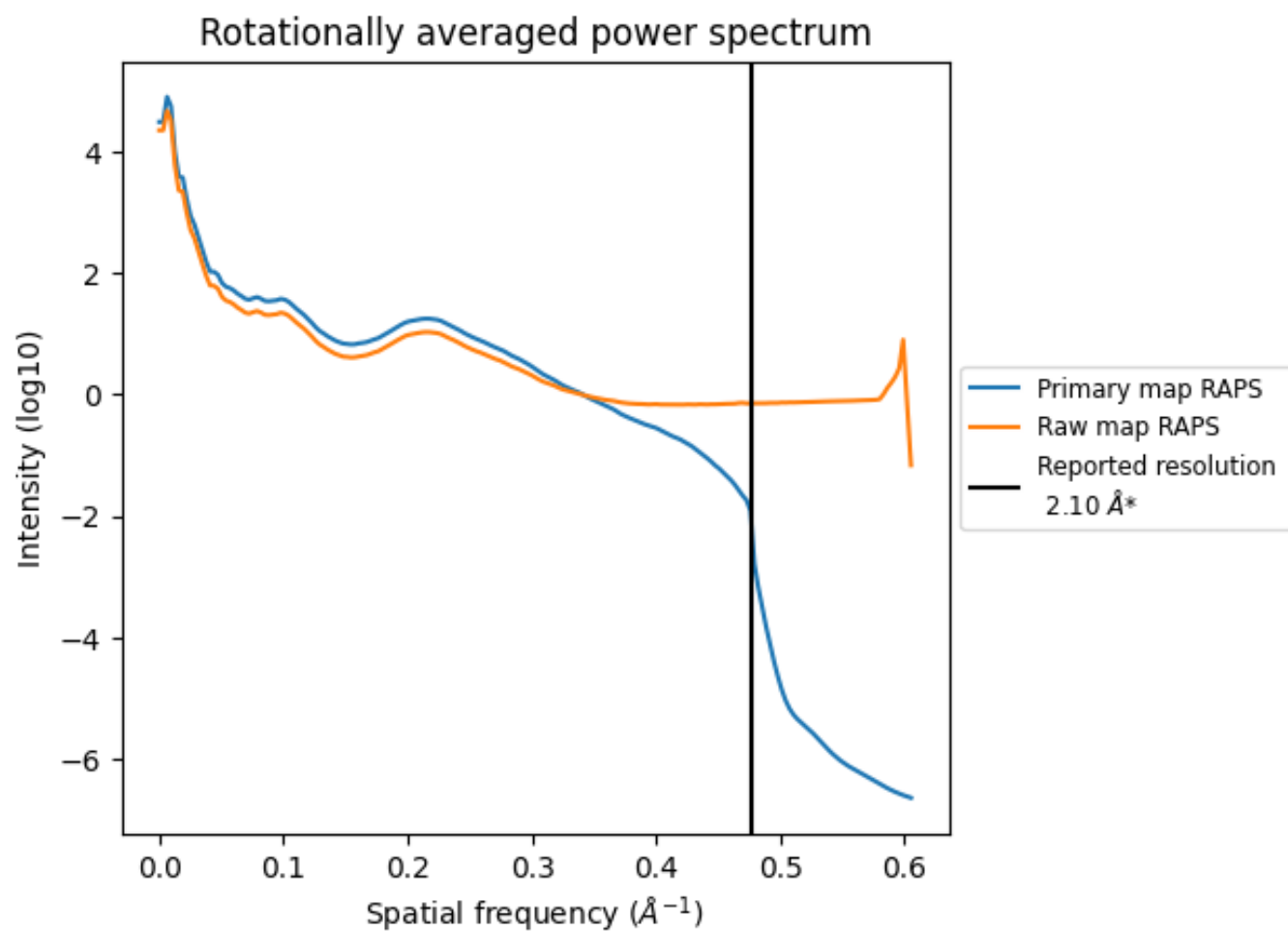
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 175 nm^3 ; this corresponds to an approximate mass of 158 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 ⓘ

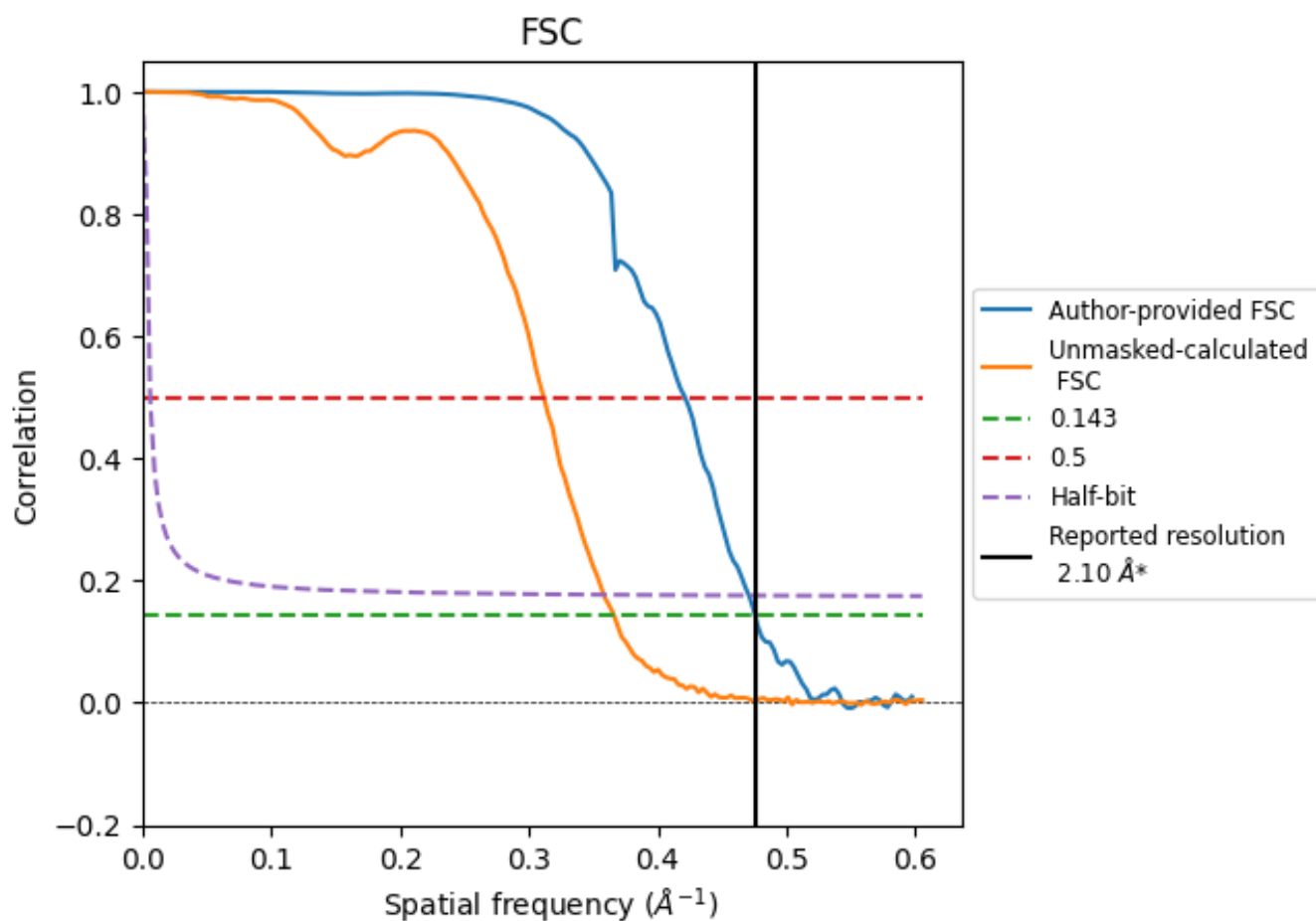


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

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 0.476 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

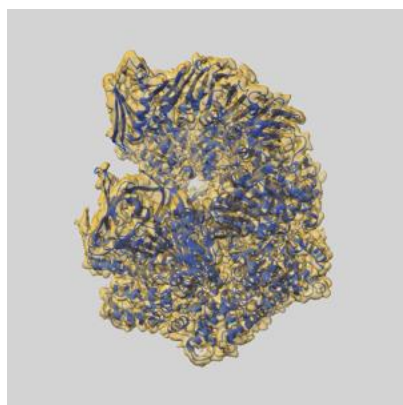
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.10	2.37	2.12
Unmasked-calculated*	2.73	3.21	2.79

*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 2.73 differs from the reported value 2.1 by more than 10 %

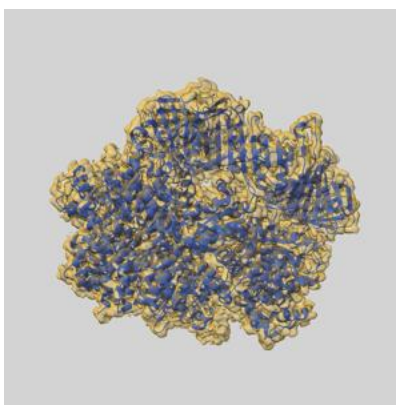
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27663 and PDB model 8DQX. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

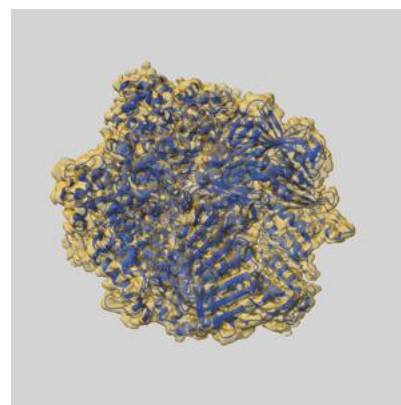
9.1 Map-model overlay [i](#)



X



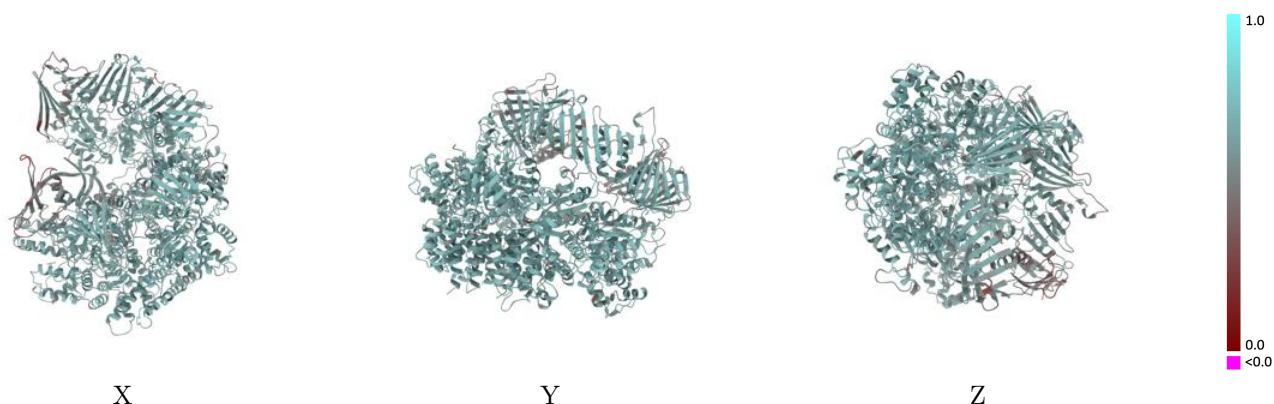
Y



Z

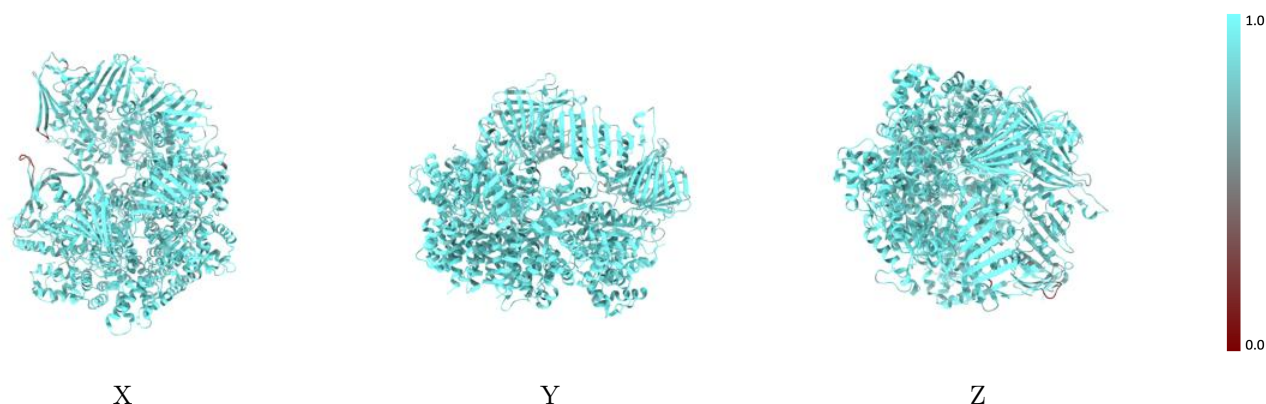
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



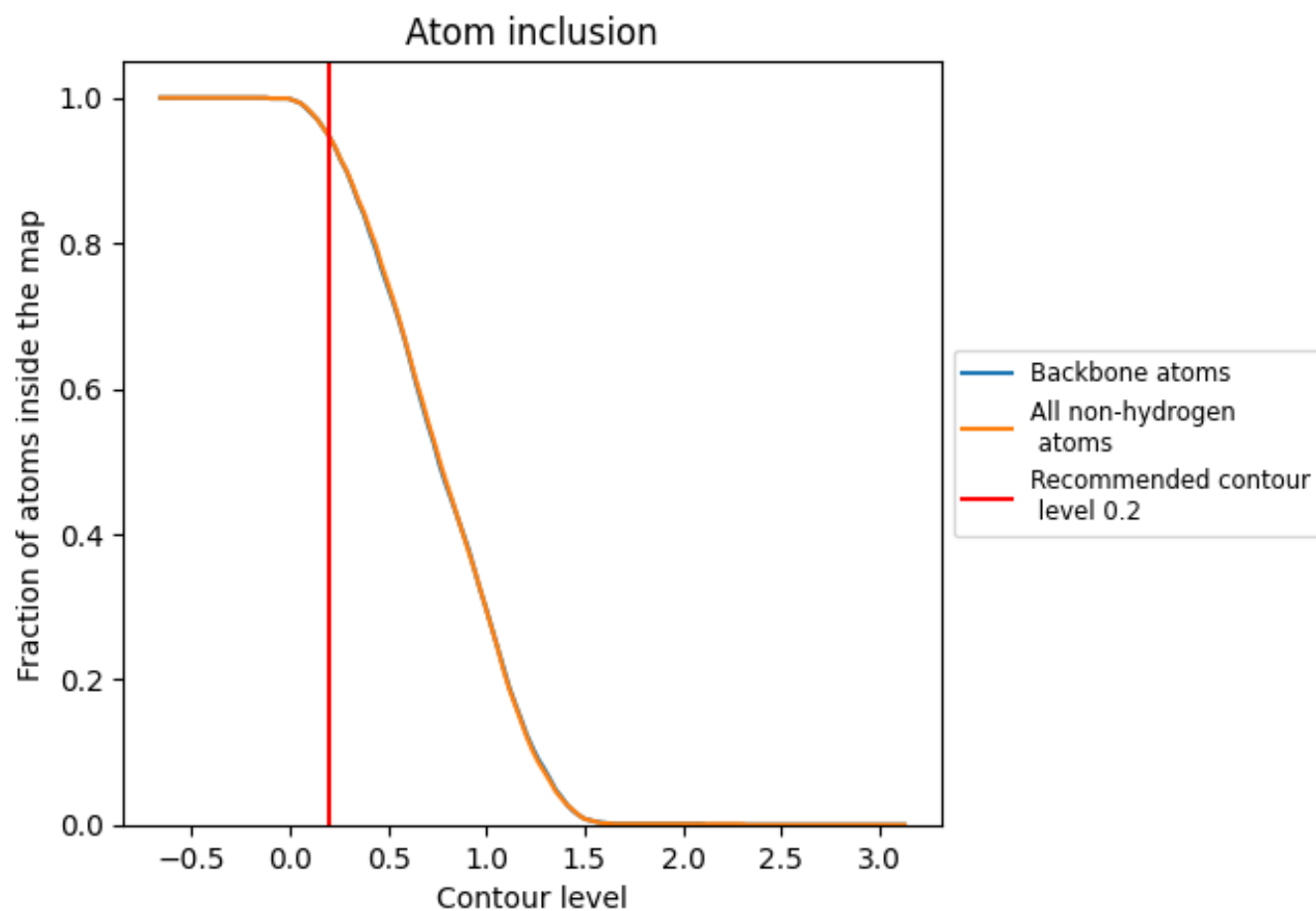
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9470	0.6210
A	0.9640	0.6280
B	0.9770	0.6560
C	0.9620	0.6460
D	0.9750	0.6590
E	0.9690	0.6500
F	0.9310	0.6050
G	0.9050	0.5610
H	0.8650	0.5250
I	0.9740	0.6310
J	0.8400	0.5160
K	0.9660	0.5920

1.0

0.0

<0.0