



Full wwPDB EM Validation Report ⓘ

Jun 9, 2026 – 10:50 AM EDT

PDB ID : 9NUL / pdb_00009nul
EMDB ID : EMD-49810
Title : SsoPfMCM:DNA class 2b from merged particles
Authors : Enemark, E.J.; Rasouli, S.; Myasnikov, A.
Deposited on : 2025-03-19
Resolution : 2.50 Å(reported)
Based on initial model : 4R7Y

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:

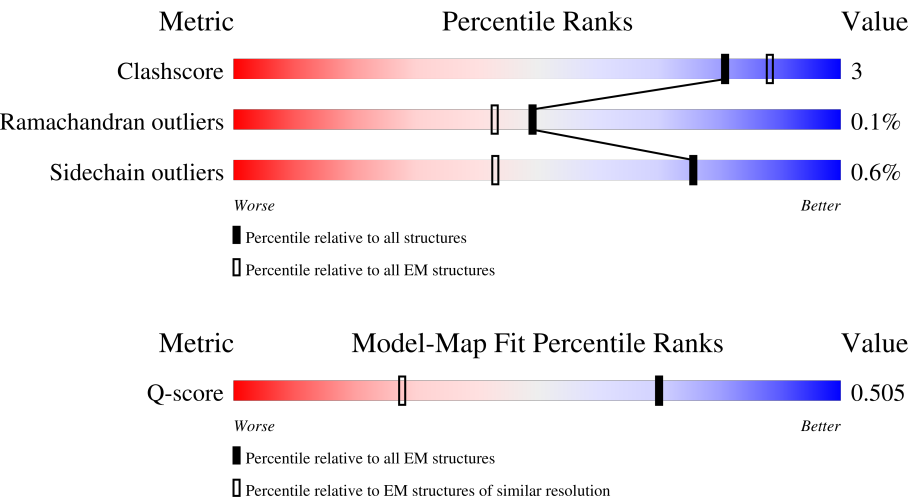
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	613	91%6%.
1	B	613	93%. .
1	C	613	92%5%.
1	D	613	91%6%.

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Mol	Chain	Length	Quality of chain
1	E	613	5% 91% 6%
1	F	613	6% 90% 7%
2	X	60	5% 27% 7% 67%
2	Y	60	10% 27% 73%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 59428 atoms, of which 29950 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 Minichromosome maintenance protein MCM,DNA helicase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	596	Total	C	H	N	O	S	0	0
			9668	3026	4912	829	887	14		
1	B	596	Total	C	H	N	O	S	0	0
			9668	3026	4912	829	887	14		
1	C	596	Total	C	H	N	O	S	0	0
			9668	3026	4912	829	887	14		
1	D	596	Total	C	H	N	O	S	0	0
			9668	3026	4912	829	887	14		
1	E	596	Total	C	H	N	O	S	0	0
			9668	3026	4912	829	887	14		
1	F	596	Total	C	H	N	O	S	0	0
			9668	3026	4912	829	887	14		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9UXG1
A	1	LEU	-	expression tag	UNP Q9UXG1
B	0	SER	-	expression tag	UNP Q9UXG1
B	1	LEU	-	expression tag	UNP Q9UXG1
C	0	SER	-	expression tag	UNP Q9UXG1
C	1	LEU	-	expression tag	UNP Q9UXG1
D	0	SER	-	expression tag	UNP Q9UXG1
D	1	LEU	-	expression tag	UNP Q9UXG1
E	0	SER	-	expression tag	UNP Q9UXG1
E	1	LEU	-	expression tag	UNP Q9UXG1
F	0	SER	-	expression tag	UNP Q9UXG1
F	1	LEU	-	expression tag	UNP Q9UXG1

- Molecule 2 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	X	20	Total	C	H	N	O	P	0	0
			633	195	226	75	118	19		
2	Y	16	Total	C	H	N	O	P	0	0
			508	156	180	60	96	16		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



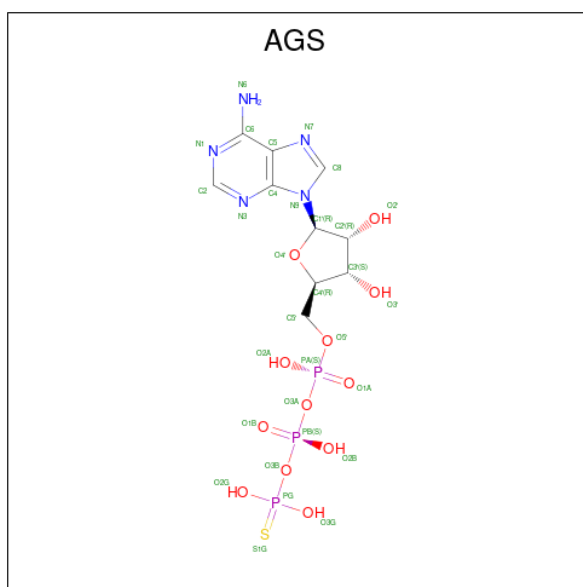
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Mol	Chain	Residues	Atoms		AltConf
4	E	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	F	1	Total	Zn	0
			1	1	

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
6	D	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	

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Mol	Chain	Residues	Atoms							AltConf
6	E	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
6	F	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	

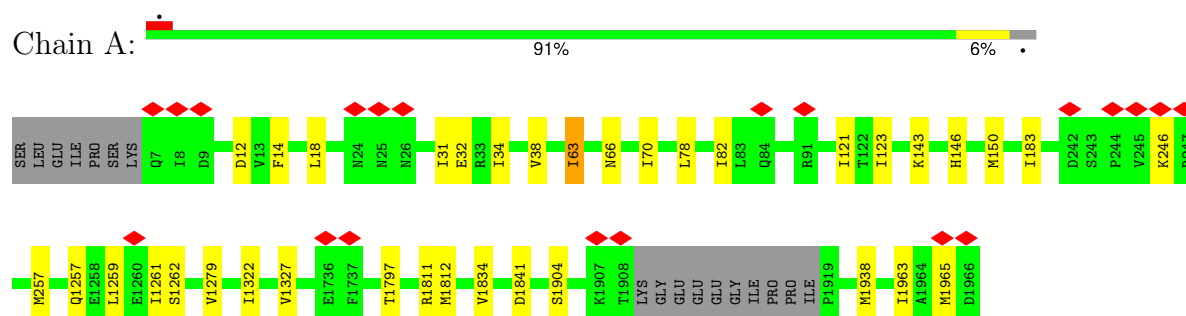
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	4	Total	O	0
			4	4	
7	B	4	Total	O	0
			4	4	
7	C	4	Total	O	0
			4	4	
7	D	3	Total	O	0
			3	3	
7	E	3	Total	O	0
			3	3	
7	F	3	Total	O	0
			3	3	

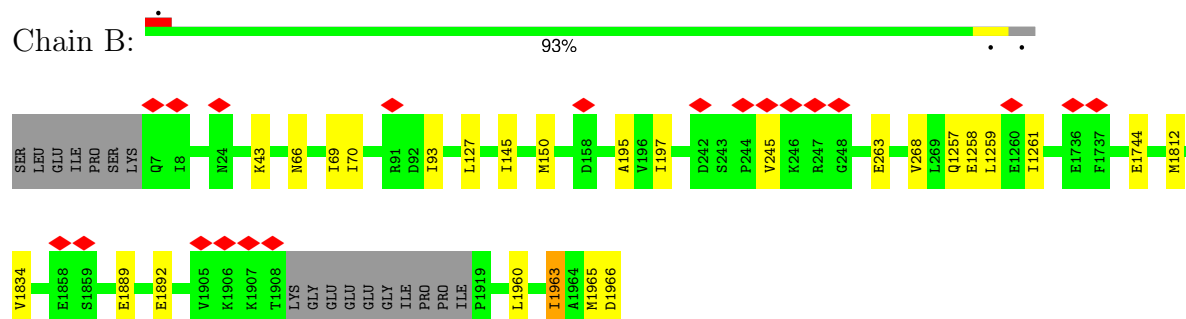
3 Residue-property plots [i](#)

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.

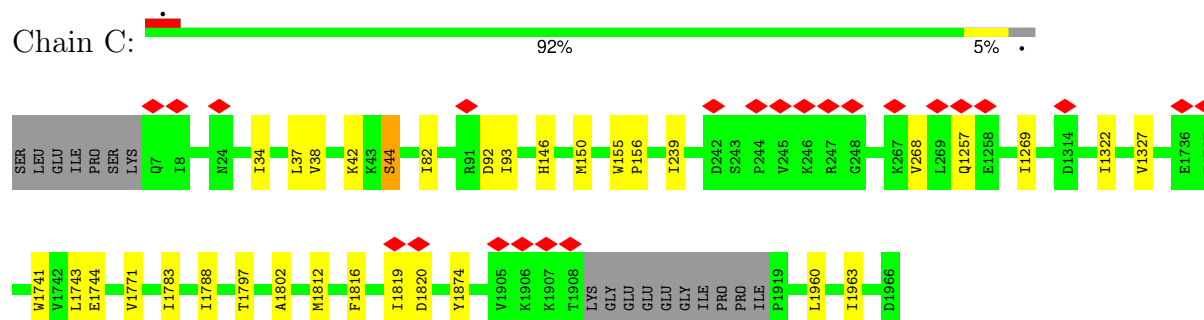
- Molecule 1: Minichromosome maintenance protein MCM,DNA helicase



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SR	LEU	GLU	IIE	PRO	SER	LVS	Q7	I8	D12	M24	Q27	I34	V38	N66	I70	I82	R91	D92	I93	I100	I103	I121	I122	I123	L127	V130	T131	K143	M150	D158	M161	P162	I183	L189	D242	S243	P244	V245					
K246	R247	G248	Q256	K267	V268	L269	Q1257	S1262	I1269	V1279	D1314	C1315	I1322	D1735	E1736	F1737	K1785	A1786	G1787	I1788	T1797	M1812	Y1874	K1906	K1907	T1908	LVS	GLY	GLY	GLU	GLU	GLY	IIE	PRO	PRO	P1919	I1920	M1938	L1960	I1963	A1964	M1965	V1966

- Chain E:  5% 91% 6% .

The diagram illustrates a complex dependency graph with components organized into three main horizontal sections. Red diamonds indicate dependencies or relationships between components.

Top Section (Left to Right):

- SER (grey)
- LEU (green)
- GLU (green)
- ILE (green)
- PRO (green)
- SER (grey)
- LYS (grey)
- Q7 (green)
- I8 (green)
- D9 (green)
- L118 (green)
- T119 (green)
- T120 (green)
- V24 (green)
- N25 (green)
- N26 (green)
- Q27 (green)
- N28 (green)
- T31 (green)
- E32 (green)
- R33 (green)
- K42 (green)
- K43 (green)
- S44 (green)
- T67 (green)
- T70 (green)
- E75 (green)
- Q84 (green)
- L85 (green)
- D86 (green)
- R91 (green)
- D92 (green)
- I93 (green)
- E94 (green)
- I103 (green)
- P104 (green)
- R105 (green)
- H146 (green)
- M150 (green)
- P155 (green)
- P156 (green)
- E157 (green)
- D158 (green)
- D242 (green)
- S243 (green)
- T244 (green)

Middle Section (Left to Right):

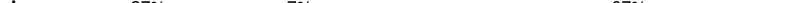
- V245 (green)
- R246 (green)
- R247 (green)
- R250 (green)
- S265 (yellow)
- E1264 (yellow)
- E1265 (yellow)
- I1268 (yellow)
- D1314 (green)
- E1736 (green)
- R1767 (green)
- D1768 (green)
- V1771 (yellow)
- A1775 (yellow)
- T1780 (yellow)
- I1781 (yellow)
- D1840 (yellow)
- D1841 (orange)
- E1858 (green)
- S1859 (yellow)
- E1860 (yellow)
- V1861 (yellow)
- V1862 (yellow)
- H1868 (yellow)
- I1894 (yellow)
- V1905 (green)
- K1906 (green)
- K1907 (green)
- T1908 (green)
- LYS (grey)
- GLY (grey)
- GUJ (grey)
- GLU (grey)
- GLY (grey)
- ILE (grey)
- PRO (grey)
- ILE (grey)
- P1919 (green)
- I1920 (green)
- T1921 (yellow)
- I1929 (yellow)

Bottom Section (Left to Right):

- S1941 (yellow)
- M1965 (green)
- D1966 (green)
- I1929 (yellow)

- Chain F:  6% 90% 7%

Category	Item	Value	Color	Label	
L237	S1904	1	Green		
	T1908	1	Red		
	LYS	1	Grey		
	GLY	1	Green		
	GLU	1	Green		
	GLU	1	Green		
	GLY	1	Green		
	ILE	1	Green		
	PRO	1	Green		
	PRO	1	Green		
D242	P1919	1	Green		
	M1938	1	Green		
	P1942	1	Green		
	I1943	1	Green		
	L1960	1	Green		
	I1963	1	Green		
	A1964	1	Green		
	M1965	1	Red		
	D1966	1	Red		
	D242	L237	1	Yellow	
D242		1	Red		
S243		1	Red		
P244		1	Red		
V245		1	Red		
K246		1	Red		
R247		1	Red		
G248		1	Green		
S249		1	Green		
R250		1	Green		
Q1257	L255	1	Yellow		
	Q1257	1	Red		
	E1260	1	Yellow		
	I1261	1	Yellow		
	S1262	1	Yellow		
	E1265	1	Yellow		
	I1268	1	Yellow		
	V1279	1	Yellow		
	L1312	1	Yellow		
	T1316	1	Yellow		
E1736	I1322	1	Yellow		
	I1349	1	Yellow		
	A1358	1	Yellow		
	E1736	1	Red		
	F1737	1	Red		
	A1747	1	Yellow		
	A1751	1	Yellow		
	R1767	1	Green		
	D1768	1	Green		
	V1771	1	Yellow		
E1859	T1796	1	Yellow		
	T1797	1	Yellow		
	R1811	1	Yellow		
	M1812	1	Yellow		
	E1859	1	Red		
	S1859	1	Red		
	H1868	1	Yellow		
	M1901	1	Yellow		
	R91	SER	1	Grey	
		LEU	1	Grey	
ILE		1	Grey		
PRO		1	Grey		
SER		1	Grey		
LYS		1	Grey		
Q7		1	Red		
I8		1	Red		
D9		1	Red		
M24		1	Green		
R91	N25	1	Green		
	M26	1	Green		
	Q27	1	Green		
	M28	1	Green		
	Y40	1	Green		
	R41	1	Green		
	K42	1	Green		
	E48	1	Green		
	Y61	1	Green		
	K68	1	Green		
R91	L69	1	Green		
	E75	1	Green		
	L78	1	Yellow		
	Q84	1	Green		
	L85	1	Green		
	R91	1	Red		
	D92	1	Red		
	I93	1	Red		
	E94	1	Green		
	T103	1	Yellow		
R91	P104	1	Green		
	R105	1	Green		
	L127	1	Yellow		
	H146	1	Yellow		
	M150	1	Yellow		
	W155	1	Yellow		
	P156	1	Yellow		
	E157	1	Green		
	D158	1	Green		
	V164	1	Yellow		
R91	A195	1	Yellow		
	T028	1	Yellow		

- Chain X: 

Year	Number of Publications
1981	1
1982	1
1983	1
1984	1
1985	1
1986	6
1987	1
1988	1
1989	1
1990	1
1991	1
1992	1
1993	1
1994	1
1995	1
1996	1
1997	1
1998	18
1999	18
2000	18
2001	18
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2004	18
2005	18
2006	18
2007	18
2008	18
2009	18
2010	18
2011	18
2012	18
2013	18
2014	18
2015	18
2016	18
2017	18
2018	18
2019	18
2020	20

- Molecule 2: DNA (60-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	471221	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	77	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.565	Depositor
Minimum map value	-0.623	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.415	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: ZN, ADP, MG, AGS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/4834	0.25	0/6529
1	B	0.09	0/4834	0.26	0/6529
1	C	0.10	0/4834	0.26	0/6529
1	D	0.09	0/4834	0.26	0/6529
1	E	0.09	0/4834	0.26	0/6529
1	F	0.09	0/4834	0.26	0/6529
2	X	0.15	0/456	0.39	0/702
2	Y	0.17	0/367	0.39	0/564
All	All	0.10	0/29827	0.26	0/40440

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	4756	4912	4922	27	0
1	B	4756	4912	4922	22	0
1	C	4756	4912	4922	27	0
1	D	4756	4912	4922	23	0
1	E	4756	4912	4922	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4756	4912	4922	33	0
2	X	407	226	227	2	0
2	Y	328	180	181	0	0
3	A	27	12	12	0	0
3	B	27	12	12	0	0
3	C	27	12	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	D	31	12	12	0	0
6	E	31	12	12	0	0
6	F	31	12	12	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
7	D	3	0	0	0	0
7	E	3	0	0	0	0
7	F	3	0	0	0	0
All	All	29478	29950	30012	157	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 3.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1812:MET:N	1:A:1812:MET:HE2	1.99	0.77
1:A:1261:ILE:HG22	1:A:1262:SER:H	1.54	0.73
1:F:1812:MET:N	1:F:1812:MET:HE2	2.04	0.73
1:F:1767:ARG:O	1:F:1771:VAL:HG13	1.89	0.72
1:A:150:MET:HA	1:A:150:MET:HE2	1.72	0.72
1:A:34:ILE:O	1:A:38:VAL:HG23	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG22	1:A:82:ILE:CD1	2.27	0.65
1:E:1264:GLU:O	1:E:1268:ILE:HG23	1.97	0.64
1:B:1965:MET:HE3	1:B:1965:MET:C	2.24	0.63
1:C:150:MET:HE2	1:C:150:MET:H	1.64	0.63
1:F:150:MET:H	1:F:150:MET:HE2	1.65	0.62
1:A:38:VAL:HG22	1:A:82:ILE:HD13	1.82	0.61
1:C:37:LEU:HD11	1:C:44:SER:H	1.67	0.60
1:E:150:MET:HA	1:E:150:MET:HE2	1.84	0.59
1:A:143:LYS:HB2	1:A:183:ILE:HD11	1.84	0.59
1:E:1767:ARG:NE	1:E:1767:ARG:H	2.01	0.58
1:B:150:MET:HE3	1:B:150:MET:HA	1.86	0.57
1:C:1812:MET:HE2	1:C:1812:MET:N	2.20	0.56
1:D:1965:MET:O	1:D:1965:MET:HE3	2.06	0.56
1:A:121:ILE:HD12	1:A:123:ILE:HD11	1.87	0.56
1:D:38:VAL:HB	1:D:82:ILE:HD11	1.87	0.56
1:F:1768:ASP:O	1:F:1771:VAL:HG22	2.06	0.56
1:E:1860:GLU:HG3	1:E:1862:VAL:HG22	1.87	0.55
1:A:1834:VAL:HG11	1:A:1963:ILE:HD12	1.88	0.55
1:C:37:LEU:HD12	1:C:42:LYS:HB2	1.88	0.55
1:D:1965:MET:HE3	1:D:1965:MET:C	2.33	0.54
1:D:150:MET:HA	1:D:150:MET:HE2	1.90	0.54
1:D:121:ILE:HD12	1:D:123:ILE:HD11	1.88	0.53
1:E:28:ASN:HB3	1:E:31:ILE:HD13	1.90	0.53
1:B:1812:MET:N	1:B:1812:MET:HE3	2.23	0.53
1:B:127:LEU:HD11	1:B:195:ALA:HB1	1.91	0.52
1:E:1840:ASP:O	1:E:1841:ASP:CB	2.57	0.52
1:C:38:VAL:CG1	1:C:82:ILE:HD11	2.39	0.52
1:D:127:LEU:HD21	1:D:130:VAL:HG23	1.91	0.52
1:E:146:HIS:O	1:E:150:MET:HE3	2.10	0.51
1:E:247:ARG:HH21	1:F:164:VAL:HG13	1.75	0.51
1:F:1312:LEU:O	1:F:1316:THR:HG22	2.11	0.51
1:A:1259:LEU:C	1:A:1261:ILE:HD12	2.35	0.51
1:B:43:LYS:HB3	1:B:93:ILE:HG21	1.93	0.51
1:E:18:LEU:HD12	1:E:19:THR:N	2.26	0.51
1:B:263:GLU:OE2	1:B:263:GLU:C	2.54	0.50
1:C:150:MET:HE2	1:C:150:MET:N	2.25	0.50
1:E:1775:ALA:HB2	1:E:1781:ILE:HD11	1.92	0.50
1:F:150:MET:HE2	1:F:150:MET:N	2.27	0.50
1:F:1260:GLU:C	1:F:1261:ILE:HD13	2.37	0.50
1:B:1812:MET:HE3	1:B:1812:MET:H	1.76	0.50
1:E:19:THR:O	1:E:31:ILE:HD11	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1257:GLN:HA	1:A:1257:GLN:OE1	2.11	0.50
1:E:43:LYS:HB3	1:E:93:ILE:HD13	1.94	0.50
1:A:146:HIS:O	1:A:150:MET:HE3	2.12	0.50
1:A:1841:ASP:OD2	1:A:1841:ASP:C	2.54	0.49
1:A:1259:LEU:HG	1:A:1261:ILE:HD13	1.94	0.49
1:B:66:ASN:O	1:B:70:ILE:HG22	2.13	0.49
1:B:1965:MET:HE3	1:B:1966:ASP:N	2.28	0.49
1:D:92:ASP:C	1:D:93:ILE:HD12	2.36	0.49
1:F:103:ILE:HG22	1:F:105:ARG:H	1.77	0.49
1:C:1812:MET:HE2	1:C:1812:MET:H	1.78	0.48
1:C:1327:VAL:HG12	1:C:1802:ALA:HB3	1.95	0.48
1:F:1261:ILE:HG22	1:F:1262:SER:H	1.78	0.48
1:C:150:MET:HE2	1:C:150:MET:HA	1.96	0.48
1:F:127:LEU:HD11	1:F:195:ALA:HB1	1.95	0.48
1:F:150:MET:HE2	1:F:150:MET:HA	1.96	0.48
1:A:1811:ARG:C	1:A:1812:MET:HE2	2.39	0.47
1:E:1767:ARG:H	1:E:1767:ARG:HE	1.61	0.47
1:F:1942:PRO:C	1:F:1943:ILE:HD12	2.39	0.47
1:C:150:MET:HE2	1:C:150:MET:CA	2.45	0.47
1:F:1767:ARG:HB2	1:F:1767:ARG:NH1	2.29	0.47
1:B:1834:VAL:HG21	1:B:1963:ILE:HD12	1.96	0.47
1:D:1785:LYS:O	1:D:1788:ILE:HG22	2.15	0.47
1:D:100:ILE:HG13	1:D:103:ILE:HD11	1.97	0.47
1:E:150:MET:HE2	1:E:150:MET:CA	2.44	0.47
1:F:150:MET:HE2	1:F:150:MET:CA	2.45	0.47
1:F:1279:VAL:HG13	1:F:1938:MET:HE1	1.96	0.47
1:C:1322:ILE:O	1:C:1797:THR:HG23	2.15	0.46
1:F:1322:ILE:O	1:F:1797:THR:HG23	2.15	0.46
1:A:1261:ILE:HG22	1:A:1262:SER:N	2.28	0.46
1:C:92:ASP:C	1:C:93:ILE:HD12	2.40	0.46
1:C:146:HIS:O	1:C:150:MET:HE3	2.16	0.46
1:C:1816:PHE:CE2	1:C:1963:ILE:HD11	2.51	0.46
1:D:66:ASN:O	1:D:70:ILE:HG22	2.15	0.46
1:C:1269:ILE:HG23	1:C:1874:TYR:CD2	2.51	0.46
1:F:1811:ARG:C	1:F:1812:MET:HE2	2.40	0.46
1:A:1322:ILE:O	1:A:1797:THR:HG23	2.16	0.45
1:F:146:HIS:O	1:F:150:MET:HE3	2.16	0.45
1:C:1816:PHE:HE2	1:C:1963:ILE:HD11	1.81	0.45
2:X:6:DC:H2'	2:X:7:DT:H72	1.98	0.45
1:A:38:VAL:HG22	1:A:82:ILE:HD11	1.99	0.45
1:D:1279:VAL:HG13	1:D:1938:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1812:MET:N	1:D:1812:MET:HE3	2.31	0.45
1:F:1265:GLU:O	1:F:1268:ILE:HG22	2.16	0.45
1:F:1942:PRO:O	1:F:1943:ILE:HD12	2.16	0.45
1:C:34:ILE:CG2	1:C:82:ILE:HD13	2.47	0.44
1:B:1834:VAL:CG2	1:B:1963:ILE:HD12	2.47	0.44
1:D:12:ASP:OD2	1:D:12:ASP:N	2.50	0.44
1:A:12:ASP:OD2	1:A:12:ASP:N	2.49	0.44
1:D:143:LYS:HB2	1:D:183:ILE:HD11	1.99	0.44
1:B:145:ILE:O	1:B:145:ILE:HG22	2.18	0.44
1:D:242:ASP:OD2	1:D:242:ASP:C	2.60	0.44
1:A:63:ILE:HA	1:A:70:ILE:HG21	2.00	0.44
1:B:69:ILE:C	1:B:69:ILE:HD12	2.43	0.44
1:D:1788:ILE:O	1:D:1788:ILE:HG23	2.16	0.44
1:F:1358:ALA:HB1	1:F:1771:VAL:HG11	2.00	0.44
2:X:18:DC:H2'	2:X:19:DT:H72	1.99	0.44
1:D:34:ILE:HG23	1:D:82:ILE:HD13	1.99	0.44
1:D:1322:ILE:O	1:D:1797:THR:HG23	2.18	0.44
1:F:85:LEU:HD23	1:F:85:LEU:O	2.17	0.43
1:B:268:VAL:HG23	1:B:1258:GLU:H	1.82	0.43
1:C:1741:TRP:HB2	1:C:1788:ILE:HD12	1.99	0.43
1:E:1265:GLU:O	1:E:1268:ILE:HG12	2.19	0.43
1:E:1840:ASP:O	1:E:1841:ASP:HB2	2.18	0.43
1:F:155:TRP:HB3	1:F:156:PRO:HD3	1.99	0.43
1:A:246:LYS:CD	1:B:245:VAL:HG22	2.48	0.43
1:B:1257:GLN:N	1:B:1257:GLN:CD	2.76	0.43
1:F:68:LYS:HG2	1:F:69:ILE:HG23	2.00	0.43
1:D:161:MET:HE3	1:D:162:PRO:HD2	2.00	0.43
1:E:1768:ASP:O	1:E:1771:VAL:HG22	2.19	0.43
1:C:268:VAL:O	1:C:268:VAL:HG13	2.19	0.43
1:F:236:ILE:HG22	1:F:237:LEU:N	2.34	0.43
1:F:1767:ARG:HB2	1:F:1767:ARG:CZ	2.48	0.43
1:F:1812:MET:HE2	1:F:1812:MET:CA	2.49	0.42
1:B:43:LYS:CB	1:B:93:ILE:HG21	2.49	0.42
1:B:127:LEU:HD12	1:B:197:ILE:HD13	2.01	0.42
1:B:1960:LEU:O	1:B:1963:ILE:HG22	2.19	0.42
1:C:155:TRP:HB3	1:C:156:PRO:HD3	2.00	0.42
1:E:1780:THR:C	1:E:1781:ILE:HD12	2.44	0.42
1:E:1894:ILE:HD13	1:E:1929:ILE:HD13	2.02	0.42
1:C:1960:LEU:HA	1:C:1963:ILE:HG22	2.02	0.42
1:F:1751:ALA:O	1:F:1796:THR:HG22	2.19	0.42
1:A:14:PHE:CE2	1:A:18:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:ILE:HG22	1:E:105:ARG:H	1.84	0.42
1:A:14:PHE:CZ	1:A:18:LEU:HD11	2.54	0.42
1:D:131:THR:HG22	1:D:1737:PHE:CD2	2.55	0.42
1:F:1349:ILE:HG21	1:F:1747:ALA:HB1	2.01	0.42
1:B:1259:LEU:C	1:B:1261:ILE:HD12	2.45	0.41
1:C:1771:VAL:O	1:C:1771:VAL:HG12	2.19	0.41
1:F:78:LEU:HD13	1:F:78:LEU:O	2.19	0.41
1:A:78:LEU:O	1:A:78:LEU:HD13	2.20	0.41
1:D:1269:ILE:HG23	1:D:1874:TYR:CD2	2.56	0.41
1:E:27:GLN:CD	1:E:27:GLN:N	2.78	0.41
1:C:1743:LEU:HD21	1:C:1783:ILE:HG21	2.03	0.41
1:A:31:ILE:HD12	1:A:32:GLU:N	2.35	0.41
1:F:1901:MET:SD	1:F:1960:LEU:HD11	2.60	0.41
1:D:1960:LEU:O	1:D:1963:ILE:HG22	2.21	0.41
1:F:1960:LEU:O	1:F:1963:ILE:HG22	2.21	0.41
1:C:239:ILE:HG21	1:D:189:LEU:HD21	2.02	0.41
1:C:1819:ILE:HG22	1:C:1820:ASP:N	2.34	0.41
1:E:27:GLN:CD	1:E:27:GLN:H	2.29	0.41
1:E:67:THR:HA	1:E:70:ILE:HG22	2.02	0.41
1:E:150:MET:HE2	1:E:150:MET:H	1.85	0.41
1:E:155:TRP:HB3	1:E:156:PRO:HD3	2.03	0.41
1:B:1744:GLU:OE2	1:B:1744:GLU:C	2.64	0.40
1:A:66:ASN:O	1:A:70:ILE:HG22	2.22	0.40
1:B:1889:GLU:O	1:B:1892:GLU:HG3	2.21	0.40
1:C:38:VAL:HG13	1:C:82:ILE:HD11	2.03	0.40
1:C:1744:GLU:OE2	1:C:1744:GLU:HA	2.22	0.40
1:E:1861:VAL:O	1:E:1861:VAL:HG12	2.22	0.40
1:A:1279:VAL:HG13	1:A:1938:MET:CE	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	592/613 (97%)	570 (96%)	22 (4%)	0	100	100
1	B	592/613 (97%)	560 (95%)	32 (5%)	0	100	100
1	C	592/613 (97%)	563 (95%)	28 (5%)	1 (0%)	43	63
1	D	592/613 (97%)	566 (96%)	25 (4%)	1 (0%)	43	63
1	E	592/613 (97%)	573 (97%)	18 (3%)	1 (0%)	43	63
1	F	592/613 (97%)	564 (95%)	27 (5%)	1 (0%)	43	63
All	All	3552/3678 (97%)	3396 (96%)	152 (4%)	4 (0%)	49	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1920	ILE
1	E	1841	ASP
1	F	250	ARG
1	C	1257	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	522/537 (97%)	517 (99%)	5 (1%)	68	86
1	B	522/537 (97%)	521 (100%)	1 (0%)	87	95
1	C	522/537 (97%)	521 (100%)	1 (0%)	87	95
1	D	522/537 (97%)	520 (100%)	2 (0%)	84	93
1	E	522/537 (97%)	516 (99%)	6 (1%)	65	84
1	F	522/537 (97%)	519 (99%)	3 (1%)	78	91
All	All	3132/3222 (97%)	3114 (99%)	18 (1%)	76	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE

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Mol	Chain	Res	Type
1	A	257	MET
1	A	1327	VAL
1	A	1904	SER
1	A	1965	MET
1	B	1963	ILE
1	C	44	SER
1	D	123	ILE
1	D	1262	SER
1	E	20	THR
1	E	44	SER
1	E	265	SER
1	E	1868	HIS
1	E	1921	THR
1	E	1941	SER
1	F	255	ILE
1	F	1868	HIS
1	F	1904	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	1778	GLN
1	A	1962	GLN
1	B	28	ASN
1	B	58	ASN
1	C	84	GLN
1	C	1881	ASN
1	D	81	HIS
1	D	84	GLN
1	D	90	GLN
1	D	198	GLN
1	D	212	GLN
1	D	1850	HIS
1	E	1778	GLN
1	F	198	GLN
1	F	1336	GLN
1	F	1962	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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$
3	ADP	B	2001	4	28,29,29	1.39	4 (14%)	43,45,45	1.88	10 (23%)
6	AGS	E	2001	4	32,33,33	0.49	1 (3%)	45,52,52	0.63	1 (2%)
3	ADP	A	2001	4	28,29,29	1.39	4 (14%)	43,45,45	1.90	11 (25%)
6	AGS	D	2001	4	32,33,33	0.48	1 (3%)	45,52,52	0.62	1 (2%)
6	AGS	F	2001	4	32,33,33	0.49	1 (3%)	45,52,52	0.63	1 (2%)
3	ADP	C	2001	4	28,29,29	1.39	4 (14%)	43,45,45	1.88	11 (25%)

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
3	ADP	B	2001	4	-	6/16/32/32	0/3/3/3
6	AGS	E	2001	4	-	4/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	2001	4	-	4/16/32/32	0/3/3/3
6	AGS	D	2001	4	-	4/21/38/38	0/3/3/3
6	AGS	F	2001	4	-	4/21/38/38	0/3/3/3
3	ADP	C	2001	4	-	6/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2001	ADP	C5-C4	4.55	1.47	1.39
3	B	2001	ADP	C5-C4	4.54	1.47	1.39
3	A	2001	ADP	C5-C4	4.54	1.47	1.39
3	A	2001	ADP	C5-C6	2.69	1.48	1.41
3	C	2001	ADP	C5-C6	2.67	1.48	1.41
3	B	2001	ADP	C5-C6	2.67	1.48	1.41
3	A	2001	ADP	C8-N7	2.40	1.36	1.31
3	C	2001	ADP	C8-N7	2.40	1.36	1.31
3	B	2001	ADP	C8-N7	2.39	1.36	1.31
3	C	2001	ADP	C5-N7	-2.30	1.34	1.39
3	B	2001	ADP	C5-N7	-2.29	1.34	1.39
3	A	2001	ADP	C5-N7	-2.28	1.34	1.39
6	D	2001	AGS	PG-S1G	2.13	1.95	1.90
6	F	2001	AGS	PG-S1G	2.11	1.95	1.90
6	E	2001	AGS	PG-S1G	2.10	1.95	1.90

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	ADP	C5-C4-N3	-5.76	118.78	126.72
3	B	2001	ADP	C5-C4-N3	-5.76	118.78	126.72
3	C	2001	ADP	C5-C4-N3	-5.76	118.79	126.72
3	B	2001	ADP	N3-C4-N9	4.60	134.98	127.17
3	C	2001	ADP	N3-C4-N9	4.58	134.96	127.17
3	A	2001	ADP	N3-C4-N9	4.56	134.92	127.17
3	A	2001	ADP	C2-N3-C4	3.87	121.28	111.83
3	B	2001	ADP	C2-N3-C4	3.86	121.27	111.83
3	C	2001	ADP	C2-N3-C4	3.86	121.26	111.83
3	A	2001	ADP	N3-C2-N1	-3.74	122.93	128.58
3	B	2001	ADP	N3-C2-N1	-3.73	122.94	128.58
3	C	2001	ADP	N3-C2-N1	-3.72	122.95	128.58
3	A	2001	ADP	C4-C5-N7	-3.58	106.49	110.58
3	C	2001	ADP	C4-C5-N7	-3.53	106.54	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	ADP	C4-C5-N7	-3.52	106.56	110.58
6	E	2001	AGS	PB-O3B-PG	-3.23	121.33	133.17
6	F	2001	AGS	PB-O3B-PG	-3.22	121.37	133.17
6	D	2001	AGS	PB-O3B-PG	-3.07	121.94	133.17
3	B	2001	ADP	C4-N9-C8	2.97	108.86	105.74
3	C	2001	ADP	C4-N9-C8	2.94	108.83	105.74
3	A	2001	ADP	C4-N9-C8	2.94	108.82	105.74
3	A	2001	ADP	C5-N7-C8	2.77	107.80	103.45
3	C	2001	ADP	C5-N7-C8	2.75	107.77	103.45
3	B	2001	ADP	C5-N7-C8	2.74	107.76	103.45
3	B	2001	ADP	N9-C8-N7	-2.36	110.58	113.94
3	A	2001	ADP	N9-C8-N7	-2.36	110.59	113.94
3	C	2001	ADP	N9-C8-N7	-2.35	110.60	113.94
3	A	2001	ADP	C6-C5-N7	2.24	136.41	132.09
3	C	2001	ADP	C6-C5-N7	2.22	136.36	132.09
3	B	2001	ADP	C6-C5-N7	2.21	136.34	132.09
3	A	2001	ADP	C3'-C2'-C1'	2.14	105.51	101.46
3	A	2001	ADP	C2-N1-C6	2.10	122.18	118.73
3	C	2001	ADP	C2-N1-C6	2.09	122.17	118.73
3	B	2001	ADP	C2-N1-C6	2.08	122.16	118.73
3	C	2001	ADP	C3'-C2'-C1'	2.04	105.32	101.46

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	ADP	C5'-O5'-PA-O1A
3	A	2001	ADP	C5'-O5'-PA-O2A
3	A	2001	ADP	C5'-O5'-PA-O3A
3	B	2001	ADP	PA-O3A-PB-O2B
3	B	2001	ADP	C5'-O5'-PA-O1A
3	B	2001	ADP	C5'-O5'-PA-O2A
3	B	2001	ADP	C5'-O5'-PA-O3A
3	C	2001	ADP	PA-O3A-PB-O2B
3	C	2001	ADP	C5'-O5'-PA-O1A
3	C	2001	ADP	C5'-O5'-PA-O2A
3	C	2001	ADP	C5'-O5'-PA-O3A
6	E	2001	AGS	O4'-C4'-C5'-O5'
6	F	2001	AGS	O4'-C4'-C5'-O5'
6	D	2001	AGS	O4'-C4'-C5'-O5'
6	E	2001	AGS	C3'-C4'-C5'-O5'
6	F	2001	AGS	C3'-C4'-C5'-O5'

Continued on next page...

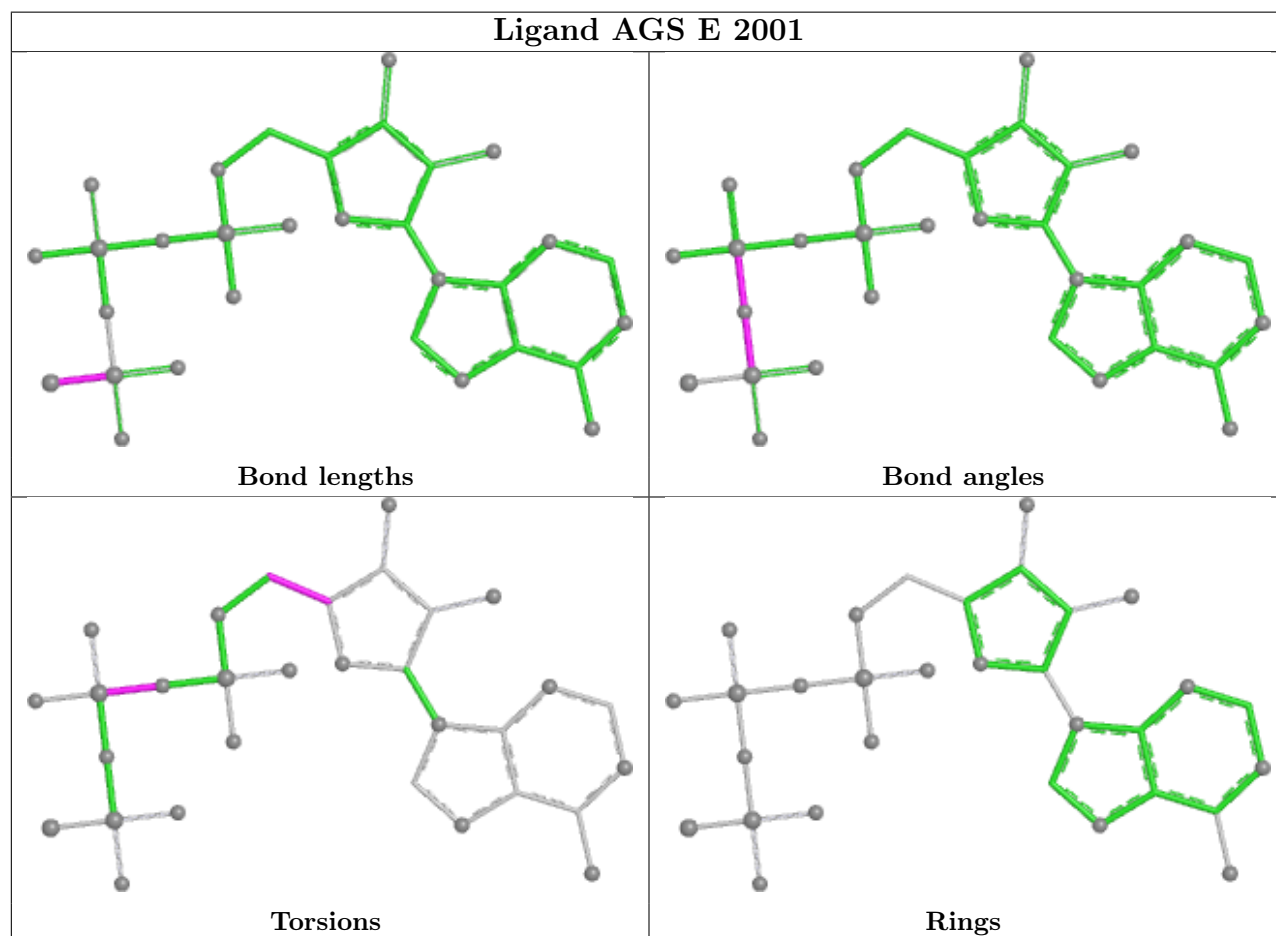
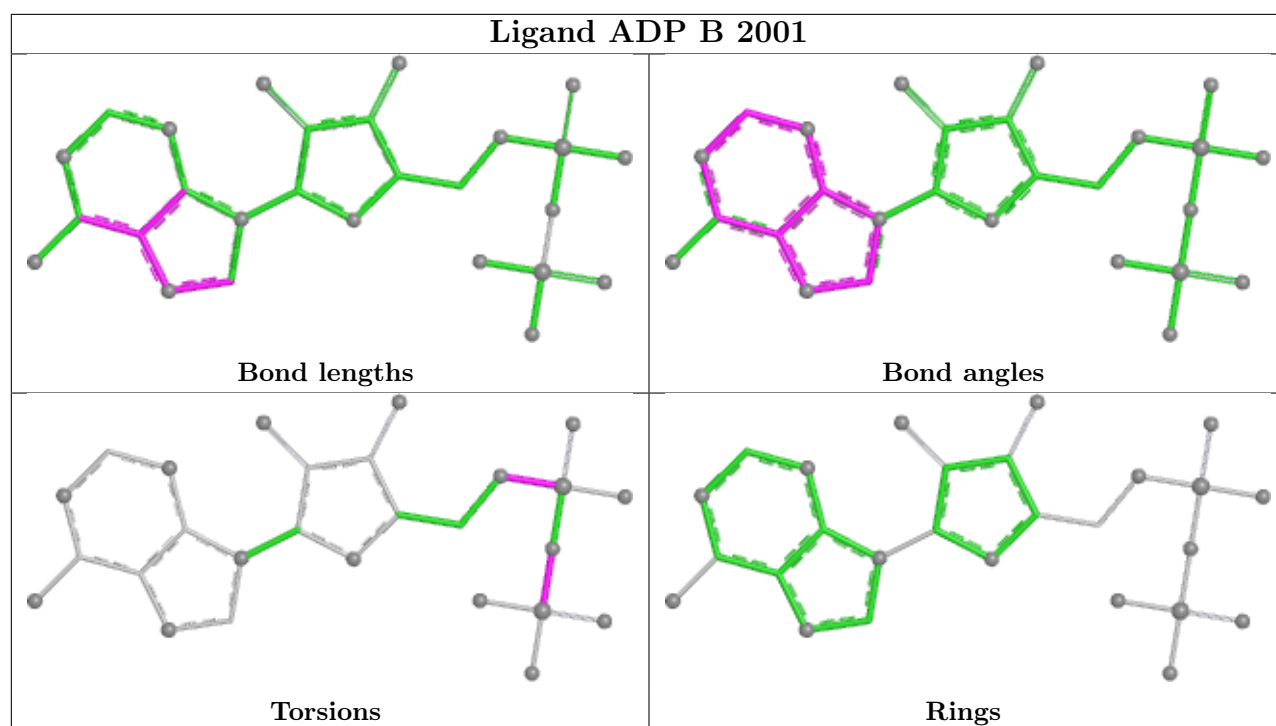
Continued from previous page...

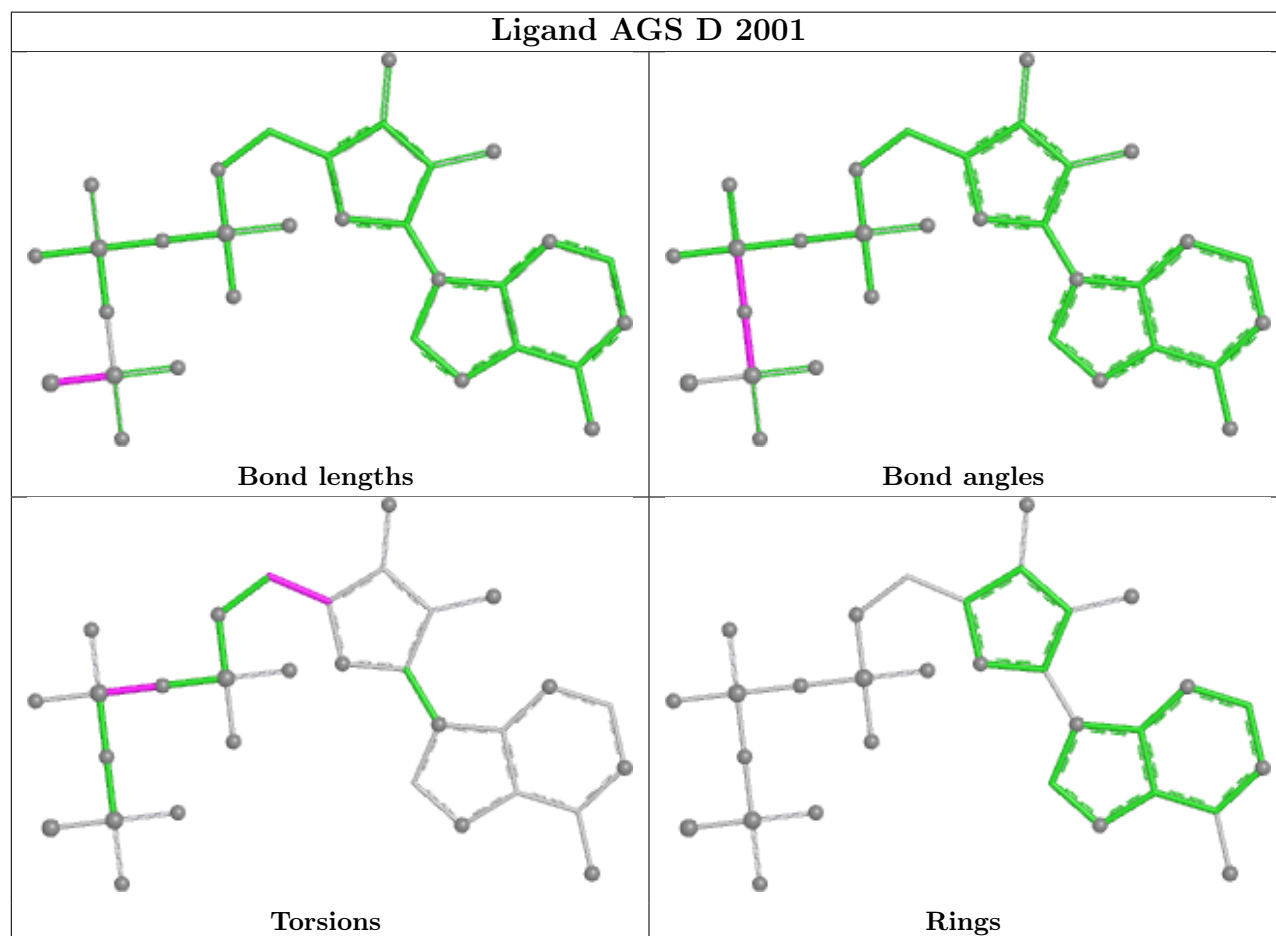
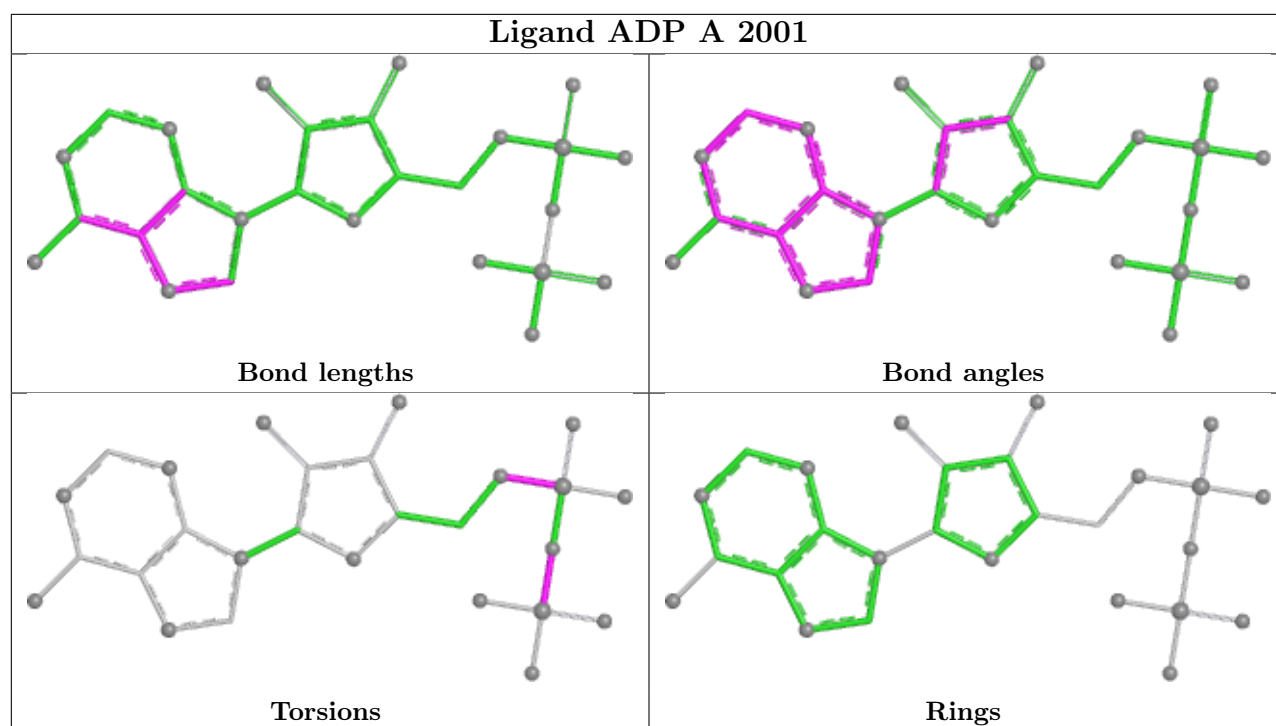
Mol	Chain	Res	Type	Atoms
6	D	2001	AGS	C3'-C4'-C5'-O5'
6	D	2001	AGS	PA-O3A-PB-O2B
3	B	2001	ADP	PA-O3A-PB-O1B
3	A	2001	ADP	PA-O3A-PB-O3B
3	B	2001	ADP	PA-O3A-PB-O3B
3	C	2001	ADP	PA-O3A-PB-O3B
6	D	2001	AGS	PA-O3A-PB-O1B
6	E	2001	AGS	PA-O3A-PB-O1B
6	E	2001	AGS	PA-O3A-PB-O2B
6	F	2001	AGS	PA-O3A-PB-O1B
6	F	2001	AGS	PA-O3A-PB-O2B
3	C	2001	ADP	PA-O3A-PB-O1B

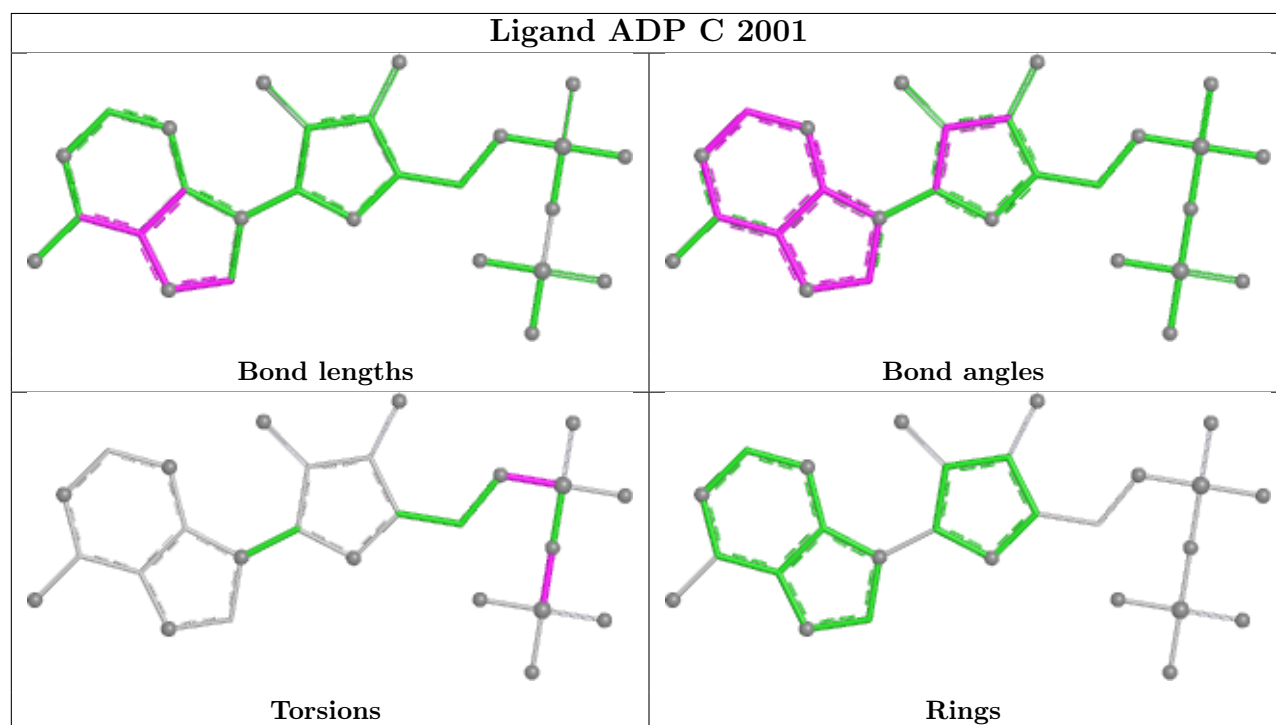
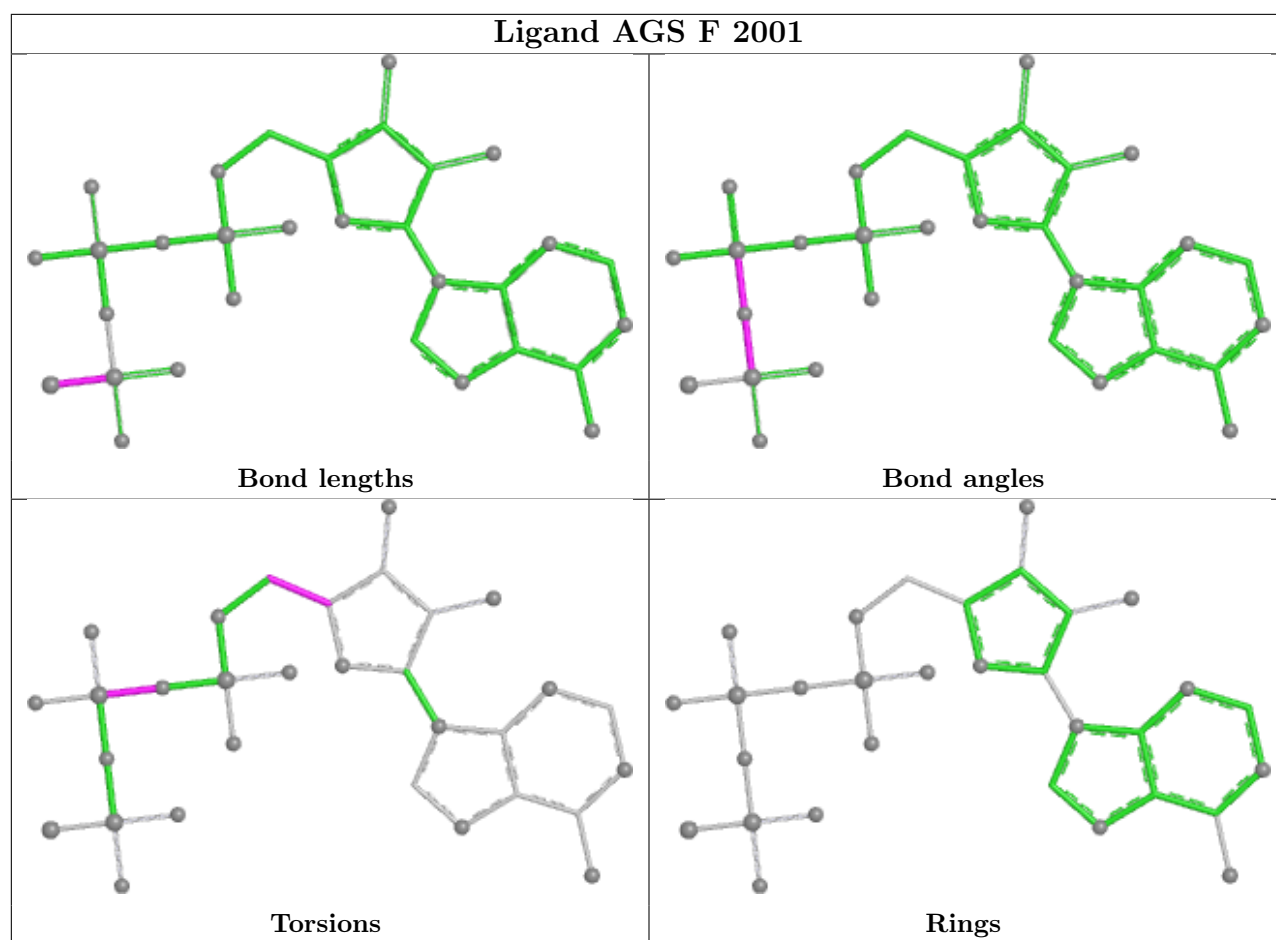
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

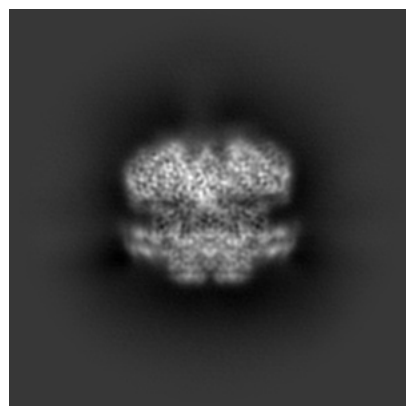
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49810. These allow visual inspection of the internal detail of the map and identification of artifacts.

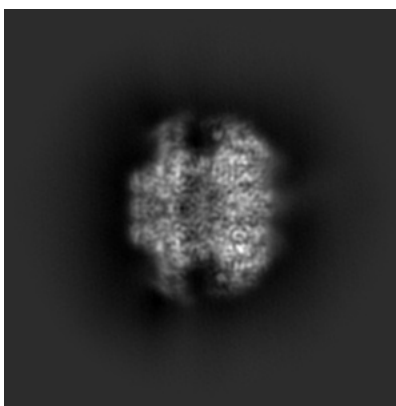
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

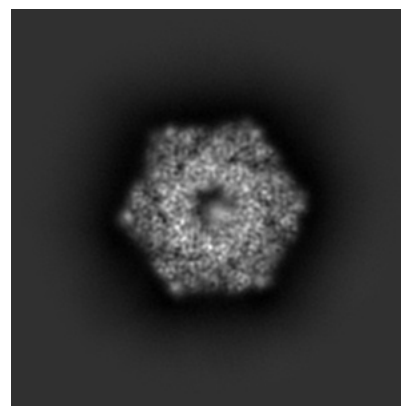
6.1.1 Primary map



X

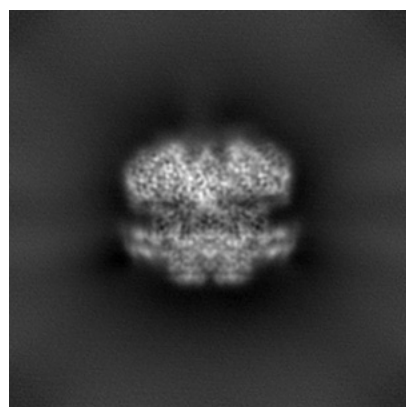


Y

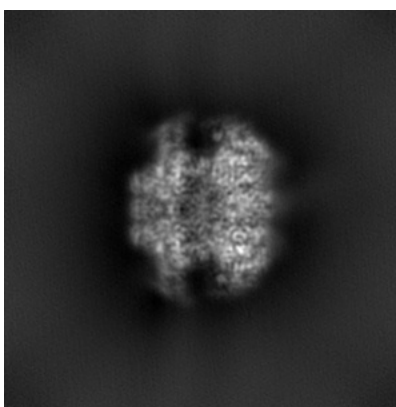


Z

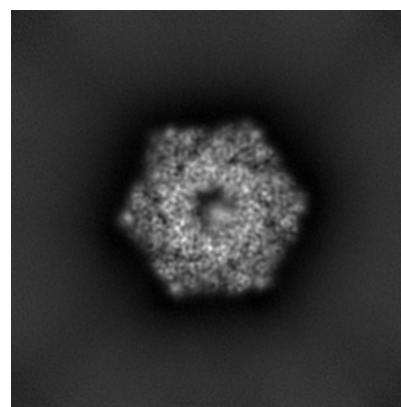
6.1.2 Raw map



X



Y

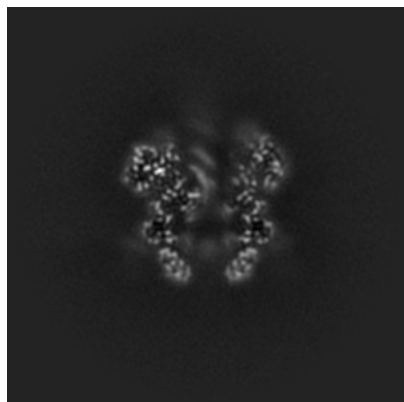


Z

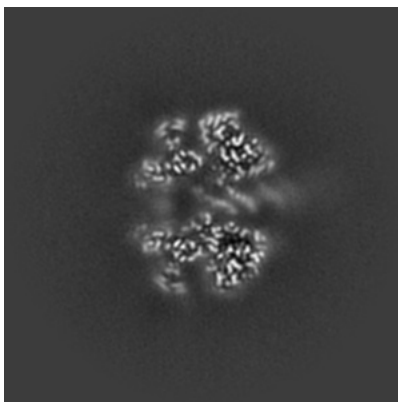
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

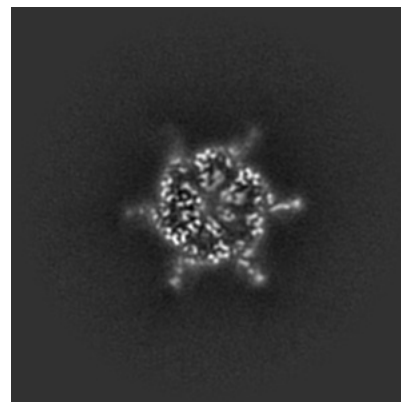
6.2.1 Primary map



X Index: 128

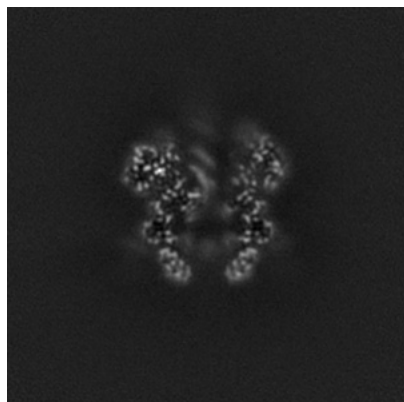


Y Index: 128

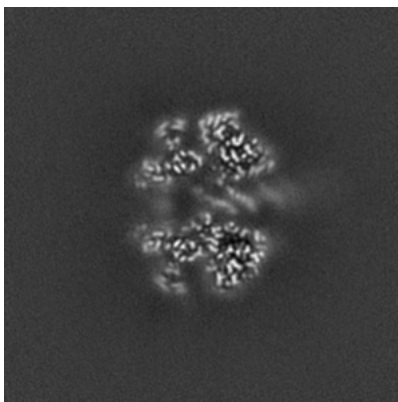


Z Index: 128

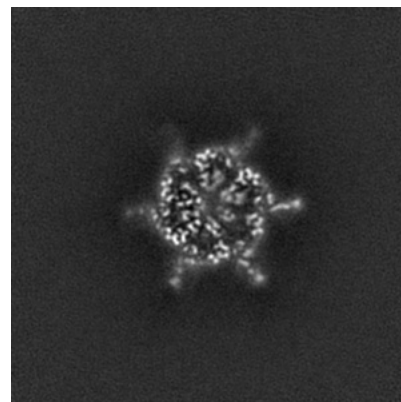
6.2.2 Raw map



X Index: 128



Y Index: 128

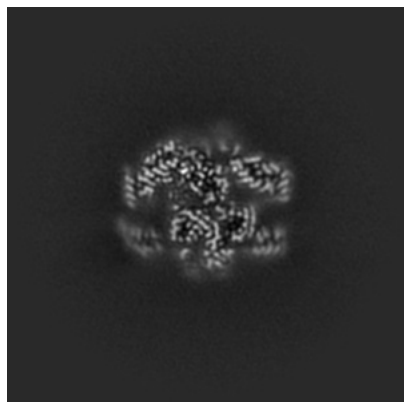


Z Index: 128

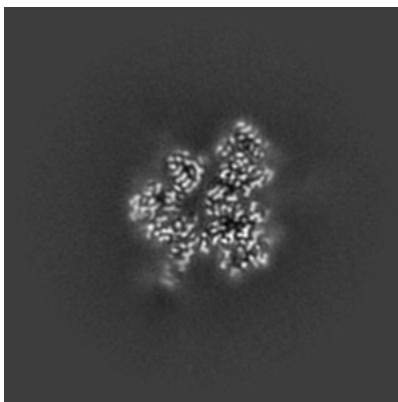
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

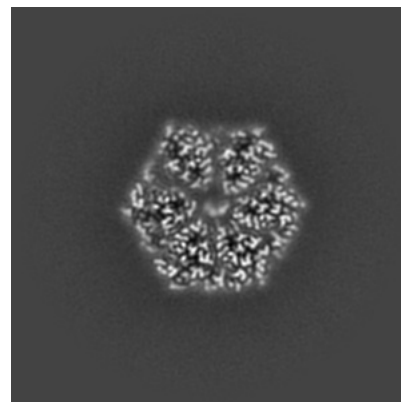
6.3.1 Primary map



X Index: 103

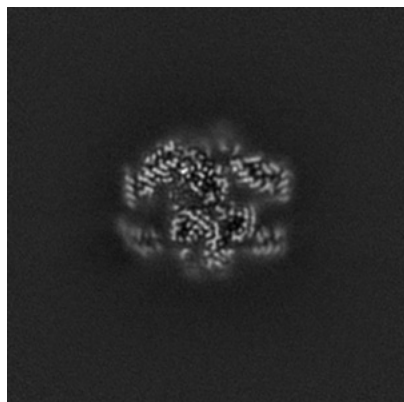


Y Index: 108

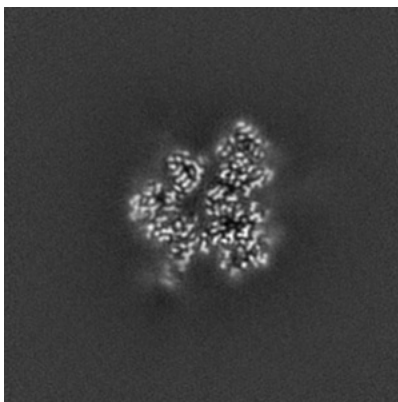


Z Index: 146

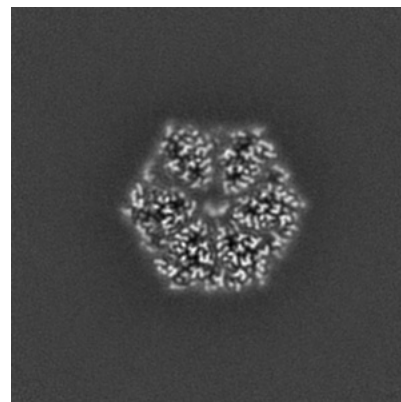
6.3.2 Raw map



X Index: 103



Y Index: 108

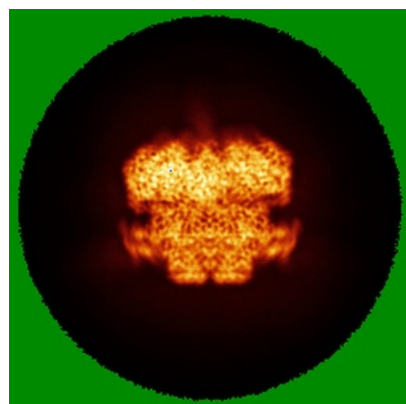


Z Index: 146

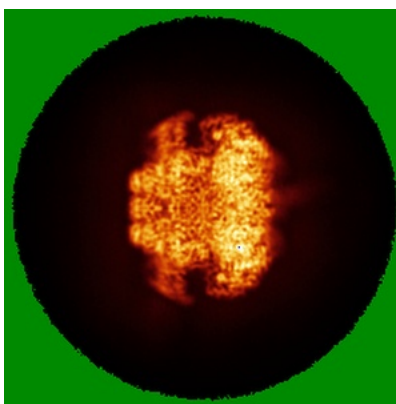
The images above show the largest variance slices of the map in three orthogonal directions.

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

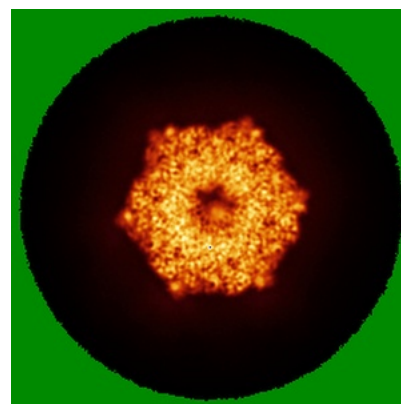
6.4.1 Primary map



X

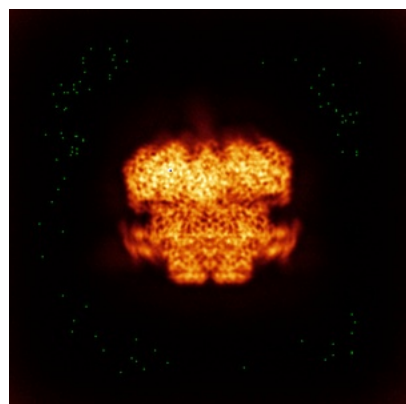


Y

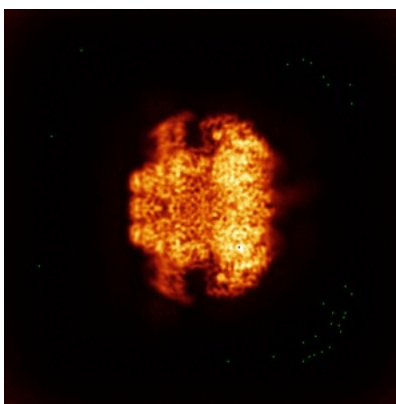


Z

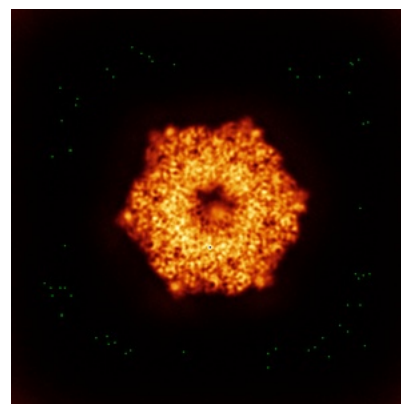
6.4.2 Raw map



X



Y

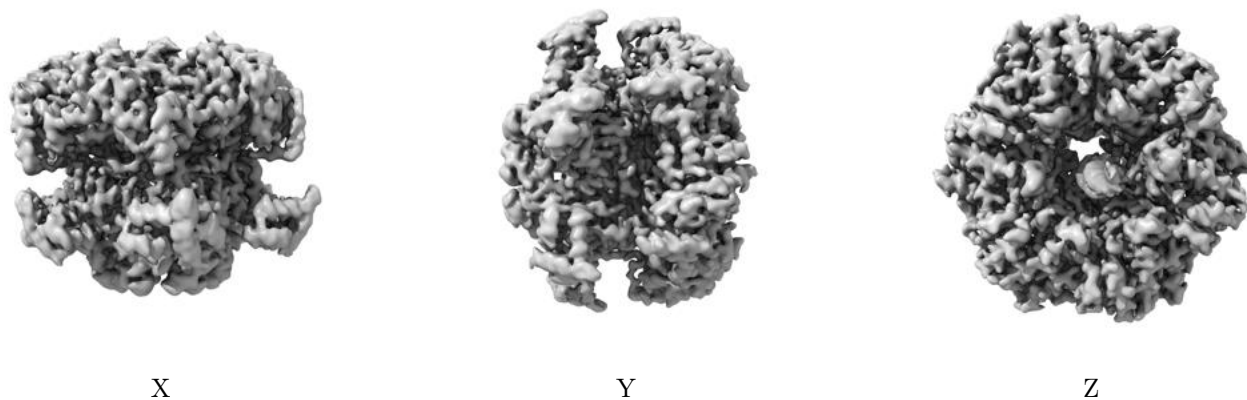


Z

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.

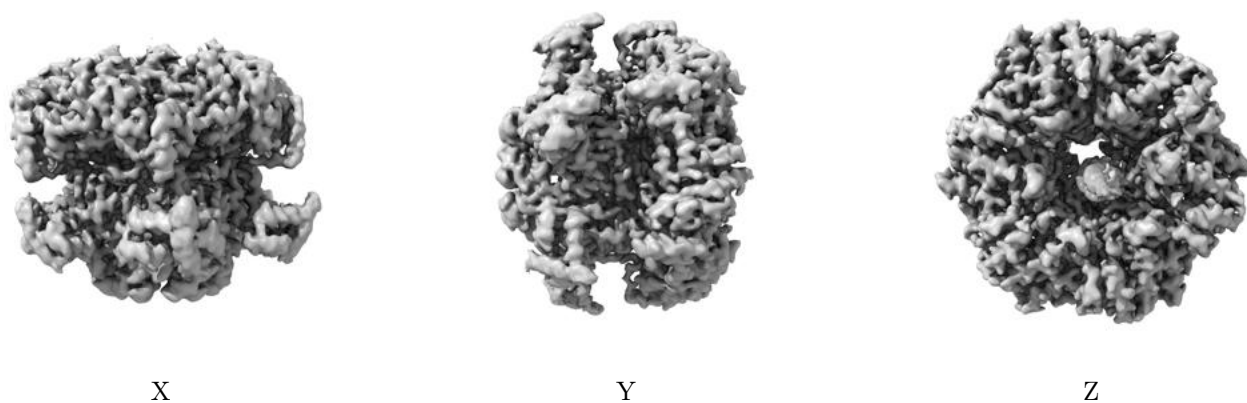
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.415. 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.

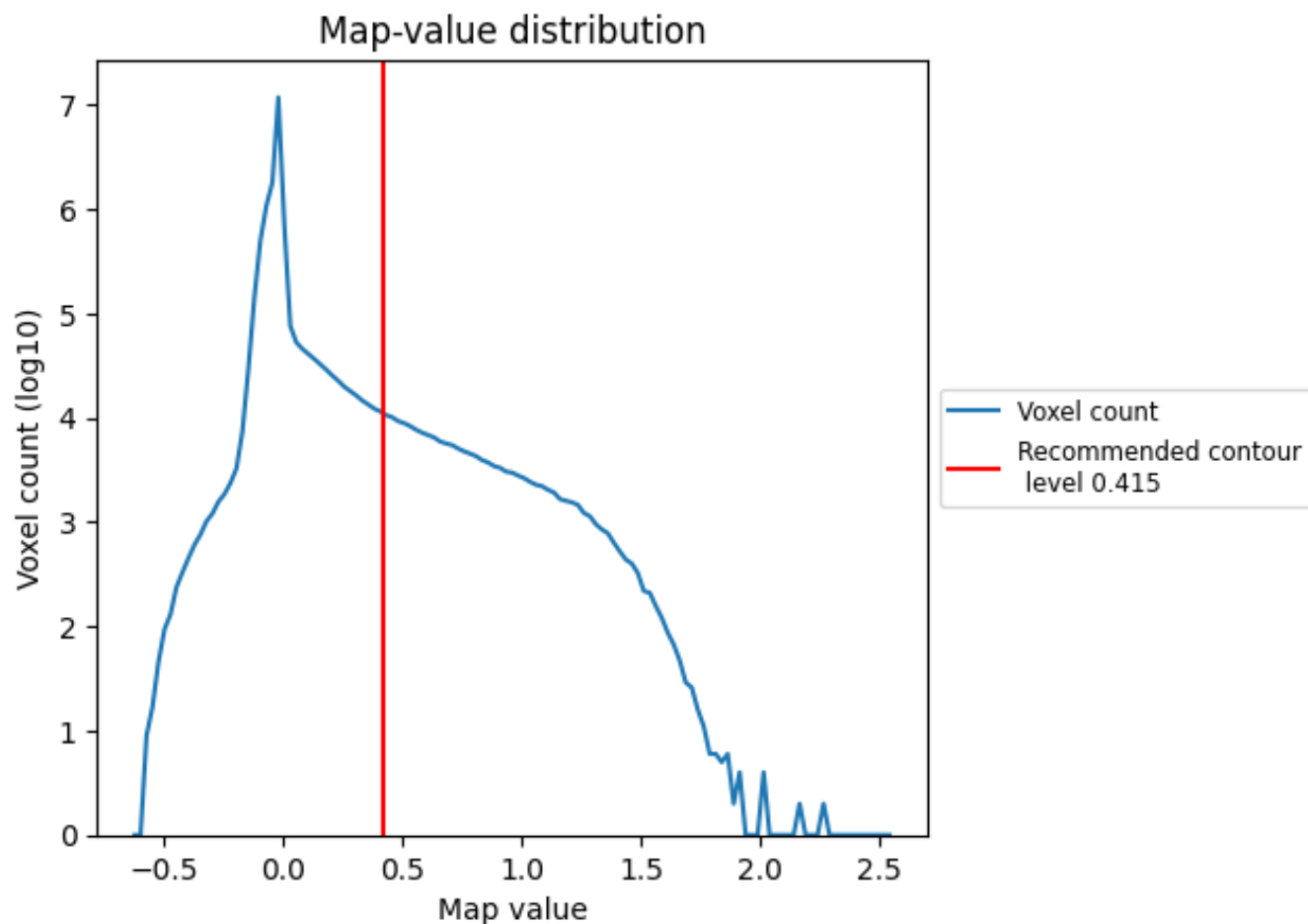
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

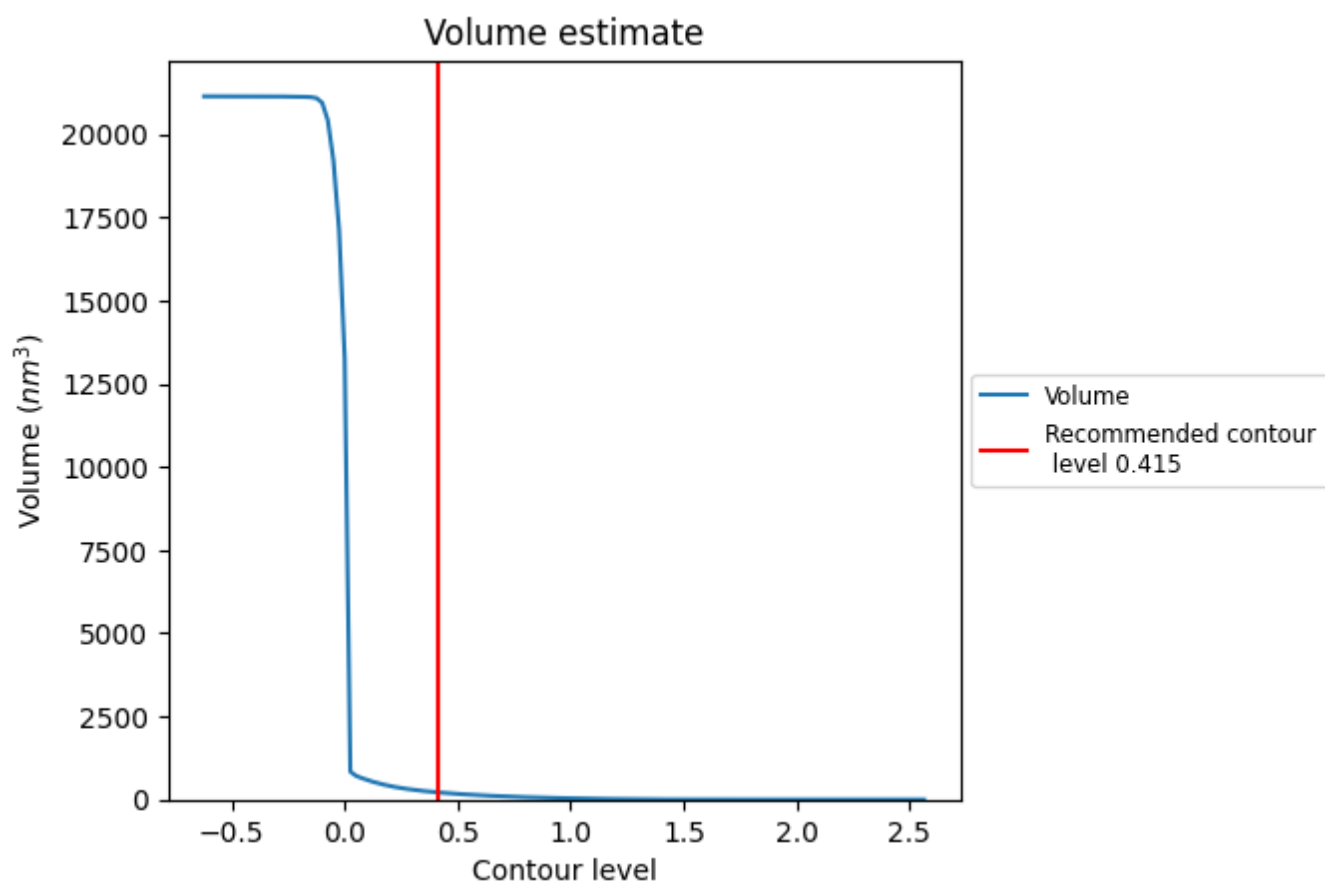
This section contains the results of statistical analysis of the map.

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.

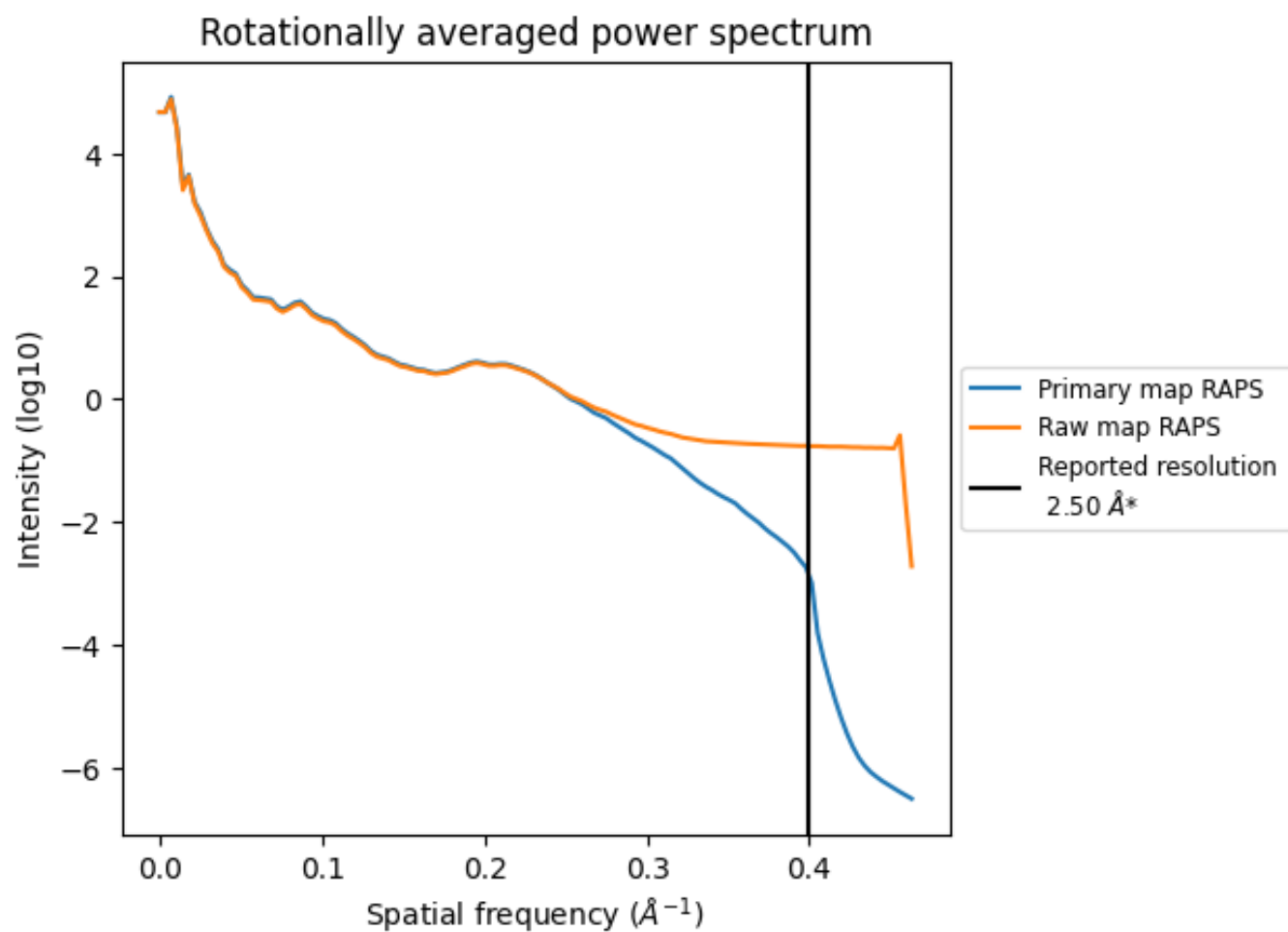
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm³; this corresponds to an approximate mass of 194 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 ⓘ

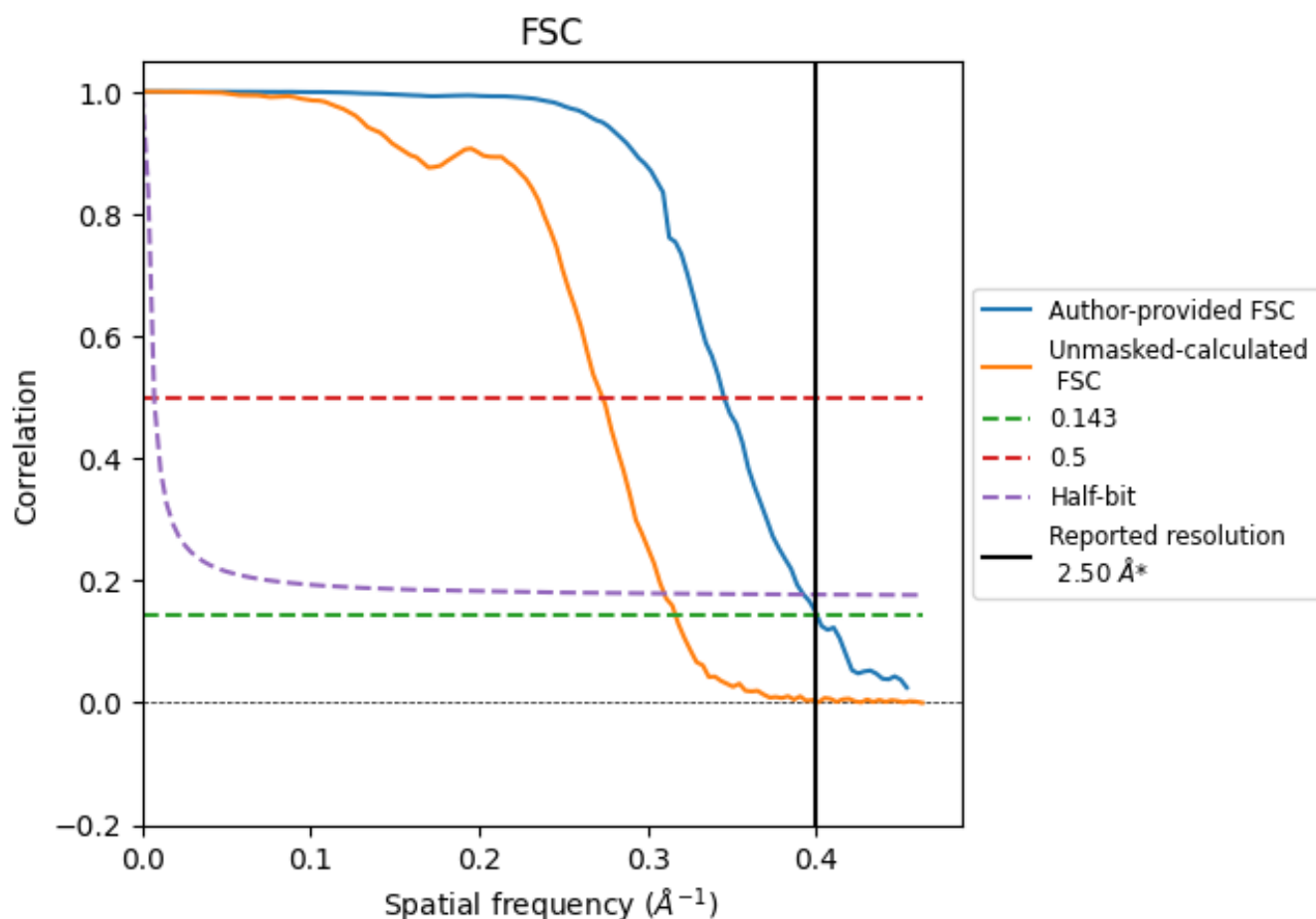


*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

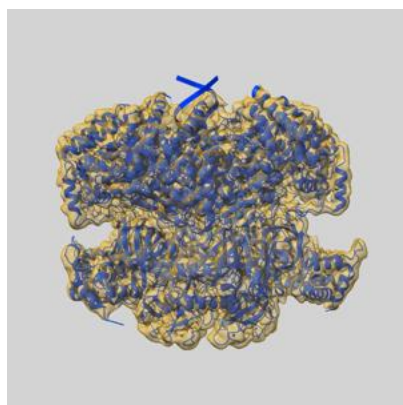
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.90	2.55
Unmasked-calculated*	3.16	3.66	3.23

*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 3.16 differs from the reported value 2.5 by more than 10 %

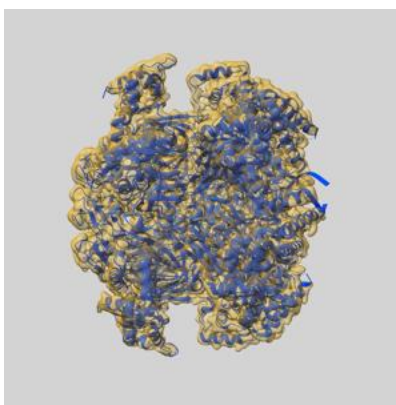
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49810 and PDB model 9NUL. Per-residue inclusion information can be found in section 3 on page 8.

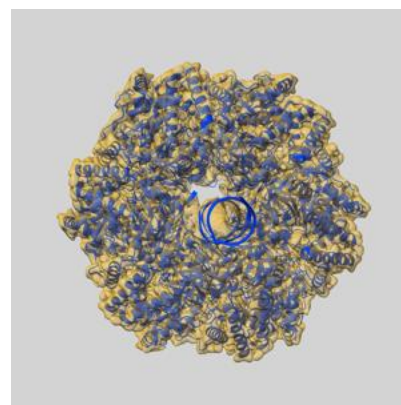
9.1 Map-model overlay [i](#)



X



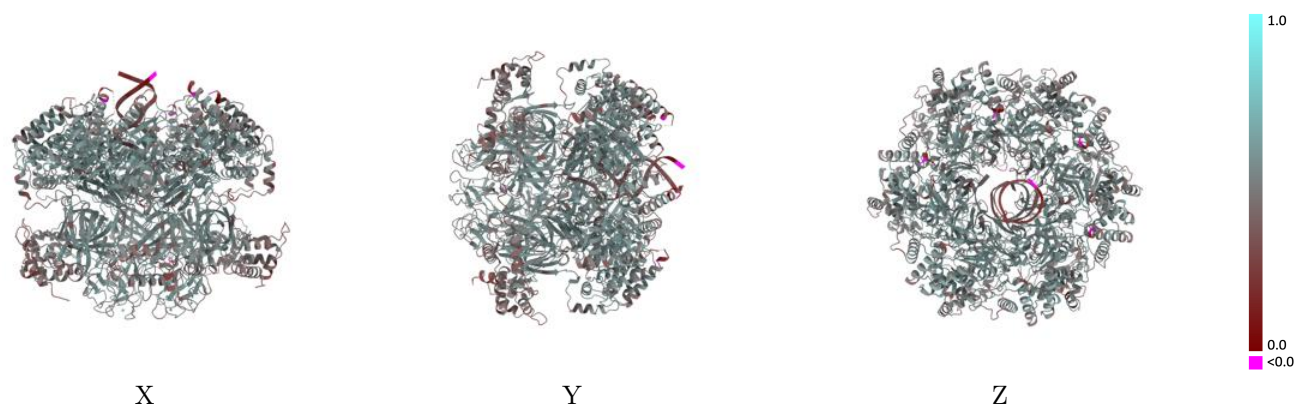
Y



Z

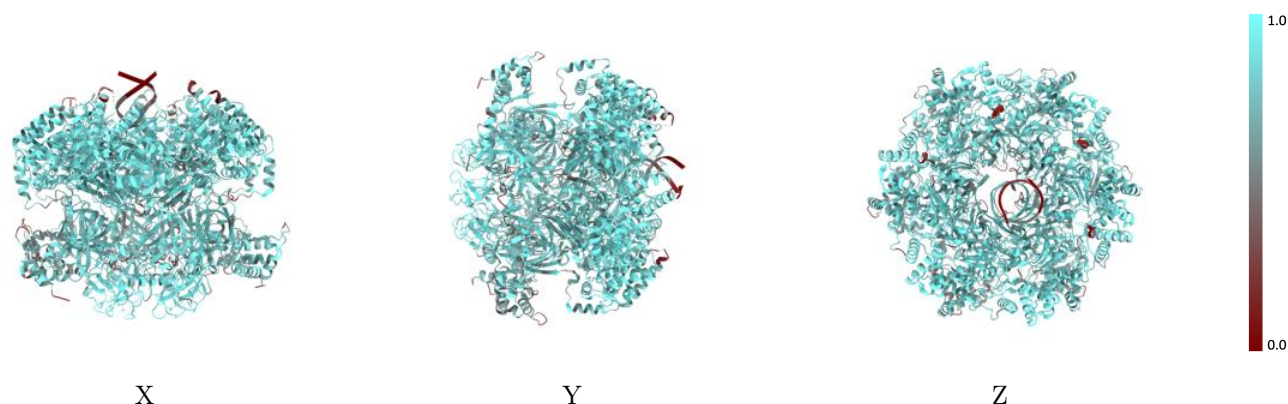
The images above show the 3D surface view of the map at the recommended contour level 0.415 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



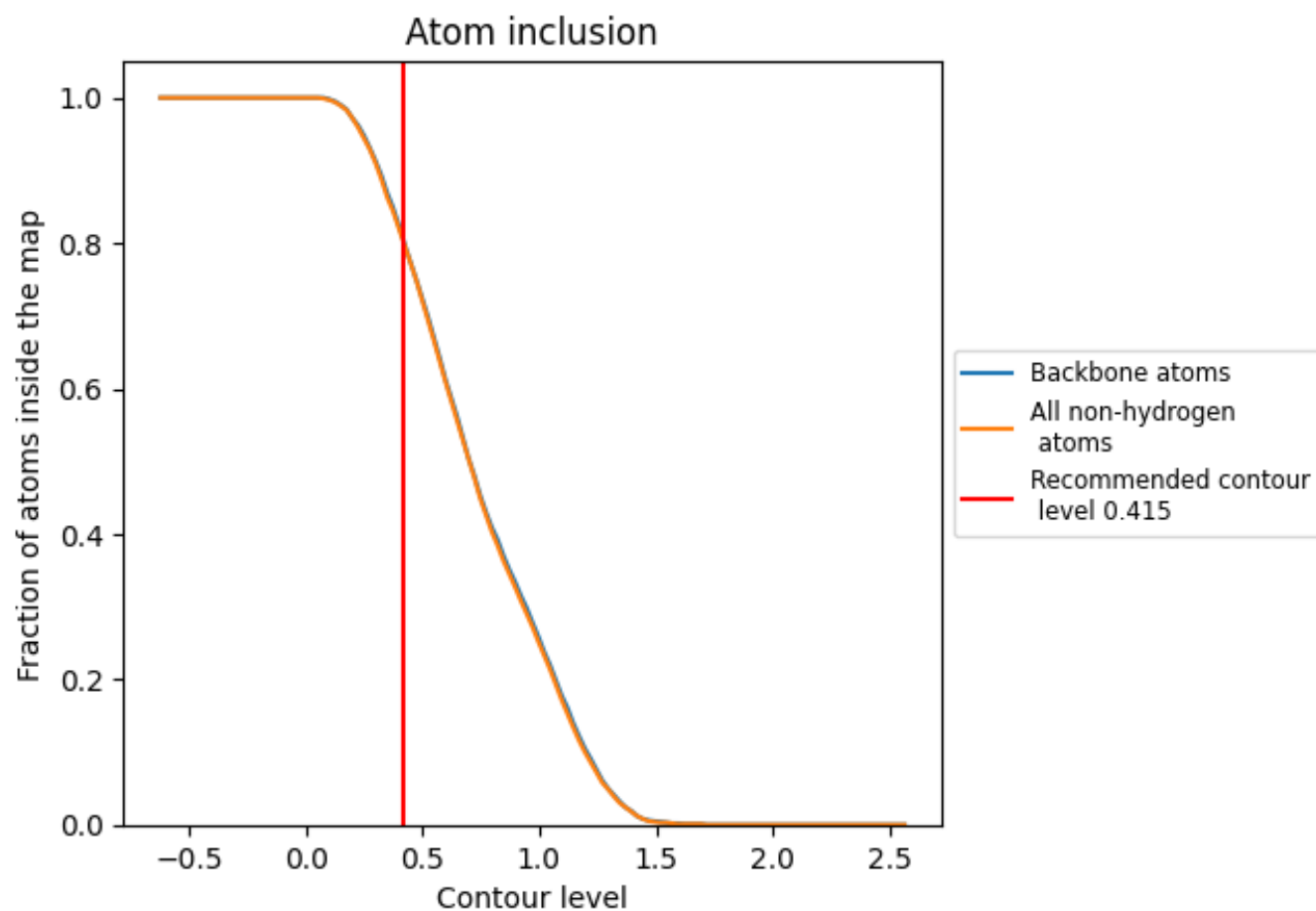
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.415).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.415) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.5050
A	0.8300	0.5170
B	0.8370	0.5100
C	0.8260	0.5000
D	0.8130	0.4980
E	0.8130	0.5130
F	0.8090	0.5140
X	0.6900	0.3920
Y	0.5120	0.3100

1.0

0.0

<0.0