



wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 01:56 PM EST

PDB ID : 6PSR
EMDB ID : EMD-20461
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TRPi1) with TraR and rpsT P2 promoter
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-07-13
Resolution : 3.40 Å(reported)

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

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<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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

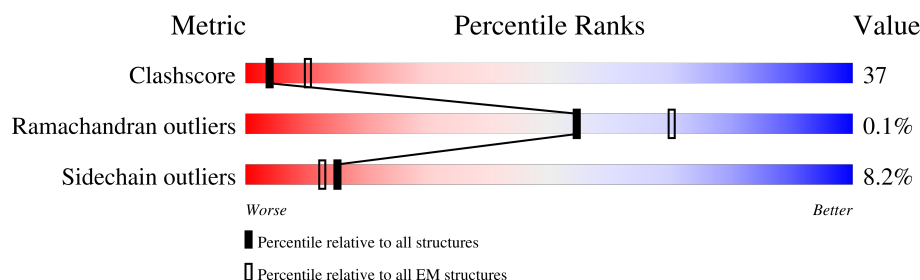
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	329	
1	H	329	
1	M	329	
2	I	1342	
3	J	1430	
4	K	91	
5	L	616	
6	N	72	

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Mol	Chain	Length	Quality of chain
7	O	85	 9% 33% 58%
8	P	85	 39% 59%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 32342 atoms, of which 156 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	230	Total	C	N	O	S	0	0
			1771	1106	314	345	6		
1	H	219	Total	C	N	O	S	0	0
			1678	1048	295	329	6		
1	M	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
			10559	6627	1841	2048	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1345	Total	C	N	O	S	0	0
			10466	6577	1867	1972	50		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	75	Total	C	N	O	S	0	0
			600	365	114	120	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	548	Total	C	N	O	S	0	0
			4407	2754	771	855	27		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP Q0P6L9
L	-1	GLU	-	expression tag	UNP Q0P6L9
L	0	PHE	-	expression tag	UNP Q0P6L9

- Molecule 6 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	72	Total	C	N	O	S	0	0
			565	350	102	108	5		

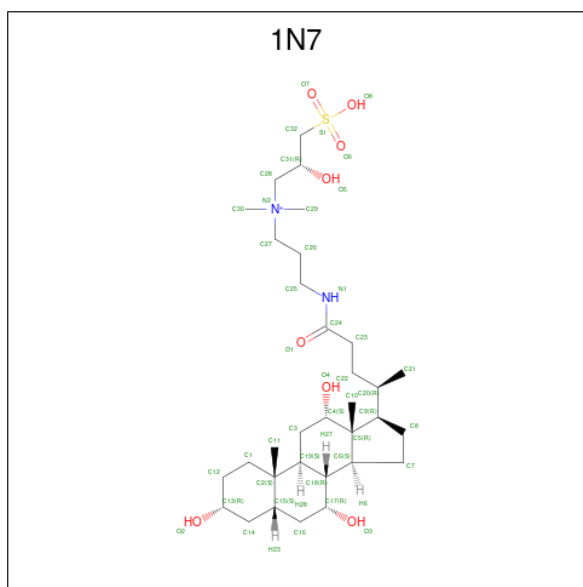
- Molecule 7 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	36	Total	C	N	O	P	0	0
			746	353	154	203	36		

- Molecule 8 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	35	Total	C	N	O	P	0	0
			710	342	111	222	35		

- Molecule 9 is CHAPSO (three-letter code: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms				AltConf
9	I	1	Total	C	H	O	0
			66	24	39	3	
9	J	1	Total	C	H	O	0
			132	48	78	6	
9	J	1	Total	C	H	O	0
			132	48	78	6	
9	L	1	Total	C	H	O	0
			66	24	39	3	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

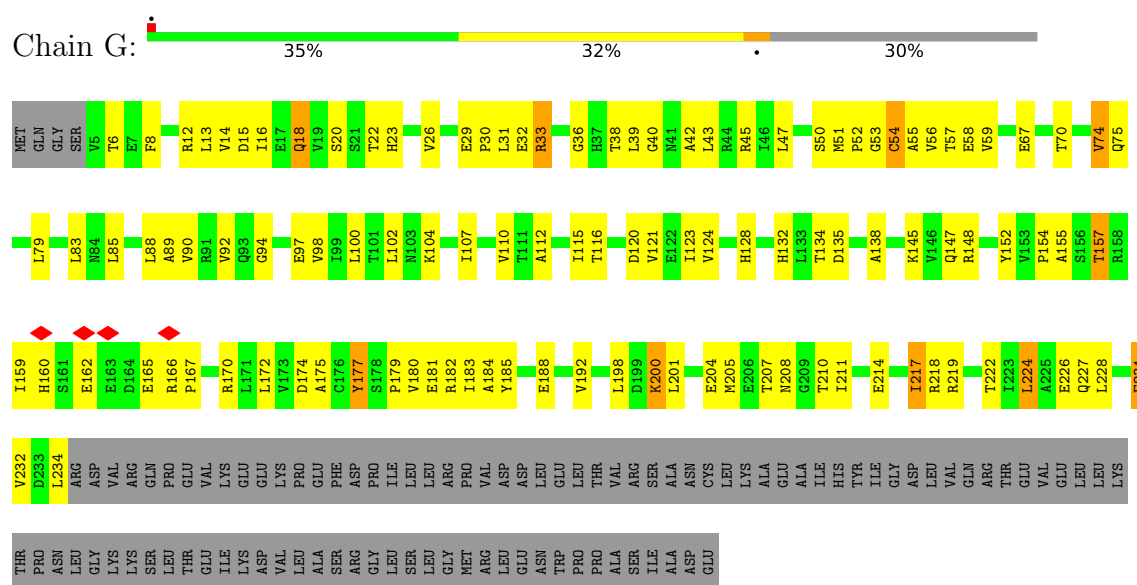
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	J	2	Total 2	Zn 2	0
11	N	1	Total 1	Zn 1	0

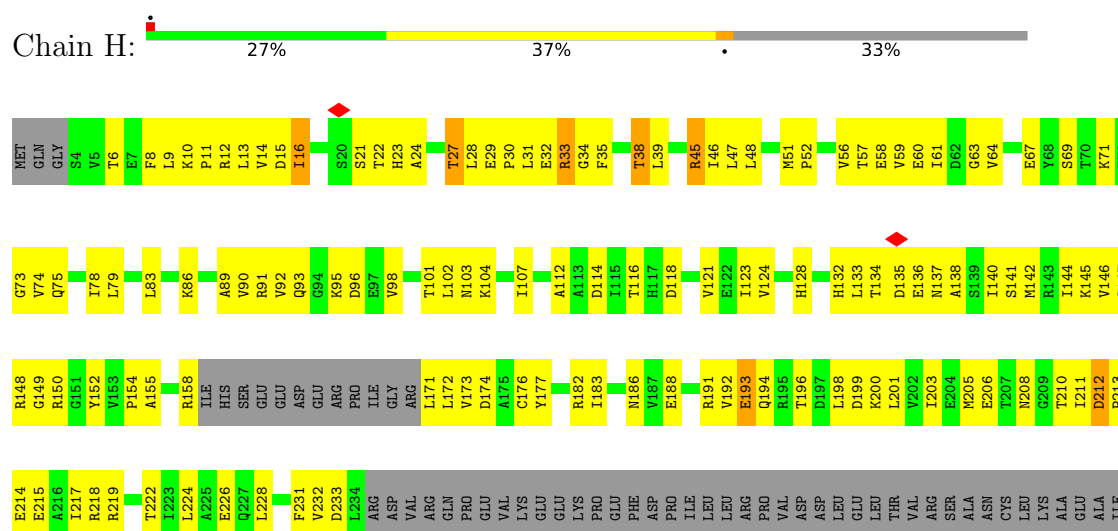
3 Residue-property plots [i](#)

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha



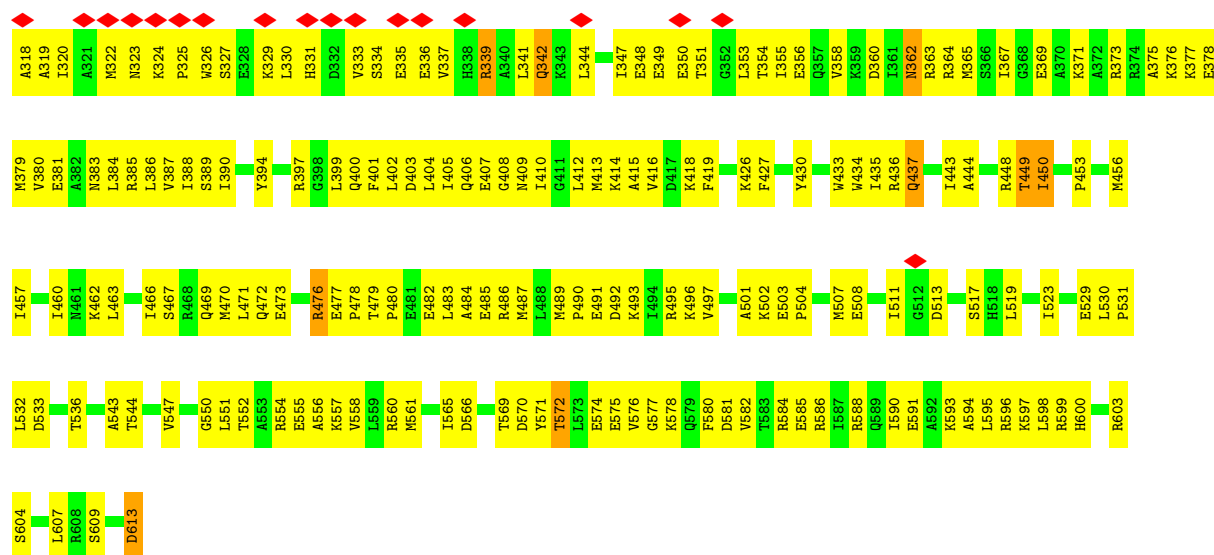
• Molecule 1: DNA-directed RNA polymerase subunit alpha







P1076	E1015	N954	S887	L746	K570	M489	L423	G358	M294	R220	G150	K76
A1077	T1016	K955	C888	M747	D571	I490	M424	L361	R297	I221	M151	R77
L1078	V1017	G956	D889	A748	T572	L491	A426	R298	M298	K222	T152	L78
K1079	A1018	P824	T890	I664	T573	M496	R425	M299	L299	L223	M153	K79
I1080		S957	G893	P750	R576	K496	P427	L299	Q300	L224	L154	H80
V1081	D1021	I958	V894			E497	T428	C366	E301	F227	E155	R81
D1082	P1022	K959	C895	I754	M551	I500	H430	G367	A302		I84	
A1083	H1023	L960	A896	I755	M582	D505	L432	L368	V303	S230	R156	
Q1084	T1024	S961	H897	V756	V583	V506	R431	P369	A305	G231	Q157	C88
G1085	M1025	R962	C757	T674	P584	V507	L433		L306	N232	Q158	G89
H1086	P1026	R963	V757	T674	L587		I434	M372	L307	K233	L160	V90
I1087	V1027	R837	V758	R678	L587		I435	A373	D308	P234	T161	E91
D1088	R963	R838	I759	Y679			A436	E375	N309	E235	E162	
V1089	R839	R842	T760	M680	I591	L510	F437	L376	G310	W236	E163	R98
L1090	R843	R844	T761	K681	V511	Y511	E438	L377	R311	L166		
I1091	R844	R845	R762	V682	Y512	Y512	P439		R312	T240	L166	R101
P1091	R845	R846	R763	V683	M513	M513	R440		G313	T241	E170	M102
G1092	R846	R847	R764	V684	L596	T514	L441		R314	V242	F172	G103
T1093	R847	R848	V769	V685	I601	R515	L442		A315	L242		H104
V1095	D847	V771	L770	M686	S602	C517	E443		I316	P243		I105
R1096	V848	Y772	Q771	R692	M604	V518	G444		T317	L245		E106
D1097	L849	F773	F773	V693	L605	N519	K445		G318	P246		L107
P1098	K850	F774	I774	S694	M606		I447		S319	P247		A108
G1099	P851	S775	T776		T607	E523	Q448		N320			
T1099	G852	T776		M697	C608	G524			R321	P251		T111
A1099	R853			N700	M525	Y609	P451		R322	L252		
Q1099	D854			R780	V526	R610	L452		L390	P253		I114
F1100	R855			K781	I611		V453		P324	P254		W115
L1101	R856			L782	E704		C454		K325	L255		F116
P1102	R857			V783	T705	G529	A459		S326			L117
G1103	V858			L784	V706	P530	D460		A328	R259		K118
T1104	R859			V785	I624	K531	F461		A329	F260		L189
K1104	R860			T786	M625		D462		K330	T262		K190
A1105	T861			A787	Y626	E534	G463		I331	S191		S191
I1106	R862			L788	T627		D464		K398	S263		R123
V1107	L863			K789	G628		I464		K399	D264		G125
G1108	R865			S793	F629		Q465		M400	L265		L126
L1109	R866			G794			M466		G336			L127
E1110	R867			T797	A633	H545	V468		R337	L268		L128
D1111	R868			R798	R634	A546			E402	Y269		D129
G1112	C869			R799	S635	V548	V468		F338	R270		M130
V1113	D870			L800	G636	K549	P471		N341	L201		P131
I1114	L871			V801	A637	V550	L472		L342	R202		L132
T1115	E873			D802	S638	I552	T473		L343	E203		R133
G1116	R874			V803	I641	T553	L474		G344	E204		D134
S1117	R875			A804		E554	E475		K345	N276		L205
L1118	S876			Q805	M644	Y555	L478		R346	N277		N206
G1119	V877			D806	V645		E479		V347	E207		E207
D1120	D878			L807	I646	D558	A490		D348	T208		T208
V1121	R879			V808	P647	A559	R481		V349	L279		N209
L1122	A879			R809	K650		A482		S350	K280		L139
T1123	R880			T737	I653	E562	A482		G351	L282		Y140
K1124	K881			R738	I654	L563	R483		R352	L282		E142
G1125	V882			E811	I654	T567	M484		E418	A287		R214
L1126	R883			D812	I656	S568	M485		S353	P288		S143
P1125	S884			L740	E566		A486		V354			Y144
A1065	V952			G742	E656	L569	T487		I355			V145
E1066	K953						M488		T356			V146
G1067									V357			I147
T1068												
A1069												
THR												
K1132												
D1133												
I1134												
T1135												
GLU												
SER												
GLY												
GLY												
THR												
R1075												



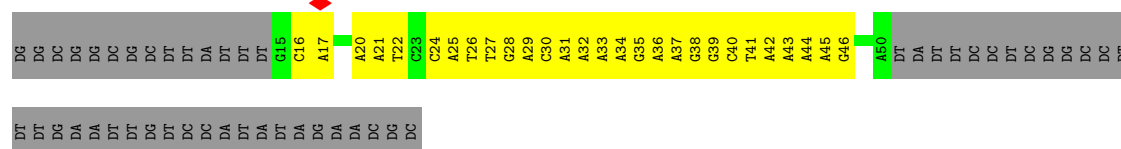
• Molecule 6: Protein TraR

Chain N: 54% 40% 6%



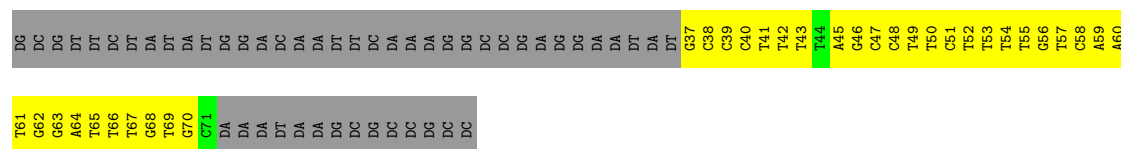
• Molecule 7: DNA (85-MER)

Chain O: 9% 33% 58%



• Molecule 8: DNA (85-MER)

Chain P: 39% 59%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98324	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	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	0.223	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1N7, ZN

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	0.41	0/1793	0.53	0/2432
1	H	0.37	0/1697	0.54	0/2301
1	M	0.25	0/579	0.47	0/784
2	I	0.43	0/10728	0.52	1/14477 (0.0%)
3	J	0.40	0/10625	0.53	1/14345 (0.0%)
4	K	0.33	0/602	0.49	0/810
5	L	0.29	0/4461	0.48	0/6004
6	N	0.39	0/575	0.49	0/778
7	O	0.61	0/842	0.88	0/1297
8	P	0.58	0/790	1.05	0/1217
All	All	0.41	0/32692	0.55	2/44445 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	2
3	J	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	53	ARG	CB-CA-C	5.29	120.97	110.40
2	I	15	PHE	C-N-CA	-5.09	111.61	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	519	ASN	Peptide
2	I	897	PRO	Peptide
3	J	53	ARG	Peptide

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	1771	0	1799	111	0
1	H	1678	0	1698	131	0
1	M	572	0	602	84	0
2	I	10559	0	10577	767	0
3	J	10466	0	10689	868	0
4	K	600	0	607	48	0
5	L	4407	0	4432	414	0
6	N	565	0	545	35	0
7	O	746	0	401	41	0
8	P	710	0	402	50	0
9	I	27	39	39	4	0
9	J	54	78	75	9	0
9	L	27	39	38	4	0
10	J	1	0	0	0	0
11	J	2	0	0	0	0
11	N	1	0	0	0	0
All	All	32186	156	31904	2388	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 37.

The worst 5 of 2388 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:L:701:1N7:C19	9:L:701:1N7:C3	1.82	1.58
9:I:1401:1N7:C3	9:I:1401:1N7:C19	1.82	1.56
9:J:1505:1N7:C3	9:J:1505:1N7:C19	1.81	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:1504:1N7:C19	9:J:1504:1N7:C3	1.84	1.50
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.34	1.08

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	228/329 (69%)	205 (90%)	23 (10%)	0	100	100
1	H	215/329 (65%)	189 (88%)	26 (12%)	0	100	100
1	M	71/329 (22%)	68 (96%)	3 (4%)	0	100	100
2	I	1338/1342 (100%)	1179 (88%)	157 (12%)	2 (0%)	51	82
3	J	1339/1430 (94%)	1197 (89%)	141 (10%)	1 (0%)	51	82
4	K	73/91 (80%)	68 (93%)	5 (7%)	0	100	100
5	L	540/616 (88%)	500 (93%)	40 (7%)	0	100	100
6	N	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
All	All	3874/4538 (85%)	3471 (90%)	400 (10%)	3 (0%)	54	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	898	GLU
3	J	854	ALA
2	I	897	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	195/286 (68%)	177 (91%)	18 (9%)	9	31
1	H	184/286 (64%)	171 (93%)	13 (7%)	14	44
1	M	65/286 (23%)	62 (95%)	3 (5%)	27	57
2	I	1153/1157 (100%)	1043 (90%)	110 (10%)	8	29
3	J	1128/1189 (95%)	1036 (92%)	92 (8%)	11	37
4	K	65/75 (87%)	59 (91%)	6 (9%)	9	31
5	L	479/543 (88%)	456 (95%)	23 (5%)	25	56
6	N	60/61 (98%)	53 (88%)	7 (12%)	5	20
All	All	3329/3883 (86%)	3057 (92%)	272 (8%)	15	37

5 of 272 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	1349	GLU
4	K	67	ARG
5	L	604	SER
2	I	815	SER
2	I	799	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	1108	GLN
5	L	129	GLN
3	J	1114	GLN
4	K	7	GLN
5	L	258	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	1N7	J	1505	-	30,30,46	4.80	14 (46%)	47,48,72	2.11	15 (31%)
9	1N7	L	701	-	30,30,46	4.86	15 (50%)	47,48,72	2.48	20 (42%)
9	1N7	I	1401	-	30,30,46	4.93	16 (53%)	47,48,72	2.08	10 (21%)
9	1N7	J	1504	-	30,30,46	5.06	16 (53%)	47,48,72	2.39	17 (36%)

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	1N7	J	1505	-	-	0/7/72/92	0/4/4/4
9	1N7	L	701	-	-	5/7/72/92	0/4/4/4
9	1N7	I	1401	-	-	5/7/72/92	0/4/4/4
9	1N7	J	1504	-	-	7/7/72/92	0/4/4/4

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	1504	1N7	C3-C19	18.21	1.84	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1401	1N7	C3-C19	17.49	1.82	1.53
9	L	701	1N7	C3-C19	17.01	1.82	1.53
9	J	1505	1N7	C3-C19	16.93	1.81	1.53
9	J	1504	1N7	C3-C4	11.93	1.73	1.53

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	701	1N7	C9-C5-C4	-7.75	110.59	117.67
9	J	1504	1N7	C9-C5-C4	-7.62	110.71	117.67
9	I	1401	1N7	C9-C5-C4	-6.66	111.58	117.67
9	L	701	1N7	C3-C19-C18	-6.35	101.58	110.88
9	J	1505	1N7	C19-C3-C4	-4.95	107.77	114.30

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1504	1N7	C21-C20-C9-C5
9	J	1504	1N7	C21-C20-C9-C8
9	I	1401	1N7	C21-C20-C9-C5
9	I	1401	1N7	C21-C20-C9-C8
9	I	1401	1N7	C22-C20-C9-C5

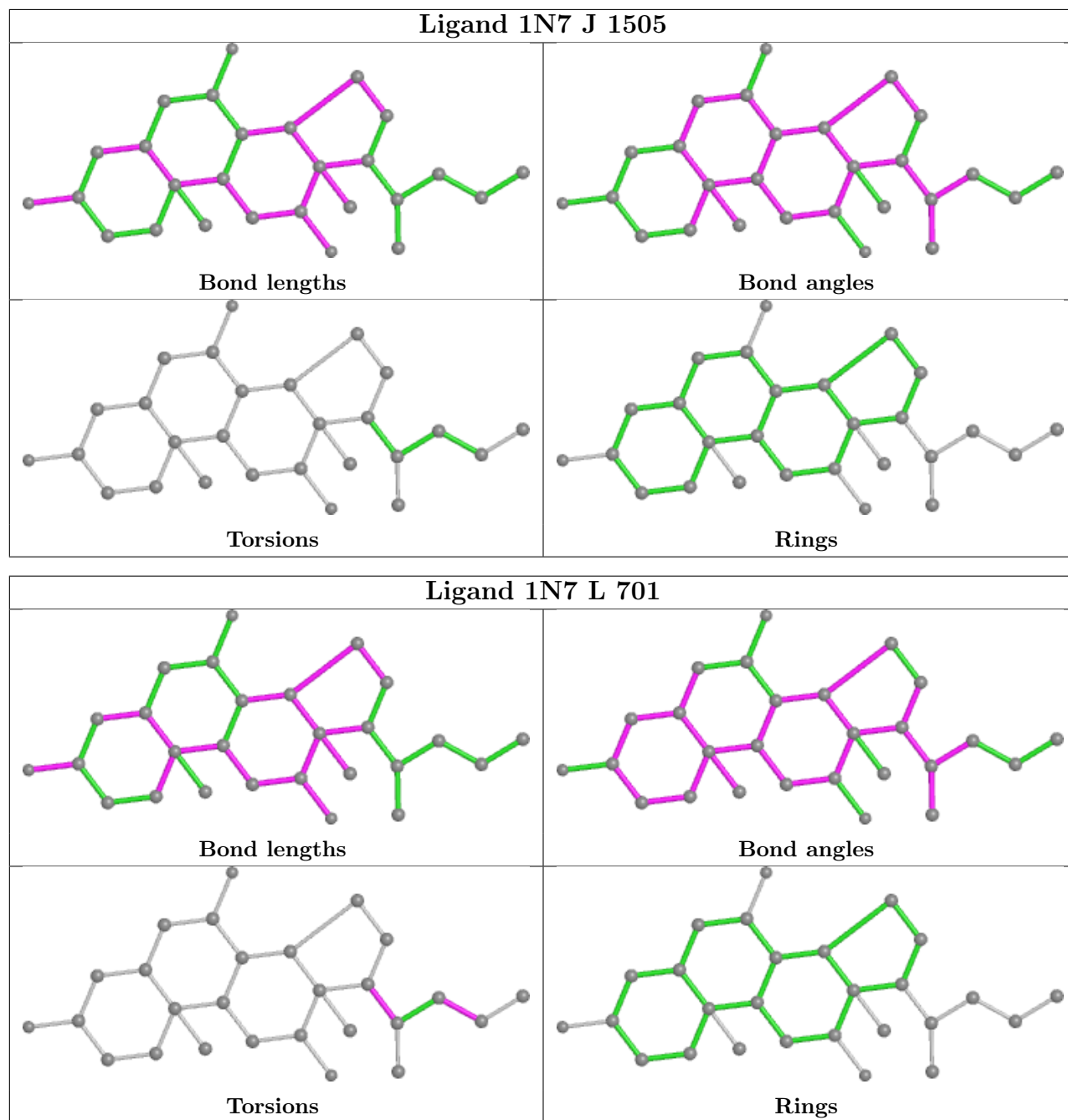
There are no ring outliers.

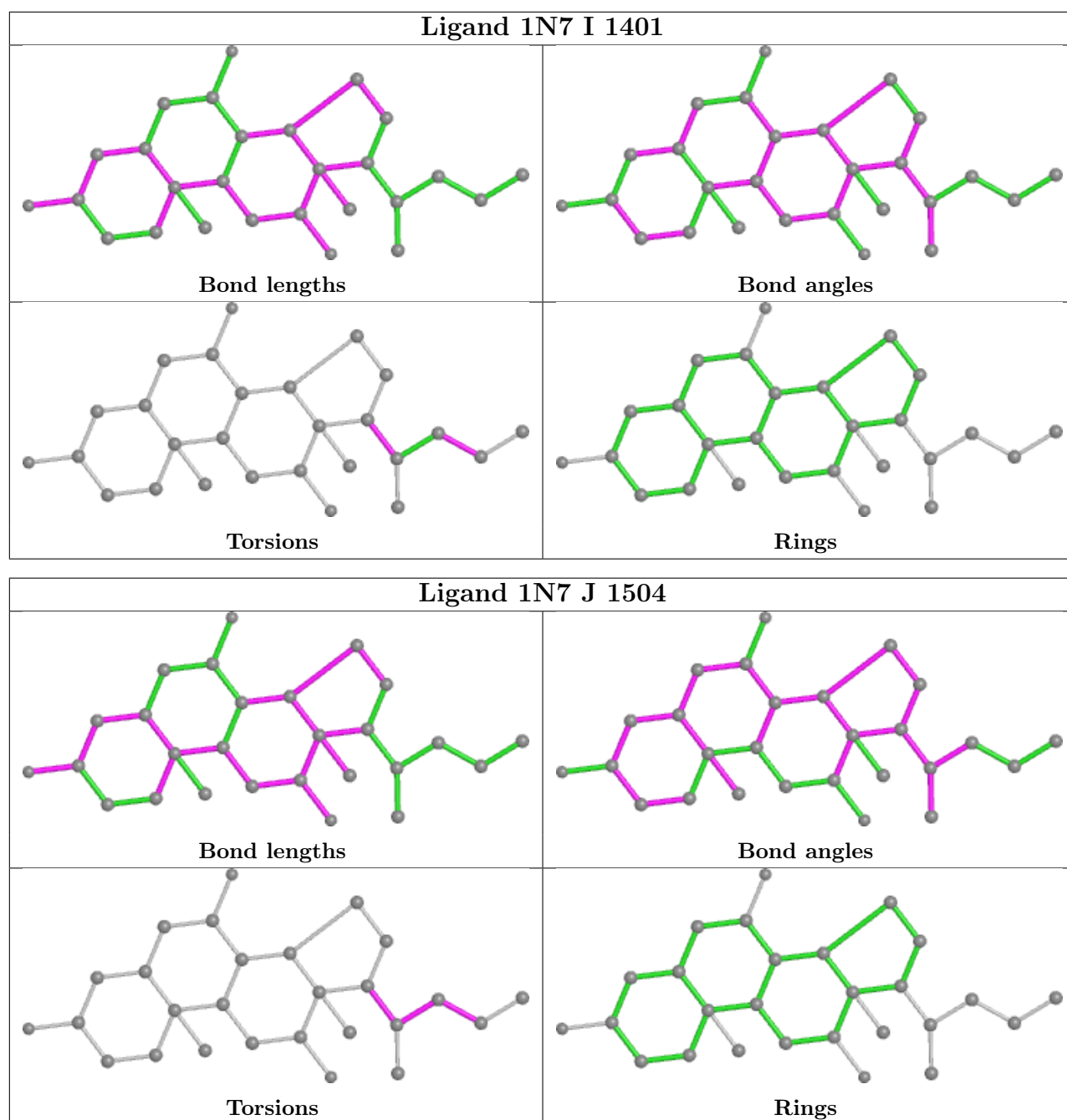
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1505	1N7	5	0
9	L	701	1N7	4	0
9	I	1401	1N7	4	0
9	J	1504	1N7	4	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.

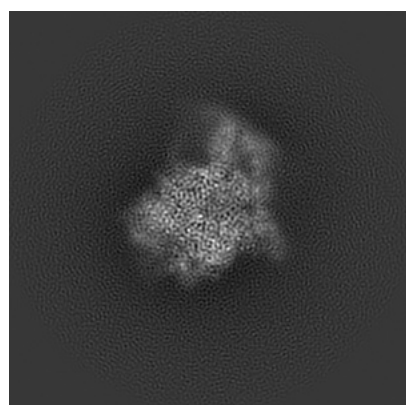
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20461. These allow visual inspection of the internal detail of the map and identification of artifacts.

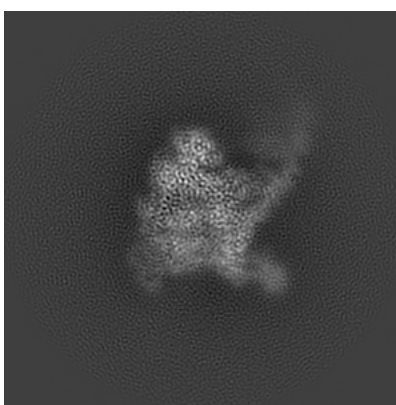
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

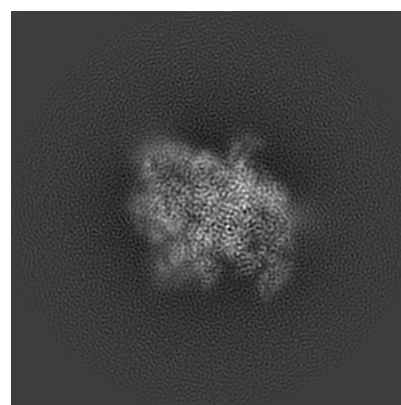
6.1.1 Primary map



X



Y

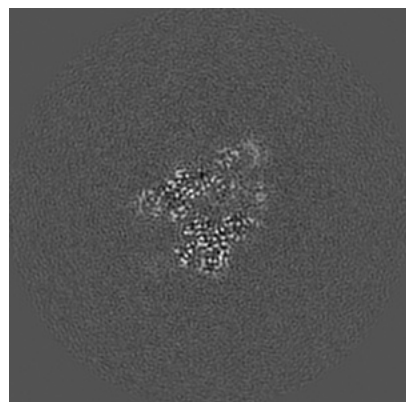


Z

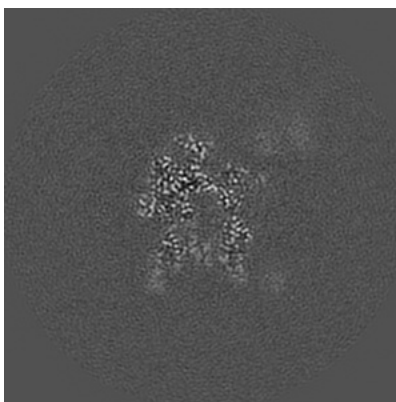
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

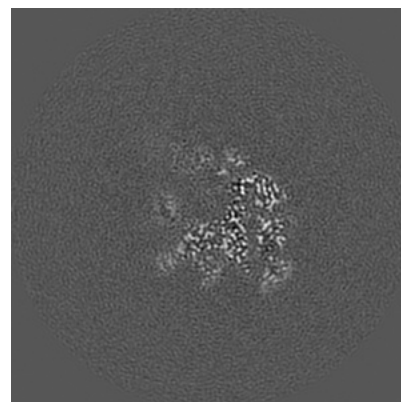
6.2.1 Primary map



X Index: 128



Y Index: 128

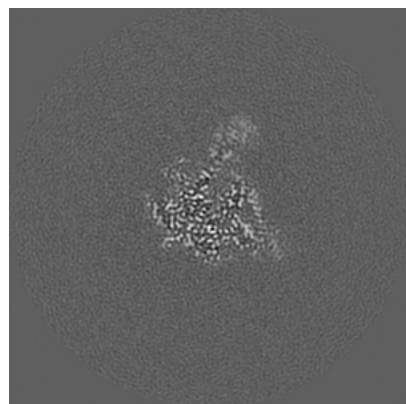


Z Index: 128

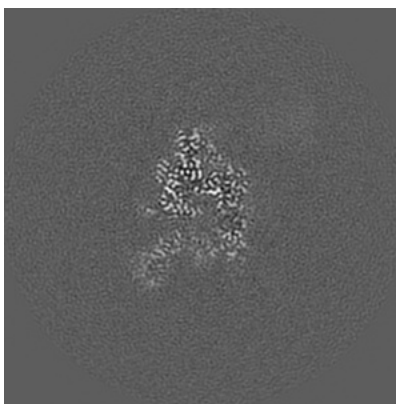
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

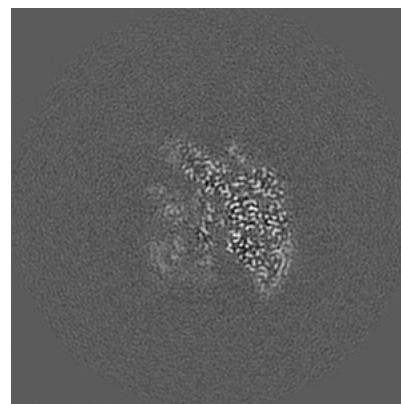
6.3.1 Primary map



X Index: 146



Y Index: 121



Z Index: 120

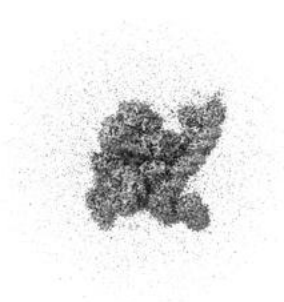
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

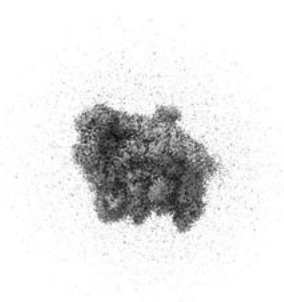
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

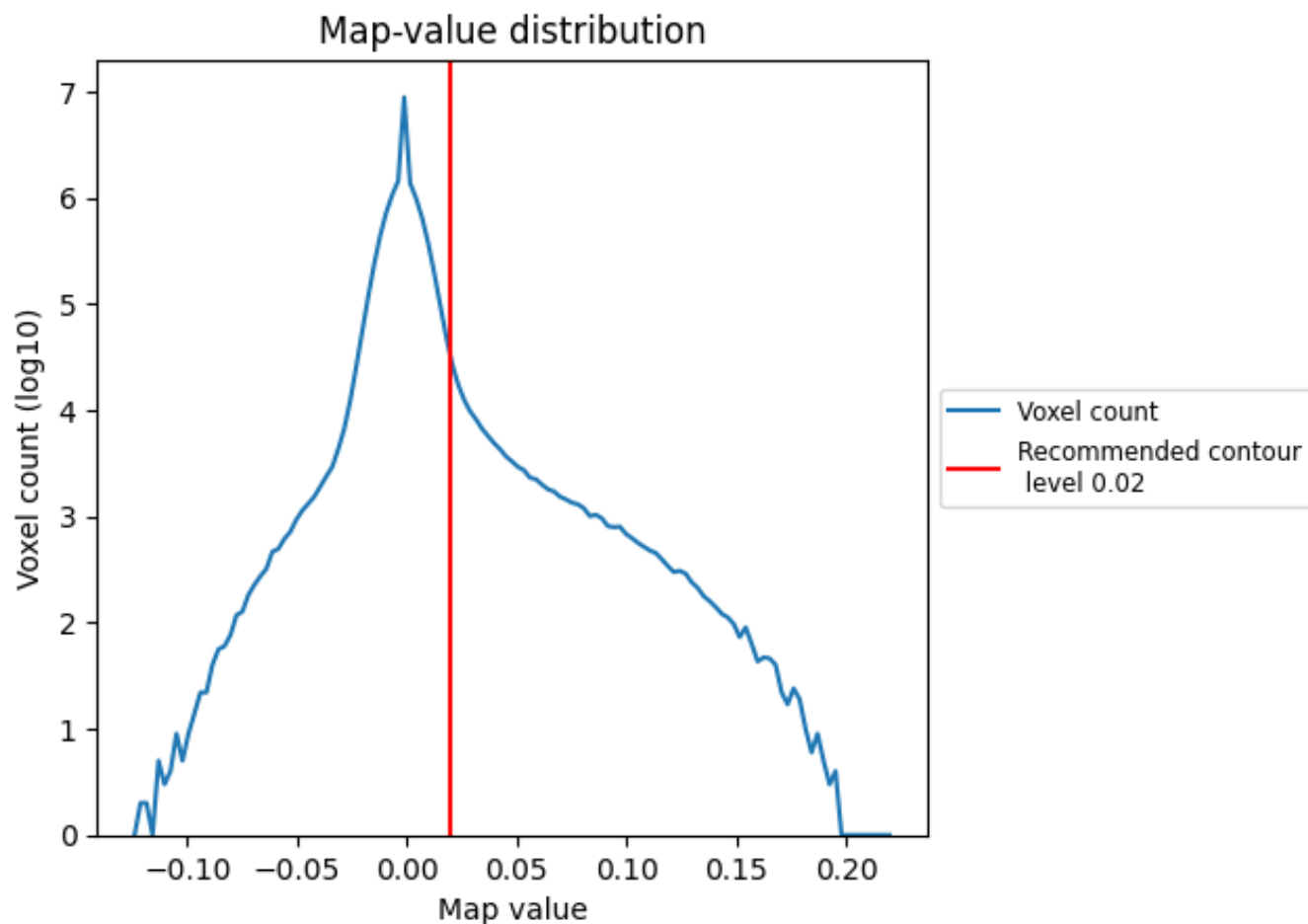
6.5 Mask visualisation

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

7 Map analysis [i](#)

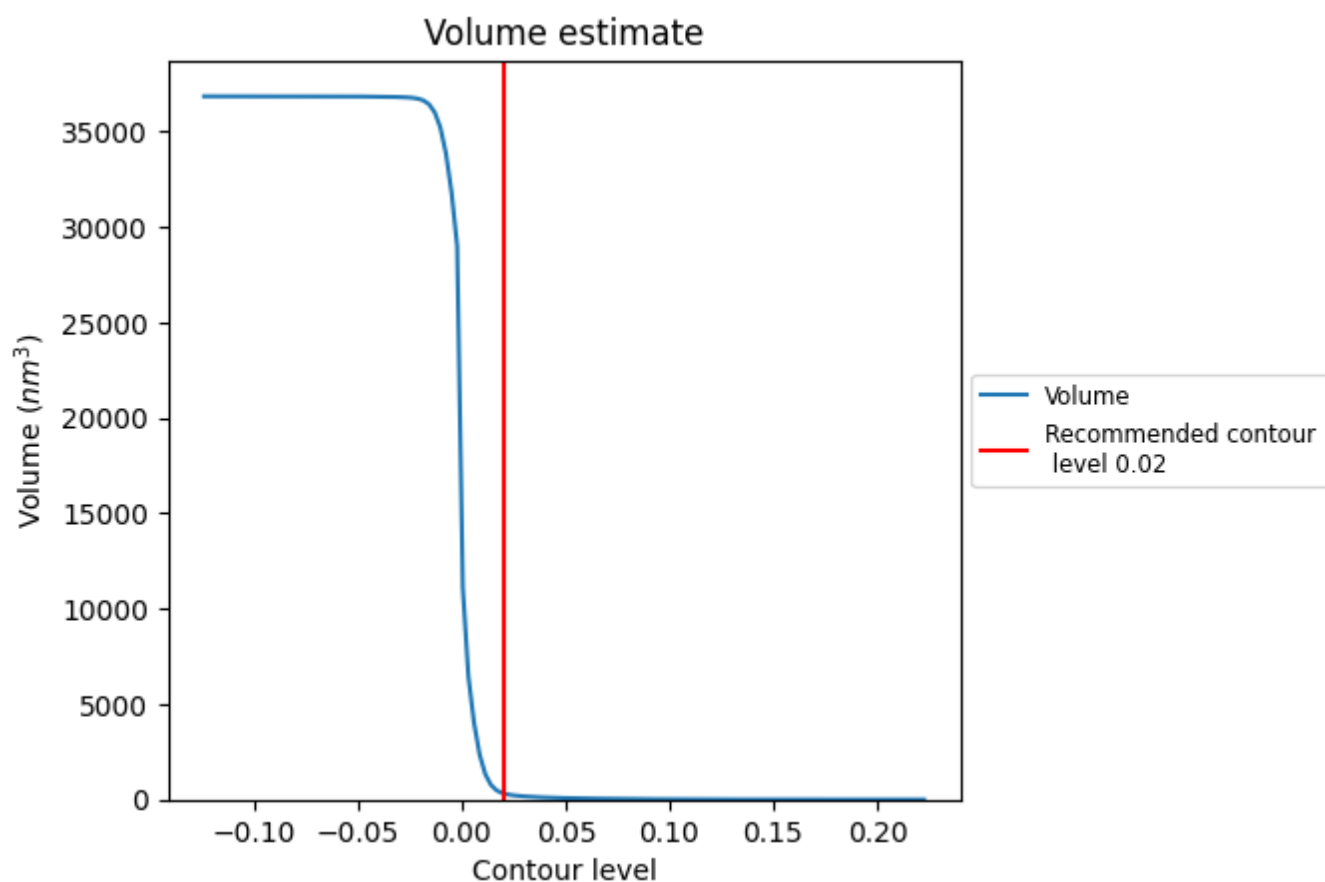
This section contains the results of statistical analysis of the map.

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.

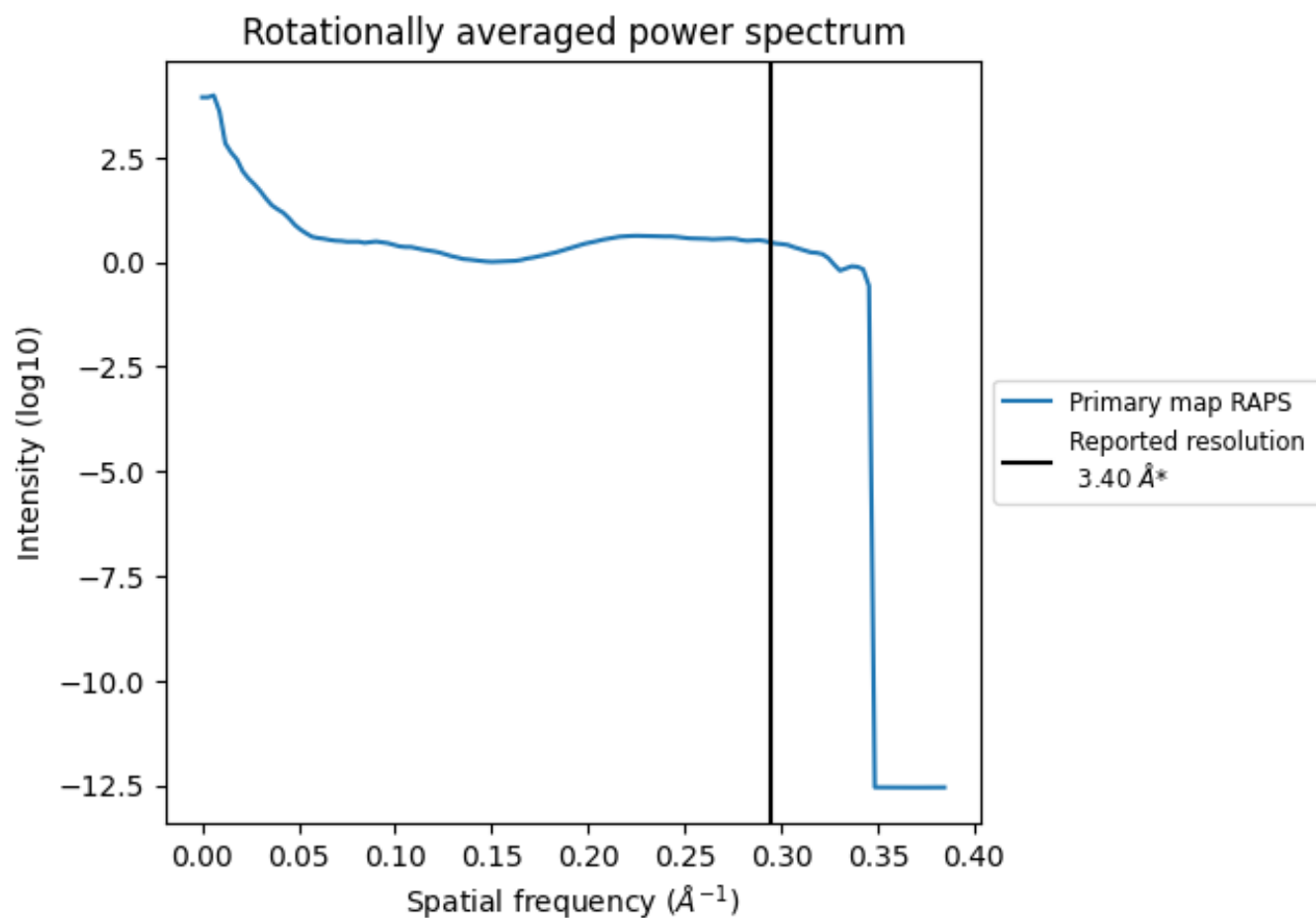
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 325 nm³; this corresponds to an approximate mass of 294 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 ⓘ

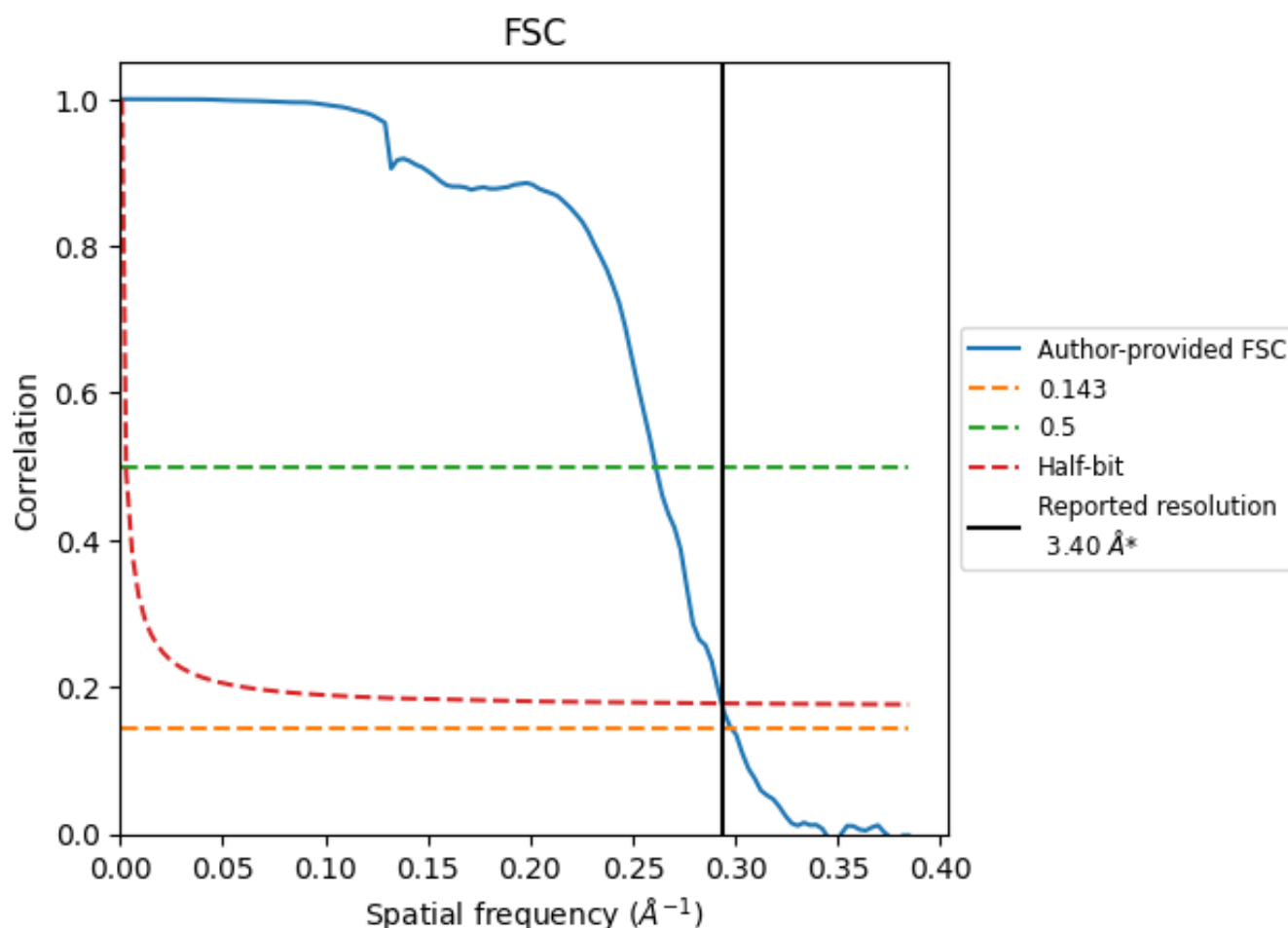


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

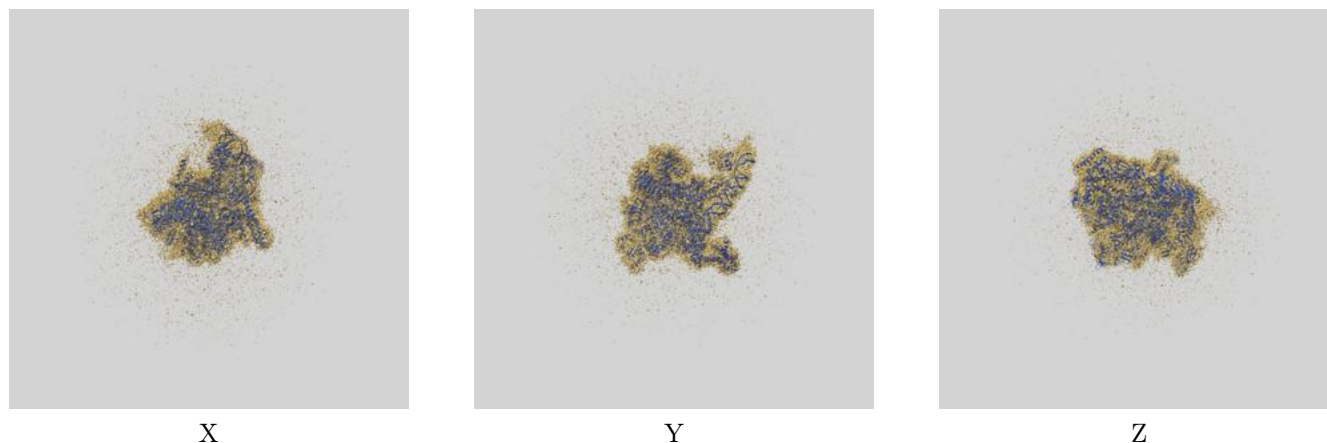
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.35	3.83	3.41
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

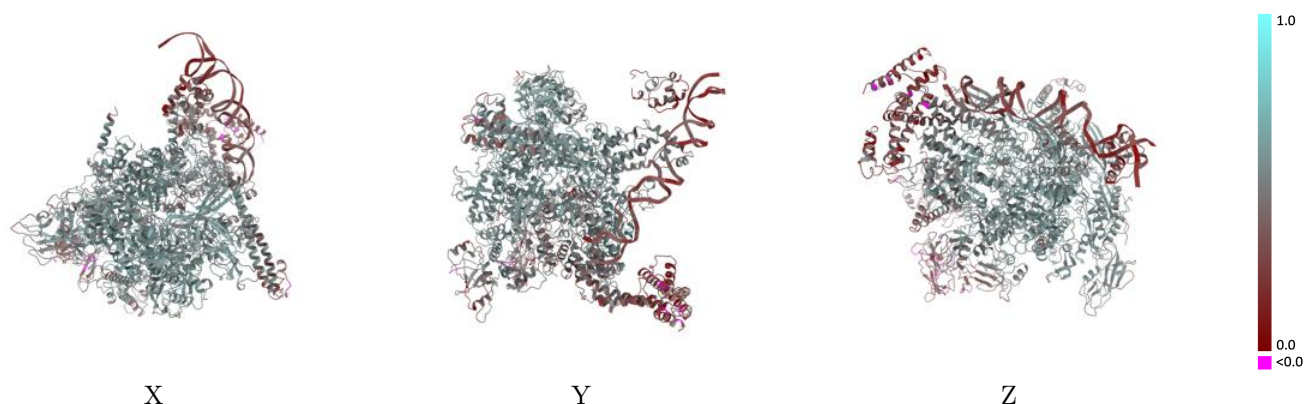
This section contains information regarding the fit between EMDB map EMD-20461 and PDB model 6PSR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



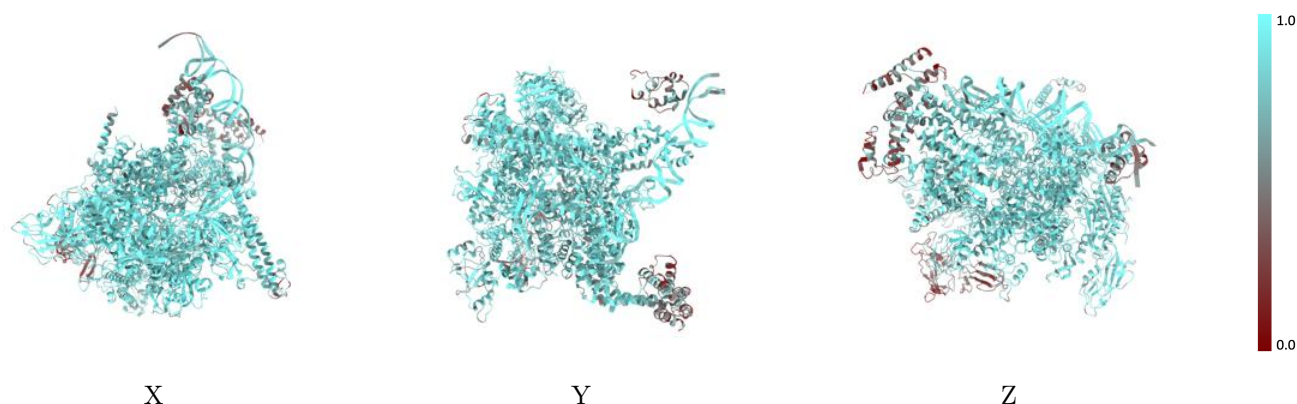
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



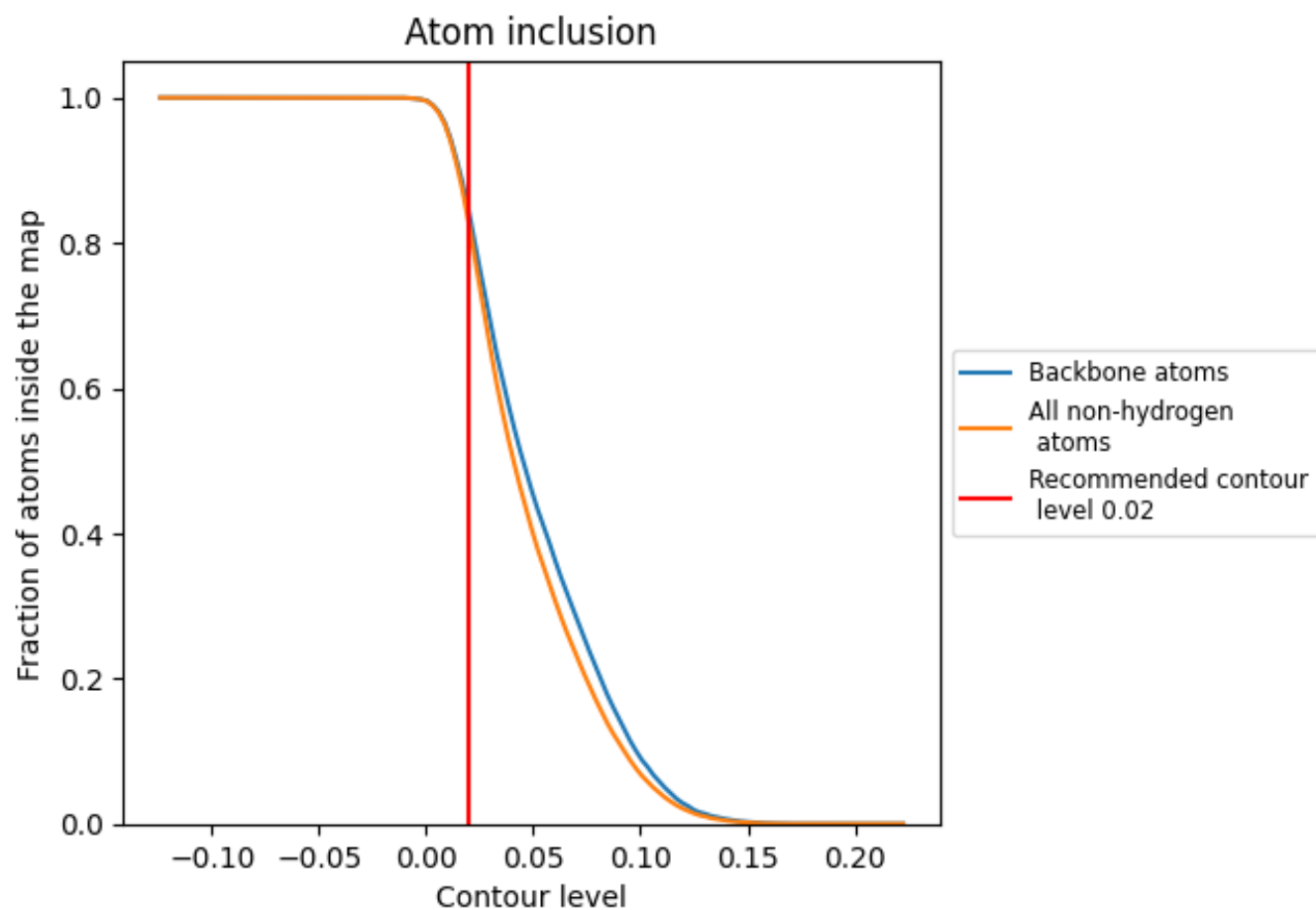
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8245	<div></div> 0.4800
G	<div></div> 0.9003	<div></div> 0.5390
H	<div></div> 0.8870	<div></div> 0.5150
I	<div></div> 0.8861	<div></div> 0.5260
J	<div></div> 0.8125	<div></div> 0.4940
K	<div></div> 0.8236	<div></div> 0.5280
L	<div></div> 0.7078	<div></div> 0.3850
M	<div></div> 0.4554	<div></div> 0.3030
N	<div></div> 0.9149	<div></div> 0.5220
O	<div></div> 0.8056	<div></div> 0.2790
P	<div></div> 0.8113	<div></div> 0.2510

1.0
0.0
<0.0