



## Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 07:40 PM EST

PDB ID : 8DQZ  
EMDB ID : EMD-27666  
Title : Intermediate state of RFC:PCNA bound to a 3' ss/dsDNA junction  
Authors : Schrecker, M.; Hite, R.K.  
Deposited on : 2022-07-20  
Resolution : 2.92 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

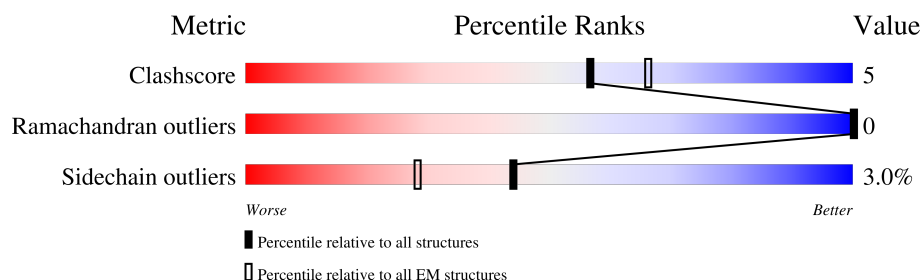
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.92 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.



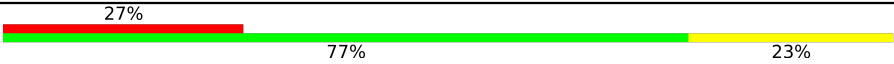

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	918	
2	B	323	
3	C	340	
4	D	353	
5	E	354	
6	F	277	
6	G	277	
6	H	277	

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Mol	Chain	Length	Quality of chain
7	I	22	
8	J	18	

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 42822 atoms, of which 21370 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	492	Total	C	H	N	O	S	0	0
			7832	2473	3942	682	717	18		

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	862	GLY	-	expression tag	UNP P38630
A	863	LEU	-	expression tag	UNP P38630
A	864	ASN	-	expression tag	UNP P38630
A	865	GLU	-	expression tag	UNP P38630
A	866	ASN	-	expression tag	UNP P38630
A	867	LEU	-	expression tag	UNP P38630
A	868	TYR	-	expression tag	UNP P38630
A	869	PHE	-	expression tag	UNP P38630
A	870	GLN	-	expression tag	UNP P38630
A	871	GLY	-	expression tag	UNP P38630
A	872	GLY	-	expression tag	UNP P38630
A	873	GLY	-	expression tag	UNP P38630
A	874	ASP	-	expression tag	UNP P38630
A	875	TYR	-	expression tag	UNP P38630
A	876	LYS	-	expression tag	UNP P38630
A	877	ASP	-	expression tag	UNP P38630
A	878	ASP	-	expression tag	UNP P38630
A	879	ASP	-	expression tag	UNP P38630
A	880	ASP	-	expression tag	UNP P38630
A	881	LYS	-	expression tag	UNP P38630
A	882	ASP	-	expression tag	UNP P38630
A	883	TYR	-	expression tag	UNP P38630
A	884	LYS	-	expression tag	UNP P38630
A	885	ASP	-	expression tag	UNP P38630
A	886	ASP	-	expression tag	UNP P38630
A	887	ASP	-	expression tag	UNP P38630
A	888	ASP	-	expression tag	UNP P38630
A	889	LYS	-	expression tag	UNP P38630

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Chain	Residue	Modelled	Actual	Comment	Reference
A	890	ASP	-	expression tag	UNP P38630
A	891	TYR	-	expression tag	UNP P38630
A	892	LYS	-	expression tag	UNP P38630
A	893	ASP	-	expression tag	UNP P38630
A	894	ASP	-	expression tag	UNP P38630
A	895	ASP	-	expression tag	UNP P38630
A	896	ASP	-	expression tag	UNP P38630
A	897	LYS	-	expression tag	UNP P38630
A	898	GLY	-	expression tag	UNP P38630
A	899	GLY	-	expression tag	UNP P38630
A	900	LYS	-	expression tag	UNP P38630
A	901	ASP	-	expression tag	UNP P38630
A	902	HIS	-	expression tag	UNP P38630
A	903	LEU	-	expression tag	UNP P38630
A	904	ILE	-	expression tag	UNP P38630
A	905	HIS	-	expression tag	UNP P38630
A	906	ASN	-	expression tag	UNP P38630
A	907	VAL	-	expression tag	UNP P38630
A	908	HIS	-	expression tag	UNP P38630
A	909	LYS	-	expression tag	UNP P38630
A	910	GLU	-	expression tag	UNP P38630
A	911	GLU	-	expression tag	UNP P38630
A	912	HIS	-	expression tag	UNP P38630
A	913	ALA	-	expression tag	UNP P38630
A	914	HIS	-	expression tag	UNP P38630
A	915	ALA	-	expression tag	UNP P38630
A	916	HIS	-	expression tag	UNP P38630
A	917	ASN	-	expression tag	UNP P38630
A	918	LYS	-	expression tag	UNP P38630

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	318	Total	C	H	N	O	S	0	0
			5084	1574	2588	444	465	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	329	Total	C	H	N	O	S	0	0
			5247	1640	2641	457	501	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	336	Total	C	H	N	O	S	0	0
			5347	1678	2688	459	512	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	354	Total	C	H	N	O	S	0	0
			5698	1765	2906	485	524	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	258	Total	C	H	N	O	S	0	0
			4055	1291	2034	319	401	10		
6	G	257	Total	C	H	N	O	S	0	0
			4047	1287	2033	318	399	10		
6	H	255	Total	C	H	N	O	S	0	0
			4023	1280	2022	315	396	10		

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	MET	-	expression tag	UNP P15873
F	-17	GLY	-	expression tag	UNP P15873
F	-16	SER	-	expression tag	UNP P15873
F	-15	SER	-	expression tag	UNP P15873
F	-14	HIS	-	expression tag	UNP P15873
F	-13	HIS	-	expression tag	UNP P15873
F	-12	HIS	-	expression tag	UNP P15873
F	-11	HIS	-	expression tag	UNP P15873
F	-10	HIS	-	expression tag	UNP P15873
F	-9	HIS	-	expression tag	UNP P15873
F	-8	SER	-	expression tag	UNP P15873
F	-7	SER	-	expression tag	UNP P15873
F	-6	GLY	-	expression tag	UNP P15873
F	-5	LEU	-	expression tag	UNP P15873
F	-4	VAL	-	expression tag	UNP P15873
F	-3	PRO	-	expression tag	UNP P15873
F	-2	ARG	-	expression tag	UNP P15873
F	-1	ALA	-	expression tag	UNP P15873
F	0	SER	-	expression tag	UNP P15873

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-18	MET	-	expression tag	UNP P15873
G	-17	GLY	-	expression tag	UNP P15873
G	-16	SER	-	expression tag	UNP P15873
G	-15	SER	-	expression tag	UNP P15873
G	-14	HIS	-	expression tag	UNP P15873
G	-13	HIS	-	expression tag	UNP P15873
G	-12	HIS	-	expression tag	UNP P15873
G	-11	HIS	-	expression tag	UNP P15873
G	-10	HIS	-	expression tag	UNP P15873
G	-9	HIS	-	expression tag	UNP P15873
G	-8	SER	-	expression tag	UNP P15873
G	-7	SER	-	expression tag	UNP P15873
G	-6	GLY	-	expression tag	UNP P15873
G	-5	LEU	-	expression tag	UNP P15873
G	-4	VAL	-	expression tag	UNP P15873
G	-3	PRO	-	expression tag	UNP P15873
G	-2	ARG	-	expression tag	UNP P15873
G	-1	ALA	-	expression tag	UNP P15873
G	0	SER	-	expression tag	UNP P15873
H	-18	MET	-	expression tag	UNP P15873
H	-17	GLY	-	expression tag	UNP P15873
H	-16	SER	-	expression tag	UNP P15873
H	-15	SER	-	expression tag	UNP P15873
H	-14	HIS	-	expression tag	UNP P15873
H	-13	HIS	-	expression tag	UNP P15873
H	-12	HIS	-	expression tag	UNP P15873
H	-11	HIS	-	expression tag	UNP P15873
H	-10	HIS	-	expression tag	UNP P15873
H	-9	HIS	-	expression tag	UNP P15873
H	-8	SER	-	expression tag	UNP P15873
H	-7	SER	-	expression tag	UNP P15873
H	-6	GLY	-	expression tag	UNP P15873
H	-5	LEU	-	expression tag	UNP P15873
H	-4	VAL	-	expression tag	UNP P15873
H	-3	PRO	-	expression tag	UNP P15873
H	-2	ARG	-	expression tag	UNP P15873
H	-1	ALA	-	expression tag	UNP P15873
H	0	SER	-	expression tag	UNP P15873

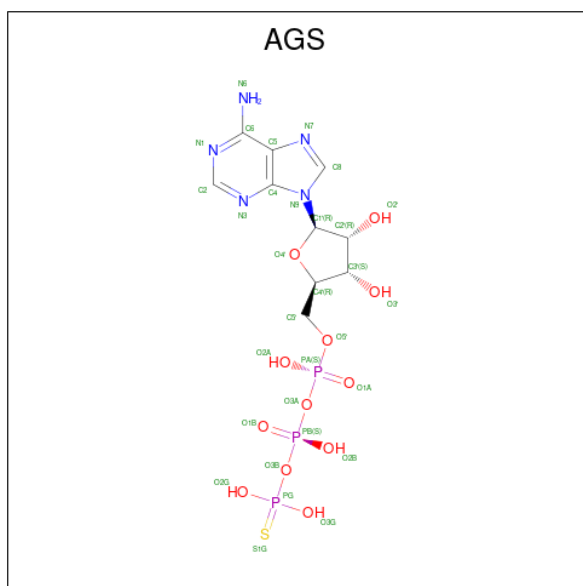
- Molecule 7 is a DNA chain called DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*CP\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*CP\*CP\*CP\*CP\*GP\*GP\*GP\*G)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	22	Total	C	H	N	O	P	0	0
			706	215	249	82	138	22		

- Molecule 8 is a DNA chain called DNA (5'-D(P\*CP\*CP\*CP\*CP\*GP\*GP\*GP\*GP\*CP\*CP\*CP\*CP\*CP\*GP\*GP\*C)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	18	Total	C	H	N	O	P	0	0
			559	168	199	66	108	18		

- Molecule 9 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



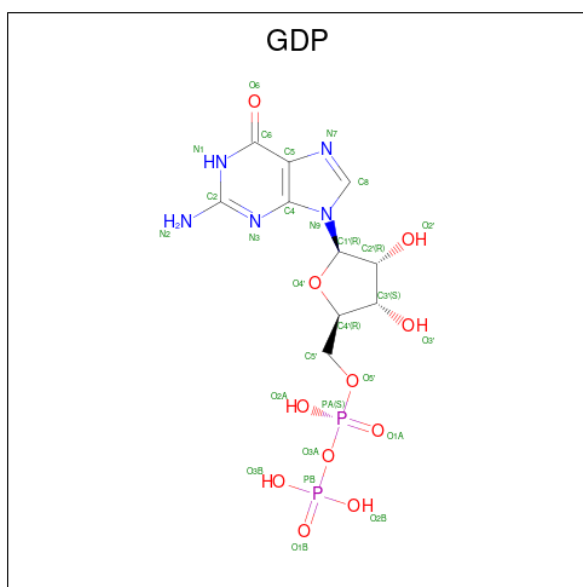
Mol	Chain	Residues	Atoms							AltConf
9	A	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	
9	B	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	
9	C	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	
9	D	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).

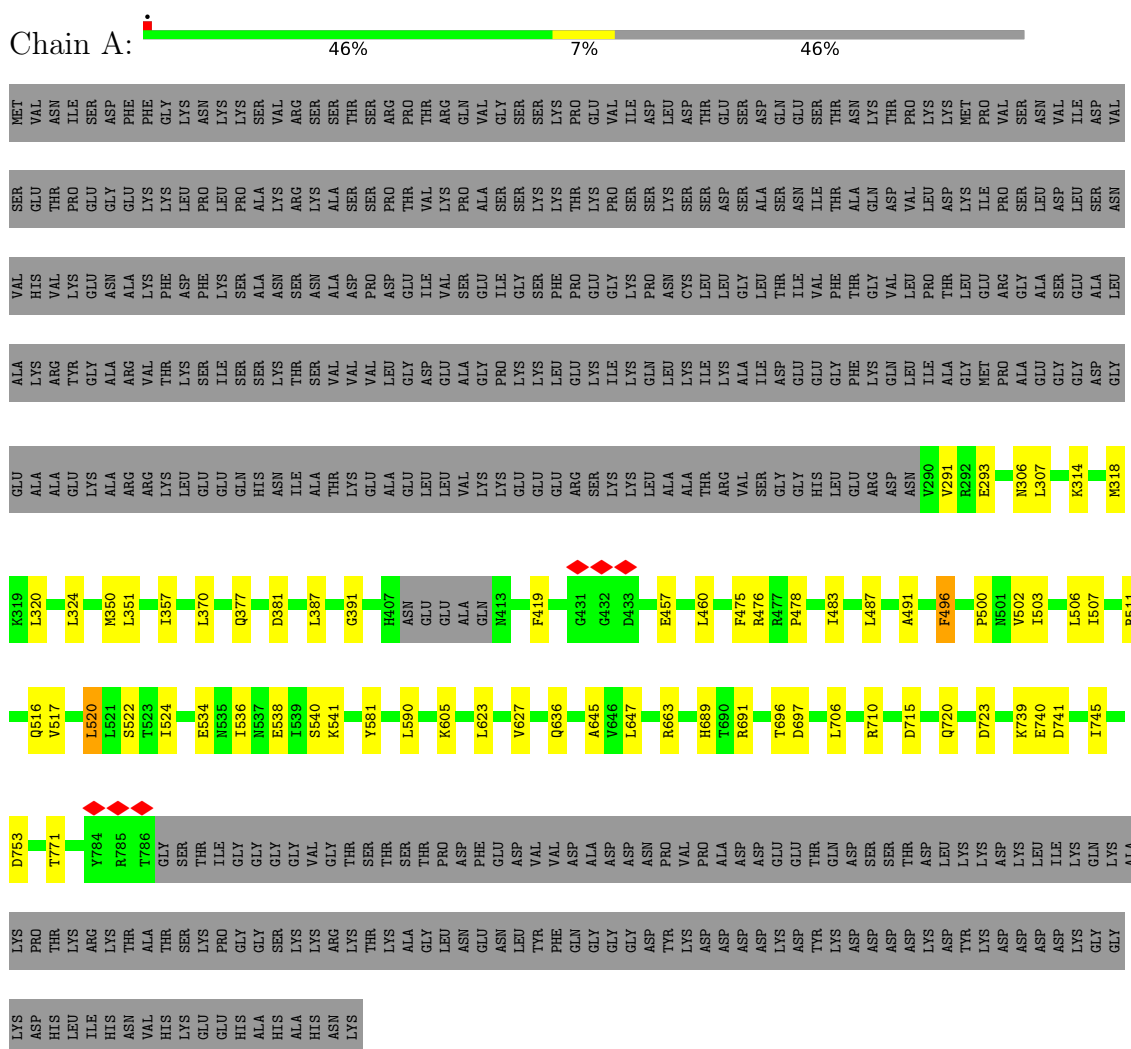


Mol	Chain	Residues	Atoms						AltConf
11	E	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	

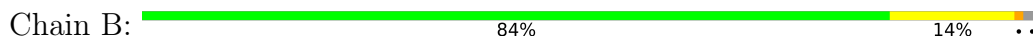
### 3 Residue-property plots

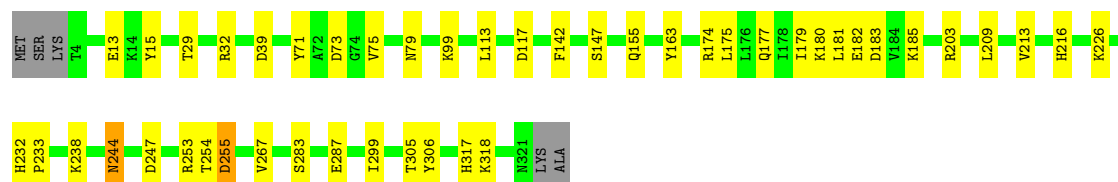
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



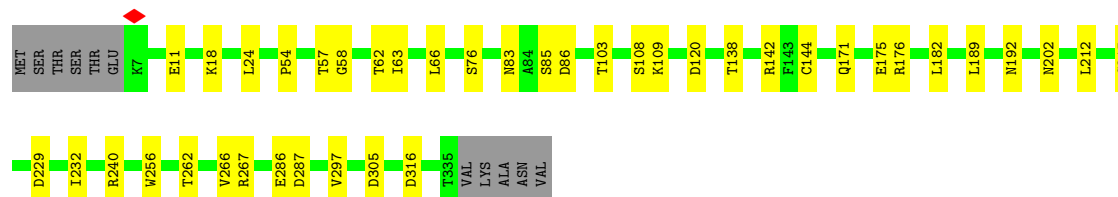
#### • Molecule 2: Replication factor C subunit 4





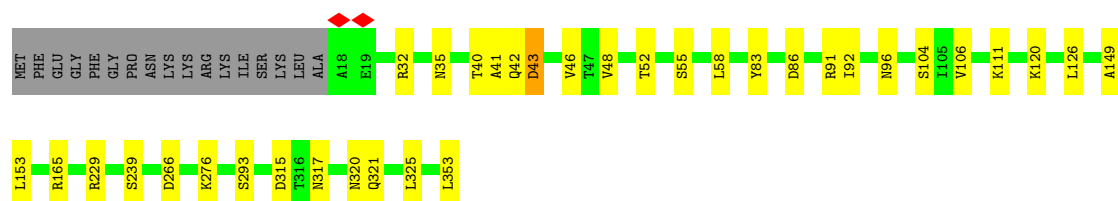
• Molecule 3: Replication factor C subunit 3

Chain C: 85% 12% .



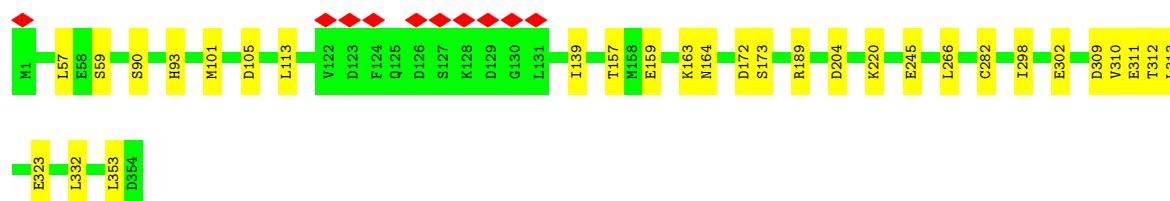
• Molecule 4: Replication factor C subunit 2

Chain D: 85% 10% 5%



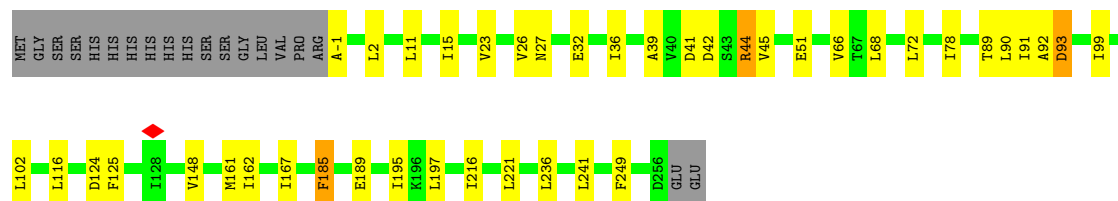
• Molecule 5: Replication factor C subunit 5

Chain E: 92% 8%




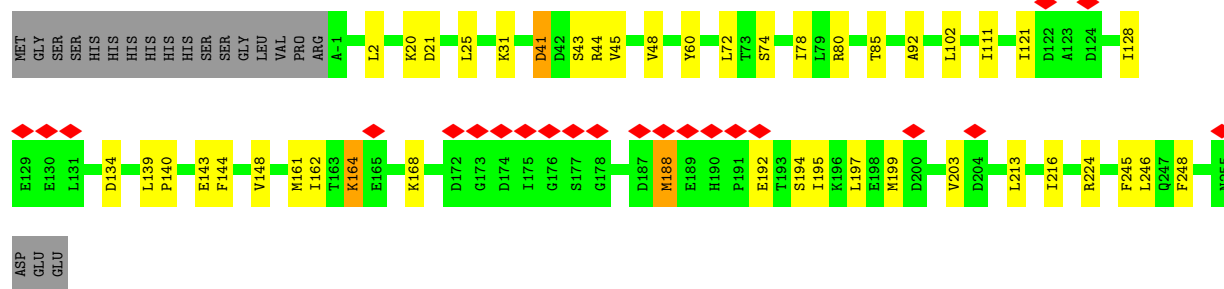
• Molecule 6: Proliferating cell nuclear antigen

Chain F: 78% 14% 7%




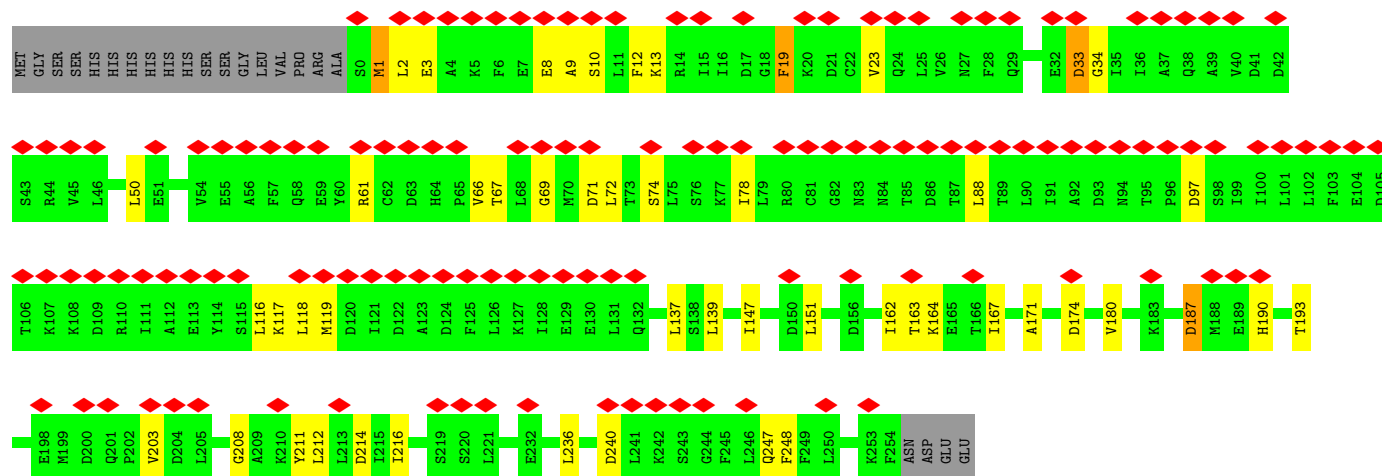
• Molecule 6: Proliferating cell nuclear antigen

Chain G: 



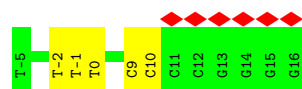
- Molecule 6: Proliferating cell nuclear antigen

Chain H: 




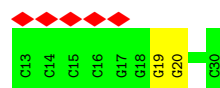
- Molecule 7: DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*CP\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*CP\*C P\*CP\*CP\*GP\*GP\*GP\*G)-3')

Chain I: 



- Molecule 8: DNA (5'-D(P\*CP\*CP\*CP\*CP\*GP\*GP\*GP\*GP\*CP\*CP\*CP\*CP\*CP\*CP\*G P\*GP\*C)-3')

Chain J: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41190	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	2.029	Depositor
Minimum map value	-0.587	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	317.184, 317.184, 317.184	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.826, 0.826, 0.826	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, MG, 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	0.25	0/3967	0.48	0/5360
2	B	0.24	0/2531	0.47	0/3414
3	C	0.24	0/2646	0.47	0/3577
4	D	0.24	0/2704	0.45	0/3657
5	E	0.25	0/2832	0.47	0/3826
6	F	0.25	0/2051	0.49	0/2767
6	G	0.25	0/2044	0.50	0/2757
6	H	0.25	0/2031	0.48	0/2739
7	I	0.51	0/511	0.93	0/789
8	J	0.52	0/401	0.79	0/614
All	All	0.26	0/21718	0.50	0/29500

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

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	3890	3942	3940	39	0
2	B	2496	2588	2588	25	0
3	C	2606	2641	2641	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2659	2688	2688	20	0
5	E	2792	2906	2906	15	0
6	F	2021	2034	2036	30	0
6	G	2014	2033	2035	35	0
6	H	2001	2022	2024	37	0
7	I	457	249	249	3	0
8	J	360	199	199	1	0
9	A	31	14	12	0	0
9	B	31	14	12	2	0
9	C	31	14	12	0	0
9	D	31	14	12	1	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	E	28	12	11	0	0
All	All	21452	21370	21365	220	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 (220) 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:15:TYR:OH	2:B:182:GLU:OE2	1.87	0.91
6:G:31:LYS:O	6:G:60:TYR:OH	1.96	0.83
1:A:487:LEU:HD12	1:A:503:ILE:HG23	1.62	0.81
1:A:324:LEU:HD12	1:A:370:LEU:HD12	1.62	0.80
4:D:48:VAL:O	4:D:52:THR:HG23	1.83	0.77
3:C:83:ASN:OD1	3:C:85:SER:OG	2.02	0.75
6:F:41:ASP:OD1	6:F:42:ASP:N	2.19	0.75
6:H:3:GLU:OE1	6:H:3:GLU:N	2.20	0.74
6:H:33:ASP:OD2	6:H:34:GLY:N	2.20	0.73
2:B:13:GLU:HG3	3:C:138:THR:HG21	1.71	0.73
5:E:172:ASP:OD1	5:E:173:SER:N	2.21	0.72
6:G:148:VAL:CG2	6:G:216:ILE:HD13	2.19	0.72
6:F:148:VAL:HG11	6:F:216:ILE:HG21	1.72	0.72
6:H:3:GLU:OE2	6:H:61:ARG:N	2.23	0.71
6:H:12:PHE:CE2	6:H:88:LEU:HD22	2.27	0.70
6:G:148:VAL:HG21	6:G:216:ILE:HD13	1.73	0.70
6:F:32:GLU:OE2	6:F:32:GLU:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:245:GLU:OE2	5:E:245:GLU:O	2.13	0.66
1:A:691:ARG:O	1:A:691:ARG:NH1	2.29	0.66
1:A:293:GLU:N	1:A:293:GLU:OE1	2.29	0.66
6:F:-1:ALA:N	6:F:93:ASP:OD1	2.29	0.65
1:A:502:VAL:HG22	1:A:536:ILE:HD11	1.79	0.64
6:F:148:VAL:HG11	6:F:216:ILE:HD13	1.80	0.63
2:B:73:ASP:O	2:B:99:LYS:NZ	2.32	0.63
6:G:192:GLU:O	6:G:224:ARG:NH1	2.32	0.63
1:A:357:ILE:HD12	1:A:475:PHE:HB3	1.82	0.61
6:F:148:VAL:CG1	6:F:216:ILE:HD13	2.30	0.60
3:C:202:ASN:O	3:C:202:ASN:ND2	2.33	0.60
6:G:128:ILE:O	6:G:128:ILE:HG23	2.02	0.59
6:G:148:VAL:HG21	6:G:216:ILE:HG21	1.85	0.59
3:C:215:CYS:SG	3:C:232:ILE:HD13	2.43	0.58
6:G:246:LEU:HD21	6:G:248:PHE:CE2	2.39	0.58
6:F:189:GLU:OE1	6:F:189:GLU:N	2.33	0.58
6:F:221:LEU:HD23	6:F:241:LEU:HD21	1.87	0.57
4:D:43:ASP:OD2	4:D:43:ASP:N	2.38	0.57
5:E:311:GLU:OE2	5:E:311:GLU:N	2.37	0.56
5:E:90:SER:HG	5:E:93:HIS:CE1	2.23	0.56
6:G:194:SER:O	6:G:224:ARG:NH2	2.37	0.56
6:H:19:PHE:HE2	6:H:50:LEU:HD22	1.70	0.56
6:G:188:MET:HA	6:G:188:MET:HE2	1.88	0.56
6:H:193:THR:HG23	6:H:193:THR:O	2.06	0.56
4:D:83:TYR:HE2	4:D:92:ILE:HD11	1.71	0.56
6:H:174:ASP:OD1	6:H:174:ASP:N	2.38	0.56
3:C:108:SER:OG	3:C:109:LYS:N	2.39	0.56
4:D:106:VAL:HG13	4:D:153:LEU:CD1	2.36	0.56
6:H:137:LEU:HD11	6:H:162:ILE:HD11	1.88	0.56
6:G:102:LEU:HD11	6:G:111:ILE:CG2	2.36	0.55
4:D:58:LEU:O	4:D:165:ARG:NE	2.39	0.55
4:D:106:VAL:HG13	4:D:153:LEU:HD13	1.87	0.55
6:G:41:ASP:OD1	6:G:43:SER:N	2.39	0.55
6:G:74:SER:O	6:G:78:ILE:HD13	2.06	0.55
4:D:106:VAL:HG21	4:D:149:ALA:HB1	1.88	0.55
1:A:350:MET:O	1:A:350:MET:HG3	2.07	0.55
5:E:313:LEU:HD22	5:E:353:LEU:HD11	1.89	0.55
1:A:627:VAL:HG21	1:A:647:LEU:CD1	2.37	0.54
4:D:32:ARG:NH2	5:E:159:GLU:OE1	2.41	0.54
6:F:26:VAL:HB	6:F:72:LEU:HD21	1.89	0.54
1:A:457:GLU:OE2	1:A:460:LEU:HD22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:163:THR:HG22	6:H:164:LYS:H	1.73	0.54
4:D:40:THR:HG23	4:D:41:ALA:N	2.23	0.54
6:G:139:LEU:HD11	6:G:144:PHE:HB2	1.89	0.53
6:G:143:GLU:OE2	6:G:195:ILE:HD11	2.07	0.53
6:H:151:LEU:HD11	6:H:171:ALA:HB3	1.90	0.53
6:H:236:LEU:HD12	6:H:248:PHE:O	2.09	0.53
6:G:148:VAL:HG23	6:G:216:ILE:HD13	1.90	0.52
6:H:212:LEU:H	6:H:212:LEU:HD22	1.75	0.52
1:A:706:LEU:HD22	1:A:745:ILE:HG23	1.91	0.52
5:E:105:ASP:N	5:E:105:ASP:OD1	2.42	0.52
4:D:293:SER:O	5:E:189:ARG:NH1	2.42	0.52
6:G:20:LYS:HA	6:G:72:LEU:HD13	1.91	0.52
1:A:503:ILE:H	1:A:503:ILE:HD12	1.74	0.52
3:C:138:THR:O	3:C:142:ARG:NH1	2.43	0.52
6:F:23:VAL:HG21	6:F:39:ALA:CB	2.39	0.52
2:B:79:ASN:N	2:B:79:ASN:OD1	2.43	0.52
6:H:236:LEU:HD11	6:H:247:GLN:HG2	1.91	0.52
5:E:113:LEU:HD23	5:E:157:THR:HG21	1.92	0.52
6:H:187:ASP:OD2	6:H:190:HIS:N	2.35	0.52
6:G:2:LEU:HB3	6:G:92:ALA:HB3	1.93	0.51
6:F:66:VAL:HG13	6:F:68:LEU:HD11	1.91	0.51
3:C:86:ASP:OD1	4:D:111:LYS:NZ	2.43	0.51
2:B:175:LEU:HD22	2:B:209:LEU:HD22	1.93	0.51
2:B:244:ASN:ND2	2:B:247:ASP:OD2	2.44	0.51
6:G:246:LEU:HD23	6:G:246:LEU:O	2.10	0.51
5:E:57:LEU:HD11	5:E:139:ILE:HD11	1.92	0.50
6:F:90:LEU:O	6:F:91:ILE:HD13	2.12	0.50
6:H:1:MET:SD	6:H:2:LEU:HD22	2.52	0.50
6:G:41:ASP:OD1	6:G:41:ASP:C	2.50	0.50
4:D:317:ASN:ND2	4:D:321:GLN:OE1	2.45	0.50
5:E:57:LEU:CD1	5:E:139:ILE:HD11	2.42	0.49
6:H:162:ILE:HG22	6:H:203:VAL:HB	1.93	0.49
1:A:320:LEU:HD22	1:A:351:LEU:HD11	1.93	0.49
1:A:710:ARG:NH1	1:A:753:ASP:O	2.45	0.49
2:B:283:SER:O	2:B:287:GLU:HG2	2.13	0.49
3:C:58:GLY:O	3:C:62:THR:OG1	2.09	0.49
6:F:68:LEU:HD22	6:F:99:ILE:HD12	1.93	0.49
6:H:212:LEU:O	6:H:216:ILE:HG12	2.12	0.49
3:C:103:THR:HG21	6:F:45:VAL:HG13	1.94	0.49
5:E:298:ILE:O	5:E:302:GLU:HG2	2.13	0.49
6:G:161:MET:SD	6:G:162:ILE:N	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ARG:NH2	9:B:402:AGS:O2A	2.46	0.49
6:H:236:LEU:HD11	6:H:247:GLN:CG	2.43	0.49
1:A:534:GLU:N	1:A:534:GLU:OE1	2.45	0.49
1:A:387:LEU:O	1:A:391:GLY:N	2.46	0.49
6:F:36:ILE:HG22	6:F:51:GLU:HG3	1.94	0.49
3:C:267:ARG:NH2	3:C:316:ASP:OD2	2.43	0.48
6:H:137:LEU:HD21	6:H:167:ILE:HD11	1.95	0.48
1:A:291:VAL:HG13	1:A:291:VAL:O	2.13	0.48
2:B:147:SER:O	2:B:155:GLN:NE2	2.46	0.48
1:A:506:LEU:HD22	1:A:520:LEU:HD21	1.95	0.48
6:H:33:ASP:OD2	6:H:33:ASP:C	2.51	0.48
6:G:164:LYS:CD	6:G:164:LYS:O	2.62	0.48
6:F:195:ILE:N	6:F:195:ILE:HD12	2.28	0.48
2:B:253:ARG:NH2	2:B:306:TYR:OH	2.47	0.48
6:G:164:LYS:O	6:G:164:LYS:HD2	2.14	0.47
3:C:202:ASN:O	3:C:202:ASN:CG	2.53	0.47
2:B:232:HIS:N	2:B:233:PRO:CD	2.77	0.47
6:F:11:LEU:O	6:F:15:ILE:HG12	2.14	0.47
6:H:137:LEU:HD21	6:H:167:ILE:CD1	2.45	0.47
2:B:15:TYR:O	2:B:174:ARG:NH2	2.46	0.47
3:C:256:TRP:NE1	4:D:320:ASN:OD1	2.44	0.47
6:G:48:VAL:HG22	6:G:248:PHE:CD1	2.50	0.47
6:H:19:PHE:CE2	6:H:50:LEU:HD22	2.48	0.47
6:F:2:LEU:HB3	6:F:92:ALA:HB3	1.97	0.47
3:C:262:THR:O	3:C:266:VAL:HG23	2.15	0.47
4:D:42:GLN:O	4:D:46:VAL:HG23	2.15	0.47
1:A:696:THR:OG1	1:A:697:ASP:N	2.48	0.46
1:A:590:LEU:HD11	7:I:-2:DT:O4	2.15	0.46
6:G:48:VAL:HG22	6:G:248:PHE:CE1	2.50	0.46
2:B:39:ASP:C	2:B:39:ASP:OD1	2.53	0.46
1:A:457:GLU:HG3	1:A:457:GLU:O	2.16	0.46
5:E:163:LYS:NZ	5:E:164:ASN:OD1	2.48	0.46
2:B:267:VAL:HG11	2:B:299:ILE:CD1	2.46	0.46
3:C:54:PRO:HD2	3:C:57:THR:HG21	1.98	0.46
4:D:96:ASN:N	4:D:96:ASN:OD1	2.48	0.46
6:H:8:GLU:OE2	6:H:10:SER:OG	2.30	0.46
2:B:113:LEU:HD12	2:B:142:PHE:CE2	2.52	0.45
1:A:350:MET:O	1:A:350:MET:CG	2.64	0.45
6:F:90:LEU:C	6:F:91:ILE:HD13	2.36	0.45
2:B:71:TYR:CD1	2:B:75:VAL:HG21	2.51	0.45
6:H:66:VAL:HG22	6:H:67:THR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:VAL:HG13	1:A:536:ILE:HG12	1.99	0.45
6:F:162:ILE:CD1	6:F:167:ILE:HD12	2.47	0.45
3:C:63:ILE:HD13	3:C:144:CYS:SG	2.57	0.45
1:A:739:LYS:HE2	1:A:771:THR:HG22	1.97	0.45
2:B:254:THR:OG1	2:B:255:ASP:OD2	2.34	0.45
6:H:208:GLY:O	6:H:212:LEU:HD22	2.17	0.45
1:A:720:GLN:HA	1:A:720:GLN:OE1	2.17	0.44
6:G:25:LEU:HB3	6:G:121:ILE:HD11	1.98	0.44
7:I:1:DT:H2'	7:I:0:DT:H72	1.99	0.44
1:A:318:MET:HA	1:A:318:MET:HE3	1.99	0.44
2:B:267:VAL:HG11	2:B:299:ILE:HD12	1.99	0.44
1:A:487:LEU:HD11	1:A:517:VAL:HG11	1.98	0.44
3:C:11:GLU:OE1	3:C:18:LYS:NZ	2.28	0.43
4:D:325:LEU:HD12	4:D:353:LEU:HD11	2.00	0.43
6:G:139:LEU:HD12	6:G:140:PRO:O	2.18	0.43
6:G:213:LEU:C	6:G:213:LEU:HD23	2.37	0.43
6:F:93:ASP:OD2	6:F:93:ASP:N	2.51	0.43
1:A:623:LEU:O	1:A:627:VAL:HG23	2.18	0.43
6:H:147:ILE:CD1	6:H:180:VAL:HG11	2.49	0.43
2:B:318:LYS:HD2	3:C:297:VAL:HG11	2.01	0.43
1:A:581:TYR:CD2	1:A:645:ALA:HB2	2.54	0.43
1:A:689:HIS:ND1	1:A:741:ASP:OD2	2.52	0.43
7:I:9:DC:H2'	7:I:10:DC:C6	2.54	0.43
6:H:23:VAL:O	6:H:72:LEU:HD21	2.19	0.43
6:H:162:ILE:HD12	6:H:167:ILE:HG12	1.99	0.43
6:H:211:TYR:O	6:H:214:ASP:OD2	2.37	0.43
1:A:377:GLN:NE2	1:A:381:ASP:OD2	2.52	0.43
1:A:500:PRO:HA	1:A:503:ILE:CD1	2.49	0.43
3:C:182:LEU:HD11	3:C:189:LEU:HB2	2.01	0.43
6:G:43:SER:HB2	6:G:45:VAL:HG12	1.99	0.43
6:F:185:PHE:C	6:F:185:PHE:CD1	2.92	0.42
3:C:24:LEU:HD11	3:C:66:LEU:HD12	2.00	0.42
4:D:83:TYR:CE2	4:D:92:ILE:HD11	2.54	0.42
6:F:78:ILE:CD1	6:F:116:LEU:HD13	2.49	0.42
1:A:506:LEU:HD22	1:A:520:LEU:CD2	2.50	0.42
3:C:189:LEU:HD13	3:C:212:LEU:HD11	2.01	0.42
6:F:197:LEU:C	6:F:197:LEU:HD13	2.40	0.42
6:H:9:ALA:O	6:H:13:LYS:HG3	2.20	0.42
2:B:29:THR:HG21	2:B:163:TYR:CE1	2.55	0.42
6:H:71:ASP:O	6:H:71:ASP:OD2	2.37	0.42
1:A:483:ILE:HD12	1:A:507:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:74:SER:O	6:H:78:ILE:HG22	2.20	0.41
6:H:97:ASP:OD1	6:H:97:ASP:N	2.54	0.41
6:F:26:VAL:HG22	6:F:27:ASN:N	2.35	0.41
6:G:85:THR:O	6:G:85:THR:OG1	2.35	0.41
2:B:209:LEU:O	2:B:213:VAL:HG23	2.20	0.41
2:B:255:ASP:OD2	2:B:255:ASP:N	2.52	0.41
2:B:305:THR:HG22	2:B:306:TYR:N	2.34	0.41
3:C:171:GLN:O	3:C:175:GLU:HG3	2.21	0.41
3:C:76:SER:O	6:F:44:ARG:NH2	2.53	0.41
1:A:520:LEU:O	1:A:524:ILE:HG12	2.21	0.41
6:H:69:GLY:O	6:H:118:LEU:HD13	2.20	0.41
4:D:229:ARG:NH2	9:D:402:AGS:O2A	2.53	0.41
6:H:116:LEU:HD23	6:H:117:LYS:O	2.20	0.41
2:B:177:GLN:O	2:B:181:LEU:HD13	2.21	0.41
4:D:91:ARG:O	4:D:92:ILE:HD13	2.21	0.41
1:A:491:ALA:HA	1:A:496:PHE:CE1	2.56	0.41
3:C:192:ASN:OD1	3:C:192:ASN:N	2.54	0.41
5:E:266:LEU:HD11	5:E:282:CYS:SG	2.61	0.41
6:F:236:LEU:HD13	6:F:249:PHE:CE2	2.56	0.41
6:H:9:ALA:HA	6:H:12:PHE:CE1	2.56	0.41
1:A:627:VAL:HG21	1:A:647:LEU:HD12	2.02	0.40
1:A:636:GLN:HA	1:A:636:GLN:NE2	2.37	0.40
2:B:179:ILE:O	2:B:183:ASP:N	2.54	0.40
6:H:12:PHE:CD2	6:H:88:LEU:HD22	2.56	0.40
8:J:19:DG:H2'	8:J:20:DG:C8	2.56	0.40
5:E:310:VAL:HG12	5:E:312:THR:H	1.87	0.40
6:F:89:THR:CG2	6:F:102:LEU:HB2	2.52	0.40
6:F:124:ASP:O	6:F:125:PHE:C	2.59	0.40
6:G:60:TYR:CD1	6:G:60:TYR:C	2.95	0.40
1:A:306:ASN:OD1	1:A:307:LEU:N	2.55	0.40
4:D:315:ASP:OD1	4:D:315:ASP:N	2.49	0.40
6:G:162:ILE:CG2	6:G:203:VAL:HG22	2.51	0.40
6:G:197:LEU:HD21	6:G:199:MET:HB2	2.03	0.40
1:A:318:MET:HA	1:A:318:MET:CE	2.51	0.40
9:B:402:AGS:HO3'	9:B:402:AGS:HO2'	1.66	0.40
6:G:245:PHE:CD1	6:G:245:PHE:N	2.89	0.40
6:F:78:ILE:HD12	6:F:116:LEU:HD13	2.03	0.40
6:G:72:LEU:HD23	6:G:72:LEU:HA	1.98	0.40
6:G:144:PHE:O	6:G:148:VAL:HG22	2.21	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	488/918 (53%)	480 (98%)	8 (2%)	0	100	100
2	B	316/323 (98%)	312 (99%)	4 (1%)	0	100	100
3	C	327/340 (96%)	323 (99%)	4 (1%)	0	100	100
4	D	334/353 (95%)	329 (98%)	5 (2%)	0	100	100
5	E	352/354 (99%)	348 (99%)	4 (1%)	0	100	100
6	F	256/277 (92%)	247 (96%)	9 (4%)	0	100	100
6	G	255/277 (92%)	247 (97%)	8 (3%)	0	100	100
6	H	253/277 (91%)	242 (96%)	11 (4%)	0	100	100
All	All	2581/3119 (83%)	2528 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	426/791 (54%)	409 (96%)	17 (4%)	31	63
2	B	279/283 (99%)	269 (96%)	10 (4%)	35	67
3	C	286/296 (97%)	279 (98%)	7 (2%)	49	78
4	D	298/312 (96%)	288 (97%)	10 (3%)	37	69
5	E	323/324 (100%)	316 (98%)	7 (2%)	52	80
6	F	231/249 (93%)	227 (98%)	4 (2%)	60	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	231/249 (93%)	223 (96%)	8 (4%)	36	68
6	H	230/249 (92%)	223 (97%)	7 (3%)	41	73
All	All	2304/2753 (84%)	2234 (97%)	70 (3%)	44	73

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	LYS
1	A	419	PHE
1	A	476	ARG
1	A	478	PRO
1	A	496	PHE
1	A	511	ARG
1	A	516	GLN
1	A	520	LEU
1	A	522	SER
1	A	538	GLU
1	A	540	SER
1	A	541	LYS
1	A	605	LYS
1	A	663	ARG
1	A	715	ASP
1	A	723	ASP
1	A	740	GLU
2	B	32	ARG
2	B	117	ASP
2	B	180	LYS
2	B	185	LYS
2	B	216	HIS
2	B	226	LYS
2	B	238	LYS
2	B	244	ASN
2	B	255	ASP
2	B	317	HIS
3	C	120	ASP
3	C	176	ARG
3	C	229	ASP
3	C	240	ARG
3	C	286	GLU
3	C	287	ASP
3	C	305	ASP

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Mol	Chain	Res	Type
4	D	35	ASN
4	D	43	ASP
4	D	55	SER
4	D	86	ASP
4	D	104	SER
4	D	120	LYS
4	D	126	LEU
4	D	239	SER
4	D	266	ASP
4	D	276	LYS
5	E	59	SER
5	E	101	MET
5	E	204	ASP
5	E	220	LYS
5	E	309	ASP
5	E	323	GLU
5	E	332	LEU
6	F	44	ARG
6	F	93	ASP
6	F	161	MET
6	F	185	PHE
6	G	21	ASP
6	G	41	ASP
6	G	44	ARG
6	G	80	ARG
6	G	134	ASP
6	G	164	LYS
6	G	168	LYS
6	G	188	MET
6	H	1	MET
6	H	19	PHE
6	H	33	ASP
6	H	119	MET
6	H	139	LEU
6	H	187	ASP
6	H	240	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
1	A	377	GLN

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Mol	Chain	Res	Type
1	A	575	ASN
1	A	636	GLN
2	B	145	ASN
2	B	320	ASN
3	C	202	ASN
3	C	315	ASN
4	D	207	GLN
4	D	302	ASN
4	D	317	ASN
5	E	118	GLN
5	E	244	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
9	AGS	A	901	10	26,33,33	3.64	12 (46%)	26,52,52	1.99	6 (23%)
9	AGS	B	402	10	26,33,33	3.64	12 (46%)	26,52,52	2.02	6 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	GDP	E	401	-	24,30,30	3.71	13 (54%)	30,47,47	1.51	6 (20%)
9	AGS	C	402	10	26,33,33	3.63	12 (46%)	26,52,52	1.98	6 (23%)
9	AGS	D	402	10	26,33,33	3.64	12 (46%)	26,52,52	2.00	6 (23%)

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	A	901	10	-	5/17/38/38	0/3/3/3
9	AGS	B	402	10	-	4/17/38/38	0/3/3/3
11	GDP	E	401	-	-	2/12/32/32	0/3/3/3
9	AGS	C	402	10	-	0/17/38/38	0/3/3/3
9	AGS	D	402	10	-	5/17/38/38	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	402	AGS	C2'-C3'	-10.59	1.24	1.53
9	A	901	AGS	C2'-C3'	-10.58	1.24	1.53
9	C	402	AGS	C2'-C3'	-10.56	1.24	1.53
9	B	402	AGS	C2'-C3'	-10.56	1.24	1.53
11	E	401	GDP	C3'-C4'	-8.54	1.31	1.53
11	E	401	GDP	O4'-C4'	7.63	1.62	1.45
9	B	402	AGS	O4'-C1'	7.38	1.51	1.41
9	A	901	AGS	O4'-C1'	7.37	1.51	1.41
9	D	402	AGS	O4'-C1'	7.37	1.51	1.41
9	C	402	AGS	O4'-C1'	7.34	1.51	1.41
11	E	401	GDP	O4'-C1'	-7.23	1.31	1.41
9	B	402	AGS	O4'-C4'	-6.04	1.31	1.45
9	A	901	AGS	O4'-C4'	-6.04	1.31	1.45
9	D	402	AGS	O4'-C4'	-5.99	1.31	1.45
9	C	402	AGS	O4'-C4'	-5.95	1.31	1.45
11	E	401	GDP	C2-N3	5.55	1.46	1.33
9	C	402	AGS	C3'-C4'	5.53	1.67	1.53
9	B	402	AGS	C3'-C4'	5.45	1.66	1.53
9	D	402	AGS	C3'-C4'	5.41	1.66	1.53
9	A	901	AGS	C3'-C4'	5.37	1.66	1.53
11	E	401	GDP	C4-N3	5.03	1.49	1.37
9	D	402	AGS	C2'-C1'	5.00	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	402	AGS	C2'-C1'	4.93	1.61	1.53
9	A	901	AGS	C2'-C1'	4.91	1.61	1.53
9	C	402	AGS	C2'-C1'	4.90	1.61	1.53
11	E	401	GDP	C2-N2	4.81	1.45	1.34
9	B	402	AGS	PG-O3G	4.22	1.68	1.54
9	D	402	AGS	PG-O3G	4.20	1.68	1.54
9	A	901	AGS	PG-O3G	4.19	1.68	1.54
9	C	402	AGS	PG-O3G	4.18	1.68	1.54
11	E	401	GDP	C6-N1	3.83	1.43	1.37
9	A	901	AGS	PG-O2G	3.82	1.67	1.54
9	B	402	AGS	PG-O2G	3.81	1.67	1.54
9	D	402	AGS	PG-O2G	3.81	1.67	1.54
9	C	402	AGS	PG-O2G	3.80	1.67	1.54
9	B	402	AGS	C6-N6	3.64	1.47	1.34
9	D	402	AGS	C6-N6	3.63	1.47	1.34
9	C	402	AGS	C6-N6	3.62	1.47	1.34
9	A	901	AGS	C6-N6	3.62	1.47	1.34
11	E	401	GDP	C5-C6	3.21	1.53	1.47
9	A	901	AGS	C5-C4	-2.97	1.33	1.40
9	B	402	AGS	C5-C4	-2.96	1.33	1.40
9	C	402	AGS	C5-C4	-2.95	1.33	1.40
11	E	401	GDP	O3'-C3'	2.95	1.49	1.43
9	D	402	AGS	C5-C4	-2.91	1.33	1.40
11	E	401	GDP	O2'-C2'	-2.90	1.36	1.43
11	E	401	GDP	C2-N1	2.79	1.44	1.37
9	D	402	AGS	O3'-C3'	2.72	1.49	1.43
9	A	901	AGS	O3'-C3'	2.71	1.49	1.43
9	B	402	AGS	O3'-C3'	2.69	1.49	1.43
9	C	402	AGS	O3'-C3'	2.69	1.49	1.43
9	D	402	AGS	O2'-C2'	2.64	1.49	1.43
9	A	901	AGS	O2'-C2'	2.64	1.49	1.43
9	B	402	AGS	O2'-C2'	2.64	1.49	1.43
9	C	402	AGS	O2'-C2'	2.63	1.49	1.43
11	E	401	GDP	C5-C4	-2.47	1.36	1.43
9	A	901	AGS	PA-O5'	2.19	1.68	1.59
9	C	402	AGS	PA-O5'	2.14	1.68	1.59
9	D	402	AGS	PA-O5'	2.14	1.67	1.59
9	B	402	AGS	PA-O5'	2.13	1.67	1.59
11	E	401	GDP	O6-C6	-2.13	1.19	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	402	AGS	N3-C2-N1	-5.52	120.05	128.68
9	D	402	AGS	N3-C2-N1	-5.52	120.06	128.68
9	A	901	AGS	N3-C2-N1	-5.51	120.07	128.68
9	C	402	AGS	N3-C2-N1	-5.49	120.10	128.68
9	A	901	AGS	C1'-N9-C4	-4.72	118.34	126.64
9	B	402	AGS	C1'-N9-C4	-4.67	118.44	126.64
9	D	402	AGS	C1'-N9-C4	-4.47	118.78	126.64
9	C	402	AGS	C1'-N9-C4	-4.42	118.88	126.64
9	A	901	AGS	C5-C6-N6	3.99	126.41	120.35
9	C	402	AGS	C5-C6-N6	3.96	126.37	120.35
9	D	402	AGS	C5-C6-N6	3.94	126.34	120.35
9	B	402	AGS	C5-C6-N6	3.94	126.34	120.35
11	E	401	GDP	C5-C6-N1	3.40	119.96	113.95
11	E	401	GDP	C3'-C2'-C1'	3.37	106.06	100.98
11	E	401	GDP	C2-N1-C6	-2.93	119.69	125.10
9	D	402	AGS	PA-O3A-PB	-2.82	123.15	132.83
9	B	402	AGS	PA-O3A-PB	-2.81	123.18	132.83
9	A	901	AGS	PA-O3A-PB	-2.78	123.28	132.83
11	E	401	GDP	C8-N7-C5	2.77	108.27	102.99
9	C	402	AGS	PA-O3A-PB	-2.67	123.66	132.83
9	B	402	AGS	C3'-C2'-C1'	2.64	104.95	100.98
11	E	401	GDP	PA-O3A-PB	-2.62	123.83	132.83
9	D	402	AGS	C3'-C2'-C1'	2.42	104.63	100.98
9	C	402	AGS	C3'-C2'-C1'	2.41	104.60	100.98
9	A	901	AGS	N6-C6-N1	-2.38	113.63	118.57
9	C	402	AGS	N6-C6-N1	-2.38	113.63	118.57
9	B	402	AGS	N6-C6-N1	-2.38	113.64	118.57
9	D	402	AGS	N6-C6-N1	-2.36	113.67	118.57
11	E	401	GDP	O6-C6-C5	-2.22	120.04	124.37
9	A	901	AGS	C3'-C2'-C1'	2.21	104.31	100.98

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	901	AGS	PB-O3B-PG-O2G
9	B	402	AGS	C5'-O5'-PA-O1A
9	B	402	AGS	C5'-O5'-PA-O2A
9	D	402	AGS	C5'-O5'-PA-O1A
9	D	402	AGS	C5'-O5'-PA-O2A
11	E	401	GDP	PA-O3A-PB-O2B
9	B	402	AGS	PA-O3A-PB-O1B
11	E	401	GDP	PA-O3A-PB-O3B

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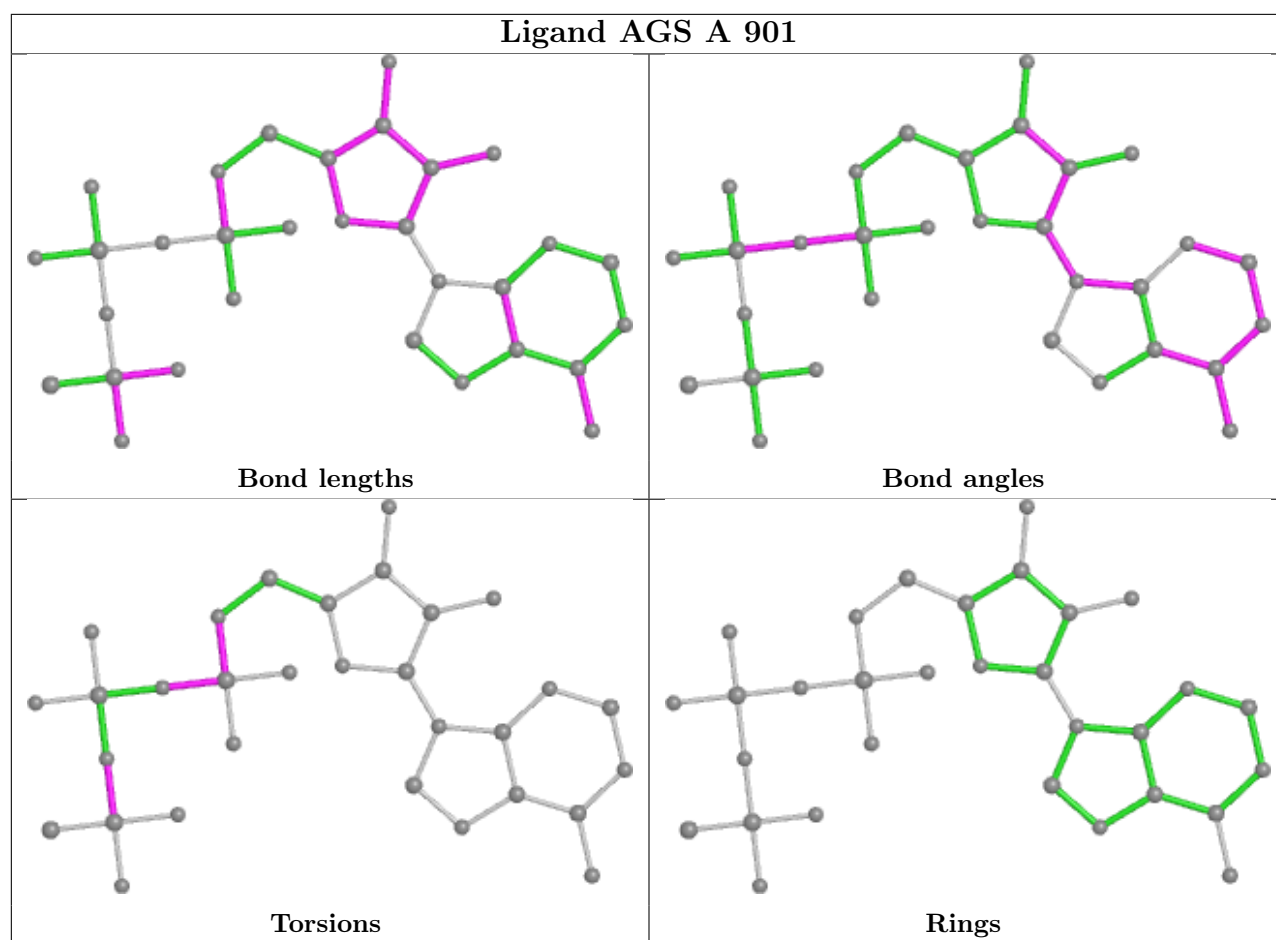
Mol	Chain	Res	Type	Atoms
9	A	901	AGS	C5'-O5'-PA-O3A
9	B	402	AGS	C5'-O5'-PA-O3A
9	D	402	AGS	C5'-O5'-PA-O3A
9	D	402	AGS	PA-O3A-PB-O2B
9	A	901	AGS	C5'-O5'-PA-O1A
9	A	901	AGS	C5'-O5'-PA-O2A
9	A	901	AGS	PB-O3A-PA-O2A
9	D	402	AGS	PA-O3A-PB-O1B

There are no ring outliers.

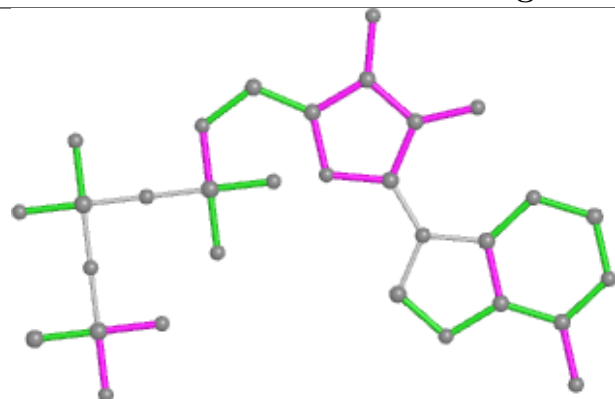
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	402	AGS	2	0
9	D	402	AGS	1	0

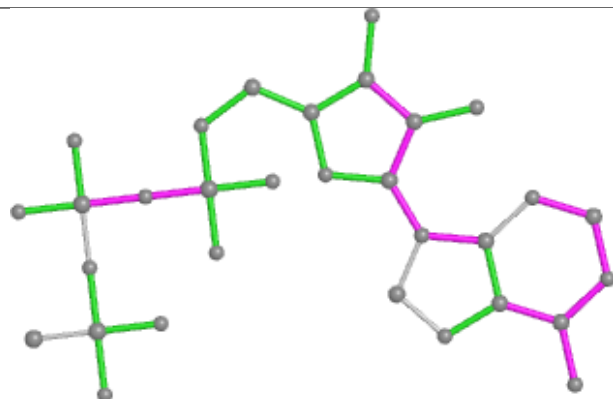
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



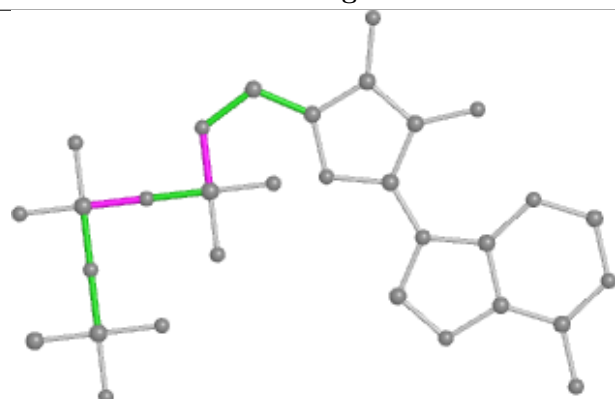
## Ligand AGS B 402



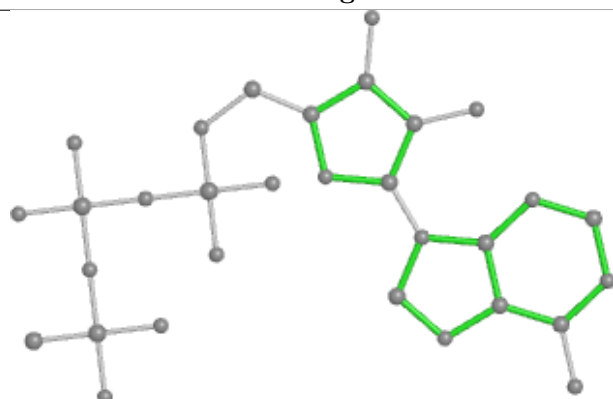
Bond lengths



Bond angles

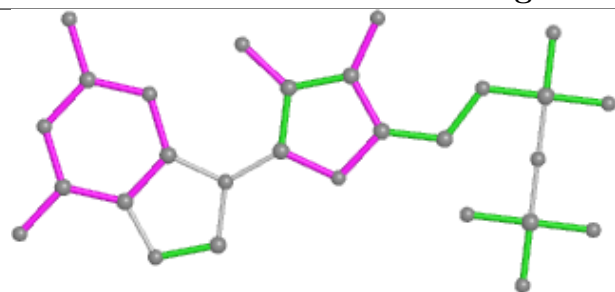


Torsions

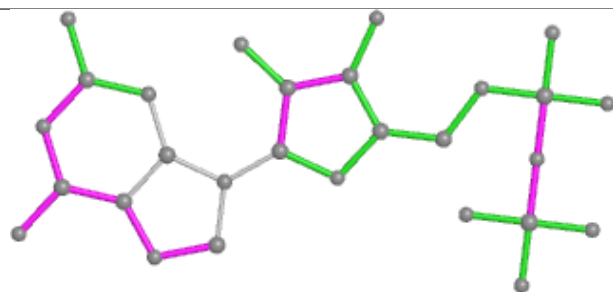


Rings

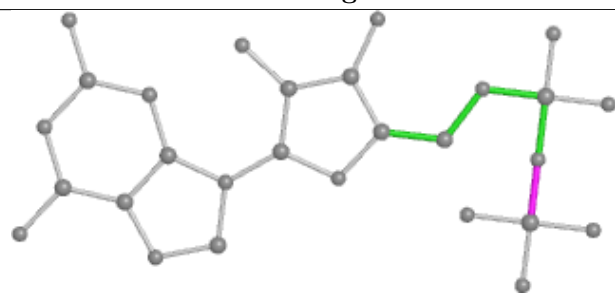
## Ligand GDP E 401



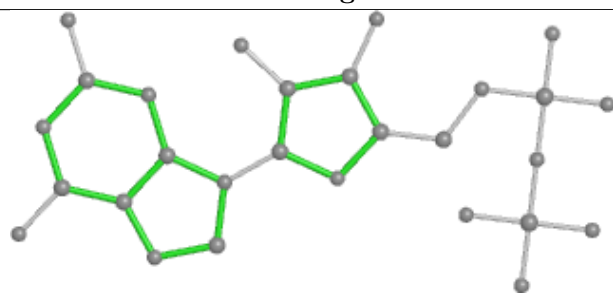
Bond lengths



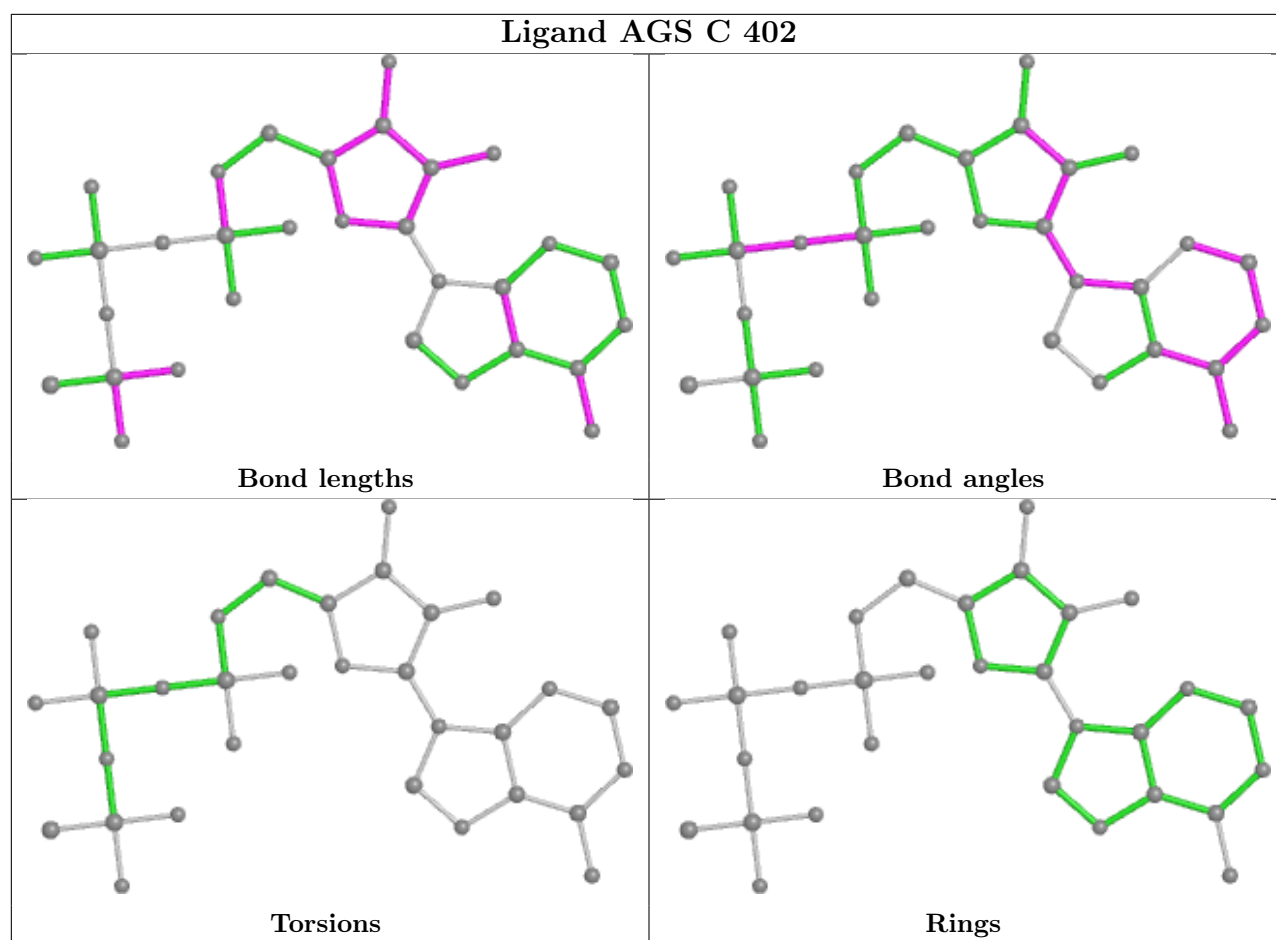
Bond angles

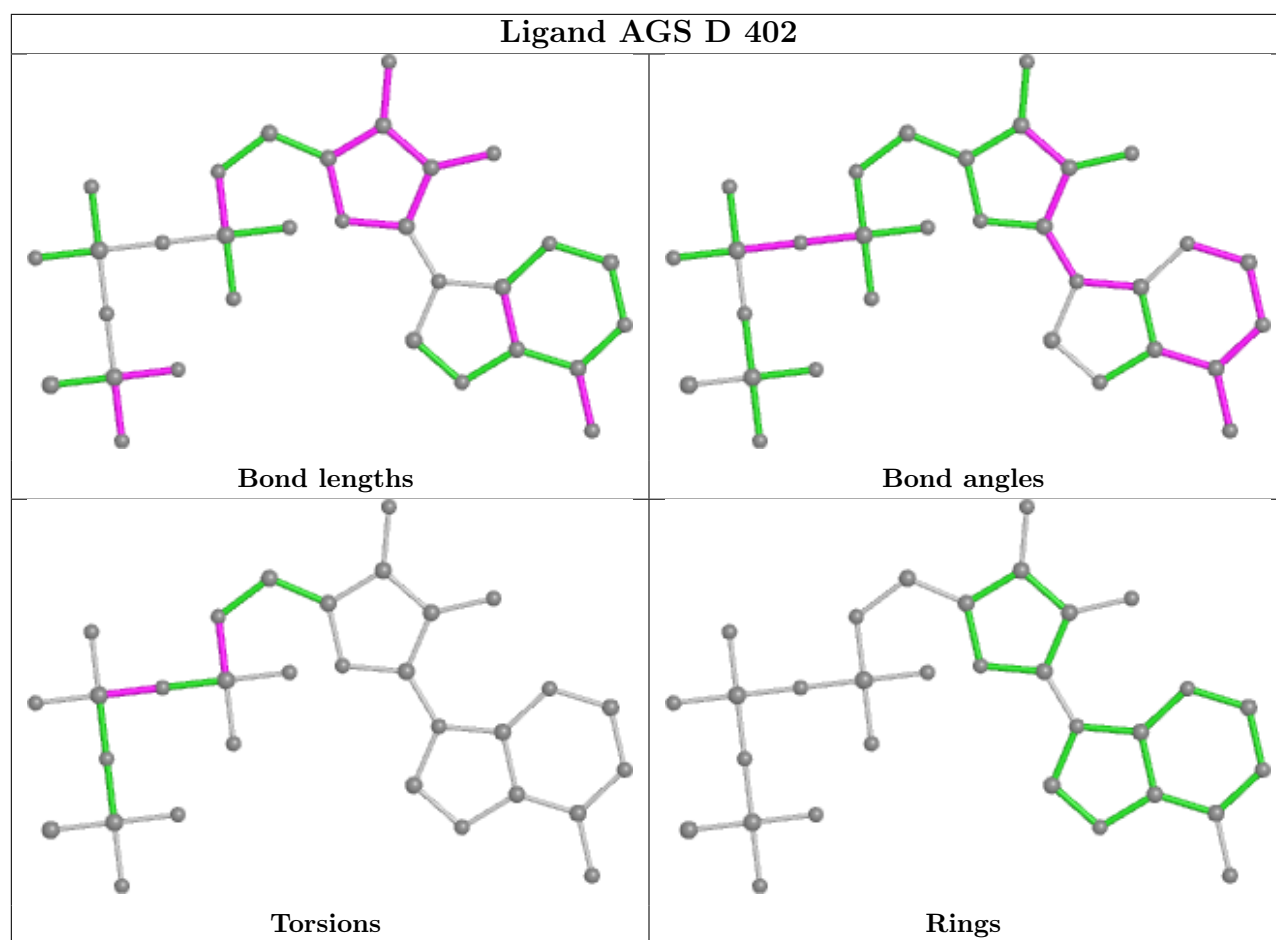


Torsions



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.



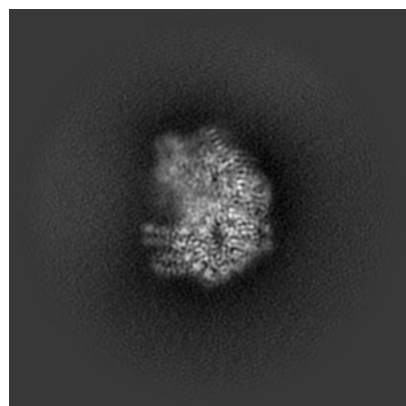
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27666. These allow visual inspection of the internal detail of the map and identification of artifacts.

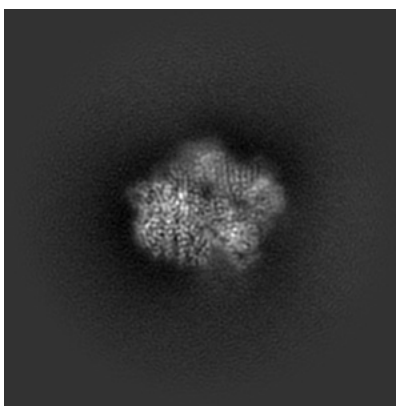
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

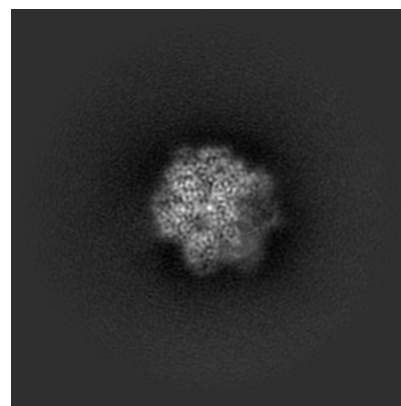
#### 6.1.1 Primary map



X

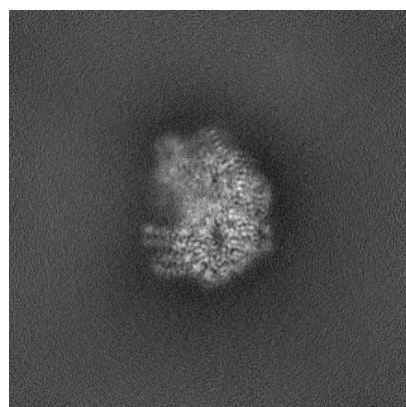


Y

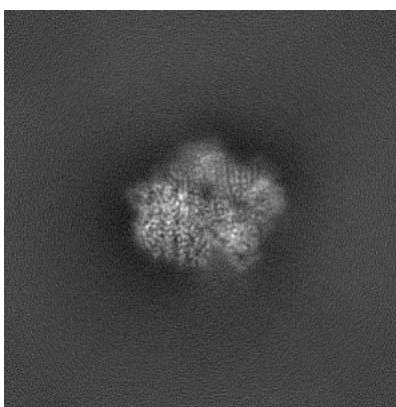


Z

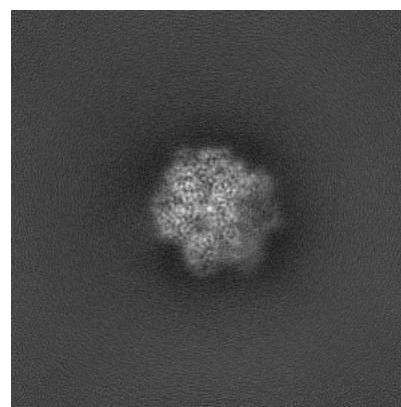
#### 6.1.2 Raw map



X



Y

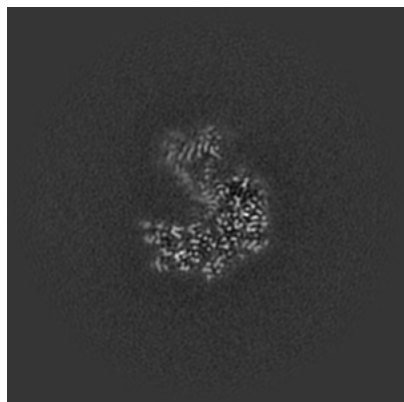


Z

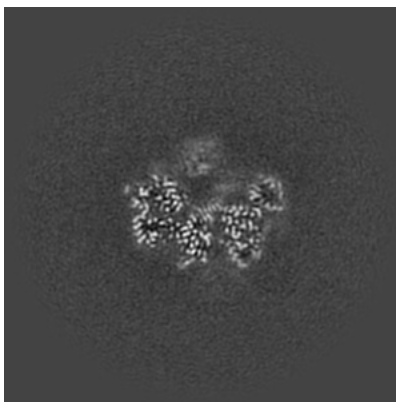
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

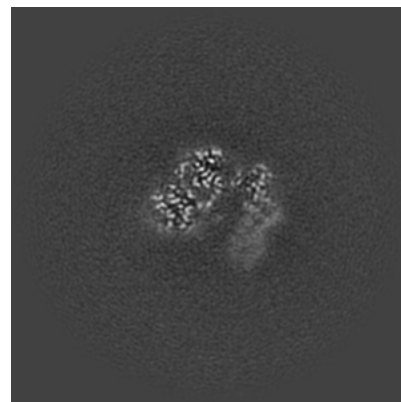
### 6.2.1 Primary map



X Index: 192

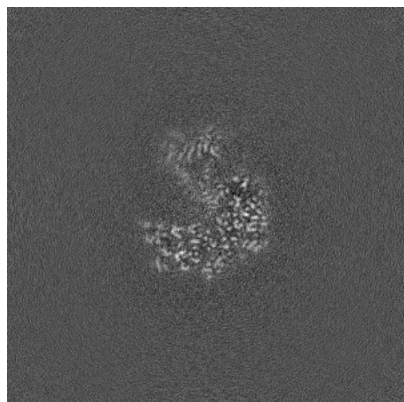


Y Index: 192

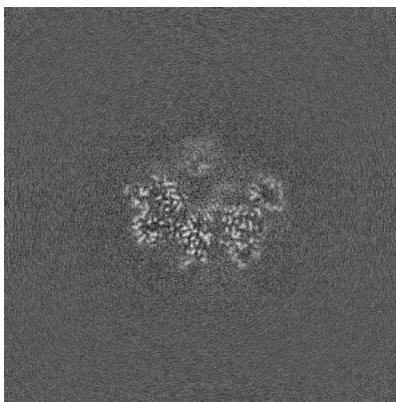


Z Index: 192

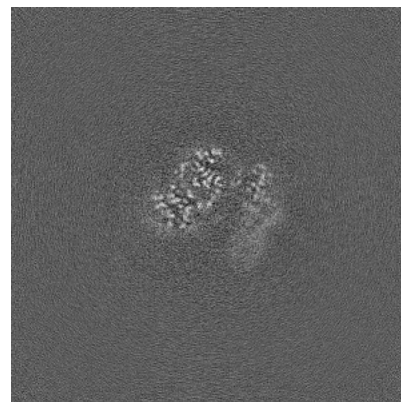
### 6.2.2 Raw map



X Index: 192



Y Index: 192

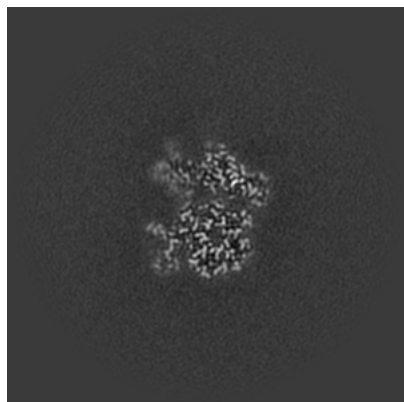


Z Index: 192

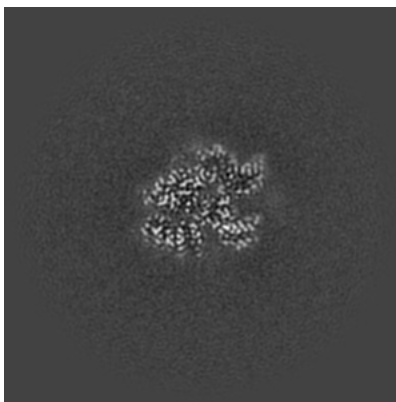
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

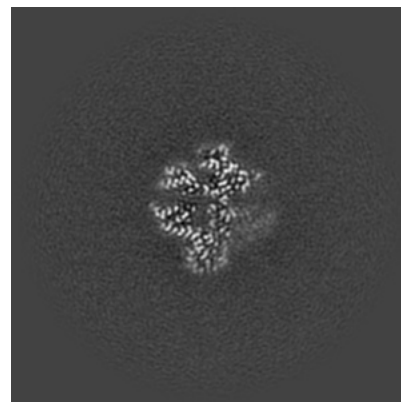
### 6.3.1 Primary map



X Index: 171

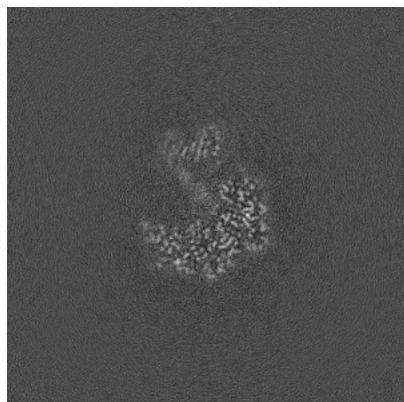


Y Index: 216

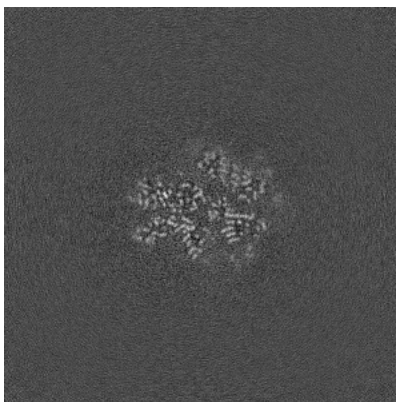


Z Index: 169

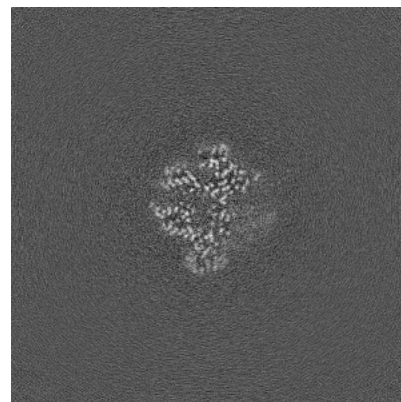
### 6.3.2 Raw map



X Index: 194



Y Index: 207

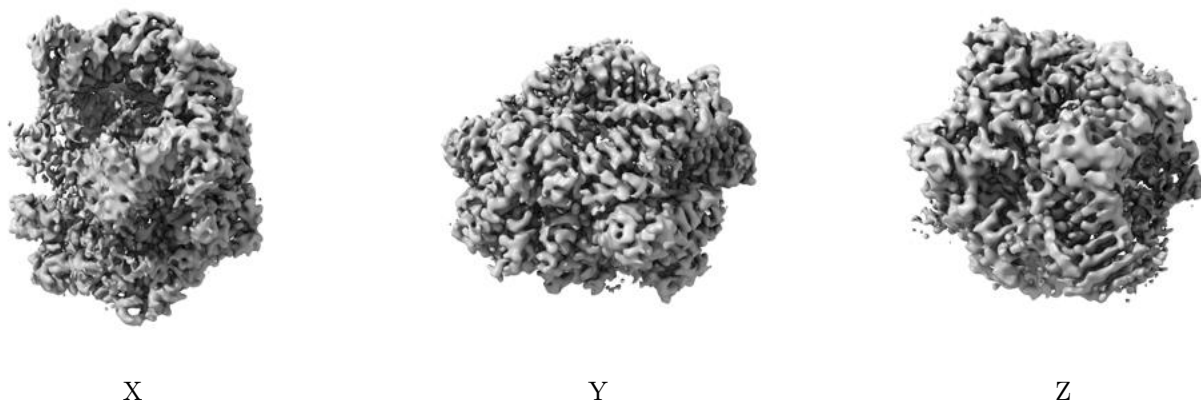


Z Index: 170

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

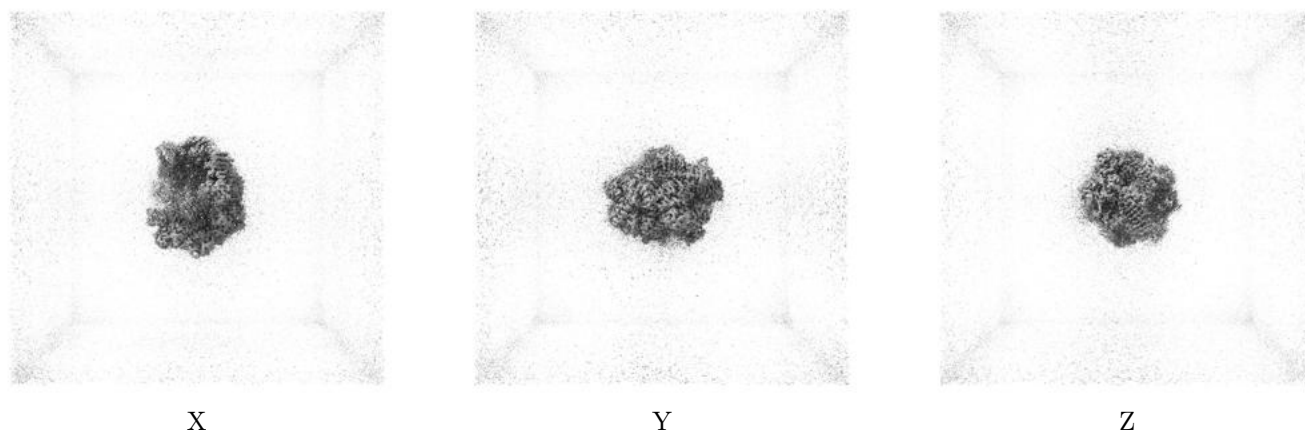
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 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.

### 6.4.2 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.

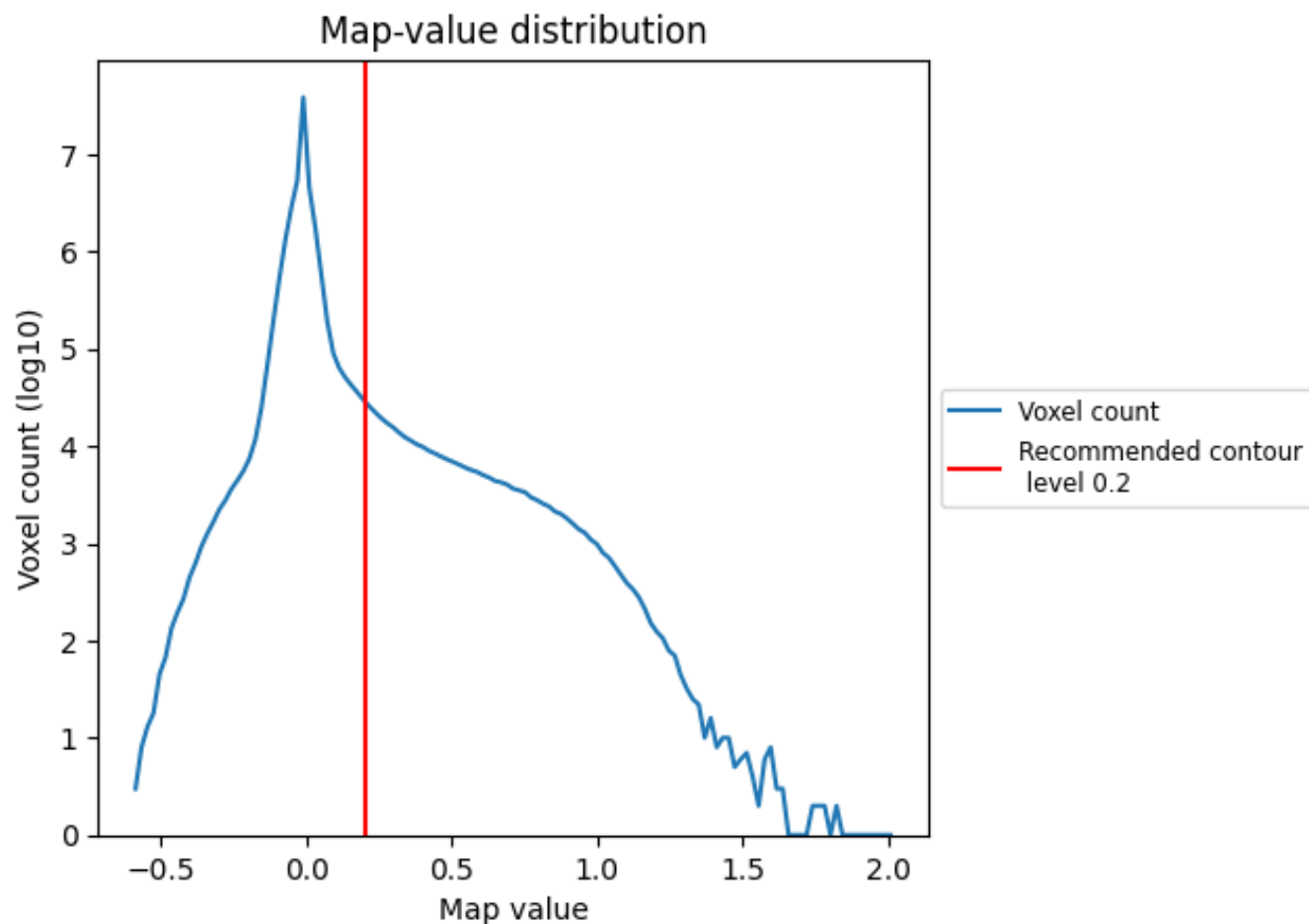
## 6.5 Mask visualisation [i](#)

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.

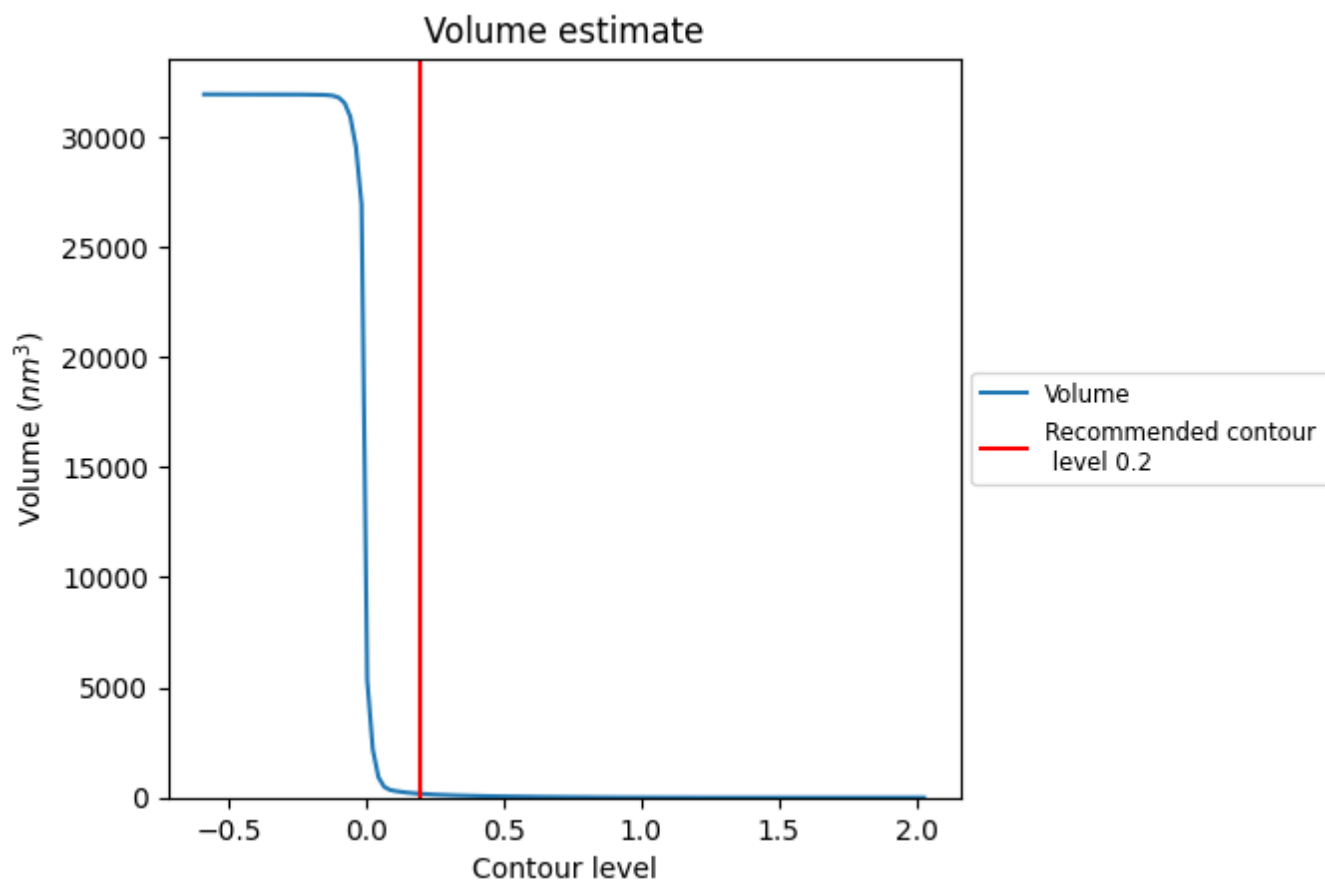
### 7.1 Map-value distribution [i](#)



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.



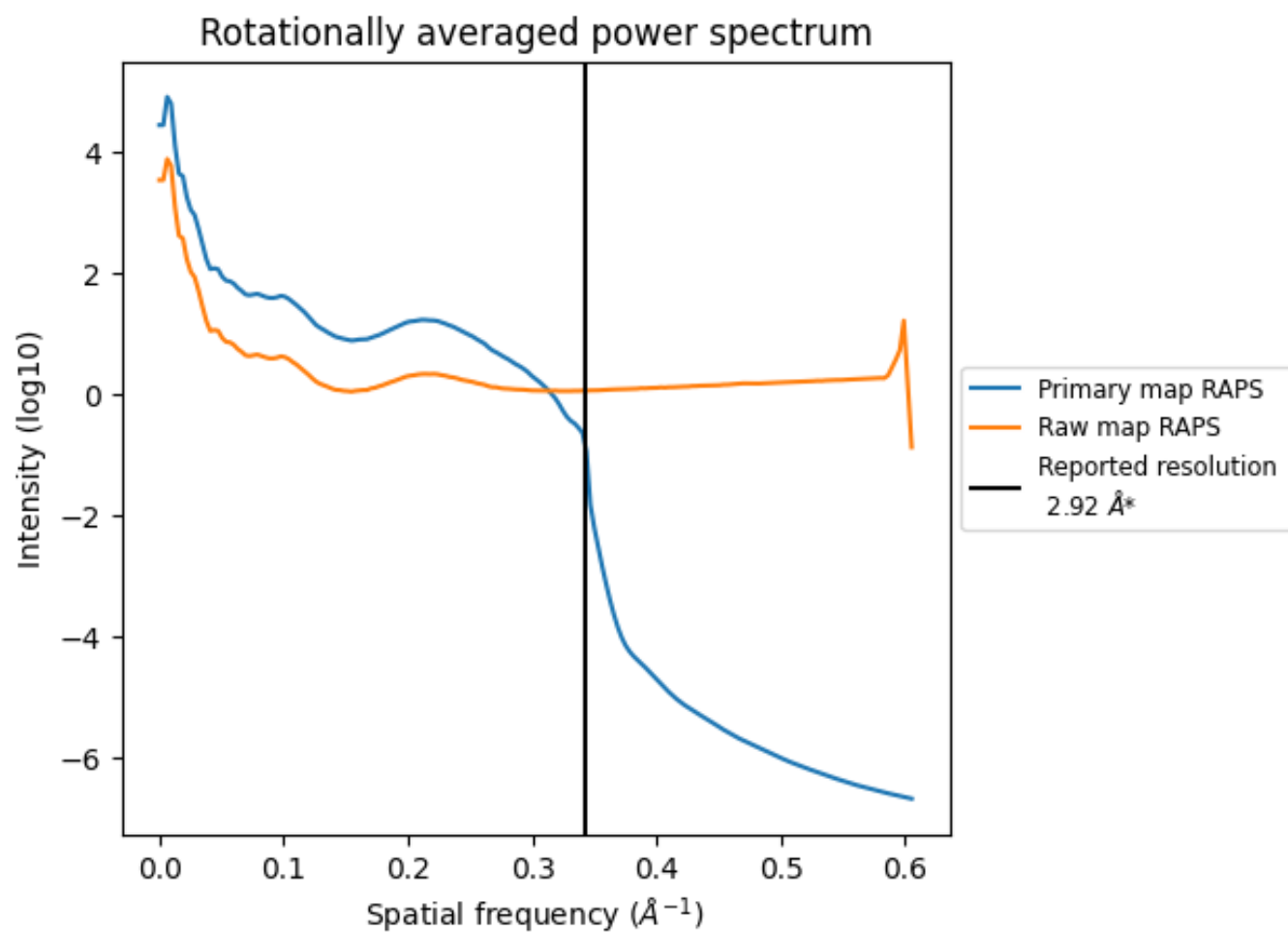
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172  $\text{nm}^3$ ; this corresponds to an approximate mass of 155 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 ⓘ

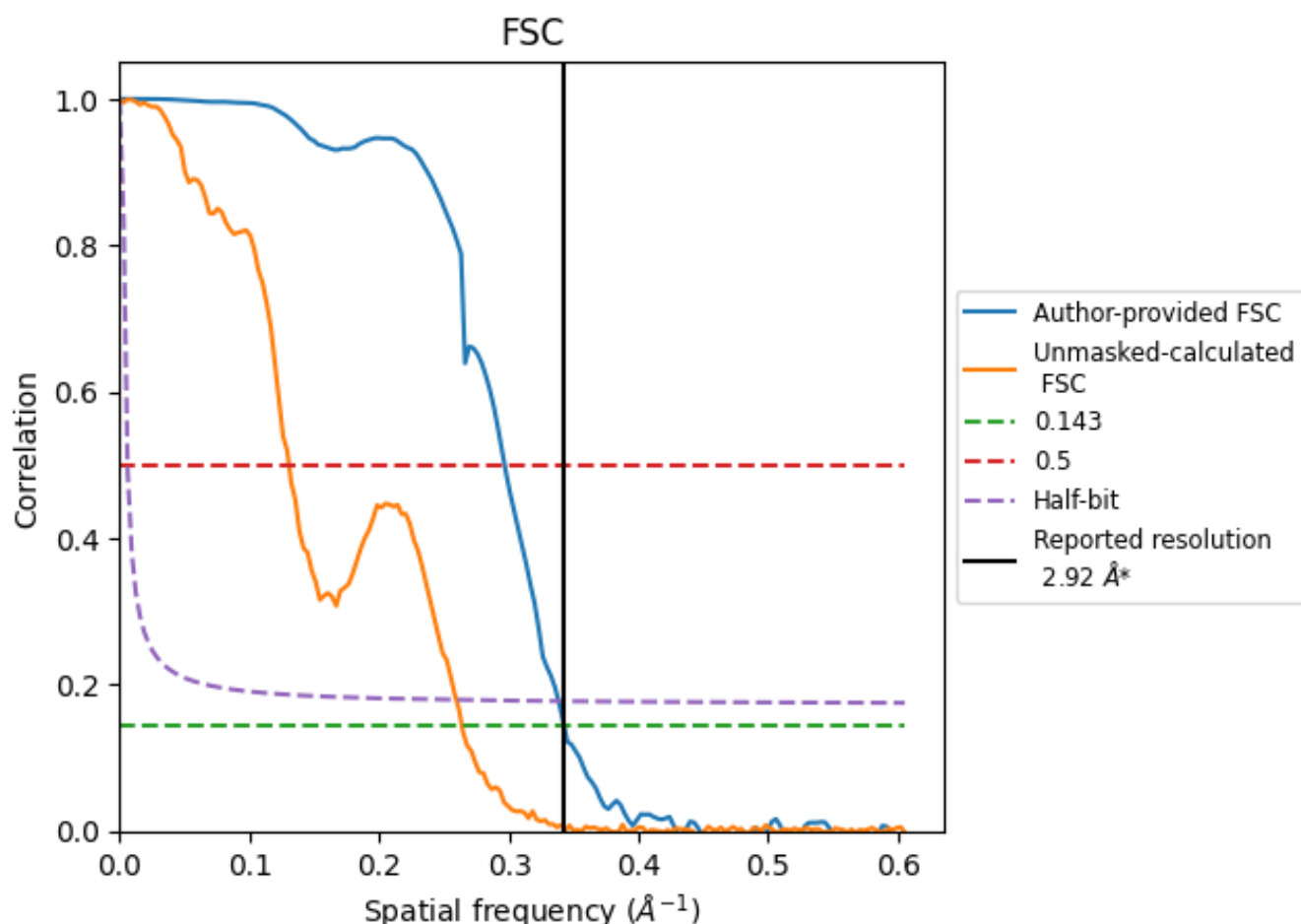


\*Reported resolution corresponds to spatial frequency of 0.342 Å<sup>-1</sup>

## 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 0.342 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

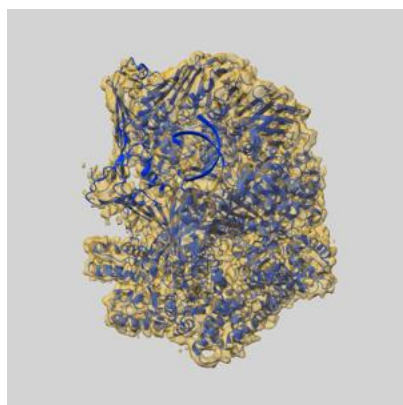
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.37	2.95
Unmasked-calculated*	3.79	7.65	3.85

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 2.92 by more than 10 %

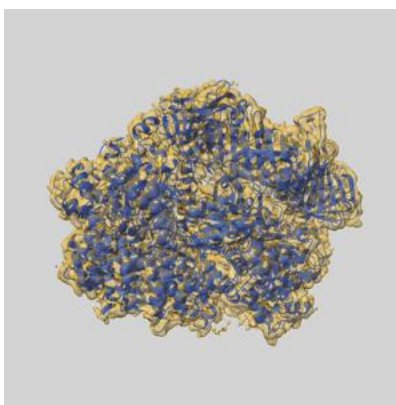
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27666 and PDB model 8DQZ. Per-residue inclusion information can be found in section 3 on page 10.

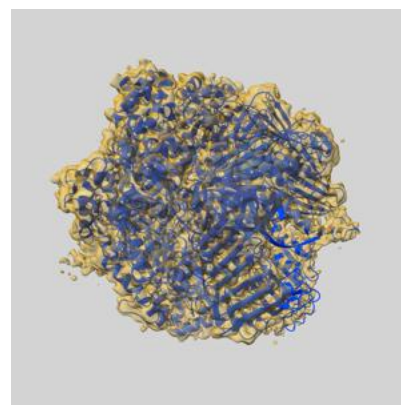
### 9.1 Map-model overlay [i](#)



X



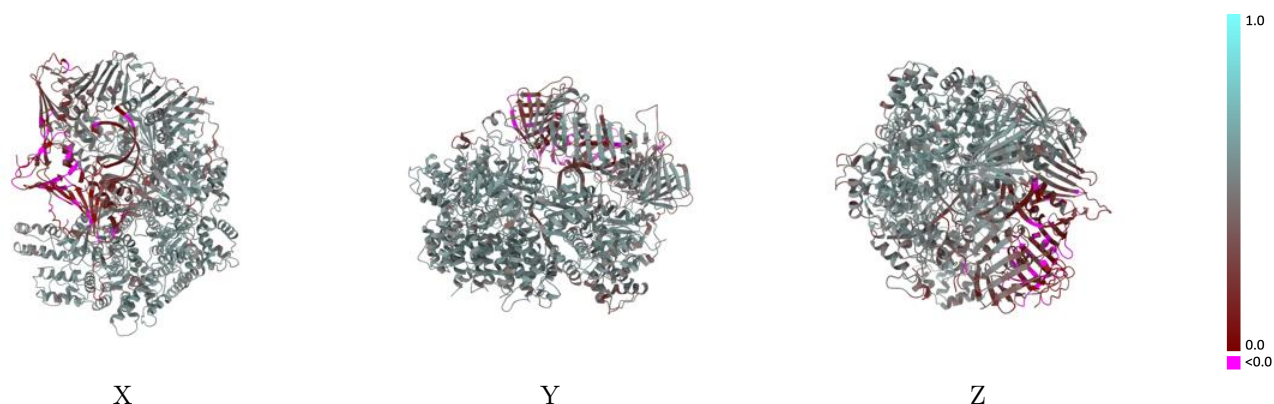
Y



Z

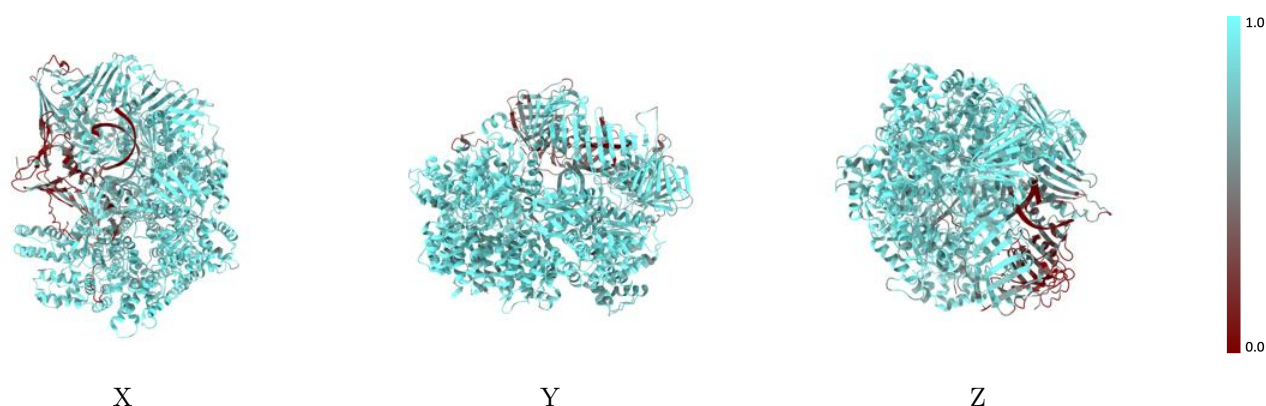
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



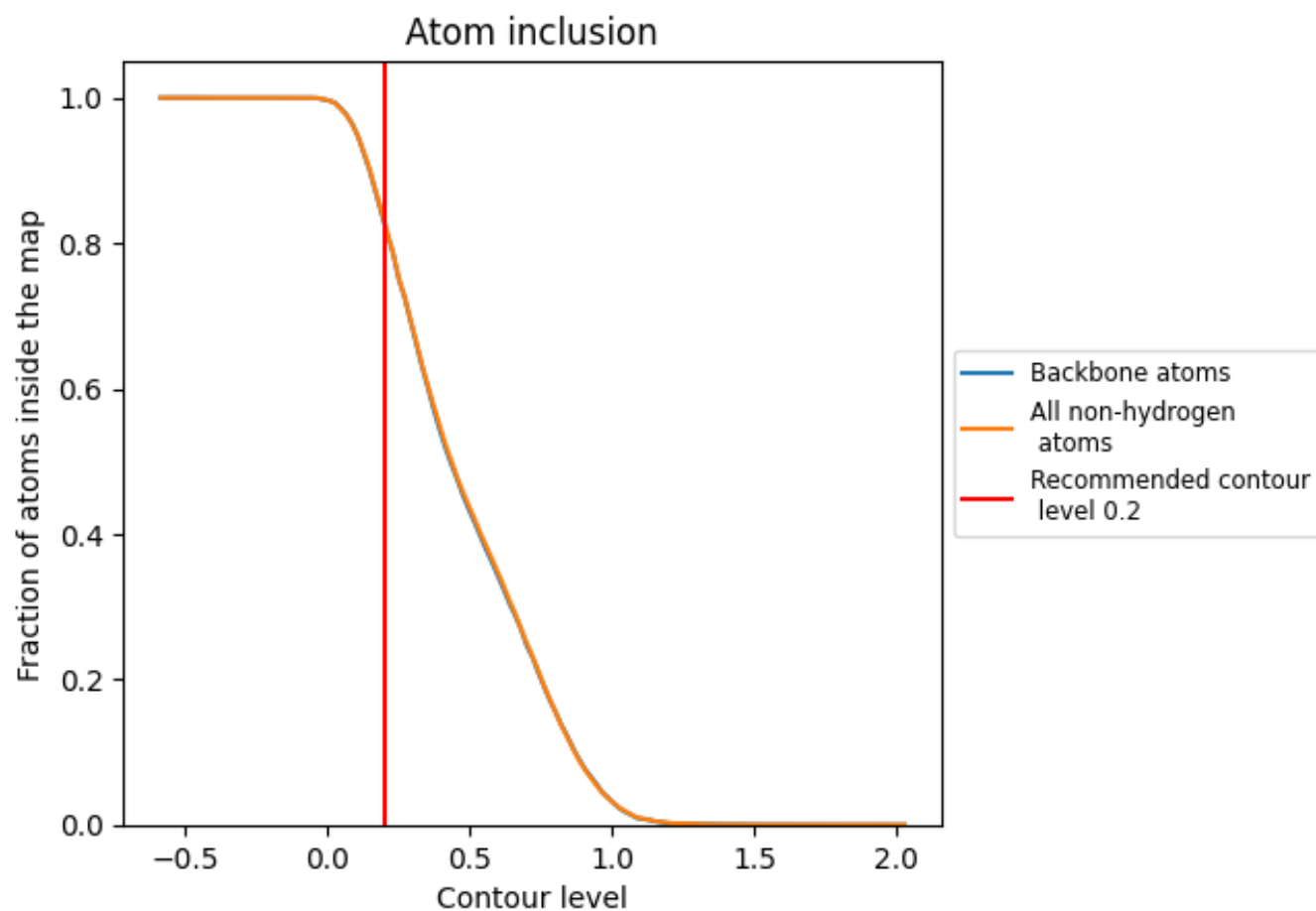
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 83% 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	<div></div> 0.8298	<div></div> 0.4700
A	<div></div> 0.8807	<div></div> 0.4970
B	<div></div> 0.9320	<div></div> 0.5400
C	<div></div> 0.9261	<div></div> 0.5450
D	<div></div> 0.9395	<div></div> 0.5510
E	<div></div> 0.9087	<div></div> 0.5310
F	<div></div> 0.8636	<div></div> 0.4820
G	<div></div> 0.7513	<div></div> 0.4020
H	<div></div> 0.3897	<div></div> 0.1540
I	<div></div> 0.6127	<div></div> 0.3090
J	<div></div> 0.5444	<div></div> 0.2890

