



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:59 AM UTC

PDB ID : 3IYD / pdb_00003iyd
EMDB ID : EMD-5127
Title : Three-dimensional EM structure of an intact activator-dependent transcription initiation complex
Authors : Hudson, B.P.; Quispe, J.; Lara, S.; Kim, Y.; Berman, H.; Arnold, E.; Ebright, R.H.; Lawson, C.L.
Deposited on : 2009-08-01
Resolution : 19.80 Å (reported)
Based on initial models : 1LB2, 3DXJ, 1SIG, 1BDF, 2AUK

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

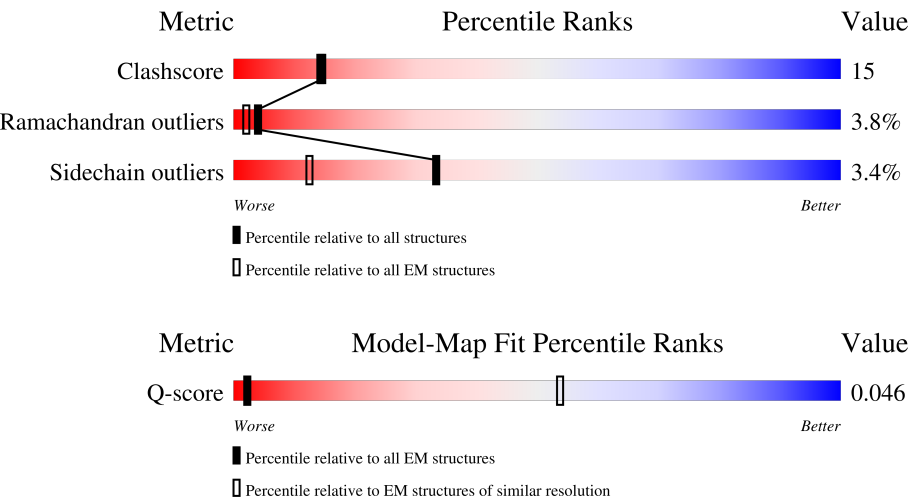
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 19.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	28 (19.40 - 20.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	8% 66% 30% ..
1	B	329	. 47% 22% . 29%
2	C	1342	. 51% 27% . 19%

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Mol	Chain	Length	Quality of chain
3	D	1413	
4	E	90	
5	F	613	
6	G	209	
6	H	209	
7	I	98	
8	J	98	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 35254 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	A	322	Total	C	N	O	S	0	0
			2496	1563	438	487	8		
1	B	235	Total	C	N	O	S	0	0
			1814	1129	320	358	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1089	Total	C	N	O	S	0	0
			8524	5351	1481	1655	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1368	Total	C	N	O	S	0	0
			10606	6657	1893	2006	50		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	HIS	-	expression tag	UNP P0A8T7
D	1409	HIS	-	expression tag	UNP P0A8T7
D	1410	HIS	-	expression tag	UNP P0A8T7
D	1411	HIS	-	expression tag	UNP P0A8T7
D	1412	HIS	-	expression tag	UNP P0A8T7
D	1413	HIS	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	479	Total	C	N	O	S	0	0
			3877	2423	693	740	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	ASN	ASP	conflict	UNP P00579
F	571	HIS	TYR	conflict	UNP P00579

- Molecule 6 is a protein called Catabolite gene activator.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	201	Total	C	N	O	S	0	0
			1591	1007	280	295	9		
6	H	201	Total	C	N	O	S	0	0
			1591	1007	280	295	9		

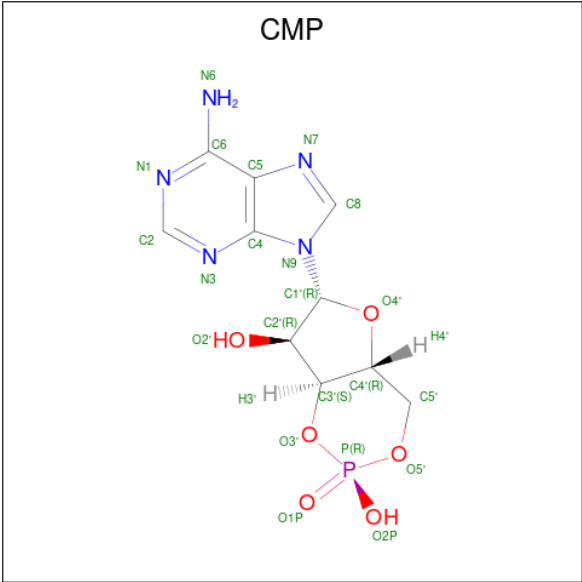
- Molecule 7 is a DNA chain called DNA (98-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	98	Total	C	N	O	P	0	0
			2006	960	366	583	97		

- Molecule 8 is a DNA chain called DNA (98-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	98	Total	C	N	O	P	0	0
			1996	958	353	588	97		

- Molecule 9 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (CCD ID: CMP) (formula: C₁₀H₁₂N₅O₆P).

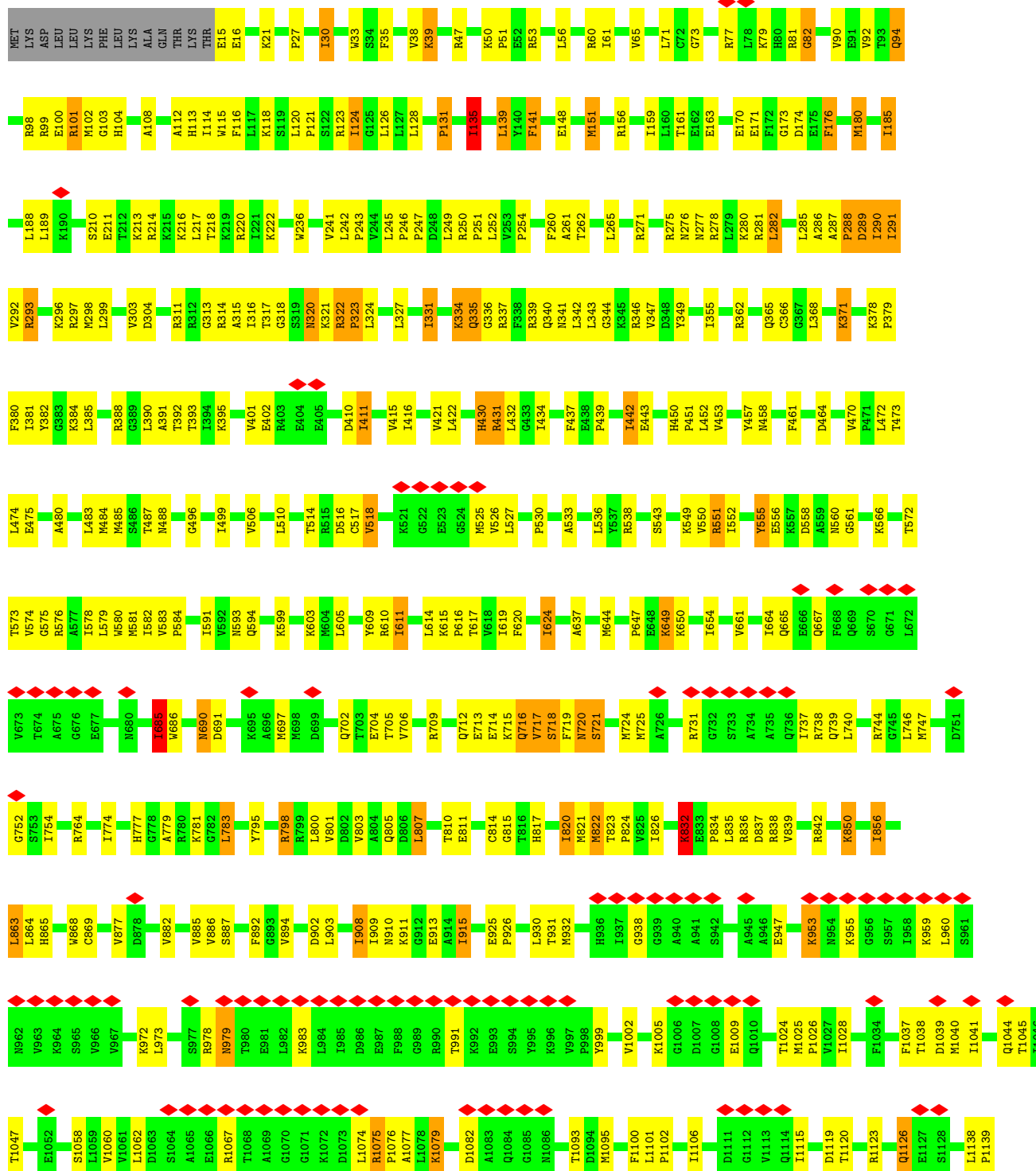


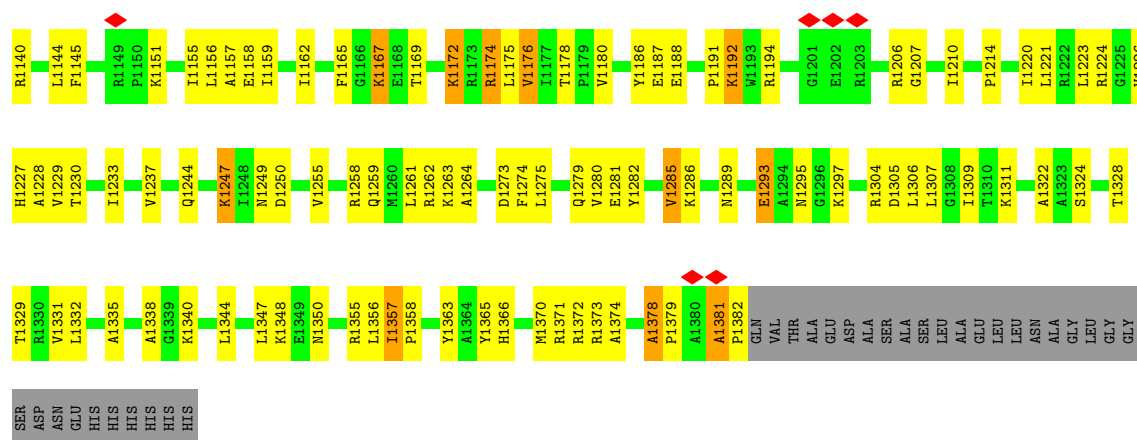
Mol	Chain	Residues	Atoms					AltConf
9	G	1	Total	C	N	O	P	0
			22	10	5	6	1	
9	H	1	Total	C	N	O	P	0
			22	10	5	6	1	



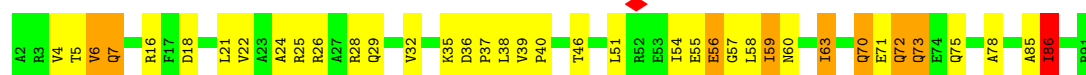


• Molecule 3: DNA-directed RNA polymerase subunit beta

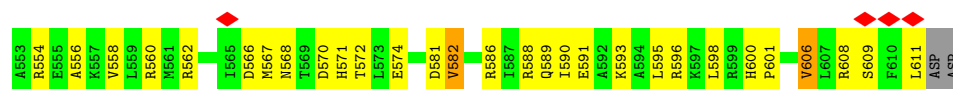
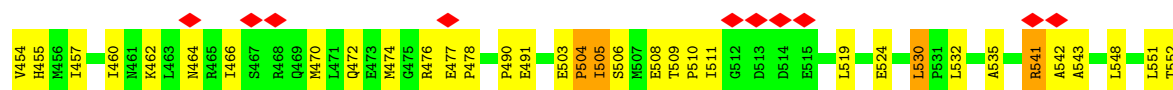
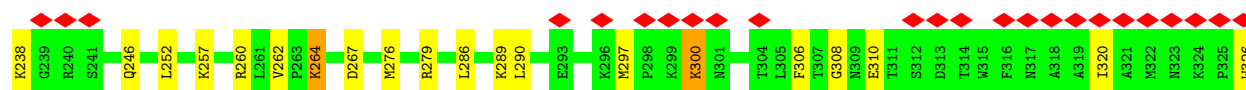
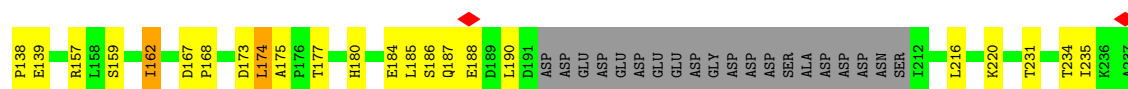
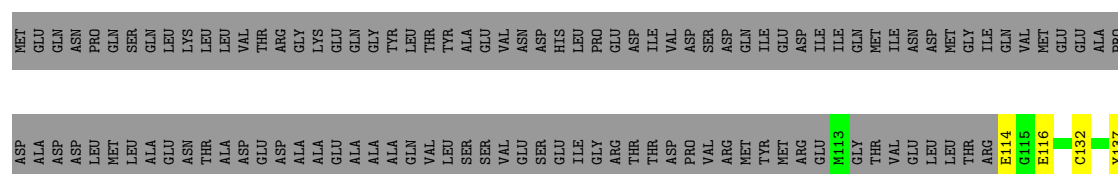




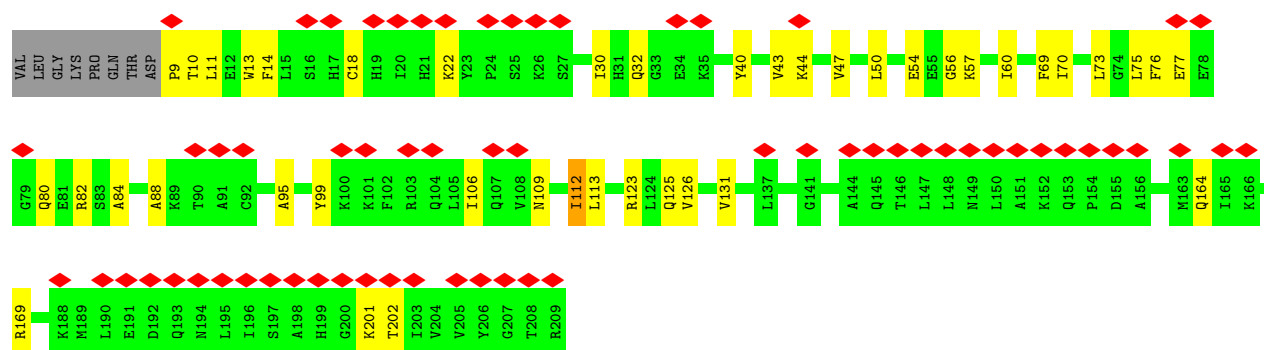
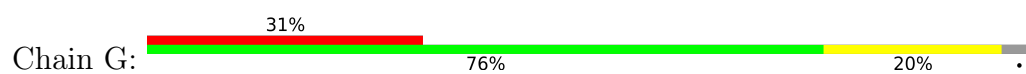
- Molecule 4: DNA-directed RNA polymerase subunit omega



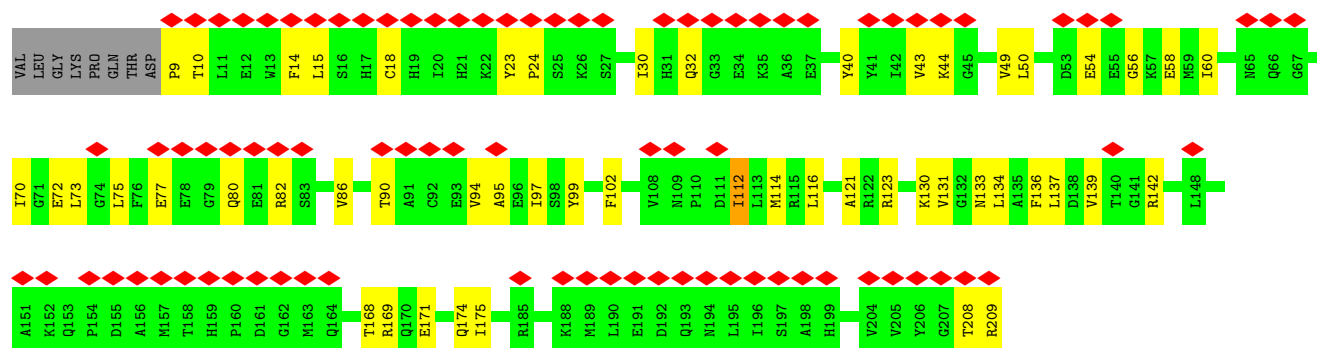
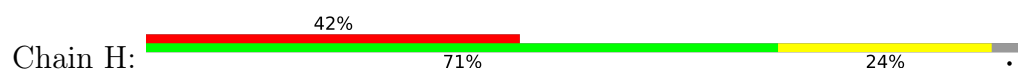
- Molecule 5: RNA polymerase sigma factor rpoD



- Molecule 6: Catabolite gene activator



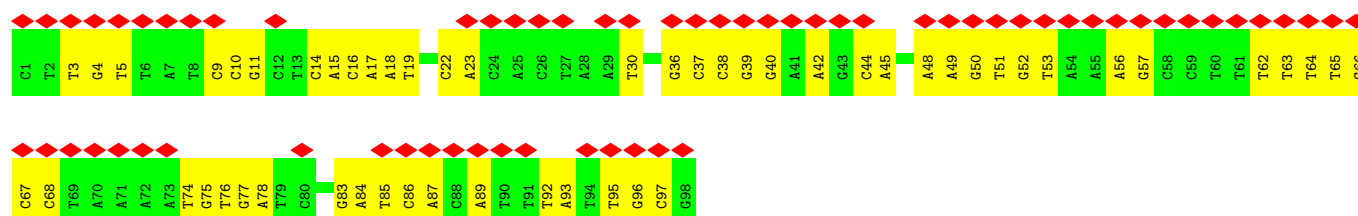
• Molecule 6: Catabolite gene activator



• Molecule 7: DNA (98-MER)



• Molecule 8: DNA (98-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14097	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	ACE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	50000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	14.395	Depositor
Minimum map value	-3.341	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.903	Depositor
Recommended contour level	2.8	Depositor
Map size ($\text{\AA}$)	371.19998, 371.19998, 371.19998	wwPDB
Map dimensions	80, 80, 80	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	4.64, 4.64, 4.64	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: CMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.24	0/2528	0.69	0/3427
1	B	0.25	0/1836	0.70	0/2488
2	C	0.24	0/8672	0.66	0/11722
3	D	0.25	0/10769	0.67	4/14544 (0.0%)
4	E	0.27	0/711	0.65	0/956
5	F	0.24	0/3931	0.64	0/5288
6	G	0.23	0/1616	0.64	0/2174
6	H	0.23	0/1616	0.64	0/2174
7	I	0.11	0/2251	0.38	0/3472
8	J	0.11	0/2236	0.36	0/3447
All	All	0.23	0/36166	0.63	4/49692 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1174	ARG	CB-CA-C	-5.27	109.52	115.79
3	D	533	ALA	CB-CA-C	-5.25	110.50	116.54
3	D	174	ASP	CA-C-O	5.02	120.85	117.94
3	D	174	ASP	CB-CA-C	-5.00	109.86	117.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2496	0	2554	77	0
1	B	1814	0	1839	62	0
2	C	8524	0	8491	299	0
3	D	10606	0	10822	411	0
4	E	709	0	719	38	0
5	F	3877	0	3929	97	0
6	G	1591	0	1632	30	0
6	H	1591	0	1632	36	0
7	I	2006	0	1108	45	0
8	J	1996	0	1111	45	0
9	G	22	0	11	3	0
9	H	22	0	11	2	0
All	All	35254	0	33859	1060	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 15.

The worst 5 of 1060 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)
9:G:679:COMP:H2	9:G:679:COMP:C2	0.97	1.49
9:H:680:COMP:C2	9:H:680:COMP:H2	0.97	1.49
4:E:59:ILE:HG12	4:E:60:ASN:H	1.45	0.81
3:D:1378:ALA:H	3:D:1379:PRO:HD3	1.45	0.81
1:A:235:ARG:H	1:A:235:ARG:HD2	1.45	0.80

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	318/329 (97%)	259 (81%)	46 (14%)	13 (4%)	2	18
1	B	233/329 (71%)	191 (82%)	38 (16%)	4 (2%)	7	36
2	C	1085/1342 (81%)	822 (76%)	217 (20%)	46 (4%)	2	17
3	D	1366/1413 (97%)	1075 (79%)	232 (17%)	59 (4%)	2	17
4	E	88/90 (98%)	68 (77%)	14 (16%)	6 (7%)	1	11
5	F	475/613 (78%)	401 (84%)	54 (11%)	20 (4%)	2	17
6	G	199/209 (95%)	172 (86%)	24 (12%)	3 (2%)	8	40
6	H	199/209 (95%)	182 (92%)	16 (8%)	1 (0%)	24	63
All	All	3963/4534 (87%)	3170 (80%)	641 (16%)	152 (4%)	4	19

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	240	PRO
1	B	52	PRO
2	C	180	ARG
2	C	332	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/286 (97%)	273 (98%)	5 (2%)	51	68
1	B	201/286 (70%)	194 (96%)	7 (4%)	32	53
2	C	936/1157 (81%)	901 (96%)	35 (4%)	30	51
3	D	1138/1174 (97%)	1090 (96%)	48 (4%)	26	48
4	E	74/74 (100%)	68 (92%)	6 (8%)	11	31
5	F	423/540 (78%)	410 (97%)	13 (3%)	35	56
6	G	173/180 (96%)	172 (99%)	1 (1%)	78	83
6	H	173/180 (96%)	172 (99%)	1 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3396/3877 (88%)	3280 (97%)	116 (3%)	33 54

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	334	LYS
5	F	418	LYS
3	D	690	ASN
5	F	405	ILE
4	E	70	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	340	GLN
5	F	579	GLN
3	D	708	ASN
5	F	469	GLN
5	F	149	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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
9	CMP	G	679	-	25,25,25	1.79	6 (24%)	37,39,39	2.10	10 (27%)
9	CMP	H	680	-	25,25,25	1.78	6 (24%)	37,39,39	2.11	10 (27%)

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
9	CMP	G	679	-	-	0/4/31/31	0/4/4/4
9	CMP	H	680	-	-	0/4/31/31	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	680	CMP	C5-C4	4.74	1.47	1.39
9	G	679	CMP	C5-C4	4.72	1.47	1.39
9	G	679	CMP	P-O5'	4.09	1.62	1.57
9	H	680	CMP	P-O5'	4.08	1.62	1.57
9	G	679	CMP	C5-C6	2.78	1.48	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	680	CMP	C5-C4-N3	-5.85	118.66	126.72
9	G	679	CMP	C5-C4-N3	-5.81	118.71	126.72
9	H	680	CMP	O3'-C3'-C4'	-5.07	106.88	110.71
9	G	679	CMP	O3'-C3'-C4'	-5.07	106.88	110.71
9	H	680	CMP	N3-C4-N9	4.62	135.03	127.17

There are no chirality outliers.

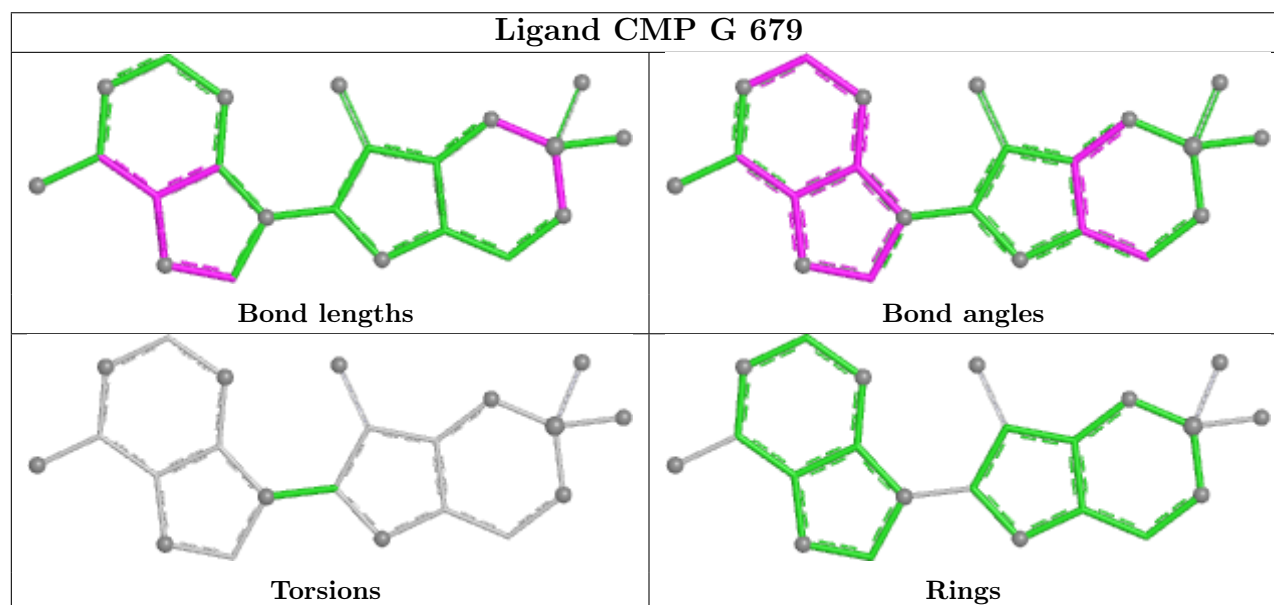
There are no torsion outliers.

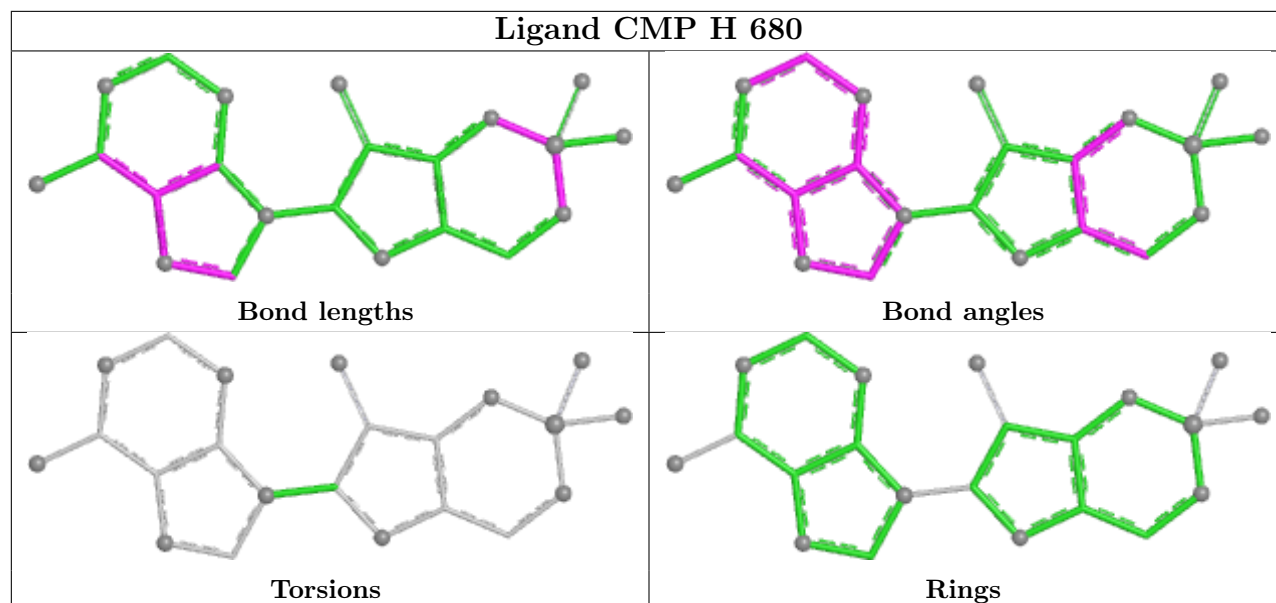
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	679	CMP	3	0
9	H	680	CMP	2	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

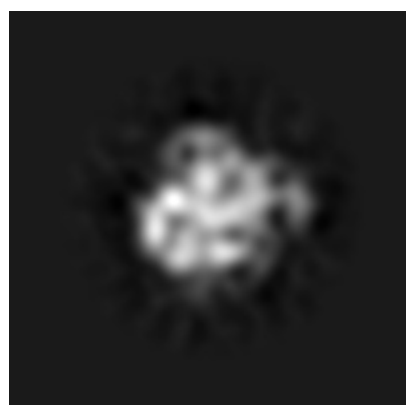
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5127. 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](#)

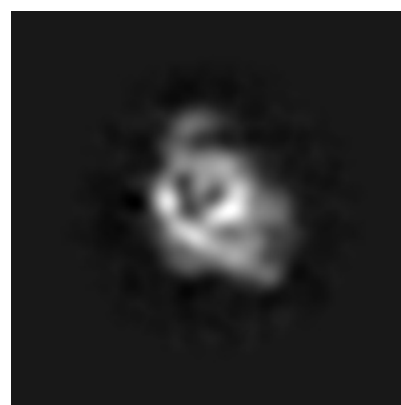
6.1.1 Primary map



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: 40



Y Index: 40



Z Index: 40

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: 44



Y Index: 39

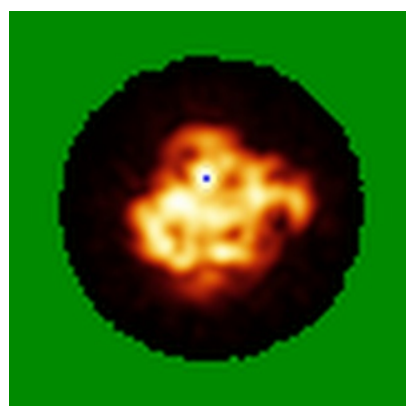


Z Index: 41

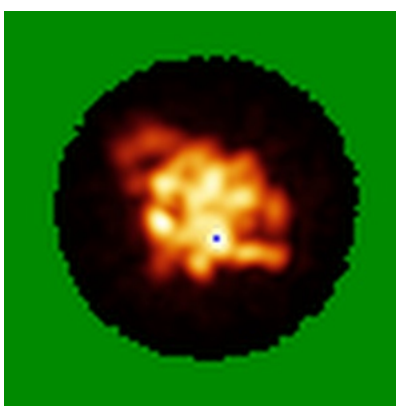
The images above show the largest variance slices of the map in three orthogonal directions.

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

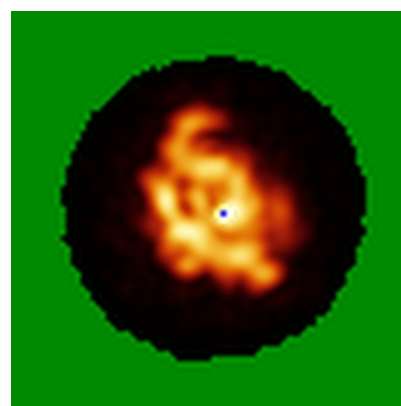
6.4.1 Primary map



X



Y

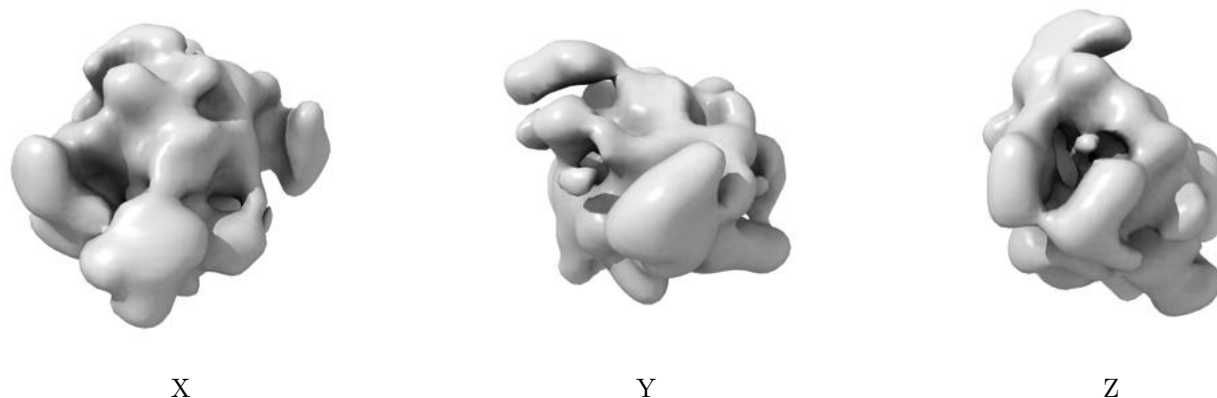


Z

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



The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

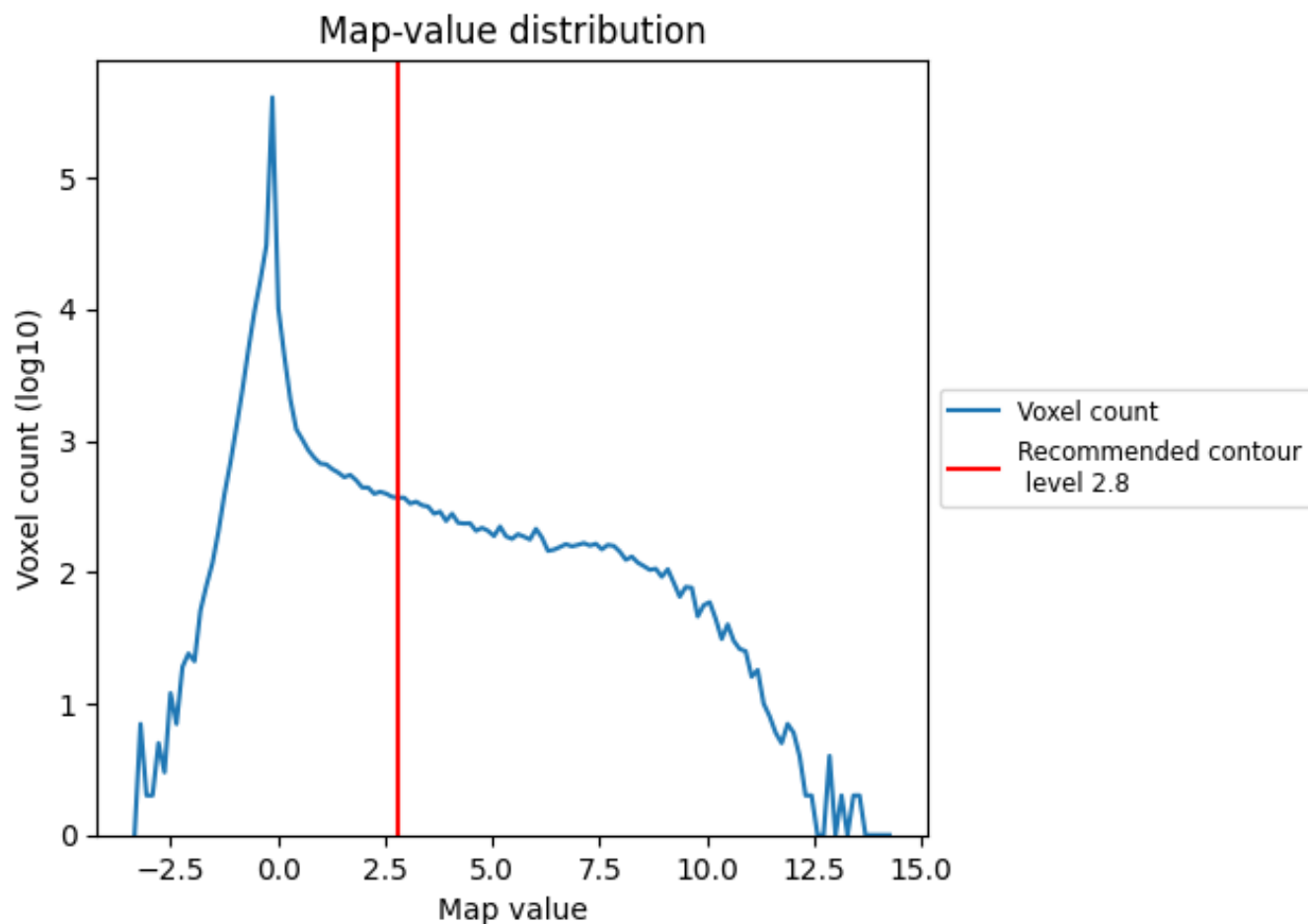
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

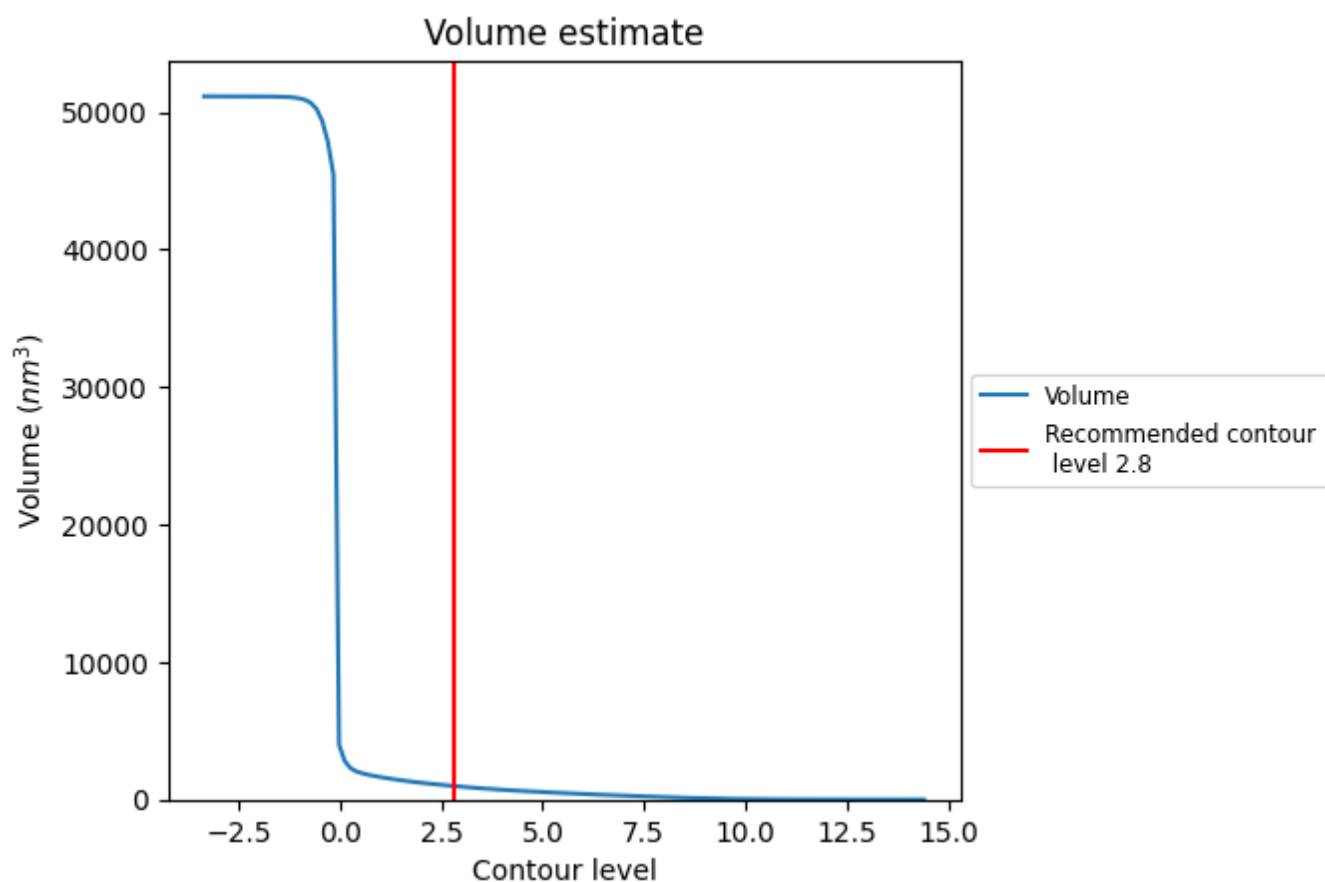
This section contains the results of statistical analysis of the map.

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.

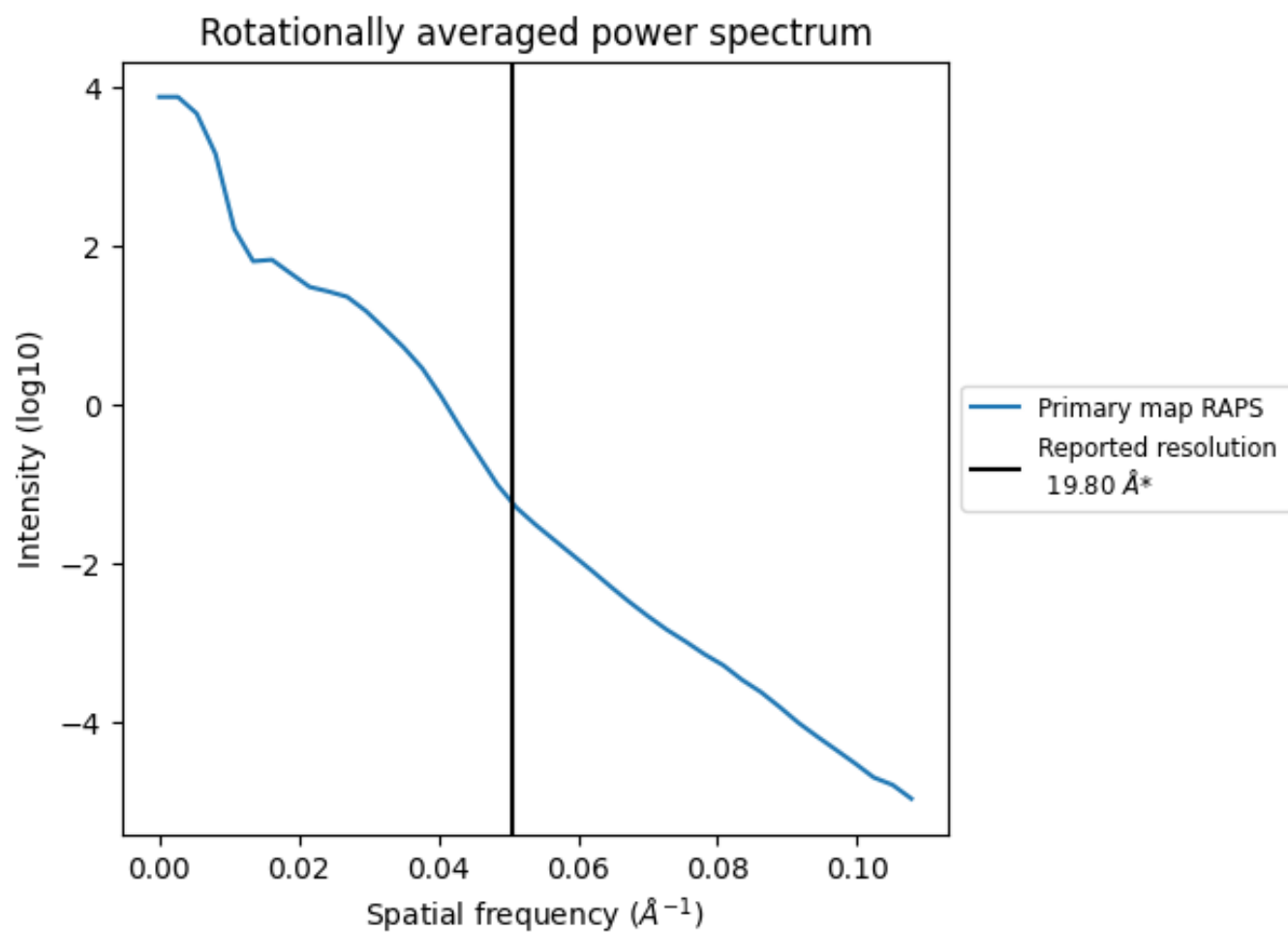
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 989 nm³; this corresponds to an approximate mass of 893 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.051 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

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-5127 and PDB model 3IYD. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

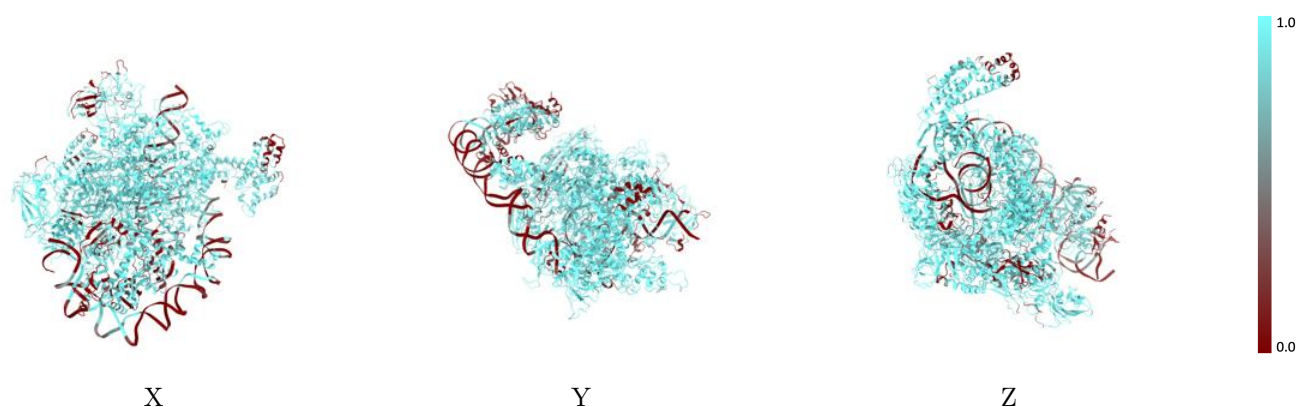
This section was not generated.

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



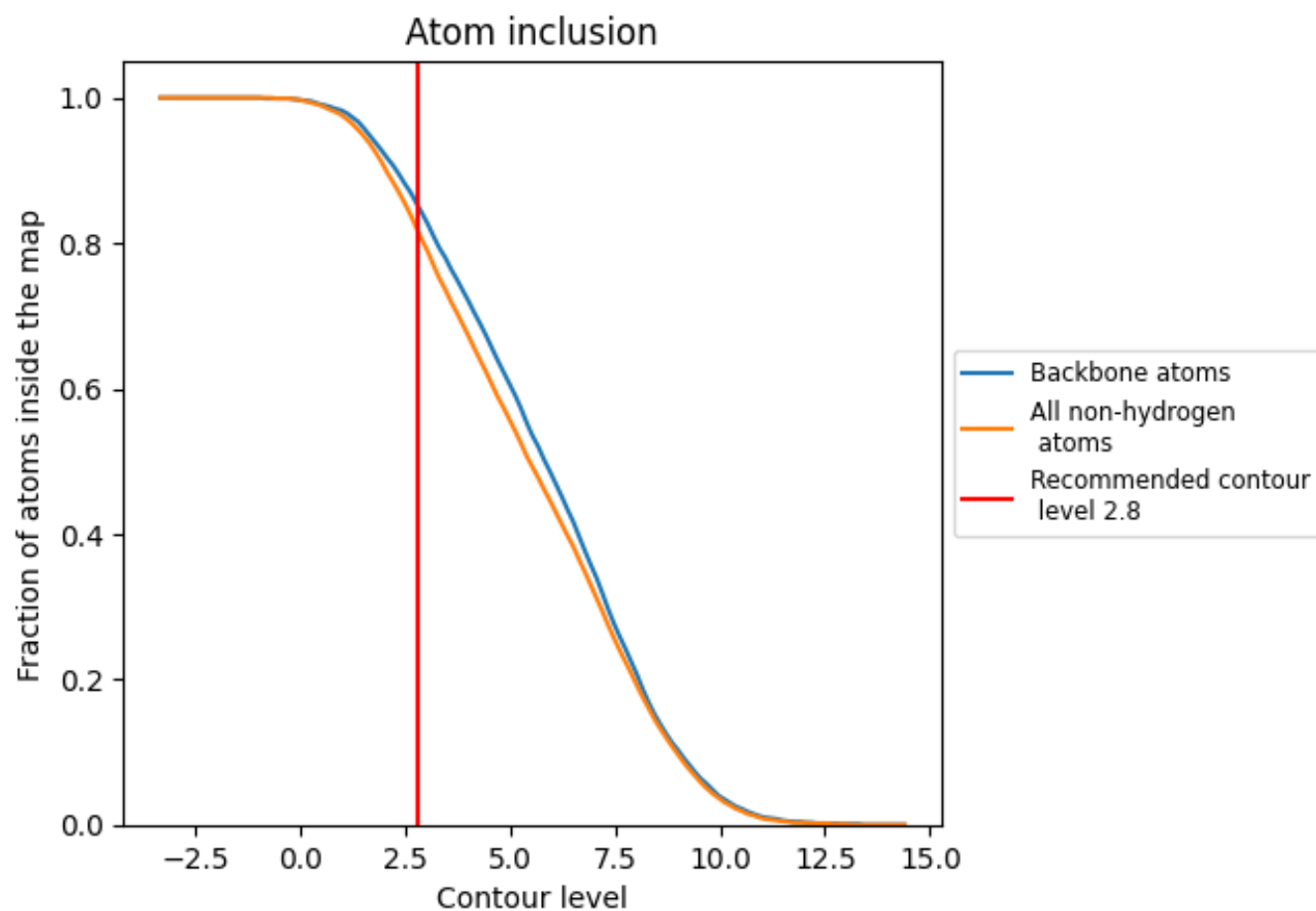
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.0460
A	0.9100	0.0450
B	0.9070	0.0500
C	0.9300	0.0460
D	0.9080	0.0500
E	0.9610	0.0370
F	0.8800	0.0590
G	0.6420	0.0480
H	0.5480	0.0440
I	0.3510	0.0250
J	0.3030	0.0170

1.0

0.0

<0.0