



Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 09:03 PM JST

PDB ID : 8XI2
EMDB ID : EMD-38362
Title : Cryo-EM structure of the Chlamydomonas C* complex
Authors : Lu, Y.; Zhan, X.
Deposited on : 2023-12-19
Resolution : 2.60 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:

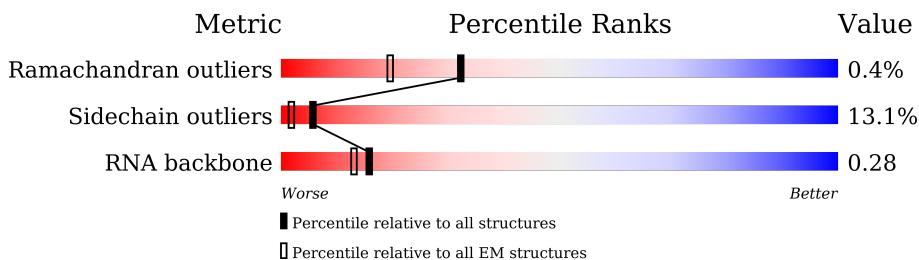
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 2.60 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.








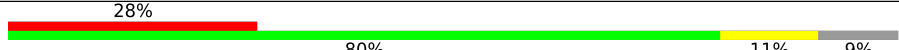
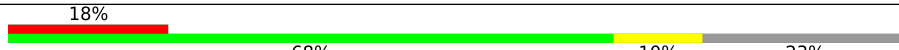

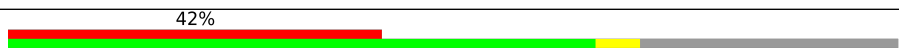




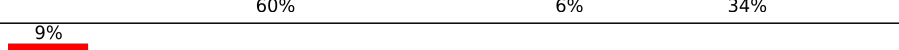
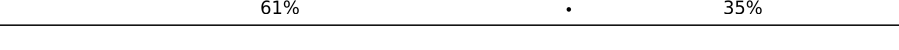
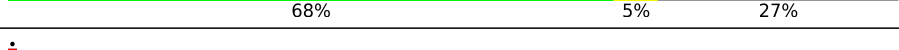


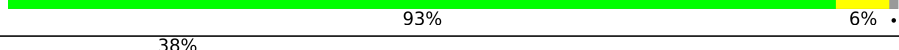

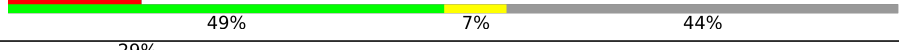
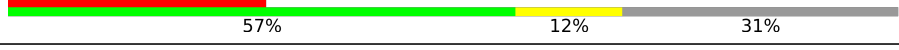
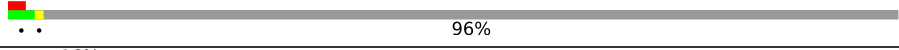


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2398	
2	B	111	
3	C	989	
4	E	362	
5	F	101	
6	q	503	
6	r	503	
6	s	503	


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Mol	Chain	Length	Quality of chain
6	t	503	
7	a	127	
8	g	77	
9	e	87	
10	f	85	
11	d	110	
12	c	114	
13	b	265	
14	I	925	
15	J	835	
16	P	235	
17	M	563	
18	T	518	
19	O	417	
20	N	233	
21	R	684	
22	H	192	
23	S	157	
24	W	576	
25	L	833	
26	K	303	
27	U	721	
28	V	928	
29	Q	1844	
30	5	7	

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Mol	Chain	Length	Quality of chain
31	3	173	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment labeled '6%', a green segment labeled '8%', a yellow segment labeled '9%', and a grey segment labeled '80%'. The segments are arranged from left to right in the order: 6%, 8%, 9%, 80%.</p>

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 73326 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 MPN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1931	15194	9743	2699	2682	70	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	86	1817	812	307	612	86	0	0

- Molecule 3 is a protein called Elongation factor Tu, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	897	6973	4431	1203	1297	42	0	0

- Molecule 4 is a protein called U5-40K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	318	2441	1524	436	465	16	0	0

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	F	92	1985	885	369	637	94	0	0

- Molecule 6 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	q	106	831	522	145	160	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	r	131	Total	C	N	O	S	0	0
			1021	638	183	196	4		
6	s	70	Total	C	N	O	S	0	0
			570	353	108	107	2		
6	t	62	Total	C	N	O	S	0	0
			504	312	95	96	1		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	90	Total	C	N	O	S	0	0
			705	444	129	126	6		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	65	Total	C	N	O	S	0	0
			512	323	90	96	3		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	80	Total	C	N	O	S	0	0
			660	420	117	119	4		

- Molecule 10 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	71	Total	C	N	O	S	0	0
			559	358	91	106	4		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	100	Total	C	N	O	S	0	0
			810	505	152	147	6		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	88	Total	C	N	O	S	0	0
			684	435	121	124	4		

- Molecule 13 is a protein called Sm domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	99	Total	C	N	O	S	0	0
			780	489	149	138	4		

- Molecule 14 is a protein called Syf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	661	Total	C	N	O	S	0	0
			4629	2900	855	861	13		

- Molecule 15 is a protein called Crooked neck protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	595	Total	C	N	O	S	0	0
			4033	2511	759	753	10		

- Molecule 16 is a protein called Cwf15/Cwc15 cell cycle control protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	104	Total	C	N	O	0	0
			867	536	175	156		

- Molecule 17 is a protein called PPIase cyclophilin-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	80	Total	C	N	O	S	0	0
			644	402	121	120	1		

- Molecule 18 is a protein called PLRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	344	Total	C	N	O	S	0	0
			2700	1705	488	490	17		

- Molecule 19 is a protein called Rbm22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	O	273	2136	1337	376	405	18	0	0

- Molecule 20 is a protein called G10 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	171	1412	897	260	248	7	0	0

- Molecule 21 is a protein called SKI-interacting protein SKIP SNW domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
21	R	260	1994	1251	361	377	2	3	0	0

- Molecule 22 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	H	40	838	375	134	289	40		0

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	S	155	1198	754	213	225	6		0

- Molecule 24 is a protein called Prp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	487	2826	1721	553	549	3		0

- Molecule 25 is a protein called Cdc5L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	L	468	3795	2349	722	712	12		0

- Molecule 26 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	K	210	Total	C	N	O	S	0	0
			1688	1045	318	321	4		

- Molecule 27 is a protein called CWF21 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	26	Total	C	N	O	S	0	0
			191	119	34	36	2		

- Molecule 28 is a protein called MI domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	186	Total	C	N	O	S	0	0
			1020	621	198	200	1		

- Molecule 29 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Q	1299	Total	C	N	O	0	0
			6423	3825	1299	1299		

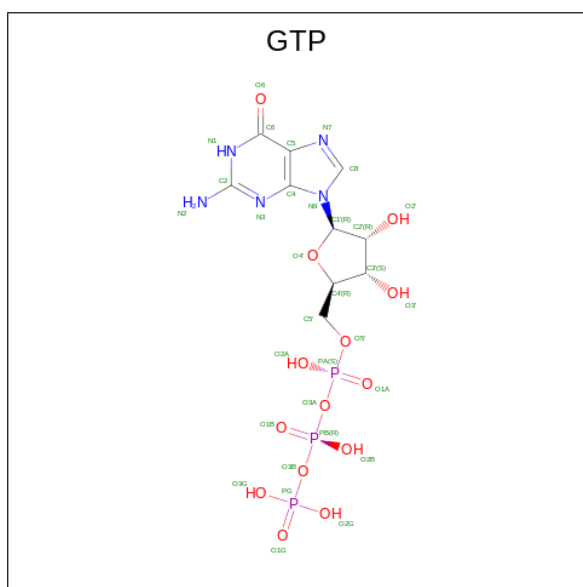
- Molecule 30 is a RNA chain called RNA (5'-R(P*CP*CP*GP*AP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	7	Total	C	N	O	P	0	0
			150	67	29	47	7		

- Molecule 31 is a RNA chain called RNA (173-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	3	34	Total	C	N	O	P	0	0
			694	311	111	238	34		

- Molecule 32 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



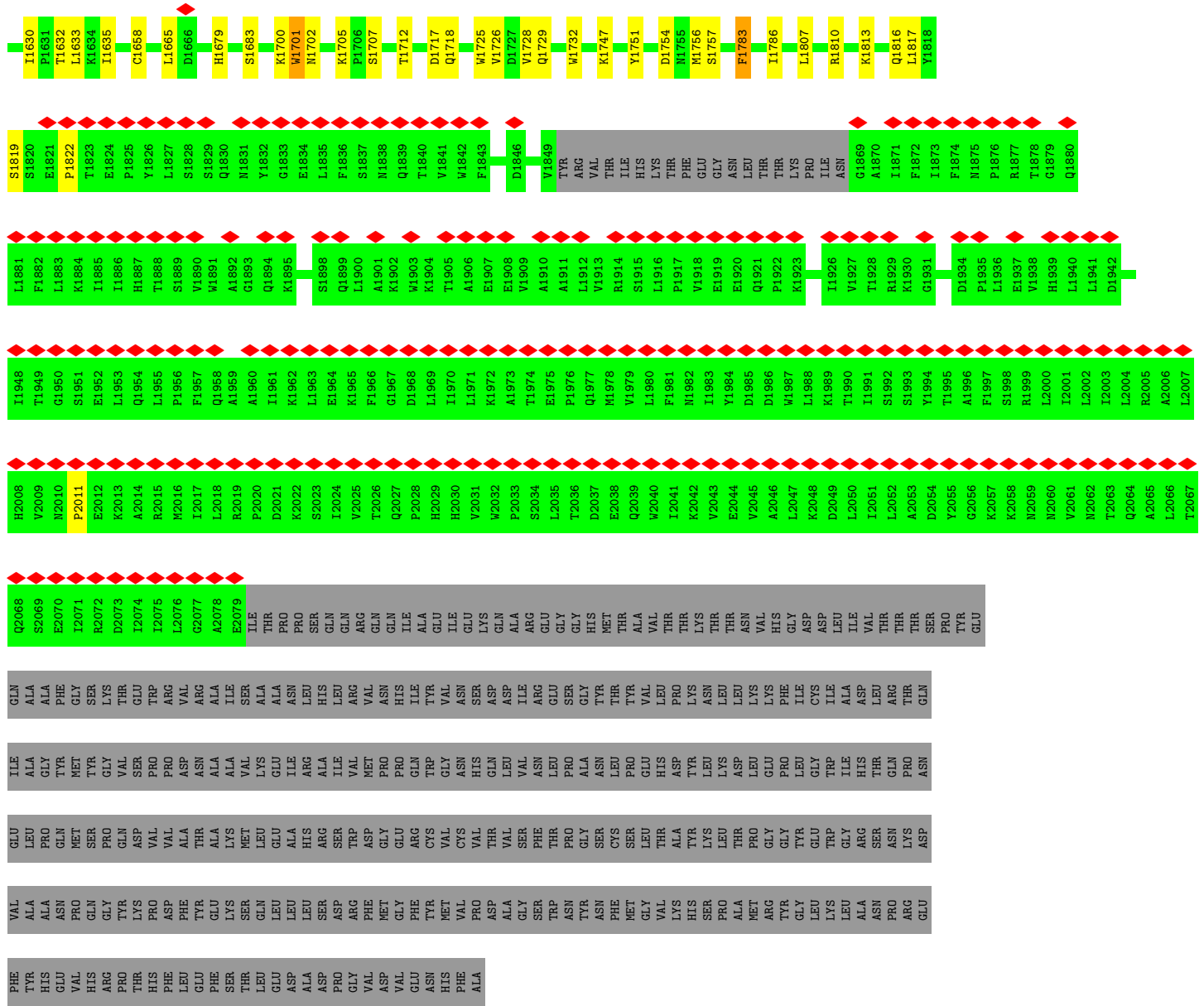
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
32	C	1	32	10	5	14	3	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

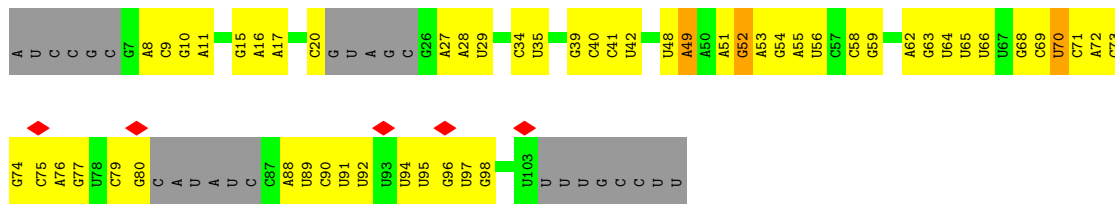
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
33	C	1	1	1	0
33	F	6	6	6	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

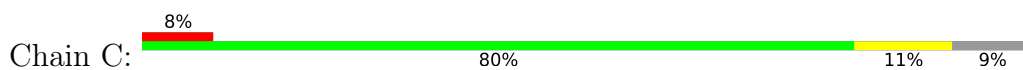
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
34	O	2	2	2	0
34	N	1	1	1	0

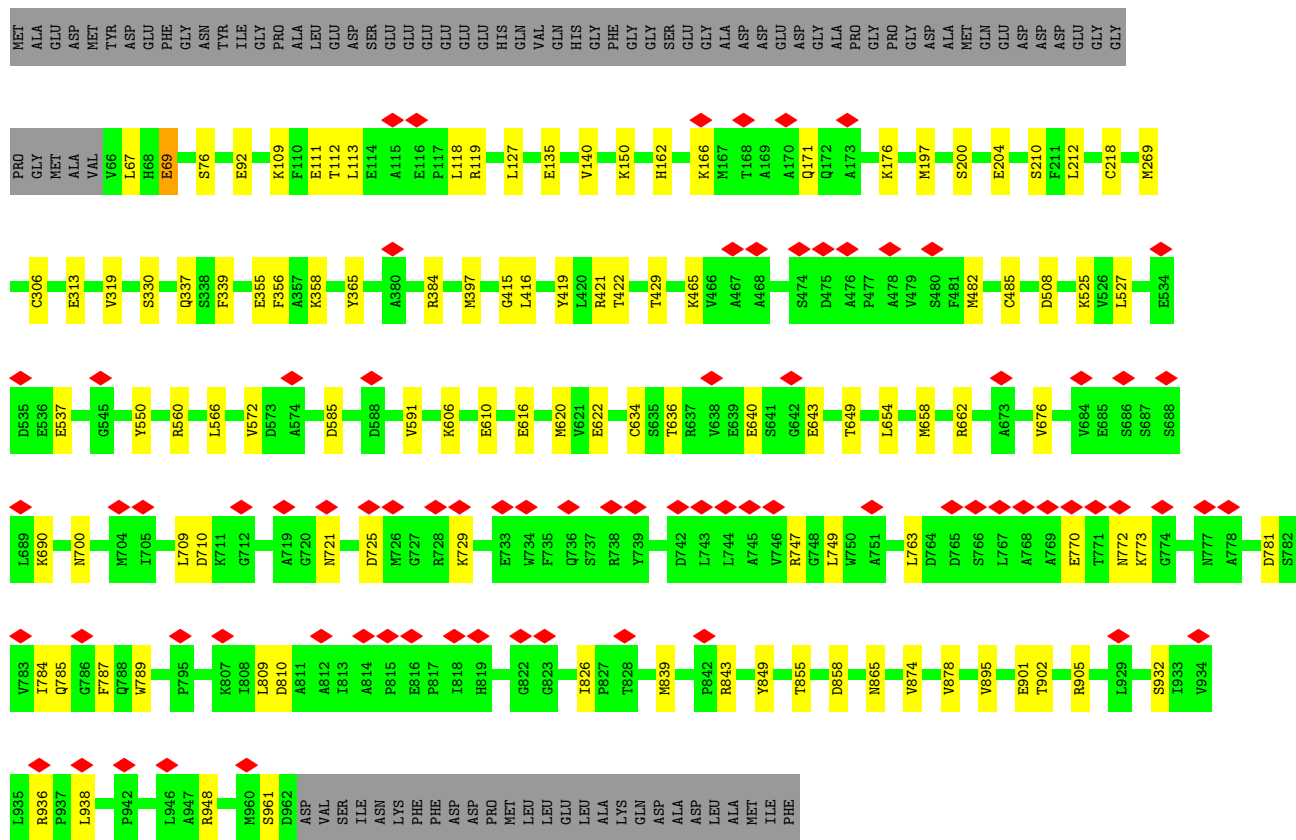


• Molecule 2: U5 snRNA

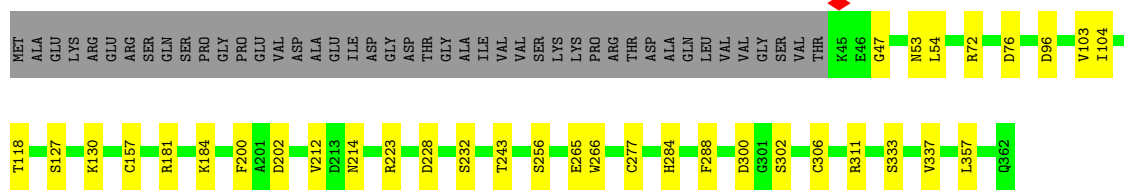


• Molecule 3: Elongation factor Tu, chloroplastic

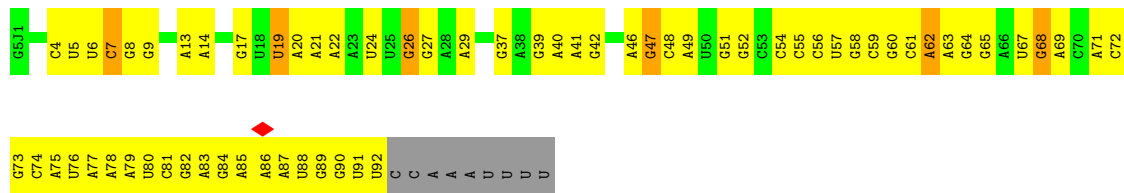
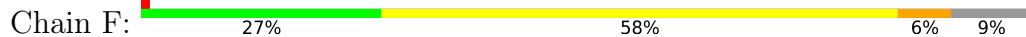




• Molecule 4: U5-40K

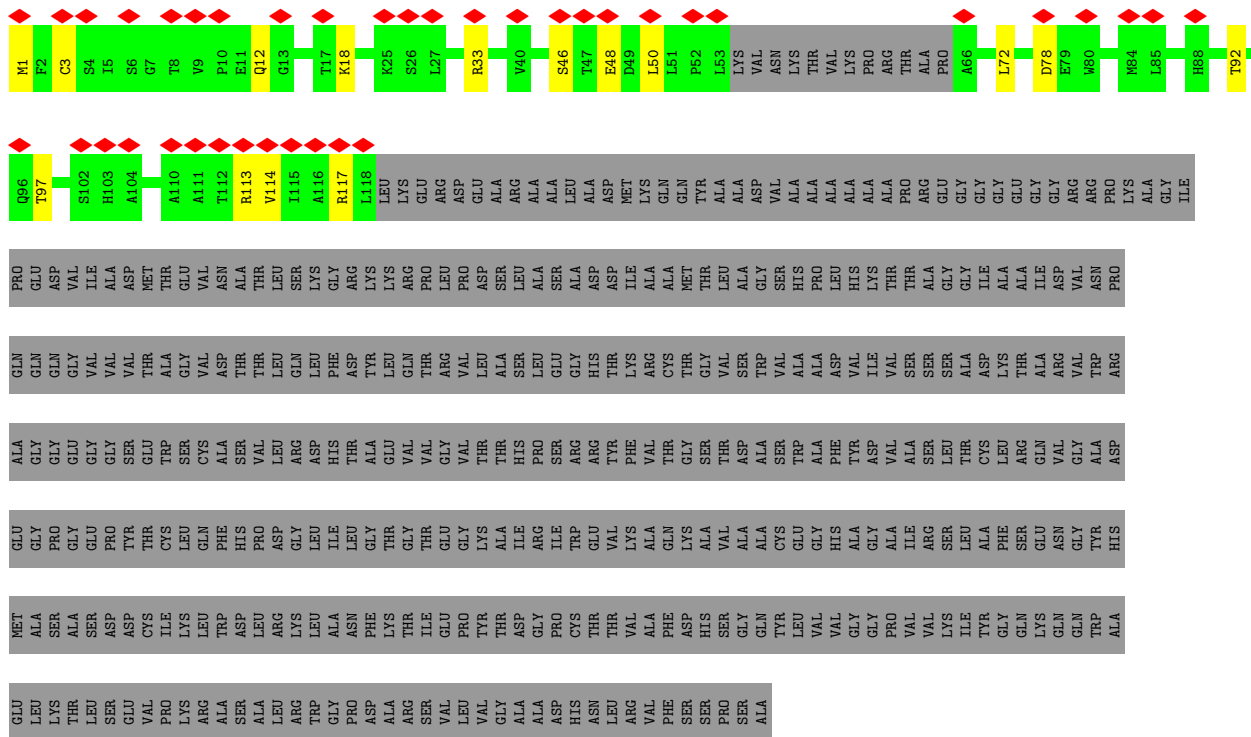


• Molecule 5: U6 snRNA

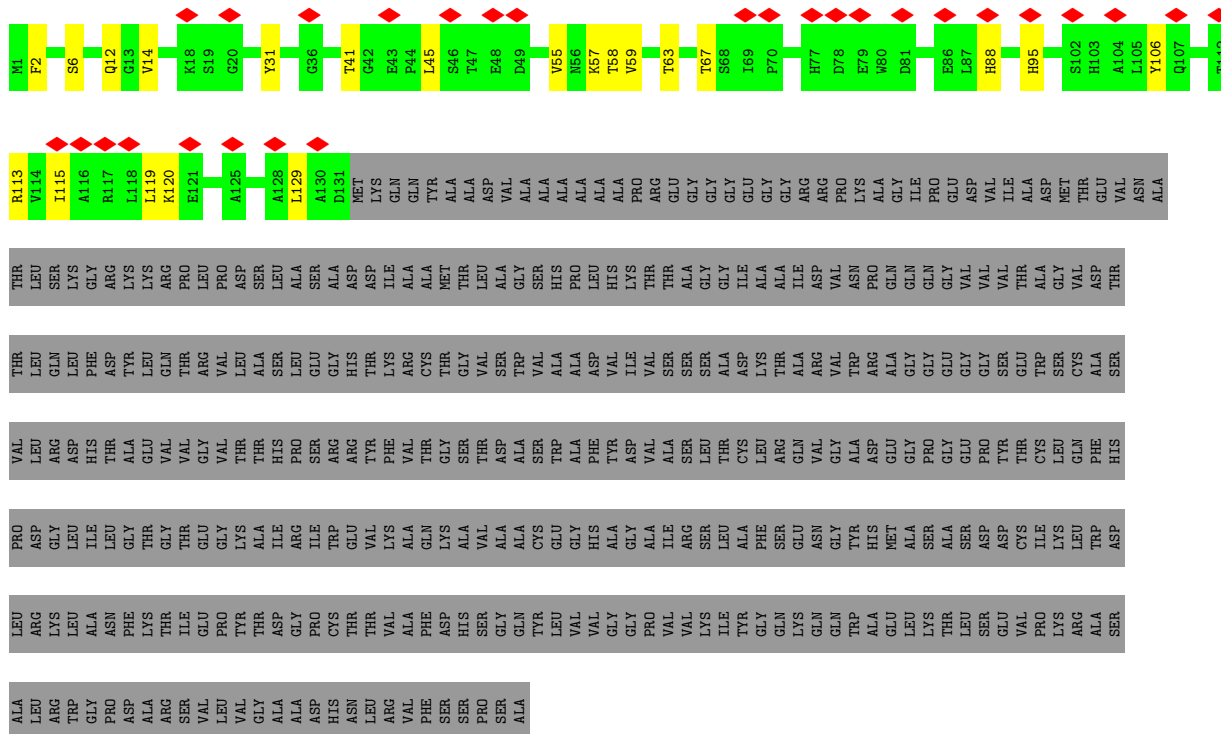


• Molecule 6: Pre-mRNA-processing factor 19



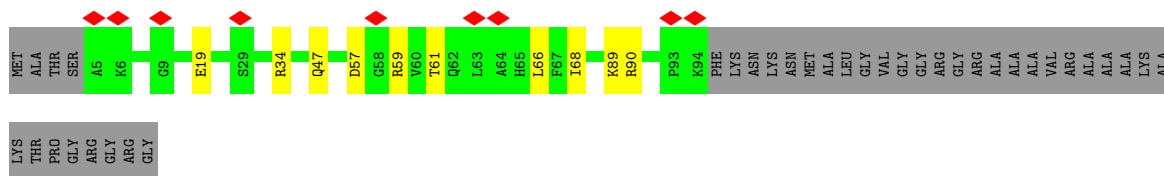


• Molecule 6: Pre-mRNA-processing factor 19

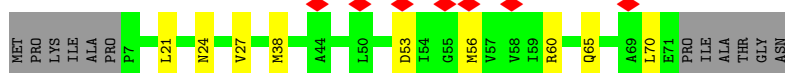


• Molecule 6: Pre-mRNA-processing factor 19

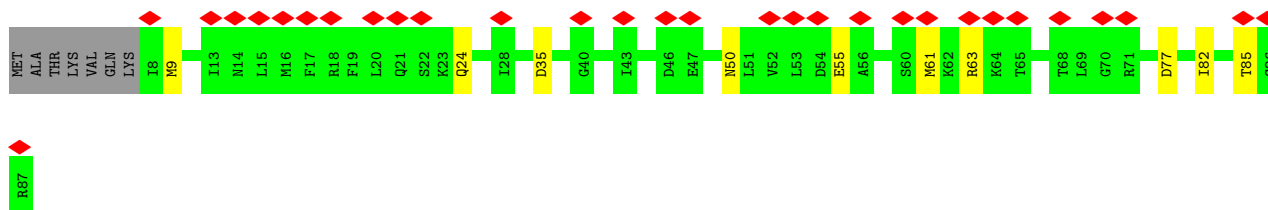
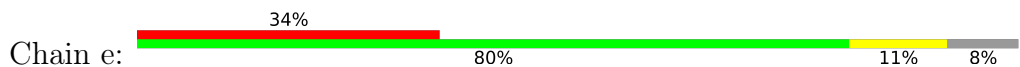
• Molecule 7: Small nuclear ribonucleoprotein Sm D3



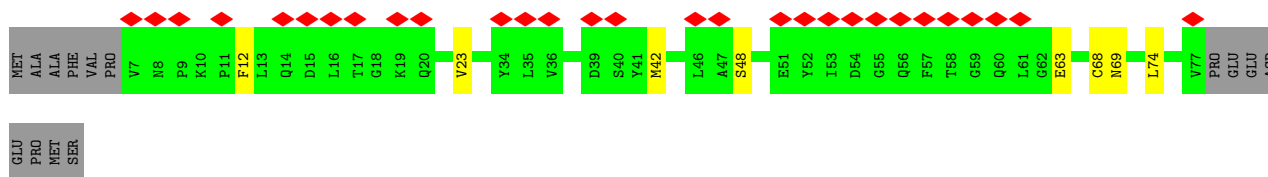
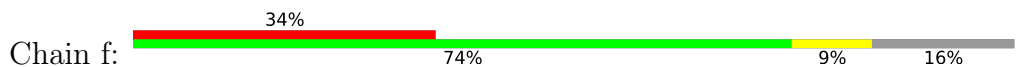
• Molecule 8: Small nuclear ribonucleoprotein G



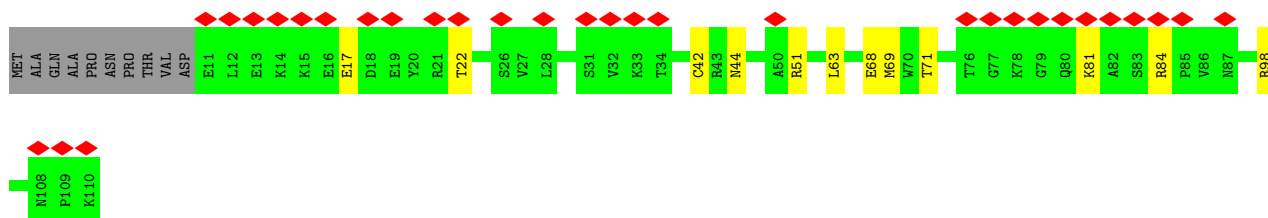
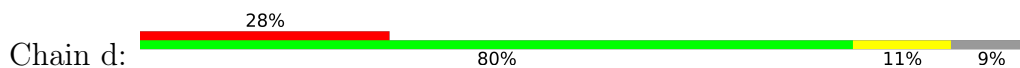
• Molecule 9: Small nuclear ribonucleoprotein E



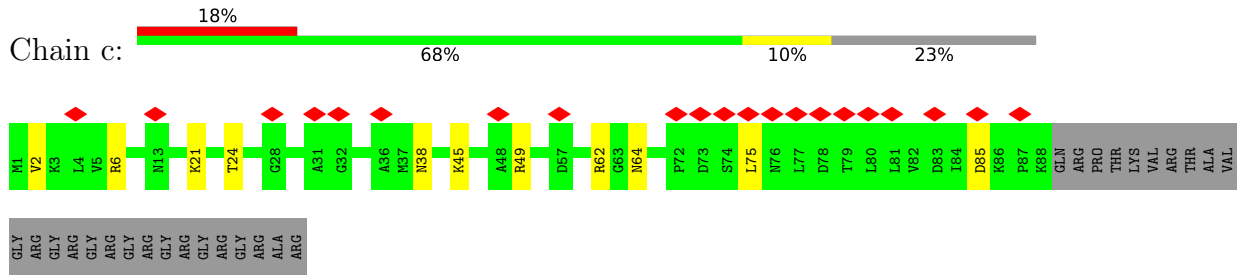
• Molecule 10: Sm protein F



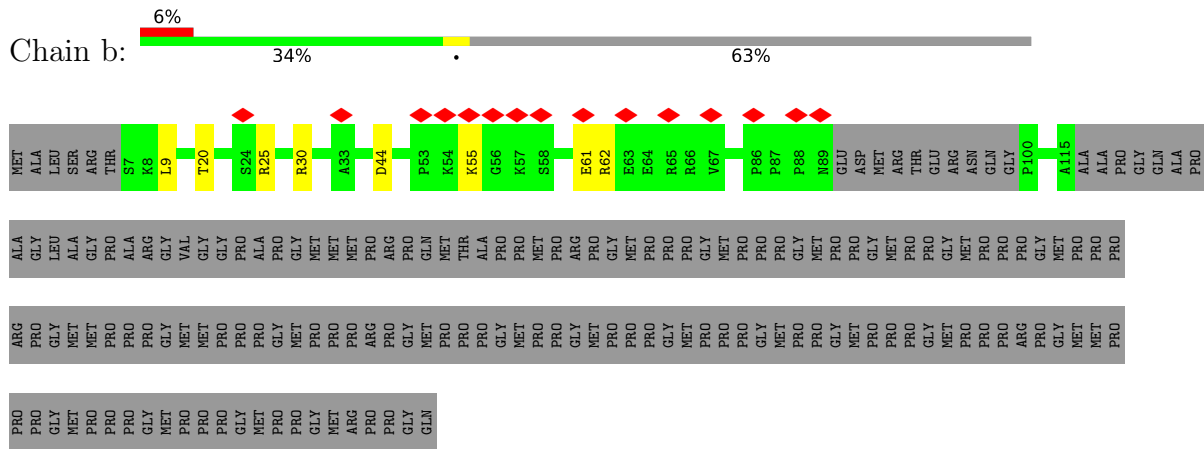
• Molecule 11: Small nuclear ribonucleoprotein Sm D2



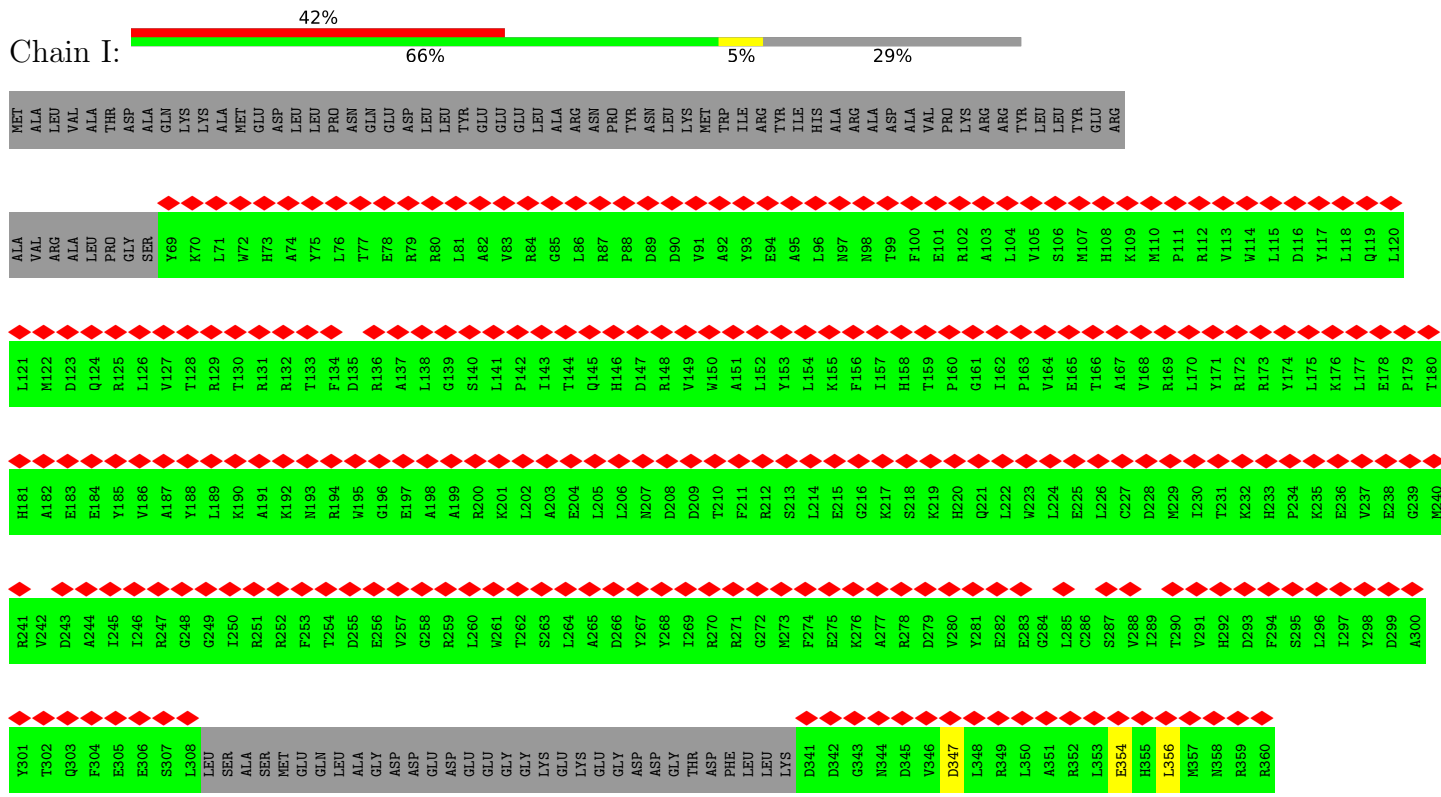
• Molecule 12: Small nuclear ribonucleoprotein Sm D1

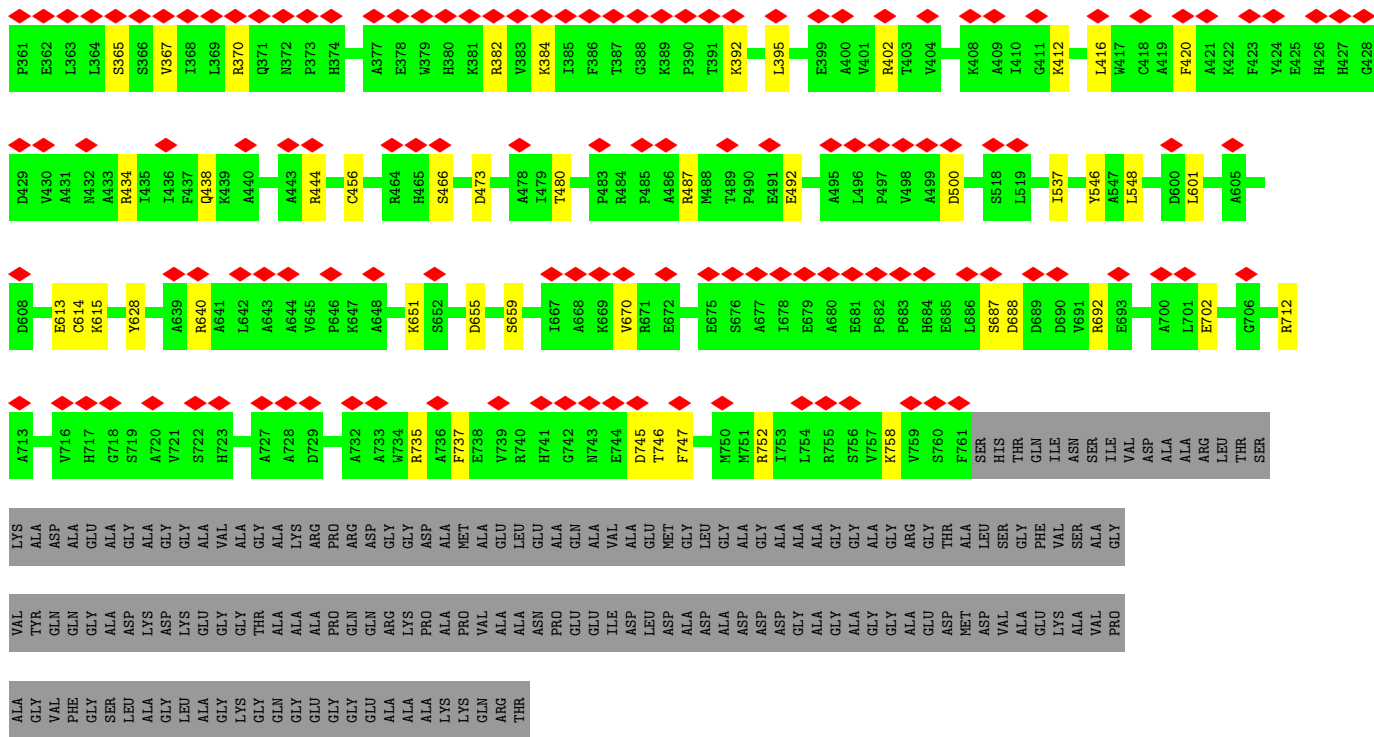


• Molecule 13: Sm domain-containing protein

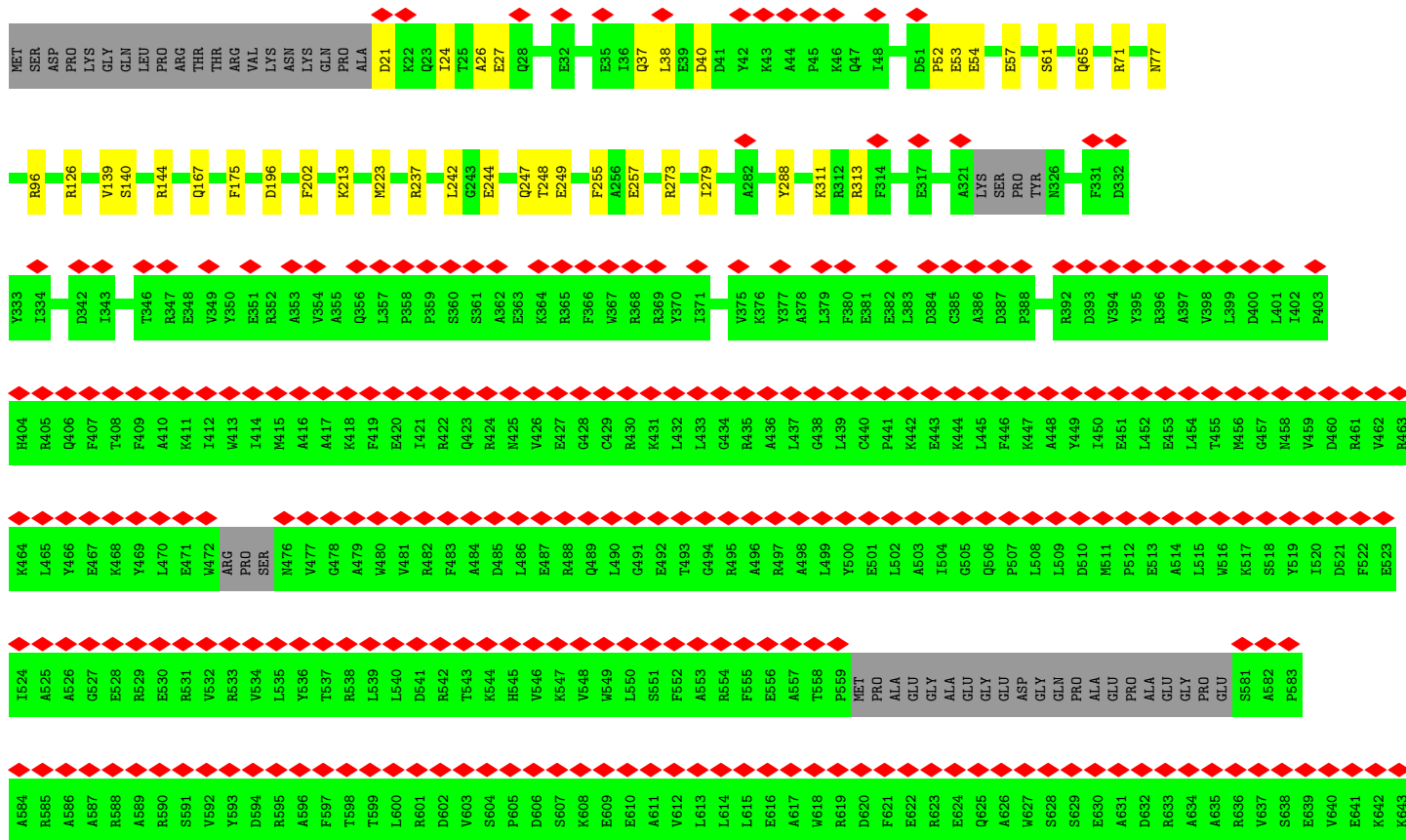


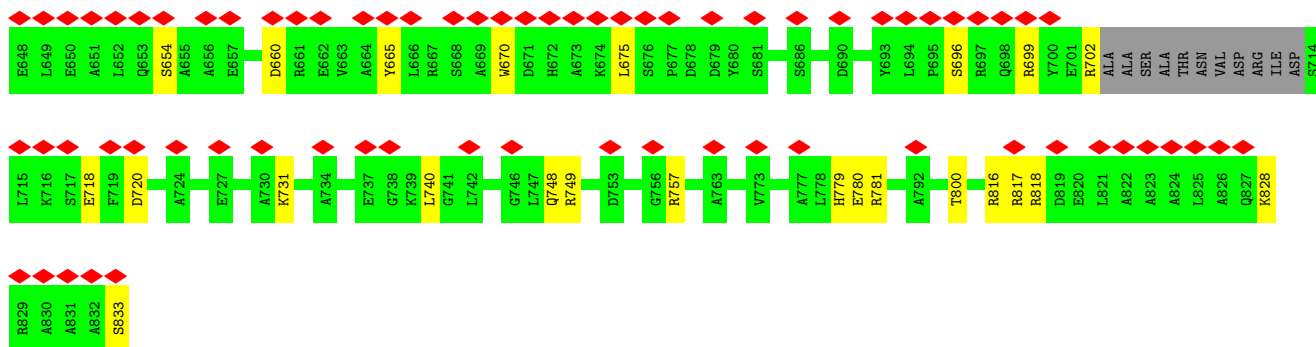
• Molecule 14: Syf1



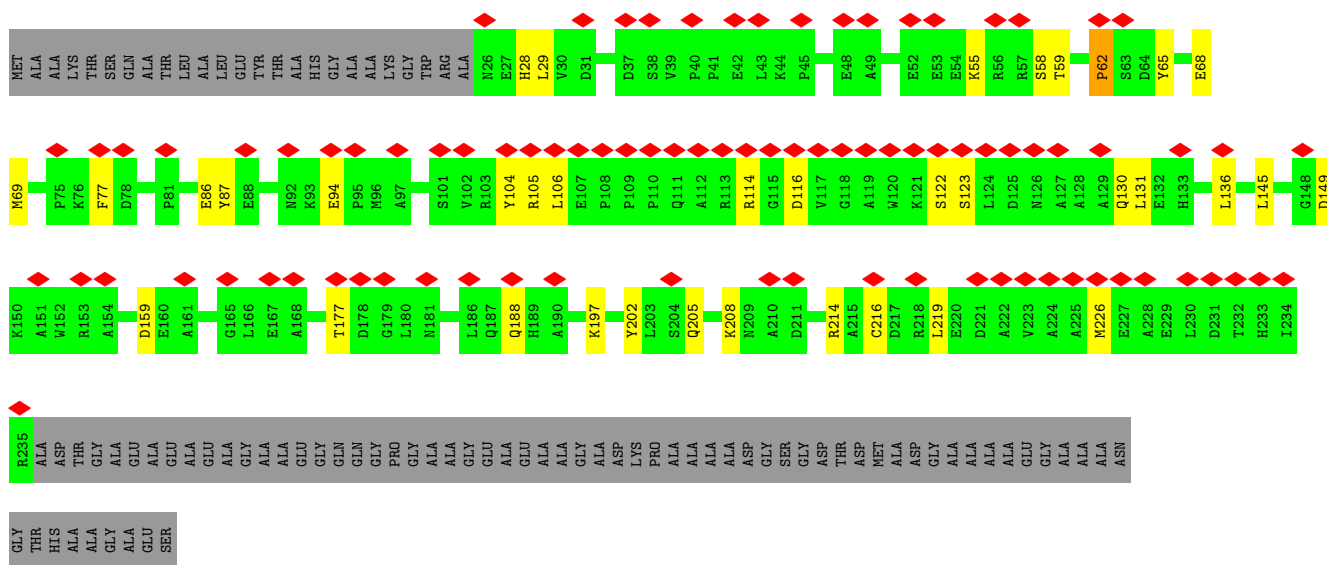


● Molecule 15: Crooked neck protein

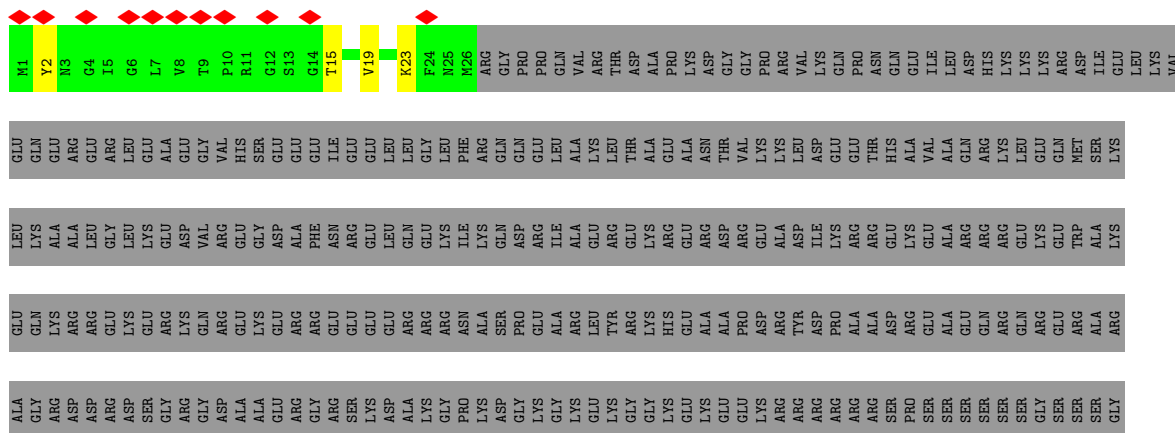




• Molecule 26: Pre-mRNA-splicing factor SPF27



• Molecule 27: CWF21 domain-containing protein



D1261	GLU	R1201	K1021	L961	S901	W841	W781	L721	D661	GLY	▲
L1262	ASP	F1202	E1022	M962	E902	C842	D782	T722	H662	ARG	▲
F1263	ALA	N1023	N1023	ASN	W903	A843	E783	G723	T663	GLY	▲
S1264	THR	M1024	M1024	ASP	D904	Y844	S784	E724	G664	ALA	▲
K1265	THR	F1025	F1025	THR	E905	T845	T785	Q725	E665	GLY	▲
L1266	GLY	K1026	K1026	GLY	L906	C846	Q786	Q726	E666	ALA	▲
M1267	ALA	A1027	A1027	ARG	R907	ASP	F787	R727	L667	ASN	▲
E1268	ALA	V1028	V1028	VAL	Q908	ASP	A788	E728	T668	GLY	▲
R1269	ALA	L1029	L1029	ARG	R909	R850	S789	L729	D669	GLN	▲
D1270	ALA	L1091	L1091	ARG	D910	R851	S790	V730	D670	GLY	▲
V1271	ALA	R1092	R1092	ASP	W911	T851	E791	C731	E671	ASN	▲
P1272	ALA	L1093	L1093	GLU	L912	R852	H792	R732	V672	ALA	▲
E1273	ALA	V1094	V1094	VAL	F913	F853	T793	Q733	N673	ALA	▲
G1213	GLU	D1095	D1095	PRO	L914	A854	Y794	L734	A674	ALA	▲
R1274	ALA	F1096	F1096	GLU	L914	R855	T795	L735	A675	GLY	▲
Y1275	ALA	L1097	L1097	GLU	L915	W856	G796	R736	A676	ARG	▲
L1276	ALA	M1036	M1036	GLU	T916	A857	E796	L736	H676	ARG	▲
G1217	GLY	N1037	N1037	THR	I917	R858	G797	W737	E677	ALA	▲
L1278	ALA	T1038	T1038	T980	R918	R859	A798	G738	E678	GLY	▲
L1279	ALA	D1039	D1039	R981	P919	M859	L799	E739	E679	SER	▲
G1280	ALA	T1040	T1040	T983	P919	A860	L799	E739	R679	PRO	▲
M1281	ALA	A1041	A1041	V984	P920	L861	A800	D740	V680	ALA	▲
GLY	GLY	L1042	L1042	T985	D921	P862	L801	D741	C681	ALA	▲
A1284	ALA	V1043	V1043	A987	ALA	T864	R802	P742	G682	GLY	▲
E1285	ALA	I1043	I1043	A987	ALA	R864	R803	M743	F683	GLY	▲
L1286	ASN	P1044	P1044	L988	ALA	A866	L804	A744	Q684	LYS	▲
D1287	PRO	W1046	W1046	D989	ALA	F866	M805	F746	R686	ALA	▲
T1227	ALA	L1047	L1047	T990	ALA	R867	L806	D746	L686	GLY	▲
G1228	ALA	H1048	H1048	A991	HIS	A868	Q807	G747	C687	ALA	▲
K1229	ALA	D1049	D1049	A992	ASP	T869	F808	F749	F688	ALA	▲
L1230	ALA	V1050	V1050	Q992	GLY	E870	L809	F750	R689	PRO	▲
D1231	ALA	F1051	F1051	Q994	ARG	W871	T810	L751	H690	PRO	▲
V1232	ALA	L1052	L1052	T995	THR	R872	W811	E752	M691	GLY	▲
A1233	ALA	G1053	G1053	D996	ASN	R873	A812	F753	Q692	ASN	▲
R1234	ALA	Y1054	Y1054	M997	ASN	P874	D813	W753	G693	ARG	▲
Q1235	ALA	G1055	G1055	T999	A938	M875	Y814	L754	V694	GLY	▲
V1236	ALA	D1056	D1056	T999	E939	W876	L815	L755	E695	GLY	▲
M1237	ALA	P1057	P1057	M1000	K940	G877	L816	A756	A696	ALA	▲
C1238	ALA	A1058	A1058	A1001	F941	E878	R817	A757	M697	SER	▲
L1240	ALA	A1059	A1059	R1002	G942	A879	S818	F758	Q698	ARG	▲
Y1241	ALA	K1060	K1060	H1003	L943	R880	F819	E759	E699	GLY	▲
M1242	ALA	Q1061	Q1061	L1004	V944	P881	H820	R760	L700	GLY	▲
M1243	ARG	ALA	ALA	S1005	Y945	A882	L821	R761	A701	ARG	▲
C1244	VAL	VAL	VAL	E1006	V946	G883	F822	R762	L702	GLY	▲
P1245	GLY	THR	THR	D1007	R947	R884	R823	S763	S703	ARG	▲
G1246	ALA	ALA	ALA	P1008	G948	T885	L824	Q764	H704	GLY	▲
Q1247	ALA	ALA	ALA	Y1009	C949	A886	E825	R765	C705	GLY	▲
R1248	ALA	ALA	ALA	A1010	E950	M887	A826	E766	G706	ARG	▲
T1249	ALA	ALA	ALA	T1011	W951	R888	T827	V767	A707	SER	▲
L1250	ALA	ALA	ALA	F1012	I952	V889	Y828	W768	F657	ARG	▲
I1251	ALA	ALA	ALA	M1013	E953	T890	E829	M769	P658	ARG	▲
I1252	ALA	ALA	ALA	L1014	R954	D891	W830	E770	A709	ARG	▲
K1314	ALA	ALA	ALA	L1015	R955	T892	R831	M771	R711	GLY	▲
M1315	ALA	ALA	ALA	M1016	D956	R893	E832	P772	D712	GLY	▲
S1255	GLY	GLY	GLY	R1017	E957	P894	D833	L773	T713	GLY	▲
M1256	LEU	THR	THR	L1018	G958	L895	L834	Y774	L714	GLY	▲
Q1257	PRO	ALA	ALA	K1019	G959	R896	D836	F775	R715	GLY	▲
A1258	PRO	ALA	ALA	P1020	R960	S897	W837	T776	R716	ARG	▲
L1259	PRO	ALA	ALA			D898	E777	G778	H717	SER	▲
M1260	PRO	ALA	ALA			W899	L718	L779	A719	SER	▲
						R900	R840	L780	S720	PRO	▲

G G D D G A C G A C A A A C D C D D C G C G G D C D D D C C A G D G G G G A D C C G A D A D C C G

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	518369	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.593	Depositor
Minimum map value	-1.565	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	404.80002, 404.80002, 404.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.92, 0.92, 0.92	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, SEP, G5J, 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	A	0.86	19/15581 (0.1%)	0.67	7/21167 (0.0%)
2	B	1.22	6/2024 (0.3%)	1.16	5/3144 (0.2%)
3	C	0.41	0/7126	0.57	1/9683 (0.0%)
4	E	0.40	0/2496	0.58	1/3382 (0.0%)
5	F	1.60	43/2188 (2.0%)	1.31	17/3409 (0.5%)
6	q	0.30	0/847	0.57	0/1148
6	r	0.31	0/1040	0.58	0/1411
6	s	0.30	0/580	0.59	0/784
6	t	0.33	0/514	0.62	0/698
7	a	0.30	0/716	0.53	0/960
8	g	0.31	0/516	0.56	0/691
9	e	0.28	0/667	0.52	0/891
10	f	0.29	0/567	0.56	0/764
11	d	0.28	0/821	0.50	0/1097
12	c	0.29	0/691	0.61	0/933
13	b	0.30	0/792	0.60	0/1059
14	I	0.28	0/4712	0.48	0/6427
15	J	0.65	0/4092	0.52	1/5574 (0.0%)
16	P	0.74	1/882 (0.1%)	0.60	0/1173
17	M	0.39	0/654	0.56	0/874
18	T	1.14	5/2773 (0.2%)	0.81	0/3765
19	O	0.54	0/2179	0.59	0/2944
20	N	0.82	0/1446	0.64	2/1944 (0.1%)
21	R	0.64	0/2020	0.59	0/2736
22	H	1.25	4/932 (0.4%)	1.29	4/1447 (0.3%)
23	S	0.43	0/1224	0.56	0/1652
24	W	0.44	2/2852 (0.1%)	0.57	2/3908 (0.1%)
25	L	0.46	0/3847	0.57	1/5158 (0.0%)
26	K	0.29	0/1717	0.55	3/2320 (0.1%)
27	U	0.32	0/194	0.60	0/259
28	V	0.28	0/1023	0.42	0/1413
29	Q	0.28	0/6411	0.48	1/8913 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	5	1.29	0/167	1.52	4/258 (1.6%)
31	3	0.55	0/771	1.19	4/1193 (0.3%)
All	All	0.69	80/75062 (0.1%)	0.68	53/103179 (0.1%)

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	11
3	C	0	1
6	s	0	1
6	t	0	1
25	L	0	1
28	V	0	1
All	All	0	16

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	W	89	PRO	N-CA	13.08	1.69	1.47
5	F	58	G	C8-N7	-7.87	1.26	1.30
5	F	58	G	C5-C4	-7.64	1.33	1.38
5	F	60	G	C8-N7	-7.22	1.26	1.30
5	F	57	U	C2-N3	-7.16	1.32	1.37
5	F	65	G	C5-C4	-7.13	1.33	1.38
5	F	47	G	C2-N3	-7.11	1.27	1.32
5	F	60	G	C6-N1	-6.90	1.34	1.39
5	F	58	G	N9-C8	-6.88	1.33	1.37
22	H	21	G	C6-N1	-6.84	1.34	1.39
5	F	62	A	N7-C5	-6.76	1.35	1.39
1	A	1092	TYR	CD2-CE2	-6.74	1.29	1.39
5	F	68	G	C8-N7	-6.66	1.26	1.30
2	B	56	U	C2-N3	-6.52	1.33	1.37
5	F	62	A	C8-N7	-6.50	1.26	1.31
5	F	63	A	C6-N1	-6.47	1.31	1.35
5	F	58	G	C6-O6	-6.38	1.18	1.24
1	A	1083	TYR	CD1-CE1	-6.29	1.29	1.39
1	A	190	GLU	CB-CG	-6.17	1.40	1.52
5	F	49	A	C5-C4	-6.11	1.34	1.38
2	B	34	C	N3-C4	-6.05	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	63	A	N9-C8	-6.03	1.32	1.37
1	A	190	GLU	CG-CD	-5.96	1.43	1.51
5	F	65	G	N1-C2	-5.89	1.33	1.37
5	F	60	G	N1-C2	-5.88	1.33	1.37
18	T	426	ASN	CB-CG	-5.86	1.37	1.51
24	W	88	GLY	C-N	5.86	1.45	1.34
5	F	60	G	N7-C5	-5.84	1.35	1.39
5	F	65	G	N9-C4	-5.80	1.33	1.38
5	F	64	G	C5-C4	-5.79	1.34	1.38
5	F	58	G	N1-C2	-5.75	1.33	1.37
1	A	1083	TYR	CD2-CE2	-5.71	1.30	1.39
1	A	154	VAL	CB-CG1	-5.70	1.40	1.52
2	B	54	G	C2-N3	-5.67	1.28	1.32
5	F	62	A	C5-C6	-5.67	1.35	1.41
2	B	51	A	C6-N1	-5.63	1.31	1.35
1	A	957	GLU	CB-CG	-5.60	1.41	1.52
5	F	64	G	C2-N3	-5.55	1.28	1.32
5	F	59	C	N3-C4	-5.51	1.30	1.33
18	T	485	GLU	CG-CD	-5.49	1.43	1.51
1	A	179	TYR	CD1-CE1	-5.49	1.31	1.39
16	P	233	TYR	CD2-CE2	-5.43	1.31	1.39
1	A	858	TYR	CD1-CE1	-5.39	1.31	1.39
5	F	47	G	C5-C4	-5.39	1.34	1.38
5	F	64	G	C8-N7	-5.38	1.27	1.30
5	F	56	C	N3-C4	-5.36	1.30	1.33
5	F	62	A	C5-C4	-5.36	1.34	1.38
18	T	202	VAL	CB-CG2	-5.36	1.41	1.52
1	A	742	GLU	CB-CG	-5.36	1.42	1.52
22	H	22	C	N3-C4	-5.34	1.30	1.33
5	F	48	C	N3-C4	-5.32	1.30	1.33
22	H	21	G	C2-N3	-5.31	1.28	1.32
1	A	283	TYR	CD1-CE1	-5.25	1.31	1.39
1	A	644	TYR	CD2-CE2	-5.23	1.31	1.39
22	H	25	A	N7-C5	-5.23	1.36	1.39
5	F	68	G	C5-C4	-5.22	1.34	1.38
5	F	59	C	N1-C6	-5.20	1.34	1.37
1	A	237	TYR	CD1-CE1	-5.20	1.31	1.39
1	A	179	TYR	CD2-CE2	-5.20	1.31	1.39
5	F	60	G	N9-C4	-5.19	1.33	1.38
1	A	1044	GLU	CB-CG	-5.18	1.42	1.52
5	F	60	G	C5-C4	-5.17	1.34	1.38
18	T	283	VAL	CB-CG2	-5.17	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	495	GLU	CB-CG	-5.16	1.42	1.52
1	A	169	TRP	CE3-CZ3	-5.15	1.29	1.38
2	B	55	A	N9-C4	-5.14	1.34	1.37
5	F	60	G	N9-C8	-5.14	1.34	1.37
1	A	973	TYR	CD2-CE2	-5.13	1.31	1.39
5	F	57	U	N3-C4	-5.13	1.33	1.38
5	F	64	G	C6-N1	-5.13	1.35	1.39
1	A	1340	GLU	CG-CD	-5.11	1.44	1.51
5	F	63	A	C8-N7	-5.08	1.27	1.31
2	B	52	G	C6-N1	-5.07	1.36	1.39
5	F	17	G	C8-N7	-5.04	1.27	1.30
5	F	47	G	N9-C4	-5.04	1.33	1.38
5	F	56	C	N1-C6	-5.03	1.34	1.37
5	F	55	C	N3-C4	-5.03	1.30	1.33
1	A	634	ASP	CB-CG	-5.01	1.41	1.51
5	F	59	C	C2-N3	-5.00	1.31	1.35
5	F	69	A	C5-C4	-5.00	1.35	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	22	C	O5'-P-OP1	-18.02	89.07	110.70
20	N	46	LEU	CA-CB-CG	7.61	132.81	115.30
1	A	843	LEU	CA-CB-CG	7.12	131.67	115.30
5	F	39	G	C5-C6-O6	-6.80	124.52	128.60
5	F	68	G	N9-C4-C5	-6.78	102.69	105.40
24	W	89	PRO	CA-N-CD	-6.59	102.28	111.50
4	E	357	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	711	LEU	CA-CB-CG	6.43	130.09	115.30
5	F	39	G	N1-C6-O6	6.41	123.74	119.90
5	F	52	G	C4-C5-N7	6.39	113.36	110.80
20	N	169	LEU	CA-CB-CG	6.37	129.96	115.30
31	3	20	A	P-O3'-C3'	6.31	127.27	119.70
5	F	65	G	C8-N9-C4	6.21	108.89	106.40
5	F	68	G	C4-C5-N7	6.11	113.24	110.80
5	F	58	G	C8-N9-C4	6.08	108.83	106.40
5	F	58	G	C5-C6-N1	6.05	114.52	111.50
22	H	4	C	N3-C2-O2	-6.03	117.68	121.90
25	L	740	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	303	LEU	CA-CB-CG	5.98	129.05	115.30
2	B	70	U	C2-N1-C1'	5.96	124.85	117.70
5	F	46	A	N1-C6-N6	-5.83	115.10	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	62	PRO	N-CA-CB	5.80	110.26	103.30
1	A	1156	LEU	CA-CB-CG	5.65	128.29	115.30
29	Q	788	ALA	N-CA-C	-5.64	95.76	111.00
30	5	-6	C	C2-N1-C1'	5.59	124.95	118.80
2	B	29	U	N3-C2-O2	-5.52	118.34	122.20
5	F	7	C	C2-N1-C1'	5.52	124.87	118.80
30	5	-2	C	C2-N3-C4	-5.51	117.14	119.90
1	A	749	LEU	CA-CB-CG	5.51	127.96	115.30
30	5	-6	C	N1-C2-O2	5.47	122.18	118.90
3	C	415	GLY	N-CA-C	-5.43	99.53	113.10
22	H	21	G	N7-C8-N9	5.43	115.81	113.10
5	F	54	C	N1-C2-O2	-5.35	115.69	118.90
5	F	47	G	N3-C4-C5	5.33	131.26	128.60
24	W	91	HIS	CB-CA-C	5.31	121.01	110.40
2	B	29	U	O4'-C1'-N1	5.25	112.40	108.20
15	J	21	ASP	CB-CG-OD2	5.25	123.03	118.30
5	F	58	G	C4-C5-C6	-5.24	115.66	118.80
5	F	26	G	N3-C4-N9	-5.20	122.88	126.00
5	F	19	U	C2-N1-C1'	5.19	123.93	117.70
1	A	1004	VAL	C-N-CA	-5.18	108.75	121.70
31	3	8	C	C5-C6-N1	5.18	123.59	121.00
5	F	63	A	N1-C6-N6	-5.17	115.50	118.60
5	F	47	G	C8-N9-C4	5.16	108.46	106.40
31	3	13	C	C6-N1-C2	-5.15	118.24	120.30
22	H	21	G	C8-N9-C4	-5.13	104.35	106.40
2	B	56	U	C2-N3-C4	-5.13	123.92	127.00
30	5	-2	C	N3-C2-O2	-5.12	118.31	121.90
1	A	1154	ARG	NE-CZ-NH2	-5.10	117.75	120.30
26	K	106	LEU	CA-CB-CG	5.09	127.02	115.30
31	3	16	U	C2-N1-C1'	5.09	123.81	117.70
2	B	49	A	O4'-C1'-N9	5.07	112.25	108.20
26	K	219	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1004	VAL	Peptide
1	A	1005	LYS	Peptide
1	A	1045	PHE	Peptide
1	A	1338	TYR	Peptide
1	A	1470	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	1480	ILE	Peptide
1	A	1701	TRP	Peptide
1	A	1751	TYR	Peptide
1	A	1783	PHE	Peptide
1	A	532	LYS	Peptide
1	A	686	GLY	Peptide
3	C	69	GLU	Peptide
25	L	670	TRP	Peptide
28	V	703	PHE	Peptide
6	s	67	THR	Peptide
6	t	67	THR	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1923/2398 (80%)	1730 (90%)	182 (10%)	11 (1%)	22	43
3	C	895/989 (90%)	816 (91%)	78 (9%)	1 (0%)	48	71
4	E	316/362 (87%)	289 (92%)	26 (8%)	1 (0%)	37	59
6	q	102/503 (20%)	102 (100%)	0	0	100	100
6	r	129/503 (26%)	120 (93%)	8 (6%)	1 (1%)	16	34
6	s	68/503 (14%)	65 (96%)	3 (4%)	0	100	100
6	t	60/503 (12%)	56 (93%)	4 (7%)	0	100	100
7	a	88/127 (69%)	86 (98%)	2 (2%)	0	100	100
8	g	63/77 (82%)	60 (95%)	3 (5%)	0	100	100
9	e	78/87 (90%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	f	69/85 (81%)	68 (99%)	1 (1%)	0	100	100
11	d	98/110 (89%)	97 (99%)	1 (1%)	0	100	100
12	c	86/114 (75%)	82 (95%)	4 (5%)	0	100	100
13	b	95/265 (36%)	89 (94%)	6 (6%)	0	100	100
14	I	657/925 (71%)	641 (98%)	16 (2%)	0	100	100
15	J	587/835 (70%)	551 (94%)	30 (5%)	6 (1%)	13	29
16	P	98/235 (42%)	90 (92%)	8 (8%)	0	100	100
17	M	74/563 (13%)	68 (92%)	6 (8%)	0	100	100
18	T	342/518 (66%)	326 (95%)	15 (4%)	1 (0%)	37	59
19	O	269/417 (64%)	245 (91%)	24 (9%)	0	100	100
20	N	167/233 (72%)	154 (92%)	13 (8%)	0	100	100
21	R	254/684 (37%)	240 (94%)	14 (6%)	0	100	100
23	S	153/157 (98%)	137 (90%)	16 (10%)	0	100	100
24	W	475/576 (82%)	431 (91%)	38 (8%)	6 (1%)	10	21
25	L	454/833 (54%)	429 (94%)	25 (6%)	0	100	100
26	K	208/303 (69%)	191 (92%)	16 (8%)	1 (0%)	25	47
27	U	24/721 (3%)	23 (96%)	1 (4%)	0	100	100
28	V	184/928 (20%)	177 (96%)	7 (4%)	0	100	100
29	Q	1275/1844 (69%)	1217 (96%)	49 (4%)	9 (1%)	19	38
All	All	9291/16398 (57%)	8654 (93%)	600 (6%)	37 (0%)	32	52

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	VAL
1	A	449	GLU
15	J	26	ALA
15	J	27	GLU
29	Q	893	ARG
1	A	246	PRO
3	C	422	THR
6	r	58	THR
15	J	37	GLN
15	J	40	ASP
15	J	53	GLU

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Mol	Chain	Res	Type
26	K	62	PRO
29	Q	155	GLU
29	Q	158	GLY
29	Q	719	ALA
29	Q	789	SER
1	A	247	LEU
1	A	528	PRO
4	E	47	GLY
24	W	86	VAL
29	Q	154	GLN
1	A	1266	MET
1	A	1717	ASP
1	A	2011	PRO
29	Q	153	LYS
1	A	1426	ASP
1	A	1718	GLN
24	W	87	LEU
24	W	92	PRO
24	W	91	HIS
29	Q	898	ASP
29	Q	1365	VAL
1	A	1822	PRO
15	J	52	PRO
24	W	84	ALA
24	W	198	GLN
18	T	247	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1505/2124 (71%)	1306 (87%)	199 (13%)	3	6
3	C	753/825 (91%)	647 (86%)	106 (14%)	3	5
4	E	264/300 (88%)	231 (88%)	33 (12%)	3	7
6	q	94/398 (24%)	79 (84%)	15 (16%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	r	113/398 (28%)	93 (82%)	20 (18%)	1	2
6	s	59/398 (15%)	54 (92%)	5 (8%)	8	18
6	t	54/398 (14%)	45 (83%)	9 (17%)	2	3
7	a	76/97 (78%)	66 (87%)	10 (13%)	3	6
8	g	58/67 (87%)	49 (84%)	9 (16%)	2	3
9	e	73/79 (92%)	63 (86%)	10 (14%)	3	5
10	f	62/75 (83%)	54 (87%)	8 (13%)	3	6
11	d	92/100 (92%)	80 (87%)	12 (13%)	3	6
12	c	78/95 (82%)	67 (86%)	11 (14%)	3	5
13	b	84/211 (40%)	76 (90%)	8 (10%)	7	14
14	I	357/743 (48%)	308 (86%)	49 (14%)	3	5
15	J	260/676 (38%)	228 (88%)	32 (12%)	4	8
16	P	88/188 (47%)	77 (88%)	11 (12%)	3	7
17	M	63/424 (15%)	56 (89%)	7 (11%)	5	10
18	T	291/416 (70%)	263 (90%)	28 (10%)	7	14
19	O	228/318 (72%)	210 (92%)	18 (8%)	10	21
20	N	148/193 (77%)	137 (93%)	11 (7%)	11	24
21	R	209/507 (41%)	179 (86%)	30 (14%)	2	5
23	S	128/130 (98%)	119 (93%)	9 (7%)	12	27
24	W	118/474 (25%)	95 (80%)	23 (20%)	1	2
25	L	388/648 (60%)	333 (86%)	55 (14%)	2	5
26	K	177/221 (80%)	144 (81%)	33 (19%)	1	2
27	U	20/572 (4%)	16 (80%)	4 (20%)	1	2
28	V	28/746 (4%)	24 (86%)	4 (14%)	2	5
All	All	5868/11821 (50%)	5099 (87%)	769 (13%)	6	6

All (769) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	95	LYS
1	A	96	TRP
1	A	108	ARG
1	A	114	GLU

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Mol	Chain	Res	Type
1	A	127	LYS
1	A	130	ARG
1	A	137	SER
1	A	145	ARG
1	A	146	VAL
1	A	148	LEU
1	A	167	MET
1	A	175	VAL
1	A	177	VAL
1	A	181	ILE
1	A	185	ILE
1	A	229	ASP
1	A	276	LYS
1	A	279	ASN
1	A	288	LEU
1	A	296	LEU
1	A	299	LEU
1	A	303	LEU
1	A	305	THR
1	A	310	ARG
1	A	311	ASN
1	A	321	PHE
1	A	331	ILE
1	A	342	ARG
1	A	368	THR
1	A	380	ASN
1	A	385	VAL
1	A	386	ARG
1	A	387	LEU
1	A	391	HIS
1	A	396	LEU
1	A	478	ARG
1	A	489	PRO
1	A	492	ASN
1	A	493	CYS
1	A	498	HIS
1	A	502	THR
1	A	503	TYR
1	A	522	LEU
1	A	529	LYS
1	A	530	SER
1	A	540	LEU

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Mol	Chain	Res	Type
1	A	547	GLN
1	A	548	SER
1	A	549	THR
1	A	587	ASN
1	A	593	THR
1	A	595	THR
1	A	596	THR
1	A	599	ARG
1	A	610	LEU
1	A	618	THR
1	A	619	LYS
1	A	633	VAL
1	A	634	ASP
1	A	640	ASP
1	A	643	GLN
1	A	675	LEU
1	A	691	VAL
1	A	706	ARG
1	A	708	ILE
1	A	712	LEU
1	A	714	ARG
1	A	729	SER
1	A	732	ILE
1	A	738	LYS
1	A	756	ASP
1	A	800	GLU
1	A	809	GLN
1	A	834	THR
1	A	866	THR
1	A	884	ARG
1	A	899	ASP
1	A	909	ARG
1	A	923	SER
1	A	935	TYR
1	A	946	LYS
1	A	952	GLN
1	A	954	SER
1	A	978	LEU
1	A	980	LYS
1	A	984	CYS
1	A	986	LEU
1	A	987	ASP

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Mol	Chain	Res	Type
1	A	993	GLU
1	A	999	LEU
1	A	1004	VAL
1	A	1005	LYS
1	A	1015	LEU
1	A	1024	ASN
1	A	1027	THR
1	A	1042	GLN
1	A	1043	SER
1	A	1059	ARG
1	A	1085	ASP
1	A	1087	SER
1	A	1091	SER
1	A	1094	LEU
1	A	1120	THR
1	A	1133	ASN
1	A	1142	LYS
1	A	1153	SER
1	A	1157	ASN
1	A	1163	PHE
1	A	1164	ARG
1	A	1188	ASN
1	A	1196	LYS
1	A	1201	ASP
1	A	1213	LEU
1	A	1224	ARG
1	A	1230	THR
1	A	1231	THR
1	A	1240	SER
1	A	1245	ASP
1	A	1246	ASN
1	A	1248	ASN
1	A	1265	ARG
1	A	1283	VAL
1	A	1285	THR
1	A	1289	THR
1	A	1319	THR
1	A	1321	THR
1	A	1322	LYS
1	A	1331	LEU
1	A	1336	THR
1	A	1340	GLU

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Mol	Chain	Res	Type
1	A	1348	LEU
1	A	1362	ARG
1	A	1365	ILE
1	A	1402	SER
1	A	1417	PHE
1	A	1421	MET
1	A	1428	LEU
1	A	1434	ARG
1	A	1441	SER
1	A	1447	GLU
1	A	1452	GLU
1	A	1456	LYS
1	A	1457	LYS
1	A	1459	GLU
1	A	1461	LYS
1	A	1465	ARG
1	A	1468	THR
1	A	1470	ASP
1	A	1472	LEU
1	A	1490	ASP
1	A	1491	ARG
1	A	1493	THR
1	A	1502	VAL
1	A	1512	THR
1	A	1513	LYS
1	A	1514	MET
1	A	1538	VAL
1	A	1545	VAL
1	A	1557	THR
1	A	1558	TYR
1	A	1590	LEU
1	A	1592	GLN
1	A	1593	ILE
1	A	1600	LEU
1	A	1601	TRP
1	A	1605	THR
1	A	1608	ARG
1	A	1630	ILE
1	A	1632	THR
1	A	1633	LEU
1	A	1635	ILE
1	A	1658	CYS

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Mol	Chain	Res	Type
1	A	1665	LEU
1	A	1679	HIS
1	A	1683	SER
1	A	1700	LYS
1	A	1701	TRP
1	A	1702	ASN
1	A	1705	LYS
1	A	1707	SER
1	A	1712	THR
1	A	1725	TRP
1	A	1726	VAL
1	A	1728	VAL
1	A	1729	GLN
1	A	1732	TRP
1	A	1747	LYS
1	A	1754	ASP
1	A	1756	MET
1	A	1757	SER
1	A	1783	PHE
1	A	1786	ILE
1	A	1807	LEU
1	A	1810	ARG
1	A	1813	LYS
1	A	1816	GLN
1	A	1817	LEU
1	A	1819	SER
3	C	67	LEU
3	C	69	GLU
3	C	76	SER
3	C	92	GLU
3	C	109	LYS
3	C	111	GLU
3	C	112	THR
3	C	113	LEU
3	C	118	LEU
3	C	119	ARG
3	C	127	LEU
3	C	135	GLU
3	C	140	VAL
3	C	150	LYS
3	C	162	HIS
3	C	166	LYS

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Mol	Chain	Res	Type
3	C	171	GLN
3	C	176	LYS
3	C	197	MET
3	C	200	SER
3	C	204	GLU
3	C	210	SER
3	C	212	LEU
3	C	218	CYS
3	C	269	MET
3	C	306	CYS
3	C	313	GLU
3	C	319	VAL
3	C	330	SER
3	C	337	GLN
3	C	339	PHE
3	C	355	GLU
3	C	356	PHE
3	C	358	LYS
3	C	365	TYR
3	C	384	ARG
3	C	397	MET
3	C	416	LEU
3	C	419	TYR
3	C	421	ARG
3	C	429	THR
3	C	465	LYS
3	C	482	MET
3	C	485	CYS
3	C	508	ASP
3	C	525	LYS
3	C	527	LEU
3	C	537	GLU
3	C	550	TYR
3	C	560	ARG
3	C	566	LEU
3	C	572	VAL
3	C	585	ASP
3	C	591	VAL
3	C	606	LYS
3	C	610	GLU
3	C	616	GLU
3	C	620	MET

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Mol	Chain	Res	Type
3	C	622	GLU
3	C	634	CYS
3	C	636	THR
3	C	640	GLU
3	C	643	GLU
3	C	649	THR
3	C	654	LEU
3	C	658	MET
3	C	662	ARG
3	C	676	VAL
3	C	690	LYS
3	C	700	ASN
3	C	709	LEU
3	C	710	ASP
3	C	721	ASN
3	C	725	ASP
3	C	729	LYS
3	C	747	ARG
3	C	749	LEU
3	C	763	LEU
3	C	770	GLU
3	C	772	ASN
3	C	773	LYS
3	C	781	ASP
3	C	784	ILE
3	C	785	GLN
3	C	787	PHE
3	C	789	TRP
3	C	809	LEU
3	C	810	ASP
3	C	826	ILE
3	C	839	MET
3	C	843	ARG
3	C	849	TYR
3	C	855	THR
3	C	858	ASP
3	C	865	ASN
3	C	874	VAL
3	C	878	VAL
3	C	895	VAL
3	C	901	GLU
3	C	902	THR

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Mol	Chain	Res	Type
3	C	905	ARG
3	C	932	SER
3	C	936	ARG
3	C	938	LEU
3	C	948	ARG
3	C	961	SER
4	E	53	ASN
4	E	54	LEU
4	E	72	ARG
4	E	76	ASP
4	E	96	ASP
4	E	103	VAL
4	E	104	ILE
4	E	118	THR
4	E	127	SER
4	E	130	LYS
4	E	157	CYS
4	E	181	ARG
4	E	184	LYS
4	E	200	PHE
4	E	202	ASP
4	E	212	VAL
4	E	214	ASN
4	E	223	ARG
4	E	228	ASP
4	E	232	SER
4	E	243	THR
4	E	256	SER
4	E	265	GLU
4	E	266	TRP
4	E	277	CYS
4	E	284	HIS
4	E	288	PHE
4	E	300	ASP
4	E	302	SER
4	E	306	CYS
4	E	311	ARG
4	E	333	SER
4	E	337	VAL
6	q	1	MET
6	q	3	CYS
6	q	12	GLN

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Mol	Chain	Res	Type
6	q	18	LYS
6	q	33	ARG
6	q	46	SER
6	q	48	GLU
6	q	50	LEU
6	q	72	LEU
6	q	78	ASP
6	q	92	THR
6	q	97	THR
6	q	113	ARG
6	q	114	VAL
6	q	117	ARG
6	r	2	PHE
6	r	6	SER
6	r	12	GLN
6	r	14	VAL
6	r	31	TYR
6	r	41	THR
6	r	45	LEU
6	r	55	VAL
6	r	57	LYS
6	r	59	VAL
6	r	63	THR
6	r	67	THR
6	r	88	HIS
6	r	95	HIS
6	r	106	TYR
6	r	113	ARG
6	r	115	ILE
6	r	119	LEU
6	r	120	LYS
6	r	129	LEU
6	s	74	SER
6	s	84	MET
6	s	85	LEU
6	s	113	ARG
6	s	131	ASP
6	t	74	SER
6	t	75	LEU
6	t	80	TRP
6	t	88	HIS
6	t	105	LEU

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Mol	Chain	Res	Type
6	t	108	HIS
6	t	117	ARG
6	t	119	LEU
6	t	123	ASP
7	a	19	GLU
7	a	34	ARG
7	a	47	GLN
7	a	57	ASP
7	a	59	ARG
7	a	61	THR
7	a	66	LEU
7	a	68	ILE
7	a	89	LYS
7	a	90	ARG
8	g	21	LEU
8	g	24	ASN
8	g	27	VAL
8	g	38	MET
8	g	53	ASP
8	g	56	MET
8	g	60	ARG
8	g	65	GLN
8	g	70	LEU
9	e	9	MET
9	e	24	GLN
9	e	35	ASP
9	e	50	ASN
9	e	55	GLU
9	e	61	MET
9	e	63	ARG
9	e	77	ASP
9	e	82	ILE
9	e	85	THR
10	f	12	PHE
10	f	23	VAL
10	f	42	MET
10	f	48	SER
10	f	63	GLU
10	f	68	CYS
10	f	69	ASN
10	f	74	LEU
11	d	17	GLU

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Mol	Chain	Res	Type
11	d	22	THR
11	d	42	CYS
11	d	44	ASN
11	d	51	ARG
11	d	63	LEU
11	d	68	GLU
11	d	69	MET
11	d	71	THR
11	d	81	LYS
11	d	84	ARG
11	d	98	ARG
12	c	2	VAL
12	c	6	ARG
12	c	21	LYS
12	c	24	THR
12	c	38	ASN
12	c	45	LYS
12	c	49	ARG
12	c	62	ARG
12	c	64	ASN
12	c	75	LEU
12	c	85	ASP
13	b	9	LEU
13	b	20	THR
13	b	25	ARG
13	b	30	ARG
13	b	44	ASP
13	b	55	LYS
13	b	61	GLU
13	b	62	ARG
14	I	347	ASP
14	I	354	GLU
14	I	356	LEU
14	I	365	SER
14	I	367	VAL
14	I	370	ARG
14	I	382	ARG
14	I	384	LYS
14	I	392	LYS
14	I	395	LEU
14	I	402	ARG
14	I	412	LYS

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Mol	Chain	Res	Type
14	I	416	LEU
14	I	420	PHE
14	I	434	ARG
14	I	438	GLN
14	I	444	ARG
14	I	456	CYS
14	I	466	SER
14	I	473	ASP
14	I	480	THR
14	I	487	ARG
14	I	492	GLU
14	I	500	ASP
14	I	537	ILE
14	I	546	TYR
14	I	548	LEU
14	I	601	LEU
14	I	613	GLU
14	I	614	CYS
14	I	615	LYS
14	I	628	TYR
14	I	640	ARG
14	I	651	LYS
14	I	655	ASP
14	I	659	SER
14	I	670	VAL
14	I	687	SER
14	I	688	ASP
14	I	692	ARG
14	I	702	GLU
14	I	712	ARG
14	I	735	ARG
14	I	737	PHE
14	I	745	ASP
14	I	746	THR
14	I	747	PHE
14	I	752	ARG
14	I	758	LYS
15	J	24	ILE
15	J	38	LEU
15	J	54	GLU
15	J	57	GLU
15	J	61	SER

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Mol	Chain	Res	Type
15	J	65	GLN
15	J	71	ARG
15	J	77	ASN
15	J	96	ARG
15	J	126	ARG
15	J	139	VAL
15	J	140	SER
15	J	144	ARG
15	J	167	GLN
15	J	175	PHE
15	J	196	ASP
15	J	202	PHE
15	J	213	LYS
15	J	223	MET
15	J	237	ARG
15	J	242	LEU
15	J	244	GLU
15	J	247	GLN
15	J	248	THR
15	J	249	GLU
15	J	255	PHE
15	J	257	GLU
15	J	273	ARG
15	J	279	ILE
15	J	288	TYR
15	J	311	LYS
15	J	313	ARG
16	P	13	ILE
16	P	40	LYS
16	P	48	GLN
16	P	62	GLU
16	P	68	ARG
16	P	194	ARG
16	P	199	ASP
16	P	204	ASN
16	P	211	LYS
16	P	231	GLN
16	P	234	ILE
17	M	447	GLN
17	M	464	GLU
17	M	484	LYS
17	M	499	MET

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Mol	Chain	Res	Type
17	M	531	ARG
17	M	535	PHE
17	M	538	LYS
18	T	190	ARG
18	T	199	MET
18	T	212	CYS
18	T	213	VAL
18	T	216	ASP
18	T	270	ASP
18	T	286	SER
18	T	306	LEU
18	T	312	ASP
18	T	314	VAL
18	T	323	LYS
18	T	353	HIS
18	T	377	SER
18	T	383	MET
18	T	388	PHE
18	T	396	GLU
18	T	414	SER
18	T	446	ARG
18	T	450	CYS
18	T	462	SER
18	T	464	GLU
18	T	465	SER
18	T	469	LEU
18	T	485	GLU
18	T	497	GLU
18	T	498	ASP
18	T	510	ARG
18	T	514	ASP
19	O	24	GLU
19	O	35	MET
19	O	49	ARG
19	O	68	VAL
19	O	70	CYS
19	O	83	CYS
19	O	110	SER
19	O	111	GLU
19	O	151	LEU
19	O	154	SER
19	O	157	TYR

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Mol	Chain	Res	Type
19	O	164	ARG
19	O	165	VAL
19	O	180	CYS
19	O	206	ASN
19	O	224	THR
19	O	233	THR
19	O	282	LYS
20	N	10	LYS
20	N	21	GLU
20	N	23	ILE
20	N	41	LYS
20	N	72	SER
20	N	82	GLU
20	N	118	SER
20	N	134	THR
20	N	146	SER
20	N	169	LEU
20	N	176	TRP
21	R	39	LEU
21	R	42	LYS
21	R	83	ILE
21	R	88	LYS
21	R	97	VAL
21	R	105	ARG
21	R	110	ASP
21	R	114	LEU
21	R	117	LYS
21	R	118	VAL
21	R	119	ASP
21	R	128	ARG
21	R	146	GLU
21	R	152	LYS
21	R	154	SER
21	R	155	SER
21	R	161	LEU
21	R	168	SER
21	R	174	THR
21	R	195	ASP
21	R	211	VAL
21	R	220	VAL
21	R	223	LEU
21	R	231	THR

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Mol	Chain	Res	Type
21	R	233	LYS
21	R	236	GLN
21	R	257	LEU
21	R	259	LYS
21	R	264	ASP
21	R	286	THR
23	S	9	ASP
23	S	28	CYS
23	S	73	LYS
23	S	80	ARG
23	S	85	THR
23	S	91	SER
23	S	133	ARG
23	S	134	LEU
23	S	146	VAL
24	W	47	THR
24	W	50	VAL
24	W	51	LEU
24	W	65	LEU
24	W	66	GLN
24	W	72	LYS
24	W	77	LEU
24	W	81	ASP
24	W	87	LEU
24	W	89	PRO
24	W	91	HIS
24	W	102	LEU
24	W	107	VAL
24	W	112	ASP
24	W	118	ILE
24	W	122	GLN
24	W	134	GLU
24	W	139	ILE
24	W	167	THR
24	W	171	ARG
24	W	202	SER
24	W	212	GLU
24	W	225	LYS
25	L	24	LYS
25	L	35	SER
25	L	38	VAL
25	L	61	GLU

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Mol	Chain	Res	Type
25	L	70	LEU
25	L	103	LEU
25	L	120	ARG
25	L	122	LEU
25	L	130	ASN
25	L	148	LYS
25	L	152	SER
25	L	161	THR
25	L	171	ARG
25	L	175	LEU
25	L	180	ARG
25	L	183	GLN
25	L	184	LEU
25	L	217	LEU
25	L	220	GLN
25	L	237	GLN
25	L	541	ASP
25	L	543	ARG
25	L	545	ARG
25	L	548	ARG
25	L	552	GLU
25	L	553	ARG
25	L	563	LYS
25	L	571	ARG
25	L	596	LEU
25	L	599	ARG
25	L	614	HIS
25	L	619	TYR
25	L	622	LYS
25	L	654	SER
25	L	660	ASP
25	L	665	TYR
25	L	675	LEU
25	L	696	SER
25	L	699	ARG
25	L	702	ARG
25	L	718	GLU
25	L	720	ASP
25	L	731	LYS
25	L	748	GLN
25	L	749	ARG
25	L	757	ARG

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Mol	Chain	Res	Type
25	L	779	HIS
25	L	780	GLU
25	L	781	ARG
25	L	800	THR
25	L	816	ARG
25	L	817	ARG
25	L	818	ARG
25	L	828	LYS
25	L	833	SER
26	K	28	HIS
26	K	29	LEU
26	K	55	LYS
26	K	58	SER
26	K	59	THR
26	K	65	TYR
26	K	68	GLU
26	K	69	MET
26	K	77	PHE
26	K	86	GLU
26	K	87	TYR
26	K	94	GLU
26	K	104	TYR
26	K	105	ARG
26	K	114	ARG
26	K	116	ASP
26	K	122	SER
26	K	123	SER
26	K	130	GLN
26	K	131	LEU
26	K	136	LEU
26	K	145	LEU
26	K	149	ASP
26	K	159	ASP
26	K	177	THR
26	K	188	GLN
26	K	197	LYS
26	K	202	TYR
26	K	205	GLN
26	K	208	LYS
26	K	214	ARG
26	K	216	CYS
26	K	226	MET

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Mol	Chain	Res	Type
27	U	2	TYR
27	U	15	THR
27	U	19	VAL
27	U	23	LYS
28	V	656	ARG
28	V	658	THR
28	V	668	ASP
28	V	669	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	124	HIS
1	A	132	HIS
1	A	269	HIS
1	A	279	ASN
1	A	311	ASN
1	A	379	ASN
1	A	391	HIS
1	A	461	ASN
1	A	481	HIS
1	A	492	ASN
1	A	496	GLN
1	A	512	GLN
1	A	521	ASN
1	A	581	HIS
1	A	625	ASN
1	A	627	GLN
1	A	648	HIS
1	A	674	HIS
1	A	728	GLN
1	A	739	GLN
1	A	744	HIS
1	A	755	HIS
1	A	809	GLN
1	A	852	GLN
1	A	855	GLN
1	A	895	ASN
1	A	939	HIS
1	A	948	HIS
1	A	952	GLN

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Mol	Chain	Res	Type
1	A	968	HIS
1	A	1024	ASN
1	A	1025	ASN
1	A	1033	ASN
1	A	1078	ASN
1	A	1133	ASN
1	A	1147	HIS
1	A	1157	ASN
1	A	1160	HIS
1	A	1175	GLN
1	A	1194	ASN
1	A	1223	ASN
1	A	1246	ASN
1	A	1282	ASN
1	A	1284	HIS
1	A	1291	GLN
1	A	1310	GLN
1	A	1325	ASN
1	A	1346	GLN
1	A	1357	ASN
1	A	1360	GLN
1	A	1401	GLN
1	A	1437	GLN
1	A	1464	ASN
1	A	1504	GLN
1	A	1521	HIS
1	A	1524	HIS
1	A	1616	GLN
1	A	1639	GLN
1	A	1702	ASN
1	A	1801	ASN
3	C	68	HIS
3	C	133	ASN
3	C	147	HIS
3	C	214	ASN
3	C	337	GLN
3	C	388	GLN
3	C	502	GLN
3	C	757	GLN
3	C	760	ASN
3	C	865	ASN
3	C	915	GLN

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Mol	Chain	Res	Type
3	C	944	GLN
4	E	100	ASN
4	E	275	ASN
4	E	284	HIS
4	E	330	HIS
6	q	83	ASN
6	q	95	HIS
6	q	99	GLN
6	r	21	HIS
6	r	56	ASN
6	r	108	HIS
6	t	88	HIS
6	t	107	GLN
7	a	16	HIS
7	a	47	GLN
7	a	84	ASN
8	g	65	GLN
9	e	21	GLN
9	e	27	GLN
9	e	50	ASN
9	e	78	ASN
11	d	44	ASN
11	d	58	HIS
11	d	80	GLN
12	c	65	ASN
12	c	76	ASN
14	I	374	HIS
14	I	393	GLN
14	I	427	HIS
14	I	432	ASN
14	I	445	HIS
14	I	453	HIS
14	I	465	HIS
14	I	512	HIS
14	I	545	ASN
14	I	553	GLN
14	I	743	ASN
15	J	154	HIS
15	J	207	GLN
15	J	224	GLN
15	J	247	GLN
16	P	38	HIS

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Mol	Chain	Res	Type
16	P	48	GLN
17	M	495	ASN
17	M	540	GLN
18	T	261	HIS
18	T	347	GLN
18	T	353	HIS
19	O	45	HIS
19	O	60	ASN
19	O	71	GLN
19	O	119	GLN
19	O	149	GLN
19	O	152	GLN
20	N	29	GLN
20	N	51	HIS
20	N	111	ASN
20	N	119	HIS
20	N	138	GLN
20	N	172	ASN
21	R	79	GLN
21	R	150	GLN
21	R	235	GLN
21	R	236	GLN
21	R	274	ASN
23	S	30	ASN
23	S	98	ASN
23	S	138	GLN
24	W	66	GLN
24	W	91	HIS
24	W	114	HIS
24	W	125	HIS
24	W	195	GLN
24	W	198	GLN
25	L	29	GLN
25	L	130	ASN
25	L	568	GLN
25	L	688	HIS
26	K	26	ASN
26	K	28	HIS
26	K	134	GLN
26	K	187	GLN
26	K	233	HIS
28	V	674	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	83/111 (74%)	48 (57%)	2 (2%)
22	H	39/192 (20%)	28 (71%)	3 (7%)
30	5	6/7 (85%)	1 (16%)	0
31	3	33/173 (19%)	16 (48%)	6 (18%)
5	F	90/101 (89%)	48 (53%)	5 (5%)
All	All	251/584 (42%)	141 (56%)	16 (6%)

All (141) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	A
2	B	9	C
2	B	10	G
2	B	11	A
2	B	15	G
2	B	16	A
2	B	17	A
2	B	20	C
2	B	27	A
2	B	28	A
2	B	35	U
2	B	39	G
2	B	40	C
2	B	41	C
2	B	42	U
2	B	48	U
2	B	49	A
2	B	52	G
2	B	53	A
2	B	58	C
2	B	59	G
2	B	62	A
2	B	63	G
2	B	64	U
2	B	65	U
2	B	66	U
2	B	68	G
2	B	69	C
2	B	70	U
2	B	71	C
2	B	72	A

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Mol	Chain	Res	Type
2	B	73	C
2	B	74	G
2	B	75	C
2	B	76	A
2	B	77	G
2	B	79	C
2	B	80	G
2	B	88	A
2	B	89	U
2	B	90	C
2	B	91	U
2	B	92	U
2	B	94	U
2	B	95	U
2	B	96	G
2	B	97	U
2	B	98	G
5	F	4	C
5	F	5	U
5	F	6	U
5	F	7	C
5	F	8	G
5	F	9	G
5	F	13	A
5	F	14	A
5	F	19	U
5	F	20	A
5	F	21	A
5	F	22	A
5	F	24	U
5	F	26	G
5	F	27	G
5	F	29	A
5	F	37	G
5	F	40	A
5	F	41	A
5	F	42	G
5	F	47	G
5	F	51	G
5	F	61	C
5	F	62	A
5	F	67	U

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Mol	Chain	Res	Type
5	F	68	G
5	F	71	A
5	F	72	C
5	F	73	G
5	F	74	C
5	F	75	A
5	F	76	U
5	F	77	A
5	F	78	A
5	F	79	A
5	F	80	U
5	F	81	C
5	F	82	G
5	F	83	A
5	F	84	G
5	F	85	A
5	F	86	A
5	F	87	A
5	F	88	U
5	F	89	G
5	F	90	G
5	F	91	U
5	F	92	U
22	H	2	U
22	H	3	A
22	H	4	C
22	H	5	C
22	H	6	U
22	H	7	U
22	H	8	U
22	H	9	C
22	H	10	U
22	H	11	C
22	H	12	G
22	H	13	G
22	H	14	C
22	H	16	U
22	H	17	U
22	H	18	U
22	H	19	U
22	H	20	G
22	H	21	G

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Mol	Chain	Res	Type
22	H	24	C
22	H	25	A
22	H	26	G
22	H	30	A
22	H	31	U
22	H	32	G
22	H	34	G
22	H	38	U
22	H	40	U
30	5	-6	C
31	3	2	U
31	3	3	A
31	3	7	G
31	3	8	C
31	3	12	G
31	3	13	C
31	3	14	A
31	3	17	A
31	3	19	U
31	3	20	A
31	3	21	C
31	3	22	U
31	3	91	A
31	3	96	U
31	3	98	U
31	3	100	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	16	A
2	B	97	U
5	F	19	U
5	F	26	G
5	F	76	U
5	F	78	A
5	F	80	U
22	H	6	U
22	H	30	A
22	H	31	U
31	3	16	U
31	3	20	A

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Mol	Chain	Res	Type
31	3	21	C
31	3	90	C
31	3	95	U
31	3	97	A

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

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
21	SEP	R	225	21	8,9,10	1.19	1 (12%)	8,12,14	1.31	2 (25%)
21	SEP	R	217	21	8,9,10	1.16	1 (12%)	8,12,14	1.38	1 (12%)

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
21	SEP	R	225	21	-	0/5/8/10	-
21	SEP	R	217	21	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	R	217	SEP	P-O1P	2.38	1.58	1.50
21	R	225	SEP	P-O1P	2.18	1.57	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	217	SEP	O2P-P-OG	3.08	114.92	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	225	SEP	OG-CB-CA	2.72	110.79	108.14
21	R	225	SEP	O3P-P-OG	2.09	112.30	106.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	R	217	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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
32	GTP	C	1001	33	26,34,34	1.11	3 (11%)	32,54,54	0.89	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	GTP	C	1001	33	-	5/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	1001	GTP	C5-C6	-2.67	1.42	1.47
32	C	1001	GTP	C8-N7	-2.23	1.31	1.35
32	C	1001	GTP	C5-C4	-2.16	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	1001	GTP	C3'-C2'-C1'	2.08	104.11	100.98

There are no chirality outliers.

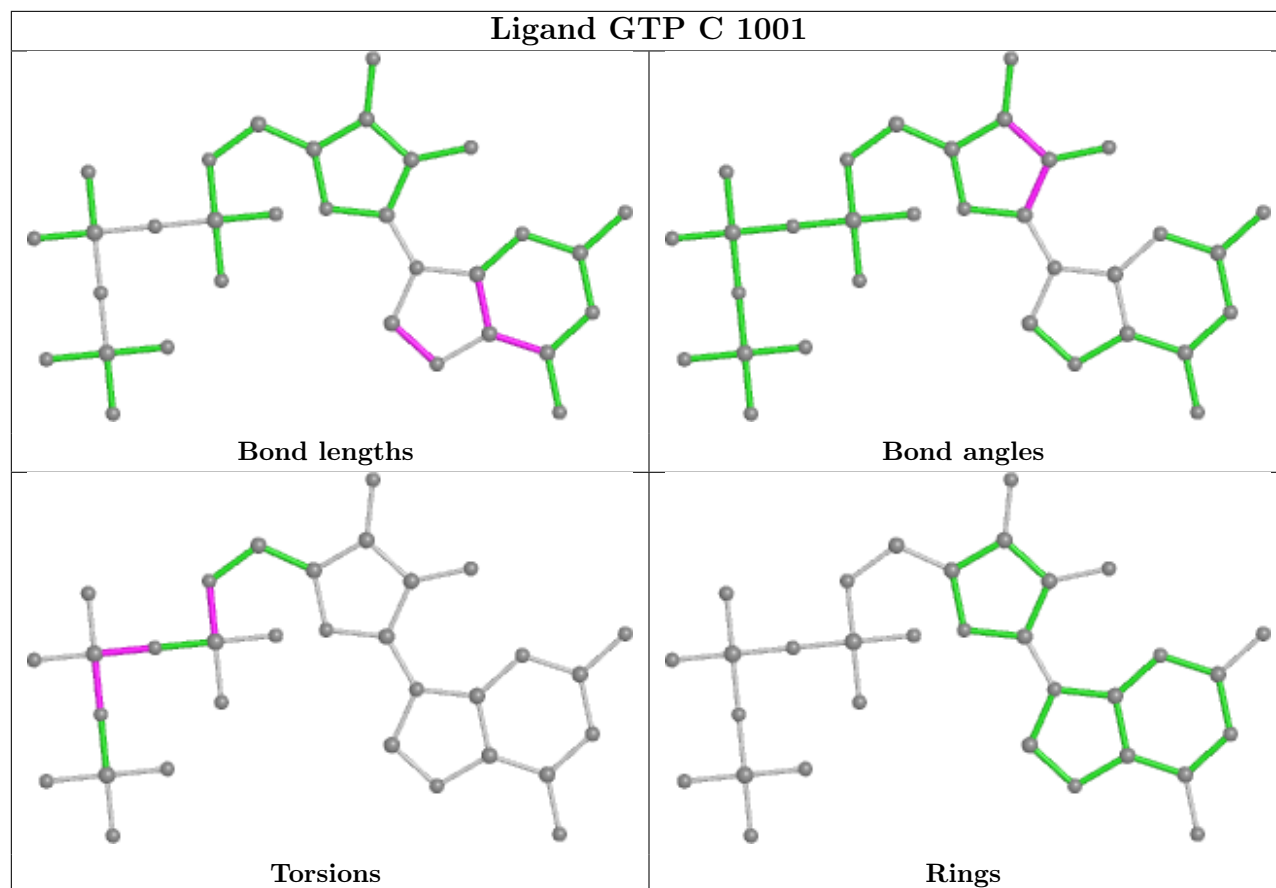
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	C	1001	GTP	C5'-O5'-PA-O1A
32	C	1001	GTP	C5'-O5'-PA-O2A
32	C	1001	GTP	PA-O3A-PB-O3B
32	C	1001	GTP	PG-O3B-PB-O2B
32	C	1001	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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.

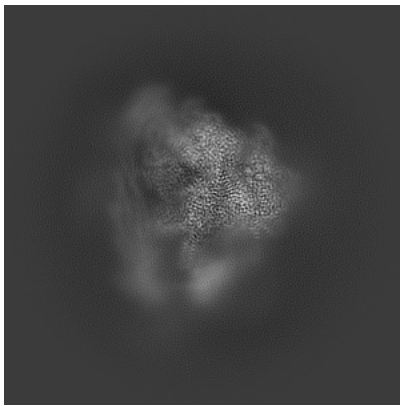
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38362. These allow visual inspection of the internal detail of the map and identification of artifacts.

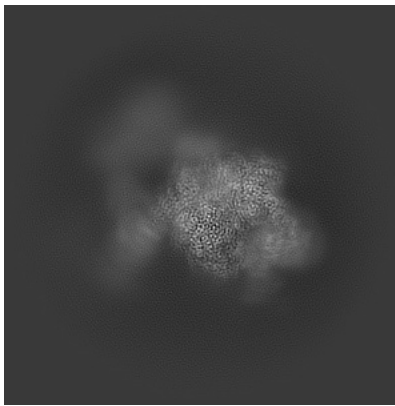
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

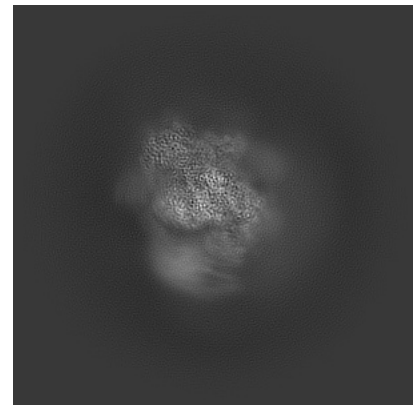
6.1.1 Primary map



X

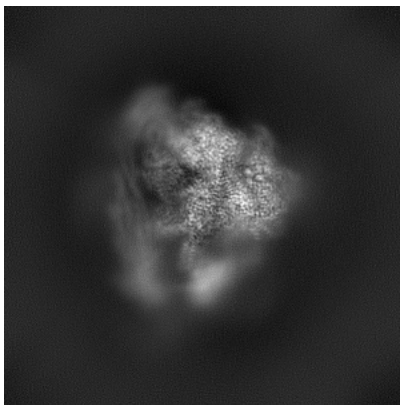


Y

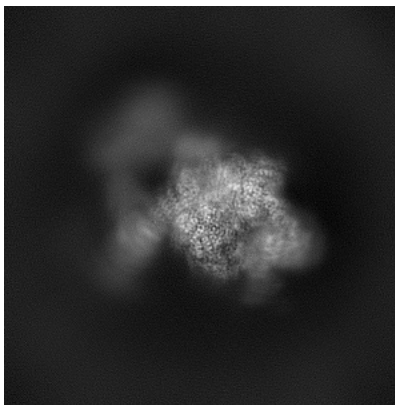


Z

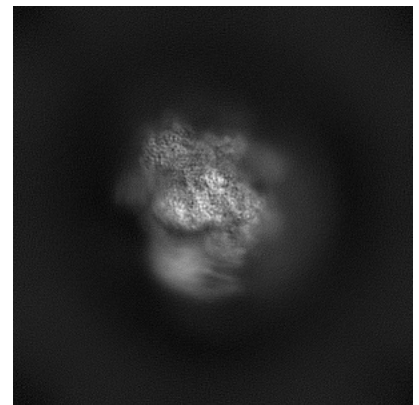
6.1.2 Raw map



X



Y

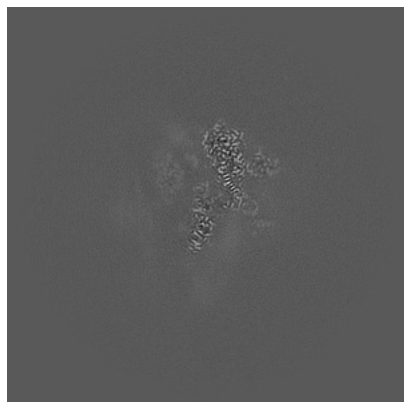


Z

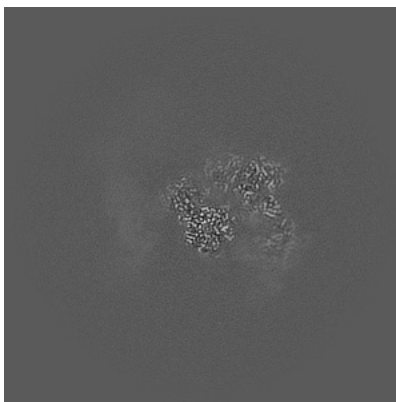
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

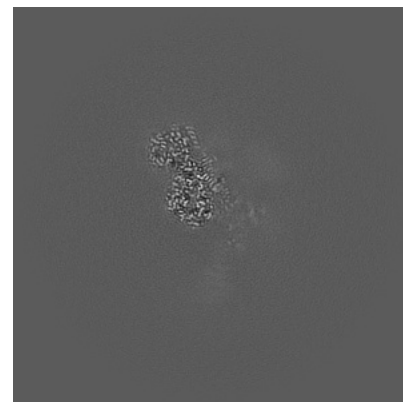
6.2.1 Primary map



X Index: 220



Y Index: 220

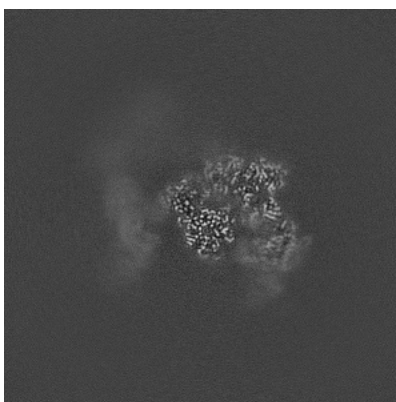


Z Index: 220

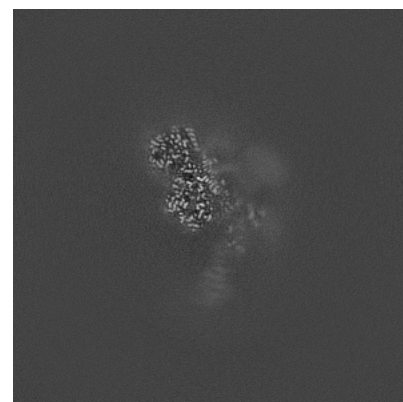
6.2.2 Raw map



X Index: 220



Y Index: 220

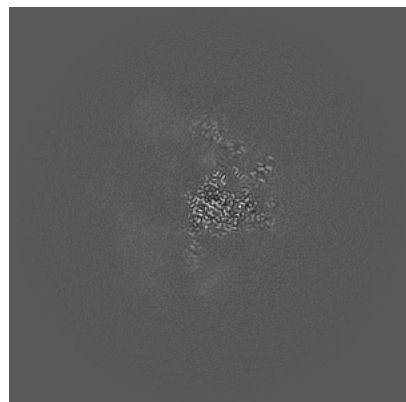


Z Index: 220

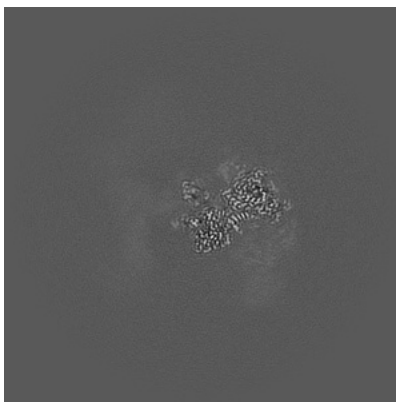
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

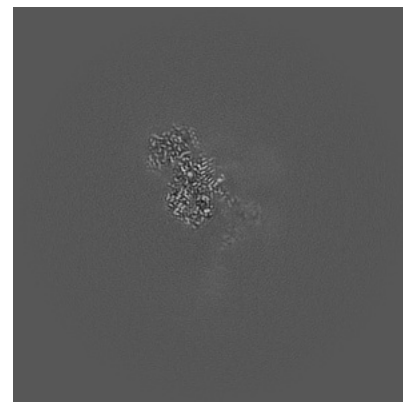
6.3.1 Primary map



X Index: 203

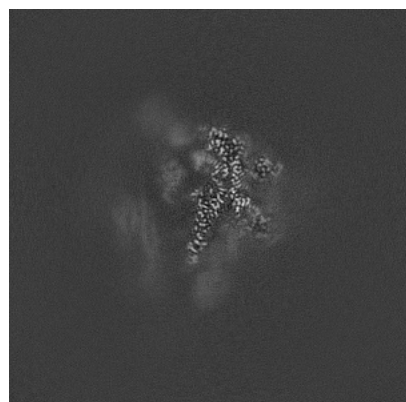


Y Index: 234

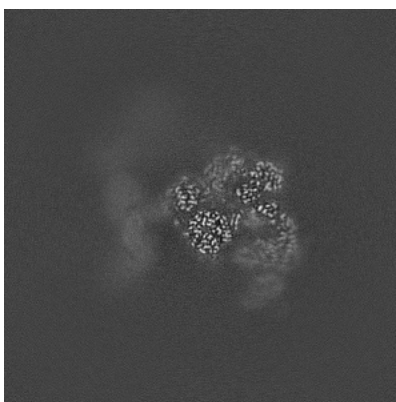


Z Index: 222

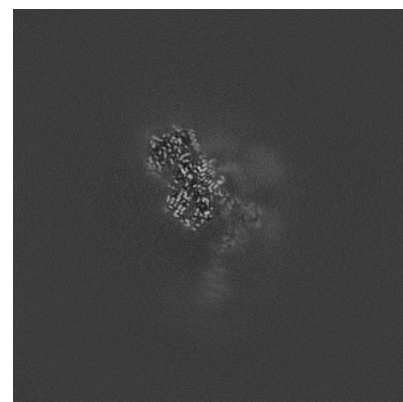
6.3.2 Raw map



X Index: 213



Y Index: 224

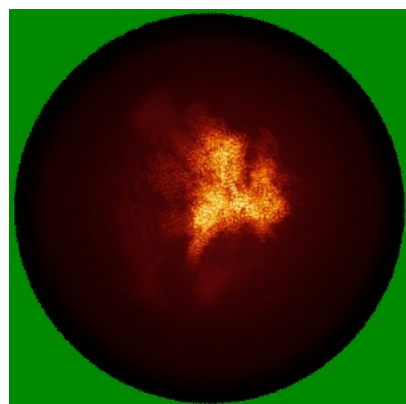


Z Index: 222

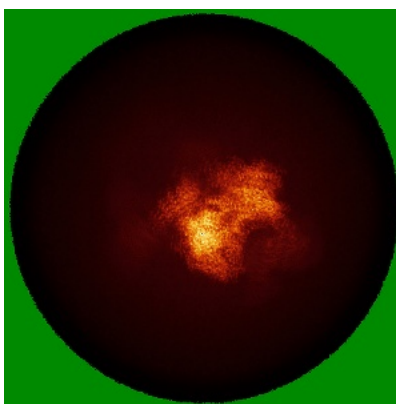
The images above show the largest variance slices of the map in three orthogonal directions.

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

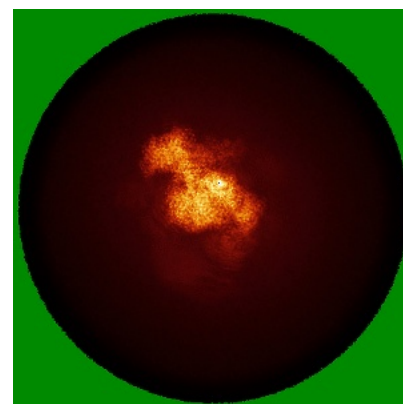
6.4.1 Primary map



X

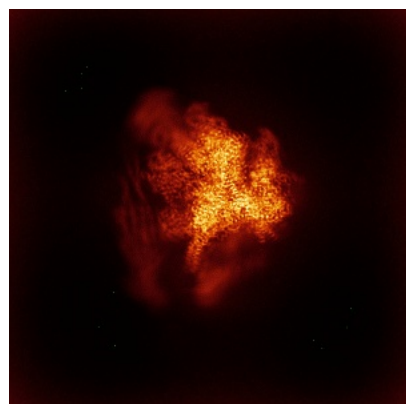


Y

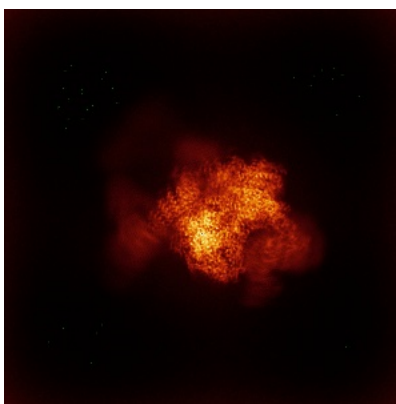


Z

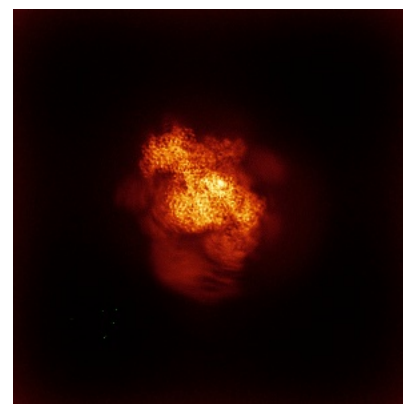
6.4.2 Raw map



X



Y

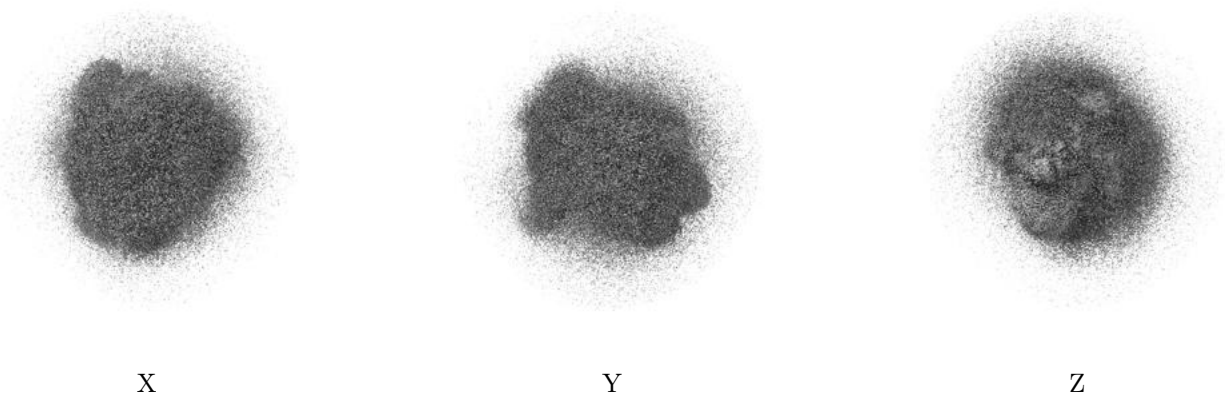


Z

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

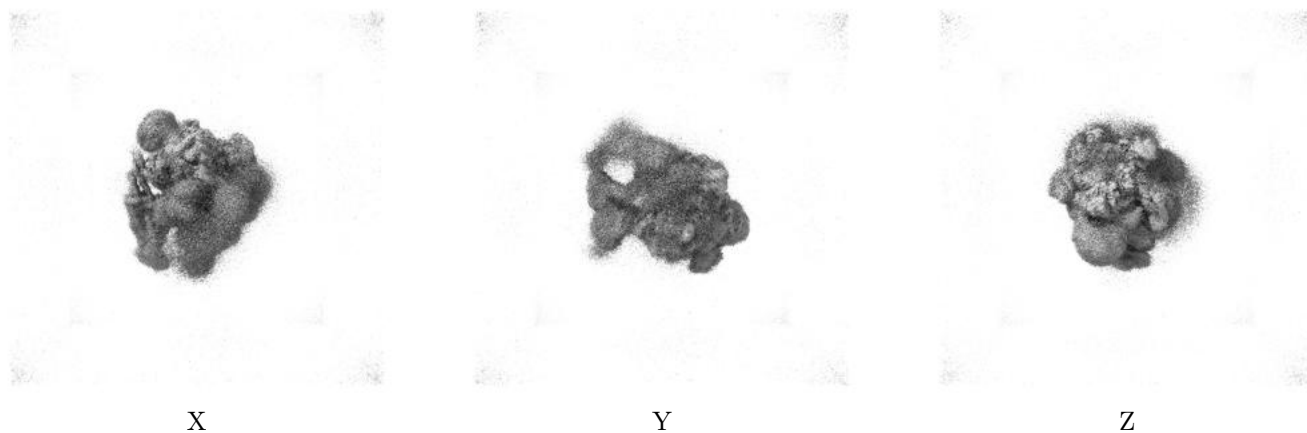
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

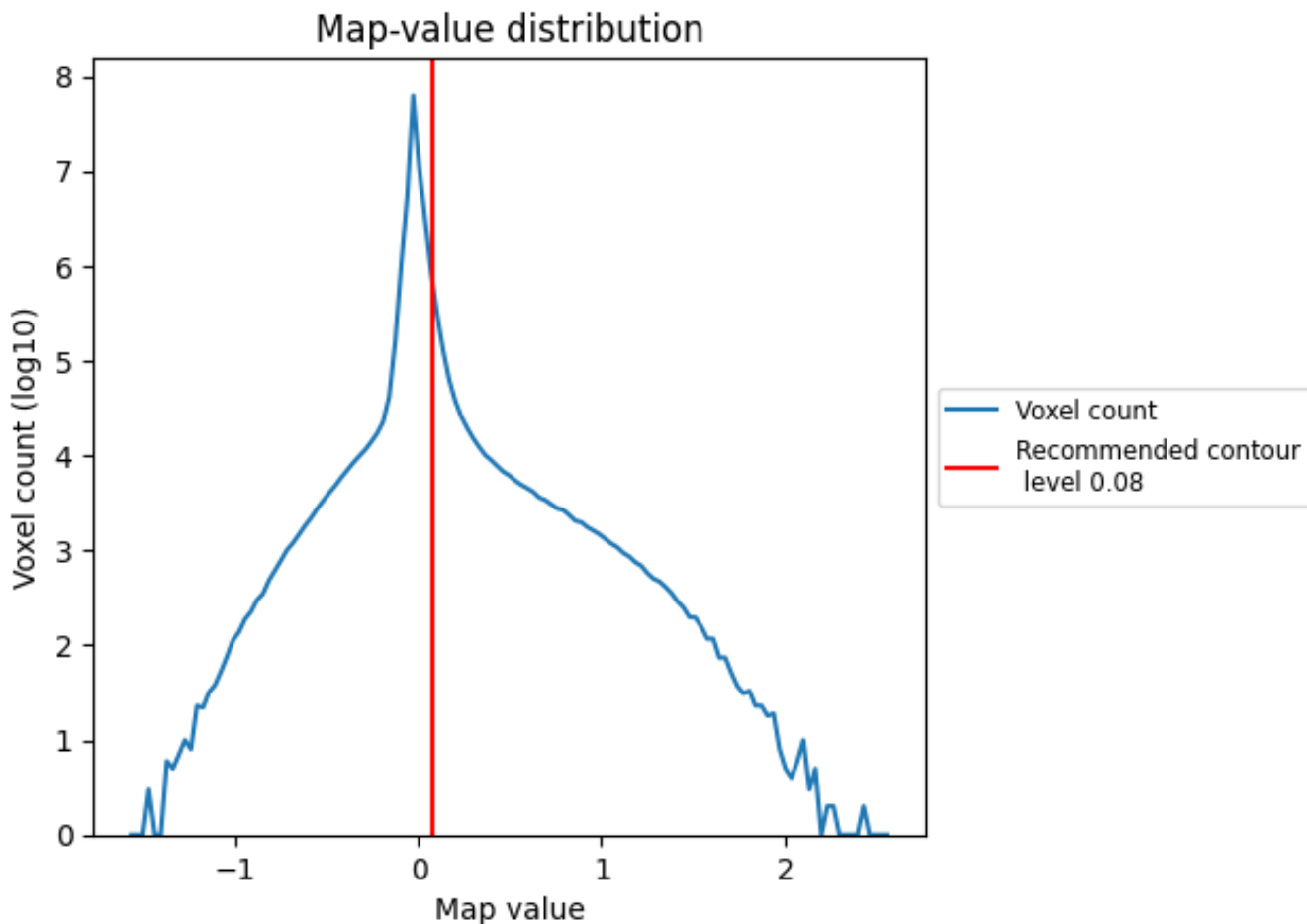
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

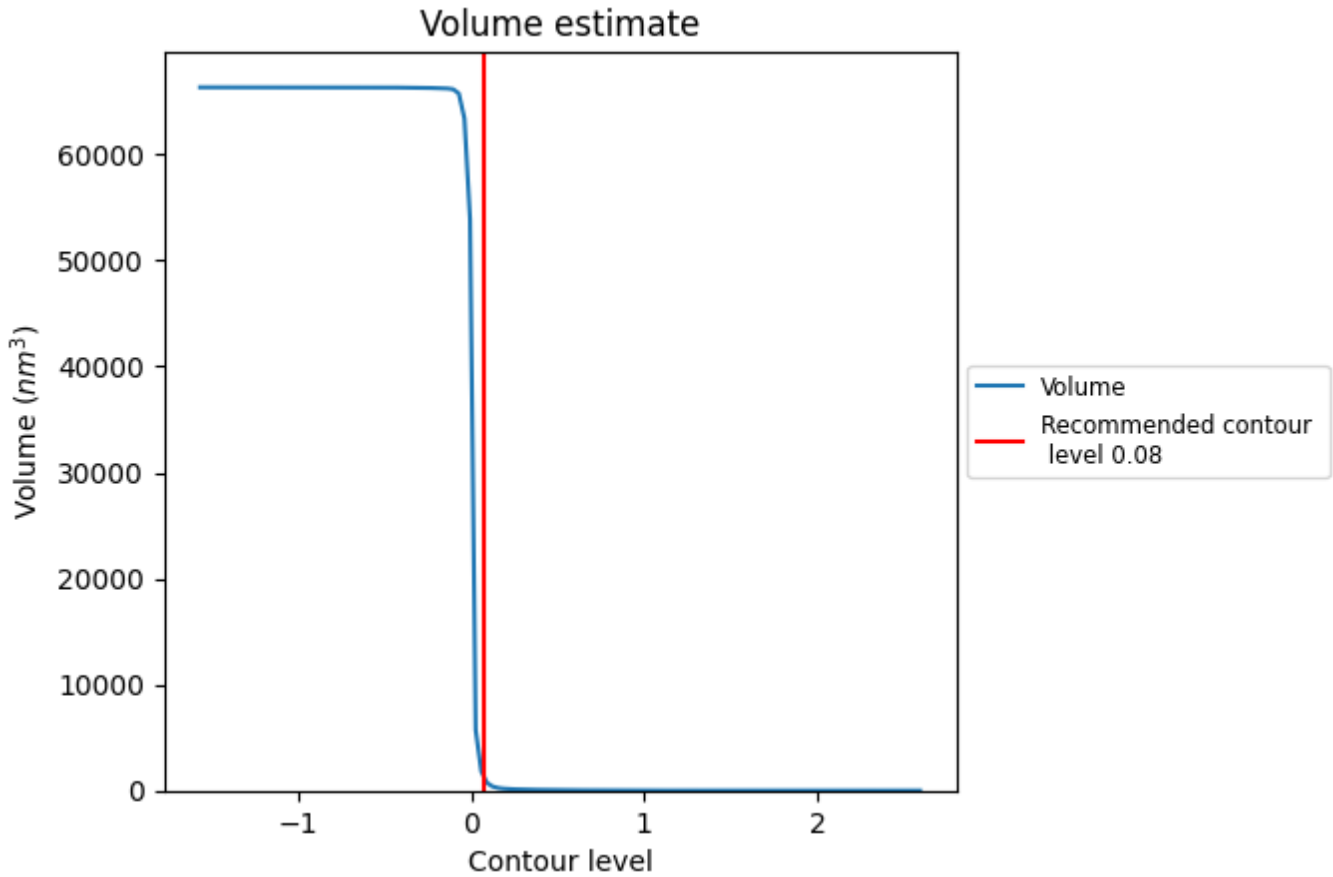
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

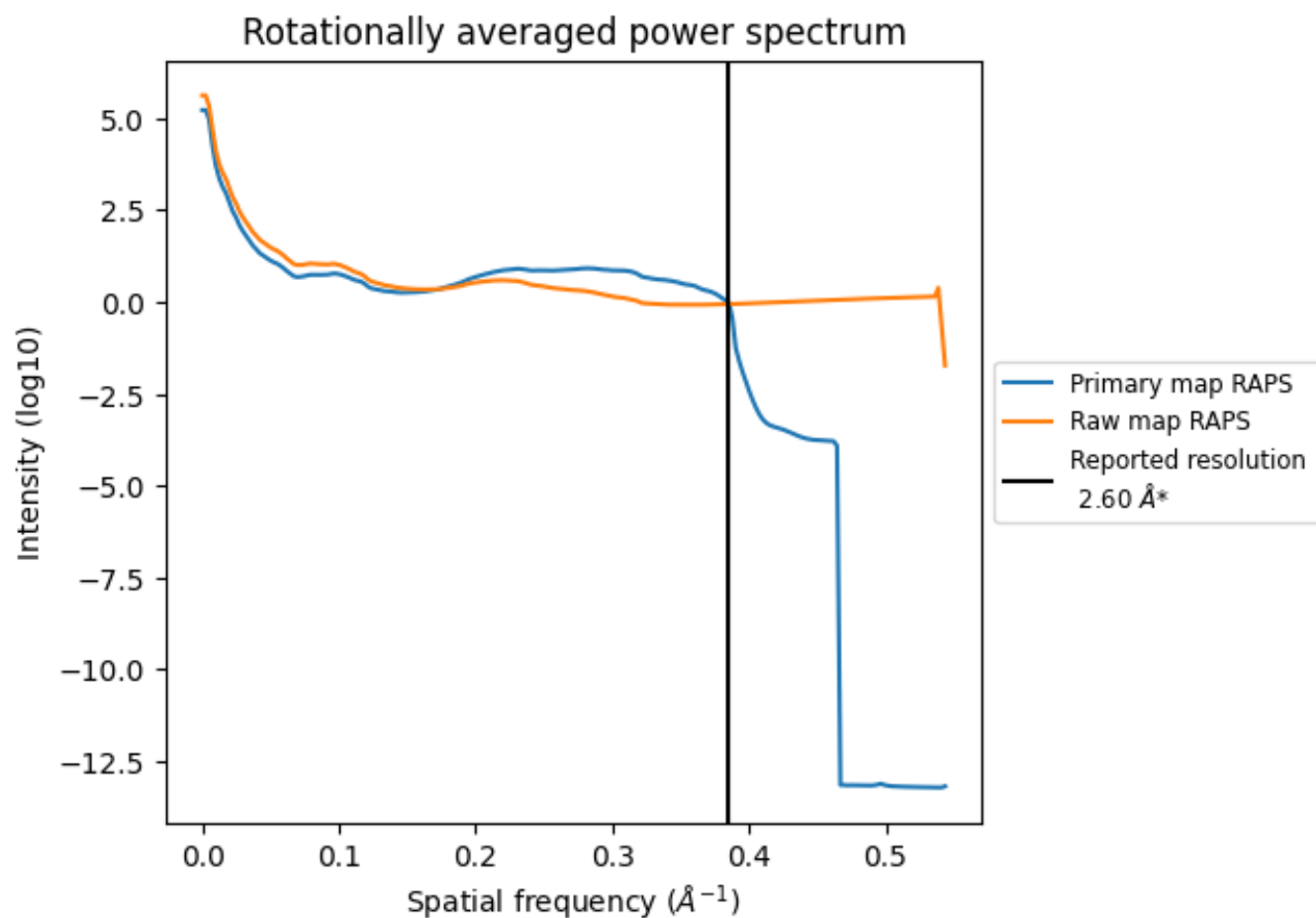
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1131 nm³; this corresponds to an approximate mass of 1022 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

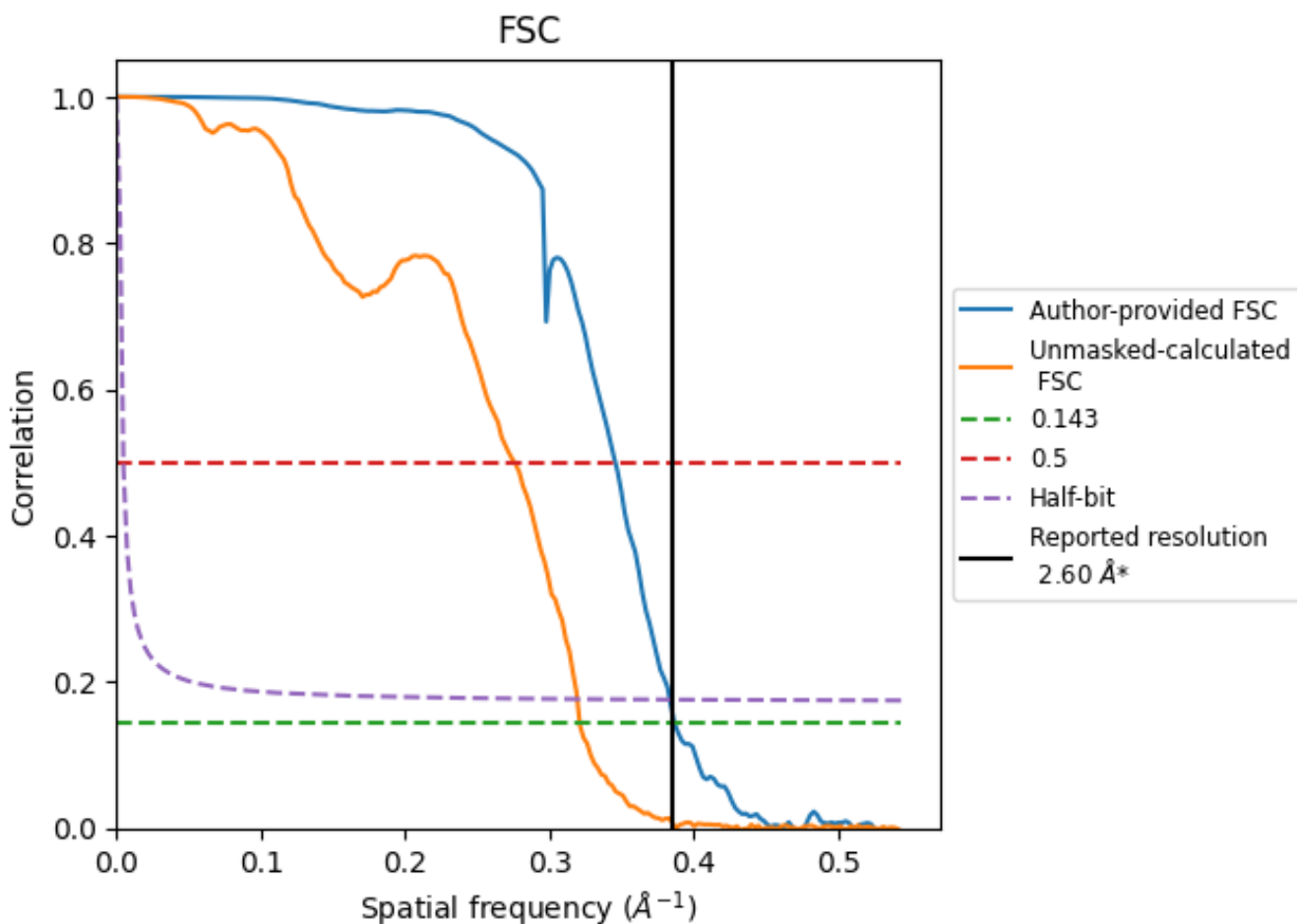


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385\AA^{-1}

8.2 Resolution estimates [i](#)

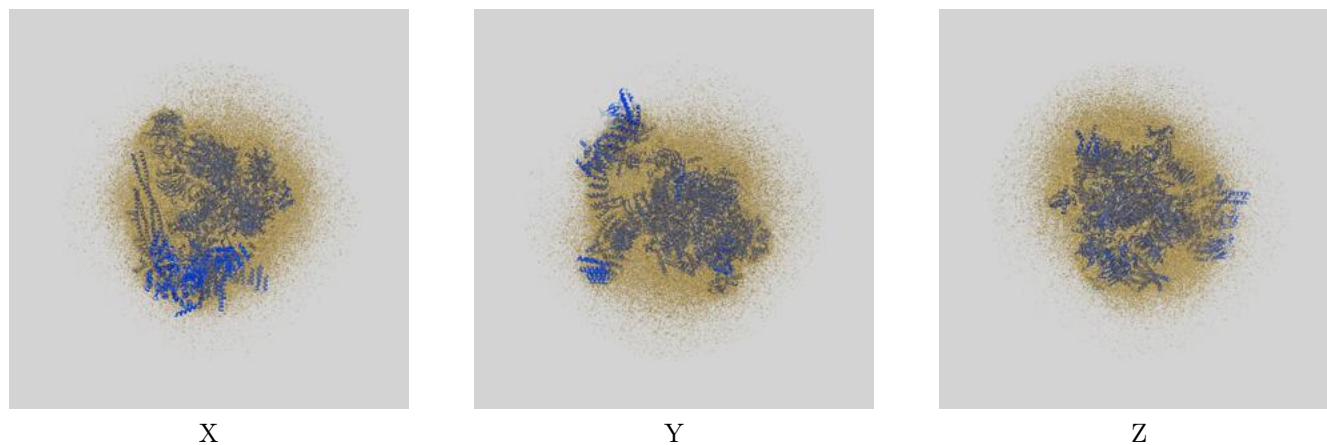
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	2.89	2.61
Unmasked-calculated*	3.12	3.63	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

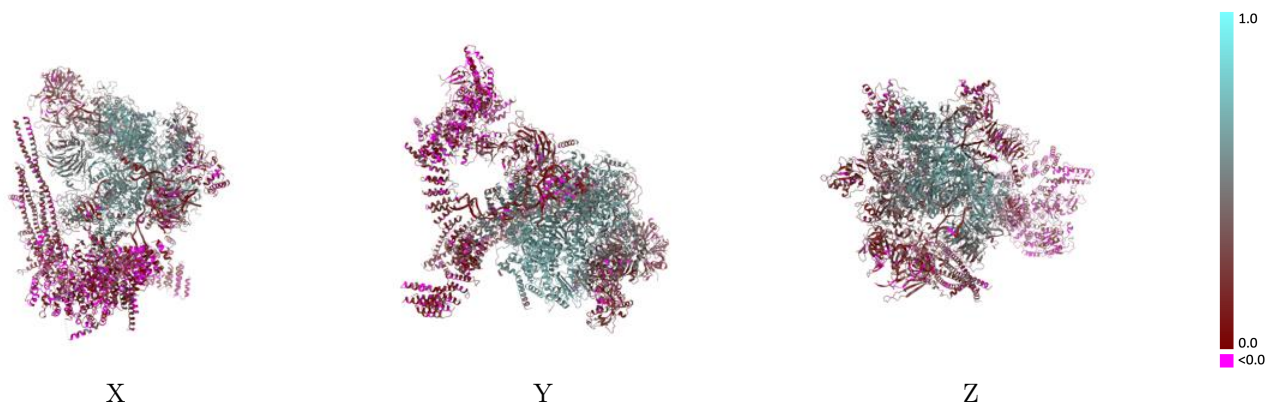
This section contains information regarding the fit between EMDB map EMD-38362 and PDB model 8XI2. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



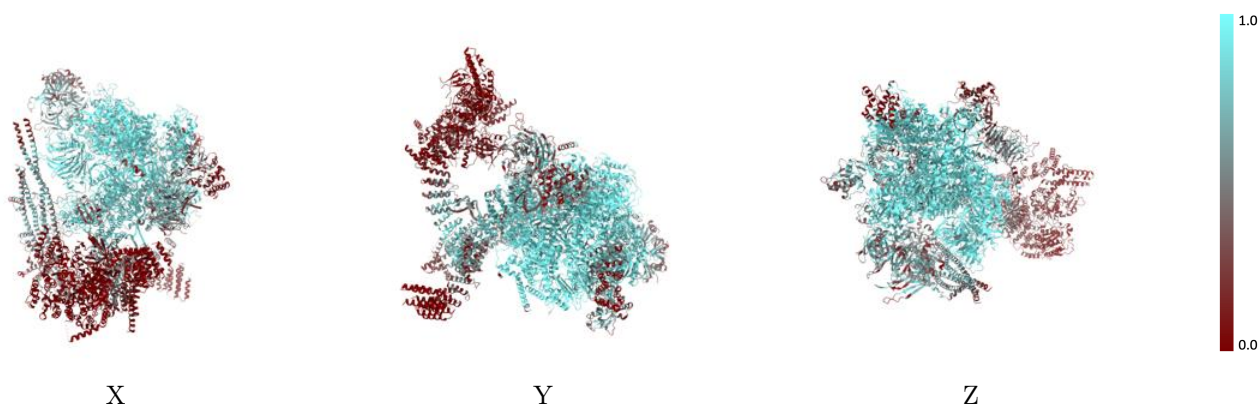
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



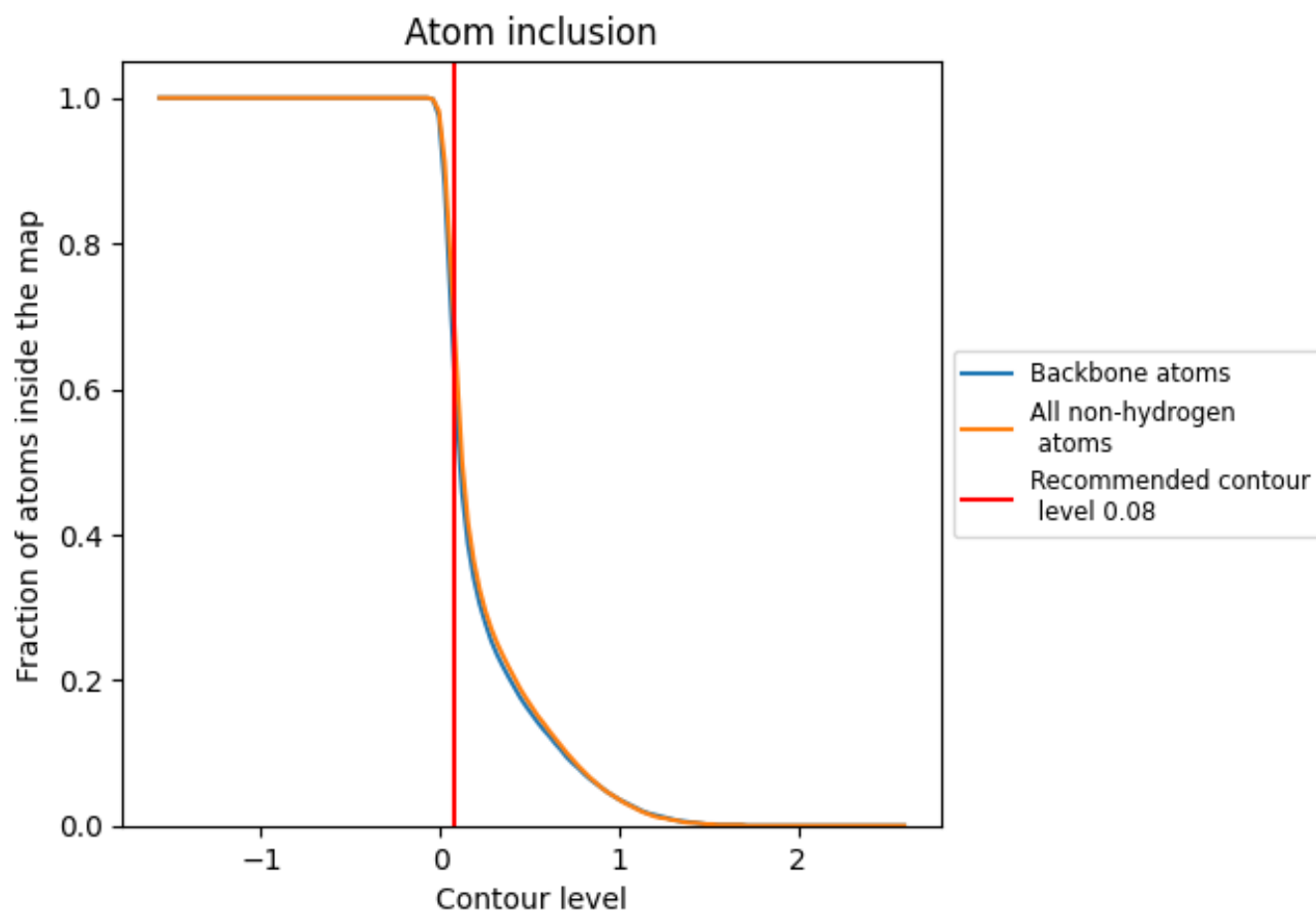
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 68% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6850	 0.3810
3	 0.7060	 0.2340
5	 0.9530	 0.6210
A	 0.8830	 0.5470
B	 0.8690	 0.3780
C	 0.7990	 0.3620
E	 0.9280	 0.4580
F	 0.9130	 0.4530
H	 0.6630	 0.2840
I	 0.4210	 0.1850
J	 0.6150	 0.3610
K	 0.4830	 0.2310
L	 0.6460	 0.3640
M	 0.7050	 0.3600
N	 0.9860	 0.6290
O	 0.7890	 0.4460
P	 0.9320	 0.5920
Q	 0.0410	 0.1050
R	 0.9330	 0.5620
S	 0.9540	 0.5290
T	 0.9960	 0.6770
U	 0.4390	 0.3290
V	 0.2680	 0.2470
W	 0.5890	 0.3040
a	 0.7190	 0.2760
b	 0.6710	 0.2880
c	 0.5790	 0.2130
d	 0.5490	 0.2310
e	 0.5280	 0.2160
f	 0.4730	 0.2010
g	 0.6610	 0.2630
q	 0.4630	 0.2050
r	 0.5790	 0.2140
s	 0.6220	 0.2370
t	 0.5040	 0.2050

