Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 01:26 PM EDT

PDB ID	:	7MKJ / pdb_00007mkj
EMDB ID	:	EMD-23897
Title	:	Cryo-EM structure of Escherichia coli RNA polymerase bound to T7A1 promoter DNA
Authors	:	Saecker, R.M.; Darst, S.A.; Chen, J.
Deposited on	:	2021-04-23
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 ⓘ 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:

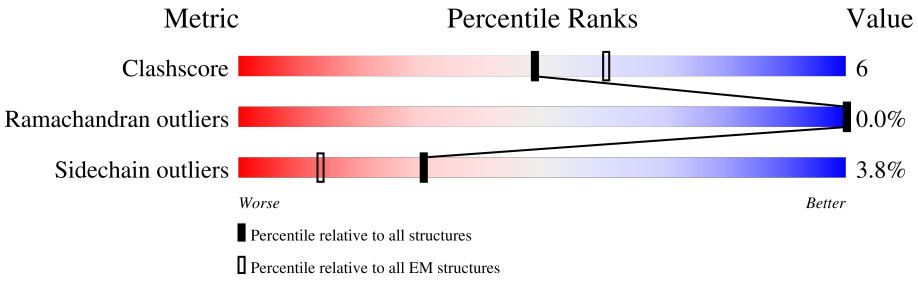
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	G	329	60% 10% 29%
1	H	329	56% 10% 33%
1	R	329	22% 20% 78%
2	I	1342	82% 17%
3	J	1407	6% 78% 16% 5%
4	K	91	65% 21% 13%
5	L	613	12% 67% 9% 23%
6	P	91	8% 47% 21% 32%

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Mol	Chain	Length	Quality of chain
7	Q	91	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32007 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	233	Total	C	N	O	S	0	0
			1808	1126	320	356	6		
1	H	222	Total	C	N	O	S	0	0
			1710	1068	301	335	6		
1	R	73	Total	C	N	O	S	0	0
			572	362	100	108	2		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1336	Total	C	N	O	S	0	0
			10386	6525	1852	1960	49		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1384	VAL	MET	conflict	UNP A0A4S1NBU2

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	471	Total	C	N	O	S	0	0
			3835	2404	686	722	23		

- Molecule 6 is a DNA chain called Nontemplate strand of T7A1 promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	62	Total	C	N	O	P	0	0
			1278	608	247	361	62		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	DC	-	insertion	GB 312369

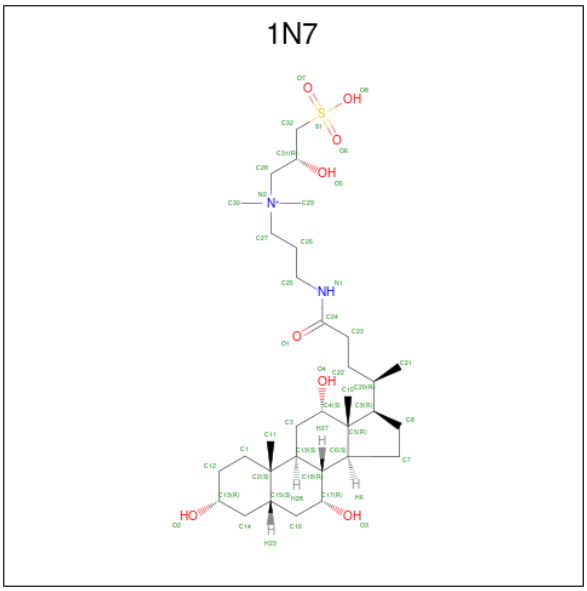
- Molecule 7 is a DNA chain called Template strand of T7A1 promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	56	Total	C	N	O	P	0	0
			1140	548	190	346	56		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	91	DG	-	insertion	GB 312369

- Molecule 8 is CHAPSO (CCD ID: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



Mol	Chain	Residues	Atoms			AltConf
8	G	1	Total	C	O	0
			27	24	3	
8	I	1	Total	C	O	0
			27	24	3	
8	J	1	Total	C	O	0
			27	24	3	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	J	1	Total	Mg	0
			1	1	

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

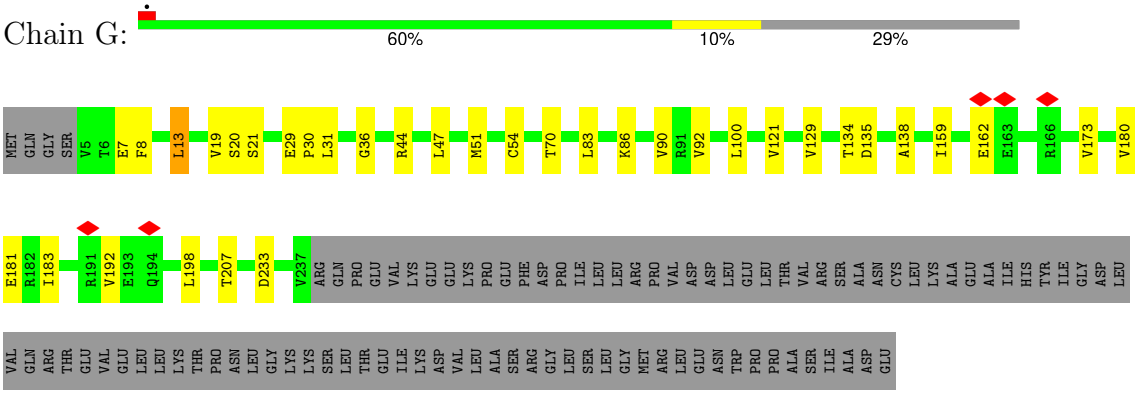
Mol	Chain	Residues	Atoms		AltConf
10	J	2	Total	Zn	0
			2	2	

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.

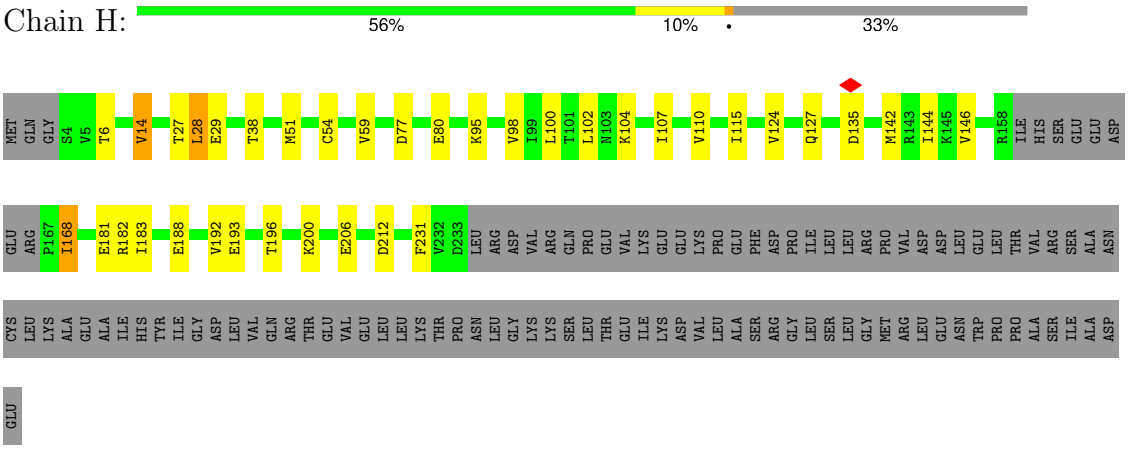
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



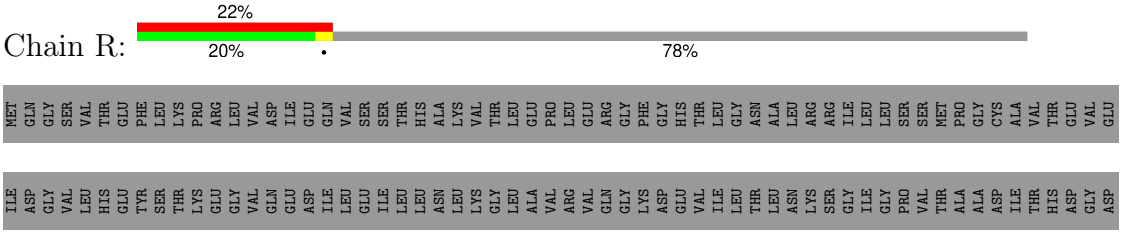
• Molecule 1: DNA-directed RNA polymerase subunit alpha

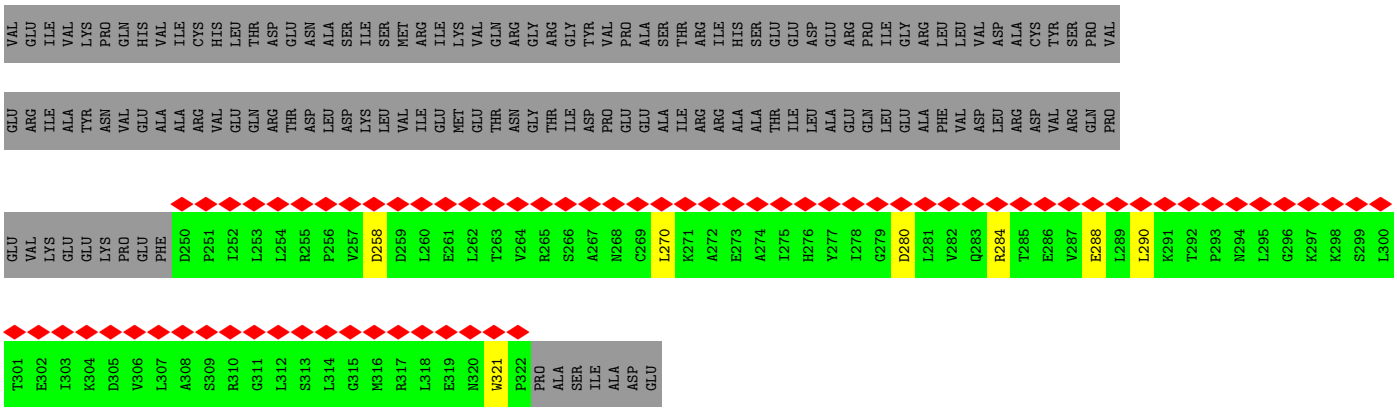
Chain H:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

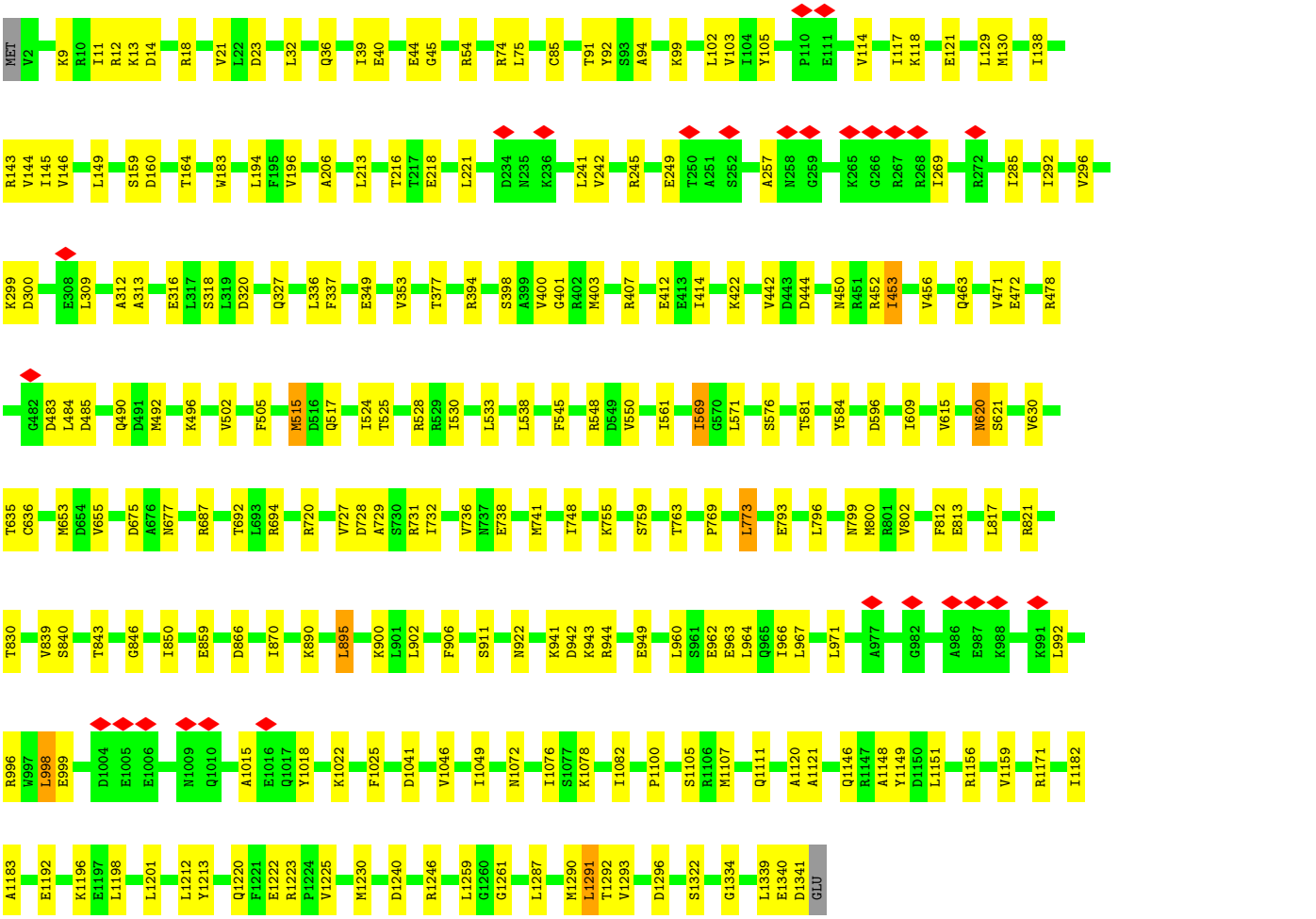
Chain R:





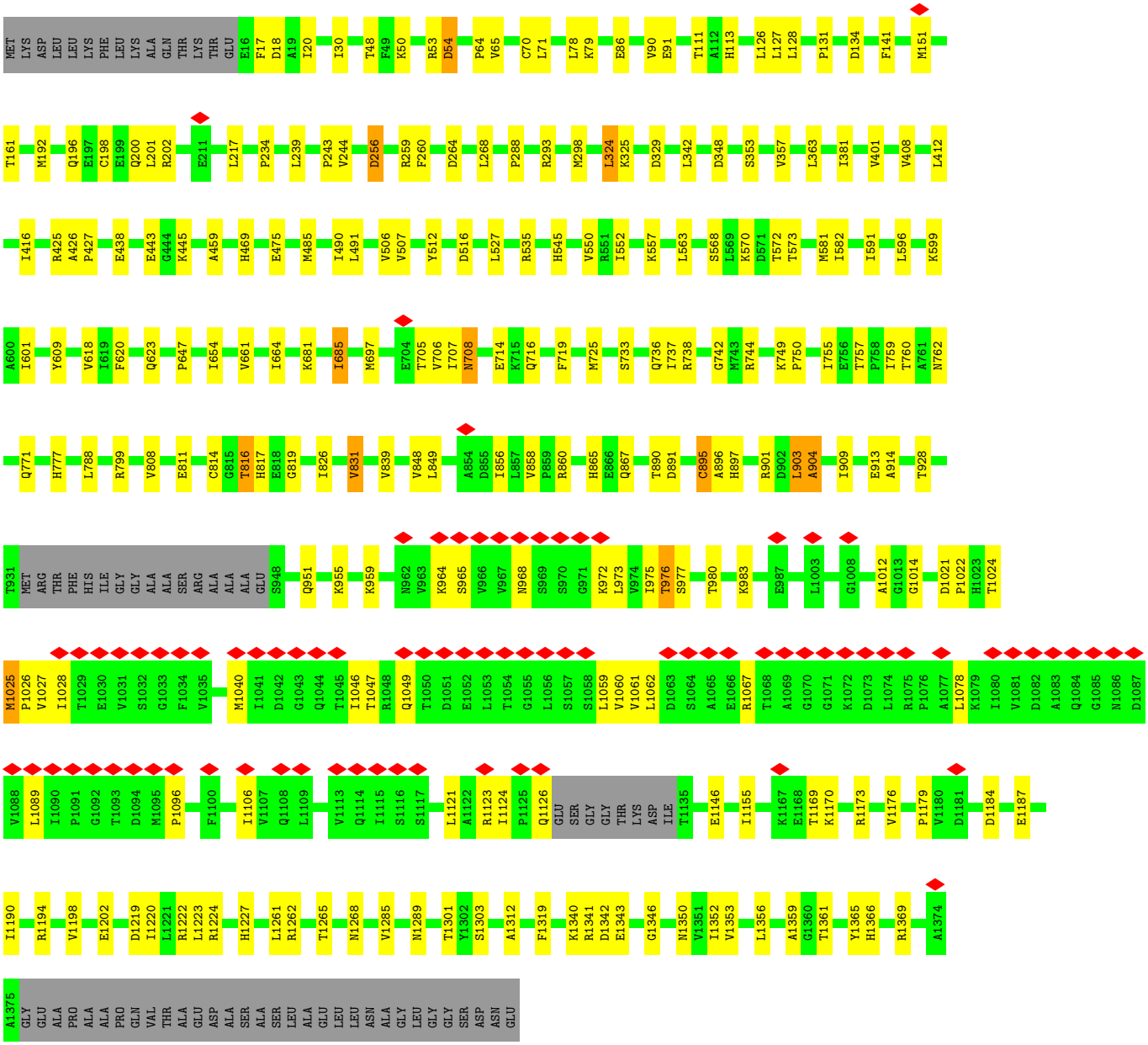
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I:



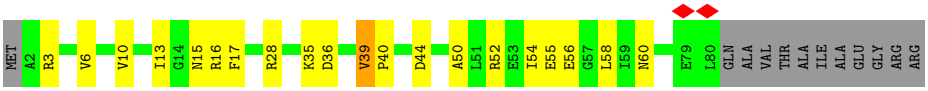
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:



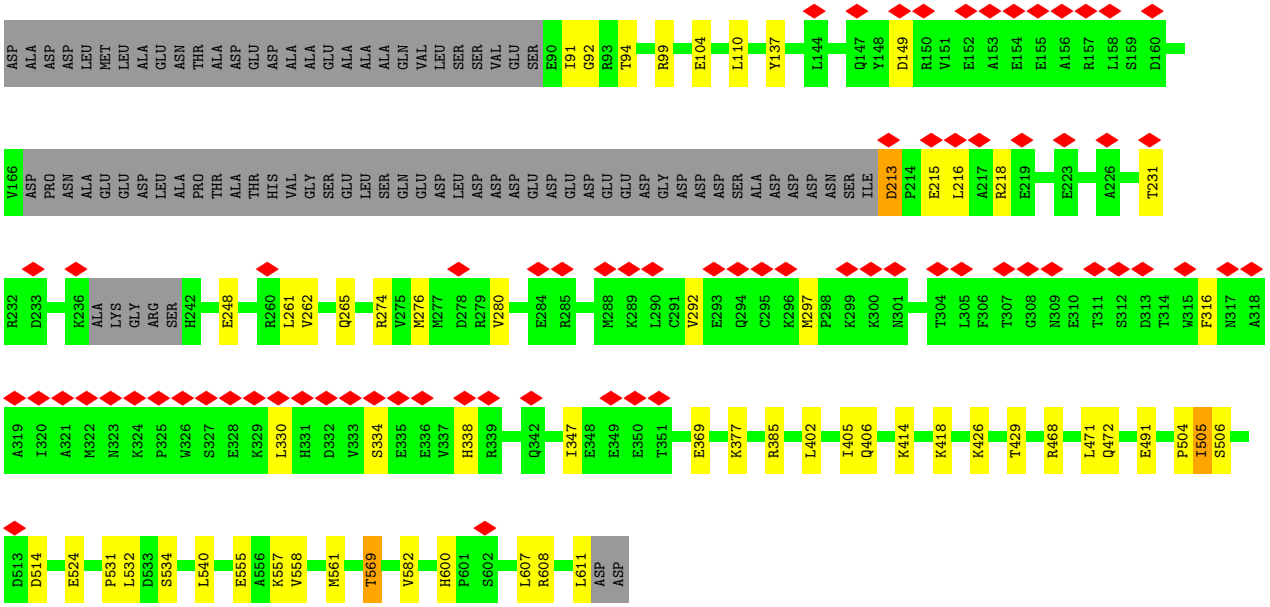
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:

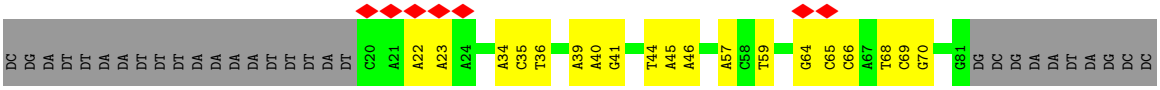


• Molecule 5: RNA polymerase sigma factor RpoD

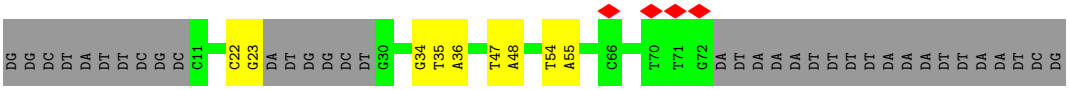
Chain L:



• Molecule 6: Nontemplate strand of T7A1 promoter DNA



• Molecule 7: Template strand of T7A1 promoter DNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	346991	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 ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.370	Depositor
Minimum map value	-3.593	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	0.34	Depositor
Map size (Å)	339.19995, 339.19995, 339.19995	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0599998, 1.0599998, 1.0599998	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1N7, ZN, 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	G	0.22	0/1830	0.43	0/2481
1	H	0.22	0/1730	0.39	0/2344
1	R	0.12	0/579	0.32	0/784
2	I	0.22	0/10736	0.41	1/14487 (0.0%)
3	J	0.21	0/10543	0.40	2/14236 (0.0%)
4	K	0.19	0/629	0.43	0/847
5	L	0.19	0/3887	0.41	0/5224
6	P	0.18	0/1438	0.37	0/2217
7	Q	0.21	0/1272	0.43	0/1958
All	All	0.21	0/32644	0.41	3/44578 (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
3	J	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1261	GLY	N-CA-C	6.55	120.21	111.03
3	J	903	LEU	CA-C-N	5.01	131.11	121.54
3	J	903	LEU	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	904	ALA	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	G	1808	0	1835	19	0
1	H	1710	0	1745	17	0
1	R	572	0	602	3	0
2	I	10567	0	10585	134	0
3	J	10386	0	10607	130	0
4	K	627	0	634	10	0
5	L	3835	0	3908	37	0
6	P	1278	0	696	15	0
7	Q	1140	0	640	6	0
8	G	27	0	38	9	0
8	I	27	0	37	7	0
8	J	27	0	38	9	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	32007	0	31365	355	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 6.

All (355) 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)
8:G:401:1N7:C3	8:G:401:1N7:C19	1.82	1.55
8:J:1504:1N7:C3	8:J:1504:1N7:C19	1.83	1.55
8:I:1401:1N7:C3	8:I:1401:1N7:C19	1.82	1.52
2:I:398:SER:HB2	2:I:401:GLY:H	1.48	0.78
8:I:1401:1N7:C3	8:I:1401:1N7:C2	2.64	0.74
8:J:1504:1N7:C3	8:J:1504:1N7:C2	2.64	0.73
8:G:401:1N7:C3	8:G:401:1N7:C2	2.65	0.71
8:I:1401:1N7:C3	8:I:1401:1N7:C18	2.68	0.70
2:I:738:GLU:HA	2:I:741:MET:HE2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.25	0.69
2:I:1246:ARG:NH1	3:J:348:ASP:OD1	2.25	0.69
3:J:507:VAL:HG23	3:J:601:ILE:HD12	1.74	0.69
1:G:7:GLU:HG2	1:G:8:PHE:H	1.58	0.69
2:I:9:LYS:HG2	2:I:1171:ARG:HH12	1.57	0.68
3:J:557:LYS:HB3	3:J:563:LEU:HD23	1.76	0.68
2:I:748:ILE:HD11	2:I:967:LEU:HA	1.76	0.67
8:J:1504:1N7:C3	8:J:1504:1N7:C18	2.70	0.67
8:G:401:1N7:C3	8:G:401:1N7:C18	2.68	0.66
3:J:955:LYS:HG2	3:J:1012:ALA:HA	1.77	0.66
2:I:103:VAL:HG12	2:I:117:ILE:HG22	1.77	0.65
2:I:528:ARG:NH2	2:I:576:SER:O	2.29	0.65
2:I:890:LYS:NZ	2:I:911:SER:O	2.29	0.65
2:I:996:ARG:NH1	2:I:999:GLU:OE1	2.30	0.65
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.77	0.64
7:Q:34:DG:H2"	7:Q:35:DT:H5"	1.79	0.64
1:H:102:LEU:HD23	1:H:142:MET:HE3	1.79	0.64
1:G:192:VAL:HG11	1:G:198:LEU:HD12	1.79	0.64
3:J:363:LEU:HD21	3:J:618:VAL:HG13	1.79	0.64
2:I:998:LEU:HD12	2:I:999:GLU:HG3	1.81	0.62
2:I:18:ARG:O	2:I:1156:ARG:NH1	2.32	0.62
3:J:1027:VAL:HG23	3:J:1121:LEU:HB2	1.82	0.62
2:I:32:LEU:HA	2:I:130:MET:HE1	1.82	0.62
3:J:475:GLU:OE2	4:K:28:ARG:NH2	2.32	0.61
5:L:94:THR:HG21	5:L:99:ARG:HD2	1.82	0.61
3:J:965:SER:HB2	3:J:973:LEU:HD11	1.82	0.61
5:L:600:HIS:NE2	1:R:258:ASP:O	2.34	0.61
2:I:242:VAL:HB	2:I:245:ARG:HD3	1.83	0.61
1:G:47:LEU:HD23	1:G:51:MET:HE3	1.82	0.61
1:G:181:GLU:O	2:I:821:ARG:NH2	2.33	0.61
3:J:1356:LEU:O	3:J:1366:HIS:NE2	2.33	0.61
6:P:64:DG:H4'	6:P:65:DC:H5'	1.83	0.60
2:I:138:ILE:HD12	2:I:143:ARG:HD3	1.82	0.60
2:I:13:LYS:NZ	2:I:1151:LEU:O	2.32	0.60
8:J:1504:1N7:H4	8:J:1504:1N7:H17	1.81	0.60
5:L:213:ASP:HB2	5:L:216:LEU:HB3	1.83	0.60
5:L:557:LYS:HE3	5:L:561:MET:HE3	1.83	0.60
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.83	0.59
3:J:909:ILE:HD11	3:J:913:GLU:HG2	1.84	0.59
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.83	0.59
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ILE:HG13	1:G:162:GLU:HA	1.84	0.58
7:Q:35:DT:H3'	7:Q:36:DA:H4'	1.86	0.58
3:J:1262:ARG:NH2	3:J:1312:ALA:O	2.36	0.58
6:P:69:DC:H2'	6:P:70:DG:C8	2.38	0.58
2:I:478:ARG:NH1	2:I:483:ASP:OD2	2.36	0.58
4:K:44:ASP:OD2	4:K:52:ARG:NH1	2.36	0.58
2:I:400:VAL:HG23	8:I:1401:1N7:H26	1.85	0.57
2:I:444:ASP:O	2:I:450:ASN:ND2	2.35	0.57
2:I:525:THR:HG21	2:I:687:ARG:HD3	1.87	0.57
2:I:902:LEU:HD13	5:L:607:LEU:HD12	1.87	0.57
5:L:231:THR:HG23	5:L:248:GLU:HB3	1.86	0.57
2:I:257:ALA:HB2	2:I:285:ILE:HG22	1.87	0.57
2:I:748:ILE:HD12	2:I:966:ILE:HG22	1.86	0.57
2:I:159:SER:HB2	2:I:442:VAL:HG11	1.87	0.57
2:I:102:LEU:HB3	2:I:118:LYS:HG3	1.87	0.56
3:J:744:ARG:HH11	3:J:759:ILE:HD11	1.70	0.56
1:G:100:LEU:HD21	1:G:121:VAL:HG11	1.87	0.56
3:J:582:ILE:HD12	3:J:623:GLN:HB3	1.86	0.56
2:I:1341:ASP:OD1	2:I:1341:ASP:N	2.39	0.56
2:I:692:THR:HA	2:I:830:THR:HG22	1.88	0.56
1:H:181:GLU:O	3:J:535:ARG:NH1	2.39	0.55
2:I:596:ASP:N	2:I:596:ASP:OD1	2.40	0.55
3:J:661:VAL:HG13	3:J:685:ILE:HD11	1.87	0.55
3:J:959:LYS:HB3	3:J:983:LYS:HB2	1.88	0.55
2:I:1341:ASP:HB3	3:J:17:PHE:HA	1.88	0.55
3:J:708:ASN:OD1	3:J:708:ASN:N	2.39	0.55
2:I:483:ASP:HB2	2:I:485:ASP:HB2	1.88	0.55
2:I:490:GLN:NE2	5:L:472:GLN:O	2.39	0.55
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.89	0.55
1:H:212:ASP:OD1	1:H:212:ASP:N	2.36	0.55
3:J:951:GLN:NE2	3:J:1014:GLY:O	2.40	0.55
1:G:83:LEU:HD23	2:I:694:ARG:HE	1.72	0.55
6:P:34:DA:H2"	6:P:35:DC:H5'	1.87	0.55
2:I:91:THR:HG23	2:I:138:ILE:HA	1.89	0.54
6:P:45:DA:H2"	6:P:46:DA:C8	2.42	0.54
3:J:744:ARG:HB2	3:J:759:ILE:HG13	1.89	0.54
3:J:353:SER:OG	3:J:445:LYS:O	2.25	0.53
2:I:213:LEU:HD22	2:I:422:LYS:HG2	1.90	0.53
5:L:429:THR:HG22	6:P:57:DA:H2'	1.90	0.53
2:I:992:LEU:HD12	2:I:996:ARG:HB3	1.90	0.53
3:J:733:SER:OG	3:J:736:GLN:OE1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:799:ARG:NH1	3:J:1146:GLU:OE2	2.41	0.53
3:J:381:ILE:HD11	3:J:412:LEU:HD13	1.91	0.53
3:J:1285:VAL:O	3:J:1289:ASN:ND2	2.42	0.53
2:I:403:MET:HE2	2:I:407:ARG:HE	1.74	0.53
2:I:496:LYS:HB3	7:Q:34:DG:H4'	1.91	0.53
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.41	0.53
2:I:821:ARG:HG2	2:I:1082:ILE:HG12	1.89	0.52
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.91	0.52
3:J:1022:PRO:O	3:J:1126:GLN:NE2	2.40	0.52
3:J:1265:THR:OG1	3:J:1303:SER:OG	2.27	0.52
5:L:402:LEU:HD23	5:L:405:ILE:HD11	1.91	0.52
1:R:284:ARG:NH1	1:R:288:GLU:OE2	2.43	0.52
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.91	0.52
3:J:256:ASP:OD2	8:J:1504:1N7:O2	2.27	0.52
2:I:14:ASP:HA	2:I:1183:ALA:HB3	1.92	0.52
2:I:1339:LEU:HD23	3:J:20:ILE:HG12	1.92	0.52
3:J:268:LEU:HD21	3:J:324:LEU:HD13	1.91	0.52
3:J:1024:THR:HG23	3:J:1123:ARG:HA	1.92	0.52
5:L:429:THR:HG22	6:P:57:DA:H8	1.74	0.52
3:J:968:ASN:OD1	3:J:972:LYS:N	2.43	0.52
3:J:438:GLU:HG3	3:J:485:MET:HE1	1.91	0.51
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.92	0.51
3:J:1060:VAL:HG22	3:J:1106:ILE:HG12	1.93	0.51
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.93	0.51
2:I:478:ARG:HG2	2:I:492:MET:HG2	1.91	0.51
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.92	0.51
1:H:135:ASP:OD1	1:H:135:ASP:N	2.44	0.51
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.93	0.51
3:J:71:LEU:HB2	3:J:90:VAL:HG21	1.92	0.51
8:G:401:1N7:H15	2:I:966:ILE:HD11	1.93	0.51
2:I:843:THR:OG1	2:I:846:GLY:O	2.25	0.51
2:I:895:LEU:HD13	2:I:900:LYS:HB3	1.92	0.51
3:J:1089:LEU:HD22	3:J:1096:PRO:HA	1.91	0.51
3:J:198:CYS:SG	3:J:202:ARG:NH1	2.84	0.51
2:I:728:ASP:OD1	2:I:729:ALA:N	2.44	0.50
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.93	0.50
2:I:23:ASP:OD1	2:I:23:ASP:N	2.42	0.50
2:I:241:LEU:HD22	2:I:285:ILE:HD13	1.93	0.50
3:J:742:GLY:O	3:J:762:ASN:ND2	2.43	0.50
3:J:759:ILE:HG22	3:J:771:GLN:HB2	1.92	0.50
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:516:ASP:OD1	3:J:516:ASP:N	2.45	0.50
1:R:280:ASP:OD1	1:R:321:TRP:NE1	2.45	0.50
2:I:1291:LEU:HD12	2:I:1292:THR:HG23	1.93	0.50
3:J:750:PRO:HG3	3:J:777:HIS:HB3	1.94	0.50
2:I:964:LEU:HD21	2:I:1022:LYS:HD2	1.94	0.50
3:J:814:CYS:SG	3:J:816:THR:OG1	2.70	0.50
7:Q:54:DT:H2"	7:Q:55:DA:C8	2.47	0.50
2:I:159:SER:OG	2:I:160:ASP:N	2.44	0.49
3:J:1021:ASP:HB3	3:J:1024:THR:HB	1.93	0.49
5:L:555:GLU:HA	5:L:558:VAL:HG12	1.95	0.49
8:G:401:1N7:C19	8:G:401:1N7:C4	2.88	0.49
3:J:1025:MET:HB2	3:J:1124:ILE:HB	1.94	0.49
2:I:1072:ASN:ND2	2:I:1111:GLN:OE1	2.39	0.49
5:L:213:ASP:OD1	5:L:213:ASP:N	2.43	0.49
1:H:192:VAL:HG12	1:H:193:GLU:H	1.77	0.49
2:I:998:LEU:HB2	2:I:1015:ALA:HB2	1.95	0.49
3:J:18:ASP:OD1	3:J:1369:ARG:NH2	2.46	0.49
1:G:135:ASP:HB3	1:G:138:ALA:HB2	1.95	0.49
3:J:568:SER:OG	3:J:570:LYS:NZ	2.44	0.49
6:P:44:DT:H2"	6:P:45:DA:C8	2.48	0.49
1:H:77:ASP:N	1:H:80:GLU:OE1	2.44	0.48
3:J:1219:ASP:OD1	3:J:1222:ARG:NH2	2.45	0.48
6:P:39:DA:H2"	6:P:40:DA:H5"	1.95	0.48
7:Q:47:DT:H2"	7:Q:48:DA:C8	2.49	0.48
1:G:20:SER:OG	1:G:21:SER:N	2.46	0.48
4:K:10:VAL:HG21	4:K:16:ARG:HE	1.78	0.48
3:J:54:ASP:OD1	3:J:54:ASP:N	2.42	0.48
3:J:1268:ASN:HB3	3:J:1301:THR:HG22	1.96	0.48
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.95	0.48
2:I:941:LYS:NZ	2:I:949:GLU:OE2	2.29	0.48
3:J:749:LYS:HE3	3:J:755:ILE:HG12	1.96	0.48
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.96	0.48
8:G:401:1N7:H4	8:G:401:1N7:H17	1.96	0.48
1:H:95:LYS:HD2	1:H:98:VAL:HB	1.95	0.48
2:I:906:PHE:HE2	5:L:608:ARG:HA	1.79	0.48
3:J:964:LYS:HB3	3:J:976:THR:HG23	1.96	0.48
8:J:1504:1N7:H13	8:J:1504:1N7:H27	1.66	0.48
2:I:1121:ALA:HB2	2:I:1182:ILE:HD12	1.96	0.47
2:I:296:VAL:HA	2:I:316:GLU:HA	1.96	0.47
2:I:620:ASN:OD1	2:I:620:ASN:N	2.47	0.47
8:I:1401:1N7:H4	8:I:1401:1N7:H17	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:53:ARG:HA	3:J:54:ASP:HA	1.59	0.47
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.96	0.47
3:J:127:LEU:HD21	3:J:234:PRO:HB3	1.96	0.47
2:I:759:SER:OG	2:I:763:THR:OG1	2.30	0.47
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.14	0.47
2:I:731:ARG:HH12	2:I:962:GLU:HG3	1.79	0.47
2:I:1213:TYR:HA	2:I:1220:GLN:HA	1.97	0.47
3:J:1341:ARG:NH1	3:J:1343:GLU:OE2	2.48	0.47
1:G:134:THR:HB	2:I:773:LEU:HD12	1.97	0.47
2:I:444:ASP:OD1	2:I:444:ASP:N	2.43	0.47
3:J:707:ILE:O	3:J:714:GLU:N	2.43	0.47
1:G:13:LEU:HB3	1:H:231:PHE:HE1	1.80	0.47
1:G:44:ARG:HG3	1:G:183:ILE:HB	1.96	0.47
1:H:104:LYS:HD3	1:H:110:VAL:HG22	1.96	0.47
3:J:1155:ILE:HD11	3:J:1194:ARG:HH11	1.80	0.47
2:I:866:ASP:OD2	2:I:944:ARG:NH1	2.47	0.46
3:J:342:LEU:HD13	3:J:1352:ILE:HG23	1.97	0.46
5:L:292:VAL:HA	5:L:297:MET:HB3	1.98	0.46
2:I:621:SER:HB2	2:I:653:MET:HE3	1.98	0.46
4:K:36:ASP:OD1	4:K:36:ASP:N	2.49	0.46
1:H:14:VAL:HB	1:H:28:LEU:HB3	1.98	0.46
2:I:800:MET:HB2	2:I:800:MET:HE3	1.71	0.46
4:K:15:ASN:C	4:K:17:PHE:H	2.24	0.46
2:I:545:PHE:HZ	3:J:788:LEU:HD11	1.80	0.46
3:J:1173:ARG:N	3:J:1190:ILE:O	2.47	0.46
3:J:654:ILE:HD13	3:J:760:THR:HB	1.98	0.46
3:J:664:ILE:HD13	3:J:681:LYS:HB3	1.98	0.46
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.45
2:I:517:GLN:HB3	2:I:759:SER:HB2	1.97	0.45
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.97	0.45
2:I:11:ILE:O	2:I:1149:TYR:OH	2.25	0.45
2:I:105:TYR:HD1	2:I:114:VAL:HG12	1.82	0.45
2:I:1259:LEU:HD11	5:L:524:GLU:HB3	1.98	0.45
5:L:262:VAL:HG23	5:L:265:GLN:H	1.80	0.45
2:I:318:SER:OG	2:I:320:ASP:OD1	2.27	0.45
2:I:484:LEU:HB2	2:I:485:ASP:HA	1.97	0.45
2:I:36:GLN:O	2:I:40:GLU:HB2	2.16	0.45
8:I:1401:1N7:C3	8:I:1401:1N7:C1	2.95	0.45
3:J:111:THR:O	3:J:239:LEU:N	2.45	0.45
3:J:914:ALA:HB2	3:J:1359:ALA:HB1	1.99	0.45
5:L:531:PRO:HA	5:L:534:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:40:DA:H2"	6:P:41:DG:H8	1.81	0.45
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.98	0.45
2:I:183:TRP:HZ3	6:P:68:DT:H1'	1.82	0.45
2:I:802:VAL:HG11	2:I:1230:MET:HB2	1.98	0.45
3:J:1220:ILE:HG23	3:J:1224:ARG:HD2	1.98	0.45
8:J:1504:1N7:C3	8:J:1504:1N7:C11	2.94	0.45
2:I:942:ASP:OD1	2:I:942:ASP:N	2.47	0.45
2:I:1105:SER:HA	3:J:736:GLN:HG2	1.99	0.45
2:I:99:LYS:HA	2:I:121:GLU:HA	1.99	0.44
2:I:453:ILE:HD13	2:I:530:ILE:HD12	1.99	0.44
3:J:325:LYS:HG3	3:J:329:ASP:HB2	1.99	0.44
1:G:86:LYS:HE3	1:G:86:LYS:HB2	1.85	0.44
2:I:960:LEU:HB3	2:I:1025:PHE:CD1	2.52	0.44
3:J:201:LEU:HD22	3:J:217:LEU:HD22	1.99	0.44
3:J:1340:LYS:HE3	3:J:1340:LYS:HB2	1.81	0.44
3:J:1184:ASP:OD1	3:J:1184:ASP:N	2.47	0.44
7:Q:22:DC:H2'	7:Q:23:DG:C8	2.52	0.44
2:I:160:ASP:OD2	2:I:164:THR:OG1	2.35	0.44
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.99	0.44
3:J:260:PHE:HB2	5:L:504:PRO:HB3	2.00	0.44
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.52	0.44
2:I:45:GLY:HA3	2:I:54:ARG:HD2	1.98	0.44
3:J:705:THR:HG21	3:J:716:GLN:HE21	1.83	0.44
8:J:1504:1N7:C3	8:J:1504:1N7:H17	2.46	0.44
3:J:79:LYS:HE2	5:L:569:THR:HB	1.99	0.44
3:J:895:CYS:SG	3:J:897:HIS:N	2.88	0.44
1:H:59:VAL:HG23	1:H:144:ILE:HA	2.00	0.44
2:I:675:ASP:OD2	2:I:677:ASN:ND2	2.45	0.44
2:I:943:LYS:HA	2:I:943:LYS:HD2	1.83	0.44
2:I:1287:LEU:O	2:I:1291:LEU:HG	2.17	0.44
2:I:1334:GLY:H	3:J:113:HIS:HE2	1.66	0.44
3:J:48:THR:O	3:J:50:LYS:N	2.45	0.44
3:J:976:THR:O	3:J:976:THR:OG1	2.30	0.44
3:J:1078:LEU:HD12	3:J:1121:LEU:HD13	1.99	0.44
5:L:414:LYS:HE3	5:L:418:LYS:HE2	1.99	0.44
1:G:180:VAL:HG12	1:G:207:THR:HG22	1.99	0.44
3:J:490:ILE:HD11	3:J:609:TYR:CD2	2.53	0.43
3:J:550:VAL:HG23	3:J:552:ILE:HG23	1.99	0.43
3:J:891:ASP:OD1	3:J:891:ASP:N	2.41	0.43
3:J:1198:VAL:HG13	3:J:1202:GLU:HB2	2.00	0.43
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:992:LEU:HD23	2:I:992:LEU:H	1.84	0.43
3:J:1040:MET:HE1	3:J:1059:LEU:HD13	2.00	0.43
4:K:3:ARG:HH21	4:K:6:VAL:HA	1.82	0.43
5:L:110:LEU:HD21	5:L:385:ARG:HD2	1.98	0.43
6:P:40:DA:H2"	6:P:41:DG:C8	2.53	0.43
3:J:697:MET:HE1	3:J:737:ILE:HG22	2.00	0.43
8:G:401:1N7:C3	8:G:401:1N7:H1	2.48	0.43
2:I:74:ARG:NH1	2:I:121:GLU:OE2	2.51	0.43
2:I:812:PHE:CD2	2:I:813:GLU:HG2	2.53	0.43
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	1.99	0.43
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.33	0.43
3:J:826:ILE:HG12	3:J:831:VAL:HG12	2.00	0.43
3:J:811:GLU:OE1	3:J:890:THR:OG1	2.27	0.43
3:J:817:HIS:CE1	3:J:860:ARG:HH12	2.36	0.43
1:G:7:GLU:CD	1:G:7:GLU:H	2.25	0.43
3:J:1319:PHE:CE1	3:J:1342:ASP:HB2	2.54	0.43
8:J:1504:1N7:C3	8:J:1504:1N7:C1	2.97	0.43
5:L:385:ARG:HB2	6:P:59:DT:H1'	2.01	0.43
1:H:29:GLU:HB3	1:H:200:LYS:HG3	2.00	0.42
4:K:13:ILE:HD11	4:K:60:ASN:HA	2.00	0.42
2:I:145:ILE:HB	2:I:456:VAL:HG22	2.01	0.42
2:I:300:ASP:OD1	2:I:313:ALA:N	2.46	0.42
2:I:144:VAL:HG23	2:I:515:MET:HG3	2.01	0.42
2:I:400:VAL:HG22	2:I:584:TYR:HB3	2.01	0.42
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	2.02	0.42
3:J:1170:LYS:HB3	3:J:1170:LYS:HE3	1.77	0.42
6:P:64:DG:C2	6:P:66:DC:H2'	2.55	0.42
2:I:249:GLU:HB2	2:I:269:ILE:HD12	2.00	0.42
4:K:3:ARG:HH12	4:K:55:GLU:CD	2.27	0.42
2:I:1340:GLU:OE2	3:J:1341:ARG:NE	2.34	0.42
3:J:975:ILE:HG22	3:J:977:SER:H	1.84	0.42
5:L:316:PHE:CZ	5:L:338:HIS:HB2	2.55	0.42
5:L:330:LEU:O	5:L:334:SER:OG	2.29	0.42
2:I:221:LEU:HD13	2:I:336:LEU:HD11	2.01	0.42
2:I:245:ARG:HG3	2:I:337:PHE:CE1	2.55	0.42
3:J:64:PRO:HG3	3:J:91:GLU:O	2.19	0.42
3:J:298:MET:SD	5:L:406:GLN:HG3	2.60	0.42
3:J:1047:THR:HG23	3:J:1049:GLN:HG3	2.02	0.42
1:H:196:THR:OG1	3:J:443:GLU:OE1	2.36	0.42
3:J:1176:VAL:HG22	3:J:1187:GLU:HB3	2.01	0.42
2:I:960:LEU:O	2:I:963:GLU:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:196:GLN:O	3:J:200:GLN:HG2	2.19	0.41
3:J:901:ARG:HG2	3:J:903:LEU:H	1.85	0.41
2:I:309:LEU:HD21	2:I:312:ALA:HB2	2.02	0.41
2:I:817:LEU:HD12	2:I:1078:LYS:HB3	2.02	0.41
2:I:1146:GLN:HE22	2:I:1159:VAL:HG13	1.86	0.41
3:J:527:LEU:HB2	3:J:550:VAL:HG12	2.02	0.41
2:I:44:GLU:OE1	2:I:44:GLU:N	2.53	0.41
3:J:895:CYS:SG	3:J:896:ALA:N	2.93	0.41
5:L:215:GLU:HG2	5:L:218:ARG:HH21	1.85	0.41
5:L:276:MET:HE3	5:L:276:MET:HB3	1.94	0.41
5:L:280:VAL:HG22	5:L:347:ILE:HD13	2.02	0.41
2:I:452:ARG:NH2	8:I:1401:1N7:H25	2.36	0.41
3:J:572:THR:OG1	3:J:573:THR:N	2.52	0.41
5:L:91:ILE:HA	5:L:92:GLY:HA2	1.58	0.41
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.01	0.41
2:I:85:CYS:SG	2:I:92:TYR:HB2	2.60	0.41
2:I:1120:ALA:HB1	2:I:1198:LEU:HB3	2.03	0.41
2:I:870:ILE:HD12	2:I:944:ARG:HG2	2.03	0.41
3:J:86:GLU:H	3:J:86:GLU:HG3	1.69	0.41
3:J:141:PHE:HB3	3:J:293:ARG:HD2	2.02	0.41
8:G:401:1N7:C3	8:G:401:1N7:C1	2.98	0.41
2:I:732:ILE:HD11	2:I:769:PRO:HB3	2.03	0.41
3:J:819:GLY:O	3:J:1227:HIS:CE1	2.74	0.41
8:G:401:1N7:H14	8:G:401:1N7:H29	1.89	0.41
1:H:102:LEU:HD13	1:H:115:ILE:HG12	2.01	0.41
2:I:1100:PRO:HB2	3:J:725:MET:HE1	2.02	0.41
3:J:697:MET:HE3	3:J:697:MET:HB2	1.89	0.41
6:P:22:DA:H2"	6:P:23:DA:C8	2.56	0.41
2:I:218:GLU:HG2	2:I:299:LYS:HA	2.03	0.41
2:I:492:MET:HB2	2:I:492:MET:HE3	1.89	0.41
1:H:182:ARG:HD2	3:J:581:MET:HE1	2.02	0.40
2:I:12:ARG:NH2	2:I:793:GLU:OE1	2.43	0.40
2:I:91:THR:OG1	2:I:138:ILE:O	2.25	0.40
3:J:30:ILE:HD13	3:J:243:PRO:HD3	2.02	0.40
3:J:582:ILE:HG22	3:J:620:PHE:HE1	1.86	0.40
3:J:647:PRO:HG3	3:J:697:MET:HB3	2.02	0.40
3:J:1062:LEU:O	3:J:1067:ARG:NH2	2.48	0.40
6:P:35:DC:H2"	6:P:36:DT:H71	2.02	0.40
2:I:906:PHE:HD2	5:L:611:LEU:HD12	1.86	0.40
3:J:264:ASP:OD1	5:L:506:SER:OG	2.32	0.40
3:J:1365:TYR:CZ	3:J:1369:ARG:HD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:426:LYS:HE3	5:L:426:LYS:HB3	1.92	0.40
5:L:491:GLU:OE1	5:L:491:GLU:N	2.53	0.40
5:L:514:ASP:OD1	5:L:514:ASP:N	2.52	0.40
2:I:1290:MET:HE1	3:J:469:HIS:HB3	2.03	0.40
2:I:1296:ASP:OD2	2:I:1322:SER:OG	2.37	0.40
3:J:259:ARG:HD3	5:L:505:ILE:HD11	2.04	0.40
1:G:70:THR:HG21	2:I:755:LYS:HE2	2.04	0.40
1:H:100:LEU:O	1:H:144:ILE:N	2.55	0.40
2:I:320:ASP:OD1	2:I:320:ASP:N	2.54	0.40
2:I:483:ASP:N	2:I:483:ASP:OD1	2.55	0.40
3:J:599:LYS:HE2	3:J:599:LYS:HB2	1.87	0.40
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.54	0.40
1:G:54:CYS:SG	1:G:92:VAL:HG22	2.62	0.40
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.03	0.40
2:I:349:GLU:O	2:I:353:VAL:HG23	2.22	0.40
2:I:548:ARG:HD2	2:I:569:ILE:O	2.22	0.40
3:J:288:PRO:HB3	5:L:377:LYS:HG3	2.04	0.40
3:J:849:LEU:HA	3:J:856:ILE:HA	2.03	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	G	231/329 (70%)	211 (91%)	20 (9%)	0	100	100
1	H	218/329 (66%)	211 (97%)	6 (3%)	1 (0%)	25	56
1	R	71/329 (22%)	70 (99%)	1 (1%)	0	100	100
2	I	1338/1342 (100%)	1252 (94%)	86 (6%)	0	100	100
3	J	1330/1407 (94%)	1262 (95%)	68 (5%)	0	100	100
4	K	77/91 (85%)	72 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	L	465/613 (76%)	451 (97%)	14 (3%)	0	100	100
All	All	3730/4440 (84%)	3529 (95%)	200 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	168	ILE

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	G	201/286 (70%)	195 (97%)	6 (3%)	36	71
1	H	190/286 (66%)	176 (93%)	14 (7%)	11	34
1	R	65/286 (23%)	63 (97%)	2 (3%)	35	70
2	I	1155/1157 (100%)	1108 (96%)	47 (4%)	26	60
3	J	1119/1168 (96%)	1081 (97%)	38 (3%)	32	67
4	K	67/75 (89%)	63 (94%)	4 (6%)	16	44
5	L	418/540 (77%)	406 (97%)	12 (3%)	37	72
All	All	3215/3798 (85%)	3092 (96%)	123 (4%)	30	63

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	13	LEU
1	G	19	VAL
1	G	90	VAL
1	G	129	VAL
1	G	173	VAL
1	G	233	ASP
1	H	6	THR
1	H	14	VAL
1	H	27	THR

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Mol	Chain	Res	Type
1	H	28	LEU
1	H	38	THR
1	H	51	MET
1	H	54	CYS
1	H	124	VAL
1	H	127	GLN
1	H	146	VAL
1	H	168	ILE
1	H	183	ILE
1	H	188	GLU
1	H	206	GLU
2	I	21	VAL
2	I	39	ILE
2	I	75	LEU
2	I	146	VAL
2	I	194	LEU
2	I	216	THR
2	I	292	ILE
2	I	327	GLN
2	I	377	THR
2	I	394	ARG
2	I	412	GLU
2	I	414	ILE
2	I	453	ILE
2	I	471	VAL
2	I	472	GLU
2	I	502	VAL
2	I	515	MET
2	I	524	ILE
2	I	538	LEU
2	I	550	VAL
2	I	561	ILE
2	I	569	ILE
2	I	581	THR
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	630	VAL
2	I	635	THR
2	I	636	CYS
2	I	655	VAL
2	I	727	VAL

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Mol	Chain	Res	Type
2	I	773	LEU
2	I	796	LEU
2	I	799	ASN
2	I	859	GLU
2	I	895	LEU
2	I	922	ASN
2	I	998	LEU
2	I	1041	ASP
2	I	1046	VAL
2	I	1076	ILE
2	I	1107	MET
2	I	1212	LEU
2	I	1225	VAL
2	I	1240	ASP
2	I	1291	LEU
2	I	1293	VAL
3	J	54	ASP
3	J	65	VAL
3	J	70	CYS
3	J	78	LEU
3	J	126	LEU
3	J	151	MET
3	J	161	THR
3	J	244	VAL
3	J	256	ASP
3	J	324	LEU
3	J	357	VAL
3	J	401	VAL
3	J	408	VAL
3	J	416	ILE
3	J	506	VAL
3	J	545	HIS
3	J	591	ILE
3	J	596	LEU
3	J	685	ILE
3	J	706	VAL
3	J	708	ASN
3	J	738	ARG
3	J	757	THR
3	J	808	VAL
3	J	816	THR
3	J	831	VAL

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Mol	Chain	Res	Type
3	J	839	VAL
3	J	895	CYS
3	J	928	THR
3	J	976	THR
3	J	1025	MET
3	J	1046	ILE
3	J	1061	VAL
3	J	1169	THR
3	J	1223	LEU
3	J	1261	LEU
3	J	1353	VAL
3	J	1361	THR
4	K	35	LYS
4	K	39	VAL
4	K	56	GLU
4	K	58	LEU
5	L	104	GLU
5	L	137	TYR
5	L	149	ASP
5	L	213	ASP
5	L	261	LEU
5	L	468	ARG
5	L	471	LEU
5	L	505	ILE
5	L	532	LEU
5	L	540	LEU
5	L	569	THR
5	L	582	VAL
1	R	270	LEU
1	R	290	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	186	ASN
1	H	18	GLN
1	H	84	ASN
1	H	227	GLN
2	I	193	ASN
2	I	214	ASN
2	I	554	HIS
2	I	573	ASN

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Mol	Chain	Res	Type
2	I	618	GLN
2	I	659	GLN
2	I	677	ASN
2	I	761	GLN
2	I	799	ASN
2	I	894	GLN
2	I	932	GLN
2	I	965	GLN
3	J	186	GLN
3	J	266	ASN
3	J	320	ASN
3	J	341	ASN
3	J	424	ASN
3	J	435	GLN
3	J	720	ASN
3	J	792	ASN
3	J	865	HIS
3	J	954	ASN
3	J	979	ASN
3	J	1218	HIS
3	J	1227	HIS
3	J	1235	ASN
3	J	1367	GLN
4	K	62	GLN
5	L	294	GLN
5	L	338	HIS
5	L	342	GLN
5	L	472	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
8	1N7	G	401	-	30,30,46	5.16	15 (50%)	47,48,72	2.22	11 (23%)
8	1N7	I	1401	-	30,30,46	5.16	16 (53%)	47,48,72	2.30	13 (27%)
8	1N7	J	1504	-	30,30,46	5.29	17 (56%)	47,48,72	2.45	19 (40%)

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
8	1N7	G	401	-	-	4/7/72/92	0/4/4/4
8	1N7	I	1401	-	-	7/7/72/92	0/4/4/4
8	1N7	J	1504	-	-	5/7/72/92	0/4/4/4

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	1N7	C3-C19	18.15	1.83	1.53
8	G	401	1N7	C3-C19	17.84	1.82	1.53
8	I	1401	1N7	C3-C19	17.69	1.82	1.53
8	J	1504	1N7	C3-C4	12.98	1.74	1.53
8	G	401	1N7	C3-C4	12.22	1.73	1.53
8	I	1401	1N7	C3-C4	12.03	1.72	1.53
8	I	1401	1N7	C5-C4	-9.41	1.40	1.54
8	G	401	1N7	C5-C4	-9.25	1.40	1.54
8	J	1504	1N7	C2-C19	-9.06	1.40	1.56
8	I	1401	1N7	C2-C19	-8.95	1.40	1.56
8	G	401	1N7	C2-C19	-8.80	1.40	1.56
8	J	1504	1N7	C5-C4	-8.63	1.41	1.54
8	I	1401	1N7	C8-C7	6.17	1.70	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	1N7	C8-C7	6.03	1.70	1.54
8	G	401	1N7	C8-C7	5.99	1.70	1.54
8	I	1401	1N7	C5-C6	-4.60	1.47	1.55
8	J	1504	1N7	C5-C9	4.49	1.63	1.55
8	J	1504	1N7	C5-C6	-4.45	1.48	1.55
8	G	401	1N7	C5-C6	-4.42	1.48	1.55
8	I	1401	1N7	C18-C6	-4.24	1.45	1.53
8	J	1504	1N7	C18-C6	-4.22	1.45	1.53
8	G	401	1N7	C18-C6	-4.17	1.45	1.53
8	I	1401	1N7	O4-C4	-4.12	1.36	1.43
8	G	401	1N7	O4-C4	-4.08	1.36	1.43
8	J	1504	1N7	O4-C4	-3.88	1.37	1.43
8	J	1504	1N7	C2-C15	3.49	1.60	1.55
8	G	401	1N7	C5-C9	3.40	1.61	1.55
8	G	401	1N7	C2-C15	3.36	1.60	1.55
8	I	1401	1N7	C2-C15	3.26	1.60	1.55
8	I	1401	1N7	C7-C6	3.24	1.61	1.54
8	G	401	1N7	C7-C6	3.20	1.60	1.54
8	J	1504	1N7	C7-C6	3.07	1.60	1.54
8	J	1504	1N7	C14-C15	-3.04	1.49	1.53
8	I	1401	1N7	C14-C15	-3.03	1.49	1.53
8	I	1401	1N7	C5-C9	2.93	1.60	1.55
8	G	401	1N7	C14-C15	-2.83	1.49	1.53
8	J	1504	1N7	C14-C13	2.67	1.56	1.52
8	J	1504	1N7	C16-C15	2.56	1.57	1.53
8	J	1504	1N7	C10-C5	2.44	1.58	1.54
8	G	401	1N7	C16-C15	2.34	1.57	1.53
8	I	1401	1N7	O2-C13	-2.31	1.36	1.43
8	G	401	1N7	O2-C13	-2.29	1.36	1.43
8	I	1401	1N7	C14-C13	2.27	1.56	1.52
8	J	1504	1N7	O2-C13	-2.26	1.36	1.43
8	G	401	1N7	C14-C13	2.23	1.55	1.52
8	J	1504	1N7	C12-C13	2.11	1.56	1.51
8	I	1401	1N7	C16-C15	2.10	1.57	1.53
8	I	1401	1N7	C20-C9	-2.01	1.51	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	401	1N7	C9-C5-C4	-7.79	110.66	117.67
8	J	1504	1N7	C9-C5-C4	-7.69	110.75	117.67
8	I	1401	1N7	C9-C5-C4	-6.95	111.41	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1401	1N7	C19-C3-C4	-5.68	106.86	114.29
8	I	1401	1N7	C6-C5-C4	5.64	112.57	107.42
8	I	1401	1N7	C7-C6-C18	-5.43	110.91	118.36
8	G	401	1N7	C7-C6-C18	-4.92	111.60	118.36
8	J	1504	1N7	C7-C6-C18	-4.55	112.11	118.36
8	G	401	1N7	C19-C3-C4	-4.51	108.39	114.29
8	J	1504	1N7	C3-C19-C2	-4.41	109.23	113.70
8	J	1504	1N7	C9-C5-C6	4.28	104.41	100.11
8	J	1504	1N7	C3-C4-C5	4.05	115.39	111.26
8	G	401	1N7	C6-C5-C4	4.05	111.11	107.42
8	I	1401	1N7	C5-C9-C20	-3.87	114.80	119.48
8	I	1401	1N7	C3-C19-C2	-3.83	109.81	113.70
8	G	401	1N7	C3-C19-C2	-3.70	109.95	113.70
8	G	401	1N7	C9-C5-C6	3.66	103.78	100.11
8	J	1504	1N7	C8-C9-C5	3.56	107.00	103.54
8	J	1504	1N7	C19-C18-C17	-3.49	107.46	111.86
8	J	1504	1N7	C5-C9-C20	3.43	123.64	119.48
8	G	401	1N7	C5-C9-C20	-3.40	115.37	119.48
8	G	401	1N7	C8-C7-C6	-3.34	98.61	105.14
8	J	1504	1N7	C22-C20-C9	3.31	117.19	110.33
8	J	1504	1N7	C14-C15-C2	-3.24	109.21	112.66
8	J	1504	1N7	C8-C9-C20	-3.22	107.31	112.18
8	G	401	1N7	C8-C9-C5	3.16	106.61	103.54
8	J	1504	1N7	C7-C6-C5	3.16	106.61	103.54
8	I	1401	1N7	C6-C18-C17	-3.12	107.71	111.85
8	J	1504	1N7	C1-C2-C19	-2.98	106.72	111.34
8	I	1401	1N7	C19-C18-C17	-2.89	108.22	111.86
8	J	1504	1N7	C15-C14-C13	-2.78	108.51	112.71
8	G	401	1N7	C3-C19-C18	-2.76	106.81	110.89
8	I	1401	1N7	C3-C19-C18	-2.70	106.90	110.89
8	J	1504	1N7	C19-C2-C15	2.66	112.21	108.51
8	J	1504	1N7	C6-C5-C4	2.61	109.80	107.42
8	I	1401	1N7	C21-C20-C9	-2.41	109.27	112.88
8	I	1401	1N7	C8-C7-C6	-2.38	100.48	105.14
8	J	1504	1N7	C19-C18-C6	-2.32	106.50	109.75
8	G	401	1N7	C6-C18-C17	-2.13	109.03	111.85
8	J	1504	1N7	C8-C7-C6	-2.12	101.00	105.14
8	I	1401	1N7	C9-C5-C6	2.10	102.22	100.11
8	I	1401	1N7	C1-C2-C19	-2.09	108.10	111.34
8	J	1504	1N7	C3-C19-C18	-2.00	107.93	110.89

There are no chirality outliers.

All (16) torsion outliers are listed below:

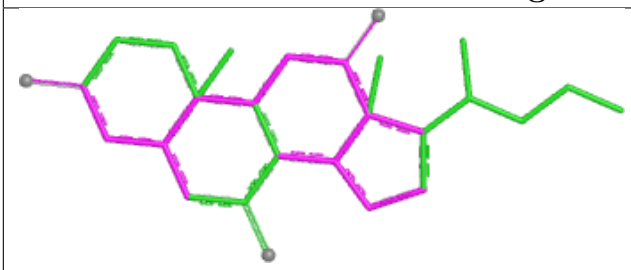
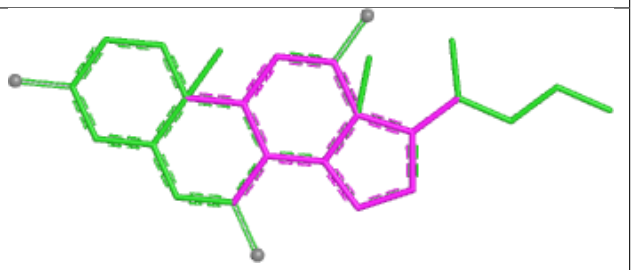
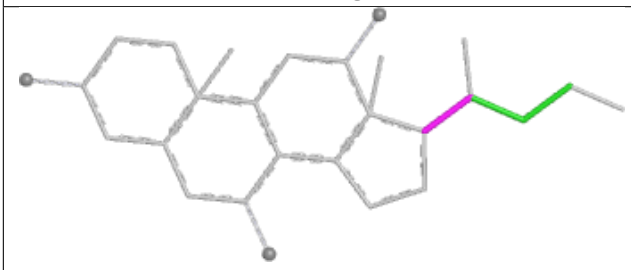
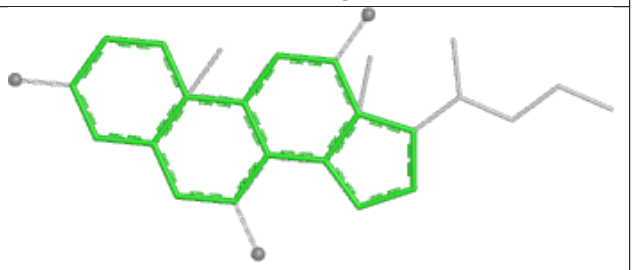
Mol	Chain	Res	Type	Atoms
8	J	1504	1N7	C22-C20-C9-C5
8	I	1401	1N7	C21-C20-C9-C5
8	G	401	1N7	C21-C20-C9-C8
8	I	1401	1N7	C21-C20-C9-C8
8	G	401	1N7	C21-C20-C9-C5
8	I	1401	1N7	C22-C20-C9-C5
8	I	1401	1N7	C21-C20-C22-C23
8	I	1401	1N7	C22-C20-C9-C8
8	J	1504	1N7	C21-C20-C9-C8
8	G	401	1N7	C22-C20-C9-C5
8	J	1504	1N7	C20-C22-C23-C24
8	I	1401	1N7	C20-C22-C23-C24
8	J	1504	1N7	C22-C20-C9-C8
8	G	401	1N7	C22-C20-C9-C8
8	J	1504	1N7	C21-C20-C9-C5
8	I	1401	1N7	C9-C20-C22-C23

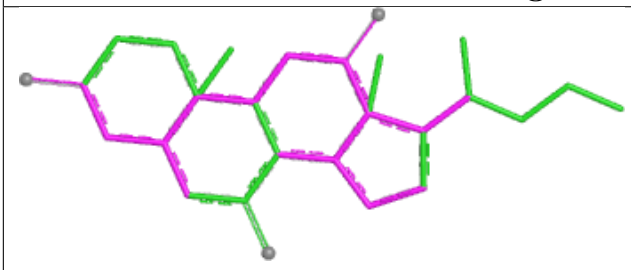
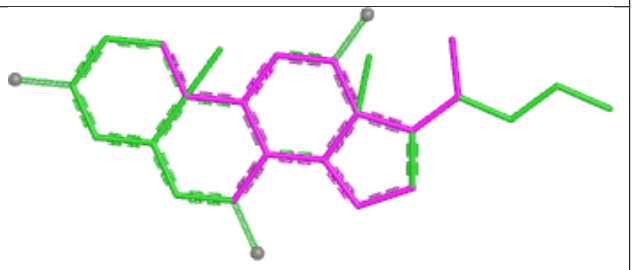
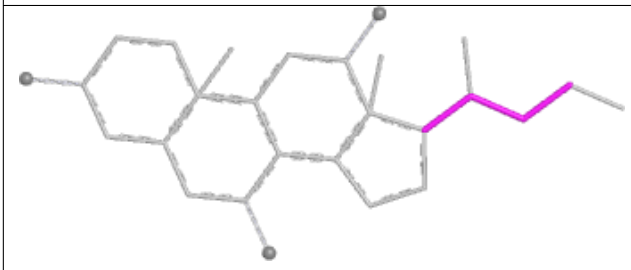
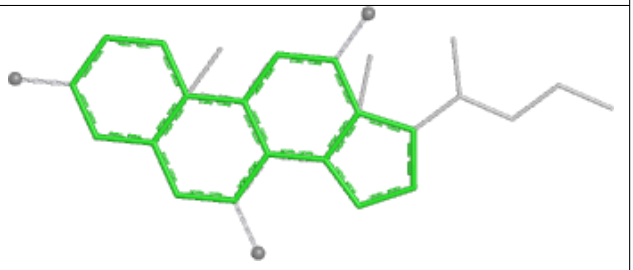
There are no ring outliers.

3 monomers are involved in 25 short contacts:

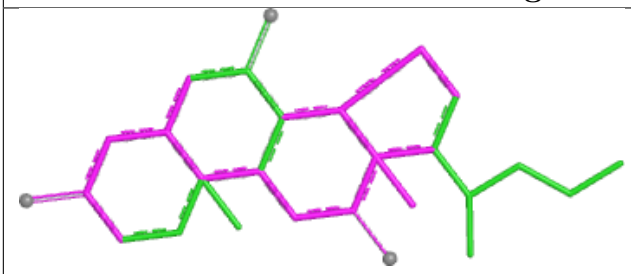
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	401	1N7	9	0
8	I	1401	1N7	7	0
8	J	1504	1N7	9	0

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.

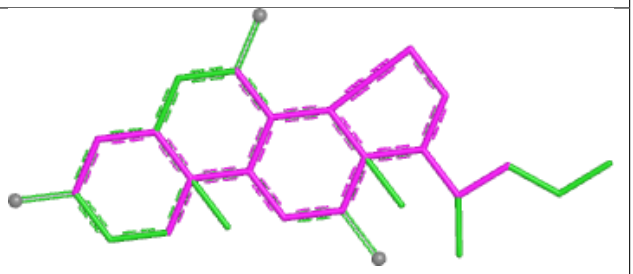
Ligand 1N7 G 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 1N7 I 1401	
	
Bond lengths	Bond angles
	
Torsions	Rings

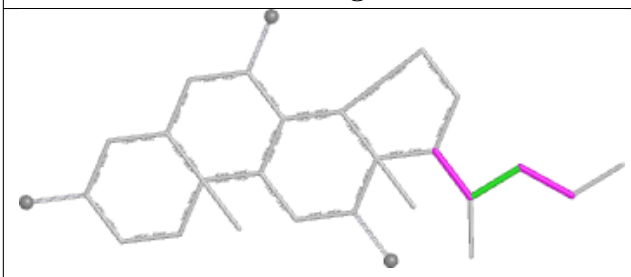
Ligand 1N7 J 1504



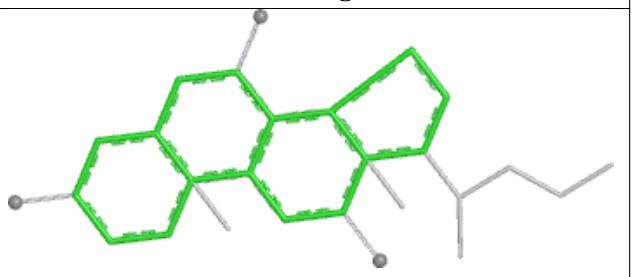
Bond lengths



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.

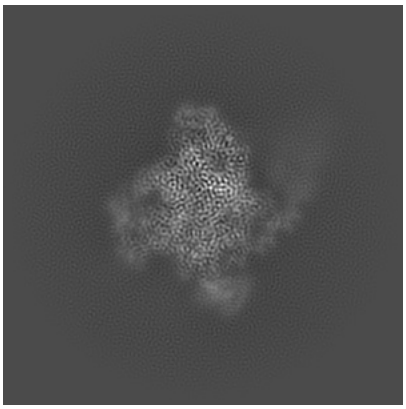
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23897. These allow visual inspection of the internal detail of the map and identification of artifacts.

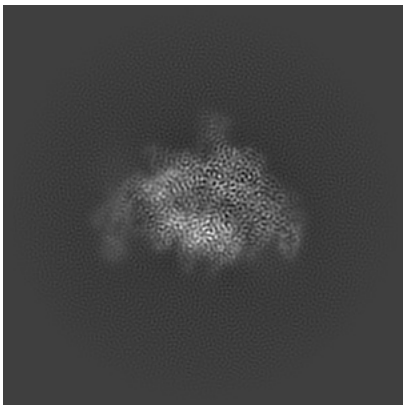
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

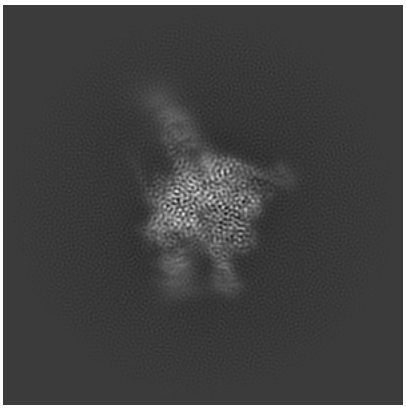
6.1.1 Primary map



X

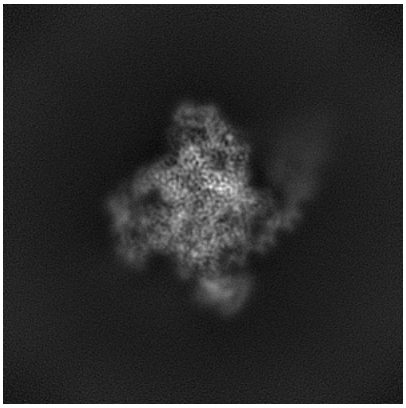


Y

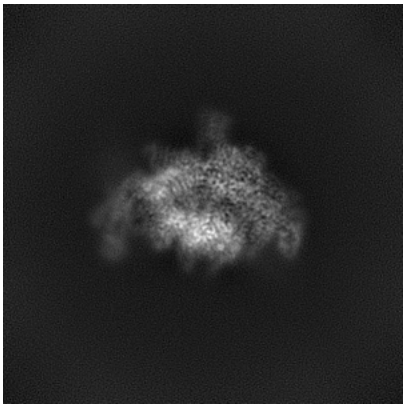


Z

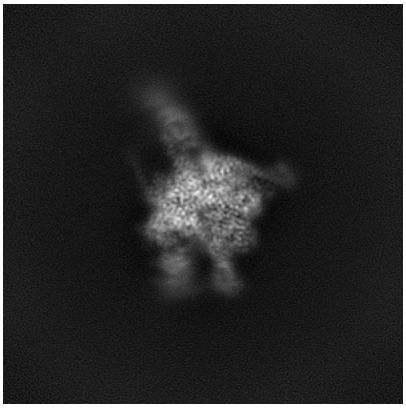
6.1.2 Raw map



X



Y

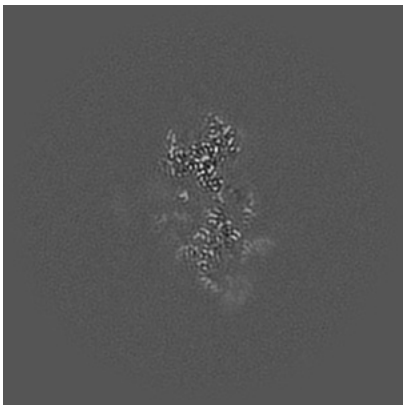


Z

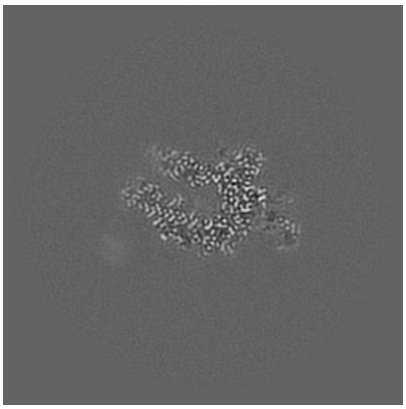
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

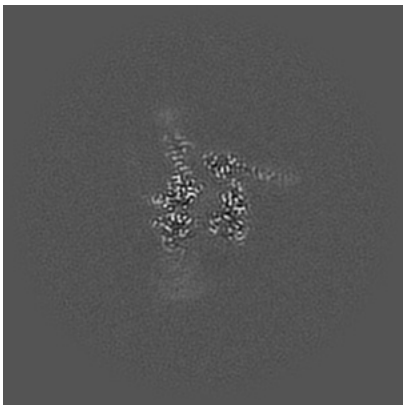
6.2.1 Primary map



X Index: 160

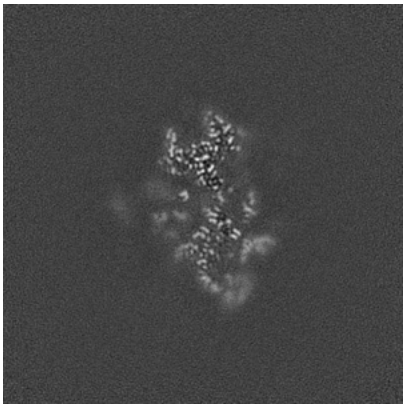


Y Index: 160

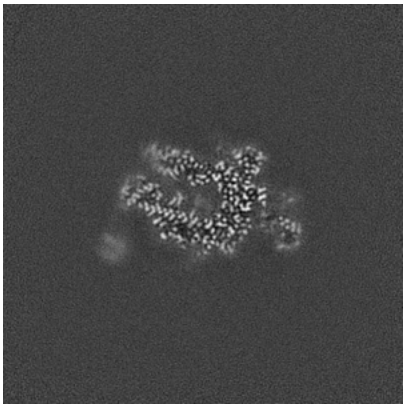


Z Index: 160

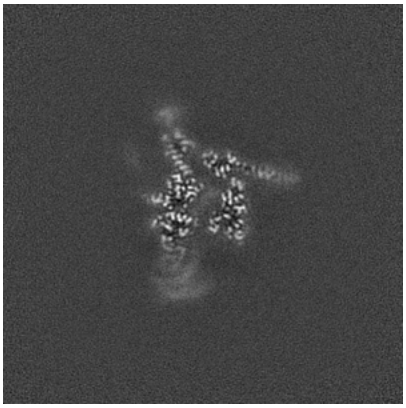
6.2.2 Raw map



X Index: 160



Y Index: 160

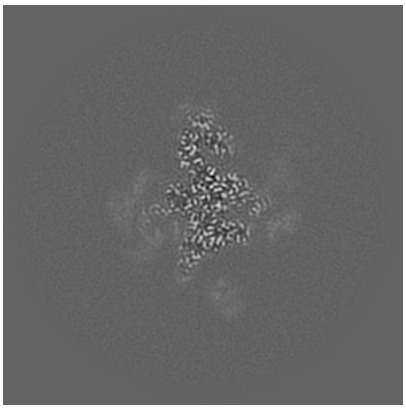


Z Index: 160

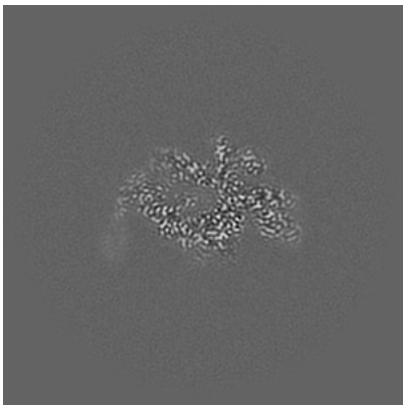
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

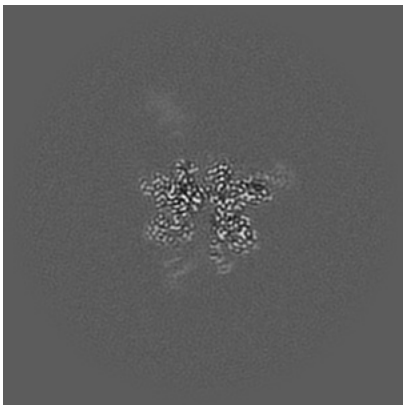
6.3.1 Primary map



X Index: 144

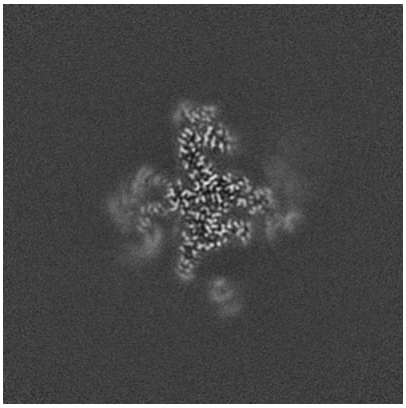


Y Index: 166

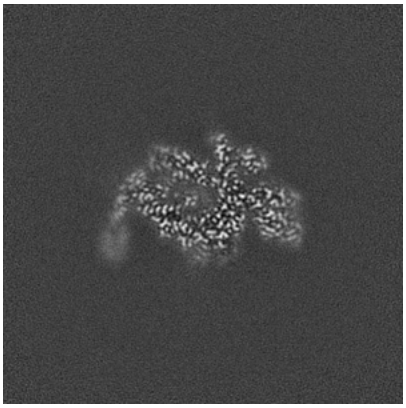


Z Index: 174

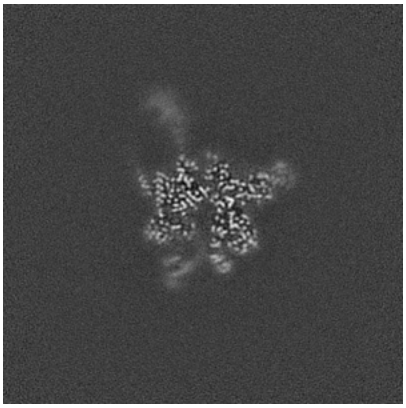
6.3.2 Raw map



X Index: 142



Y Index: 166

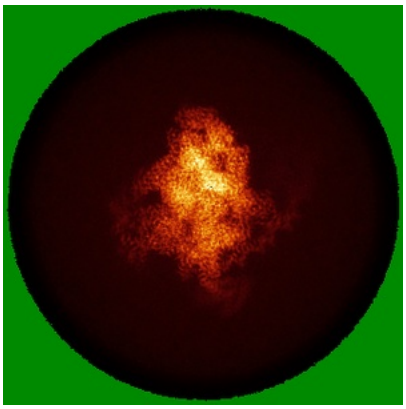


Z Index: 173

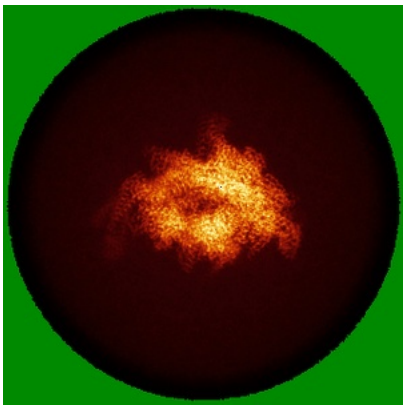
The images above show the largest variance slices of the map in three orthogonal directions.

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

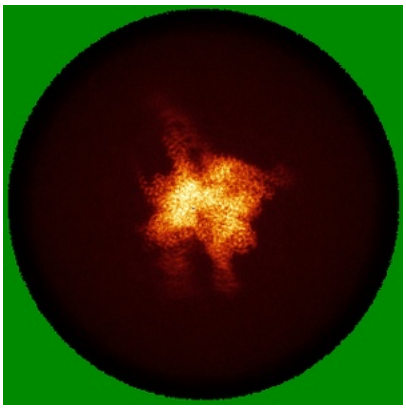
6.4.1 Primary map



X

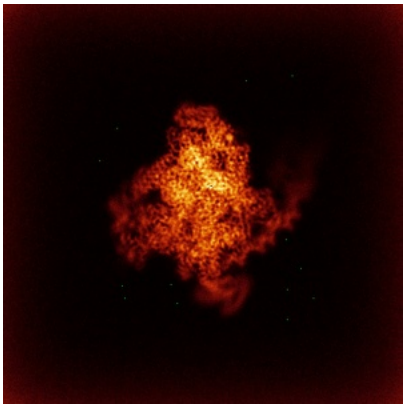


Y

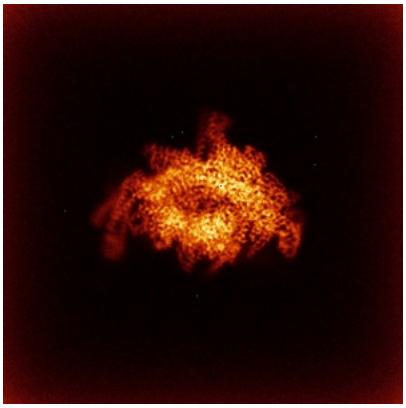


Z

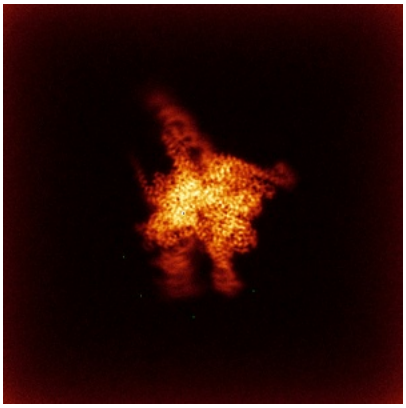
6.4.2 Raw map



X



Y

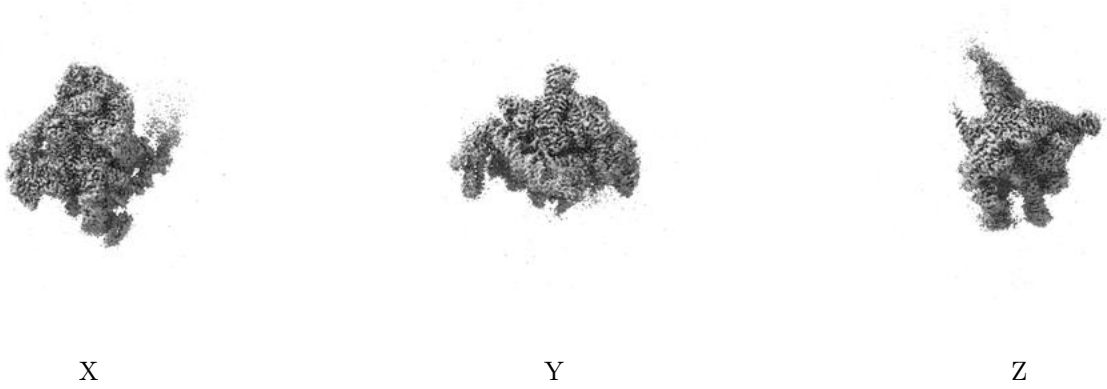


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.34. 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.

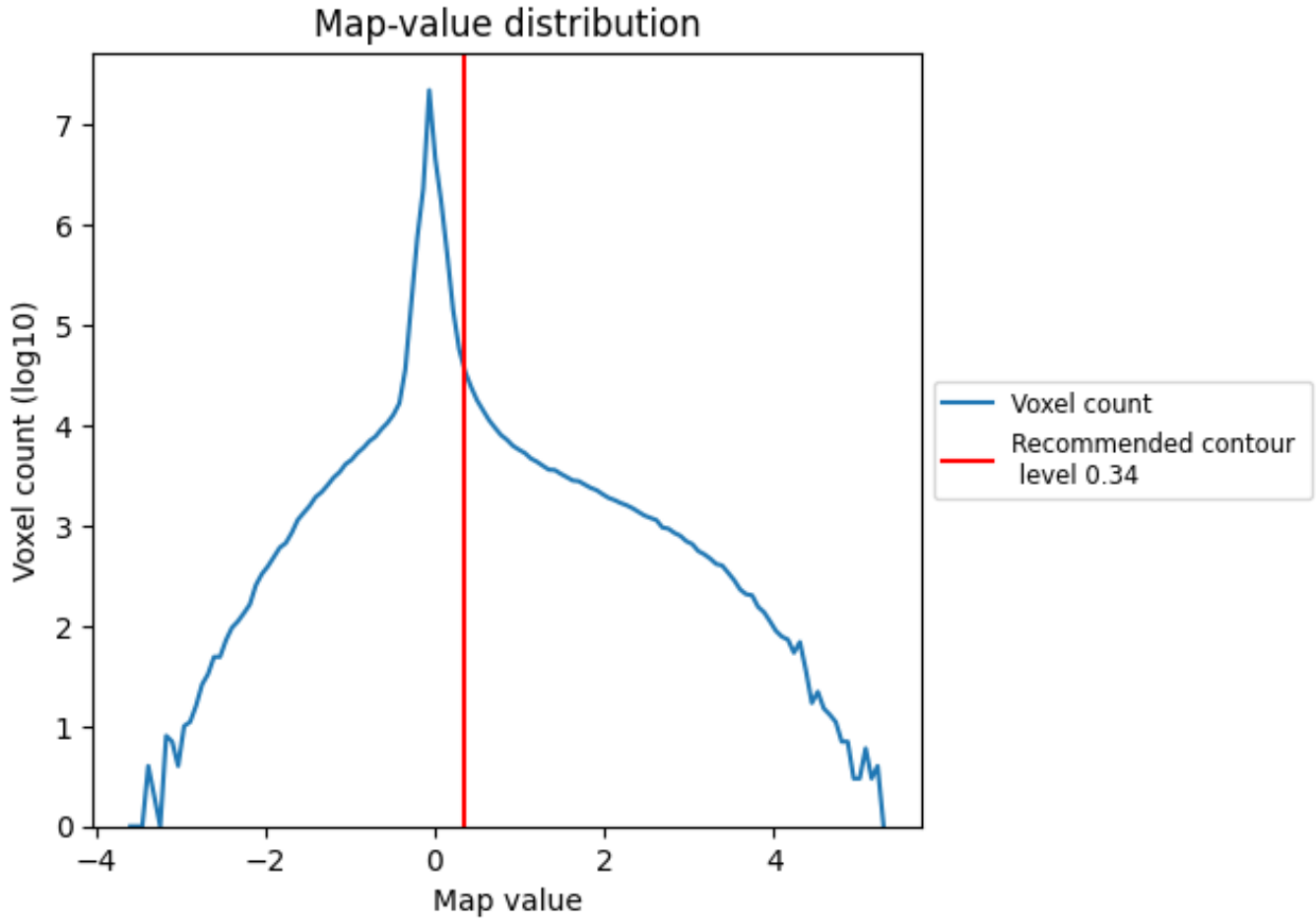
6.6 Mask visualisation (i)

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

7 Map analysis

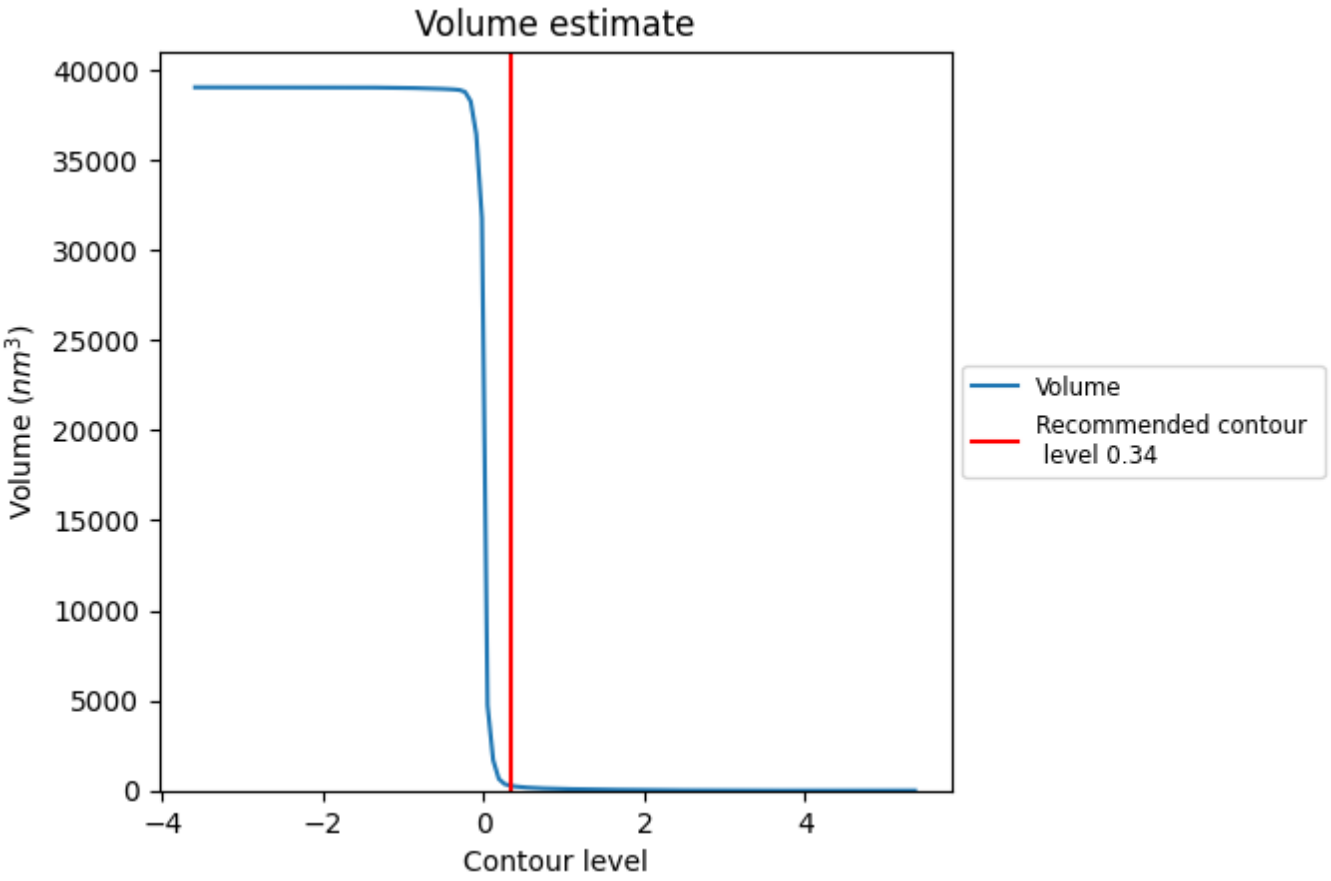
This section contains the results of statistical analysis of the map.

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.

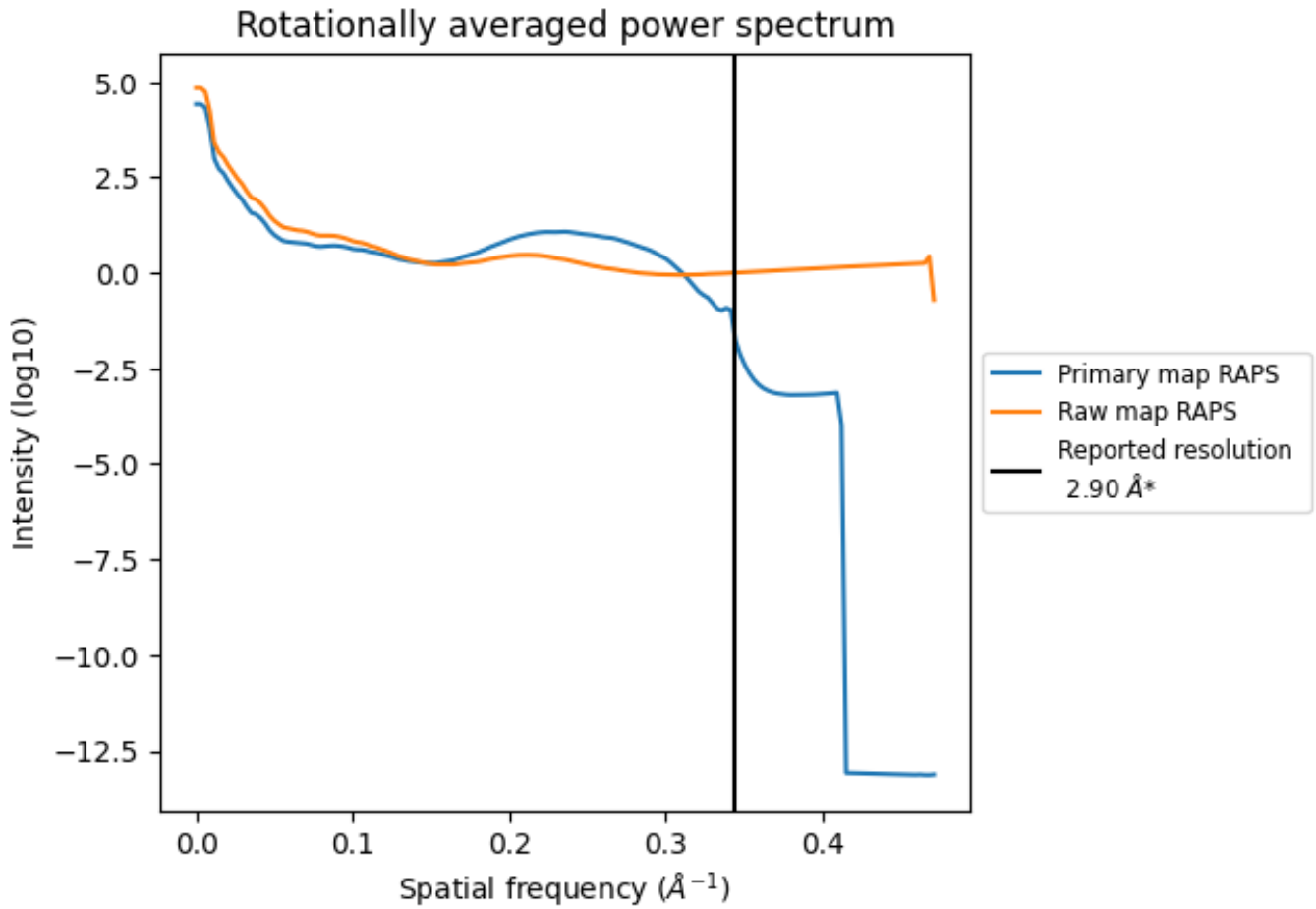
7.2 Volume estimate



The volume at the recommended contour level is 265 nm^3; this corresponds to an approximate mass of 239 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)

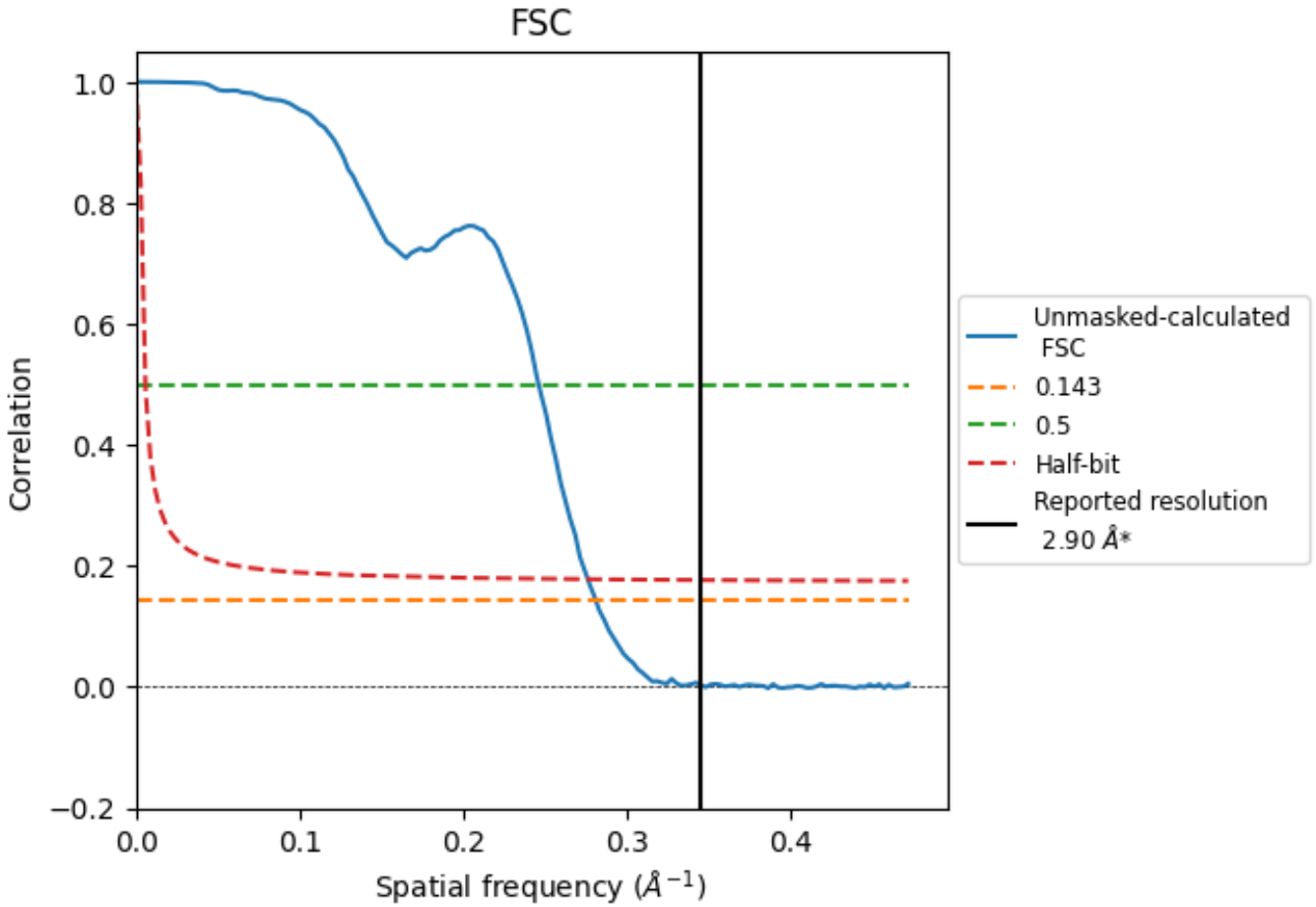


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

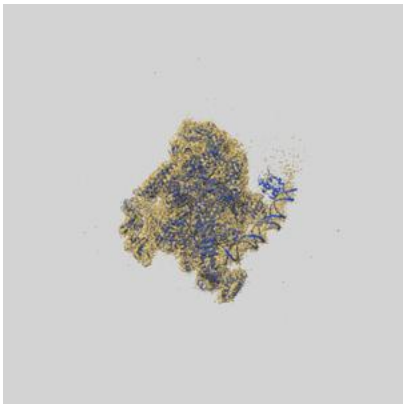
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.56	4.07	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.56 differs from the reported value 2.9 by more than 10 %

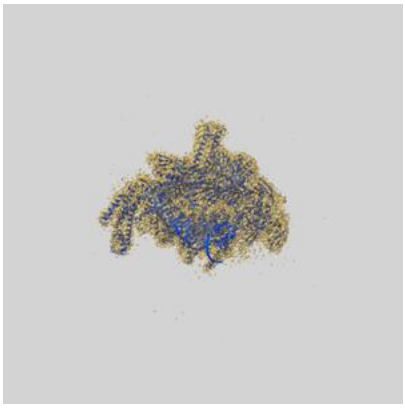
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23897 and PDB model 7MKJ. Per-residue inclusion information can be found in section 3 on page 7.

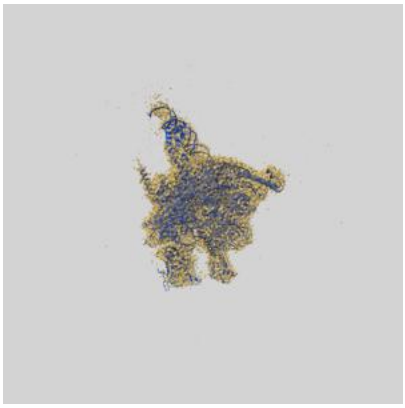
9.1 Map-model overlay



X



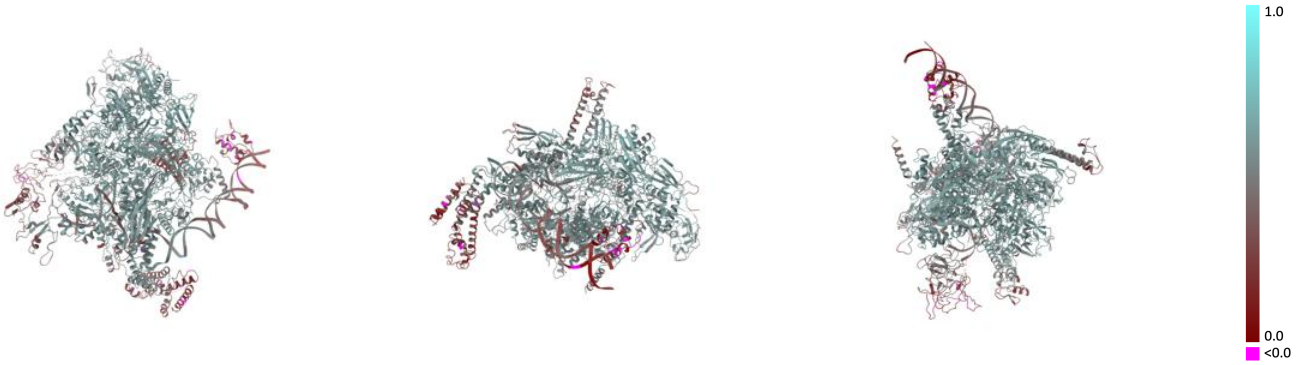
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.34 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.

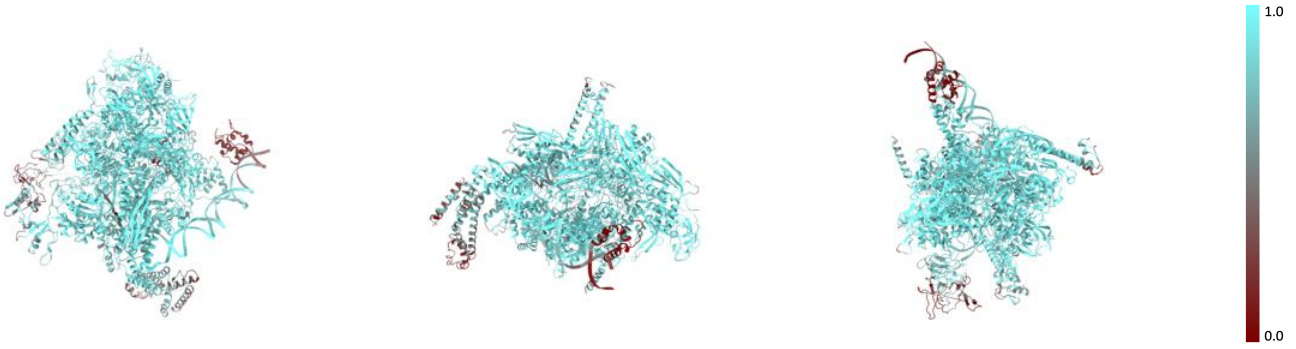
9.2 Q-score mapped to coordinate model (i)



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.

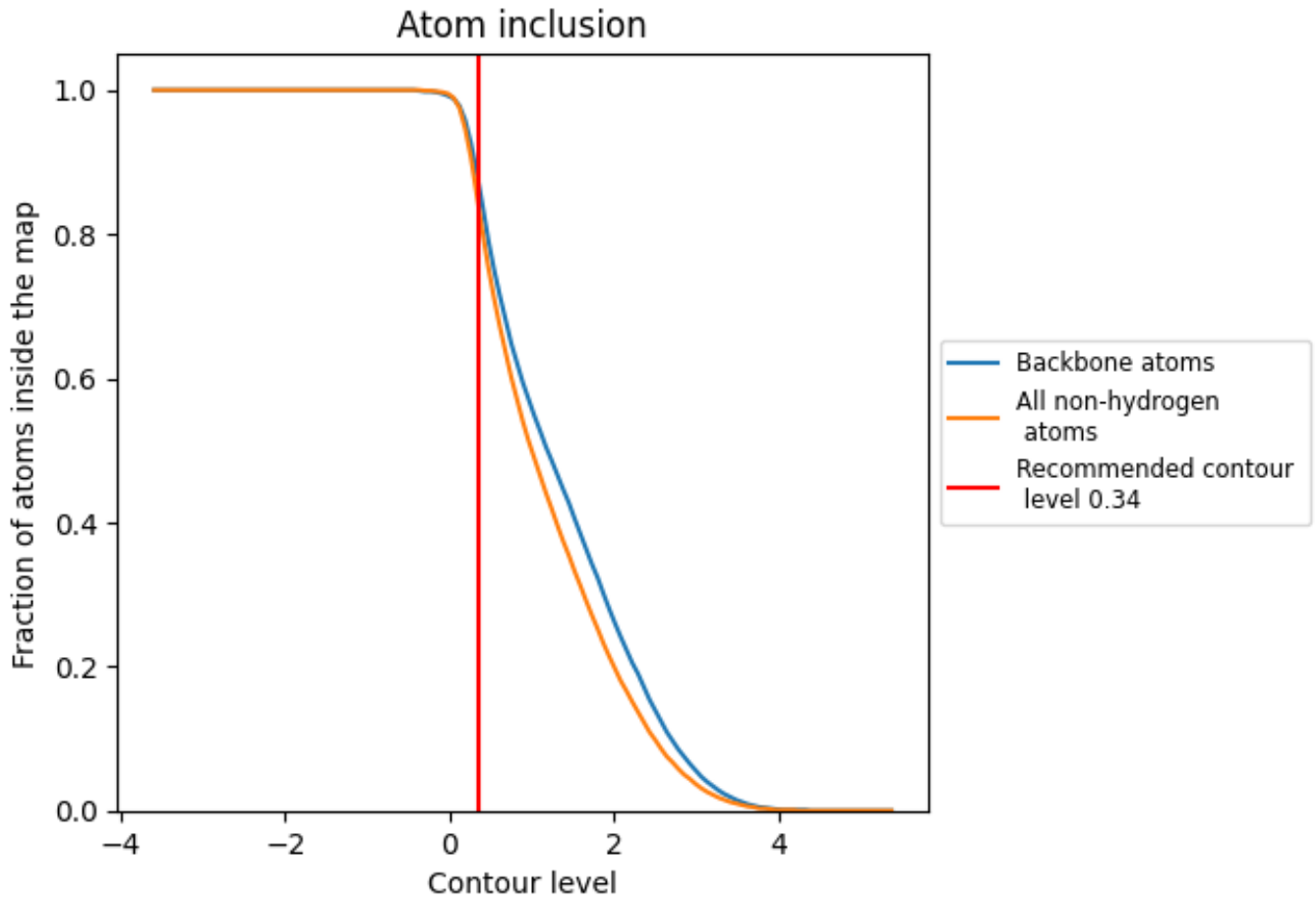
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.34).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8460	0.5090
G	0.9120	0.5540
H	0.9180	0.5470
I	0.9050	0.5480
J	0.8640	0.5280
K	0.8490	0.5350
L	0.7390	0.4290
P	0.7610	0.4010
Q	0.7630	0.3890
R	0.0660	0.1550