



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:07 AM UTC

PDB ID : 8QCF / pdb_00008qcf
EMDB ID : EMD-18329
Title : yeast cytoplasmic exosome-Ski2 complex degrading a RNA substrate
Authors : Keidel, A.; Koegel, A.; Reichelt, P.; Kowalinski, E.; Schaefer, I.B.; Conti, E.
Deposited on : 2023-08-25
Resolution : 2.55 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:

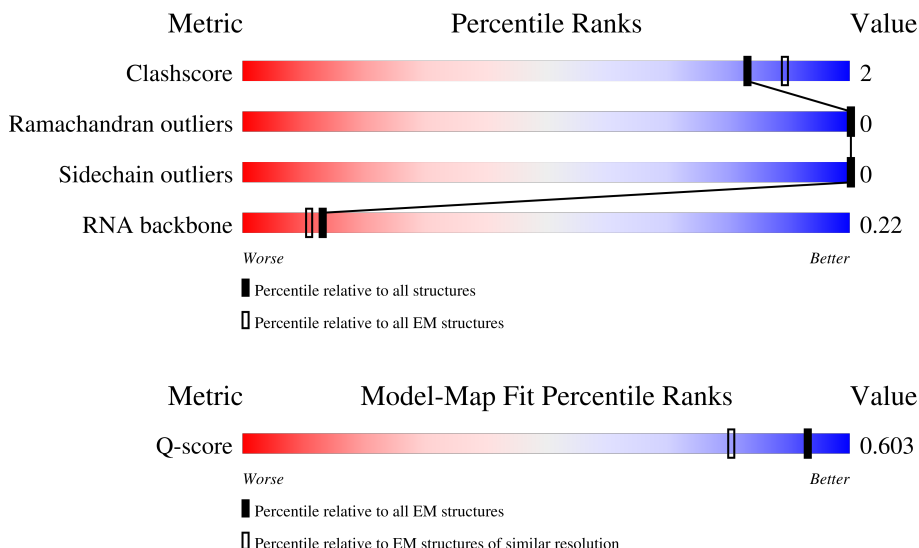
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.55 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.



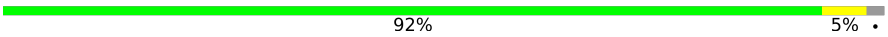
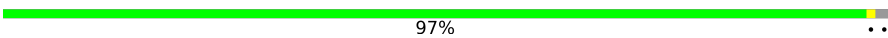
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7475 (2.05 - 3.05)

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	B	305	
2	C	249	
3	D	394	

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Mol	Chain	Length	Quality of chain
4	E	226	 92% 5%
5	F	268	 97% ..
6	G	250	 80% . 16%
7	H	244	 89% . 7%
8	I	364	 72% . 26%
9	J	295	 74% . 23%
10	K	1005	 39% 79% 12% 9%
11	L	353	 21% . 78%
12	M	1040	 12% 58% 5% 37%
13	N	78	 32% 21% 23% 56%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 30751 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 Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	297	Total	C	N	O	S	0	0
			2261	1425	383	437	16		

- Molecule 2 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	241	Total	C	N	O	S	0	0
			1881	1176	334	363	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P46948
C	-1	PRO	-	expression tag	UNP P46948
C	0	HIS	-	expression tag	UNP P46948

- Molecule 3 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	305	Total	C	N	O	S	0	0
			2358	1496	403	449	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	102	SER	ALA	conflict	UNP P25359
D	363	MET	VAL	conflict	UNP P25359

- Molecule 4 is a protein called RRP46 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	221	Total	C	N	O	S	0	0
			1691	1063	287	332	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ALA	-	expression tag	UNP A0A6A5PYM9
E	-1	ALA	-	expression tag	UNP A0A6A5PYM9
E	0	SER	-	expression tag	UNP A0A6A5PYM9

- Molecule 5 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	263	Total	C	N	O	S	0	0
			1998	1276	331	387	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP Q12277
F	-1	PRO	-	expression tag	UNP Q12277
F	0	HIS	-	expression tag	UNP Q12277
F	138	ILE	VAL	conflict	UNP Q12277

- Molecule 6 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	209	Total	C	N	O	S	0	0
			1581	994	267	310	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	161	THR	MET	conflict	UNP P48240

- Molecule 7 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	228	Total	C	N	O	S	0	0
			1765	1127	288	340	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	GLY	-	expression tag	UNP Q08285
H	-2	PRO	-	expression tag	UNP Q08285

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	ASP	-	expression tag	UNP Q08285
H	0	SER	-	expression tag	UNP Q08285

- Molecule 8 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	268	Total	C	N	O	S	0	0
			2084	1306	374	392	12		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	THR	-	expression tag	UNP P38792
I	-3	GLY	-	expression tag	UNP P38792
I	-2	GLY	-	expression tag	UNP P38792
I	-1	ARG	-	expression tag	UNP P38792
I	0	SER	-	expression tag	UNP P38792

- Molecule 9 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	227	Total	C	N	O	S	0	0
			1689	1056	297	329	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	expression tag	UNP P53859
J	-1	PRO	-	expression tag	UNP P53859
J	0	HIS	-	expression tag	UNP P53859

- Molecule 10 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	915	Total	C	N	O	S	0	0
			7231	4579	1267	1350	35		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	GLY	-	expression tag	UNP Q08162

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	PRO	-	expression tag	UNP Q08162
K	-1	ASP	-	expression tag	UNP Q08162
K	0	SER	-	expression tag	UNP Q08162

- Molecule 11 is a protein called Superkiller protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	79	Total	C	N	O	S	0	0
			618	398	103	114	3		

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-105	GLY	-	expression tag	UNP Q08491
L	-104	PRO	-	expression tag	UNP Q08491
L	-103	ASP	-	expression tag	UNP Q08491
L	-102	SER	-	expression tag	UNP Q08491
L	-101	MET	-	expression tag	UNP Q08491
L	-100	SER	-	expression tag	UNP Q08491
L	-99	ALA	-	expression tag	UNP Q08491
L	-98	GLY	-	expression tag	UNP Q08491
L	-97	LEU	-	expression tag	UNP Q08491
L	-96	GLU	-	expression tag	UNP Q08491
L	-95	VAL	-	expression tag	UNP Q08491
L	-94	LEU	-	expression tag	UNP Q08491
L	-93	PHE	-	expression tag	UNP Q08491
L	-92	GLN	-	expression tag	UNP Q08491
L	-91	GLY	-	expression tag	UNP Q08491
L	-90	PRO	-	expression tag	UNP Q08491
L	-89	ASP	-	expression tag	UNP Q08491
L	-88	SER	-	expression tag	UNP Q08491
L	-87	ALA	-	expression tag	UNP Q08491
L	-86	THR	-	expression tag	UNP Q08491
L	-85	HIS	-	expression tag	UNP Q08491
L	-84	ILE	-	expression tag	UNP Q08491
L	-83	LYS	-	expression tag	UNP Q08491
L	-82	PHE	-	expression tag	UNP Q08491
L	-81	SER	-	expression tag	UNP Q08491
L	-80	LYS	-	expression tag	UNP Q08491
L	-79	ARG	-	expression tag	UNP Q08491
L	-78	ASP	-	expression tag	UNP Q08491
L	-77	GLU	-	expression tag	UNP Q08491

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-76	ASP	-	expression tag	UNP Q08491
L	-75	GLY	-	expression tag	UNP Q08491
L	-74	LYS	-	expression tag	UNP Q08491
L	-73	GLU	-	expression tag	UNP Q08491
L	-72	LEU	-	expression tag	UNP Q08491
L	-71	ALA	-	expression tag	UNP Q08491
L	-70	GLY	-	expression tag	UNP Q08491
L	-69	ALA	-	expression tag	UNP Q08491
L	-68	THR	-	expression tag	UNP Q08491
L	-67	MET	-	expression tag	UNP Q08491
L	-66	GLU	-	expression tag	UNP Q08491
L	-65	LEU	-	expression tag	UNP Q08491
L	-64	ARG	-	expression tag	UNP Q08491
L	-63	ASP	-	expression tag	UNP Q08491
L	-62	SER	-	expression tag	UNP Q08491
L	-61	SER	-	expression tag	UNP Q08491
L	-60	GLY	-	expression tag	UNP Q08491
L	-59	LYS	-	expression tag	UNP Q08491
L	-58	THR	-	expression tag	UNP Q08491
L	-57	ILE	-	expression tag	UNP Q08491
L	-56	SER	-	expression tag	UNP Q08491
L	-55	THR	-	expression tag	UNP Q08491
L	-54	TRP	-	expression tag	UNP Q08491
L	-53	ILE	-	expression tag	UNP Q08491
L	-52	SER	-	expression tag	UNP Q08491
L	-51	ASP	-	expression tag	UNP Q08491
L	-50	GLY	-	expression tag	UNP Q08491
L	-49	GLN	-	expression tag	UNP Q08491
L	-48	VAL	-	expression tag	UNP Q08491
L	-47	LYS	-	expression tag	UNP Q08491
L	-46	ASP	-	expression tag	UNP Q08491
L	-45	PHE	-	expression tag	UNP Q08491
L	-44	TYR	-	expression tag	UNP Q08491
L	-43	LEU	-	expression tag	UNP Q08491
L	-42	TYR	-	expression tag	UNP Q08491
L	-41	PRO	-	expression tag	UNP Q08491
L	-40	GLY	-	expression tag	UNP Q08491
L	-39	LYS	-	expression tag	UNP Q08491
L	-38	TYR	-	expression tag	UNP Q08491
L	-37	THR	-	expression tag	UNP Q08491
L	-36	PHE	-	expression tag	UNP Q08491
L	-35	VAL	-	expression tag	UNP Q08491

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-34	GLU	-	expression tag	UNP Q08491
L	-33	THR	-	expression tag	UNP Q08491
L	-32	ALA	-	expression tag	UNP Q08491
L	-31	ALA	-	expression tag	UNP Q08491
L	-30	PRO	-	expression tag	UNP Q08491
L	-29	ASP	-	expression tag	UNP Q08491
L	-28	GLY	-	expression tag	UNP Q08491
L	-27	TYR	-	expression tag	UNP Q08491
L	-26	GLU	-	expression tag	UNP Q08491
L	-25	VAL	-	expression tag	UNP Q08491
L	-24	ALA	-	expression tag	UNP Q08491
L	-23	THR	-	expression tag	UNP Q08491
L	-22	ALA	-	expression tag	UNP Q08491
L	-21	ILE	-	expression tag	UNP Q08491
L	-20	THR	-	expression tag	UNP Q08491
L	-19	PHE	-	expression tag	UNP Q08491
L	-18	THR	-	expression tag	UNP Q08491
L	-17	VAL	-	expression tag	UNP Q08491
L	-16	ASN	-	expression tag	UNP Q08491
L	-15	GLU	-	expression tag	UNP Q08491
L	-14	GLN	-	expression tag	UNP Q08491
L	-13	GLY	-	expression tag	UNP Q08491
L	-12	GLN	-	expression tag	UNP Q08491
L	-11	VAL	-	expression tag	UNP Q08491
L	-10	THR	-	expression tag	UNP Q08491
L	-9	VAL	-	expression tag	UNP Q08491
L	-8	ASN	-	expression tag	UNP Q08491
L	-7	GLY	-	expression tag	UNP Q08491
L	-6	SER	-	expression tag	UNP Q08491
L	-5	GLY	-	expression tag	UNP Q08491
L	-4	SER	-	expression tag	UNP Q08491
L	-3	GLY	-	expression tag	UNP Q08491
L	-2	SER	-	expression tag	UNP Q08491
L	-1	GLY	-	expression tag	UNP Q08491
L	0	SER	-	expression tag	UNP Q08491
L	237	GLY	PRO	conflict	UNP Q08491
L	238	SER	LYS	conflict	UNP Q08491
L	240	TRP	-	expression tag	UNP Q08491
L	241	SER	-	expression tag	UNP Q08491
L	242	HIS	-	expression tag	UNP Q08491
L	243	PRO	-	expression tag	UNP Q08491
L	244	GLN	-	expression tag	UNP Q08491

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Chain	Residue	Modelled	Actual	Comment	Reference
L	245	PHE	-	expression tag	UNP Q08491
L	246	GLU	-	expression tag	UNP Q08491
L	247	LYS	-	expression tag	UNP Q08491

- Molecule 12 is a protein called Antiviral helicase SKI2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	657	Total	C	N	O	S	0	0
			5050	3252	854	918	26		

There are 201 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	445	GLN	GLU	conflict	UNP P35207
M	835	GLY	LYS	conflict	UNP P35207
M	836	SER	GLU	conflict	UNP P35207
M	837	ARG	-	insertion	UNP P35207
M	838	GLY	-	insertion	UNP P35207
M	839	LEU	-	insertion	UNP P35207
M	840	SER	THR	conflict	UNP P35207
M	842	LEU	GLN	conflict	UNP P35207
M	844	ASP	GLU	conflict	UNP P35207
M	845	TYR	HIS	conflict	UNP P35207
M	848	ARG	GLN	conflict	UNP P35207
M	849	LEU	ILE	conflict	UNP P35207
M	850	ALA	LYS	conflict	UNP P35207
M	853	LYS	GLN	conflict	UNP P35207
M	854	ASP	GLU	conflict	UNP P35207
M	855	THR	-	expression tag	UNP P35207
M	856	GLU	-	expression tag	UNP P35207
M	857	PHE	-	expression tag	UNP P35207
M	858	ILE	-	expression tag	UNP P35207
M	859	ASP	-	expression tag	UNP P35207
M	860	GLN	-	expression tag	UNP P35207
M	861	ASN	-	expression tag	UNP P35207
M	862	HIS	-	expression tag	UNP P35207
M	863	ASN	-	expression tag	UNP P35207
M	864	VAL	-	expression tag	UNP P35207
M	865	LEU	-	expression tag	UNP P35207
M	866	LEU	-	expression tag	UNP P35207
M	867	LYS	-	expression tag	UNP P35207
M	868	GLY	-	expression tag	UNP P35207

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Chain	Residue	Modelled	Actual	Comment	Reference
M	869	ARG	-	expression tag	UNP P35207
M	870	VAL	-	expression tag	UNP P35207
M	871	ALA	-	expression tag	UNP P35207
M	872	CYS	-	expression tag	UNP P35207
M	873	GLU	-	expression tag	UNP P35207
M	874	ILE	-	expression tag	UNP P35207
M	875	ASN	-	expression tag	UNP P35207
M	876	SER	-	expression tag	UNP P35207
M	877	GLY	-	expression tag	UNP P35207
M	878	TYR	-	expression tag	UNP P35207
M	879	GLU	-	expression tag	UNP P35207
M	880	LEU	-	expression tag	UNP P35207
M	881	VAL	-	expression tag	UNP P35207
M	882	LEU	-	expression tag	UNP P35207
M	883	THR	-	expression tag	UNP P35207
M	884	GLU	-	expression tag	UNP P35207
M	885	LEU	-	expression tag	UNP P35207
M	886	ILE	-	expression tag	UNP P35207
M	887	LEU	-	expression tag	UNP P35207
M	888	ASP	-	expression tag	UNP P35207
M	889	ASN	-	expression tag	UNP P35207
M	890	PHE	-	expression tag	UNP P35207
M	891	LEU	-	expression tag	UNP P35207
M	892	GLY	-	expression tag	UNP P35207
M	893	SER	-	expression tag	UNP P35207
M	894	PHE	-	expression tag	UNP P35207
M	895	GLU	-	expression tag	UNP P35207
M	896	PRO	-	expression tag	UNP P35207
M	897	GLU	-	expression tag	UNP P35207
M	898	GLU	-	expression tag	UNP P35207
M	899	ILE	-	expression tag	UNP P35207
M	900	VAL	-	expression tag	UNP P35207
M	901	ALA	-	expression tag	UNP P35207
M	902	LEU	-	expression tag	UNP P35207
M	903	LEU	-	expression tag	UNP P35207
M	904	SER	-	expression tag	UNP P35207
M	905	VAL	-	expression tag	UNP P35207
M	906	PHE	-	expression tag	UNP P35207
M	907	VAL	-	expression tag	UNP P35207
M	908	TYR	-	expression tag	UNP P35207
M	909	GLU	-	expression tag	UNP P35207
M	910	GLY	-	expression tag	UNP P35207

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Chain	Residue	Modelled	Actual	Comment	Reference
M	911	LYS	-	expression tag	UNP P35207
M	912	THR	-	expression tag	UNP P35207
M	913	ARG	-	expression tag	UNP P35207
M	914	GLU	-	expression tag	UNP P35207
M	915	GLU	-	expression tag	UNP P35207
M	916	GLU	-	expression tag	UNP P35207
M	917	PRO	-	expression tag	UNP P35207
M	918	PRO	-	expression tag	UNP P35207
M	919	ILE	-	expression tag	UNP P35207
M	920	VAL	-	expression tag	UNP P35207
M	921	THR	-	expression tag	UNP P35207
M	922	PRO	-	expression tag	UNP P35207
M	923	ARG	-	expression tag	UNP P35207
M	924	LEU	-	expression tag	UNP P35207
M	925	ALA	-	expression tag	UNP P35207
M	926	LYS	-	expression tag	UNP P35207
M	927	GLY	-	expression tag	UNP P35207
M	928	LYS	-	expression tag	UNP P35207
M	929	GLN	-	expression tag	UNP P35207
M	930	ARG	-	expression tag	UNP P35207
M	931	ILE	-	expression tag	UNP P35207
M	932	GLU	-	expression tag	UNP P35207
M	933	GLU	-	expression tag	UNP P35207
M	934	ILE	-	expression tag	UNP P35207
M	935	TYR	-	expression tag	UNP P35207
M	936	LYS	-	expression tag	UNP P35207
M	937	LYS	-	expression tag	UNP P35207
M	938	MET	-	expression tag	UNP P35207
M	939	LEU	-	expression tag	UNP P35207
M	940	CYS	-	expression tag	UNP P35207
M	941	VAL	-	expression tag	UNP P35207
M	942	PHE	-	expression tag	UNP P35207
M	943	ASN	-	expression tag	UNP P35207
M	944	THR	-	expression tag	UNP P35207
M	945	HIS	-	expression tag	UNP P35207
M	946	GLN	-	expression tag	UNP P35207
M	947	ILE	-	expression tag	UNP P35207
M	948	PRO	-	expression tag	UNP P35207
M	949	LEU	-	expression tag	UNP P35207
M	950	THR	-	expression tag	UNP P35207
M	951	GLN	-	expression tag	UNP P35207
M	952	ASP	-	expression tag	UNP P35207

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Chain	Residue	Modelled	Actual	Comment	Reference
M	953	GLU	-	expression tag	UNP P35207
M	954	ALA	-	expression tag	UNP P35207
M	955	GLU	-	expression tag	UNP P35207
M	956	PHE	-	expression tag	UNP P35207
M	957	LEU	-	expression tag	UNP P35207
M	958	ASP	-	expression tag	UNP P35207
M	959	ARG	-	expression tag	UNP P35207
M	960	LYS	-	expression tag	UNP P35207
M	961	ARG	-	expression tag	UNP P35207
M	962	PHE	-	expression tag	UNP P35207
M	963	ALA	-	expression tag	UNP P35207
M	964	MET	-	expression tag	UNP P35207
M	965	MET	-	expression tag	UNP P35207
M	966	ASN	-	expression tag	UNP P35207
M	967	VAL	-	expression tag	UNP P35207
M	968	VAL	-	expression tag	UNP P35207
M	969	TYR	-	expression tag	UNP P35207
M	970	GLU	-	expression tag	UNP P35207
M	971	TRP	-	expression tag	UNP P35207
M	972	ALA	-	expression tag	UNP P35207
M	973	ARG	-	expression tag	UNP P35207
M	974	GLY	-	expression tag	UNP P35207
M	975	LEU	-	expression tag	UNP P35207
M	976	SER	-	expression tag	UNP P35207
M	977	PHE	-	expression tag	UNP P35207
M	978	LYS	-	expression tag	UNP P35207
M	979	GLU	-	expression tag	UNP P35207
M	980	ILE	-	expression tag	UNP P35207
M	981	MET	-	expression tag	UNP P35207
M	982	GLU	-	expression tag	UNP P35207
M	983	MET	-	expression tag	UNP P35207
M	984	SER	-	expression tag	UNP P35207
M	985	PRO	-	expression tag	UNP P35207
M	986	GLU	-	expression tag	UNP P35207
M	987	ALA	-	expression tag	UNP P35207
M	988	GLU	-	expression tag	UNP P35207
M	989	GLY	-	expression tag	UNP P35207
M	990	THR	-	expression tag	UNP P35207
M	991	VAL	-	expression tag	UNP P35207
M	992	VAL	-	expression tag	UNP P35207
M	993	ARG	-	expression tag	UNP P35207
M	994	VAL	-	expression tag	UNP P35207

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Chain	Residue	Modelled	Actual	Comment	Reference
M	995	ILE	-	expression tag	UNP P35207
M	996	THR	-	expression tag	UNP P35207
M	997	TRP	-	expression tag	UNP P35207
M	998	LEU	-	expression tag	UNP P35207
M	999	ASP	-	expression tag	UNP P35207
M	1000	GLU	-	expression tag	UNP P35207
M	1001	ILE	-	expression tag	UNP P35207
M	1002	CYS	-	expression tag	UNP P35207
M	1003	ARG	-	expression tag	UNP P35207
M	1004	GLU	-	expression tag	UNP P35207
M	1005	VAL	-	expression tag	UNP P35207
M	1006	LYS	-	expression tag	UNP P35207
M	1007	THR	-	expression tag	UNP P35207
M	1008	ALA	-	expression tag	UNP P35207
M	1009	SER	-	expression tag	UNP P35207
M	1010	ILE	-	expression tag	UNP P35207
M	1011	ILE	-	expression tag	UNP P35207
M	1012	ILE	-	expression tag	UNP P35207
M	1013	GLY	-	expression tag	UNP P35207
M	1014	ASN	-	expression tag	UNP P35207
M	1015	SER	-	expression tag	UNP P35207
M	1016	THR	-	expression tag	UNP P35207
M	1017	LEU	-	expression tag	UNP P35207
M	1018	HIS	-	expression tag	UNP P35207
M	1019	MET	-	expression tag	UNP P35207
M	1020	LYS	-	expression tag	UNP P35207
M	1021	MET	-	expression tag	UNP P35207
M	1022	SER	-	expression tag	UNP P35207
M	1023	ARG	-	expression tag	UNP P35207
M	1024	ALA	-	expression tag	UNP P35207
M	1025	GLN	-	expression tag	UNP P35207
M	1026	GLU	-	expression tag	UNP P35207
M	1027	LEU	-	expression tag	UNP P35207
M	1028	ILE	-	expression tag	UNP P35207
M	1029	LYS	-	expression tag	UNP P35207
M	1030	ARG	-	expression tag	UNP P35207
M	1031	ASP	-	expression tag	UNP P35207
M	1032	ILE	-	expression tag	UNP P35207
M	1033	VAL	-	expression tag	UNP P35207
M	1034	PHE	-	expression tag	UNP P35207
M	1035	ALA	-	expression tag	UNP P35207
M	1036	ALA	-	expression tag	UNP P35207

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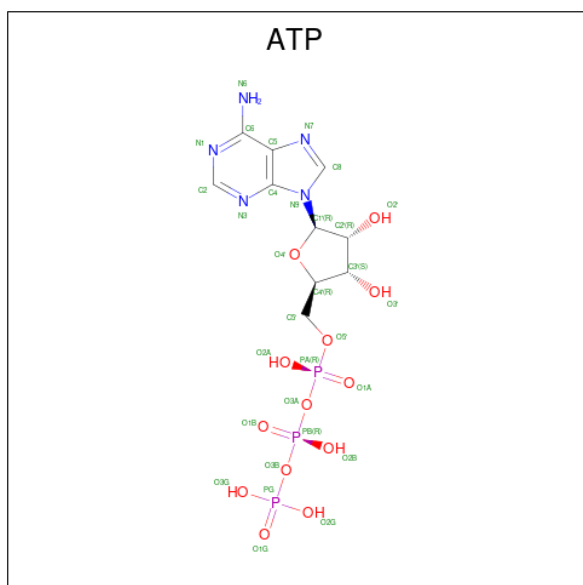
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Chain	Residue	Modelled	Actual	Comment	Reference
M	1037	SER	-	expression tag	UNP P35207
M	1038	LEU	-	expression tag	UNP P35207
M	1039	TYR	-	expression tag	UNP P35207
M	1040	LEU	-	expression tag	UNP P35207

- Molecule 13 is a RNA chain called RNA (5'hairpin 60U).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	34	Total	C	N	O	P	0	0
			513	222	27	230	34		

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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.

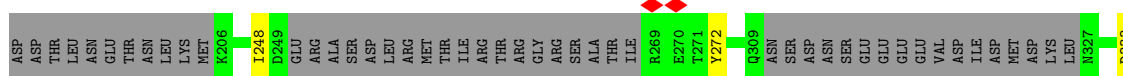
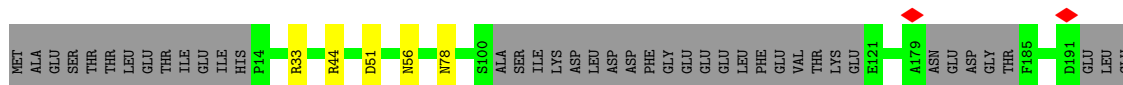
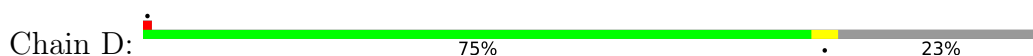
- Molecule 1: Exosome complex component RRP45



- Molecule 2: Exosome complex component SKI6



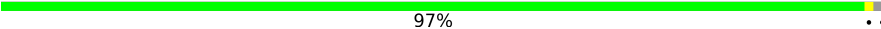
- Molecule 3: Exosome complex component RRP43



- Molecule 4: RRP46 isoform 1



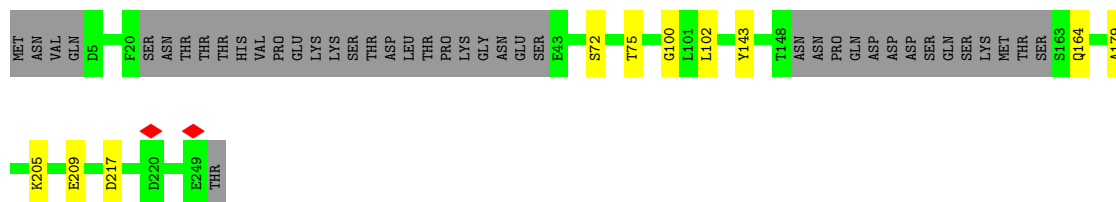
- Molecule 5: Exosome complex component RRP42

Chain F:  97%



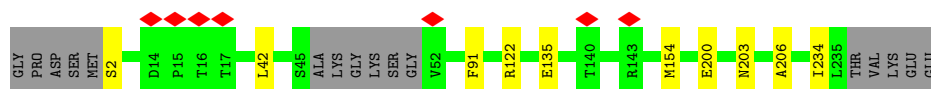
- Molecule 6: Exosome complex component MTR3

Chain G:  80%



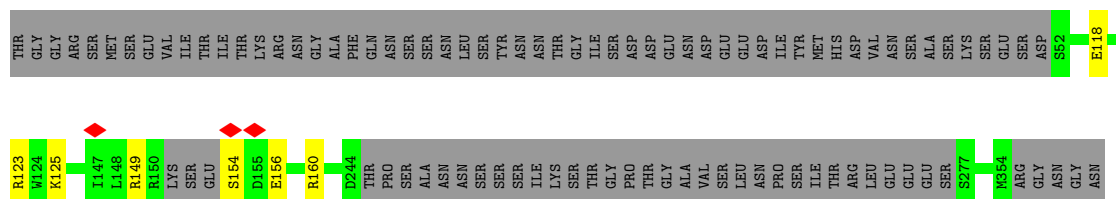
- Molecule 7: Exosome complex component RRP40

Chain H:  89%



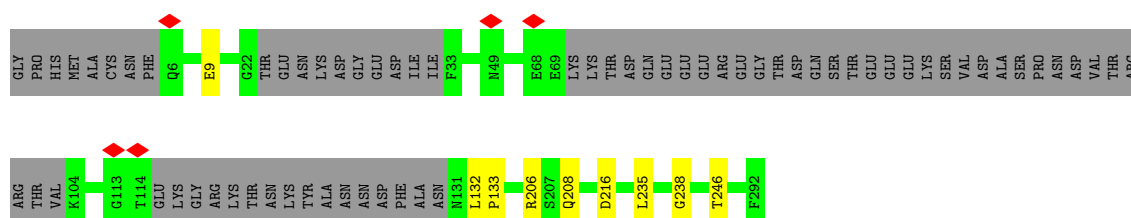
- Molecule 8: Exosome complex component RRP4

Chain I:  72%



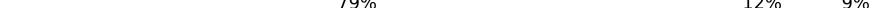
- Molecule 9: Exosome complex component CSL4

Chain J:  74%



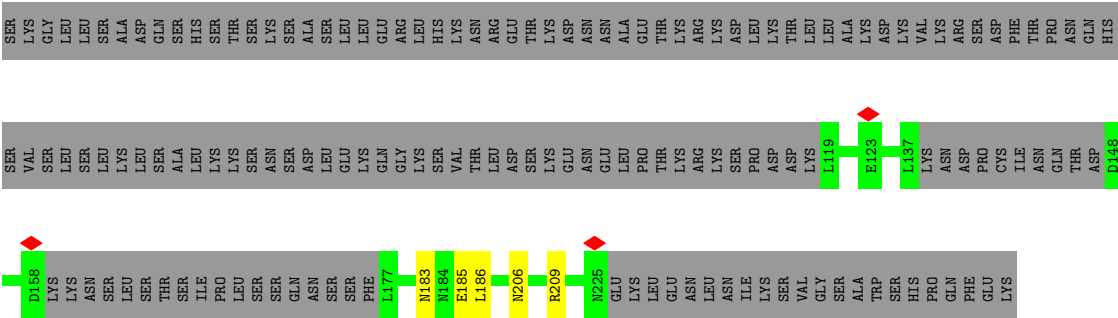
- Molecule 10: Exosome complex exonuclease DIS3

Chain K:  39%

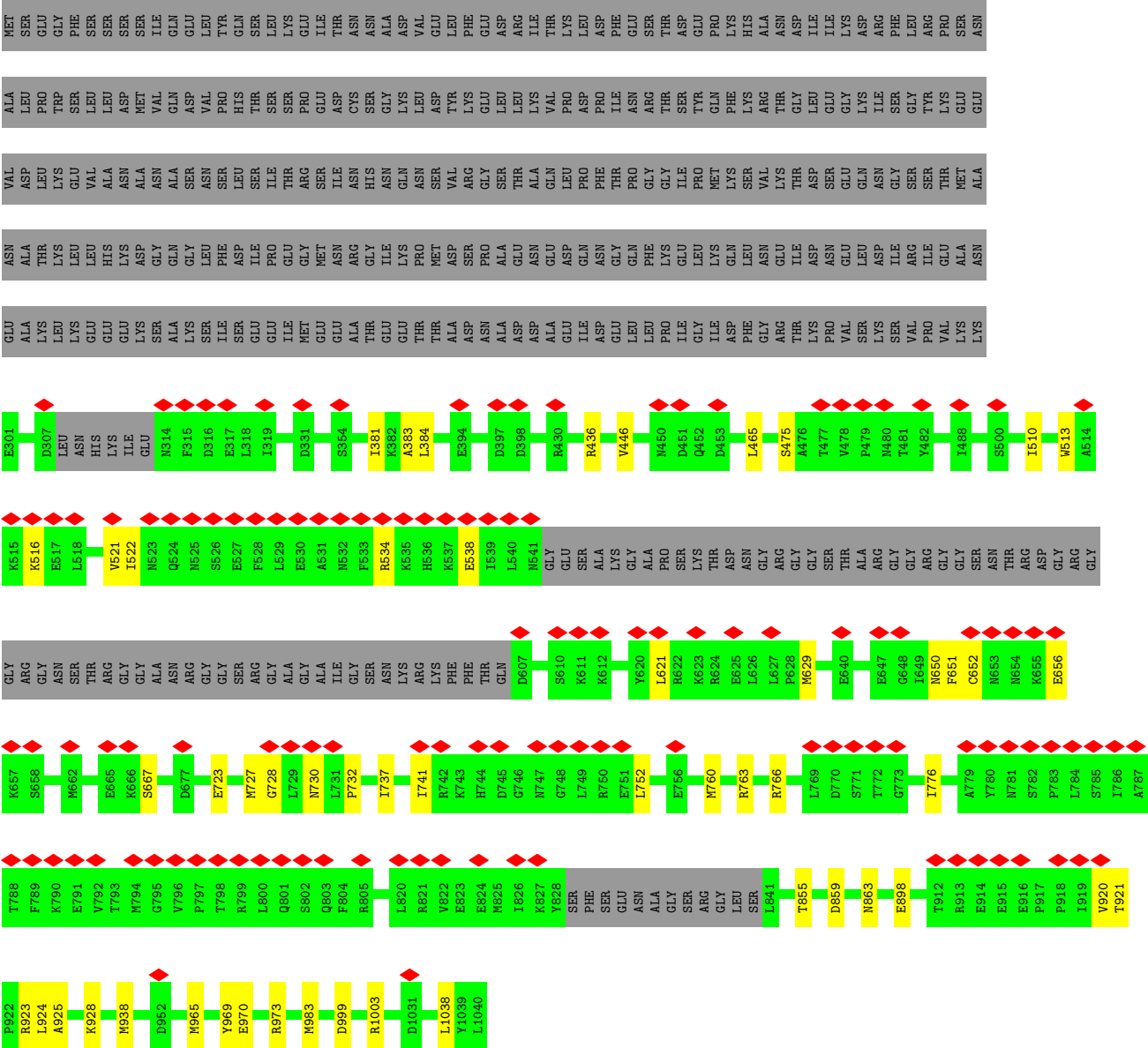
Chain K:  79%

Chain K: 12%

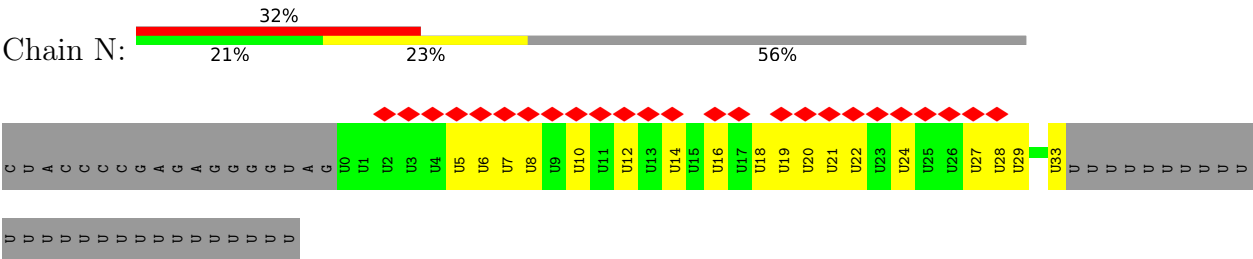
Chain K: 9%



● Molecule 12: Antiviral helicase SKI2



● Molecule 13: RNA (5'hairpin 60U)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	338757	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 ($e^-/\text{\AA}^2$)	63.36	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.155	Depositor
Minimum map value	-3.001	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.156	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	306.432, 306.432, 306.432	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85120004, 0.85120004, 0.85120004	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: ATP

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	B	0.13	0/2296	0.28	0/3104
2	C	0.14	0/1905	0.27	0/2569
3	D	0.13	0/2392	0.29	0/3238
4	E	0.15	0/1709	0.31	0/2319
5	F	0.13	0/2037	0.31	0/2776
6	G	0.13	0/1602	0.28	0/2163
7	H	0.11	0/1801	0.28	0/2446
8	I	0.11	0/2117	0.26	0/2859
9	J	0.11	0/1714	0.29	0/2321
10	K	0.09	0/7371	0.25	0/10000
11	L	0.09	0/631	0.25	0/859
12	M	0.09	0/5154	0.23	0/7006
13	N	0.06	0/559	0.12	0/860
All	All	0.11	0/31288	0.26	0/42520

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	B	2261	0	2232	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1881	0	1915	4	0
3	D	2358	0	2400	6	0
4	E	1691	0	1745	6	0
5	F	1998	0	1998	3	0
6	G	1581	0	1547	6	0
7	H	1765	0	1727	6	0
8	I	2084	0	2098	5	0
9	J	1689	0	1685	6	0
10	K	7231	0	7181	67	0
11	L	618	0	569	3	0
12	M	5050	0	4851	29	0
13	N	513	0	258	1	0
14	M	31	0	11	0	0
All	All	30751	0	30217	144	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 2.

All (144) 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)
12:M:521:VAL:HG13	12:M:522:ILE:HD12	1.66	0.77
10:K:275:GLN:OE1	10:K:315:GLN:NE2	2.23	0.72
10:K:112:ILE:HG21	10:K:181:TYR:HE2	1.56	0.71
8:I:123:ARG:NH2	13:N:8:U:O2'	2.22	0.71
3:D:51:ASP:OD1	3:D:391:ARG:NH2	2.24	0.71
10:K:120:GLU:OE2	10:K:170:ASN:ND2	2.25	0.69
4:E:36:PRO:HB3	4:E:87:LEU:HB2	1.74	0.69
12:M:928:LYS:HD2	12:M:965:MET:HE1	1.74	0.68
12:M:970:GLU:HG3	12:M:983:MET:HE1	1.76	0.67
10:K:309:ARG:O	10:K:398:ARG:NH2	2.26	0.67
8:I:149:ARG:O	12:M:436:ARG:NH1	2.29	0.65
10:K:474:ILE:HG22	10:K:475:GLU:HG2	1.79	0.64
3:D:248:ILE:HD11	3:D:272:TYR:HB3	1.79	0.64
10:K:503:LEU:HD13	10:K:607:LEU:HD23	1.80	0.64
10:K:308:ASN:ND2	10:K:392:VAL:O	2.32	0.63
10:K:514:THR:O	10:K:535:ARG:NH2	2.31	0.63
1:B:11:GLU:HG3	7:H:154:MET:HE1	1.83	0.61
5:F:224:SER:OG	6:G:217:ASP:N	2.34	0.60
1:B:262:MET:HG3	2:C:211:GLU:HG2	1.83	0.59
10:K:671:THR:OG1	10:K:675:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:939:ILE:HD13	10:K:1000:LEU:HB2	1.85	0.58
10:K:530:LYS:HD3	10:K:864:TYR:HD1	1.67	0.58
12:M:723:GLU:HG3	12:M:760:MET:HE2	1.85	0.58
12:M:730:ASN:HA	12:M:763:ARG:HH22	1.68	0.58
3:D:357:TYR:OH	3:D:382:ARG:NH1	2.37	0.58
10:K:629:GLU:HB2	10:K:638:ASN:HB2	1.85	0.58
10:K:770:LEU:O	10:K:775:ASN:N	2.35	0.58
10:K:694:LEU:HD12	10:K:787:ALA:HB2	1.85	0.58
10:K:721:LEU:HD23	10:K:723:THR:H	1.69	0.57
10:K:699:PRO:HB3	10:K:717:ILE:HG23	1.86	0.57
6:G:205:LYS:HD2	6:G:209:GLU:HG3	1.85	0.57
12:M:652:CYS:HB3	12:M:656:GLU:HB2	1.85	0.57
6:G:72:SER:HB2	6:G:143:TYR:HB3	1.88	0.55
10:K:553:ALA:HB3	10:K:569:HIS:HB2	1.88	0.55
1:B:239:LEU:HB2	1:B:272:ILE:HD13	1.89	0.55
10:K:778:ILE:HA	10:K:789:SER:HB3	1.89	0.55
12:M:732:PRO:HB2	12:M:766:ARG:HG2	1.89	0.54
12:M:920:VAL:HG23	12:M:921:THR:H	1.73	0.54
12:M:741:ILE:HA	12:M:752:LEU:HD12	1.89	0.54
10:K:641:PHE:HZ	10:K:737:SER:HB3	1.73	0.54
10:K:870:THR:HA	10:K:876:LYS:HD3	1.91	0.53
1:B:167:ILE:HG22	1:B:176:VAL:HA	1.91	0.53
10:K:749:THR:O	10:K:857:GLN:NE2	2.41	0.53
11:L:206:ASN:OD1	11:L:209:ARG:NH2	2.42	0.52
10:K:525:ASP:HB3	10:K:528:LEU:HB2	1.91	0.52
10:K:942:ASP:OD1	10:K:943:ASN:N	2.42	0.52
12:M:621:LEU:HD22	12:M:629:MET:HE2	1.92	0.52
12:M:667:SER:HB2	12:M:1038:LEU:HD21	1.91	0.51
10:K:959:LYS:HG3	10:K:974:TYR:HE1	1.75	0.51
12:M:999:ASP:OD2	12:M:1003:ARG:NH1	2.44	0.51
12:M:381:ILE:HG22	12:M:383:ALA:H	1.75	0.51
12:M:737:ILE:HG12	12:M:776:ILE:HB	1.94	0.50
10:K:196:THR:OG1	10:K:198:ASP:OD1	2.28	0.50
10:K:810:THR:HA	10:K:813:MET:HE1	1.94	0.50
10:K:538:LEU:HD13	10:K:649:ARG:HG3	1.93	0.50
12:M:384:LEU:HD21	12:M:728:GLY:HA3	1.94	0.50
10:K:921:VAL:HG21	10:K:958:TYR:HB3	1.94	0.49
12:M:446:VAL:HB	12:M:475:SER:HB3	1.95	0.48
10:K:798:ASP:OD1	10:K:798:ASP:N	2.45	0.48
12:M:855:THR:HG21	12:M:938:MET:HE1	1.94	0.48
1:B:239:LEU:HD23	1:B:245:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:242:ASN:OD1	2:C:243:ALA:N	2.47	0.48
10:K:962:PHE:HZ	10:K:971:ARG:HH21	1.61	0.48
7:H:200:GLU:OE1	7:H:203:ASN:ND2	2.43	0.48
1:B:269:TYR:HA	1:B:272:ILE:HG12	1.96	0.48
2:C:212:ASN:O	2:C:216:ILE:HG12	2.14	0.48
12:M:650:ASN:OD1	12:M:651:PHE:N	2.47	0.48
10:K:549:ASP:OD1	10:K:549:ASP:N	2.41	0.47
12:M:898:GLU:HB3	12:M:924:LEU:HD21	1.97	0.47
3:D:33:ARG:HB3	11:L:186:LEU:HD12	1.96	0.47
10:K:831:HIS:CD2	10:K:834:LEU:H	2.33	0.47
10:K:112:ILE:HD13	10:K:181:TYR:CE2	2.50	0.47
10:K:188:TYR:O	10:K:190:ILE:HG13	2.15	0.46
10:K:606:MET:O	10:K:610:THR:HB	2.16	0.46
6:G:100:GLY:O	6:G:102:LEU:N	2.48	0.46
12:M:923:ARG:C	12:M:925:ALA:H	2.24	0.46
10:K:721:LEU:HD23	10:K:722:ALA:N	2.31	0.45
10:K:802:ASN:O	10:K:806:ARG:HG3	2.16	0.45
9:J:132:LEU:HD12	9:J:133:PRO:HD2	1.97	0.45
4:E:84:PRO:C	4:E:85:ARG:HD3	2.41	0.45
10:K:904:GLY:HA2	10:K:907:MET:HG2	1.98	0.45
10:K:982:GLN:HE22	10:K:984:ARG:HG2	1.82	0.45
4:E:140:LYS:O	4:E:142:THR:N	2.49	0.45
10:K:761:THR:O	10:K:764:GLU:HG3	2.16	0.45
9:J:9:GLU:OE1	9:J:9:GLU:N	2.40	0.45
10:K:225:LEU:HD12	10:K:231:ILE:HD11	1.98	0.44
3:D:56:ASN:OD1	3:D:78:ASN:ND2	2.47	0.44
10:K:727:VAL:O	10:K:731:MET:HG2	2.16	0.44
1:B:269:TYR:CD1	1:B:272:ILE:HD11	2.52	0.44
2:C:29:ILE:HD11	2:C:145:LEU:HB3	2.00	0.44
10:K:760:SER:O	10:K:764:GLU:N	2.45	0.44
8:I:154:SER:C	8:I:156:GLU:H	2.25	0.44
12:M:920:VAL:HG23	12:M:921:THR:N	2.32	0.44
12:M:723:GLU:HG2	12:M:727:MET:HE3	2.00	0.44
10:K:786:LEU:O	10:K:790:LEU:HG	2.17	0.43
7:H:122:ARG:NH1	7:H:135:GLU:OE2	2.51	0.43
12:M:859:ASP:OD2	12:M:863:ASN:HB2	2.19	0.43
9:J:216:ASP:OD1	9:J:216:ASP:N	2.52	0.43
10:K:883:ASN:O	10:K:887:LYS:HG2	2.18	0.43
10:K:888:HIS:NE2	10:K:892:GLN:OE1	2.51	0.43
6:G:164:GLN:OE1	6:G:164:GLN:N	2.51	0.43
9:J:235:LEU:HD11	9:J:246:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:542:ILE:HG13	10:K:652:PHE:HB2	2.01	0.43
10:K:867:LEU:HD23	10:K:872:ARG:HG3	2.01	0.43
9:J:206:ARG:HH11	9:J:208:GLN:HE21	1.66	0.43
10:K:873:ASP:HB3	10:K:876:LYS:HG3	2.01	0.43
10:K:928:VAL:O	10:K:937:GLY:N	2.50	0.43
4:E:132:ALA:HB1	4:E:205:LEU:HD23	2.00	0.43
11:L:183:ASN:C	11:L:185:GLU:H	2.27	0.43
4:E:208:ASN:OD1	4:E:211:ARG:NH2	2.52	0.42
12:M:510:ILE:HB	12:M:522:ILE:HB	2.01	0.42
5:F:67:VAL:HB	5:F:72:GLU:HG3	2.01	0.42
1:B:209:ASN:ND2	1:B:217:GLU:OE2	2.49	0.42
6:G:75:THR:HG23	6:G:179:ALA:HB2	2.01	0.42
10:K:669:GLU:HA	10:K:672:MET:HE2	2.00	0.42
10:K:181:TYR:HB3	10:K:192:VAL:HG11	2.01	0.42
10:K:845:PRO:HA	10:K:851:ASP:HB2	2.02	0.42
10:K:841:HIS:HB3	10:K:851:ASP:OD1	2.20	0.42
10:K:61:PRO:HB2	10:K:65:ASN:HA	2.02	0.42
1:B:2:ALA:HB3	7:H:91:PHE:HA	2.01	0.41
10:K:737:SER:HA	10:K:740:ARG:HE	1.85	0.41
10:K:658:GLN:HB2	10:K:721:LEU:HD21	2.02	0.41
10:K:788:ASP:O	10:K:792:ARG:HG2	2.20	0.41
1:B:50:LYS:HE3	1:B:50:LYS:HB2	1.97	0.41
10:K:78:GLU:HA	10:K:85:LYS:H	1.85	0.41
10:K:112:ILE:HG21	10:K:181:TYR:CE2	2.46	0.41
12:M:513:TRP:CZ2	12:M:516:LYS:HA	2.54	0.41
10:K:911:GLU:OE1	10:K:911:GLU:N	2.52	0.41
10:K:964:PRO:HG2	10:K:967:SER:O	2.21	0.41
4:E:7:ILE:HD11	4:E:118:LEU:HB3	2.03	0.41
7:H:2:SER:N	7:H:42:LEU:O	2.54	0.41
10:K:311:PHE:CD2	10:K:431:LEU:HD22	2.55	0.41
5:F:169:LEU:HD12	10:K:265:MET:HB3	2.03	0.41
10:K:521:ALA:HA	10:K:524:LYS:HE3	2.02	0.41
12:M:534:ARG:O	12:M:538:GLU:HG2	2.21	0.41
12:M:969:TYR:CZ	12:M:973:ARG:HD2	2.56	0.41
1:B:81:THR:HG22	1:B:138:VAL:HB	2.03	0.41
3:D:44:ARG:HH12	3:D:333:ASP:HB3	1.86	0.41
8:I:160:ARG:NH2	9:J:238:GLY:O	2.53	0.41
7:H:206:ALA:HB2	7:H:234:ILE:HD13	2.03	0.40
10:K:301:ILE:HG22	10:K:307:LEU:HD12	2.03	0.40
10:K:672:MET:O	10:K:675:ARG:HG2	2.21	0.40
12:M:465:LEU:HD23	12:M:465:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:118:GLU:HB2	8:I:125:LYS:HB2	2.04	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	B	295/305 (97%)	286 (97%)	9 (3%)	0	100	100
2	C	239/249 (96%)	235 (98%)	4 (2%)	0	100	100
3	D	293/394 (74%)	284 (97%)	9 (3%)	0	100	100
4	E	219/226 (97%)	213 (97%)	6 (3%)	0	100	100
5	F	261/268 (97%)	245 (94%)	16 (6%)	0	100	100
6	G	203/250 (81%)	201 (99%)	2 (1%)	0	100	100
7	H	224/244 (92%)	218 (97%)	6 (3%)	0	100	100
8	I	262/364 (72%)	257 (98%)	5 (2%)	0	100	100
9	J	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
10	K	901/1005 (90%)	858 (95%)	43 (5%)	0	100	100
11	L	73/353 (21%)	71 (97%)	2 (3%)	0	100	100
12	M	649/1040 (62%)	627 (97%)	22 (3%)	0	100	100
All	All	3838/4993 (77%)	3709 (97%)	129 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	B	247/266 (93%)	247 (100%)	0	100	100
2	C	211/220 (96%)	211 (100%)	0	100	100
3	D	262/350 (75%)	262 (100%)	0	100	100
4	E	195/198 (98%)	195 (100%)	0	100	100
5	F	229/242 (95%)	229 (100%)	0	100	100
6	G	170/219 (78%)	170 (100%)	0	100	100
7	H	196/212 (92%)	196 (100%)	0	100	100
8	I	230/314 (73%)	230 (100%)	0	100	100
9	J	180/242 (74%)	180 (100%)	0	100	100
10	K	796/904 (88%)	796 (100%)	0	100	100
11	L	65/315 (21%)	65 (100%)	0	100	100
12	M	509/910 (56%)	509 (100%)	0	100	100
All	All	3290/4392 (75%)	3290 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	191	HIS
1	B	215	ASN
2	C	30	ASN
2	C	77	ASN
3	D	239	GLN
4	E	93	GLN
4	E	187	ASN
5	F	136	HIS
5	F	196	ASN
6	G	235	ASN
6	G	247	ASN
7	H	32	GLN
8	I	92	ASN
8	I	133	HIS
9	J	242	ASN

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Mol	Chain	Res	Type
10	K	167	ASN
10	K	275	GLN
10	K	315	GLN
10	K	387	GLN
10	K	640	ASN
10	K	748	GLN
12	M	495	ASN
12	M	619	ASN
12	M	659	GLN
12	M	809	ASN
12	M	863	ASN
12	M	945	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	N	33/78 (42%)	17 (51%)	0

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	N	5	U
13	N	6	U
13	N	7	U
13	N	10	U
13	N	12	U
13	N	14	U
13	N	16	U
13	N	18	U
13	N	19	U
13	N	20	U
13	N	21	U
13	N	22	U
13	N	24	U
13	N	27	U
13	N	28	U
13	N	29	U
13	N	33	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
14	ATP	M	1101	-	32,33,33	3.26	11 (34%)	48,52,52	1.80	10 (20%)

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
14	ATP	M	1101	-	-	8/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1101	ATP	O4'-C1'	8.88	1.62	1.42
14	M	1101	ATP	O4'-C4'	-7.78	1.27	1.45
14	M	1101	ATP	C2'-C1'	-7.19	1.30	1.53
14	M	1101	ATP	PB-O3B	5.40	1.65	1.59
14	M	1101	ATP	PB-O3A	5.11	1.65	1.59
14	M	1101	ATP	PA-O3A	5.11	1.65	1.59
14	M	1101	ATP	C6-N6	4.40	1.45	1.34
14	M	1101	ATP	O2'-C2'	3.33	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1101	ATP	C8-N9	-2.87	1.32	1.37
14	M	1101	ATP	O3'-C3'	-2.61	1.36	1.43
14	M	1101	ATP	C5-N7	-2.39	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1101	ATP	C5-C4-N3	-5.46	119.20	126.72
14	M	1101	ATP	N3-C2-N1	-4.87	121.21	128.58
14	M	1101	ATP	N3-C4-N9	4.39	134.64	127.17
14	M	1101	ATP	C2-N3-C4	3.72	120.92	111.83
14	M	1101	ATP	N9-C8-N7	-3.12	109.50	113.94
14	M	1101	ATP	C4-N9-C8	2.94	108.83	105.74
14	M	1101	ATP	C5-N7-C8	2.82	107.89	103.45
14	M	1101	ATP	C4-C5-N7	-2.59	107.62	110.58
14	M	1101	ATP	C3'-C2'-C1'	2.30	105.82	101.46
14	M	1101	ATP	C4'-O4'-C1'	-2.28	104.44	109.47

There are no chirality outliers.

All (8) torsion outliers are listed below:

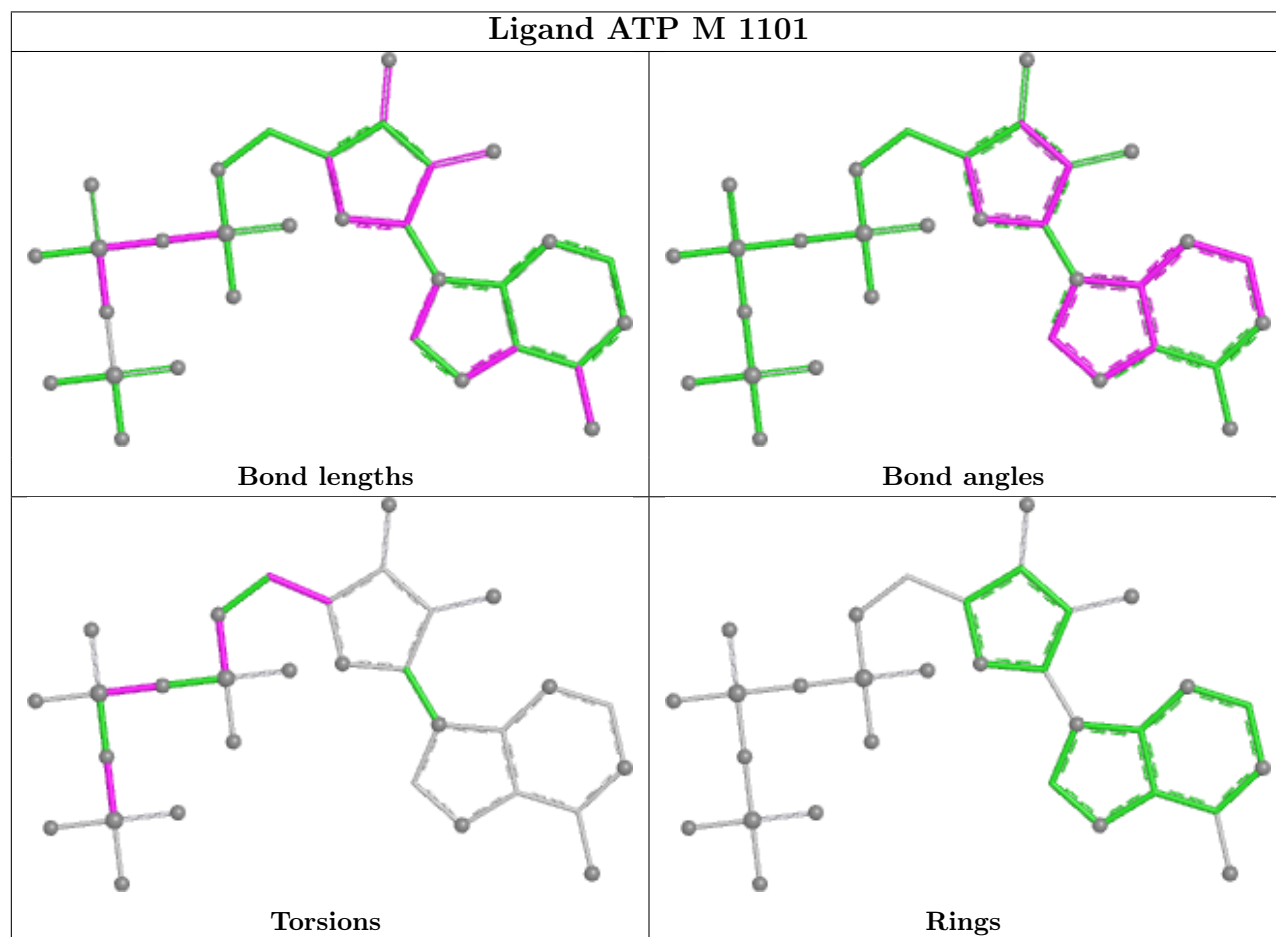
Mol	Chain	Res	Type	Atoms
14	M	1101	ATP	C5'-O5'-PA-O1A
14	M	1101	ATP	C5'-O5'-PA-O2A
14	M	1101	ATP	C5'-O5'-PA-O3A
14	M	1101	ATP	O4'-C4'-C5'-O5'
14	M	1101	ATP	C3'-C4'-C5'-O5'
14	M	1101	ATP	PB-O3B-PG-O1G
14	M	1101	ATP	PA-O3A-PB-O2B
14	M	1101	ATP	PA-O3A-PB-O1B

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.

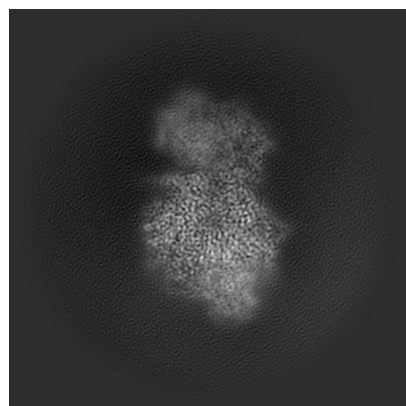
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18329. These allow visual inspection of the internal detail of the map and identification of artifacts.

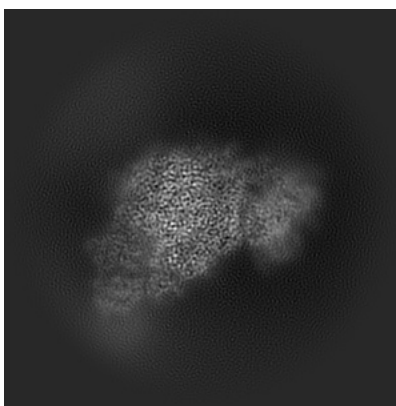
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

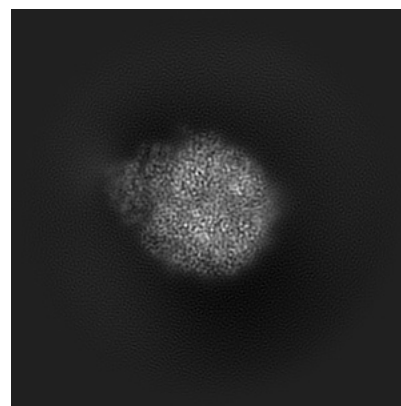
6.1.1 Primary map



X

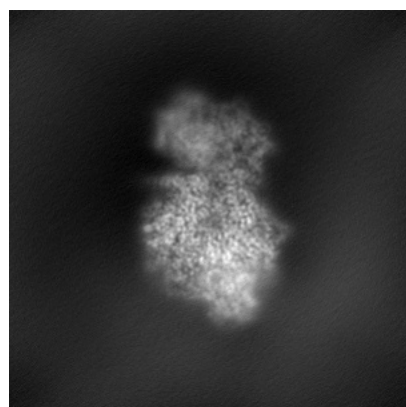


Y

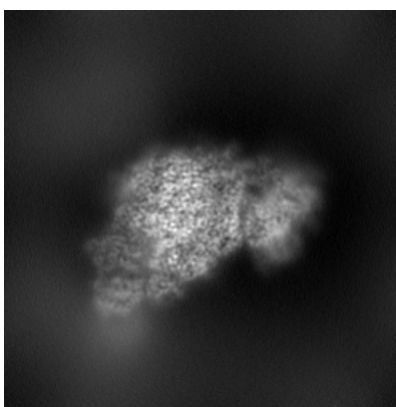


Z

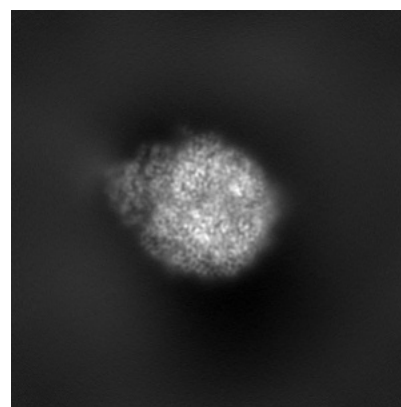
6.1.2 Raw map



X



Y

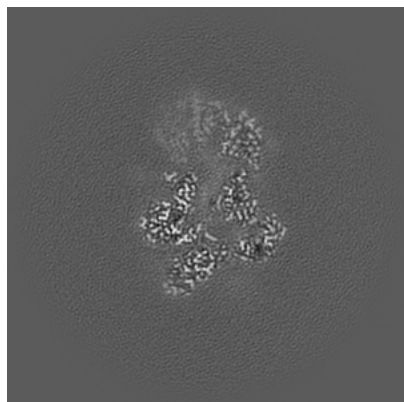


Z

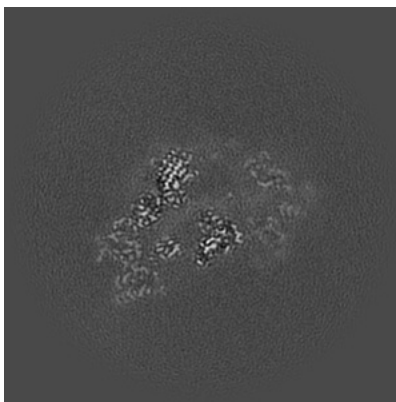
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

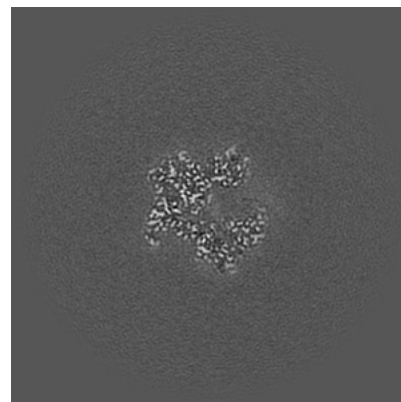
6.2.1 Primary map



X Index: 180

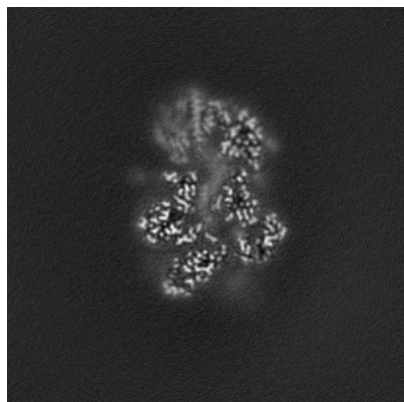


Y Index: 180

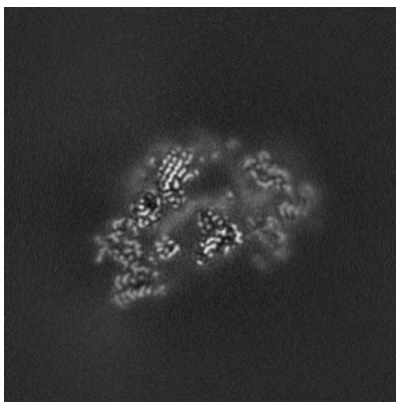


Z Index: 180

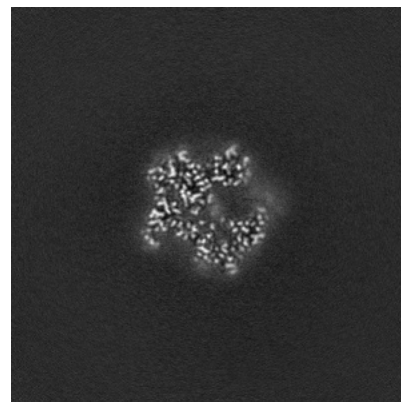
6.2.2 Raw map



X Index: 180



Y Index: 180

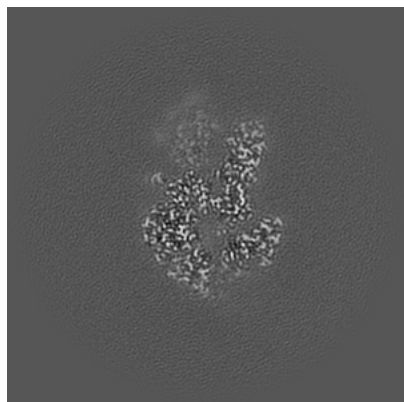


Z Index: 180

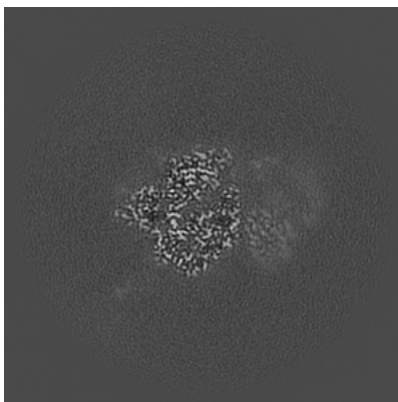
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

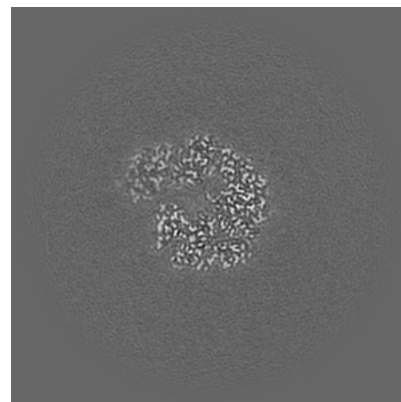
6.3.1 Primary map



X Index: 167

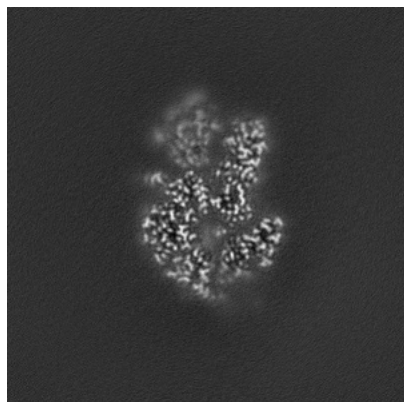


Y Index: 165

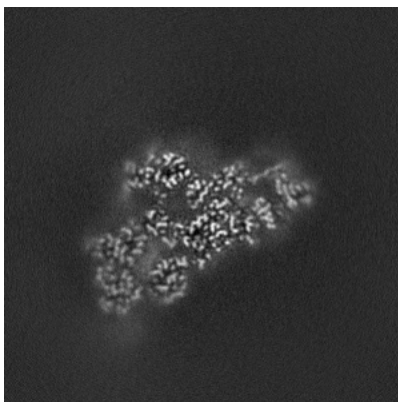


Z Index: 149

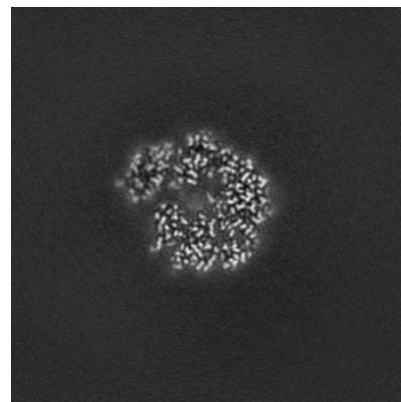
6.3.2 Raw map



X Index: 167



Y Index: 200

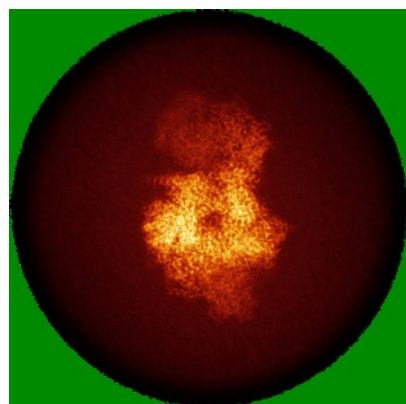


Z Index: 150

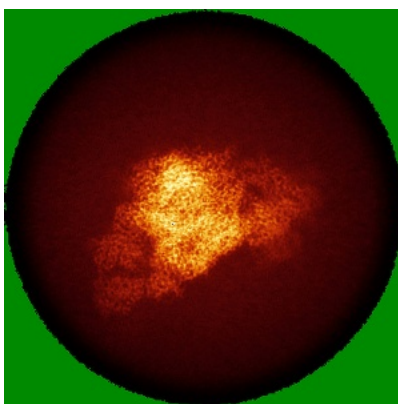
The images above show the largest variance slices of the map in three orthogonal directions.

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

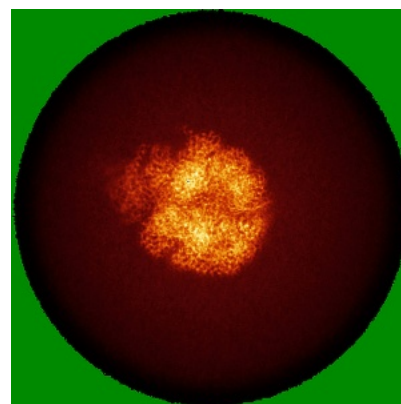
6.4.1 Primary map



X

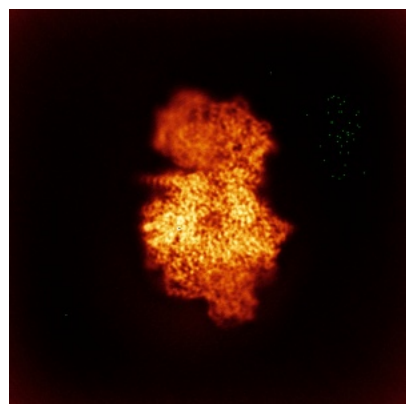


Y

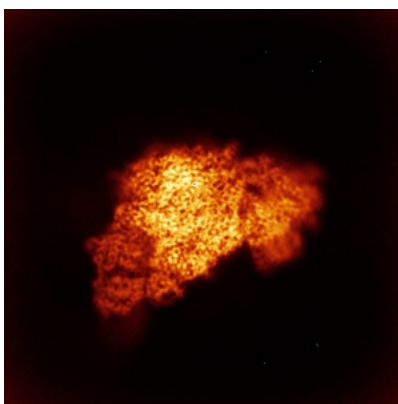


Z

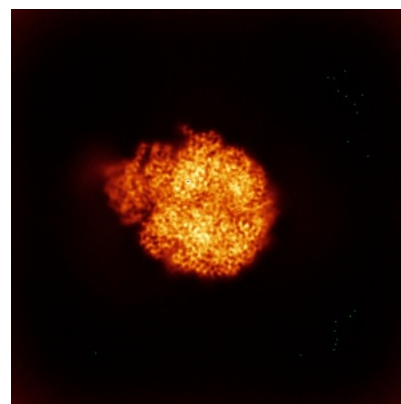
6.4.2 Raw map



X



Y

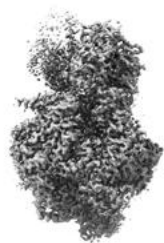


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



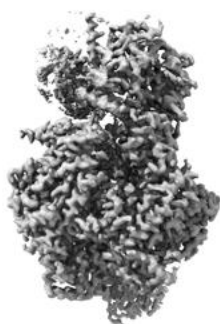
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

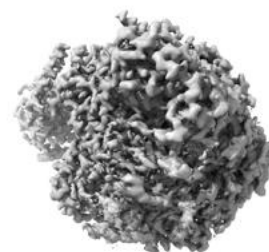
6.5.2 Raw map



X



Y



Z

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.

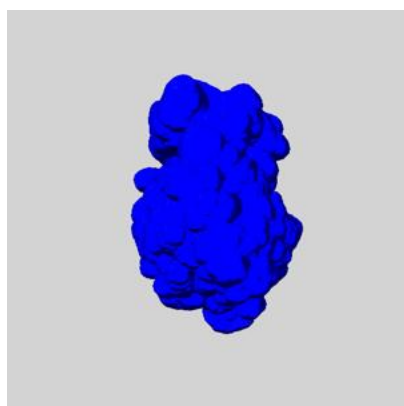
6.6 Mask visualisation [i](#)

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

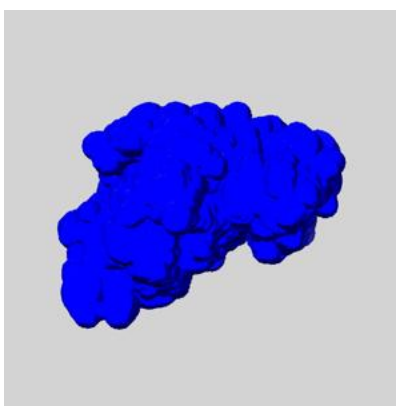
A mask typically either:

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

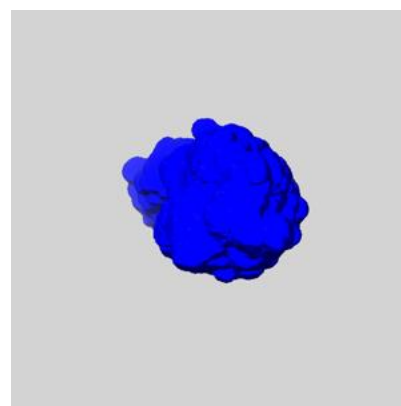
6.6.1 emd_18329_msk_1.map [i](#)



X



Y

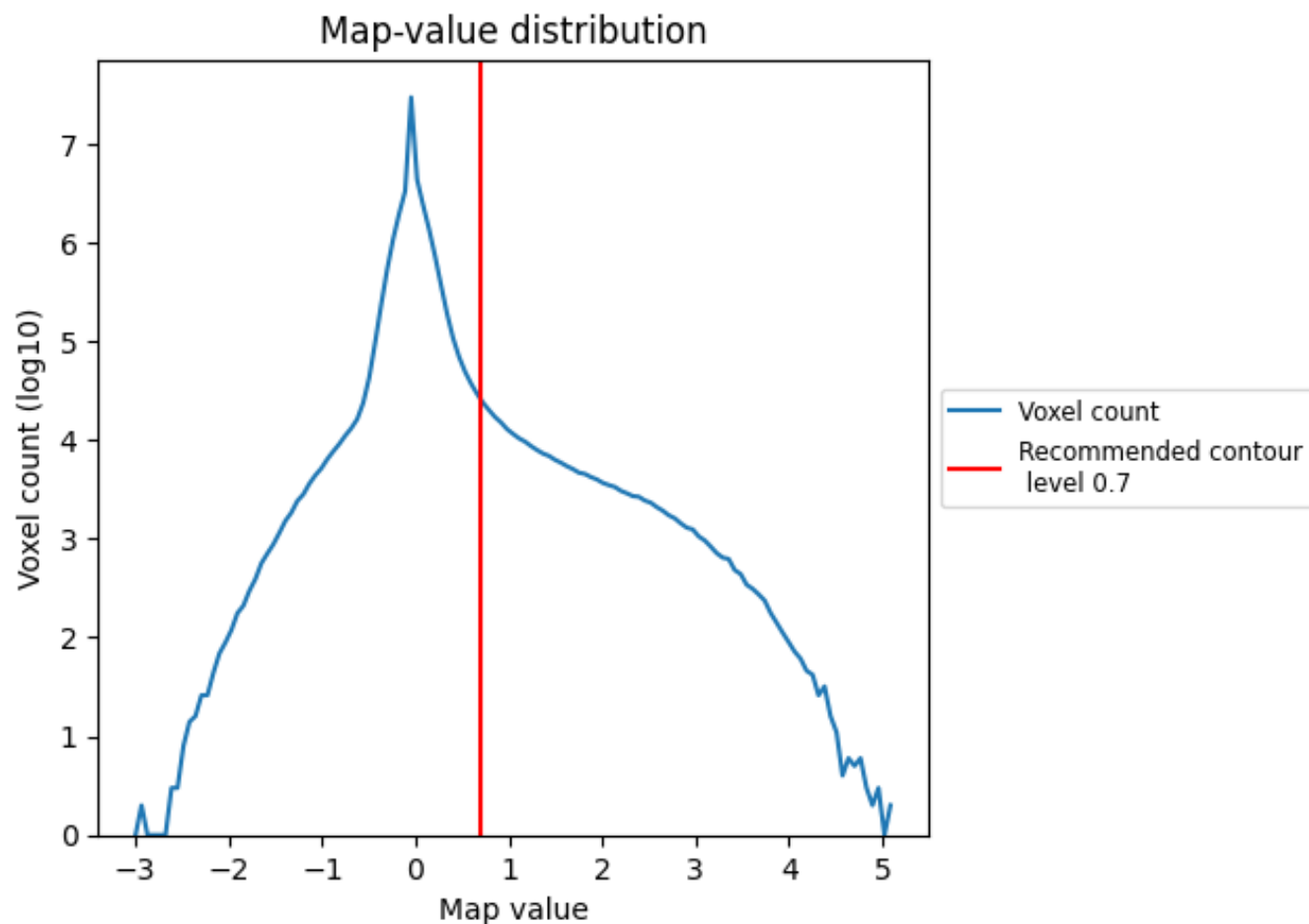


Z

7 Map analysis [i](#)

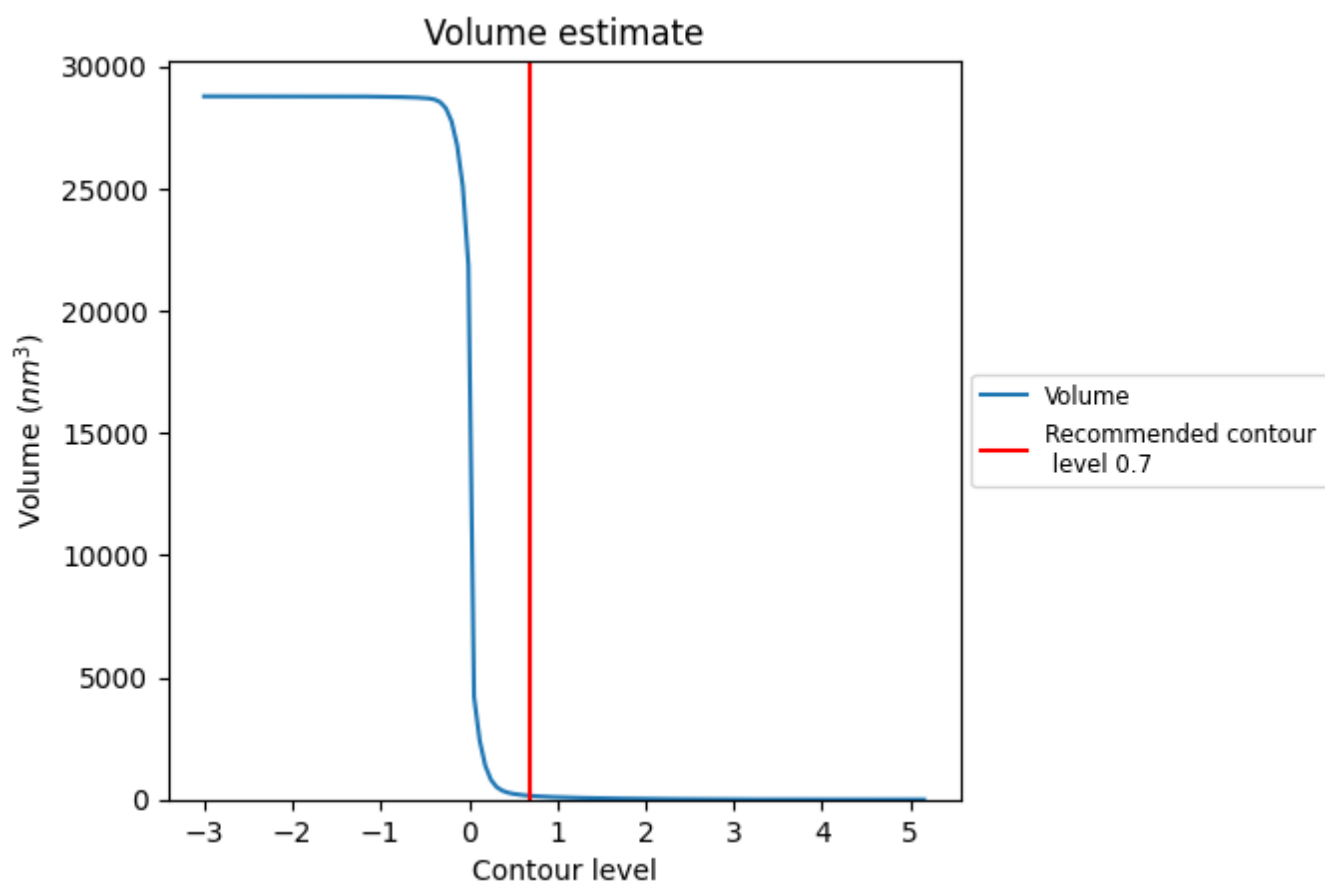
This section contains the results of statistical analysis of the map.

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.

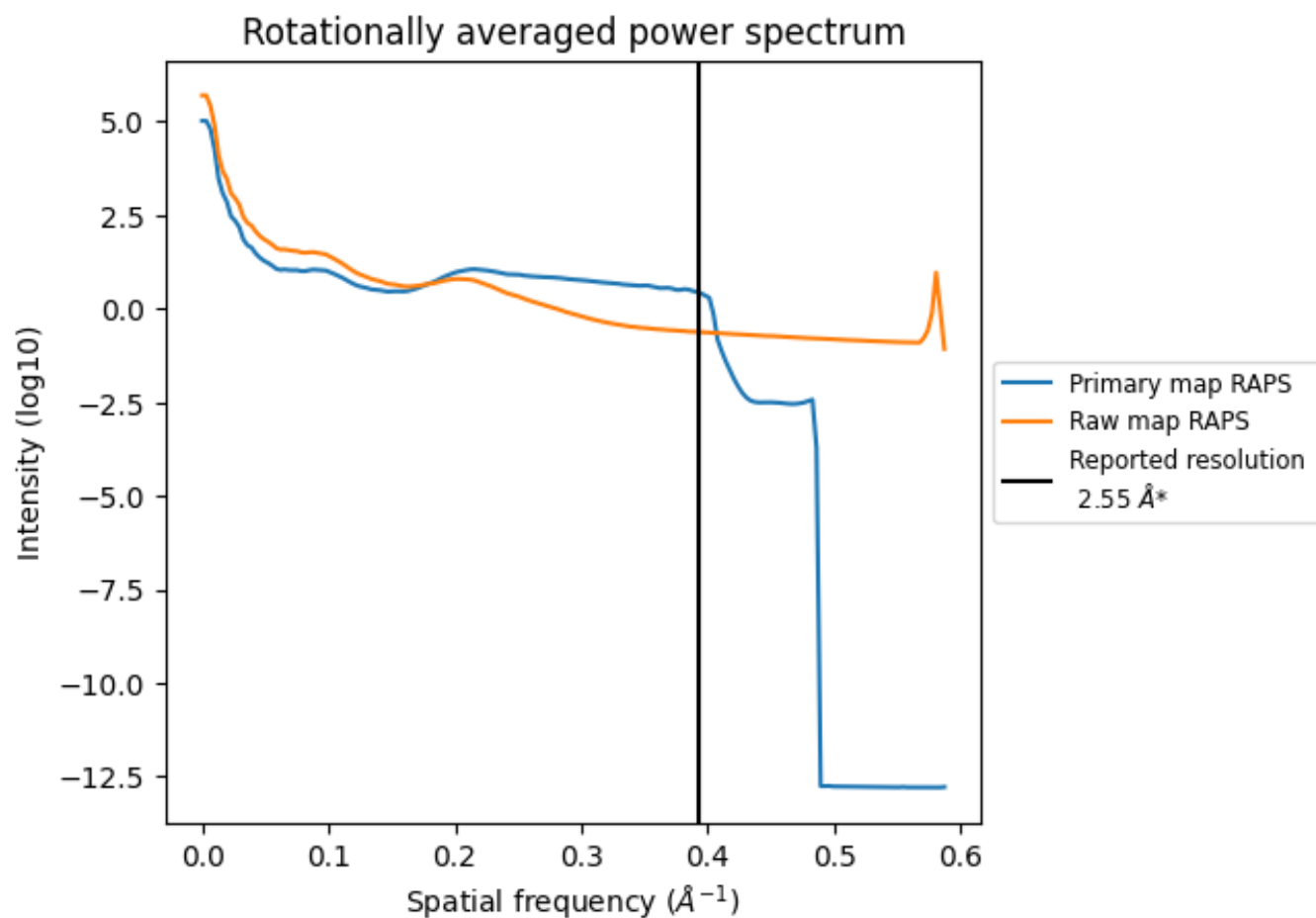
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 138 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 ⓘ

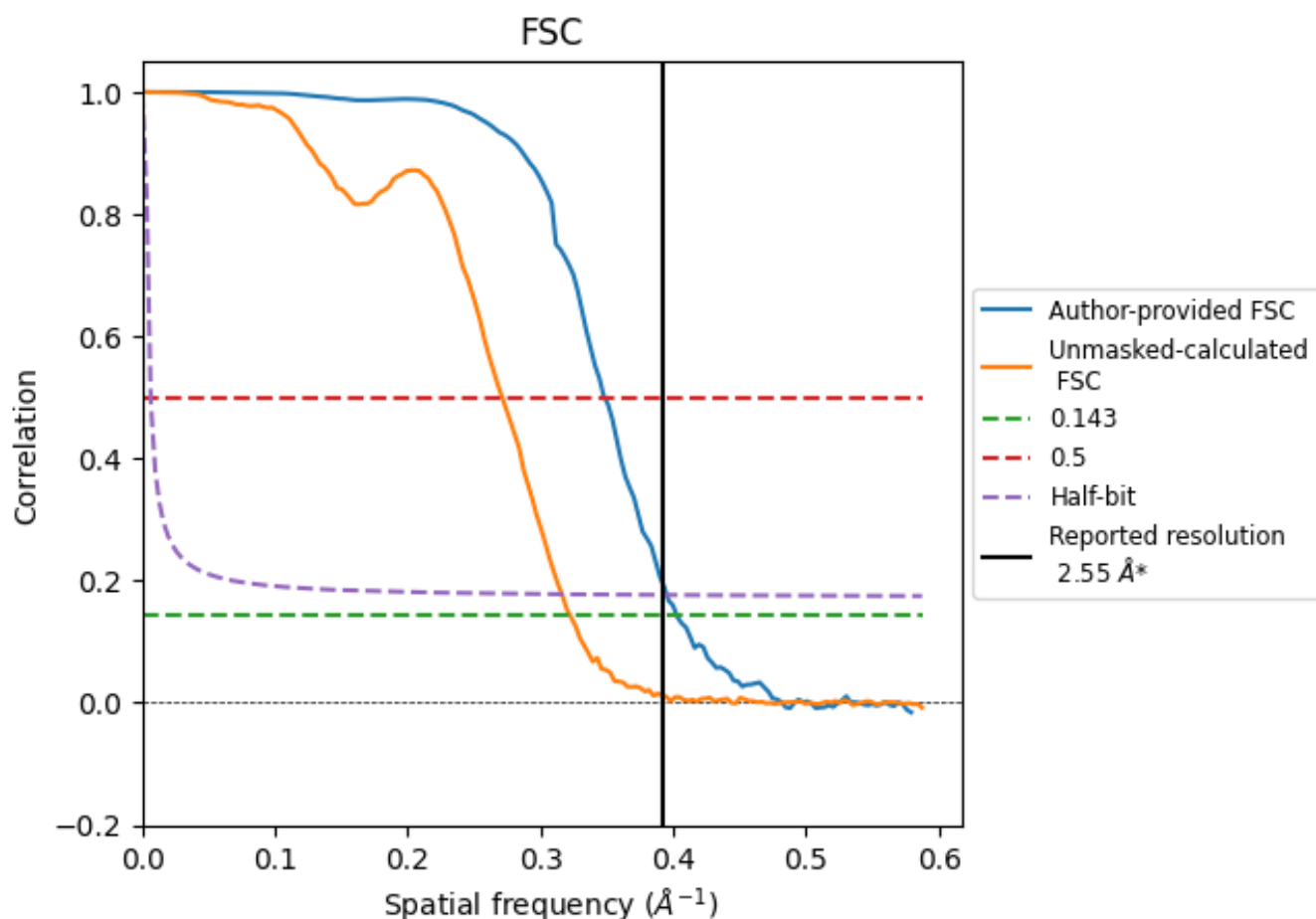


*Reported resolution corresponds to spatial frequency of 0.392 Å⁻¹

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 $0.392 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

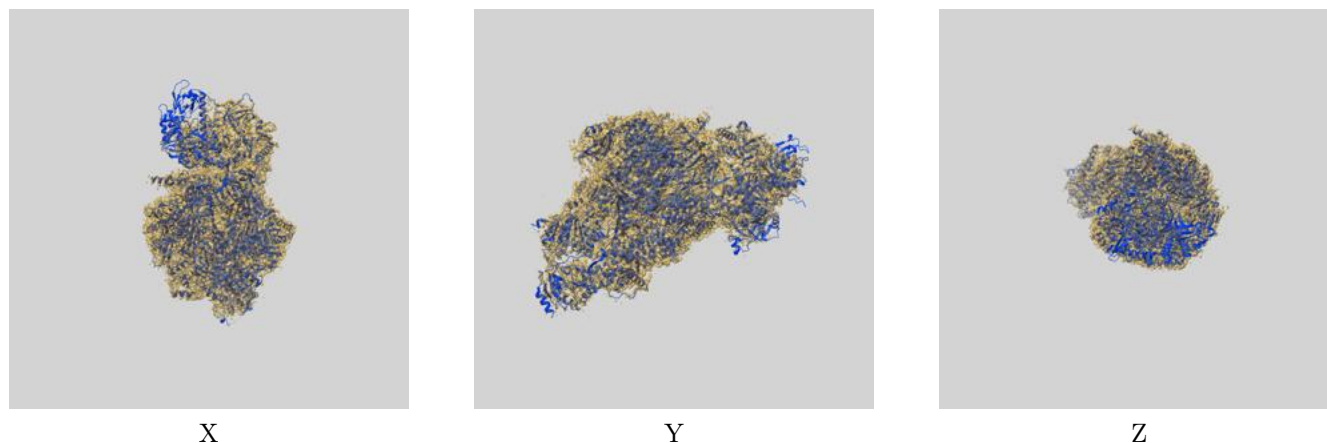
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.48	2.87	2.53
Unmasked-calculated*	3.10	3.69	3.16

*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 3.10 differs from the reported value 2.55 by more than 10 %

9 Map-model fit [i](#)

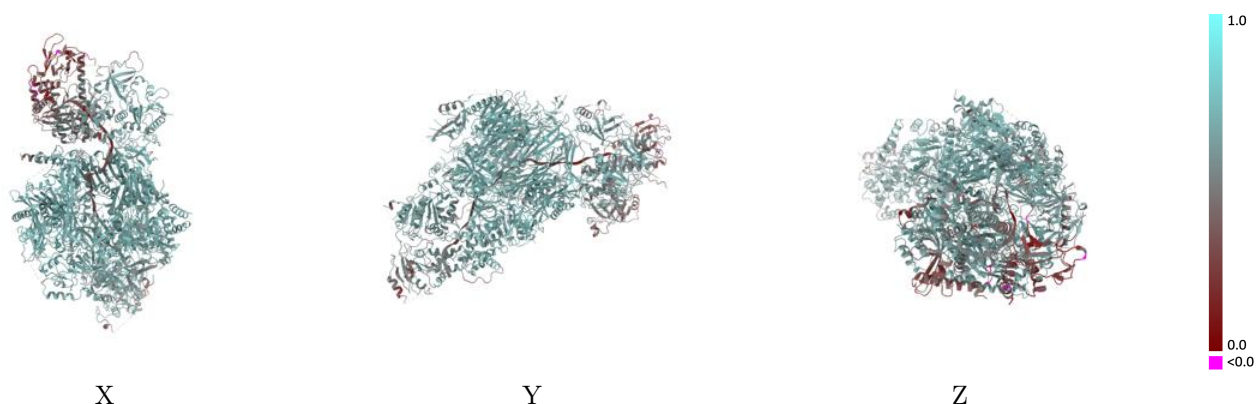
This section contains information regarding the fit between EMDB map EMD-18329 and PDB model 8QCF. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



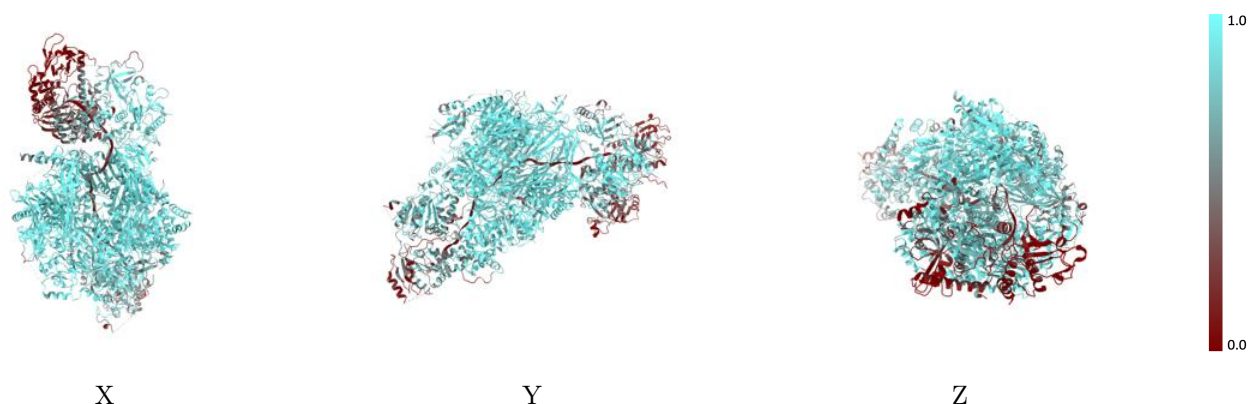
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



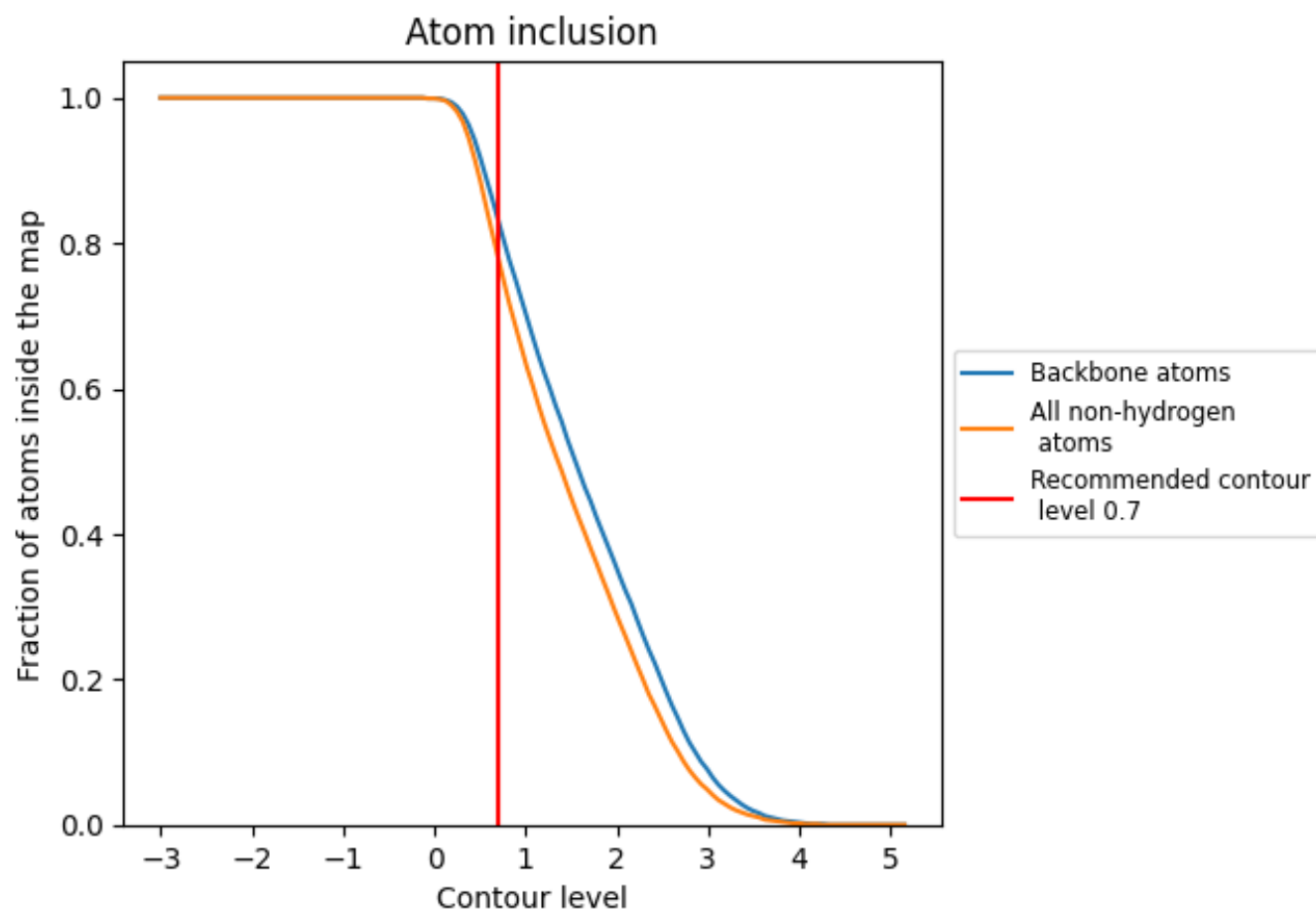
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.6030
B	0.9430	0.6670
C	0.9580	0.6790
D	0.9320	0.6650
E	0.9640	0.6790
F	0.9400	0.6590
G	0.9390	0.6610
H	0.9090	0.6560
I	0.9310	0.6620
J	0.9070	0.6490
K	0.5030	0.4880
L	0.8060	0.5930
M	0.6850	0.5860
N	0.3080	0.3580

