Full wwPDB EM Validation Report ⓘ

Feb 27, 2023 – 04:25 pm GMT

PDB ID	:	7Z15
EMDB ID	:	EMD-14441
Title	:	E. coli C-P lyase bound to a PhnK/PhnL dual ABC dimer and ADP + Pi
Authors	:	Amstrup, S.K.; Sofos, N.; Karlsen, J.L.; Skjerning, R.B.; Boesen, T.; Enghild, J.J.; Hove-Jensen, B.; Brodersen, D.E.
Deposited on	:	2022-02-24
Resolution	:	1.93 Å(reported)
Based on initial model	:	4XB6

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:

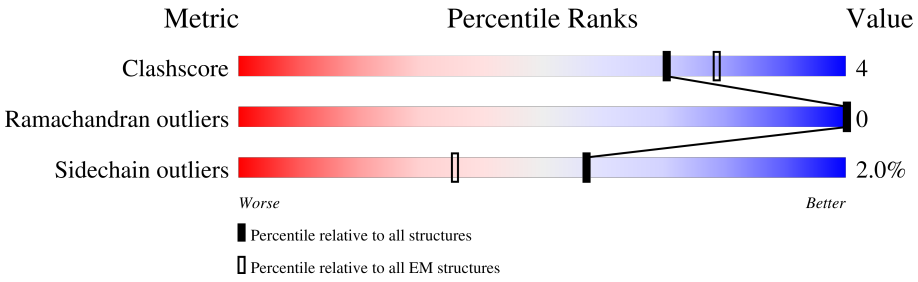
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 1.93 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.



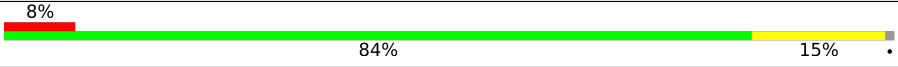
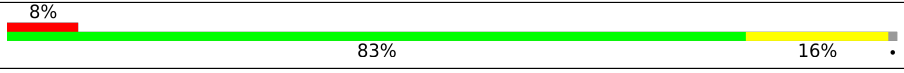
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	150	82% 13% • 5%
1	E	150	82% 13% • 5%
2	B	194	84% 15% ••
2	F	194	84% 15% ••
3	C	354	92% 8%
3	G	354	90% 10%
4	D	281	90% 9% •
4	H	281	88% 10% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	291	
5	J	291	
6	K	226	
6	L	226	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 46176 atoms, of which 22421 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 Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnG.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	143	Total	C	H	N	O	S	0	0
			2195	682	1091	209	207	6		
1	E	143	Total	C	H	N	O	S	0	0
			2195	682	1091	209	207	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	LEU	GLN	conflict	UNP P16685
E	85	LEU	GLN	conflict	UNP P16685

- Molecule 2 is a protein called Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnH.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	193	Total	C	H	N	O	S	0	0
			2961	926	1494	256	278	7		
2	F	193	Total	C	H	N	O	S	0	0
			2961	926	1494	256	278	7		

- Molecule 3 is a protein called Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnI.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	353	Total	C	H	N	O	S	0	0
			5412	1713	2679	478	531	11		
3	G	353	Total	C	H	N	O	S	0	0
			5413	1713	2680	478	531	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	264	ASP	GLY	conflict	UNP P16687
C	351	LYS	GLN	conflict	UNP P16687
G	264	ASP	GLY	conflict	UNP P16687
G	351	LYS	GLN	conflict	UNP P16687

- Molecule 4 is a protein called Alpha-D-ribose 1-methylphosphonate 5-phosphate C-P lyase.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	278	Total	C	H	N	O	S	0	0
			4365	1399	2153	378	421	14		
4	H	278	Total	C	H	N	O	S	0	0
			4365	1399	2153	378	421	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	103	LEU	VAL	conflict	UNP P16688
H	103	LEU	VAL	conflict	UNP P16688

- Molecule 5 is a protein called Putative phosphonates utilization ATP-binding protein PhnK.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	253	Total	C	H	N	O	S	0	0
			3950	1232	1985	360	368	5		
5	J	253	Total	C	H	N	O	S	0	0
			3950	1232	1985	360	368	5		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	253	GLU	-	expression tag	UNP P16678
I	254	ASN	-	expression tag	UNP P16678
I	255	LEU	-	expression tag	UNP P16678
I	256	TYR	-	expression tag	UNP P16678
I	257	PHE	-	expression tag	UNP P16678
I	258	GLN	-	expression tag	UNP P16678
I	259	GLY	-	expression tag	UNP P16678
I	260	GLN	-	expression tag	UNP P16678
I	261	PHE	-	expression tag	UNP P16678
I	262	GLY	-	expression tag	UNP P16678
I	263	SER	-	expression tag	UNP P16678
I	264	TRP	-	expression tag	UNP P16678
I	265	SER	-	expression tag	UNP P16678

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	266	HIS	-	expression tag	UNP P16678
I	267	PRO	-	expression tag	UNP P16678
I	268	GLN	-	expression tag	UNP P16678
I	269	PHE	-	expression tag	UNP P16678
I	270	GLU	-	expression tag	UNP P16678
I	271	LYS	-	expression tag	UNP P16678
I	272	GLY	-	expression tag	UNP P16678
I	273	GLY	-	expression tag	UNP P16678
I	274	GLY	-	expression tag	UNP P16678
I	275	SER	-	expression tag	UNP P16678
I	276	GLY	-	expression tag	UNP P16678
I	277	GLY	-	expression tag	UNP P16678
I	278	GLY	-	expression tag	UNP P16678
I	279	SER	-	expression tag	UNP P16678
I	280	GLY	-	expression tag	UNP P16678
I	281	GLY	-	expression tag	UNP P16678
I	282	GLY	-	expression tag	UNP P16678
I	283	SER	-	expression tag	UNP P16678
I	284	TRP	-	expression tag	UNP P16678
I	285	SER	-	expression tag	UNP P16678
I	286	HIS	-	expression tag	UNP P16678
I	287	PRO	-	expression tag	UNP P16678
I	288	GLN	-	expression tag	UNP P16678
I	289	PHE	-	expression tag	UNP P16678
I	290	GLU	-	expression tag	UNP P16678
I	291	LYS	-	expression tag	UNP P16678
J	253	GLU	-	expression tag	UNP P16678
J	254	ASN	-	expression tag	UNP P16678
J	255	LEU	-	expression tag	UNP P16678
J	256	TYR	-	expression tag	UNP P16678
J	257	PHE	-	expression tag	UNP P16678
J	258	GLN	-	expression tag	UNP P16678
J	259	GLY	-	expression tag	UNP P16678
J	260	GLN	-	expression tag	UNP P16678
J	261	PHE	-	expression tag	UNP P16678
J	262	GLY	-	expression tag	UNP P16678
J	263	SER	-	expression tag	UNP P16678
J	264	TRP	-	expression tag	UNP P16678
J	265	SER	-	expression tag	UNP P16678
J	266	HIS	-	expression tag	UNP P16678
J	267	PRO	-	expression tag	UNP P16678
J	268	GLN	-	expression tag	UNP P16678

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	269	PHE	-	expression tag	UNP P16678
J	270	GLU	-	expression tag	UNP P16678
J	271	LYS	-	expression tag	UNP P16678
J	272	GLY	-	expression tag	UNP P16678
J	273	GLY	-	expression tag	UNP P16678
J	274	GLY	-	expression tag	UNP P16678
J	275	SER	-	expression tag	UNP P16678
J	276	GLY	-	expression tag	UNP P16678
J	277	GLY	-	expression tag	UNP P16678
J	278	GLY	-	expression tag	UNP P16678
J	279	SER	-	expression tag	UNP P16678
J	280	GLY	-	expression tag	UNP P16678
J	281	GLY	-	expression tag	UNP P16678
J	282	GLY	-	expression tag	UNP P16678
J	283	SER	-	expression tag	UNP P16678
J	284	TRP	-	expression tag	UNP P16678
J	285	SER	-	expression tag	UNP P16678
J	286	HIS	-	expression tag	UNP P16678
J	287	PRO	-	expression tag	UNP P16678
J	288	GLN	-	expression tag	UNP P16678
J	289	PHE	-	expression tag	UNP P16678
J	290	GLU	-	expression tag	UNP P16678
J	291	LYS	-	expression tag	UNP P16678

- Molecule 6 is a protein called Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnL.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	224	Total	C	H	N	O	S	0	0
			3503	1090	1776	319	313	5		
6	L	224	Total	C	H	N	O	S	0	0
			3503	1090	1776	319	313	5		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

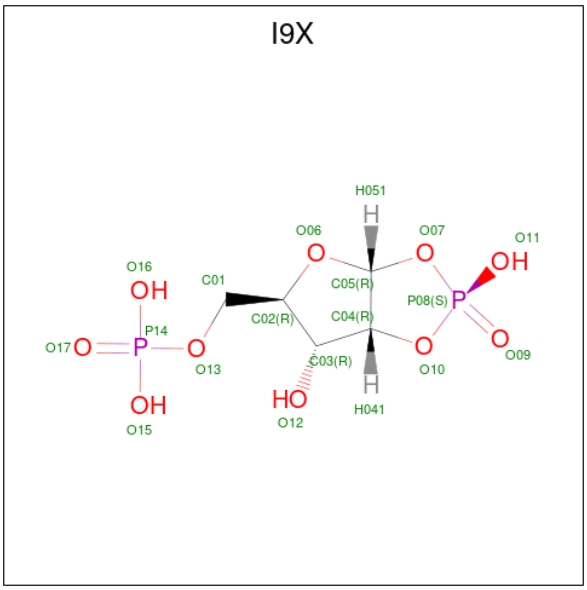
Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total	Zn	0
			1	1	
7	D	1	Total	Zn	0
			1	1	
7	G	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

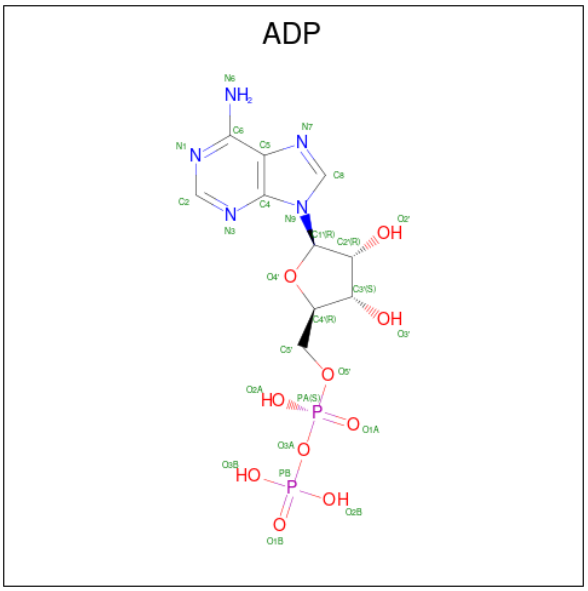
Mol	Chain	Residues	Atoms	AltConf
7	H	1	Total Zn 1 1	0

- Molecule 8 is alpha-D-ribose-1,2-cyclic-phosphate-5-phosphate (three-letter code: I9X) (formula: $C_5H_{10}O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



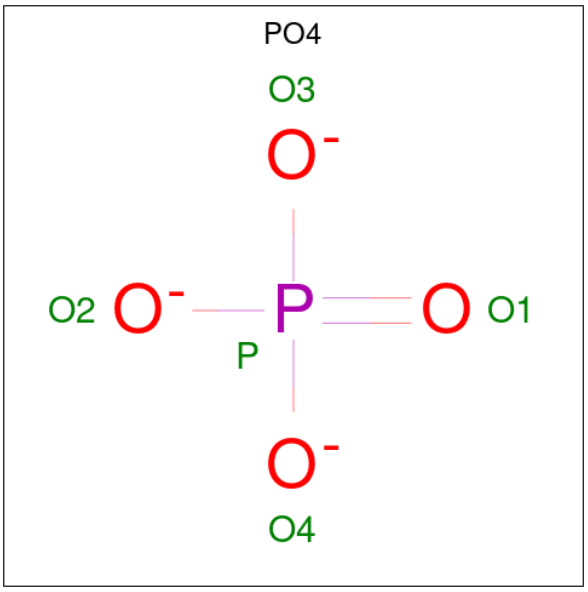
Mol	Chain	Residues	Atoms	AltConf
8	D	1	Total C H O P 25 5 8 10 2	0
8	H	1	Total C H O P 25 5 8 10 2	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
9	I	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
9	J	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	I	1	Total	O	P	0
			5	4	1	

Continued on next page...

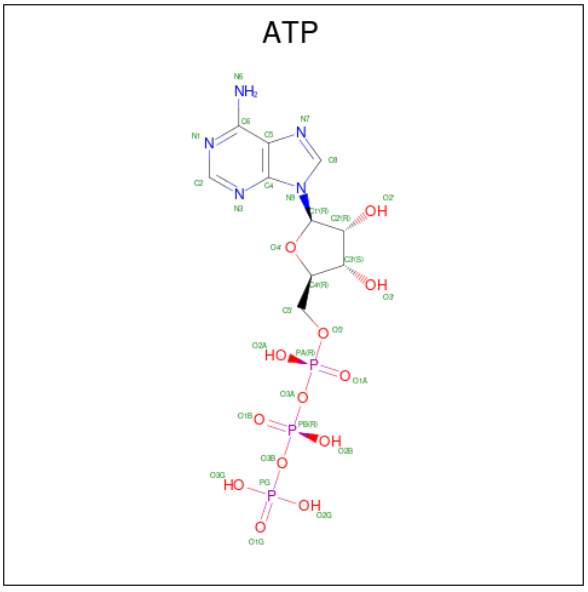
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
10	J	1	Total O P 5 4 1	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
11	I	1	Total Mg 1 1	0
11	J	1	Total Mg 1 1	0
11	K	1	Total Mg 1 1	0
11	L	1	Total Mg 1 1	0

- Molecule 12 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
12	K	1	Total C H N O P 43 10 12 5 13 3	0
12	L	1	Total C H N O P 43 10 12 5 13 3	0

- Molecule 13 is water.

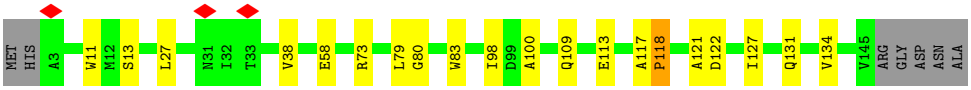
Mol	Chain	Residues	Atoms	AltConf
13	A	58	Total O 58 58	0
13	B	73	Total O 73 73	0
13	C	210	Total O 210 210	0
13	D	170	Total O 170 170	0
13	E	56	Total O 56 56	0
13	F	73	Total O 73 73	0
13	G	220	Total O 220 220	0
13	H	162	Total O 162 162	0
13	I	69	Total O 69 69	0
13	J	69	Total O 69 69	0
13	K	5	Total O 5 5	0
13	L	6	Total O 6 6	0

3 Residue-property plots (i)

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.

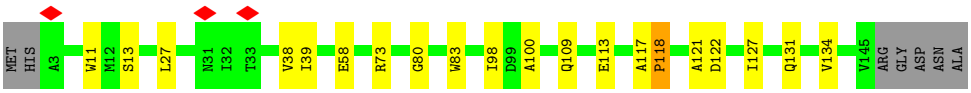
• Molecule 1: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnG

Chain A:



• Molecule 1: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnG

Chain E:

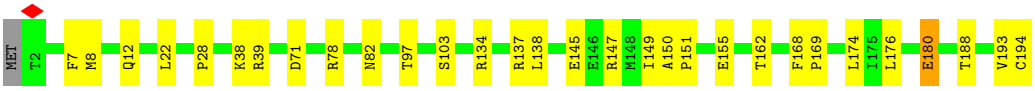


• Molecule 2: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnH

Chain B:

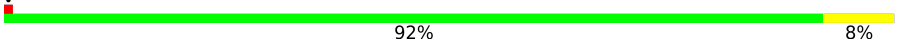
• Molecule 2: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnH

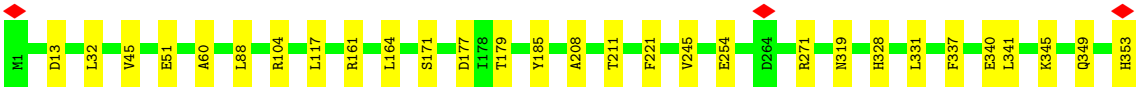
Chain F:



• Molecule 3: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnI

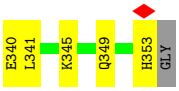
Chain C:





• Molecule 3: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnI

Chain G:

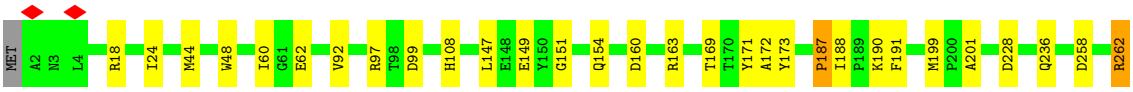


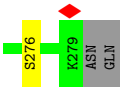
• Molecule 4: Alpha-D-ribose 1-methylphosphonate 5-phosphate C-P lyase

Chain D:

• Molecule 4: Alpha-D-ribose 1-methylphosphonate 5-phosphate C-P lyase

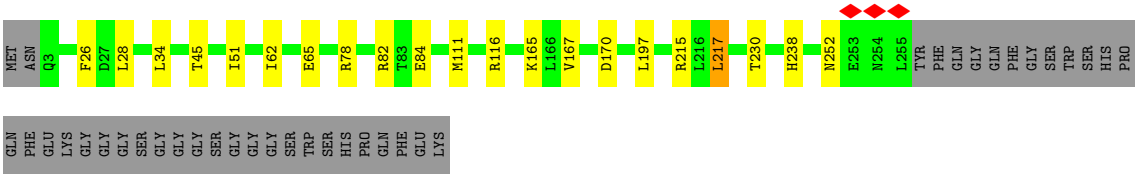
Chain H:





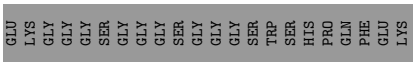
• Molecule 5: Putative phosphonates utilization ATP-binding protein PhnK

Chain I:



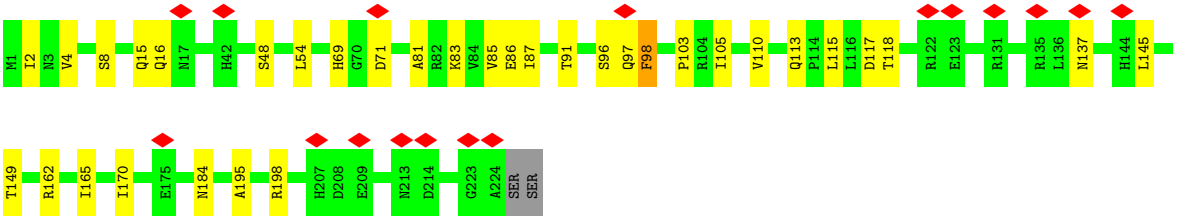
• Molecule 5: Putative phosphonates utilization ATP-binding protein PhnK

Chain J:



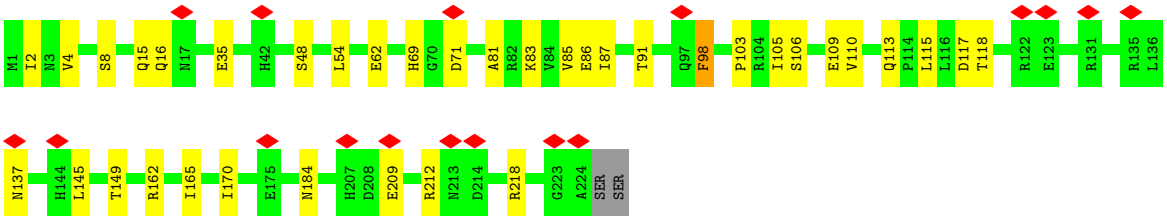
• Molecule 6: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnL

Chain K:



• Molecule 6: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnL

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	222056	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 ($e^-/Å^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	135000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.971	Depositor
Minimum map value	-1.543	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	401.136, 401.136, 401.136	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8357, 0.8357, 0.8357	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: MG, ADP, ZN, ATP, I9X, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.56	3/1120 (0.3%)	0.68	0/1516
1	E	0.56	3/1120 (0.3%)	0.68	0/1516
2	B	0.76	8/1495 (0.5%)	0.70	1/2044 (0.0%)
2	F	0.74	6/1495 (0.4%)	0.69	1/2044 (0.0%)
3	C	0.48	3/2787 (0.1%)	0.61	1/3779 (0.0%)
3	G	0.62	8/2787 (0.3%)	0.66	4/3779 (0.1%)
4	D	0.52	3/2265 (0.1%)	0.62	2/3078 (0.1%)
4	H	0.68	9/2265 (0.4%)	0.66	2/3078 (0.1%)
5	I	0.62	4/1999 (0.2%)	0.69	2/2714 (0.1%)
5	J	0.46	0/1999	0.64	2/2714 (0.1%)
6	K	0.38	0/1758	0.60	0/2391
6	L	0.35	0/1758	0.58	0/2391
All	All	0.57	47/22848 (0.2%)	0.65	15/31044 (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
4	D	0	1
4	H	0	1
All	All	0	2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	151	GLY	C-O	-13.97	1.01	1.23
4	H	151	GLY	C-O	-13.92	1.01	1.23
3	G	258	GLY	C-O	-12.66	1.03	1.23
3	G	245	VAL	C-O	-11.18	1.02	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	245	VAL	C-O	-11.16	1.02	1.23
5	I	26	PHE	C-O	-10.14	1.04	1.23
4	H	190	LYS	C-O	-10.10	1.04	1.23
2	B	97	THR	C-O	-8.89	1.06	1.23
2	F	97	THR	C-O	-8.79	1.06	1.23
2	B	151	PRO	C-O	-8.72	1.05	1.23
2	F	151	PRO	C-O	-8.66	1.05	1.23
4	H	173	TYR	C-O	-8.51	1.07	1.23
2	F	149	ILE	C-O	-7.82	1.08	1.23
2	B	149	ILE	C-O	-7.67	1.08	1.23
2	B	181	ARG	C-O	-7.64	1.08	1.23
3	G	339	ALA	C-O	-7.55	1.08	1.23
4	H	187	PRO	C-O	-7.39	1.08	1.23
4	H	149	GLU	C-O	-7.31	1.09	1.23
4	D	149	GLU	C-O	-7.25	1.09	1.23
3	G	336	ASP	C-O	-6.92	1.10	1.23
1	E	13	SER	C-O	-6.62	1.10	1.23
1	A	13	SER	C-O	-6.62	1.10	1.23
3	G	340	GLU	C-O	-6.28	1.11	1.23
4	H	172	ALA	CA-CB	-6.26	1.39	1.52
1	A	83	TRP	C-O	-6.25	1.11	1.23
3	C	340	GLU	C-O	-6.22	1.11	1.23
1	E	83	TRP	C-O	-6.19	1.11	1.23
1	A	118	PRO	C-O	-6.18	1.10	1.23
4	H	188	ILE	C-O	-6.13	1.11	1.23
1	E	118	PRO	C-O	-6.13	1.10	1.23
2	B	138	LEU	C-O	-5.85	1.12	1.23
4	H	171	TYR	C-O	-5.82	1.12	1.23
3	G	257	ASN	C-O	-5.78	1.12	1.23
2	F	138	LEU	C-O	-5.78	1.12	1.23
2	F	150	ALA	C-O	-5.72	1.12	1.23
5	I	230	THR	C-O	-5.70	1.12	1.23
3	G	164	LEU	C-O	-5.69	1.12	1.23
3	C	164	LEU	C-O	-5.62	1.12	1.23
3	G	220	PRO	C-O	-5.61	1.12	1.23
5	I	217	LEU	C-O	-5.57	1.12	1.23
5	I	28	LEU	C-O	-5.54	1.12	1.23
2	B	151	PRO	N-CA	-5.51	1.37	1.47
4	H	169	THR	C-O	-5.38	1.13	1.23
4	D	171	TYR	C-O	-5.31	1.13	1.23
2	B	150	ALA	C-O	-5.20	1.13	1.23
2	F	151	PRO	N-CA	-5.19	1.38	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	SER	CA-CB	-5.00	1.45	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	171	TYR	CB-CA-C	8.48	127.35	110.40
4	D	171	TYR	CB-CA-C	8.41	127.22	110.40
4	D	262	ARG	NE-CZ-NH1	6.69	123.64	120.30
4	H	262	ARG	NE-CZ-NH1	6.62	123.61	120.30
3	G	217	ARG	NE-CZ-NH1	6.52	123.56	120.30
5	J	82	ARG	NE-CZ-NH1	6.38	123.49	120.30
5	I	82	ARG	NE-CZ-NH1	6.24	123.42	120.30
5	J	215	ARG	NE-CZ-NH1	6.09	123.34	120.30
5	I	215	ARG	NE-CZ-NH1	6.09	123.34	120.30
3	G	220	PRO	N-CA-CB	5.70	110.14	103.30
2	B	137	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	F	137	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	G	221	PHE	CB-CA-C	-5.33	99.74	110.40
3	G	257	ASN	CB-CA-C	5.28	120.96	110.40
3	C	221	PHE	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	18	ARG	Sidechain
4	H	18	ARG	Sidechain

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	A	1104	1091	1091	12	0
1	E	1104	1091	1091	12	0
2	B	1467	1494	1494	17	0
2	F	1467	1494	1494	15	0
3	C	2733	2679	2679	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2733	2680	2679	16	0
4	D	2212	2153	2153	14	0
4	H	2212	2153	2153	14	0
5	I	1965	1985	1983	9	0
5	J	1965	1985	1983	11	0
6	K	1727	1776	1776	24	0
6	L	1727	1776	1776	25	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	D	17	8	0	0	0
8	H	17	8	0	0	0
9	I	27	12	12	1	0
9	J	27	12	12	1	0
10	I	5	0	0	0	0
10	J	5	0	0	0	0
11	I	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
12	K	31	12	12	1	0
12	L	31	12	12	1	0
13	A	58	0	0	1	0
13	B	73	0	0	2	0
13	C	210	0	0	3	0
13	D	170	0	0	4	0
13	E	56	0	0	1	0
13	F	73	0	0	2	0
13	G	220	0	0	2	0
13	H	162	0	0	4	0
13	I	69	0	0	1	0
13	J	69	0	0	1	0
13	K	5	0	0	2	0
13	L	6	0	0	2	0
All	All	23755	22421	22400	161	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 4.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:MET:HE2	2:B:150:ALA:HB2	1.71	0.71
4:D:258:ASP:OD1	3:G:161:ARG:NH2	2.23	0.71
3:C:161:ARG:NH2	4:H:258:ASP:OD1	2.24	0.71
2:F:7:PHE:O	13:F:201:HOH:O	2.12	0.68
4:D:191:PHE:O	13:D:1101:HOH:O	2.12	0.68
4:H:191:PHE:O	13:H:1101:HOH:O	2.12	0.68
3:C:13:ASP:OD1	13:C:1101:HOH:O	2.12	0.67
1:A:121:ALA:O	13:A:201:HOH:O	2.13	0.67
2:B:7:PHE:O	13:B:201:HOH:O	2.13	0.67
1:E:121:ALA:O	13:E:201:HOH:O	2.13	0.66
1:A:58:GLU:OE2	3:C:171:SER:OG	2.11	0.66
1:E:58:GLU:OE2	3:G:171:SER:OG	2.11	0.66
2:F:22:LEU:HD13	13:H:1240:HOH:O	1.96	0.65
9:J:1000:ADP:O2A	13:J:1101:HOH:O	2.15	0.65
6:K:105:ILE:O	13:K:1101:HOH:O	2.16	0.63
5:J:45:THR:OG1	5:J:170:ASP:OD2	2.17	0.62
5:J:167:VAL:HG23	5:J:197:LEU:HD11	1.80	0.62
5:I:167:VAL:HG23	5:I:197:LEU:HD11	1.81	0.62
2:B:22:LEU:HD13	13:D:1240:HOH:O	1.97	0.62
2:B:33:ALA:O	13:B:202:HOH:O	2.16	0.62
5:I:45:THR:OG1	5:I:170:ASP:OD2	2.17	0.61
6:L:48:SER:OG	12:L:1000:ATP:O1G	2.14	0.61
6:L:105:ILE:O	13:L:1101:HOH:O	2.16	0.61
6:L:103:PRO:O	13:L:1101:HOH:O	2.16	0.61
6:K:115:LEU:O	6:K:118:THR:OG1	2.18	0.60
6:K:103:PRO:O	13:K:1101:HOH:O	2.16	0.60
2:F:39:ARG:O	13:F:202:HOH:O	2.17	0.59
9:I:1000:ADP:O2A	13:I:1101:HOH:O	2.17	0.59
3:G:88:LEU:O	13:G:1101:HOH:O	2.17	0.59
6:L:110:VAL:O	6:L:162:ARG:NH1	2.35	0.59
6:K:110:VAL:O	6:K:162:ARG:NH1	2.35	0.59
6:L:115:LEU:O	6:L:118:THR:OG1	2.18	0.58
4:D:112:GLU:OE1	13:D:1102:HOH:O	2.17	0.58
5:J:65:GLU:OE2	5:J:165:LYS:NZ	2.23	0.58
3:C:88:LEU:O	13:C:1104:HOH:O	2.17	0.58
5:I:65:GLU:OE2	5:I:165:LYS:NZ	2.23	0.56
6:K:48:SER:OG	12:K:1000:ATP:O1G	2.14	0.56
6:K:113:GLN:NE2	6:K:117:ASP:OD1	2.39	0.56
3:C:208:ALA:O	3:C:211:THR:OG1	2.20	0.55
6:L:113:GLN:NE2	6:L:117:ASP:OD1	2.39	0.55
4:H:160:ASP:OD1	4:H:163:ARG:NH2	2.41	0.54
4:D:160:ASP:OD1	4:D:163:ARG:NH2	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:98:PHE:HD1	6:L:98:PHE:C	2.12	0.53
4:H:97:ARG:NH1	4:H:99:ASP:OD1	2.42	0.53
4:D:97:ARG:NH1	4:D:99:ASP:OD1	2.42	0.53
1:E:38:VAL:O	1:E:38:VAL:HG23	2.08	0.53
6:K:98:PHE:HD1	6:K:98:PHE:C	2.12	0.52
6:L:98:PHE:C	6:L:98:PHE:CD1	2.83	0.52
6:K:69:HIS:HD1	6:K:91:THR:HG1	1.57	0.52
1:A:38:VAL:O	1:A:38:VAL:HG23	2.08	0.52
1:A:58:GLU:HA	1:A:58:GLU:OE1	2.10	0.52
6:L:2:ILE:HD11	6:L:170:ILE:HG23	1.92	0.52
2:B:135:MET:CE	2:B:150:ALA:HB2	2.39	0.51
1:E:58:GLU:HA	1:E:58:GLU:OE1	2.10	0.51
3:G:208:ALA:O	3:G:211:THR:OG1	2.20	0.51
5:I:34:LEU:HD21	5:I:217:LEU:HD11	1.91	0.51
6:K:2:ILE:HD11	6:K:170:ILE:HG23	1.92	0.51
6:L:69:HIS:HD1	6:L:91:THR:HG1	1.58	0.51
2:B:134:ARG:HG2	2:B:134:ARG:HH11	1.75	0.51
3:G:337:PHE:CE2	3:G:341:LEU:HD11	2.46	0.51
6:K:98:PHE:C	6:K:98:PHE:CD1	2.83	0.51
2:F:134:ARG:HG2	2:F:134:ARG:HH11	1.75	0.50
3:G:82:ARG:NH2	13:H:1106:HOH:O	2.41	0.50
5:J:252:ASN:O	6:K:98:PHE:HE2	1.95	0.50
3:C:337:PHE:CE2	3:C:341:LEU:HD11	2.46	0.49
4:H:228:ASP:OD1	5:J:116:ARG:NE	2.41	0.49
6:L:162:ARG:O	6:L:165:ILE:HG22	2.13	0.49
4:H:199:MET:HG2	4:H:201:ALA:H	1.78	0.48
2:B:174:LEU:HD21	2:B:176:LEU:HD21	1.95	0.48
4:D:199:MET:HG2	4:D:201:ALA:H	1.78	0.48
4:D:147:LEU:HD13	5:I:78:ARG:HG3	1.95	0.48
5:J:34:LEU:HD11	5:J:217:LEU:HG	1.94	0.48
2:F:162:THR:HG21	2:F:193:VAL:HG23	1.94	0.48
6:K:162:ARG:O	6:K:165:ILE:HG22	2.13	0.48
1:E:134:VAL:CG1	3:G:117:LEU:HD21	2.44	0.48
1:E:127:ILE:O	1:E:131:GLN:HG2	2.14	0.48
5:I:252:ASN:O	6:L:98:PHE:HE2	1.95	0.48
3:C:185:TYR:OH	13:C:1102:HOH:O	2.16	0.47
2:F:174:LEU:HD21	2:F:176:LEU:HD21	1.95	0.47
4:H:154:GLN:HB3	5:J:111:MET:HE3	1.96	0.47
4:D:154:GLN:HB3	5:I:111:MET:HE3	1.95	0.47
3:G:177:ASP:OD1	3:G:179:THR:OG1	2.25	0.47
1:A:134:VAL:CG1	3:C:117:LEU:HD21	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:O	1:A:131:GLN:HG2	2.14	0.47
2:B:162:THR:HG21	2:B:193:VAL:HG23	1.96	0.46
6:K:149:THR:HG21	6:L:15:GLN:HB3	1.97	0.46
4:D:228:ASP:OD1	5:I:116:ARG:NE	2.42	0.46
1:E:117:ALA:HB3	1:E:118:PRO:HD3	1.97	0.46
4:H:147:LEU:HD13	5:J:78:ARG:HG3	1.96	0.46
2:F:82:ASN:O	2:F:82:ASN:OD1	2.34	0.46
6:L:81:ALA:O	6:L:85:VAL:HG23	2.16	0.46
6:K:4:VAL:HG21	6:K:54:LEU:HD11	1.98	0.46
2:B:12:GLN:HG3	4:D:62:GLU:OE2	2.16	0.46
4:D:44:MET:N	4:D:44:MET:SD	2.89	0.46
1:E:27:LEU:HD13	1:E:98:ILE:HD11	1.99	0.45
4:H:44:MET:N	4:H:44:MET:SD	2.89	0.45
5:J:51:ILE:HA	5:J:62:ILE:HD13	1.99	0.45
1:A:117:ALA:HB3	1:A:118:PRO:HD3	1.97	0.45
2:B:82:ASN:O	2:B:82:ASN:OD1	2.34	0.45
3:G:51:GLU:OE1	3:G:319:ASN:ND2	2.50	0.45
4:H:60:ILE:HD11	4:H:92:VAL:HG21	1.98	0.45
6:L:4:VAL:HG21	6:L:54:LEU:HD11	1.98	0.45
2:B:134:ARG:NH2	2:B:193:VAL:HG11	2.32	0.45
2:B:135:MET:SD	2:B:148:MET:HB3	2.57	0.45
3:C:51:GLU:OE1	3:C:319:ASN:ND2	2.50	0.45
2:F:168:PHE:CG	2:F:169:PRO:HA	2.52	0.45
5:I:51:ILE:HA	5:I:62:ILE:HD13	1.99	0.45
1:A:27:LEU:HD13	1:A:98:ILE:HD11	1.99	0.45
4:D:24:ILE:HG22	13:D:1240:HOH:O	2.16	0.45
5:J:34:LEU:HD21	5:J:217:LEU:HD11	2.00	0.44
6:K:15:GLN:HB3	6:L:149:THR:HG21	1.98	0.44
4:H:108:HIS:CD2	4:H:187:PRO:HB2	2.53	0.44
2:B:168:PHE:CG	2:B:169:PRO:HA	2.52	0.44
2:B:180:GLU:H	2:B:180:GLU:CD	2.21	0.44
3:C:254:GLU:OE1	3:C:271:ARG:NH2	2.46	0.44
1:A:109:GLN:O	1:A:113:GLU:HG3	2.18	0.43
4:D:60:ILE:HD11	4:D:92:VAL:HG21	1.98	0.43
1:E:109:GLN:O	1:E:113:GLU:HG3	2.18	0.43
6:K:16:GLN:O	6:K:16:GLN:HG3	2.19	0.43
6:L:209:GLU:OE1	6:L:212:ARG:NH1	2.51	0.43
1:A:134:VAL:HG12	3:C:117:LEU:HD11	1.99	0.43
1:E:134:VAL:HG12	3:G:117:LEU:HD11	1.99	0.43
3:G:254:GLU:OE1	3:G:271:ARG:NH2	2.46	0.43
6:L:137:ASN:ND2	6:L:184:ASN:OD1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:GLN:HG3	4:H:62:GLU:OE2	2.18	0.43
6:L:87:ILE:O	6:L:91:THR:N	2.47	0.43
2:B:162:THR:HG21	2:B:193:VAL:CG2	2.48	0.43
4:H:24:ILE:HG22	13:H:1240:HOH:O	2.19	0.43
6:L:16:GLN:O	6:L:16:GLN:HG3	2.19	0.43
2:F:180:GLU:H	2:F:180:GLU:CD	2.21	0.43
3:G:185:TYR:OH	13:G:1102:HOH:O	2.21	0.43
6:K:137:ASN:ND2	6:K:184:ASN:OD1	2.48	0.43
3:C:45:VAL:HG13	3:C:60:ALA:HB3	2.01	0.42
3:G:45:VAL:HG13	3:G:60:ALA:HB3	2.01	0.42
6:K:16:GLN:HB2	6:L:145:LEU:HD13	2.01	0.42
2:F:28:PRO:O	2:F:147:ARG:NH2	2.49	0.42
6:L:35:GLU:OE2	6:L:218:ARG:NH2	2.51	0.42
3:G:341:LEU:O	3:G:345:LYS:HG3	2.20	0.42
2:F:162:THR:HG21	2:F:193:VAL:CG2	2.50	0.42
3:C:177:ASP:OD1	3:C:179:THR:OG1	2.25	0.41
6:L:106:SER:OG	6:L:109:GLU:OE2	2.34	0.41
2:F:145:GLU:HA	2:F:145:GLU:OE1	2.21	0.41
2:F:168:PHE:CD1	2:F:169:PRO:HA	2.55	0.41
1:E:80:GLY:HA3	1:E:100:ALA:HB2	2.03	0.41
6:K:81:ALA:O	6:K:85:VAL:HG23	2.19	0.41
6:K:96:SER:OG	6:K:97:GLN:N	2.53	0.41
2:B:168:PHE:CE1	2:B:188:THR:HG22	2.55	0.41
3:C:331:LEU:HD21	4:D:48:TRP:CE3	2.56	0.41
3:C:341:LEU:O	3:C:345:LYS:HG3	2.20	0.41
6:K:87:ILE:O	6:K:91:THR:N	2.47	0.41
2:F:168:PHE:CE1	2:F:188:THR:HG22	2.55	0.41
3:C:32:LEU:HD22	3:G:32:LEU:CD2	2.51	0.41
1:A:73:ARG:HG3	1:A:79:LEU:HD23	2.03	0.40
2:B:145:GLU:HA	2:B:145:GLU:OE1	2.21	0.40
6:K:145:LEU:HD13	6:L:16:GLN:CB	2.51	0.40
6:K:145:LEU:HD13	6:L:16:GLN:HB2	2.02	0.40
3:G:331:LEU:HD21	4:H:48:TRP:CE3	2.56	0.40
5:J:36:ILE:HB	5:J:202:VAL:HG22	2.03	0.40
6:K:195:ALA:O	6:K:198:ARG:HG2	2.22	0.40
1:A:80:GLY:HA3	1:A:100:ALA:HB2	2.03	0.40
1:E:39:ILE:HD11	1:E:73:ARG:CZ	2.52	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	A	141/150 (94%)	139 (99%)	2 (1%)	0	100	100
1	E	141/150 (94%)	139 (99%)	2 (1%)	0	100	100
2	B	191/194 (98%)	188 (98%)	3 (2%)	0	100	100
2	F	191/194 (98%)	188 (98%)	3 (2%)	0	100	100
3	C	351/354 (99%)	347 (99%)	4 (1%)	0	100	100
3	G	351/354 (99%)	348 (99%)	3 (1%)	0	100	100
4	D	276/281 (98%)	268 (97%)	8 (3%)	0	100	100
4	H	276/281 (98%)	267 (97%)	9 (3%)	0	100	100
5	I	251/291 (86%)	250 (100%)	1 (0%)	0	100	100
5	J	251/291 (86%)	250 (100%)	1 (0%)	0	100	100
6	K	222/226 (98%)	217 (98%)	5 (2%)	0	100	100
6	L	222/226 (98%)	218 (98%)	4 (2%)	0	100	100
All	All	2864/2992 (96%)	2819 (98%)	45 (2%)	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	A	110/115 (96%)	108 (98%)	2 (2%)	59	47
1	E	110/115 (96%)	108 (98%)	2 (2%)	59	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	163/164 (99%)	156 (96%)	7 (4%)	29 14
2	F	163/164 (99%)	155 (95%)	8 (5%)	25 10
3	C	286/286 (100%)	282 (99%)	4 (1%)	67 58
3	G	286/286 (100%)	282 (99%)	4 (1%)	67 58
4	D	241/244 (99%)	238 (99%)	3 (1%)	71 64
4	H	241/244 (99%)	238 (99%)	3 (1%)	71 64
5	I	214/242 (88%)	212 (99%)	2 (1%)	78 75
5	J	214/242 (88%)	212 (99%)	2 (1%)	78 75
6	K	186/188 (99%)	181 (97%)	5 (3%)	44 31
6	L	186/188 (99%)	180 (97%)	6 (3%)	39 25
All	All	2400/2478 (97%)	2352 (98%)	48 (2%)	57 42

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TRP
1	A	122	ASP
2	B	8	MET
2	B	38	LYS
2	B	71	ASP
2	B	78	ARG
2	B	103	SER
2	B	155	GLU
2	B	180	GLU
3	C	104	ARG
3	C	328	HIS
3	C	349	GLN
3	C	353	HIS
4	D	236	GLN
4	D	262	ARG
4	D	276	SER
1	E	11	TRP
1	E	122	ASP
2	F	8	MET
2	F	38	LYS
2	F	71	ASP
2	F	78	ARG
2	F	103	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	155	GLU
2	F	180	GLU
2	F	194	CYS
3	G	104	ARG
3	G	328	HIS
3	G	349	GLN
3	G	353	HIS
4	H	236	GLN
4	H	262	ARG
4	H	276	SER
5	I	84	GLU
5	I	238	HIS
5	J	84	GLU
5	J	238	HIS
6	K	8	SER
6	K	71	ASP
6	K	83	LYS
6	K	86	GLU
6	K	98	PHE
6	L	8	SER
6	L	62	GLU
6	L	71	ASP
6	L	83	LYS
6	L	86	GLU
6	L	98	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
10	PO4	J	1001	11	4,4,4	0.97	0	6,6,6	0.46	0
8	I9X	H	1001	7	16,18,18	5.76	7 (43%)	24,29,29	1.13	2 (8%)
8	I9X	D	1001	7	16,18,18	5.77	7 (43%)	24,29,29	1.14	2 (8%)
9	ADP	I	1000	11	24,29,29	0.92	1 (4%)	29,45,45	1.41	5 (17%)
9	ADP	J	1000	11	24,29,29	0.91	1 (4%)	29,45,45	1.41	5 (17%)
12	ATP	L	1000	11	26,33,33	0.61	0	31,52,52	1.05	2 (6%)
10	PO4	I	1001	11	4,4,4	0.97	0	6,6,6	0.46	0
12	ATP	K	1000	11	26,33,33	0.61	0	31,52,52	1.05	2 (6%)

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
8	I9X	H	1001	7	-	0/6/32/32	0/2/2/2
8	I9X	D	1001	7	-	0/6/32/32	0/2/2/2
9	ADP	I	1000	11	-	1/12/32/32	0/3/3/3
9	ADP	J	1000	11	-	1/12/32/32	0/3/3/3
12	ATP	L	1000	11	-	6/18/38/38	0/3/3/3
12	ATP	K	1000	11	-	6/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1001	I9X	C03-C04	-13.83	1.22	1.52
8	H	1001	I9X	C03-C04	-13.83	1.22	1.52
8	H	1001	I9X	O07-C05	-11.34	1.21	1.46
8	D	1001	I9X	O07-C05	-11.31	1.22	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1001	I9X	C05-C04	9.71	1.72	1.53
8	H	1001	I9X	C05-C04	9.70	1.72	1.53
8	D	1001	I9X	C03-C02	7.77	1.72	1.53
8	H	1001	I9X	C03-C02	7.75	1.72	1.53
8	H	1001	I9X	O06-C05	4.31	1.49	1.41
8	D	1001	I9X	O06-C05	4.28	1.49	1.41
8	D	1001	I9X	O06-C02	-4.11	1.35	1.45
8	H	1001	I9X	O06-C02	-4.11	1.35	1.45
8	D	1001	I9X	C01-C02	-2.97	1.42	1.51
8	H	1001	I9X	C01-C02	-2.95	1.42	1.51
9	J	1000	ADP	C5-C4	2.30	1.47	1.40
9	I	1000	ADP	C5-C4	2.29	1.47	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	1000	ADP	N3-C2-N1	-3.72	122.87	128.68
9	I	1000	ADP	N3-C2-N1	-3.71	122.88	128.68
9	J	1000	ADP	PA-O3A-PB	-2.90	122.86	132.83
9	I	1000	ADP	PA-O3A-PB	-2.89	122.91	132.83
9	J	1000	ADP	C4-C5-N7	-2.63	106.66	109.40
8	D	1001	I9X	O07-P08-O09	-2.62	108.83	115.76
8	H	1001	I9X	O07-P08-O09	-2.62	108.84	115.76
9	I	1000	ADP	C4-C5-N7	-2.58	106.71	109.40
8	D	1001	I9X	O10-P08-O09	-2.45	109.31	115.76
8	H	1001	I9X	O10-P08-O09	-2.42	109.37	115.76
12	L	1000	ATP	C5-C6-N6	2.27	123.80	120.35
12	K	1000	ATP	C5-C6-N6	2.25	123.77	120.35
9	I	1000	ADP	C3'-C2'-C1'	2.06	104.08	100.98
9	J	1000	ADP	C3'-C2'-C1'	2.06	104.08	100.98
12	L	1000	ATP	PB-O3B-PG	2.05	139.88	132.83
12	K	1000	ATP	PB-O3B-PG	2.02	139.77	132.83
9	I	1000	ADP	C2-N1-C6	2.01	122.19	118.75
9	J	1000	ADP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	K	1000	ATP	C5'-O5'-PA-O2A
12	L	1000	ATP	C5'-O5'-PA-O2A
12	K	1000	ATP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	L	1000	ATP	C3'-C4'-C5'-O5'
12	K	1000	ATP	O4'-C4'-C5'-O5'
12	L	1000	ATP	O4'-C4'-C5'-O5'
12	K	1000	ATP	C5'-O5'-PA-O3A
12	L	1000	ATP	C5'-O5'-PA-O3A
12	K	1000	ATP	PA-O3A-PB-O1B
12	L	1000	ATP	PA-O3A-PB-O1B
12	K	1000	ATP	C5'-O5'-PA-O1A
12	L	1000	ATP	C5'-O5'-PA-O1A
9	I	1000	ADP	PA-O3A-PB-O2B
9	J	1000	ADP	PA-O3A-PB-O2B

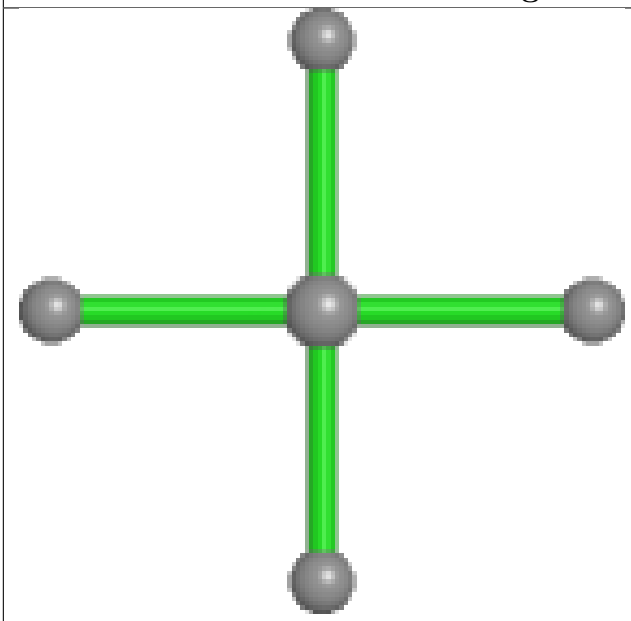
There are no ring outliers.

4 monomers are involved in 4 short contacts:

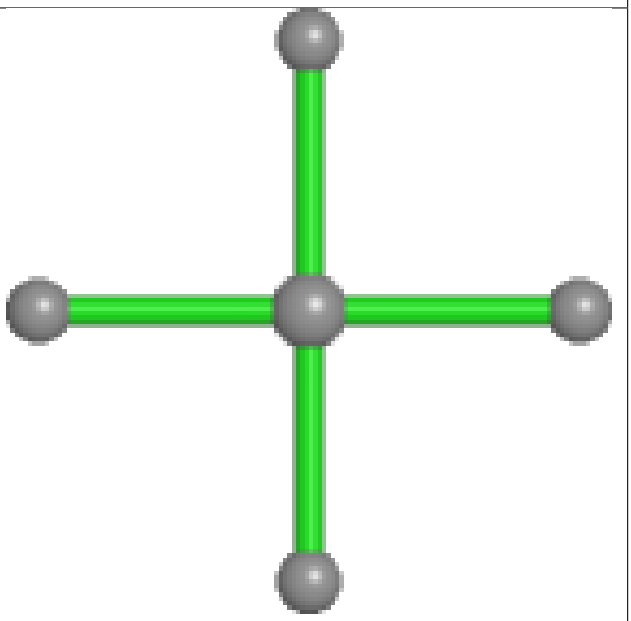
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1000	ADP	1	0
9	J	1000	ADP	1	0
12	L	1000	ATP	1	0
12	K	1000	ATP	1	0

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 then 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.

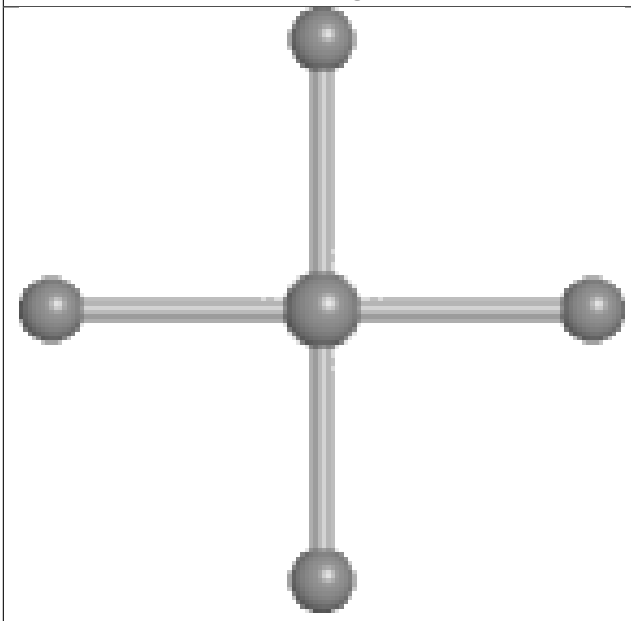
Ligand PO4 J 1001



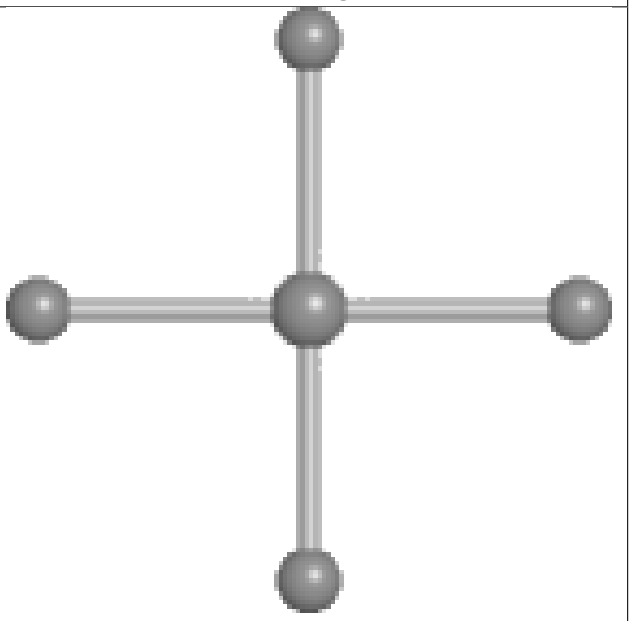
Bond lengths



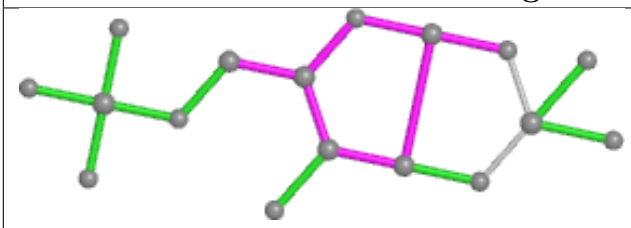
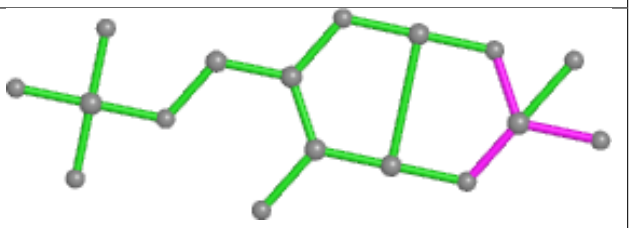
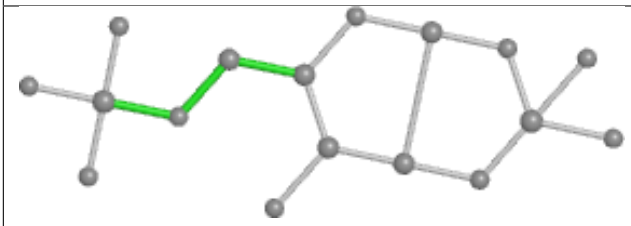
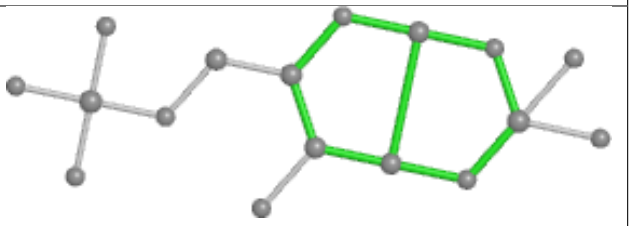
Bond angles

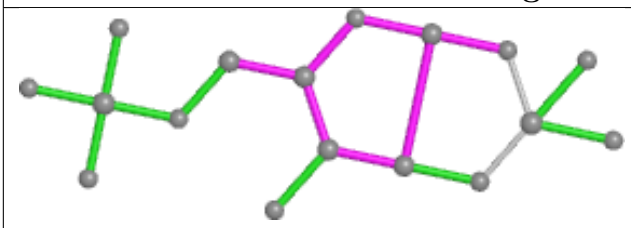
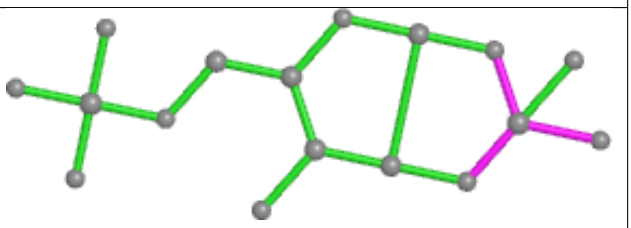
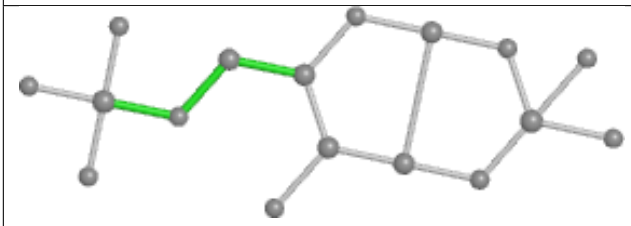
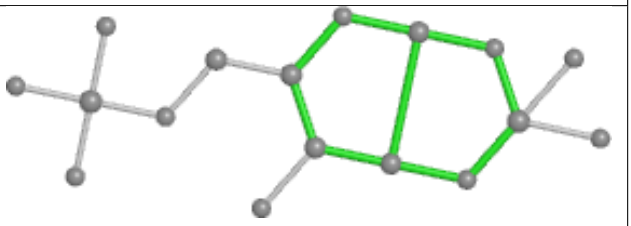


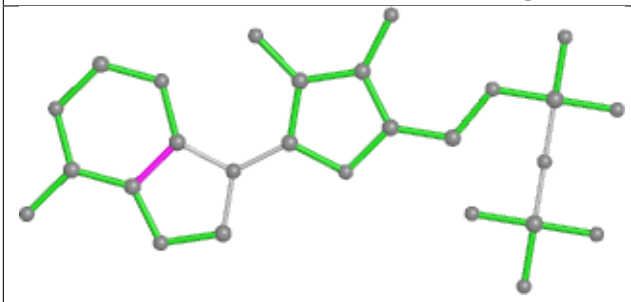
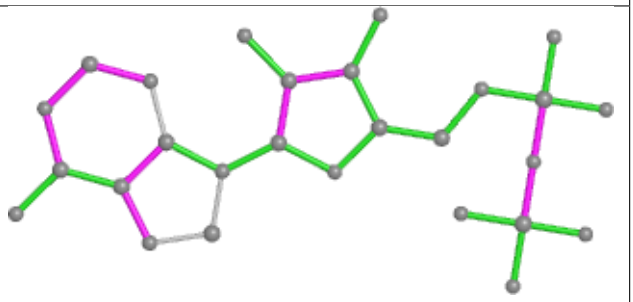
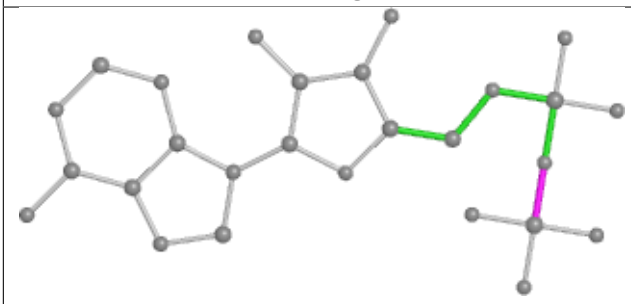
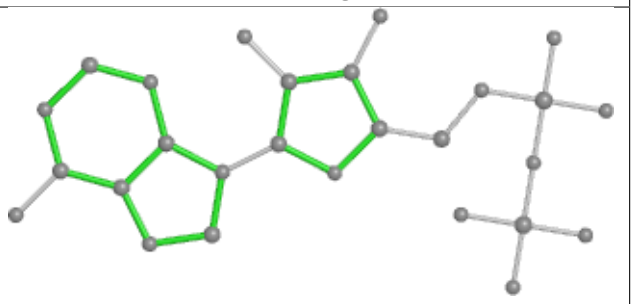
Torsions

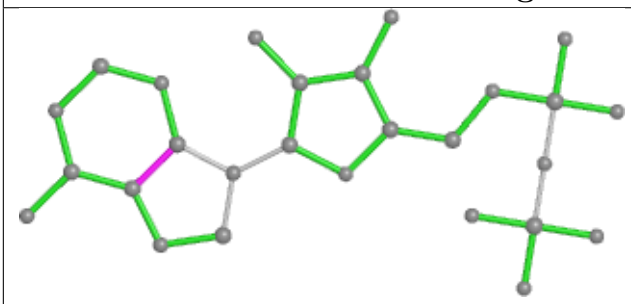
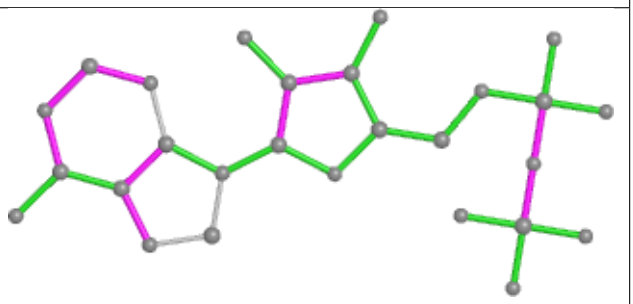
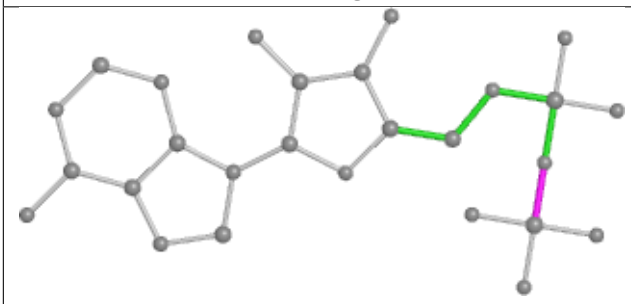
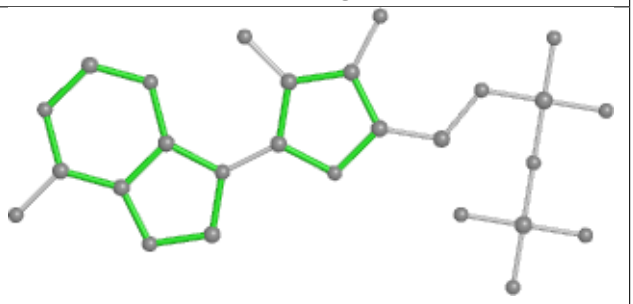


Rings

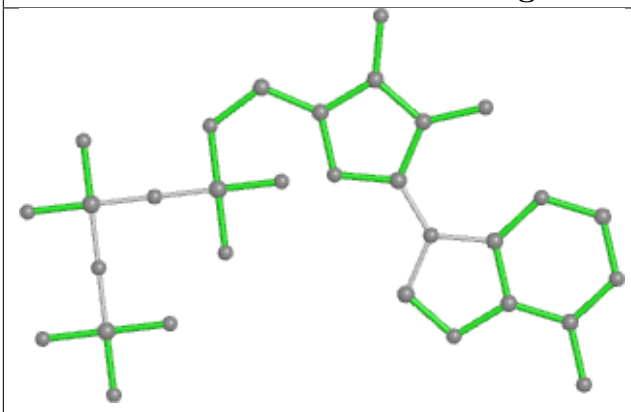
Ligand I9X H 1001	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand I9X D 1001	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

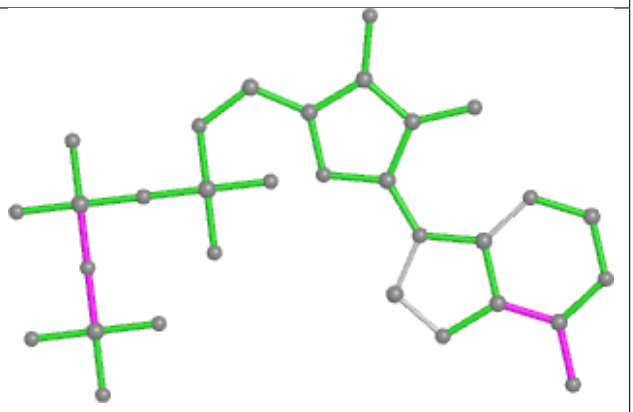
Ligand ADP I 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP J 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

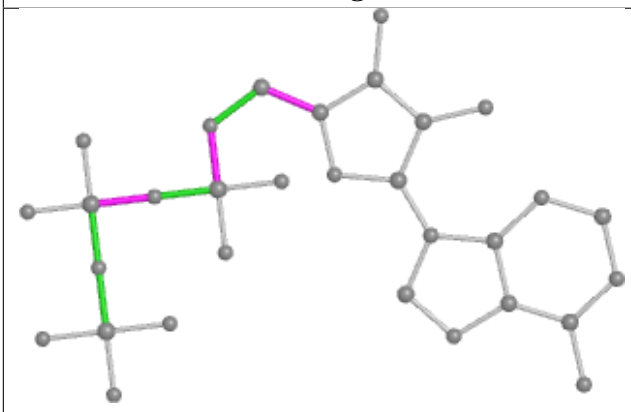
Ligand ATP L 1000



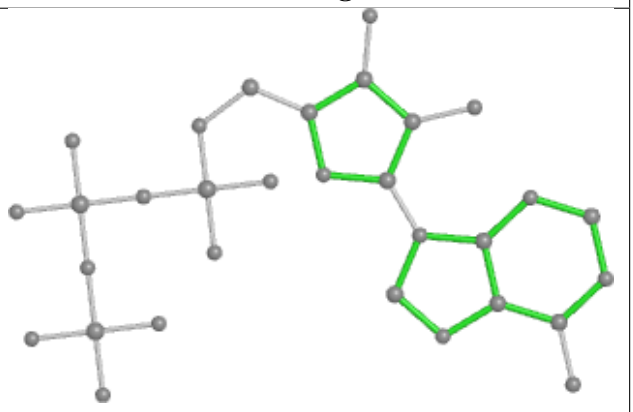
Bond lengths



Bond angles

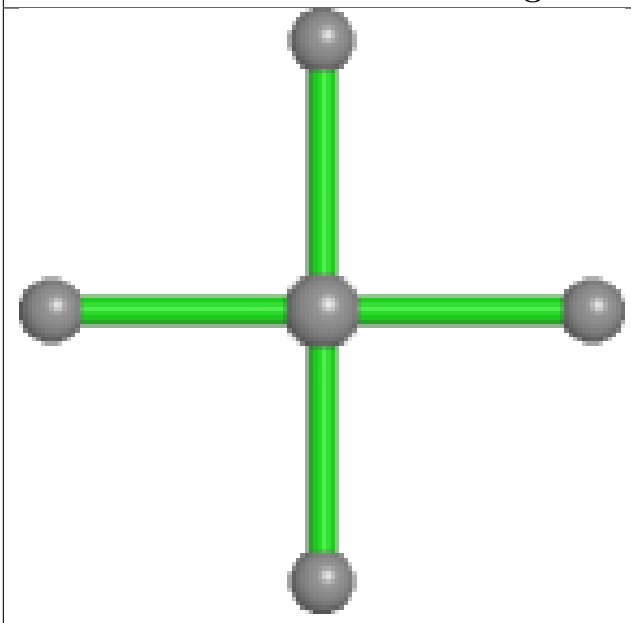


Torsions

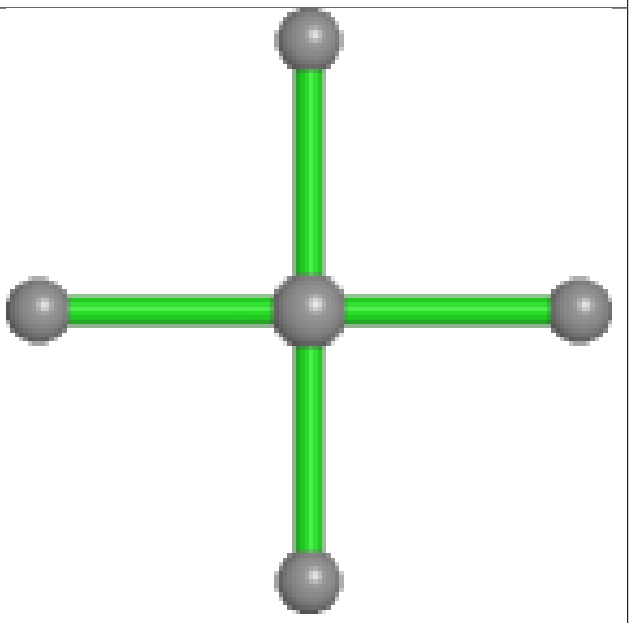


Rings

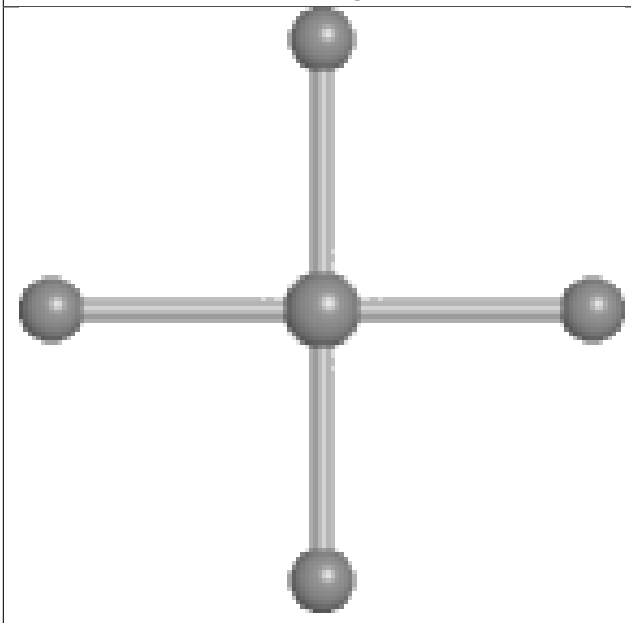
Ligand PO4 I 1001



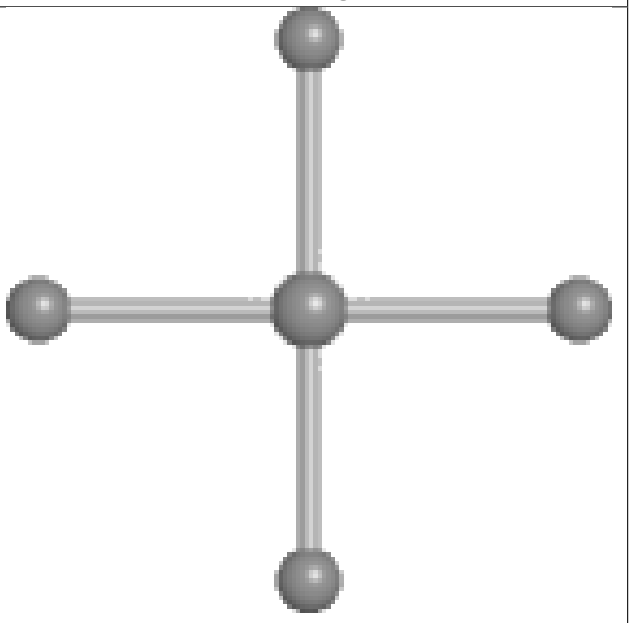
Bond lengths



Bond angles

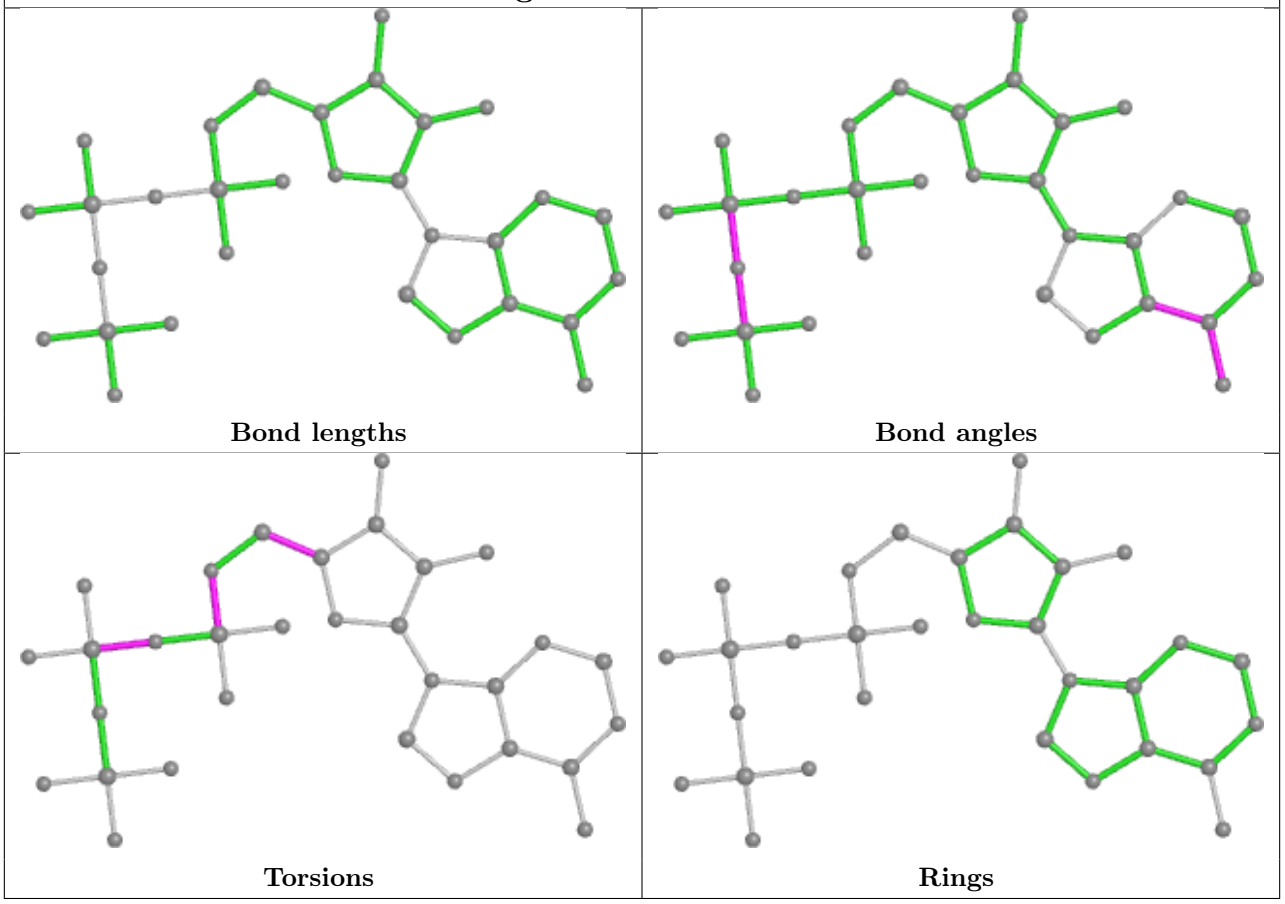


Torsions



Rings

Ligand ATP K 1000



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.

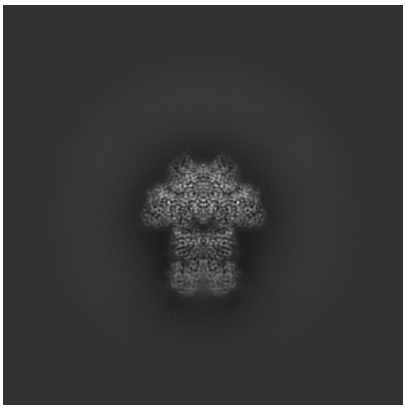
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14441. These allow visual inspection of the internal detail of the map and identification of artifacts.

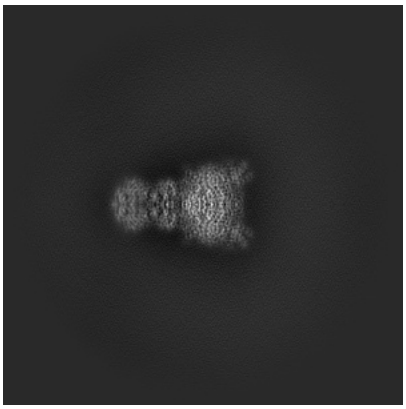
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

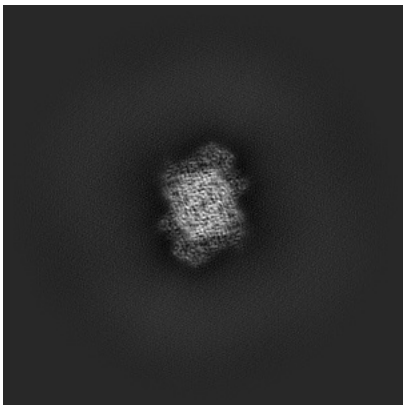
6.1.1 Primary map



X

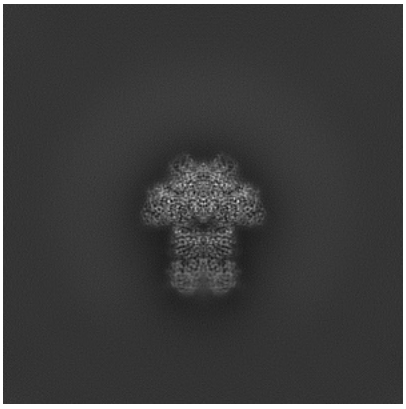


Y

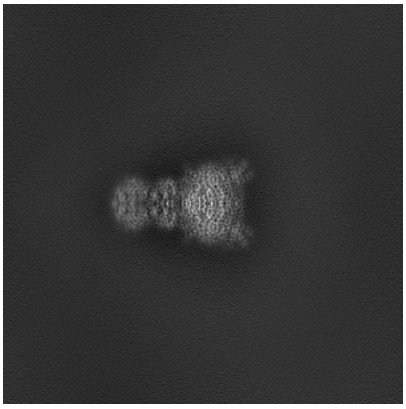


Z

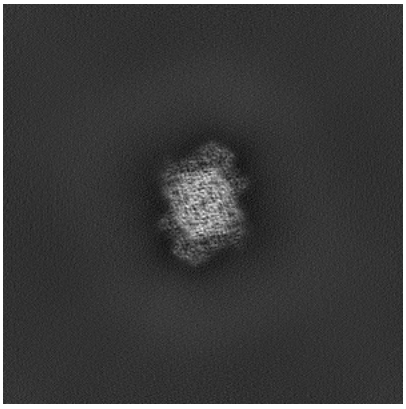
6.1.2 Raw map



X



Y

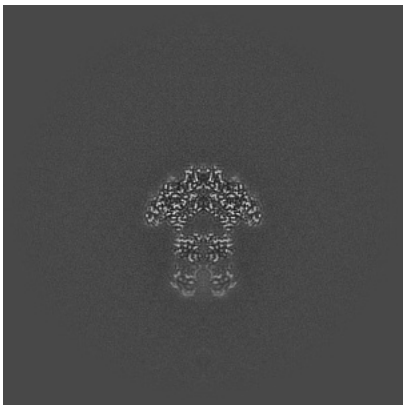


Z

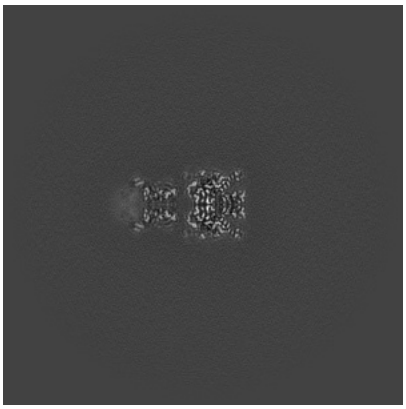
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

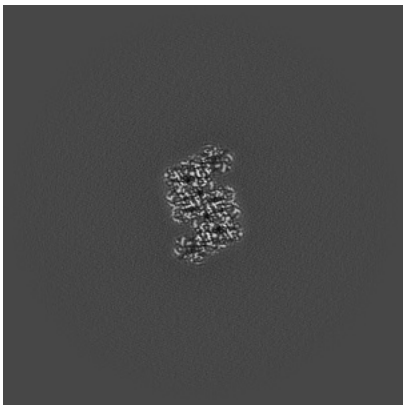
6.2.1 Primary map



X Index: 240

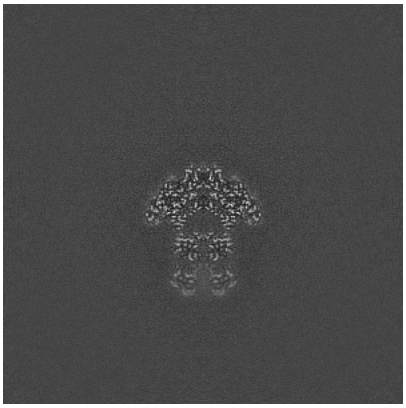


Y Index: 240

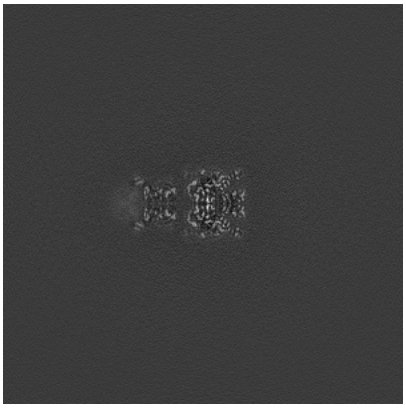


Z Index: 240

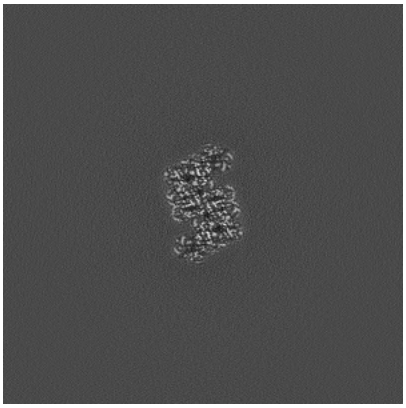
6.2.2 Raw map



X Index: 240



Y Index: 240

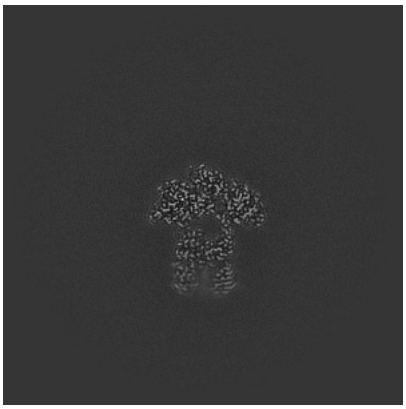


Z Index: 240

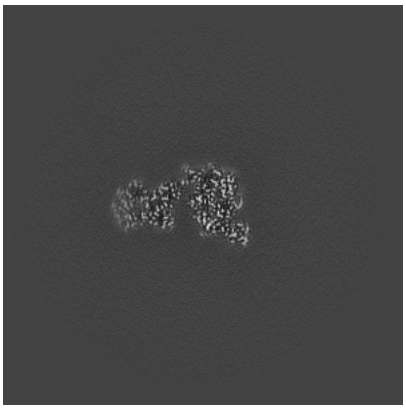
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

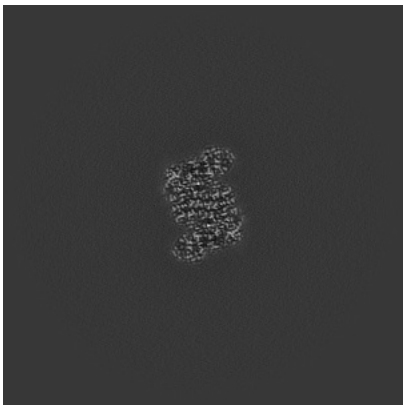
6.3.1 Primary map



X Index: 246

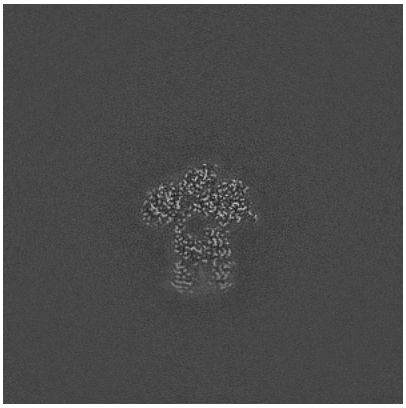


Y Index: 226

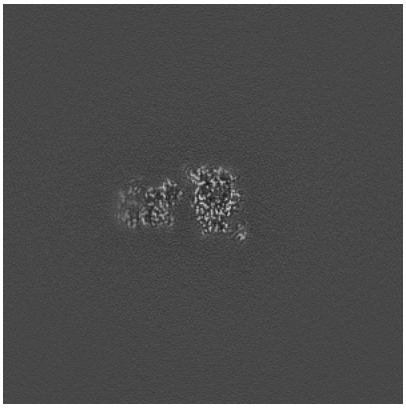


Z Index: 246

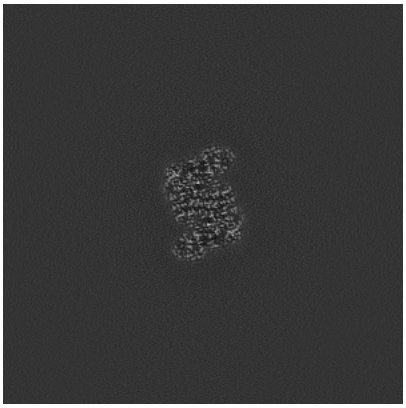
6.3.2 Raw map



X Index: 233



Y Index: 231



Z Index: 246

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

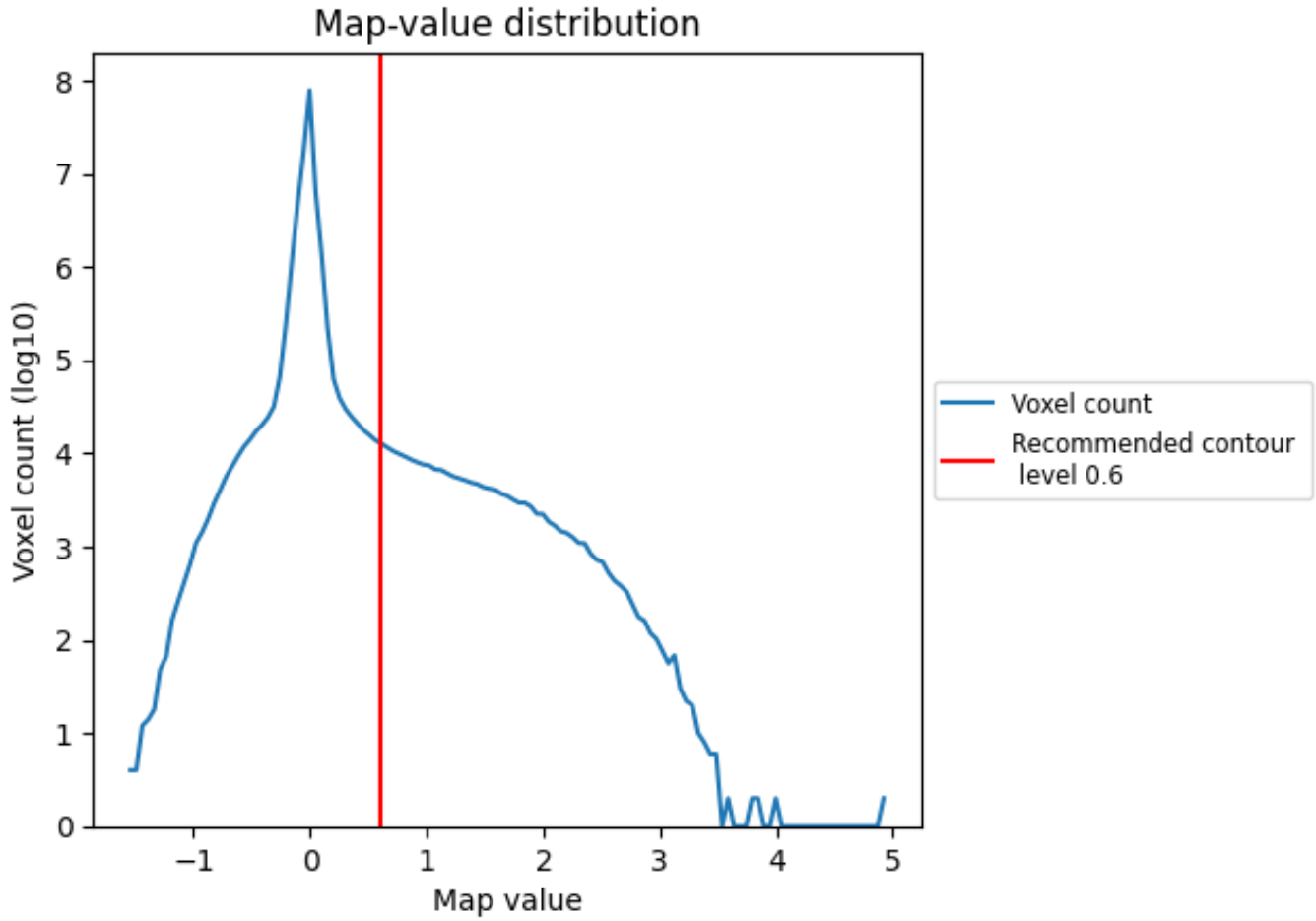
6.5 Mask visualisation (i)

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

7 Map analysis

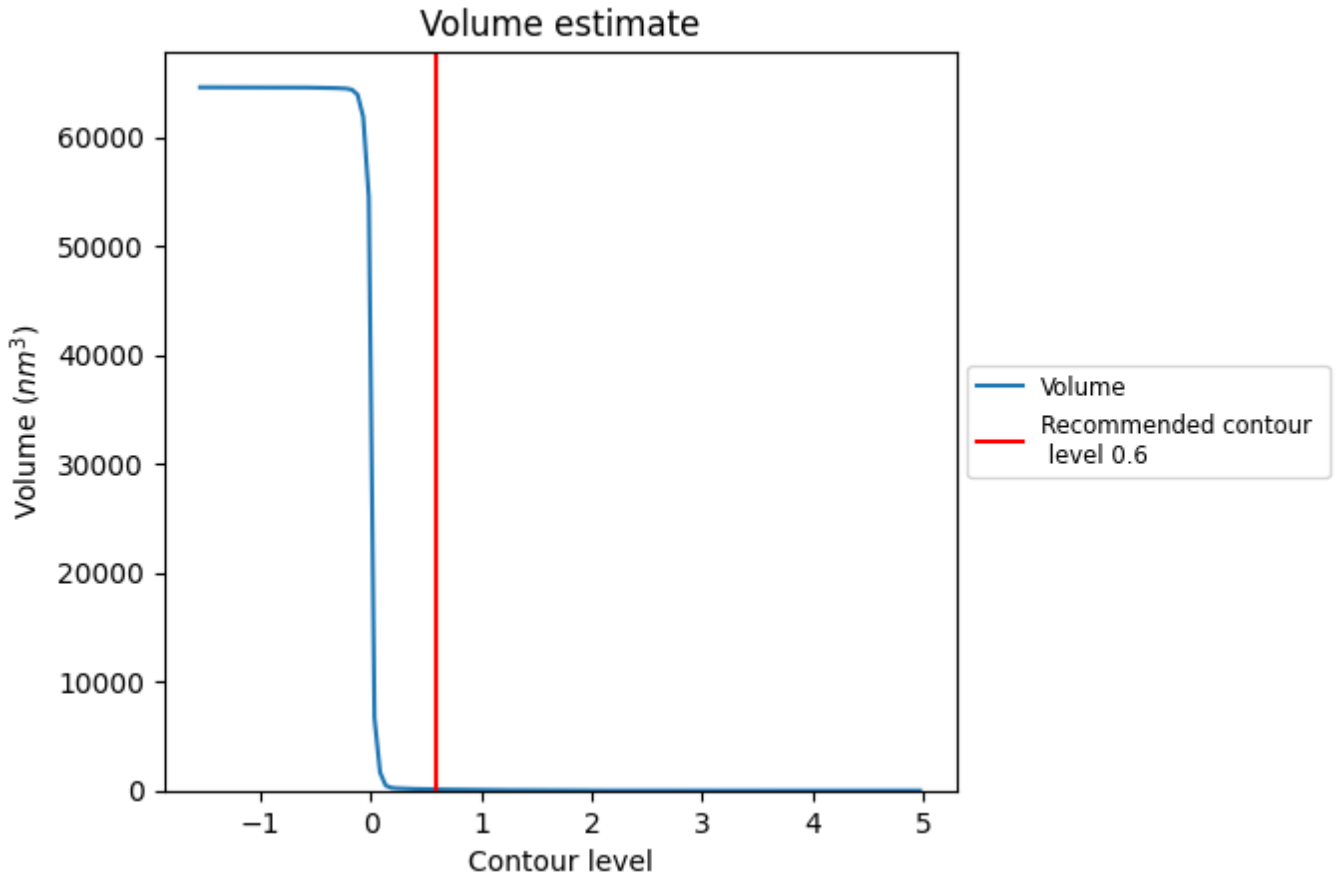
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

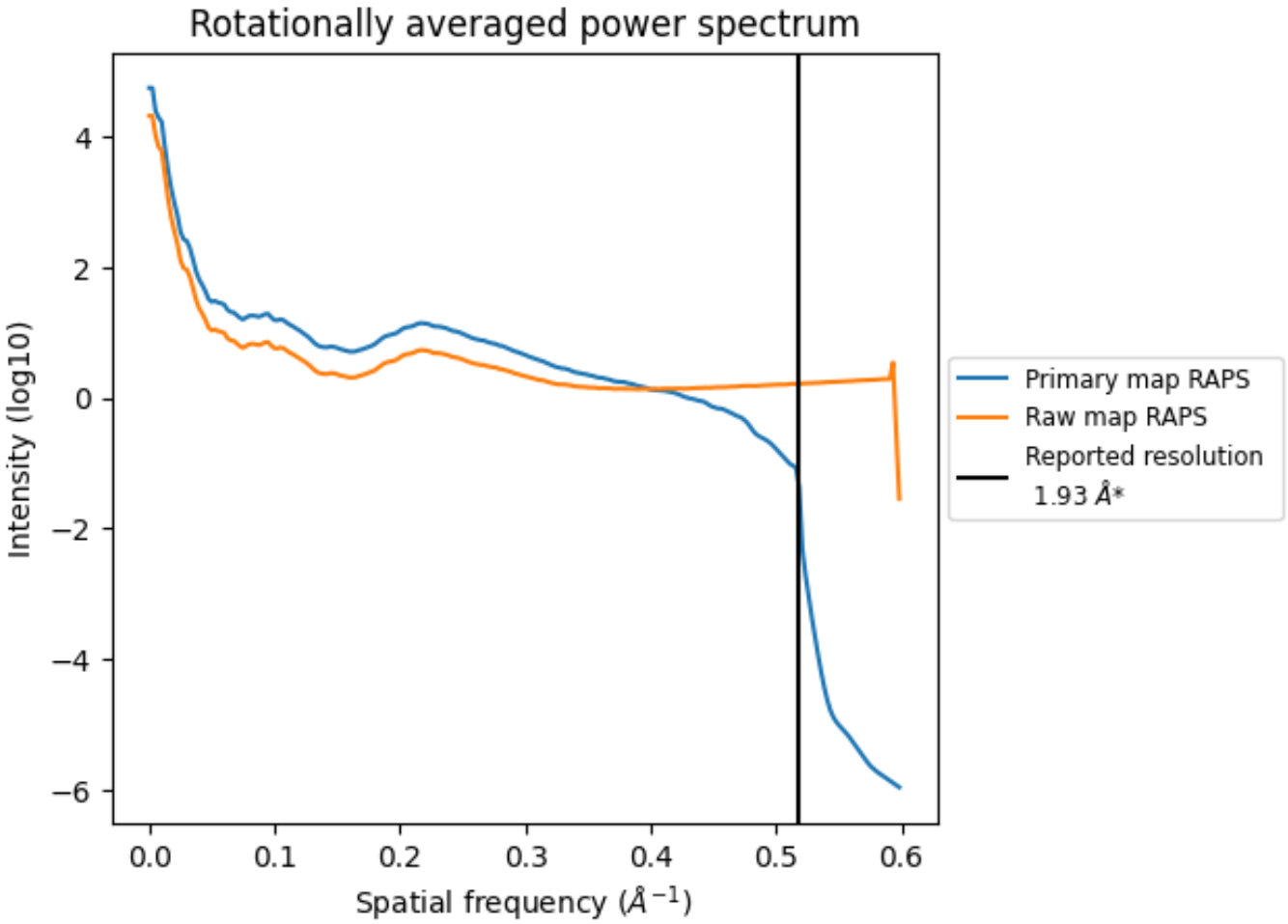
7.2 Volume estimate



The volume at the recommended contour level is 108 nm^3; this corresponds to an approximate mass of 97 kDa.

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

7.3 Rotationally averaged power spectrum (i)

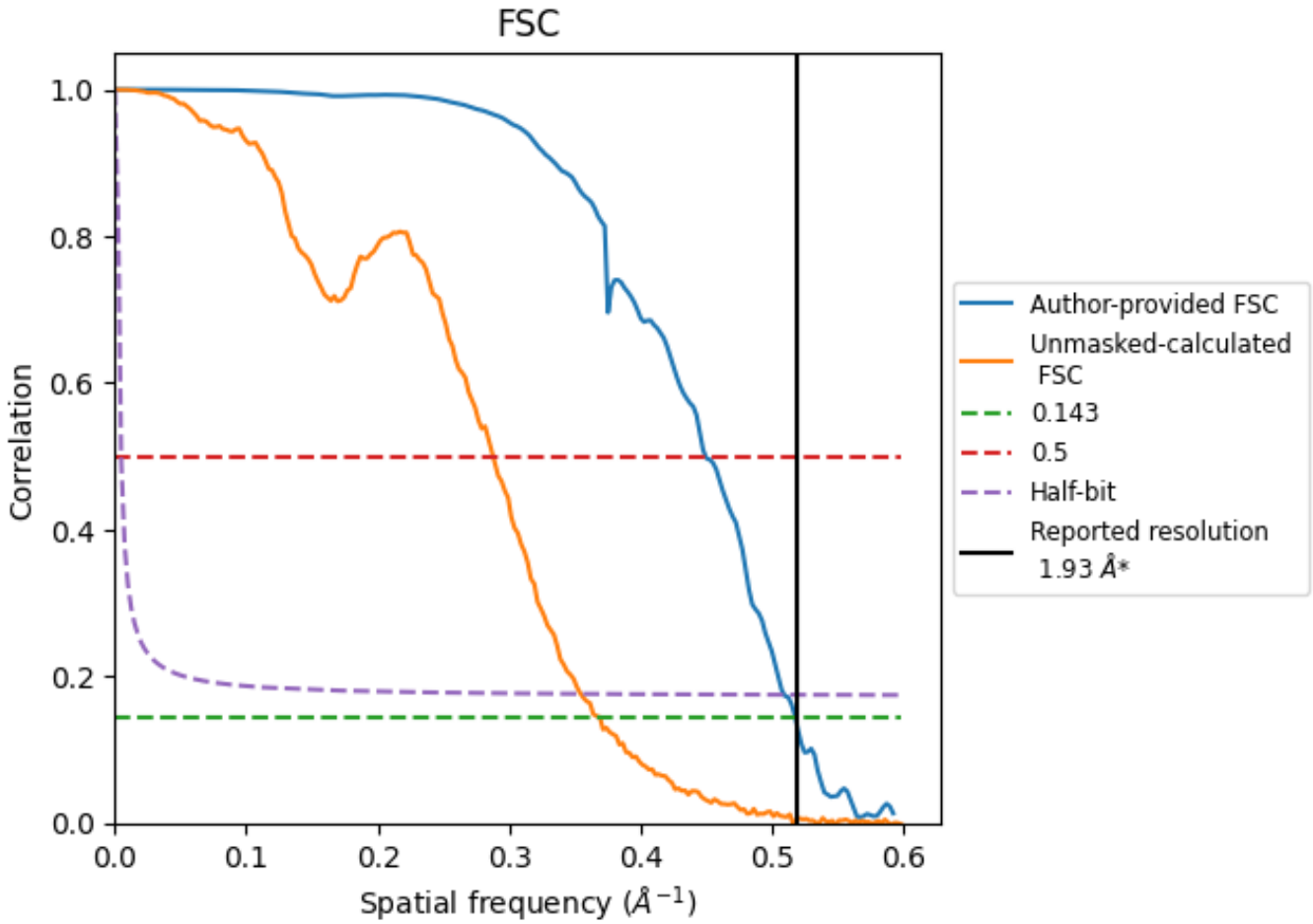


*Reported resolution corresponds to spatial frequency of 0.518 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.518 Å^{-1}

8.2 Resolution estimates (i)

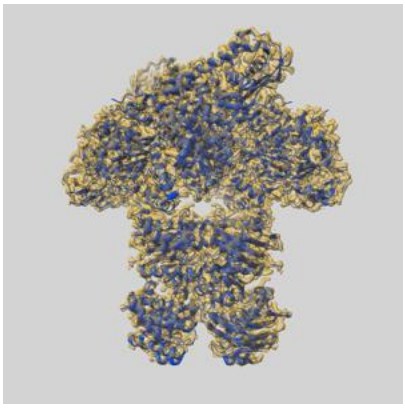
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.93	-	-
Author-provided FSC curve	1.93	2.23	1.96
Unmasked-calculated*	2.71	3.48	2.82

*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 2.71 differs from the reported value 1.93 by more than 10 %

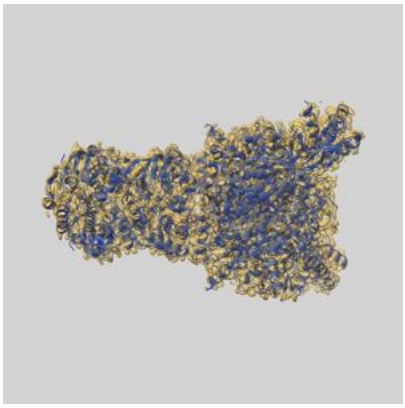
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14441 and PDB model 7Z15. Per-residue inclusion information can be found in section 3 on page 12.

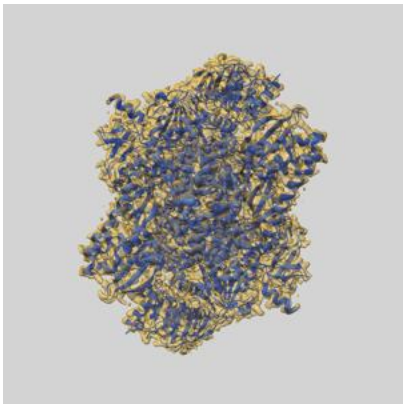
9.1 Map-model overlay



X



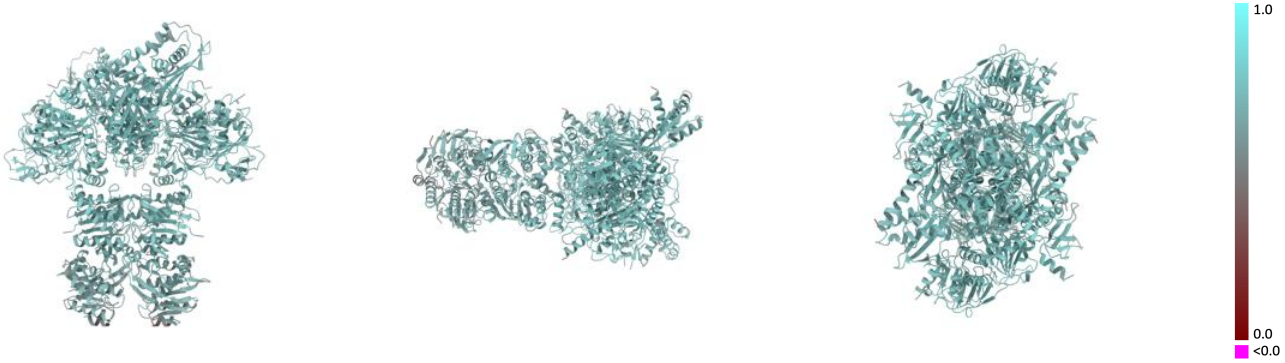
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

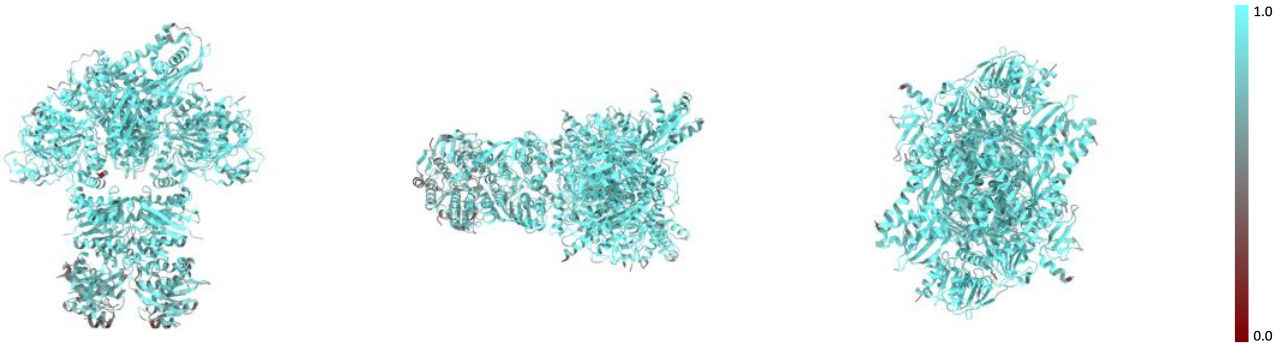
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

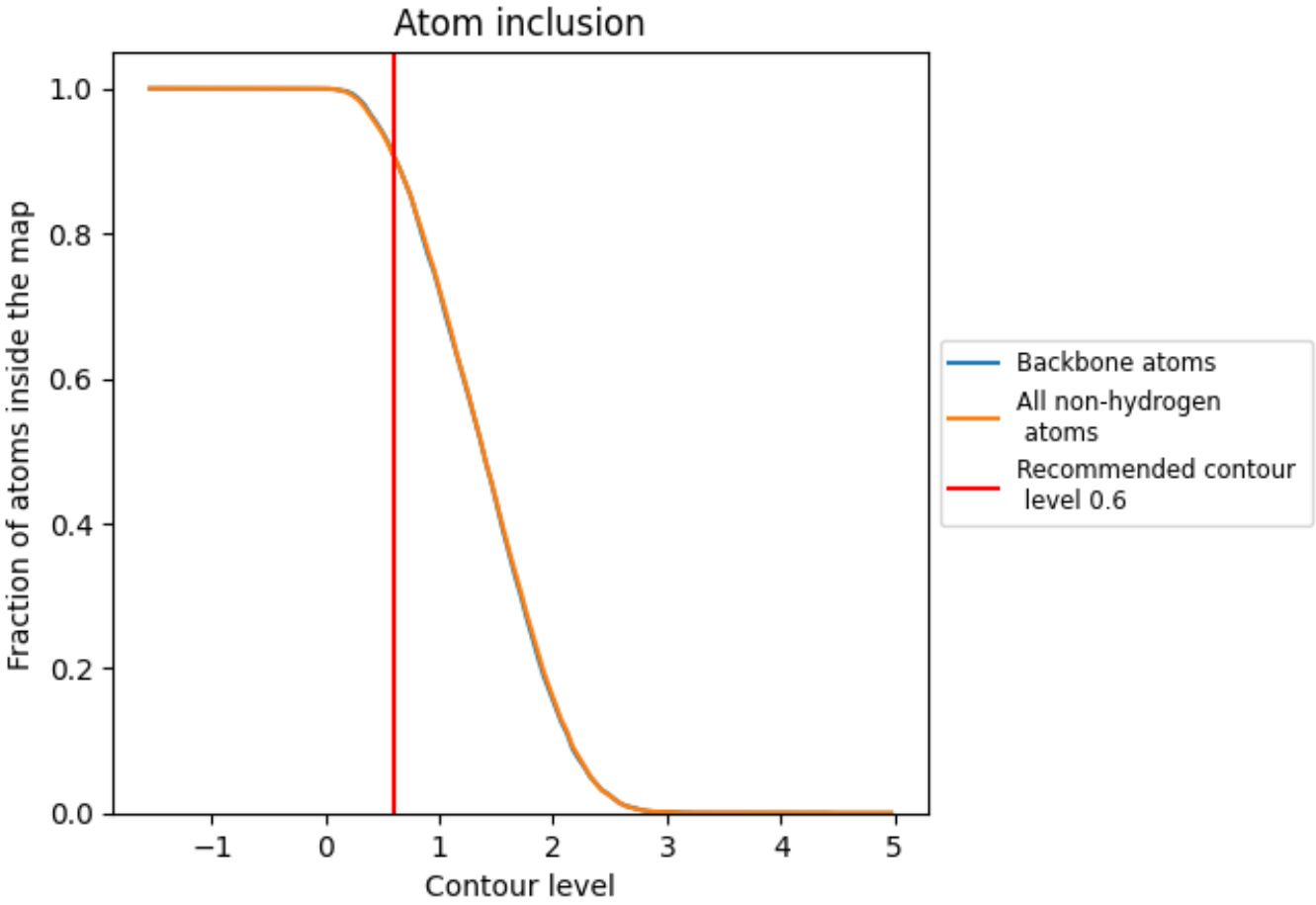
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9063	0.6880
A	0.9011	0.6800
B	0.9176	0.6890
C	0.9507	0.7130
D	0.9587	0.7210
E	0.9011	0.6790
F	0.9204	0.6880
G	0.9503	0.7150
H	0.9587	0.7200
I	0.9191	0.6900
J	0.9180	0.6890
K	0.7417	0.6100
L	0.7423	0.6100