



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:51 PM UTC

PDB ID : 7PLO / pdb_00007plo
EMDB ID : EMD-13494
Title : H. sapiens replisome-CUL2/LRR1 complex
Authors : Jones, M.J.; Yeeles, J.T.P.; Deegan, T.D.; Jenkyn-Bedford, M.
Deposited on : 2021-09-01
Resolution : 2.80 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:

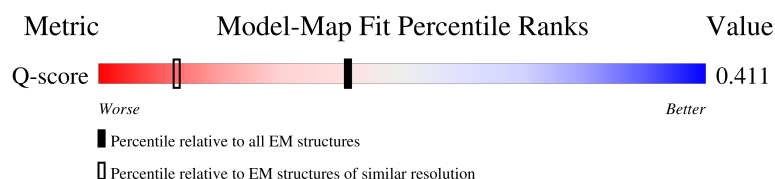
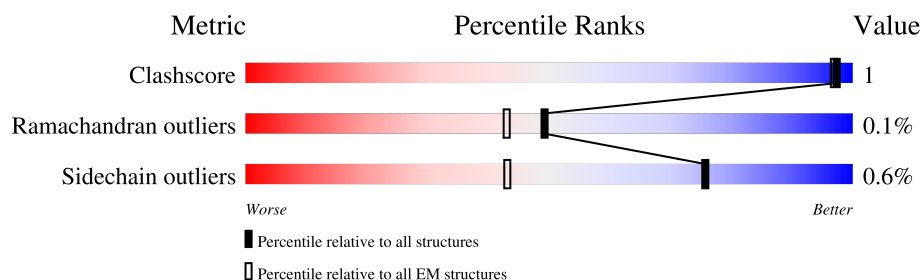
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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.



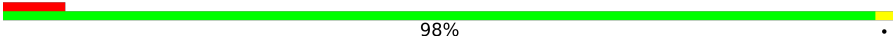
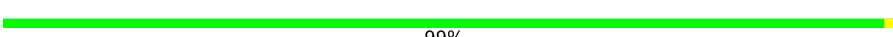
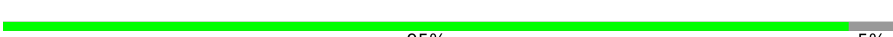
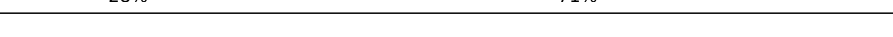
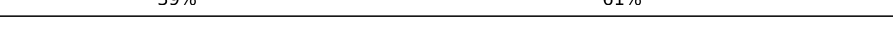
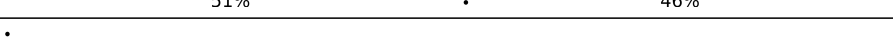
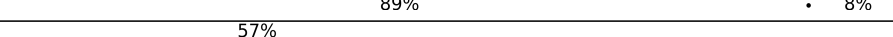
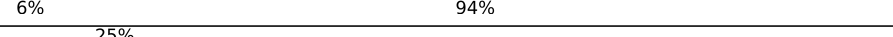
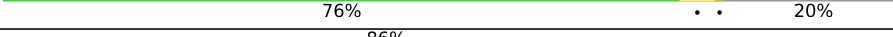
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	2	904	77% 22%
2	3	808	76% 23%
3	4	863	70% 28%
4	5	734	83% 16%

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Mol	Chain	Length	Quality of chain
5	6	821	
6	7	719	
7	A	527	
8	B	2286	
9	C	569	
10	D	196	
11	E	185	
12	F	216	
13	G	262	
14	H	1161	
14	I	1161	
14	J	1161	
15	K	1209	
16	L	301	
17	M	85	
18	N	41	
19	O	414	
20	P	118	
21	Q	1371	
22	R	112	
23	S	745	
24	T	108	

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 158151 atoms, of which 78735 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	2	703	Total	C	H	N	O	S	0	0
			11174	3513	5593	994	1042	32		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	3	623	Total	C	H	N	O	S	0	0
			9768	3041	4901	858	942	26		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	4	619	Total	C	H	N	O	S	0	0
			9905	3100	4980	873	925	27		

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	5	614	Total	C	H	N	O	S	0	0
			9671	3007	4868	856	905	35		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	6	631	Total	C	H	N	O	S	0	0
			10043	3146	5036	889	946	26		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	7	608	Total	C	H	N	O	S	0	0
			9715	3033	4884	856	912	30		

- Molecule 7 is a protein called DNA polymerase epsilon subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	527	Total	C	H	N	O	S	0	0
			8359	2702	4160	697	780	20		

- Molecule 8 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	804	Total	C	H	N	O	S	0	0
			12969	4162	6472	1116	1176	43		

- Molecule 9 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	534	Total	C	H	N	O	S	0	0
			8645	2764	4298	745	807	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	135Z	ASP	-	linker	UNP O75419
C	136A	TYR	-	linker	UNP O75419
C	136B	LYS	-	linker	UNP O75419
C	136C	ASP	-	linker	UNP O75419
C	136D	ASP	-	linker	UNP O75419
C	136E	ASP	-	linker	UNP O75419

- Molecule 10 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	196	Total	C	H	N	O	S	0	0
			3219	1016	1606	290	295	12		

- Molecule 11 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	176	Total	C	H	N	O	S	0	0
			2887	916	1456	242	264	9		

- Molecule 12 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	F	194	Total	C	H	N	O	S	0	0
			3046	979	1500	268	293	6		

- Molecule 13 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	G	203	Total	C	H	N	O	S	0	0
			3379	1065	1700	290	314	10		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-38	MET	-	initiating methionine	UNP Q9BRT9
G	-37	TRP	-	expression tag	UNP Q9BRT9
G	-36	SER	-	expression tag	UNP Q9BRT9
G	-35	HIS	-	expression tag	UNP Q9BRT9
G	-34	PRO	-	expression tag	UNP Q9BRT9
G	-33	GLN	-	expression tag	UNP Q9BRT9
G	-32	PHE	-	expression tag	UNP Q9BRT9
G	-31	GLU	-	expression tag	UNP Q9BRT9
G	-30	LYS	-	expression tag	UNP Q9BRT9
G	-29	GLY	-	expression tag	UNP Q9BRT9
G	-28	GLY	-	expression tag	UNP Q9BRT9
G	-27	GLY	-	expression tag	UNP Q9BRT9
G	-26	SER	-	expression tag	UNP Q9BRT9
G	-25	GLY	-	expression tag	UNP Q9BRT9
G	-24	GLY	-	expression tag	UNP Q9BRT9
G	-23	GLY	-	expression tag	UNP Q9BRT9
G	-22	SER	-	expression tag	UNP Q9BRT9
G	-21	GLY	-	expression tag	UNP Q9BRT9
G	-20	GLY	-	expression tag	UNP Q9BRT9
G	-19	SER	-	expression tag	UNP Q9BRT9
G	-18	ALA	-	expression tag	UNP Q9BRT9
G	-17	TRP	-	expression tag	UNP Q9BRT9
G	-16	SER	-	expression tag	UNP Q9BRT9
G	-15	HIS	-	expression tag	UNP Q9BRT9
G	-14	PRO	-	expression tag	UNP Q9BRT9
G	-13	GLN	-	expression tag	UNP Q9BRT9
G	-12	PHE	-	expression tag	UNP Q9BRT9
G	-11	GLU	-	expression tag	UNP Q9BRT9
G	-10	LYS	-	expression tag	UNP Q9BRT9
G	-9	SER	-	expression tag	UNP Q9BRT9
G	-8	GLY	-	expression tag	UNP Q9BRT9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	LEU	-	expression tag	UNP Q9BRT9
G	-6	GLU	-	expression tag	UNP Q9BRT9
G	-5	VAL	-	expression tag	UNP Q9BRT9
G	-4	LEU	-	expression tag	UNP Q9BRT9
G	-3	PHE	-	expression tag	UNP Q9BRT9
G	-2	GLN	-	expression tag	UNP Q9BRT9
G	-1	GLY	-	expression tag	UNP Q9BRT9
G	0	PRO	-	expression tag	UNP Q9BRT9

- Molecule 14 is a protein called WD repeat and HMG-box DNA-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	H	401	Total	C	H	N	O	S	0	0
			6307	2011	3138	552	585	21		
14	I	451	Total	C	H	N	O	S	0	0
			7116	2269	3534	624	666	23		
14	J	401	Total	C	H	N	O	S	0	0
			6307	2011	3138	552	585	21		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-31	MET	-	initiating methionine	UNP O75717
H	-30	ASP	-	expression tag	UNP O75717
H	-29	TYR	-	expression tag	UNP O75717
H	-28	LYS	-	expression tag	UNP O75717
H	-27	ASP	-	expression tag	UNP O75717
H	-26	ASP	-	expression tag	UNP O75717
H	-25	ASP	-	expression tag	UNP O75717
H	-24	ASP	-	expression tag	UNP O75717
H	-23	LYS	-	expression tag	UNP O75717
H	-22	ASP	-	expression tag	UNP O75717
H	-21	TYR	-	expression tag	UNP O75717
H	-20	LYS	-	expression tag	UNP O75717
H	-19	ASP	-	expression tag	UNP O75717
H	-18	ASP	-	expression tag	UNP O75717
H	-17	ASP	-	expression tag	UNP O75717
H	-16	ASP	-	expression tag	UNP O75717
H	-15	LYS	-	expression tag	UNP O75717
H	-14	ASP	-	expression tag	UNP O75717
H	-13	TYR	-	expression tag	UNP O75717
H	-12	LYS	-	expression tag	UNP O75717

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	ASP	-	expression tag	UNP O75717
H	-10	ASP	-	expression tag	UNP O75717
H	-9	ASP	-	expression tag	UNP O75717
H	-8	ASP	-	expression tag	UNP O75717
H	-7	LYS	-	expression tag	UNP O75717
H	-6	GLU	-	expression tag	UNP O75717
H	-5	ASN	-	expression tag	UNP O75717
H	-4	LEU	-	expression tag	UNP O75717
H	-3	TYR	-	expression tag	UNP O75717
H	-2	PHE	-	expression tag	UNP O75717
H	-1	GLN	-	expression tag	UNP O75717
H	0	GLY	-	expression tag	UNP O75717
I	-31	MET	-	initiating methionine	UNP O75717
I	-30	ASP	-	expression tag	UNP O75717
I	-29	TYR	-	expression tag	UNP O75717
I	-28	LYS	-	expression tag	UNP O75717
I	-27	ASP	-	expression tag	UNP O75717
I	-26	ASP	-	expression tag	UNP O75717
I	-25	ASP	-	expression tag	UNP O75717
I	-24	ASP	-	expression tag	UNP O75717
I	-23	LYS	-	expression tag	UNP O75717
I	-22	ASP	-	expression tag	UNP O75717
I	-21	TYR	-	expression tag	UNP O75717
I	-20	LYS	-	expression tag	UNP O75717
I	-19	ASP	-	expression tag	UNP O75717
I	-18	ASP	-	expression tag	UNP O75717
I	-17	ASP	-	expression tag	UNP O75717
I	-16	ASP	-	expression tag	UNP O75717
I	-15	LYS	-	expression tag	UNP O75717
I	-14	ASP	-	expression tag	UNP O75717
I	-13	TYR	-	expression tag	UNP O75717
I	-12	LYS	-	expression tag	UNP O75717
I	-11	ASP	-	expression tag	UNP O75717
I	-10	ASP	-	expression tag	UNP O75717
I	-9	ASP	-	expression tag	UNP O75717
I	-8	ASP	-	expression tag	UNP O75717
I	-7	LYS	-	expression tag	UNP O75717
I	-6	GLU	-	expression tag	UNP O75717
I	-5	ASN	-	expression tag	UNP O75717
I	-4	LEU	-	expression tag	UNP O75717
I	-3	TYR	-	expression tag	UNP O75717
I	-2	PHE	-	expression tag	UNP O75717

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLN	-	expression tag	UNP O75717
I	0	GLY	-	expression tag	UNP O75717
J	-31	MET	-	initiating methionine	UNP O75717
J	-30	ASP	-	expression tag	UNP O75717
J	-29	TYR	-	expression tag	UNP O75717
J	-28	LYS	-	expression tag	UNP O75717
J	-27	ASP	-	expression tag	UNP O75717
J	-26	ASP	-	expression tag	UNP O75717
J	-25	ASP	-	expression tag	UNP O75717
J	-24	ASP	-	expression tag	UNP O75717
J	-23	LYS	-	expression tag	UNP O75717
J	-22	ASP	-	expression tag	UNP O75717
J	-21	TYR	-	expression tag	UNP O75717
J	-20	LYS	-	expression tag	UNP O75717
J	-19	ASP	-	expression tag	UNP O75717
J	-18	ASP	-	expression tag	UNP O75717
J	-17	ASP	-	expression tag	UNP O75717
J	-16	ASP	-	expression tag	UNP O75717
J	-15	LYS	-	expression tag	UNP O75717
J	-14	ASP	-	expression tag	UNP O75717
J	-13	TYR	-	expression tag	UNP O75717
J	-12	LYS	-	expression tag	UNP O75717
J	-11	ASP	-	expression tag	UNP O75717
J	-10	ASP	-	expression tag	UNP O75717
J	-9	ASP	-	expression tag	UNP O75717
J	-8	ASP	-	expression tag	UNP O75717
J	-7	LYS	-	expression tag	UNP O75717
J	-6	GLU	-	expression tag	UNP O75717
J	-5	ASN	-	expression tag	UNP O75717
J	-4	LEU	-	expression tag	UNP O75717
J	-3	TYR	-	expression tag	UNP O75717
J	-2	PHE	-	expression tag	UNP O75717
J	-1	GLN	-	expression tag	UNP O75717
J	0	GLY	-	expression tag	UNP O75717

- Molecule 15 is a protein called Protein timeless homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K	639	Total	C	H	N	O	S	0	0
			10492	3343	5247	933	943	26		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP Q9UNS1

- Molecule 16 is a protein called TIMELESS-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L	86	Total	C	H	N	O	S	0	0
			1479	465	753	138	120	3		

- Molecule 17 is a DNA chain called Leading strand DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	M	33	Total	C	H	N	O	P	0	0
			1064	330	382	108	211	33		

- Molecule 18 is a DNA chain called Lagging strand DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	N	22	Total	C	H	N	O	P	0	0
			686	211	248	74	131	22		

- Molecule 19 is a protein called Leucine-rich repeat protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	O	382	Total	C	H	N	O	S	0	0
			5747	1837	2859	513	522	16		

- Molecule 20 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	P	82	Total	C	H	N	O	S	0	0
			1236	397	609	105	122	3		

- Molecule 21 is a protein called Claspins.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	Q	79	Total	C	H	N	O	S	0	0
			1384	431	701	133	117	2		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1340	LEU	-	expression tag	UNP Q9HAW4

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1341	GLU	-	expression tag	UNP Q9HAW4
Q	1342	VAL	-	expression tag	UNP Q9HAW4
Q	1343	LEU	-	expression tag	UNP Q9HAW4
Q	1344	PHE	-	expression tag	UNP Q9HAW4
Q	1345	GLN	-	expression tag	UNP Q9HAW4
Q	1346	GLY	-	expression tag	UNP Q9HAW4
Q	1347	PRO	-	expression tag	UNP Q9HAW4
Q	1348	ASP	-	expression tag	UNP Q9HAW4
Q	1349	TYR	-	expression tag	UNP Q9HAW4
Q	1350	LYS	-	expression tag	UNP Q9HAW4
Q	1351	ASP	-	expression tag	UNP Q9HAW4
Q	1352	ASP	-	expression tag	UNP Q9HAW4
Q	1353	ASP	-	expression tag	UNP Q9HAW4
Q	1354	ASP	-	expression tag	UNP Q9HAW4
Q	1355	LYS	-	expression tag	UNP Q9HAW4
Q	1356	ASP	-	expression tag	UNP Q9HAW4
Q	1357	TYR	-	expression tag	UNP Q9HAW4
Q	1358	LYS	-	expression tag	UNP Q9HAW4
Q	1359	ASP	-	expression tag	UNP Q9HAW4
Q	1360	ASP	-	expression tag	UNP Q9HAW4
Q	1361	ASP	-	expression tag	UNP Q9HAW4
Q	1362	ASP	-	expression tag	UNP Q9HAW4
Q	1363	LYS	-	expression tag	UNP Q9HAW4
Q	1364	ASP	-	expression tag	UNP Q9HAW4
Q	1365	TYR	-	expression tag	UNP Q9HAW4
Q	1366	LYS	-	expression tag	UNP Q9HAW4
Q	1367	ASP	-	expression tag	UNP Q9HAW4
Q	1368	ASP	-	expression tag	UNP Q9HAW4
Q	1369	ASP	-	expression tag	UNP Q9HAW4
Q	1370	ASP	-	expression tag	UNP Q9HAW4
Q	1371	LYS	-	expression tag	UNP Q9HAW4

- Molecule 22 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	R	90	Total	C	H	N	O	S	0	0
			1381	446	686	112	131	6		

- Molecule 23 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	S	671	Total	C	H	N	O	S	0	0
			10694	3408	5302	925	1017	42		

- Molecule 24 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	T	86	Total	C	H	N	O	S	0	0
			1330	429	645	127	120	9		

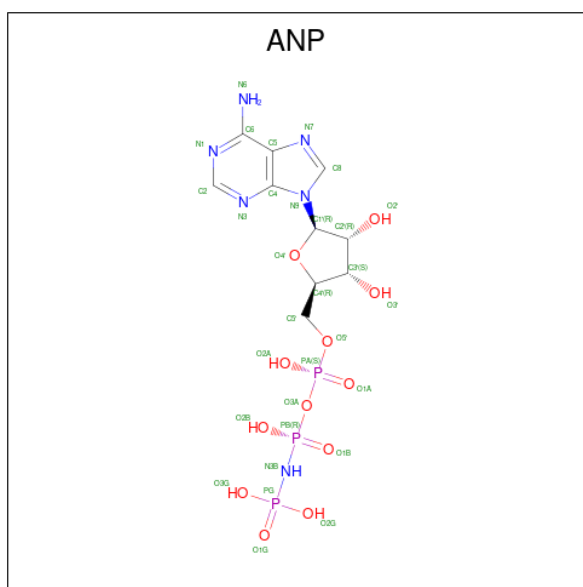
- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
25	2	1	Total	Zn	0
			1	1	
25	4	1	Total	Zn	0
			1	1	
25	5	1	Total	Zn	0
			1	1	
25	6	1	Total	Zn	0
			1	1	
25	7	1	Total	Zn	0
			1	1	
25	T	3	Total	Zn	0
			3	3	

- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

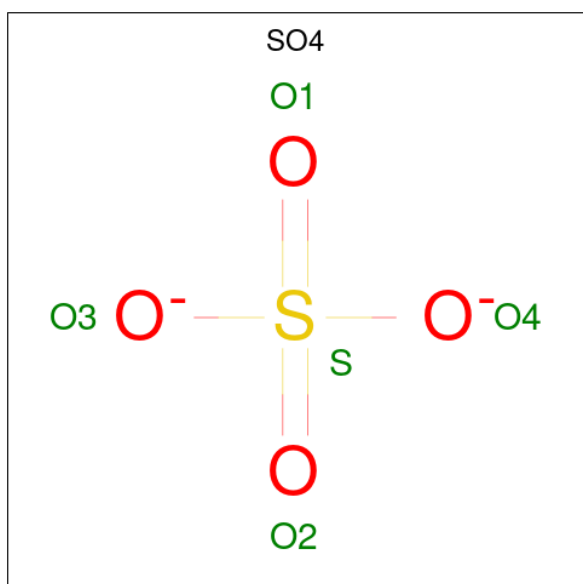
Mol	Chain	Residues	Atoms		AltConf
26	2	1	Total	Mg	0
			1	1	
26	3	1	Total	Mg	0
			1	1	
26	5	1	Total	Mg	0
			1	1	

- Molecule 27 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf	
27	2	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
27	3	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
27	5	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	

- Molecule 28 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).

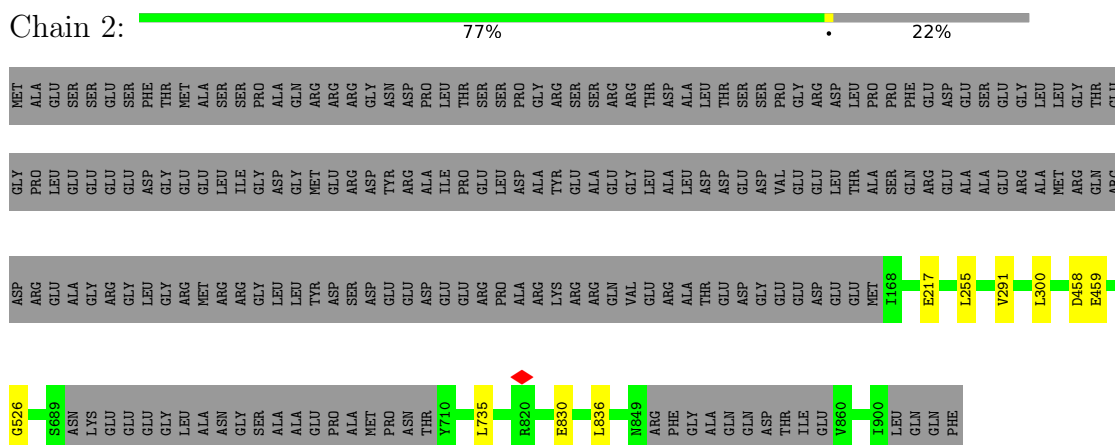


Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	O	S	0
			5	4	1	

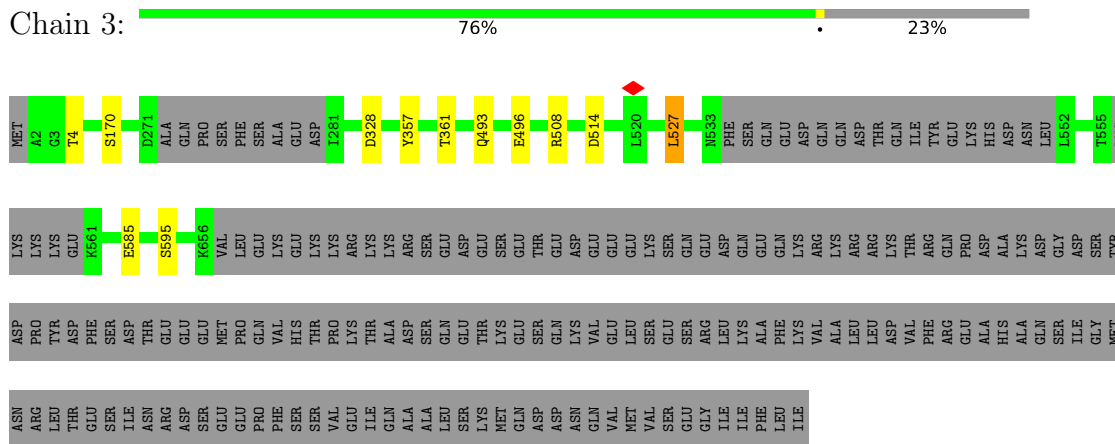
3 Residue-property plots

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.

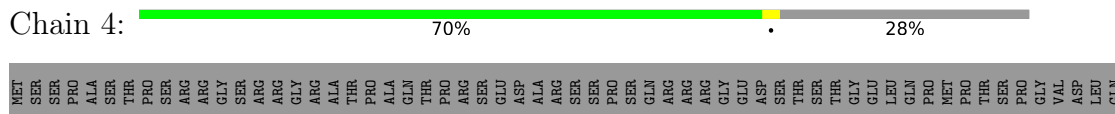
- Molecule 1: DNA replication licensing factor MCM2

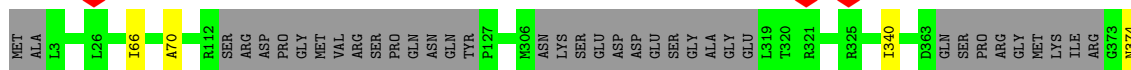


- Molecule 2: DNA replication licensing factor MCM3

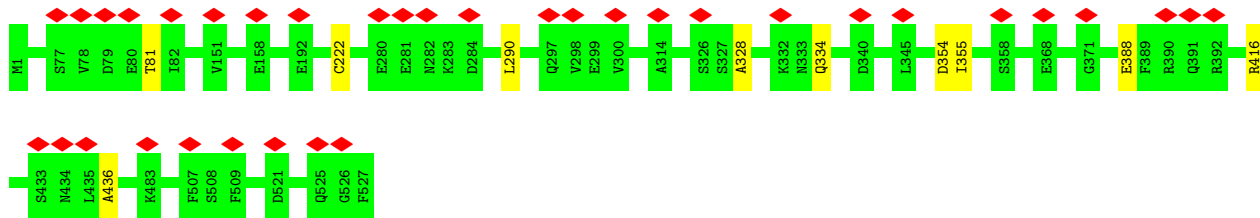


- Molecule 3: DNA replication licensing factor MCM4

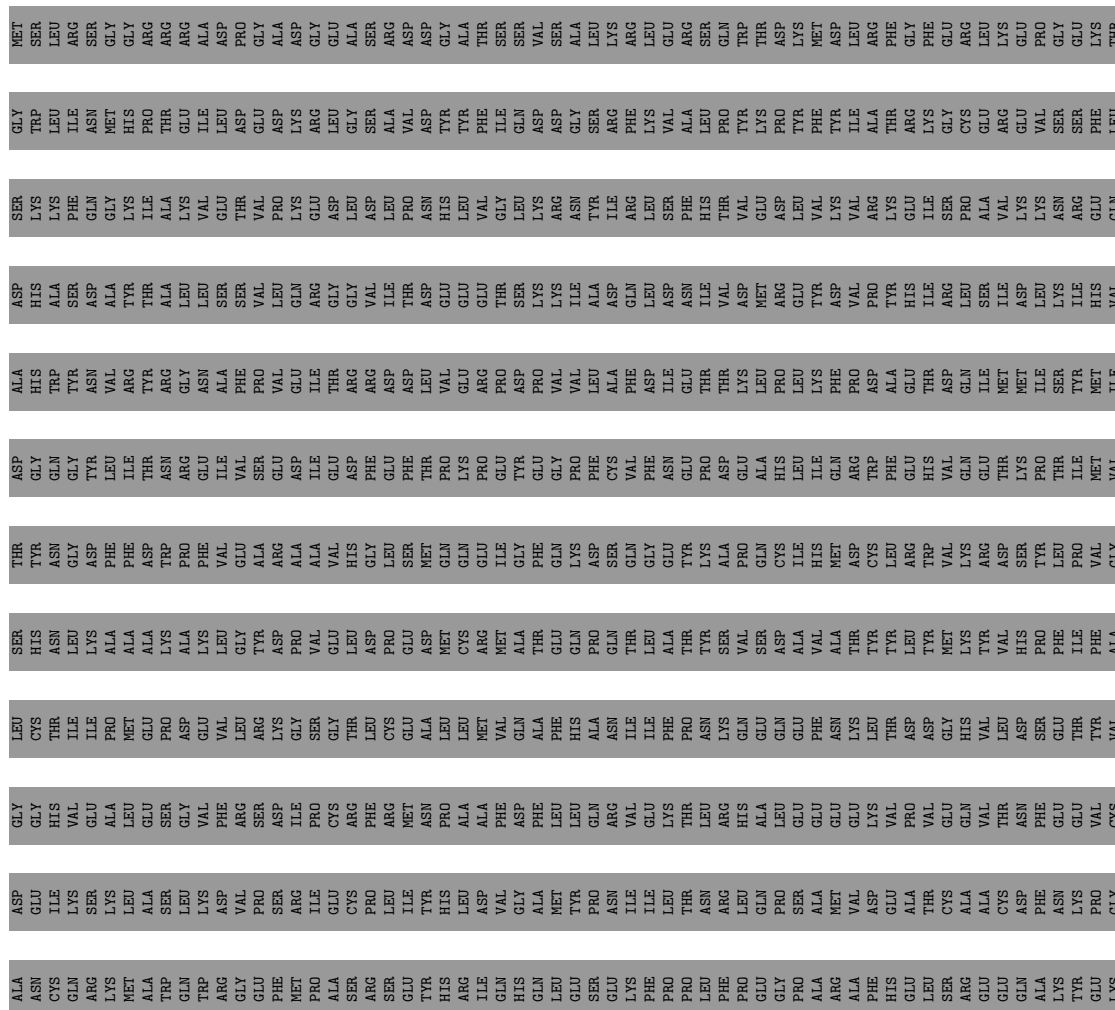




- Molecule 7: DNA polymerase epsilon subunit 2

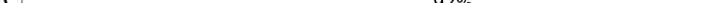


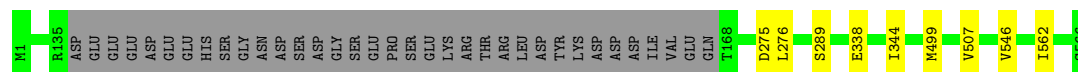
- Molecule 8: DNA polymerase epsilon catalytic subunit A





- Molecule 9: Cell division control protein 45 homolog

Chain C:  92% • 6%

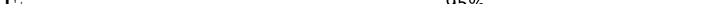


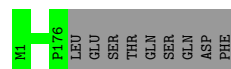
- Molecule 10: DNA replication complex GINS protein PSF1

Chain D: 99%

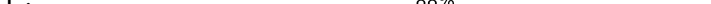


- Molecule 11: DNA replication complex GINS protein PSF2

Chain E:  95% 5%

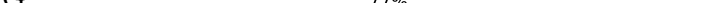


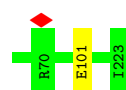
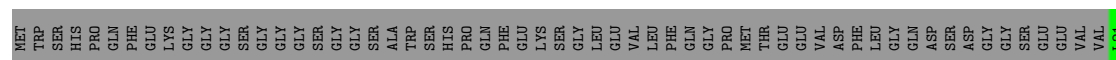
- Molecule 12: DNA replication complex GINS protein PSF3

Chain F:  88% : 10%



- Molecule 13: DNA replication complex GINS protein SLD5

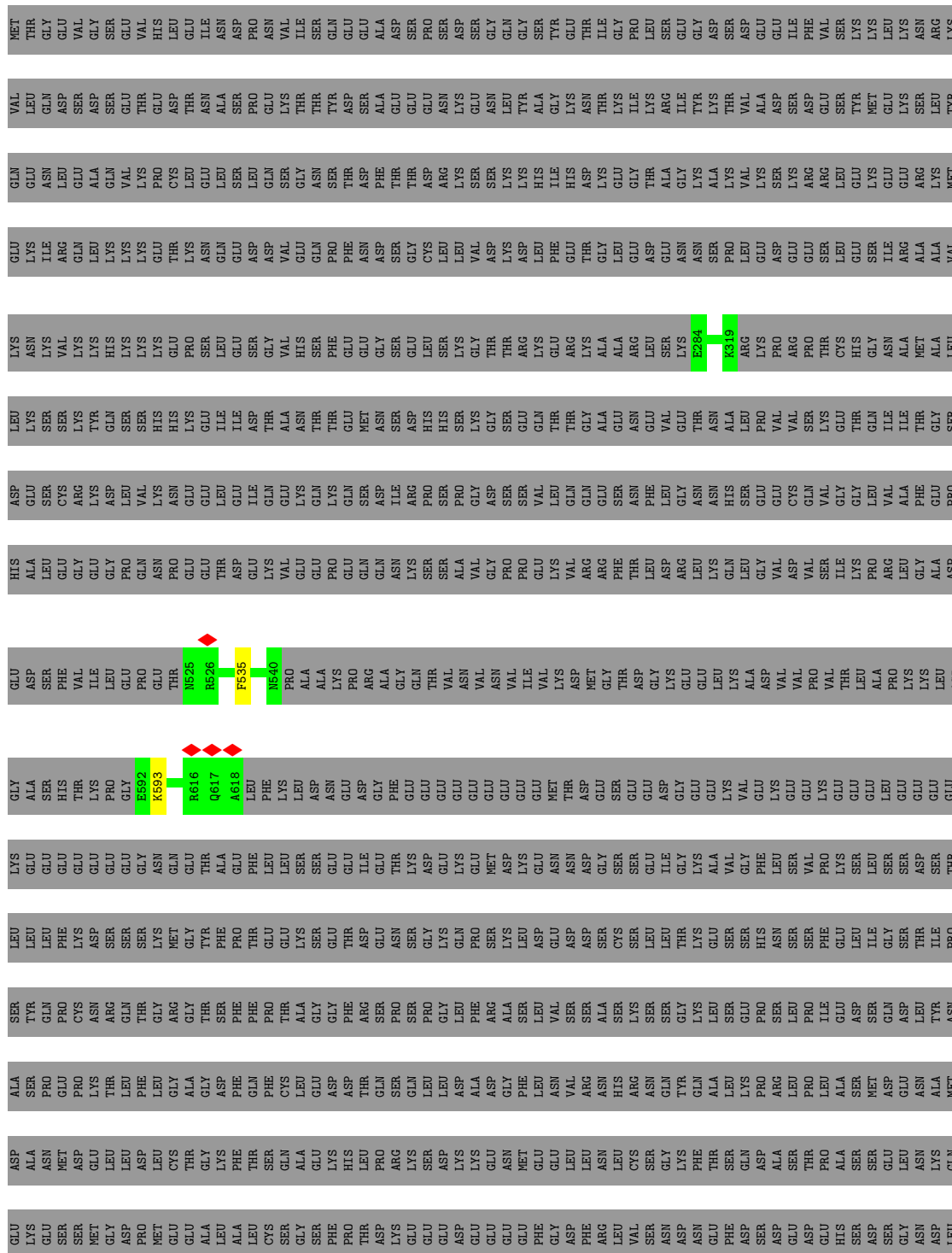
Chain G:  77% 23%

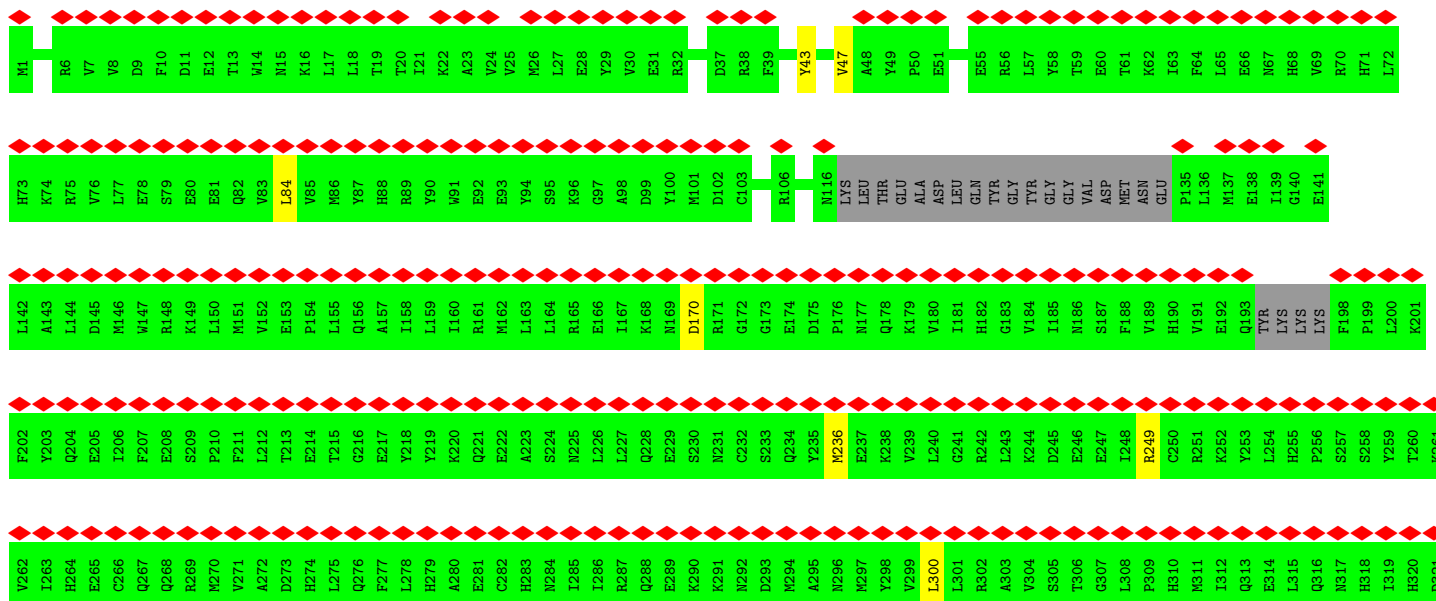


[illegible]



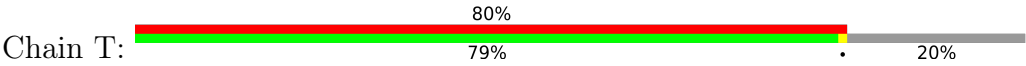






E322	K382	R442	ASP	G562	M622	A682	S742
G323	S383	L443	LEU	E563	I623	A683	Y743
L324	V384	I444	ILE	V564	M624	I684	V744
R325	C385	H445	S506	K565	HIS	V685	A745
A326	K386	G446	F507	M566	ASP	R686	
T327	A387	L447	Q508	N567	GLU	M687	
S328	P388	S448	I509	TYR	LYS	M688	
N329	E389	M449	Y510	LEU	GLU	K689	
L330	L390	S450	Y511	GLY	ASP	A690	
T331	L391	M451	V512	LYS	ILE	R691	
Q332	L392	D452	L513	PRO	ASP	R692	
E333	K393	S453	Q513	TYR	ALA	K693	
N334	Y394	E454	A514	V574	E635	L694	
M335	C395	E455	G515	A575	S636	R695	
P336	D396	A456	A516	M576	S637	H696	
T337	N397	M457	W517	V577	F638	M697	
L338	L398	I458	P518	T578	S639	A698	
F339	L399	I459	L519	T579	L640	L699	
V340	K400	K460	T520	Y580	N641	I700	
E341	K401	L461	Q521	Q581	M642	Q701	
S342	S402	L462	A522	M582	N643	E702	
V343	A403	Q463	P523	A583	F644	V703	
L344	K404	A464	SER	V584	SER	I704	
E345	G405	C465	LEU	LEU	LYS	S705	
V346	M406	G466	THR	ALA	ARG	Q706	
H347	T407	G467	PHE	ALA	THR	S707	
G348	E408	E468	ALA	ASN	LYS	R708	
K349	N409	F469	ILE	ASN	PHE	A709	
F350	E410	T470	PS30	ASN	LYS	R710	
V351	V411	S471	Q531	THR	ILE	F711	
Q352	E412	K472	L533	V594	THR	M712	
L353	D413	L473	E534	S595	MET	P713	
I354	R414	H474	K535	Y596	GLN	S714	
N355	L415	R475	S536	K597	LYS	I715	
T356	L416	M476	V537	E598	ASP	S716	
V357	S417	Y477	Q538	L599	T661	M717	
L358	F418	T478	M539	Q600	P662	I718	
N359	I419	D479	F540	D601	Q663	K719	
G360	T420	M480	E541	S602	E664	T720	
D361	V421	S481	L542	T603	M665	C721	
Q362	F422	V482	F543	Q604	Q667	I722	
H363	K423	A484	Y544	M605	T668	E723	
F364	Y424	A484	Q546	M606	R669	V724	
M365	I425	D485	H547	K608	A671	L725	
S366	D426	L486	F548	E609	V672	I726	
A367	D427	N487	SS49	L610	D673	D727	
L368	K428	N488	G550	T611	E674	K728	
D369	D429	K489	R551	K612	D675	Q729	
K370	V430	F490	K552	T613	R676	Y730	
A371	F431	N491	L553	I614	K677	I731	
L372	Q432	N492	L554	K615	M678	E732	
T373	K433	F493	W555	S616	Y679	R733	
S374	F434	I494	L556	L617	L680	S734	
V375	Y435	K495	H557	L618	Q681	Q735	
V376	A436	N496	Y558	D619	A736	A736	
N377	R437	Q497	L559	V620	S737	A738	
Y378	M438	D498	C560	K621	E740	E740	
R379	T439	T499	T561			Y741	
E380	A440	V500					
P381	K441	ILE					

• Molecule 24: E3 ubiquitin-protein ligase RBX1



MET	A17	A61
ALA	G18	S62
ALA	K19	A63
MET	K20	T64
ASP	R21	S65
VAL	F22	E66
ASP	E23	E67
THR	V24	C68
PRO	K25	T69
SER	W27	GLY
GLY	N28	V70
THR	A29	A71
ASN	V30	W72
SER	A31	G73
GLY	L32	V74
A17	W33	C75
G18	A34	N76
K19	V35	H77
K20	D36	A78
R21	I37	F79
F22	V38	H80
E23	V39	S81
V24	D40	H82
K25	N41	C83
W27	N42	I84
N28	C42	S85
A29	A43	R86
V30	I44	W87
A31	C45	L88
L32	R46	R89
W33	N47	T90
A34	H48	R91
V35	T49	Q92
D36	M50	V93
I37	D51	C94
V38	L52	P95
V39	C53	L96
D40	I54	D97
N41	E55	N98
N42	C56	C99
C42	Q57	E100
A43	A58	W101
I44	N59	E102
C45	Q60	PHE
R46		GLN
N47		LYS
H48		TYR
T49		GLY
M50		HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232000	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 ($e^-/\text{\AA}^2$)	38.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.336	Depositor
Minimum map value	-0.180	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0181	Depositor
Map size (Å)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, ANP, MG

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	2	0.24	0/5684	0.45	0/7676
2	3	0.22	0/4939	0.43	0/6669
3	4	0.22	0/5009	0.44	0/6769
4	5	0.21	0/4877	0.43	0/6564
5	6	0.21	0/5088	0.44	0/6866
6	7	0.23	0/4905	0.46	0/6621
7	A	0.29	0/4310	0.55	2/5853 (0.0%)
8	B	0.31	0/6647	0.59	0/9011
9	C	0.21	0/4439	0.38	0/5992
10	D	0.22	0/1645	0.42	0/2210
11	E	0.24	0/1462	0.42	0/1981
12	F	0.21	0/1580	0.43	0/2133
13	G	0.26	0/1711	0.47	0/2305
14	H	0.26	0/3244	0.47	0/4395
14	I	0.23	0/3664	0.44	0/4959
14	J	0.24	0/3244	0.47	0/4395
15	K	0.23	0/5350	0.43	0/7209
16	L	0.24	0/741	0.48	0/988
17	M	0.34	0/760	0.63	0/1172
18	N	0.36	0/488	0.57	0/747
19	O	0.23	0/2933	0.48	0/3962
20	P	0.21	0/634	0.47	0/851
21	Q	0.25	0/693	0.47	0/919
22	R	0.24	0/709	0.42	0/956
23	S	0.27	0/5484	0.51	0/7384
24	T	0.33	0/702	0.57	0/952
All	All	0.25	0/80942	0.47	2/109539 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	A	436	ALA	CA-C-N	5.26	125.48	120.43
7	A	436	ALA	C-N-CA	5.26	125.48	120.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	B	1723	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5581	5593	5593	6	0
2	3	4867	4901	4901	8	0
3	4	4925	4980	4980	7	0
4	5	4803	4868	4868	4	0
5	6	5007	5036	5036	5	0
6	7	4831	4884	4884	4	0
7	A	4199	4160	4160	3	0
8	B	6497	6472	6471	11	0
9	C	4347	4298	4296	4	0
10	D	1613	1606	1606	1	0
11	E	1431	1456	1456	0	0
12	F	1546	1500	1500	1	0
13	G	1679	1700	1700	1	0
14	H	3169	3138	3138	3	0
14	I	3582	3534	3534	3	0
14	J	3169	3138	3138	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	5245	5247	5246	14	0
16	L	726	753	753	2	0
17	M	682	382	384	0	0
18	N	438	248	249	1	0
19	O	2888	2859	2859	5	0
20	P	627	609	609	0	0
21	Q	683	701	701	2	0
22	R	695	686	685	2	0
23	S	5392	5302	5295	11	0
24	T	685	645	645	0	0
25	2	1	0	0	0	0
25	4	1	0	0	0	0
25	5	1	0	0	0	0
25	6	1	0	0	0	0
25	7	1	0	0	0	0
25	T	3	0	0	0	0
26	2	1	0	0	0	0
26	3	1	0	0	0	0
26	5	1	0	0	0	0
27	2	31	13	13	1	0
27	3	31	13	13	1	0
27	5	31	13	13	0	0
28	A	5	0	0	0	0
All	All	79416	78735	78726	93	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 1.

All (93) 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)
4:5:495:TRP:O	4:5:503:ASN:ND2	2.24	0.71
22:R:17:MET:SD	22:R:17:MET:N	2.69	0.65
23:S:170:ASP:OD1	23:S:249:ARG:NH2	2.33	0.62
23:S:500:VAL:HG22	23:S:539:MET:HE3	1.85	0.58
8:B:1367:TYR:HD2	8:B:1431:VAL:HG21	1.69	0.58
15:K:52:ARG:NH1	15:K:88:ASN:O	2.37	0.58
14:H:789:THR:O	14:H:793:VAL:HG23	2.03	0.58
15:K:738:MET:HE3	15:K:799:VAL:HG11	1.84	0.58
15:K:451:ASN:ND2	15:K:512:MET:SD	2.77	0.57
15:K:9:GLU:N	15:K:9:GLU:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:10:DC:OP1	19:O:22:ARG:NH1	2.37	0.57
23:S:599:LEU:HB2	23:S:614:ILE:HD12	1.88	0.56
8:B:1655:ILE:O	8:B:1659:ASN:ND2	2.39	0.55
2:3:595:SER:OG	6:7:527:ARG:NH1	2.40	0.54
15:K:738:MET:CE	15:K:799:VAL:HG11	2.38	0.53
5:6:82:GLU:O	5:6:86:VAL:HG22	2.09	0.52
3:4:155:THR:HG22	3:4:157:VAL:HG23	1.92	0.51
23:S:599:LEU:HB2	23:S:614:ILE:CD1	2.40	0.51
8:B:2236:CYS:SG	8:B:2237:SER:N	2.83	0.51
2:3:585:GLU:N	2:3:585:GLU:OE1	2.44	0.51
2:3:508:ARG:NH2	2:3:514:ASP:O	2.43	0.51
23:S:43:TYR:O	23:S:47:VAL:HG23	2.11	0.51
5:6:362:ASP:OD2	5:6:366:ARG:NH1	2.43	0.51
2:3:527:LEU:HD12	12:F:99:VAL:HG22	1.92	0.50
5:6:363:GLU:N	5:6:363:GLU:OE1	2.45	0.49
15:K:797:THR:O	15:K:800:VAL:HG22	2.11	0.49
15:K:182:ASP:O	15:K:332:ARG:NH2	2.46	0.49
3:4:155:THR:HG23	3:4:229:TYR:CZ	2.48	0.48
14:I:668:CYS:SG	14:I:669:LYS:N	2.86	0.48
16:L:146:ASP:OD1	16:L:146:ASP:N	2.45	0.48
14:H:534:ASP:OD1	14:H:535:ILE:N	2.46	0.48
14:I:503:SER:OG	14:I:509:SER:N	2.46	0.48
1:2:735:LEU:HD22	4:5:541:VAL:HG22	1.96	0.48
15:K:780:LEU:HD22	15:K:803:MET:HE1	1.96	0.48
23:S:500:VAL:HG22	23:S:539:MET:CE	2.43	0.47
9:C:499:MET:SD	9:C:499:MET:N	2.88	0.47
19:O:197:GLY:O	19:O:223:THR:OG1	2.27	0.47
3:4:289:VAL:HG21	3:4:382:VAL:CG1	2.44	0.47
8:B:1867:ASN:OD1	8:B:1868:PHE:N	2.44	0.47
15:K:802:GLU:C	15:K:803:MET:HE2	2.40	0.46
2:3:4:THR:HG1	2:3:170:SER:HG	1.55	0.46
9:C:507:VAL:HG12	9:C:546:VAL:HG22	1.98	0.46
19:O:402:SER:OG	19:O:403:LEU:N	2.48	0.46
23:S:622:MET:SD	23:S:622:MET:N	2.84	0.46
15:K:348:GLU:N	15:K:348:GLU:OE1	2.48	0.46
22:R:75:MET:O	22:R:78:THR:OG1	2.34	0.46
1:2:217:GLU:OE1	1:2:217:GLU:N	2.49	0.46
2:3:493:GLN:NE2	2:3:496:GLU:OE2	2.47	0.46
7:A:328:ALA:O	7:A:334:GLN:NE2	2.49	0.45
8:B:1389:PRO:HG3	8:B:1683:LEU:HD13	1.97	0.45
3:4:232:GLU:N	3:4:232:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:66:ILE:HD12	19:O:111:HIS:HB2	1.98	0.45
4:5:537:ILE:O	4:5:541:VAL:HG23	2.17	0.44
6:7:404:THR:HG21	6:7:433:ALA:HB2	1.99	0.44
3:4:175:ASP:OD1	3:4:175:ASP:N	2.50	0.44
27:3:1500:ANP:N3B	27:3:1500:ANP:O2A	2.51	0.44
9:C:276:LEU:HD22	9:C:344:ILE:HG21	2.00	0.43
15:K:182:ASP:OD1	15:K:183:ALA:N	2.51	0.43
14:J:603:LEU:HD23	14:J:614:LEU:HD13	2.00	0.43
8:B:2103:GLU:OE1	8:B:2103:GLU:N	2.50	0.43
19:O:54:ASP:N	19:O:54:ASP:OD1	2.52	0.43
23:S:407:THR:O	23:S:411:VAL:HG23	2.18	0.43
2:3:328:ASP:OD1	2:3:328:ASP:N	2.52	0.43
15:K:14:CYS:SG	15:K:60:ILE:HG21	2.58	0.43
1:2:830:GLU:OE1	1:2:830:GLU:N	2.51	0.42
14:J:462:GLN:NE2	14:J:463:ASP:OD2	2.50	0.42
7:A:388:GLU:OE1	7:A:388:GLU:N	2.50	0.42
10:D:88:ARG:NE	13:G:101:GLU:OE1	2.45	0.42
1:2:291:VAL:O	21:Q:593:LYS:NZ	2.45	0.42
8:B:1406:MET:SD	8:B:1407:TYR:N	2.92	0.42
8:B:1799:VAL:HG22	8:B:1821:PHE:CE2	2.53	0.42
23:S:615:LYS:HA	23:S:618:LEU:HD23	2.02	0.42
5:6:477:MET:HG2	5:6:499:ILE:HD12	2.02	0.42
23:S:236:MET:HE1	23:S:300:LEU:HD22	2.02	0.42
3:4:694:ALA:HA	3:4:698:ILE:HD13	2.02	0.42
6:7:66:ILE:O	6:7:70:ALA:HA	2.19	0.41
8:B:1431:VAL:HG11	8:B:1684:LEU:HD21	2.02	0.41
8:B:1684:LEU:H	8:B:1684:LEU:HD23	1.85	0.41
7:A:354:ASP:OD1	7:A:355:ILE:N	2.49	0.41
14:H:719:ALA:O	14:H:720:THR:OG1	2.37	0.41
15:K:46:ASP:OD1	15:K:47:GLU:N	2.54	0.41
1:2:458:ASP:OD1	1:2:459:GLU:N	2.53	0.41
6:7:374:ASN:O	6:7:611:ARG:NH1	2.54	0.41
1:2:526:GLY:H	27:2:1003:ANP:HNB1	1.69	0.41
5:6:322:ALA:HB1	21:Q:535:PHE:CE1	2.56	0.41
15:K:789:VAL:HG13	16:L:78:LEU:HD12	2.01	0.41
3:4:442:SER:O	3:4:446:VAL:HG23	2.21	0.41
8:B:1405:ASP:OD1	8:B:1406:MET:N	2.52	0.41
9:C:338:GLU:OE1	9:C:338:GLU:N	2.51	0.41
2:3:357:TYR:CE1	2:3:361:THR:HG21	2.56	0.40
4:5:77:LEU:CD2	4:5:88:LEU:HD12	2.51	0.40
23:S:401:LYS:NZ	23:S:446:GLY:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:525:TRP:CZ3	14:I:527:ILE:HD12	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	697/904 (77%)	673 (97%)	24 (3%)	0	100	100
2	3	615/808 (76%)	598 (97%)	17 (3%)	0	100	100
3	4	611/863 (71%)	598 (98%)	13 (2%)	0	100	100
4	5	608/734 (83%)	592 (97%)	16 (3%)	0	100	100
5	6	623/821 (76%)	606 (97%)	16 (3%)	1 (0%)	43	72
6	7	600/719 (83%)	584 (97%)	16 (3%)	0	100	100
7	A	525/527 (100%)	501 (95%)	24 (5%)	0	100	100
8	B	792/2286 (35%)	714 (90%)	74 (9%)	4 (0%)	24	55
9	C	530/569 (93%)	519 (98%)	11 (2%)	0	100	100
10	D	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
11	E	174/185 (94%)	171 (98%)	3 (2%)	0	100	100
12	F	190/216 (88%)	185 (97%)	5 (3%)	0	100	100
13	G	201/262 (77%)	196 (98%)	5 (2%)	0	100	100
14	H	399/1161 (34%)	381 (96%)	18 (4%)	0	100	100
14	I	447/1161 (38%)	436 (98%)	11 (2%)	0	100	100
14	J	399/1161 (34%)	386 (97%)	13 (3%)	0	100	100
15	K	635/1209 (52%)	617 (97%)	18 (3%)	0	100	100
16	L	84/301 (28%)	80 (95%)	4 (5%)	0	100	100
19	O	374/414 (90%)	346 (92%)	28 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	P	70/118 (59%)	65 (93%)	5 (7%)	0	100	100
21	Q	73/1371 (5%)	72 (99%)	1 (1%)	0	100	100
22	R	86/112 (77%)	85 (99%)	1 (1%)	0	100	100
23	S	653/745 (88%)	619 (95%)	34 (5%)	0	100	100
24	T	84/108 (78%)	76 (90%)	8 (10%)	0	100	100
All	All	9664/16951 (57%)	9289 (96%)	370 (4%)	5 (0%)	49	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	B	1725	VAL
8	B	1431	VAL
8	B	1656	PRO
5	6	44	ILE
8	B	1918	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	618/781 (79%)	615 (100%)	3 (0%)	81	93
2	3	535/707 (76%)	534 (100%)	1 (0%)	87	96
3	4	548/753 (73%)	544 (99%)	4 (1%)	76	91
4	5	522/625 (84%)	521 (100%)	1 (0%)	87	96
5	6	555/724 (77%)	553 (100%)	2 (0%)	84	94
6	7	527/619 (85%)	526 (100%)	1 (0%)	87	96
7	A	471/471 (100%)	467 (99%)	4 (1%)	73	90
8	B	725/2012 (36%)	715 (99%)	10 (1%)	59	85
9	C	487/520 (94%)	484 (99%)	3 (1%)	78	92
10	D	174/174 (100%)	173 (99%)	1 (1%)	78	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	E	160/169 (95%)	160 (100%)	0	100	100
12	F	167/186 (90%)	165 (99%)	2 (1%)	63	87
13	G	188/233 (81%)	188 (100%)	0	100	100
14	H	345/1018 (34%)	343 (99%)	2 (1%)	78	92
14	I	390/1018 (38%)	387 (99%)	3 (1%)	73	90
14	J	345/1018 (34%)	343 (99%)	2 (1%)	78	92
15	K	563/1055 (53%)	558 (99%)	5 (1%)	70	89
16	L	77/274 (28%)	77 (100%)	0	100	100
19	O	303/380 (80%)	299 (99%)	4 (1%)	61	86
20	P	67/103 (65%)	67 (100%)	0	100	100
21	Q	72/1230 (6%)	72 (100%)	0	100	100
22	R	77/96 (80%)	74 (96%)	3 (4%)	28	64
23	S	590/681 (87%)	587 (100%)	3 (0%)	81	93
24	T	72/90 (80%)	71 (99%)	1 (1%)	59	85
All	All	8578/14937 (57%)	8523 (99%)	55 (1%)	76	92

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	255	LEU
1	2	300	LEU
1	2	836	LEU
2	3	527	LEU
3	4	587	LEU
3	4	666	LEU
3	4	708	GLN
3	4	781	VAL
4	5	649	LEU
5	6	173	LYS
5	6	254	VAL
6	7	340	ILE
7	A	81	THR
7	A	222	CYS
7	A	290	LEU
7	A	416	ARG
8	B	1366	PHE
8	B	1423	ILE

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Mol	Chain	Res	Type
8	B	1560	ASP
8	B	1588	GLN
8	B	1694	LEU
8	B	1729	LEU
8	B	1817	GLN
8	B	1903	LEU
8	B	1915	LEU
8	B	1918	ASP
9	C	275	ASP
9	C	289	SER
9	C	562	ILE
10	D	156	TYR
12	F	68	LEU
12	F	169	ASP
14	H	601	VAL
14	H	797	ILE
14	I	459	ASN
14	I	497	ILE
14	I	762	GLN
14	J	447	MET
14	J	756	GLN
15	K	124	PHE
15	K	137	LEU
15	K	348	GLU
15	K	422	MET
15	K	466	ARG
19	O	58	THR
19	O	159	LEU
19	O	174	LEU
19	O	184	LEU
22	R	17	MET
22	R	18	TYR
22	R	84	THR
23	S	84	LEU
23	S	610	LEU
23	S	618	LEU
24	T	44	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	201	ASN

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Mol	Chain	Res	Type
1	2	321	GLN
1	2	343	GLN
1	2	371	GLN
1	2	430	ASN
1	2	471	GLN
1	2	777	HIS
1	2	849	ASN
2	3	110	HIS
2	3	310	HIS
3	4	300	GLN
3	4	305	GLN
3	4	407	ASN
3	4	606	GLN
4	5	524	HIS
5	6	59	ASN
5	6	121	HIS
5	6	162	GLN
5	6	176	GLN
7	A	55	GLN
7	A	282	ASN
7	A	410	GLN
8	B	1627	HIS
8	B	2068	GLN
8	B	2098	ASN
8	B	2189	ASN
8	B	2264	HIS
9	C	173	GLN
9	C	246	GLN
9	C	261	ASN
9	C	308	GLN
9	C	408	ASN
9	C	427	GLN
9	C	428	GLN
9	C	437	ASN
10	D	115	ASN
10	D	138	GLN
14	H	486	ASN
14	H	656	ASN
14	H	663	ASN
14	H	794	ASN
14	I	476	HIS
14	I	486	ASN

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Mol	Chain	Res	Type
14	I	512	HIS
14	I	656	ASN
15	K	168	HIS
15	K	229	GLN
15	K	323	GLN
15	K	417	ASN
15	K	526	GLN
16	L	63	ASN
19	O	65	ASN
19	O	208	ASN
21	Q	315	HIS
23	S	317	ASN
23	S	487	ASN
24	T	82	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SO4	A	601	-	4,4,4	0.23	0	6,6,6	0.07	0
27	ANP	3	1500	26	33,33,33	0.96	4 (12%)	45,52,52	0.56	0
27	ANP	5	801	26	33,33,33	0.98	4 (12%)	45,52,52	0.49	0
27	ANP	2	1003	26	33,33,33	0.92	4 (12%)	45,52,52	0.55	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
27	ANP	3	1500	26	-	5/18/38/38	0/3/3/3
27	ANP	5	801	26	-	3/18/38/38	0/3/3/3
27	ANP	2	1003	26	-	2/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	801	ANP	PB-O3A	-2.86	1.55	1.59
27	3	1500	ANP	PB-O3A	-2.83	1.55	1.59
27	2	1003	ANP	PB-O3A	-2.48	1.56	1.59
27	5	801	ANP	PG-O1G	2.47	1.49	1.46
27	2	1003	ANP	PG-O1G	2.44	1.49	1.46
27	5	801	ANP	PG-N3B	2.39	1.69	1.63
27	3	1500	ANP	PG-O1G	2.38	1.49	1.46
27	5	801	ANP	PB-O1B	2.35	1.49	1.46
27	2	1003	ANP	PB-O1B	2.32	1.49	1.46
27	3	1500	ANP	PG-N3B	2.30	1.69	1.63
27	2	1003	ANP	PG-N3B	2.28	1.69	1.63
27	3	1500	ANP	PB-O1B	2.25	1.49	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	2	1003	ANP	PB-N3B-PG-O1G
27	3	1500	ANP	PG-N3B-PB-O1B
27	3	1500	ANP	PG-N3B-PB-O3A
27	3	1500	ANP	C5'-O5'-PA-O1A

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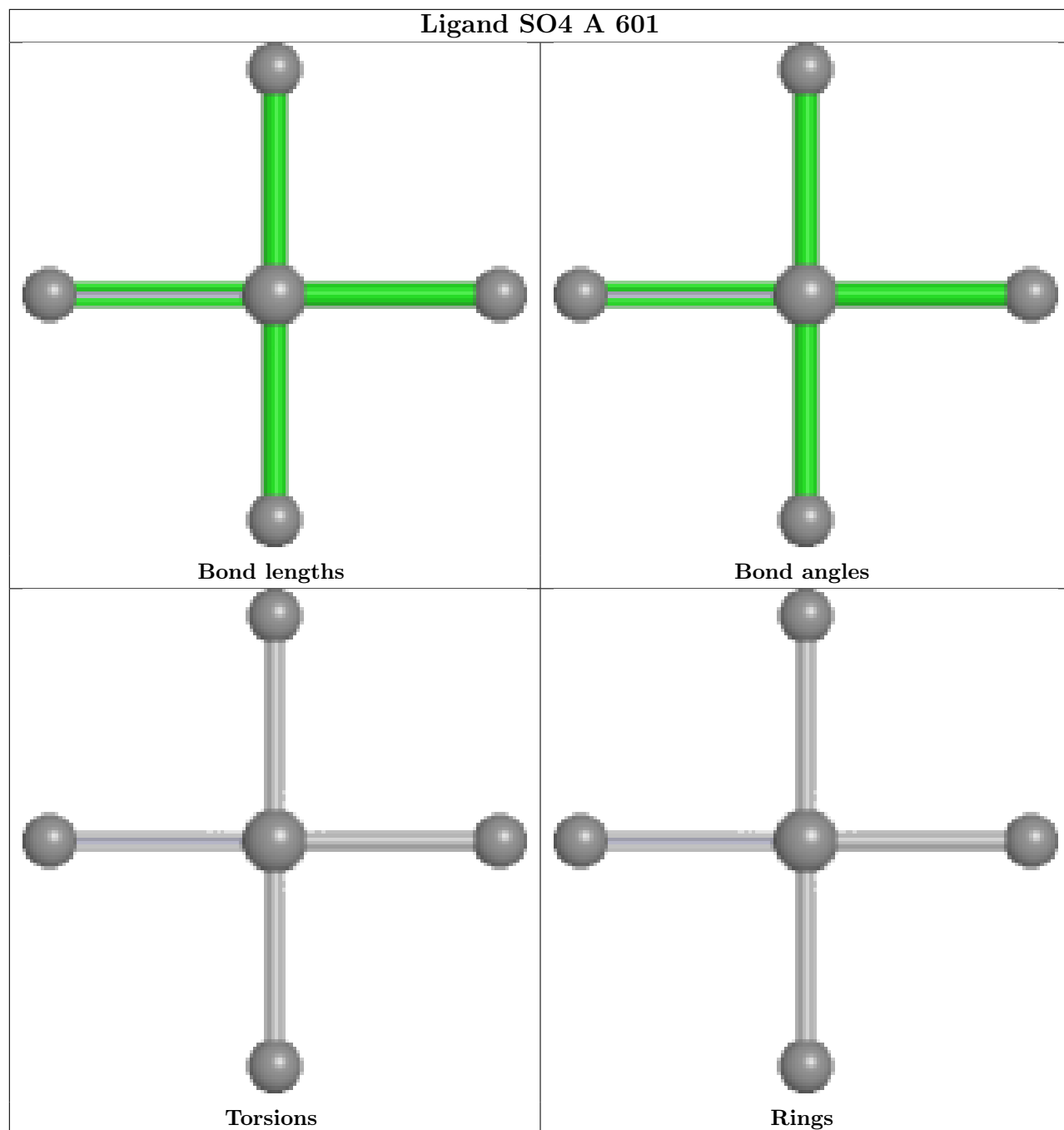
Mol	Chain	Res	Type	Atoms
27	3	1500	ANP	C5'-O5'-PA-O2A
27	3	1500	ANP	C5'-O5'-PA-O3A
27	5	801	ANP	PB-N3B-PG-O1G
27	5	801	ANP	PG-N3B-PB-O1B
27	5	801	ANP	PG-N3B-PB-O3A
27	2	1003	ANP	PA-O3A-PB-O1B

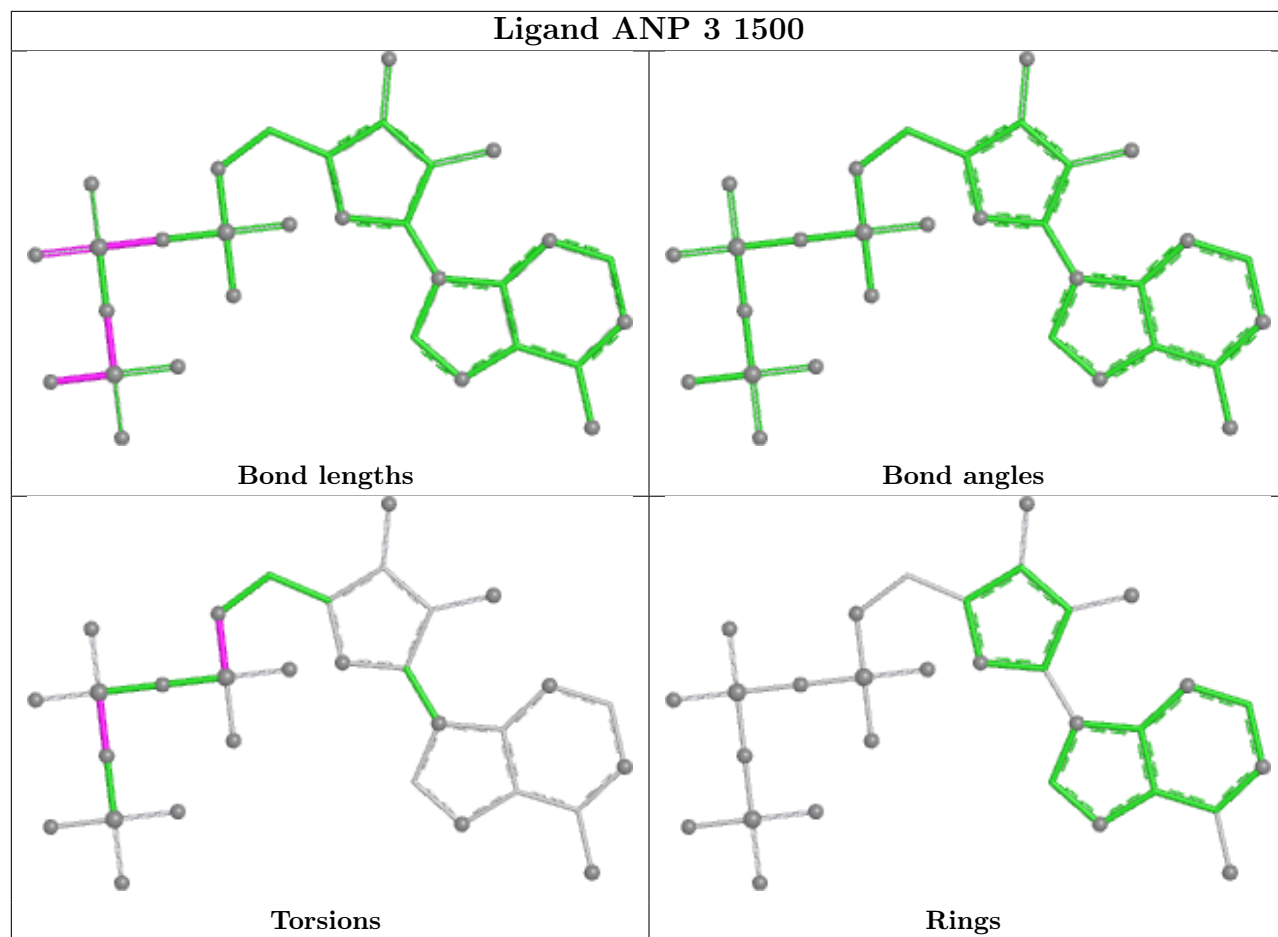
There are no ring outliers.

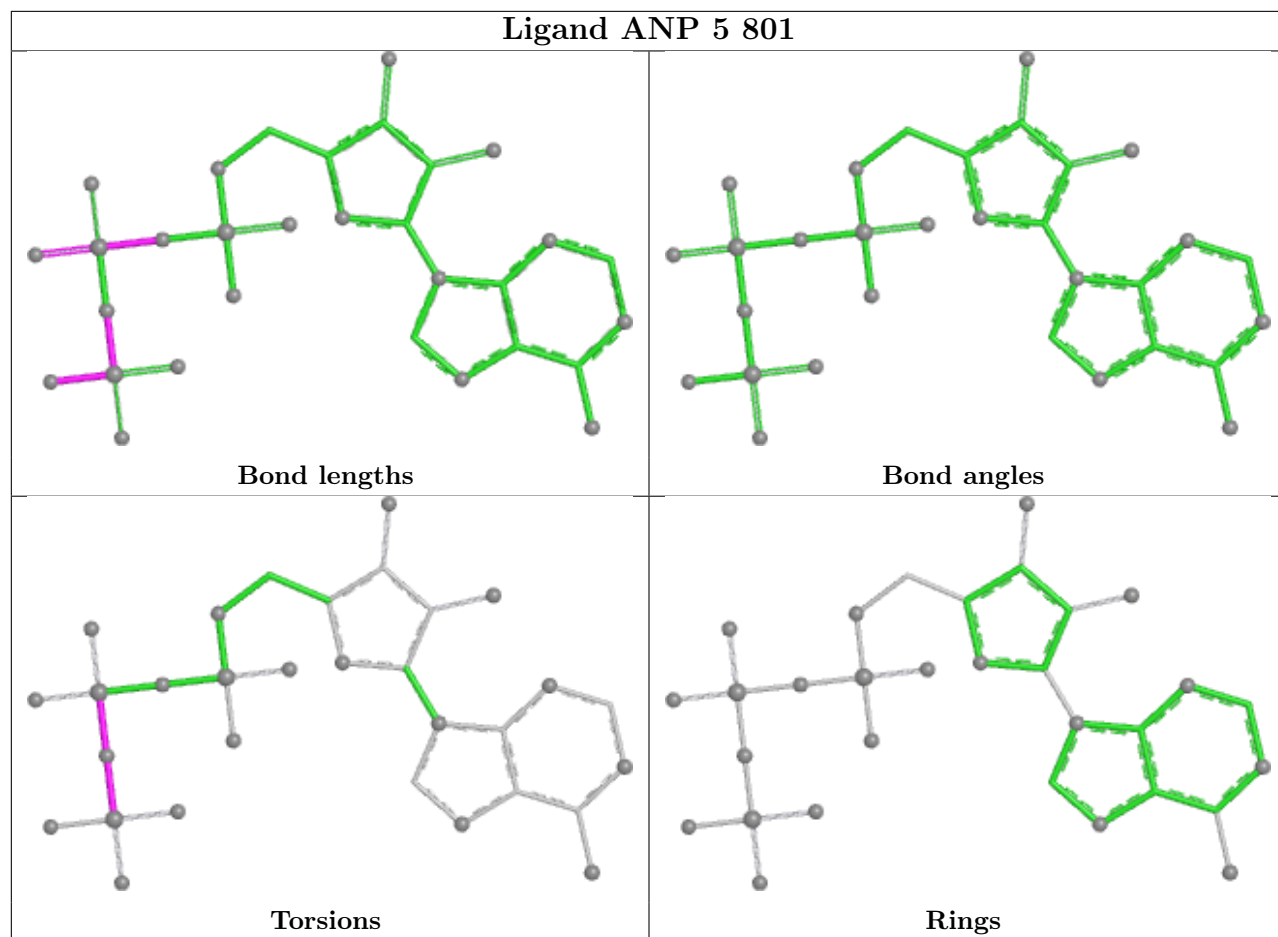
2 monomers are involved in 2 short contacts:

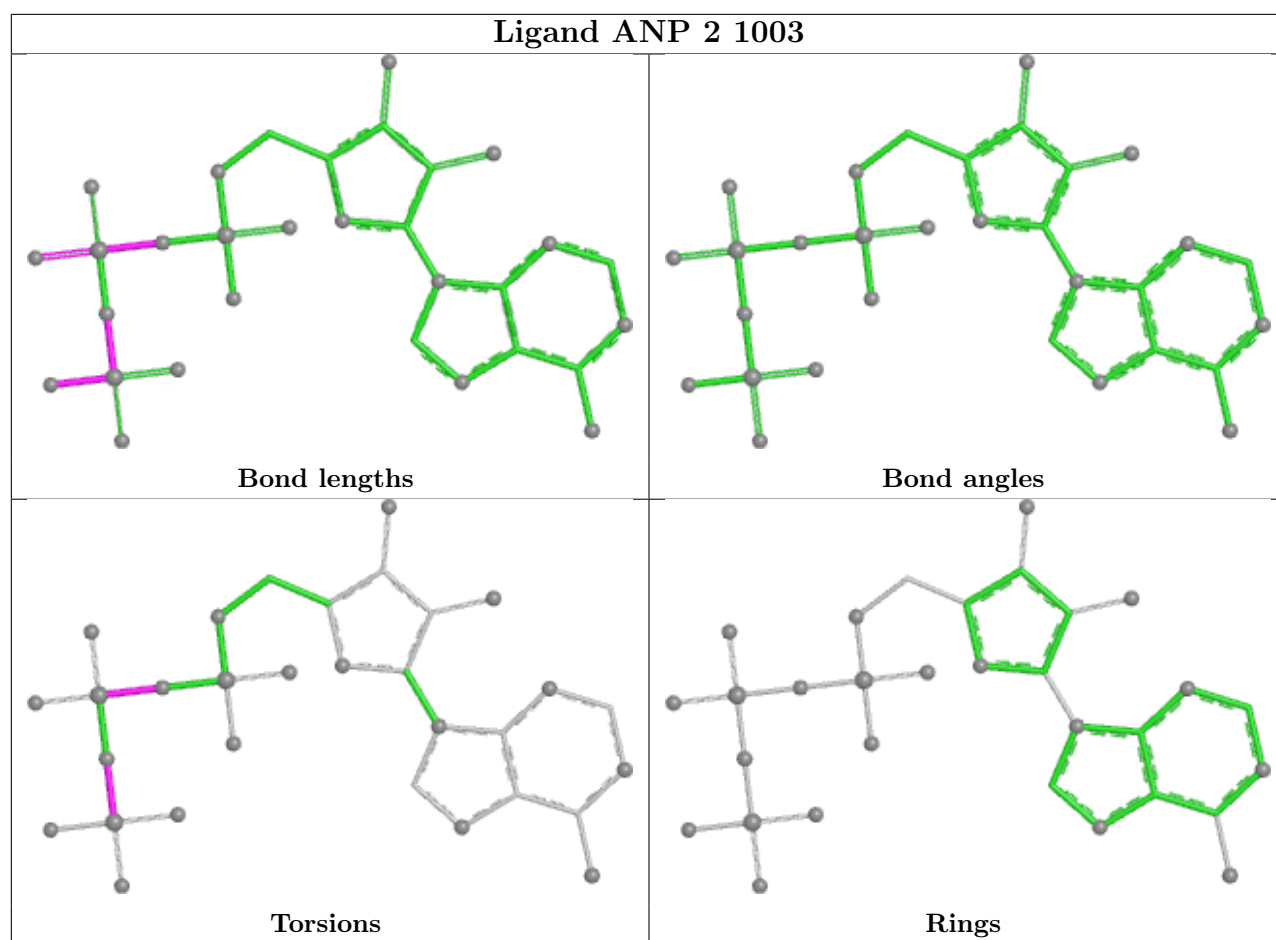
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	3	1500	ANP	1	0
27	2	1003	ANP	1	0

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.

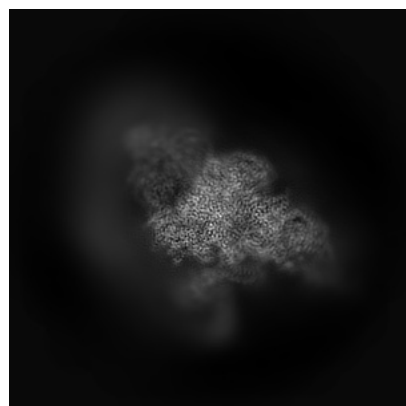
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13494. These allow visual inspection of the internal detail of the map and identification of artifacts.

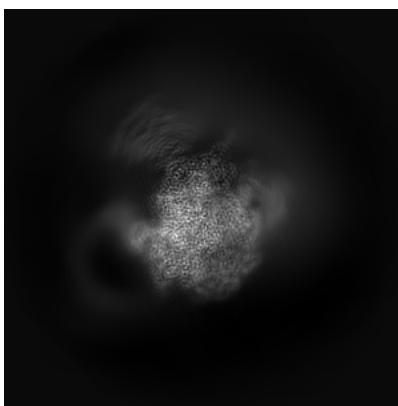
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

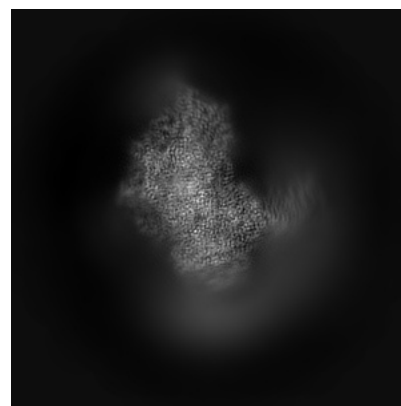
6.1.1 Primary map



X

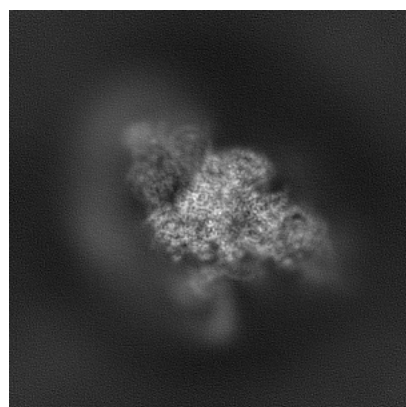


Y

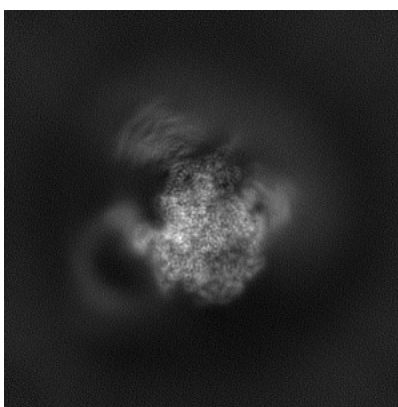


Z

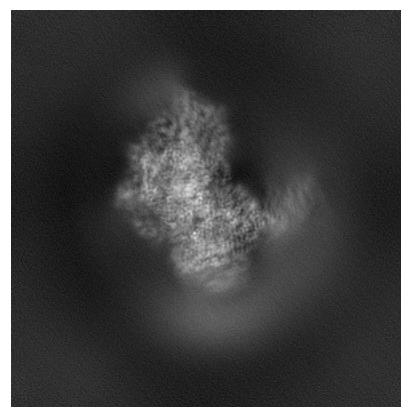
6.1.2 Raw map



X



Y

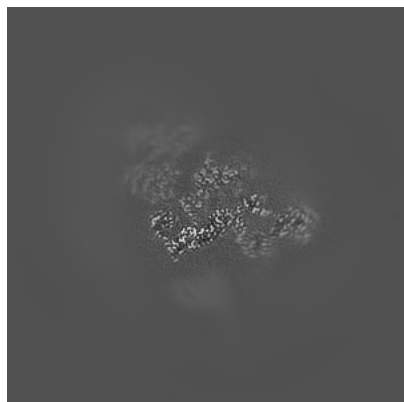


Z

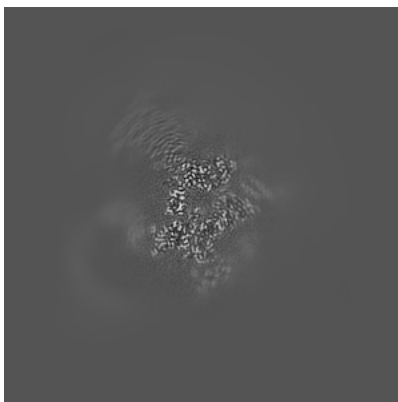
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

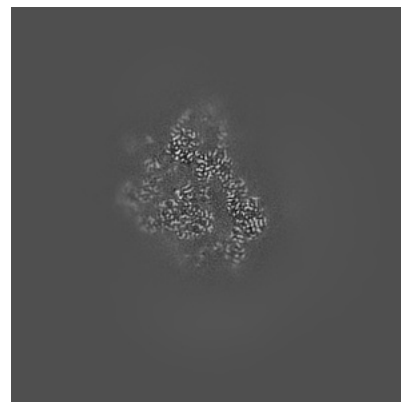
6.2.1 Primary map



X Index: 200

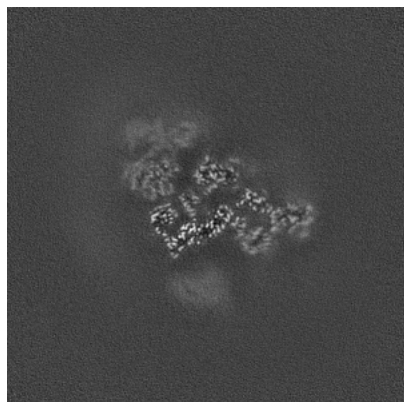


Y Index: 200

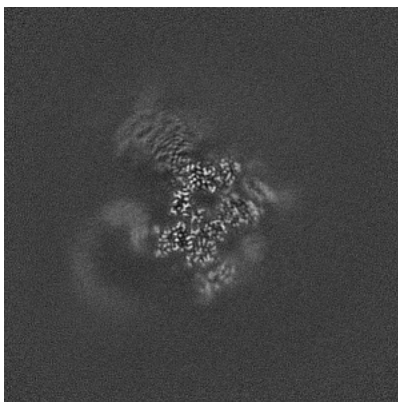


Z Index: 200

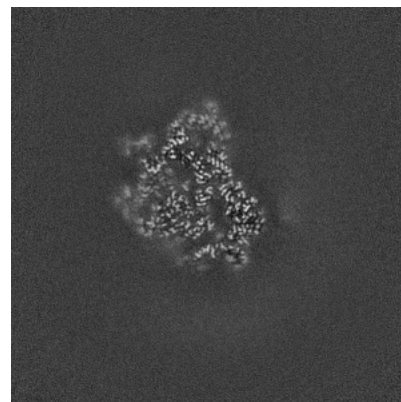
6.2.2 Raw map



X Index: 200



Y Index: 200

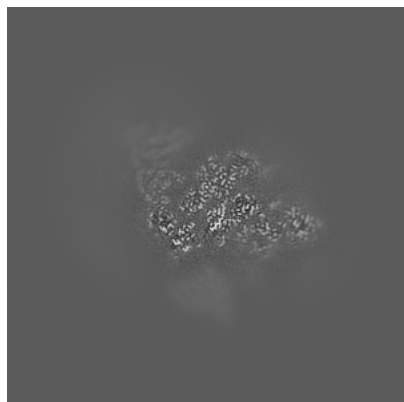


Z Index: 200

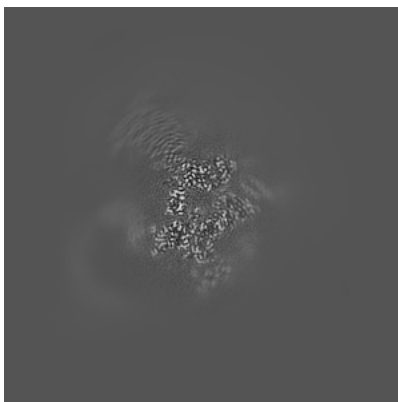
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

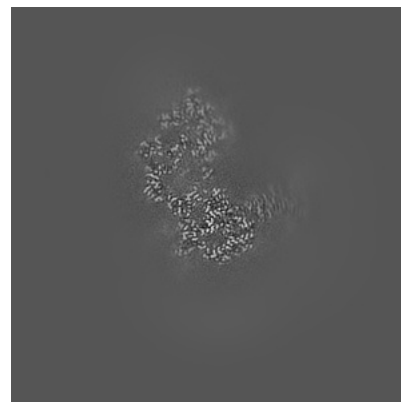
6.3.1 Primary map



X Index: 191

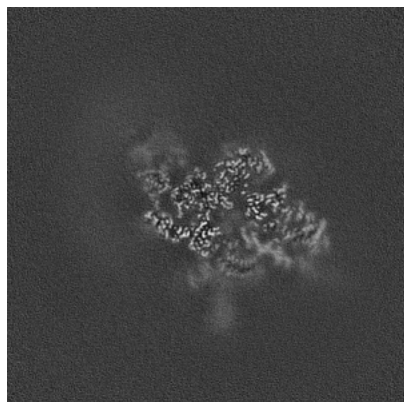


Y Index: 200

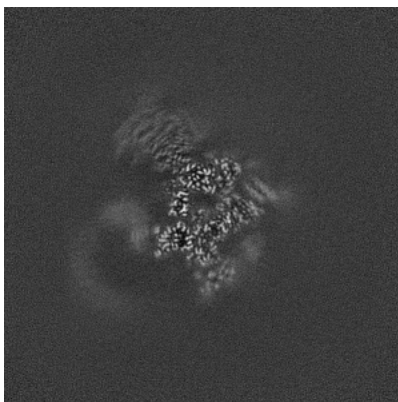


Z Index: 174

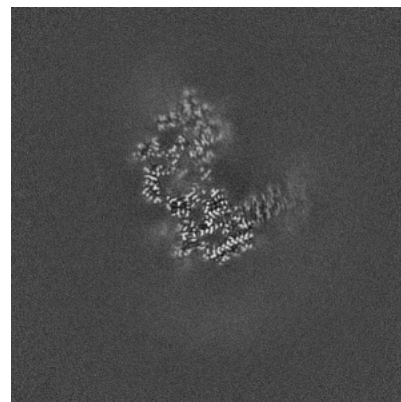
6.3.2 Raw map



X Index: 175



Y Index: 199

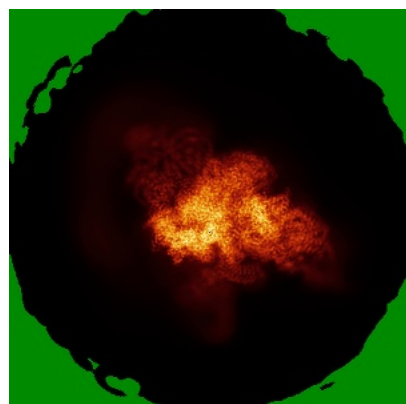


Z Index: 178

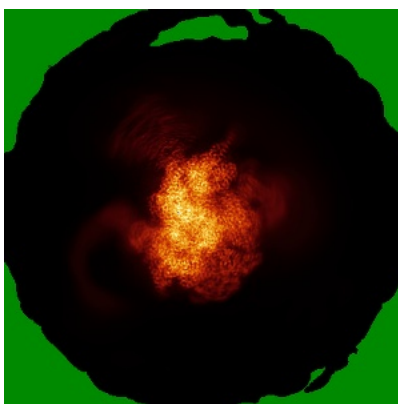
The images above show the largest variance slices of the map in three orthogonal directions.

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

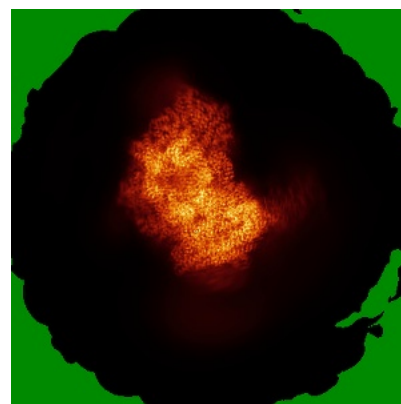
6.4.1 Primary map



X

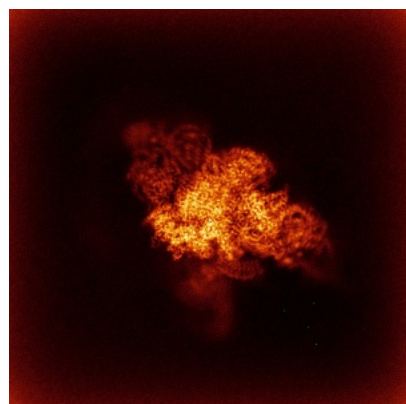


Y

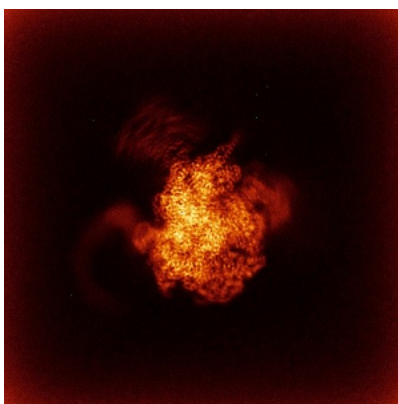


Z

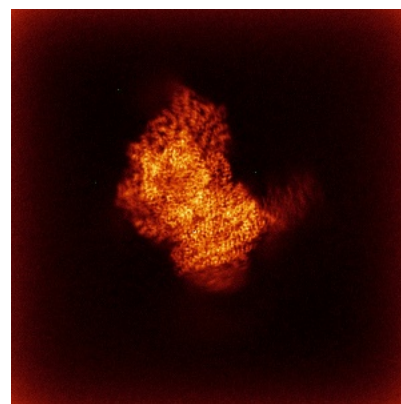
6.4.2 Raw map



X



Y

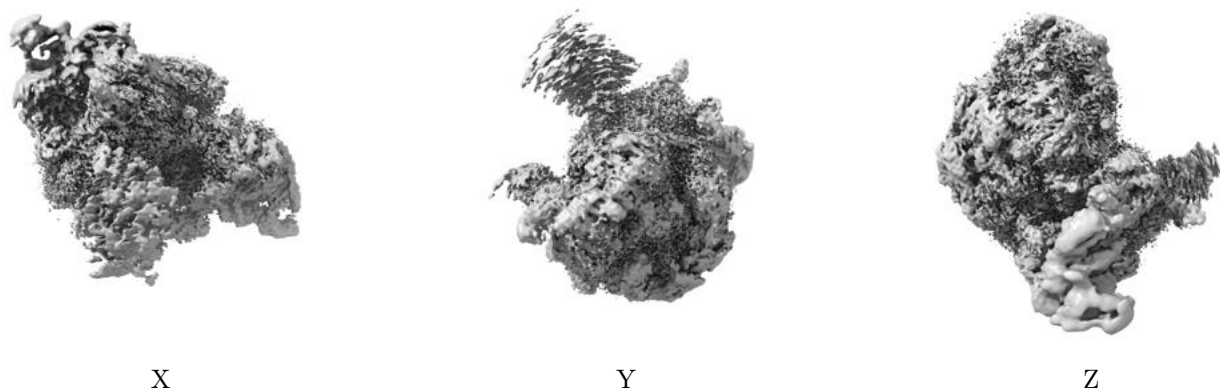


Z

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.

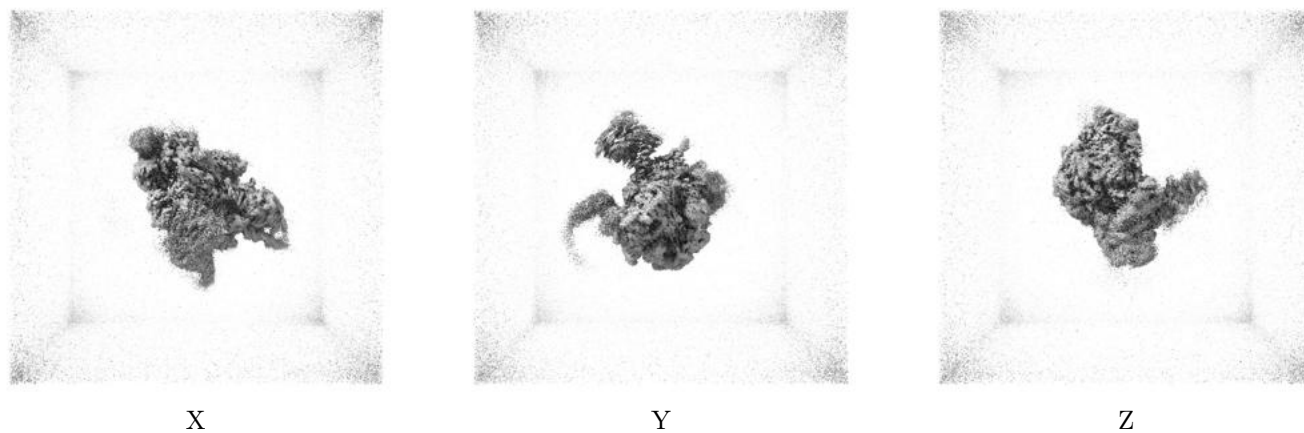
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0181. 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.

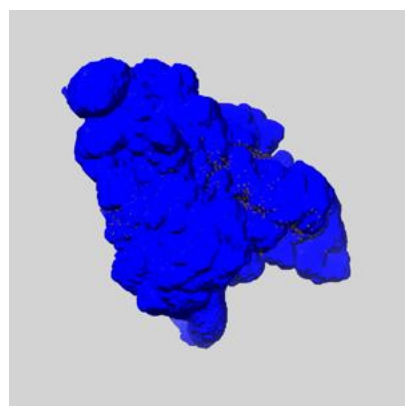
6.6 Mask visualisation [i](#)

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

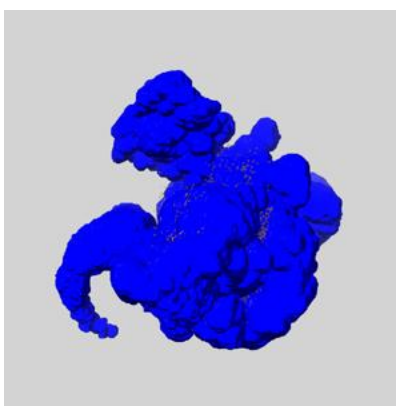
A mask typically either:

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

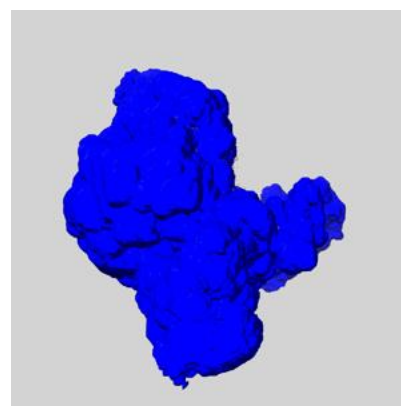
6.6.1 emd_13494_msk_1.map [i](#)



X



Y

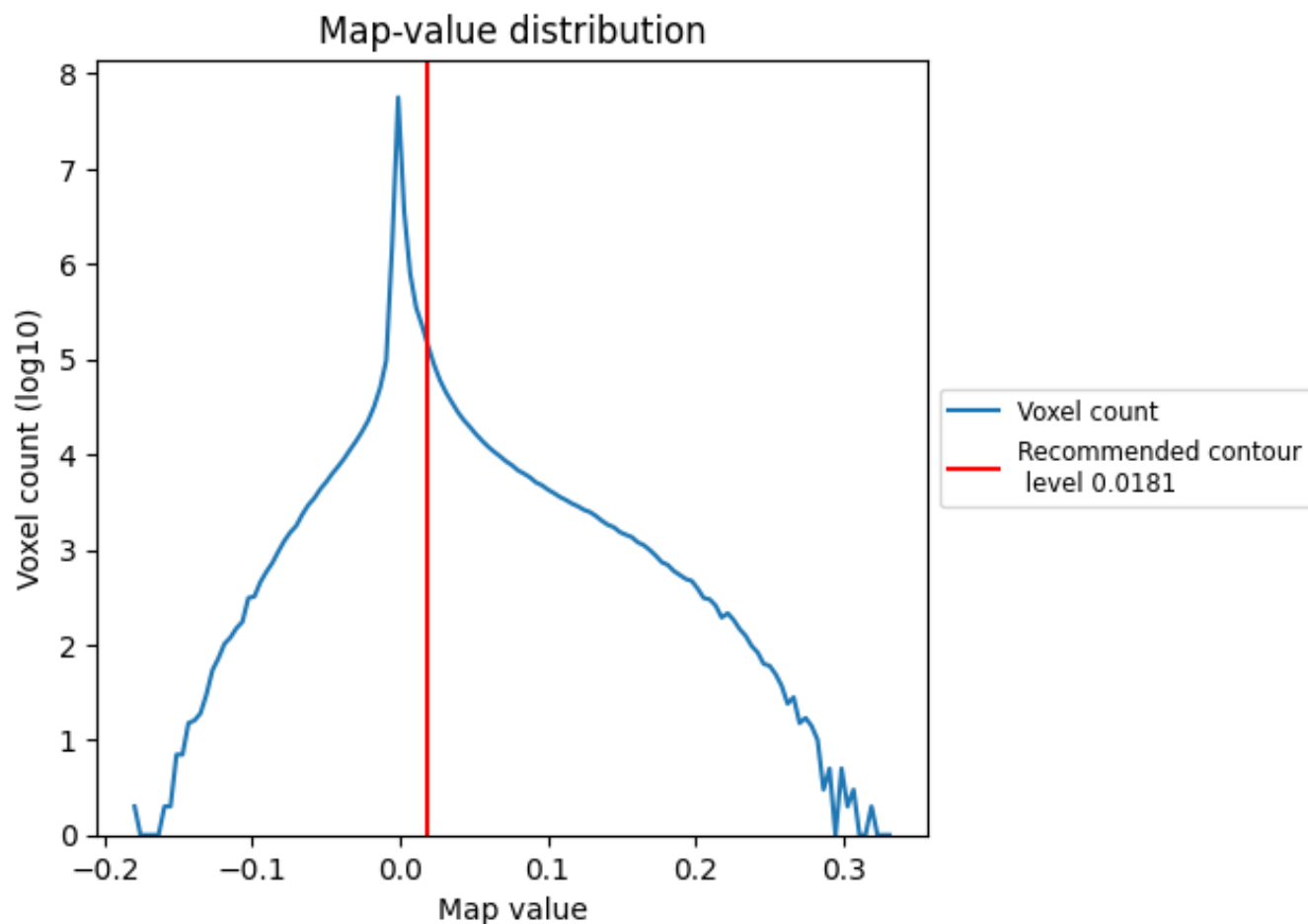


Z

7 Map analysis [i](#)

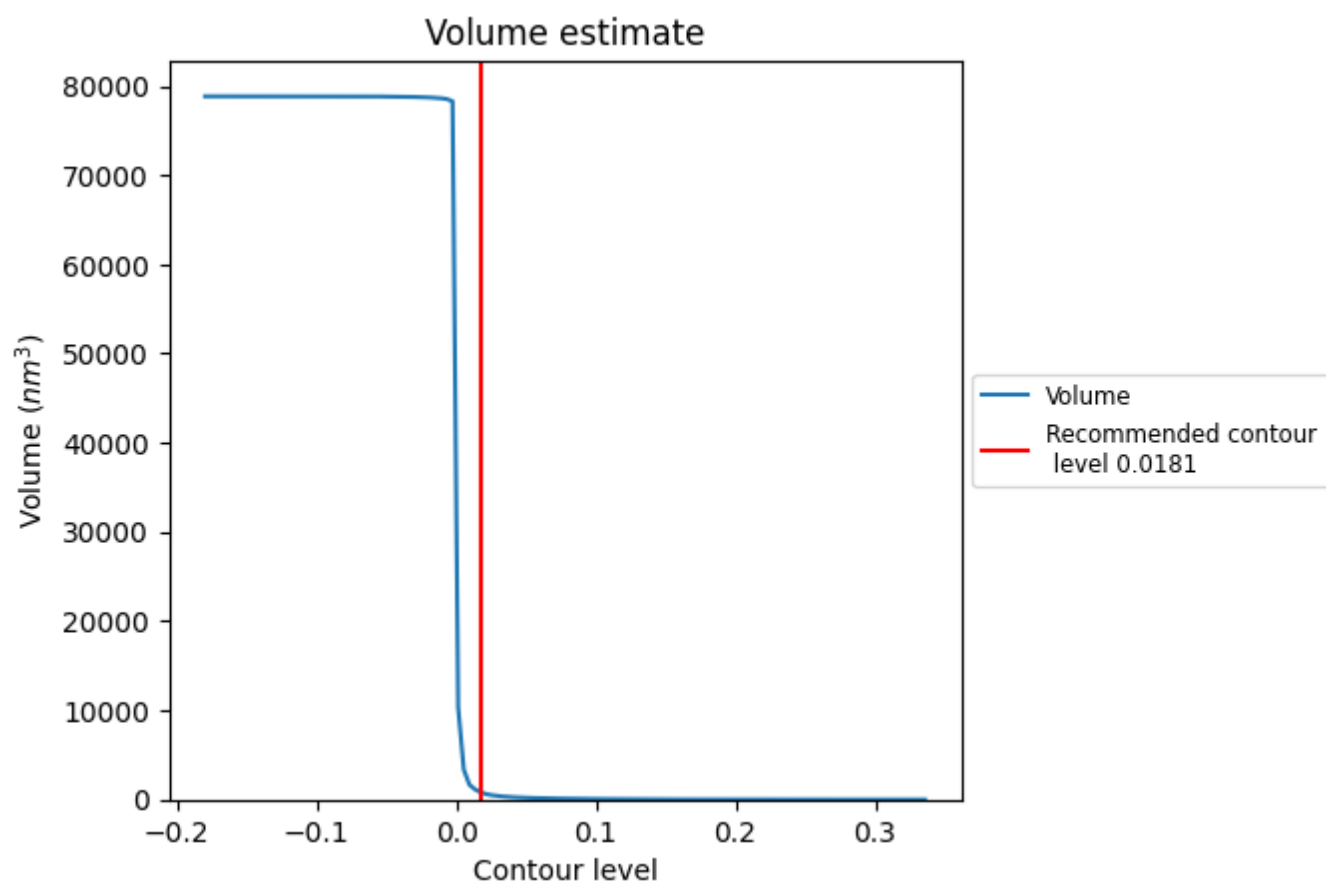
This section contains the results of statistical analysis of the map.

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.

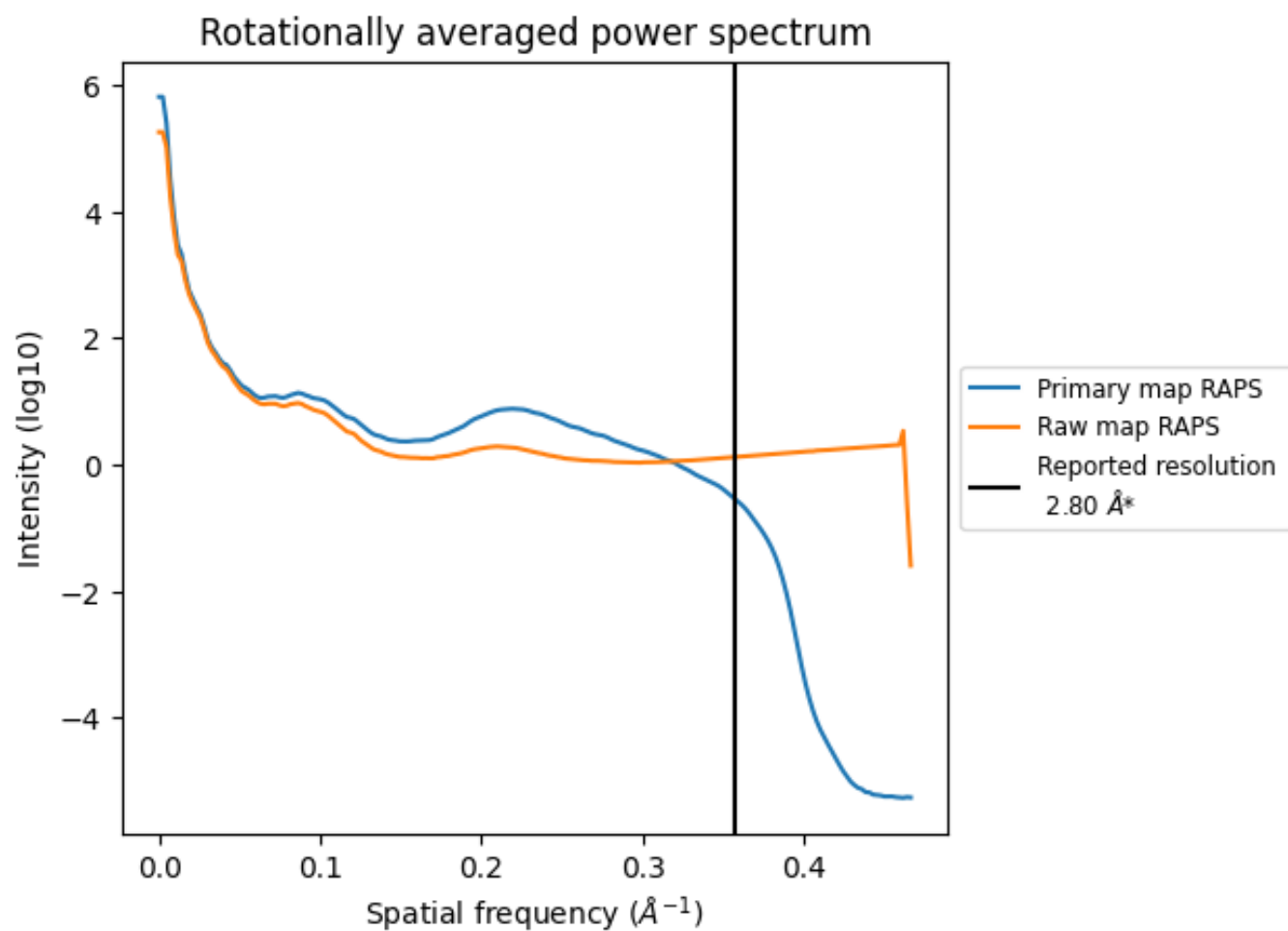
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 791 nm^3 ; this corresponds to an approximate mass of 714 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 ⓘ

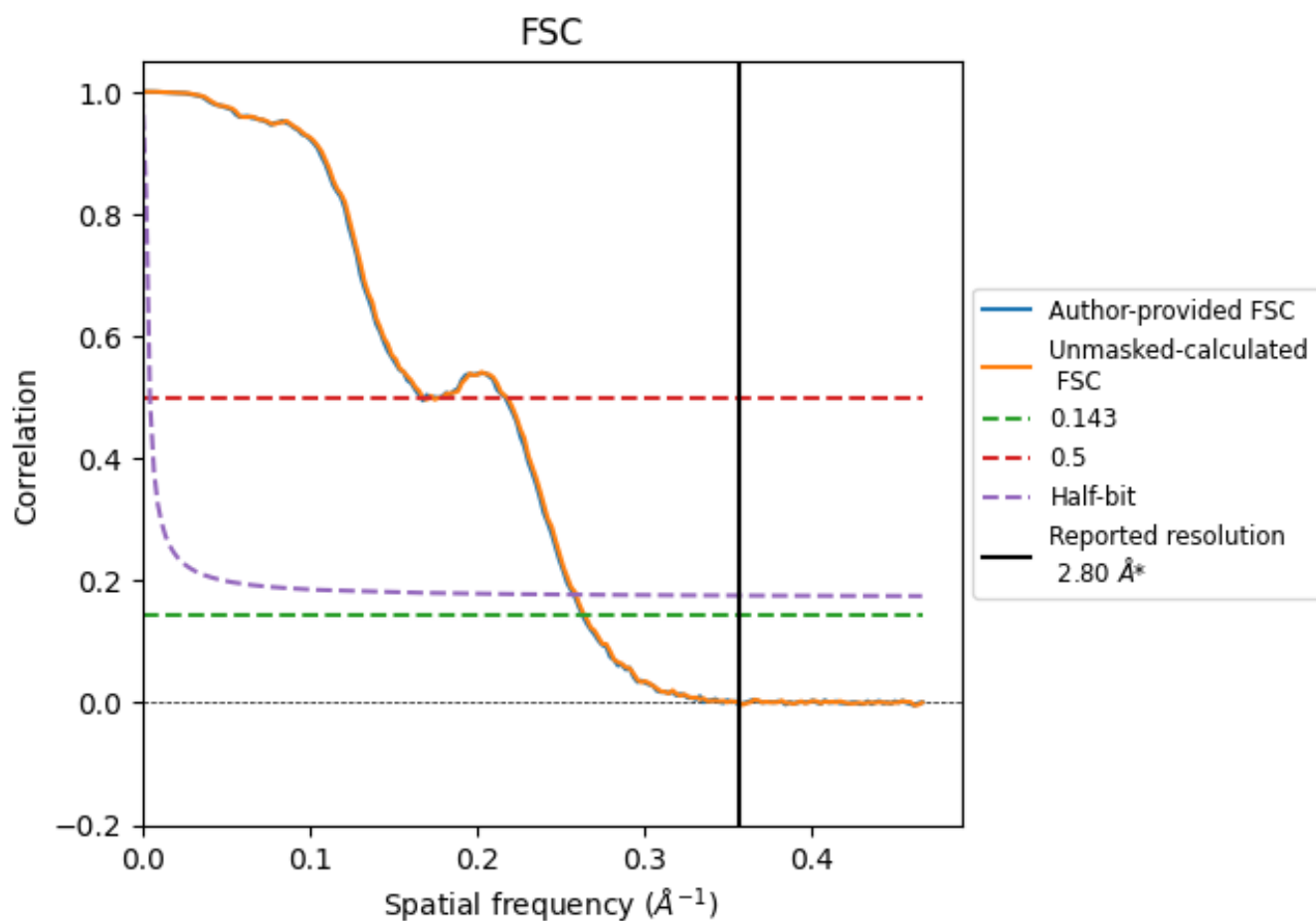


*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	3.80	6.01	3.88
Unmasked-calculated*	3.78	5.97	3.86

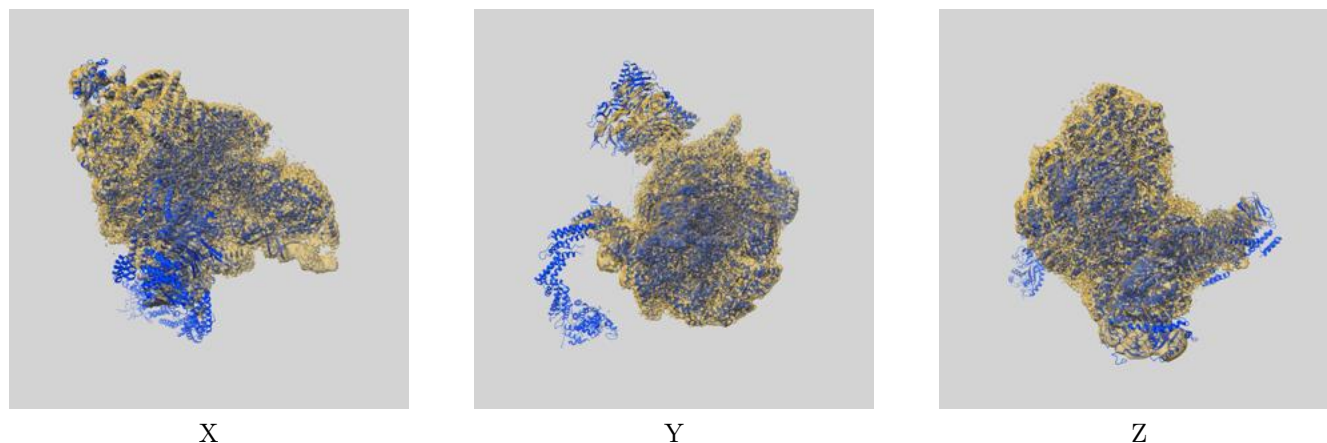
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.8 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

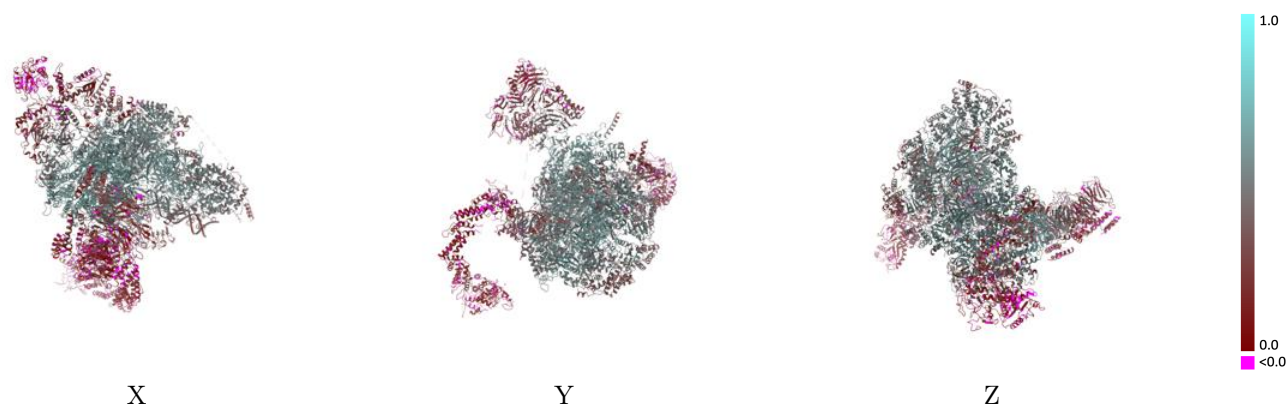
This section contains information regarding the fit between EMDB map EMD-13494 and PDB model 7PLO. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



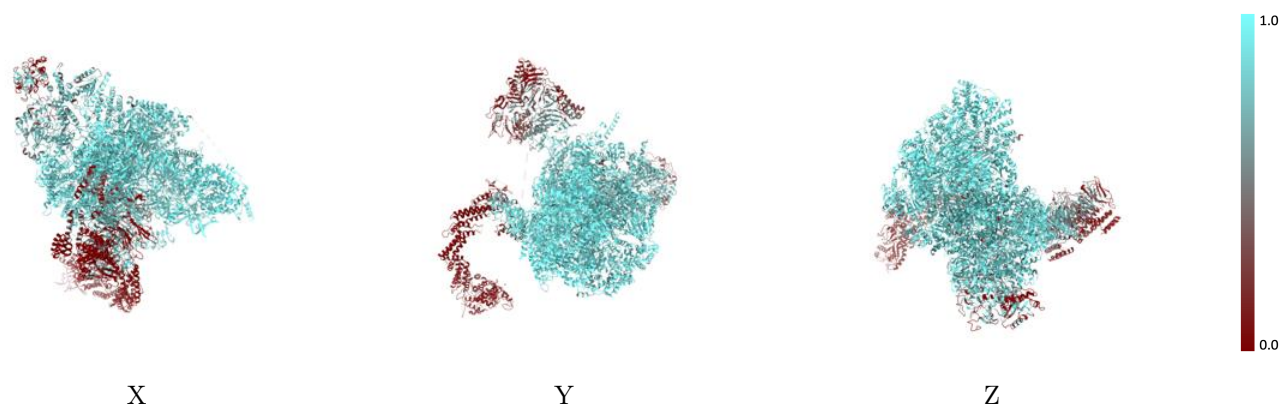
The images above show the 3D surface view of the map at the recommended contour level 0.0181 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



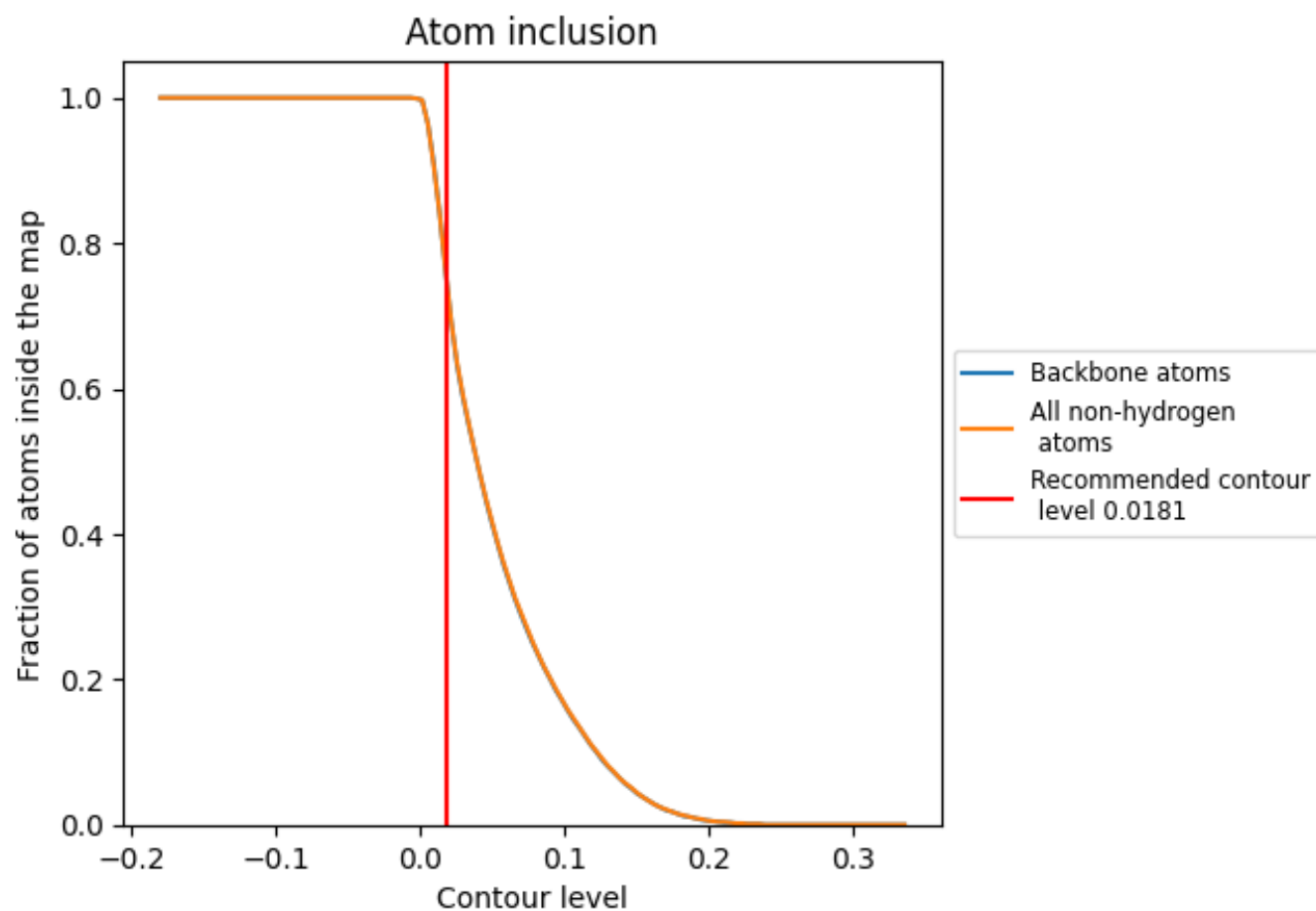
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0181).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 76% 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 (0.0181) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.4110
2	 0.9500	 0.5360
3	 0.9620	 0.5560
4	 0.9530	 0.5050
5	 0.9650	 0.5900
6	 0.9540	 0.5380
7	 0.9380	 0.4840
A	 0.7870	 0.3490
B	 0.5930	 0.1670
C	 0.9650	 0.5710
D	 0.9620	 0.5810
E	 0.9810	 0.6270
F	 0.9760	 0.6000
G	 0.9580	 0.5880
H	 0.2870	 0.2220
I	 0.4830	 0.3120
J	 0.1680	 0.1840
K	 0.9660	 0.4950
L	 0.9460	 0.4740
M	 0.9740	 0.4180
N	 0.9730	 0.3940
O	 0.9120	 0.3890
P	 0.1640	 0.0760
Q	 0.8030	 0.3700
R	 0.6160	 0.1180
S	 0.0450	 0.0700
T	 0.0000	 0.0450

