Full wwPDB EM Validation Report ⓘ

Mar 4, 2024 – 09:55 AM EST

PDB ID	:	6MDM
EMDB ID	:	EMD-9100
Title	:	The 20S supercomplex engaging the SNAP-25 N-terminus (class 1)
Authors	:	White, K.I.; Zhao, M.; Brunger, A.T.
Deposited on	:	2018-09-04
Resolution	:	4.40 Å(reported)
Based on initial model	:	3J96

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:

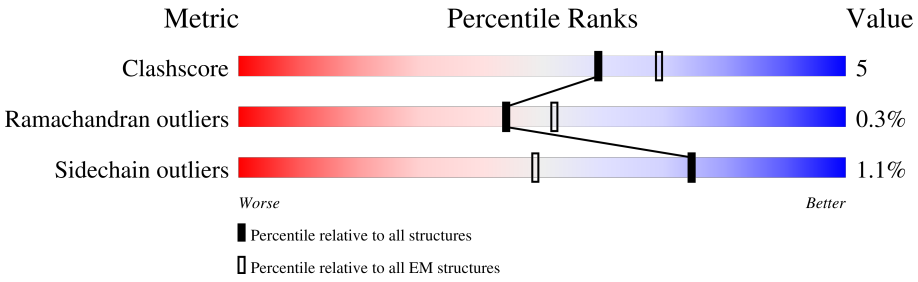
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.40 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	768	13% 78% 12% 9%
1	B	768	16% 76% 15% • 8%
1	C	768	9% 78% 14% 8%
1	D	768	23% 81% 12% 7%
1	E	768	6% 58% 9% 33%
1	F	768	29% 53% 8% 39%
2	H	207	5% 64% 6% 29%
3	I	256	19% 7% 74%

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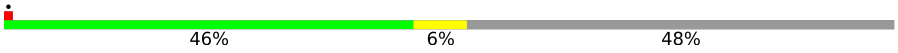
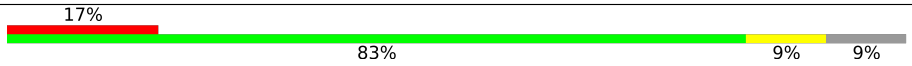
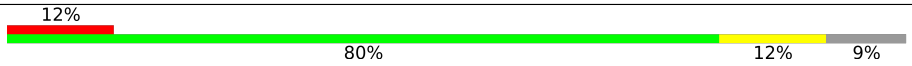
Mol	Chain	Length	Quality of chain
4	J	117	
5	K	313	
5	L	313	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 73303 atoms, of which 36736 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 Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	699	Total	C	H	N	O	S	0	0
			11004	3450	5558	947	1019	30		
1	B	704	Total	C	H	N	O	S	0	0
			11079	3472	5597	953	1027	30		
1	C	709	Total	C	H	N	O	S	0	0
			11164	3499	5638	960	1037	30		
1	D	713	Total	C	H	N	O	S	0	0
			11232	3519	5675	964	1043	31		
1	E	514	Total	C	H	N	O	S	0	0
			8130	2539	4120	701	748	22		
1	F	466	Total	C	H	N	O	S	0	0
			7007	2220	3500	615	657	15		

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP P18708
A	-22	GLY	-	expression tag	UNP P18708
A	-21	HIS	-	expression tag	UNP P18708
A	-20	HIS	-	expression tag	UNP P18708
A	-19	HIS	-	expression tag	UNP P18708
A	-18	HIS	-	expression tag	UNP P18708
A	-17	HIS	-	expression tag	UNP P18708
A	-16	HIS	-	expression tag	UNP P18708
A	-15	ASP	-	expression tag	UNP P18708
A	-14	TYR	-	expression tag	UNP P18708
A	-13	ASP	-	expression tag	UNP P18708
A	-12	ILE	-	expression tag	UNP P18708
A	-11	PRO	-	expression tag	UNP P18708
A	-10	THR	-	expression tag	UNP P18708
A	-9	THR	-	expression tag	UNP P18708
A	-8	GLU	-	expression tag	UNP P18708
A	-7	ASN	-	expression tag	UNP P18708
A	-6	LEU	-	expression tag	UNP P18708

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	TYR	-	expression tag	UNP P18708
A	-4	PHE	-	expression tag	UNP P18708
A	-3	GLN	-	expression tag	UNP P18708
A	-2	GLY	-	expression tag	UNP P18708
A	-1	ALA	-	expression tag	UNP P18708
A	0	HIS	-	expression tag	UNP P18708
A	458	ILE	LYS	conflict	UNP P18708
B	-23	MET	-	initiating methionine	UNP P18708
B	-22	GLY	-	expression tag	UNP P18708
B	-21	HIS	-	expression tag	UNP P18708
B	-20	HIS	-	expression tag	UNP P18708
B	-19	HIS	-	expression tag	UNP P18708
B	-18	HIS	-	expression tag	UNP P18708
B	-17	HIS	-	expression tag	UNP P18708
B	-16	HIS	-	expression tag	UNP P18708
B	-15	ASP	-	expression tag	UNP P18708
B	-14	TYR	-	expression tag	UNP P18708
B	-13	ASP	-	expression tag	UNP P18708
B	-12	ILE	-	expression tag	UNP P18708
B	-11	PRO	-	expression tag	UNP P18708
B	-10	THR	-	expression tag	UNP P18708
B	-9	THR	-	expression tag	UNP P18708
B	-8	GLU	-	expression tag	UNP P18708
B	-7	ASN	-	expression tag	UNP P18708
B	-6	LEU	-	expression tag	UNP P18708
B	-5	TYR	-	expression tag	UNP P18708
B	-4	PHE	-	expression tag	UNP P18708
B	-3	GLN	-	expression tag	UNP P18708
B	-2	GLY	-	expression tag	UNP P18708
B	-1	ALA	-	expression tag	UNP P18708
B	0	HIS	-	expression tag	UNP P18708
B	458	ILE	LYS	conflict	UNP P18708
C	-23	MET	-	initiating methionine	UNP P18708
C	-22	GLY	-	expression tag	UNP P18708
C	-21	HIS	-	expression tag	UNP P18708
C	-20	HIS	-	expression tag	UNP P18708
C	-19	HIS	-	expression tag	UNP P18708
C	-18	HIS	-	expression tag	UNP P18708
C	-17	HIS	-	expression tag	UNP P18708
C	-16	HIS	-	expression tag	UNP P18708
C	-15	ASP	-	expression tag	UNP P18708
C	-14	TYR	-	expression tag	UNP P18708

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	ASP	-	expression tag	UNP P18708
C	-12	ILE	-	expression tag	UNP P18708
C	-11	PRO	-	expression tag	UNP P18708
C	-10	THR	-	expression tag	UNP P18708
C	-9	THR	-	expression tag	UNP P18708
C	-8	GLU	-	expression tag	UNP P18708
C	-7	ASN	-	expression tag	UNP P18708
C	-6	LEU	-	expression tag	UNP P18708
C	-5	TYR	-	expression tag	UNP P18708
C	-4	PHE	-	expression tag	UNP P18708
C	-3	GLN	-	expression tag	UNP P18708
C	-2	GLY	-	expression tag	UNP P18708
C	-1	ALA	-	expression tag	UNP P18708
C	0	HIS	-	expression tag	UNP P18708
C	458	ILE	LYS	conflict	UNP P18708
D	-23	MET	-	initiating methionine	UNP P18708
D	-22	GLY	-	expression tag	UNP P18708
D	-21	HIS	-	expression tag	UNP P18708
D	-20	HIS	-	expression tag	UNP P18708
D	-19	HIS	-	expression tag	UNP P18708
D	-18	HIS	-	expression tag	UNP P18708
D	-17	HIS	-	expression tag	UNP P18708
D	-16	HIS	-	expression tag	UNP P18708
D	-15	ASP	-	expression tag	UNP P18708
D	-14	TYR	-	expression tag	UNP P18708
D	-13	ASP	-	expression tag	UNP P18708
D	-12	ILE	-	expression tag	UNP P18708
D	-11	PRO	-	expression tag	UNP P18708
D	-10	THR	-	expression tag	UNP P18708
D	-9	THR	-	expression tag	UNP P18708
D	-8	GLU	-	expression tag	UNP P18708
D	-7	ASN	-	expression tag	UNP P18708
D	-6	LEU	-	expression tag	UNP P18708
D	-5	TYR	-	expression tag	UNP P18708
D	-4	PHE	-	expression tag	UNP P18708
D	-3	GLN	-	expression tag	UNP P18708
D	-2	GLY	-	expression tag	UNP P18708
D	-1	ALA	-	expression tag	UNP P18708
D	0	HIS	-	expression tag	UNP P18708
D	458	ILE	LYS	conflict	UNP P18708
E	-23	MET	-	initiating methionine	UNP P18708
E	-22	GLY	-	expression tag	UNP P18708

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-21	HIS	-	expression tag	UNP P18708
E	-20	HIS	-	expression tag	UNP P18708
E	-19	HIS	-	expression tag	UNP P18708
E	-18	HIS	-	expression tag	UNP P18708
E	-17	HIS	-	expression tag	UNP P18708
E	-16	HIS	-	expression tag	UNP P18708
E	-15	ASP	-	expression tag	UNP P18708
E	-14	TYR	-	expression tag	UNP P18708
E	-13	ASP	-	expression tag	UNP P18708
E	-12	ILE	-	expression tag	UNP P18708
E	-11	PRO	-	expression tag	UNP P18708
E	-10	THR	-	expression tag	UNP P18708
E	-9	THR	-	expression tag	UNP P18708
E	-8	GLU	-	expression tag	UNP P18708
E	-7	ASN	-	expression tag	UNP P18708
E	-6	LEU	-	expression tag	UNP P18708
E	-5	TYR	-	expression tag	UNP P18708
E	-4	PHE	-	expression tag	UNP P18708
E	-3	GLN	-	expression tag	UNP P18708
E	-2	GLY	-	expression tag	UNP P18708
E	-1	ALA	-	expression tag	UNP P18708
E	0	HIS	-	expression tag	UNP P18708
E	458	ILE	LYS	conflict	UNP P18708
F	-23	MET	-	initiating methionine	UNP P18708
F	-22	GLY	-	expression tag	UNP P18708
F	-21	HIS	-	expression tag	UNP P18708
F	-20	HIS	-	expression tag	UNP P18708
F	-19	HIS	-	expression tag	UNP P18708
F	-18	HIS	-	expression tag	UNP P18708
F	-17	HIS	-	expression tag	UNP P18708
F	-16	HIS	-	expression tag	UNP P18708
F	-15	ASP	-	expression tag	UNP P18708
F	-14	TYR	-	expression tag	UNP P18708
F	-13	ASP	-	expression tag	UNP P18708
F	-12	ILE	-	expression tag	UNP P18708
F	-11	PRO	-	expression tag	UNP P18708
F	-10	THR	-	expression tag	UNP P18708
F	-9	THR	-	expression tag	UNP P18708
F	-8	GLU	-	expression tag	UNP P18708
F	-7	ASN	-	expression tag	UNP P18708
F	-6	LEU	-	expression tag	UNP P18708
F	-5	TYR	-	expression tag	UNP P18708

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	PHE	-	expression tag	UNP P18708
F	-3	GLN	-	expression tag	UNP P18708
F	-2	GLY	-	expression tag	UNP P18708
F	-1	ALA	-	expression tag	UNP P18708
F	0	HIS	-	expression tag	UNP P18708
F	458	ILE	LYS	conflict	UNP P18708

- Molecule 2 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	147	Total	C	H	N	O	S	0	0
			2301	690	1130	218	251	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	MET	-	initiating methionine	UNP P60881
H	-1	ALA	-	expression tag	UNP P60881
H	0	SER	-	expression tag	UNP P60881

- Molecule 3 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	I	66	Total	C	H	N	O	S	0	0
			1060	331	524	91	109	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	145	SER	CYS	conflict	UNP P32851

- Molecule 4 is a protein called Vesicle-associated membrane protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	J	61	Total	C	H	N	O	S	0	0
			984	301	491	93	98	1		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-27	MET	-	initiating methionine	UNP P63045

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-26	ALA	-	expression tag	UNP P63045
J	-25	SER	-	expression tag	UNP P63045
J	-24	TYR	-	expression tag	UNP P63045
J	-23	TYR	-	expression tag	UNP P63045
J	-22	HIS	-	expression tag	UNP P63045
J	-21	HIS	-	expression tag	UNP P63045
J	-20	HIS	-	expression tag	UNP P63045
J	-19	HIS	-	expression tag	UNP P63045
J	-18	HIS	-	expression tag	UNP P63045
J	-17	HIS	-	expression tag	UNP P63045
J	-16	ASP	-	expression tag	UNP P63045
J	-15	TYR	-	expression tag	UNP P63045
J	-14	ASP	-	expression tag	UNP P63045
J	-13	ILE	-	expression tag	UNP P63045
J	-12	PRO	-	expression tag	UNP P63045
J	-11	THR	-	expression tag	UNP P63045
J	-10	SER	-	expression tag	UNP P63045
J	-9	GLU	-	expression tag	UNP P63045
J	-8	ASN	-	expression tag	UNP P63045
J	-7	LEU	-	expression tag	UNP P63045
J	-6	TYR	-	expression tag	UNP P63045
J	-5	PHE	-	expression tag	UNP P63045
J	-4	GLN	-	expression tag	UNP P63045
J	-3	GLY	-	expression tag	UNP P63045
J	-2	ALA	-	expression tag	UNP P63045
J	-1	SER	-	expression tag	UNP P63045
J	0	HIS	-	expression tag	UNP P63045

- Molecule 5 is a protein called Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	286	Total	C	H	N	O	S	0	0
			4430	1421	2179	372	441	17		
5	L	286	Total	C	H	N	O	S	0	0
			4447	1424	2192	373	441	17		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-17	MET	-	initiating methionine	UNP P54921
K	-16	HIS	-	expression tag	UNP P54921
K	-15	HIS	-	expression tag	UNP P54921

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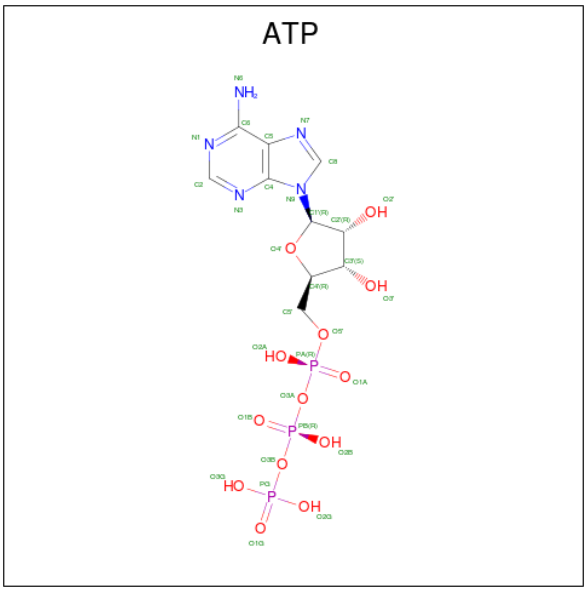
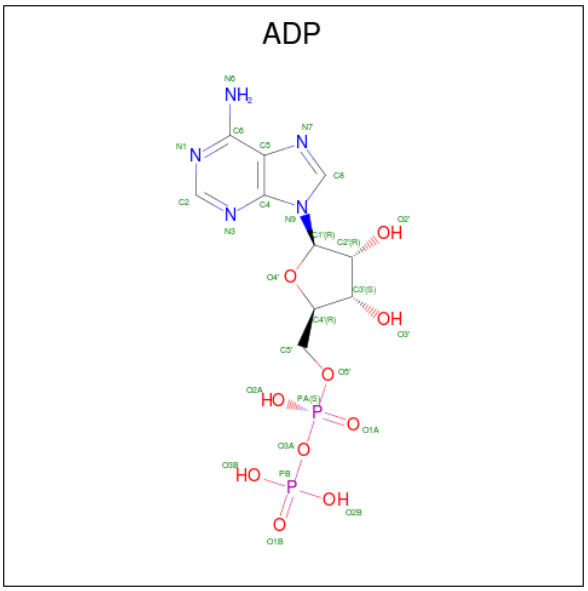
Chain	Residue	Modelled	Actual	Comment	Reference
K	-14	HIS	-	expression tag	UNP P54921
K	-13	HIS	-	expression tag	UNP P54921
K	-12	HIS	-	expression tag	UNP P54921
K	-11	HIS	-	expression tag	UNP P54921
K	-10	HIS	-	expression tag	UNP P54921
K	-9	HIS	-	expression tag	UNP P54921
K	-8	HIS	-	expression tag	UNP P54921
K	-7	HIS	-	expression tag	UNP P54921
K	-6	GLU	-	expression tag	UNP P54921
K	-5	ASN	-	expression tag	UNP P54921
K	-4	LEU	-	expression tag	UNP P54921
K	-3	TYR	-	expression tag	UNP P54921
K	-2	PHE	-	expression tag	UNP P54921
K	-1	GLN	-	expression tag	UNP P54921
K	0	GLY	-	expression tag	UNP P54921
L	-17	MET	-	initiating methionine	UNP P54921
L	-16	HIS	-	expression tag	UNP P54921
L	-15	HIS	-	expression tag	UNP P54921
L	-14	HIS	-	expression tag	UNP P54921
L	-13	HIS	-	expression tag	UNP P54921
L	-12	HIS	-	expression tag	UNP P54921
L	-11	HIS	-	expression tag	UNP P54921
L	-10	HIS	-	expression tag	UNP P54921
L	-9	HIS	-	expression tag	UNP P54921
L	-8	HIS	-	expression tag	UNP P54921
L	-7	HIS	-	expression tag	UNP P54921
L	-6	GLU	-	expression tag	UNP P54921
L	-5	ASN	-	expression tag	UNP P54921
L	-4	LEU	-	expression tag	UNP P54921
L	-3	TYR	-	expression tag	UNP P54921
L	-2	PHE	-	expression tag	UNP P54921
L	-1	GLN	-	expression tag	UNP P54921
L	0	GLY	-	expression tag	UNP P54921

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



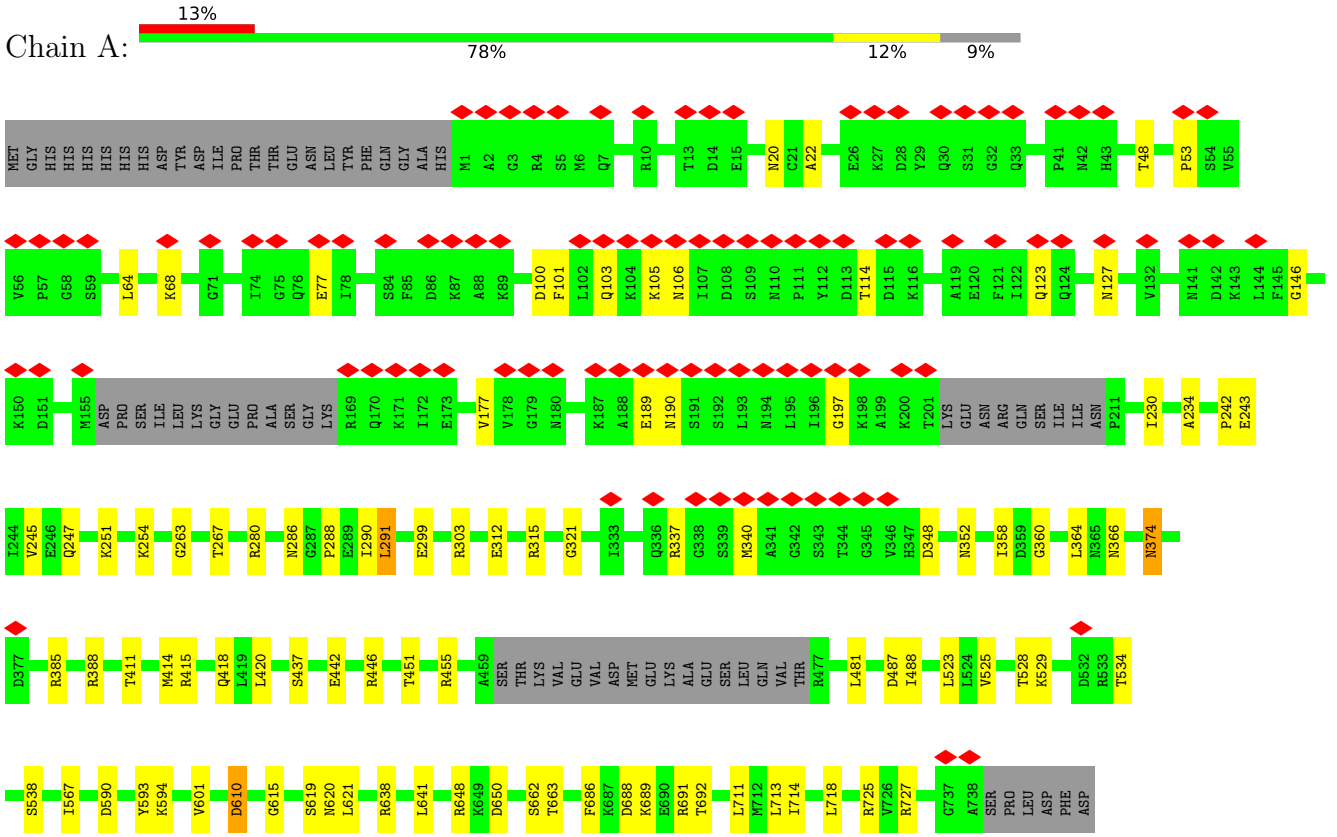
Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
7	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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.

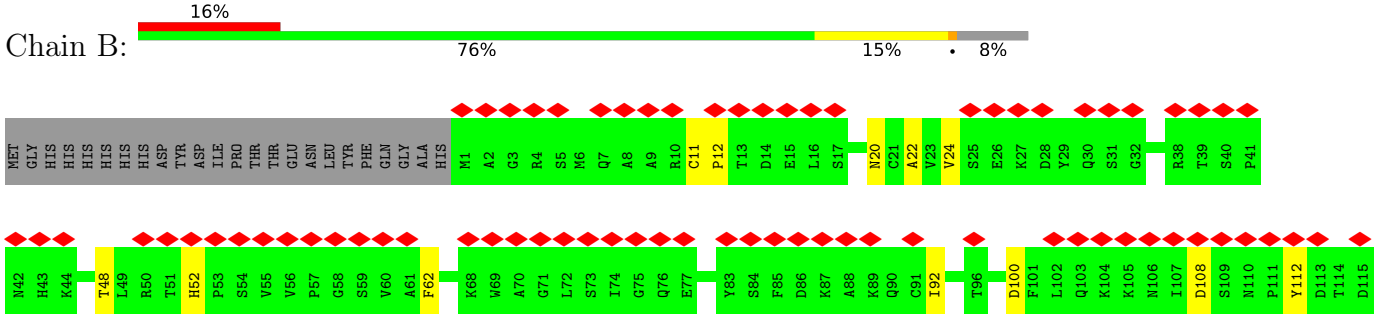
• Molecule 1: Vesicle-fusing ATPase

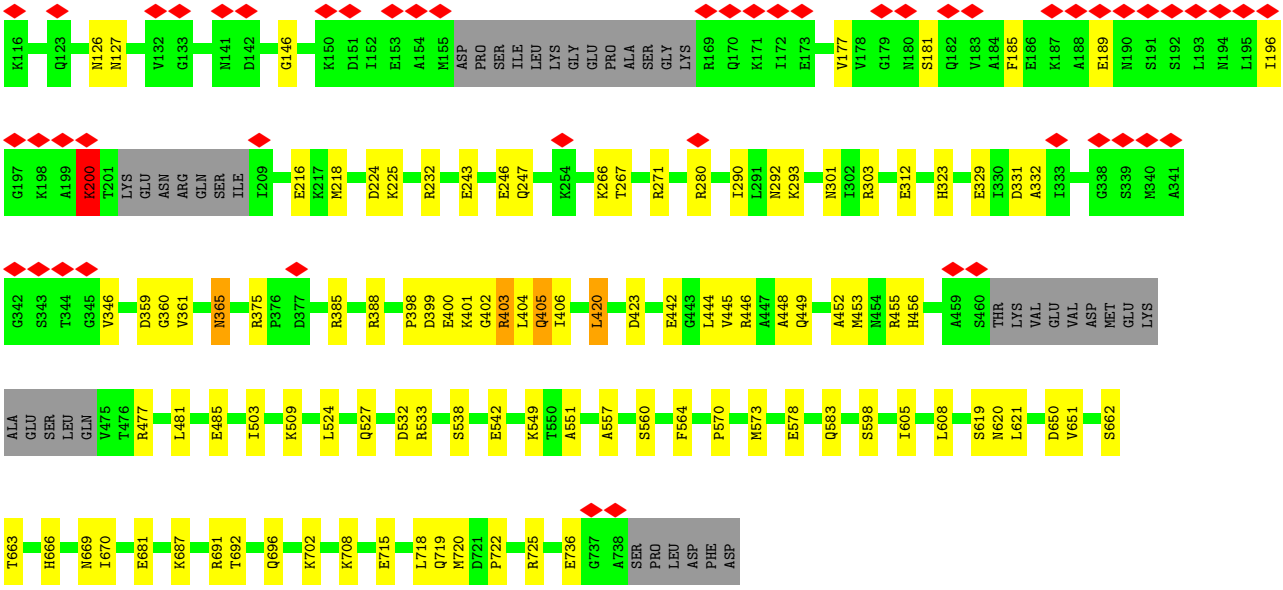
Chain A:



• Molecule 1: Vesicle-fusing ATPase

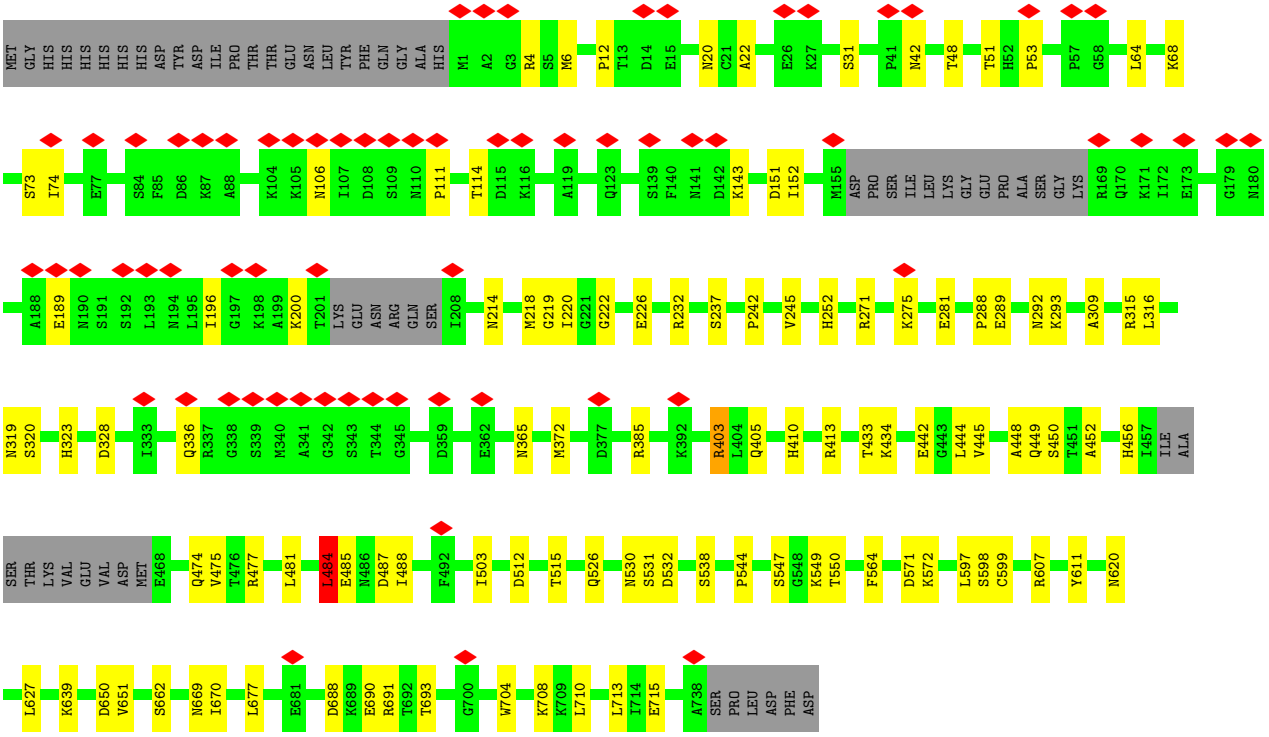
Chain B:





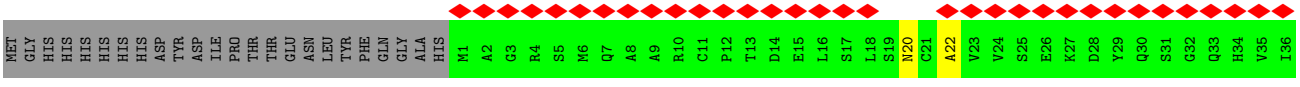
• Molecule 1: Vesicle-fusing ATPase

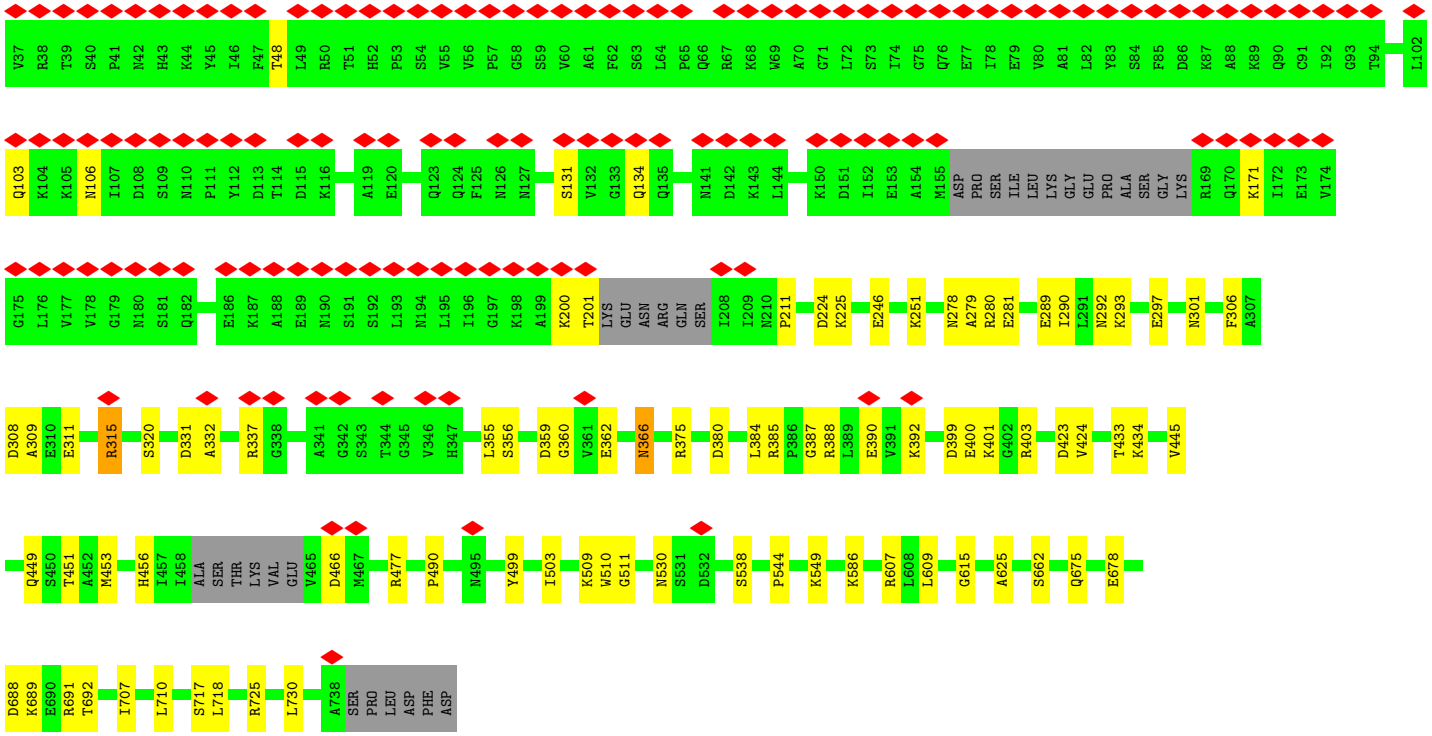
Chain C:



• Molecule 1: Vesicle-fusing ATPase

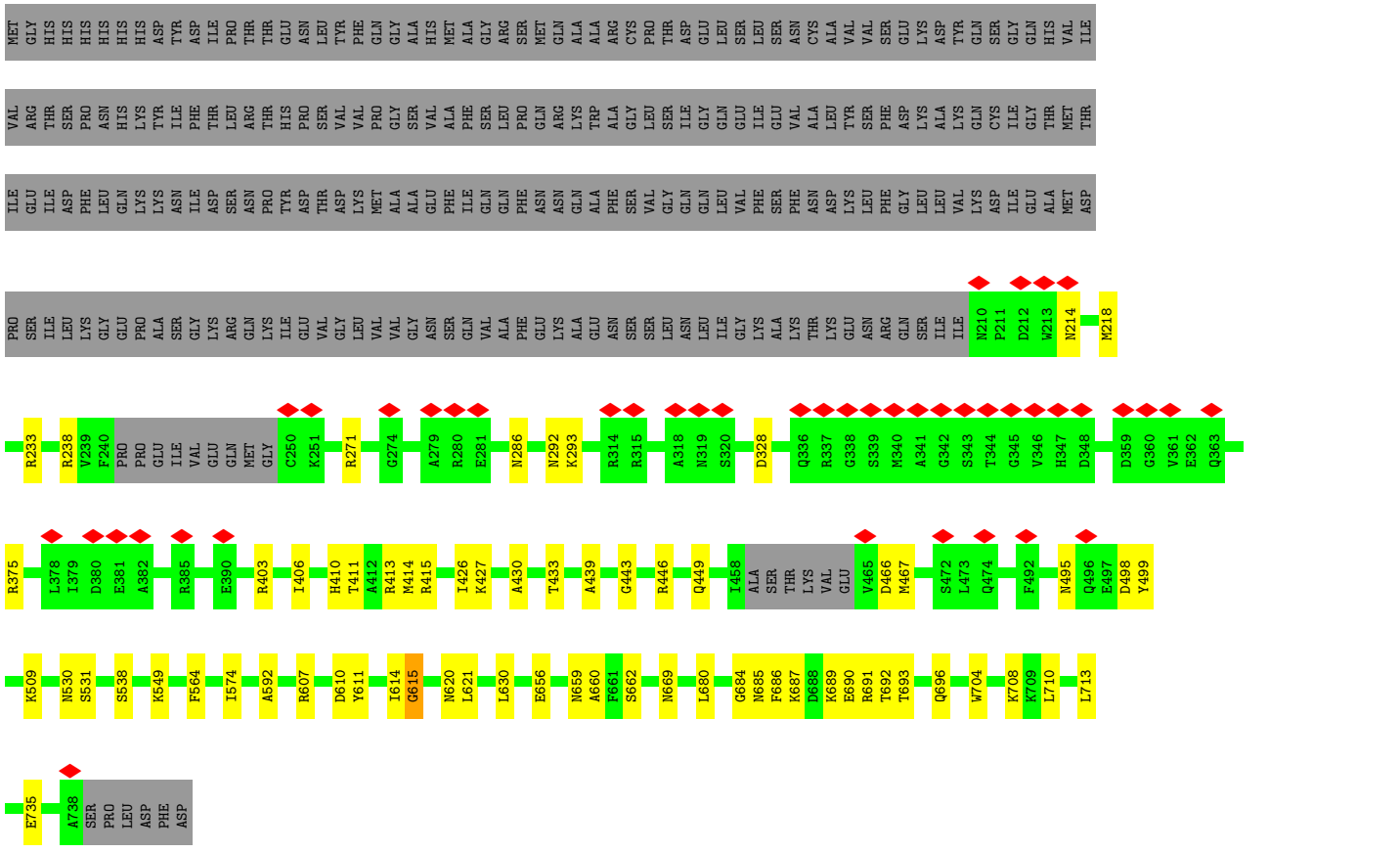
Chain D:





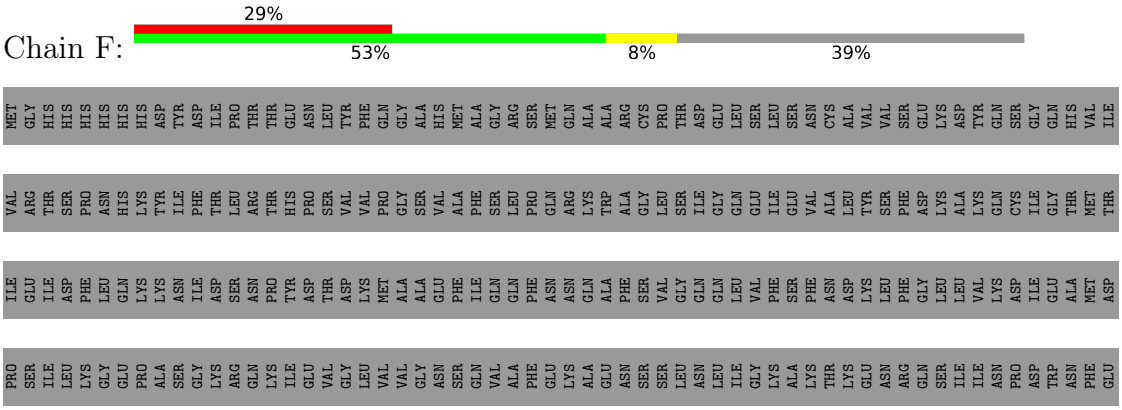
• Molecule 1: Vesicle-fusing ATPase

Chain E:



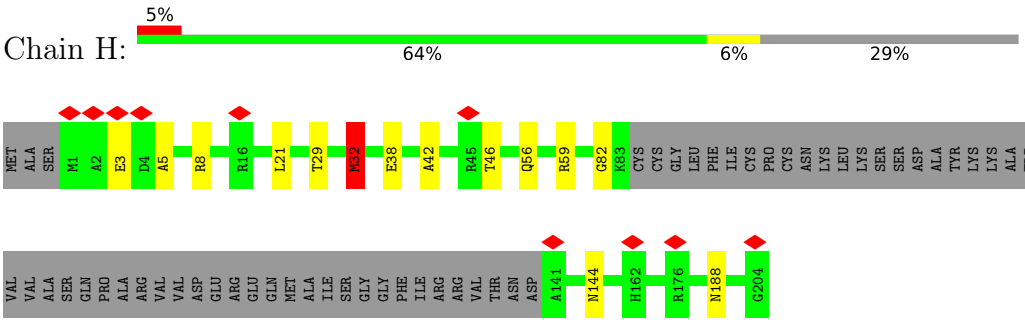
• Molecule 1: Vesicle-fusing ATPase

Chain F:



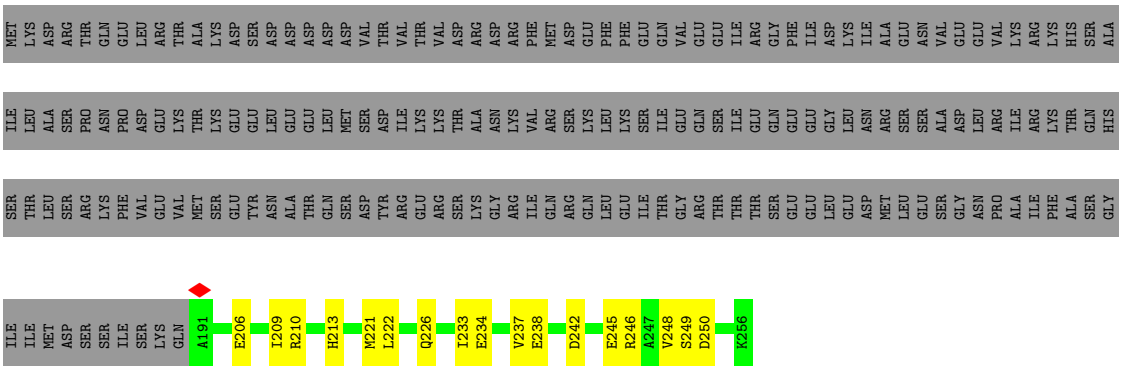
• Molecule 2: Synaptosomal-associated protein 25

Chain H:

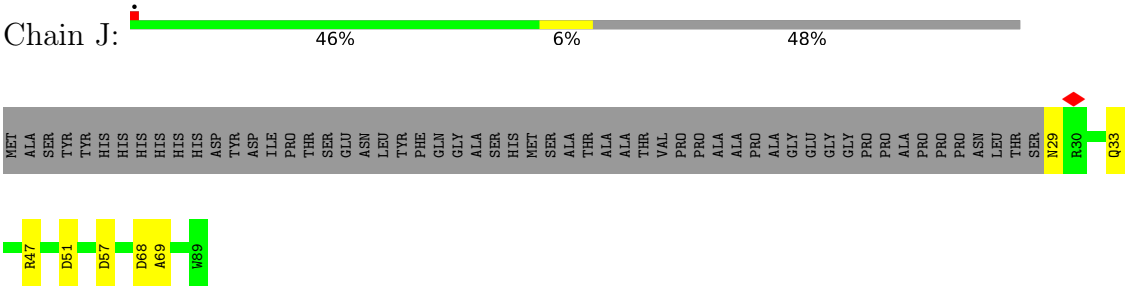


• Molecule 3: Syntaxin-1A

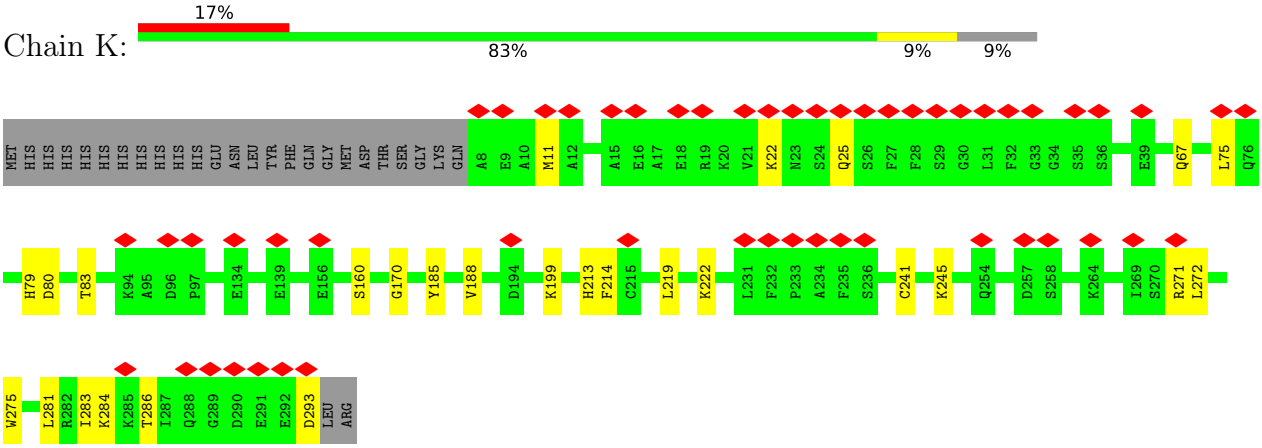
Chain I:



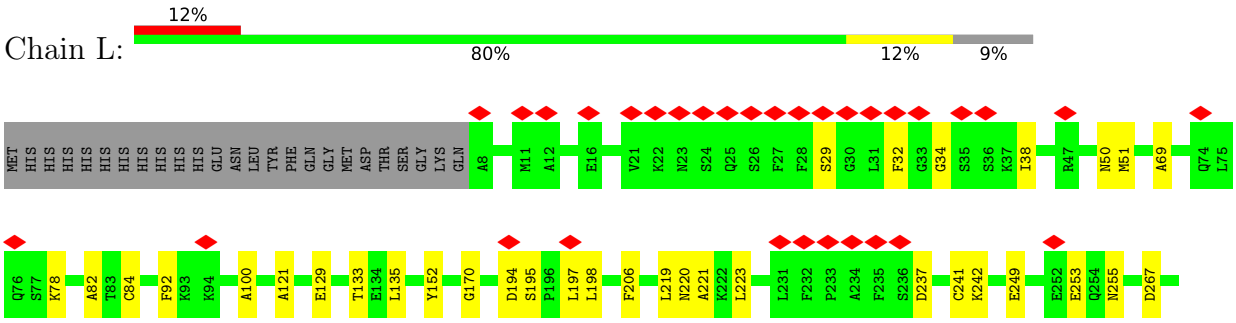
• Molecule 4: Vesicle-associated membrane protein 2

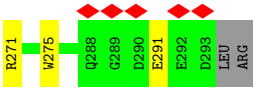


• Molecule 5: Alpha-soluble NSF attachment protein



• Molecule 5: Alpha-soluble NSF attachment protein




R271
W275
Q288
G289
D290
E291
E292
D293
LEU
ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55150	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was carried out in Relion with reconstruction step.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	301.3, 301.3, 301.3	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	0/5531	0.81	7/7450 (0.1%)
1	B	0.62	0/5567	0.86	6/7501 (0.1%)
1	C	0.61	0/5611	0.83	3/7559 (0.0%)
1	D	0.57	0/5642	0.81	5/7601 (0.1%)
1	E	0.54	0/4068	0.84	4/5477 (0.1%)
1	F	0.54	0/3553	0.82	4/4796 (0.1%)
2	H	0.41	0/1171	0.77	0/1557
3	I	0.43	0/541	0.72	1/723 (0.1%)
4	J	0.42	0/496	0.73	0/664
5	K	0.44	0/2291	0.73	2/3082 (0.1%)
5	L	0.44	0/2295	0.72	2/3086 (0.1%)
All	All	0.56	0/36766	0.81	34/49496 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	H	0	1
5	K	0	3
5	L	0	2
All	All	0	7

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	420	LEU	CB-CG-CD2	9.59	127.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	484	LEU	CB-CG-CD2	9.01	126.32	111.00
1	E	610	ASP	CB-CG-OD1	7.81	125.33	118.30
1	E	615	GLY	N-CA-C	-7.37	94.67	113.10
1	D	730	LEU	CA-CB-CG	7.26	132.00	115.30
1	B	200	LYS	CD-CE-NZ	-7.20	95.13	111.70
1	F	698	VAL	CG1-CB-CG2	7.15	122.34	110.90
1	B	346	VAL	CA-CB-CG2	6.94	121.31	110.90
1	A	610	ASP	CB-CG-OD1	6.70	124.33	118.30
1	F	591	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	615	GLY	N-CA-C	-6.34	97.25	113.10
1	F	615	GLY	N-CA-C	-6.23	97.53	113.10
1	A	615	GLY	N-CA-C	-6.22	97.54	113.10
1	B	403	ARG	NE-CZ-NH1	6.17	123.39	120.30
5	K	67	GLN	CA-CB-CG	6.14	126.90	113.40
1	C	444	LEU	CA-CB-CG	6.10	129.32	115.30
1	D	306	PHE	CB-CG-CD1	6.03	125.02	120.80
1	A	481	LEU	CB-CG-CD1	6.01	121.21	111.00
1	D	306	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	A	291	LEU	CA-CB-CG	5.55	128.06	115.30
1	F	629	LEU	CA-CB-CG	5.49	127.92	115.30
1	B	346	VAL	CG1-CB-CG2	5.40	119.53	110.90
1	A	713	LEU	CA-CB-CG	5.39	127.70	115.30
1	E	271	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	D	609	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	641	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	481	LEU	CA-CB-CG	5.20	127.25	115.30
1	C	403	ARG	NE-CZ-NH1	5.18	122.89	120.30
3	I	222	LEU	CA-CB-CG	5.13	127.09	115.30
5	L	197	LEU	CA-CB-CG	5.13	127.10	115.30
1	E	238	ARG	NE-CZ-NH2	5.12	122.86	120.30
5	K	67	GLN	N-CA-CB	5.10	119.78	110.60
5	L	198	LEU	CA-CB-CG	5.09	127.00	115.30
1	B	444	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	405	GLN	Sidechain
2	H	32	MET	Peptide
5	K	213	HIS	Peptide
5	K	214	PHE	Peptide

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Mol	Chain	Res	Type	Group
5	K	75	LEU	Peptide
5	L	135	LEU	Peptide
5	L	206	PHE	Peptide

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	5446	5558	5576	57	0
1	B	5482	5597	5613	77	0
1	C	5526	5638	5657	71	0
1	D	5557	5675	5690	54	0
1	E	4010	4120	4134	39	0
1	F	3507	3500	3503	32	0
2	H	1171	1130	1134	8	0
3	I	536	524	527	11	0
4	J	493	491	491	4	0
5	K	2251	2179	2188	14	0
5	L	2255	2192	2199	17	0
6	A	31	12	12	0	0
6	B	62	24	24	7	0
6	C	62	24	24	5	0
6	D	62	24	24	2	0
6	E	31	12	12	2	0
6	F	31	12	12	2	0
7	A	27	12	12	1	0
7	E	27	12	12	1	0
All	All	36567	36736	36844	349	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 5.

All (349) 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)
1:D:510:TRP:O	1:D:675:GLN:NE2	2.04	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ARG:NH1	1:D:433:THR:O	2.07	0.87
1:D:718:LEU:O	1:D:725:ARG:NH1	2.09	0.86
1:C:669:ASN:ND2	1:C:704:TRP:O	2.09	0.86
1:D:538:SER:O	1:D:662:SER:OG	1.95	0.85
1:A:538:SER:O	1:A:662:SER:OG	1.94	0.85
2:H:42:ALA:O	2:H:46:THR:OG1	1.95	0.84
1:B:453:MET:O	1:B:456:HIS:ND1	2.12	0.81
1:C:106:ASN:O	1:C:143:LYS:NZ	2.12	0.81
1:B:687:LYS:O	1:B:691:ARG:NH2	2.14	0.81
1:C:512:ASP:O	1:C:515:THR:OG1	1.99	0.80
1:A:251:LYS:O	1:B:446:ARG:NH1	2.15	0.80
1:D:509:LYS:NZ	1:D:511:GLY:O	2.15	0.80
1:A:103:GLN:OE1	1:A:106:ASN:ND2	2.15	0.80
1:B:681:GLU:OE1	1:B:691:ARG:NH2	2.15	0.79
1:E:403:ARG:NH1	1:E:433:THR:O	2.15	0.79
5:K:271:ARG:NH1	5:K:272:LEU:O	2.16	0.78
5:L:267:ASP:O	5:L:271:ARG:NH1	2.16	0.78
1:D:320:SER:N	1:D:366:ASN:OD1	2.17	0.77
1:F:538:SER:O	1:F:662:SER:OG	2.01	0.77
1:C:564:PHE:O	1:C:598:SER:OG	2.03	0.76
1:C:550:THR:OG1	6:C:801:ATP:O1A	2.02	0.76
2:H:56:GLN:OE1	2:H:59:ARG:NH2	2.18	0.76
1:C:410:HIS:NE2	1:C:442:GLU:OE2	2.19	0.75
1:E:607:ARG:NH2	1:E:611:TYR:O	2.19	0.75
1:B:196:ILE:O	1:B:200:LYS:NZ	2.19	0.74
1:B:360:GLY:O	1:C:271:ARG:NH1	2.21	0.73
1:B:557:ALA:O	1:B:560:SER:OG	2.06	0.73
1:D:103:GLN:OE1	1:D:106:ASN:ND2	2.21	0.73
1:A:352:ASN:ND2	1:B:329:GLU:OE1	2.21	0.72
1:E:414:MET:SD	1:E:449:GLN:NE2	2.63	0.72
1:B:542:GLU:OE1	1:B:666:HIS:ND1	2.14	0.72
1:A:688:ASP:O	1:A:692:THR:OG1	2.06	0.72
3:I:226:GLN:NE2	4:J:57:ASP:OD1	2.22	0.72
1:D:311:GLU:OE1	1:D:315:ARG:NH1	2.23	0.72
5:K:283:ILE:O	5:K:286:THR:OG1	2.07	0.71
1:F:607:ARG:NH2	1:F:611:TYR:O	2.22	0.71
1:E:735:GLU:OE1	1:E:735:GLU:N	2.22	0.71
1:E:411:THR:OG1	1:E:415:ARG:NH1	2.24	0.71
1:B:359:ASP:OD2	1:B:385:ARG:NH2	2.24	0.71
1:B:303:ARG:NH2	1:C:288:PRO:O	2.24	0.70
1:C:538:SER:OG	1:C:662:SER:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:ARG:NH2	1:C:611:TYR:O	2.25	0.70
1:E:233:ARG:NH1	1:F:487:ASP:O	2.24	0.70
1:C:677:LEU:O	1:C:691:ARG:NH2	2.24	0.70
1:B:22:ALA:N	1:B:48:THR:O	2.22	0.69
1:D:717:SER:OG	1:D:725:ARG:O	2.09	0.69
1:A:415:ARG:O	1:A:418:GLN:NE2	2.26	0.69
1:C:538:SER:O	1:C:662:SER:OG	2.06	0.68
1:D:356:SER:OG	1:E:328:ASP:OD2	2.07	0.68
1:B:385:ARG:NH2	6:C:802:ATP:O1B	2.26	0.68
1:C:22:ALA:N	1:C:48:THR:O	2.27	0.68
1:A:686:PHE:O	1:A:691:ARG:NH2	2.26	0.68
1:B:538:SER:O	1:B:662:SER:OG	2.06	0.67
1:C:214:ASN:ND2	1:D:466:ASP:OD1	2.26	0.67
1:D:289:GLU:N	1:D:289:GLU:OE1	2.28	0.67
1:A:385:ARG:NH2	6:B:801:ATP:O1B	2.26	0.67
1:C:403:ARG:NE	1:C:433:THR:O	2.26	0.67
1:C:403:ARG:NH1	1:C:434:LYS:O	2.27	0.67
1:B:692:THR:O	1:B:696:GLN:NE2	2.28	0.67
1:A:451:THR:O	1:A:455:ARG:N	2.28	0.67
1:D:22:ALA:N	1:D:48:THR:O	2.28	0.66
1:E:439:ALA:O	1:E:443:GLY:N	2.28	0.66
1:C:442:GLU:OE1	6:C:802:ATP:O2'	2.13	0.66
5:L:129:GLU:O	5:L:133:THR:OG1	2.08	0.66
1:C:708:LYS:NZ	6:C:801:ATP:O3A	2.30	0.65
1:F:300:ALA:O	1:F:304:LYS:N	2.28	0.65
1:B:266:LYS:NZ	6:B:801:ATP:O2B	2.28	0.65
1:C:544:PRO:O	1:C:547:SER:OG	2.08	0.64
1:B:189:GLU:OE1	1:B:189:GLU:N	2.30	0.64
1:E:430:ALA:O	1:E:433:THR:OG1	2.10	0.64
1:A:523:LEU:O	1:B:719:GLN:NE2	2.31	0.64
1:B:405:GLN:HG2	1:B:406:ILE:N	2.13	0.64
5:K:25:GLN:N	5:K:25:GLN:OE1	2.32	0.63
1:A:718:LEU:O	1:A:725:ARG:NH1	2.32	0.63
1:B:718:LEU:O	1:B:725:ARG:NH1	2.32	0.63
1:B:402:GLY:O	1:B:405:GLN:NE2	2.32	0.63
5:L:50:ASN:OD1	5:L:51:MET:N	2.32	0.62
1:B:620:ASN:OD1	1:B:621:LEU:N	2.32	0.62
1:D:387:GLY:N	1:D:390:GLU:OE2	2.32	0.62
1:E:630:LEU:HD23	1:E:660:ALA:HB1	1.82	0.62
1:D:538:SER:OG	1:D:662:SER:N	2.33	0.62
1:E:549:LYS:N	6:E:801:ATP:O2A	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ASN:OD1	1:A:621:LEU:N	2.33	0.61
1:A:415:ARG:NH2	1:A:420:LEU:O	2.33	0.61
1:B:400:GLU:O	1:B:404:LEU:N	2.33	0.61
1:D:278:ASN:OD1	1:D:279:ALA:N	2.33	0.61
5:L:241:CYS:SG	5:L:242:LYS:N	2.74	0.61
1:E:410:HIS:NE2	7:E:802:ADP:N7	2.49	0.60
1:F:447:ALA:O	1:F:450:SER:N	2.35	0.60
1:D:308:ASP:OD1	1:D:309:ALA:N	2.34	0.60
1:D:403:ARG:NH2	1:D:434:LYS:O	2.35	0.59
5:L:220:ASN:OD1	5:L:221:ALA:N	2.35	0.59
1:C:189:GLU:N	1:C:189:GLU:OE1	2.36	0.59
1:E:466:ASP:OD1	1:E:467:MET:N	2.36	0.59
1:E:692:THR:O	1:E:696:GLN:NE2	2.35	0.59
1:C:31:SER:OG	1:C:51:THR:N	2.34	0.59
1:D:675:GLN:NE2	1:D:678:GLU:OE2	2.36	0.59
1:B:267:THR:N	6:B:801:ATP:O1A	2.35	0.58
1:C:710:LEU:O	1:C:713:LEU:N	2.36	0.58
1:A:267:THR:OG1	7:A:802:ADP:O2A	2.18	0.58
1:B:11:CYS:N	1:B:62:PHE:O	2.36	0.58
1:A:534:THR:OG1	1:B:715:GLU:OE1	2.21	0.58
1:D:355:LEU:O	1:D:388:ARG:NH1	2.34	0.58
5:L:34:GLY:O	5:L:38:ILE:N	2.34	0.58
1:B:246:GLU:O	1:C:413:ARG:NH2	2.36	0.58
1:E:690:GLU:O	1:E:693:THR:OG1	2.18	0.58
1:A:610:ASP:OD1	1:A:619:SER:N	2.34	0.57
1:E:498:ASP:OD1	1:E:499:TYR:N	2.37	0.57
1:A:299:GLU:OE1	1:A:303:ARG:NH2	2.37	0.57
1:D:246:GLU:O	1:E:413:ARG:NH2	2.38	0.57
1:D:544:PRO:O	1:D:549:LYS:NZ	2.38	0.57
1:F:399:ASP:O	1:F:402:GLY:N	2.37	0.57
1:C:232:ARG:NH2	1:D:451:THR:OG1	2.38	0.57
1:B:303:ARG:NE	1:C:289:GLU:OE1	2.38	0.57
4:J:29:ASN:O	4:J:33:GLN:NE2	2.38	0.57
1:B:100:ASP:O	1:B:146:GLY:N	2.36	0.57
1:D:359:ASP:OD1	1:D:360:GLY:N	2.38	0.57
5:L:78:LYS:O	5:L:82:ALA:N	2.38	0.57
1:B:532:ASP:OD1	1:B:533:ARG:N	2.38	0.56
1:D:337:ARG:NE	1:D:380:ASP:OD2	2.38	0.56
1:D:445:VAL:O	1:D:449:GLN:NE2	2.39	0.56
1:D:499:TYR:O	1:D:503:ILE:N	2.37	0.56
1:A:280:ARG:NH1	1:A:321:GLY:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:LYS:NZ	1:C:281:GLU:OE2	2.35	0.56
1:C:531:SER:OG	1:C:532:ASP:N	2.38	0.56
5:K:170:GLY:O	5:K:275:TRP:NE1	2.39	0.56
2:H:56:GLN:NE2	3:I:234:GLU:OE1	2.39	0.56
1:B:267:THR:OG1	6:B:801:ATP:O1A	2.15	0.55
1:C:650:ASP:OD1	1:C:651:VAL:N	2.38	0.55
1:D:200:LYS:O	1:D:201:THR:OG1	2.17	0.55
1:B:720:MET:O	1:B:725:ARG:NH2	2.38	0.55
1:B:650:ASP:OD1	1:B:651:VAL:N	2.40	0.55
1:B:399:ASP:OD2	1:B:401:LYS:NZ	2.29	0.55
1:F:302:ILE:O	1:F:357:LYS:NZ	2.40	0.55
5:K:241:CYS:O	5:K:245:LYS:N	2.34	0.55
1:B:127:ASN:N	1:B:177:VAL:O	2.40	0.54
1:E:538:SER:OG	1:E:662:SER:N	2.35	0.54
1:C:385:ARG:NH2	6:D:802:ATP:O3A	2.41	0.54
1:D:224:ASP:OD1	1:D:225:LYS:N	2.40	0.54
4:J:68:ASP:OD1	4:J:69:ALA:N	2.40	0.54
1:A:22:ALA:N	1:A:48:THR:O	2.40	0.54
1:F:495:ASN:O	1:F:496:GLN:NE2	2.41	0.54
3:I:246:ARG:O	3:I:249:SER:OG	2.23	0.54
1:A:340:MET:SD	1:B:583:GLN:NE2	2.79	0.53
1:F:311:GLU:OE1	1:F:314:ARG:NH2	2.40	0.53
1:B:503:ILE:HG22	1:B:551:ALA:HB1	1.90	0.53
1:B:485:GLU:N	1:B:485:GLU:OE1	2.40	0.53
1:D:362:GLU:OE1	1:D:362:GLU:N	2.40	0.53
1:B:549:LYS:NZ	6:B:802:ATP:O3G	2.41	0.53
1:B:232:ARG:O	1:C:450:SER:OG	2.27	0.53
1:D:280:ARG:HE	1:D:281:GLU:H	1.57	0.53
1:C:73:SER:OG	1:C:74:ILE:N	2.40	0.53
1:E:687:LYS:N	1:E:690:GLU:OE2	2.38	0.53
3:I:246:ARG:NH1	5:K:79:HIS:O	2.42	0.53
1:C:598:SER:OG	1:C:599:CYS:N	2.42	0.52
5:L:237:ASP:O	5:L:241:CYS:N	2.36	0.52
5:L:255:ASN:N	5:L:291:GLU:OE2	2.43	0.52
1:A:230:ILE:O	1:A:234:ALA:HB3	2.08	0.52
1:A:312:GLU:OE1	1:A:315:ARG:NH1	2.42	0.52
1:B:420:LEU:O	1:B:420:LEU:HG	2.09	0.52
1:E:686:PHE:O	1:E:691:ARG:NE	2.41	0.52
1:A:662:SER:OG	1:A:663:THR:N	2.43	0.52
1:B:578:GLU:OE2	1:B:619:SER:OG	2.25	0.52
1:B:292:ASN:OD1	1:B:293:LYS:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASP:OD1	1:D:332:ALA:N	2.43	0.52
1:F:549:LYS:NZ	6:F:801:ATP:O2G	2.42	0.52
1:A:263:GLY:O	1:A:437:SER:OG	2.27	0.52
1:B:331:ASP:OD1	1:B:332:ALA:N	2.43	0.52
1:D:399:ASP:OD1	1:D:400:GLU:N	2.40	0.52
1:B:722:PRO:HA	1:B:725:ARG:HE	1.75	0.51
1:C:292:ASN:OD1	1:C:293:LYS:N	2.43	0.51
1:B:216:GLU:OE1	1:B:216:GLU:N	2.43	0.51
1:E:530:ASN:OD1	1:E:531:SER:N	2.44	0.51
1:C:627:LEU:HD11	1:D:607:ARG:HD3	1.91	0.51
1:F:407:LEU:O	1:F:411:THR:N	2.42	0.51
3:I:238:GLU:O	3:I:242:ASP:N	2.40	0.51
1:A:348:ASP:OD2	1:B:375:ARG:NH2	2.43	0.51
2:H:38:GLU:OE2	3:I:213:HIS:NE2	2.44	0.51
5:L:249:GLU:O	5:L:253:GLU:N	2.43	0.51
1:A:374:ASN:ND2	1:A:374:ASN:O	2.43	0.51
1:D:251:LYS:O	1:E:446:ARG:NH2	2.42	0.51
1:F:522:GLU:HA	1:F:525:VAL:HG12	1.92	0.51
1:C:456:HIS:HE2	1:C:474:GLN:C	2.14	0.51
1:F:591:ASP:OD1	1:F:592:ALA:N	2.44	0.51
1:F:592:ALA:O	1:F:595:SER:OG	2.23	0.50
1:F:669:ASN:ND2	1:F:704:TRP:O	2.44	0.50
1:F:224:ASP:O	1:F:228:SER:N	2.43	0.50
4:J:47:ARG:NH1	4:J:51:ASP:OD1	2.44	0.50
1:A:254:LYS:NZ	1:A:364:LEU:O	2.43	0.50
1:C:448:ALA:HB2	1:C:481:LEU:HB2	1.92	0.50
1:D:423:ASP:OD1	1:D:424:VAL:N	2.45	0.50
1:F:659:ASN:OD1	1:F:660:ALA:N	2.44	0.50
5:K:293:ASP:OD1	5:K:293:ASP:N	2.44	0.50
1:E:669:ASN:ND2	1:E:704:TRP:O	2.43	0.50
1:F:688:ASP:OD1	1:F:689:LYS:N	2.45	0.50
1:F:708:LYS:NZ	6:F:801:ATP:O3A	2.43	0.49
1:A:360:GLY:O	1:B:271:ARG:NH2	2.46	0.49
1:B:605:ILE:O	1:B:608:LEU:N	2.45	0.49
1:C:309:ALA:HB2	1:C:323:HIS:CG	2.47	0.49
1:B:243:GLU:OE1	1:B:247:GLN:NE2	2.46	0.49
1:C:669:ASN:OD1	1:C:670:ILE:N	2.46	0.49
1:A:127:ASN:N	1:A:177:VAL:O	2.43	0.49
1:E:656:GLU:OE2	1:F:648:ARG:NH2	2.43	0.49
1:A:64:LEU:O	1:A:68:LYS:N	2.44	0.49
1:B:216:GLU:HG2	1:B:218:MET:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:VAL:O	1:B:449:GLN:NE2	2.45	0.49
1:A:650:ASP:OD1	1:A:650:ASP:N	2.45	0.49
1:B:108:ASP:OD2	1:B:112:TYR:OH	2.26	0.49
1:C:452:ALA:O	1:C:456:HIS:N	2.44	0.49
5:L:170:GLY:O	5:L:275:TRP:NE1	2.46	0.49
1:D:707:ILE:O	1:D:710:LEU:N	2.46	0.48
1:A:442:GLU:O	1:A:446:ARG:N	2.42	0.48
1:A:100:ASP:OD1	1:A:101:PHE:N	2.46	0.48
1:A:189:GLU:OE1	1:A:190:ASN:ND2	2.47	0.48
1:B:224:ASP:OD1	1:B:225:LYS:N	2.47	0.48
1:B:736:GLU:N	1:B:736:GLU:OE1	2.46	0.48
1:C:690:GLU:O	1:C:693:THR:N	2.44	0.48
1:A:487:ASP:OD1	1:A:488:ILE:N	2.47	0.48
1:F:650:ASP:OD1	1:F:651:VAL:N	2.46	0.48
1:C:484:LEU:HD13	1:C:485:GLU:HB3	1.96	0.48
1:B:92:ILE:O	1:B:181:SER:OG	2.12	0.47
5:K:281:LEU:HA	5:K:284:LYS:HG2	1.96	0.47
1:C:64:LEU:O	1:C:68:LYS:N	2.41	0.47
1:C:336:GLN:OE1	1:D:375:ARG:NH2	2.46	0.47
2:H:42:ALA:O	2:H:46:THR:CB	2.61	0.47
1:A:525:VAL:O	1:A:528:THR:OG1	2.26	0.47
1:B:442:GLU:HA	1:B:445:VAL:HG12	1.95	0.47
5:K:80:ASP:O	5:K:83:THR:OG1	2.25	0.47
5:K:185:TYR:HA	5:K:188:VAL:HG12	1.96	0.47
1:C:226:GLU:OE1	1:C:226:GLU:N	2.45	0.47
1:B:402:GLY:HA2	1:B:405:GLN:OE1	2.15	0.47
1:E:689:LYS:O	1:E:692:THR:OG1	2.22	0.47
1:F:697:GLN:OE1	1:F:697:GLN:N	2.48	0.47
5:L:219:LEU:O	5:L:223:LEU:N	2.47	0.47
1:A:288:PRO:HA	1:A:291:LEU:HD13	1.97	0.47
1:D:688:ASP:OD1	1:D:691:ARG:NH1	2.48	0.47
1:E:292:ASN:OD1	1:E:293:LYS:N	2.45	0.47
1:D:131:SER:N	1:D:134:GLN:OE1	2.48	0.46
1:F:720:MET:O	1:F:725:ARG:NE	2.37	0.46
1:E:620:ASN:OD1	1:E:621:LEU:N	2.49	0.46
1:E:708:LYS:NZ	6:E:801:ATP:O1B	2.49	0.46
1:C:475:VAL:O	1:C:477:ARG:NH1	2.49	0.46
2:H:29:THR:HA	2:H:32:MET:HG3	1.97	0.46
1:E:426:ILE:HG13	1:E:427:LYS:HD3	1.96	0.46
1:E:614:ILE:HD12	1:E:615:GLY:N	2.31	0.46
1:A:100:ASP:O	1:A:146:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:GLU:O	1:D:301:ASN:ND2	2.49	0.45
1:B:312:GLU:OE1	1:B:323:HIS:NE2	2.27	0.45
1:C:242:PRO:O	1:C:245:VAL:HG12	2.16	0.45
1:E:406:ILE:O	1:E:410:HIS:ND1	2.31	0.45
3:I:206:GLU:HA	3:I:209:ILE:HG22	1.97	0.45
1:B:361:VAL:O	1:C:271:ARG:NE	2.49	0.45
1:C:531:SER:OG	1:C:532:ASP:O	2.35	0.45
1:A:123:GLN:OE1	1:A:123:GLN:N	2.50	0.45
1:C:385:ARG:NH2	6:D:802:ATP:O3B	2.48	0.45
1:C:571:ASP:OD1	1:C:572:LYS:N	2.50	0.45
1:D:292:ASN:OD1	1:D:293:LYS:N	2.44	0.45
5:L:29:SER:OG	5:L:32:PHE:O	2.21	0.45
1:C:242:PRO:HA	1:C:245:VAL:HG12	1.99	0.45
1:A:114:THR:HG1	1:A:197:GLY:HA3	1.81	0.45
1:C:597:LEU:HA	1:C:639:LYS:O	2.16	0.44
1:D:453:MET:O	1:D:456:HIS:N	2.50	0.44
1:B:564:PHE:HD2	1:B:598:SER:HG	1.65	0.44
1:A:77:GLU:OE1	1:A:77:GLU:N	2.50	0.44
1:B:385:ARG:HE	1:B:388:ARG:NH1	2.15	0.44
1:C:487:ASP:OD1	1:C:488:ILE:N	2.50	0.44
1:C:526:GLN:O	1:C:530:ASN:ND2	2.51	0.44
1:A:243:GLU:O	1:A:247:GLN:NE2	2.43	0.44
1:B:185:PHE:H	1:B:200:LYS:HB2	1.82	0.44
1:C:445:VAL:O	1:C:449:GLN:NE2	2.50	0.44
1:D:384:LEU:HB3	1:D:392:LYS:HE3	1.99	0.44
1:C:237:SER:HB3	1:C:252:HIS:ND1	2.32	0.44
1:E:710:LEU:HA	1:E:713:LEU:CD2	2.48	0.43
1:F:686:PHE:O	1:F:691:ARG:NH2	2.51	0.43
2:H:59:ARG:NH1	5:K:160:SER:OG	2.51	0.43
3:I:245:GLU:HA	3:I:248:VAL:HG22	2.00	0.43
1:B:524:LEU:O	1:B:527:GLN:HB3	2.19	0.43
1:A:242:PRO:HA	1:A:245:VAL:HG12	2.01	0.43
1:A:688:ASP:OD1	1:A:689:LYS:N	2.51	0.43
3:I:242:ASP:OD1	3:I:246:ARG:NH2	2.44	0.43
5:K:11:MET:SD	5:K:11:MET:N	2.91	0.43
5:L:121:ALA:O	5:L:152:TYR:OH	2.32	0.43
1:A:593:TYR:O	1:A:638:ARG:HD3	2.18	0.43
1:B:538:SER:OG	1:B:662:SER:N	2.46	0.43
1:D:359:ASP:OD1	1:D:388:ARG:NH2	2.52	0.43
1:E:564:PHE:HE2	1:E:592:ALA:HB2	1.83	0.43
1:F:620:ASN:OD1	1:F:621:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ASP:O	1:A:594:LYS:NZ	2.43	0.43
1:C:538:SER:O	1:C:662:SER:N	2.52	0.43
1:A:648:ARG:NH1	1:F:656:GLU:OE1	2.52	0.42
1:D:251:LYS:O	1:E:446:ARG:NH1	2.49	0.42
1:F:614:ILE:HD12	1:F:615:GLY:N	2.34	0.42
1:B:290:ILE:HD12	1:B:290:ILE:H	1.83	0.42
1:C:690:GLU:OE1	1:C:690:GLU:N	2.52	0.42
1:C:549:LYS:NZ	6:C:801:ATP:O3G	2.47	0.42
1:F:349:THR:O	1:F:353:GLN:N	2.43	0.42
5:L:92:PHE:HB2	5:L:100:ALA:HB2	2.00	0.42
1:A:388:ARG:NH1	6:B:801:ATP:O1B	2.52	0.42
1:F:300:ALA:O	1:F:304:LYS:HG2	2.20	0.42
1:F:585:MET:O	1:F:589:PHE:HB2	2.19	0.42
1:C:4:ARG:NE	1:C:6:MET:SD	2.93	0.42
1:E:680:LEU:O	1:E:684:GLY:N	2.46	0.42
5:K:219:LEU:O	5:K:222:LYS:N	2.52	0.42
1:A:286:ASN:OD1	1:A:288:PRO:HD2	2.19	0.42
1:B:708:LYS:NZ	6:B:802:ATP:O3B	2.42	0.42
1:C:531:SER:O	1:C:639:LYS:NZ	2.51	0.42
1:A:411:THR:O	1:A:414:MET:N	2.53	0.42
1:B:365:ASN:ND2	1:B:365:ASN:O	2.50	0.42
1:B:452:ALA:HA	1:B:455:ARG:HE	1.85	0.42
1:C:111:PRO:HB2	1:C:196:ILE:HD12	2.02	0.42
1:C:222:GLY:N	1:C:405:GLN:OE1	2.47	0.42
1:D:689:LYS:O	1:D:692:THR:OG1	2.35	0.42
2:H:3:GLU:OE2	2:H:5:ALA:HB2	2.19	0.42
1:C:151:ASP:OD1	1:C:152:ILE:N	2.53	0.42
1:D:359:ASP:OD2	1:D:385:ARG:NH1	2.43	0.42
1:A:230:ILE:O	1:A:234:ALA:N	2.51	0.41
1:A:254:LYS:HE2	1:A:358:ILE:O	2.19	0.41
5:L:194:ASP:OD1	5:L:195:SER:N	2.52	0.41
1:D:290:ILE:HD12	1:D:290:ILE:H	1.86	0.41
1:D:356:SER:O	1:E:286:ASN:ND2	2.53	0.41
1:D:434:LYS:HE2	1:D:434:LYS:HA	2.02	0.41
3:I:233:ILE:O	3:I:237:VAL:N	2.52	0.41
1:A:290:ILE:HG13	1:A:290:ILE:O	2.21	0.41
1:A:711:LEU:HA	1:A:714:ILE:HG12	2.02	0.41
1:B:398:PRO:O	1:B:403:ARG:NH1	2.52	0.41
1:B:662:SER:OG	1:B:663:THR:N	2.52	0.41
1:C:503:ILE:HD12	1:C:503:ILE:O	2.21	0.41
1:D:586:LYS:HE2	1:E:574:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:THR:HG21	1:C:200:LYS:HG2	2.01	0.41
1:C:328:ASP:HA	1:C:372:MET:HG2	2.02	0.41
1:F:319:ASN:OD1	1:F:320:SER:N	2.51	0.41
1:A:528:THR:OG1	1:A:529:LYS:N	2.53	0.41
1:C:218:MET:O	1:C:220:ILE:N	2.54	0.41
1:C:319:ASN:O	1:C:320:SER:OG	2.35	0.41
1:A:414:MET:O	1:A:418:GLN:N	2.54	0.41
1:C:315:ARG:HD2	1:C:316:LEU:HD12	2.03	0.41
1:F:499:TYR:OH	1:F:554:ALA:O	2.36	0.41
1:B:527:GLN:NE2	1:C:715:GLU:O	2.52	0.40
1:B:24:VAL:O	1:B:52:HIS:N	2.54	0.40
1:B:570:PRO:HA	1:B:573:MET:HG2	2.02	0.40
5:L:69:ALA:HB2	5:L:84:CYS:HB2	2.03	0.40
1:B:185:PHE:O	1:B:200:LYS:HB2	2.20	0.40
1:A:567:ILE:HD13	1:A:601:VAL:CG1	2.51	0.40
1:B:448:ALA:HB2	1:B:481:LEU:HB2	2.03	0.40
1:B:669:ASN:OD1	1:B:670:ILE:N	2.54	0.40
1:D:625:ALA:HB1	1:E:574:ILE:HD11	2.04	0.40
1:D:337:ARG:HE	1:E:375:ARG:HH12	1.70	0.40
3:I:250:ASP:OD1	5:K:79:HIS:NE2	2.55	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	691/768 (90%)	668 (97%)	21 (3%)	2 (0%)	41	76
1	B	696/768 (91%)	669 (96%)	25 (4%)	2 (0%)	41	76
1	C	701/768 (91%)	683 (97%)	14 (2%)	4 (1%)	25	65
1	D	705/768 (92%)	671 (95%)	32 (4%)	2 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	508/768 (66%)	501 (99%)	7 (1%)	0	100 100
1	F	454/768 (59%)	435 (96%)	18 (4%)	1 (0%)	47 81
2	H	143/207 (69%)	135 (94%)	6 (4%)	2 (1%)	11 47
3	I	64/256 (25%)	62 (97%)	2 (3%)	0	100 100
4	J	59/117 (50%)	58 (98%)	1 (2%)	0	100 100
5	K	284/313 (91%)	254 (89%)	30 (11%)	0	100 100
5	L	284/313 (91%)	261 (92%)	23 (8%)	0	100 100
All	All	4589/5814 (79%)	4397 (96%)	179 (4%)	13 (0%)	44 76

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	688	ASP
1	C	219	GLY
1	B	12	PRO
1	D	490	PRO
2	H	21	LEU
2	H	82	GLY
1	B	423	ASP
1	A	105	LYS
1	F	451	THR
1	C	53	PRO
1	D	211	PRO
1	A	53	PRO
1	C	12	PRO

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	596/658 (91%)	591 (99%)	5 (1%)	81 89
1	B	601/658 (91%)	592 (98%)	9 (2%)	65 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	606/658 (92%)	601 (99%)	5 (1%)	81 89
1	D	610/658 (93%)	603 (99%)	7 (1%)	73 85
1	E	438/658 (67%)	432 (99%)	6 (1%)	67 81
1	F	361/658 (55%)	357 (99%)	4 (1%)	73 85
2	H	127/177 (72%)	123 (97%)	4 (3%)	40 63
3	I	60/235 (26%)	58 (97%)	2 (3%)	38 61
4	J	52/96 (54%)	52 (100%)	0	100 100
5	K	234/260 (90%)	232 (99%)	2 (1%)	78 88
5	L	235/260 (90%)	235 (100%)	0	100 100
All	All	3920/4976 (79%)	3876 (99%)	44 (1%)	74 85

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	337	ARG
1	A	366	ASN
1	A	374	ASN
1	A	727	ARG
1	B	20	ASN
1	B	126	ASN
1	B	200	LYS
1	B	280	ARG
1	B	301	ASN
1	B	365	ASN
1	B	477	ARG
1	B	509	LYS
1	B	702	LYS
1	C	20	ASN
1	C	42	ASN
1	C	365	ASN
1	C	484	LEU
1	C	620	ASN
1	D	20	ASN
1	D	171	LYS
1	D	315	ARG
1	D	366	ASN
1	D	401	LYS
1	D	477	ARG

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Mol	Chain	Res	Type
1	D	530	ASN
1	E	214	ASN
1	E	218	MET
1	E	495	ASN
1	E	509	LYS
1	E	659	ASN
1	E	685	ASN
1	F	375	ARG
1	F	453	MET
1	F	454	ASN
1	F	591	ASP
2	H	8	ARG
2	H	32	MET
2	H	144	ASN
2	H	188	ASN
3	I	210	ARG
3	I	221	MET
5	K	22	LYS
5	K	199	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	106	ASN
1	A	190	ASN
1	A	347	HIS
1	A	530	ASN
1	B	106	ASN
1	B	126	ASN
1	B	252	HIS
1	B	365	ASN
1	B	435	ASN
1	B	505	ASN
1	B	546	HIS
1	B	696	GLN
1	B	719	GLN
1	C	42	ASN
1	C	103	GLN
1	C	128	GLN
1	C	141	ASN
1	C	347	HIS

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Mol	Chain	Res	Type
1	C	374	ASN
1	C	474	GLN
1	C	530	ASN
1	C	696	GLN
1	D	106	ASN
1	D	252	HIS
1	D	301	ASN
1	D	363	GLN
1	D	435	ASN
1	D	456	HIS
1	D	675	GLN
1	E	214	ASN
1	E	252	HIS
1	E	486	ASN
1	E	719	GLN
1	F	286	ASN
1	F	313	GLN
3	I	239	HIS
5	L	57	ASN
5	L	63	ASN
5	L	254	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ATP	C	801	-	26,33,33	0.89	1 (3%)	31,52,52	1.97	8 (25%)
7	ADP	E	802	-	24,29,29	1.05	2 (8%)	29,45,45	1.61	8 (27%)
6	ATP	B	801	-	26,33,33	0.86	0	31,52,52	1.65	6 (19%)
6	ATP	B	802	-	26,33,33	0.98	0	31,52,52	1.93	8 (25%)
6	ATP	F	801	-	26,33,33	0.85	0	31,52,52	1.93	7 (22%)
6	ATP	A	801	-	26,33,33	1.01	1 (3%)	31,52,52	2.25	6 (19%)
6	ATP	C	802	-	26,33,33	0.95	0	31,52,52	1.78	6 (19%)
7	ADP	A	802	-	24,29,29	0.89	1 (4%)	29,45,45	1.70	6 (20%)
6	ATP	D	801	-	26,33,33	0.96	1 (3%)	31,52,52	1.73	5 (16%)
6	ATP	D	802	-	26,33,33	1.09	2 (7%)	31,52,52	1.92	8 (25%)
6	ATP	E	801	-	26,33,33	0.97	1 (3%)	31,52,52	1.85	7 (22%)

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
6	ATP	C	801	-	-	5/18/38/38	0/3/3/3
7	ADP	E	802	-	-	4/12/32/32	0/3/3/3
6	ATP	B	801	-	-	1/18/38/38	0/3/3/3
6	ATP	B	802	-	-	0/18/38/38	0/3/3/3
6	ATP	F	801	-	-	4/18/38/38	0/3/3/3
6	ATP	A	801	-	-	4/18/38/38	0/3/3/3
6	ATP	C	802	-	-	1/18/38/38	0/3/3/3
7	ADP	A	802	-	-	6/12/32/32	0/3/3/3
6	ATP	D	801	-	-	2/18/38/38	0/3/3/3
6	ATP	D	802	-	-	4/18/38/38	0/3/3/3
6	ATP	E	801	-	-	2/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	802	ADP	O4'-C1'	2.58	1.44	1.41
6	D	802	ATP	C2'-C1'	-2.46	1.50	1.53
6	D	801	ATP	C2'-C1'	-2.26	1.50	1.53
7	E	802	ADP	C5-C4	2.25	1.46	1.40
6	E	801	ATP	O4'-C1'	2.18	1.44	1.41
6	D	802	ATP	C5-N7	-2.15	1.31	1.39
6	A	801	ATP	C5-C4	2.15	1.46	1.40
6	C	801	ATP	C2'-C1'	-2.13	1.50	1.53
7	A	802	ADP	C5-C4	2.06	1.46	1.40

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	801	ATP	PA-O3A-PB	-7.39	107.48	132.83
6	A	801	ATP	PB-O3B-PG	-6.20	111.56	132.83
6	D	802	ATP	PB-O3B-PG	-5.99	112.29	132.83
6	C	801	ATP	PA-O3A-PB	-5.58	113.68	132.83
6	E	801	ATP	PB-O3B-PG	-5.49	113.97	132.83
6	F	801	ATP	PB-O3B-PG	-5.48	114.03	132.83
6	B	802	ATP	PA-O3A-PB	-5.37	114.39	132.83
6	C	801	ATP	PB-O3B-PG	-5.36	114.43	132.83
6	D	802	ATP	PA-O3A-PB	-5.09	115.37	132.83
6	D	801	ATP	PB-O3B-PG	-4.98	115.74	132.83
6	C	802	ATP	PB-O3B-PG	-4.90	116.00	132.83
6	A	801	ATP	O4'-C1'-C2'	-4.80	99.92	106.93
7	A	802	ADP	PA-O3A-PB	-4.69	116.73	132.83
6	B	802	ATP	PB-O3B-PG	-4.37	117.82	132.83
6	F	801	ATP	PA-O3A-PB	-4.10	118.74	132.83
6	F	801	ATP	C4-C5-N7	-3.93	105.30	109.40
6	E	801	ATP	PA-O3A-PB	-3.81	119.75	132.83
7	E	802	ADP	C3'-C2'-C1'	3.74	106.61	100.98
6	C	801	ATP	N3-C2-N1	-3.69	122.92	128.68
6	B	801	ATP	C3'-C2'-C1'	3.61	106.41	100.98
6	B	801	ATP	O4'-C1'-C2'	-3.60	101.67	106.93
7	A	802	ADP	C3'-C2'-C1'	3.58	106.36	100.98
6	D	801	ATP	N3-C2-N1	-3.56	123.11	128.68
6	C	802	ATP	PA-O3A-PB	-3.50	120.80	132.83
6	B	802	ATP	N3-C2-N1	-3.36	123.42	128.68
6	B	801	ATP	N3-C2-N1	-3.35	123.44	128.68
6	D	801	ATP	PA-O3A-PB	-3.26	121.64	132.83
7	A	802	ADP	N3-C2-N1	-3.24	123.62	128.68
6	F	801	ATP	N3-C2-N1	-3.23	123.63	128.68
6	C	802	ATP	N3-C2-N1	-3.19	123.69	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	801	ATP	N3-C2-N1	-3.07	123.88	128.68
6	B	801	ATP	PB-O3B-PG	-3.03	122.42	132.83
7	E	802	ADP	PA-O3A-PB	-2.97	122.65	132.83
6	E	801	ATP	C2'-C3'-C4'	2.82	108.11	102.64
6	B	801	ATP	PA-O3A-PB	-2.80	123.20	132.83
6	D	802	ATP	N3-C2-N1	-2.79	124.32	128.68
6	E	801	ATP	C3'-C2'-C1'	2.77	105.15	100.98
6	B	802	ATP	N6-C6-N1	2.76	124.31	118.57
6	A	801	ATP	N3-C2-N1	-2.75	124.37	128.68
7	A	802	ADP	O4'-C1'-C2'	-2.67	103.02	106.93
6	C	801	ATP	C4-C5-N7	-2.66	106.62	109.40
7	A	802	ADP	C4-C5-N7	-2.64	106.65	109.40
6	D	801	ATP	C4-C5-N7	-2.63	106.66	109.40
7	E	802	ADP	N3-C2-N1	-2.59	124.62	128.68
6	D	801	ATP	O4'-C1'-C2'	-2.56	103.18	106.93
6	C	802	ATP	C3'-C2'-C1'	2.55	104.81	100.98
6	F	801	ATP	O2A-PA-O1A	2.51	124.63	112.24
6	C	801	ATP	O5'-C5'-C4'	2.50	117.61	108.99
6	D	802	ATP	N6-C6-N1	2.47	123.70	118.57
7	E	802	ADP	N6-C6-N1	2.47	123.70	118.57
7	A	802	ADP	O3B-PB-O2B	2.47	117.06	107.64
6	D	802	ATP	C1'-N9-C4	2.46	130.97	126.64
6	A	801	ATP	O3G-PG-O2G	2.41	116.84	107.64
6	E	801	ATP	O5'-C5'-C4'	2.35	117.09	108.99
6	B	802	ATP	O5'-C5'-C4'	2.33	117.03	108.99
7	E	802	ADP	O2A-PA-O1A	2.33	123.75	112.24
6	F	801	ATP	O5'-C5'-C4'	2.33	117.00	108.99
6	B	802	ATP	O4'-C4'-C3'	2.29	109.65	105.11
7	E	802	ADP	C1'-N9-C4	2.27	130.63	126.64
7	E	802	ADP	C2'-C3'-C4'	2.24	107.00	102.64
6	B	802	ATP	O3G-PG-O2G	2.22	116.11	107.64
6	A	801	ATP	C3'-C2'-C1'	2.20	104.29	100.98
6	B	802	ATP	O2A-PA-O1A	2.18	123.04	112.24
6	C	802	ATP	C4-C5-N7	-2.17	107.14	109.40
6	D	802	ATP	O4'-C1'-C2'	-2.17	103.76	106.93
6	D	802	ATP	O3G-PG-O2G	2.17	115.91	107.64
6	C	801	ATP	O2A-PA-O1A	2.13	122.77	112.24
6	E	801	ATP	C4-C5-N7	-2.12	107.19	109.40
6	F	801	ATP	O4'-C1'-C2'	2.12	110.02	106.93
6	B	801	ATP	O3G-PG-O2G	2.10	115.68	107.64
6	C	801	ATP	C3'-C2'-C1'	2.10	104.14	100.98
6	C	801	ATP	O3G-PG-O2G	2.08	115.60	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	802	ATP	C4-C5-N7	-2.06	107.26	109.40
6	C	802	ATP	O4'-C4'-C5'	2.03	116.05	109.37
7	E	802	ADP	O4'-C4'-C5'	2.01	115.98	109.37

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	ATP	C5'-O5'-PA-O3A
6	A	801	ATP	C3'-C4'-C5'-O5'
6	C	801	ATP	C5'-O5'-PA-O3A
6	C	802	ATP	PB-O3A-PA-O5'
6	D	801	ATP	C5'-O5'-PA-O2A
6	D	801	ATP	C5'-O5'-PA-O3A
6	D	802	ATP	C5'-O5'-PA-O2A
6	D	802	ATP	C5'-O5'-PA-O3A
6	E	801	ATP	C5'-O5'-PA-O2A
6	E	801	ATP	C5'-O5'-PA-O3A
6	F	801	ATP	C5'-O5'-PA-O2A
7	A	802	ADP	C5'-O5'-PA-O1A
7	A	802	ADP	C5'-O5'-PA-O2A
7	E	802	ADP	C5'-O5'-PA-O3A
6	C	801	ATP	O4'-C4'-C5'-O5'
6	A	801	ATP	O4'-C4'-C5'-O5'
6	C	801	ATP	C3'-C4'-C5'-O5'
7	E	802	ADP	C3'-C4'-C5'-O5'
7	A	802	ADP	PB-O3A-PA-O1A
6	B	801	ATP	PB-O3B-PG-O1G
6	A	801	ATP	C5'-O5'-PA-O2A
6	C	801	ATP	C5'-O5'-PA-O1A
7	E	802	ADP	C5'-O5'-PA-O2A
6	D	802	ATP	PA-O3A-PB-O2B
6	F	801	ATP	C5'-O5'-PA-O3A
7	A	802	ADP	C5'-O5'-PA-O3A
6	F	801	ATP	O4'-C4'-C5'-O5'
7	E	802	ADP	O4'-C4'-C5'-O5'
6	C	801	ATP	PB-O3A-PA-O2A
6	D	802	ATP	PA-O3A-PB-O1B
6	F	801	ATP	PB-O3A-PA-O1A
7	A	802	ADP	PB-O3A-PA-O2A
7	A	802	ADP	O4'-C4'-C5'-O5'

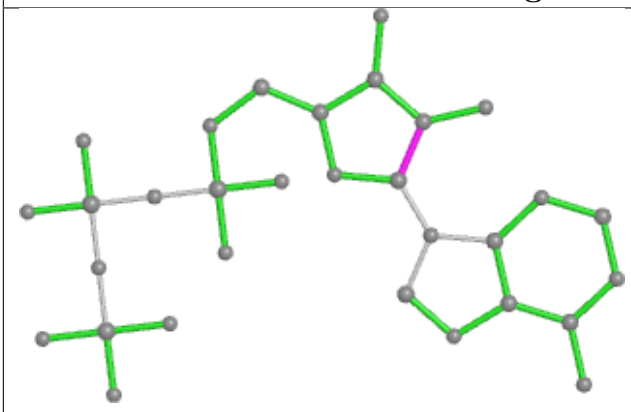
There are no ring outliers.

9 monomers are involved in 20 short contacts:

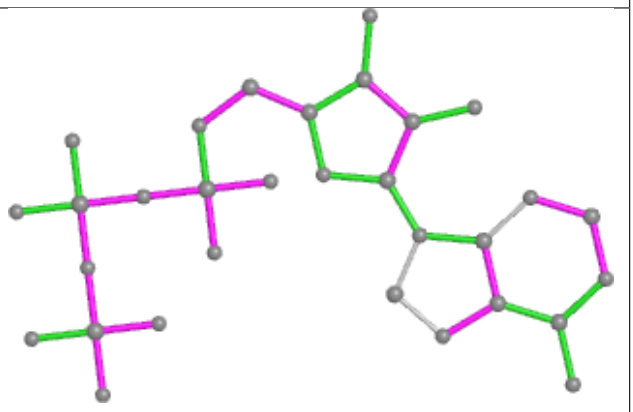
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	801	ATP	3	0
7	E	802	ADP	1	0
6	B	801	ATP	5	0
6	B	802	ATP	2	0
6	F	801	ATP	2	0
6	C	802	ATP	2	0
7	A	802	ADP	1	0
6	D	802	ATP	2	0
6	E	801	ATP	2	0

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.

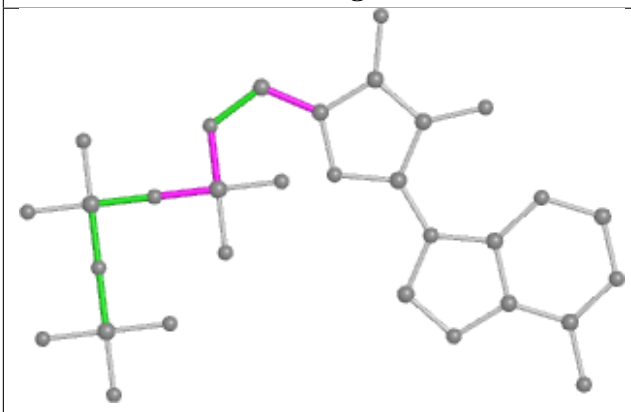
Ligand ATP C 801



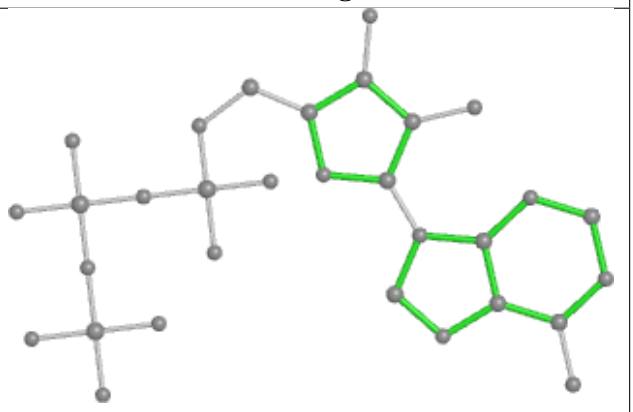
Bond lengths



Bond angles

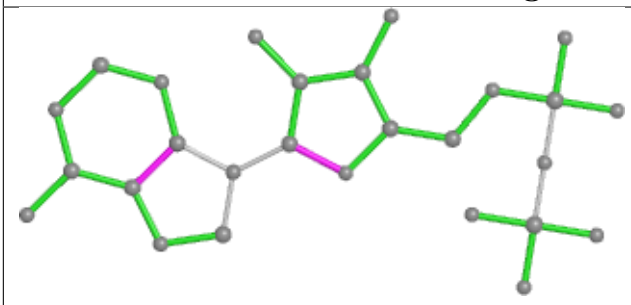


Torsions

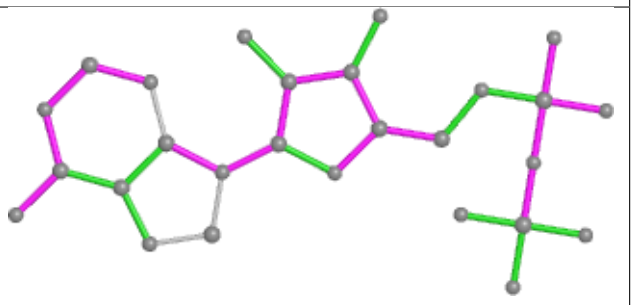


Rings

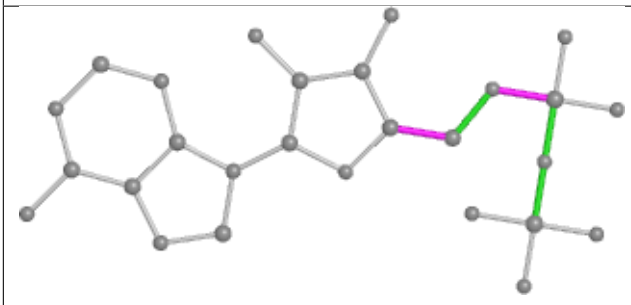
Ligand ADP E 802



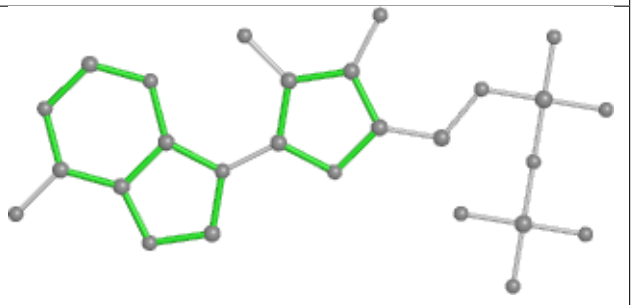
Bond lengths



Bond angles

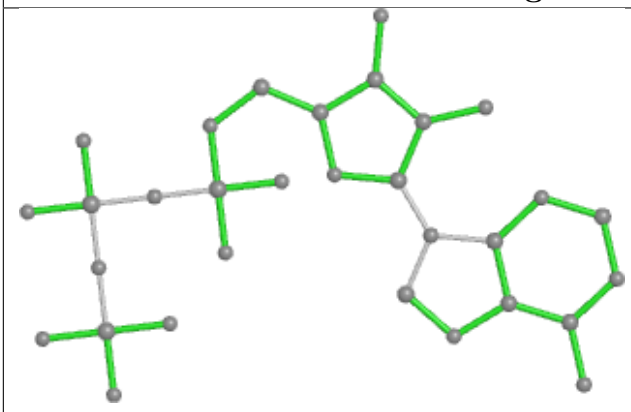


Torsions

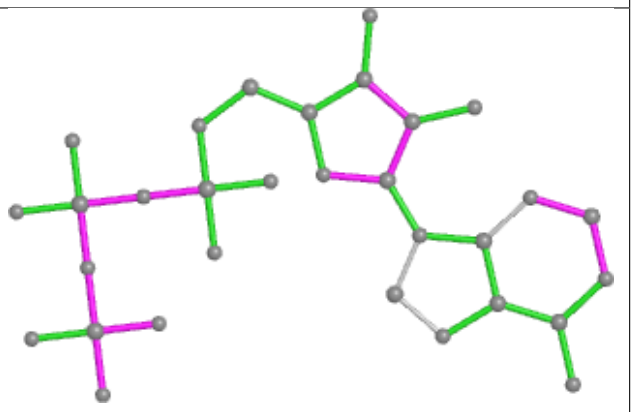


Rings

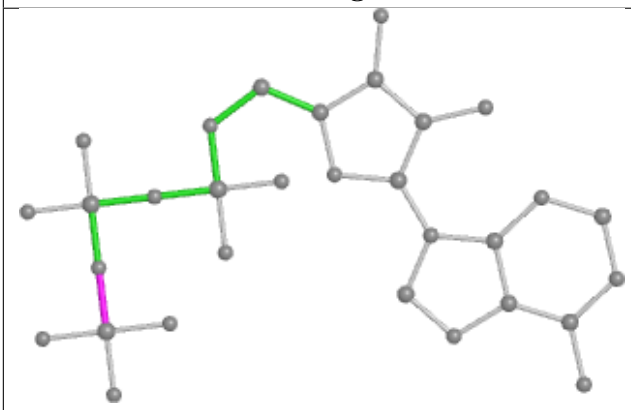
Ligand ATP B 801



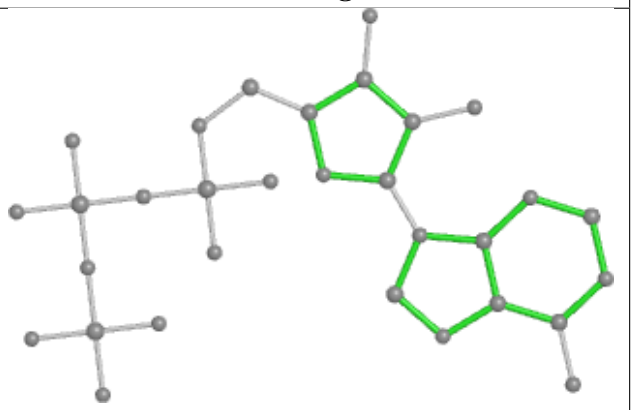
Bond lengths



Bond angles

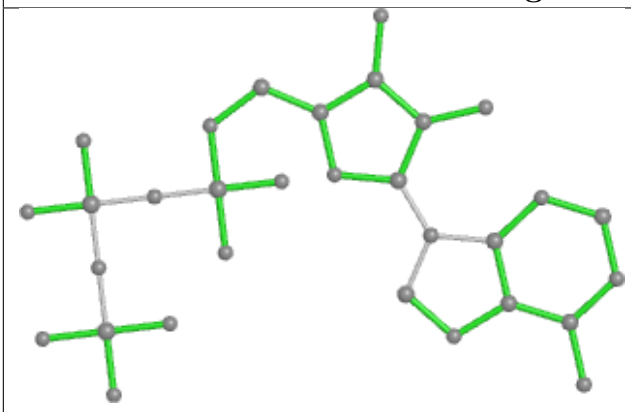


Torsions

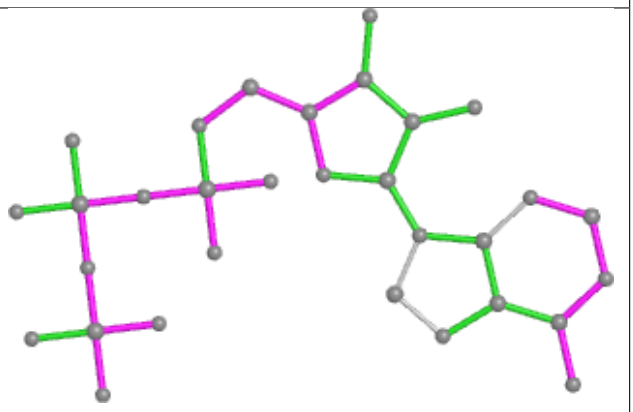


Rings

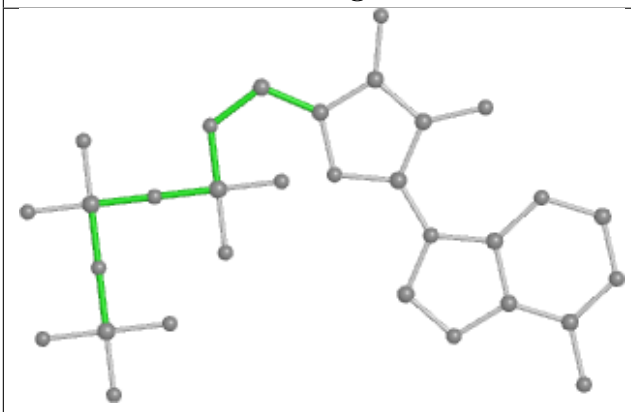
Ligand ATP B 802



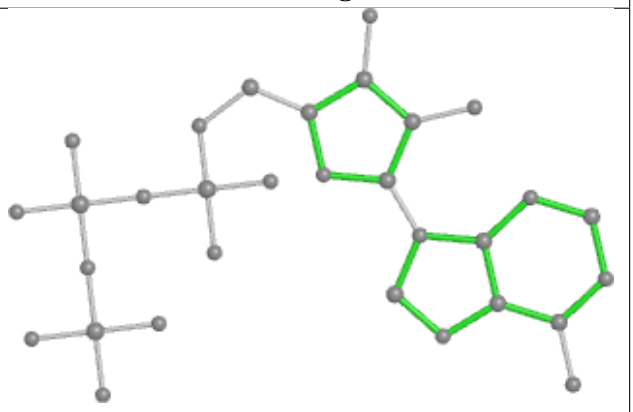
Bond lengths



Bond angles

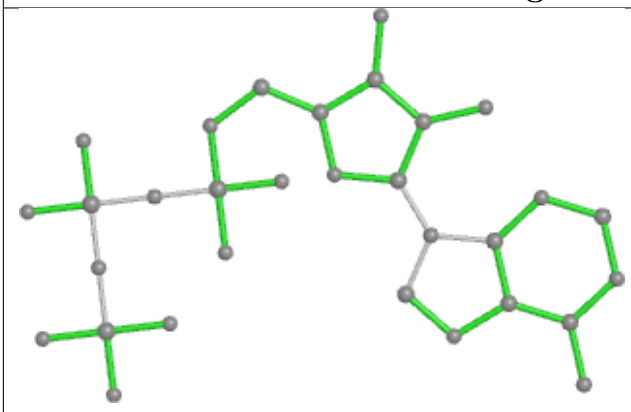


Torsions

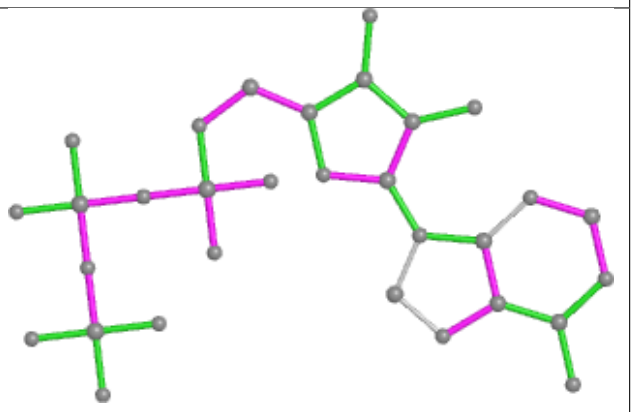


Rings

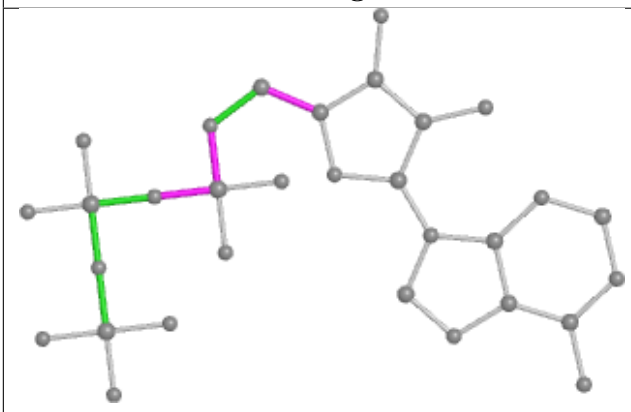
Ligand ATP F 801



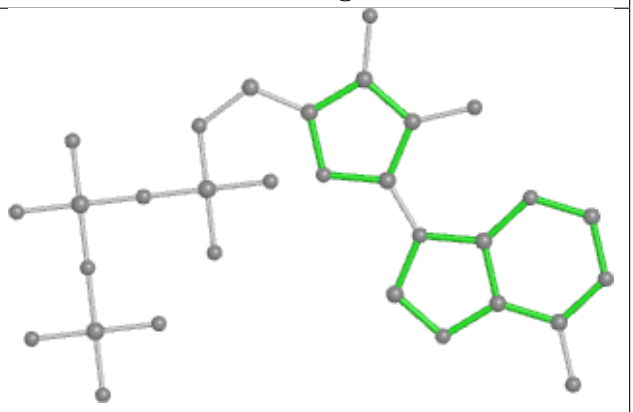
Bond lengths



Bond angles

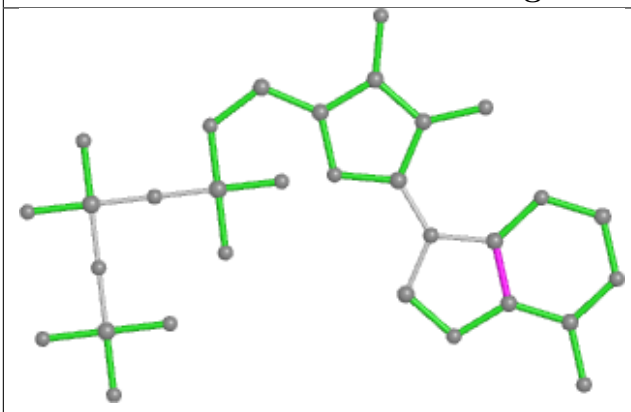


Torsions

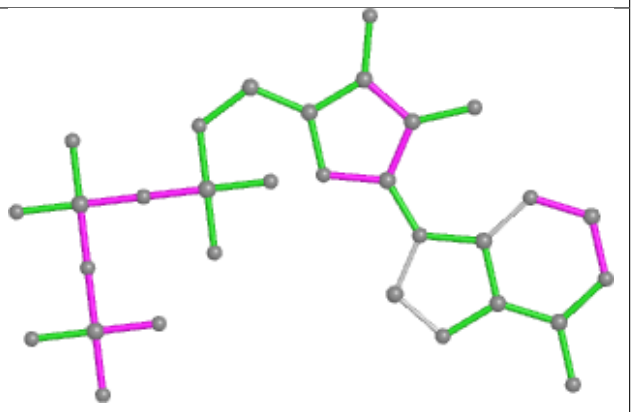


Rings

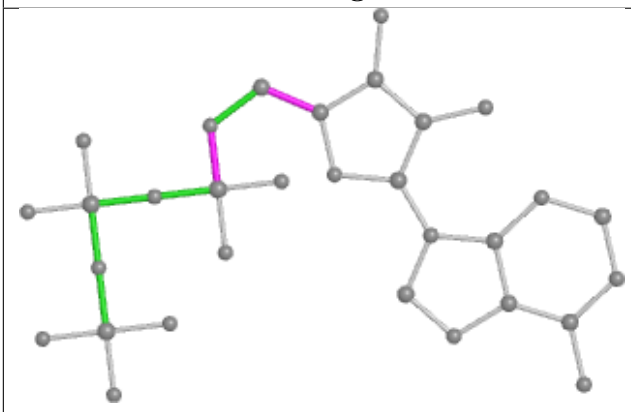
Ligand ATP A 801



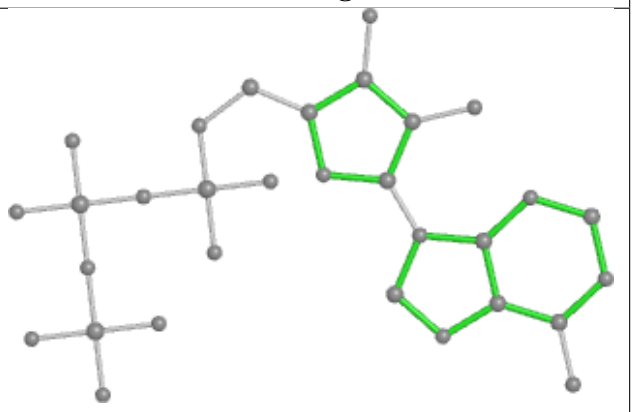
Bond lengths



Bond angles

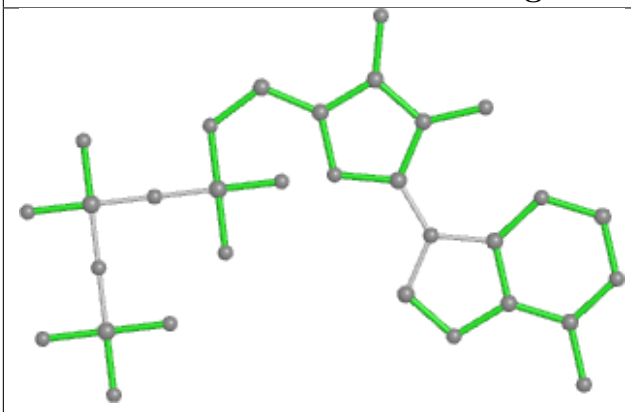


Torsions

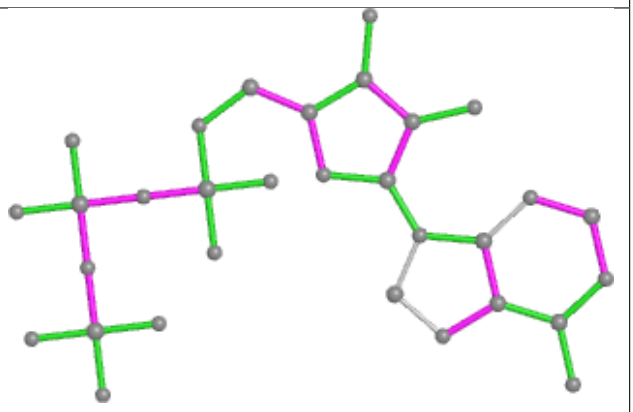


Rings

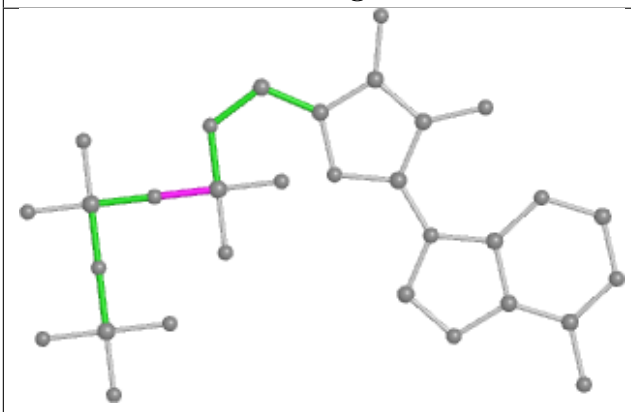
Ligand ATP C 802



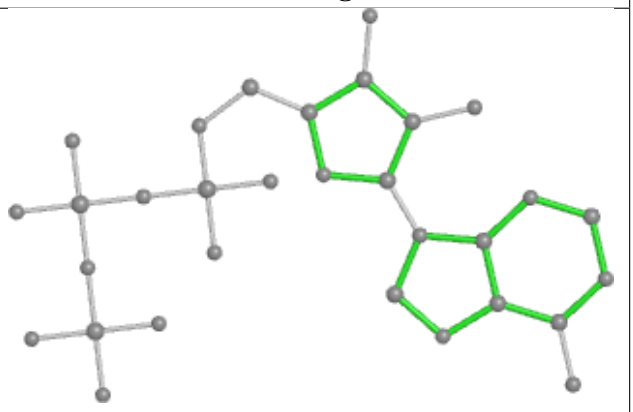
Bond lengths



Bond angles

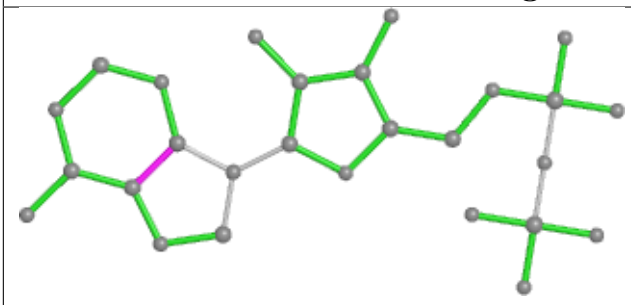


Torsions

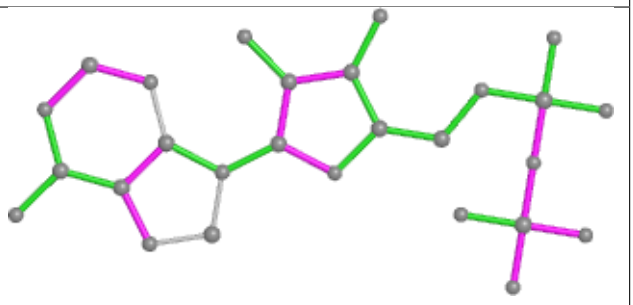


Rings

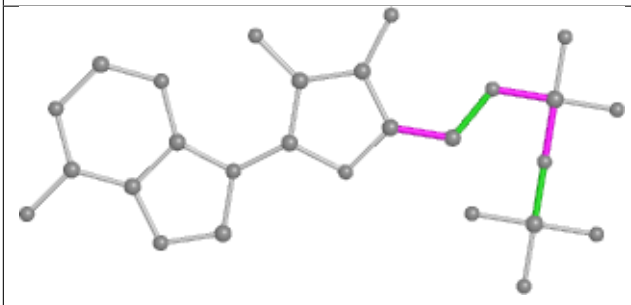
Ligand ADP A 802



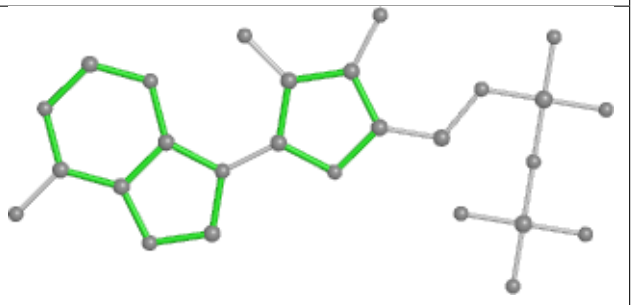
Bond lengths



Bond angles

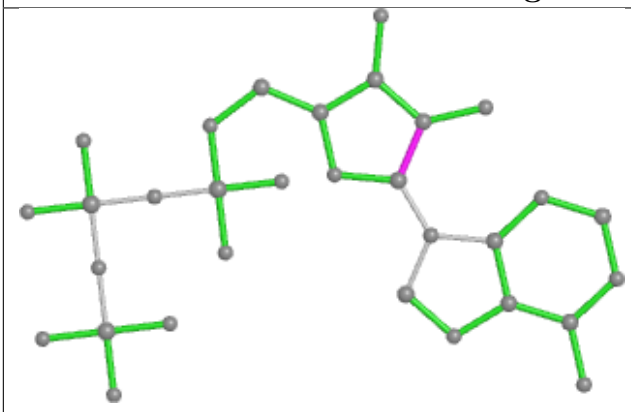


Torsions

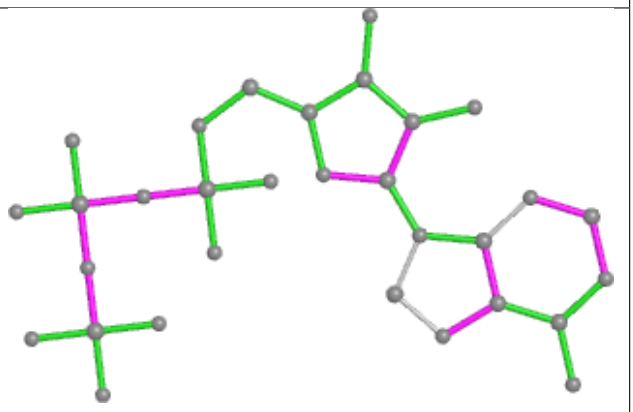


Rings

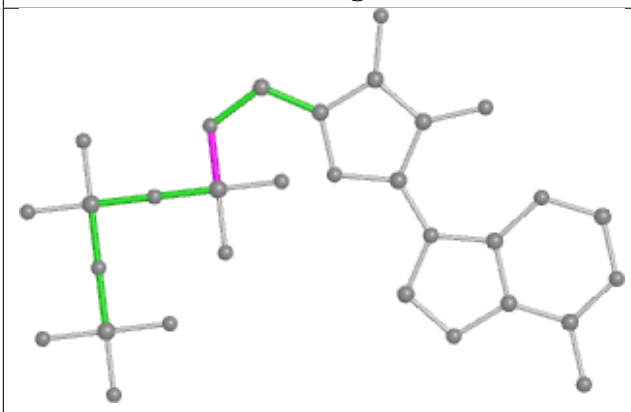
Ligand ATP D 801



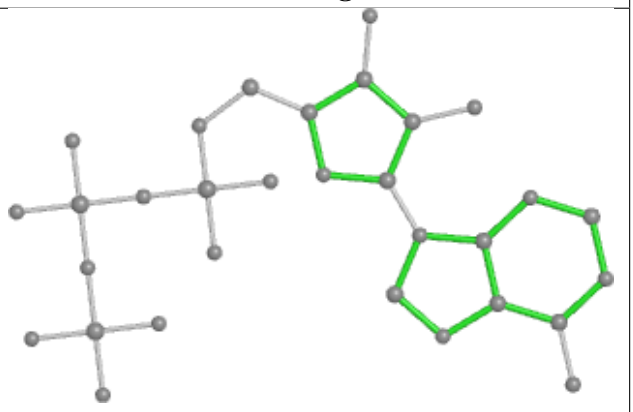
Bond lengths



Bond angles

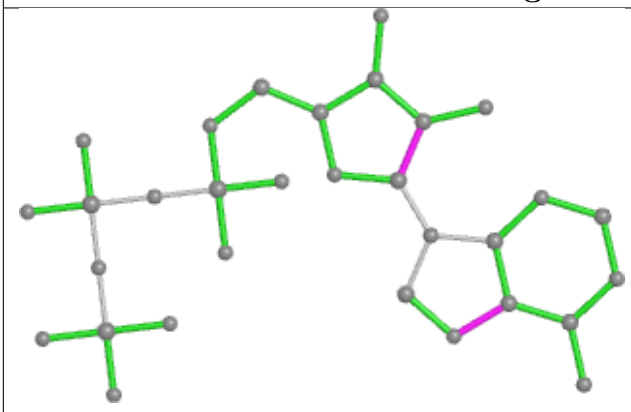


Torsions

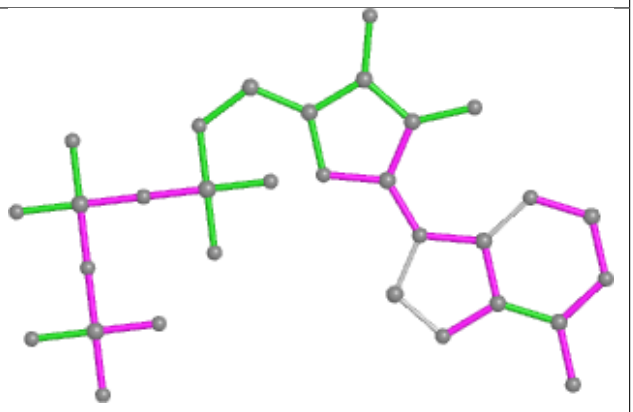


Rings

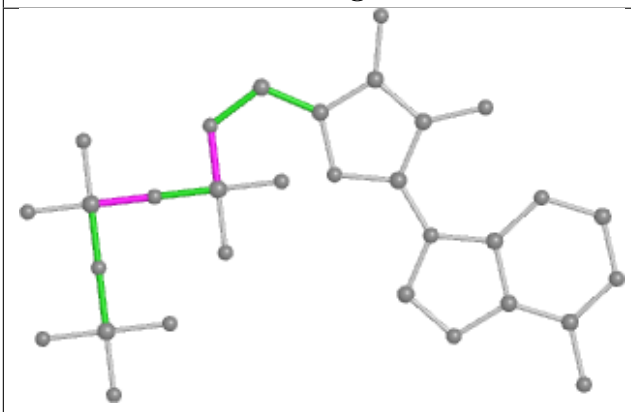
Ligand ATP D 802



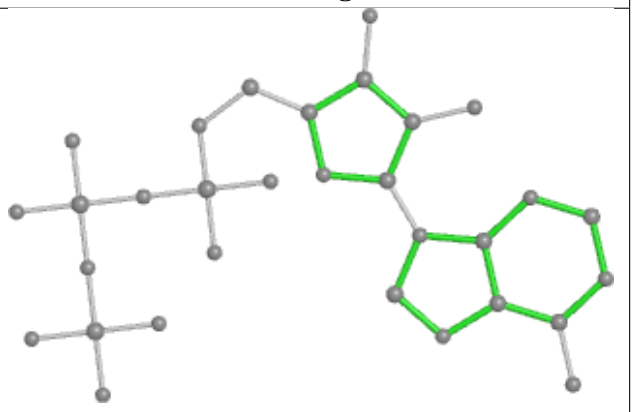
Bond lengths



Bond angles

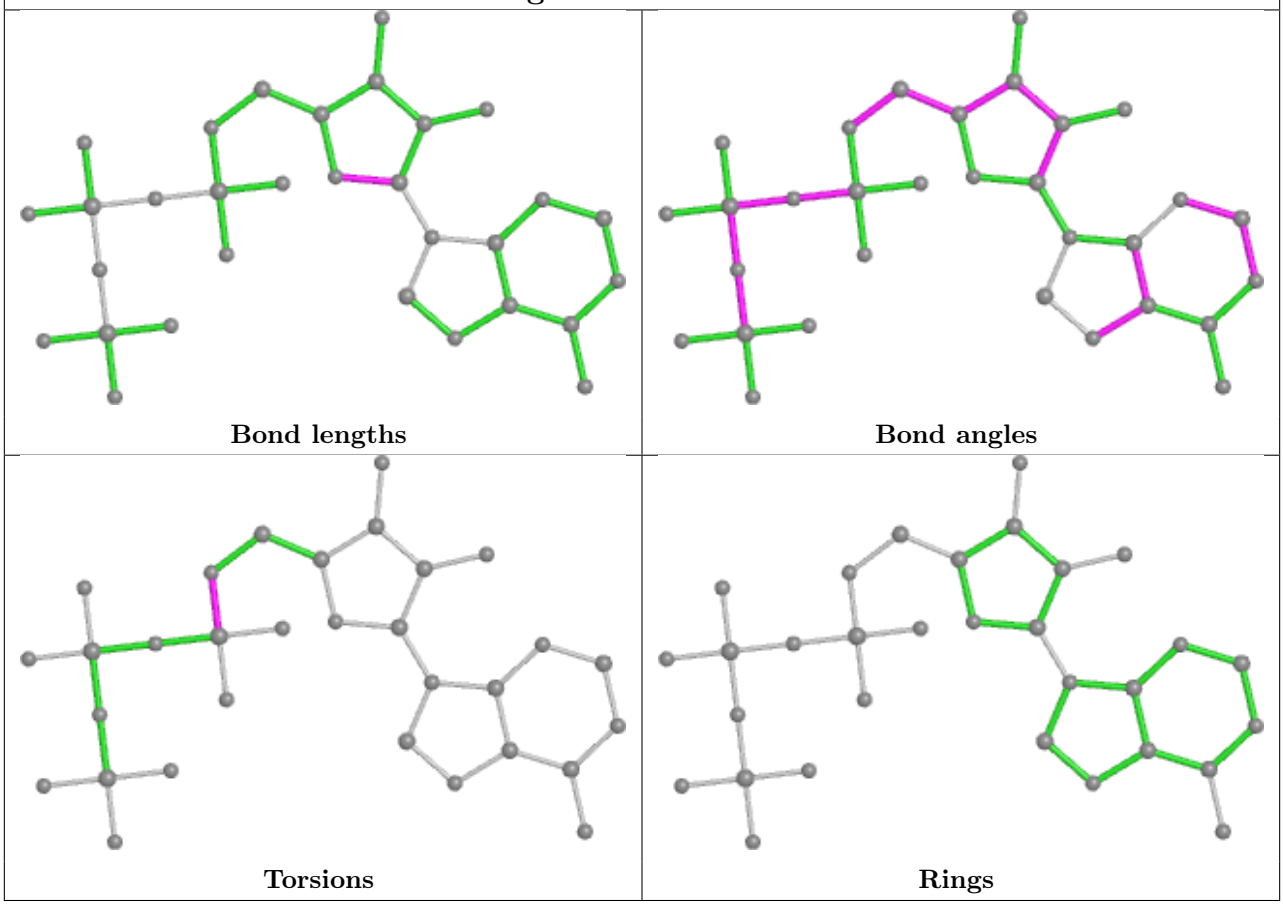


Torsions



Rings

Ligand ATP E 801



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

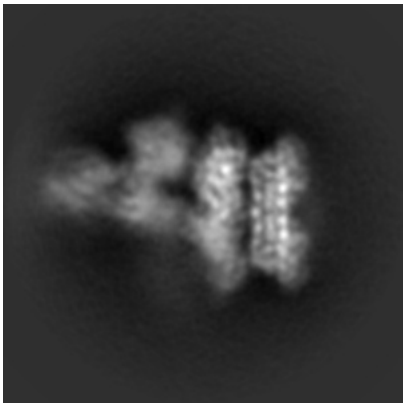
This section contains visualisations of the EMDB entry EMD-9100. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

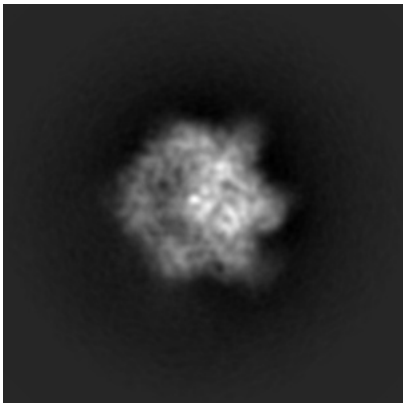
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

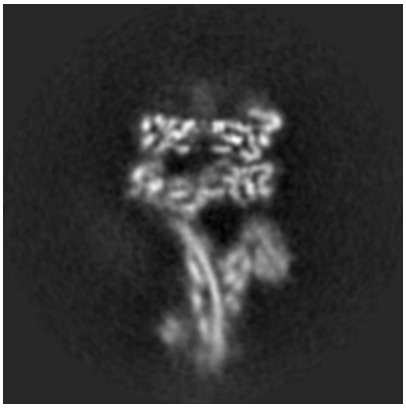


Z

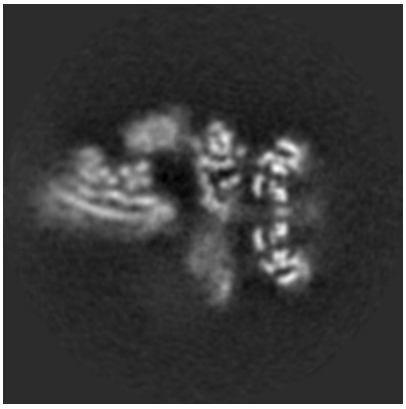
The images above show the map projected in three orthogonal directions.

6.2 Central slices

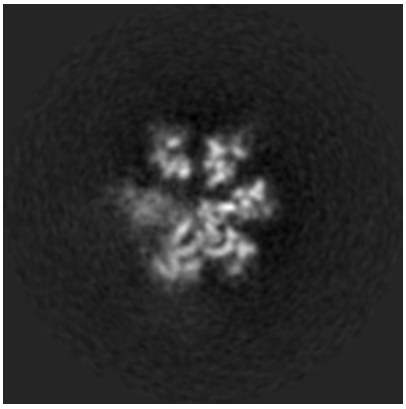
6.2.1 Primary map



X Index: 115



Y Index: 115

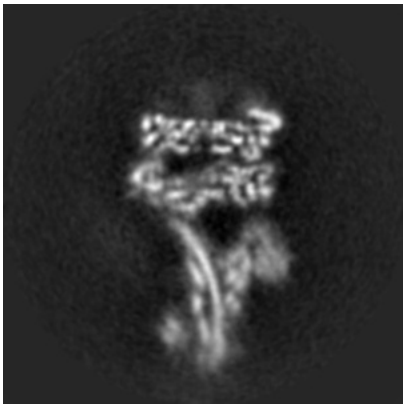


Z Index: 115

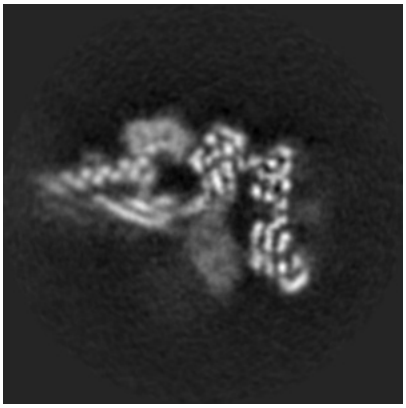
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

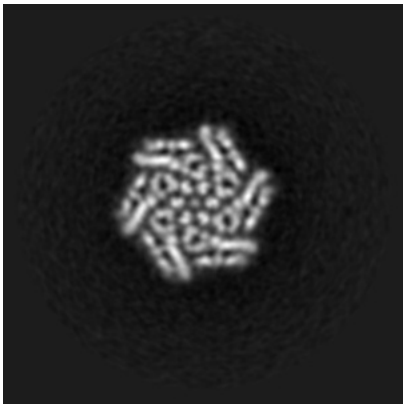
6.3.1 Primary map



X Index: 116



Y Index: 109

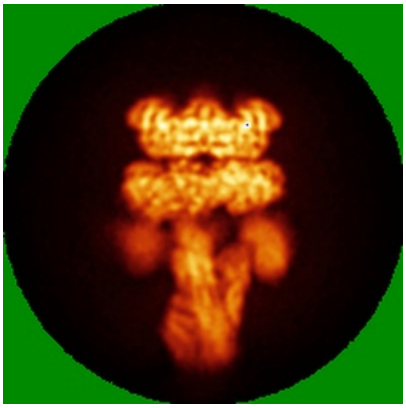


Z Index: 160

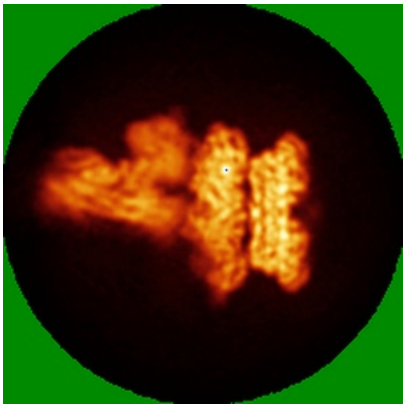
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

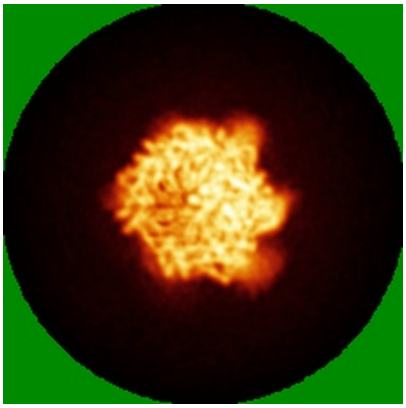
6.4.1 Primary map



X



Y

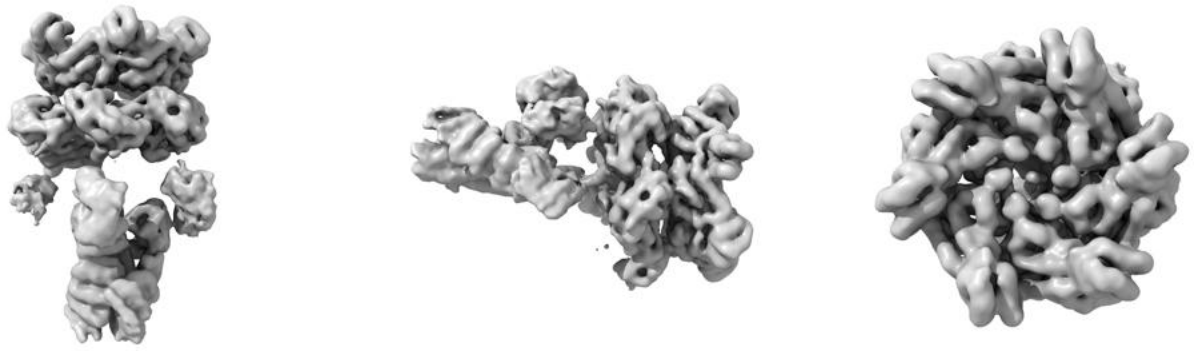


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

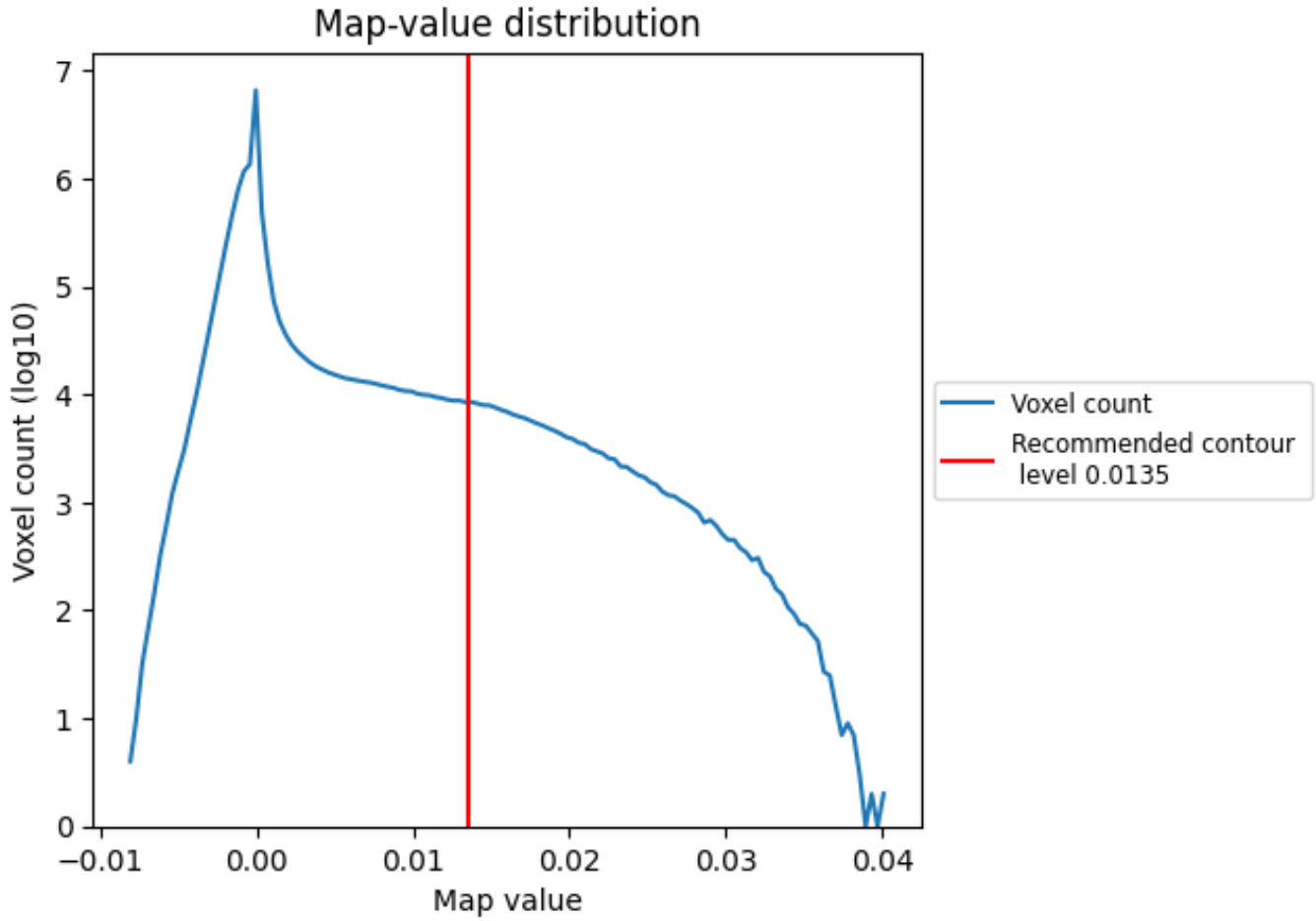
6.6 Mask visualisation (i)

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

7 Map analysis

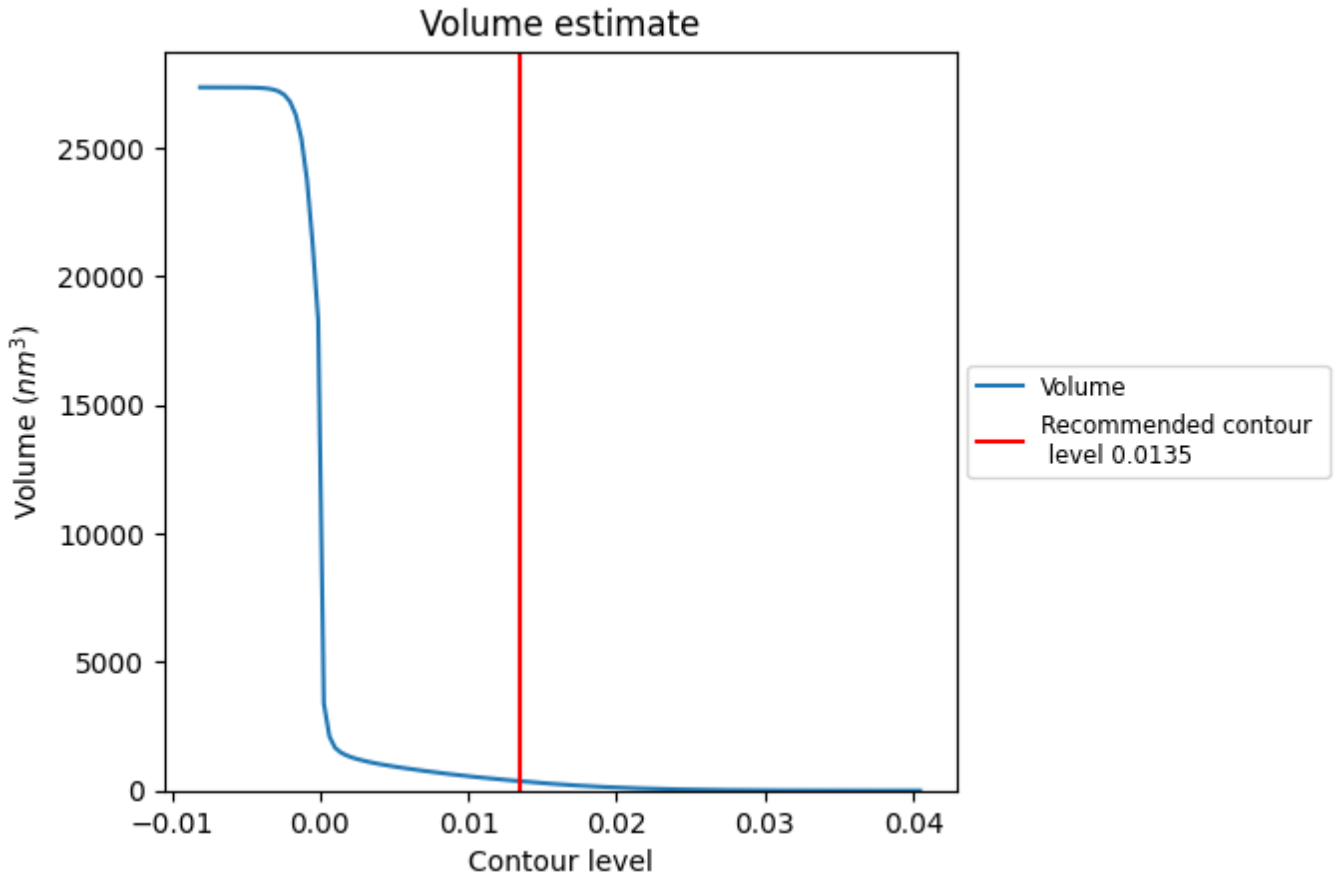
This section contains the results of statistical analysis of the map.

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.

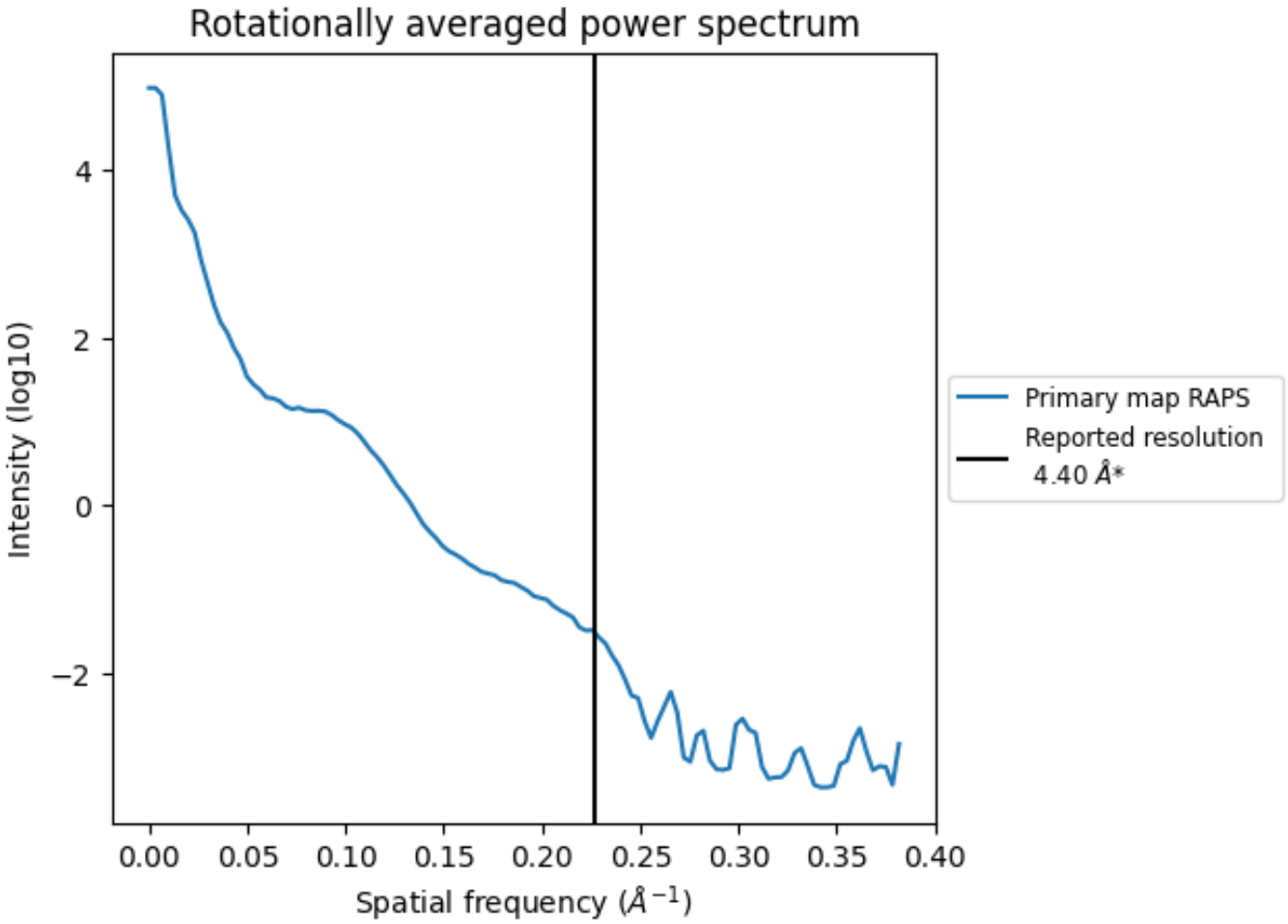
7.2 Volume estimate



The volume at the recommended contour level is 365 nm^3; this corresponds to an approximate mass of 330 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)

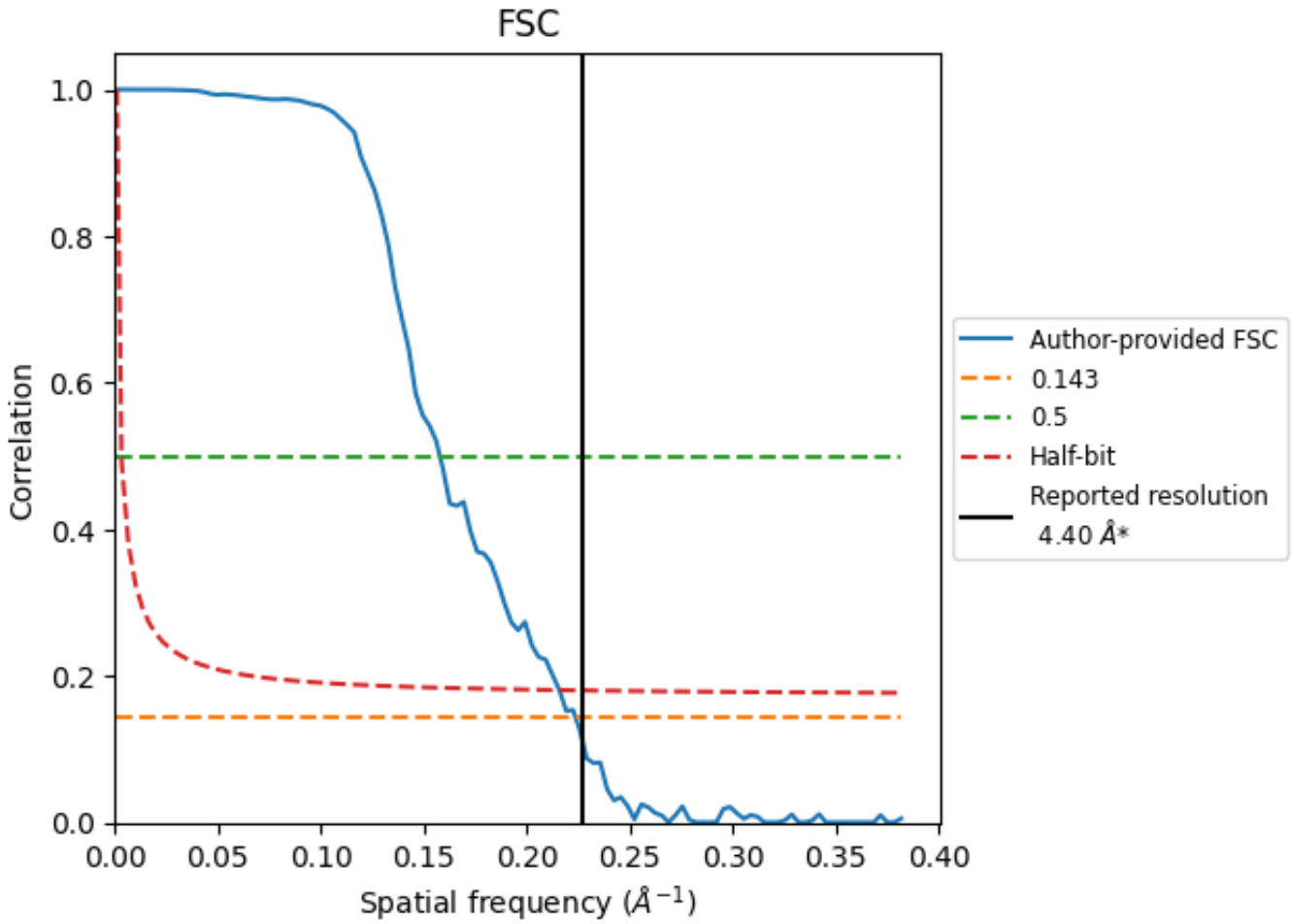


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

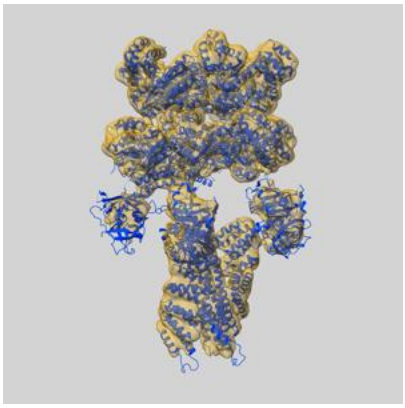
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.47	6.34	4.63
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

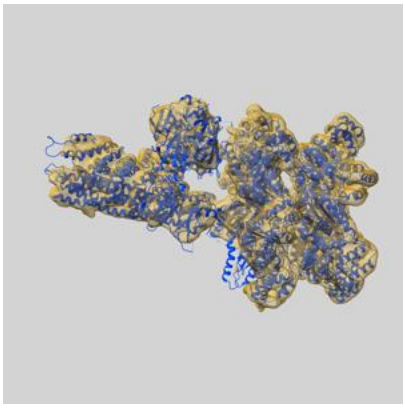
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9100 and PDB model 6MDM. Per-residue inclusion information can be found in section 3 on page 13.

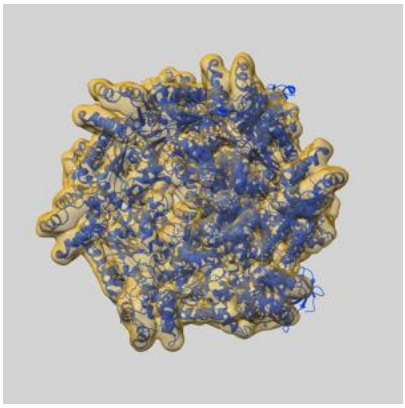
9.1 Map-model overlay



X



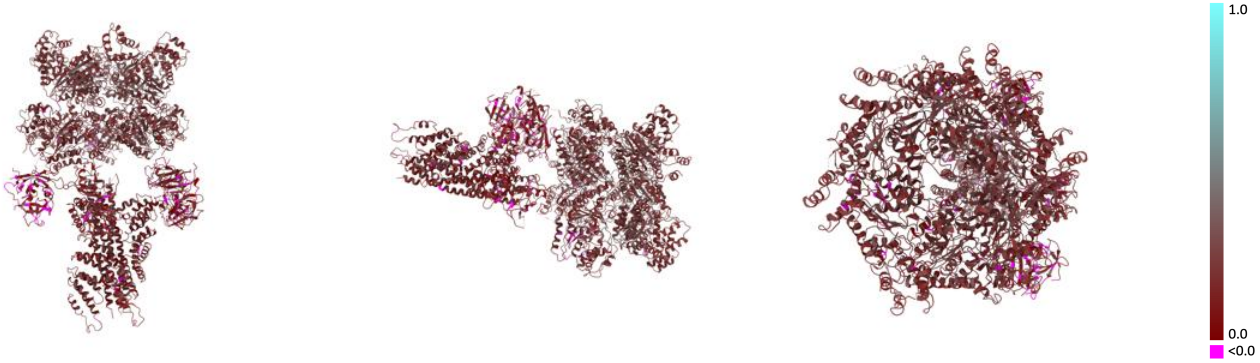
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135 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.

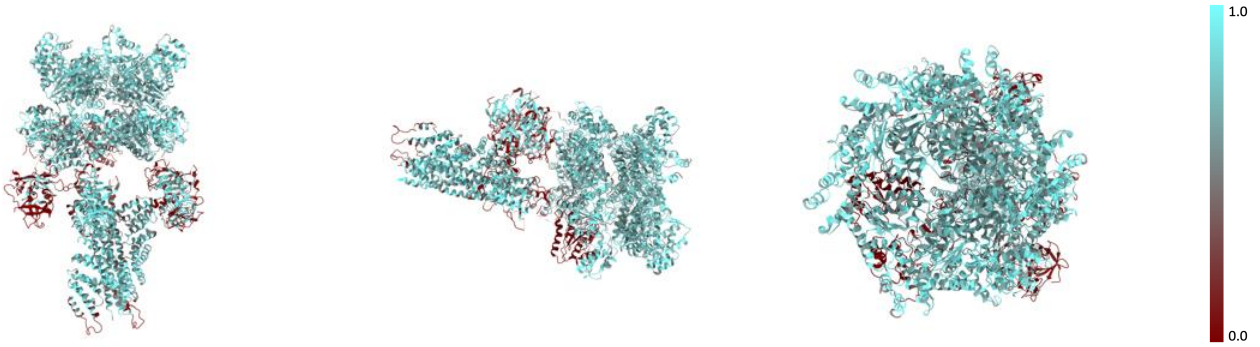
9.2 Q-score mapped to coordinate model



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.

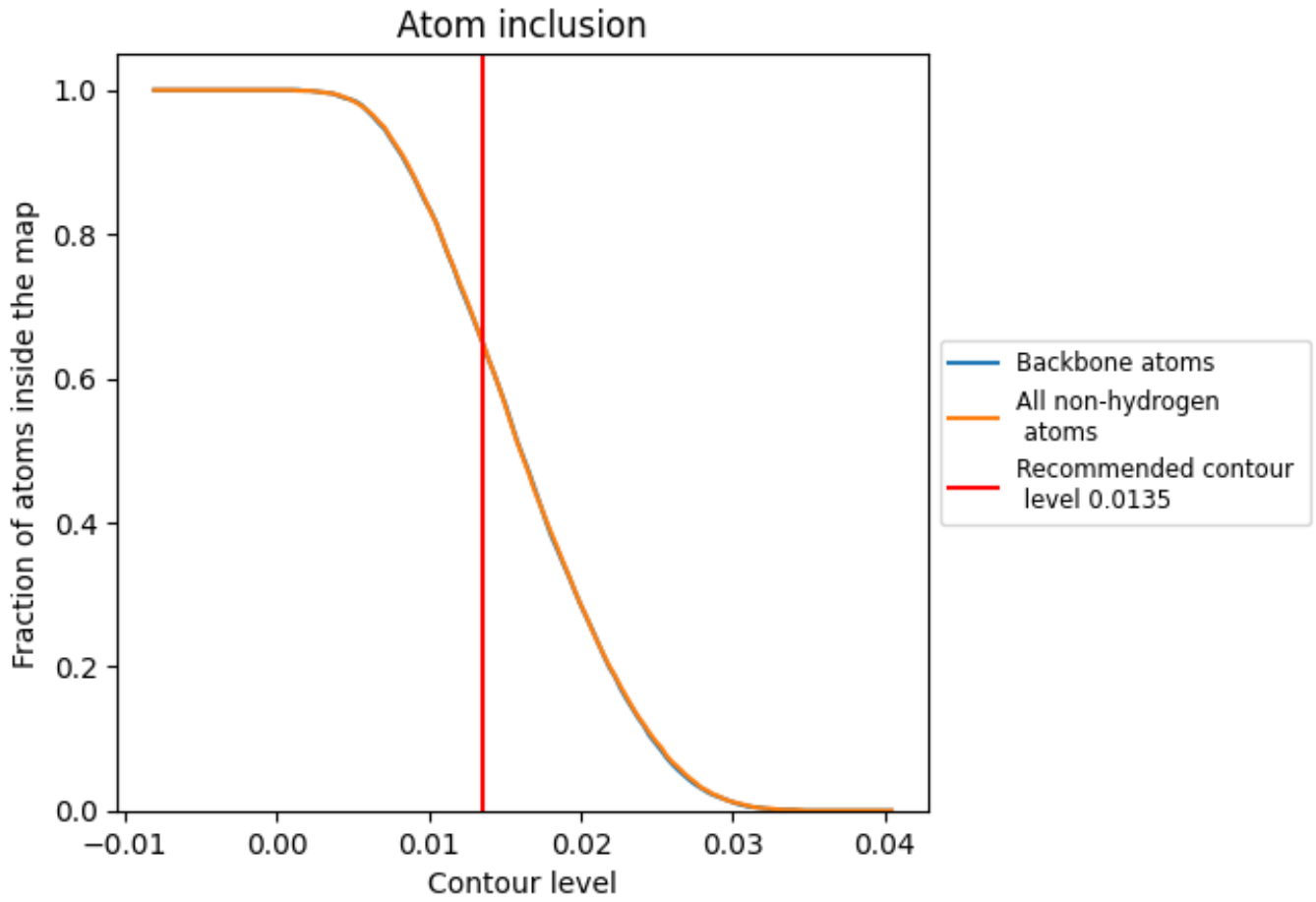
9.3 Atom inclusion mapped to coordinate model



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 (0.0135).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6520	0.2070
A	0.6780	0.2100
B	0.6630	0.2140
C	0.7280	0.2260
D	0.6090	0.1980
E	0.7270	0.2230
F	0.4330	0.2030
H	0.7370	0.1870
I	0.7600	0.1760
J	0.7890	0.1840
K	0.6550	0.1780
L	0.6940	0.1830