WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Feb 4, 2024 – 03:38 PM EST

PDB ID	:	8DQW
EMDB ID	:	EMD-27662
Title	:	Open state of Rad24-RFC:9-1-1 bound to a 5' ss/dsDNA junction
Authors	:	Schrecker, M.; Hite, R.K.
Deposited on	:	2022-07-20
Resolution	:	2.10 Å(reported)
Based on initial model	:	7ST9

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 (i) 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 (i)) were used in the production of this report:

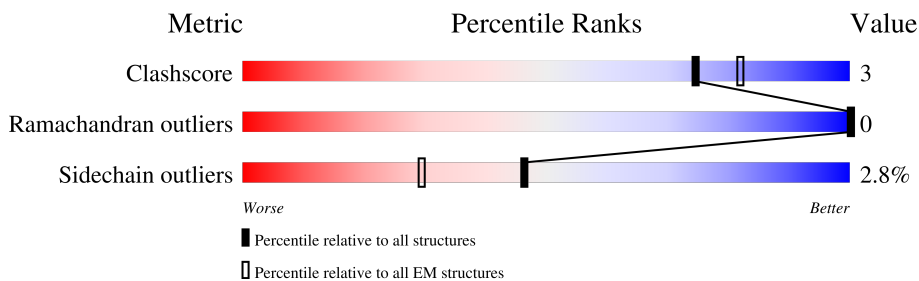|		
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.10 Å.

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

Metric	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		2.8%

Worse   *Better*

▌Percentile relative to all structures

▯Percentile relative to all EM structures

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	B	323	88% 10% •
2	C	340	89% 7% • •
3	D	353	90% 5% • 5%
4	E	354	89% 11%
5	F	401	67% 5% 27%
6	G	646	47% 5% 47%
7	H	474	56% 10% • 33%
8	A	696	5% 68% 7% 25%

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Mol	Chain	Length	Quality of chain
9	J	70	31% 64%
10	I	20	40% 10% 50%

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 46632 atoms, of which 23003 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 4.

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

- Molecule 2 is a protein called Replication factor C subunit 3.

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

- Molecule 3 is a protein called Replication factor C subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	335	Total 5318	C 1671	H 2672	N 457	O 508	S 10	0	0

- Molecule 4 is a protein called Replication factor C subunit 5.

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

- Molecule 5 is a protein called DNA damage checkpoint control protein RAD17.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	293	Total 4624	C 1475	H 2308	N 375	O 454	S 12	0	0

- Molecule 6 is a protein called DDC1 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	340	Total 5440	C 1745	H 2710	N 450	O 521	S 14	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-33	MET	-	initiating methionine	UNP A0A8H4BUG7
G	-32	ASP	-	expression tag	UNP A0A8H4BUG7
G	-31	TYR	-	expression tag	UNP A0A8H4BUG7
G	-30	LYS	-	expression tag	UNP A0A8H4BUG7
G	-29	ASP	-	expression tag	UNP A0A8H4BUG7
G	-28	ASP	-	expression tag	UNP A0A8H4BUG7
G	-27	ASP	-	expression tag	UNP A0A8H4BUG7
G	-26	ASP	-	expression tag	UNP A0A8H4BUG7
G	-25	LYS	-	expression tag	UNP A0A8H4BUG7
G	-24	ASP	-	expression tag	UNP A0A8H4BUG7
G	-23	TYR	-	expression tag	UNP A0A8H4BUG7
G	-22	LYS	-	expression tag	UNP A0A8H4BUG7
G	-21	ASP	-	expression tag	UNP A0A8H4BUG7
G	-20	ASP	-	expression tag	UNP A0A8H4BUG7
G	-19	ASP	-	expression tag	UNP A0A8H4BUG7
G	-18	ASP	-	expression tag	UNP A0A8H4BUG7
G	-17	LYS	-	expression tag	UNP A0A8H4BUG7
G	-16	ASP	-	expression tag	UNP A0A8H4BUG7
G	-15	TYR	-	expression tag	UNP A0A8H4BUG7
G	-14	LYS	-	expression tag	UNP A0A8H4BUG7
G	-13	ASP	-	expression tag	UNP A0A8H4BUG7
G	-12	ASP	-	expression tag	UNP A0A8H4BUG7
G	-11	ASP	-	expression tag	UNP A0A8H4BUG7
G	-10	ASP	-	expression tag	UNP A0A8H4BUG7
G	-9	LYS	-	expression tag	UNP A0A8H4BUG7
G	-8	LEU	-	expression tag	UNP A0A8H4BUG7
G	-7	GLU	-	expression tag	UNP A0A8H4BUG7
G	-6	VAL	-	expression tag	UNP A0A8H4BUG7
G	-5	LEU	-	expression tag	UNP A0A8H4BUG7
G	-4	PHE	-	expression tag	UNP A0A8H4BUG7
G	-3	GLN	-	expression tag	UNP A0A8H4BUG7
G	-2	GLY	-	expression tag	UNP A0A8H4BUG7
G	-1	PRO	-	expression tag	UNP A0A8H4BUG7
G	0	GLY	-	expression tag	UNP A0A8H4BUG7

- Molecule 7 is a protein called DNA damage checkpoint control protein MEC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	H	316	5057	1599	2537	437	463	21	0	0

- Molecule 8 is a protein called RAD24 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	A	522	8507	2706	4234	741	804	22	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	660	GLY	-	expression tag	UNP A0A8H8UM36
A	661	LEU	-	expression tag	UNP A0A8H8UM36
A	662	ASN	-	expression tag	UNP A0A8H8UM36
A	663	LEU	-	expression tag	UNP A0A8H8UM36
A	664	GLU	-	expression tag	UNP A0A8H8UM36
A	665	VAL	-	expression tag	UNP A0A8H8UM36
A	666	LEU	-	expression tag	UNP A0A8H8UM36
A	667	PHE	-	expression tag	UNP A0A8H8UM36
A	668	GLN	-	expression tag	UNP A0A8H8UM36
A	669	GLY	-	expression tag	UNP A0A8H8UM36
A	670	PRO	-	expression tag	UNP A0A8H8UM36
A	671	GLY	-	expression tag	UNP A0A8H8UM36
A	672	GLY	-	expression tag	UNP A0A8H8UM36
A	673	ASP	-	expression tag	UNP A0A8H8UM36
A	674	TYR	-	expression tag	UNP A0A8H8UM36
A	675	LYS	-	expression tag	UNP A0A8H8UM36
A	676	ASP	-	expression tag	UNP A0A8H8UM36
A	677	ASP	-	expression tag	UNP A0A8H8UM36
A	678	ASP	-	expression tag	UNP A0A8H8UM36
A	679	ASP	-	expression tag	UNP A0A8H8UM36
A	680	LYS	-	expression tag	UNP A0A8H8UM36
A	681	ASP	-	expression tag	UNP A0A8H8UM36
A	682	TYR	-	expression tag	UNP A0A8H8UM36
A	683	LYS	-	expression tag	UNP A0A8H8UM36
A	684	ASP	-	expression tag	UNP A0A8H8UM36
A	685	ASP	-	expression tag	UNP A0A8H8UM36
A	686	ASP	-	expression tag	UNP A0A8H8UM36
A	687	ASP	-	expression tag	UNP A0A8H8UM36
A	688	LYS	-	expression tag	UNP A0A8H8UM36
A	689	ASP	-	expression tag	UNP A0A8H8UM36
A	690	TYR	-	expression tag	UNP A0A8H8UM36
A	691	LYS	-	expression tag	UNP A0A8H8UM36
A	692	ASP	-	expression tag	UNP A0A8H8UM36
A	693	ASP	-	expression tag	UNP A0A8H8UM36
A	694	ASP	-	expression tag	UNP A0A8H8UM36
A	695	ASP	-	expression tag	UNP A0A8H8UM36
A	696	LYS	-	expression tag	UNP A0A8H8UM36

- 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*TP*CP*CP*CP*TP*TP*CP*C) -3').

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
10	I	10	309	94	113	29	63	10	0	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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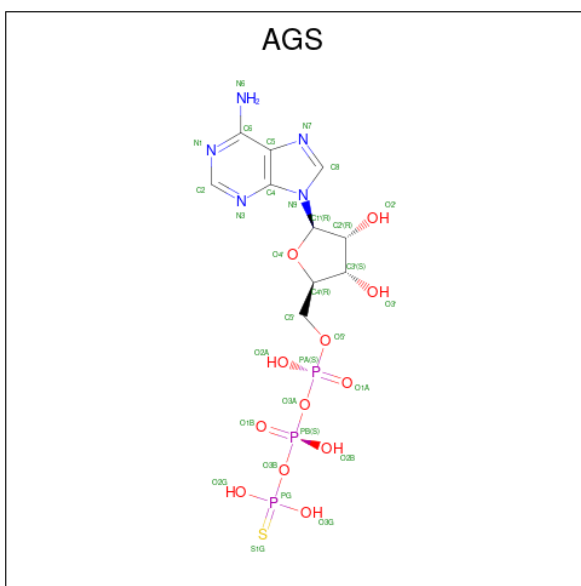
Mol	Chain	Residues	Atoms							AltConf
12	B	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	
12	C	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	
12	D	1	Total	C	H	N	O	P	S	0
			45	10	14	5	12	3	1	
12	A	1	Total	C	H	N	O	P	S	0
			44	10	13	5	12	3	1	

- Molecule 13 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
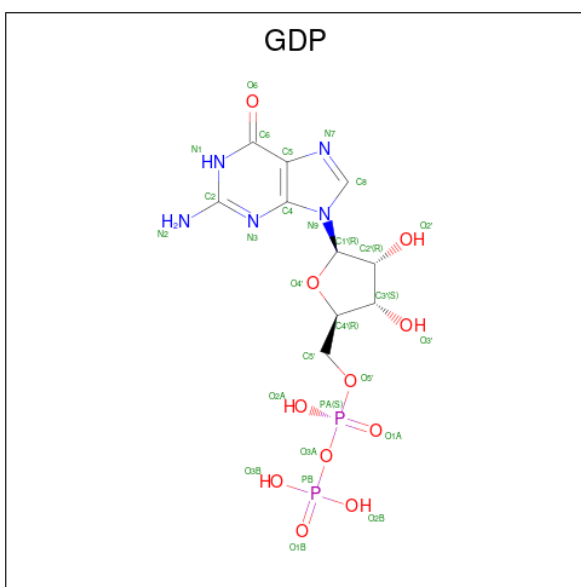
Mol	Chain	Residues	Atoms						AltConf
13	E	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
14	B	53	Total	O	0
			53	53	
14	C	79	Total	O	0
			79	79	
14	D	106	Total	O	0
			106	106	
14	E	55	Total	O	0
			55	55	

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Mol	Chain	Residues	Atoms		AltConf
14	F	21	Total 21	O 21	0
14	G	29	Total 29	O 29	0
14	H	4	Total 4	O 4	0
14	A	64	Total 64	O 64	0
14	J	15	Total 15	O 15	0
14	I	3	Total 3	O 3	0

3　Residue-property plots ⓘ

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

• Molecule 1: Replication factor C subunit 4

Chain B:

• Molecule 2: Replication factor C subunit 3

Chain C:

• Molecule 3: Replication factor C subunit 2

Chain D:

• Molecule 4: Replication factor C subunit 5

Chain E:

• Molecule 5: DNA damage checkpoint control protein RAD17

Chain F:

67% 5% 27%

• Molecule 6: DDC1 isoform 1

Chain G:

47% 5% 47%

• Molecule 7: DNA damage checkpoint control protein MEC3

Chain H:

56% 10% 33%

F205 M224 L230 Y256 I262 H263 L264 K268 K269 LYS GLU HIS GLY ASN GLU GLY D277 D278 L300 D301 I304 GLN ARG GLN GLU GLY LEU THR ASP ASN PRO SER GLN ASN GLN HIS ILE ASP THR ASP GLY ARG GLN GLU GLY GLY SER LEU PRO ILE ILE GLU ALA

ASP LYS PRO MET SER SER LEU TYR THR ASN THR ARG ASP ARG GLU MET GLU GLU ASN ILE ARG TYR ASP GLU ASP LEU LEU ARG ILE GLU GLU ASP SER SER ILE ALA ASP THR ARG GLY ASN ILE TYR THR ALA ASP SER THR SER GLY ASP THR PHE ASN D390 V393 Q400 S403

S404 T405 H406 E407 K420 F425 A431 I432 E436 S437 C438 V439 F440 R446 G447 S448 LEU GLU ASP SER SER GLU ASP VAL GLU K457 E460 I464 L474

● Molecule 8: RAD24 isoform 1

Chain A:

5%
68% 7% 25%

MET ASP SER THR ASN LEU ASN LYS ARG PRO LEU LEU GLN TYR SER LEU SER SER LEU GLY SER GLN ILE THR LYS TRP SER SER SER ARG PRO THR SER PRO VAL ARG LYS ALA ARG SER THR GLU ASN ASP PHE LEU SER LYS GLN ASP THR SER SER ILE LEU PRO SER ILE ASN ASP

ASP GLY G63 E64 Y67 K101 L107 S114 K115 S116 I119 K124 N135 M163 E168 E187 T224 E227 I228 P229 E230 N231 D232 N233 N234 Y242 T243 F244 P258 L273 K274 K278 M285 A305 Q306 T323 I337 S338 Y339

D356 L363 S367 N368 L370 E382 C403 N409 E415 G420 K426 R429 F443 P444 E461 D462 K507 N508 L509 PRO SER GLY SER SER GLY PRO LYS GLN THR MET D521 K522 F523 S524 D525 I526 M527 D534 S547 VAL GLU ASP GLY LEU ALA

PRO LEU MET ASP ASN ASP SER ASN ASN CYS D564 R573 R576 M579 E585 R586 N587 V588 M589 M590 A591 N592 D593 D594 L595 E596 D597 E598 E599 T600 S601 F602 N603 D604 D605 D609 S610 D611 SER ASP ASN SER ASN ASN ILE GLY ASN GLU THR PHE GLY ARG SER ASP GLU

ASP GLU SER LEU CYS GLU ILE LEU SER GLN ARG GLN PRO ARG LYS ALA PRO VAL ILE LEU SER GLU SER LEU ASP SER ASP LEU GLU ILE LEU GLY LEU ASN LEU GLU VAL LEU PHE GLY GLY PRO GLY GLY ASP TYR LYS ASP ASP ASP ASP LYS ASP ASP ASP ASP LYS

ASP TYR LYS ASP ASP ASP LYS

● Molecule 9: DNA (50-MER)

Chain J:

31% 64%

DG DG DA DC DG DA DG DT DC DA G11 T21 T22 T23 T24 T25 T33 T34 T35 DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT

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

Chain I:

40% 10% 50%

C1 T7 T8 C9 C10 DT DG DA DC DT DC DG DT DC DC

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	938420	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 $(e^-/\text{Å}^2)$	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.112	Depositor
Minimum map value	-0.758	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.050	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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	B	0.25	0/2507	0.48	0/3381
2	C	0.24	0/2625	0.47	0/3551
3	D	0.24	0/2691	0.46	0/3640
4	E	0.24	0/2832	0.48	0/3826
5	F	0.25	0/2352	0.48	0/3168
6	G	0.24	0/2782	0.45	0/3768
7	H	0.24	0/2564	0.49	0/3459
8	A	0.24	0/4359	0.45	0/5873
9	J	0.53	0/572	1.07	0/883
10	I	0.50	0/216	0.95	0/329
All	All	0.26	0/23500	0.50	0/31878

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	B	2472	2555	2555	18	0
2	C	2585	2611	2611	15	0
3	D	2646	2672	2672	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	2792	2906	2906	25	0
5	F	2316	2308	2308	13	0
6	G	2730	2710	2712	19	0
7	H	2520	2537	2537	27	0
8	A	4273	4234	4233	29	0
9	J	514	290	291	2	0
10	I	196	113	114	1	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
12	A	31	13	12	3	0
12	B	31	14	12	0	0
12	C	31	14	12	0	0
12	D	31	14	12	0	0
13	E	28	12	11	1	0
14	A	64	0	0	6	0
14	B	53	0	0	2	0
14	C	79	0	0	2	0
14	D	106	0	0	3	0
14	E	55	0	0	2	0
14	F	21	0	0	1	0
14	G	29	0	0	3	0
14	H	4	0	0	0	0
14	I	3	0	0	0	0
14	J	15	0	0	1	0
All	All	23629	23003	22998	147	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 (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:100:GLU:OE1	14:D:501:HOH:O	1.98	0.82
12:A:901:AGS:O2B	14:A:1001:HOH:O	1.98	0.80
6:G:234:SER:OG	6:G:347:ASP:O	2.01	0.79
5:F:238:ASP:OD1	14:F:501:HOH:O	2.03	0.77
6:G:65:GLU:OE2	14:G:701:HOH:O	2.03	0.76
6:G:1:MET:O	14:G:701:HOH:O	2.02	0.75
8:A:224:THR:OG1	12:A:901:AGS:O3G	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:100:GLU:OE2	14:D:502:HOH:O	2.05	0.74
7:H:20:ARG:NH1	7:H:108:ASP:OD2	2.20	0.74
8:A:116:SER:OG	14:A:1002:HOH:O	2.05	0.73
7:H:446:ARG:NH1	7:H:460:GLU:O	2.21	0.73
1:B:87:ASP:OD2	14:B:501:HOH:O	2.06	0.72
3:D:338:ASN:OD1	4:E:301:LYS:NZ	2.22	0.71
6:G:325:LYS:NZ	8:A:168:GLU:OE2	2.24	0.70
12:A:901:AGS:O2G	14:A:1001:HOH:O	2.10	0.70
8:A:415:GLU:OE2	14:A:1003:HOH:O	2.10	0.69
2:C:207:ARG:NH1	14:C:502:HOH:O	2.23	0.69
7:H:98:ASP:OD1	7:H:99:SER:N	2.26	0.68
2:C:124:ASN:ND2	14:C:503:HOH:O	2.26	0.68
8:A:163:MET:O	14:A:1004:HOH:O	2.12	0.67
1:B:187:THR:OG1	1:B:189:ASP:OD1	2.06	0.67
8:A:461:GLU:OE1	8:A:573:ARG:NH1	2.28	0.67
1:B:128:ARG:NH1	14:B:502:HOH:O	2.29	0.66
7:H:20:ARG:HD2	7:H:23:ILE:HD11	1.77	0.65
2:C:218:THR:OG1	2:C:235:CYS:SG	2.53	0.65
6:G:29:ASP:OD1	14:G:702:HOH:O	2.15	0.64
8:A:523:PHE:HB3	8:A:526:ILE:HD12	1.79	0.63
8:A:363:LEU:O	8:A:367:SER:OG	2.11	0.63
8:A:228:ILE:HD11	8:A:244:PHE:HB2	1.81	0.63
6:G:21:TYR:O	6:G:25:THR:HG23	1.98	0.62
3:D:236:GLN:NE2	14:D:504:HOH:O	2.35	0.59
4:E:286:LEU:HD11	4:E:346:ILE:HD12	1.85	0.59
8:A:527:MET:SD	8:A:527:MET:N	2.74	0.59
9:J:21:DT:H71	9:J:22:DT:N3	2.17	0.58
7:H:38:ASN:OD1	7:H:39:SER:N	2.37	0.58
1:B:149:LYS:NZ	8:A:230:GLU:O	2.36	0.58
6:G:276:ASP:N	6:G:276:ASP:OD1	2.37	0.57
2:C:39:LYS:N	2:C:39:LYS:HD3	2.20	0.57
6:G:269:ALA:HB2	6:G:281:ALA:HB2	1.87	0.56
6:G:81:ILE:HD12	6:G:91:LEU:HD11	1.88	0.56
5:F:119:LEU:HD21	5:F:121:PHE:CE1	2.41	0.55
7:H:230:LEU:HD11	7:H:431:ALA:HB1	1.87	0.55
1:B:246:GLU:HA	1:B:246:GLU:OE1	2.06	0.55
1:B:13:GLU:HG3	2:C:138:THR:HG21	1.89	0.55
6:G:50:THR:HG21	6:G:328:ASP:OD2	2.06	0.55
5:F:323:GLU:OE2	6:G:133:ARG:NH1	2.38	0.54
2:C:217:ALA:O	3:D:51:LYS:HE2	2.08	0.54
8:A:356:ASP:OD2	8:A:429:ARG:NE	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:THR:HG23	2:C:39:LYS:HE2	1.91	0.53
1:B:287:GLU:HB3	1:B:319:LEU:HD22	1.89	0.53
8:A:369:ASN:OD1	8:A:370:LEU:N	2.41	0.53
4:E:70:ILE:HD11	4:E:86:ASN:HB3	1.90	0.52
4:E:258:ASP:N	4:E:258:ASP:OD1	2.42	0.52
3:D:219:ARG:NH1	3:D:257:GLU:OE2	2.43	0.52
6:G:169:ARG:NH2	6:G:224:ALA:O	2.42	0.52
6:G:241:LEU:HD22	6:G:326:LEU:HD11	1.91	0.51
7:H:43:THR:HG22	7:H:45:ILE:CD1	2.41	0.51
4:E:131:LEU:HD11	7:H:436:GLU:O	2.11	0.51
6:G:28:ASP:OD1	6:G:29:ASP:N	2.43	0.51
7:H:230:LEU:HD12	7:H:432:ILE:O	2.11	0.51
4:E:73:ARG:NH1	4:E:112:LEU:HD13	2.26	0.50
1:B:317:HIS:CE1	2:C:293:GLU:OE1	2.63	0.50
2:C:119:ALA:HB3	2:C:145:VAL:HG13	1.94	0.50
4:E:30:SER:OG	4:E:56:LEU:HD12	2.12	0.49
1:B:47:ILE:HD13	1:B:161:LEU:HB2	1.93	0.49
7:H:400:GLN:NE2	7:H:405:THR:O	2.45	0.49
3:D:227:ASP:OD2	4:E:183:SER:OG	2.26	0.49
5:F:78:ASP:OD2	5:F:78:ASP:C	2.51	0.49
3:D:194:ALA:HA	3:D:221:LEU:HD13	1.95	0.49
5:F:64:ARG:NH2	5:F:70:TYR:O	2.46	0.49
1:B:267:VAL:HG11	1:B:299:ILE:HD12	1.96	0.48
7:H:262:ILE:HD12	7:H:264:LEU:HD21	1.94	0.48
5:F:21:ILE:O	5:F:25:LEU:HD23	2.14	0.48
8:A:187:GLU:OE2	14:A:1001:HOH:O	2.20	0.48
5:F:95:VAL:HG11	7:H:256:TYR:CE2	2.48	0.48
8:A:382:GLU:OE1	8:A:444:PRO:HA	2.14	0.48
4:E:122:VAL:O	7:H:65:THR:HG21	2.15	0.47
7:H:269:LYS:N	7:H:278:ASP:O	2.41	0.47
2:C:86:ASP:OD1	3:D:111:LYS:NZ	2.47	0.47
6:G:76:ASN:OD1	6:G:76:ASN:N	2.46	0.47
3:D:24:GLN:HG2	7:H:393:VAL:HG11	1.96	0.47
6:G:277:LEU:HD21	6:G:280:ASN:OD1	2.14	0.47
8:A:337:ILE:HD11	8:A:363:LEU:HD11	1.96	0.47
3:D:24:GLN:HE21	4:E:34:ARG:HD3	1.80	0.47
7:H:15:ASP:HB3	7:H:76:VAL:HG13	1.96	0.47
4:E:8:TYR:OH	4:E:209:GLU:OE1	2.24	0.46
4:E:221:ARG:HH11	4:E:221:ARG:HG2	1.80	0.46
8:A:273:LEU:HD23	8:A:305:ALA:HA	1.97	0.46
1:B:287:GLU:CB	1:B:319:LEU:HD22	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:232:VAL:O	4:E:236:MET:HG3	2.16	0.46
4:E:309:ASP:OD1	14:E:501:HOH:O	2.21	0.46
8:A:274:LYS:O	8:A:278:LYS:HG3	2.15	0.46
5:F:153:SER:N	5:F:259:MET:O	2.46	0.46
4:E:301:LYS:NZ	14:E:503:HOH:O	2.38	0.46
8:A:101:LYS:NZ	8:A:258:PRO:O	2.47	0.46
7:H:21:THR:O	7:H:25:THR:HG23	2.16	0.46
5:F:106:CYS:HG	5:F:121:PHE:HE1	1.62	0.45
2:C:256:TRP:NE1	3:D:320:ASN:OD1	2.42	0.45
7:H:425:PHE:CZ	7:H:464:ILE:HD12	2.52	0.45
10:I:7:DT:H2'	10:I:8:DT:H72	1.99	0.45
2:C:68:ARG:O	2:C:72:GLY:N	2.50	0.44
3:D:116:LEU:HD11	5:F:133:SER:HB3	2.00	0.44
1:B:277:LEU:O	1:B:285:ARG:NH1	2.45	0.44
5:F:35:ASP:H	5:F:86:ILE:HG22	1.82	0.44
7:H:390:ASP:OD1	7:H:390:ASP:N	2.51	0.44
7:H:50:SER:OG	7:H:94:GLU:OE2	2.36	0.43
4:E:17:SER:OG	13:E:401:GDP:N1	2.50	0.43
8:A:107:LEU:HD11	8:A:119:ILE:HD11	2.00	0.43
8:A:242:TYR:OH	8:A:369:ASN:O	2.19	0.43
1:B:232:HIS:N	1:B:233:PRO:CD	2.81	0.43
8:A:339:TYR:HA	8:A:370:LEU:HD21	1.99	0.43
2:C:120:ASP:N	2:C:120:ASP:OD1	2.51	0.43
8:A:403:CYS:SG	8:A:420:GLY:HA2	2.59	0.43
1:B:100:LYS:NZ	6:G:76:ASN:OD1	2.52	0.43
1:B:20:LEU:HA	1:B:23:ILE:HD12	2.01	0.42
1:B:267:VAL:HG11	1:B:299:ILE:CD1	2.48	0.42
1:B:67:LEU:HD13	1:B:75:VAL:HG23	2.02	0.42
7:H:43:THR:HG22	7:H:45:ILE:HD11	2.00	0.42
4:E:123:ASP:OD2	4:E:124:PHE:N	2.53	0.42
2:C:146:LEU:HD12	2:C:146:LEU:N	2.34	0.42
8:A:306:GLN:HA	8:A:306:GLN:OE1	2.20	0.42
7:H:22:THR:HG23	7:H:70:CYS:SG	2.59	0.42
1:B:61:CYS:O	1:B:65:GLU:HG3	2.19	0.42
5:F:223:ASP:OD1	5:F:226:THR:HG22	2.19	0.42
6:G:226:GLU:OE1	6:G:355:HIS:NE2	2.53	0.42
7:H:45:ILE:HD12	7:H:69:TRP:CE3	2.55	0.42
4:E:101:MET:HG3	4:E:108:VAL:HG21	2.01	0.42
4:E:277:ASN:O	4:E:281:GLU:HG3	2.20	0.42
2:C:171:GLN:NE2	2:C:175:GLU:OE2	2.52	0.41
4:E:105:ASP:N	4:E:105:ASP:OD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:323:THR:O	8:A:323:THR:HG22	2.20	0.41
4:E:83:LEU:C	4:E:83:LEU:HD12	2.41	0.41
7:H:159:THR:HG21	7:H:202:MET:CE	2.50	0.41
6:G:45:ASN:CG	6:G:50:THR:HG22	2.41	0.41
3:D:153:LEU:O	3:D:157:MET:HG3	2.20	0.41
7:H:224:MET:HE3	7:H:224:MET:O	2.21	0.41
7:H:3:LEU:HD23	7:H:82:VAL:HG22	2.03	0.41
8:A:228:ILE:HD12	8:A:228:ILE:N	2.36	0.41
4:E:280:ILE:N	4:E:280:ILE:HD13	2.36	0.41
8:A:443:PHE:CD1	8:A:444:PRO:HD2	2.56	0.41
9:J:33:DT:OP2	14:J:101:HOH:O	2.22	0.41
4:E:140:ILE:HB	4:E:169:MET:HG2	2.03	0.40
4:E:138:VAL:HG21	4:E:165:ILE:HD11	2.04	0.40
7:H:3:LEU:HD21	7:H:91:ILE:HD12	2.03	0.40
8:A:462:ASP:OD2	8:A:576:ARG:NH1	2.55	0.40
4:E:283:ARG:NH1	8:A:382:GLU:HG2	2.37	0.40
5:F:29:THR:N	5:F:30:PRO:HD2	2.36	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	B	313/323 (97%)	306 (98%)	7 (2%)	0	100	100
2	C	325/340 (96%)	321 (99%)	4 (1%)	0	100	100
3	D	333/353 (94%)	330 (99%)	3 (1%)	0	100	100
4	E	352/354 (99%)	345 (98%)	7 (2%)	0	100	100
5	F	289/401 (72%)	285 (99%)	4 (1%)	0	100	100
6	G	332/646 (51%)	326 (98%)	6 (2%)	0	100	100
7	H	304/474 (64%)	303 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	A	516/696 (74%)	503 (98%)	13 (2%)	0	100	100
All	All	2764/3587 (77%)	2719 (98%)	45 (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	B	275/283 (97%)	269 (98%)	6 (2%)	52	57
2	C	283/296 (96%)	274 (97%)	9 (3%)	39	41
3	D	296/312 (95%)	289 (98%)	7 (2%)	49	53
4	E	323/324 (100%)	318 (98%)	5 (2%)	65	71
5	F	265/369 (72%)	259 (98%)	6 (2%)	50	55
6	G	313/592 (53%)	302 (96%)	11 (4%)	36	38
7	H	286/424 (68%)	273 (96%)	13 (4%)	27	27
8	A	482/645 (75%)	468 (97%)	14 (3%)	42	46
All	All	2523/3245 (78%)	2452 (97%)	71 (3%)	46	47

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	LYS
1	B	69	ARG
1	B	148	ASN
1	B	222	ASP
1	B	223	ASN
1	B	229	ASP
2	C	39	LYS
2	C	40	PHE
2	C	69	GLU
2	C	78	MET

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Mol	Chain	Res	Type
2	C	81	GLU
2	C	120	ASP
2	C	132	ARG
2	C	195	LYS
2	C	234	GLU
3	D	51	LYS
3	D	57	ASN
3	D	80	LYS
3	D	100	GLU
3	D	202	ARG
3	D	212	CYS
3	D	219	ARG
4	E	69	LYS
4	E	90	SER
4	E	204	ASP
4	E	309	ASP
4	E	352	CYS
5	F	52	ASN
5	F	78	ASP
5	F	82	LEU
5	F	155	GLU
5	F	224	SER
5	F	323	GLU
6	G	1	MET
6	G	9	GLU
6	G	29	ASP
6	G	48	ASP
6	G	75	GLU
6	G	106	ARG
6	G	107	LYS
6	G	168	ARG
6	G	250	ASP
6	G	370	LYS
6	G	379	SER
7	H	50	SER
7	H	126	MET
7	H	205	PHE
7	H	224	MET
7	H	268	LYS
7	H	300	LEU
7	H	301	ASP
7	H	403	SER

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Mol	Chain	Res	Type
7	H	407	GLU
7	H	420	LYS
7	H	438	CYS
7	H	440	PHE
7	H	446	ARG
8	A	64	GLU
8	A	67	TYR
8	A	114	SER
8	A	124	LYS
8	A	227	GLU
8	A	242	TYR
8	A	285	MET
8	A	409	ASN
8	A	426	LYS
8	A	523	PHE
8	A	527	MET
8	A	534	ASP
8	A	579	MET
8	A	593	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	GLN
1	B	60	HIS
1	B	155	GLN
1	B	250	GLN
1	B	317	HIS
2	C	124	ASN
2	C	140	ASN
3	D	24	GLN
3	D	236	GLN
3	D	317	ASN
4	E	227	ASN
4	E	336	ASN
5	F	79	HIS
6	G	57	GLN
6	G	132	ASN
7	H	57	ASN
8	A	77	GLN
8	A	298	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	AGS	C	402	11	26,33,33	3.62	12 (46%)	26,52,52	2.02	7 (26%)
12	AGS	A	901	11	26,33,33	3.62	12 (46%)	26,52,52	1.94	5 (19%)
13	GDP	E	401	-	24,30,30	3.69	13 (54%)	30,47,47	1.49	6 (20%)
12	AGS	B	402	11	26,33,33	3.63	12 (46%)	26,52,52	2.00	6 (23%)
12	AGS	D	402	11	26,33,33	3.64	12 (46%)	26,52,52	1.96	7 (26%)

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
12	AGS	C	402	11	-	2/17/38/38	0/3/3/3
12	AGS	A	901	11	-	7/17/38/38	0/3/3/3
13	GDP	E	401	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	AGS	B	402	11	-	<mark>3/17/38/38</mark>	0/3/3/3
12	AGS	D	402	11	-	<mark>4/17/38/38</mark>	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	402	AGS	C2'-C3'	-10.59	1.24	1.53
12	B	402	AGS	C2'-C3'	-10.51	1.24	1.53
12	C	402	AGS	C2'-C3'	-10.46	1.24	1.53
12	A	901	AGS	C2'-C3'	-10.46	1.24	1.53
13	E	401	GDP	C3'-C4'	-8.56	1.31	1.53
13	E	401	GDP	O4'-C4'	7.67	1.62	1.45
12	D	402	AGS	O4'-C1'	7.44	1.51	1.41
12	B	402	AGS	O4'-C1'	7.36	1.51	1.41
12	C	402	AGS	O4'-C1'	7.32	1.51	1.41
12	A	901	AGS	O4'-C1'	7.19	1.51	1.41
13	E	401	GDP	O4'-C1'	-7.08	1.31	1.41
12	A	901	AGS	O4'-C4'	-6.02	1.31	1.45
12	C	402	AGS	O4'-C4'	-6.01	1.31	1.45
12	D	402	AGS	O4'-C4'	-5.98	1.31	1.45
12	B	402	AGS	O4'-C4'	-5.97	1.31	1.45
13	E	401	GDP	C2-N3	5.52	1.46	1.33
12	A	901	AGS	C3'-C4'	5.52	1.67	1.53
12	B	402	AGS	C3'-C4'	5.51	1.67	1.53
12	C	402	AGS	C3'-C4'	5.51	1.67	1.53
12	D	402	AGS	C3'-C4'	5.50	1.67	1.53
12	A	901	AGS	C2'-C1'	5.05	1.61	1.53
12	D	402	AGS	C2'-C1'	5.01	1.61	1.53
13	E	401	GDP	C4-N3	5.00	1.49	1.37
12	B	402	AGS	C2'-C1'	5.00	1.61	1.53
12	C	402	AGS	C2'-C1'	4.92	1.61	1.53
13	E	401	GDP	C2-N2	4.76	1.45	1.34
12	D	402	AGS	PG-O3G	4.18	1.68	1.54
12	B	402	AGS	PG-O3G	4.17	1.68	1.54
12	C	402	AGS	PG-O3G	4.17	1.68	1.54
12	A	901	AGS	PG-O3G	4.16	1.68	1.54
13	E	401	GDP	C6-N1	3.86	1.43	1.37
12	B	402	AGS	PG-O2G	3.79	1.67	1.54
12	A	901	AGS	PG-O2G	3.76	1.67	1.54
12	C	402	AGS	PG-O2G	3.72	1.67	1.54
12	D	402	AGS	PG-O2G	3.70	1.66	1.54
12	C	402	AGS	C6-N6	3.64	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	901	AGS	C6-N6	3.64	1.47	1.34
12	B	402	AGS	C6-N6	3.61	1.47	1.34
12	D	402	AGS	C6-N6	3.61	1.47	1.34
13	E	401	GDP	C5-C6	3.20	1.53	1.47
12	B	402	AGS	C5-C4	-2.92	1.33	1.40
12	D	402	AGS	C5-C4	-2.92	1.33	1.40
12	A	901	AGS	C5-C4	-2.92	1.33	1.40
13	E	401	GDP	O3'-C3'	2.91	1.49	1.43
13	E	401	GDP	O2'-C2'	-2.91	1.36	1.43
12	C	402	AGS	C5-C4	-2.85	1.33	1.40
13	E	401	GDP	C2-N1	2.79	1.44	1.37
12	A	901	AGS	O3'-C3'	2.70	1.49	1.43
12	B	402	AGS	O3'-C3'	2.69	1.49	1.43
12	D	402	AGS	O3'-C3'	2.67	1.49	1.43
12	B	402	AGS	O2'-C2'	2.64	1.49	1.43
12	C	402	AGS	O2'-C2'	2.64	1.49	1.43
12	C	402	AGS	O3'-C3'	2.63	1.49	1.43
12	A	901	AGS	O2'-C2'	2.63	1.49	1.43
12	D	402	AGS	O2'-C2'	2.62	1.49	1.43
13	E	401	GDP	C5-C4	-2.50	1.36	1.43
12	A	901	AGS	PA-O5'	2.17	1.68	1.59
13	E	401	GDP	O6-C6	-2.15	1.18	1.23
12	B	402	AGS	PA-O5'	2.13	1.67	1.59
12	D	402	AGS	PA-O5'	2.10	1.67	1.59
12	C	402	AGS	PA-O5'	2.06	1.67	1.59

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	901	AGS	N3-C2-N1	-5.53	120.04	128.68
12	B	402	AGS	N3-C2-N1	-5.50	120.09	128.68
12	C	402	AGS	N3-C2-N1	-5.47	120.13	128.68
12	D	402	AGS	N3-C2-N1	-5.44	120.17	128.68
12	B	402	AGS	C1'-N9-C4	-4.35	118.99	126.64
12	C	402	AGS	C1'-N9-C4	-4.33	119.03	126.64
12	A	901	AGS	C1'-N9-C4	-4.05	119.53	126.64
12	D	402	AGS	C1'-N9-C4	-4.05	119.53	126.64
12	D	402	AGS	C5-C6-N6	3.94	126.35	120.35
12	A	901	AGS	C5-C6-N6	3.94	126.34	120.35
12	B	402	AGS	C5-C6-N6	3.94	126.34	120.35
12	C	402	AGS	C5-C6-N6	3.87	126.23	120.35
13	E	401	GDP	C5-C6-N1	3.35	119.86	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	401	GDP	C3'-C2'-C1'	3.18	105.77	100.98
12	C	402	AGS	C3'-C2'-C1'	3.09	105.63	100.98
13	E	401	GDP	C2-N1-C6	-2.90	119.76	125.10
13	E	401	GDP	C8-N7-C5	2.87	108.45	102.99
12	B	402	AGS	C3'-C2'-C1'	2.79	105.18	100.98
12	A	901	AGS	PA-O3A-PB	-2.66	123.69	132.83
12	D	402	AGS	PA-O3A-PB	-2.65	123.74	132.83
12	C	402	AGS	PA-O3A-PB	-2.63	123.81	132.83
12	B	402	AGS	PA-O3A-PB	-2.57	124.02	132.83
12	D	402	AGS	C3'-C2'-C1'	2.46	104.68	100.98
12	D	402	AGS	N6-C6-N1	-2.41	113.57	118.57
12	A	901	AGS	N6-C6-N1	-2.39	113.62	118.57
12	B	402	AGS	N6-C6-N1	-2.36	113.68	118.57
13	E	401	GDP	PA-O3A-PB	-2.29	124.97	132.83
12	C	402	AGS	N6-C6-N1	-2.27	113.86	118.57
13	E	401	GDP	O6-C6-C5	-2.22	120.04	124.37
12	C	402	AGS	C2'-C3'-C4'	2.08	106.68	102.64
12	D	402	AGS	O4'-C1'-C2'	-2.00	104.00	106.93

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	901	AGS	C5'-O5'-PA-O1A
12	A	901	AGS	C5'-O5'-PA-O2A
12	A	901	AGS	O4'-C4'-C5'-O5'
12	A	901	AGS	C3'-C4'-C5'-O5'
12	B	402	AGS	C5'-O5'-PA-O3A
12	D	402	AGS	C5'-O5'-PA-O3A
12	B	402	AGS	C5'-O5'-PA-O1A
12	D	402	AGS	C5'-O5'-PA-O1A
12	C	402	AGS	PA-O3A-PB-O2B
13	E	401	GDP	PB-O3A-PA-O2A
12	A	901	AGS	PG-O3B-PB-O2B
12	D	402	AGS	PA-O3A-PB-O1B
12	A	901	AGS	PA-O3A-PB-O1B
12	A	901	AGS	C5'-O5'-PA-O3A
13	E	401	GDP	O4'-C4'-C5'-O5'
12	B	402	AGS	PA-O3A-PB-O2B
12	C	402	AGS	PA-O3A-PB-O1B
12	D	402	AGS	PA-O3A-PB-O2B
13	E	401	GDP	PB-O3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	901	AGS	3	0
13	E	401	GDP	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 A 901

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP E 401

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
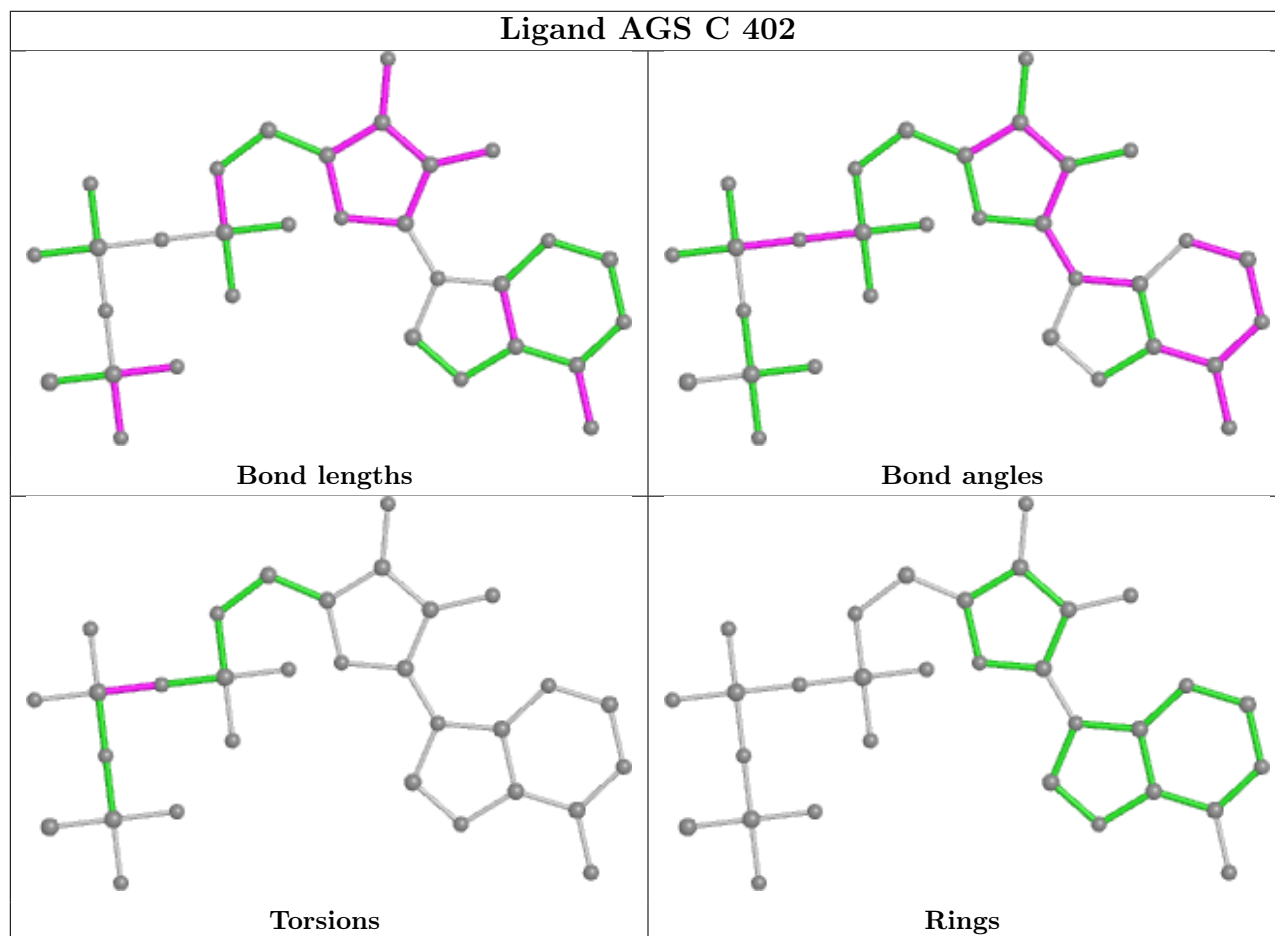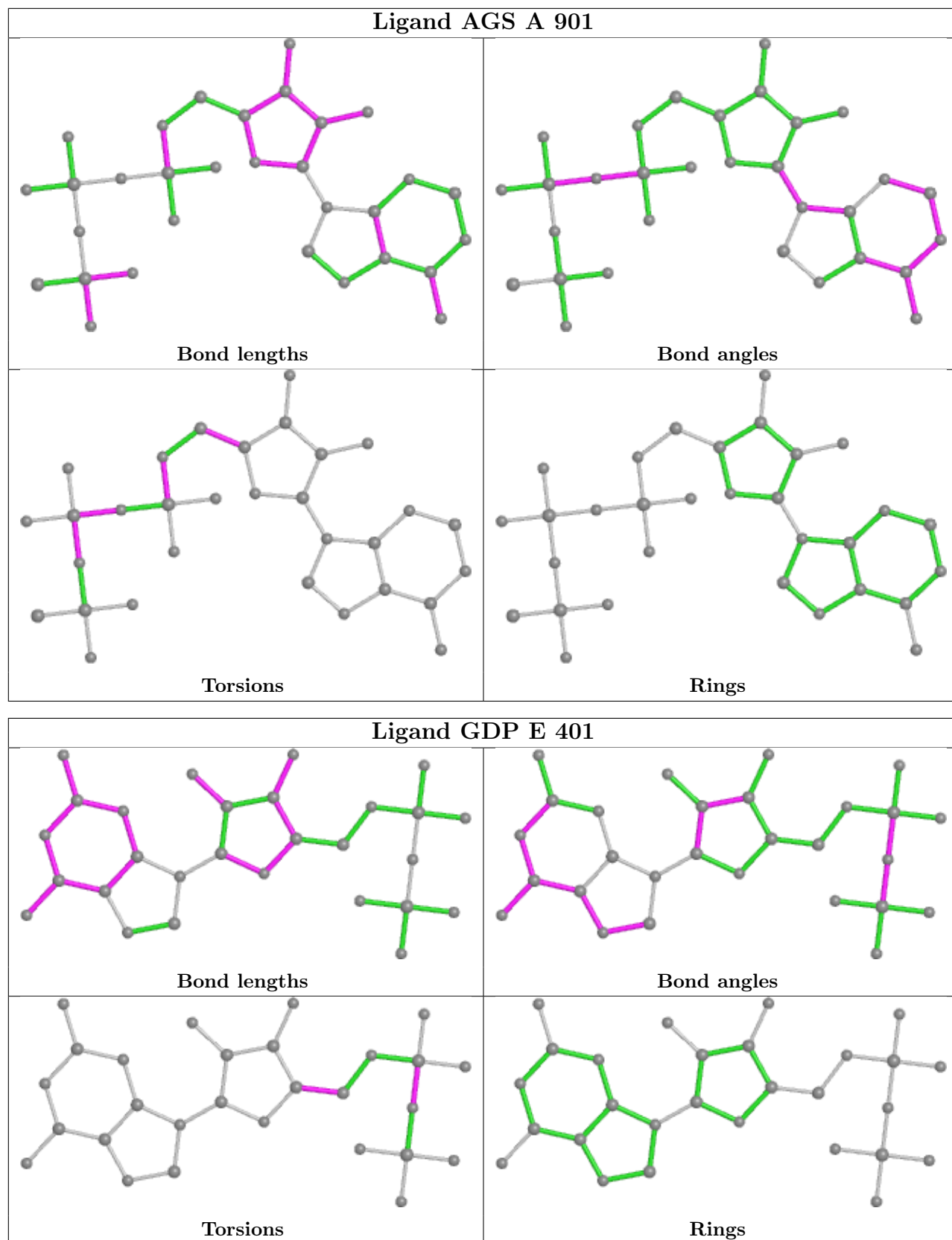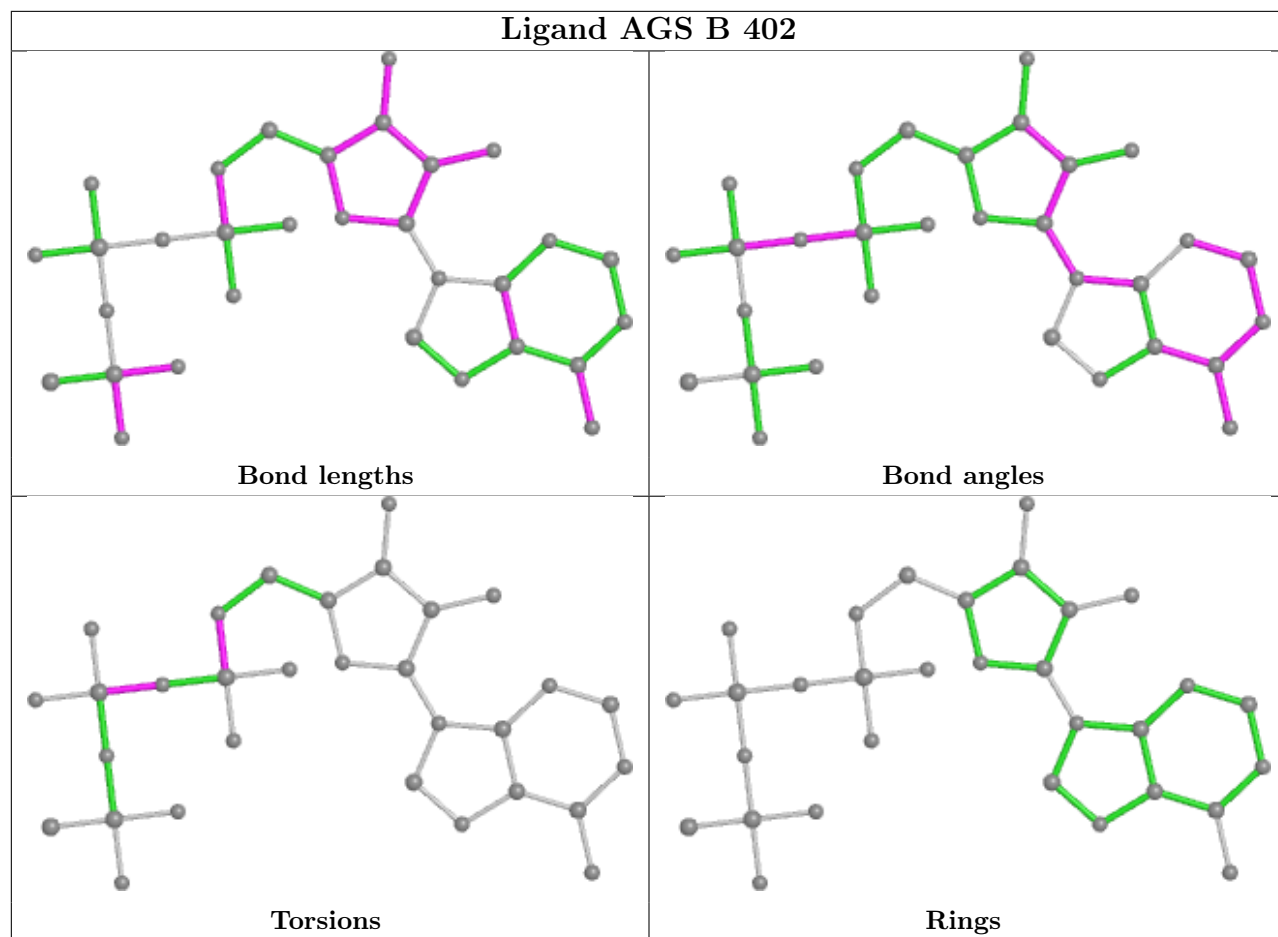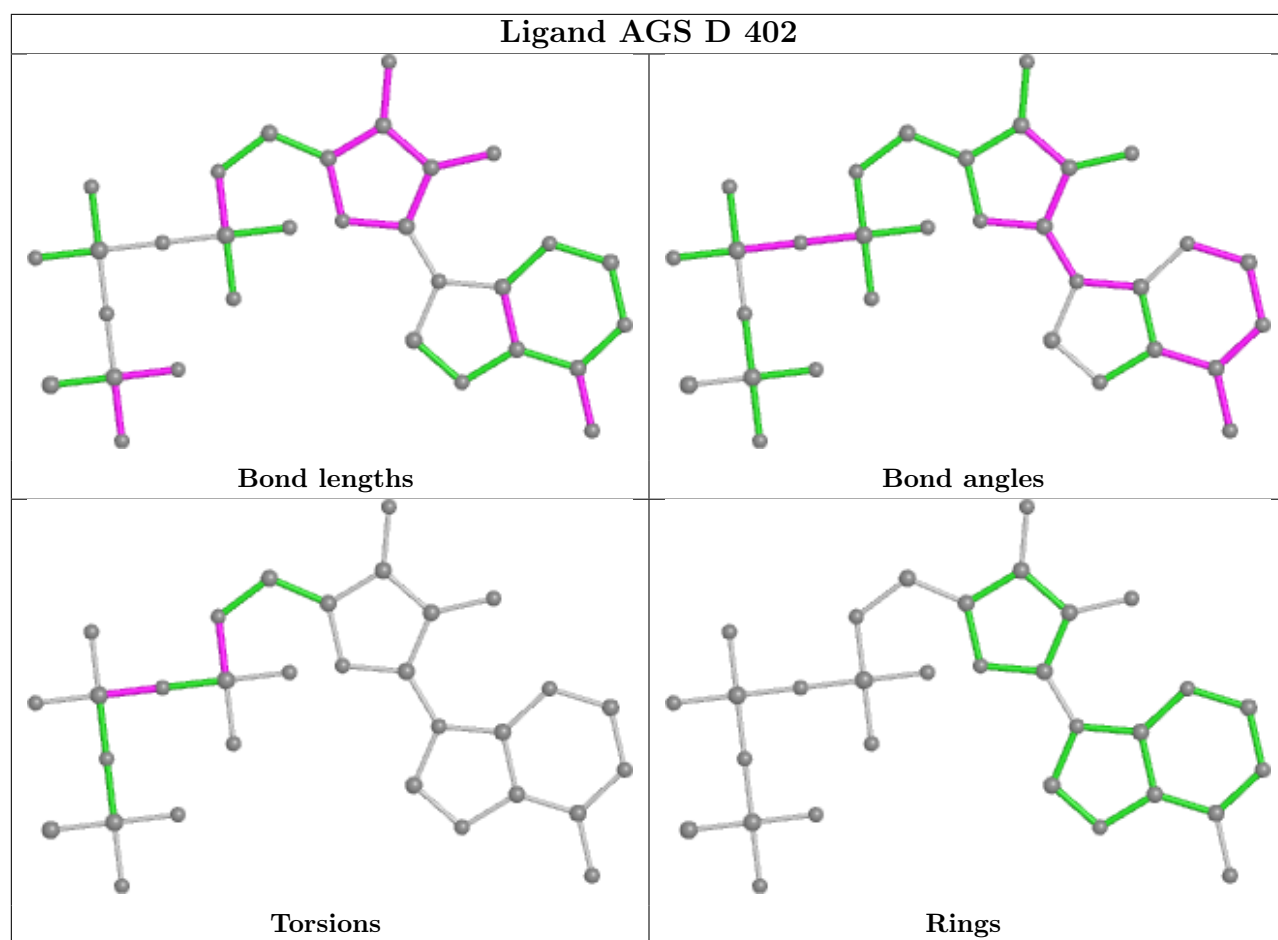
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-27662. 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 ⓘ
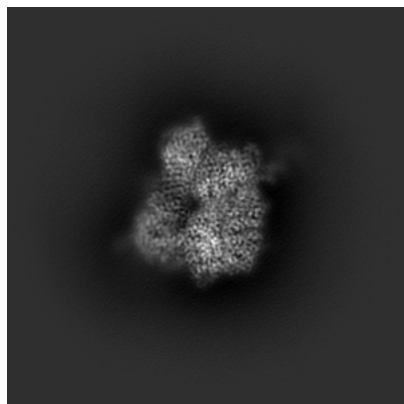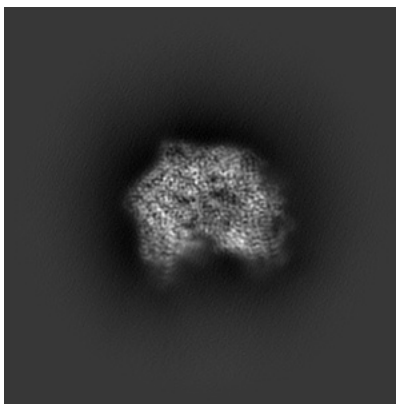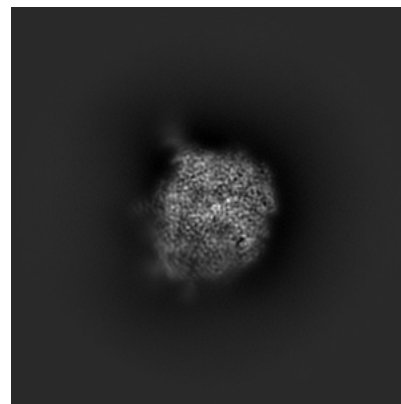
6.1.1 Primary map

X Y Z

6.1.2 Raw map

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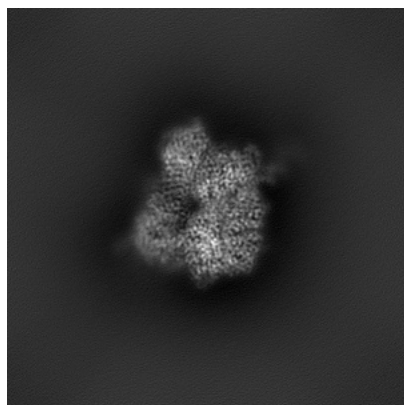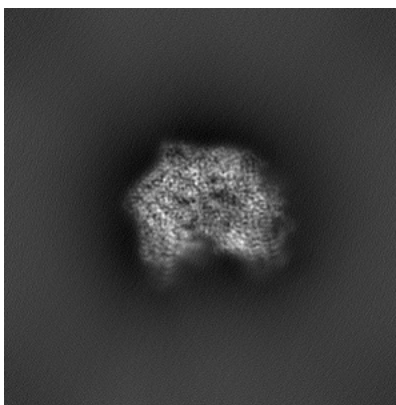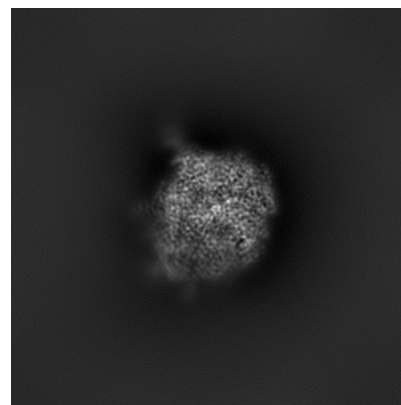
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
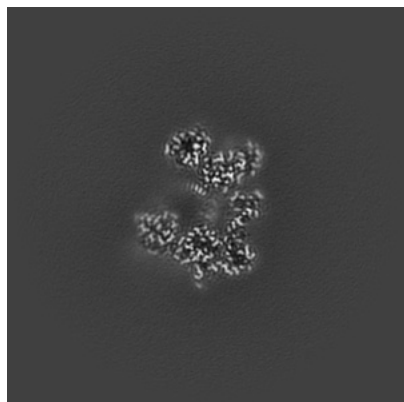
6.2.1 Primary map
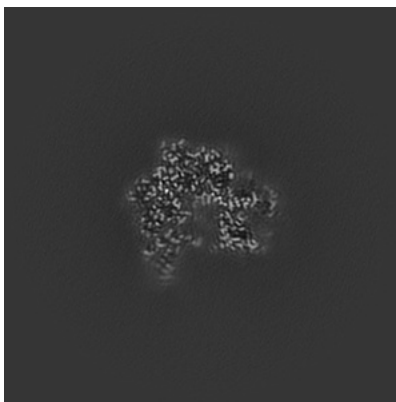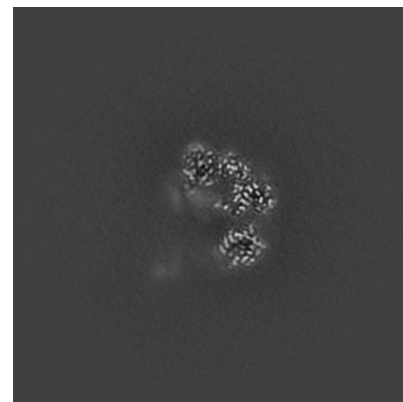
X Index: 192   Y Index: 192   Z Index: 192

6.2.2 Raw map
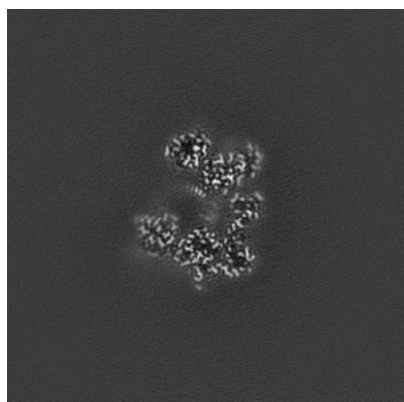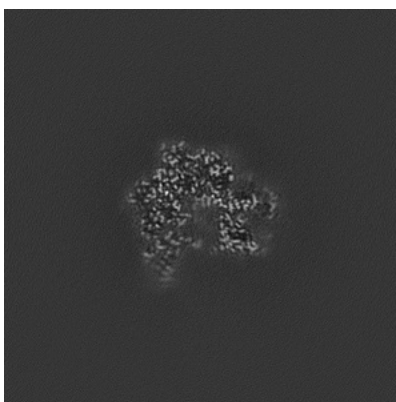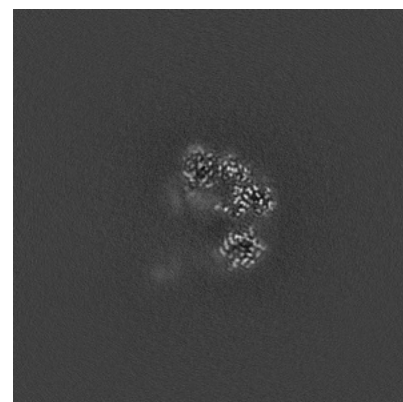
X Index: 192   Y Index: 192   Z Index: 192

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

6.3　Largest variance slices ⓘ

6.3.1　Primary map
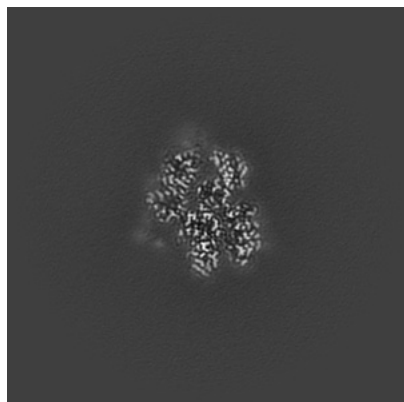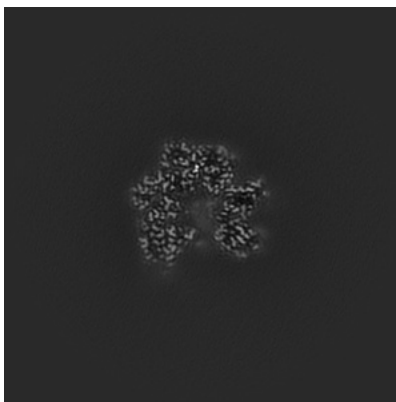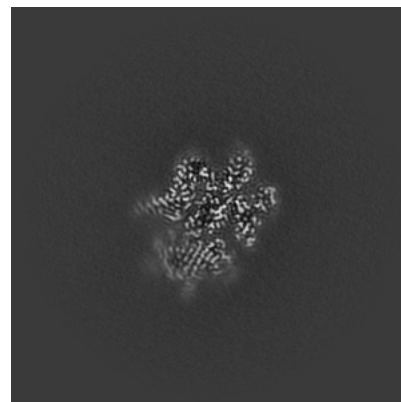
| X Index: 215 | Y Index: 199 | Z Index: 160 |

6.3.2　Raw map
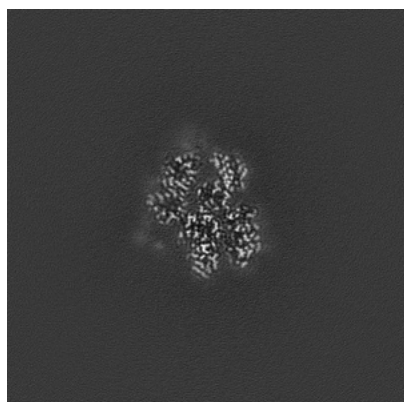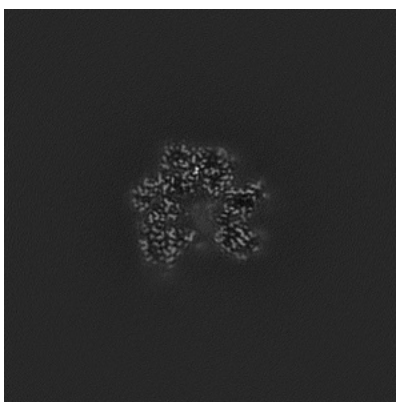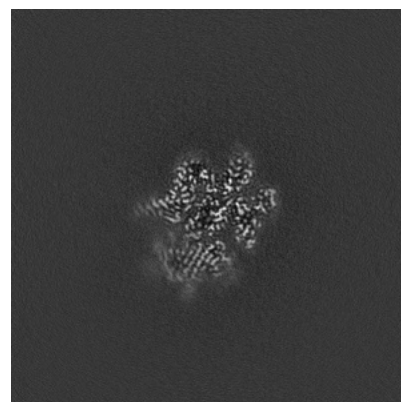
| X Index: 215 | Y Index: 199 | Z Index: 160 |

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
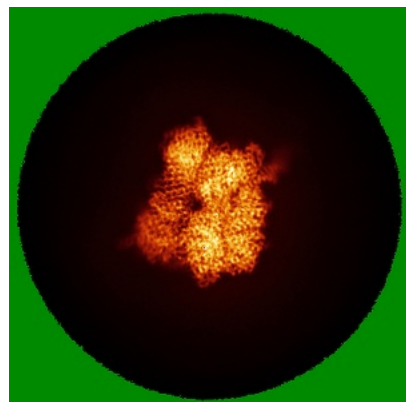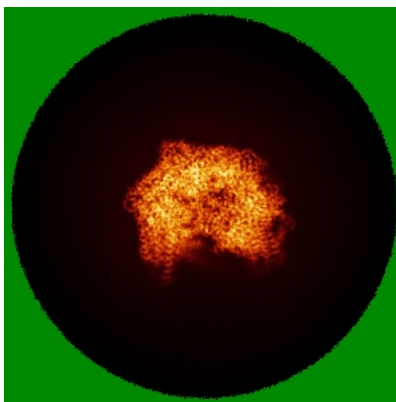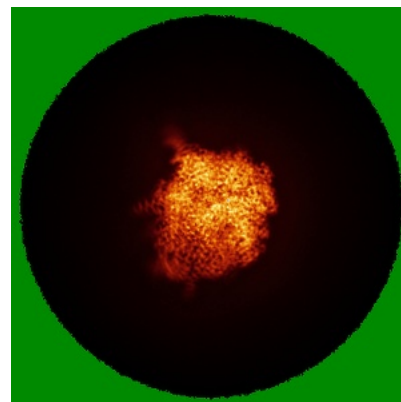
| X | Y | Z |

6.4.2 Raw map

| X | Y | Z |
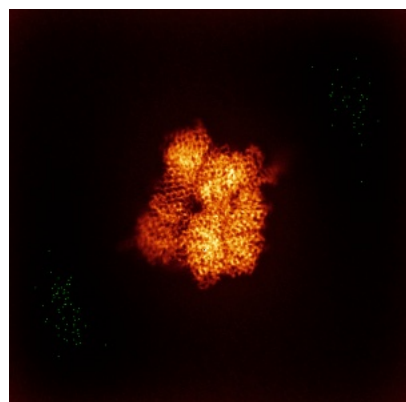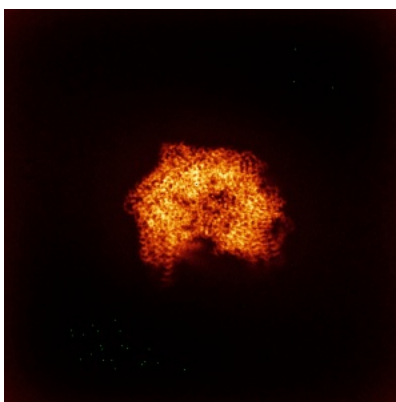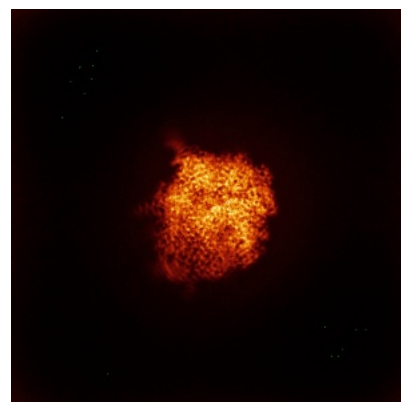
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

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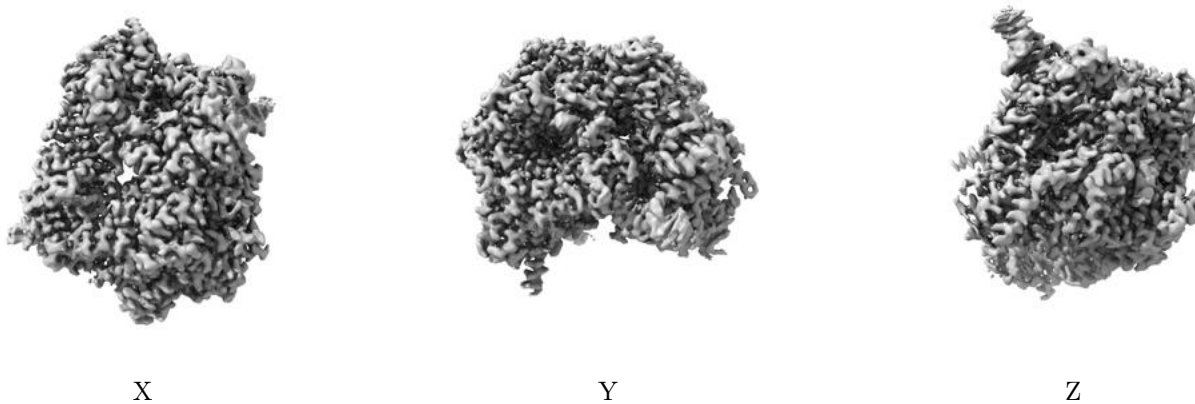
The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

| X | Y | Z |
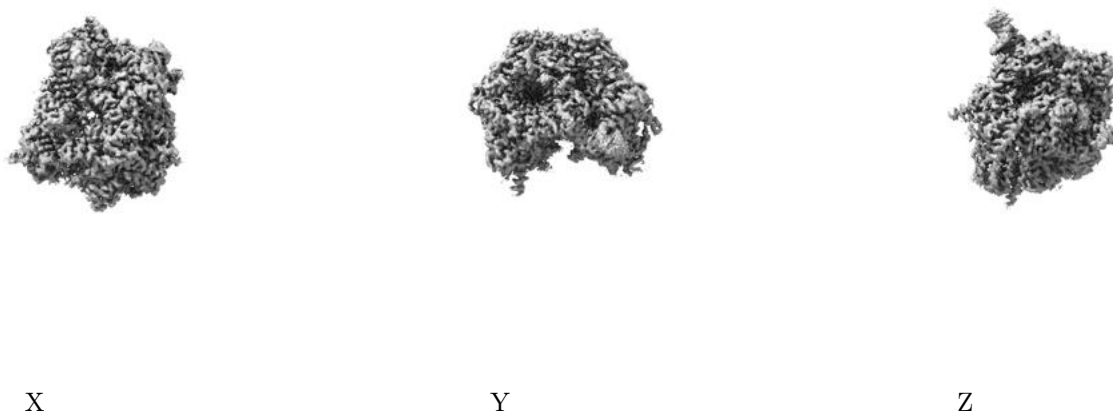
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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 ⓘ
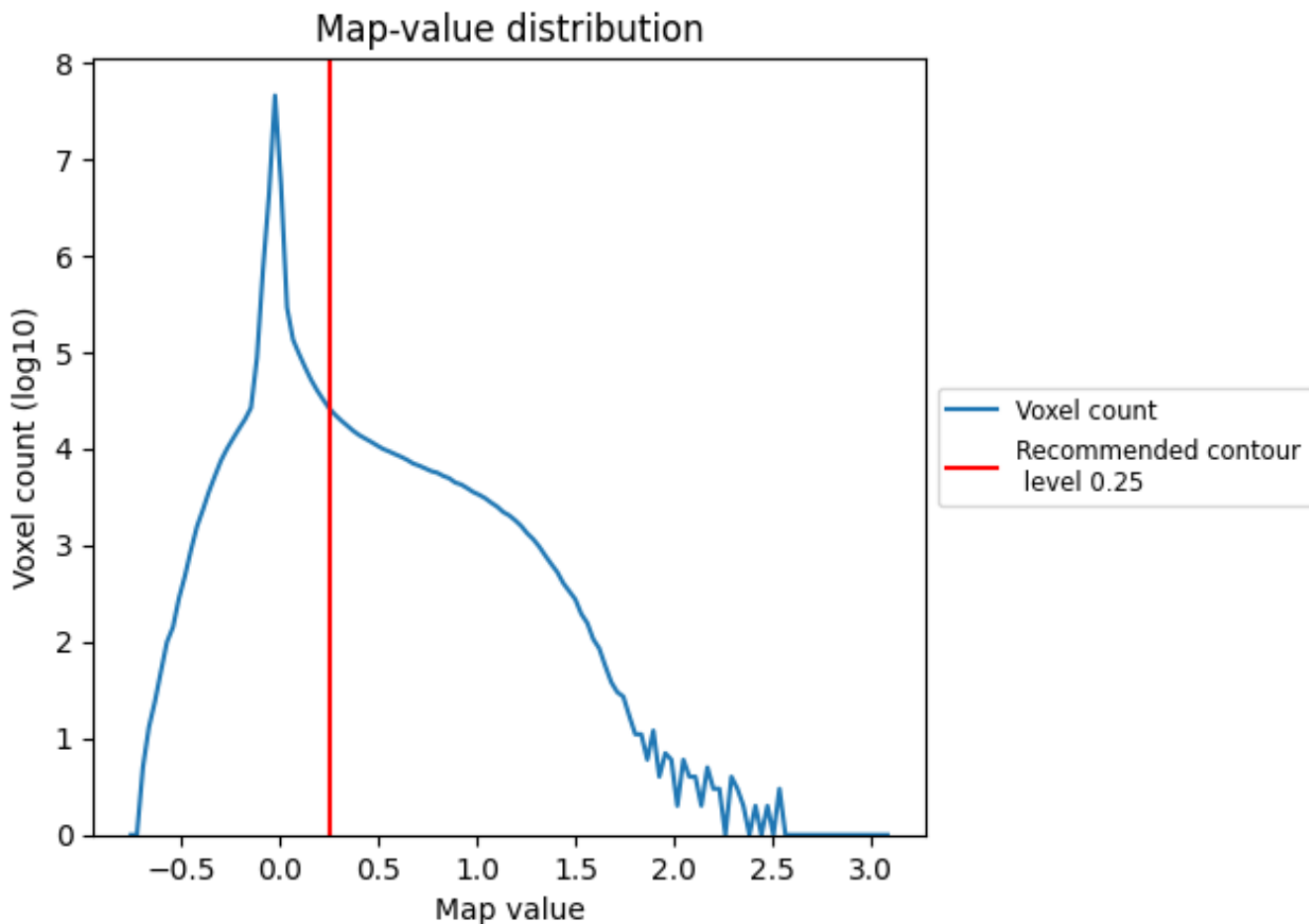
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
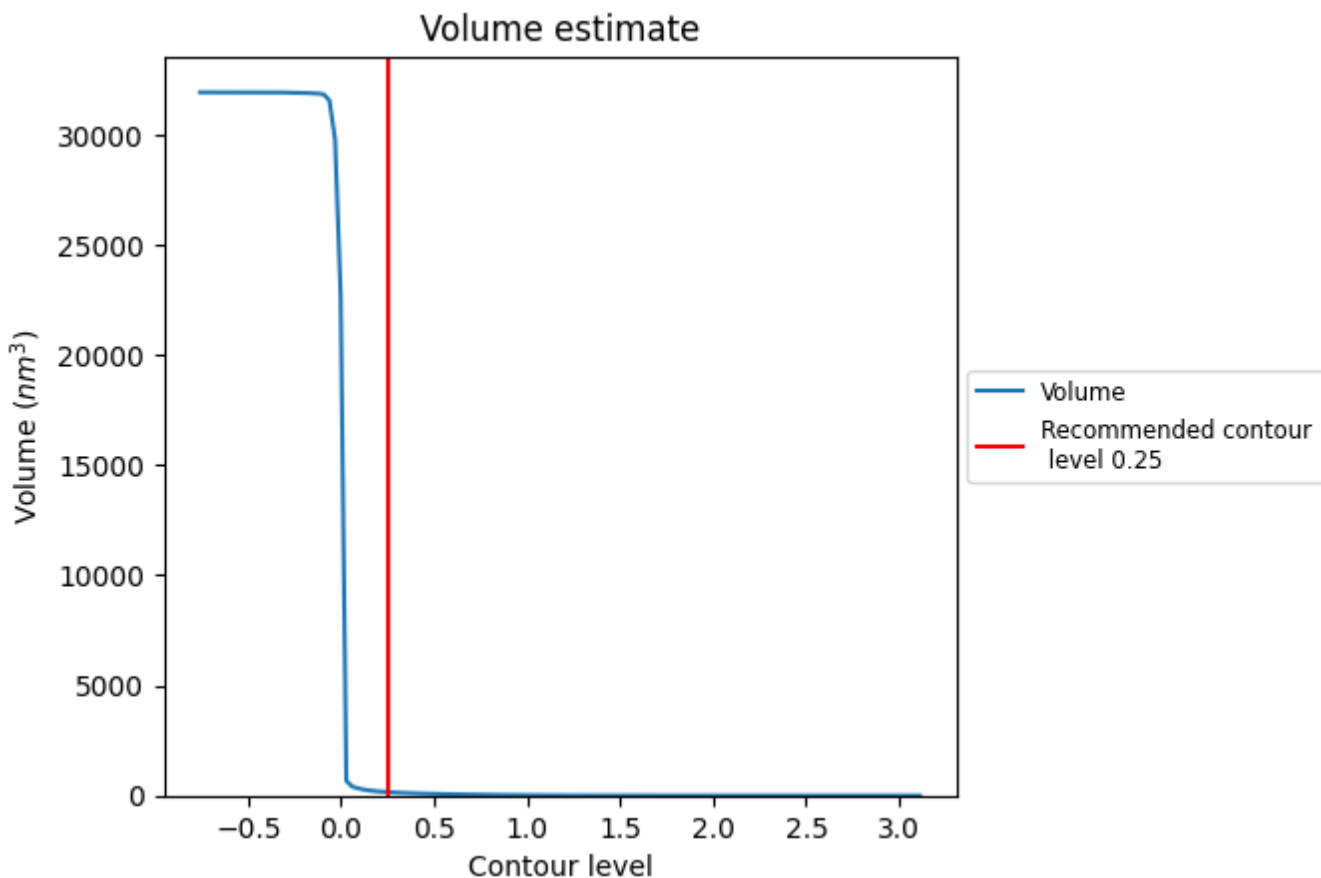
The volume at the recommended contour level is 156 nm^3; this corresponds to an approximate mass of 140 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ
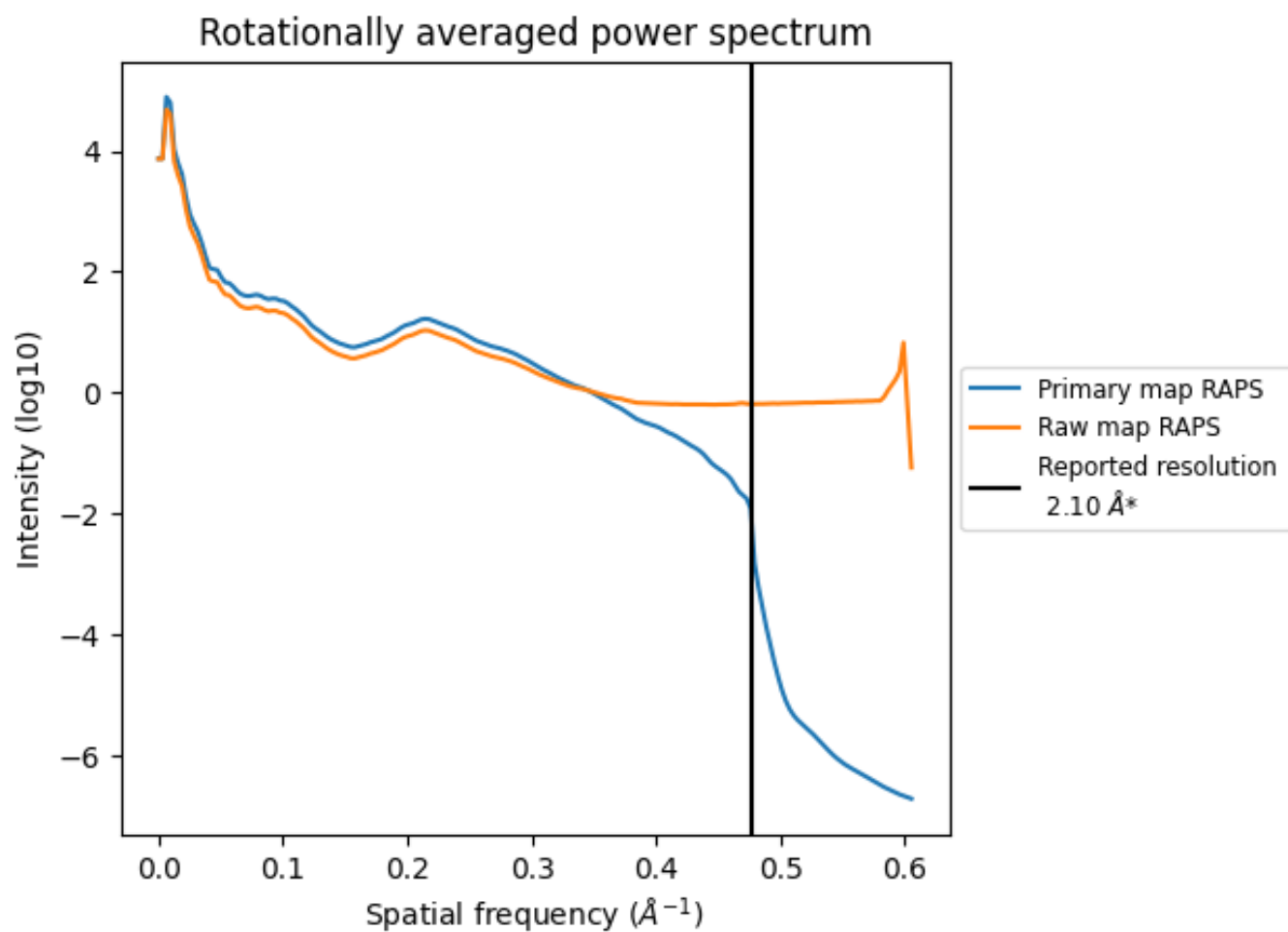
*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)
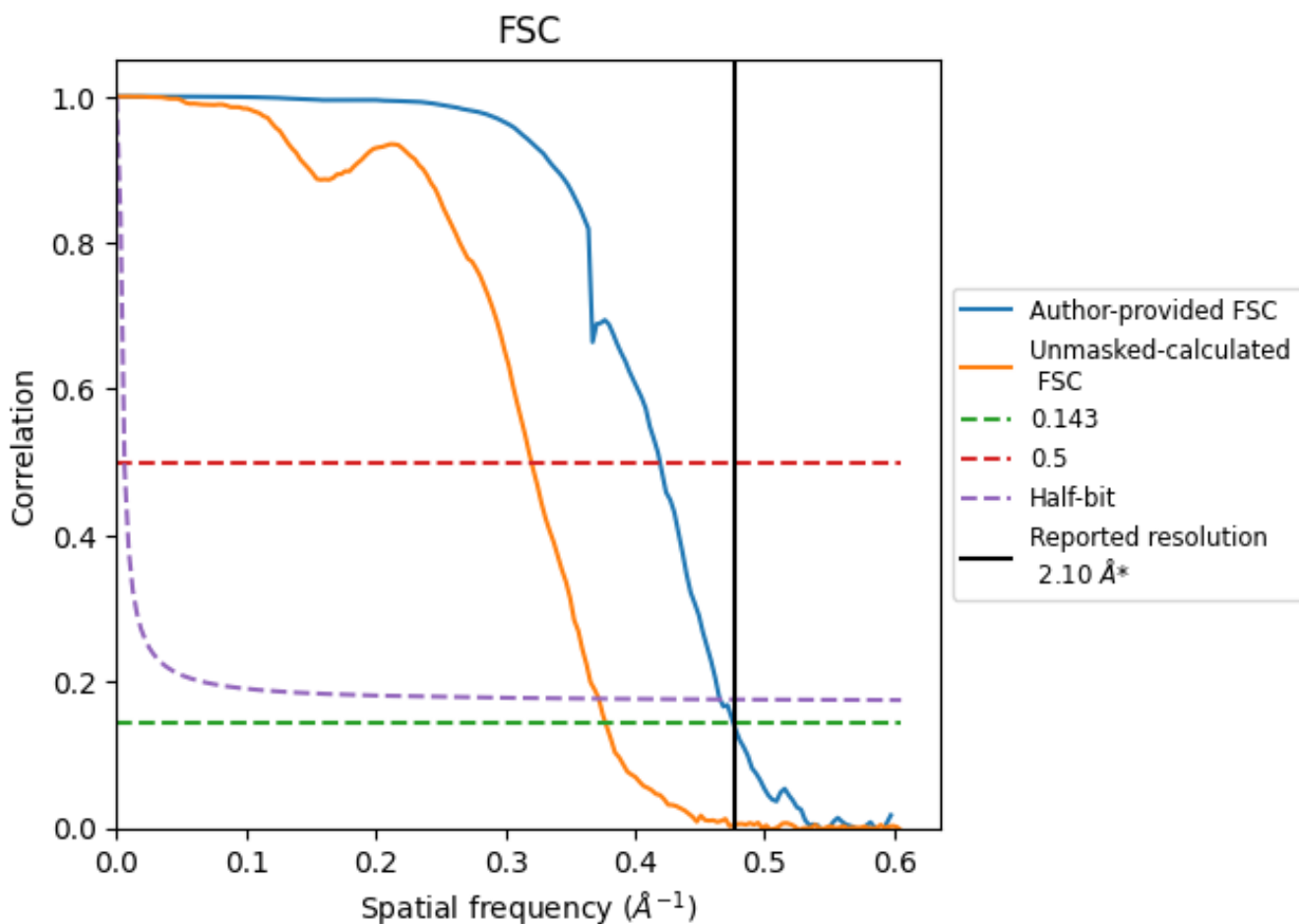
*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.10	2.39	2.15
Unmasked-calculated*	2.65	3.12	2.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.65 differs from the reported value 2.1 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-27662 and PDB model 8DQW. Per-residue inclusion information can be found in section 3 on page 10.

9.1   Map-model overlay ⓘ

X   Y   Z
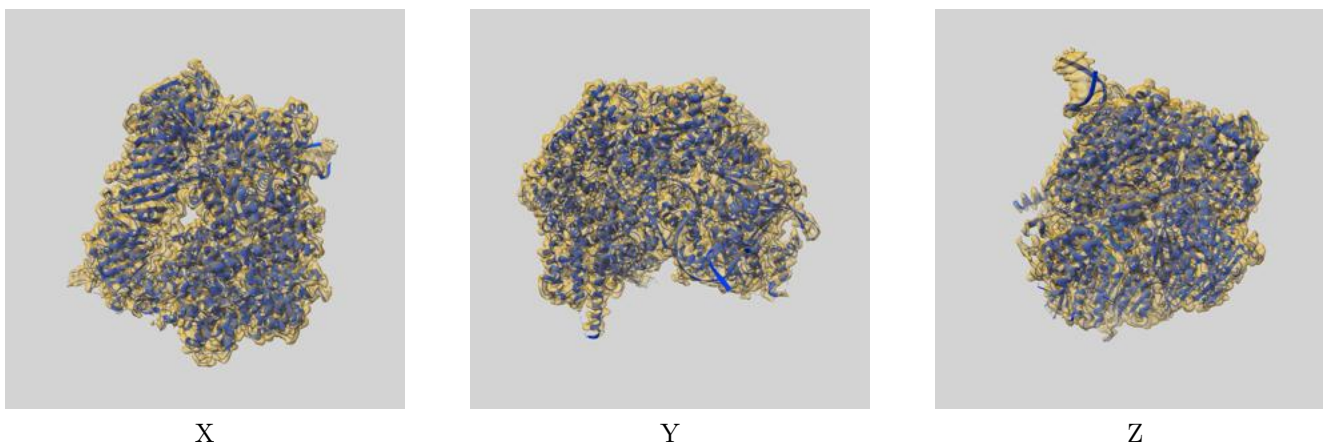
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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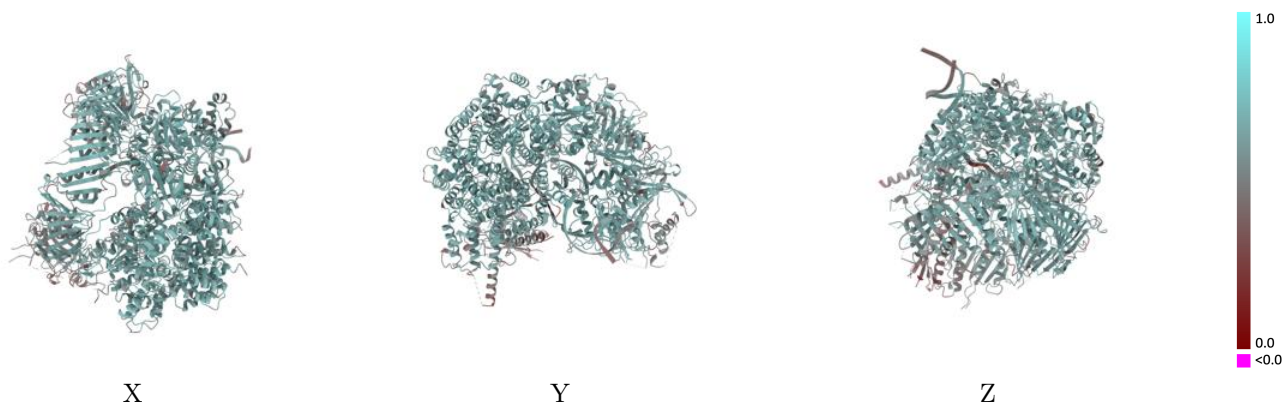
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
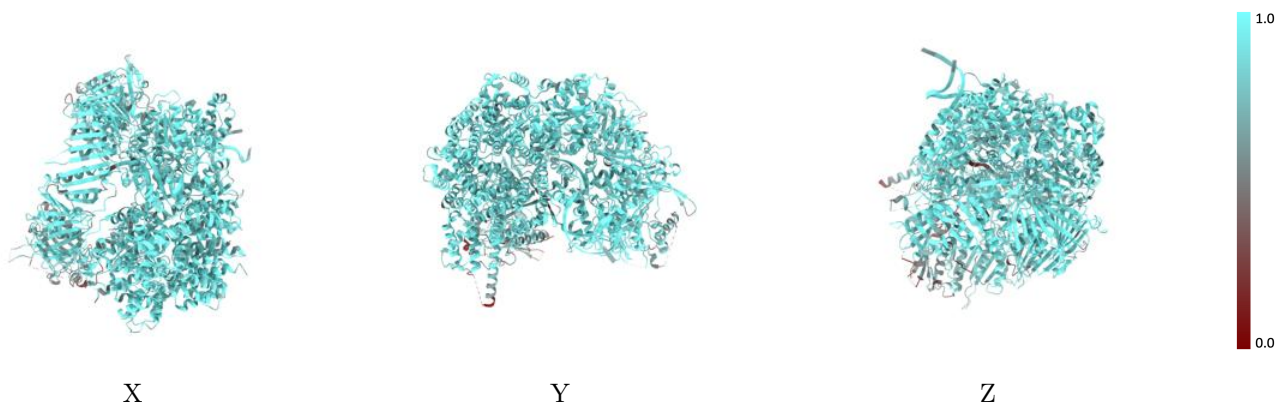
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion ⓘ
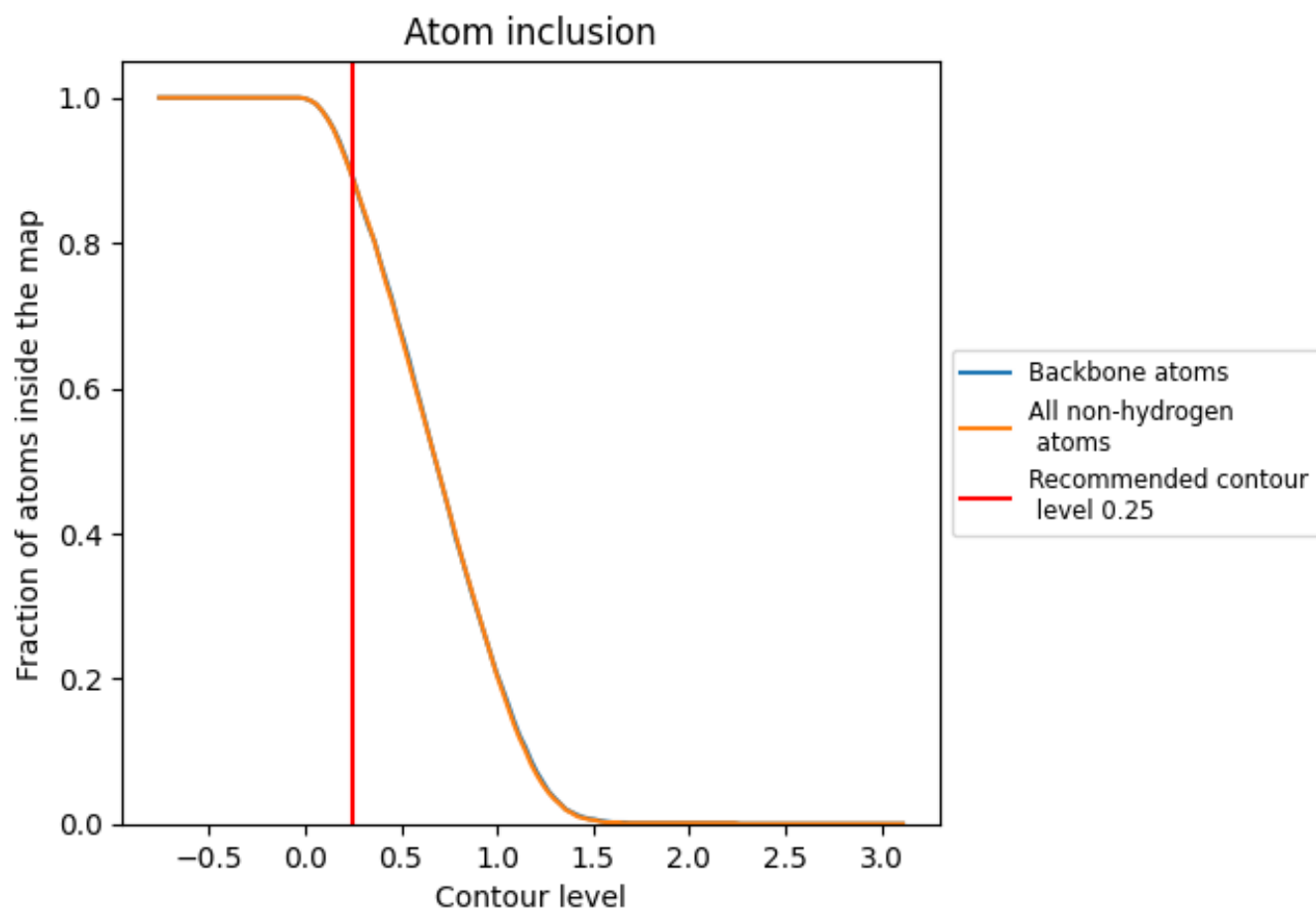
At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary (i)

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	0.8880	0.6020
A	0.8500	0.5820
B	0.9410	0.6410
C	0.9360	0.6380
D	0.9500	0.6530
E	0.9350	0.6330
F	0.8990	0.6030
G	0.8760	0.5860
H	0.7840	0.5050
I	0.8930	0.5320
J	0.8290	0.5300

1.0

0.0
<0.0