wwPDB EM Validation Summary Report ⓘ

Nov 26, 2022 – 12:16 PM EST

PDB ID	:	7STB
EMDB ID	:	EMD-25423
Title	:	Closed state of Rad24-RFC:9-1-1 bound to a 5' ss/dsDNA junction
Authors	:	Castaneda, J.C.; Schrecker, M.; Remus, D.; Hite, R.K.
Deposited on	:	2021-11-12
Resolution	:	2.72 Å(reported)
Based on initial models	:	3A1J, 1SXJ

This is a wwPDB EM Validation Summary 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:

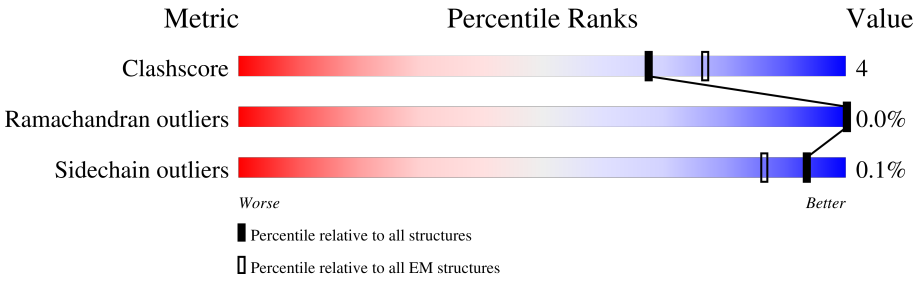
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.72 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 >=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 <=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	696	5% 69% 5% 26%
2	B	323	86% 11%
3	C	340	84% 12%
4	D	353	85% 9% 6%
5	E	354	86% 10%
6	F	401	5% 60% 12% 28%
7	G	646	48% 47%
8	H	474	56% 6% 38%

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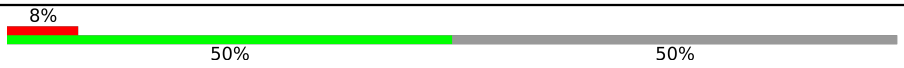
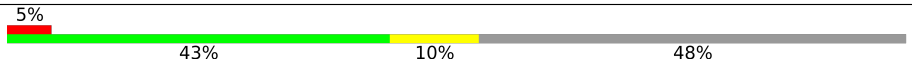
Mol	Chain	Length	Quality of chain
9	J	50	
10	I	21	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 45429 atoms, of which 22615 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 Checkpoint protein RAD24.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	515	8378	2669	4172	733	783	21	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	660	GLY	-	expression tag	UNP P32641
A	661	LEU	-	expression tag	UNP P32641
A	662	ASN	-	expression tag	UNP P32641
A	663	LEU	-	expression tag	UNP P32641
A	664	GLU	-	expression tag	UNP P32641
A	665	VAL	-	expression tag	UNP P32641
A	666	LEU	-	expression tag	UNP P32641
A	667	PHE	-	expression tag	UNP P32641
A	668	GLN	-	expression tag	UNP P32641
A	669	GLY	-	expression tag	UNP P32641
A	670	PRO	-	expression tag	UNP P32641
A	671	GLY	-	expression tag	UNP P32641
A	672	GLY	-	expression tag	UNP P32641
A	673	ASP	-	expression tag	UNP P32641
A	674	TYR	-	expression tag	UNP P32641
A	675	LYS	-	expression tag	UNP P32641
A	676	ASP	-	expression tag	UNP P32641
A	677	ASP	-	expression tag	UNP P32641
A	678	ASP	-	expression tag	UNP P32641
A	679	ASP	-	expression tag	UNP P32641
A	680	LYS	-	expression tag	UNP P32641
A	681	ASP	-	expression tag	UNP P32641
A	682	TYR	-	expression tag	UNP P32641
A	683	LYS	-	expression tag	UNP P32641
A	684	ASP	-	expression tag	UNP P32641
A	685	ASP	-	expression tag	UNP P32641
A	686	ASP	-	expression tag	UNP P32641
A	687	ASP	-	expression tag	UNP P32641

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Chain	Residue	Modelled	Actual	Comment	Reference
A	688	LYS	-	expression tag	UNP P32641
A	689	ASP	-	expression tag	UNP P32641
A	690	TYR	-	expression tag	UNP P32641
A	691	LYS	-	expression tag	UNP P32641
A	692	ASP	-	expression tag	UNP P32641
A	693	ASP	-	expression tag	UNP P32641
A	694	ASP	-	expression tag	UNP P32641
A	695	ASP	-	expression tag	UNP P32641
A	696	LYS	-	expression tag	UNP P32641

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	315	Total	C	H	N	O	S	0	0
			5027	1558	2555	441	460	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	327	Total	C	H	N	O	S	0	0
			5196	1628	2611	451	498	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	333	Total	C	H	N	O	S	0	0
			5304	1665	2668	455	506	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	342	Total	C	H	N	O	S	0	0
			5525	1711	2822	471	503	18		

- Molecule 6 is a protein called DNA damage checkpoint control protein RAD17.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	288	Total	C	H	N	O	S	0	0
			4539	1451	2265	365	447	11		

- Molecule 7 is a protein called DNA damage checkpoint protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	340	Total	C	H	N	O	S	0	0
			5428	1742	2701	450	521	14		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-33	MET	-	expression tag	UNP Q08949
G	-32	ASP	-	expression tag	UNP Q08949
G	-31	TYR	-	expression tag	UNP Q08949
G	-30	LYS	-	expression tag	UNP Q08949
G	-29	ASP	-	expression tag	UNP Q08949
G	-28	ASP	-	expression tag	UNP Q08949
G	-27	ASP	-	expression tag	UNP Q08949
G	-26	ASP	-	expression tag	UNP Q08949
G	-25	LYS	-	expression tag	UNP Q08949
G	-24	ASP	-	expression tag	UNP Q08949
G	-23	TYR	-	expression tag	UNP Q08949
G	-22	LYS	-	expression tag	UNP Q08949
G	-21	ASP	-	expression tag	UNP Q08949
G	-20	ASP	-	expression tag	UNP Q08949
G	-19	ASP	-	expression tag	UNP Q08949
G	-18	ASP	-	expression tag	UNP Q08949
G	-17	LYS	-	expression tag	UNP Q08949
G	-16	ASP	-	expression tag	UNP Q08949
G	-15	TYR	-	expression tag	UNP Q08949
G	-14	LYS	-	expression tag	UNP Q08949
G	-13	ASP	-	expression tag	UNP Q08949
G	-12	ASP	-	expression tag	UNP Q08949
G	-11	ASP	-	expression tag	UNP Q08949
G	-10	ASP	-	expression tag	UNP Q08949
G	-9	LYS	-	expression tag	UNP Q08949
G	-8	LEU	-	expression tag	UNP Q08949
G	-7	GLU	-	expression tag	UNP Q08949
G	-6	VAL	-	expression tag	UNP Q08949
G	-5	LEU	-	expression tag	UNP Q08949
G	-4	PHE	-	expression tag	UNP Q08949
G	-3	GLN	-	expression tag	UNP Q08949
G	-2	GLY	-	expression tag	UNP Q08949
G	-1	PRO	-	expression tag	UNP Q08949
G	0	GLY	-	expression tag	UNP Q08949

- Molecule 8 is a protein called DNA damage checkpoint control protein MEC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	293	4710	1496	2365	406	423	20	0	0

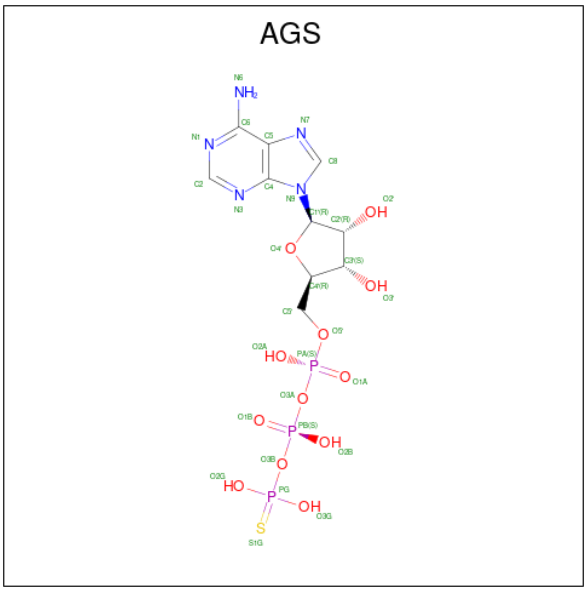
- Molecule 9 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
9	J	25	804	249	290	78	162	25	0	0

- Molecule 10 is a DNA chain called DNA (5'-D(P*CP*GP*CP*TP*CP*CP*TP*TP*CP*CP*TP*GP*AP*CP*TP*CP*GP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
10	I	11	303	94	106	29	64	10	0	1

- Molecule 11 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
11	A	1	43	10	12	5	12	3	1	0
11	B	1	43	10	12	5	12	3	1	0
11	C	1	43	10	12	5	12	3	1	0

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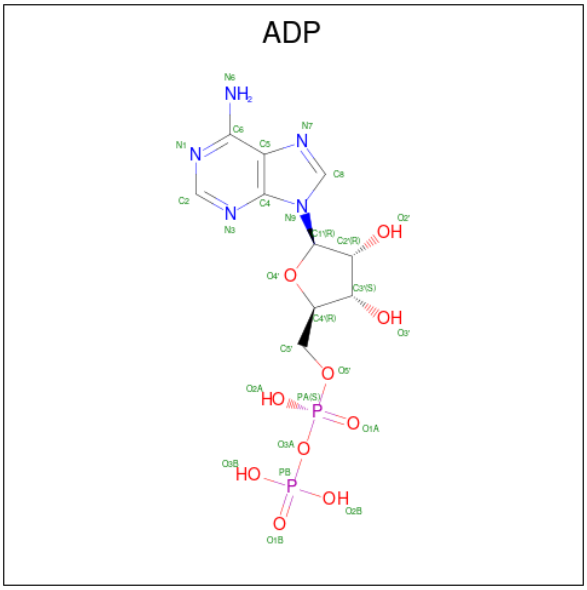
Mol	Chain	Residues	Atoms							AltConf
11	D	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

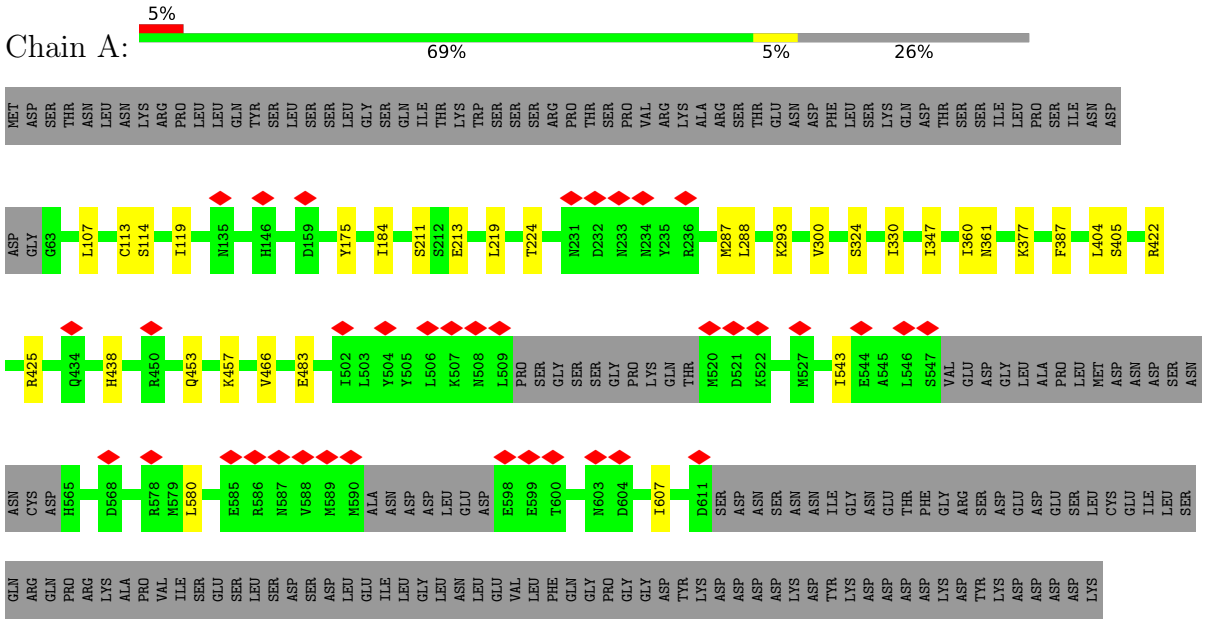


Mol	Chain	Residues	Atoms						AltConf
13	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

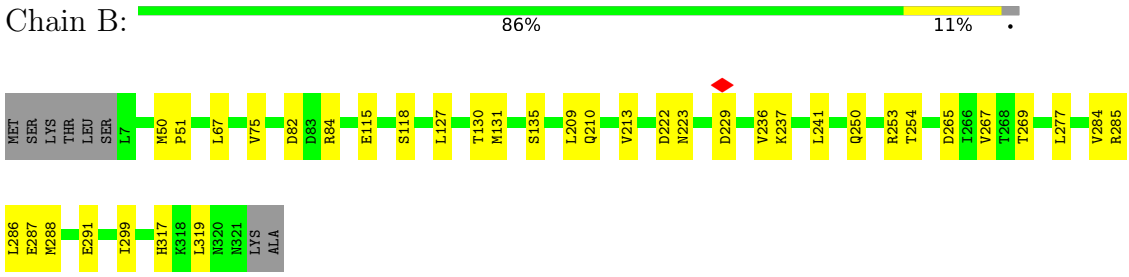
3 Residue-property plots (i)

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.

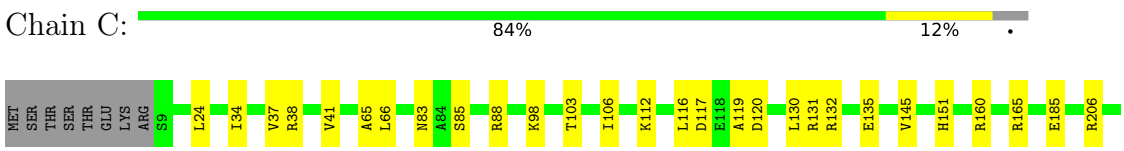
• Molecule 1: Checkpoint protein RAD24



• Molecule 2: Replication factor C subunit 4

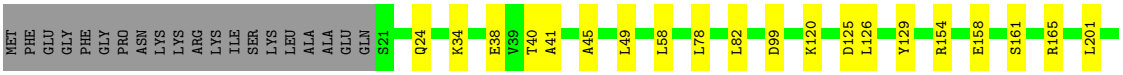


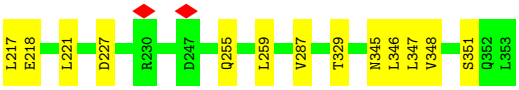
• Molecule 3: Replication factor C subunit 3



• Molecule 4: Replication factor C subunit 2

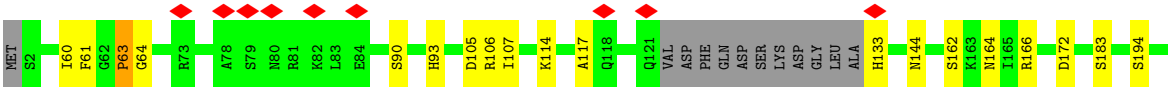
Chain D:





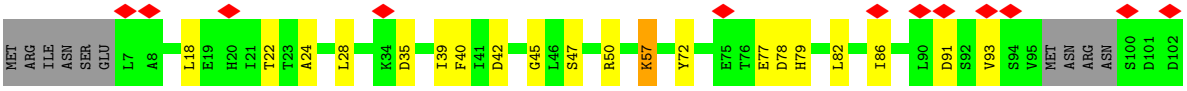
• Molecule 5: Replication factor C subunit 5

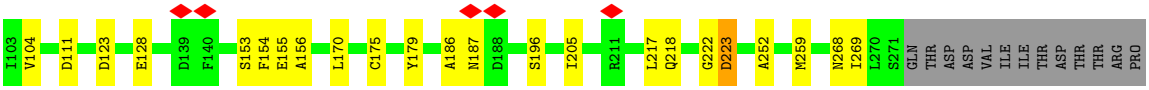
Chain E:

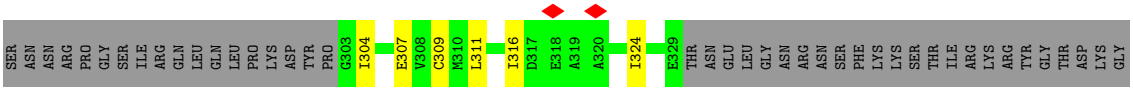


• Molecule 6: DNA damage checkpoint control protein RAD17

Chain F:

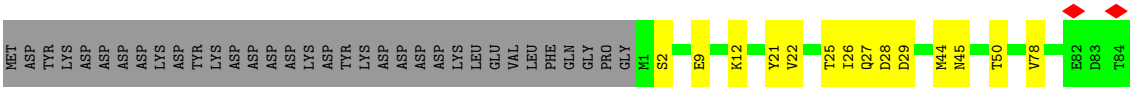


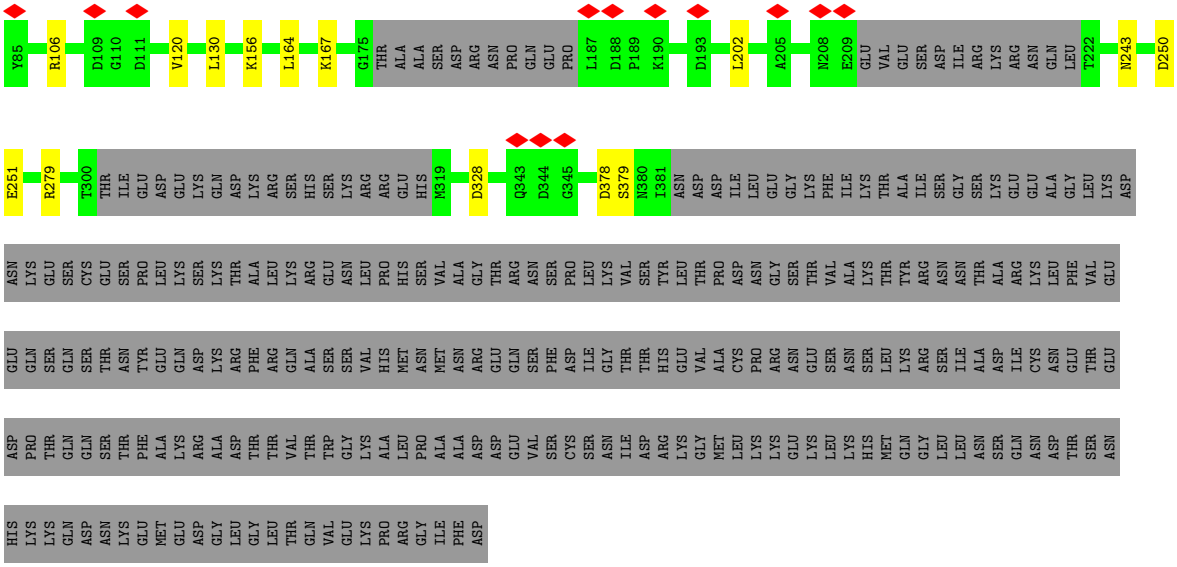




• Molecule 7: DNA damage checkpoint protein 1

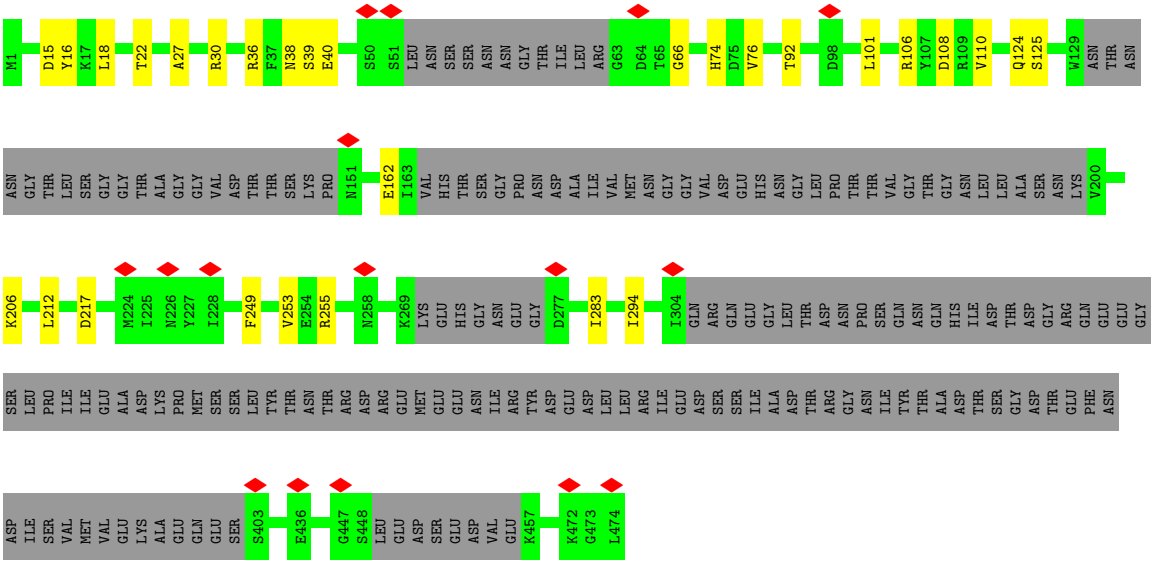
Chain G:





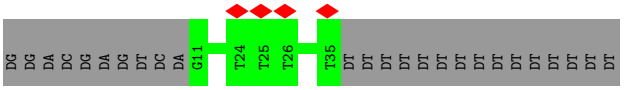
• Molecule 8: DNA damage checkpoint control protein MEC3

Chain H:



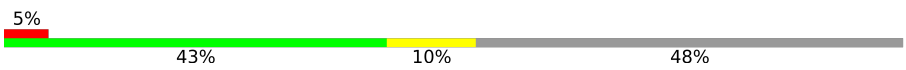
• Molecule 9: DNA (50-MER)

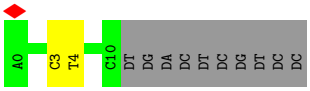
Chain J:



• Molecule 10: DNA (5'-D(P*CP*GP*CP*TP*CP*CP*TP*TP*CP*CP*TP*GP*AP*CP*TP*CP*GP*TP*CP*C)-3')

Chain I:




A0
C3
T4
C10
DT
DG
DA
DC
DT
DC
DG
DT
DC
DC

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	237512	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 ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.870	Depositor
Minimum map value	-0.847	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	317.184, 317.184, 317.184	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 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	0.24	0/4291	0.44	0/5780
2	B	0.23	0/2507	0.46	0/3381
3	C	0.24	0/2625	0.46	0/3551
4	D	0.23	0/2681	0.45	0/3626
5	E	0.25	0/2741	0.51	2/3702 (0.1%)
6	F	0.25	0/2308	0.47	0/3108
7	G	0.24	0/2779	0.45	0/3764
8	H	0.24	0/2388	0.48	0/3221
9	J	0.53	0/572	1.08	0/883
10	I	0.62	0/217	0.96	0/332
All	All	0.26	0/23109	0.50	2/31348 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	63	PRO	CA-N-CD	-10.40	96.94	111.50
5	E	63	PRO	N-CD-CG	-5.90	94.36	103.20

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	4206	4172	4172	24	0
2	B	2472	2555	2555	25	0
3	C	2585	2611	2611	31	0
4	D	2636	2668	2669	24	0
5	E	2703	2822	2822	26	0
6	F	2274	2265	2265	34	0
7	G	2727	2701	2703	18	0
8	H	2345	2365	2365	19	0
9	J	514	290	291	0	0
10	I	197	106	114	1	0
11	A	31	12	12	2	0
11	B	31	12	12	1	0
11	C	31	12	12	2	0
11	D	31	12	12	1	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
13	E	27	12	12	1	0
All	All	22814	22615	22627	178	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 4.

The worst 5 of 178 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:211:SER:OG	1:A:213:GLU:OE1	1.91	0.89
7:G:22:VAL:O	7:G:25:THR:OG1	1.99	0.81
1:A:175:TYR:OH	7:G:251:GLU:OE1	1.99	0.80
3:C:132:ARG:NH1	3:C:135:GLU:OE1	2.17	0.78
2:B:131:MET:O	2:B:135:SER:OG	2.00	0.77

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	507/696 (73%)	491 (97%)	16 (3%)	0	100	100
2	B	313/323 (97%)	307 (98%)	6 (2%)	0	100	100
3	C	325/340 (96%)	322 (99%)	3 (1%)	0	100	100
4	D	331/353 (94%)	322 (97%)	9 (3%)	0	100	100
5	E	338/354 (96%)	329 (97%)	9 (3%)	0	100	100
6	F	282/401 (70%)	271 (96%)	10 (4%)	1 (0%)	34	58
7	G	332/646 (51%)	321 (97%)	11 (3%)	0	100	100
8	H	279/474 (59%)	272 (98%)	7 (2%)	0	100	100
All	All	2707/3587 (76%)	2635 (97%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	223	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	472/645 (73%)	472 (100%)	0	100	100
2	B	275/283 (97%)	274 (100%)	1 (0%)	91	96
3	C	283/296 (96%)	283 (100%)	0	100	100
4	D	296/312 (95%)	296 (100%)	0	100	100
5	E	313/324 (97%)	313 (100%)	0	100	100
6	F	260/369 (70%)	259 (100%)	1 (0%)	91	96
7	G	312/592 (53%)	311 (100%)	1 (0%)	92	97
8	H	265/424 (62%)	265 (100%)	0	100	100
All	All	2476/3245 (76%)	2473 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	210	GLN
6	F	57	LYS
7	G	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN

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	$\#\|Z\| > 2$
11	AGS	C	402	12	26,33,33	0.70	1 (3%)	26,52,52	1.03	2 (7%)
11	AGS	B	402	12	26,33,33	0.71	1 (3%)	26,52,52	1.01	2 (7%)
11	AGS	D	402	12	26,33,33	0.70	1 (3%)	26,52,52	1.02	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	AGS	A	901	12	26,33,33	0.71	1 (3%)	26,52,52	1.06	2 (7%)
13	ADP	E	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	AGS	C	402	12	-	6/17/38/38	0/3/3/3
11	AGS	B	402	12	-	3/17/38/38	0/3/3/3
11	AGS	D	402	12	-	5/17/38/38	0/3/3/3
11	AGS	A	901	12	-	5/17/38/38	0/3/3/3
13	ADP	E	401	-	-	3/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	401	ADP	C5-C4	2.35	1.47	1.40
11	B	402	AGS	PG-S1G	2.10	1.95	1.90
11	A	901	AGS	PG-S1G	2.09	1.95	1.90
11	D	402	AGS	PG-S1G	2.08	1.95	1.90
11	C	402	AGS	PG-S1G	2.06	1.95	1.90

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	402	AGS	PA-O3A-PB	-3.69	120.17	132.83
11	A	901	AGS	PA-O3A-PB	-3.68	120.21	132.83
13	E	401	ADP	N3-C2-N1	-3.67	122.95	128.68
11	D	402	AGS	PA-O3A-PB	-3.57	120.58	132.83
13	E	401	ADP	PA-O3A-PB	-3.54	120.68	132.83

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	402	AGS	C5'-O5'-PA-O1A
11	C	402	AGS	C5'-O5'-PA-O2A
11	C	402	AGS	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	D	402	AGS	C5'-O5'-PA-O3A
13	E	401	ADP	C5'-O5'-PA-O1A

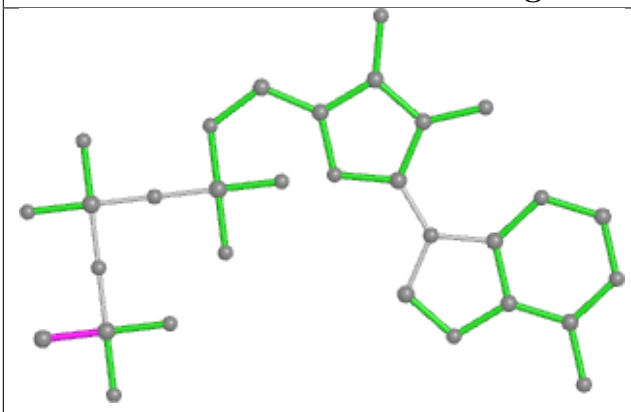
There are no ring outliers.

5 monomers are involved in 7 short contacts:

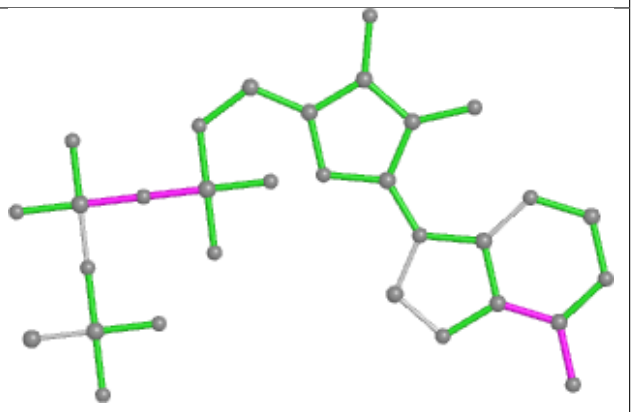
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	402	AGS	2	0
11	B	402	AGS	1	0
11	D	402	AGS	1	0
11	A	901	AGS	2	0
13	E	401	ADP	1	0

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 then 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.

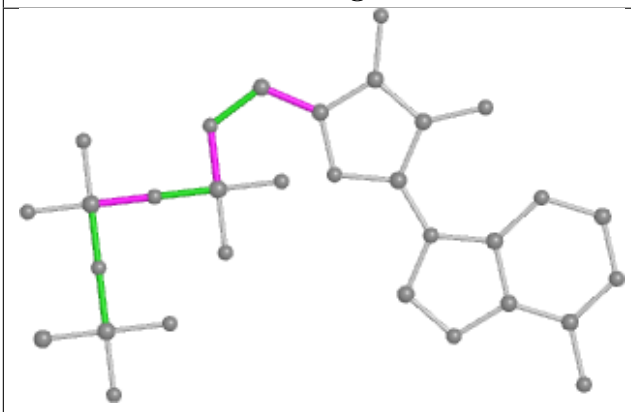
Ligand AGS C 402



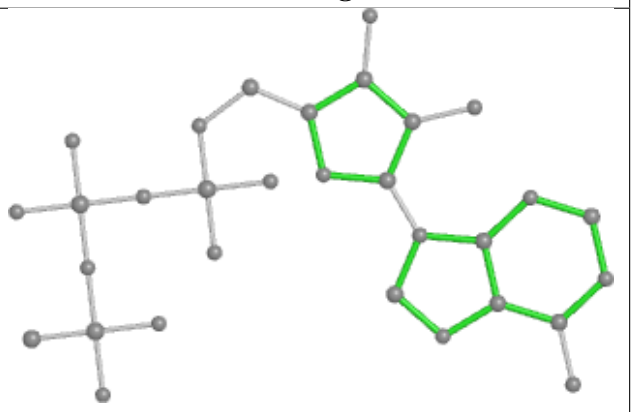
Bond lengths



Bond angles

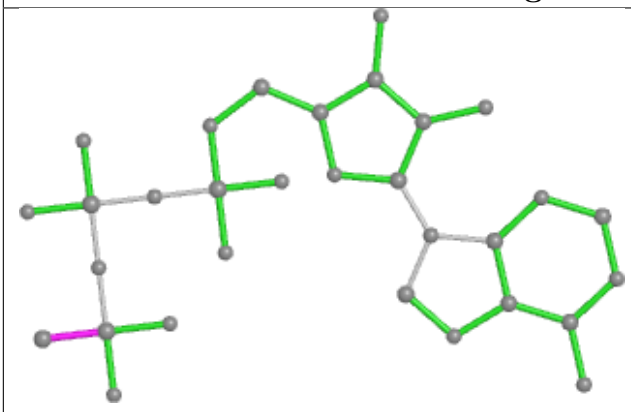


Torsions

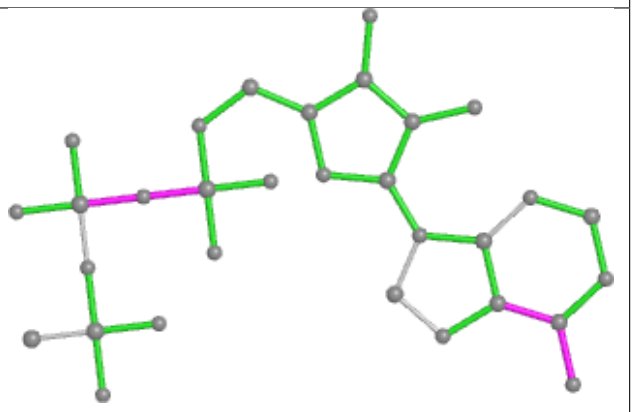


Rings

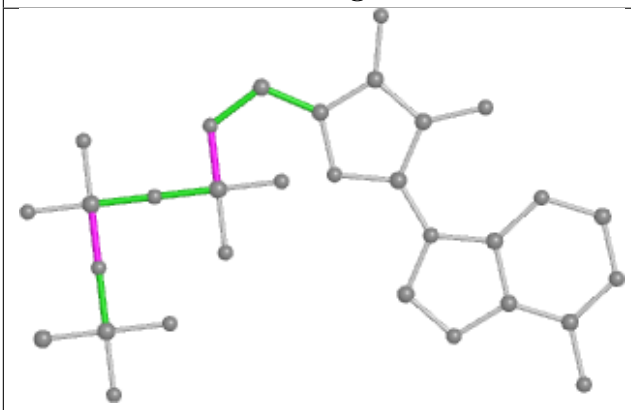
Ligand AGS B 402



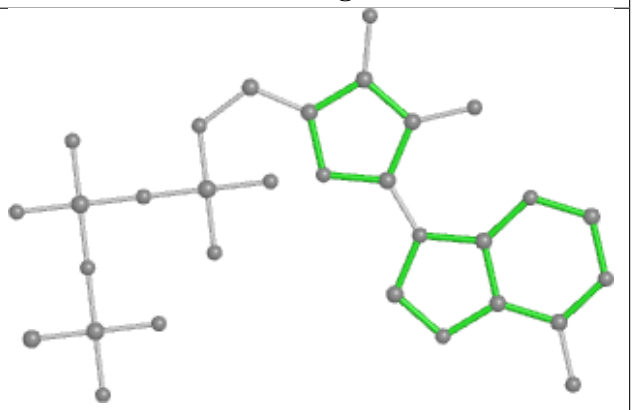
Bond lengths



Bond angles

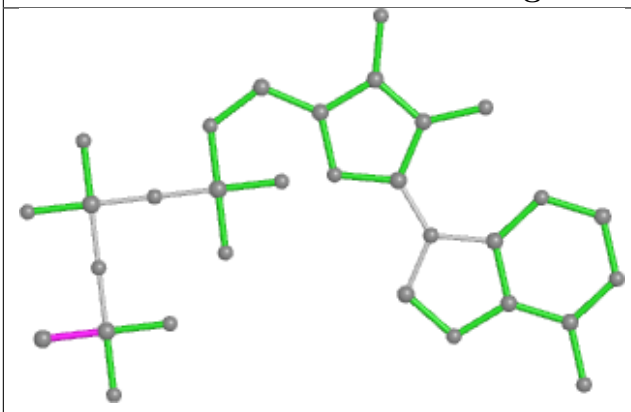


Torsions

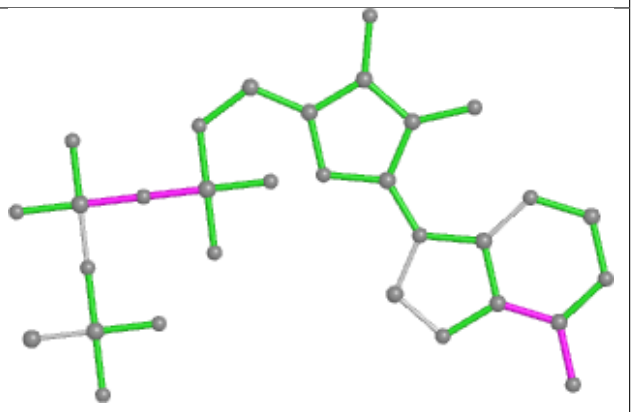


Rings

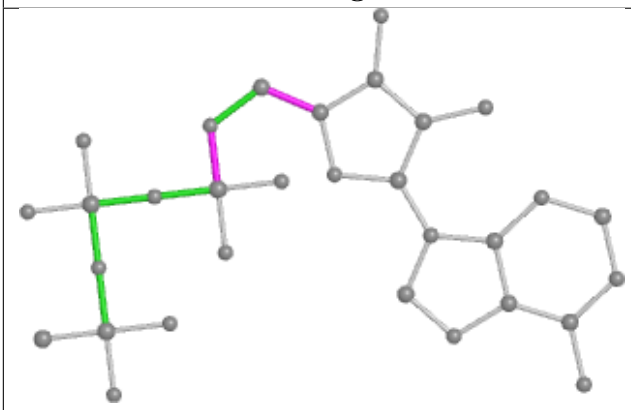
Ligand AGS D 402



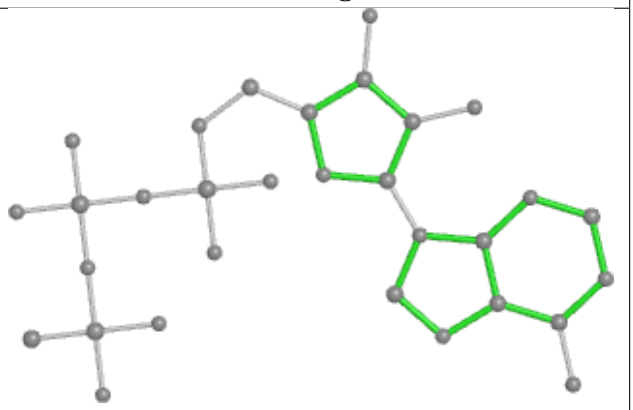
Bond lengths



Bond angles

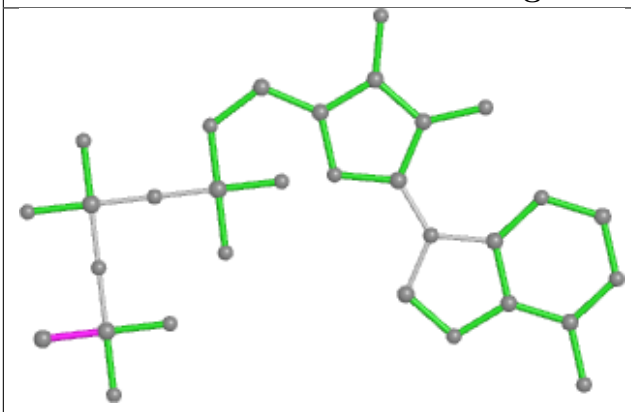


Torsions

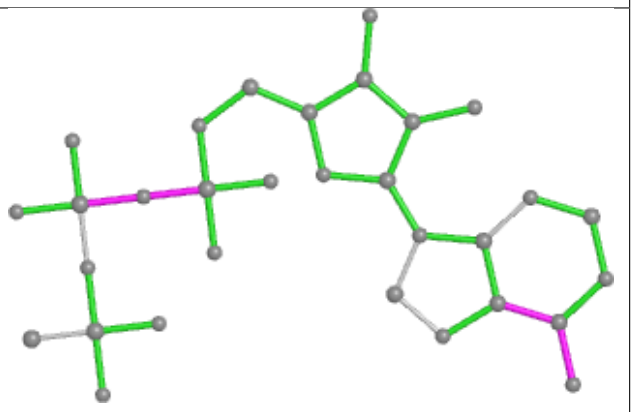


Rings

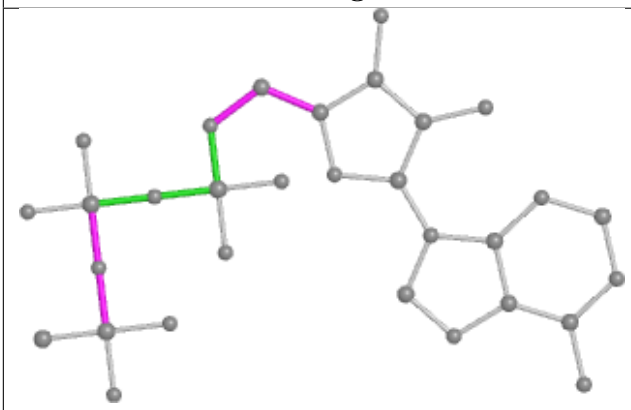
Ligand AGS A 901



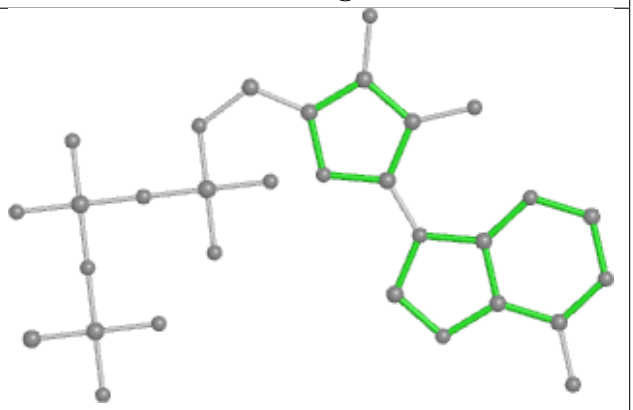
Bond lengths



Bond angles

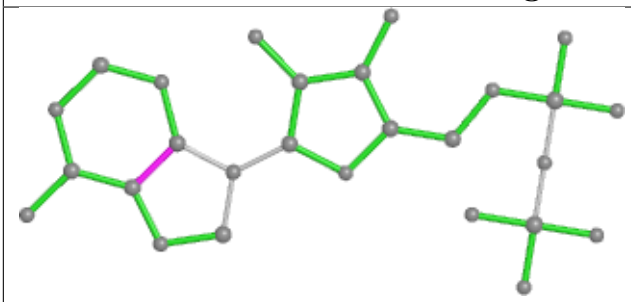


Torsions

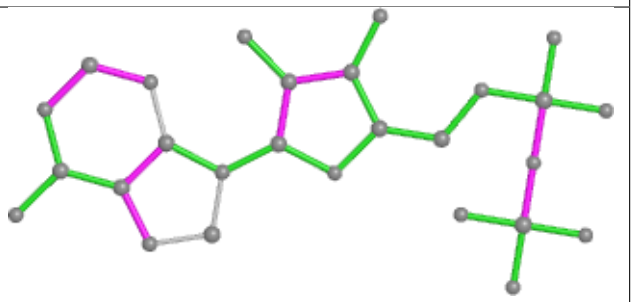


Rings

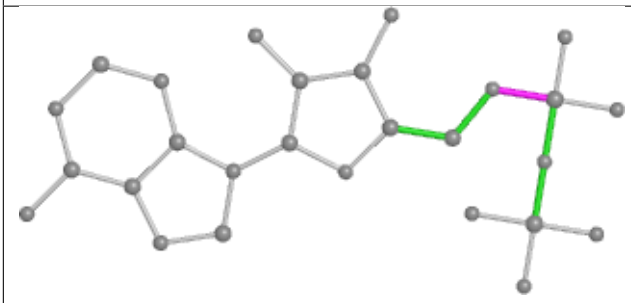
Ligand ADP E 401



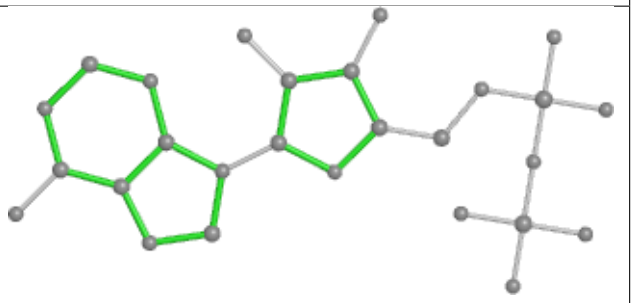
Bond lengths



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.

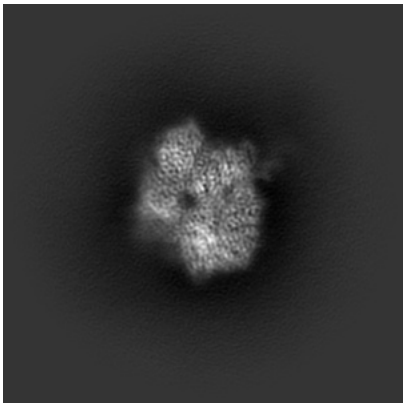
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25423. These allow visual inspection of the internal detail of the map and identification of artifacts.

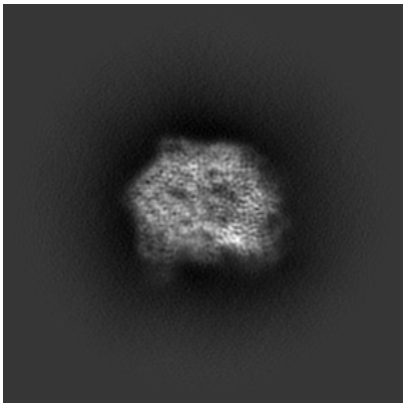
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

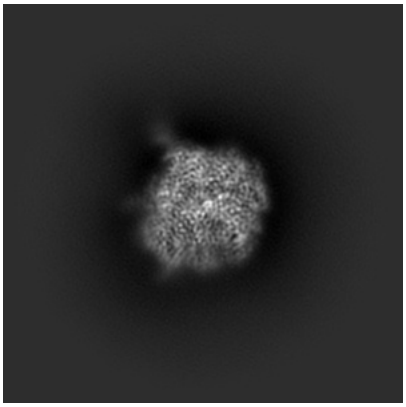
6.1.1 Primary map



X



Y

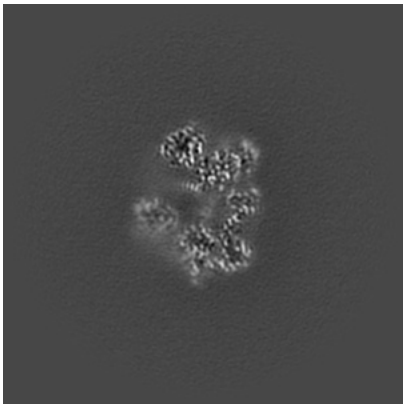


Z

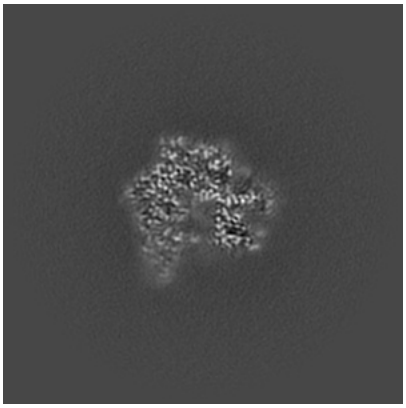
The images above show the map projected in three orthogonal directions.

6.2 Central slices

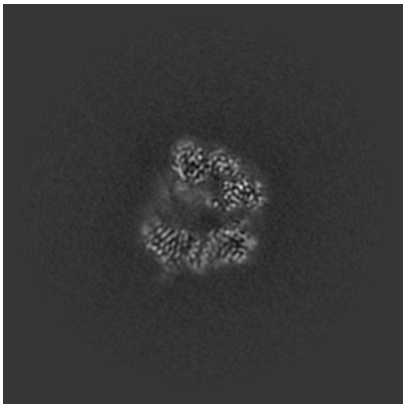
6.2.1 Primary map



X Index: 192



Y Index: 192

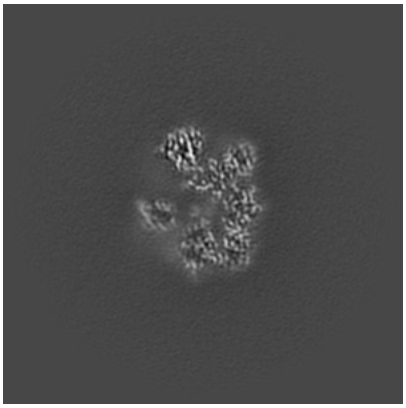


Z Index: 192

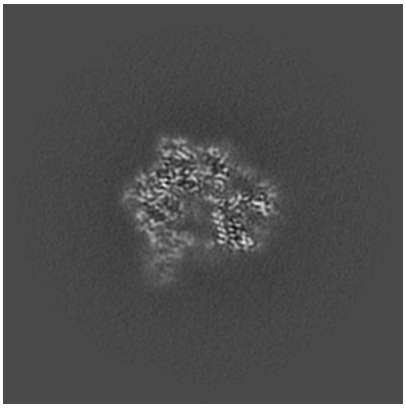
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

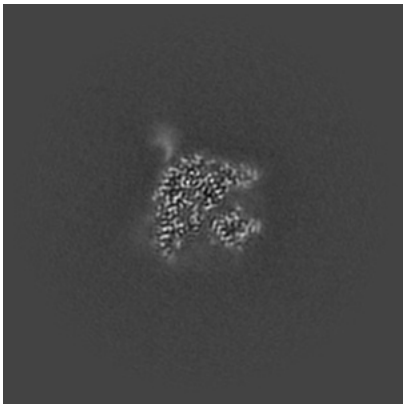
6.3.1 Primary map



X Index: 185



Y Index: 189

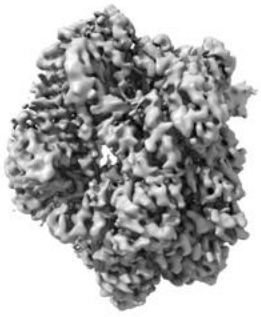


Z Index: 226

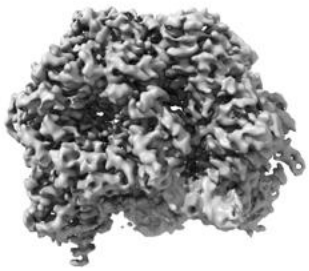
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

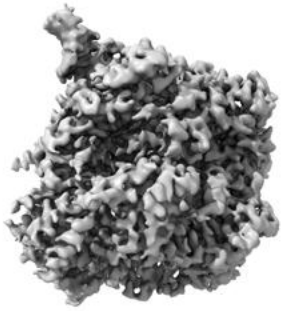
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

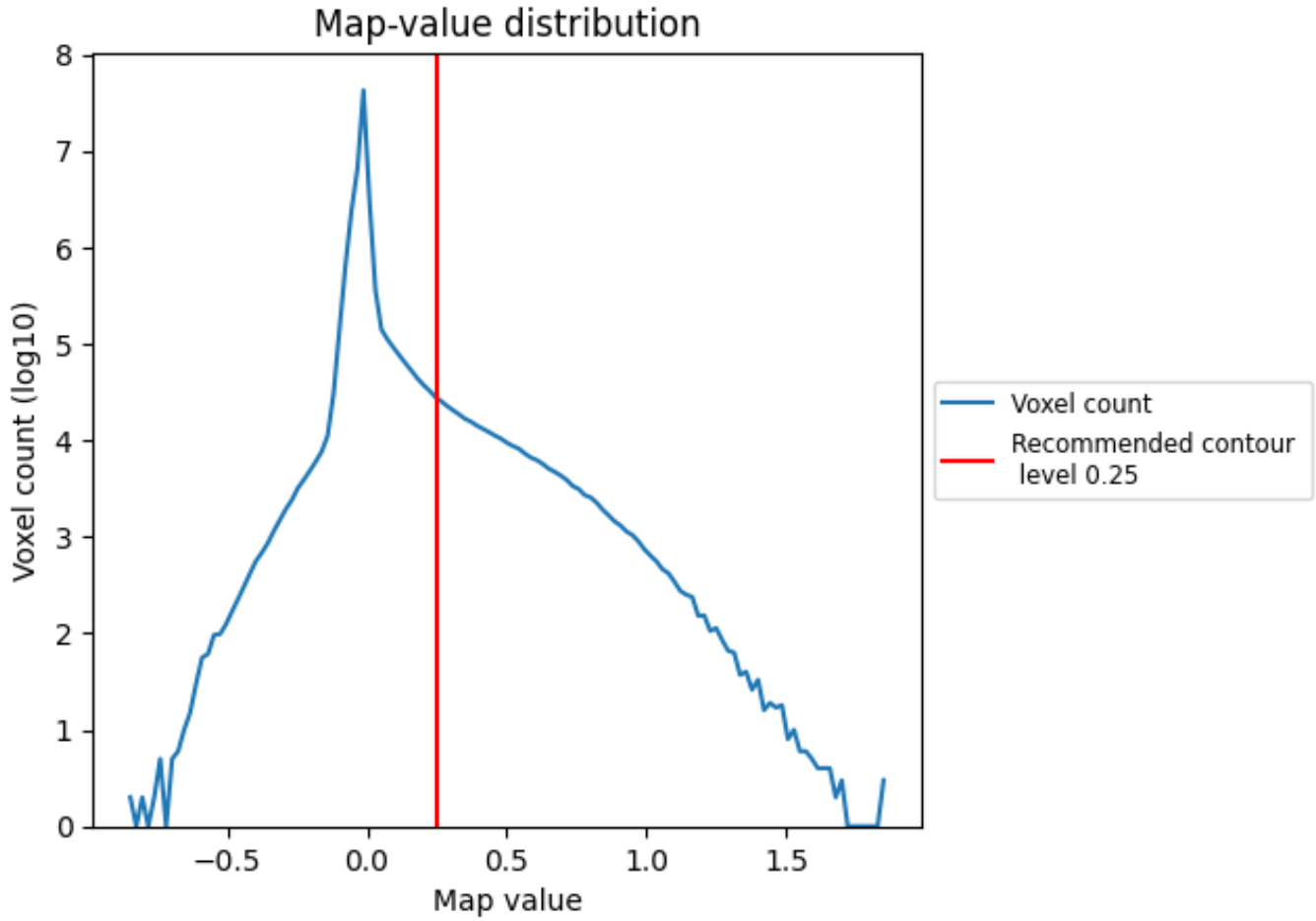
6.5 Mask visualisation (i)

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

7 Map analysis

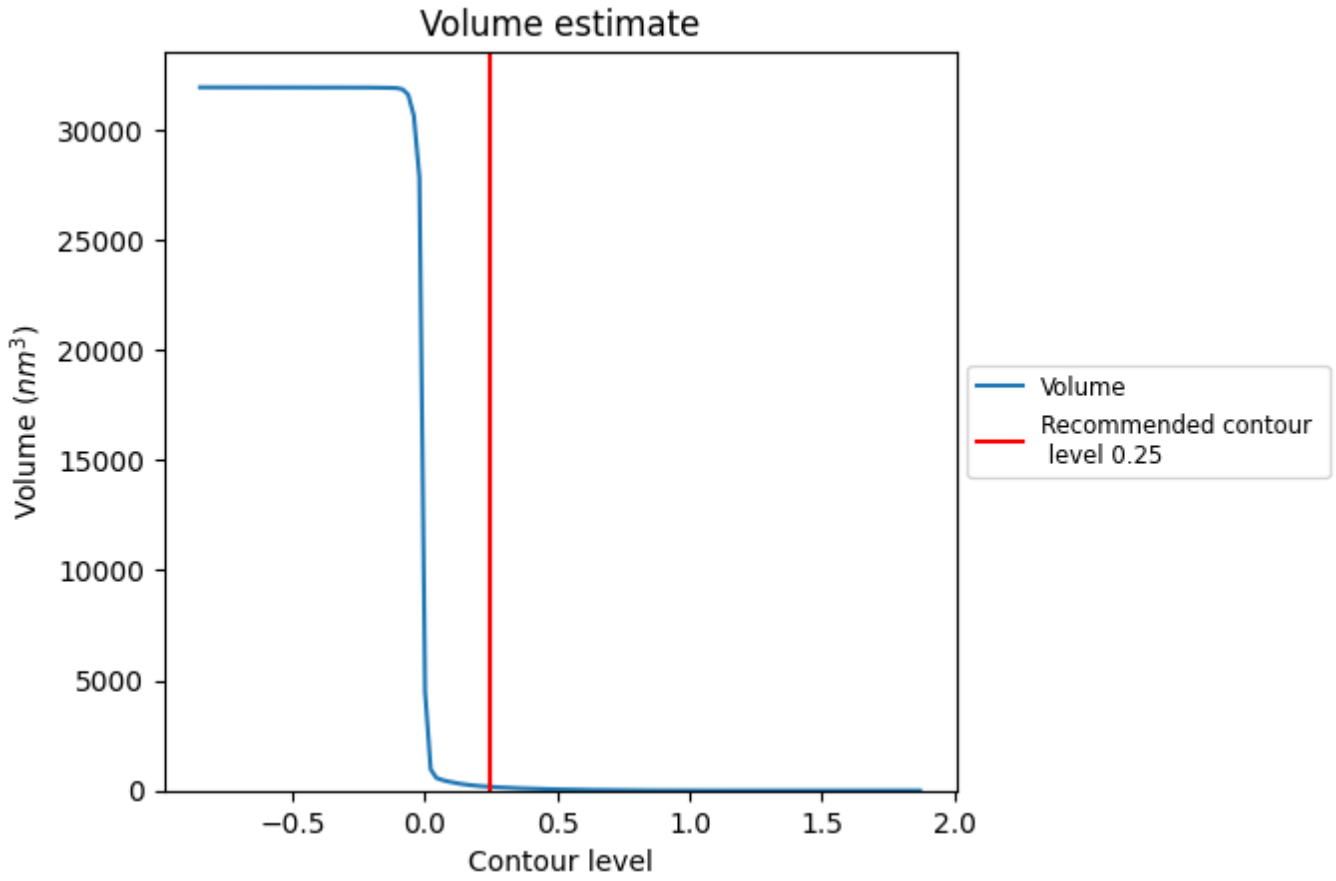
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

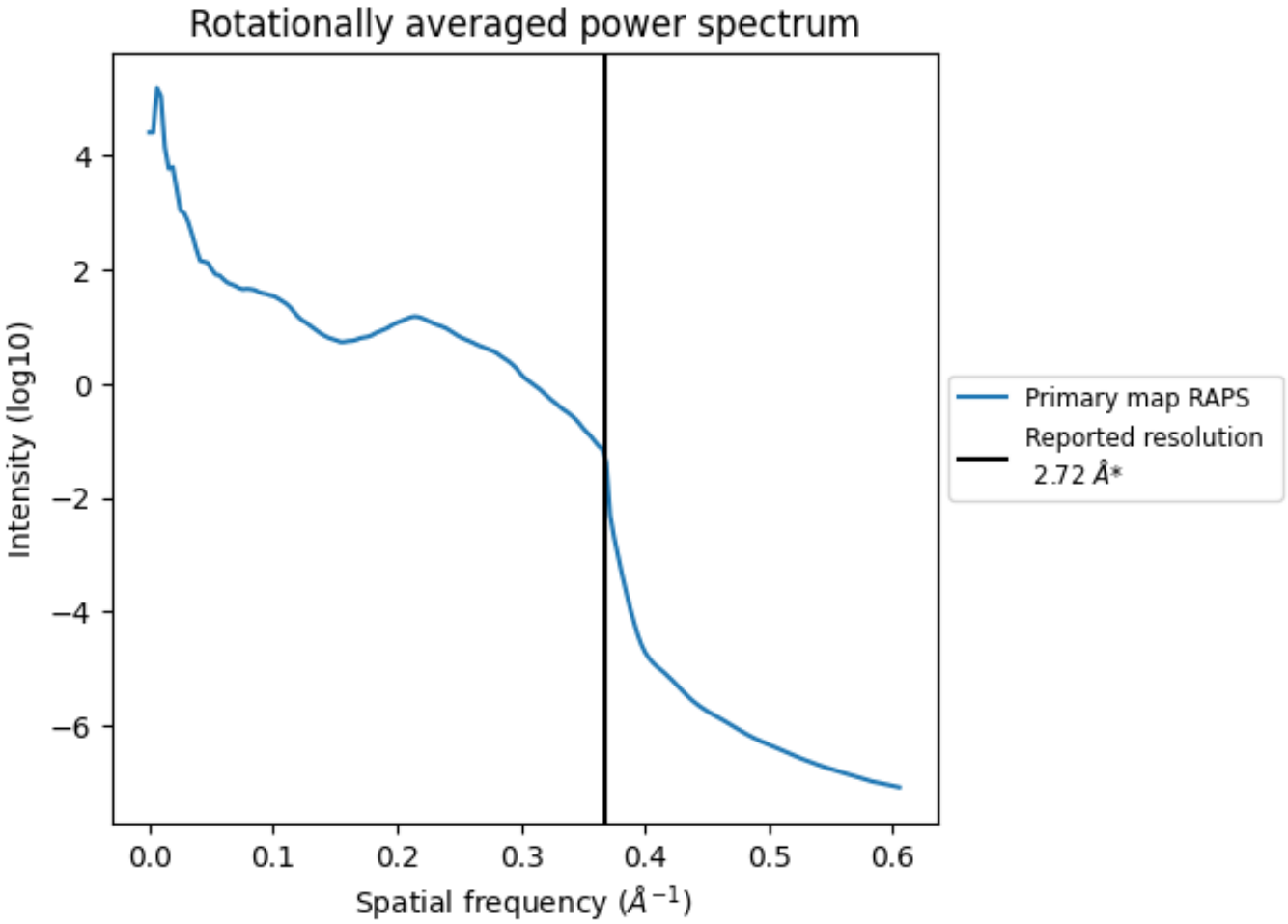
7.2 Volume estimate (i)



The volume at the recommended contour level is 168 nm^3; this corresponds to an approximate mass of 152 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

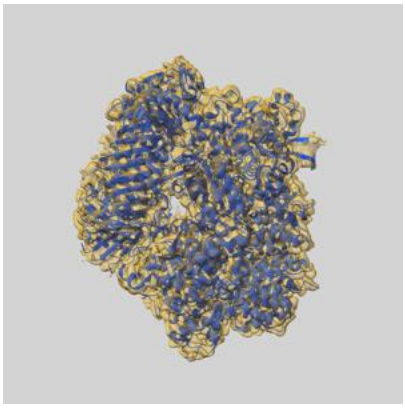
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

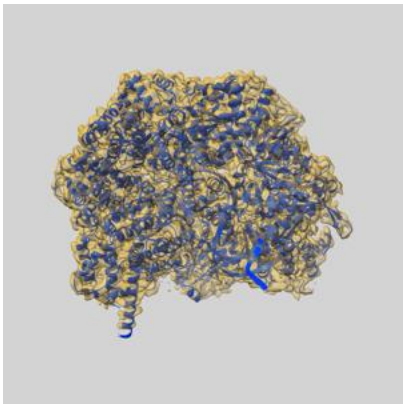
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25423 and PDB model 7STB. Per-residue inclusion information can be found in section 3 on page 9.

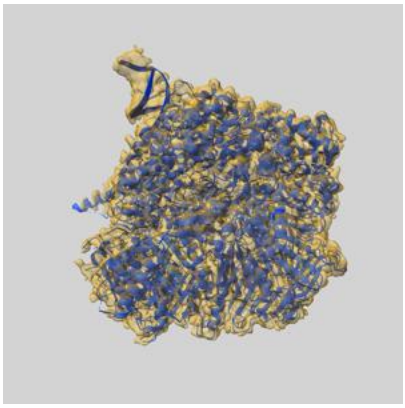
9.1 Map-model overlay



X



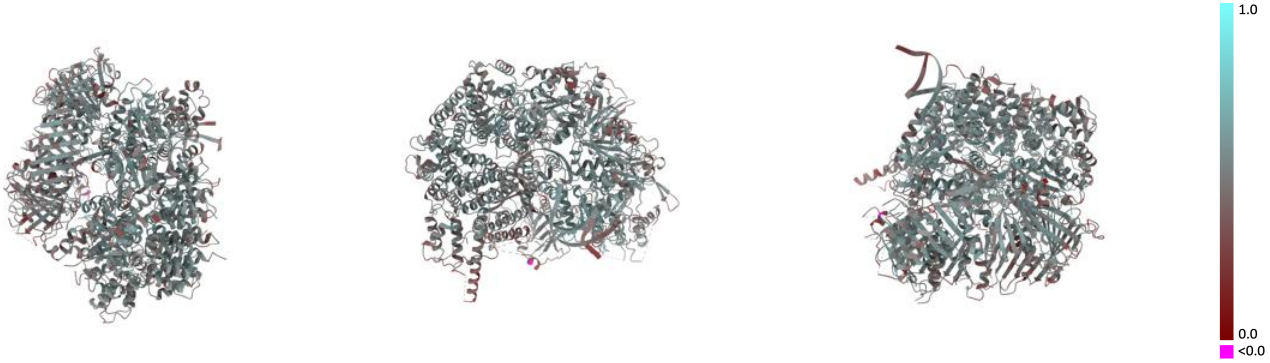
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

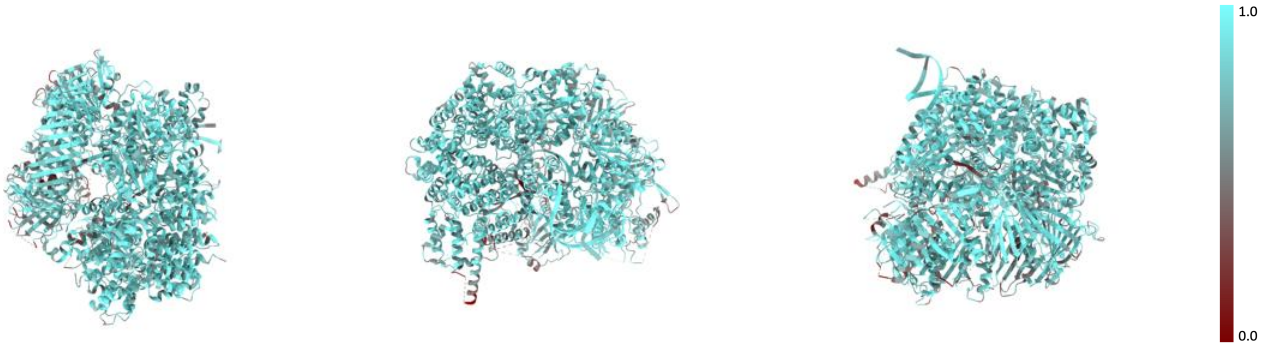
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

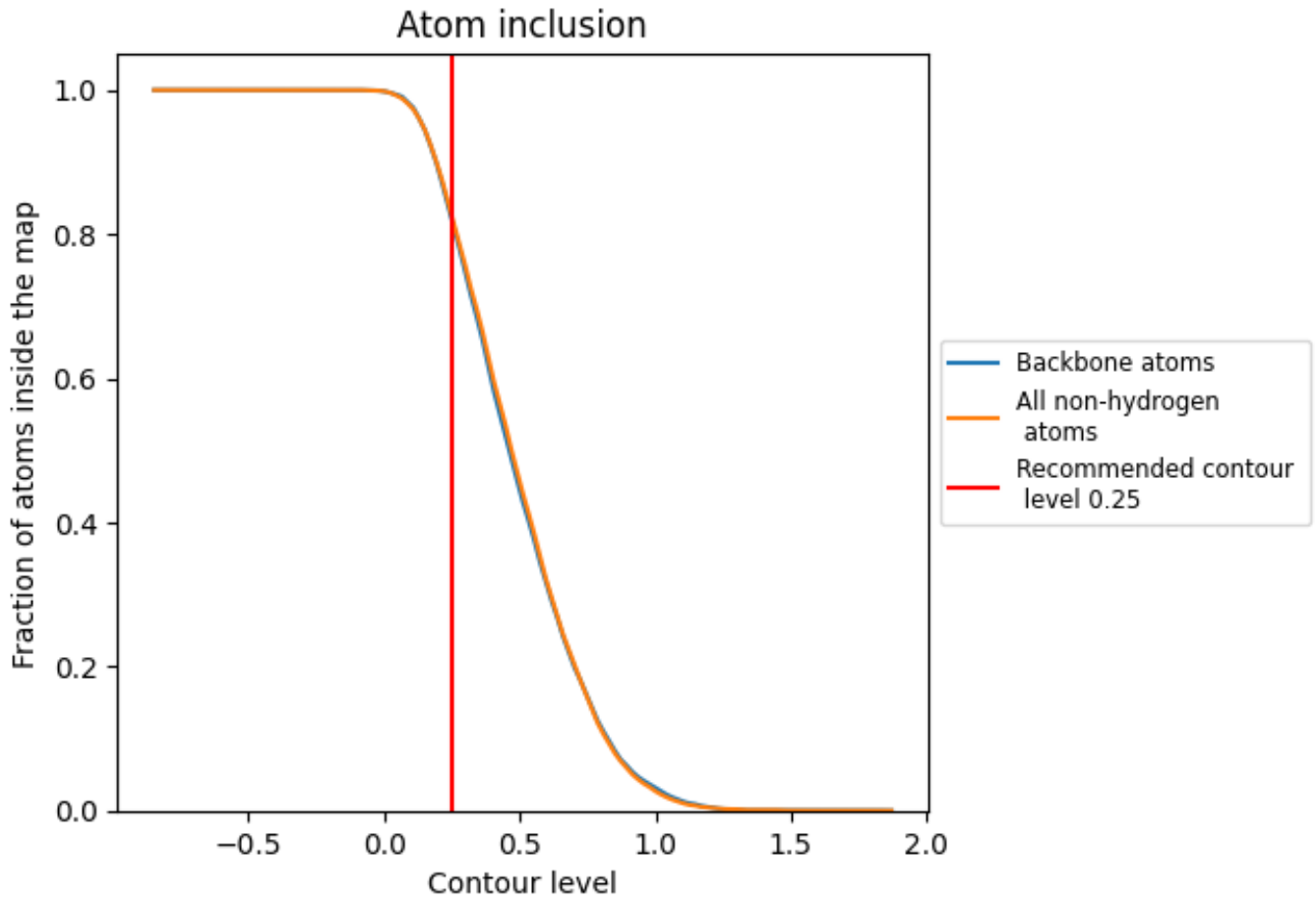
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 82% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8256	0.4930
A	0.8111	0.4890
B	0.8729	0.5130
C	0.8635	0.5070
D	0.8912	0.5210
E	0.8250	0.4860
F	0.7737	0.4560
G	0.8361	0.5120
H	0.7651	0.4630
I	0.8731	0.4470
J	0.7802	0.4790