Full wwPDB EM Validation Report (i)

Mar 9, 2024 – 07:44 AM EST

PDB ID	:	6OF2
EMDB ID	:	EMD-20040
Title	:	Precursor ribosomal RNA processing complex, State 2.
Authors	:	Pillon, M.C.; Hsu, A.L.; Krahn, J.M.; Williams, J.G.; Goslen, K.H.; Sobhany, M.; Borgnia, M.J.; Stanley, R.E.
Deposited on	:	2019-03-28
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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 (1)) were used in the production of this report:

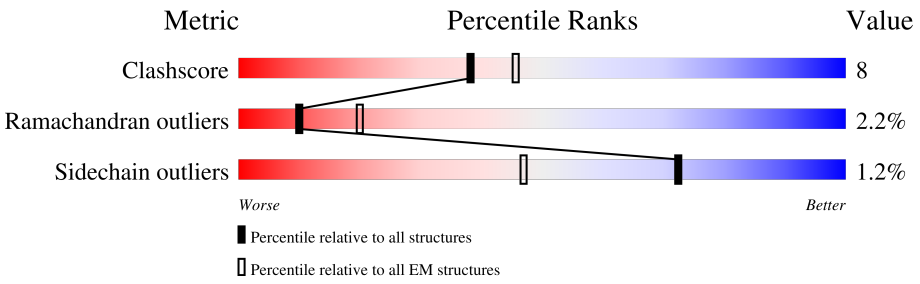
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	391	6% 41% 6% 53%
1	D	391	6% 41% 6% 53%
2	B	640	17% 63% 18% • 18%
2	E	640	18% 63% 18% • 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11062 atoms, of which 0 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 Ribonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	183	1451	928	258	259	6	0	0
1	D	183	1451	928	258	259	6	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP G0SGE9
A	-26	SER	-	expression tag	UNP G0SGE9
A	-25	TYR	-	expression tag	UNP G0SGE9
A	-24	TYR	-	expression tag	UNP G0SGE9
A	-23	HIS	-	expression tag	UNP G0SGE9
A	-22	HIS	-	expression tag	UNP G0SGE9
A	-21	HIS	-	expression tag	UNP G0SGE9
A	-20	HIS	-	expression tag	UNP G0SGE9
A	-19	HIS	-	expression tag	UNP G0SGE9
A	-18	HIS	-	expression tag	UNP G0SGE9
A	-17	ASP	-	expression tag	UNP G0SGE9
A	-16	TYR	-	expression tag	UNP G0SGE9
A	-15	ASP	-	expression tag	UNP G0SGE9
A	-14	ILE	-	expression tag	UNP G0SGE9
A	-13	PRO	-	expression tag	UNP G0SGE9
A	-12	THR	-	expression tag	UNP G0SGE9
A	-11	THR	-	expression tag	UNP G0SGE9
A	-10	GLU	-	expression tag	UNP G0SGE9
A	-9	ASN	-	expression tag	UNP G0SGE9
A	-8	LEU	-	expression tag	UNP G0SGE9
A	-7	TYR	-	expression tag	UNP G0SGE9
A	-6	PHE	-	expression tag	UNP G0SGE9
A	-5	GLN	-	expression tag	UNP G0SGE9
A	-4	GLY	-	expression tag	UNP G0SGE9
A	-3	ALA	-	expression tag	UNP G0SGE9
A	-2	MET	-	expression tag	UNP G0SGE9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G0SGE9
A	0	SER	-	expression tag	UNP G0SGE9
D	-27	MET	-	initiating methionine	UNP G0SGE9
D	-26	SER	-	expression tag	UNP G0SGE9
D	-25	TYR	-	expression tag	UNP G0SGE9
D	-24	TYR	-	expression tag	UNP G0SGE9
D	-23	HIS	-	expression tag	UNP G0SGE9
D	-22	HIS	-	expression tag	UNP G0SGE9
D	-21	HIS	-	expression tag	UNP G0SGE9
D	-20	HIS	-	expression tag	UNP G0SGE9
D	-19	HIS	-	expression tag	UNP G0SGE9
D	-18	HIS	-	expression tag	UNP G0SGE9
D	-17	ASP	-	expression tag	UNP G0SGE9
D	-16	TYR	-	expression tag	UNP G0SGE9
D	-15	ASP	-	expression tag	UNP G0SGE9
D	-14	ILE	-	expression tag	UNP G0SGE9
D	-13	PRO	-	expression tag	UNP G0SGE9
D	-12	THR	-	expression tag	UNP G0SGE9
D	-11	THR	-	expression tag	UNP G0SGE9
D	-10	GLU	-	expression tag	UNP G0SGE9
D	-9	ASN	-	expression tag	UNP G0SGE9
D	-8	LEU	-	expression tag	UNP G0SGE9
D	-7	TYR	-	expression tag	UNP G0SGE9
D	-6	PHE	-	expression tag	UNP G0SGE9
D	-5	GLN	-	expression tag	UNP G0SGE9
D	-4	GLY	-	expression tag	UNP G0SGE9
D	-3	ALA	-	expression tag	UNP G0SGE9
D	-2	MET	-	expression tag	UNP G0SGE9
D	-1	GLY	-	expression tag	UNP G0SGE9
D	0	SER	-	expression tag	UNP G0SGE9

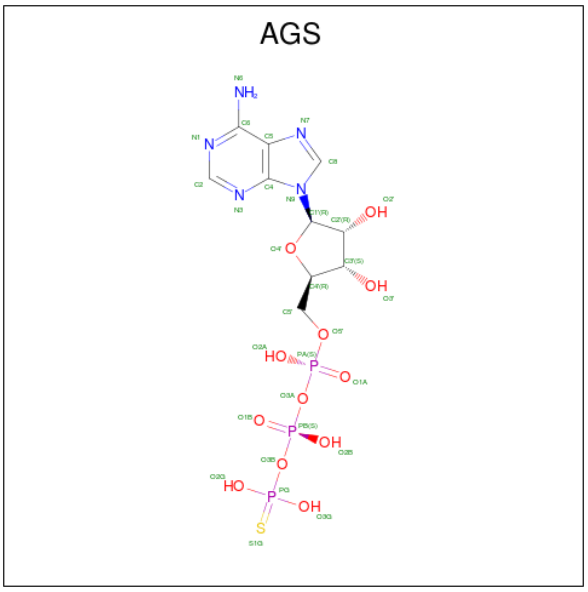
- Molecule 2 is a protein called CLP1_P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	528	4048	2586	702	739	21	0	0
2	E	528	4048	2586	702	739	21	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	109	MET	-	initiating methionine	UNP G0S263
E	109	MET	-	initiating methionine	UNP G0S263

- Molecule 3 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	N	O	P	S	
3	B	1	31	10	5	12	3	1	0
			Total	C	N	O	P	S	
3	E	1	31	10	5	12	3	1	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

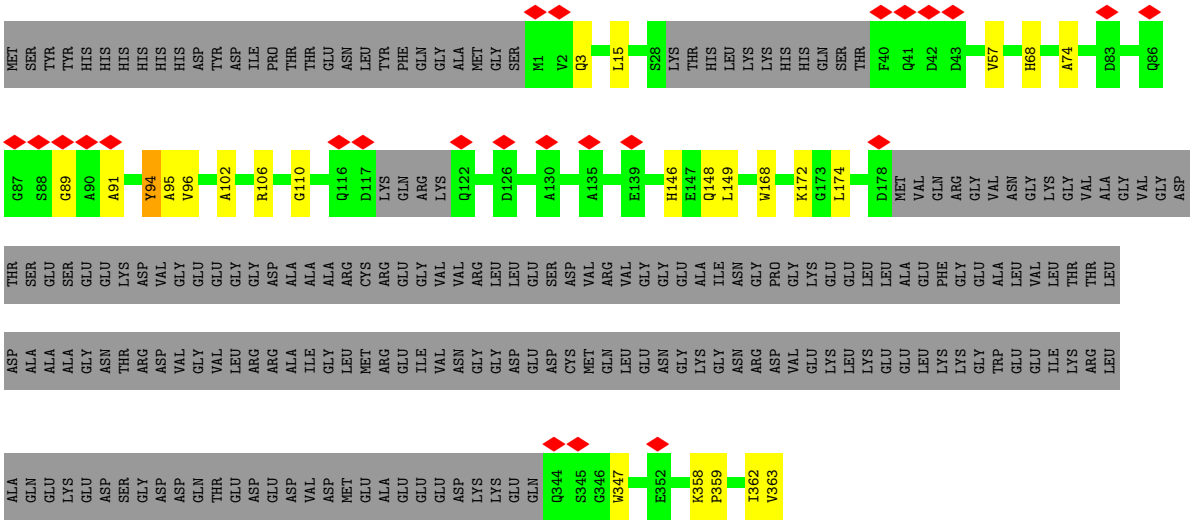
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	B	1	1	1	0
			Total	Mg	
4	E	1	1	1	0

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.

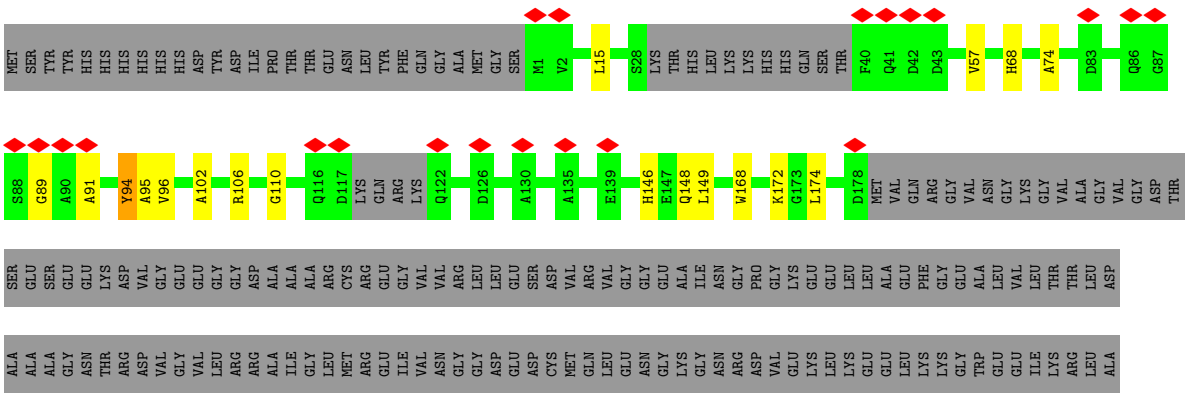
- Molecule 1: Ribonuclease

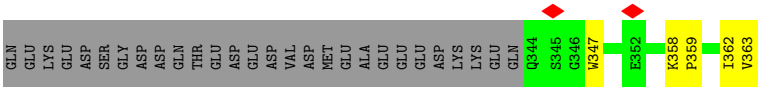
Chain A:



- Molecule 1: Ribonuclease

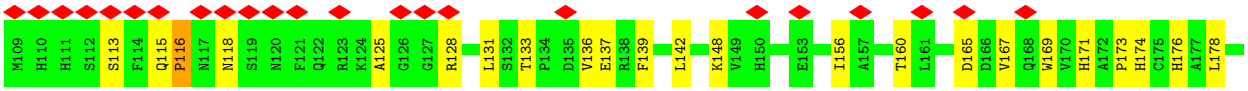
Chain D:

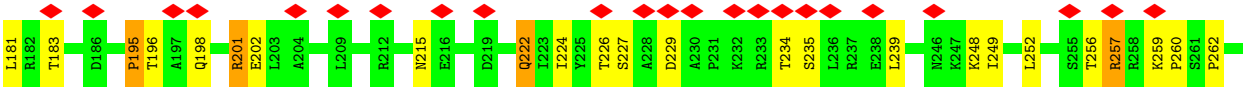


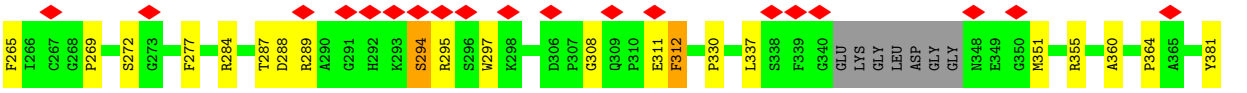


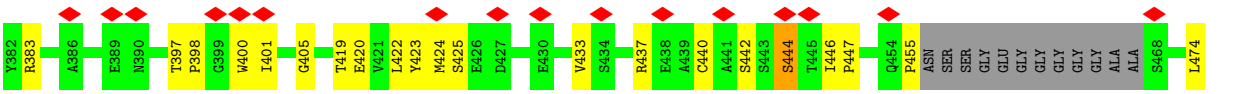
• Molecule 2: CLP1_P domain-containing protein

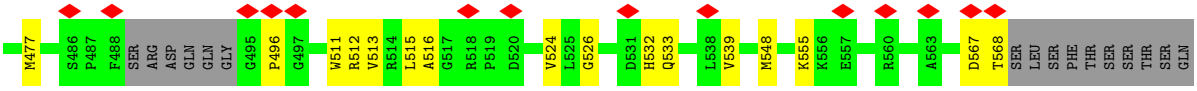
Chain B:

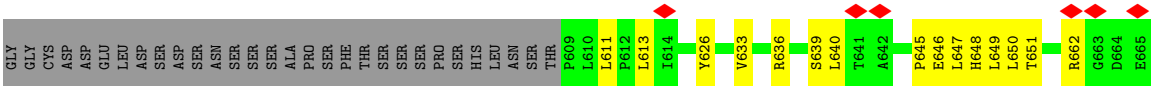


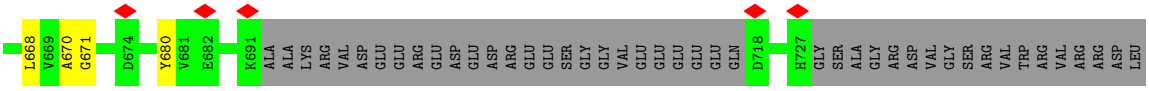






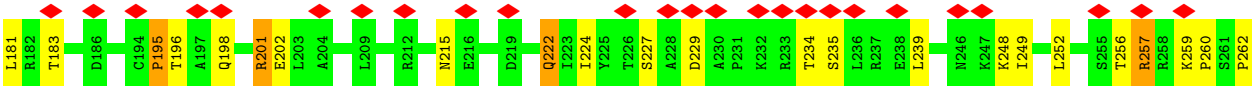


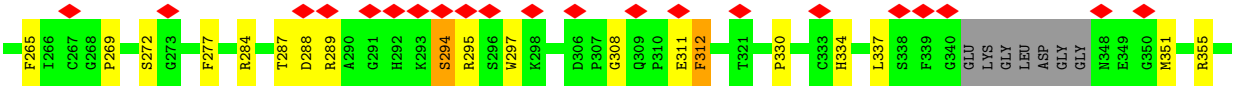


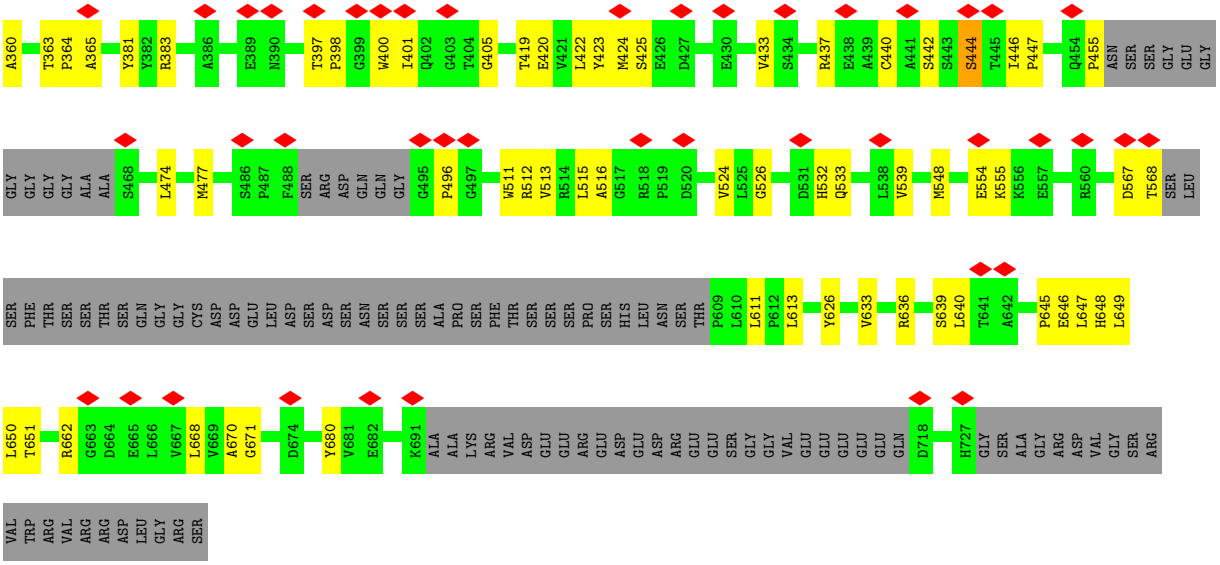


• Molecule 2: CLP1_P domain-containing protein

Chain E:






A360 T363 P364 A365 Y381 Y382 R383 A386 E389 N390 T397 P398 G399 W400 I401 Q402 G403 T404 G405 T419 E420 V421 L422 Y423 M424 S425 E426 D427 E430 V433 S434 R437 E438 A439 C440 A441 S442 S443 S444 T445 I446 P447 Q454 P455 ASN SER SER GLY GLU GLY
GLY GLY GLY GLY ALA ALA S468 L474 M477 S486 P487 F488 SER ARG ASP GLN GLN GLY G495 P496 G497 W511 R512 V513 R514 L515 A516 G517 R518 P519 D520 V524 L525 G526 D531 H532 Q533 L538 V539 M548 E554 K555 K556 E557 R560 D567 T568 SER LEU
SER PHE THR SER SER THR SER GLN GLY GLY CYS ASP ASP GLU LEU ASP SER ASP SER ASN SER SER SER ALA PRO SER PHE THR SER SER SER PRO SER HIS LEU ASN SER THR P609 L610 L611 P612 L613 Y626 V633 R636 S639 L640 T641 A642 P645 E646 L647 H648 L649
L650 T651 R662 G663 D664 E665 L666 V667 L668 V669 A670 G671 D674 Y680 V681 E682 K691 ALA ALA ALA LYS ARG VAL ASP GLU GLU ARG GLU ASP GLU ASP ARG GLU GLU GLU SER GLY GLY VAL GLU GLU GLU GLU GLU GLN D718 H727 GLY SER ALA GLY ARG ASP VAL GLY SER ARG
VAL TRP ARG VAL ARG ARG ASP LEU GLY ARG SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70561	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	28.107	Depositor
Minimum map value	-0.787	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.705	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	241.92001, 241.92001, 241.92001	wwPDB
Map dimensions	224, 224, 224	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: AGS, MG

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	0.35	0/1490	0.44	0/2021
1	D	0.35	0/1490	0.44	0/2021
2	B	0.32	0/4158	0.55	1/5683 (0.0%)
2	E	0.32	0/4158	0.55	1/5683 (0.0%)
All	All	0.33	0/11296	0.53	2/15408 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	455	PRO	N-CA-CB	6.10	110.62	103.30
2	B	455	PRO	N-CA-CB	6.06	110.58	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	295	ARG	Peptide
2	E	295	ARG	Peptide

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	1451	0	1402	16	0
1	D	1451	0	1402	15	0
2	B	4048	0	4024	75	0
2	E	4048	0	4024	78	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
All	All	11062	0	10876	175	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 8.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:160:THR:H	2:E:287:THR:HG21	1.38	0.87
2:B:160:THR:H	2:B:287:THR:HG21	1.38	0.85
1:D:91:ALA:HB1	1:D:95:ALA:HB3	1.59	0.83
1:A:91:ALA:HB1	1:A:95:ALA:HB3	1.59	0.82
2:B:222:GLN:NE2	2:B:229:ASP:OD2	2.17	0.77
1:A:106:ARG:NH1	1:D:146:HIS:O	2.17	0.77
2:E:222:GLN:NE2	2:E:229:ASP:OD2	2.17	0.76
2:E:165:ASP:OD1	2:E:289:ARG:NH2	2.22	0.72
2:B:165:ASP:OD1	2:B:289:ARG:NH2	2.22	0.72
2:E:116:PRO:HG2	2:E:224:ILE:O	1.91	0.71
2:B:239:LEU:HA	3:B:801:AGS:H2	1.70	0.71
2:E:239:LEU:HA	3:E:801:AGS:H2	1.70	0.71
2:B:116:PRO:HG2	2:B:224:ILE:O	1.91	0.70
1:A:146:HIS:O	1:D:106:ARG:NH1	2.25	0.70
2:B:115:GLN:HB2	2:B:116:PRO:HD3	1.74	0.70
2:E:115:GLN:HB2	2:E:116:PRO:HD3	1.74	0.69
2:E:257:ARG:HH11	2:E:257:ARG:HB3	1.57	0.69
2:B:272:SER:OG	2:B:424:MET:O	2.11	0.69
2:B:257:ARG:HH11	2:B:257:ARG:HB3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:272:SER:OG	2:E:424:MET:O	2.11	0.67
2:B:113:SER:HG	2:B:226:THR:HG1	1.42	0.66
1:A:363:VAL:HG11	2:B:639:SER:HB3	1.77	0.65
2:E:633:VAL:HG13	2:E:651:THR:HG22	1.81	0.63
2:B:633:VAL:HG13	2:B:651:THR:HG22	1.81	0.63
2:E:512:ARG:NE	2:E:646:GLU:OE1	2.32	0.62
2:B:512:ARG:NE	2:B:646:GLU:OE1	2.32	0.62
2:E:633:VAL:HG11	2:E:649:LEU:HD22	1.82	0.62
2:B:277:PHE:HE2	2:B:422:LEU:HD13	1.66	0.61
2:B:567:ASP:OD1	2:B:568:THR:N	2.33	0.61
2:E:567:ASP:OD1	2:E:568:THR:N	2.33	0.61
2:B:633:VAL:HG11	2:B:649:LEU:HD22	1.82	0.60
2:E:277:PHE:HE2	2:E:422:LEU:HD13	1.66	0.60
2:B:355:ARG:HD2	2:B:381:TYR:CE1	2.39	0.58
2:E:355:ARG:HD2	2:E:381:TYR:CE1	2.39	0.57
2:B:265:PHE:CZ	2:B:397:THR:HG21	2.40	0.57
2:E:265:PHE:CZ	2:E:397:THR:HG21	2.40	0.56
2:B:524:VAL:HG22	2:B:526:GLY:H	1.71	0.56
2:E:419:THR:HG22	2:E:420:GLU:HG3	1.87	0.56
2:B:515:LEU:HD11	2:B:647:LEU:HG	1.88	0.56
2:E:636:ARG:HD2	2:E:650:LEU:HD23	1.88	0.56
2:E:515:LEU:HD11	2:E:647:LEU:HG	1.88	0.55
2:E:524:VAL:HG22	2:E:526:GLY:H	1.71	0.55
2:B:636:ARG:HD2	2:B:650:LEU:HD23	1.88	0.55
2:B:419:THR:HG22	2:B:420:GLU:HG3	1.88	0.55
2:B:548:MET:HE3	2:B:668:LEU:HB3	1.89	0.54
2:B:259:LYS:HB3	2:B:260:PRO:HD2	1.89	0.54
2:E:548:MET:HE3	2:E:668:LEU:HB3	1.90	0.54
2:E:259:LYS:HB3	2:E:260:PRO:HD2	1.89	0.54
1:A:102:ALA:HB2	1:D:102:ALA:HB2	1.90	0.53
1:A:358:LYS:O	2:B:636:ARG:NH2	2.41	0.53
2:B:289:ARG:HG2	2:B:294:SER:O	2.08	0.52
2:E:234:THR:OG1	2:E:235:SER:N	2.42	0.52
2:E:289:ARG:HG2	2:E:294:SER:O	2.08	0.52
2:E:440:CYS:SG	2:E:446:ILE:HB	2.50	0.52
1:A:68:HIS:NE2	1:A:110:GLY:HA3	2.26	0.51
2:B:440:CYS:SG	2:B:446:ILE:HB	2.50	0.51
2:E:173:PRO:HG2	2:E:330:PRO:HG2	1.93	0.51
2:B:234:THR:OG1	2:B:235:SER:N	2.42	0.51
2:E:555:LYS:HD2	2:E:626:TYR:HD2	1.76	0.51
2:E:248:LYS:HE3	2:E:252:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:555:LYS:HD2	2:B:626:TYR:HD2	1.76	0.51
2:B:248:LYS:HE3	2:B:252:LEU:HD21	1.92	0.50
1:D:68:HIS:NE2	1:D:110:GLY:HA3	2.26	0.50
2:B:169:TRP:NE1	2:B:496:PRO:HB3	2.27	0.50
2:B:173:PRO:HG2	2:B:330:PRO:HG2	1.92	0.50
2:E:169:TRP:NE1	2:E:496:PRO:HB3	2.27	0.50
2:E:195:PRO:HG2	2:E:196:THR:H	1.77	0.49
2:E:474:LEU:HA	2:E:477:MET:HE3	1.95	0.49
2:B:174:HIS:HE1	2:B:234:THR:O	1.96	0.48
2:E:400:TRP:HB3	2:E:405:GLY:HA3	1.95	0.48
2:B:115:GLN:CB	2:B:116:PRO:HD3	2.44	0.48
2:B:474:LEU:HA	2:B:477:MET:HE3	1.96	0.48
2:E:442:SER:C	2:E:444:SER:H	2.17	0.48
2:B:337:LEU:HD13	2:B:351:MET:HB3	1.96	0.47
2:E:513:VAL:CG2	2:E:647:LEU:HB2	2.44	0.47
2:E:174:HIS:HE1	2:E:234:THR:O	1.96	0.47
2:B:400:TRP:HB3	2:B:405:GLY:HA3	1.95	0.47
2:B:142:LEU:HD12	2:B:178:LEU:HD21	1.97	0.47
2:B:516:ALA:HB2	2:B:645:PRO:HD2	1.97	0.47
2:B:442:SER:C	2:B:444:SER:H	2.17	0.47
2:B:195:PRO:HG2	2:B:196:THR:H	1.77	0.47
2:B:513:VAL:CG2	2:B:647:LEU:HB2	2.45	0.47
2:E:433:VAL:HG12	2:E:437:ARG:HH12	1.80	0.47
2:B:433:VAL:HG12	2:B:437:ARG:HH12	1.81	0.46
1:D:359:PRO:HG2	1:D:362:ILE:HD12	1.98	0.46
2:E:337:LEU:HD13	2:E:351:MET:HB3	1.96	0.46
2:E:224:ILE:HG12	2:E:229:ASP:HB2	1.97	0.46
2:B:201:ARG:HH11	2:B:201:ARG:HG2	1.81	0.46
2:B:224:ILE:HG12	2:B:229:ASP:HB2	1.97	0.46
2:E:516:ALA:HB2	2:E:645:PRO:HD2	1.97	0.46
2:E:142:LEU:HD12	2:E:178:LEU:HD21	1.97	0.46
2:E:115:GLN:CB	2:E:116:PRO:HD3	2.44	0.45
2:B:169:TRP:CD1	2:B:496:PRO:HB3	2.52	0.45
2:B:636:ARG:HH11	2:B:636:ARG:HG3	1.82	0.45
2:E:201:ARG:HG2	2:E:201:ARG:HH11	1.81	0.45
1:A:359:PRO:HG2	1:A:362:ILE:HD12	1.98	0.45
2:E:169:TRP:CD1	2:E:496:PRO:HB3	2.52	0.45
2:E:548:MET:SD	2:E:670:ALA:HB2	2.56	0.45
1:A:347:TRP:CZ3	2:B:649:LEU:HD11	2.51	0.45
2:E:178:LEU:H	2:E:178:LEU:HD12	1.82	0.45
2:B:548:MET:SD	2:B:670:ALA:HB2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:419:THR:O	2:E:447:PRO:HD2	2.18	0.44
2:B:539:VAL:HG21	2:B:613:LEU:CD1	2.47	0.44
1:D:149:LEU:H	1:D:149:LEU:HD12	1.82	0.44
2:E:355:ARG:NH2	2:E:554:GLU:OE2	2.41	0.44
2:E:636:ARG:HH11	2:E:636:ARG:HG3	1.82	0.44
2:B:156:ILE:HG12	2:B:181:LEU:HD13	2.00	0.44
2:B:178:LEU:H	2:B:178:LEU:HD12	1.82	0.44
2:B:269:PRO:HB3	2:B:401:ILE:HD13	1.99	0.44
2:B:287:THR:O	2:B:289:ARG:HG3	2.18	0.44
2:E:136:VAL:HA	2:E:183:THR:O	2.18	0.44
2:E:156:ILE:HG12	2:E:181:LEU:HD13	2.00	0.44
1:A:149:LEU:H	1:A:149:LEU:HD12	1.81	0.43
2:B:419:THR:O	2:B:447:PRO:HD2	2.18	0.43
2:E:539:VAL:HG21	2:E:613:LEU:CD1	2.47	0.43
2:E:252:LEU:HD22	2:E:420:GLU:OE1	2.18	0.43
2:E:269:PRO:HB3	2:E:401:ILE:HD13	2.00	0.43
2:B:136:VAL:HA	2:B:183:THR:O	2.18	0.43
2:E:133:THR:HB	2:E:137:GLU:OE1	2.19	0.43
1:A:3:GLN:H	1:A:3:GLN:HG2	1.67	0.42
2:B:125:ALA:O	2:B:128:ARG:HG2	2.19	0.42
2:B:148:LYS:HD2	2:B:167:VAL:HG22	2.01	0.42
2:E:201:ARG:NH2	2:E:215:ASN:OD1	2.52	0.42
2:E:148:LYS:HD2	2:E:167:VAL:HG22	2.01	0.42
2:B:133:THR:HB	2:B:137:GLU:OE1	2.19	0.42
2:B:360:ALA:HB1	2:B:671:GLY:HA3	2.01	0.42
2:E:131:LEU:HD12	2:E:131:LEU:O	2.19	0.42
2:B:131:LEU:HD12	2:B:131:LEU:O	2.19	0.42
2:B:611:LEU:O	2:B:613:LEU:N	2.53	0.42
2:E:198:GLN:HE22	2:E:202:GLU:HG3	1.84	0.42
2:E:201:ARG:HG2	2:E:201:ARG:NH1	2.34	0.42
2:B:532:HIS:ND1	2:B:533:GLN:O	2.41	0.42
1:D:347:TRP:CZ3	2:E:649:LEU:HD11	2.55	0.42
1:D:363:VAL:HG11	2:E:639:SER:HB3	2.01	0.42
2:B:201:ARG:HG2	2:B:201:ARG:NH1	2.34	0.42
2:B:252:LEU:HD22	2:B:420:GLU:OE1	2.18	0.42
2:E:287:THR:O	2:E:289:ARG:HG3	2.18	0.42
2:E:532:HIS:ND1	2:E:533:GLN:O	2.41	0.42
1:D:91:ALA:HB3	1:D:96:VAL:HG23	2.01	0.42
2:E:423:TYR:CE2	2:E:425:SER:HB3	2.55	0.42
1:A:91:ALA:HB3	1:A:96:VAL:HG23	2.01	0.42
2:B:256:THR:OG1	2:B:262:PRO:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:GLN:HE22	2:B:202:GLU:HG3	1.85	0.42
2:B:423:TYR:CE2	2:B:425:SER:HB3	2.55	0.42
2:E:125:ALA:O	2:E:128:ARG:HG2	2.19	0.42
2:E:139:PHE:N	2:E:139:PHE:CD2	2.87	0.42
2:B:511:TRP:HB2	2:B:649:LEU:O	2.21	0.41
2:E:222:GLN:HE21	2:E:222:GLN:HB2	1.62	0.41
2:E:249:ILE:HG21	2:E:284:ARG:HD3	2.00	0.41
2:B:201:ARG:NH2	2:B:215:ASN:OD1	2.52	0.41
1:D:168:TRP:CZ3	1:D:172:LYS:HD2	2.55	0.41
1:D:358:LYS:O	2:E:636:ARG:NH2	2.52	0.41
2:B:249:ILE:HG21	2:B:284:ARG:HD3	2.00	0.41
2:E:171:HIS:C	2:E:173:PRO:HD3	2.41	0.41
2:E:611:LEU:O	2:E:613:LEU:N	2.53	0.41
1:A:57:VAL:HG11	1:A:74:ALA:HB2	2.02	0.41
2:B:171:HIS:C	2:B:173:PRO:HD3	2.40	0.41
1:A:94:TYR:HD1	1:A:94:TYR:HA	1.75	0.41
1:A:168:TRP:CZ3	1:A:172:LYS:HD2	2.55	0.41
2:E:360:ALA:HB1	2:E:671:GLY:HA3	2.01	0.41
2:E:511:TRP:HB2	2:E:649:LEU:O	2.21	0.41
1:D:15:LEU:HD21	1:D:174:LEU:HD13	2.03	0.41
1:D:57:VAL:HG11	1:D:74:ALA:HB2	2.02	0.41
2:E:311:GLU:O	2:E:312:PHE:HB2	2.21	0.41
1:A:15:LEU:HD21	1:A:174:LEU:HD13	2.03	0.41
2:E:256:THR:OG1	2:E:262:PRO:HG2	2.20	0.40
2:B:139:PHE:CD2	2:B:139:PHE:N	2.87	0.40
1:D:94:TYR:HD1	1:D:94:TYR:HA	1.75	0.40
2:E:287:THR:HA	2:E:297:TRP:CD1	2.56	0.40
2:E:363:THR:C	2:E:365:ALA:H	2.25	0.40
2:B:287:THR:HA	2:B:297:TRP:CD1	2.56	0.40
2:B:383:ARG:HA	2:B:383:ARG:HE	1.86	0.40
2:E:383:ARG:HE	2:E:383:ARG:HA	1.86	0.40
2:B:311:GLU:O	2:B:312:PHE:HB2	2.21	0.40
2:E:334:HIS:O	2:E:334:HIS:ND1	2.53	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	175/391 (45%)	154 (88%)	19 (11%)	2 (1%)	14 42
1	D	175/391 (45%)	154 (88%)	19 (11%)	2 (1%)	14 42
2	B	516/640 (81%)	400 (78%)	103 (20%)	13 (2%)	5 21
2	E	516/640 (81%)	400 (78%)	103 (20%)	13 (2%)	5 21
All	All	1382/2062 (67%)	1108 (80%)	244 (18%)	30 (2%)	10 24

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	116	PRO
2	B	176	HIS
2	B	195	PRO
2	B	294	SER
2	B	398	PRO
2	E	116	PRO
2	E	176	HIS
2	E	195	PRO
2	E	294	SER
2	E	398	PRO
1	A	148	GLN
2	B	444	SER
2	B	662	ARG
1	D	148	GLN
2	E	444	SER
2	E	662	ARG
1	A	89	GLY
2	B	118	ASN
2	B	227	SER
1	D	89	GLY
2	E	118	ASN
2	E	227	SER

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Mol	Chain	Res	Type
2	B	288	ASP
2	B	312	PHE
2	E	288	ASP
2	E	312	PHE
2	B	308	GLY
2	E	308	GLY
2	B	364	PRO
2	E	364	PRO

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	144/316 (46%)	143 (99%)	1 (1%)	84	95
1	D	144/316 (46%)	143 (99%)	1 (1%)	84	95
2	B	446/542 (82%)	440 (99%)	6 (1%)	69	90
2	E	446/542 (82%)	440 (99%)	6 (1%)	69	90
All	All	1180/1716 (69%)	1166 (99%)	14 (1%)	72	91

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
2	B	201	ARG
2	B	222	GLN
2	B	257	ARG
2	B	640	LEU
2	B	648	HIS
2	B	680	TYR
1	D	94	TYR
2	E	201	ARG
2	E	222	GLN
2	E	257	ARG
2	E	640	LEU
2	E	648	HIS

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Mol	Chain	Res	Type
2	E	680	TYR

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

Mol	Chain	Res	Type
1	A	146	HIS
2	B	120	ASN
2	B	174	HIS
2	B	198	GLN
2	B	222	GLN
2	B	327	ASN
1	D	3	GLN
1	D	146	HIS
2	E	120	ASN
2	E	174	HIS
2	E	198	GLN
2	E	222	GLN
2	E	327	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	AGS	E	801	4	26,33,33	0.80	0	26,52,52	1.29	2 (7%)
3	AGS	B	801	4	26,33,33	0.80	0	26,52,52	1.29	2 (7%)

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	AGS	E	801	4	-	1/17/38/38	0/3/3/3
3	AGS	B	801	4	-	1/17/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	801	AGS	PA-O3A-PB	-4.20	118.40	132.83
3	E	801	AGS	PA-O3A-PB	-4.20	118.42	132.83
3	B	801	AGS	C5-C6-N6	2.31	123.87	120.35
3	E	801	AGS	C5-C6-N6	2.28	123.81	120.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	AGS	PA-O3A-PB-O2B
3	E	801	AGS	PA-O3A-PB-O2B

There are no ring outliers.

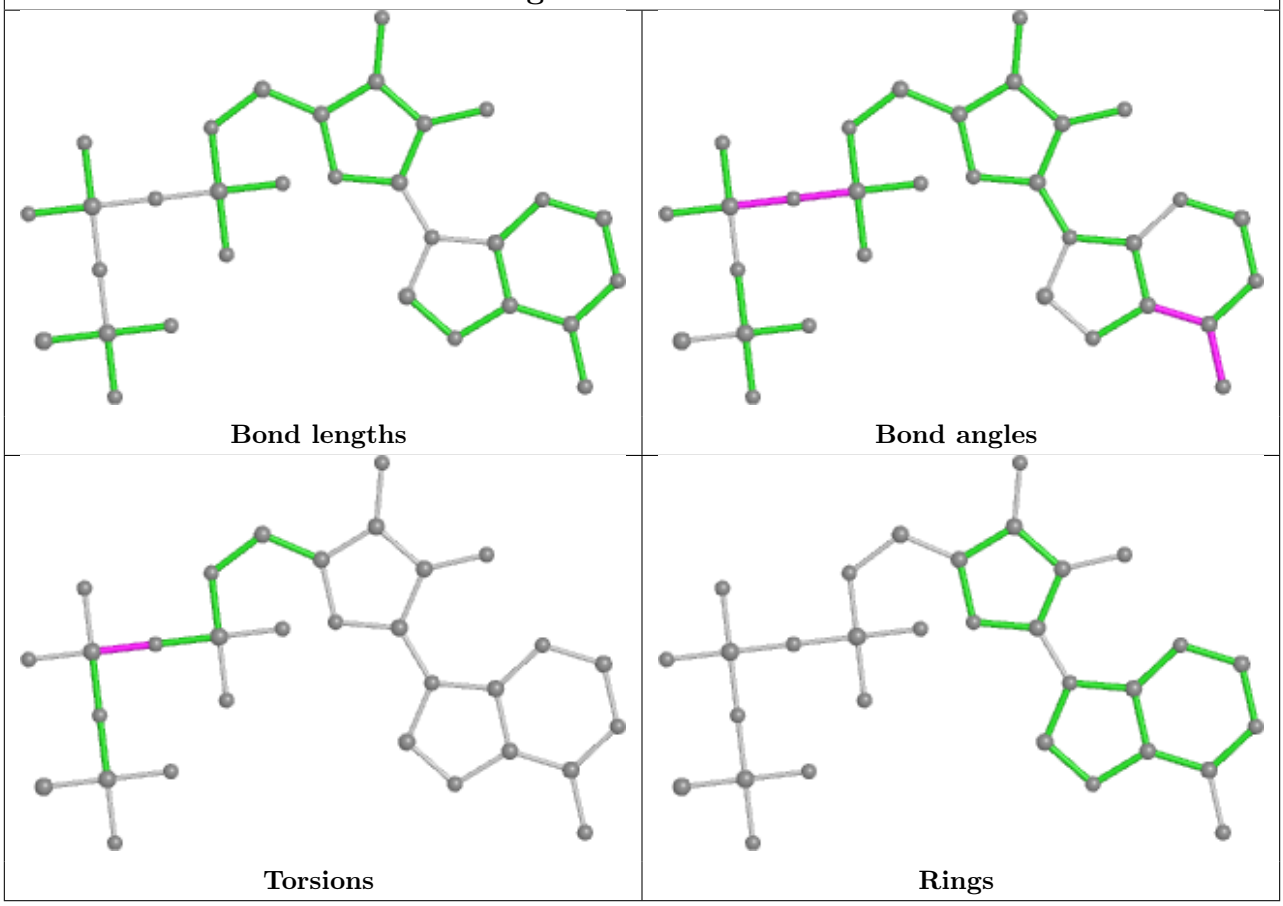
2 monomers are involved in 2 short contacts:

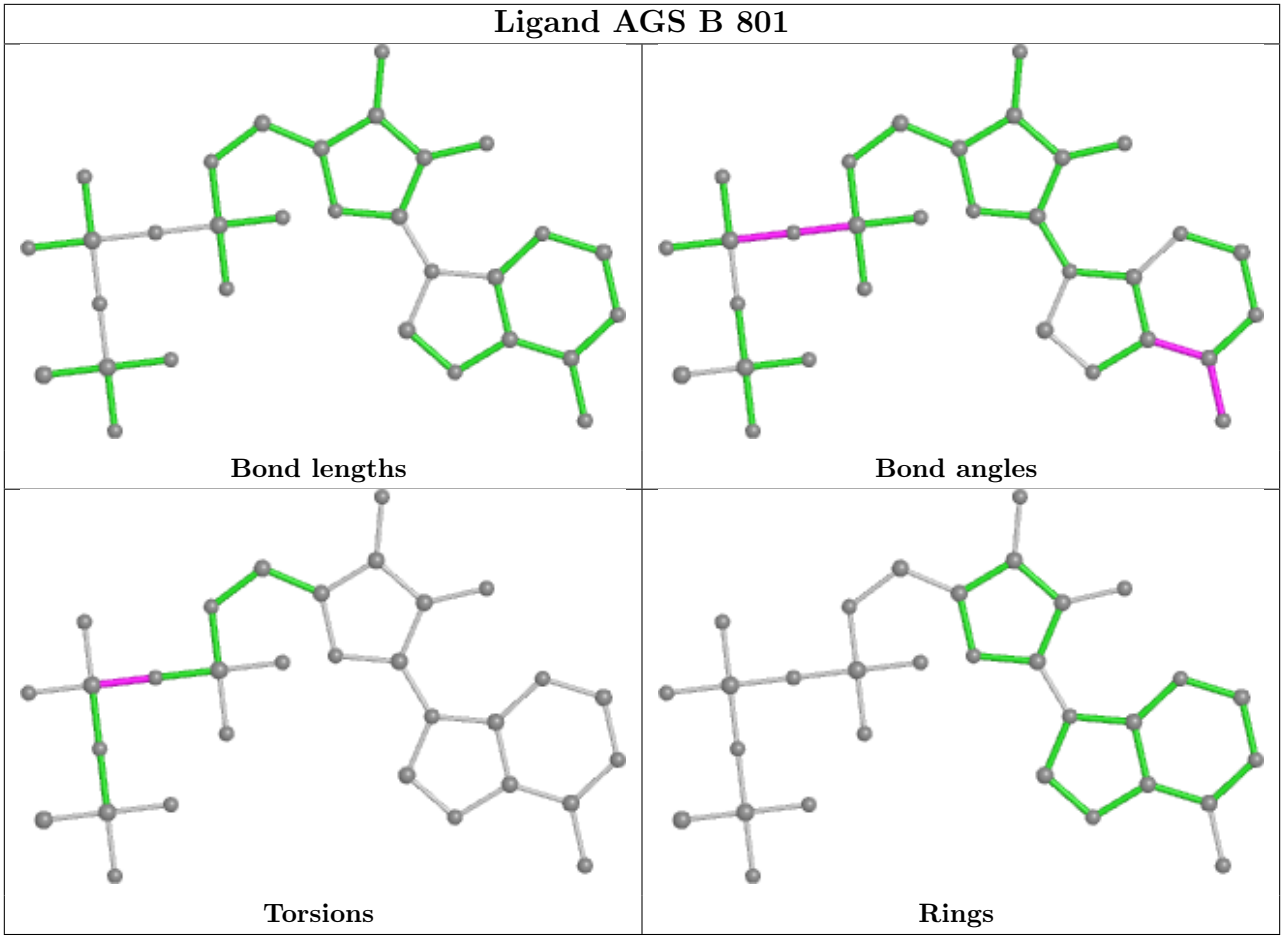
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	801	AGS	1	0
3	B	801	AGS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 E 801





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.

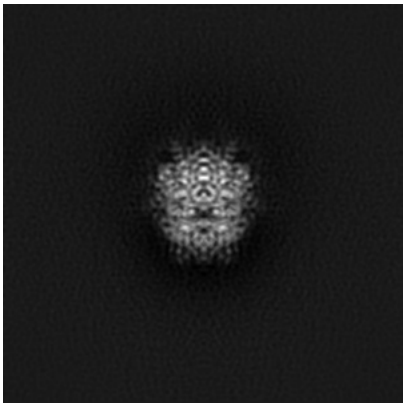
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20040. These allow visual inspection of the internal detail of the map and identification of artifacts.

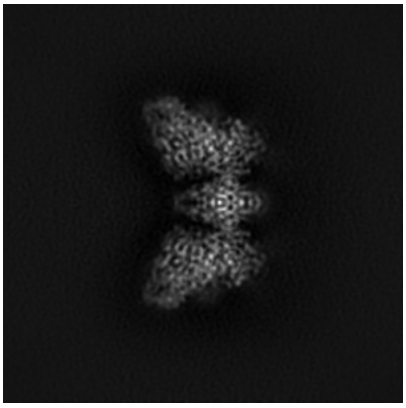
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

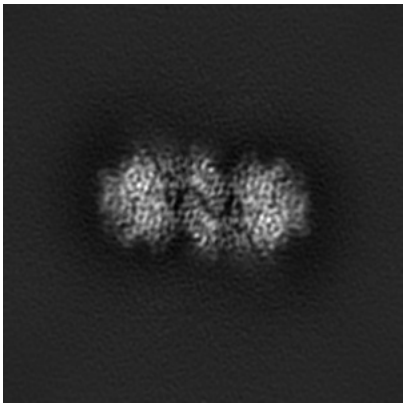
6.1.1 Primary map



X



Y



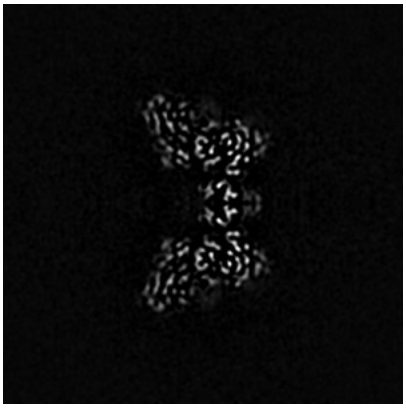
Z

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

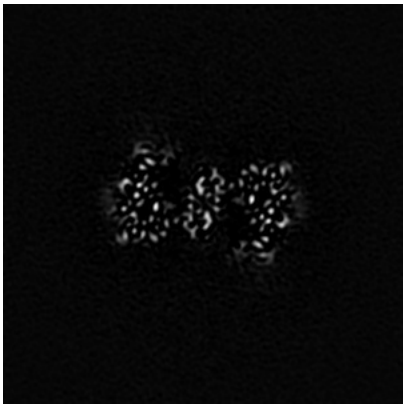
6.2 Central slices (i)

6.2.1 Primary map

X Index: 112



Y Index: 112

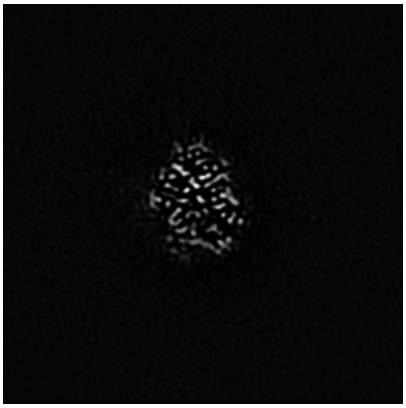


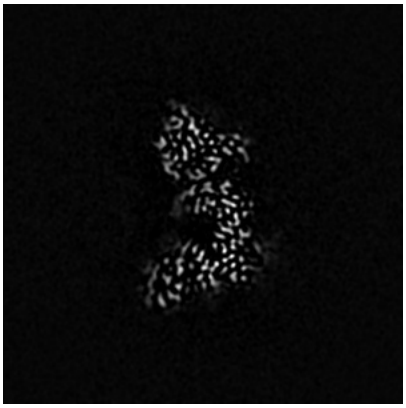
Z Index: 112

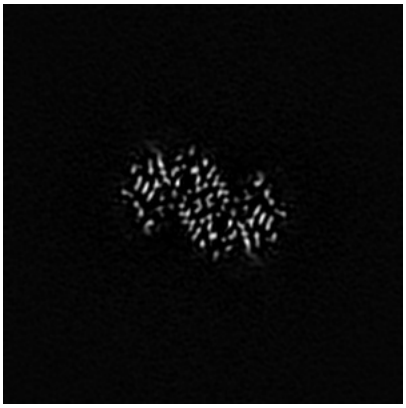
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 146

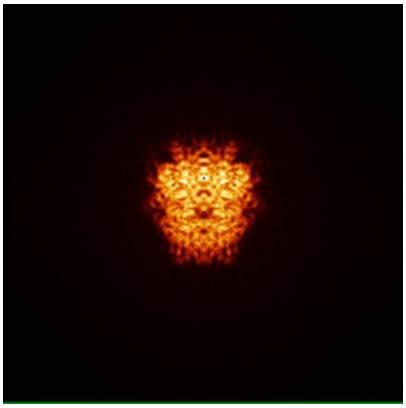

Y Index: 122

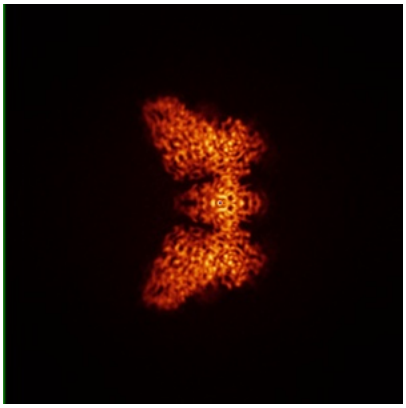

Z Index: 124

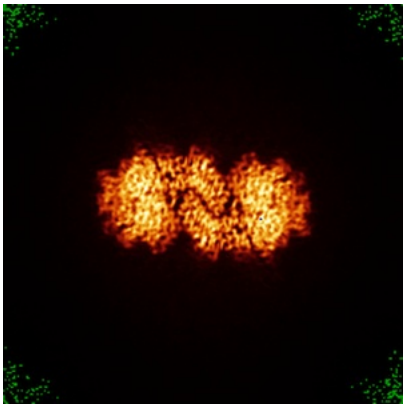
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

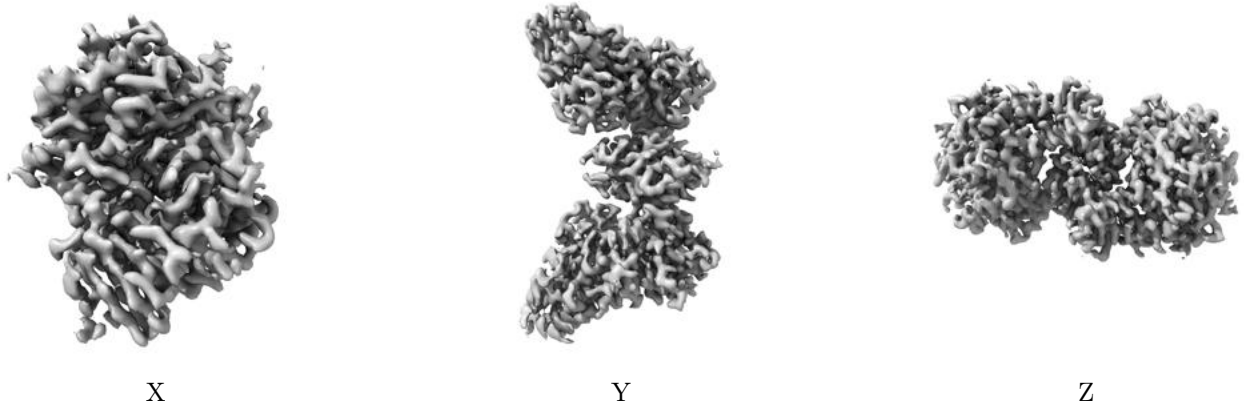

Y


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

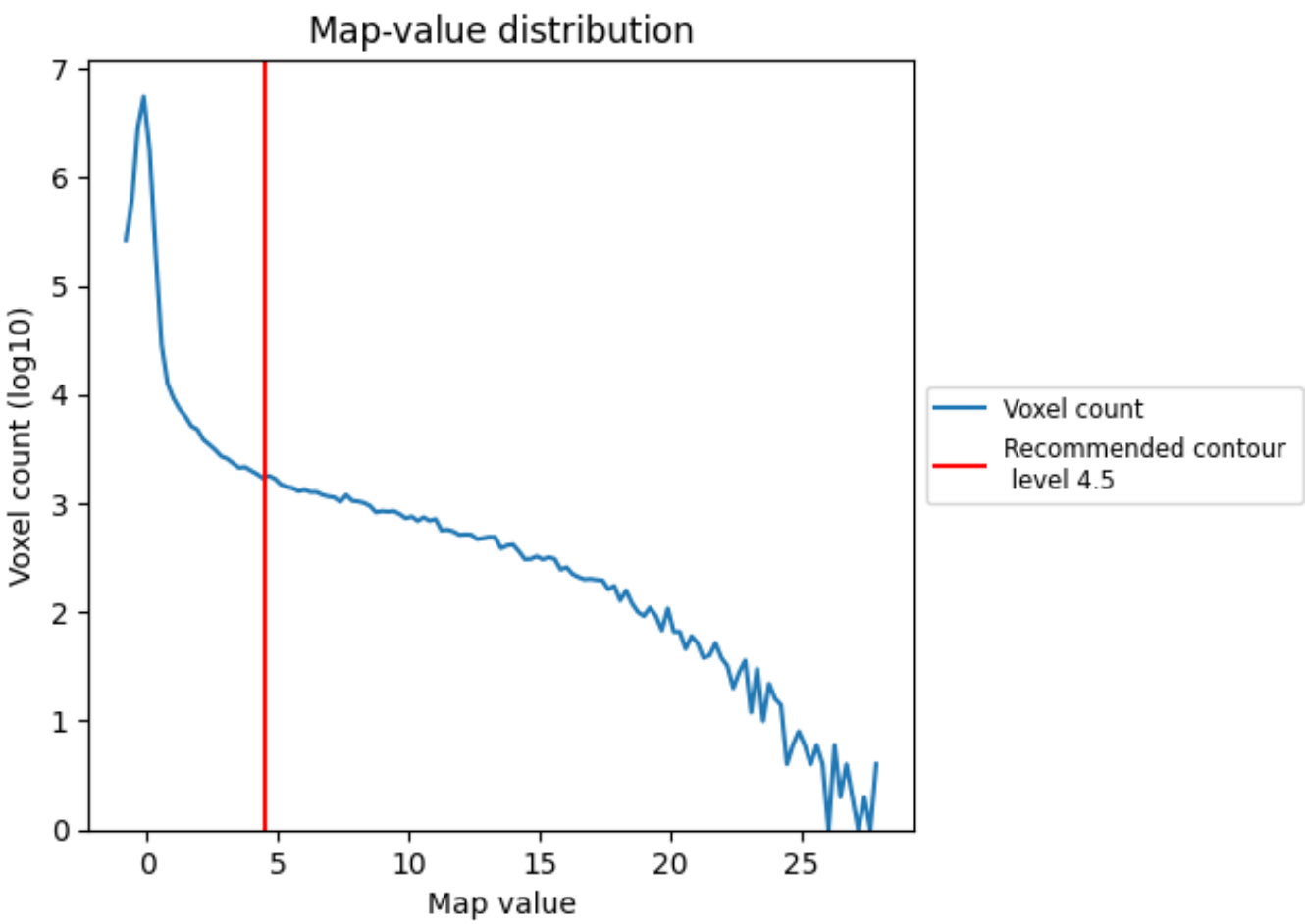
6.6 Mask visualisation (i)

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

7 Map analysis (i)

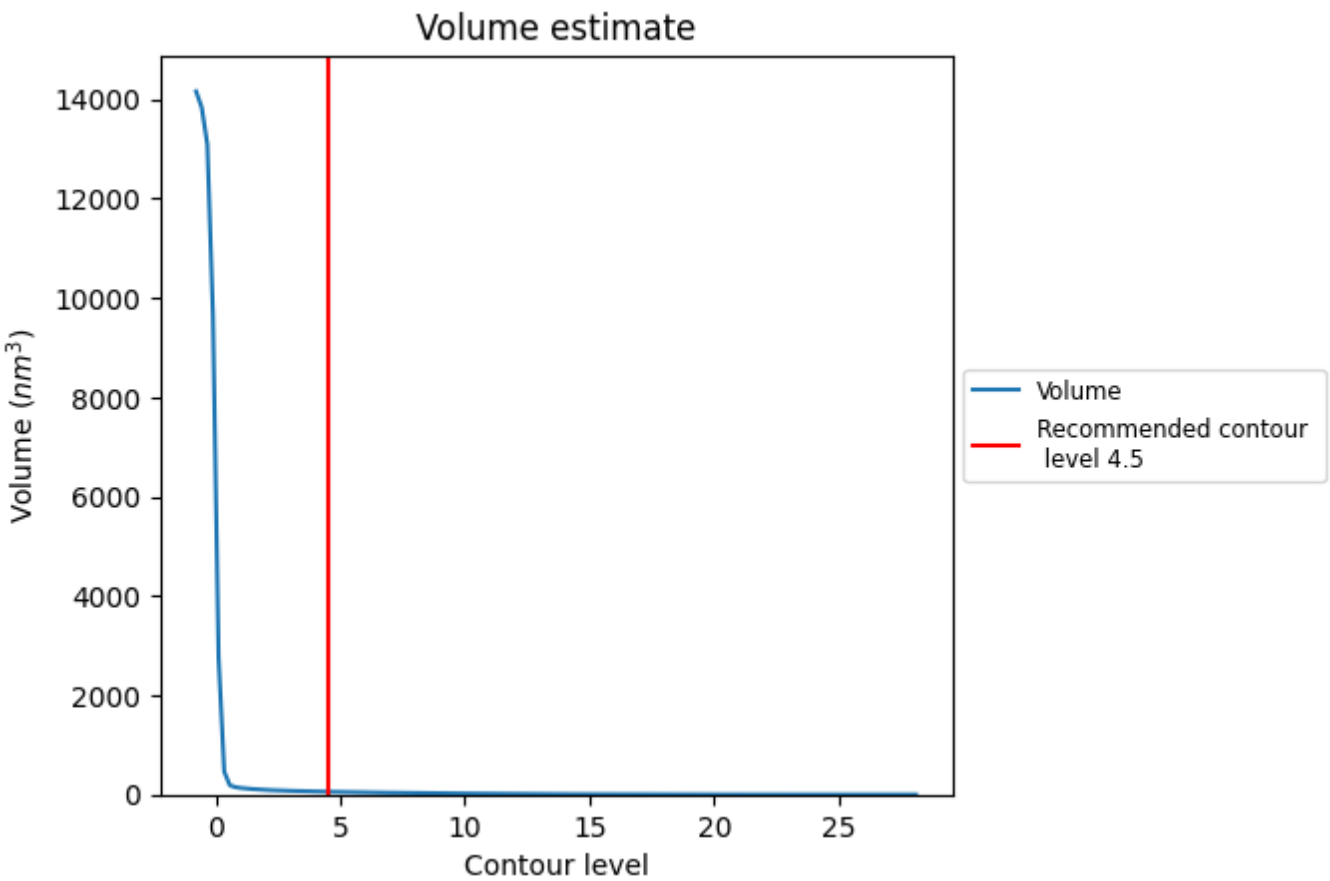
This section contains the results of statistical analysis of the map.

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.

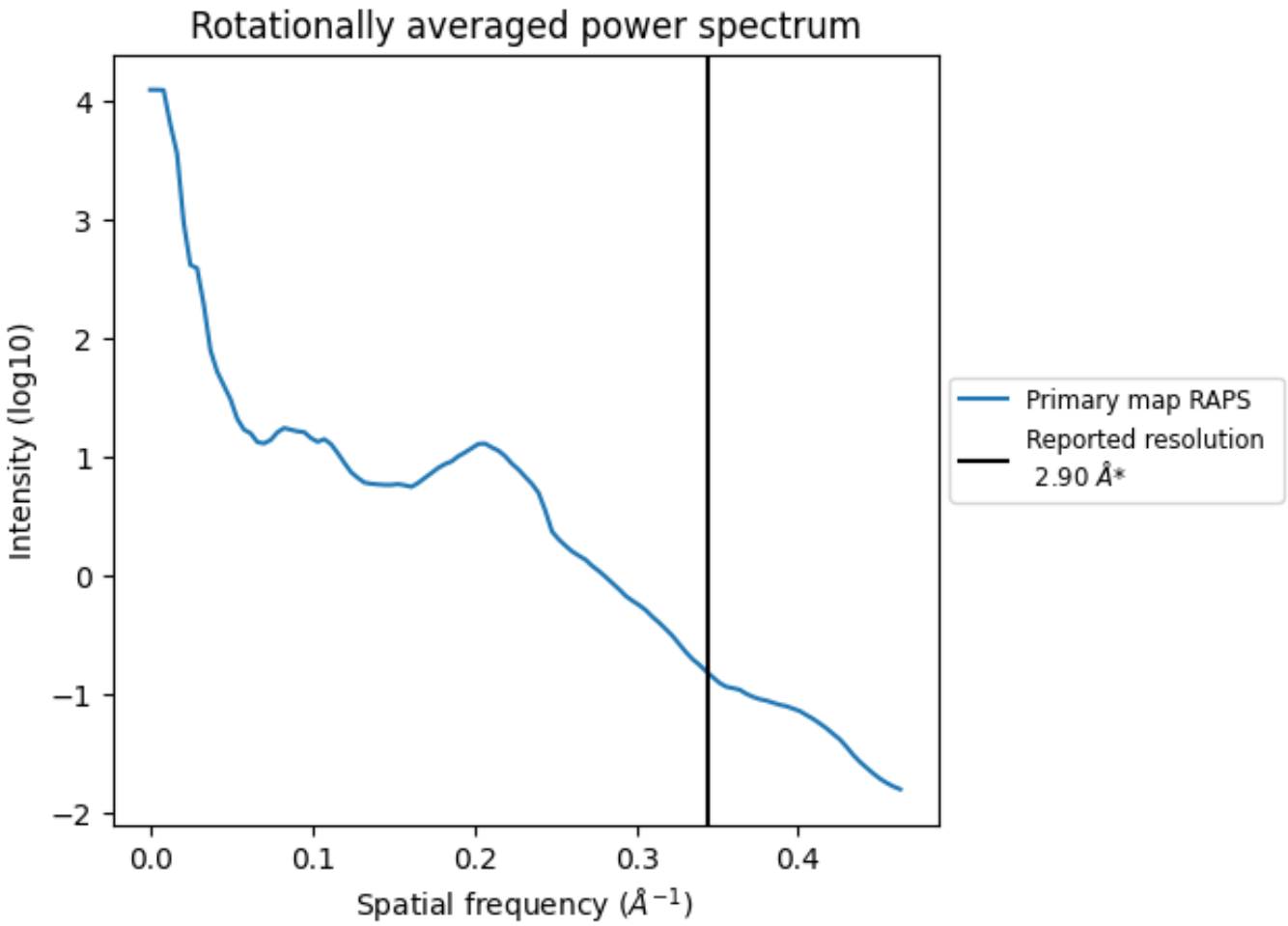
7.2 Volume estimate (i)



The volume at the recommended contour level is 57 nm^3; this corresponds to an approximate mass of 51 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 0.345 Å^{-1}

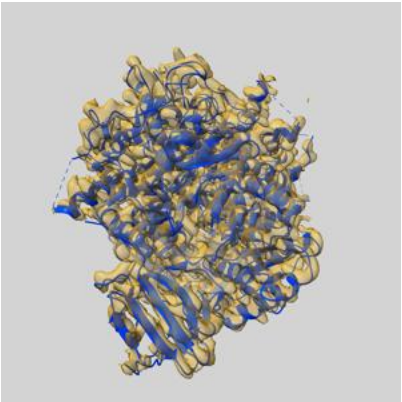
8 Fourier-Shell correlation (i)

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

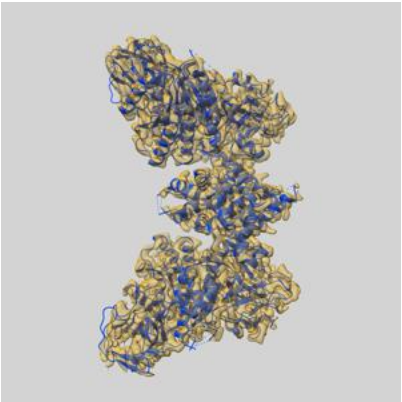
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20040 and PDB model 6OF2. Per-residue inclusion information can be found in section 3 on page 6.

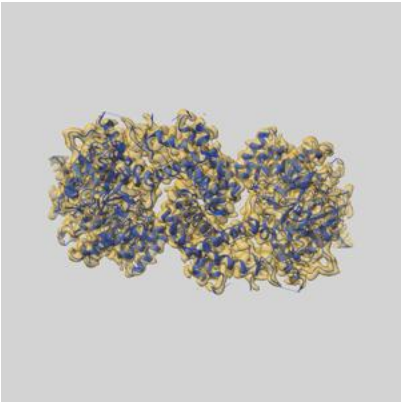
9.1 Map-model overlay (i)



X



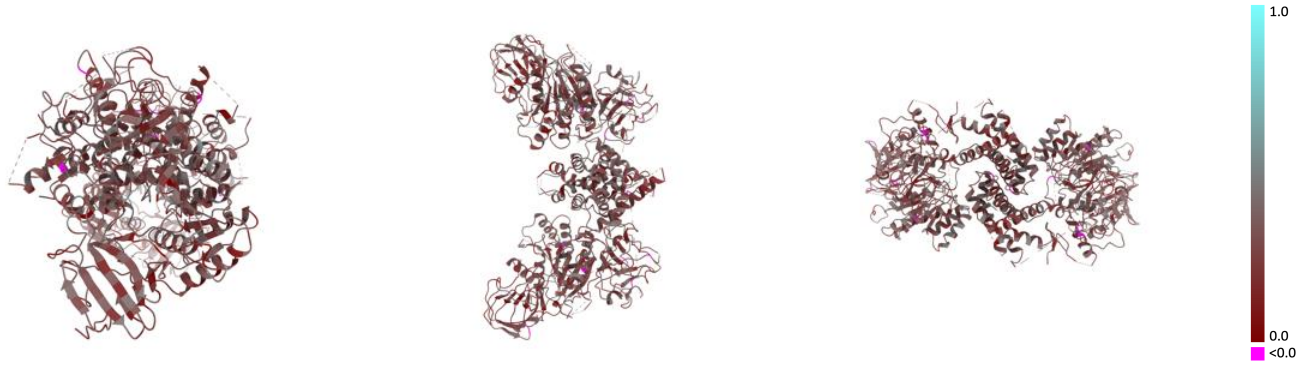
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 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.

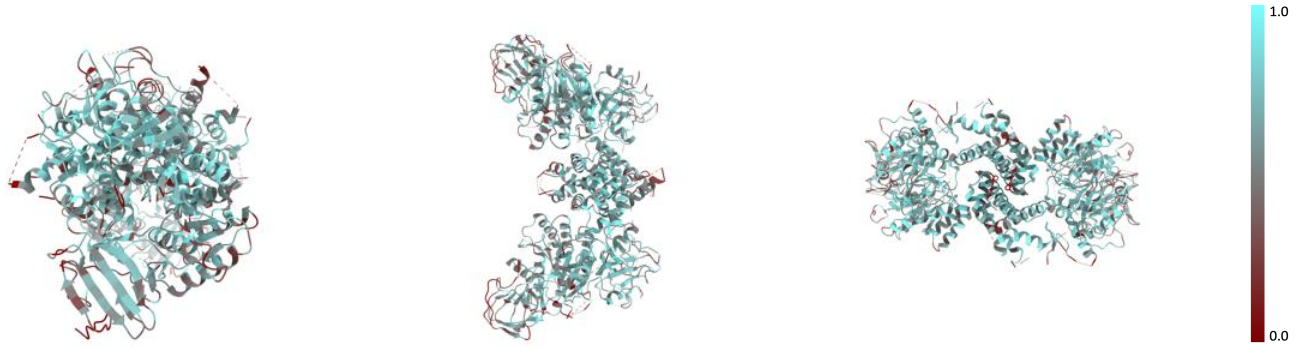
9.2 Q-score mapped to coordinate model (i)



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.

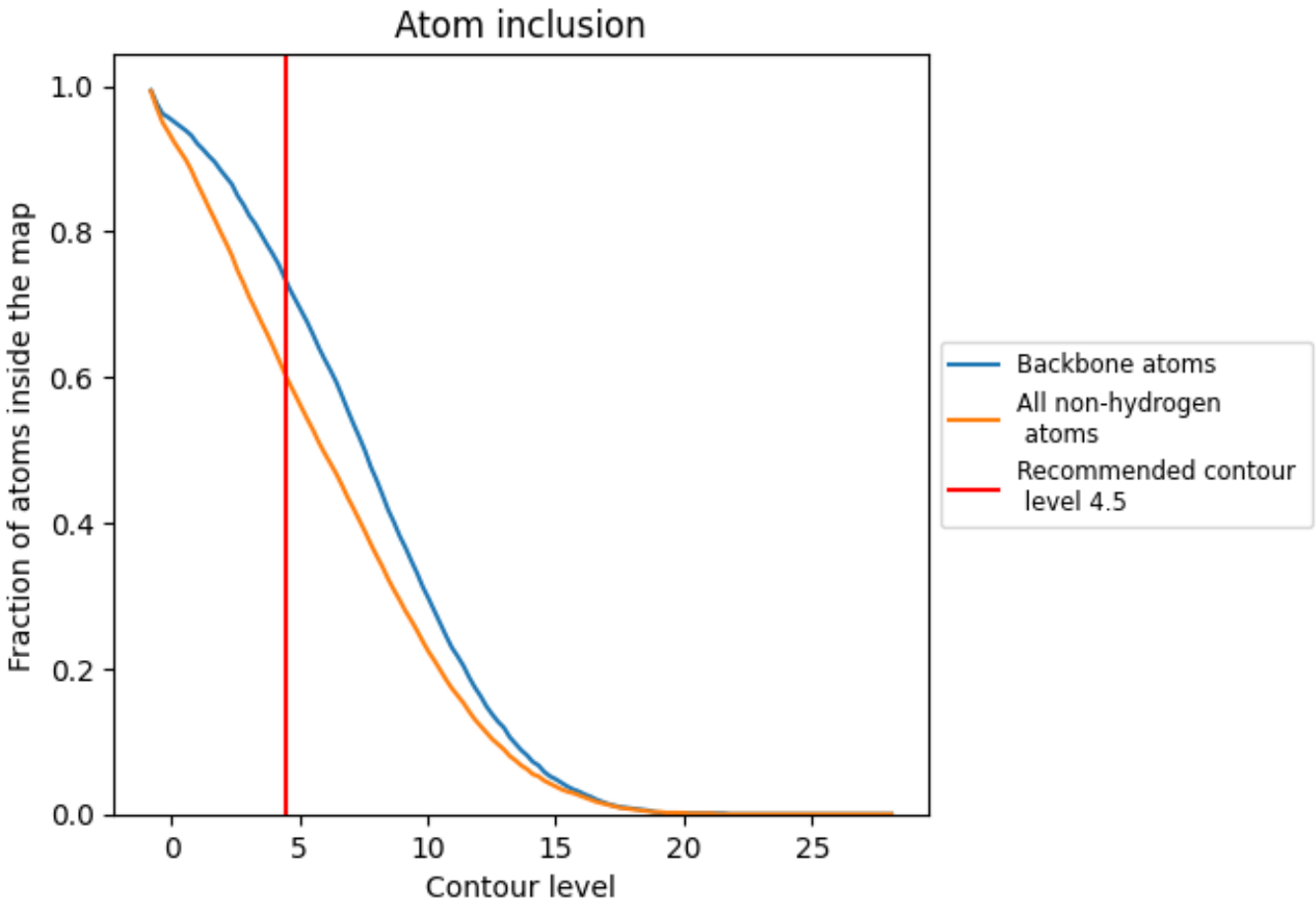
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 60% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6000	0.3000
A	0.6370	0.3210
B	0.5940	0.3040
D	0.6270	0.3110
E	0.5850	0.2840