



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:15 AM UTC

PDB ID : 6GMH / pdb_00006gmh
EMDB ID : EMD-0031
Title : Structure of activated transcription complex Pol II-DSIF-PAF-SPT6
Authors : Vos, S.M.; Farnung, L.; Boehing, M.; Linden, A.; Wigge, C.; Urlaub, H.; Cramer, P.
Deposited on : 2018-05-26
Resolution : 3.10 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:

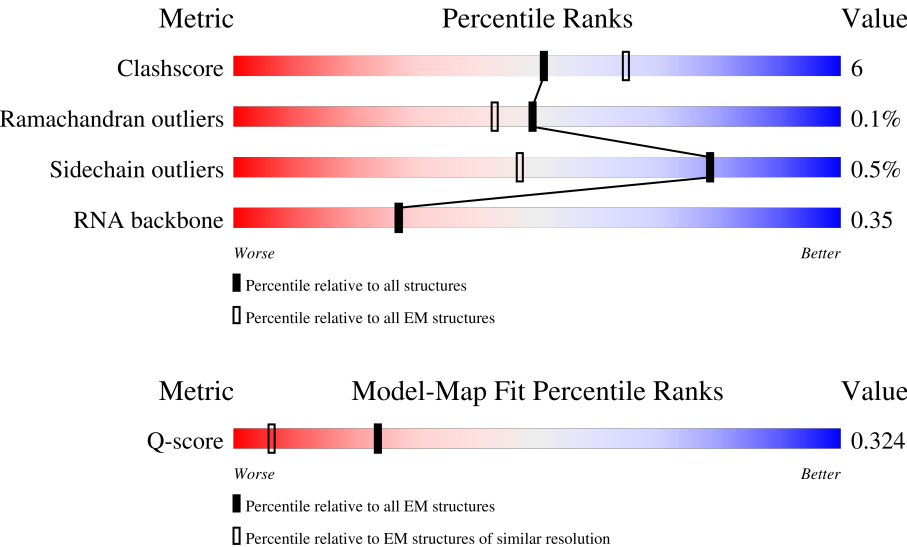
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.10 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.



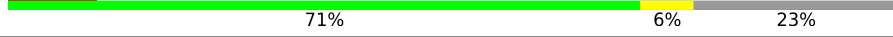
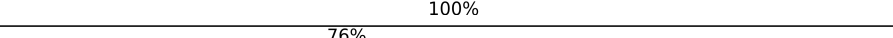
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1970	
2	B	1174	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1726	
14	N	48	
15	P	46	
16	Q	1178	
17	T	48	
18	U	776	
19	V	613	
20	W	305	
21	X	16	
22	Y	121	
23	Z	1087	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 50239 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 RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1441	Total	C	N	O	P	S	
			11371	7151	2033	2115	2	70	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1132	Total	C	N	O	S		
			9052	5725	1592	1671	64	0	0

- Molecule 3 is a protein called RNA polymerase II subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S		
			2115	1324	365	420	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S		
			1004	630	170	200	4	0	0

- Molecule 5 is a protein called RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S		
			1720	1089	300	323	8	0	0

- Molecule 6 is a protein called RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S		
			657	418	113	121	5	0	0

- Molecule 7 is a protein called RNA polymerase II subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			949	587	169	182	11		

- Molecule 10 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6,Transcription elongation factor SPT6,Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	1002	Total	C	N	O	S	0	0
			4737	2583	1071	1076	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	37	Total	C	N	O	P	0	0
			773	361	158	217	37		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	21	Total	C	N	O	P	0	0
			452	202	87	142	21		

- Molecule 16 is a protein called CTR9,RNA polymerase-associated protein CTR9 homolog,RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	884	Total	C	N	O	S	0	0
			4116	2199	953	961	3		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	GLN	-	expression tag	UNP Q6PD62

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	48	Total	C	N	O	P	0	0
			974	462	168	296	48		

- Molecule 18 is a protein called LEO1,LEO1,RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	U	110	Total	C	N	O	0	0
			440	220	110	110		

- Molecule 19 is a protein called PAF1,RNA polymerase II-associated factor 1 homolog,RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	81	Total	C	N	O	0	0
			324	162	81	81		

- Molecule 20 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	300	Total	C	N	O	S	0	0
			2333	1483	392	454	4		

- Molecule 21 is a protein called CDC73.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	X	16	Total	C	N	O	0	0
			63	32	16	15		

- Molecule 22 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 23 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	486	Total	C	N	O	S	0	0
			3878	2465	684	712	17		

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total 2	Zn 2	0
24	B	1	Total 1	Zn 1	0
24	C	1	Total 1	Zn 1	0
24	I	2	Total 2	Zn 2	0
24	J	1	Total 1	Zn 1	0
24	L	1	Total 1	Zn 1	0
24	Y	1	Total 1	Zn 1	0

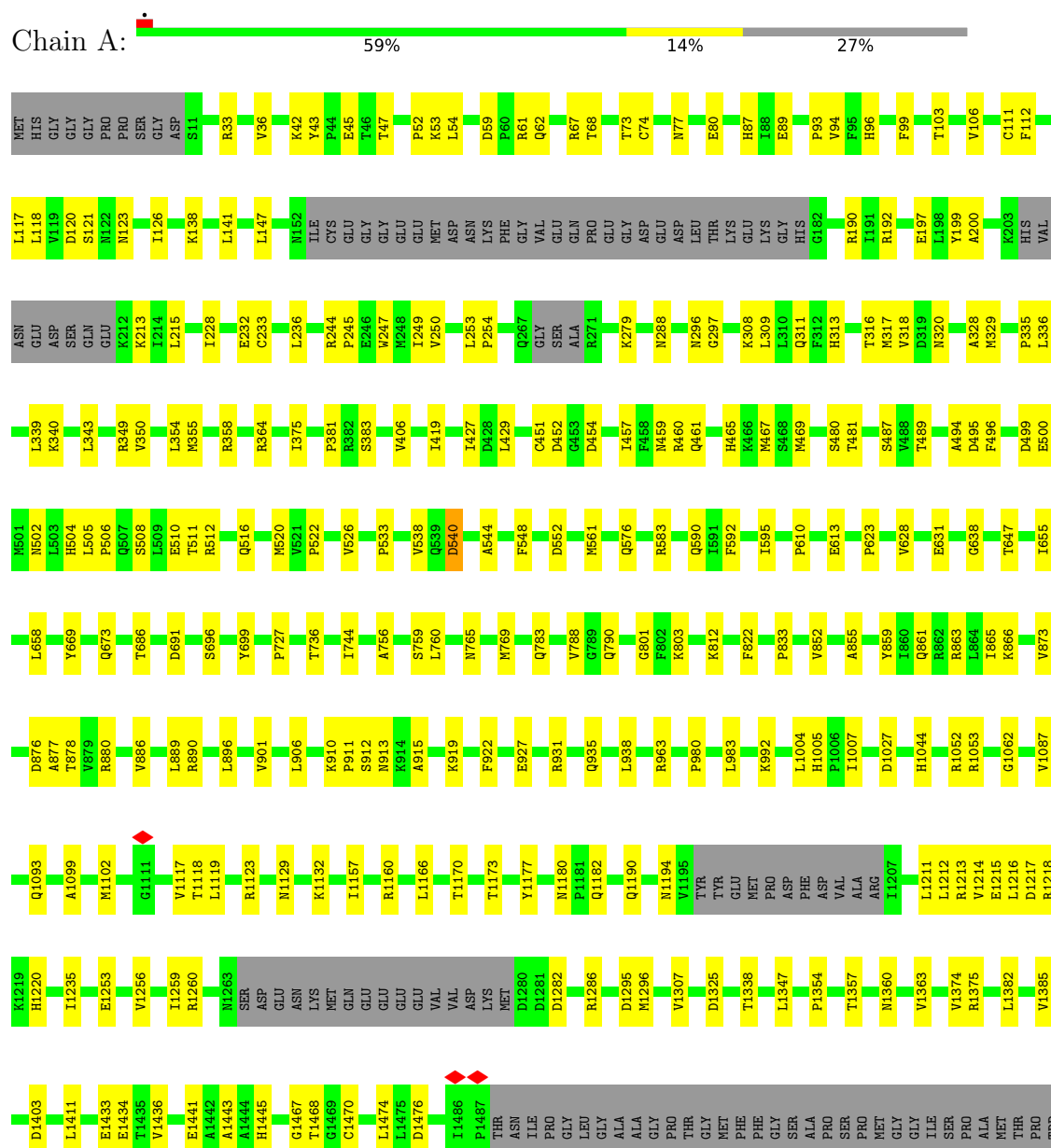
- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total 1	Mg 1	0

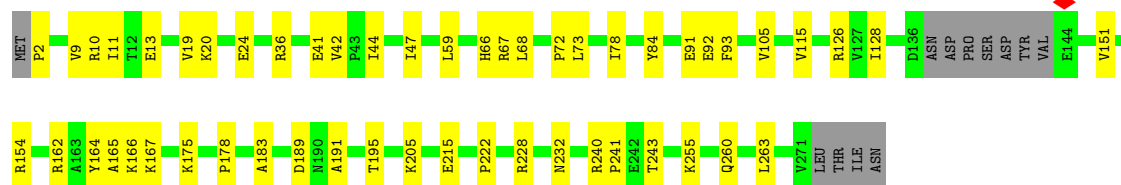
3 Residue-property plots

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: RPB1



Chain C:  77% 19%



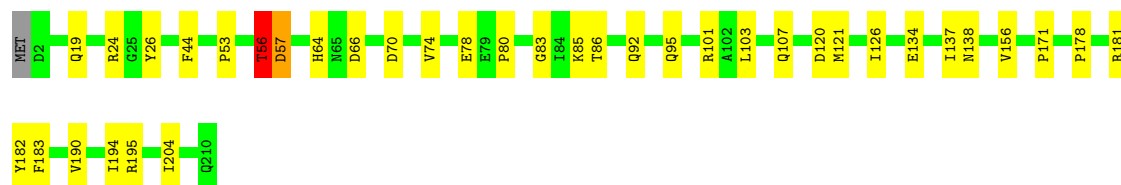
- Molecule 4: RNA polymerase II subunit D

Chain D:  77% 11% 11%



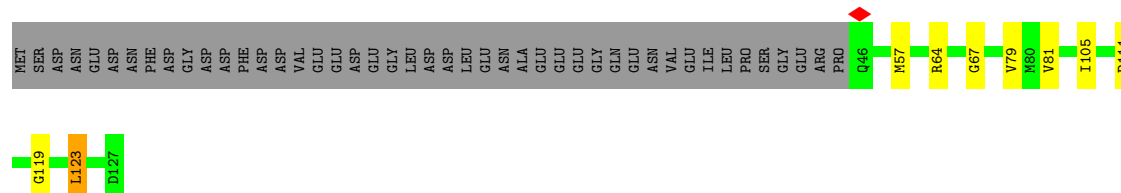
- Molecule 5: RNA polymerase II subunit E

Chain E:  82% 17%



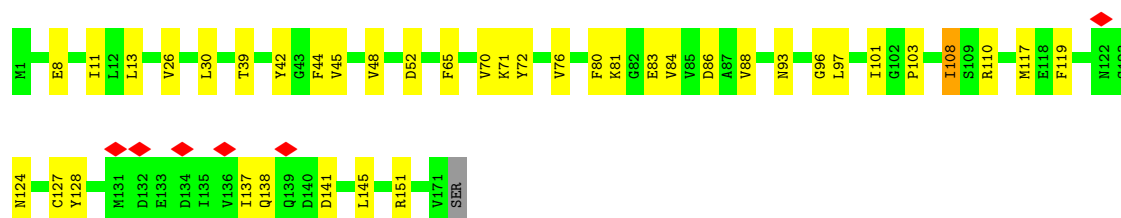
- Molecule 6: RNA polymerase II subunit F

Chain F:  57% 6% 35%

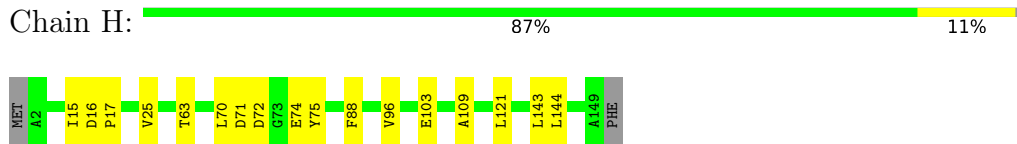


- Molecule 7: RNA polymerase II subunit G

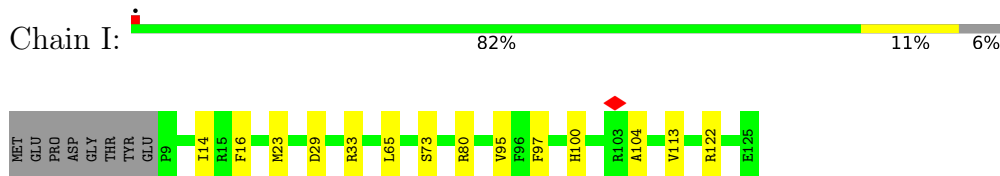
Chain G:  77% 22%



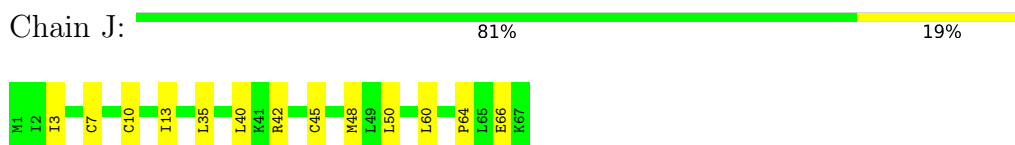
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



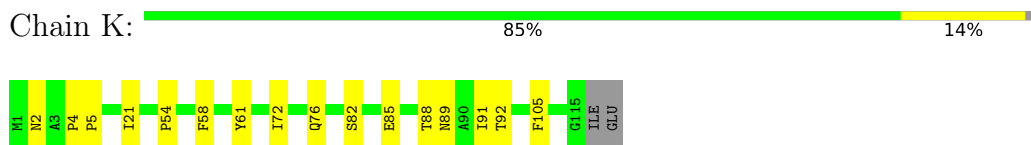
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



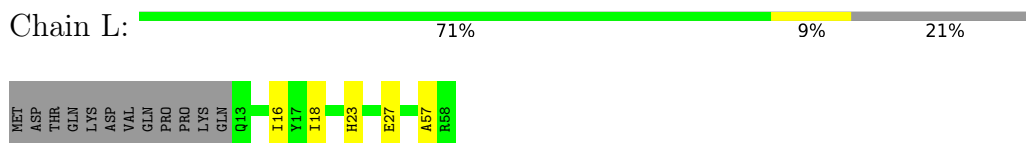
- Molecule 10: RPB10



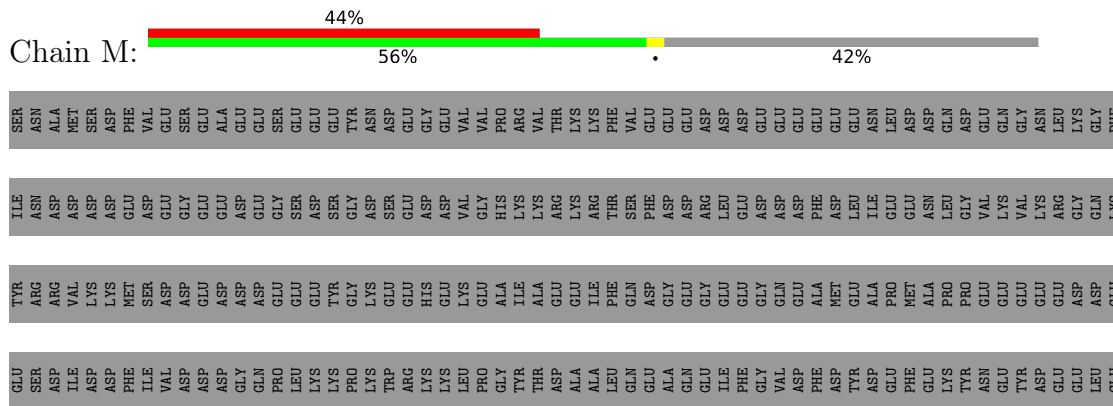
- Molecule 11: RPB11



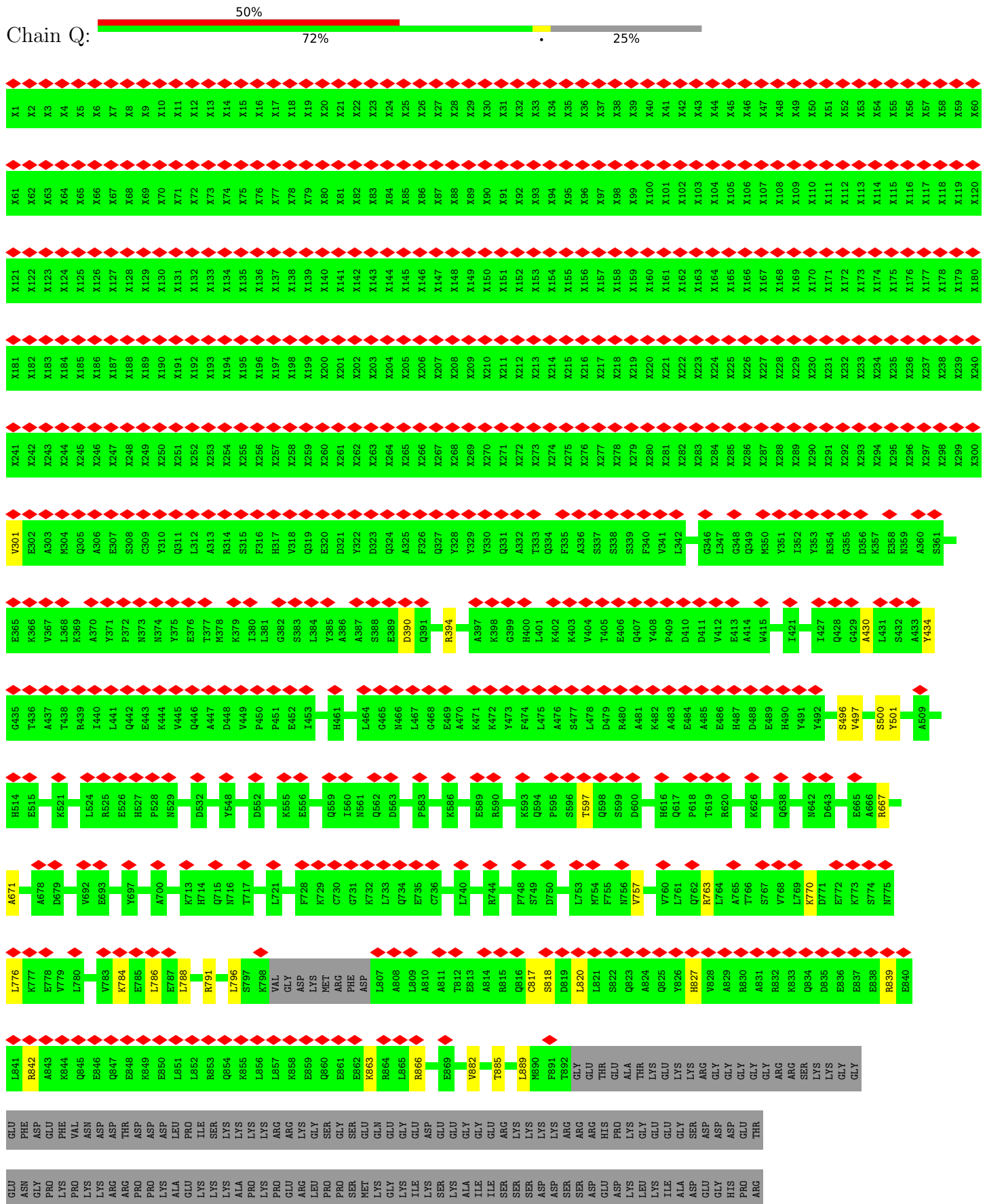
- Molecule 12: RPB12



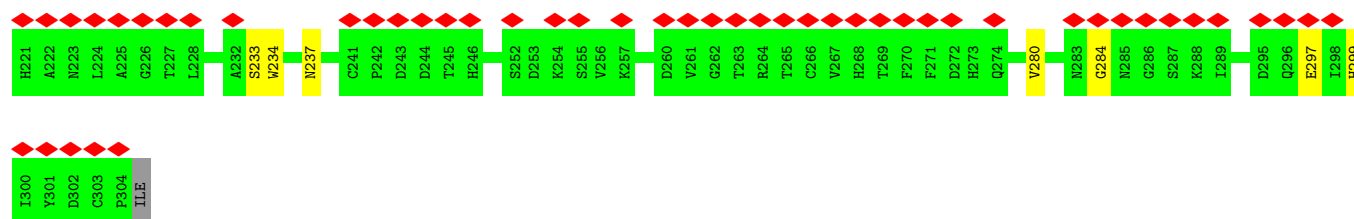
- Molecule 13: Transcription elongation factor SPT6, Transcription elongation factor SPT6, Transcription elongation factor SPT6



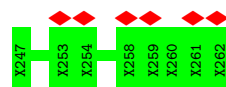
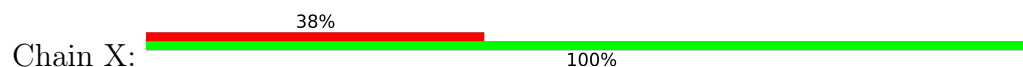
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ASP	SER	TYR	ILE	E1051	V1052	L1053	D1054	G1055	S1056	R1057	V1058	H1059	P1060	E1061	T1062	Y1063	E1064	W1065	A1066	R1067	K1068	M1069	E1070	V1071	D1072	A1073	L1074	E1075	V1076	D1077	E1078	S1079	A1080	E1081	D1082	A1083	M1084	P1085	A1086	G1087	A1088	L1089	E1090	E1091	I1092	L1093	E1094	M1095	P1096	E1097	R1098	L1099	K1100	D1101	L1102	L1103	L1104	D1105	A1106
F298	Q299	L300	R301	S302	I303	P304	V305	K306	G307	A308	E309	D310	N391	D392	E314	E315	E316	A317	D318	Y321	R322	T327	P328	T329	T330	S331	L332	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	ARG	GLY	GLN	PRO	R441	A442	L443	N448	S349	R290	A291	T292	D293	L294	P295	E296	R297						
F378	F379	R380	R381	E382	F383	V384	E385	F386	ARG	E387	L388	H389	I390	N391	D392	T404	M412	A422	Y423	Q424	Y425	E426	Q427	I428	S429	A430	L432	GLN	GLU	SER	CYS	ASP	LEU	THR	ASP	GLY	ARG	GLY	GLN	PRO	R441	A442	L443	N448	S349	R290	A291	T292	D293	L294	P295	E296	R297						
GLN	ASN	ALA	ALA	LYS	ALA	SER	ARG	LYS	LEU	LYS	ARG	VAL	GLU	GLY	ASP	GLU	GLY	GLU	ALA	ASP	GLU	GLU	GLN	GLY	PRO	GLU	LEU	LYS	GLY	ALA	SER	ARG	GLN	PHE	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR								
F539	P543	E544	D545	E548	N549	L550	R551	D552	S553	Y554	Q555	R556	H557	T558	E559	E560	Q561	F562	P563	A564	E565	P566	L567	E568	L569	A570	K571	D572	TYR	VAL	CYS	SER	ASP	GLN	PHE	PRO	T580	P581	E582	A583	V584	L585	Y590	L601	I618	T619	P620	T621	K622	K623	G624	R625	K626	V628					
D629	E630	A631	Y635	S636	F637	K638	V639	L640	K641	F653	L658	A659	E660	D661	E662	G663	L664	L665	T666	T667	D668	L669	S670	G675	VAL	GLU	ASP	GLY	TYR	VAL	CYS	SER	ASP	GLN	PHE	PRO	T684	E688	L689	K690	Q691	R695	D696	E697	F698	S699	H700	Q701	E704	W705	N706	R707	Q708	R709	E714				
Y722	M725	A726	L734	Y740	C745	S746	R747	K748	L749	Y750	L753	R754	V755	A756	P757	Y758	R759	T760	D761	Q762	Q763	VAL	GLU	GLU	ASP	ASP	PHE	MET	ASP	GLU	ASN	ASN	Q775	G776	K777	G778	I779	R780	L784	A785	T786	S787	S788	A789	R790	D791	H792	P793	V794	F795	C796	A797							
L798	V799	R800	G801	E802	G803	E804	V805	T806	D807	F808	L809	R810	L811	P812	H813	F814	LYS	ARG	ARG	THR	ALA	TRP	ARG	GLU	E824	E825	R826	E827	K828	K829	A830	Q831	D832	L833	E834	T835	L836	K837	K838	F839	L840	L841	N842	K843	K844	P845	H846	V847	W848	T849	G852	E853	N854	R855	D856	A857	Q858		
M859	L860	I861	E862	D863	V864	K865	R866	L867	V868	H869	E870	L871	D872	Q873	G874	Q875	Q876	L877	S878	S879	T880	G881	V882	E883	L884	V885	D886	H887	E888	L889	A890	L891	L892	Y893	M894	N895	S896	K897	K898	S899	E900	A901	E902	F903	R904	D905	Y906	P907	P908	Y909	Q912	A913	V914	S915	L916	A917	R918	R919	
I920	Q921	D922	E926	F927	A928	Q929	V930	C931	S932	SER	ASP	E935	D936	T937	L938	C939	L940	K941	F942	H943	P944	L945	A946	E947	D948	H949	V949	K950	V951	E952	E953	L954	L955	N956	A957	L958	Y959	C960	I963	V966	N967	E968	V969	G970	V971	D972	V973	N974	R975	A976	I977	A978	H979	P980	Y981	S982	Q983		
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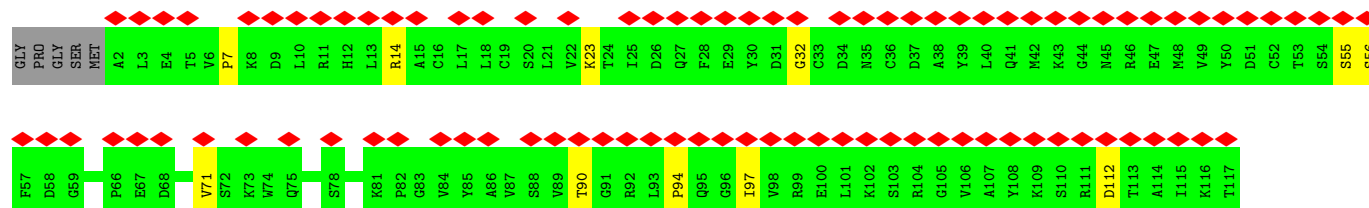
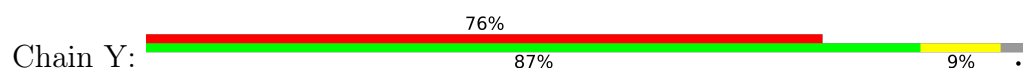




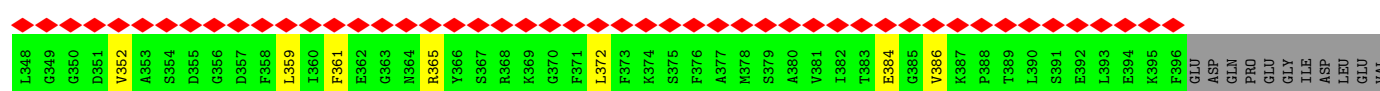
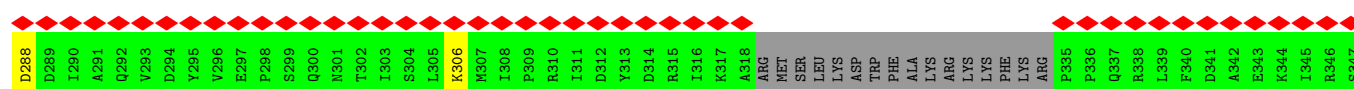
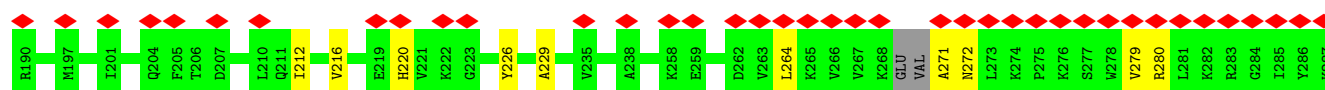
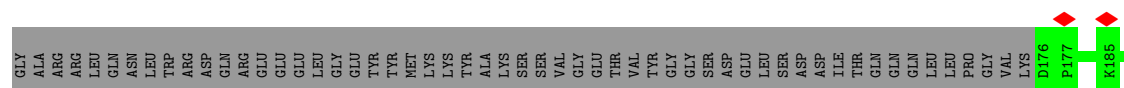
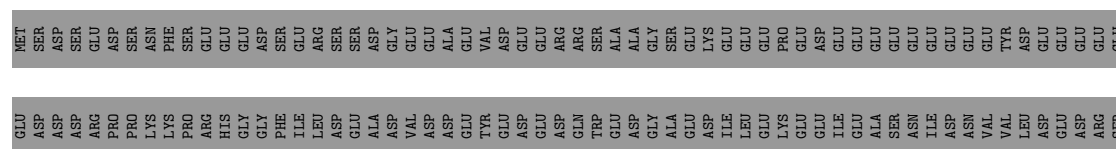
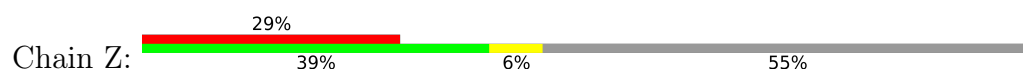
- Molecule 21: CDC73



- Molecule 22: Transcription elongation factor SPT4



- Molecule 23: Transcription elongation factor SPT5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	374964	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0157	Depositor
Map size (Å)	377.64, 377.64, 377.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.049, 1.049, 1.049	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, SEP, ZN, TPO

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	0.33	0/11558	0.65	5/15601 (0.0%)
2	B	0.36	0/9232	0.63	0/12462
3	C	0.35	0/2158	0.54	0/2931
4	D	0.26	0/1017	0.58	0/1368
5	E	0.31	0/1751	0.65	2/2366 (0.1%)
6	F	0.28	0/667	0.48	0/901
7	G	0.28	0/1364	0.64	0/1853
8	H	0.33	0/1207	0.61	0/1628
9	I	0.27	0/972	0.64	2/1316 (0.2%)
10	J	0.37	0/542	0.51	0/730
11	K	0.34	0/939	0.57	0/1271
12	L	0.36	0/394	0.70	0/524
13	M	0.18	0/4724	0.53	4/6031 (0.1%)
14	N	0.22	0/870	0.40	0/1341
15	P	0.25	0/506	0.49	1/787 (0.1%)
16	Q	0.20	0/2923	0.50	1/3746 (0.0%)
17	T	0.27	0/1087	0.45	0/1674
20	W	0.18	0/2392	0.53	0/3257
22	Y	0.17	0/927	0.45	0/1250
23	Z	0.20	0/3946	0.52	0/5314
All	All	0.29	0/49176	0.59	15/66351 (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
1	A	0	2
2	B	0	3
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	2
7	G	0	1
13	M	0	3
All	All	0	12

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	56	THR	CA-C-N	6.21	133.40	121.54
5	E	56	THR	C-N-CA	6.21	133.40	121.54
1	A	112	PHE	CA-C-N	5.89	132.79	121.54
1	A	112	PHE	C-N-CA	5.89	132.79	121.54
13	M	1082	ASP	N-CA-C	-5.83	105.43	113.18
9	I	104	ALA	CA-C-N	5.52	129.10	120.82
9	I	104	ALA	C-N-CA	5.52	129.10	120.82
1	A	1434	GLU	CA-C-N	5.48	132.01	121.54
1	A	1434	GLU	C-N-CA	5.48	132.01	121.54
13	M	977	ILE	N-CA-C	-5.40	108.01	113.20
15	P	36	G	P-O3'-C3'	5.23	128.05	120.20
1	A	910	LYS	N-CA-C	5.15	121.20	109.81
16	Q	597	THR	N-CA-C	5.15	116.93	110.91
13	M	1339	ASN	CA-C-N	5.08	128.43	120.82
13	M	1339	ASN	C-N-CA	5.08	128.43	120.82

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	ARG	Peptide
1	A	538	VAL	Peptide
2	B	629	GLU	Peptide
2	B	71	ALA	Peptide
2	B	98	HIS	Peptide
3	C	91	GLU	Peptide
5	E	56	THR	Peptide
5	E	57	ASP	Peptide
7	G	124	ASN	Peptide
13	M	1145	ASN	Peptide
13	M	1251	LYS	Peptide
13	M	1252	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	A	11371	0	11489	190	0
2	B	9052	0	9081	134	0
3	C	2115	0	2057	34	0
4	D	1004	0	980	12	0
5	E	1720	0	1737	26	0
6	F	657	0	684	8	0
7	G	1333	0	1321	27	0
8	H	1186	0	1147	11	0
9	I	949	0	879	10	0
10	J	533	0	554	10	0
11	K	920	0	942	11	0
12	L	388	0	393	5	0
13	M	4737	0	2252	21	0
14	N	773	0	412	3	0
15	P	452	0	229	5	0
16	Q	4116	0	1657	20	0
17	T	974	0	541	9	0
18	U	440	0	18	0	0
19	V	324	0	15	1	0
20	W	2333	0	2246	22	0
21	X	63	0	2	0	0
22	Y	911	0	904	8	0
23	Z	3878	0	3941	39	0
24	A	2	0	0	0	0
24	B	1	0	0	0	0
24	C	1	0	0	0	0
24	I	2	0	0	0	0
24	J	1	0	0	0	0
24	L	1	0	0	0	0
24	Y	1	0	0	0	0
25	A	1	0	0	0	0
All	All	50239	0	43481	510	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 (510) 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)
5:E:85:LYS:NZ	14:N:41:DC:OP2	1.92	1.03
2:B:816:GLU:OE2	2:B:869:LYS:NZ	2.00	0.95
9:I:65:LEU:O	9:I:122:ARG:NH1	2.06	0.88
1:A:803:LYS:O	1:A:812:LYS:NZ	2.12	0.83
1:A:355:MET:SD	2:B:1091:ARG:NH1	2.50	0.82
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.13	0.81
13:M:1454:LYS:NZ	13:M:1456:THR:OG1	2.15	0.79
1:A:358:ARG:NH1	17:T:27:DT:OP1	2.17	0.78
1:A:1375:ARG:NH1	1:A:1403:ASP:OD1	2.18	0.77
2:B:1131:ARG:NH1	23:Z:535:GLU:OE1	2.18	0.77
2:B:859:ARG:NH1	2:B:860:VAL:O	2.19	0.76
1:A:927:GLU:OE2	1:A:931:ARG:NH2	2.14	0.75
16:Q:885:THR:O	16:Q:889:LEU:HB2	1.87	0.75
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.72	0.71
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.72	0.71
1:A:686:THR:HG21	2:B:1041:ILE:HA	1.74	0.70
1:A:33:ARG:HH21	2:B:1141:ARG:HE	1.40	0.69
16:Q:784:LYS:NZ	20:W:64:GLN:OE1	2.26	0.68
1:A:87:HIS:NE2	1:A:89:GLU:OE2	2.27	0.68
2:B:592:ARG:NE	2:B:663:GLU:OE2	2.18	0.68
2:B:274:ARG:NH1	2:B:311:ILE:O	2.26	0.67
7:G:97:LEU:HB3	7:G:108:ILE:HG23	1.76	0.67
22:Y:23:LYS:NZ	22:Y:32:GLY:O	2.26	0.66
4:D:114:LEU:HD22	7:G:84:VAL:HG11	1.78	0.66
2:B:473:LEU:HD11	2:B:1052:LYS:HD3	1.76	0.65
2:B:819:SER:H	2:B:827:GLU:HB2	1.61	0.65
23:Z:529:ASP:HB2	23:Z:553:LEU:HD13	1.78	0.65
6:F:57:MET:HB2	6:F:123:LEU:HD13	1.79	0.65
3:C:92:GLU:OE1	23:Z:711:ARG:NH1	2.30	0.65
1:A:861:GLN:HE21	1:A:865:ILE:HD11	1.61	0.65
1:A:54:LEU:HB3	1:A:61:ARG:HH12	1.62	0.64
4:D:60:VAL:HG13	7:G:103:PRO:HB3	1.79	0.64
1:A:199:TYR:HB3	1:A:215:LEU:HD23	1.80	0.64
2:B:282:ARG:HH11	9:I:16:PHE:HD2	1.45	0.64
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.30	0.64
23:Z:417:GLU:OE2	23:Z:516:ARG:NH1	2.31	0.64
2:B:91:ILE:HD11	2:B:124:LEU:HD12	1.80	0.63
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.80	0.63
3:C:47:ILE:HD11	3:C:68:LEU:HB3	1.80	0.63
1:A:459:ASN:HB3	1:A:469:MET:HG2	1.81	0.63
1:A:865:ILE:HD13	2:B:1092:ASP:OD2	1.99	0.63
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1441:LYS:NZ	13:M:1445:GLU:OE2	2.31	0.63
1:A:381:PRO:HB3	1:A:480:SER:HA	1.81	0.62
3:C:47:ILE:HA	3:C:165:ALA:HA	1.81	0.62
1:A:576:GLN:O	1:A:590:GLN:NE2	2.32	0.62
1:A:865:ILE:HG21	2:B:1092:ASP:OD2	2.00	0.62
2:B:458:LYS:HB2	2:B:461:GLN:HB2	1.81	0.62
3:C:41:GLU:OE1	3:C:255:LYS:NZ	2.27	0.62
23:Z:306:LYS:HA	23:Z:372:LEU:O	2.01	0.61
2:B:98:HIS:HB2	2:B:108:MET:HB2	1.83	0.61
1:A:200:ALA:O	1:A:213:LYS:HA	2.01	0.60
23:Z:479:LYS:HD3	23:Z:521:CYS:HB2	1.83	0.60
2:B:354:SER:HG	2:B:357:CYS:HG	1.48	0.60
23:Z:220:HIS:NE2	23:Z:384:GLU:OE1	2.34	0.60
1:A:457:ILE:HG22	1:A:504:HIS:HB2	1.84	0.60
23:Z:450:ILE:HG23	23:Z:452:PRO:HD3	1.84	0.59
20:W:35:VAL:HB	20:W:47:TRP:HB2	1.83	0.59
23:Z:639:LYS:HB2	23:Z:642:HIS:HD2	1.68	0.59
2:B:344:GLN:NE2	2:B:354:SER:O	2.36	0.59
2:B:565:THR:HG22	2:B:610:ARG:HB3	1.85	0.59
2:B:32:SER:HB3	2:B:643:LEU:HD21	1.83	0.59
3:C:154:ARG:NH1	10:J:60:LEU:O	2.36	0.59
16:Q:763:ARG:HH12	20:W:65:LEU:HD11	1.68	0.59
13:M:1357:ILE:HG21	13:M:1408:LEU:HD13	1.85	0.59
23:Z:439:LYS:O	23:Z:452:PRO:HA	2.03	0.59
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.84	0.59
1:A:318:VAL:HG12	1:A:339:LEU:HD12	1.85	0.58
1:A:727:PRO:HA	1:A:736:THR:HG21	1.84	0.58
1:A:1190:GLN:O	1:A:1194:ASN:HB2	2.03	0.58
7:G:8:GLU:HA	7:G:70:VAL:O	2.03	0.58
1:A:94:VAL:HG13	1:A:311:GLN:HG2	1.83	0.58
1:A:47:THR:HA	1:A:52:PRO:HA	1.85	0.58
1:A:1218:ARG:NH1	1:A:1253:GLU:HA	2.18	0.58
20:W:36:VAL:HG22	20:W:46:VAL:HG22	1.86	0.58
1:A:520:MET:HG3	1:A:522:PRO:HD2	1.85	0.58
1:A:783:GLN:HG3	1:A:788:VAL:HA	1.86	0.58
1:A:919:LYS:HE2	1:A:1053:ARG:HH12	1.67	0.58
1:A:320:ASN:ND2	1:A:336:LEU:O	2.37	0.58
9:I:73:SER:HA	9:I:95:VAL:HG11	1.86	0.57
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.33	0.57
23:Z:595:HIS:N	23:Z:598:ASP:OD2	2.37	0.57
1:A:866:LYS:HZ3	2:B:1091:ARG:HH22	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:LYS:NZ	12:L:57:ALA:HB3	2.19	0.57
1:A:45:GLU:HB2	1:A:53:LYS:NZ	2.19	0.57
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.87	0.57
1:A:886:VAL:HG13	5:E:171:PRO:HD3	1.86	0.57
2:B:483:ARG:NH2	2:B:527:ALA:O	2.38	0.57
23:Z:549:VAL:HG11	23:Z:635:MET:HE2	1.87	0.57
2:B:725:GLN:NE2	2:B:937:SER:O	2.38	0.57
1:A:138:LYS:NZ	1:A:1441:GLU:OE2	2.26	0.57
4:D:67:TYR:OH	7:G:86:ASP:O	2.22	0.56
23:Z:279:VAL:HA	23:Z:386:VAL:HG21	1.87	0.56
2:B:549:SER:HG	2:B:577:HIS:HE2	1.51	0.56
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.86	0.56
23:Z:444:ASP:H	23:Z:448:ILE:HG23	1.70	0.56
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.88	0.56
4:D:100:LEU:HD21	4:D:118:LEU:HD11	1.87	0.56
16:Q:763:ARG:HH22	16:Q:788:LEU:HD23	1.70	0.56
20:W:206:VAL:HG22	20:W:216:ILE:HG12	1.88	0.56
23:Z:272:ASN:HD21	23:Z:384:GLU:HB2	1.70	0.56
1:A:1552:SER:HB3	13:M:1509:ARG:HH12	1.70	0.56
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.88	0.56
2:B:191:GLU:OE2	2:B:743:ARG:NH2	2.39	0.56
2:B:692:THR:OG1	9:I:80:ARG:NH1	2.39	0.56
1:A:922:PHE:HA	1:A:1052:ARG:HD3	1.87	0.55
16:Q:885:THR:O	16:Q:889:LEU:CB	2.53	0.55
2:B:806:PHE:O	2:B:1050:ARG:NH1	2.39	0.55
9:I:29:ASP:O	9:I:33:ARG:HA	2.05	0.55
5:E:64:HIS:ND1	5:E:66:ASP:OD1	2.38	0.55
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.37	0.55
1:A:866:LYS:NZ	2:B:1091:ARG:HH22	2.05	0.55
1:A:42:LYS:O	1:A:288:ASN:ND2	2.40	0.54
23:Z:552:ARG:HB3	23:Z:559:GLN:HB2	1.89	0.54
1:A:855:ALA:HB3	2:B:494:LYS:NZ	2.23	0.54
1:A:919:LYS:HE2	1:A:1053:ARG:NH1	2.22	0.54
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.72	0.54
16:Q:763:ARG:NH1	20:W:65:LEU:HD21	2.23	0.54
20:W:75:THR:OG1	20:W:116:PRO:O	2.26	0.54
1:A:1552:SER:HB3	13:M:1509:ARG:NH1	2.21	0.53
1:A:279:LYS:HZ1	1:A:328:ALA:HB1	1.73	0.53
1:A:358:ARG:NH2	2:B:1076:GLU:OE1	2.41	0.53
1:A:111:CYS:HB2	1:A:118:LEU:HB3	1.90	0.53
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:ARG:HH11	2:B:771:GLU:HG3	1.73	0.53
1:A:877:ALA:HB3	1:A:890:ARG:NH1	2.23	0.53
1:A:1123:ARG:NH2	1:A:1360:ASN:OD1	2.42	0.53
10:J:10:CYS:SG	10:J:42:ARG:NH2	2.78	0.53
1:A:43:TYR:HB3	1:A:53:LYS:NZ	2.24	0.53
1:A:138:LYS:HG3	1:A:1441:GLU:OE2	2.09	0.53
5:E:134:GLU:OE2	5:E:181:ARG:NH2	2.42	0.53
1:A:1347:LEU:HD22	1:A:1354:PRO:HA	1.90	0.53
2:B:280:SER:OG	2:B:281:ASP:N	2.42	0.53
1:A:1212:LEU:HD22	1:A:1259:ILE:HD12	1.91	0.52
2:B:603:MET:HG3	2:B:614:ILE:HG12	1.91	0.52
7:G:138:GLN:N	7:G:141:ASP:OD2	2.29	0.52
1:A:1375:ARG:NH1	5:E:195:ARG:HH22	2.07	0.52
2:B:92:TYR:HB2	2:B:125:TYR:HB2	1.90	0.52
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.92	0.52
1:A:343:LEU:HA	1:A:349:ARG:H	1.74	0.52
2:B:872:THR:HA	2:B:889:LYS:HG2	1.89	0.52
2:B:225:LEU:HD22	2:B:228:SER:HB2	1.91	0.52
2:B:927:ARG:HH11	2:B:1054:MET:HE2	1.74	0.52
6:F:105:ILE:HG22	6:F:119:GLY:HA2	1.92	0.52
7:G:81:LYS:HD3	23:Z:473:LYS:NZ	2.24	0.52
20:W:297:GLU:OE1	20:W:299:HIS:NE2	2.43	0.52
23:Z:441:LEU:HB3	23:Z:451:MET:HB2	1.92	0.52
1:A:866:LYS:HZ3	2:B:1091:ARG:NH2	2.08	0.52
1:A:1005:HIS:HD2	1:A:1007:ILE:HG22	1.74	0.52
2:B:790:GLN:O	2:B:968:ASN:ND2	2.43	0.52
1:A:1546:PHE:HB3	13:M:1515:TYR:CZ	2.45	0.51
2:B:760:THR:OG1	2:B:764:MET:SD	2.62	0.51
1:A:106:VAL:HG22	1:A:236:LEU:HD11	1.93	0.51
1:A:508:SER:HB2	1:A:511:THR:HG22	1.92	0.51
3:C:175:LYS:HZ2	12:L:57:ALA:HB3	1.74	0.51
9:I:14:ILE:HD13	9:I:23:MET:HE2	1.91	0.51
3:C:205:LYS:NZ	3:C:215:GLU:O	2.35	0.51
1:A:1286:ARG:HH22	2:B:252:ILE:HA	1.75	0.51
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.26	0.51
3:C:67:ARG:NH1	10:J:3:ILE:O	2.40	0.51
1:A:1173:THR:HG22	1:A:1214:VAL:HG12	1.93	0.51
20:W:43:LEU:HD22	20:W:61:GLU:HG2	1.93	0.51
1:A:67:ARG:NE	15:P:35:A:OP1	2.44	0.51
3:C:10:ARG:HH22	3:C:228:ARG:HH22	1.59	0.51
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:PRO:O	1:A:647:THR:OG1	2.29	0.50
22:Y:71:VAL:HG13	23:Z:264:LEU:HD11	1.93	0.50
1:A:197:GLU:OE2	1:A:308:LYS:NZ	2.45	0.50
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.94	0.50
20:W:24:TRP:HE1	20:W:284:GLY:H	1.60	0.50
22:Y:14:ARG:HA	22:Y:55:SER:HA	1.93	0.50
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.92	0.50
2:B:624:PRO:HA	2:B:663:GLU:O	2.11	0.50
7:G:101:ILE:HD11	7:G:145:LEU:HD11	1.94	0.50
1:A:190:ARG:HH12	1:A:192:ARG:HH22	1.59	0.50
2:B:587:LEU:HB3	2:B:603:MET:HE3	1.94	0.50
2:B:1029:TYR:HA	2:B:1036:LYS:HA	1.94	0.50
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.93	0.50
22:Y:7:PRO:HG3	22:Y:23:LYS:HA	1.94	0.50
1:A:583:ARG:NH1	3:C:222:PRO:O	2.45	0.50
1:A:1177:TYR:OH	1:A:1282:ASP:OD2	2.27	0.50
2:B:627:ILE:HD11	2:B:663:GLU:HG3	1.93	0.50
13:M:1462:ILE:HA	13:M:1473:LEU:O	2.12	0.50
1:A:228:ILE:O	1:A:244:ARG:NH2	2.34	0.49
3:C:47:ILE:HG22	3:C:165:ALA:HB2	1.94	0.49
1:A:613:GLU:OE2	1:A:623:PRO:HD2	2.12	0.49
1:A:913:ASN:N	1:A:1325:ASP:O	2.38	0.49
1:A:1347:LEU:HD21	1:A:1357:THR:HB	1.94	0.49
2:B:505:LEU:HD22	2:B:509:VAL:HB	1.94	0.49
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.95	0.49
23:Z:361:PHE:O	23:Z:365:ARG:HB2	2.12	0.49
1:A:67:ARG:HD3	1:A:68:THR:HG23	1.94	0.49
1:A:880:ARG:HG2	1:A:886:VAL:HA	1.95	0.49
2:B:1038:THR:HA	3:C:195:THR:HA	1.93	0.49
7:G:80:PHE:HD2	7:G:83:GLU:OE2	1.96	0.49
11:K:61:TYR:HA	11:K:72:ILE:O	2.13	0.49
5:E:74:VAL:HG12	5:E:103:LEU:HB2	1.95	0.49
23:Z:280:ARG:HH21	23:Z:288:ASP:HB3	1.78	0.49
8:H:72:ASP:HB3	8:H:74:GLU:H	1.77	0.49
11:K:85:GLU:HA	11:K:88:THR:HG22	1.94	0.49
1:A:244:ARG:HD2	1:A:245:PRO:HD2	1.94	0.49
1:A:631:GLU:OE2	1:A:992:LYS:NZ	2.36	0.49
1:A:1375:ARG:HH11	5:E:195:ARG:HH12	1.60	0.49
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.94	0.49
1:A:495:ASP:N	1:A:499:ASP:OD2	2.42	0.49
1:A:1533:PRO:HD3	13:M:1471:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ILE:HB	2:B:139:GLN:HB3	1.94	0.49
2:B:1060:HIS:HB3	2:B:1078:ARG:HG3	1.94	0.49
3:C:72:PRO:HG3	10:J:13:ILE:HD11	1.95	0.49
5:E:19:GLN:OE1	5:E:138:ASN:ND2	2.41	0.49
7:G:8:GLU:HG2	7:G:71:LYS:HG2	1.95	0.49
9:I:97:PHE:HB2	9:I:100:HIS:HE2	1.76	0.49
20:W:165:SER:O	20:W:172:ILE:HA	2.12	0.49
1:A:790:GLN:HA	1:A:822:PHE:HA	1.94	0.48
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.95	0.48
2:B:124:LEU:HD13	2:B:152:ILE:HD11	1.95	0.48
4:D:112:LYS:HD2	4:D:119:GLU:HG2	1.95	0.48
9:I:29:ASP:O	9:I:33:ARG:CA	2.61	0.48
1:A:296:ASN:OD1	1:A:297:GLY:N	2.46	0.48
2:B:130:LYS:O	2:B:141:GLN:HA	2.13	0.48
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.95	0.48
2:B:223:SER:OG	2:B:350:HIS:ND1	2.39	0.48
2:B:677:MET:H	2:B:682:LEU:HD22	1.79	0.48
3:C:24:GLU:OE2	3:C:228:ARG:HG2	2.13	0.48
8:H:88:PHE:HD2	8:H:144:LEU:HD12	1.78	0.48
9:I:113:VAL:HG22	9:I:122:ARG:HG2	1.95	0.48
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.96	0.48
5:E:92:GLN:HG2	5:E:95:GLN:HE21	1.78	0.48
16:Q:863:LYS:HG2	16:Q:866:ARG:HH22	1.77	0.48
22:Y:90:THR:HG23	22:Y:112:ASP:OD2	2.13	0.48
1:A:500:GLU:OE2	2:B:1058:LYS:HD3	2.14	0.48
5:E:178:PRO:O	5:E:182:TYR:HB2	2.13	0.48
16:Q:791:ARG:HB3	20:W:106:PRO:HB3	1.96	0.48
7:G:30:LEU:HD22	7:G:70:VAL:HG11	1.95	0.48
23:Z:479:LYS:HG3	23:Z:489:THR:HG22	1.94	0.48
1:A:487:SER:OG	1:A:673:GLN:NE2	2.47	0.48
1:A:45:GLU:HB2	1:A:53:LYS:HZ3	1.78	0.48
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.95	0.48
4:D:34:ASN:O	4:D:68:THR:OG1	2.31	0.48
16:Q:786:LEU:HD21	16:Q:820:LEU:HB3	1.96	0.48
1:A:383:SER:H	11:K:2:ASN:HD21	1.61	0.48
2:B:864:ASP:OD1	23:Z:725:LYS:NZ	2.47	0.48
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.94	0.48
2:B:272:VAL:O	2:B:276:LEU:HB2	2.14	0.48
20:W:126:HIS:HA	20:W:150:PHE:HD1	1.79	0.48
1:A:540:ASP:OD2	2:B:790:GLN:HG2	2.14	0.47
1:A:1528:TYR:CG	13:M:1469:PRO:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:ASP:HB2	6:F:105:ILE:HG23	1.96	0.47
2:B:513:GLU:OE2	2:B:730:LYS:NZ	2.46	0.47
2:B:744:MET:SD	2:B:906:GLN:NE2	2.79	0.47
1:A:36:VAL:HG23	2:B:1138:ARG:NH1	2.29	0.47
22:Y:56:SER:HB3	23:Z:271:ALA:HA	1.96	0.47
1:A:451:CYS:SG	1:A:452:ASP:N	2.87	0.47
2:B:341:GLU:HG3	2:B:345:LYS:NZ	2.29	0.47
14:N:42:DT:O4	17:T:6:DC:N4	2.47	0.47
1:A:855:ALA:HB3	2:B:494:LYS:HZ1	1.79	0.47
2:B:88:PHE:HZ	2:B:412:LEU:HD21	1.80	0.47
10:J:35:LEU:HD11	10:J:50:LEU:HD12	1.95	0.47
5:E:194:ILE:HG13	5:E:204:ILE:HG22	1.95	0.47
11:K:82:SER:HB3	11:K:85:GLU:HG2	1.97	0.47
23:Z:490:GLY:HA3	23:Z:502:LEU:HD13	1.97	0.47
1:A:233:CYS:HA	1:A:236:LEU:HB3	1.95	0.47
1:A:861:GLN:HE22	1:A:1093:GLN:HA	1.80	0.47
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.46	0.47
2:B:949:TYR:HB3	2:B:953:ASP:HB2	1.96	0.47
6:F:79:VAL:HG22	6:F:81:VAL:H	1.78	0.47
7:G:151:ARG:HE	23:Z:491:LEU:HG	1.80	0.47
20:W:83:SER:OG	20:W:85:ASP:OD1	2.24	0.47
1:A:77:ASN:H	1:A:80:GLU:HB3	1.79	0.47
1:A:1467:GLY:H	1:A:1470:CYS:HB2	1.80	0.47
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.21	0.47
14:N:35:DA:OP2	14:N:35:DA:H2'	2.15	0.47
1:A:190:ARG:NH1	1:A:192:ARG:HH22	2.12	0.47
2:B:117:ASN:ND2	2:B:188:ASN:O	2.39	0.47
4:D:84:ARG:O	4:D:88:LEU:HB2	2.15	0.47
7:G:117:MET:HE2	7:G:137:ILE:HD12	1.96	0.47
23:Z:216:VAL:HB	23:Z:226:TYR:HB2	1.97	0.47
23:Z:588:ASP:OD1	23:Z:592:ASN:N	2.42	0.47
23:Z:714:GLN:HB2	23:Z:749:ARG:HG2	1.97	0.47
1:A:1123:ARG:HG2	1:A:1385:VAL:HG11	1.98	0.46
2:B:570:ASN:HD21	2:B:616:THR:HB	1.80	0.46
16:Q:430:ALA:O	16:Q:434:TYR:N	2.47	0.46
17:T:24:DG:H2'	17:T:25:DA:C8	2.50	0.46
2:B:994:GLY:HA2	10:J:50:LEU:HD11	1.96	0.46
9:I:29:ASP:O	9:I:33:ARG:N	2.48	0.46
17:T:33:DC:H2''	17:T:34:DT:H5''	1.96	0.46
1:A:880:ARG:NH1	6:F:111:PRO:HB2	2.31	0.46
2:B:157:ARG:NH2	2:B:177:CYS:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HB2	1:A:250:VAL:HG23	1.98	0.46
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.96	0.46
1:A:329:MET:HA	1:A:335:PRO:HA	1.96	0.46
1:A:1375:ARG:NH1	5:E:195:ARG:HH12	2.13	0.46
2:B:905:ASP:HB2	2:B:924:ARG:HG3	1.97	0.46
2:B:1069:ILE:HD11	15:P:37:G:OP1	2.16	0.46
1:A:43:TYR:HB3	1:A:53:LYS:HZ2	1.81	0.46
2:B:1066:PRO:HB3	15:P:35:A:H62	1.80	0.46
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.98	0.46
5:E:44:PHE:HB3	5:E:53:PRO:HB3	1.97	0.46
7:G:127:CYS:SG	7:G:128:TYR:N	2.89	0.46
13:M:1357:ILE:HG12	13:M:1369:VAL:HG22	1.98	0.46
1:A:358:ARG:HH12	17:T:27:DT:P	2.38	0.46
2:B:252:ILE:HG22	2:B:303:PRO:HB3	1.98	0.46
23:Z:472:PHE:HE1	23:Z:520:LEU:HB2	1.81	0.46
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.80	0.46
13:M:1511:PHE:O	13:M:1515:TYR:N	2.48	0.46
17:T:39:DC:H2"	17:T:40:DT:H72	1.98	0.46
1:A:1099:ALA:HA	1:A:1102:MET:HE3	1.97	0.45
7:G:80:PHE:HB2	7:G:83:GLU:HG3	1.98	0.45
1:A:516:GLN:HA	1:A:520:MET:HE2	1.98	0.45
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.98	0.45
1:A:1170:THR:HA	1:A:1216:LEU:HA	1.99	0.45
2:B:274:ARG:NH1	2:B:312:GLN:HA	2.31	0.45
1:A:375:ILE:HD13	1:A:669:TYR:HD2	1.81	0.45
3:C:44:ILE:HD12	3:C:178:PRO:HB3	1.97	0.45
3:C:93:PHE:HE1	3:C:166:LYS:HZ3	1.65	0.45
7:G:81:LYS:HD3	23:Z:473:LYS:HZ1	1.80	0.45
8:H:63:THR:HB	8:H:70:LEU:HD23	1.97	0.45
10:J:40:LEU:HD22	10:J:45:CYS:HB3	1.98	0.45
23:Z:352:VAL:HG23	23:Z:359:LEU:HD21	1.98	0.45
1:A:93:PRO:HB3	1:A:249:ILE:HD13	1.98	0.45
23:Z:479:LYS:NZ	23:Z:521:CYS:O	2.50	0.45
1:A:228:ILE:HG23	1:A:232:GLU:HG2	1.99	0.45
1:A:1529:GLY:H	13:M:1396:ALA:HB2	1.81	0.45
8:H:25:VAL:HG21	8:H:121:LEU:HD22	1.96	0.45
2:B:54:SER:HA	2:B:57:ARG:HG2	1.99	0.45
7:G:138:GLN:HG2	7:G:141:ASP:OD2	2.16	0.45
1:A:889:LEU:O	1:A:890:ARG:NE	2.48	0.45
20:W:193:ILE:HA	20:W:209:SER:HA	1.99	0.45
1:A:1282:ASP:N	1:A:1282:ASP:OD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:94:PRO:HD2	22:Y:97:ILE:HD12	1.98	0.45
1:A:244:ARG:HB3	1:A:247:TRP:CD2	2.52	0.45
1:A:502:ASN:OD1	1:A:502:ASN:N	2.46	0.45
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.49	0.45
13:M:1426:LEU:HD22	13:M:1462:ILE:HD13	1.99	0.45
23:Z:433:LEU:HD13	23:Z:461:LEU:HD13	1.97	0.45
2:B:1062:ARG:HH12	2:B:1066:PRO:HD2	1.82	0.45
11:K:89:ASN:HA	11:K:92:THR:HG22	1.99	0.45
1:A:480:SER:HB3	11:K:2:ASN:HB2	1.99	0.44
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.99	0.44
16:Q:882:VAL:HA	16:Q:885:THR:HG22	1.98	0.44
16:Q:839:ARG:HA	16:Q:842:ARG:HG2	1.99	0.44
23:Z:554:GLU:OE1	23:Z:557:THR:OG1	2.36	0.44
1:A:906:LEU:HD23	1:A:1044:HIS:HD2	1.82	0.44
2:B:388:TYR:HE1	2:B:391:LYS:HZ2	1.63	0.44
5:E:70:ASP:OD1	5:E:70:ASP:N	2.49	0.44
16:Q:817:CYS:SG	16:Q:818:SER:N	2.91	0.44
7:G:39:THR:HG23	7:G:42:TYR:H	1.82	0.44
20:W:110:TRP:CG	20:W:111:THR:H	2.36	0.44
1:A:526:VAL:HA	1:A:533:PRO:HA	1.99	0.44
2:B:98:HIS:CE1	2:B:116:ARG:NH1	2.85	0.44
2:B:796:MET:HE2	2:B:796:MET:HB3	1.87	0.44
17:T:30:DG:H2'	17:T:31:DT:C6	2.53	0.44
1:A:696:SER:HA	1:A:699:TYR:HB2	1.98	0.44
1:A:1217:ASP:OD2	1:A:1220:HIS:HD2	2.01	0.44
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.99	0.44
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.48	0.44
2:B:206:TYR:HA	2:B:383:ASP:OD2	2.17	0.44
16:Q:667:ARG:O	16:Q:671:ALA:N	2.51	0.44
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.83	0.44
3:C:78:ILE:HD11	3:C:126:ARG:HD2	1.99	0.44
1:A:454:ASP:HA	1:A:512:ARG:HH22	1.83	0.44
1:A:510:GLU:HG3	6:F:67:GLY:HA3	2.00	0.44
1:A:552:ASP:HB3	8:H:25:VAL:HG12	2.00	0.44
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.98	0.44
1:A:912:SER:HB3	1:A:915:ALA:H	1.83	0.44
2:B:927:ARG:NH1	2:B:1054:MET:HE2	2.32	0.44
1:A:912:SER:O	1:A:963:ARG:NH2	2.51	0.43
2:B:778:SER:O	2:B:1045:PRO:HA	2.18	0.43
1:A:120:ASP:O	1:A:123:ASN:N	2.52	0.43
7:G:45:VAL:HG22	7:G:76:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1422:PHE:HB3	13:M:1494:PHE:CE1	2.54	0.43
1:A:852:VAL:HG13	2:B:494:LYS:HD3	2.00	0.43
1:A:253:LEU:HD12	1:A:254:PRO:HD2	2.00	0.43
1:A:1211:LEU:HB3	1:A:1260:ARG:NH1	2.33	0.43
2:B:330:VAL:HG13	2:B:331:THR:HG23	2.00	0.43
10:J:7:CYS:HA	10:J:48:MET:HE2	2.00	0.43
13:M:1450:THR:HB	13:M:1459:PRO:HG3	2.00	0.43
16:Q:770:LYS:O	16:Q:827:HIS:NE2	2.52	0.43
1:A:756:ALA:O	1:A:759:SER:OG	2.33	0.43
2:B:212:ASP:OD1	2:B:212:ASP:N	2.51	0.43
1:A:350:VAL:HA	1:A:354:LEU:HD12	2.00	0.43
1:A:496:PHE:HB2	2:B:791:GLU:O	2.19	0.43
1:A:833:PRO:HG3	2:B:1002:PHE:CG	2.53	0.43
1:A:1295:ASP:OD1	1:A:1295:ASP:N	2.51	0.43
1:A:364:ARG:NE	1:A:500:GLU:OE1	2.48	0.43
1:A:364:ARG:HD2	2:B:1084:LEU:HD11	2.00	0.43
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.99	0.43
1:A:1474:LEU:HB2	6:F:105:ILE:HG13	2.00	0.43
5:E:24:ARG:NH2	5:E:182:TYR:O	2.42	0.43
13:M:1364:GLU:OE1	13:M:1365:ASN:ND2	2.52	0.43
19:V:204:UNK:O	19:V:332:UNK:N	2.52	0.43
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.19	0.43
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.01	0.43
7:G:13:LEU:O	7:G:65:PHE:HA	2.19	0.43
7:G:52:ASP:H	7:G:72:TYR:HA	1.84	0.43
22:Y:14:ARG:HG2	22:Y:55:SER:HB3	2.01	0.43
3:C:162:ARG:NH1	3:C:164:TYR:HE2	2.17	0.42
5:E:120:ASP:OD1	5:E:121:MET:N	2.52	0.42
8:H:16:ASP:OD1	8:H:16:ASP:N	2.52	0.42
2:B:108:MET:HE3	2:B:120:TYR:HA	2.01	0.42
2:B:132:VAL:O	2:B:139:GLN:HA	2.18	0.42
2:B:937:SER:OG	2:B:938:ARG:N	2.52	0.42
4:D:60:VAL:HG11	7:G:44:PHE:CE2	2.54	0.42
16:Q:497:VAL:O	16:Q:501:TYR:N	2.51	0.42
10:J:64:PRO:O	12:L:23:HIS:NE2	2.48	0.42
11:K:4:PRO:HA	11:K:5:PRO:HD3	1.91	0.42
1:A:1375:ARG:HD2	5:E:195:ARG:NH1	2.34	0.42
2:B:124:LEU:HD22	2:B:152:ILE:HG13	2.01	0.42
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.01	0.42
2:B:873:LEU:HD12	2:B:874:PRO:HD2	2.00	0.42
3:C:240:ARG:HB2	3:C:243:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.01	0.42
13:M:824:GLU:N	15:P:29:C:OP2	2.53	0.42
16:Q:496:SER:O	16:Q:500:SER:N	2.43	0.42
1:A:99:PHE:O	1:A:103:THR:OG1	2.30	0.42
1:A:873:VAL:HG23	1:A:1087:VAL:HG21	2.02	0.42
1:A:901:VAL:HA	1:A:980:PRO:HA	2.02	0.42
1:A:1525:TPO:O1P	13:M:1340:PHE:HB2	2.20	0.42
2:B:731:GLN:NE2	15:P:44:A:O3'	2.53	0.42
4:D:70:ARG:NH1	7:G:88:VAL:HG11	2.34	0.42
4:D:70:ARG:HH12	7:G:88:VAL:HG11	1.82	0.42
5:E:26:TYR:HA	5:E:64:HIS:HA	2.01	0.42
8:H:15:ILE:HD12	8:H:15:ILE:HA	1.97	0.42
20:W:189:HIS:CE1	20:W:215:LYS:HD2	2.53	0.42
1:A:279:LYS:HZ1	1:A:328:ALA:CB	2.33	0.42
1:A:313:HIS:HA	1:A:316:THR:HG22	2.01	0.42
2:B:581:GLU:OE2	2:B:585:ASN:ND2	2.52	0.42
20:W:65:LEU:HD12	20:W:85:ASP:HB3	2.02	0.42
1:A:769:MET:SD	2:B:973:PRO:HG3	2.60	0.42
1:A:1215:GLU:OE2	1:A:1256:VAL:HG22	2.20	0.42
2:B:770:ARG:NH1	2:B:771:GLU:HG3	2.34	0.42
23:Z:639:LYS:HB2	23:Z:642:HIS:CD2	2.52	0.42
1:A:253:LEU:HD11	1:A:317:MET:HE1	2.01	0.42
1:A:406:VAL:HG13	1:A:429:LEU:HD21	2.02	0.42
3:C:47:ILE:HG23	3:C:73:LEU:HD11	2.00	0.42
7:G:110:ARG:HG3	7:G:119:PHE:CZ	2.55	0.42
1:A:544:ALA:O	1:A:548:PHE:HB2	2.20	0.42
1:A:561:MET:HE3	1:A:561:MET:HB2	1.85	0.42
1:A:1180:ASN:ND2	1:A:1182:GLN:HE21	2.18	0.42
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.55	0.42
1:A:658:LEU:HD23	1:A:658:LEU:HA	1.88	0.42
5:E:24:ARG:NE	5:E:183:PHE:O	2.53	0.42
10:J:66:GLU:HG2	12:L:18:ILE:HD13	2.02	0.42
20:W:237:ASN:HB3	20:W:280:VAL:HG22	2.01	0.42
23:Z:212:ILE:HG22	23:Z:229:ALA:HB2	2.02	0.42
1:A:481:THR:HG22	2:B:1055:VAL:HG21	2.01	0.41
2:B:796:MET:HB2	2:B:948:GLN:HG2	2.02	0.41
2:B:801:VAL:HG13	2:B:929:PRO:HD2	2.02	0.41
2:B:870:THR:HA	2:B:891:ASP:HA	2.01	0.41
5:E:101:ARG:HD3	5:E:126:ILE:HG13	2.01	0.41
5:E:156:VAL:HG22	5:E:190:VAL:HG12	2.01	0.41
1:A:461:GLN:HG2	17:T:26:DG:H1'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:ARG:NE	1:A:1215:GLU:OE2	2.52	0.41
2:B:513:GLU:HG2	2:B:525:ASN:HD22	1.85	0.41
2:B:735:VAL:HG23	2:B:754:PRO:HG2	2.01	0.41
1:A:691:ASP:OD2	1:A:765:ASN:HB2	2.20	0.41
2:B:474:THR:OG1	2:B:732:ALA:O	2.33	0.41
1:A:1547:SEP:O	1:A:1547:SEP:OG	2.39	0.41
2:B:513:GLU:HG3	2:B:726:SER:HB3	2.03	0.41
2:B:601:VAL:HG22	2:B:616:THR:HG23	2.01	0.41
5:E:83:GLY:H	5:E:86:THR:HG1	1.66	0.41
1:A:59:ASP:HB3	1:A:62:GLN:HB2	2.02	0.41
17:T:27:DT:H2'	17:T:28:DG:H8	1.85	0.41
1:A:876:ASP:HB2	1:A:878:THR:HG22	2.02	0.41
1:A:1117:VAL:HG23	1:A:1119:LEU:HG	2.03	0.41
13:M:749:LEU:O	13:M:753:LEU:N	2.54	0.41
16:Q:757:VAL:HA	16:Q:796:LEU:HD12	2.01	0.41
20:W:146:THR:HG22	20:W:182:LEU:HD22	2.03	0.41
1:A:505:LEU:HD12	1:A:506:PRO:HD2	2.03	0.41
1:A:1157:ILE:HD12	1:A:1160:ARG:HH11	1.85	0.41
1:A:1347:LEU:HB3	5:E:137:ILE:HD12	2.03	0.41
1:A:1547:SEP:HA	1:A:1548:PRO:HD3	1.74	0.41
2:B:67:LEU:HD11	2:B:416:ARG:HG3	2.02	0.41
16:Q:763:ARG:NH1	20:W:65:LEU:HD11	2.34	0.41
1:A:126:ILE:HD11	1:A:147:LEU:HD22	2.02	0.41
1:A:935:GLN:HB2	1:A:938:LEU:HD13	2.03	0.41
1:A:1132:LYS:HE3	1:A:1363:VAL:HG11	2.03	0.41
1:A:1307:VAL:HG13	1:A:1338:THR:HG22	2.02	0.41
2:B:903:ILE:O	2:B:924:ARG:N	2.54	0.41
7:G:93:ASN:HB3	7:G:96:GLY:H	1.85	0.41
23:Z:420:PHE:CD1	23:Z:470:LYS:HE3	2.56	0.41
1:A:610:PRO:HG2	1:A:613:GLU:HB2	2.03	0.41
2:B:807:ARG:NH1	3:C:66:HIS:CD2	2.89	0.41
3:C:84:TYR:CZ	3:C:167:LYS:HE3	2.56	0.41
4:D:111:SER:HB2	4:D:131:LEU:HD21	2.02	0.41
1:A:983:LEU:HD23	1:A:983:LEU:HA	1.89	0.41
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	2.02	0.41
2:B:956:PHE:HB3	2:B:962:THR:HG22	2.03	0.41
4:D:104:CYS:SG	4:D:135:GLN:NE2	2.93	0.41
1:A:141:LEU:HD13	1:A:1445:HIS:HE1	1.86	0.40
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.57	0.40
1:A:1546:PHE:HB3	13:M:1515:TYR:CE1	2.56	0.40
2:B:556:ILE:H	2:B:556:ILE:HG13	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:561:ILE:HD11	2:B:573:TRP:HH2	1.86	0.40
3:C:13:GLU:HB3	3:C:20:LYS:HB3	2.02	0.40
1:A:1533:PRO:HD3	13:M:1471:LYS:HZ3	1.86	0.40
2:B:86:LEU:HD23	2:B:130:LYS:HB3	2.03	0.40
3:C:189:ASP:O	3:C:191:ALA:N	2.55	0.40
16:Q:390:ASP:O	16:Q:394:ARG:N	2.53	0.40
1:A:859:TYR:OH	1:A:1433:GLU:OE2	2.30	0.40
8:H:71:ASP:OD1	8:H:71:ASP:N	2.53	0.40
12:L:16:ILE:HG12	12:L:27:GLU:HG2	2.03	0.40
20:W:233:SER:OG	20:W:234:TRP:N	2.52	0.40
1:A:73:THR:OG1	1:A:74:CYS:N	2.52	0.40
2:B:998:ASP:OD2	2:B:1000:THR:HG22	2.21	0.40
1:A:54:LEU:CB	1:A:61:ARG:HH12	2.31	0.40
1:A:863:ARG:NH1	1:A:1129:ASN:HD21	2.19	0.40
1:A:1296:MET:HE2	1:A:1296:MET:HB3	1.93	0.40
1:A:1375:ARG:HH12	5:E:195:ARG:HH22	1.69	0.40
23:Z:427:GLU:OE2	23:Z:469:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1425/1970 (72%)	1340 (94%)	82 (6%)	3 (0%)	43	73
2	B	1122/1174 (96%)	1062 (95%)	59 (5%)	1 (0%)	48	78
3	C	259/275 (94%)	245 (95%)	14 (5%)	0	100	100
4	D	124/142 (87%)	122 (98%)	2 (2%)	0	100	100
5	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	24	57
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
7	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	146/150 (97%)	135 (92%)	11 (8%)	0	100	100
9	I	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	44/58 (76%)	38 (86%)	6 (14%)	0	100	100
13	M	970/1726 (56%)	918 (95%)	52 (5%)	0	100	100
16	Q	581/1178 (49%)	555 (96%)	25 (4%)	1 (0%)	43	73
20	W	298/305 (98%)	278 (93%)	20 (7%)	0	100	100
22	Y	114/121 (94%)	114 (100%)	0	0	100	100
23	Z	476/1087 (44%)	466 (98%)	9 (2%)	1 (0%)	43	73
All	All	6308/9004 (70%)	5995 (95%)	306 (5%)	7 (0%)	49	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	57	ASP
1	A	911	PRO
2	B	492	ASP
1	A	540	ASP
23	Z	506	LEU
1	A	121	SER
16	Q	301	VAL

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	1257/1747 (72%)	1249 (99%)	8 (1%)	78	83
2	B	992/1027 (97%)	988 (100%)	4 (0%)	84	86
3	C	240/252 (95%)	237 (99%)	3 (1%)	61	77
4	D	109/126 (86%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	70 (99%)	1 (1%)	59	76
7	G	146/153 (95%)	144 (99%)	2 (1%)	59	76
8	H	129/131 (98%)	127 (98%)	2 (2%)	55	75
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	103 (99%)	1 (1%)	68	79
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	154/1514 (10%)	153 (99%)	1 (1%)	78	83
16	Q	121/752 (16%)	120 (99%)	1 (1%)	73	81
20	W	255/260 (98%)	254 (100%)	1 (0%)	84	86
22	Y	102/105 (97%)	102 (100%)	0	100	100
23	Z	427/940 (45%)	427 (100%)	0	100	100
All	All	4502/7639 (59%)	4478 (100%)	24 (0%)	78	85

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	309	LEU
1	A	655	ILE
1	A	744	ILE
1	A	760	LEU
1	A	1166	LEU
1	A	1235	ILE
1	A	1382	LEU
2	B	128	ILE
2	B	556	ILE
2	B	612	ILE
2	B	896	LEU
3	C	11	ILE
3	C	128	ILE
3	C	263	LEU
6	F	123	LEU
7	G	48	VAL
7	G	108	ILE
8	H	96	VAL

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Mol	Chain	Res	Type
8	H	143	LEU
11	K	21	ILE
13	M	1515	TYR
16	Q	776	LEU
20	W	154	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	ASN
1	A	410	ASN
1	A	504	HIS
1	A	704	ASN
1	A	711	GLN
1	A	757	GLN
1	A	861	GLN
1	A	884	ASN
1	A	904	GLN
1	A	926	ASN
1	A	935	GLN
1	A	995	HIS
1	A	1005	HIS
1	A	1032	GLN
1	A	1044	HIS
1	A	1082	HIS
1	A	1093	GLN
1	A	1129	ASN
1	A	1182	GLN
1	A	1194	ASN
1	A	1220	HIS
1	A	1248	ASN
1	A	1332	GLN
1	A	1457	ASN
2	B	23	GLN
2	B	98	HIS
2	B	460	HIS
2	B	471	ASN
2	B	582	GLN
2	B	654	GLN
2	B	725	GLN
2	B	777	ASN
2	B	797	ASN

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Mol	Chain	Res	Type
2	B	1040	GLN
2	B	1053	HIS
2	B	1101	GLN
2	B	1120	ASN
2	B	1133	HIS
3	C	66	HIS
3	C	83	GLN
3	C	145	GLN
3	C	157	GLN
3	C	232	ASN
4	D	129	GLN
4	D	135	GLN
5	E	71	GLN
5	E	95	GLN
5	E	189	GLN
7	G	14	HIS
7	G	53	ASN
7	G	60	GLN
7	G	93	ASN
13	M	1365	ASN
13	M	1514	HIS
16	Q	756	ASN
16	Q	775	ASN
16	Q	781	ASN
16	Q	834	GLN
20	W	13	GLN
20	W	98	GLN
20	W	173	ASN
20	W	184	HIS
20	W	189	HIS
20	W	221	HIS
20	W	223	ASN
20	W	273	HIS
20	W	274	GLN
22	Y	12	HIS
22	Y	45	ASN
23	Z	272	ASN
23	Z	519	GLN
23	Z	534	HIS
23	Z	616	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/46 (43%)	8 (40%)	3 (15%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	27	A
15	P	29	C
15	P	30	C
15	P	31	G
15	P	33	A
15	P	36	G
15	P	37	G
15	P	39	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	36	G
15	P	38	G

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	1525	1	8,10,11	1.58	1 (12%)	10,14,16	2.25	1 (10%)
1	SEP	A	1547	13,1	8,9,10	1.75	3 (37%)	7,12,14	1.15	1 (14%)

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
1	TPO	A	1525	1	-	0/9/11/13	-
1	SEP	A	1547	13,1	-	2/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.73	1.62	1.50
1	A	1525	TPO	P-O1P	3.39	1.61	1.50
1	A	1547	SEP	P-O2P	2.09	1.62	1.54
1	A	1547	SEP	P-O3P	2.07	1.62	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	P-OG1-CB	-6.70	105.11	123.33
1	A	1547	SEP	OG-CB-CA	2.46	110.53	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1547	SEP	N-CA-CB-OG
1	A	1547	SEP	C-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1525	TPO	1	0
1	A	1547	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	U	3
19	V	3
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	492:UNK	C	498:UNK	N	29.01
1	V	293:UNK	C	307:UNK	N	14.62
1	U	429:UNK	C	448:UNK	N	12.83
1	V	227:UNK	C	250:UNK	N	9.56
1	V	260:UNK	C	285:UNK	N	6.58
1	M	1334:UNK	C	1338:ILE	N	6.19
1	U	397:UNK	C	416:UNK	N	3.22

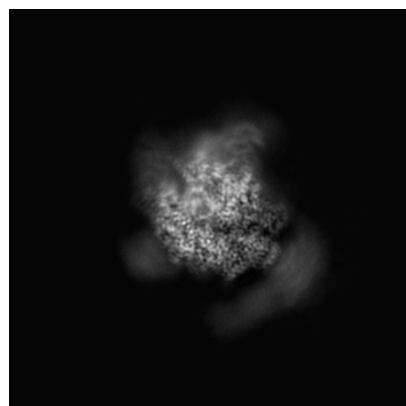
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0031. These allow visual inspection of the internal detail of the map and identification of artifacts.

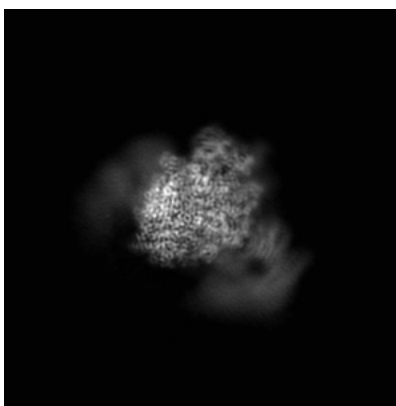
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

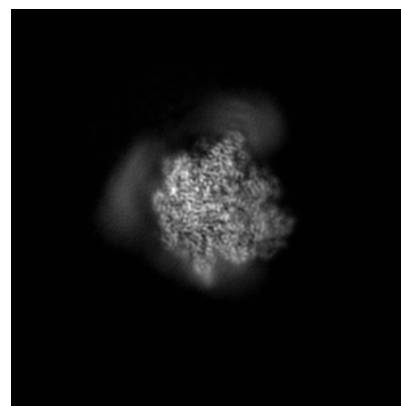
6.1.1 Primary map



X

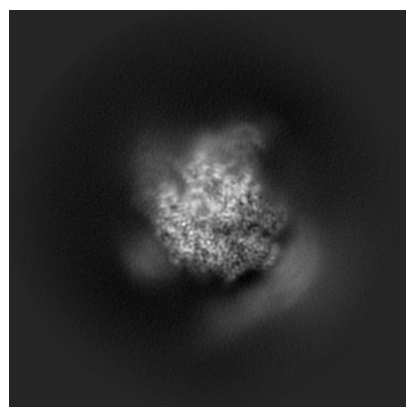


Y

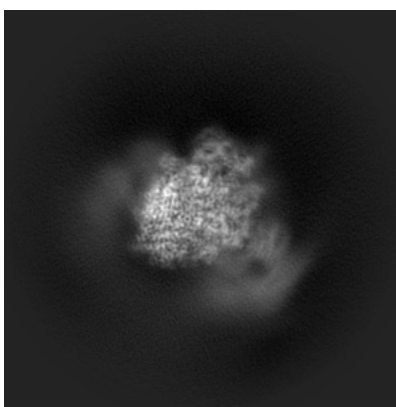


Z

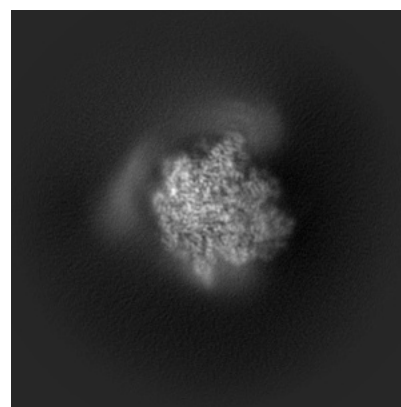
6.1.2 Raw map



X



Y

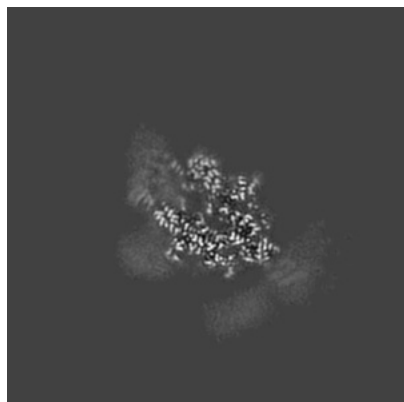


Z

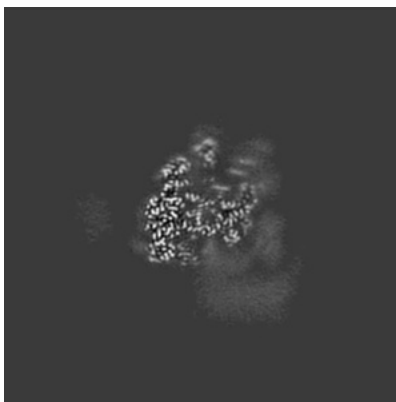
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

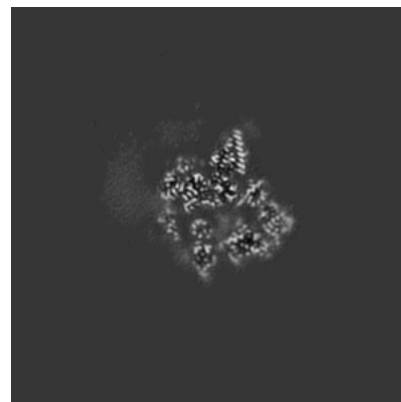
6.2.1 Primary map



X Index: 180

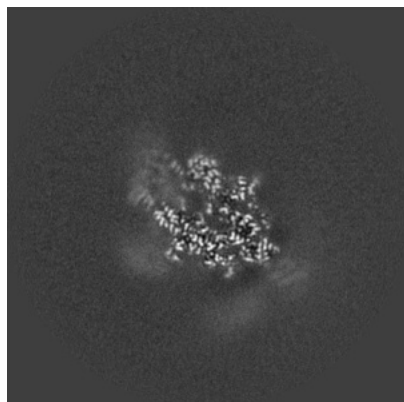


Y Index: 180

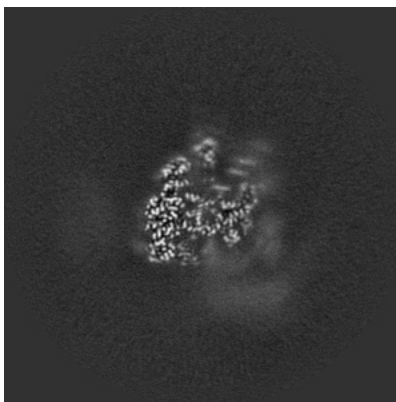


Z Index: 180

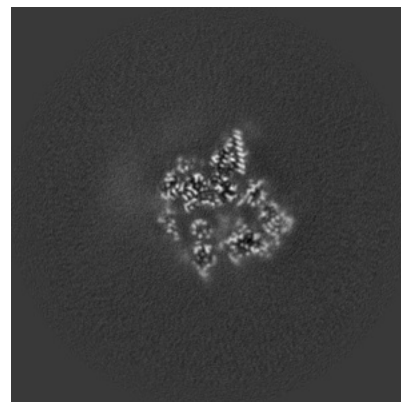
6.2.2 Raw map



X Index: 180



Y Index: 180

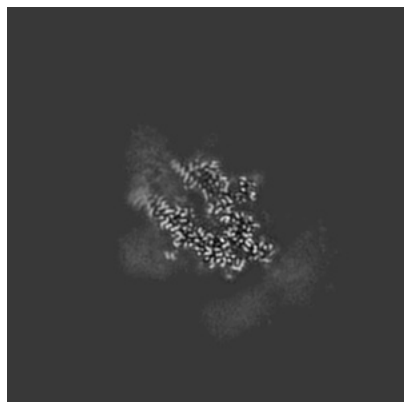


Z Index: 180

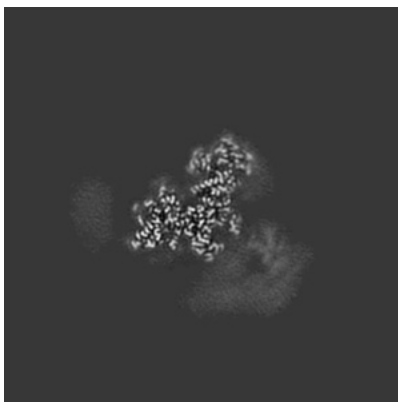
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

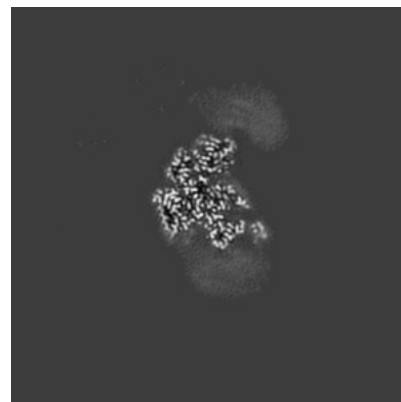
6.3.1 Primary map



X Index: 177

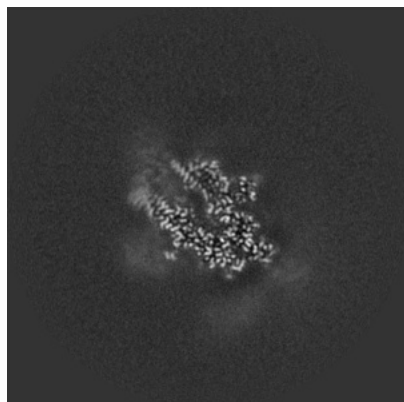


Y Index: 198

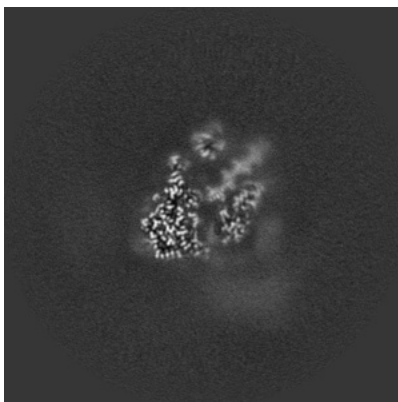


Z Index: 143

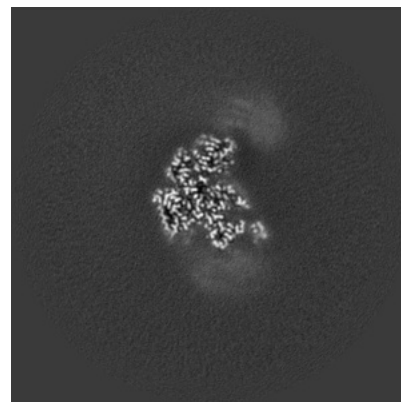
6.3.2 Raw map



X Index: 177



Y Index: 173

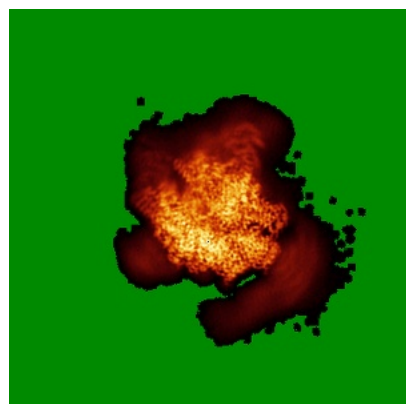


Z Index: 143

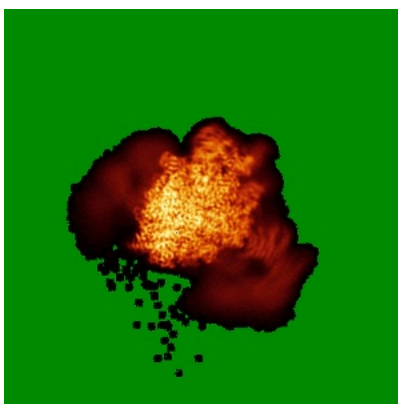
The images above show the largest variance slices of the map in three orthogonal directions.

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

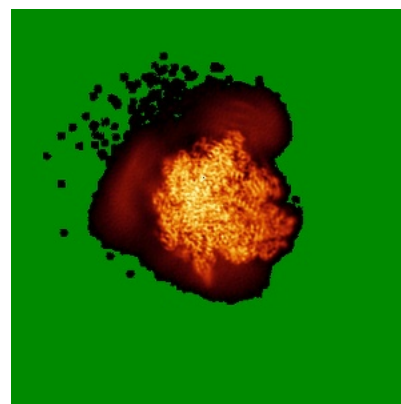
6.4.1 Primary map



X

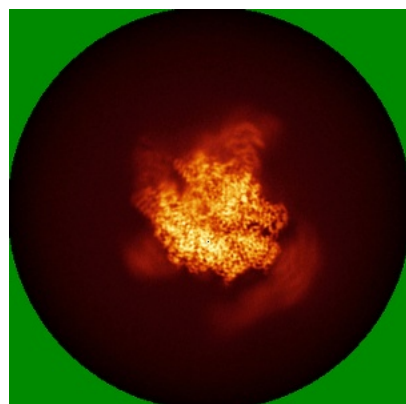


Y

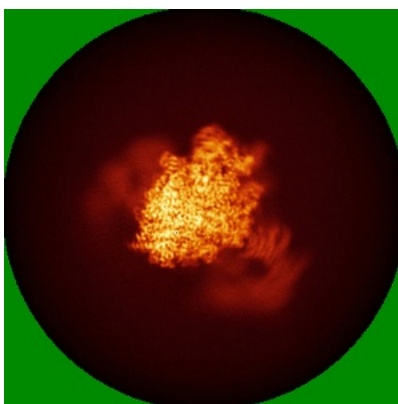


Z

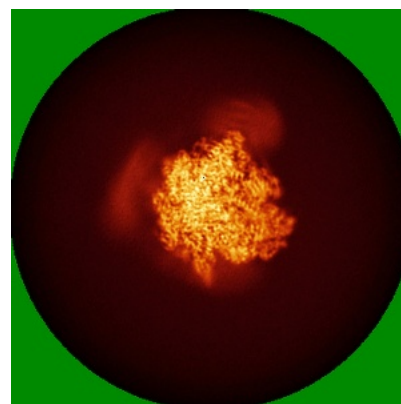
6.4.2 Raw map



X



Y



Z

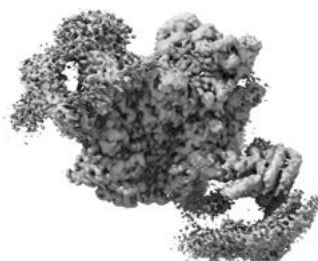
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.0157. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

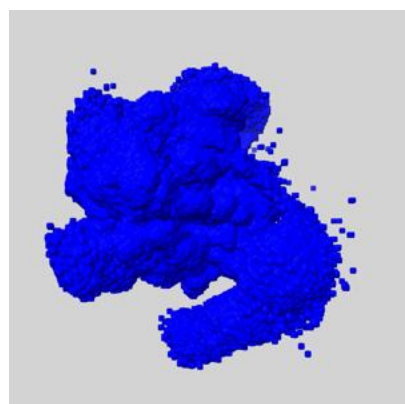
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

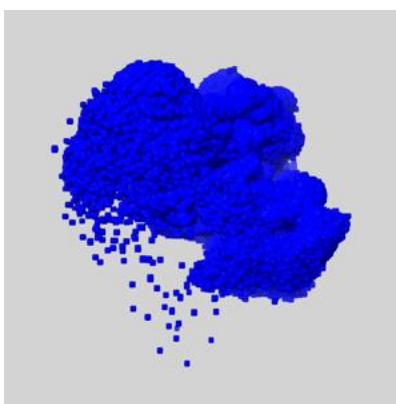
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

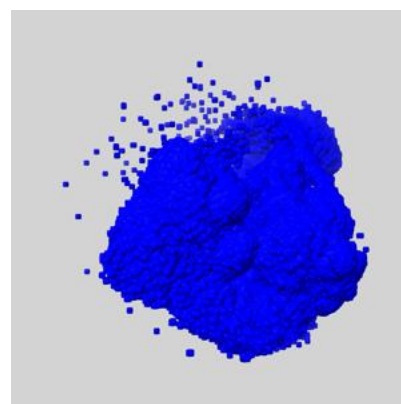
6.6.1 emd_0031_msk_1.map [i](#)



X



Y

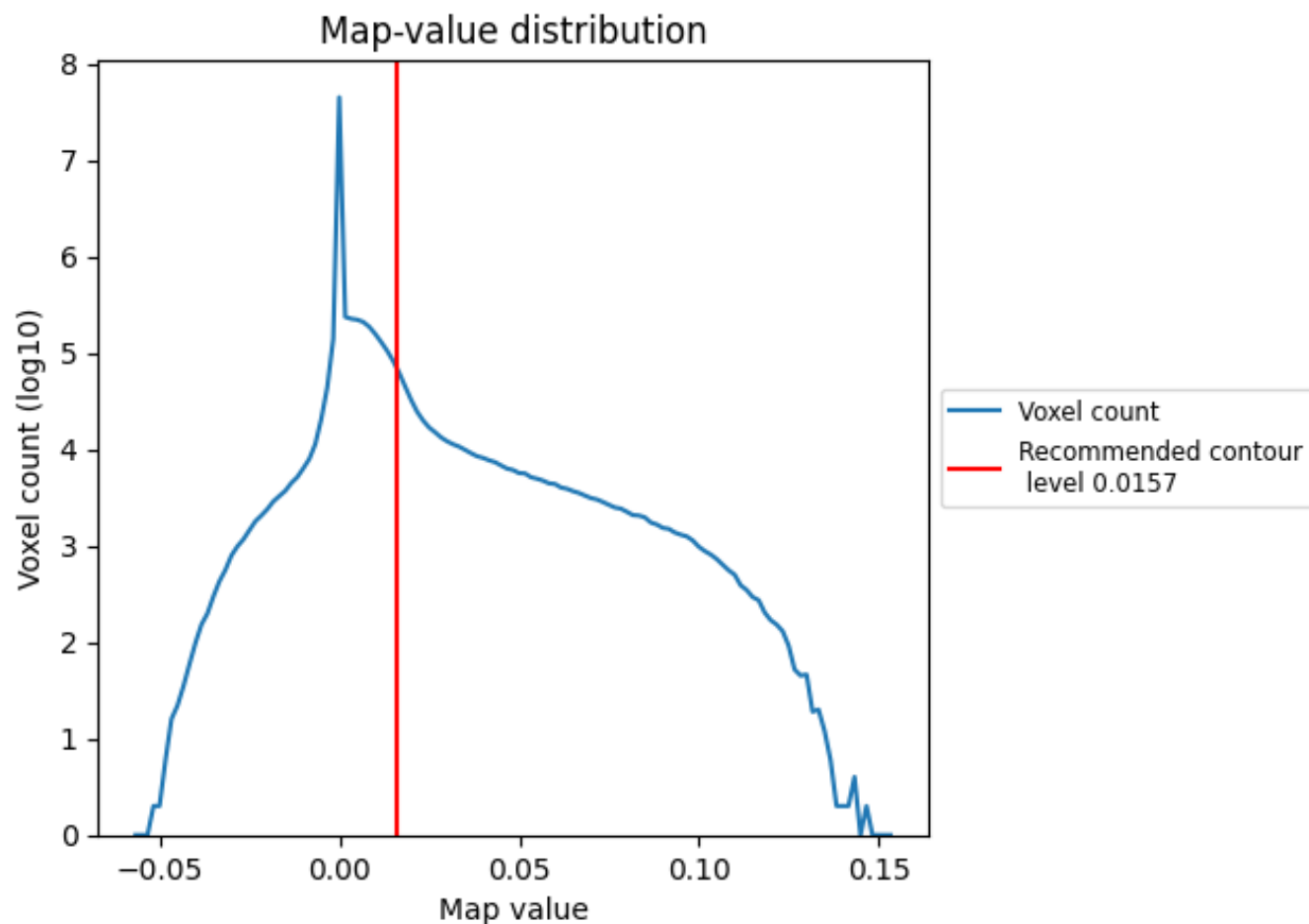


Z

7 Map analysis [i](#)

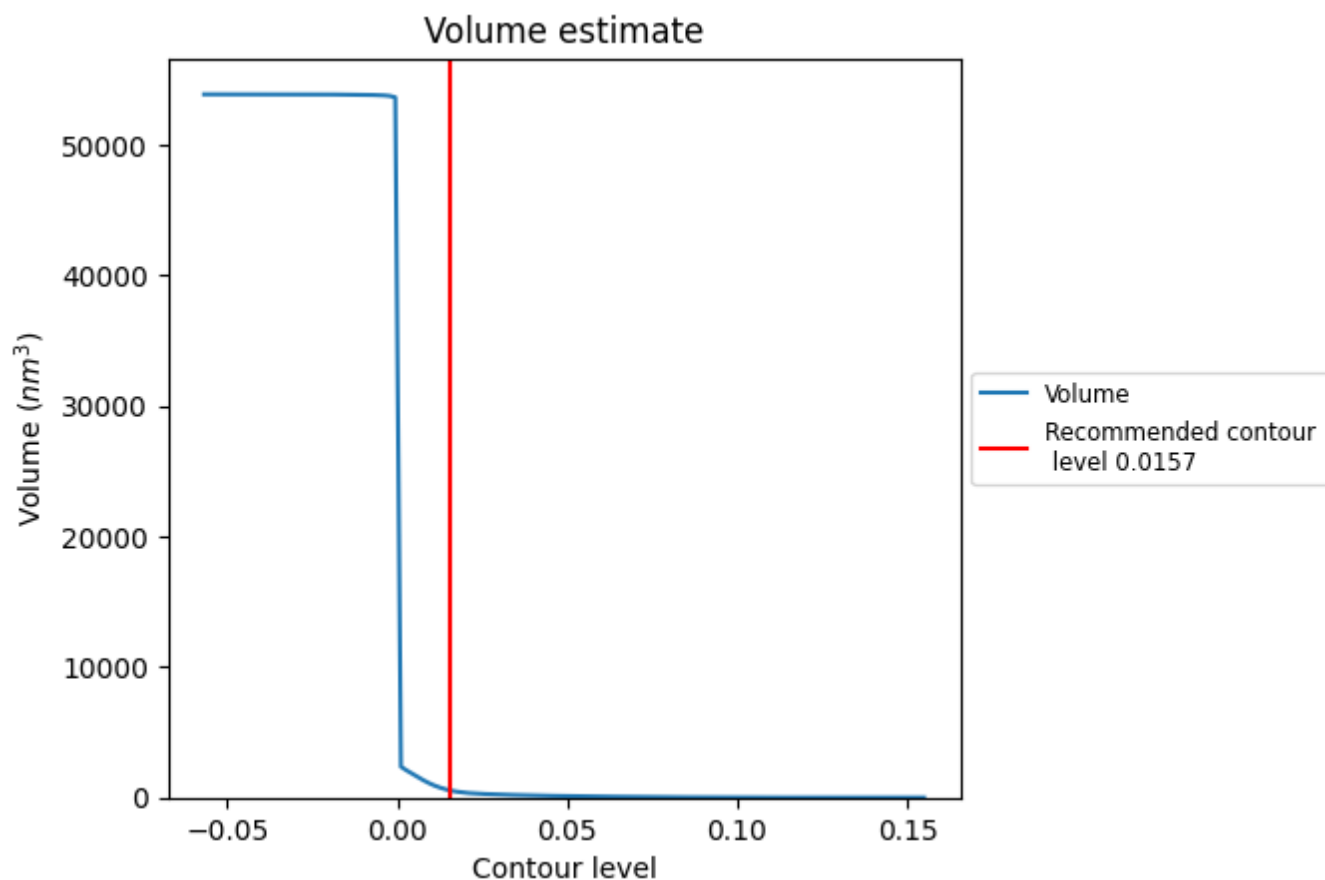
This section contains the results of statistical analysis of the map.

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.

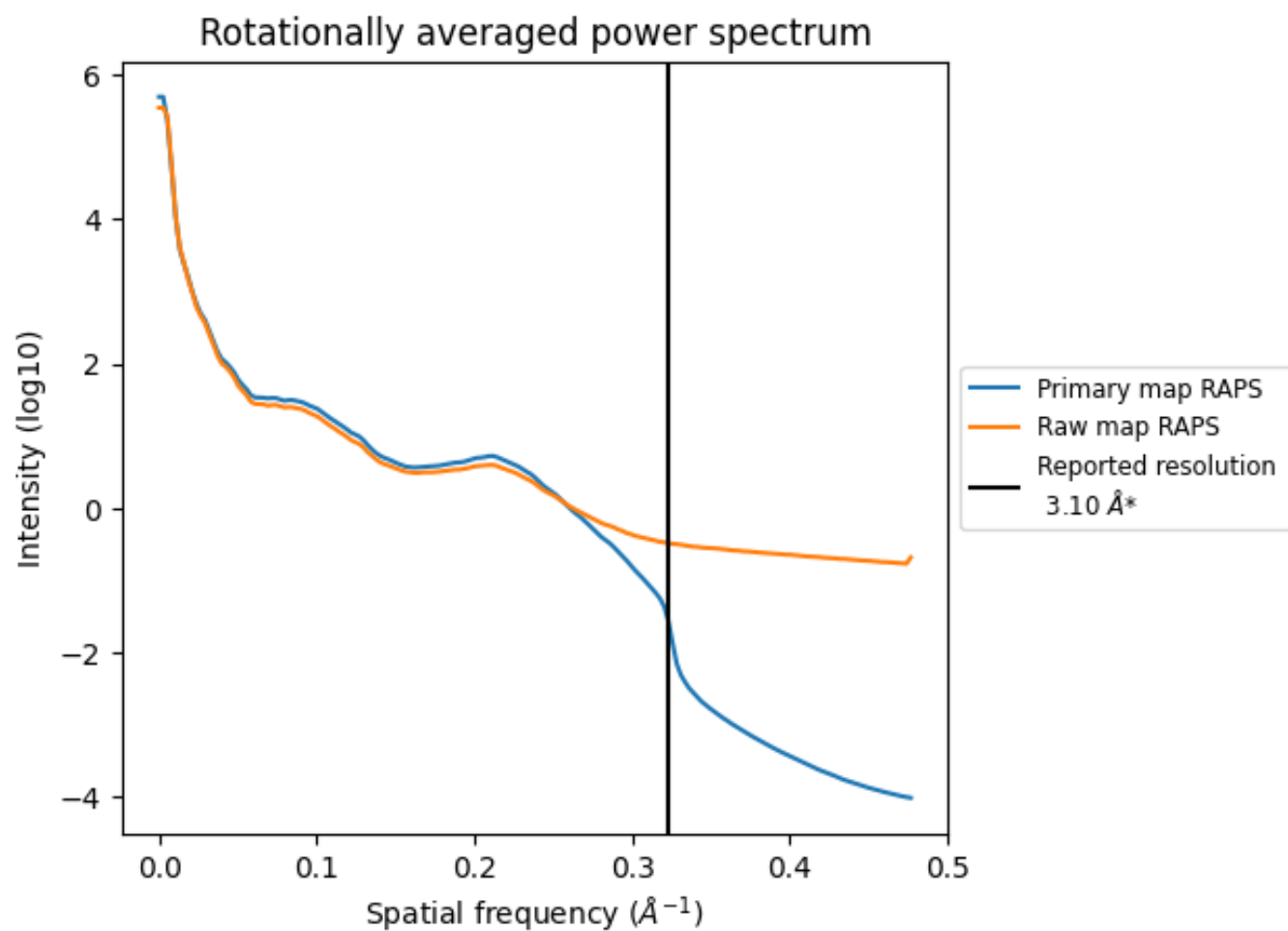
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 541 nm³; this corresponds to an approximate mass of 489 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 ⓘ

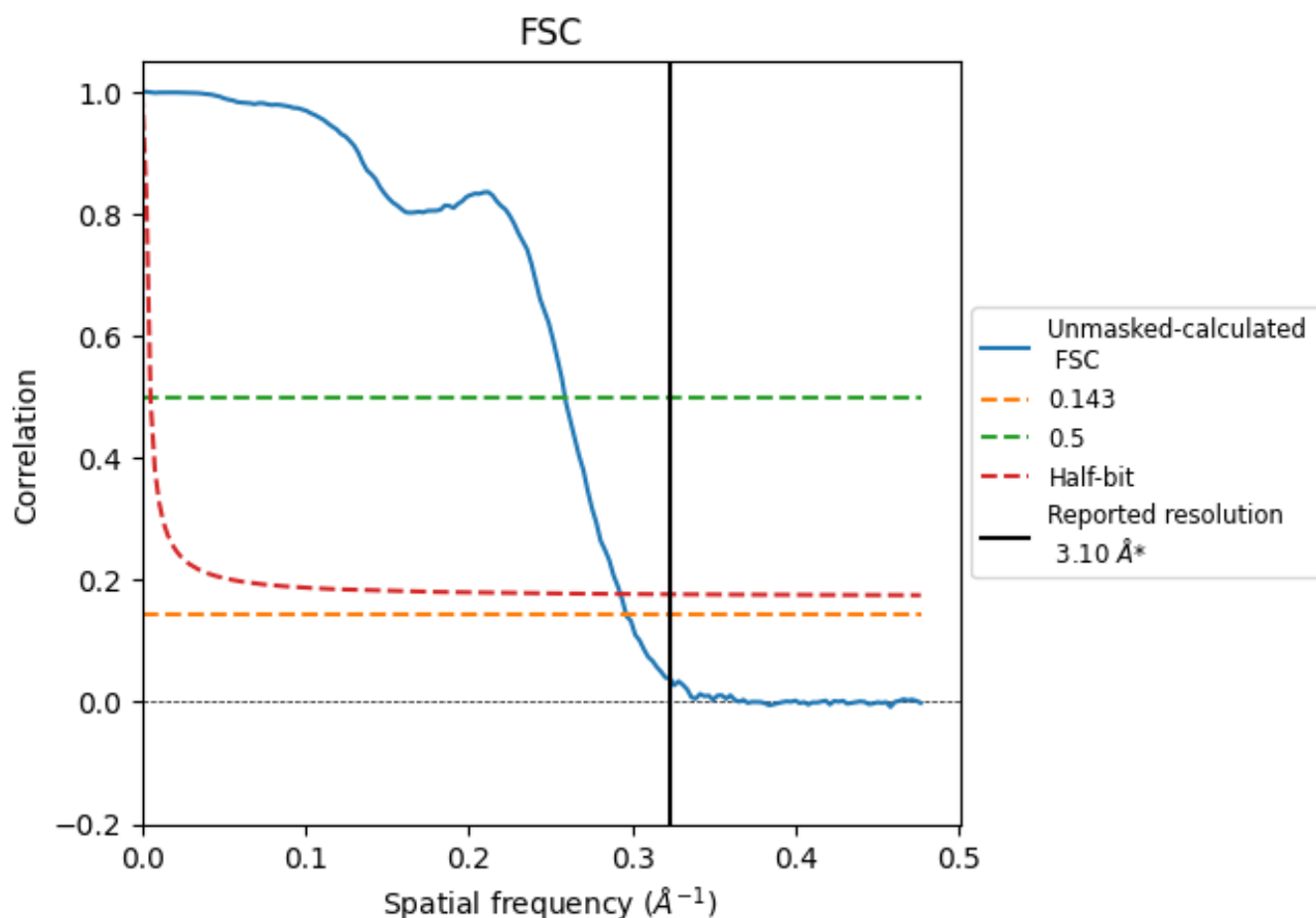


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

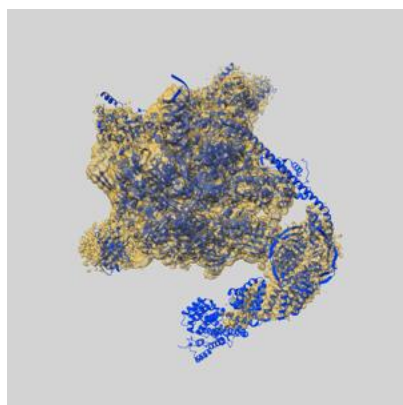
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	3.86	3.42

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

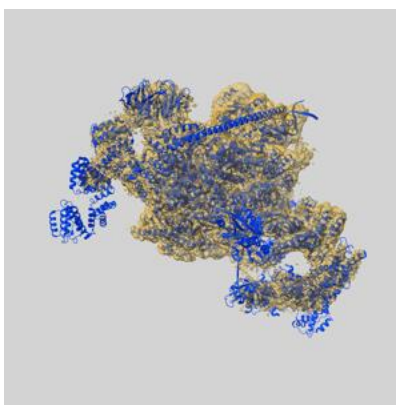
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0031 and PDB model 6GMH. Per-residue inclusion information can be found in section [3](#) on page [9](#).

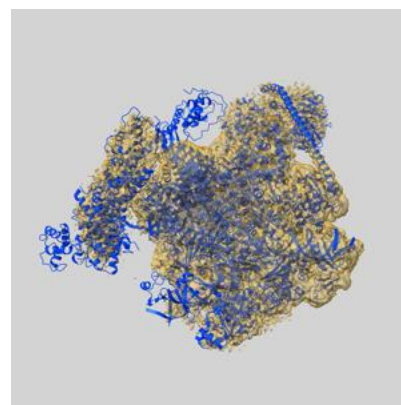
9.1 Map-model overlay [i](#)



X



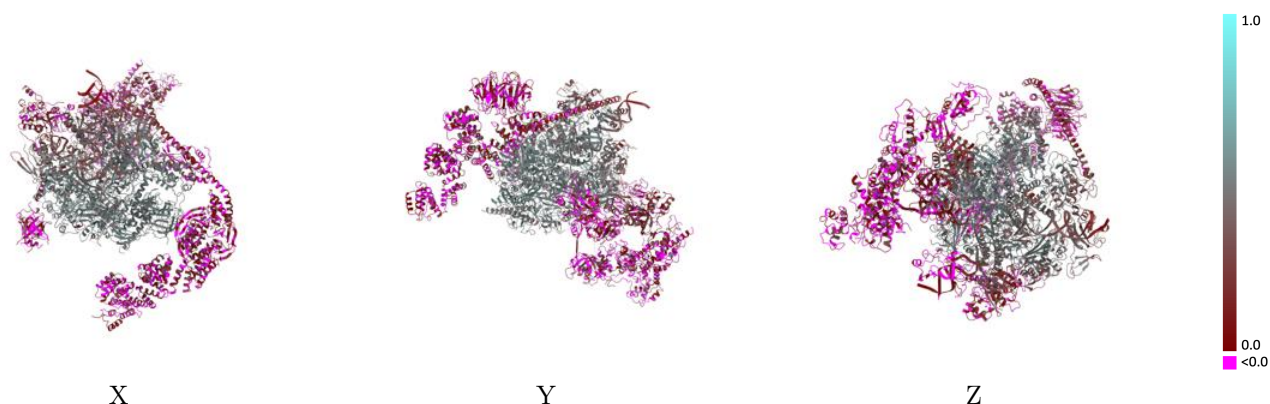
Y



Z

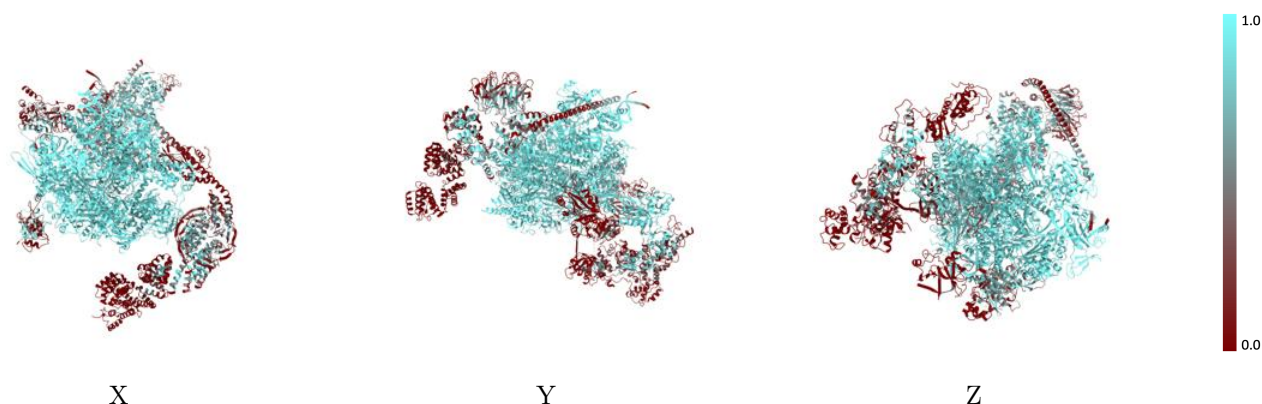
The images above show the 3D surface view of the map at the recommended contour level 0.0157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



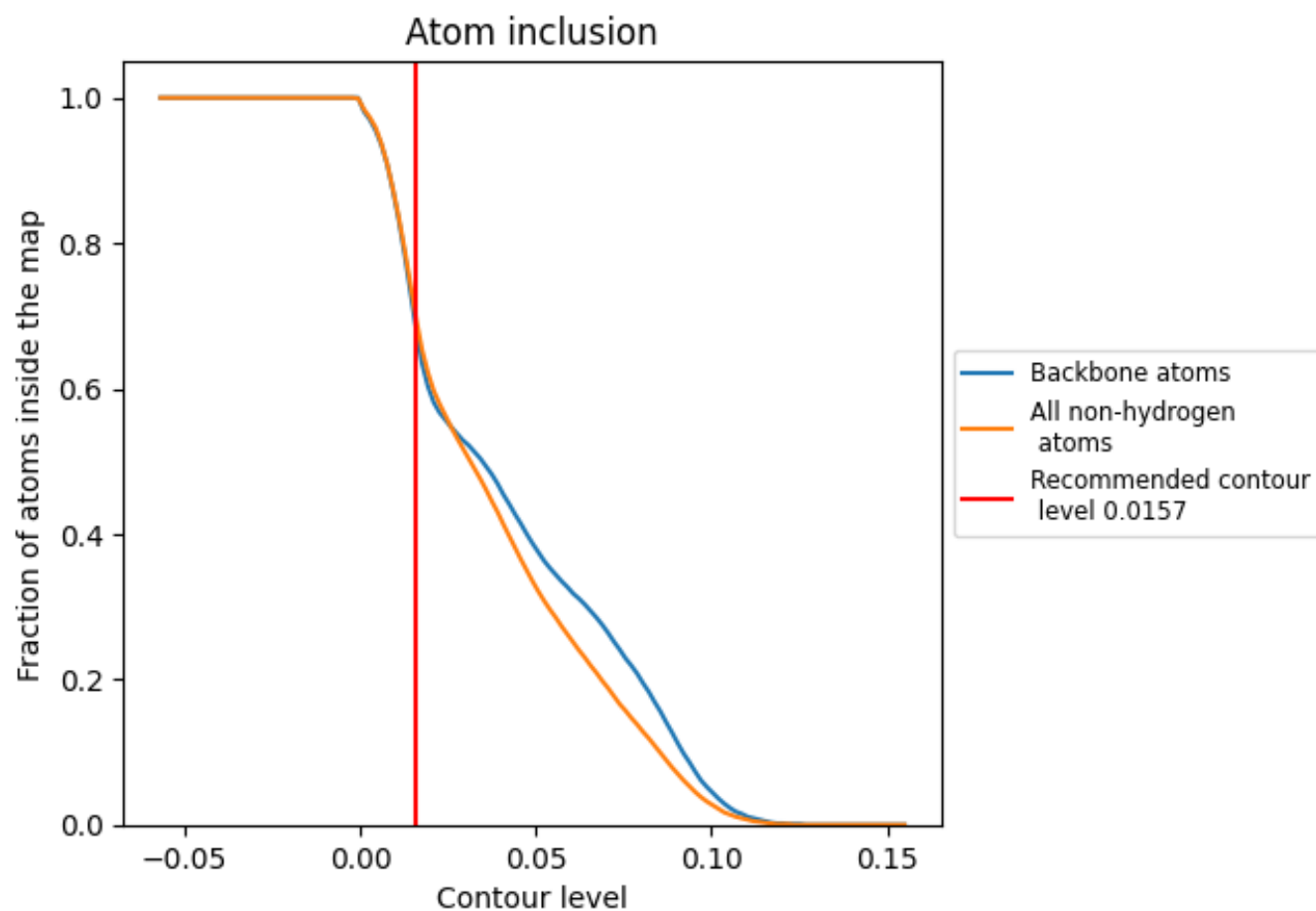
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0157).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 70% 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 (0.0157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7030	 0.3240
A	 0.9290	 0.4710
B	 0.9540	 0.4950
C	 0.9460	 0.5090
D	 0.8230	 0.2100
E	 0.9540	 0.4400
F	 0.9330	 0.5000
G	 0.8430	 0.2540
H	 0.9280	 0.4960
I	 0.9400	 0.4270
J	 0.9600	 0.5360
K	 0.9620	 0.5230
L	 0.9410	 0.4820
M	 0.1680	 0.0280
N	 0.8370	 0.2560
P	 0.7010	 0.2670
Q	 0.2770	 0.0810
T	 0.8400	 0.3330
U	 0.3480	 0.0230
V	 0.4380	 0.0630
W	 0.3520	 0.0410
X	 0.5710	 0.1690
Y	 0.2040	 0.1250
Z	 0.3030	 0.1100

