



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:33 AM UTC

PDB ID : 8HSL / pdb_00008hsl
EMDB ID : EMD-35000
Title : Thermus thermophilus RNA polymerase bound with an inverted Rho hexamer
Authors : Murayama, Y.; Ehara, H.; Sekine, S.
Deposited on : 2022-12-19
Resolution : 5.80 Å(reported)

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

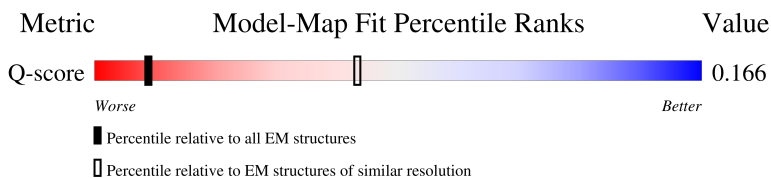
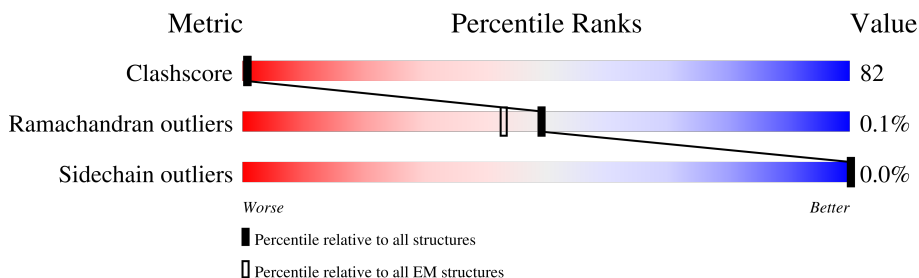
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 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	511 (5.30 - 6.30)

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	G	315	22% 8% 65% 27%
1	H	315	36% 7% 65% 27%
2	I	1119	41% 14% 84% .
3	J	1532	30% 10% 73% 17%

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Mol	Chain	Length	Quality of chain
4	K	99	
5	A	428	
5	B	428	
5	C	428	
5	D	428	
5	E	428	
5	F	428	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BEF	A	1002	-	-	X	-
9	BEF	F	1002	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 40350 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	229	Total	C	N	O	S	0	0
			1806	1153	313	337	3		
1	H	229	Total	C	N	O	S	0	0
			1806	1153	313	337	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1096	Total	C	N	O	S	0	0
			8644	5468	1543	1609	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1278	Total	C	N	O	S	0	0
			10078	6384	1783	1883	28		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1525	ASP	-	expression tag	UNP Q8RQE8
J	1526	TYR	-	expression tag	UNP Q8RQE8
J	1527	LYS	-	expression tag	UNP Q8RQE8
J	1528	ASP	-	expression tag	UNP Q8RQE8
J	1529	ASP	-	expression tag	UNP Q8RQE8
J	1530	ASP	-	expression tag	UNP Q8RQE8
J	1531	ASP	-	expression tag	UNP Q8RQE8
J	1532	LYS	-	expression tag	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	95	Total	C	N	O	S	0	0
			770	491	133	142	4		

- Molecule 5 is a protein called Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		
5	B	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		
5	C	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		
5	D	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		
5	E	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		
5	F	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q5SJE9
A	0	PRO	-	expression tag	UNP Q5SJE9
B	-1	GLY	-	expression tag	UNP Q5SJE9
B	0	PRO	-	expression tag	UNP Q5SJE9
C	-1	GLY	-	expression tag	UNP Q5SJE9
C	0	PRO	-	expression tag	UNP Q5SJE9
D	-1	GLY	-	expression tag	UNP Q5SJE9
D	0	PRO	-	expression tag	UNP Q5SJE9
E	-1	GLY	-	expression tag	UNP Q5SJE9
E	0	PRO	-	expression tag	UNP Q5SJE9
F	-1	GLY	-	expression tag	UNP Q5SJE9
F	0	PRO	-	expression tag	UNP Q5SJE9

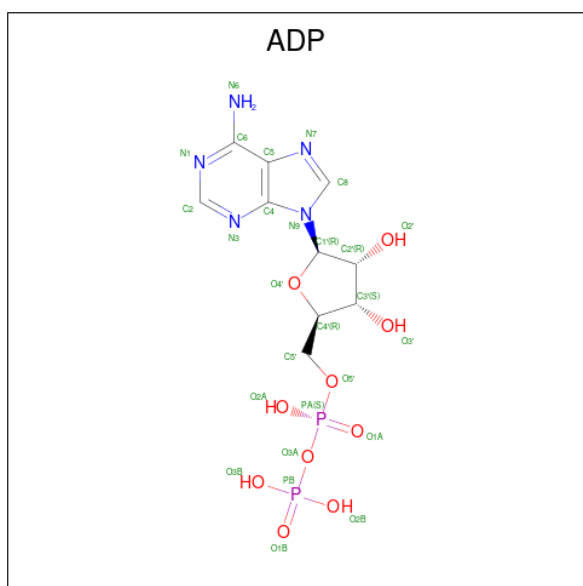
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	J	1	Total	Zn	0
			1	1	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	J	1	Total 1	Mg 1	0
7	A	1	Total 1	Mg 1	0
7	B	1	Total 1	Mg 1	0
7	C	1	Total 1	Mg 1	0
7	D	1	Total 1	Mg 1	0
7	E	1	Total 1	Mg 1	0
7	F	1	Total 1	Mg 1	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



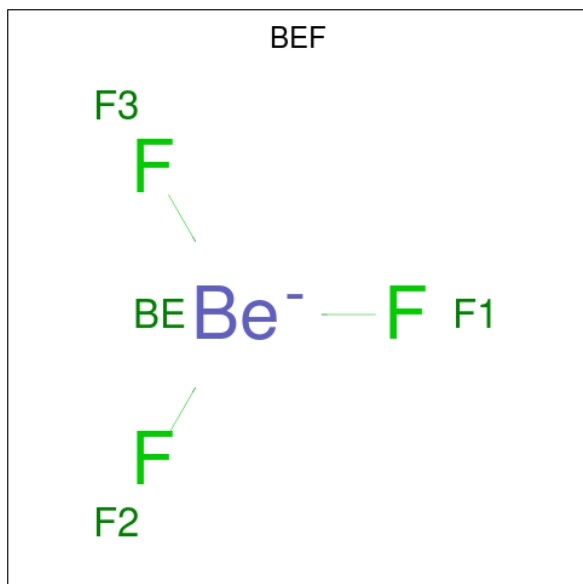
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 27	C 10	N 5	O 10	P 2	0
8	B	1	Total 27	C 10	N 5	O 10	P 2	0
8	C	1	Total 27	C 10	N 5	O 10	P 2	0
8	D	1	Total 27	C 10	N 5	O 10	P 2	0
8	E	1	Total 27	C 10	N 5	O 10	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
8	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 9 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).

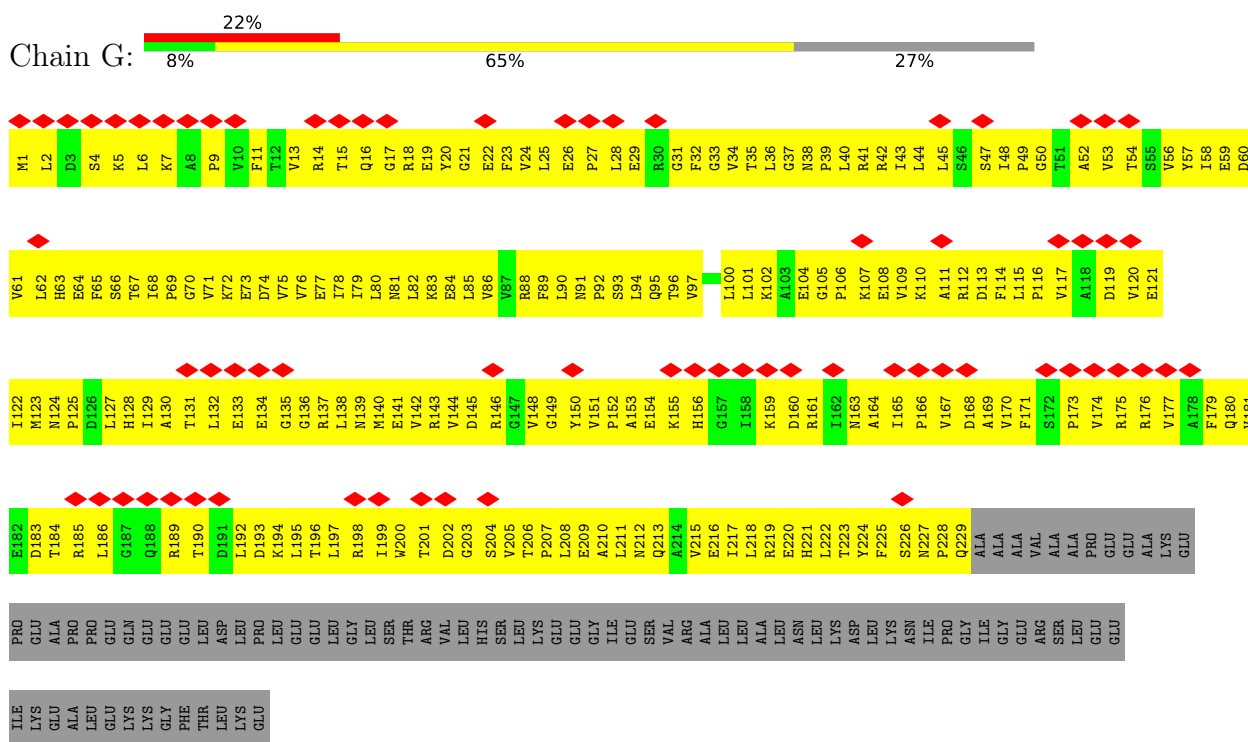


Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	Be	F	0
			4	1	3	
9	B	1	Total	Be	F	0
			4	1	3	
9	C	1	Total	Be	F	0
			4	1	3	
9	D	1	Total	Be	F	0
			4	1	3	
9	E	1	Total	Be	F	0
			4	1	3	
9	F	1	Total	Be	F	0
			4	1	3	

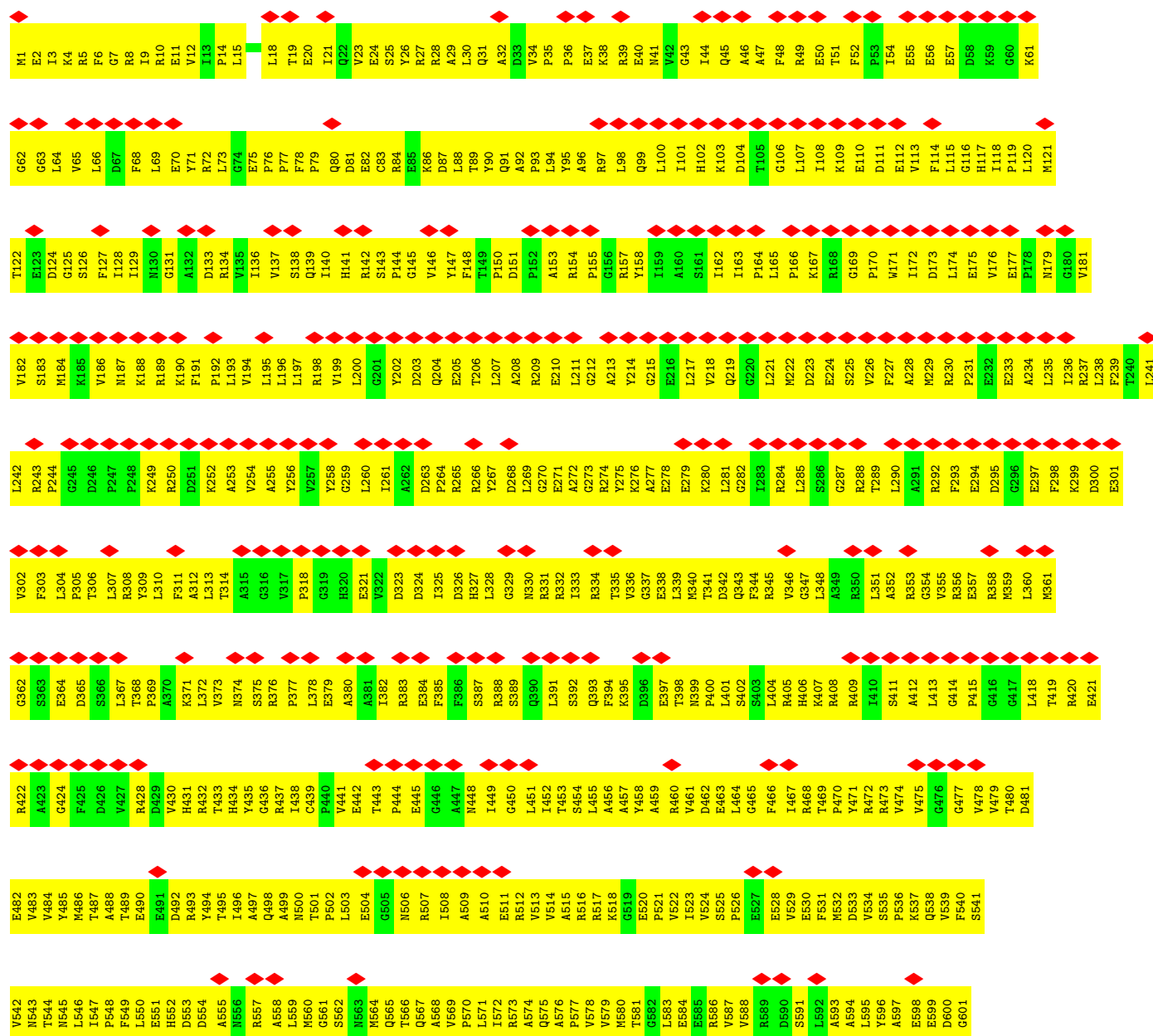
3 Residue-property plots

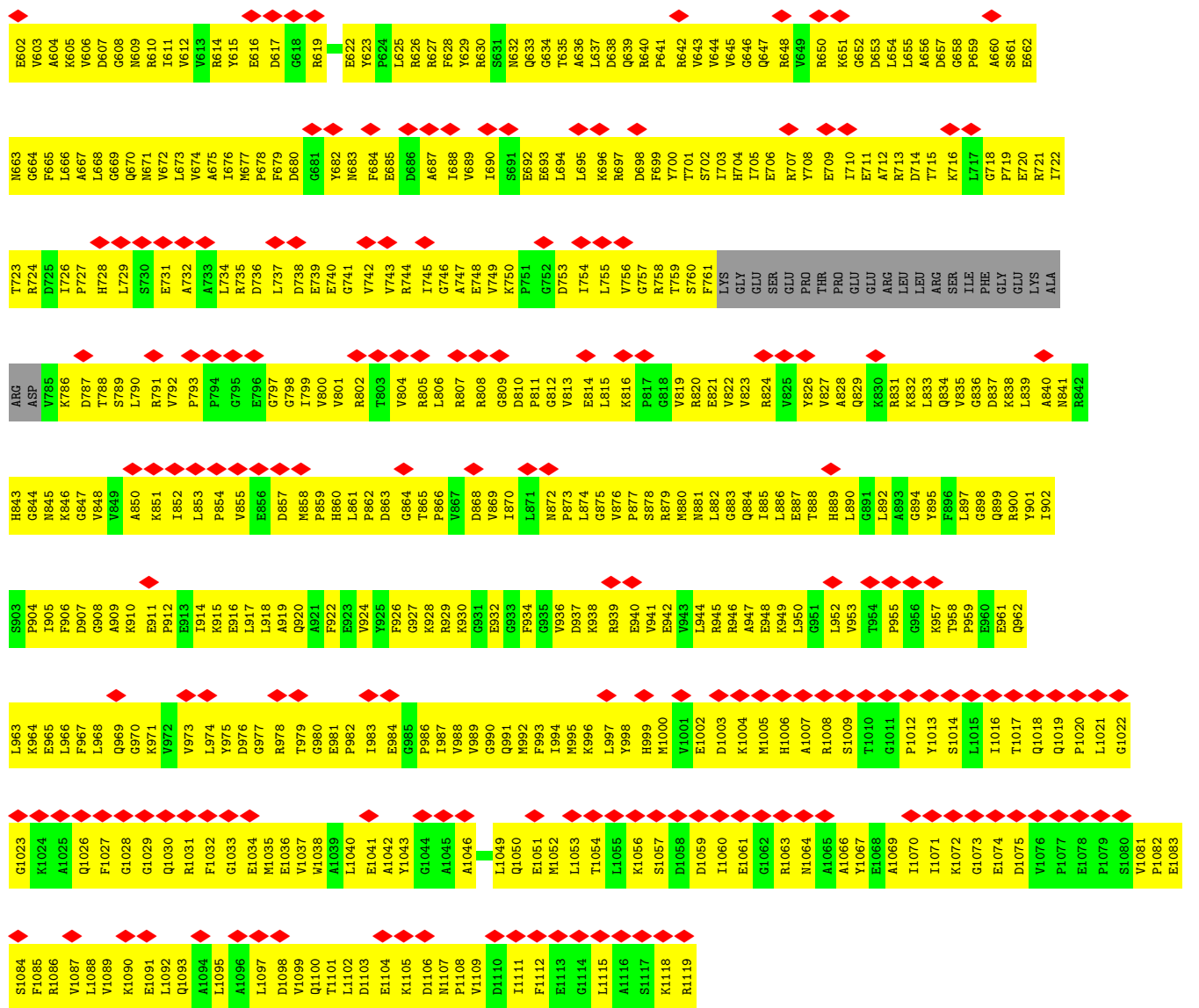
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

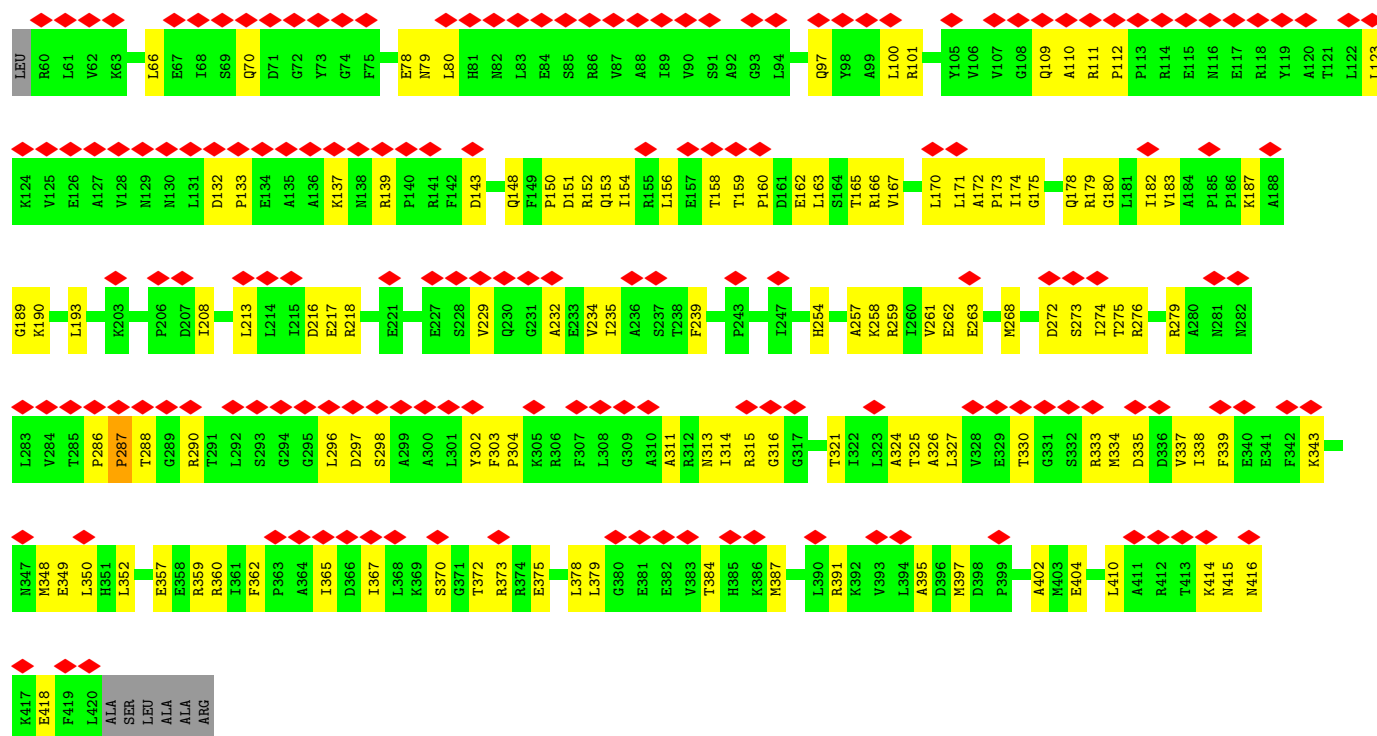


- Molecule 2: DNA-directed RNA polymerase subunit beta

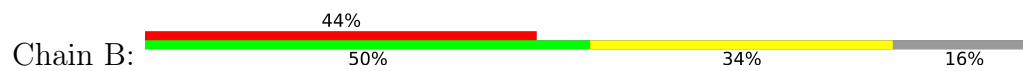




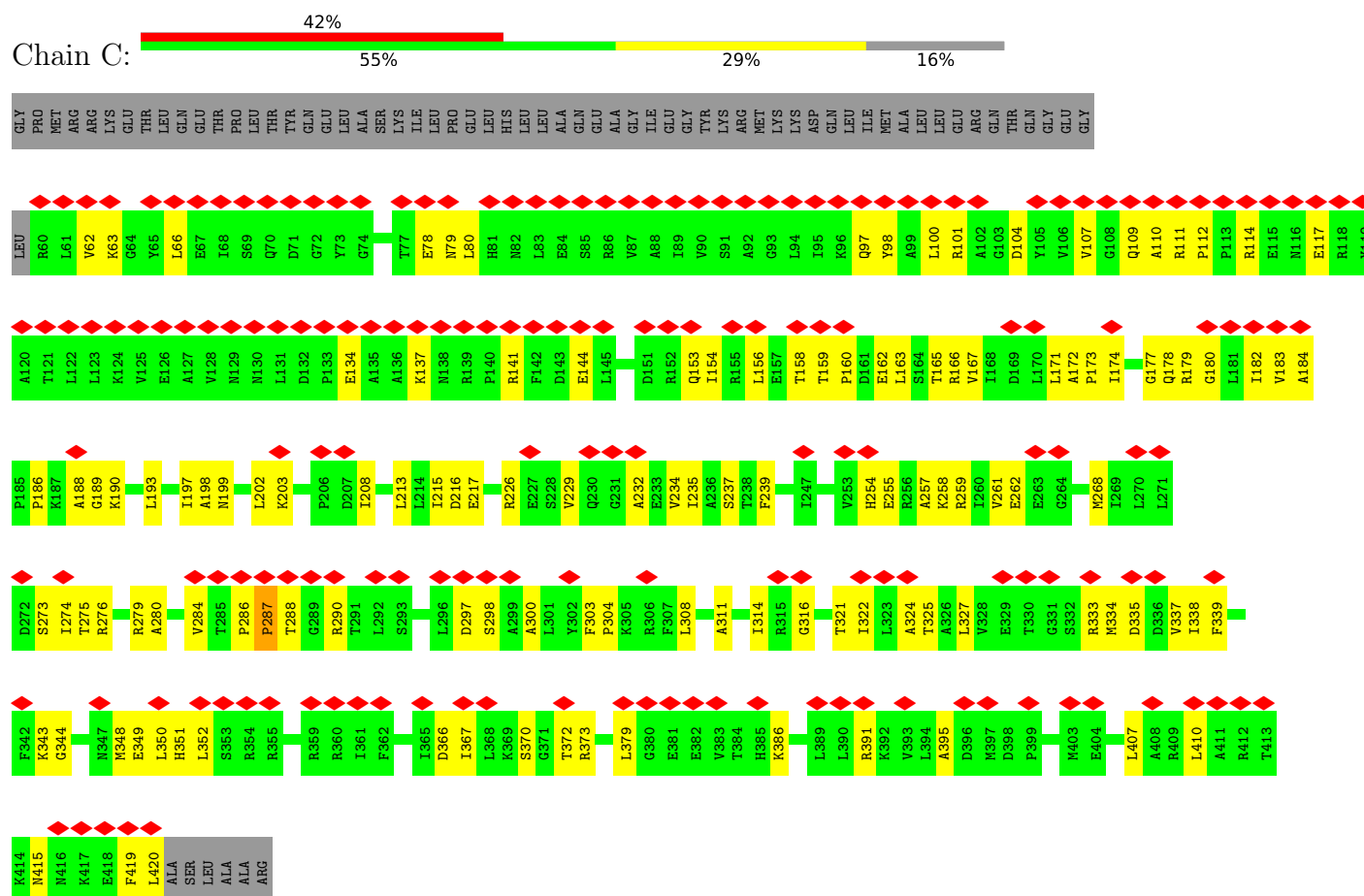




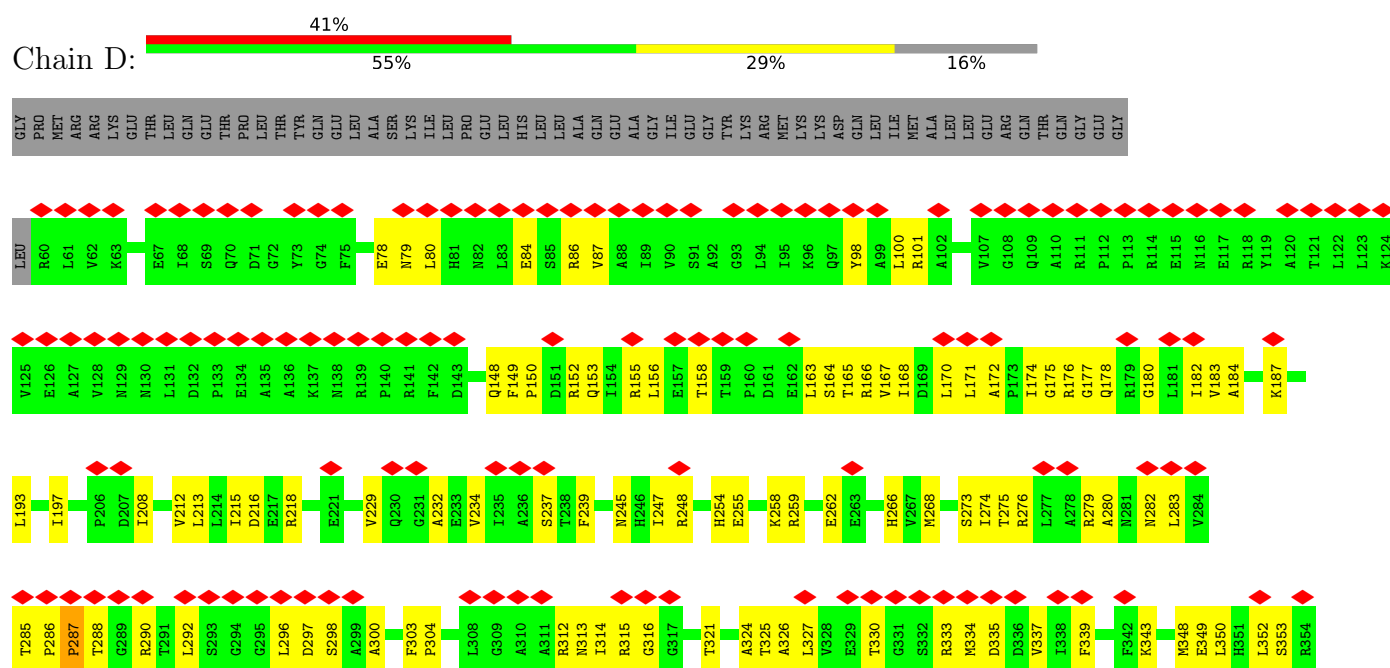
• Molecule 5: Transcription termination factor Rho

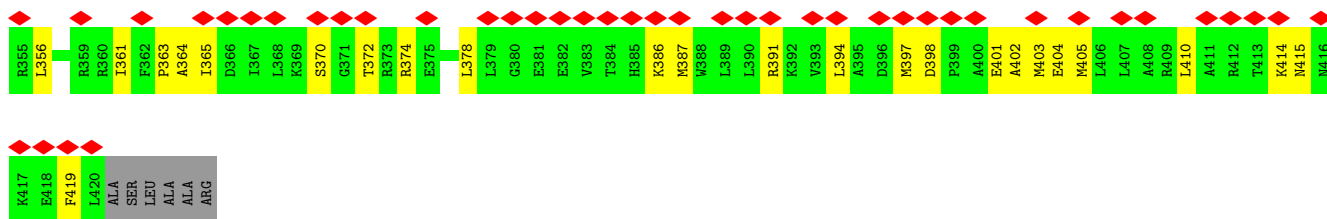


• Molecule 5: Transcription termination factor Rho



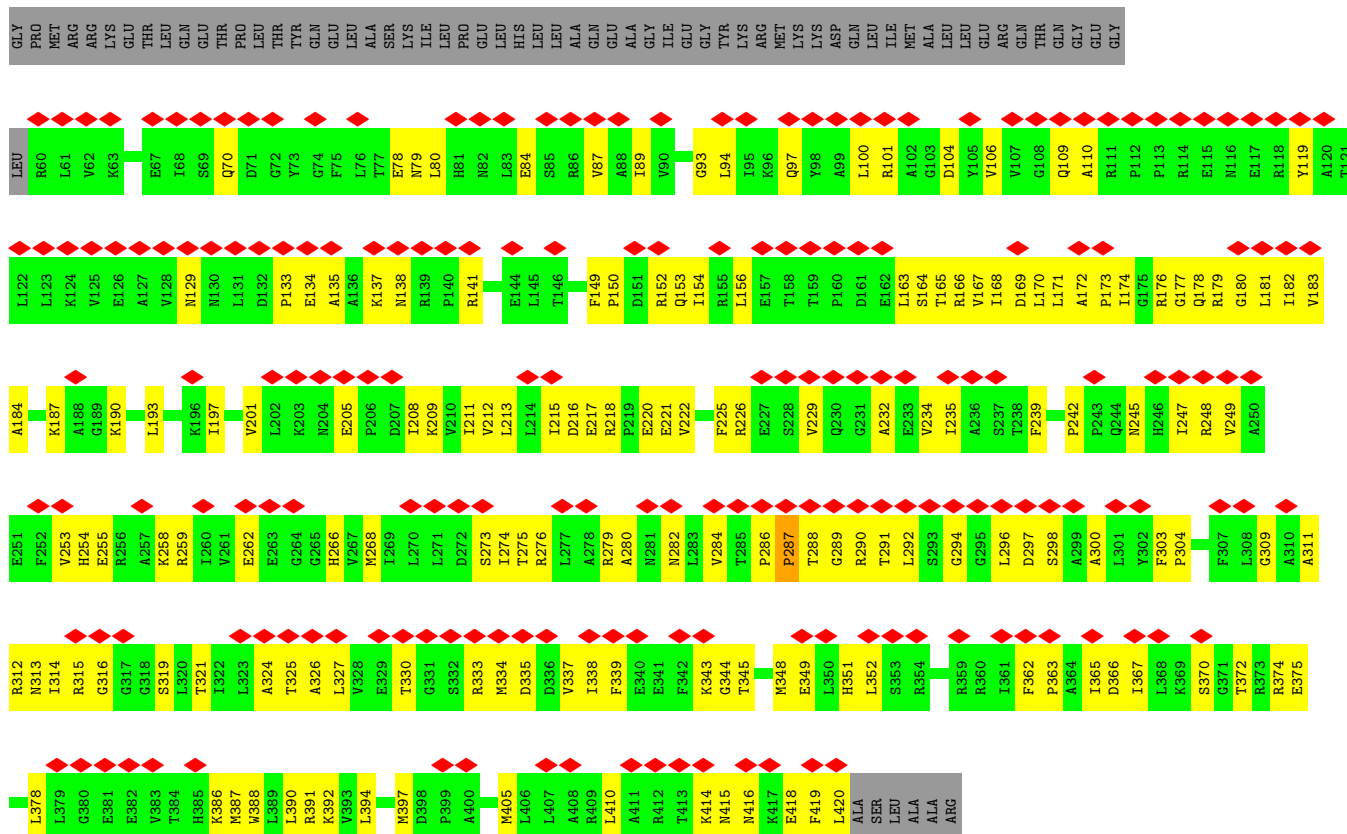
• Molecule 5: Transcription termination factor Rho





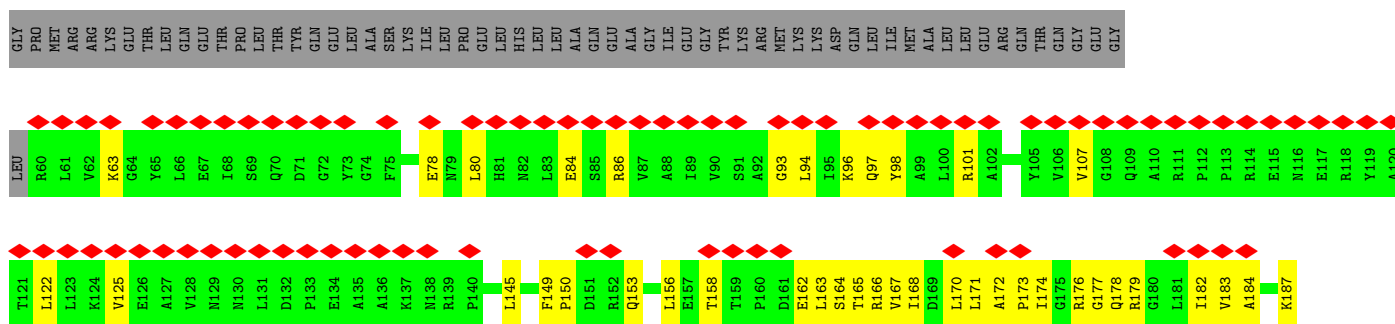
• Molecule 5: Transcription termination factor Rho

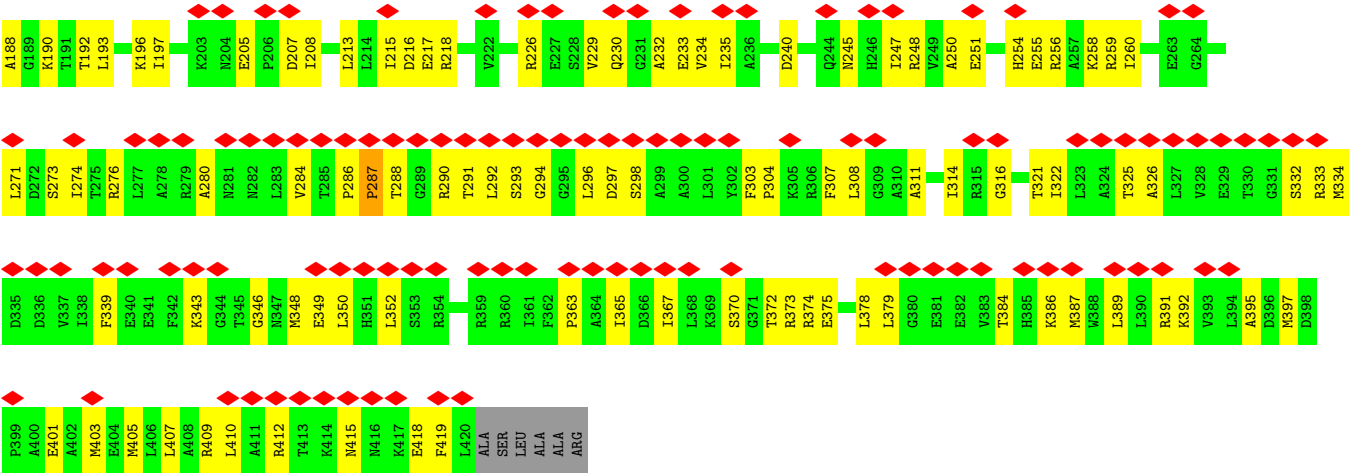
Chain E: 45% 46% 38% 16%



• Molecule 5: Transcription termination factor Rho

Chain F: 46% 52% 32% 16%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147189	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size ($\text{\AA}$)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, BEF, ADP

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	0.24	0/1838	0.46	0/2498
1	H	0.21	0/1838	0.44	0/2498
2	I	0.21	0/8808	0.44	0/11910
3	J	0.22	0/10246	0.49	0/13842
4	K	0.20	0/784	0.53	0/1057
5	A	0.19	0/2886	0.42	0/3900
5	B	0.19	0/2886	0.40	0/3900
5	C	0.18	0/2886	0.38	0/3900
5	D	0.20	0/2886	0.41	0/3900
5	E	0.22	0/2886	0.47	0/3900
5	F	0.21	0/2886	0.44	0/3900
All	All	0.21	0/40830	0.45	0/55205

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1806	0	1861	489	0
1	H	1806	0	1861	529	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	8644	0	8749	2257	0
3	J	10078	0	10316	2708	0
4	K	770	0	784	211	0
5	A	2842	0	2925	120	0
5	B	2842	0	2925	135	0
5	C	2842	0	2925	114	0
5	D	2842	0	2925	107	0
5	E	2842	0	2926	157	0
5	F	2842	0	2925	133	0
6	J	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	J	1	0	0	0	0
8	A	27	0	12	4	0
8	B	27	0	12	0	0
8	C	27	0	12	3	0
8	D	27	0	12	1	0
8	E	27	0	12	2	0
8	F	27	0	12	3	0
9	A	4	0	0	2	0
9	B	4	0	0	1	0
9	C	4	0	0	1	0
9	D	4	0	0	0	0
9	E	4	0	0	1	0
9	F	4	0	0	2	0
All	All	40350	0	41194	6663	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 82.

The worst 5 of 6663 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:699:VAL:HA	3:J:718:PRO:HD3	1.23	1.17
3:J:792:ILE:HG13	3:J:860:LEU:HD21	1.26	1.16
3:J:800:LYS:HE3	3:J:804:LEU:HB3	1.23	1.16
2:I:755:LEU:HB2	2:I:790:LEU:HG	1.15	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:VAL:HB	1:H:169:ALA:HB3	1.22	1.13

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	227/315 (72%)	211 (93%)	16 (7%)	0	100	100
1	H	227/315 (72%)	213 (94%)	14 (6%)	0	100	100
2	I	1092/1119 (98%)	975 (89%)	117 (11%)	0	100	100
3	J	1270/1532 (83%)	1138 (90%)	131 (10%)	1 (0%)	48	83
4	K	93/99 (94%)	87 (94%)	6 (6%)	0	100	100
5	A	359/428 (84%)	345 (96%)	13 (4%)	1 (0%)	36	72
5	B	359/428 (84%)	345 (96%)	13 (4%)	1 (0%)	36	72
5	C	359/428 (84%)	345 (96%)	13 (4%)	1 (0%)	36	72
5	D	359/428 (84%)	345 (96%)	13 (4%)	1 (0%)	36	72
5	E	359/428 (84%)	343 (96%)	15 (4%)	1 (0%)	36	72
5	F	359/428 (84%)	343 (96%)	15 (4%)	1 (0%)	36	72
All	All	5063/5948 (85%)	4690 (93%)	366 (7%)	7 (0%)	49	83

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	287	PRO
5	B	287	PRO
5	C	287	PRO
5	D	287	PRO
5	E	287	PRO

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	G	202/273 (74%)	202 (100%)	0	100	100
1	H	202/273 (74%)	201 (100%)	1 (0%)	81	83
2	I	921/941 (98%)	921 (100%)	0	100	100
3	J	1079/1287 (84%)	1079 (100%)	0	100	100
4	K	84/88 (96%)	84 (100%)	0	100	100
5	A	304/359 (85%)	304 (100%)	0	100	100
5	B	304/359 (85%)	304 (100%)	0	100	100
5	C	304/359 (85%)	304 (100%)	0	100	100
5	D	304/359 (85%)	304 (100%)	0	100	100
5	E	304/359 (85%)	304 (100%)	0	100	100
5	F	304/359 (85%)	304 (100%)	0	100	100
All	All	4312/5016 (86%)	4311 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	227	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	696	HIS
3	J	1195	GLN
5	D	138	ASN
3	J	729	HIS
3	J	976	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 ⓘ

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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
9	BEF	B	1002	8	0,3,3	-	-	-		
8	ADP	E	1000	7	28,29,29	1.42	4 (14%)	43,45,45	1.92	12 (27%)
8	ADP	F	1000	7	28,29,29	1.38	4 (14%)	43,45,45	1.95	10 (23%)
8	ADP	B	1000	9,7	28,29,29	1.41	4 (14%)	43,45,45	1.91	11 (25%)
9	BEF	E	1002	-	0,3,3	-	-	-		
8	ADP	A	1000	9,7	28,29,29	1.37	5 (17%)	43,45,45	1.91	11 (25%)
8	ADP	C	1000	7	28,29,29	1.41	4 (14%)	43,45,45	1.92	10 (23%)
9	BEF	A	1002	8	0,3,3	-	-	-		
8	ADP	D	1000	7	28,29,29	1.38	4 (14%)	43,45,45	1.90	11 (25%)
9	BEF	F	1002	-	0,3,3	-	-	-		
9	BEF	C	1002	-	0,3,3	-	-	-		
9	BEF	D	1002	-	0,3,3	-	-	-		

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	ADP	E	1000	7	-	6/16/32/32	0/3/3/3
8	ADP	F	1000	7	-	5/16/32/32	0/3/3/3
8	ADP	B	1000	9,7	-	4/16/32/32	0/3/3/3
8	ADP	A	1000	9,7	-	1/16/32/32	0/3/3/3
8	ADP	C	1000	7	-	2/16/32/32	0/3/3/3
8	ADP	D	1000	7	-	2/16/32/32	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1000	ADP	C5-C4	4.69	1.47	1.39
8	B	1000	ADP	C5-C4	4.65	1.47	1.39
8	E	1000	ADP	C5-C4	4.59	1.47	1.39
8	D	1000	ADP	C5-C4	4.57	1.47	1.39
8	F	1000	ADP	C5-C4	4.54	1.47	1.39

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1000	ADP	C5-C4-N3	-6.08	118.34	126.72
8	B	1000	ADP	C5-C4-N3	-5.96	118.51	126.72
8	F	1000	ADP	C5-C4-N3	-5.91	118.58	126.72
8	E	1000	ADP	C5-C4-N3	-5.89	118.61	126.72
8	D	1000	ADP	C5-C4-N3	-5.82	118.70	126.72

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

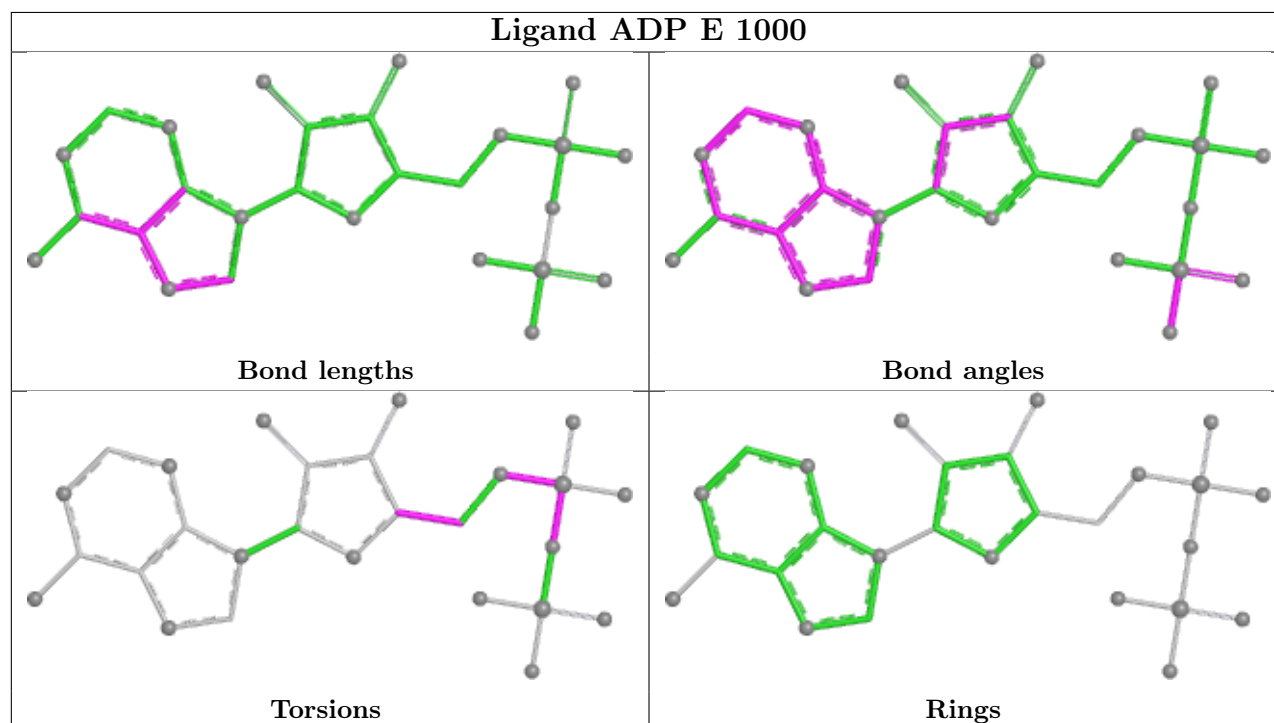
Mol	Chain	Res	Type	Atoms
8	B	1000	ADP	C5'-O5'-PA-O1A
8	B	1000	ADP	C5'-O5'-PA-O2A
8	B	1000	ADP	C5'-O5'-PA-O3A
8	C	1000	ADP	C5'-O5'-PA-O1A
8	C	1000	ADP	C5'-O5'-PA-O3A

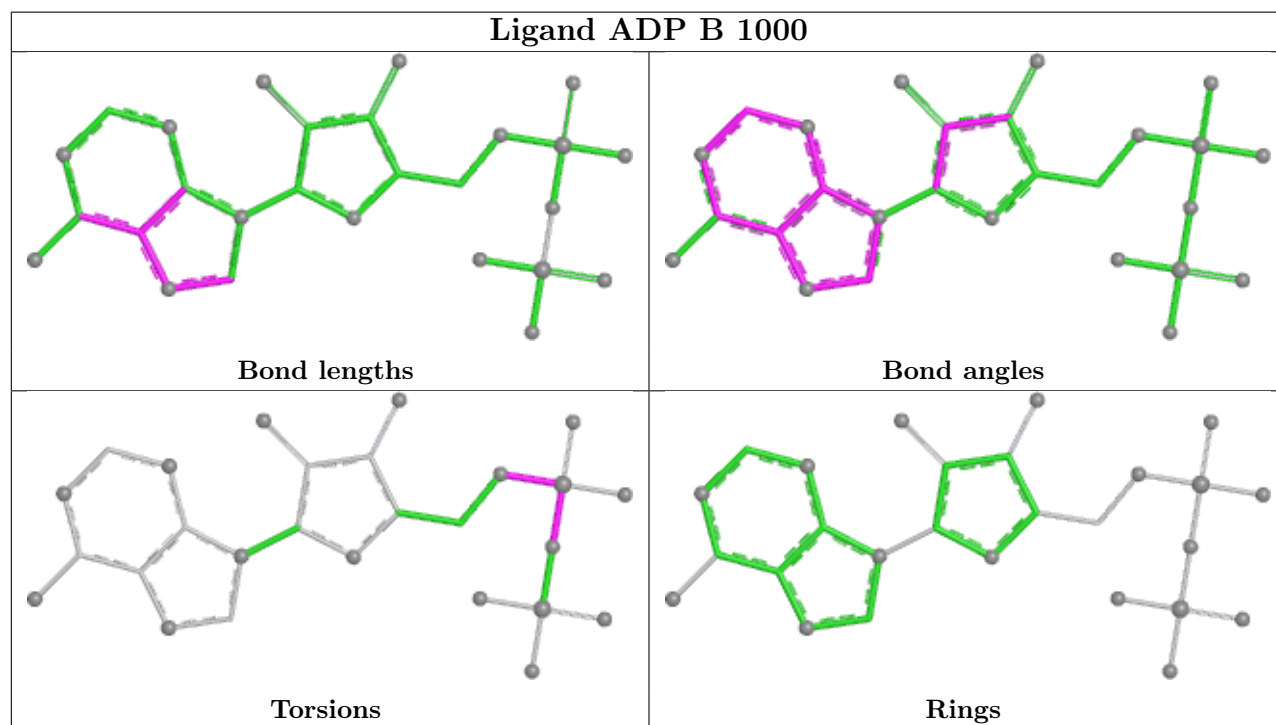
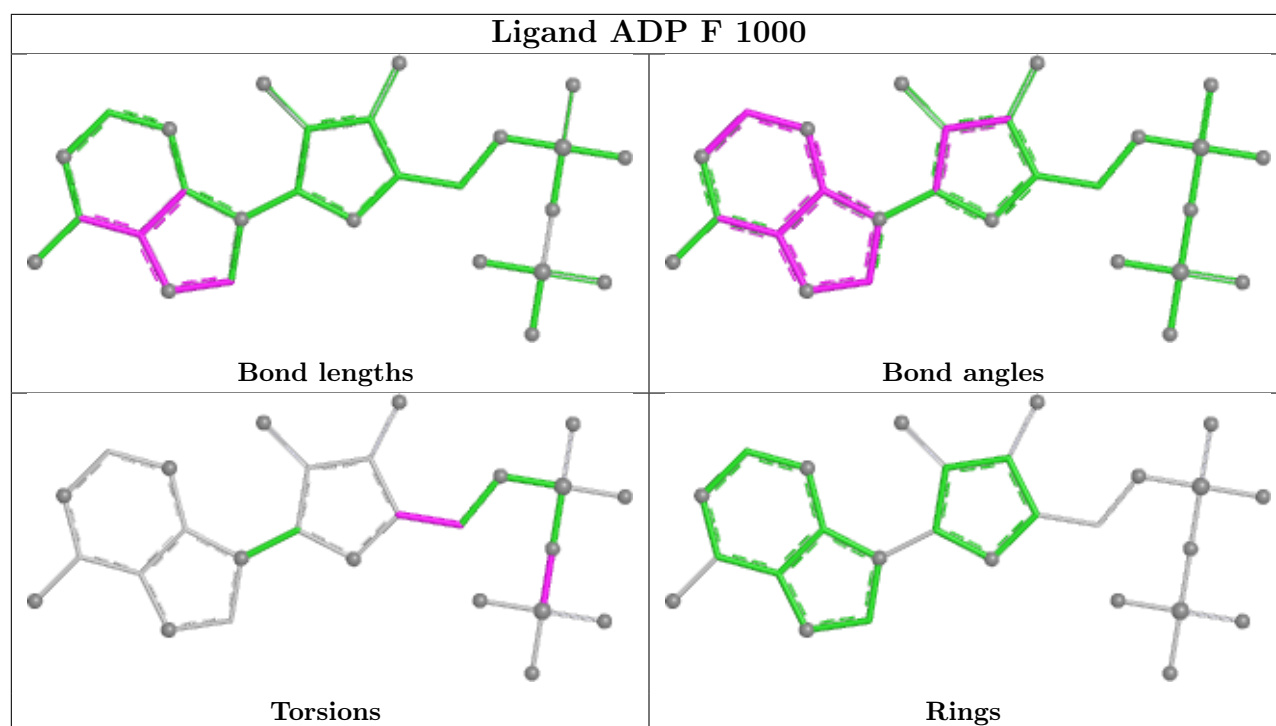
There are no ring outliers.

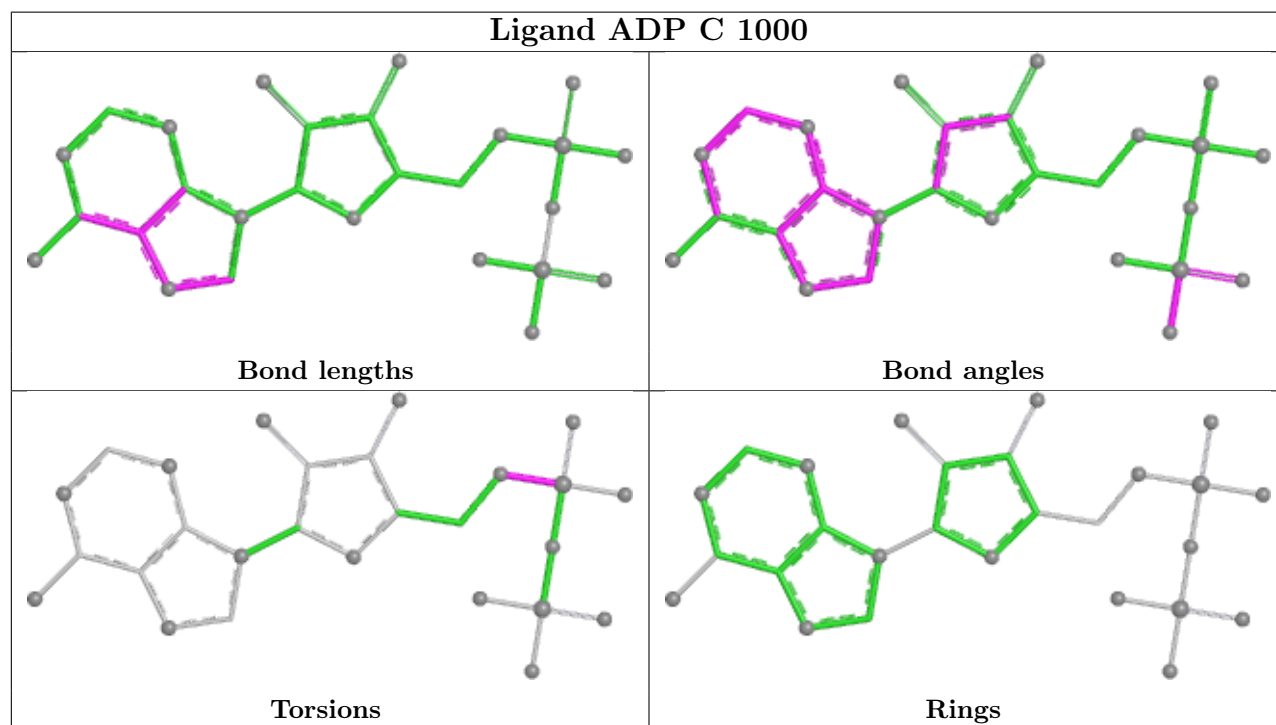
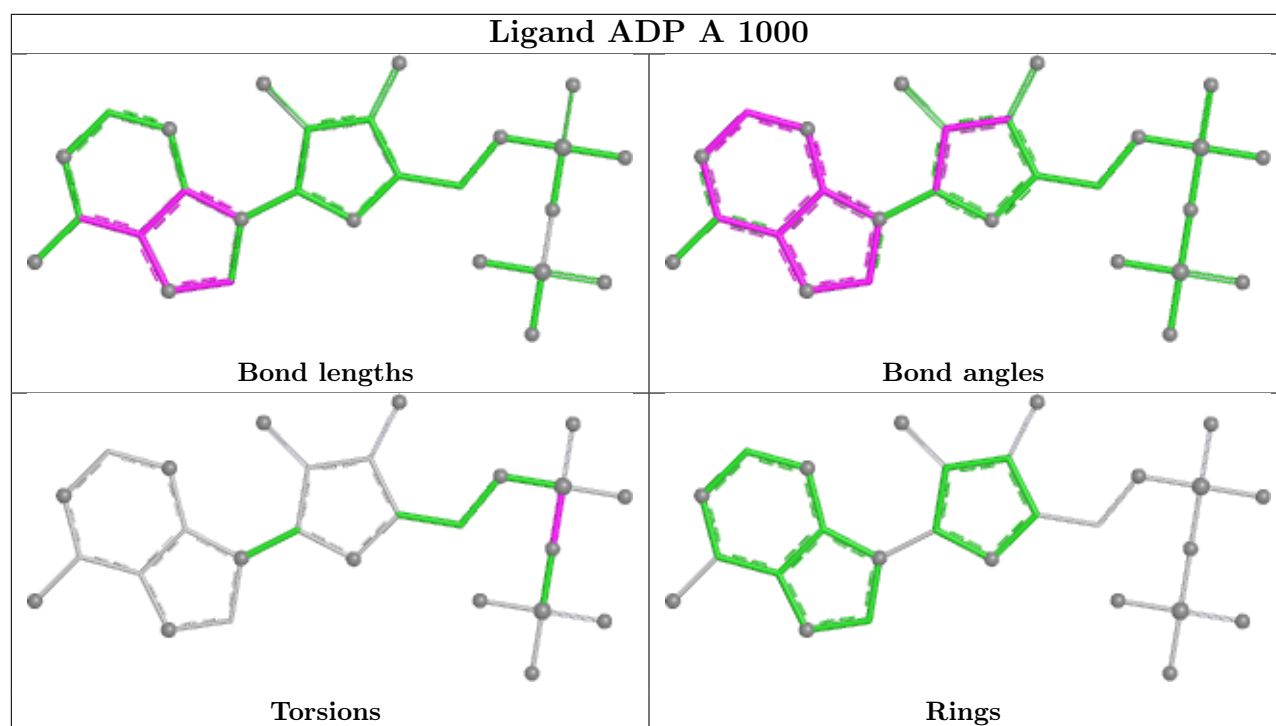
10 monomers are involved in 16 short contacts:

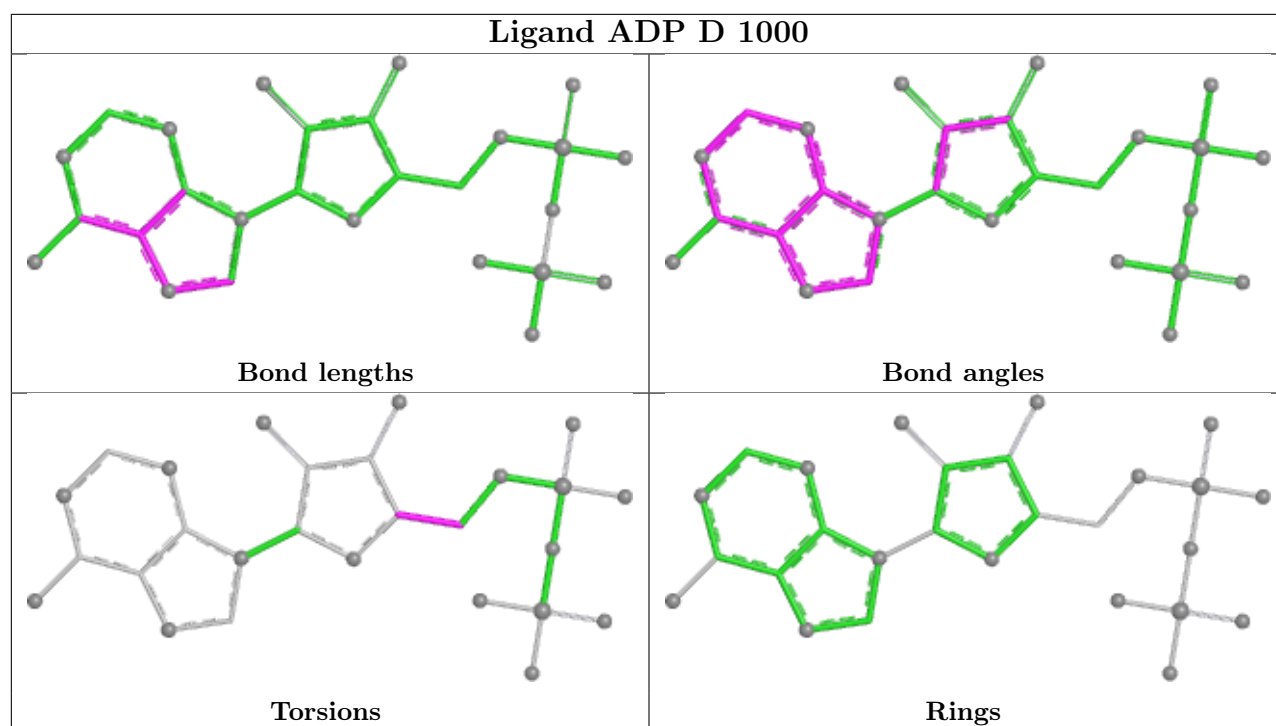
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1002	BEF	1	0
8	E	1000	ADP	2	0
8	F	1000	ADP	3	0
9	E	1002	BEF	1	0
8	A	1000	ADP	4	0
8	C	1000	ADP	3	0
9	A	1002	BEF	2	0
8	D	1000	ADP	1	0
9	F	1002	BEF	2	0
9	C	1002	BEF	1	0

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 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.

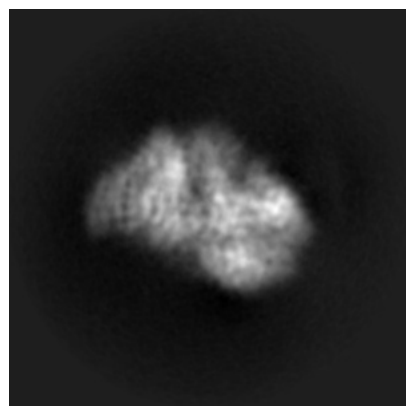
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35000. These allow visual inspection of the internal detail of the map and identification of artifacts.

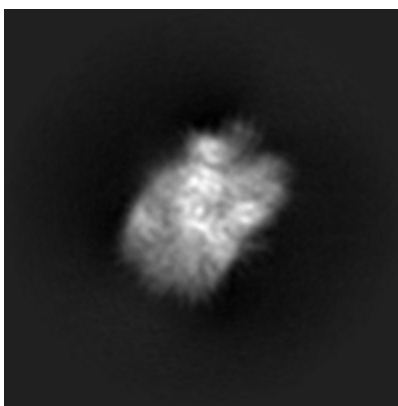
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

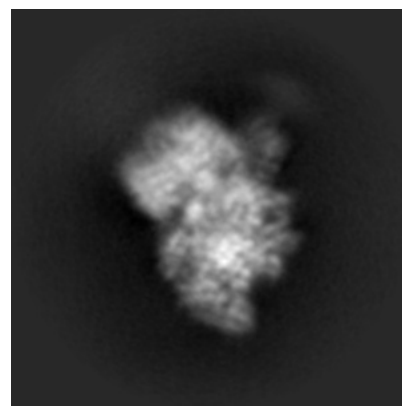
6.1.1 Primary map



X

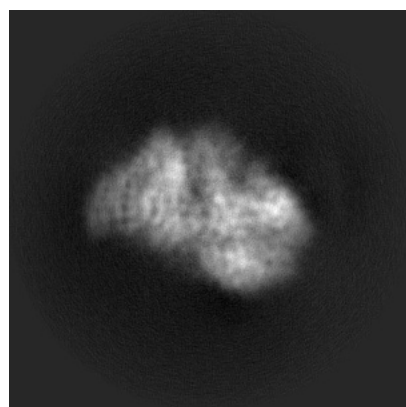


Y

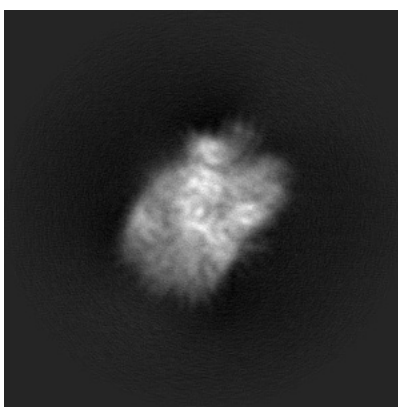


Z

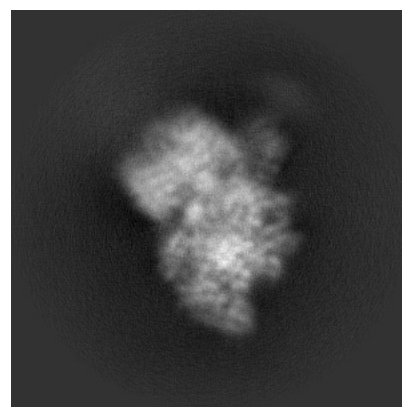
6.1.2 Raw map



X



Y

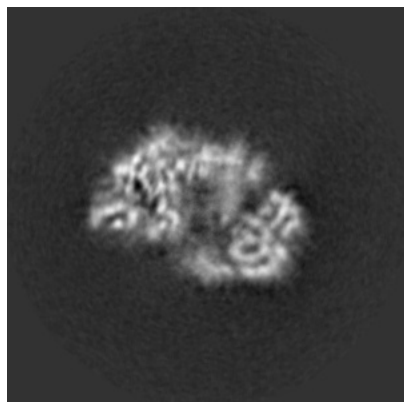


Z

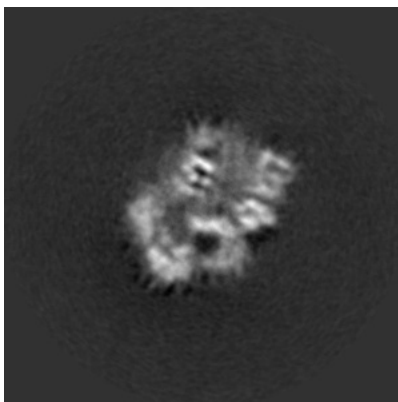
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

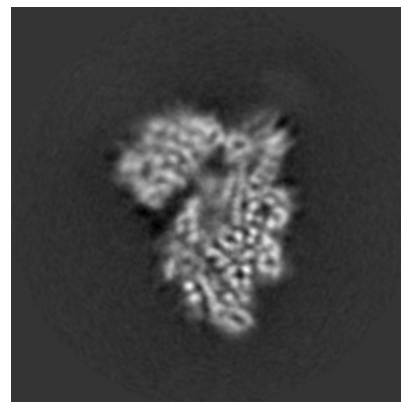
6.2.1 Primary map



X Index: 160

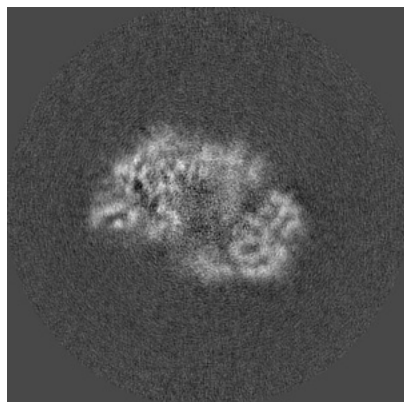


Y Index: 160

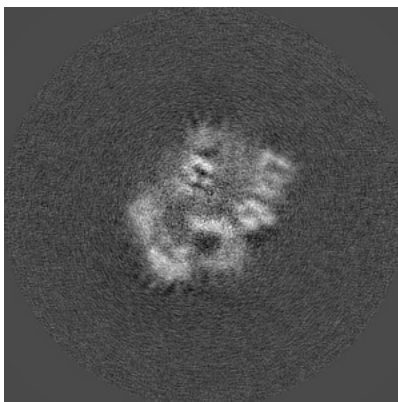


Z Index: 160

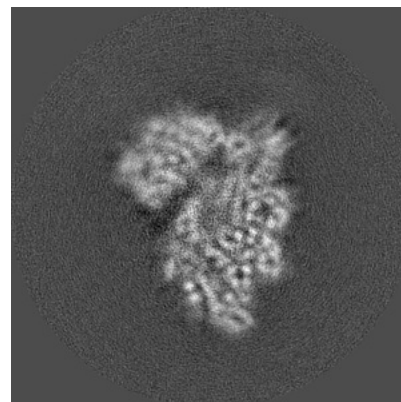
6.2.2 Raw map



X Index: 160



Y Index: 160

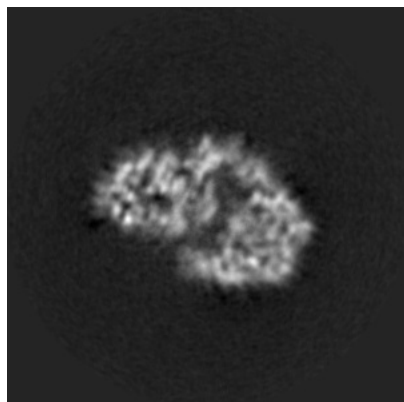


Z Index: 160

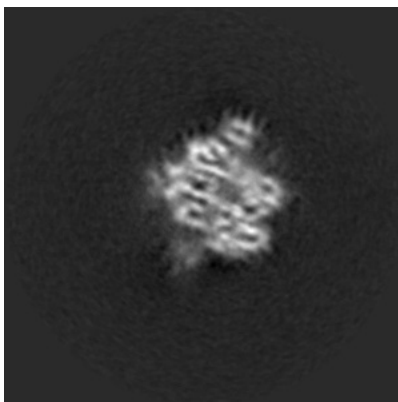
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

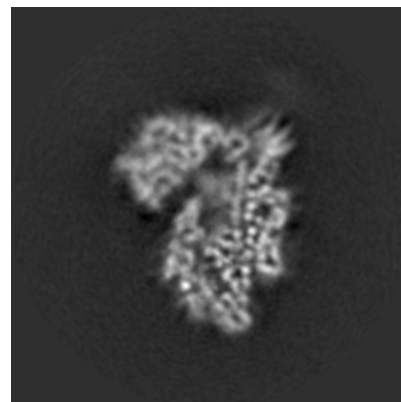
6.3.1 Primary map



X Index: 149

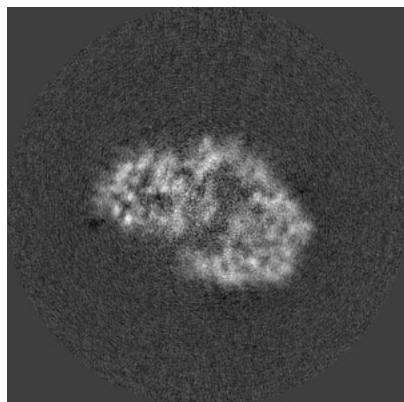


Y Index: 132

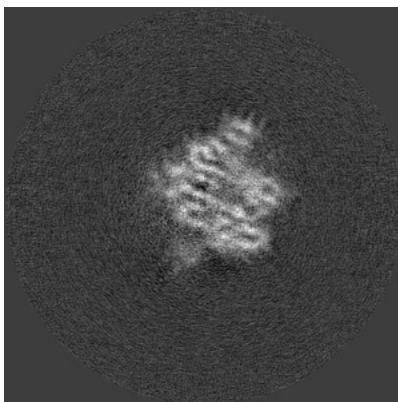


Z Index: 163

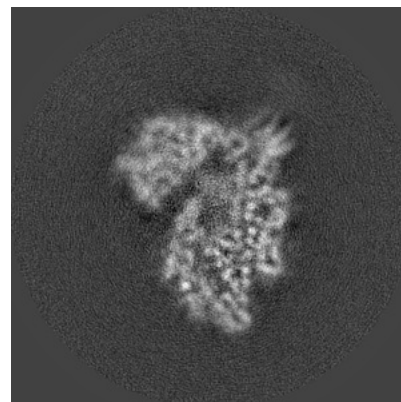
6.3.2 Raw map



X Index: 149



Y Index: 133

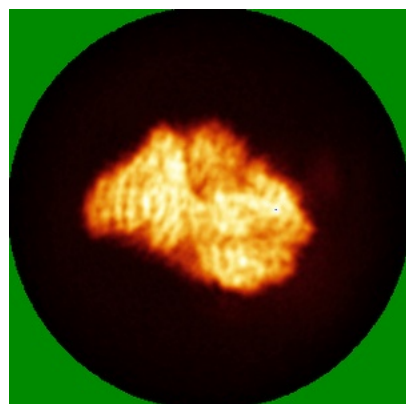


Z Index: 163

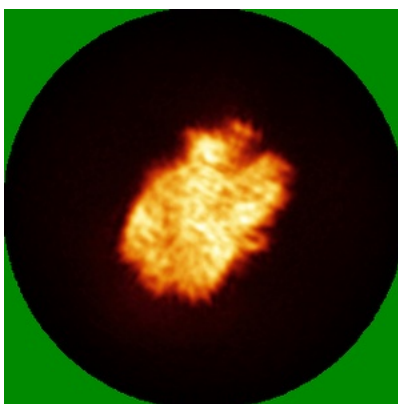
The images above show the largest variance slices of the map in three orthogonal directions.

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

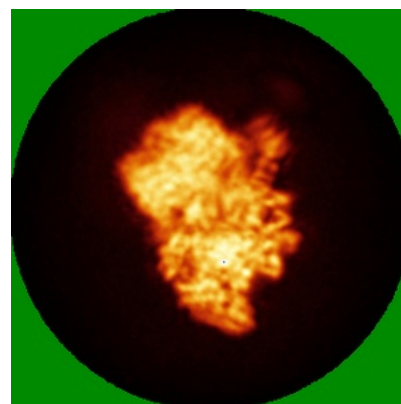
6.4.1 Primary map



X

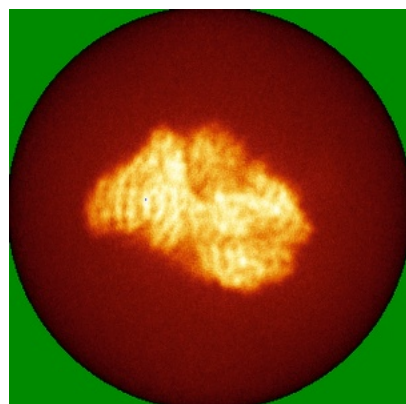


Y

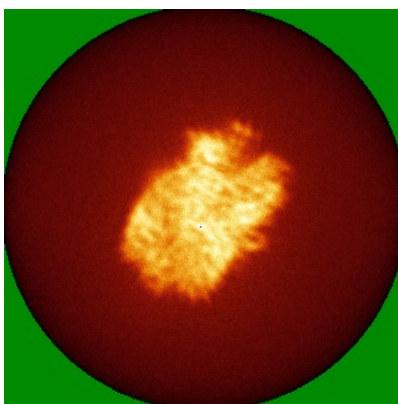


Z

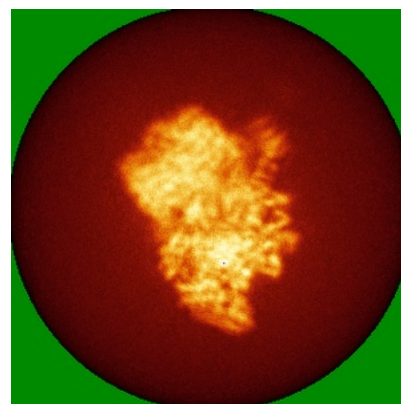
6.4.2 Raw map



X



Y

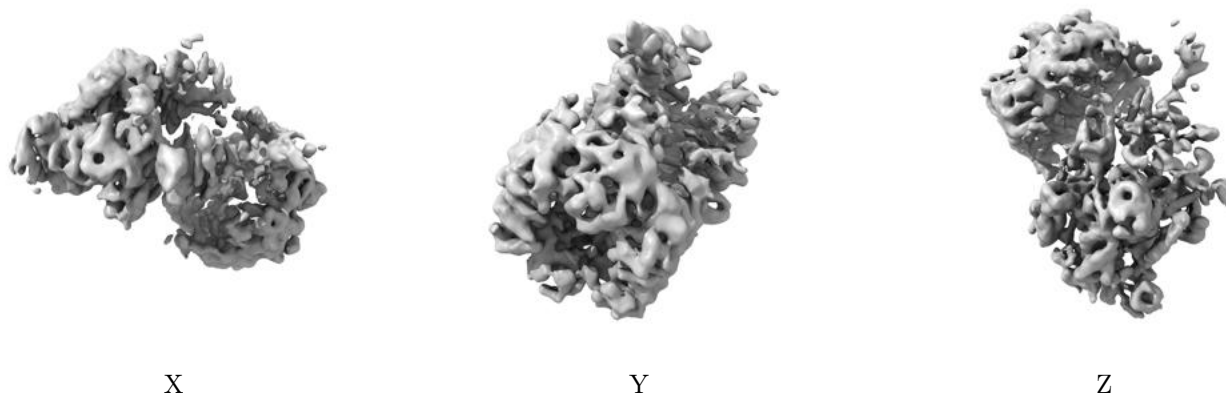


Z

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.

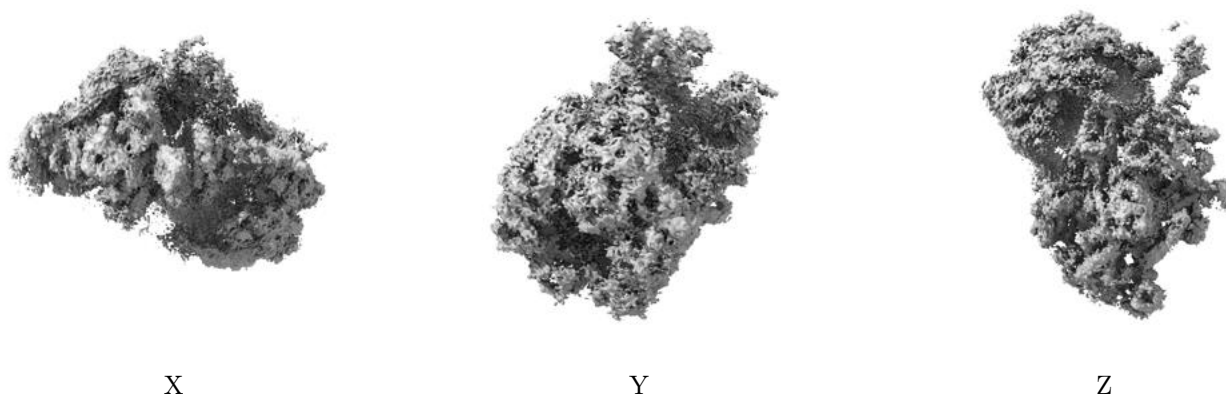
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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



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.

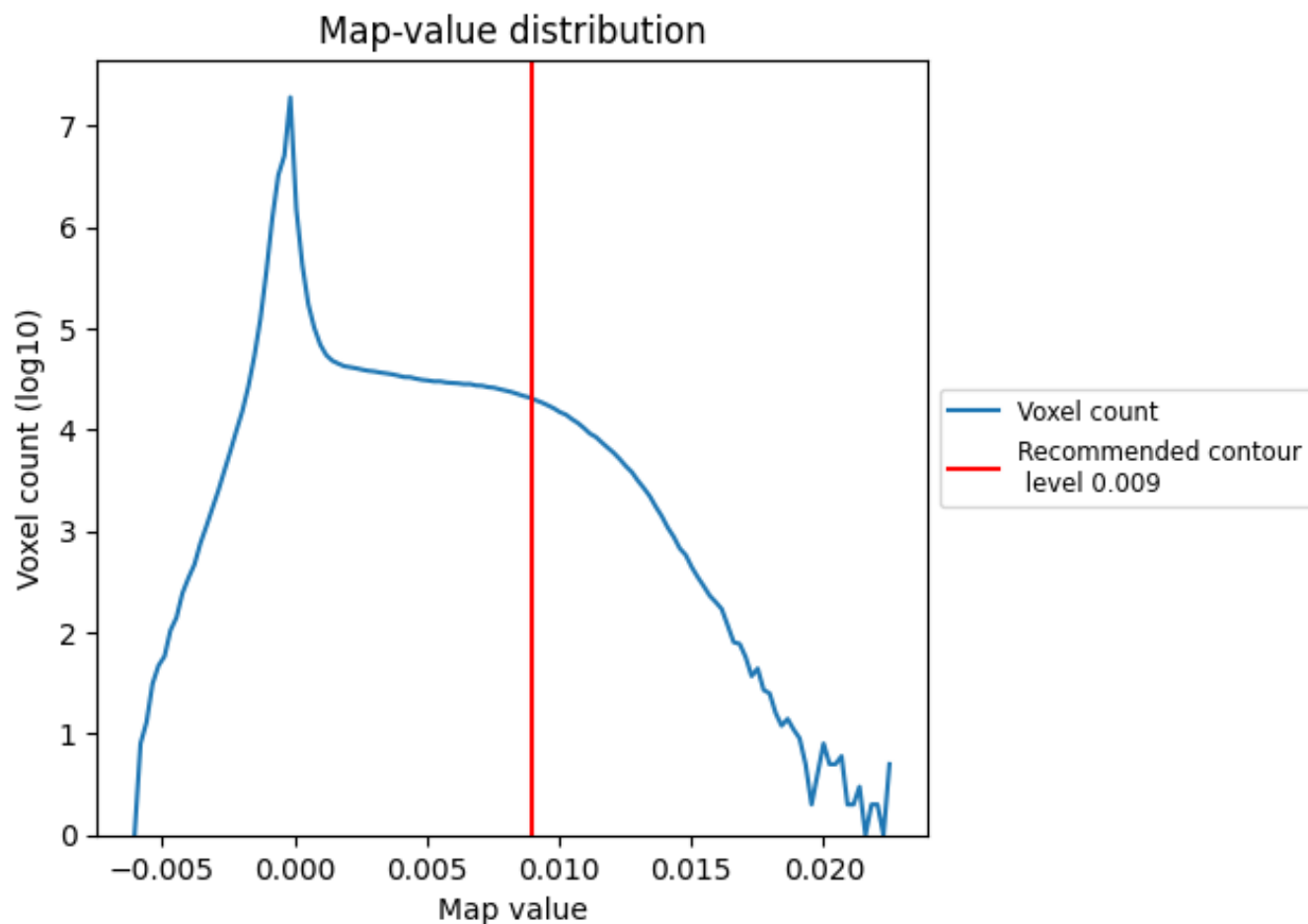
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

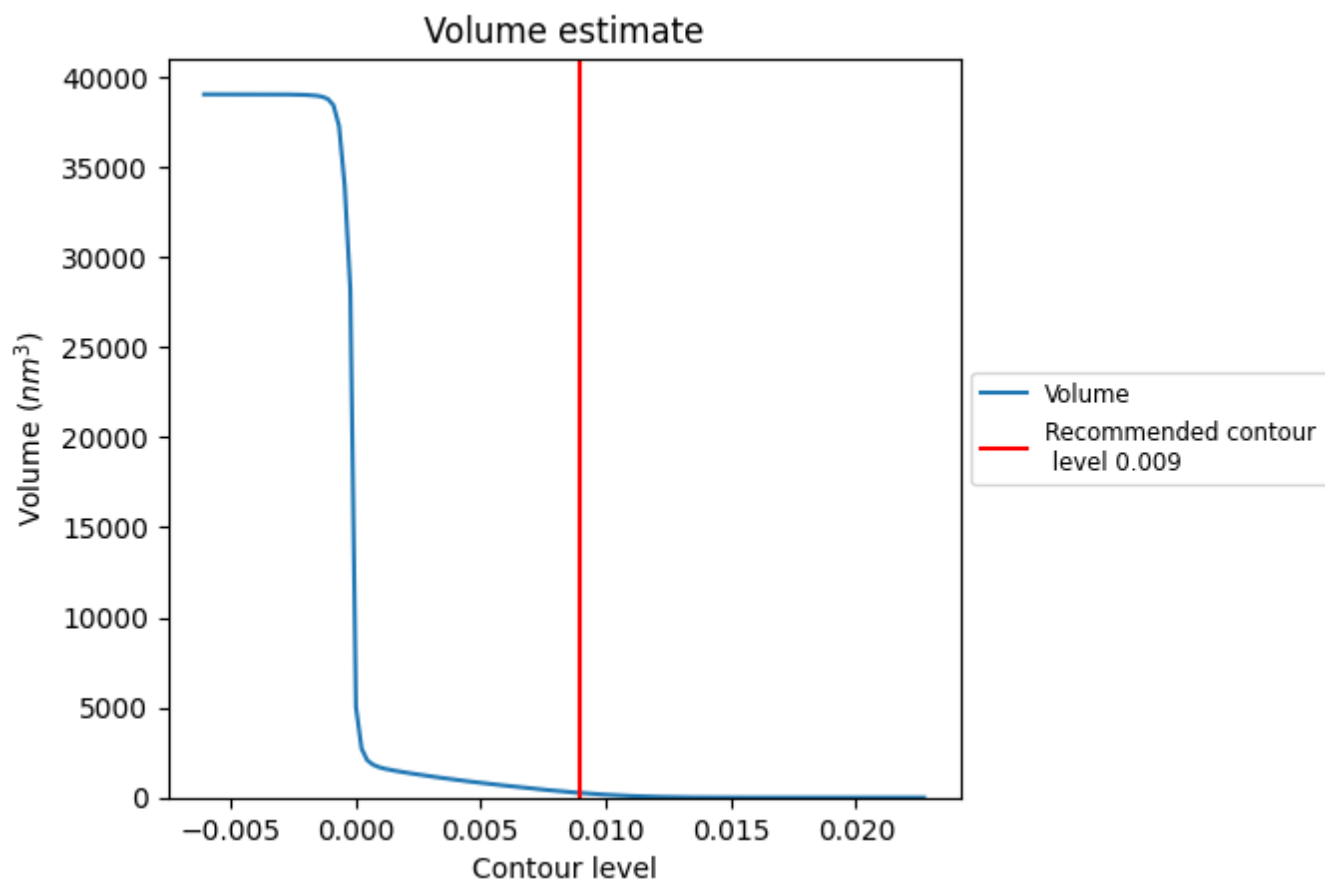
This section contains the results of statistical analysis of the map.

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.

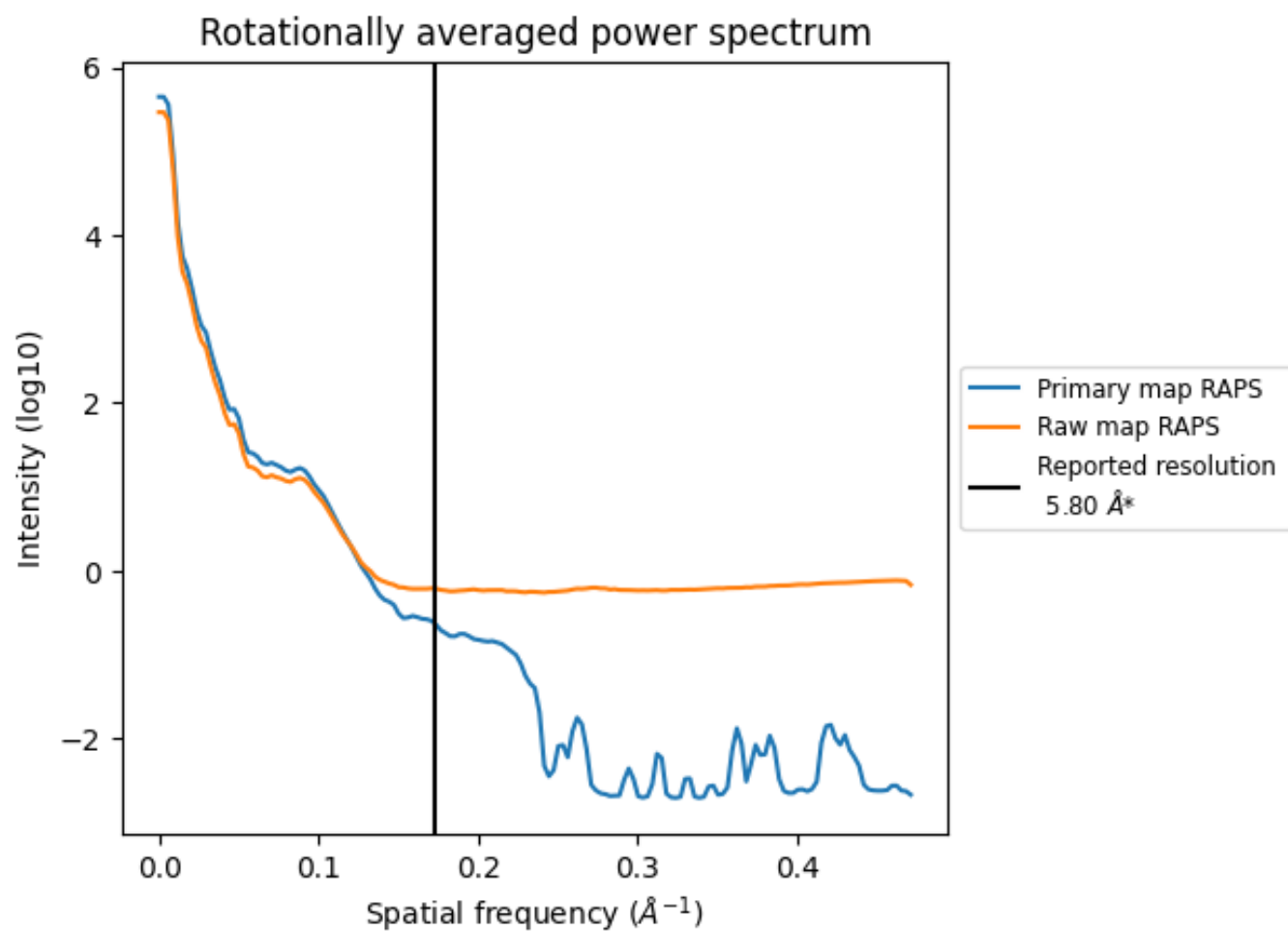
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 256 nm³; this corresponds to an approximate mass of 231 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 ⓘ

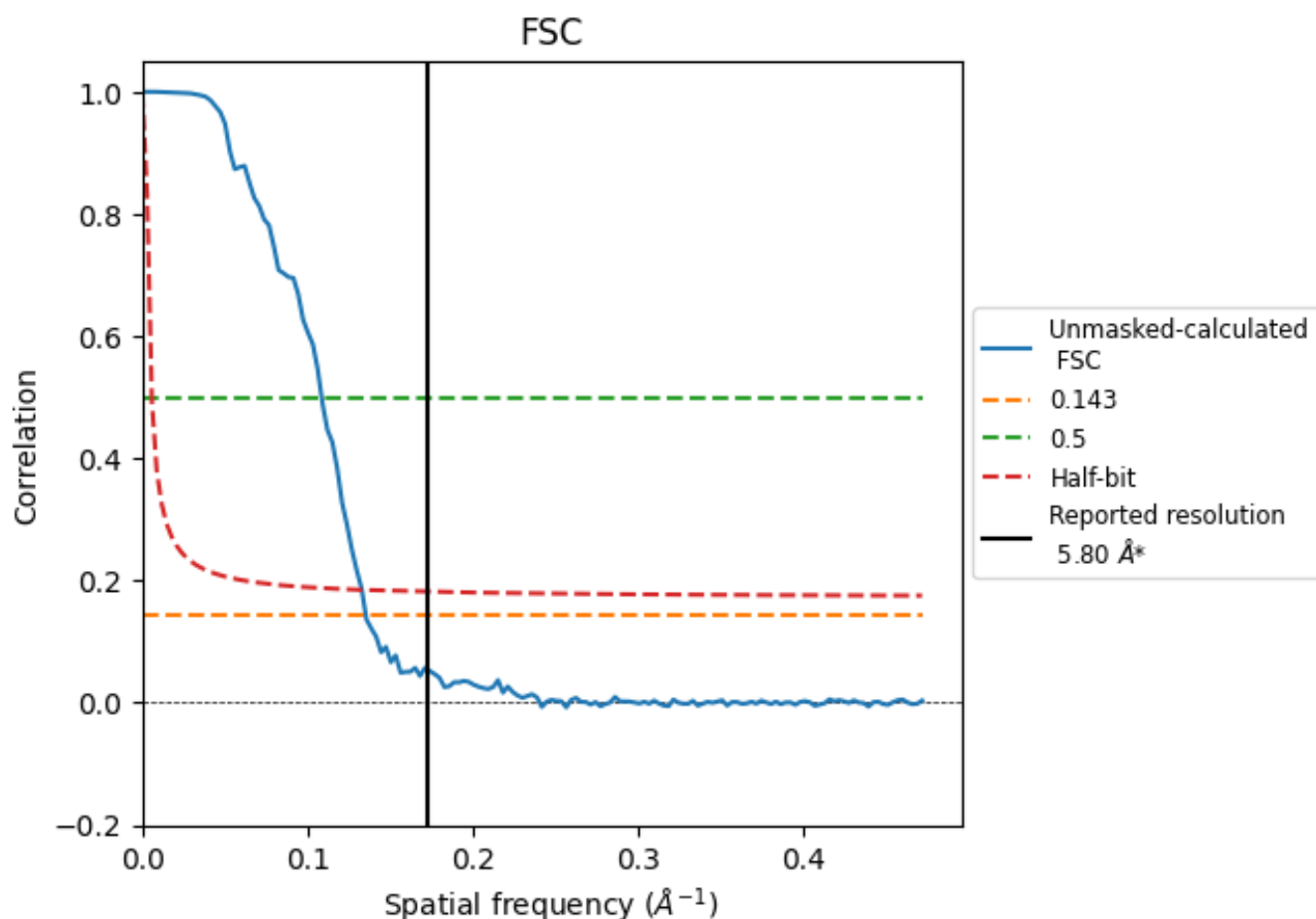


*Reported resolution corresponds to spatial frequency of 0.172 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.172 Å⁻¹

8.2 Resolution estimates [i](#)

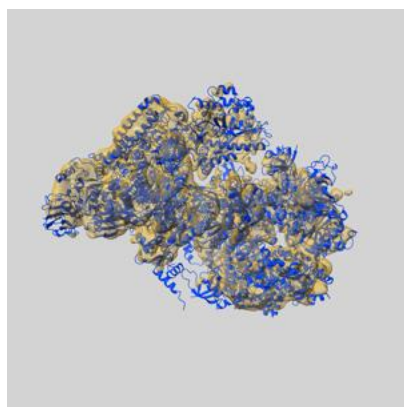
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.40	9.22	7.53

*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 7.40 differs from the reported value 5.8 by more than 10 %

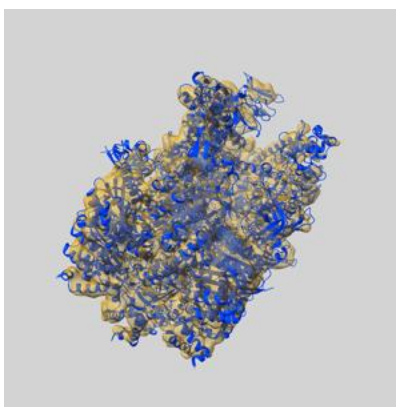
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35000 and PDB model 8HSL. Per-residue inclusion information can be found in section [3](#) on page [8](#).

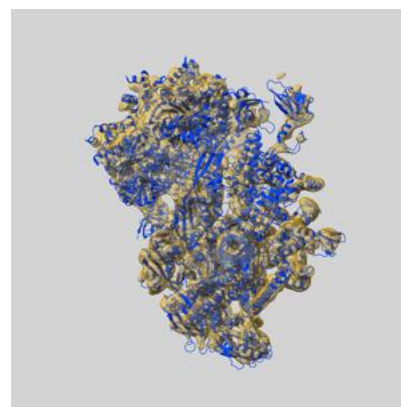
9.1 Map-model overlay [i](#)



X



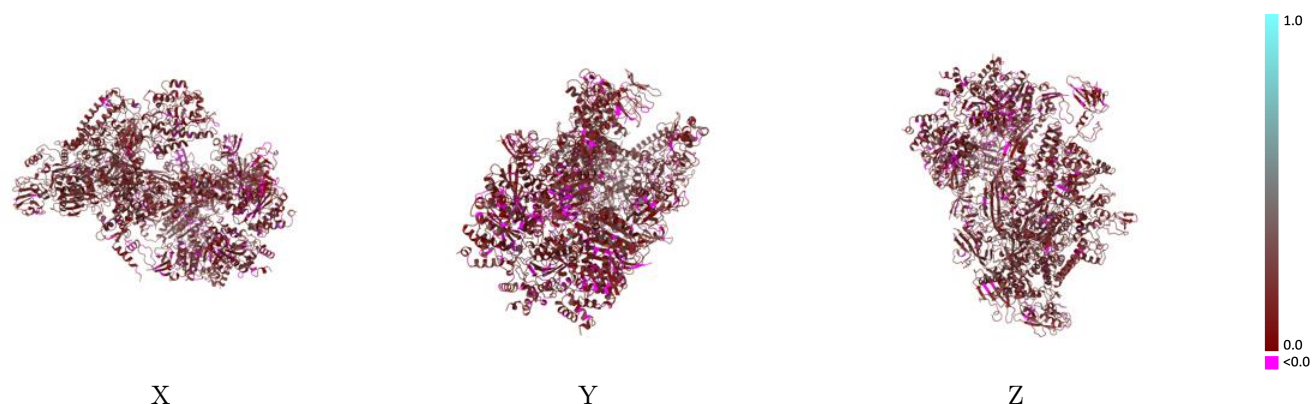
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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](#)

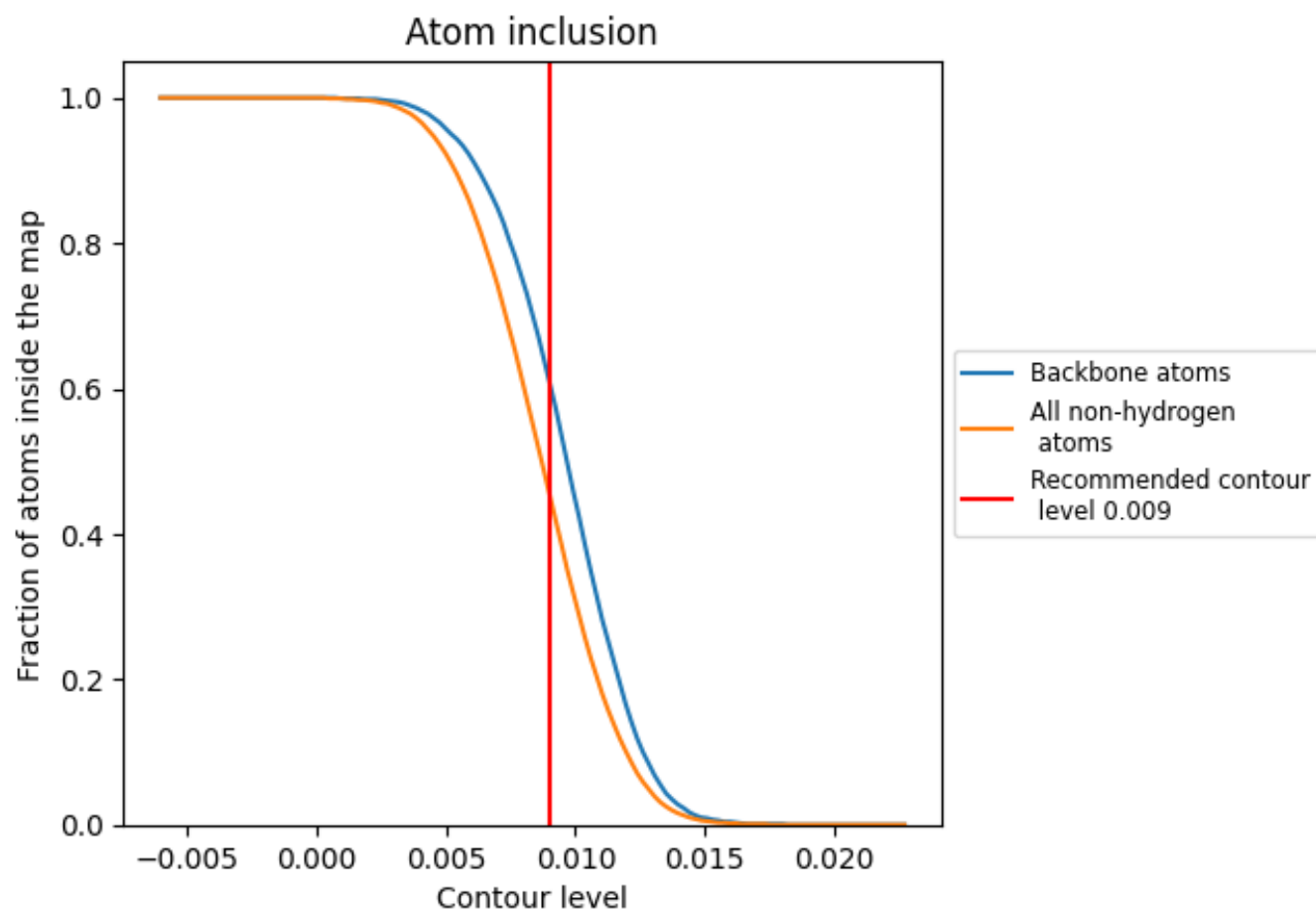


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 46% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4550	0.1660
A	0.4520	0.1240
B	0.3950	0.1400
C	0.3960	0.1290
D	0.4150	0.1270
E	0.3960	0.1330
F	0.3960	0.1210
G	0.5380	0.2090
H	0.4000	0.1910
I	0.4770	0.1980
J	0.5060	0.1930
K	0.4990	0.1580

1.0

0.0

<0.0