



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 03:29 PM UTC

PDB ID : 8Q91 / pdb_00008q91
EMDB ID : EMD-18267
Title : Structure of the human 20S U5 snRNP core
Authors : Schneider, S.; Galej, W.P.
Deposited on : 2023-08-19
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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

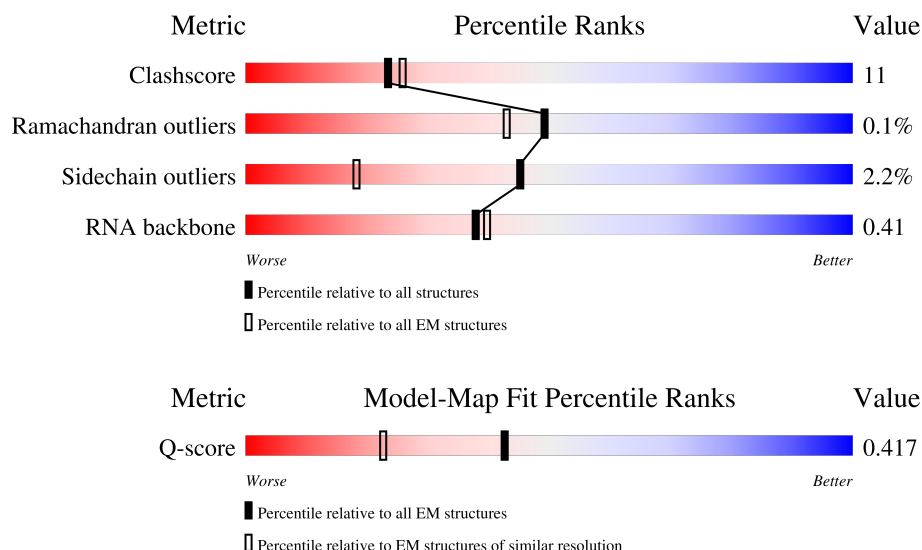
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



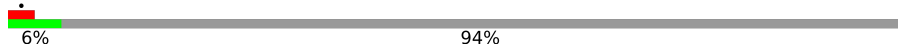
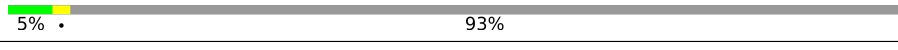
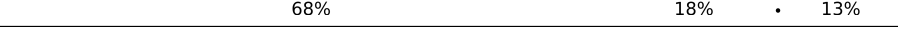
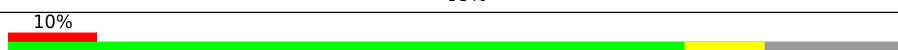
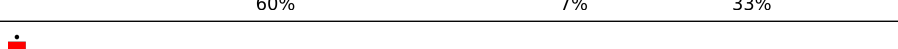
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	F	341	
2	A	2335	
3	5	117	

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Mol	Chain	Length	Quality of chain
4	E	941	 6% 94%
5	D	820	 5% 93%
6	C	972	 68% 18% 13%
7	B	2136	 99%
8	m	86	 10% 76% 9% 15%
9	n	76	 22% 86% 12%
10	i	119	 65% 32%
11	j	118	 16% 80% 17%
12	k	126	 60% 7% 33%
13	h	240	 28% 70%
14	l	92	 5% 75% 8% 16%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 26706 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 CD2 antigen cytoplasmic tail-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	140	Total	C	N	O	S	0	0
			887	552	165	169	1		

- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1627	Total	C	N	O	S	0	0
			13247	8535	2321	2333	58		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	104	Total	C	N	O	P	0	0
			2192	983	372	734	103		

- Molecule 4 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	60	Total	C	N	O	0	0
			300	180	60	60		

- Molecule 5 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	54	Total	C	N	O	0	0
			455	294	78	83		

- Molecule 6 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	847	Total	C	N	O	S	0	0
			6629	4238	1108	1250	33		

- Molecule 7 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	27	Total	C	N	O	S	0	0
			201	123	38	39	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	m	73	Total	C	N	O	0	0
			356	210	73	73		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	n	74	Total	C	N	O	0	0
			364	215	74	75		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	i	81	Total	C	N	O	0	0
			401	239	81	81		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	j	98	Total	C	N	O	0	0
			487	291	98	98		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	k	84	Total	C	N	O	0	0
			414	246	84	84		

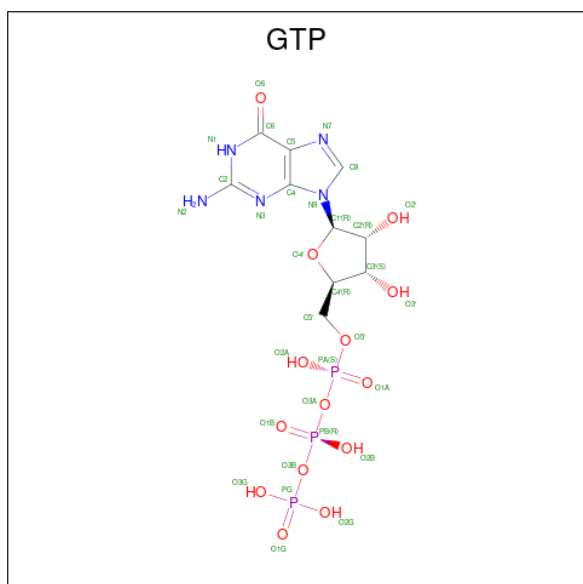
- Molecule 13 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	h	73	Total	C	N	O	0	0
			360	214	73	73		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	1	77	Total	C	N	O	0	0
			381	227	77	77		

- Molecule 15 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

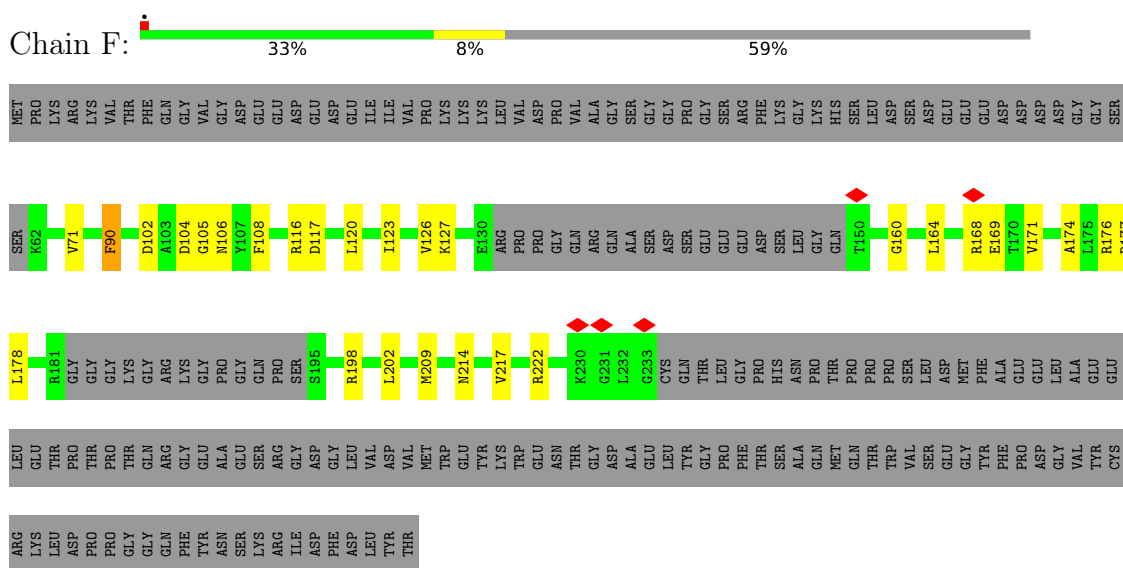


Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

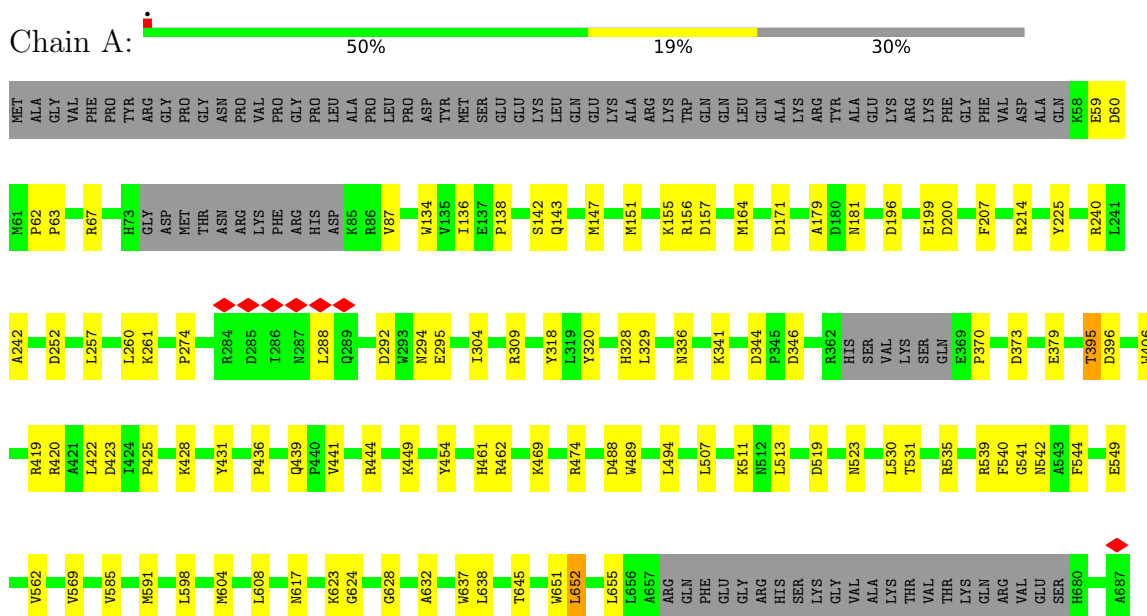
3 Residue-property plots

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

• Molecule 1: CD2 antigen cytoplasmic tail-binding protein 2



• Molecule 2: Pre-mRNA-processing-splicing factor 8



LEU	THR	LYS	ALA	P1738	Y1660	I1585	SER	I1411	M1330	E1193	P1065	N974	Q860	P898
ILE	ILE	GLY	ILE	A1739	W1661	H1586	MET	W1412	M1333	CL194	Q1066	N976	R861	E899
ALA	PHE	LEU	PHE	L1740	I1662	D1413	TRP	D1413	V1333	R1201	N1069	Y975	L864	G700
ASP	PHE	ASP	ASP	R1746	D1663	G1415	LYS	G1415	L1334	T1202	F1071	S979	G865	I701
TVR	ALA	PRO	ASN	R1747	W1668	L1593	LEU	R1418	I1395	E1205	Q1075	R980	L866	K702
GLY	PHE	GLU	ARG	R1748	W1668	L1593	THR	R1418	P1336	E1206	D1076	L992	L867	Q703
LYS	THR	VAL	GLY	Y1754	Y1671	F1597	ASN	T1421	L1340	F1207	A1077	N994	E868	N704
ASN	THR	GLN	SER	SER	D1672	E1600	ALA	D1426	W1342	T1208	A1078	R995	E876	C719
GLN	THR	LEU	GLY	GLY	S1673	E1600	GLN	R1427	R1346	H1209	A1082	L996	A877	N723
LEU	THR	LEU	ARG	THR	I1676	L1604	ARG	H1428	Q1345	M1218	H1083	L997	R880	L731
ASP	PHE	ASP	SER	SER	E1605	E1605	SER	R1429	T1346	E1219	F1088	V1001	L881	P732
LEU	LEU	LEU	LEU	GLY	I1606	I1606	LEU	T1429	D1347	W1220	C1089	H1003	L885	C772
ALA	LEU	PRO	ASN	ASN	E1607	E1607	GLN	D1433	G1349	T1221	R1090	D1002	L896	L776
LEU	ALA	TYR	GLN	GLN	Q1610	Q1610	GLN	K1434	G1349	R1231	Y1091	N1004	M899	G777
THR	THR	LEU	ILE	ILE	K1611	K1611	ILE	G1435	I1386	V1232	I1092	I1005	D900	R778
SER	SER	SER	SER	SER	E1612	E1612	ASP	R1439	F1353	D1234	H1096	A1006	Y902	L780
GLN	GLN	GLN	ASN	ASN	H1615	H1615	GLU	Q1444	R1354	M1237	R1100	M1009	V906	R781
VAL	VAL	GLY	TYR	TYR	R1617	R1617	GLY	Y1445	S1355	N1242	A1103	T1010	V908	L782
LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	Y1446	GLY	R1243	R1107	V1016	P913	E804
LEU	LYS	LEU	LEU	LEU	LEU	LEU	LEU	L1448	MET	V1244	R1107	I1017	E805	E806
PRO	ARG	PRO	PHE	PHE	S1697	S1697	ASP	K1449	SER	W1257	R1107	N1018	A806	V807
LEU	ARG	LEU	LEU	LEU	P1698	P1698	ASP	Y1459	GLU	T1268	I1126	Y1019	A808	A808
GLY	GLY	GLY	GLY	GLY	I1699	I1699	GLY	H1460	GLU	E1276	V1126	K1020	V809	V809
VAL	VAL	VAL	VAL	VAL	G1700	G1700	VAL	Y1466	L1364	E1283	G1127	M1021	T810	T811
ALA	ALA	ALA	ALA	ALA	W1701	W1701	ALA	L1467	I1385	L1284	Y1128	D1022	T812	T813
LEU	LEU	LEU	LEU	LEU	L1702	L1702	LEU	E1468	I1385	E1284	N1129	H1024	Q924	V814
ASP	ASP	ASP	ASP	ASP	A1627	A1627	ASP	N1469	I1369	L1284	N1130	T1025	L926	H815
LYS	LYS	LYS	LYS	LYS	D1628	D1628	LYS	Y1466	ASP	V1289	R1136	T1026	Q924	Y832
LEU	LEU	LEU	LEU	LEU	I1630	I1630	LEU	N1469	LYS	T1297	D1137	L1031	Y925	D835
GLY	GLY	GLY	GLY	GLY	L1631	L1631	GLY	M1474	ASP	K1300	K1144	R1032	P947	K837
THR	THR	THR	THR	THR	Q1552	Q1552	THR	L1474	GLU	V1307	V1147	G1033	R934	L841
ASP	ASP	ASP	ASP	ASP	L1555	L1555	ASP	L1478	GLY	M1308	V1153	L1034	E818	E848
GLY	GLY	GLY	GLY	GLY	G1559	G1559	GLY	L1478	GLY	P1309	W1153	Y1043	P938	R855
LEU	LEU	LEU	LEU	LEU	I1560	I1560	LEU	E1482	GLY	S1309	W1170	Y1044	W939	L856
ALA	ALA	ALA	ALA	ALA	H1563	H1563	ALA	I1484	GLY	R1310	E1171	G1045	I940	N857
THR	THR	THR	THR	THR	P1567	P1567	THR	T1493	GLY	F1311	W1172	L1046	P829	
THR	THR	THR	THR	THR	I1571	I1571	THR	W1498	GLY	P1312	S1173	D1049	Y832	
ASP	ASP	ASP	ASP	ASP	S1572	S1572	ASP	E1499	GLY	E1309	W1170	L1046	E946	
GLY	GLY	GLY	GLY	GLY	L1573	L1573	GLY	G1500	GLY	R1310	E1171	L1046	E946	
ASN	ASN	ASN	ASN	ASN	I1574	I1574	ASN	E1499	GLY	F1312	W1172	D1049	E946	
LEU	LEU	LEU	LEU	LEU	Q1575	Q1575	LEU	G1500	GLY	P1314	S1173	L1046	E946	
THR	THR	THR	THR	THR	I1577	I1577	THR	L1501	GLY	V1314	W1172	D1049	E946	
THR	THR	THR	THR	THR	F1577	F1577	THR	E1504	GLY	V1315	S1173	L1046	E946	
LYS	LYS	LYS	LYS	LYS	R1578	R1578	LYS	K1505	GLY	T1318	W1179	L1055	P948	
PRO	PRO	PRO	PRO	PRO	A1579	A1579	PRO	ALA	GLY	P1319	K1180	H1056	P948	
ILE	ILE	ILE	ILE	ILE	H1580	H1580	ILE	SER	GLY	K1320	S1179	L1055	P948	
VAL	VAL	VAL	VAL	VAL	L1581	L1581	VAL	GLY	GLY	E1321	K1180	H1056	P948	
ARG	ARG	ARG	ARG	ARG	W1582	W1582	ARG	PHE	GLY	L1322	W1187	E1060	L961	
LYS	LYS	LYS	LYS	LYS	Q1583	Q1583	LYS	GLY	GLY	G1323	N1188	M1061	L962	
ARG	ARG	ARG	ARG	ARG	K1584	K1584	ARG	GLY	GLY	G1324	C1190	A1062	L962	
ARG	ARG	ARG	ARG	ARG			ARG	GLY	GLY				V965	



WORLD WIDE
PDB
PROTEIN DATA BANK

ILE	ARG	GLU	TRP	TRP	ALA	ALA
GLY	THR	CYS	LEU	VAL	ALA	ALA
ASP	VAL	PRO	LEU	GLN	ARG	GLN
ILE	LYS	ASN	LEU	ASP	SER	VAL
LEU	ILE	SER	SER	ASN	ILE	PHE
ARG	ASP	GLY	ARG	ILE	LEU	PRO
LEU	SER	ILE	LEU	ARG	ALA	SER
VAL	ASP	LEU	GLU	ALA	LEU	LYS
ALA	LEU	TRP	GLU	GLN	ALA	LYS
GLY	GLY	SER	LYS	GLN	PHE	SER
ARG	ASP	GLU	ILE	ASP	GLN	VAL
ILE	ALA	ALA	GLY	LEU	ALA	TRP
LYS	TRP	ILE	GLN	CYS	ASN	LEU
ASN	ALA	PHE	LEU	GLU	PRO	ARG
THR	PHE	LEU	THR	GLU	ASN	ALA
PHE	THR	GLU	ARG	ALA	SER	ALA
	TYR	ALA	ALA	LEU	GLU	TYR
	LYS	ARG	ARG	ARG	GLU	PHE
	PHE	PRO	ALA	HIS	ILE	GLU
	GLU	GLN	ILE	TYR	TRP	LYS
	LEU	ARG	LEU	GLU	ASN	ASN
	GLN	ARG	GLU	ASP	ALA	HIS
	HIS	THR	LYS	PHE	ALA	GLY
	GLY	LYS	SER	PRO	VAL	THR
	THR	SER	ARG	LYS	LYS	ARG
	GLU	VAL	LEU	LEU	GLU	GLU
	GLU	ASP	LYS	TRP	SER	LEU
	GLN	ALA	ASN	MET	GLU	GLU
	GLN	LEU	PRO	MET	GLU	ALA
	GLU	LYS	LYS	LYS	ASN	ALA
	GLU	LYS	ASN	GLY	ASP	LEU
	VAL	CYS	PRO	ILE	TYR	LEU
	ARG	GLU	GLY	ILE	GLU	GLN
	LYS	HIS	LEU	GLU	ARG	ALA
	ARG	ASP	TRP	GLU	ALA	VAL
	CYS	PRO	LEU	GLN	ALA	VAL
	GLU	HIS	GLU	LYS	ARG	ALA
	SER	VAL	SER	GLU	ARG	HIS
	ALA	LEU	VAL	MET	LEU	CYS
	GLU	LEU	LEU	ARG	LEU	PRO
	PRO	ALA	LEU	GLU	ALA	LYS
	ARG	VAL	GLU	LYS	LYS	ALA
	HIS	ALA	TYR	ALA	ALA	ALA
	GLY	LYS	ARG	ARG	ARG	VAL
	LEU	LEU	PHE	GLY	SER	LEU
	TRP	TRP	LEU	TYR	ALA	TRP
	CYS	SER	LYS	ASN	ALA	LEU
	ALA	GLN	ASN	GLN	PRO	MET
	VAL	ARG	ILE	GLY	THR	GLY
	SER	LYS	ALA	LEU	ARG	LYS
	LYS	ILE	ASN	LYS	VAL	SER
	ASP	THR	THR	LYS	PHE	LYS
	ILE	LYS	LEU	CYS	MET	TRP
	ALA	ALA	MET	PRO	LYS	LEU
	ASN	ARG	ALA	HIS	SER	ALA
	TRP	THR	LYS	SER	GLY	GLY
	GLN	TRP	ALA	THR	VAL	ASP
	LYS	PHE	GLN	PRO	LYS	PRO
	THR	HIS	THR	LEU	THR	THR

- Molecule 5: Probable ATP-dependent RNA helicase DDX23

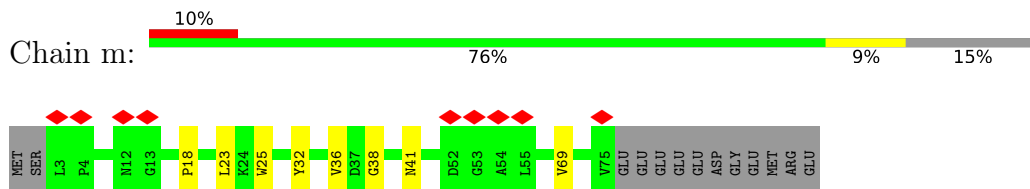
Chain D: 5% • 93%

[illegible]

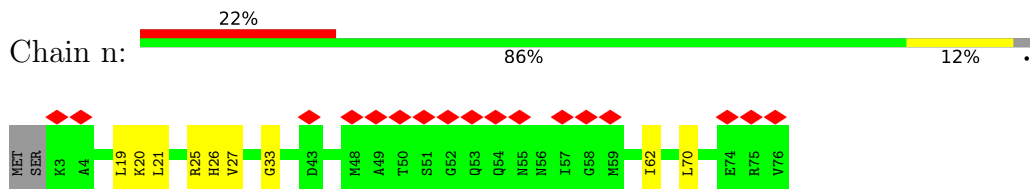


[illegible]

- Molecule 8: Small nuclear ribonucleoprotein F

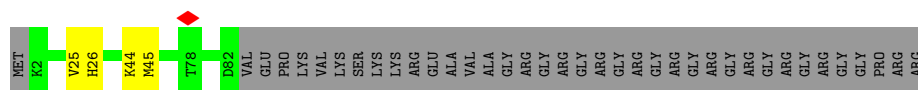


- Molecule 9: Small nuclear ribonucleoprotein G

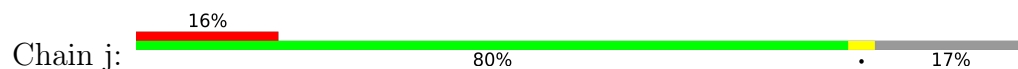


- Molecule 10: Small nuclear ribonucleoprotein Sm D1

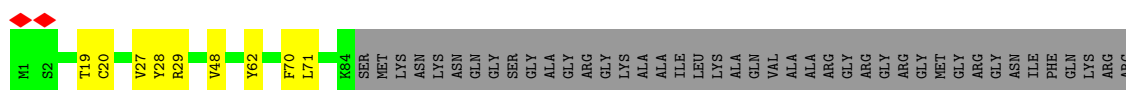




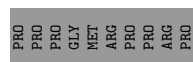
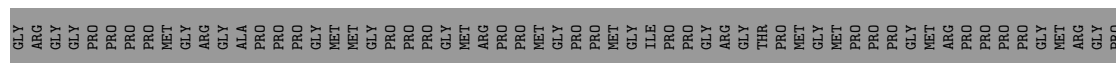
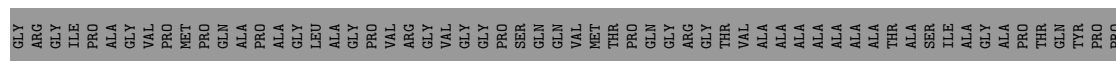
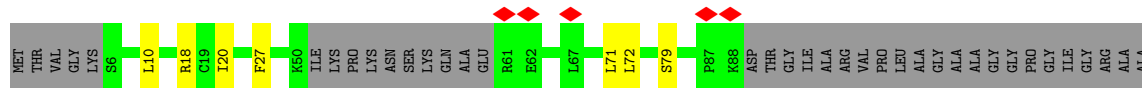
- Molecule 11: Small nuclear ribonucleoprotein Sm D2



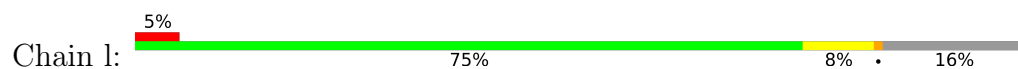
- Molecule 12: Small nuclear ribonucleoprotein Sm D3



- Molecule 13: Small nuclear ribonucleoprotein-associated proteins B and B'



- Molecule 14: Small nuclear ribonucleoprotein E



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76918	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 ($e^-/\text{\AA}^2$)	40.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.051	Depositor
Minimum map value	-0.392	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	526.6296, 526.6296, 526.6296	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0449, 1.0449, 1.0449	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

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	F	0.21	0/896	0.44	0/1224
2	A	0.17	0/13608	0.38	1/18483 (0.0%)
3	5	0.12	0/2444	0.30	0/3798
4	E	0.10	0/298	0.27	0/414
5	D	0.17	0/464	0.44	0/620
6	C	0.18	0/6777	0.39	4/9214 (0.0%)
7	B	0.19	0/202	0.50	0/268
8	m	0.30	0/355	0.63	0/490
9	n	0.19	0/363	0.54	0/501
10	i	0.35	0/400	0.60	0/556
11	j	0.17	0/485	0.47	0/674
12	k	0.23	0/413	0.45	0/573
13	h	0.21	0/358	0.57	1/495 (0.2%)
14	l	0.22	0/380	0.82	2/528 (0.4%)
All	All	0.18	0/27443	0.40	8/37838 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	15	VAL	CA-C-N	7.75	135.25	121.76
14	l	15	VAL	C-N-CA	7.75	135.25	121.76
6	C	144	CYS	N-CA-CB	7.07	120.47	109.94
13	h	10	LEU	N-CA-C	-5.82	105.44	112.54
2	A	867	ILE	CA-CB-CG1	5.49	119.73	110.40
6	C	144	CYS	CB-CA-C	-5.19	102.51	110.81
6	C	143	THR	CA-C-N	-5.14	113.61	120.54
6	C	143	THR	C-N-CA	-5.14	113.61	120.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	887	0	714	30	0
2	A	13247	0	12877	344	0
3	5	2192	0	1111	42	0
4	E	300	0	132	0	0
5	D	455	0	450	13	0
6	C	6629	0	6607	124	0
7	B	201	0	214	10	0
8	m	356	0	156	5	0
9	n	364	0	160	6	0
10	i	401	0	165	2	0
11	j	487	0	199	2	0
12	k	414	0	185	6	0
13	h	360	0	149	4	0
14	l	381	0	159	5	0
15	C	32	0	12	1	0
All	All	26706	0	23290	552	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 11.

All (552) 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)
2:A:1474:MET:HE3	2:A:1474:MET:HA	1.51	0.91
2:A:885:LEU:HD21	2:A:922:LEU:HD21	1.53	0.89
2:A:1365:ILE:HG13	2:A:1474:MET:HE1	1.55	0.86
2:A:1307:MET:HE3	2:A:1307:MET:H	1.39	0.86
2:A:813:THR:HG21	2:A:996:LEU:HD11	1.59	0.84
2:A:1237:MET:HG2	2:A:1284:LEU:HD13	1.66	0.78
2:A:975:VAL:HG11	2:A:1153:VAL:HG21	1.66	0.78
6:C:829:GLU:HG3	6:C:907:VAL:HG22	1.66	0.77
2:A:1314:VAL:HG13	2:A:1478:LEU:HD23	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1368:LEU:HD11	2:A:1467:LEU:HD23	1.67	0.76
12:k:70:PHE:HA	13:h:72:LEU:HA	1.68	0.76
2:A:200:ASP:OD1	2:A:240:ARG:NH2	2.19	0.75
2:A:1365:ILE:CG1	2:A:1474:MET:HE1	2.16	0.75
5:D:243:LYS:HG3	5:D:244:SER:H	1.52	0.75
2:A:1032:ARG:HD3	2:A:1445:TYR:HE2	1.50	0.74
2:A:1622:MET:O	2:A:1687:TYR:OH	2.05	0.74
2:A:1171:GLU:OE2	2:A:1171:GLU:N	2.18	0.73
2:A:1622:MET:SD	2:A:1622:MET:N	2.62	0.73
2:A:292:ASP:OD2	2:A:1130:ASN:ND2	2.22	0.72
2:A:370:PRO:HG2	6:C:304:LEU:HD21	1.69	0.72
6:C:406:GLU:OE1	6:C:406:GLU:N	2.22	0.72
2:A:530:LEU:HG	2:A:535:ARG:HG3	1.71	0.72
2:A:1701:VAL:HA	2:A:1716:GLY:HA3	1.70	0.72
2:A:585:VAL:HG11	2:A:637:TRP:CZ2	2.25	0.72
2:A:1573:LEU:HA	2:A:1576:ILE:HG22	1.72	0.72
3:5:88:A:N6	8:m:38:GLY:O	2.23	0.71
5:D:243:LYS:HG3	5:D:244:SER:N	2.05	0.71
2:A:329:LEU:HB3	6:C:177:ARG:HD3	1.72	0.71
1:F:164:LEU:O	1:F:198:ARG:NH2	2.23	0.70
2:A:974:ASN:OD1	2:A:1100:ARG:NH1	2.25	0.70
3:5:19:A:N3	3:5:21:A:N6	2.40	0.69
2:A:1543:ASN:O	2:A:1563:HIS:ND1	2.25	0.69
2:A:1576:ILE:HG23	2:A:1577:PHE:HD1	1.57	0.69
2:A:1712:HIS:HB3	2:A:1734:MET:HE1	1.75	0.69
2:A:1626:CYS:SG	2:A:1627:ALA:N	2.66	0.69
2:A:1289:VAL:HG21	7:B:42:SER:HA	1.72	0.69
2:A:776:LEU:HA	2:A:779:LEU:HD12	1.74	0.68
6:C:147:ASP:HA	6:C:150:ILE:HB	1.75	0.68
2:A:1544:ARG:HG3	2:A:1672:ASP:OD2	1.93	0.68
6:C:846:VAL:HG22	6:C:887:LEU:HD11	1.75	0.68
2:A:549:GLU:HB3	2:A:591:MET:HG2	1.75	0.68
2:A:1493:THR:HA	2:A:1747:ILE:HD11	1.75	0.68
2:A:1330:MET:HE2	2:A:1330:MET:HA	1.76	0.67
2:A:1660:TYR:OH	2:A:1717:ASN:O	2.09	0.67
1:F:117:ASP:OD2	2:A:541:GLY:N	2.27	0.66
6:C:143:THR:O	6:C:144:CYS:C	2.39	0.66
2:A:877:ALA:O	2:A:881:ILE:HG12	1.96	0.65
2:A:1032:ARG:HD3	2:A:1445:TYR:CE2	2.32	0.65
5:D:275:GLU:OE1	5:D:275:GLU:N	2.30	0.65
2:A:1069:ASN:OD1	2:A:1075:GLN:NE2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:171:ASP:OD2	2:A:523:ASN:ND2	2.30	0.64
6:C:159:LYS:NZ	6:C:160:ARG:O	2.29	0.64
2:A:341:LYS:O	5:D:301:ARG:NH1	2.30	0.64
2:A:1625:SER:OG	2:A:1663:ASP:OD2	2.14	0.64
2:A:1631:LEU:HD12	2:A:1660:TYR:HB3	1.80	0.64
6:C:436:GLN:OE1	6:C:437:HIS:NE2	2.30	0.64
2:A:855:ARG:HH12	2:A:857:ASN:HB3	1.62	0.64
2:A:992:LEU:HD13	2:A:996:LEU:HD23	1.80	0.64
6:C:137:HIS:O	6:C:142:LYS:NZ	2.31	0.64
2:A:881:ILE:HD12	2:A:918:THR:HA	1.80	0.63
2:A:1330:MET:HE1	2:A:1369:TYR:H	1.64	0.63
2:A:1411:SER:HA	2:A:1414:ARG:HD3	1.80	0.63
1:F:102:ASP:OD1	1:F:106:ASN:N	2.28	0.63
1:F:105:GLY:HA3	2:A:1532:ARG:HD2	1.79	0.63
2:A:1737:ASN:HB3	2:A:1740:LEU:HB2	1.80	0.63
1:F:168:ARG:H	1:F:222:ARG:HD3	1.64	0.62
2:A:143:GLN:NE2	2:A:207:PHE:O	2.27	0.62
2:A:1544:ARG:HG2	2:A:1546:ASN:H	1.64	0.62
2:A:813:THR:HG21	2:A:996:LEU:CD1	2.30	0.62
6:C:215:VAL:HG11	6:C:242:LEU:HD22	1.82	0.62
1:F:120:LEU:HD22	2:A:539:ARG:HD2	1.82	0.62
10:i:26:HIS:O	10:i:44:LYS:N	2.30	0.61
1:F:209:MET:HE3	1:F:209:MET:O	2.00	0.61
11:j:69:ASN:N	11:j:97:SER:O	2.30	0.61
8:m:23:LEU:HA	8:m:69:VAL:HA	1.82	0.61
2:A:474:ARG:NH2	3:5:14:U:OP2	2.33	0.61
2:A:1555:LEU:HD11	2:A:1574:ILE:HD11	1.82	0.61
6:C:685:ILE:HD11	6:C:808:ILE:HD11	1.83	0.61
2:A:856:LEU:O	2:A:861:ARG:NH2	2.34	0.60
6:C:144:CYS:HB3	6:C:312:SER:HB2	1.83	0.60
2:A:899:MET:HE2	2:A:899:MET:HA	1.84	0.60
6:C:335:ASN:ND2	6:C:338:GLU:OE1	2.34	0.60
2:A:1687:TYR:O	2:A:1693:SER:OG	2.20	0.60
6:C:697:ALA:O	6:C:701:GLU:HG2	2.01	0.60
2:A:1342:TRP:CZ2	2:A:1353:PHE:HB2	2.36	0.60
2:A:309:ARG:NH1	5:D:285:ASP:OD2	2.29	0.59
2:A:1434:LYS:O	2:A:1439:ARG:NH2	2.28	0.59
6:C:473:PRO:HB2	6:C:571:ASN:HD21	1.67	0.59
2:A:1342:TRP:CE2	2:A:1353:PHE:HB2	2.38	0.59
2:A:1427:ARG:HD3	2:A:1428:HIS:H	1.68	0.59
6:C:512:GLU:OE1	6:C:562:THR:OG1	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:772:CYS:O	2:A:776:LEU:HG	2.03	0.58
2:A:881:ILE:HG23	2:A:918:THR:HG23	1.85	0.58
6:C:407:GLU:OE1	6:C:418:LEU:HD21	2.03	0.58
6:C:170:ILE:HG22	6:C:536:ARG:HE	1.68	0.58
6:C:473:PRO:O	6:C:498:SER:OG	2.20	0.58
2:A:608:LEU:HD13	2:A:632:ALA:HB1	1.84	0.58
2:A:585:VAL:HG11	2:A:637:TRP:HZ2	1.69	0.58
2:A:1082:ALA:O	2:A:1083:HIS:ND1	2.37	0.58
2:A:304:ILE:HG21	5:D:250:ILE:HD13	1.86	0.58
6:C:140:HIS:NE2	6:C:233:GLU:OE1	2.36	0.58
2:A:1536:LEU:O	2:A:1539:SER:OG	2.18	0.57
6:C:144:CYS:O	6:C:148:CYS:N	2.29	0.57
2:A:507:LEU:HD11	2:A:652:LEU:HD11	1.86	0.57
2:A:1703:ILE:HG12	2:A:1714:ALA:HB2	1.86	0.57
5:D:285:ASP:OD1	5:D:287:ASN:N	2.37	0.57
11:j:44:ILE:N	11:j:52:LEU:O	2.32	0.57
6:C:169:ASP:HB3	6:C:174:GLU:HB3	1.87	0.57
2:A:1444:GLN:HG3	2:A:1445:TYR:HD1	1.69	0.57
3:5:67:A:H2'	3:5:68:C:C6	2.39	0.57
5:D:282:THR:HG22	5:D:283:SER:H	1.69	0.57
2:A:252:ASP:OD1	2:A:252:ASP:N	2.38	0.57
2:A:147:MET:O	2:A:151:MET:HG3	2.04	0.57
2:A:1218:ASN:HB3	2:A:1221:THR:HG22	1.86	0.57
5:D:245:LYS:H	5:D:245:LYS:HD2	1.69	0.57
2:A:856:LEU:HD13	2:A:860:GLN:HB3	1.87	0.56
2:A:1676:ILE:HD13	2:A:1706:ASP:HB2	1.87	0.56
3:5:57:G:O2'	3:5:58:U:O5'	2.16	0.56
2:A:899:MET:HB2	2:A:906:VAL:HG13	1.86	0.56
2:A:1607:GLU:N	2:A:1632:PHE:O	2.37	0.56
2:A:1610:GLN:NE2	2:A:1612:GLU:OE1	2.37	0.56
2:A:1410:ASP:OD1	2:A:1410:ASP:N	2.34	0.56
3:5:17:U:H2'	3:5:18:C:C6	2.40	0.56
6:C:147:ASP:C	6:C:149:LEU:N	2.62	0.56
2:A:1090:ARG:NH1	2:A:1091:TYR:O	2.38	0.56
2:A:544:PHE:HA	2:A:651:TRP:CH2	2.41	0.56
3:5:111:A:H2'	3:5:112:A:C8	2.41	0.56
12:k:20:CYS:N	12:k:28:TYR:O	2.38	0.56
2:A:776:LEU:O	2:A:780:THR:HG23	2.06	0.55
2:A:1474:MET:HE2	2:A:1478:LEU:HD12	1.87	0.55
6:C:147:ASP:C	6:C:149:LEU:H	2.14	0.55
2:A:899:MET:HE3	2:A:1448:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1188:ASN:HD21	2:A:1233:ASP:CG	2.15	0.55
2:A:1560:ILE:HG21	2:A:1573:LEU:HD13	1.88	0.55
6:C:449:ILE:HD12	6:C:465:MET:HE3	1.89	0.55
6:C:455:GLY:O	6:C:459:SER:OG	2.23	0.55
6:C:573:GLU:OE1	6:C:573:GLU:N	2.31	0.55
1:F:117:ASP:HB3	1:F:120:LEU:HB3	1.87	0.55
2:A:1076:ASP:OD1	2:A:1077:ILE:N	2.40	0.55
2:A:1482:GLU:CD	2:A:1483:GLY:N	2.65	0.55
2:A:1597:PHE:HE1	2:A:1604:LEU:HD12	1.72	0.55
6:C:394:ARG:NH1	6:C:394:ARG:HB3	2.22	0.55
1:F:209:MET:CE	1:F:214:ASN:HB3	2.38	0.54
3:5:117:A:O2'	8:m:25:TRP:O	2.18	0.54
2:A:531:THR:O	2:A:535:ARG:N	2.40	0.54
2:A:827:PHE:HD2	2:A:1005:ILE:HD11	1.72	0.54
2:A:1093:ASP:N	2:A:1093:ASP:OD1	2.40	0.54
2:A:1747:ILE:HD12	2:A:1748:ARG:N	2.23	0.54
6:C:479:THR:HA	6:C:562:THR:HG22	1.90	0.54
2:A:494:LEU:HD21	2:A:562:VAL:HG21	1.89	0.54
2:A:899:MET:HB2	2:A:906:VAL:CG1	2.38	0.54
2:A:1630:LEU:HD21	2:A:1696:PRO:HG3	1.90	0.54
6:C:159:LYS:HG3	6:C:164:ASP:HA	1.89	0.54
2:A:1579:ALA:O	2:A:1584:LYS:NZ	2.40	0.54
2:A:1311:PHE:HE1	2:A:1315:VAL:HG21	1.72	0.54
6:C:173:THR:O	6:C:177:ARG:HG2	2.08	0.54
2:A:996:LEU:HB3	2:A:1043:TYR:HE2	1.71	0.54
1:F:123:ILE:O	1:F:127:LYS:N	2.40	0.53
2:A:156:ARG:NH1	2:A:157:ASP:OD1	2.41	0.53
1:F:71:VAL:HG23	2:A:1575:GLN:HB2	1.90	0.53
2:A:1127:GLY:O	2:A:1170:TRP:NE1	2.34	0.53
9:n:70:LEU:O	12:k:62:TYR:N	2.38	0.53
2:A:151:MET:HE1	2:A:628:GLY:C	2.33	0.53
3:5:47:A:O2'	3:5:48:A:O5'	2.26	0.53
2:A:939:TRP:NE1	2:A:1049:ASP:OD2	2.40	0.53
6:C:724:TRP:HZ3	6:C:732:ILE:HD11	1.73	0.53
2:A:1333:VAL:HG23	7:B:40:VAL:HG13	1.89	0.53
2:A:805:GLU:O	2:A:809:VAL:HG12	2.08	0.53
2:A:950:LEU:HD12	2:A:1379:PHE:CD1	2.43	0.53
2:A:1002:ASP:OD2	2:A:1004:ASN:ND2	2.42	0.53
1:F:90:PHE:CD1	2:A:1574:ILE:HG13	2.44	0.53
2:A:1334:LEU:HD13	2:A:1364:LEU:HD23	1.91	0.53
13:h:20:ILE:N	13:h:79:SER:O	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:946:GLU:OE1	2:A:951:LEU:HD23	2.08	0.53
2:A:67:ARG:HD3	2:A:179:ALA:HB2	1.91	0.52
2:A:1586:HIS:NE2	2:A:1628:ASP:OD2	2.41	0.52
2:A:1031:ILE:HB	2:A:1034:LEU:HG	1.91	0.52
6:C:945:GLU:OE2	6:C:946:ASP:HB2	2.10	0.52
2:A:1313:PRO:HG2	2:A:1335:ILE:HD12	1.91	0.52
6:C:133:THR:HG21	6:C:219:LEU:HD23	1.92	0.52
2:A:1019:TYR:O	2:A:1021:ASP:N	2.42	0.52
2:A:1368:LEU:HD11	2:A:1467:LEU:CD2	2.37	0.52
2:A:940:ILE:HD11	2:A:1046:LEU:HB2	1.92	0.52
3:5:69:A:H2'	3:5:70:A:O4'	2.09	0.52
3:5:109:G:H2'	3:5:110:C:C6	2.44	0.52
6:C:177:ARG:HG3	6:C:177:ARG:HH11	1.73	0.52
6:C:391:SER:OG	6:C:391:SER:O	2.25	0.52
2:A:1612:GLU:HG2	2:A:1627:ALA:HB3	1.90	0.52
2:A:1661:TRP:NE1	2:A:1697:SER:O	2.42	0.52
9:n:19:LEU:O	9:n:27:VAL:N	2.41	0.52
2:A:436:PRO:HG2	2:A:439:GLN:HG3	1.92	0.52
6:C:692:LEU:HD22	6:C:696:LEU:HD23	1.90	0.52
2:A:549:GLU:CB	2:A:591:MET:HG2	2.39	0.52
2:A:1094:ARG:HH22	2:A:1190:CYS:H	1.58	0.52
6:C:780:CYS:O	6:C:941:LYS:NZ	2.43	0.52
2:A:425:PRO:HB2	2:A:428:LYS:HB2	1.92	0.51
2:A:926:LEU:HD11	2:A:1009:MET:HE1	1.92	0.51
2:A:1368:LEU:HG	2:A:1372:ILE:HD11	1.92	0.51
1:F:176:ARG:NE	2:A:59:GLU:HB3	2.26	0.51
2:A:1017:ILE:HD11	2:A:1026:ASN:HB2	1.92	0.51
2:A:1391:LEU:O	2:A:1394:GLN:HG3	2.11	0.51
2:A:1607:GLU:HB2	2:A:1634:SER:HB3	1.93	0.51
2:A:379:GLU:OE1	2:A:379:GLU:N	2.42	0.51
2:A:923:ASP:OD2	2:A:1439:ARG:NH1	2.32	0.51
2:A:1641:ARG:HG2	2:A:1642:PRO:HD2	1.92	0.51
6:C:674:CYS:SG	6:C:822:MET:HE2	2.51	0.51
6:C:308:CYS:HB2	6:C:433:MET:HE2	1.92	0.51
7:B:62:GLN:N	7:B:62:GLN:OE1	2.43	0.51
2:A:1692:MET:HE3	2:A:1692:MET:O	2.11	0.51
1:F:209:MET:HE2	1:F:217:VAL:HG22	1.93	0.51
2:A:946:GLU:HG3	2:A:950:LEU:HD22	1.93	0.51
2:A:1447:VAL:HG12	2:A:1449:LYS:H	1.76	0.51
6:C:203:MET:HA	6:C:203:MET:HE3	1.93	0.51
2:A:134:TRP:HZ2	3:5:58:U:OP2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:919:ASP:OD2	2:A:1012:LYS:NZ	2.41	0.50
2:A:1678:ARG:HH12	2:A:1681:ARG:HD3	1.77	0.50
10:i:25:VAL:HA	10:i:45:MET:HA	1.94	0.50
2:A:837:LYS:O	2:A:841:LEU:HG	2.11	0.50
2:A:1465:TRP:HD1	2:A:1467:LEU:HD11	1.76	0.50
12:k:71:LEU:N	13:h:71:LEU:O	2.42	0.50
6:C:144:CYS:O	6:C:145:PHE:C	2.54	0.50
2:A:1474:MET:HE2	2:A:1478:LEU:CD1	2.42	0.50
2:A:1504:GLU:N	2:A:1504:GLU:OE1	2.45	0.50
2:A:420:ARG:NH1	3:5:57:G:H5'	2.27	0.50
2:A:591:MET:HE3	2:A:598:LEU:HD21	1.93	0.50
2:A:1257:THR:HG21	2:A:1320:LYS:HE3	1.93	0.50
2:A:1322:LEU:HD12	2:A:1498:TRP:CZ2	2.45	0.50
2:A:461:HIS:HD2	3:5:27:U:H3	1.59	0.50
2:A:1129:ASN:ND2	2:A:1173:SER:O	2.43	0.50
2:A:1193:GLU:HB3	2:A:1231:ARG:HB2	1.94	0.50
6:C:692:LEU:HD21	6:C:744:ILE:HD12	1.94	0.50
9:n:20:LYS:HA	9:n:26:HIS:HA	1.93	0.50
2:A:1013:ASN:HA	2:A:1031:ILE:HG12	1.94	0.50
2:A:1283:GLU:N	2:A:1283:GLU:OE1	2.45	0.50
6:C:620:LYS:NZ	6:C:622:GLU:OE1	2.45	0.50
2:A:841:LEU:HD21	2:A:1429:THR:HG22	1.93	0.49
2:A:865:GLY:O	2:A:868:GLU:HG3	2.12	0.49
6:C:145:PHE:HA	6:C:148:CYS:HB2	1.93	0.49
2:A:318:TYR:O	6:C:645:ARG:NH1	2.45	0.49
2:A:815:HIS:HA	2:A:818:GLU:OE1	2.11	0.49
2:A:1641:ARG:HH21	2:A:1651:VAL:HG22	1.76	0.49
3:5:17:U:H3	3:5:60:G:H1	1.59	0.49
2:A:1392:LYS:O	2:A:1395:GLU:HG3	2.12	0.49
3:5:56:C:H2'	3:5:57:G:H5'	1.94	0.49
3:5:65:G:O6	3:5:66:A:N6	2.46	0.49
2:A:142:SER:HA	2:A:242:ALA:HB2	1.94	0.49
2:A:419:ARG:NH2	2:A:423:ASP:O	2.46	0.49
2:A:829:PRO:HD2	2:A:832:TYR:CD2	2.46	0.49
2:A:1576:ILE:HG23	2:A:1577:PHE:CD1	2.43	0.49
6:C:158:ARG:HH12	6:C:160:ARG:CG	2.26	0.49
2:A:155:LYS:NZ	2:A:624:GLY:O	2.46	0.49
2:A:779:LEU:HA	2:A:782:LEU:HD12	1.94	0.49
2:A:1307:MET:H	2:A:1307:MET:CE	2.19	0.49
2:A:1559:GLY:HA2	2:A:1622:MET:HE3	1.94	0.49
2:A:1728:GLN:O	2:A:1732:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:530:LEU:HG	2:A:535:ARG:CG	2.42	0.49
2:A:1482:GLU:C	2:A:1482:GLU:OE1	2.56	0.49
3:5:36:C:O2	3:5:44:A:N6	2.46	0.49
2:A:1629:ILE:HB	2:A:1662:ILE:HB	1.94	0.49
2:A:1318:THR:HB	2:A:1324:GLY:HA3	1.95	0.49
6:C:561:LYS:NZ	6:C:615:PRO:O	2.43	0.49
2:A:1061:MET:CE	2:A:1088:PHE:HB3	2.43	0.48
2:A:778:ARG:O	2:A:782:LEU:HG	2.12	0.48
2:A:1560:ILE:HD13	2:A:1573:LEU:HD13	1.95	0.48
6:C:148:CYS:SG	6:C:312:SER:HB2	2.53	0.48
2:A:469:LYS:NZ	3:5:59:G:N7	2.59	0.48
2:A:1300:LYS:HG2	2:A:1311:PHE:CD2	2.48	0.48
1:F:71:VAL:HG22	2:A:1574:ILE:HG22	1.94	0.48
2:A:1597:PHE:HZ	2:A:1719:PHE:HZ	1.59	0.48
6:C:362:THR:OG1	6:C:363:SER:N	2.47	0.48
1:F:174:ALA:HA	1:F:177:ARG:HG2	1.96	0.48
2:A:1125:ILE:HD13	2:A:1147:VAL:HG11	1.95	0.48
14:l:31:ILE:N	14:l:45:GLY:O	2.46	0.48
2:A:1393:ARG:O	2:A:1397:ILE:HG13	2.13	0.48
6:C:674:CYS:SG	6:C:818:SER:HB2	2.53	0.48
2:A:651:TRP:NE1	2:A:655:LEU:HD22	2.28	0.48
2:A:867:ILE:HD12	2:A:868:GLU:N	2.29	0.48
6:C:177:ARG:HG3	6:C:177:ARG:NH1	2.28	0.48
6:C:720:THR:HG23	6:C:721:LYS:HD3	1.96	0.48
2:A:976:MET:HG2	2:A:1187:PHE:HB3	1.96	0.48
6:C:261:ASP:OD2	6:C:311:SER:OG	2.26	0.48
2:A:1368:LEU:HD12	2:A:1368:LEU:HA	1.52	0.48
2:A:1645:LEU:HD21	2:A:1730:MET:HE2	1.95	0.48
6:C:603:MET:HB2	6:C:651:ILE:HD11	1.95	0.48
2:A:944:ASP:OD2	2:A:1435:GLY:N	2.40	0.48
2:A:1672:ASP:OD1	2:A:1673:SER:HB3	2.14	0.48
3:5:12:U:H3	3:5:65:G:H1	1.60	0.48
6:C:357:THR:OG1	6:C:359:LYS:O	2.32	0.48
2:A:136:ILE:HG22	2:A:138:PRO:HD2	1.96	0.47
2:A:1013:ASN:O	2:A:1026:ASN:ND2	2.39	0.47
6:C:696:LEU:HD13	6:C:722:TYR:CE2	2.49	0.47
2:A:979:SER:OG	2:A:980:ARG:N	2.47	0.47
2:A:1090:ARG:HG2	2:A:1091:TYR:O	2.14	0.47
2:A:1621:LYS:HD3	2:A:1624:SER:OG	2.14	0.47
6:C:212:SER:O	6:C:216:THR:HG23	2.13	0.47
14:l:44:GLU:O	14:l:61:ALA:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:274:PRO:HA	5:D:282:THR:HG22	1.96	0.47
3:5:63:A:H2'	3:5:64:G:H8	1.79	0.47
6:C:483:SER:HB2	6:C:490:PHE:CE2	2.49	0.47
2:A:288:LEU:O	2:A:1136:ARG:NH2	2.48	0.47
6:C:110:PRO:HD2	6:C:537:TYR:CE2	2.50	0.47
6:C:236:MET:O	6:C:239:THR:OG1	2.29	0.47
1:F:209:MET:HE1	1:F:214:ASN:HB3	1.97	0.47
2:A:1137:ASP:OD1	2:A:1137:ASP:N	2.48	0.47
2:A:1342:TRP:CG	2:A:1482:GLU:OE1	2.68	0.47
2:A:1544:ARG:HH21	2:A:1671:TYR:HB3	1.79	0.47
2:A:1625:SER:OG	2:A:1626:CYS:N	2.47	0.47
6:C:146:VAL:CG1	6:C:186:VAL:HG21	2.45	0.47
6:C:213:ASP:OD1	6:C:213:ASP:N	2.47	0.47
6:C:320:LEU:HD21	6:C:344:TRP:HB2	1.97	0.47
6:C:534:VAL:HG12	6:C:535:ALA:H	1.79	0.47
9:n:33:GLY:HA3	14:l:15:VAL:O	2.14	0.47
2:A:913:PRO:HA	2:A:916:LYS:HB2	1.96	0.47
2:A:1559:GLY:HA2	2:A:1622:MET:CE	2.44	0.47
2:A:1606:ILE:HG12	2:A:1637:TRP:HZ2	1.80	0.47
6:C:670:SER:HB2	6:C:822:MET:HB2	1.97	0.47
2:A:1209:HIS:O	7:B:51:ARG:NH1	2.48	0.47
2:A:1433:ASP:HB3	2:A:1460:HIS:HE1	1.79	0.47
2:A:344:ASP:HB3	2:A:346:ASP:OD1	2.14	0.47
2:A:488:ASP:OD1	2:A:489:TRP:N	2.48	0.47
2:A:1653:ASP:HB3	2:A:1655:THR:HG22	1.97	0.47
6:C:727:LEU:O	6:C:731:SER:OG	2.20	0.47
9:n:62:ILE:HA	14:l:86:LEU:HA	1.97	0.47
2:A:260:LEU:HD21	2:A:454:TYR:CZ	2.50	0.46
2:A:997:LEU:O	2:A:1001:VAL:HG12	2.14	0.46
6:C:146:VAL:HG11	6:C:186:VAL:HG21	1.96	0.46
6:C:167:TYR:HA	6:C:536:ARG:CZ	2.46	0.46
6:C:830:PRO:HG2	6:C:877:ALA:HB3	1.97	0.46
2:A:1103:ALA:O	2:A:1107:ARG:HG3	2.14	0.46
2:A:1660:TYR:OH	2:A:1701:VAL:HB	2.15	0.46
12:k:19:THR:HA	12:k:29:ARG:HA	1.96	0.46
2:A:1066:GLN:OE1	2:A:1066:GLN:N	2.48	0.46
2:A:511:LYS:HB2	2:A:513:LEU:CD2	2.45	0.46
2:A:976:MET:HE1	2:A:1096:HIS:HB3	1.97	0.46
1:F:116:ARG:CZ	2:A:542:ASN:HD21	2.28	0.46
2:A:908:VAL:HG11	2:A:1448:LEU:CD2	2.46	0.46
2:A:1426:ASP:OD2	2:A:1459:ARG:NH1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1615:HIS:ND1	2:A:1617:ARG:HG3	2.30	0.46
3:5:12:U:H2'	3:5:13:C:C6	2.51	0.46
6:C:647:MET:HE3	6:C:647:MET:HB2	1.80	0.46
2:A:164:MET:HG2	2:A:569:VAL:HG11	1.98	0.46
2:A:1560:ILE:HG12	2:A:1668:TRP:CD1	2.51	0.46
2:A:1581:LEU:HD12	2:A:1746:ARG:HH11	1.81	0.46
3:5:49:A:H2'	3:5:50:G:H8	1.81	0.46
2:A:214:ARG:HG3	2:A:225:TYR:CD1	2.51	0.46
2:A:828:PRO:HG3	2:A:925:TYR:CE2	2.51	0.46
2:A:1061:MET:HE2	2:A:1088:PHE:HB3	1.98	0.46
2:A:1179:SER:O	2:A:1201:ARG:NH1	2.38	0.46
2:A:864:LEU:O	2:A:867:ILE:HD12	2.16	0.45
2:A:896:ILE:HD12	2:A:896:ILE:O	2.16	0.45
2:A:1064:PRO:HB2	2:A:1066:GLN:OE1	2.16	0.45
2:A:1202:THR:O	2:A:1202:THR:HG22	2.16	0.45
1:F:178:LEU:HD21	1:F:198:ARG:HB3	1.98	0.45
2:A:993:LEU:O	2:A:997:LEU:HG	2.16	0.45
2:A:1537:TRP:HD1	2:A:1538:TRP:NE1	2.15	0.45
2:A:1559:GLY:HA3	2:A:1582:TRP:CH2	2.51	0.45
3:5:63:A:H2'	3:5:64:G:C8	2.52	0.45
3:5:96:A:O2'	3:5:97:G:OP1	2.29	0.45
9:n:21:LEU:N	9:n:25:ARG:O	2.46	0.45
1:F:169:GLU:OE2	1:F:177:ARG:HD3	2.17	0.45
3:5:16:U:H2'	3:5:17:U:C6	2.52	0.45
2:A:1276:GLU:CD	2:A:1375:TRP:H	2.24	0.45
2:A:948:PRO:O	2:A:951:LEU:HB2	2.17	0.45
2:A:1600:GLU:HG2	2:A:1725:LEU:HD13	1.98	0.45
6:C:139:HIS:HE1	6:C:178:GLY:O	2.00	0.45
6:C:687:MET:HE1	6:C:816:VAL:HG22	1.99	0.45
2:A:1374:PRO:HG3	7:B:52:MET:HB3	1.99	0.45
2:A:1474:MET:HA	2:A:1474:MET:CE	2.34	0.45
2:A:1501:LEU:HD12	2:A:1754:TYR:C	2.42	0.45
2:A:1567:PRO:O	2:A:1571:ILE:HG22	2.18	0.45
2:A:1644:LEU:HD11	2:A:1678:ARG:NH2	2.31	0.45
6:C:148:CYS:SG	6:C:312:SER:O	2.75	0.45
1:F:102:ASP:HB3	1:F:108:PHE:CE2	2.52	0.44
2:A:395:THR:HG22	2:A:396:ASP:H	1.81	0.44
2:A:1747:ILE:HD12	2:A:1747:ILE:C	2.41	0.44
3:5:23:C:H5''	3:5:24:G:H2'	1.98	0.44
2:A:809:VAL:O	2:A:813:THR:HG22	2.16	0.44
2:A:1624:SER:CB	2:A:1692:MET:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:VAL:HG23	1:F:202:LEU:HD11	1.99	0.44
2:A:336:ASN:O	6:C:262:ARG:NH2	2.50	0.44
2:A:598:LEU:HD12	2:A:598:LEU:HA	1.75	0.44
6:C:192:ASP:N	6:C:196:LYS:O	2.49	0.44
7:B:41:LEU:HD23	7:B:41:LEU:HA	1.76	0.44
6:C:534:VAL:HG12	6:C:535:ALA:N	2.33	0.44
2:A:835:ASP:OD1	2:A:836:THR:N	2.51	0.44
2:A:1076:ASP:OD1	2:A:1078:ALA:N	2.30	0.44
2:A:1589:ILE:HA	2:A:1733:ILE:HD11	1.99	0.44
2:A:1552:GLN:HG2	2:A:1563:HIS:CD2	2.52	0.44
6:C:614:TYR:HB2	6:C:617:LEU:HB2	1.98	0.44
6:C:230:ASP:HB3	6:C:233:GLU:HB2	1.99	0.44
6:C:733:TRP:NE1	6:C:747:ASP:OD2	2.51	0.44
2:A:1276:GLU:OE1	2:A:1375:TRP:N	2.50	0.44
2:A:1585:ILE:HD13	2:A:1739:ALA:HB1	2.00	0.44
3:5:34:U:H2'	3:5:35:U:C6	2.53	0.44
2:A:329:LEU:HB3	6:C:177:ARG:CD	2.43	0.43
2:A:962:LEU:HB2	2:A:965:VAL:HB	2.00	0.43
3:5:110:C:H2'	3:5:111:A:H8	1.83	0.43
5:D:254:TYR:OH	6:C:657:ASP:OD2	2.34	0.43
6:C:687:MET:HE3	6:C:687:MET:HB3	1.79	0.43
6:C:713:LYS:O	6:C:716:GLU:HG2	2.18	0.43
6:C:724:TRP:CZ3	6:C:732:ILE:HD11	2.51	0.43
2:A:260:LEU:HD21	2:A:454:TYR:CE2	2.53	0.43
2:A:922:LEU:HD13	2:A:922:LEU:HA	1.86	0.43
2:A:934:ARG:HB3	2:A:934:ARG:CZ	2.49	0.43
2:A:1049:ASP:OD1	2:A:1090:ARG:HD3	2.17	0.43
2:A:1469:ASN:HB2	7:B:57:GLN:HG2	2.01	0.43
6:C:461:LEU:HD21	6:C:475:MET:HE2	1.99	0.43
6:C:715:GLY:HA2	6:C:729:ALA:HB1	1.99	0.43
2:A:902:TYR:HB2	2:A:1242:ASN:CG	2.44	0.43
2:A:1346:THR:OG1	2:A:1348:VAL:HG12	2.18	0.43
6:C:158:ARG:HD3	6:C:158:ARG:O	2.19	0.43
1:F:102:ASP:OD1	1:F:105:GLY:N	2.52	0.43
2:A:428:LYS:HA	2:A:431:TYR:CE2	2.54	0.43
2:A:1382:SER:HA	2:A:1415:GLY:HA2	2.00	0.43
2:A:1427:ARG:NH1	2:A:1428:HIS:HB2	2.34	0.43
2:A:1730:MET:O	2:A:1733:ILE:HG22	2.18	0.43
3:5:8:G:C2'	3:5:9:G:H5'	2.49	0.43
3:5:113:G:H2'	3:5:114:G:H8	1.83	0.43
2:A:996:LEU:HB3	2:A:1043:TYR:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1639:VAL:HG11	2:A:1699:THR:HG21	2.00	0.43
3:5:17:U:H2'	3:5:18:C:H6	1.83	0.43
6:C:109:LEU:CD2	6:C:116:MET:HG3	2.48	0.43
2:A:1448:LEU:HD23	2:A:1448:LEU:HA	1.78	0.43
2:A:1559:GLY:HA3	2:A:1582:TRP:CZ2	2.54	0.43
2:A:1576:ILE:HD11	2:A:1746:ARG:C	2.43	0.43
3:5:9:G:H8	3:5:9:G:OP2	2.01	0.43
6:C:181:ILE:HG22	6:C:182:LYS:HG3	2.01	0.43
6:C:818:SER:O	6:C:822:MET:HG2	2.19	0.43
1:F:164:LEU:HB3	1:F:202:LEU:HD23	2.00	0.43
2:A:1418:ARG:O	2:A:1421:THR:HG22	2.19	0.43
8:m:18:PRO:HA	8:m:32:TYR:HA	2.00	0.43
2:A:196:ASP:HB3	2:A:199:GLU:HG2	2.01	0.42
2:A:422:LEU:H	2:A:422:LEU:HD23	1.82	0.42
2:A:1308:PRO:HB3	2:A:1548:TYR:CE1	2.54	0.42
1:F:164:LEU:HD23	1:F:202:LEU:CA	2.49	0.42
1:F:176:ARG:HE	2:A:59:GLU:HB3	1.83	0.42
2:A:804:GLU:HA	2:A:807:VAL:HG22	2.00	0.42
2:A:1056:HIS:O	2:A:1060:GLU:HG3	2.20	0.42
2:A:638:LEU:HD23	2:A:638:LEU:HA	1.90	0.42
2:A:1010:THR:HA	2:A:1013:ASN:OD1	2.19	0.42
2:A:1180:LYS:O	2:A:1201:ARG:NH2	2.52	0.42
2:A:1322:LEU:HD23	2:A:1484:ILE:HD13	2.01	0.42
2:A:1531:ASN:OD1	2:A:1531:ASN:N	2.52	0.42
5:D:273:VAL:HG23	5:D:273:VAL:O	2.19	0.42
13:h:18:ARG:HA	13:h:27:PHE:O	2.18	0.42
2:A:1615:HIS:HB3	2:A:1617:ARG:NH1	2.34	0.42
6:C:719:GLN:HG2	6:C:724:TRP:O	2.19	0.42
6:C:934:MET:HE3	6:C:938:ARG:HD2	2.02	0.42
1:F:117:ASP:OD2	2:A:540:PHE:N	2.53	0.42
2:A:876:GLU:OE1	2:A:880:ARG:NH1	2.52	0.42
3:5:60:G:H2'	3:5:61:A:C8	2.54	0.42
2:A:171:ASP:O	2:A:519:ASP:HB2	2.19	0.42
2:A:507:LEU:HD11	2:A:652:LEU:CD1	2.47	0.42
2:A:1310:ARG:NH2	2:A:1336:PRO:HG2	2.34	0.42
3:5:112:A:H2'	3:5:113:G:C8	2.54	0.42
6:C:166:CYS:C	6:C:168:THR:H	2.27	0.42
6:C:713:LYS:HA	6:C:716:GLU:CD	2.44	0.42
2:A:934:ARG:HB3	2:A:934:ARG:NH1	2.35	0.42
2:A:1593:LEU:HD12	2:A:1593:LEU:HA	1.87	0.42
2:A:62:PRO:HA	2:A:63:PRO:HD3	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:719:CYS:O	2:A:723:ASN:N	2.53	0.42
2:A:810:TYR:O	2:A:814:VAL:HG13	2.20	0.42
2:A:1017:ILE:HD11	2:A:1026:ASN:CB	2.49	0.42
6:C:446:LYS:HB3	6:C:447:PRO:HD3	2.00	0.42
12:k:27:VAL:O	12:k:48:VAL:HA	2.19	0.42
2:A:406:TRP:CZ2	6:C:266:GLU:HG2	2.55	0.42
2:A:462:ARG:NH2	3:5:51:A:OP2	2.53	0.42
2:A:876:GLU:CD	2:A:880:ARG:HH12	2.28	0.42
2:A:1009:MET:HE2	2:A:1009:MET:HB3	1.62	0.42
3:5:76:A:H2'	3:5:77:G:C8	2.55	0.42
6:C:186:VAL:HG22	6:C:535:ALA:HB2	2.01	0.42
6:C:254:THR:HB	6:C:433:MET:SD	2.60	0.42
2:A:1022:MET:SD	2:A:1023:ASN:N	2.93	0.41
2:A:1342:TRP:CE2	2:A:1482:GLU:CD	2.98	0.41
2:A:1589:ILE:C	2:A:1589:ILE:HD12	2.45	0.41
3:5:51:A:H2'	3:5:52:U:C6	2.55	0.41
6:C:236:MET:HE2	6:C:236:MET:HA	2.02	0.41
6:C:738:ASP:OD1	6:C:775:ARG:NH2	2.47	0.41
6:C:836:VAL:HG22	6:C:897:SER:HB3	2.02	0.41
1:F:160:GLY:O	1:F:164:LEU:HB2	2.20	0.41
2:A:320:TYR:OH	6:C:881:PHE:HB3	2.20	0.41
2:A:1639:VAL:HG21	2:A:1699:THR:HG21	2.02	0.41
5:D:285:ASP:O	5:D:291:LYS:HD3	2.20	0.41
6:C:676:ALA:HB3	6:C:815:VAL:HB	2.01	0.41
6:C:946:ASP:OD1	6:C:947:VAL:N	2.51	0.41
2:A:1394:GLN:HA	2:A:1397:ILE:HD11	2.02	0.41
2:A:1543:ASN:OD1	2:A:1543:ASN:C	2.64	0.41
3:5:7:U:C2	3:5:8:G:C8	3.07	0.41
2:A:881:ILE:O	2:A:885:LEU:HD23	2.20	0.41
8:m:36:VAL:HA	8:m:41:ASN:O	2.20	0.41
2:A:1624:SER:HB3	2:A:1692:MET:HG3	2.01	0.41
6:C:166:CYS:O	6:C:168:THR:N	2.54	0.41
6:C:370:VAL:HA	6:C:374:LEU:HB2	2.02	0.41
2:A:261:LYS:HD2	2:A:328:HIS:HB3	2.03	0.41
2:A:1006:ALA:O	2:A:1010:THR:HG23	2.20	0.41
3:5:29:A:H2'	3:5:30:A:H8	1.86	0.41
6:C:481:MET:HE3	6:C:481:MET:HB3	1.89	0.41
6:C:531:TRP:HB3	6:C:538:HIS:HB3	2.01	0.41
6:C:863:ILE:HD11	6:C:870:THR:HG23	2.03	0.41
2:A:1031:ILE:O	2:A:1032:ARG:HG2	2.21	0.41
2:A:1320:LYS:HA	2:A:1324:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1393:ARG:HA	2:A:1403:LEU:HD21	2.02	0.41
2:A:1394:GLN:O	2:A:1397:ILE:HD12	2.21	0.41
2:A:1585:ILE:O	2:A:1589:ILE:HG23	2.21	0.41
2:A:1680:ALA:HB2	2:A:1704:ALA:HB3	2.01	0.41
2:A:617:ASN:HB3	2:A:623:LYS:HD2	2.03	0.41
2:A:811:THR:HA	2:A:814:VAL:HG22	2.02	0.41
2:A:1013:ASN:HA	2:A:1031:ILE:CG1	2.50	0.41
2:A:1465:TRP:CD1	2:A:1467:LEU:HD11	2.55	0.41
2:A:1498:TRP:HA	2:A:1501:LEU:HD23	2.02	0.41
6:C:434:CYS:O	6:C:438:ILE:HB	2.20	0.41
6:C:589:LYS:HG3	6:C:628:VAL:HG13	2.02	0.41
2:A:257:LEU:HD12	2:A:257:LEU:HA	1.93	0.41
2:A:604:MET:HB2	2:A:604:MET:HE2	1.81	0.41
2:A:1369:TYR:O	7:B:52:MET:HG3	2.20	0.41
2:A:1412:TRP:CE3	2:A:1412:TRP:HA	2.56	0.41
2:A:1589:ILE:HD12	2:A:1590:VAL:N	2.35	0.41
2:A:1723:LYS:HB3	2:A:1724:PRO:HD3	2.01	0.41
3:5:96:A:H2	3:5:97:G:C4	2.39	0.41
3:5:111:A:H2'	3:5:112:A:H8	1.84	0.41
6:C:299:ILE:O	6:C:306:ASN:ND2	2.54	0.41
6:C:399:LEU:HB2	6:C:401:ILE:HD12	2.03	0.41
6:C:925:PRO:HD2	6:C:928:HIS:NE2	2.36	0.41
2:A:946:GLU:HG3	2:A:950:LEU:HB3	2.04	0.40
2:A:994:ASN:HA	2:A:1010:THR:HG21	2.03	0.40
2:A:1345:GLN:OE1	2:A:1711:LEU:HA	2.21	0.40
6:C:147:ASP:O	6:C:149:LEU:N	2.54	0.40
6:C:302:PRO:HG2	6:C:344:TRP:CD2	2.56	0.40
6:C:751:PRO:HA	6:C:756:LYS:HD3	2.02	0.40
1:F:102:ASP:CG	1:F:104:ASP:H	2.28	0.40
2:A:1045:GLY:HA3	2:A:1090:ARG:CZ	2.51	0.40
2:A:1555:LEU:HD21	2:A:1574:ILE:HD12	2.03	0.40
2:A:1645:LEU:HB2	2:A:1714:ALA:H	1.86	0.40
6:C:145:PHE:CA	6:C:148:CYS:HB2	2.51	0.40
1:F:90:PHE:HD1	1:F:90:PHE:HA	1.76	0.40
2:A:441:VAL:HG23	2:A:444:ARG:HH21	1.85	0.40
2:A:820:ARG:NH1	2:A:1063:GLY:O	2.43	0.40
2:A:938:PRO:HB2	2:A:1071:PHE:HA	2.02	0.40
2:A:996:LEU:C	2:A:1043:TYR:HH	2.29	0.40
2:A:1016:VAL:HA	2:A:1025:THR:HA	2.03	0.40
7:B:48:GLU:HG2	7:B:49:GLY:N	2.37	0.40
7:B:51:ARG:N	7:B:54:ASP:OD2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:l:58:LEU:O	14:l:76:ARG:HA	2.21	0.40
2:A:295:GLU:HG3	2:A:1144:LYS:HG3	2.03	0.40
2:A:901:LEU:H	2:A:901:LEU:HD22	1.86	0.40
2:A:1403:LEU:HD13	2:A:1403:LEU:HA	1.93	0.40
6:C:122:LEU:HD23	6:C:122:LEU:HA	1.93	0.40
6:C:158:ARG:HD3	6:C:158:ARG:C	2.46	0.40
6:C:343:LEU:HD13	6:C:373:ILE:HD11	2.04	0.40
2:A:449:LYS:HA	2:A:449:LYS:HD3	1.87	0.40
2:A:1626:CYS:HG	2:A:1627:ALA:H	1.66	0.40
6:C:313:GLN:HB2	15:C:1001:GTP:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	134/341 (39%)	123 (92%)	10 (8%)	1 (1%)	18	49
2	A	1615/2335 (69%)	1558 (96%)	56 (4%)	1 (0%)	48	78
4	E	56/941 (6%)	56 (100%)	0	0	100	100
5	D	50/820 (6%)	49 (98%)	1 (2%)	0	100	100
6	C	845/972 (87%)	813 (96%)	31 (4%)	1 (0%)	48	78
7	B	25/2136 (1%)	25 (100%)	0	0	100	100
8	m	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
9	n	72/76 (95%)	64 (89%)	8 (11%)	0	100	100
10	i	79/119 (66%)	73 (92%)	6 (8%)	0	100	100
11	j	94/118 (80%)	84 (89%)	10 (11%)	0	100	100
12	k	82/126 (65%)	78 (95%)	4 (5%)	0	100	100
13	h	69/240 (29%)	67 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
All	All	3267/8402 (39%)	3130 (96%)	134 (4%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1020	LYS
6	C	148	CYS
1	F	126	VAL

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	F	58/281 (21%)	57 (98%)	1 (2%)	53	74
2	A	1384/2108 (66%)	1357 (98%)	27 (2%)	48	72
5	D	48/721 (7%)	44 (92%)	4 (8%)	10	35
6	C	737/866 (85%)	721 (98%)	16 (2%)	45	71
7	B	22/1908 (1%)	21 (96%)	1 (4%)	24	56
All	All	2249/5884 (38%)	2200 (98%)	49 (2%)	45	71

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	90	PHE
2	A	60	ASP
2	A	87	VAL
2	A	181	ASN
2	A	294	ASN
2	A	373	ASP
2	A	395	THR
2	A	645	THR
2	A	652	LEU

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Mol	Chain	Res	Type
2	A	1017	ILE
2	A	1023	ASN
2	A	1024	HIS
2	A	1055	LEU
2	A	1194	CYS
2	A	1234	ASP
2	A	1244	VAL
2	A	1268	ILE
2	A	1297	THR
2	A	1340	LEU
2	A	1385	VAL
2	A	1403	LEU
2	A	1426	ASP
2	A	1539	SER
2	A	1597	PHE
2	A	1630	LEU
2	A	1635	TYR
2	A	1672	ASP
2	A	1710	ASN
5	D	244	SER
5	D	246	GLU
5	D	284	ILE
5	D	298	LEU
6	C	109	LEU
6	C	112	THR
6	C	147	ASP
6	C	162	ASP
6	C	255	VAL
6	C	357	THR
6	C	498	SER
6	C	520	GLU
6	C	525	CYS
6	C	587	VAL
6	C	660	VAL
6	C	668	GLU
6	C	674	CYS
6	C	714	LEU
6	C	735	PHE
6	C	878	ILE
7	B	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	294	ASN
2	A	300	ASN
2	A	328	HIS
2	A	357	ASN
2	A	434	HIS
2	A	517	HIS
2	A	542	ASN
2	A	994	ASN
2	A	1096	HIS
2	A	1159	ASN
2	A	1188	ASN
2	A	1246	GLN
2	A	1282	GLN
2	A	1710	ASN
6	C	139	HIS
6	C	280	HIS
6	C	335	ASN
6	C	337	GLN
6	C	451	HIS
6	C	571	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	5	101/117 (86%)	34 (33%)	4 (3%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	5	4	C
3	5	5	U
3	5	6	C
3	5	9	G
3	5	20	G
3	5	21	A
3	5	22	U
3	5	23	C
3	5	24	G
3	5	25	C
3	5	26	A
3	5	28	A
3	5	36	C

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Mol	Chain	Res	Type
3	5	38	C
3	5	47	A
3	5	48	A
3	5	57	G
3	5	58	U
3	5	59	G
3	5	66	A
3	5	67	A
3	5	69	A
3	5	71	C
3	5	75	G
3	5	78	U
3	5	86	C
3	5	94	U
3	5	95	G
3	5	97	G
3	5	98	G
3	5	105	U
3	5	106	U
3	5	107	U
3	5	108	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	5	57	G
3	5	58	U
3	5	96	A
3	5	105	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
15	GTP	C	1001	-	33,34,34	0.60	0	50,54,54	0.62	0

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
15	GTP	C	1001	-	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	1001	GTP	O4'-C4'-C5'-O5'
15	C	1001	GTP	C3'-C4'-C5'-O5'

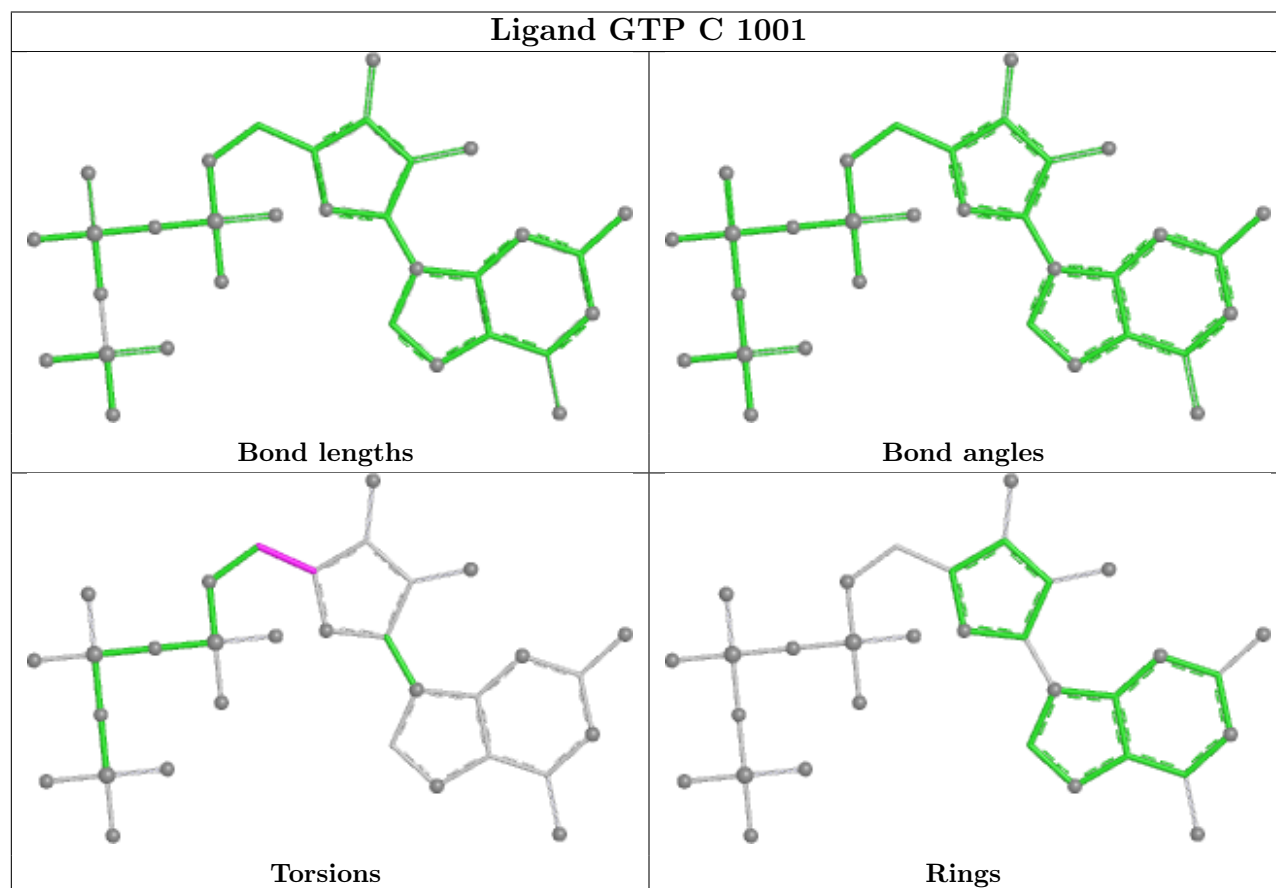
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	1001	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

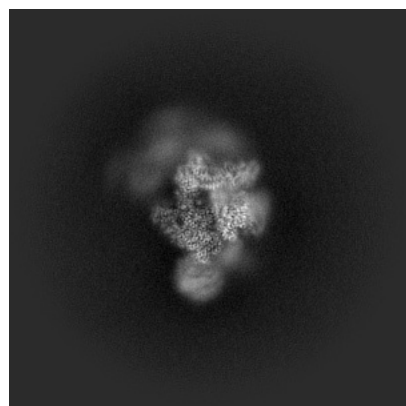
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18267. These allow visual inspection of the internal detail of the map and identification of artifacts.

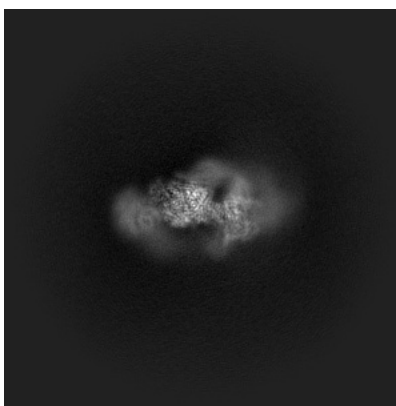
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

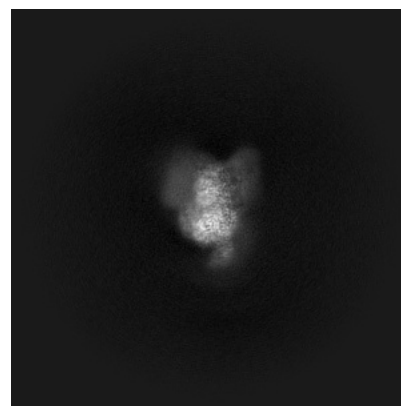
6.1.1 Primary map



X

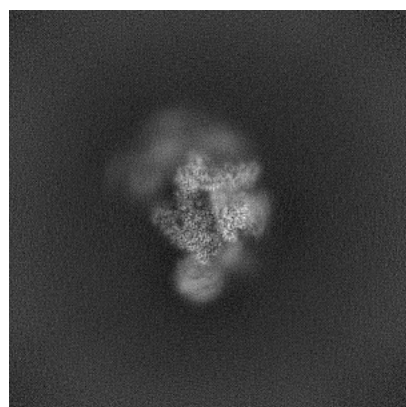


Y

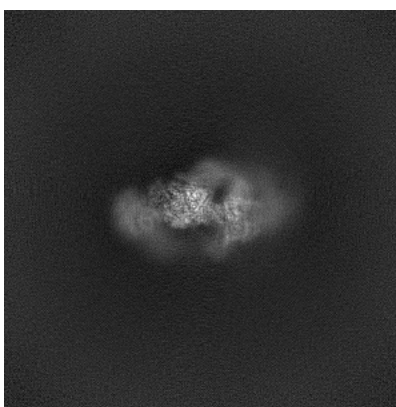


Z

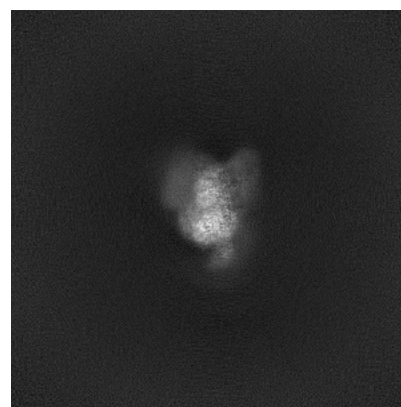
6.1.2 Raw map



X



Y

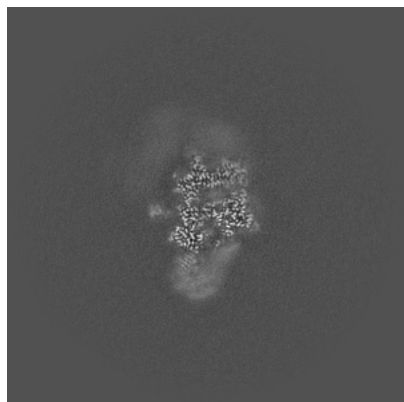


Z

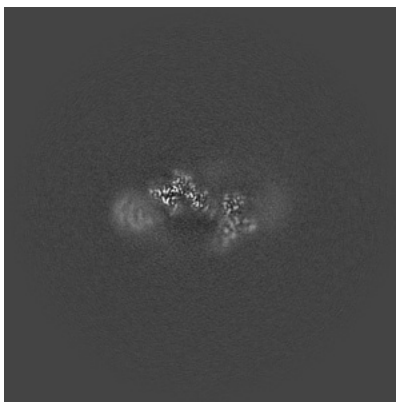
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

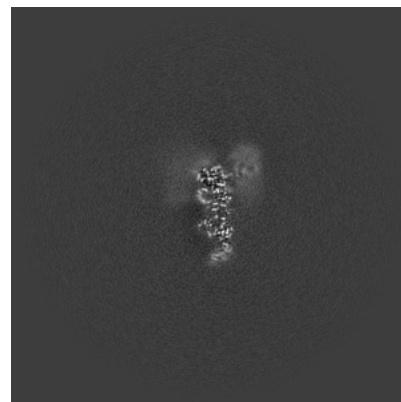
6.2.1 Primary map



X Index: 252

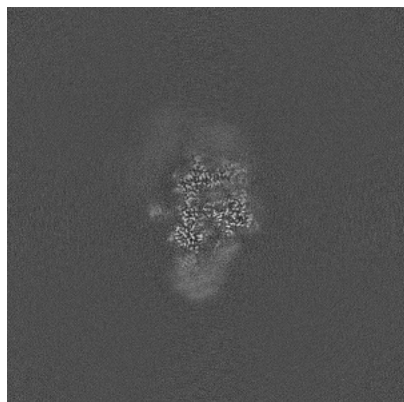


Y Index: 252

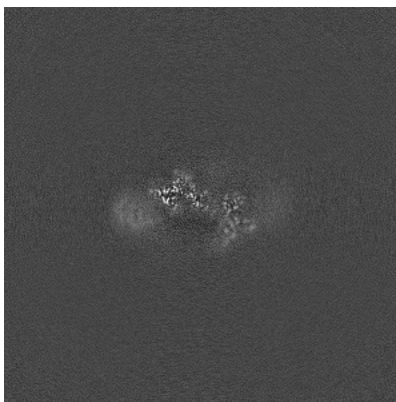


Z Index: 252

6.2.2 Raw map



X Index: 252



Y Index: 252

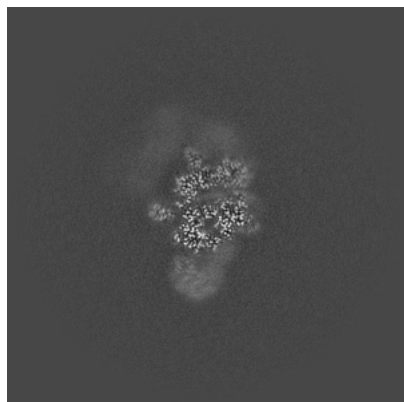


Z Index: 252

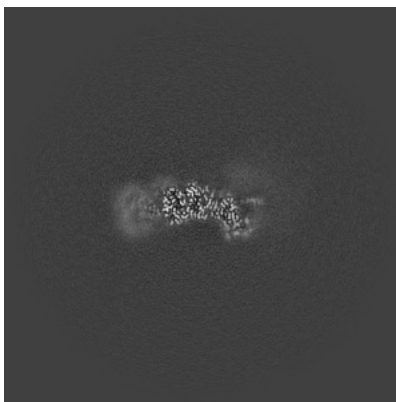
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

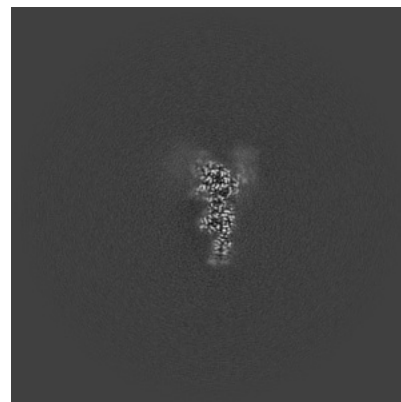
6.3.1 Primary map



X Index: 256

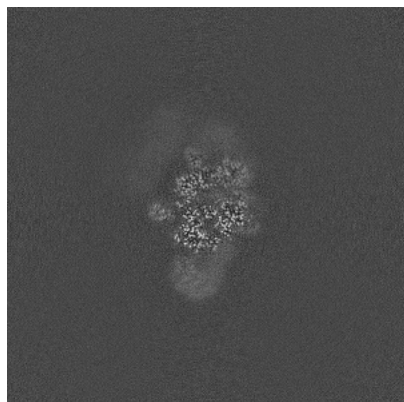


Y Index: 228

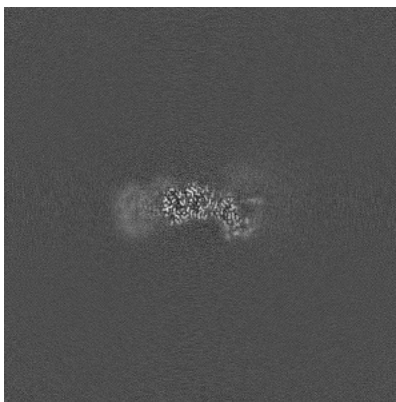


Z Index: 241

6.3.2 Raw map



X Index: 256



Y Index: 228

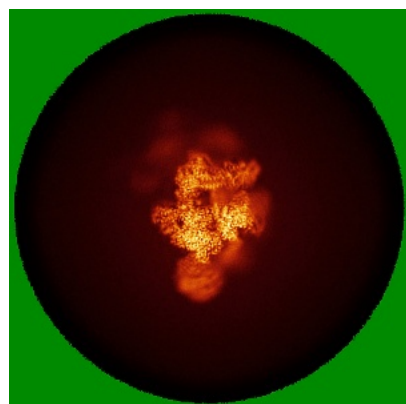


Z Index: 241

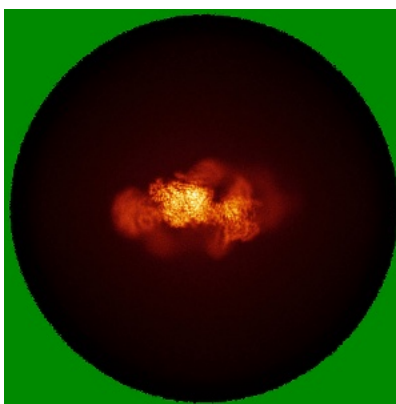
The images above show the largest variance slices of the map in three orthogonal directions.

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

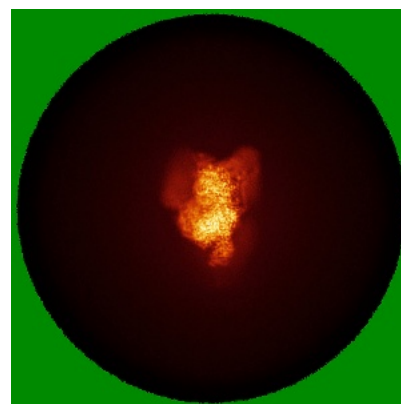
6.4.1 Primary map



X

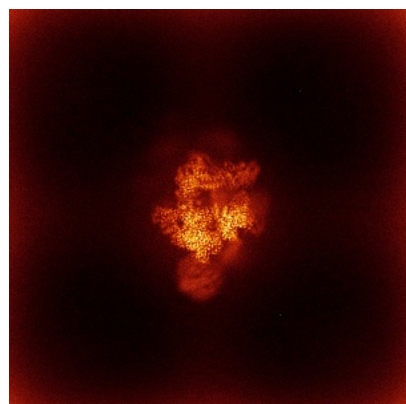


Y

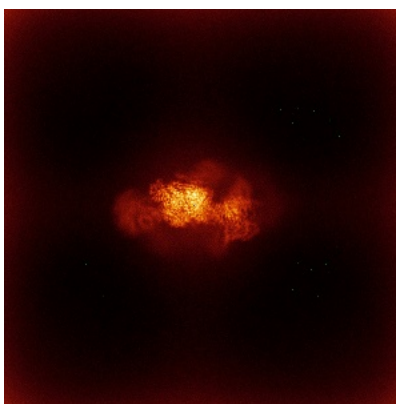


Z

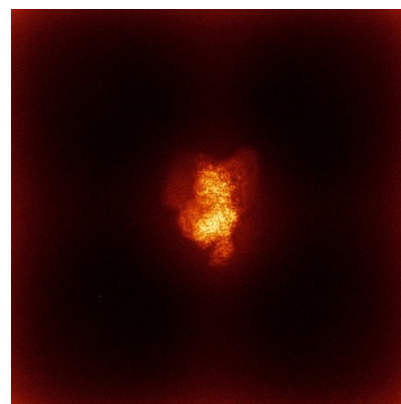
6.4.2 Raw map



X



Y

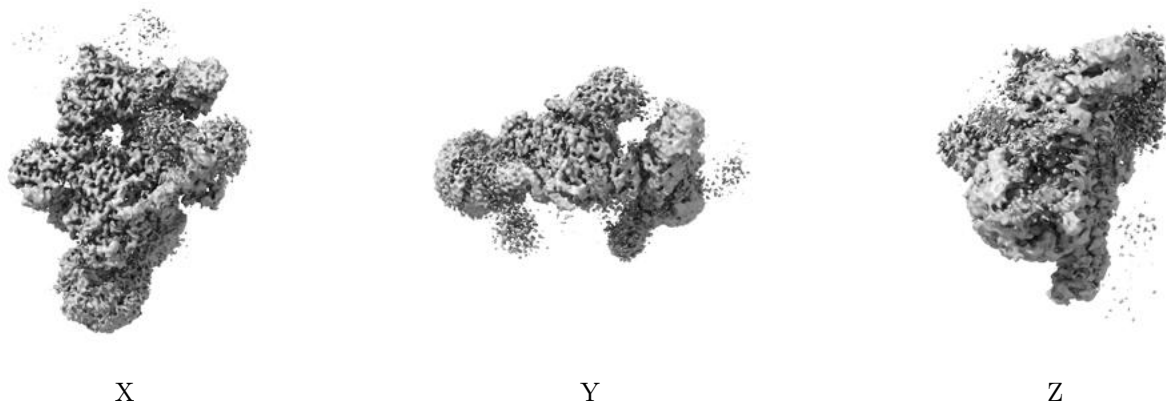


Z

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.

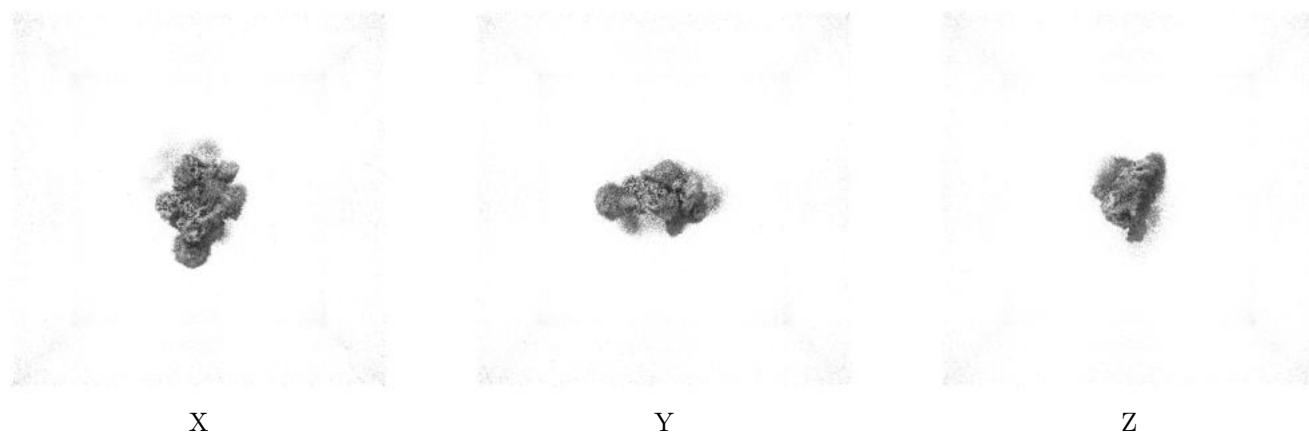
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

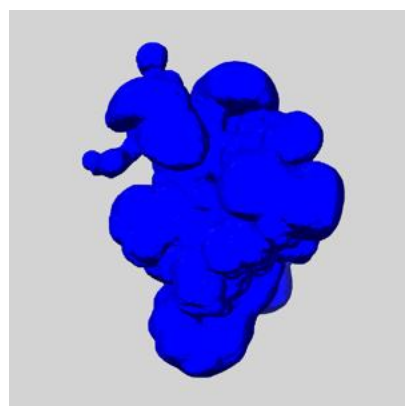
6.6 Mask visualisation [i](#)

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

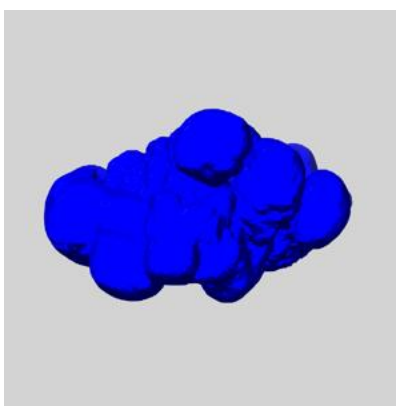
A mask typically either:

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

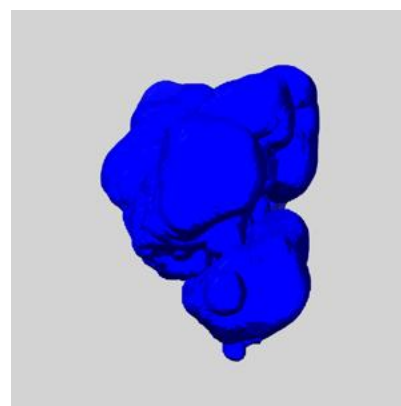
6.6.1 emd_18267_msk_1.map [i](#)



X



Y

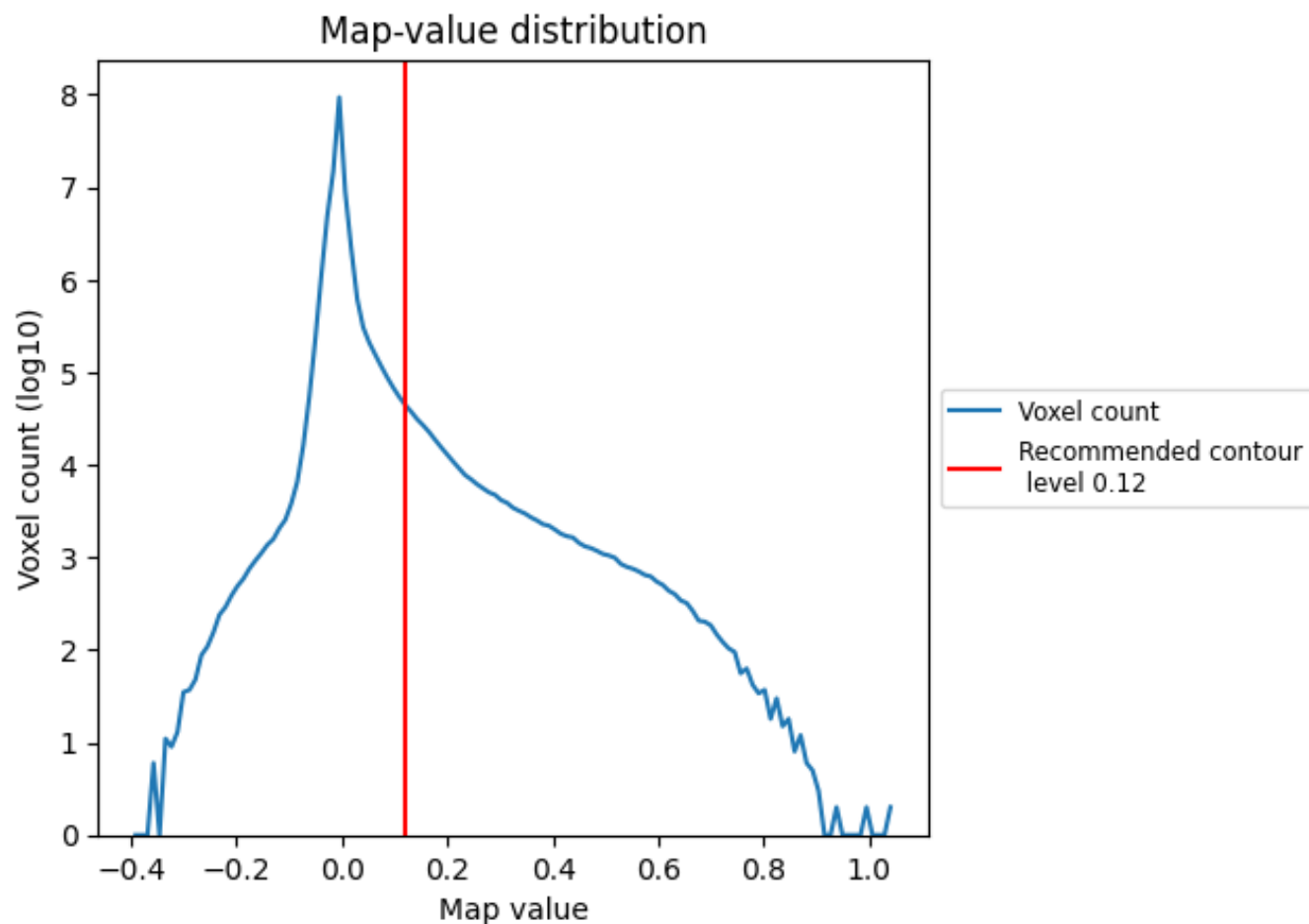


Z

7 Map analysis [i](#)

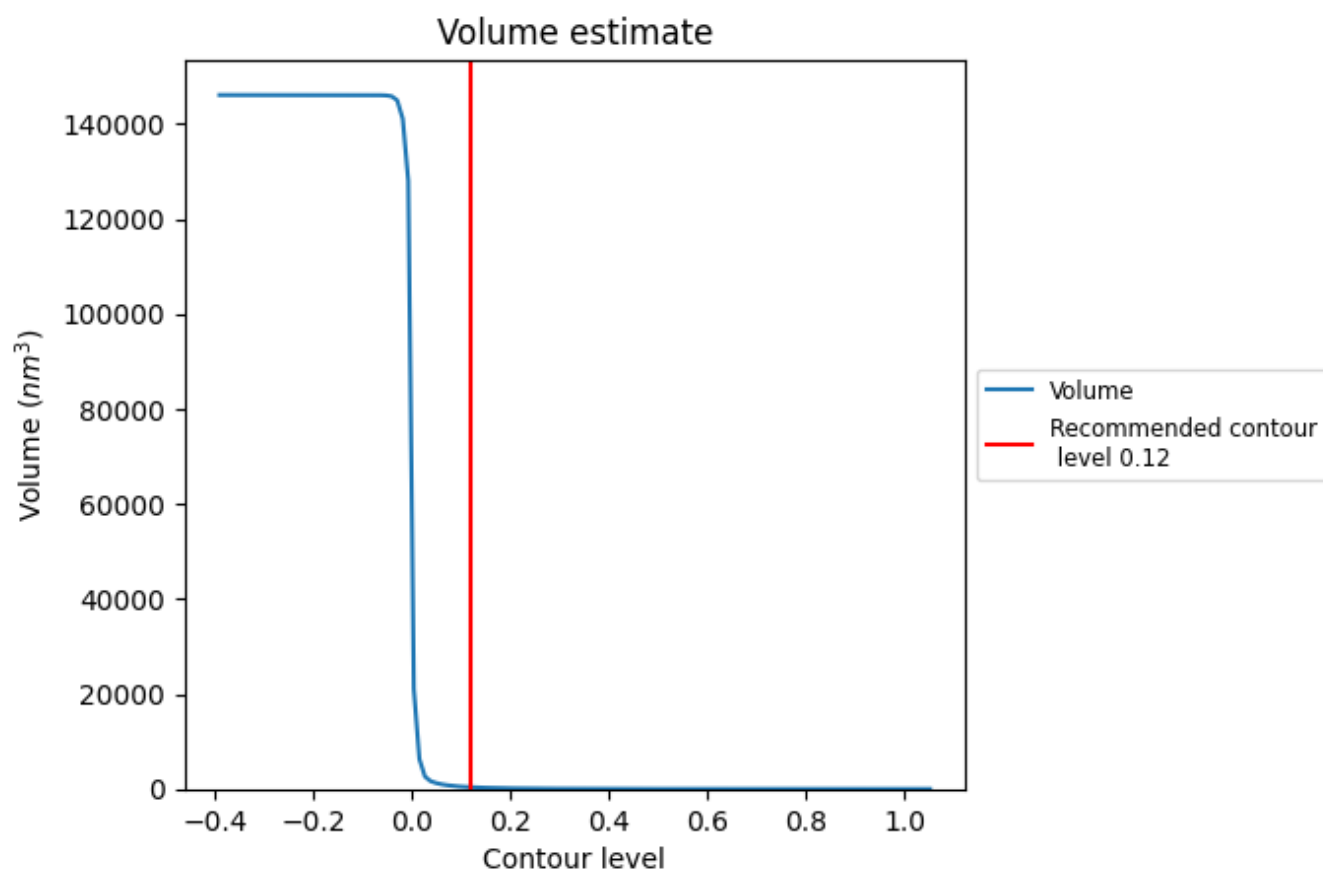
This section contains the results of statistical analysis of the map.

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.

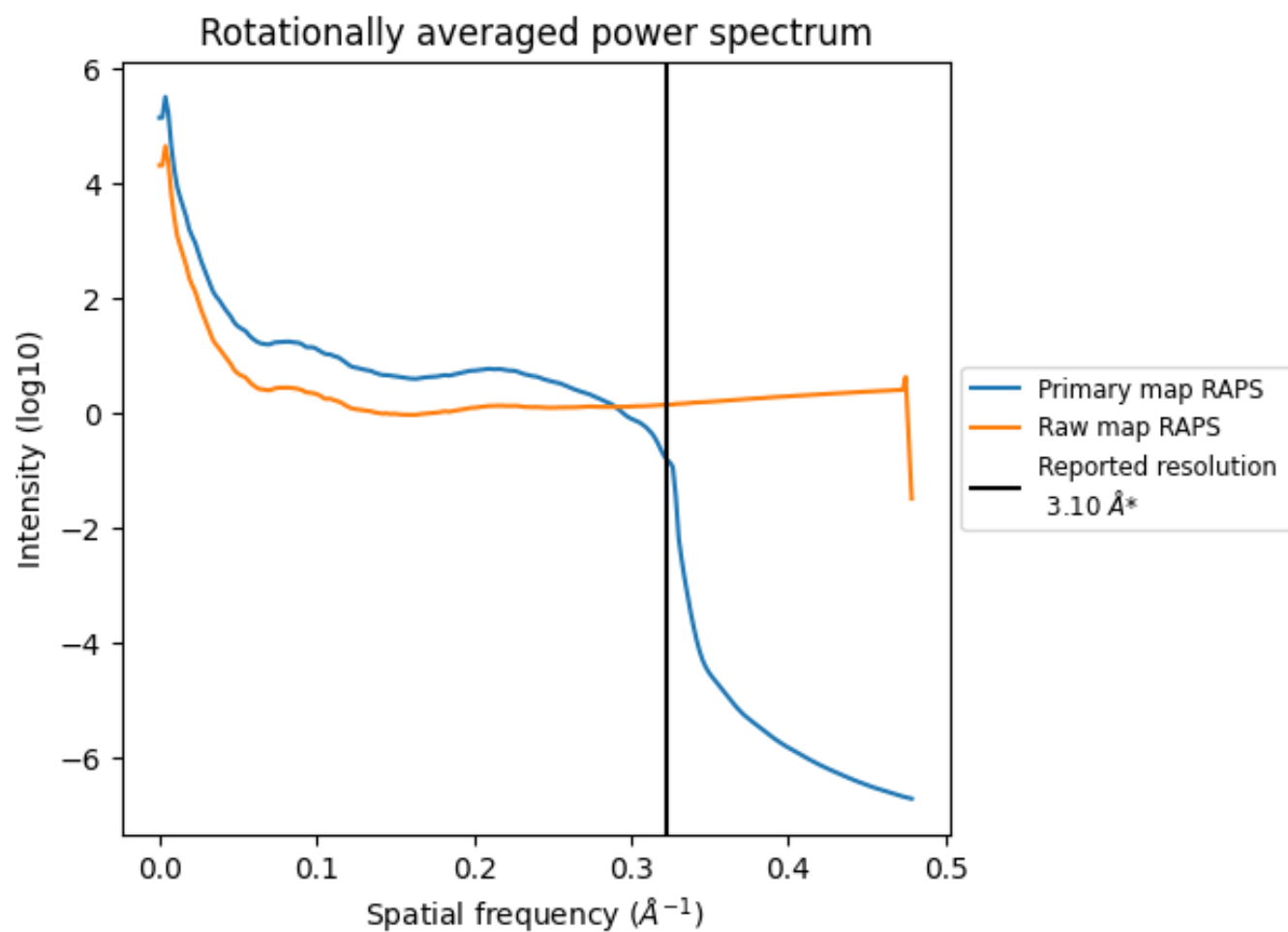
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm^3 ; this corresponds to an approximate mass of 327 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 ⓘ

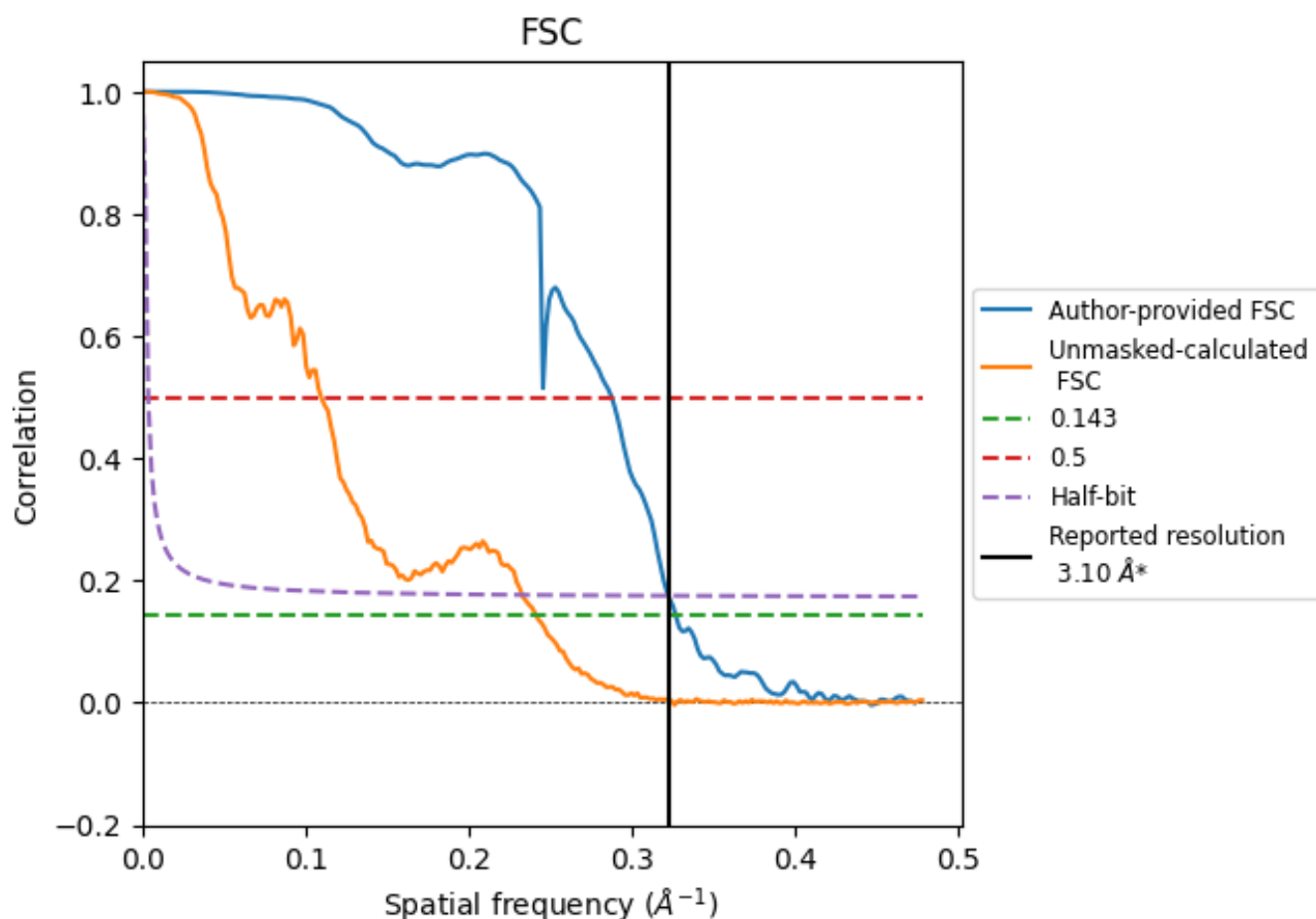


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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

8.2 Resolution estimates [i](#)

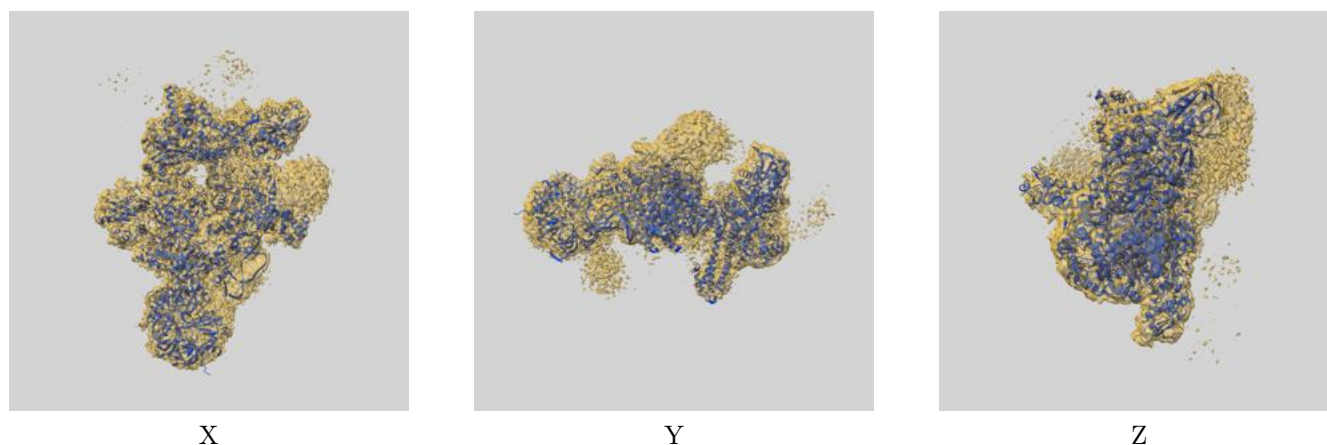
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.47	3.10
Unmasked-calculated*	4.14	9.11	4.29

*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 4.14 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

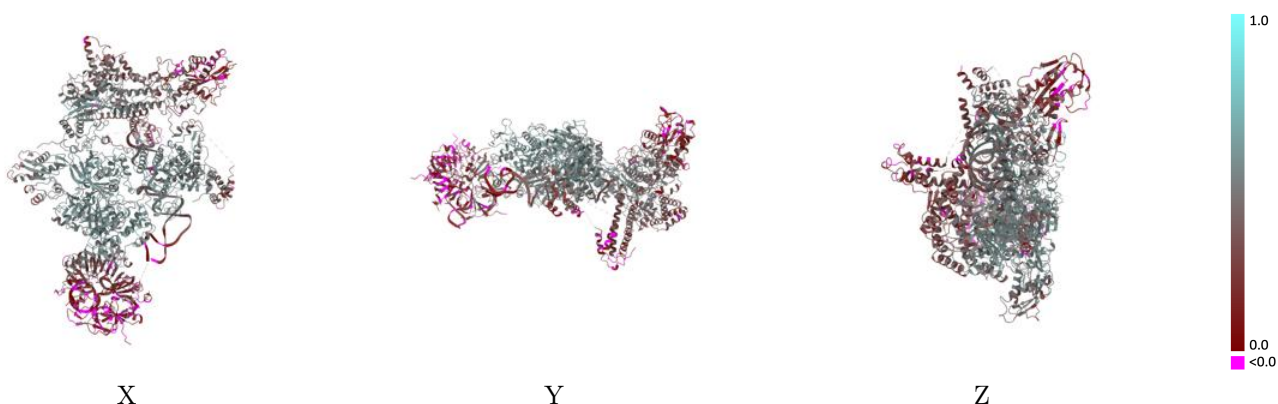
This section contains information regarding the fit between EMDB map EMD-18267 and PDB model 8Q91. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



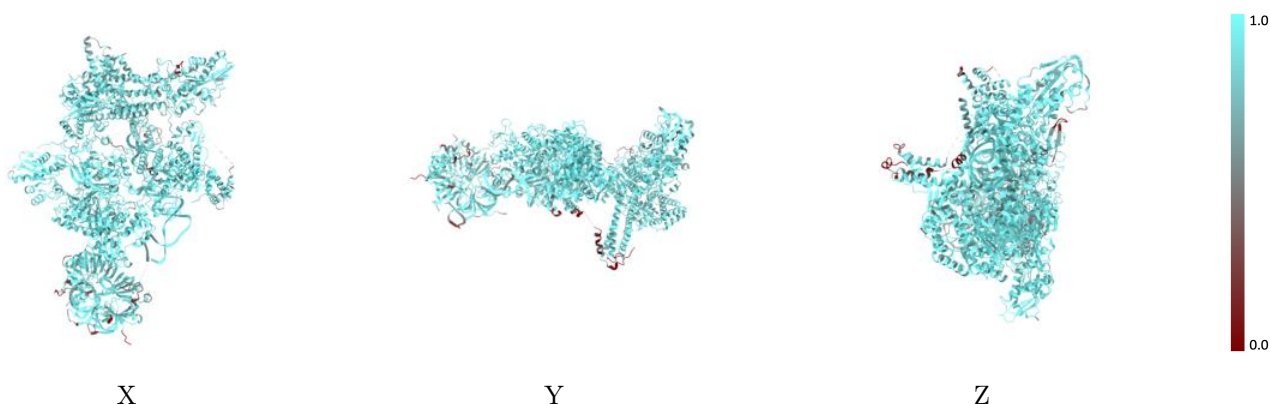
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



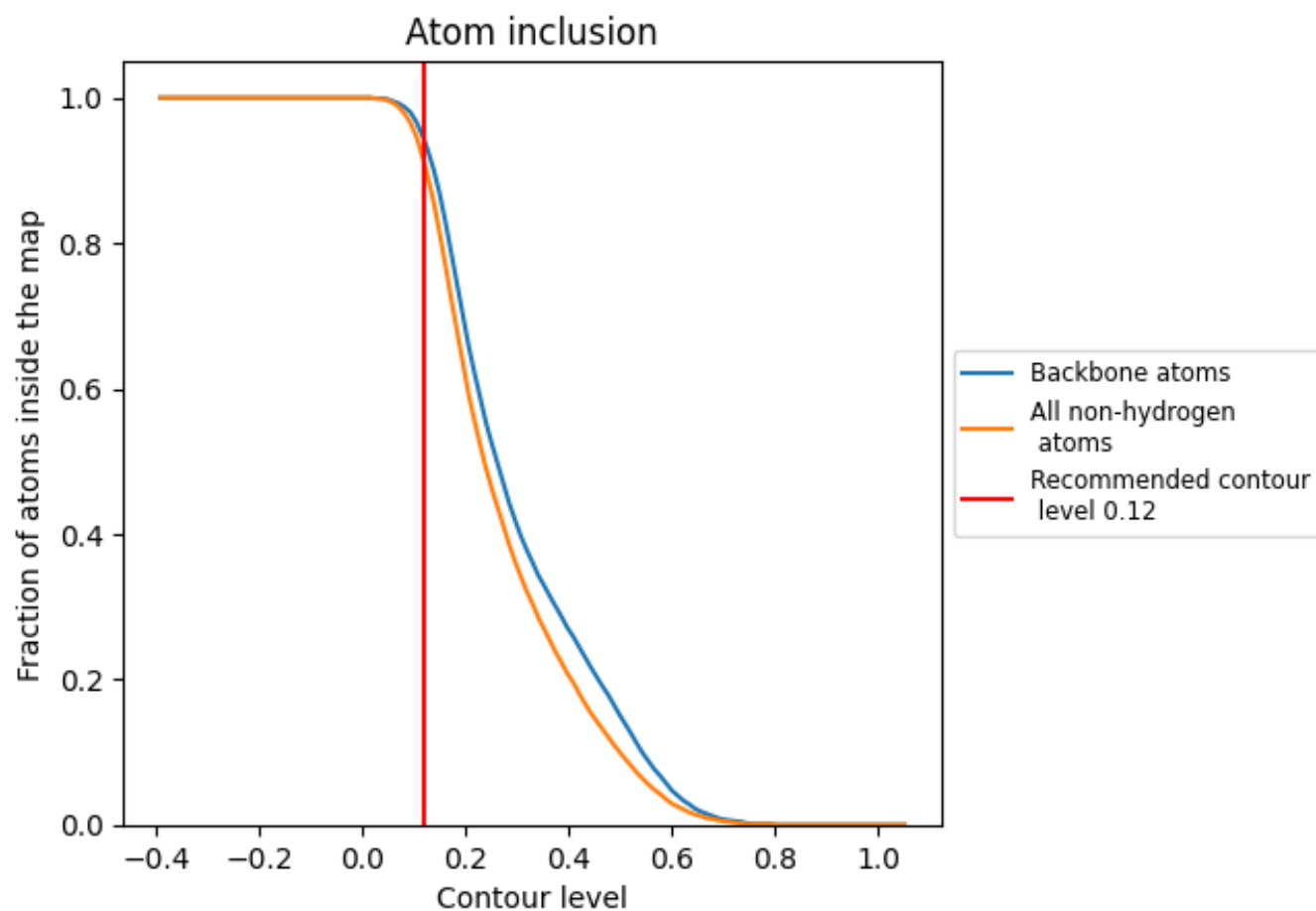
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.4170
5	0.8850	0.2720
A	0.9190	0.4350
B	0.7870	0.4280
C	0.9590	0.5270
D	0.8880	0.5120
E	0.4570	0.2020
F	0.8490	0.3660
h	0.8940	0.2550
i	0.9250	0.1800
j	0.7700	0.0980
k	0.9350	0.3980
l	0.8920	0.1310
m	0.8480	0.0930
n	0.7450	0.2620

