Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:50 AM UTC

PDB ID	:	6MDN / pdb_00006mdn
EMDB ID	:	EMD-9101
Title	:	The 20S supercomplex engaging the SNAP-25 N-terminus (class 2)
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:

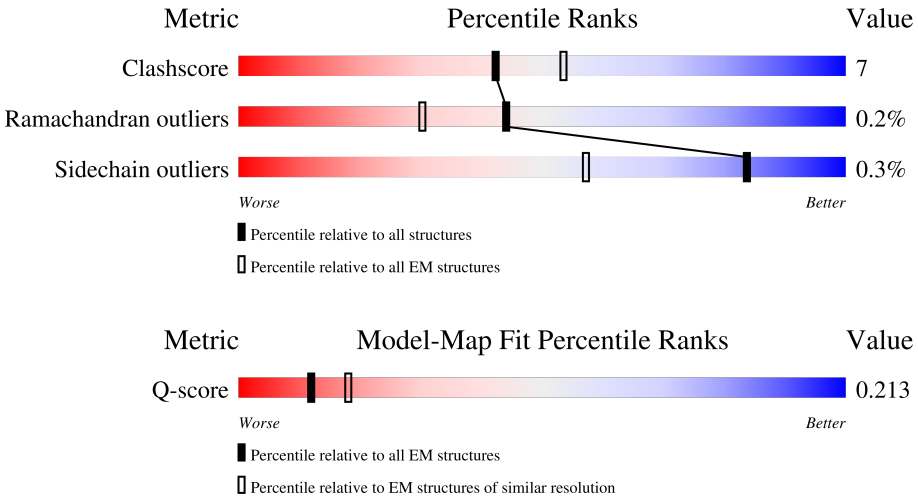
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	56% 10% 33%
1	B	768	9% 77% 15% 8%
1	C	768	18% 73% 19% 8%
1	D	768	11% 76% 17% 7%

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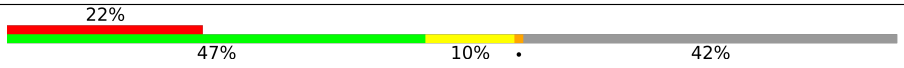
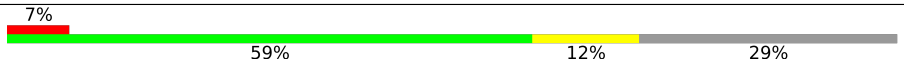
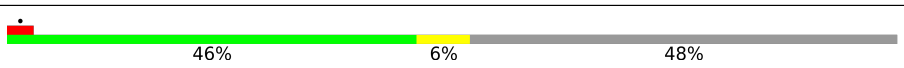
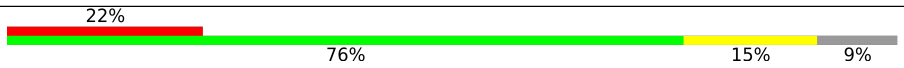
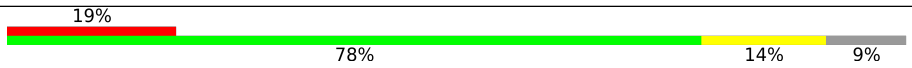
Mol	Chain	Length	Quality of chain
1	E	768	
1	F	768	
2	H	207	
3	I	256	
4	J	117	
5	K	313	
5	L	313	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 73042 atoms, of which 36628 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	511	Total	C	H	N	O	S	0	0
			8082	2525	4099	696	740	22		
1	B	707	Total	C	H	N	O	S	0	0
			11129	3486	5624	957	1032	30		
1	C	709	Total	C	H	N	O	S	0	0
			11167	3499	5641	960	1037	30		
1	D	713	Total	C	H	N	O	S	0	0
			11232	3519	5675	964	1043	31		
1	E	697	Total	C	H	N	O	S	0	0
			10987	3436	5559	944	1018	30		
1	F	449	Total	C	H	N	O	S	0	0
			6748	2140	3372	588	633	15		

There are 276 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
A	724	TYR	-	expression tag	UNP P18708
A	725	ARG	-	expression tag	UNP P18708
A	726	VAL	-	expression tag	UNP P18708
A	727	ARG	-	expression tag	UNP P18708
A	728	LYS	-	expression tag	UNP P18708
A	729	PHE	-	expression tag	UNP P18708
A	730	LEU	-	expression tag	UNP P18708
A	731	ALA	-	expression tag	UNP P18708
A	732	LEU	-	expression tag	UNP P18708
A	733	LEU	-	expression tag	UNP P18708
A	734	ARG	-	expression tag	UNP P18708
A	735	GLU	-	expression tag	UNP P18708
A	736	GLU	-	expression tag	UNP P18708
A	737	GLY	-	expression tag	UNP P18708
A	738	ALA	-	expression tag	UNP P18708
A	739	SER	-	expression tag	UNP P18708
A	740	PRO	-	expression tag	UNP P18708
A	741	LEU	-	expression tag	UNP P18708
A	742	ASP	-	expression tag	UNP P18708
A	743	PHE	-	expression tag	UNP P18708
A	744	ASP	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	724	TYR	-	expression tag	UNP P18708
B	725	ARG	-	expression tag	UNP P18708
B	726	VAL	-	expression tag	UNP P18708
B	727	ARG	-	expression tag	UNP P18708
B	728	LYS	-	expression tag	UNP P18708
B	729	PHE	-	expression tag	UNP P18708
B	730	LEU	-	expression tag	UNP P18708
B	731	ALA	-	expression tag	UNP P18708
B	732	LEU	-	expression tag	UNP P18708
B	733	LEU	-	expression tag	UNP P18708
B	734	ARG	-	expression tag	UNP P18708
B	735	GLU	-	expression tag	UNP P18708
B	736	GLU	-	expression tag	UNP P18708
B	737	GLY	-	expression tag	UNP P18708
B	738	ALA	-	expression tag	UNP P18708
B	739	SER	-	expression tag	UNP P18708
B	740	PRO	-	expression tag	UNP P18708
B	741	LEU	-	expression tag	UNP P18708
B	742	ASP	-	expression tag	UNP P18708
B	743	PHE	-	expression tag	UNP P18708
B	744	ASP	-	expression tag	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
C	724	TYR	-	expression tag	UNP P18708
C	725	ARG	-	expression tag	UNP P18708
C	726	VAL	-	expression tag	UNP P18708
C	727	ARG	-	expression tag	UNP P18708
C	728	LYS	-	expression tag	UNP P18708
C	729	PHE	-	expression tag	UNP P18708
C	730	LEU	-	expression tag	UNP P18708
C	731	ALA	-	expression tag	UNP P18708
C	732	LEU	-	expression tag	UNP P18708
C	733	LEU	-	expression tag	UNP P18708
C	734	ARG	-	expression tag	UNP P18708
C	735	GLU	-	expression tag	UNP P18708
C	736	GLU	-	expression tag	UNP P18708
C	737	GLY	-	expression tag	UNP P18708
C	738	ALA	-	expression tag	UNP P18708
C	739	SER	-	expression tag	UNP P18708
C	740	PRO	-	expression tag	UNP P18708
C	741	LEU	-	expression tag	UNP P18708
C	742	ASP	-	expression tag	UNP P18708
C	743	PHE	-	expression tag	UNP P18708
C	744	ASP	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	724	TYR	-	expression tag	UNP P18708
D	725	ARG	-	expression tag	UNP P18708
D	726	VAL	-	expression tag	UNP P18708
D	727	ARG	-	expression tag	UNP P18708
D	728	LYS	-	expression tag	UNP P18708
D	729	PHE	-	expression tag	UNP P18708
D	730	LEU	-	expression tag	UNP P18708
D	731	ALA	-	expression tag	UNP P18708
D	732	LEU	-	expression tag	UNP P18708
D	733	LEU	-	expression tag	UNP P18708
D	734	ARG	-	expression tag	UNP P18708
D	735	GLU	-	expression tag	UNP P18708
D	736	GLU	-	expression tag	UNP P18708
D	737	GLY	-	expression tag	UNP P18708
D	738	ALA	-	expression tag	UNP P18708
D	739	SER	-	expression tag	UNP P18708
D	740	PRO	-	expression tag	UNP P18708
D	741	LEU	-	expression tag	UNP P18708
D	742	ASP	-	expression tag	UNP P18708
D	743	PHE	-	expression tag	UNP P18708
D	744	ASP	-	expression tag	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
E	724	TYR	-	expression tag	UNP P18708
E	725	ARG	-	expression tag	UNP P18708
E	726	VAL	-	expression tag	UNP P18708
E	727	ARG	-	expression tag	UNP P18708
E	728	LYS	-	expression tag	UNP P18708
E	729	PHE	-	expression tag	UNP P18708
E	730	LEU	-	expression tag	UNP P18708
E	731	ALA	-	expression tag	UNP P18708
E	732	LEU	-	expression tag	UNP P18708
E	733	LEU	-	expression tag	UNP P18708
E	734	ARG	-	expression tag	UNP P18708
E	735	GLU	-	expression tag	UNP P18708
E	736	GLU	-	expression tag	UNP P18708
E	737	GLY	-	expression tag	UNP P18708
E	738	ALA	-	expression tag	UNP P18708
E	739	SER	-	expression tag	UNP P18708
E	740	PRO	-	expression tag	UNP P18708
E	741	LEU	-	expression tag	UNP P18708
E	742	ASP	-	expression tag	UNP P18708

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Chain	Residue	Modelled	Actual	Comment	Reference
E	743	PHE	-	expression tag	UNP P18708
E	744	ASP	-	expression tag	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
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
F	724	TYR	-	expression tag	UNP P18708
F	725	ARG	-	expression tag	UNP P18708
F	726	VAL	-	expression tag	UNP P18708
F	727	ARG	-	expression tag	UNP P18708
F	728	LYS	-	expression tag	UNP P18708
F	729	PHE	-	expression tag	UNP P18708
F	730	LEU	-	expression tag	UNP P18708
F	731	ALA	-	expression tag	UNP P18708
F	732	LEU	-	expression tag	UNP P18708
F	733	LEU	-	expression tag	UNP P18708
F	734	ARG	-	expression tag	UNP P18708
F	735	GLU	-	expression tag	UNP P18708
F	736	GLU	-	expression tag	UNP P18708
F	737	GLY	-	expression tag	UNP P18708
F	738	ALA	-	expression tag	UNP P18708

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Chain	Residue	Modelled	Actual	Comment	Reference
F	739	SER	-	expression tag	UNP P18708
F	740	PRO	-	expression tag	UNP P18708
F	741	LEU	-	expression tag	UNP P18708
F	742	ASP	-	expression tag	UNP P18708
F	743	PHE	-	expression tag	UNP P18708
F	744	ASP	-	expression tag	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
			2295	690	1124	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
			1063	331	527	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 45 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
J	73	GLY	-	expression tag	UNP P63045
J	74	ALA	-	expression tag	UNP P63045
J	75	SER	-	expression tag	UNP P63045
J	76	GLN	-	expression tag	UNP P63045
J	77	PHE	-	expression tag	UNP P63045
J	78	GLU	-	expression tag	UNP P63045
J	79	THR	-	expression tag	UNP P63045
J	80	SER	-	expression tag	UNP P63045
J	81	ALA	-	expression tag	UNP P63045
J	82	ALA	-	expression tag	UNP P63045
J	83	LYS	-	expression tag	UNP P63045
J	84	LEU	-	expression tag	UNP P63045
J	85	LYS	-	expression tag	UNP P63045
J	86	ARG	-	expression tag	UNP P63045
J	87	LYS	-	expression tag	UNP P63045

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Chain	Residue	Modelled	Actual	Comment	Reference
J	88	TYR	-	expression tag	UNP P63045
J	89	TRP	-	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
			4436	1421	2185	372	441	17		
5	L	286	Total	C	H	N	O	S	0	0
			4454	1424	2199	373	441	17		

There are 70 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
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
K	279	MET	-	expression tag	UNP P54921
K	280	LEU	-	expression tag	UNP P54921
K	281	LEU	-	expression tag	UNP P54921
K	282	ARG	-	expression tag	UNP P54921
K	283	ILE	-	expression tag	UNP P54921
K	284	LYS	-	expression tag	UNP P54921
K	285	LYS	-	expression tag	UNP P54921
K	286	THR	-	expression tag	UNP P54921
K	287	ILE	-	expression tag	UNP P54921
K	288	GLN	-	expression tag	UNP P54921

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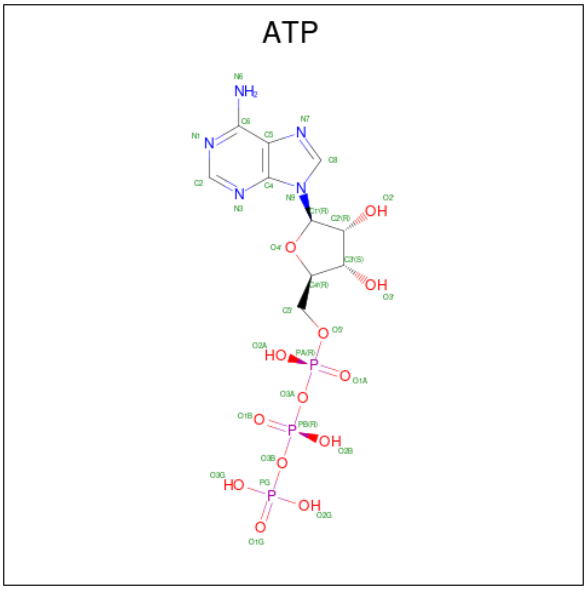
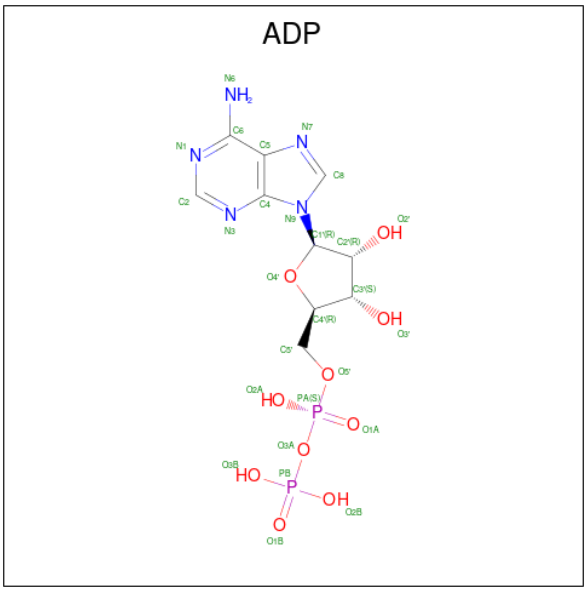
Chain	Residue	Modelled	Actual	Comment	Reference
K	289	GLY	-	expression tag	UNP P54921
K	290	ASP	-	expression tag	UNP P54921
K	291	GLU	-	expression tag	UNP P54921
K	292	GLU	-	expression tag	UNP P54921
K	293	ASP	-	expression tag	UNP P54921
K	294	LEU	-	expression tag	UNP P54921
K	295	ARG	-	expression tag	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
L	279	MET	-	expression tag	UNP P54921
L	280	LEU	-	expression tag	UNP P54921
L	281	LEU	-	expression tag	UNP P54921
L	282	ARG	-	expression tag	UNP P54921
L	283	ILE	-	expression tag	UNP P54921
L	284	LYS	-	expression tag	UNP P54921
L	285	LYS	-	expression tag	UNP P54921
L	286	THR	-	expression tag	UNP P54921
L	287	ILE	-	expression tag	UNP P54921
L	288	GLN	-	expression tag	UNP P54921
L	289	GLY	-	expression tag	UNP P54921
L	290	ASP	-	expression tag	UNP P54921
L	291	GLU	-	expression tag	UNP P54921
L	292	GLU	-	expression tag	UNP P54921
L	293	ASP	-	expression tag	UNP P54921
L	294	LEU	-	expression tag	UNP P54921
L	295	ARG	-	expression tag	UNP P54921

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

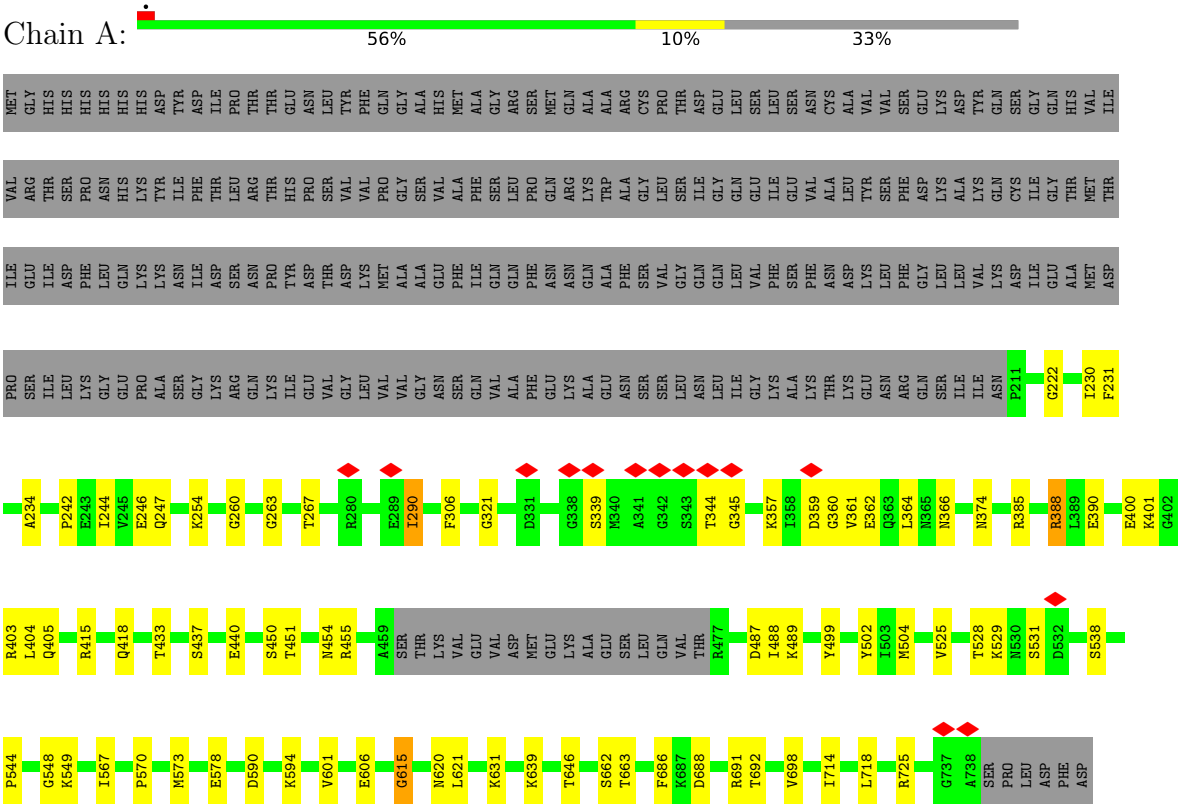


Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
7	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

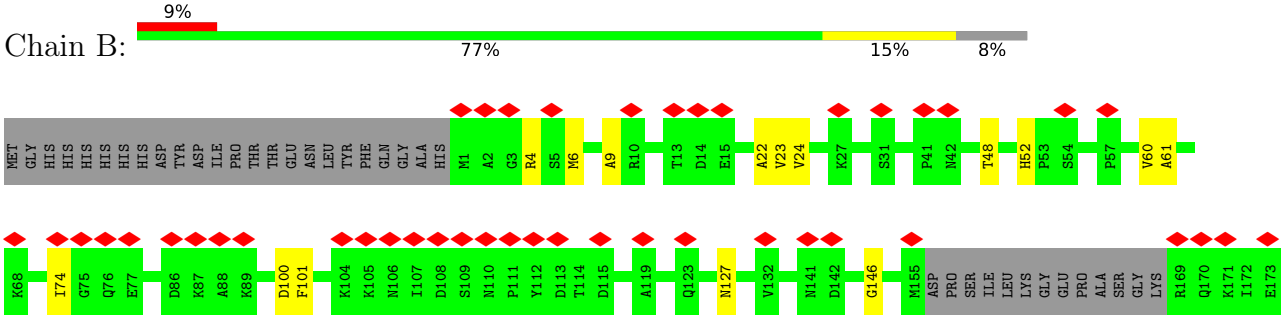
3 Residue-property plots (i)

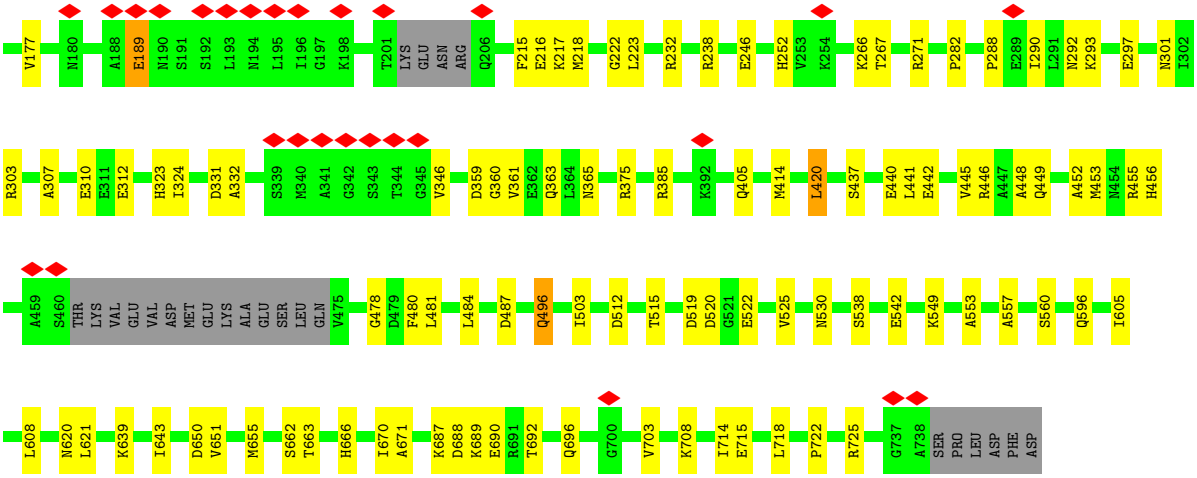
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



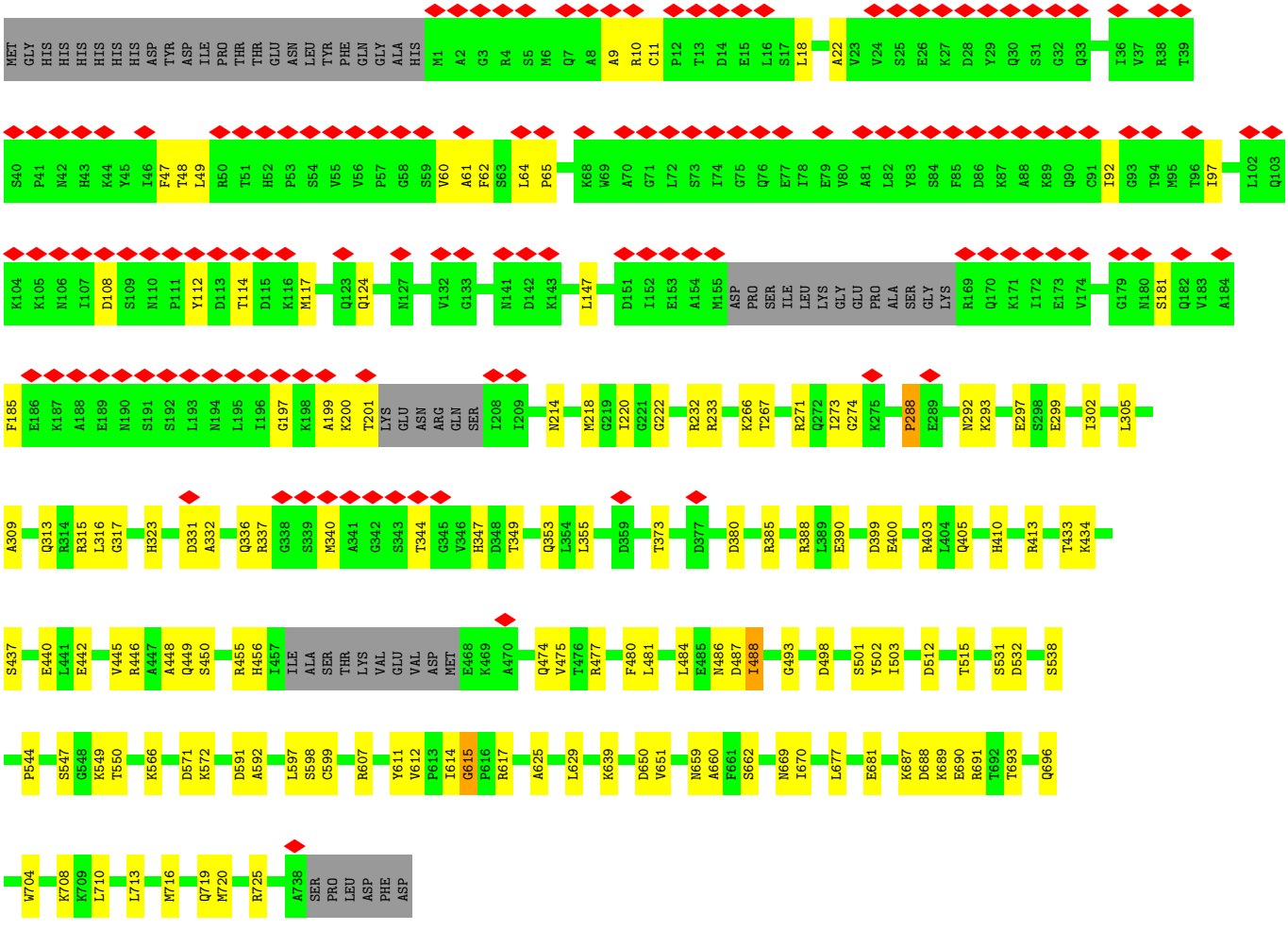
• Molecule 1: Vesicle-fusing ATPase





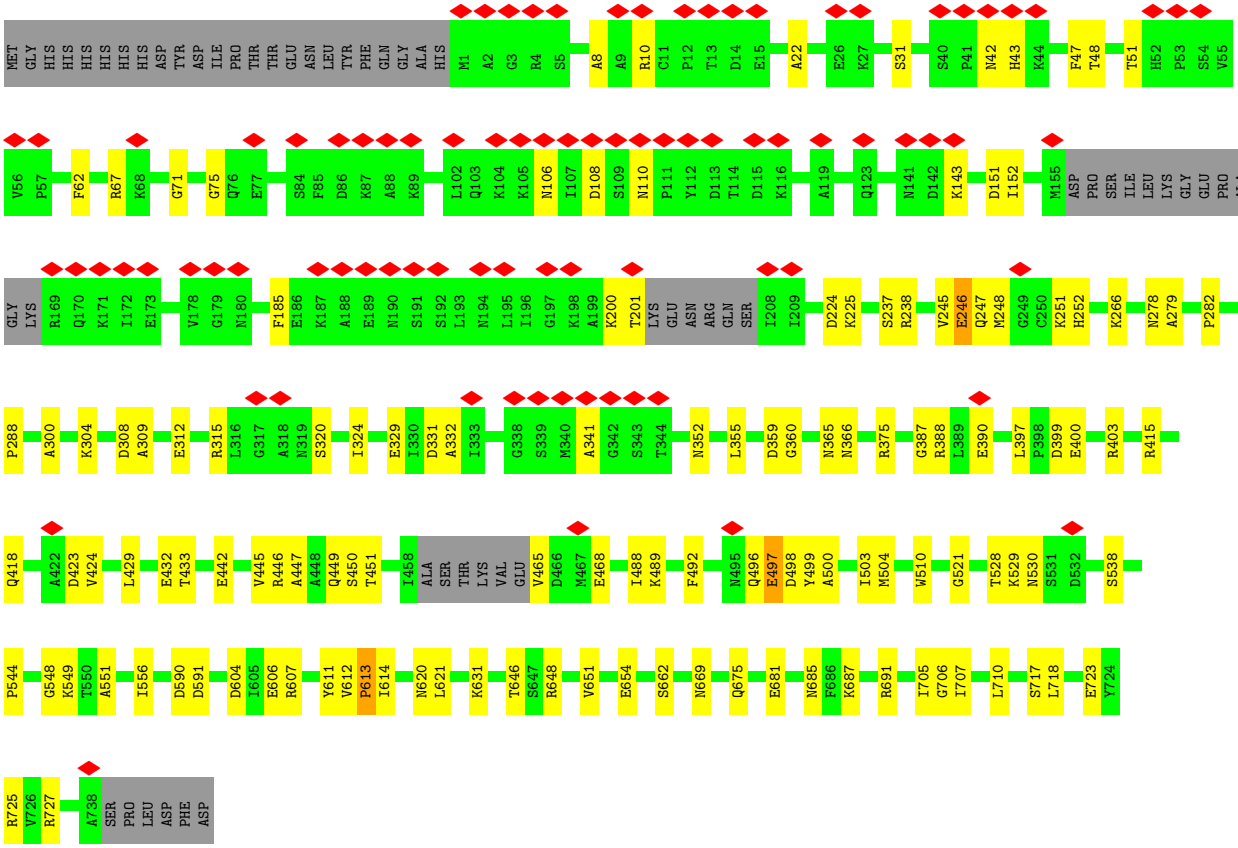
• Molecule 1: Vesicle-fusing ATPase

Chain C:



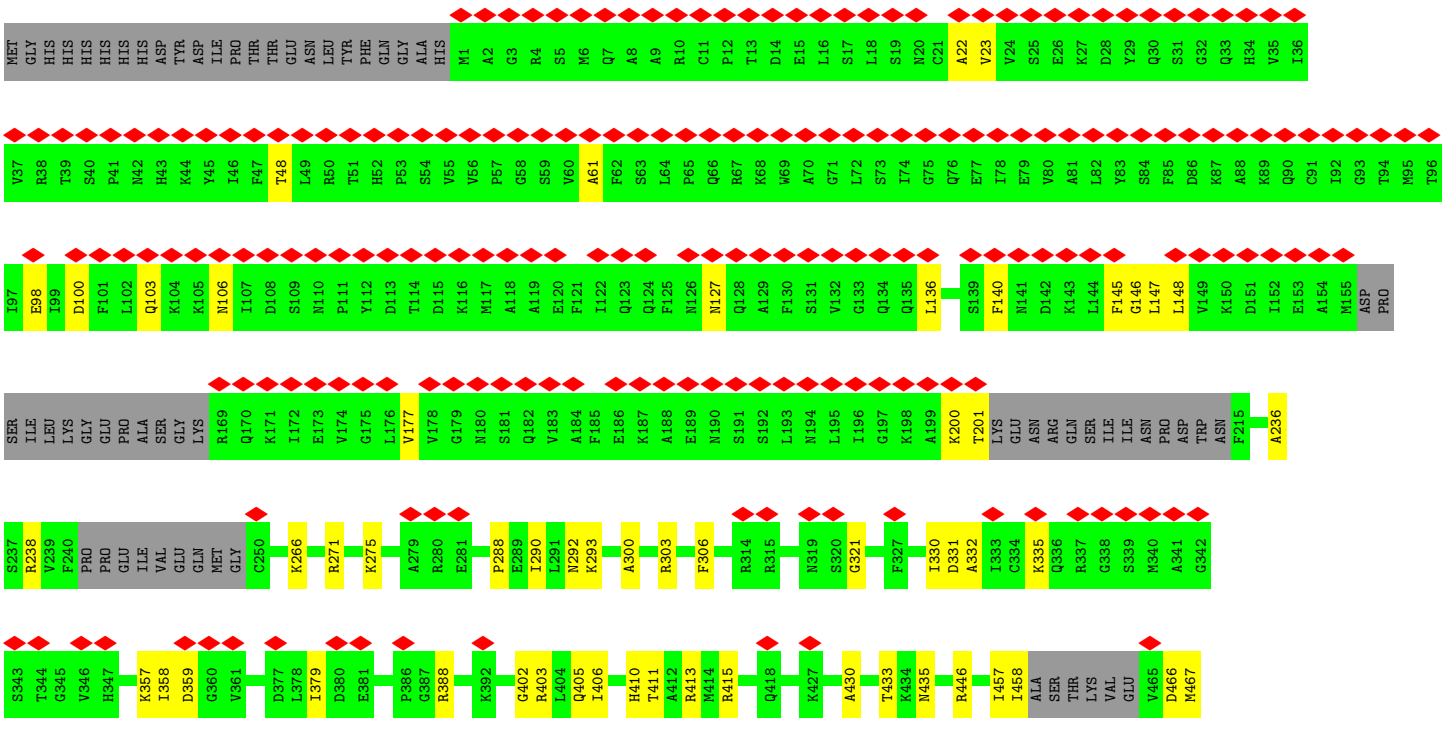
• Molecule 1: Vesicle-fusing ATPase

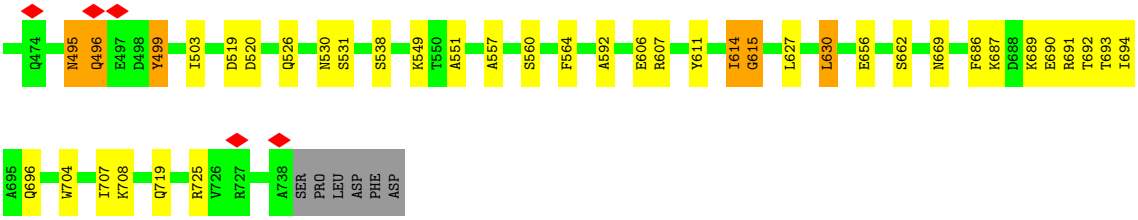
Chain D:



• Molecule 1: Vesicle-fusing ATPase

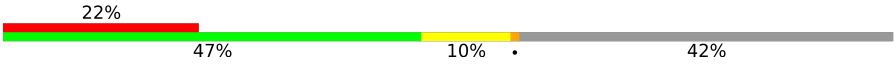
Chain E:

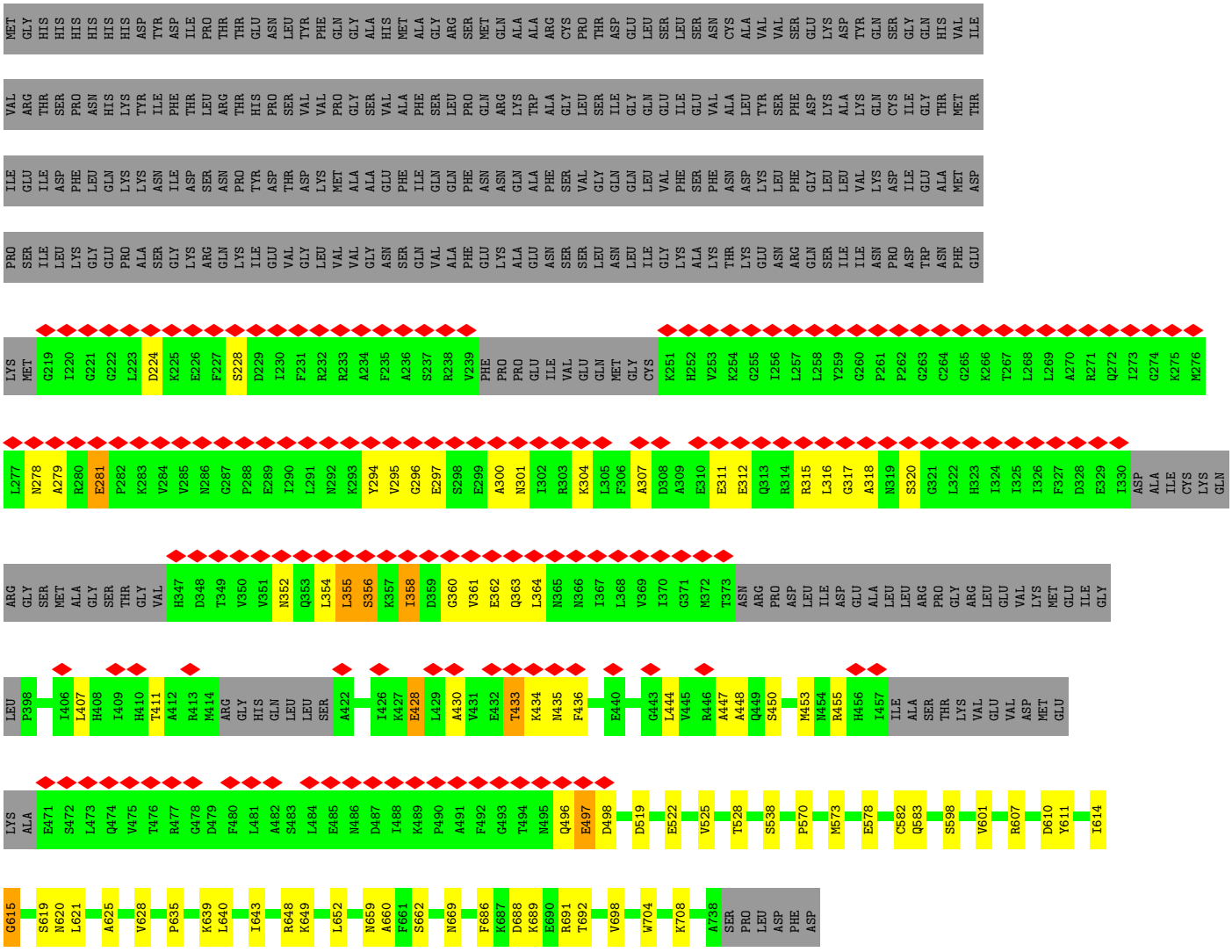




• Molecule 1: Vesicle-fusing ATPase

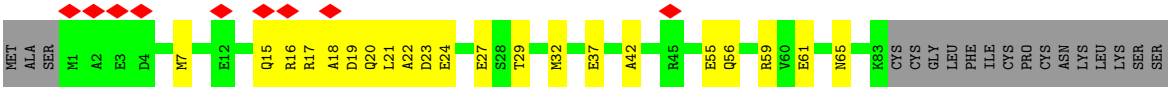
Chain F:

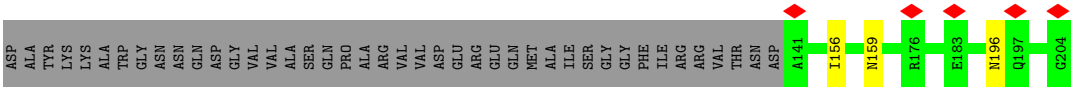




• Molecule 2: Synaptosomal-associated protein 25

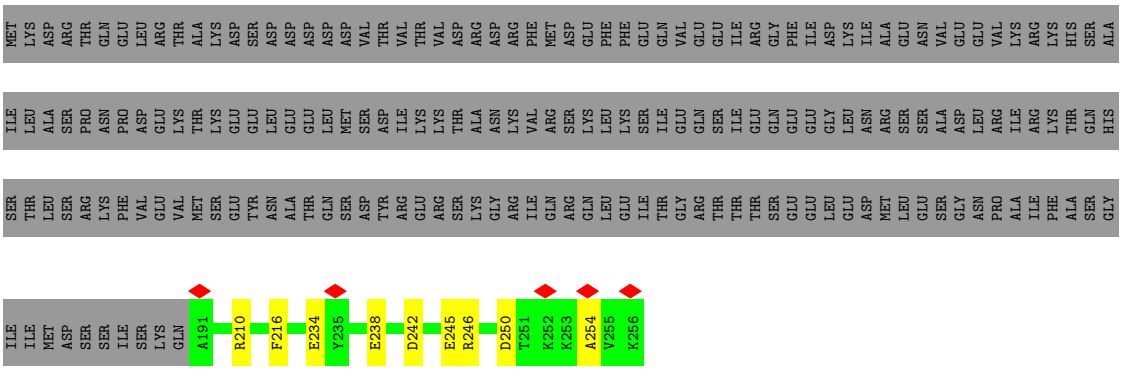
Chain H:





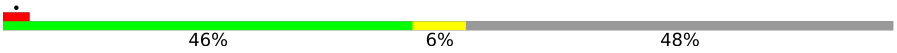
• Molecule 3: Syntaxin-1A

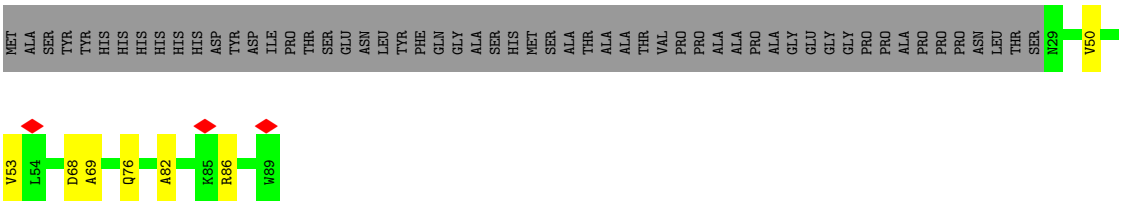
Chain I:



• Molecule 4: Vesicle-associated membrane protein 2

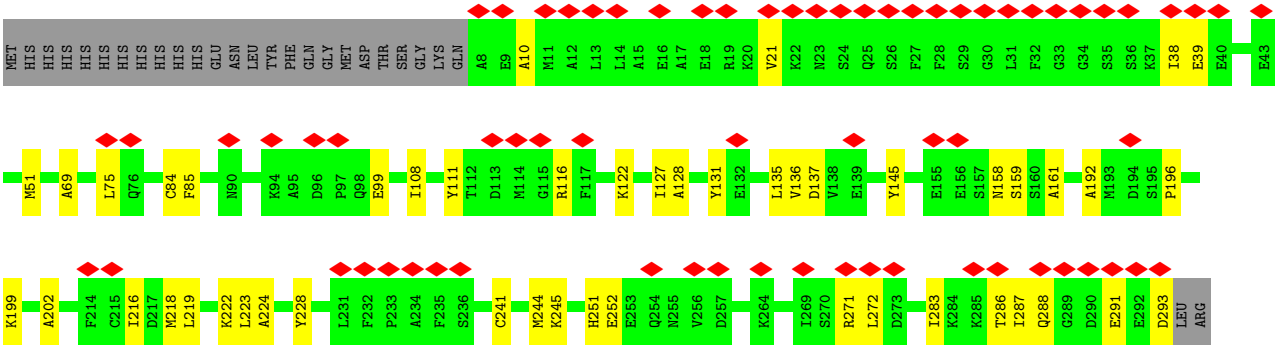
Chain J:





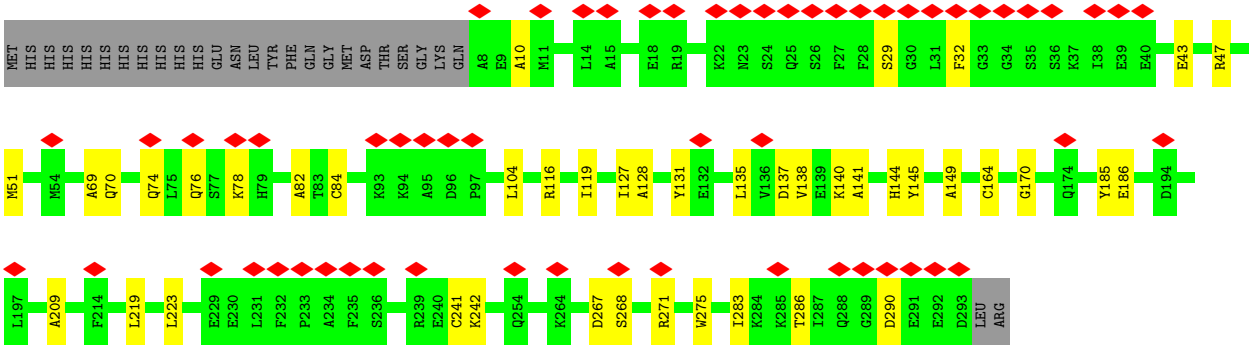
• Molecule 5: Alpha-soluble NSF attachment protein

Chain K:



• Molecule 5: Alpha-soluble NSF attachment protein

Chain L:


MET HIS HIS HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY MET ASP THR SER GLY LYS GLN A8 E9 A10 M11 L14 A15 E18 R19 K22 N23 S24 Q25 S26 F27 F28 S29 G30 L31 F32 G33 G34 S35 S36 K37 I38 E39 E40 E43 R47
M51 M54 A69 Q70 Q74 L75 Q76 S77 K78 H79 A82 T83 C84 K93 K94 A95 D96 P97 L104 R116 I119 I127 A128 Y131 E132 L135 Y136 D137 V138 E139 K140 A141 H144 Y145 A149 C164 G170 Q174 Y185 E186 D194
L197 A209 F214 L219 L223 E229 E230 L231 F232 P233 A234 F235 S236 R239 E240 C241 K242 Q254 K264 D267 S268 R271 W275 I283 K284 K285 T286 I287 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	62723	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	0.85	0/4044	0.99	1/5447 (0.0%)
1	B	0.81	0/5590	0.94	5/7532 (0.1%)
1	C	0.77	0/5611	0.91	2/7559 (0.0%)
1	D	0.73	0/5642	0.88	2/7601 (0.0%)
1	E	0.64	0/5507	0.91	4/7412 (0.1%)
1	F	0.66	0/3420	1.02	8/4615 (0.2%)
2	H	0.47	0/1171	0.80	0/1557
3	I	0.49	0/541	0.75	0/723
4	J	0.45	0/496	0.80	0/664
5	K	0.44	0/2291	0.77	1/3082 (0.0%)
5	L	0.41	0/2295	0.73	0/3086
All	All	0.70	0/36608	0.90	23/49278 (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
1	A	0	4
1	B	0	2
1	C	0	4
1	D	0	3
1	E	0	4
1	F	0	1
5	K	0	3
5	L	0	2
All	All	0	23

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	495	ASN	N-CA-C	10.06	121.83	111.07
1	F	318	ALA	N-CA-C	9.51	121.65	111.28
1	E	496	GLN	N-CA-C	8.08	122.39	111.24
1	F	615	GLY	N-CA-C	-8.07	95.88	112.34
1	E	615	GLY	N-CA-C	-7.33	97.38	112.34
1	A	615	GLY	N-CA-C	-6.49	99.09	112.34
1	E	335	LYS	N-CA-C	-6.38	99.81	109.95
1	B	189	GLU	CA-C-N	6.13	134.54	124.31
1	B	189	GLU	C-N-CA	6.13	134.54	124.31
1	F	358	ILE	N-CA-C	5.92	116.69	110.72
1	C	488	ILE	CA-C-N	-5.69	113.70	121.61
1	C	488	ILE	C-N-CA	-5.69	113.70	121.61
1	B	346	VAL	CA-CB-CG2	5.60	119.91	110.40
1	D	687	LYS	CB-CG-CD	5.50	123.95	111.30
1	F	698	VAL	CG1-CB-CG2	5.46	122.80	110.80
1	F	281	GLU	N-CA-C	-5.17	102.03	109.48
5	K	252	GLU	N-CA-CB	5.14	117.53	110.07
1	F	317	GLY	N-CA-C	5.13	118.89	112.73
1	B	420	LEU	CD1-CG-CD2	5.12	122.05	110.80
1	B	346	VAL	CG1-CB-CG2	5.03	121.88	110.80
1	D	614	ILE	N-CA-C	-5.03	97.66	106.61
1	F	363	GLN	N-CA-C	-5.02	105.81	111.28
1	F	433	THR	N-CA-C	5.02	118.50	112.38

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	ILE	Peptide
1	A	388	ARG	Peptide
1	A	615	GLY	Peptide
1	A	698	VAL	Peptide
1	B	288	PRO	Peptide
1	B	496	GLN	Peptide
1	C	199	ALA	Mainchain
1	C	214	ASN	Peptide
1	C	288	PRO	Peptide
1	C	615	GLY	Peptide
1	D	612	VAL	Peptide
1	D	613	PRO	Peptide
1	D	685	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	379	ILE	Peptide
1	E	388	ARG	Peptide
1	E	614	ILE	Peptide
1	E	725	ARG	Peptide
1	F	279	ALA	Mainchain
5	K	135	LEU	Peptide
5	K	75	LEU	Peptide
5	K	99	GLU	Peptide
5	L	135	LEU	Peptide
5	L	76	GLN	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	3983	4099	4109	50	0
1	B	5505	5624	5637	77	0
1	C	5526	5641	5657	101	0
1	D	5557	5675	5690	81	0
1	E	5428	5559	5568	67	0
1	F	3376	3372	3374	65	0
2	H	1171	1124	1134	14	0
3	I	536	527	527	7	0
4	J	493	491	491	5	0
5	K	2251	2185	2188	27	0
5	L	2255	2199	2199	23	0
6	A	31	12	12	1	0
6	B	62	24	24	10	0
6	C	62	24	24	8	0
6	D	62	24	24	5	0
6	E	31	12	12	4	0
6	F	31	12	12	1	0
7	A	27	12	12	1	0
7	E	27	12	12	2	0
All	All	36414	36628	36706	487	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 7.

All (487) 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:F:315:ARG:HG2	1:F:316:LEU:CD1	1.63	1.28
1:F:278:ASN:CB	1:F:281:GLU:CB	2.15	1.23
1:E:435:ASN:ND2	1:E:495:ASN:HD22	1.35	1.22
1:F:315:ARG:C	1:F:316:LEU:HD12	1.69	1.14
1:E:435:ASN:CG	1:E:495:ASN:HD22	1.61	1.09
1:E:435:ASN:CG	1:E:495:ASN:ND2	2.12	1.08
1:F:315:ARG:HG2	1:F:316:LEU:HD11	1.37	1.04
1:F:355:LEU:O	1:F:358:ILE:HG12	1.64	0.98
1:F:430:ALA:O	1:F:433:THR:HG23	1.70	0.91
1:E:435:ASN:ND2	1:E:495:ASN:ND2	2.15	0.90
1:F:315:ARG:HG2	1:F:316:LEU:HD12	1.53	0.89
1:F:315:ARG:CG	1:F:316:LEU:CD1	2.51	0.89
1:C:669:ASN:ND2	1:C:704:TRP:O	2.06	0.88
1:C:299:GLU:OE2	1:C:349:THR:OG1	1.94	0.85
1:D:510:TRP:O	1:D:675:GLN:NE2	2.10	0.84
1:F:355:LEU:O	1:F:358:ILE:CG1	2.25	0.83
1:F:315:ARG:O	1:F:316:LEU:HD12	1.78	0.83
1:D:718:LEU:O	1:D:725:ARG:NH1	2.11	0.83
5:K:219:LEU:O	5:K:223:LEU:N	2.12	0.82
1:B:359:ASP:OD2	1:B:385:ARG:NH2	2.12	0.82
1:A:538:SER:O	1:A:662:SER:OG	1.98	0.82
1:E:669:ASN:ND2	1:E:704:TRP:O	2.12	0.82
1:D:403:ARG:NH1	1:D:433:THR:O	2.13	0.81
3:I:245:GLU:OE1	5:K:116:ARG:NH1	2.13	0.81
1:C:538:SER:O	1:C:662:SER:OG	1.99	0.81
1:A:254:LYS:NZ	1:A:364:LEU:O	2.14	0.80
1:A:390:GLU:OE1	1:B:446:ARG:NH2	2.15	0.80
1:C:344:THR:OG1	1:D:341:ALA:O	1.98	0.80
1:C:677:LEU:O	1:C:691:ARG:NH2	2.13	0.79
1:A:688:ASP:O	1:A:692:THR:OG1	1.99	0.79
1:B:453:MET:O	1:B:456:HIS:ND1	2.14	0.79
1:E:607:ARG:NH2	1:E:611:TYR:O	2.15	0.79
1:D:538:SER:O	1:D:662:SER:OG	2.01	0.79
5:K:283:ILE:O	5:K:286:THR:OG1	2.02	0.78
5:L:219:LEU:O	5:L:223:LEU:N	2.16	0.78
1:F:430:ALA:O	1:F:433:THR:CG2	2.31	0.77
1:D:544:PRO:O	1:D:549:LYS:NZ	2.17	0.77
1:F:686:PHE:O	1:F:691:ARG:NH2	2.16	0.77
1:B:538:SER:O	1:B:662:SER:OG	2.02	0.77
1:D:606:GLU:OE2	1:D:646:THR:OG1	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:GLU:OE1	1:F:315:ARG:NH2	2.18	0.77
1:C:292:ASN:ND2	1:C:297:GLU:OE2	2.18	0.76
1:A:544:PRO:O	1:A:549:LYS:NZ	2.18	0.76
1:C:200:LYS:O	1:C:201:THR:HB	1.85	0.76
1:C:108:ASP:OD2	1:C:112:TYR:OH	2.03	0.76
1:B:363:GLN:OE1	1:C:271:ARG:NH2	2.19	0.75
1:F:538:SER:O	1:F:662:SER:OG	2.04	0.75
1:A:385:ARG:NH2	6:B:801:ATP:O1B	2.20	0.75
1:B:708:LYS:NZ	6:B:802:ATP:O3B	2.18	0.75
1:E:557:ALA:O	1:E:560:SER:OG	2.03	0.75
1:A:686:PHE:O	1:A:691:ARG:NH2	2.19	0.75
1:C:531:SER:O	1:C:639:LYS:NZ	2.13	0.74
1:C:410:HIS:NE2	1:C:442:GLU:OE2	2.21	0.74
1:C:232:ARG:NH2	1:D:451:THR:OG1	2.21	0.74
1:A:531:SER:O	1:A:639:LYS:NZ	2.17	0.74
1:D:388:ARG:NH2	7:E:802:ADP:O1B	2.20	0.74
1:B:557:ALA:O	1:B:560:SER:OG	2.05	0.73
1:C:549:LYS:NZ	6:C:801:ATP:O3G	2.21	0.73
1:D:320:SER:N	1:D:366:ASN:OD1	2.22	0.73
1:B:542:GLU:OE1	1:B:666:HIS:ND1	2.22	0.73
1:D:251:LYS:O	1:E:446:ARG:NH2	2.22	0.73
1:C:475:VAL:O	1:C:477:ARG:NH1	2.22	0.73
1:A:415:ARG:O	1:A:418:GLN:NE2	2.22	0.72
1:F:360:GLY:O	1:F:362:GLU:N	2.23	0.72
3:I:242:ASP:OD1	3:I:246:ARG:NE	2.21	0.72
2:H:56:GLN:OE1	2:H:59:ARG:NH2	2.22	0.72
1:C:498:ASP:O	1:C:501:SER:OG	2.07	0.71
1:E:526:GLN:OE1	1:E:530:ASN:ND2	2.23	0.71
1:E:430:ALA:O	1:E:433:THR:OG1	2.07	0.71
5:K:196:PRO:O	5:K:199:LYS:NZ	2.19	0.71
1:E:519:ASP:OD1	1:E:520:ASP:N	2.24	0.71
2:H:196:ASN:ND2	4:J:76:GLN:OE1	2.24	0.71
5:K:288:GLN:O	5:K:293:ASP:N	2.24	0.71
1:B:312:GLU:OE1	1:B:323:HIS:NE2	2.22	0.71
1:D:442:GLU:OE1	1:D:446:ARG:NH1	2.24	0.71
1:D:329:GLU:N	1:D:329:GLU:OE1	2.24	0.70
1:B:385:ARG:NH2	6:C:802:ATP:O2B	2.24	0.70
1:A:451:THR:O	1:A:455:ARG:N	2.23	0.70
1:B:360:GLY:O	1:C:271:ARG:NH1	2.24	0.70
1:E:238:ARG:NH1	1:E:321:GLY:O	2.24	0.70
1:B:718:LEU:O	1:B:725:ARG:NH1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:VAL:O	1:D:449:GLN:NE2	2.25	0.69
1:B:512:ASP:O	1:B:515:THR:OG1	2.10	0.69
1:B:267:THR:N	6:B:801:ATP:O1A	2.26	0.68
1:D:22:ALA:N	1:D:48:THR:O	2.27	0.68
1:A:222:GLY:N	1:A:405:GLN:OE1	2.27	0.68
1:F:669:ASN:ND2	1:F:704:TRP:O	2.27	0.68
1:E:687:LYS:N	1:E:690:GLU:OE2	2.27	0.68
1:C:512:ASP:O	1:C:515:THR:OG1	2.11	0.67
1:E:656:GLU:OE1	1:F:648:ARG:NH2	2.28	0.67
1:E:411:THR:OG1	1:E:415:ARG:NH1	2.28	0.67
5:K:288:GLN:NE2	5:K:291:GLU:OE1	2.27	0.67
1:B:303:ARG:NH2	1:C:288:PRO:O	2.28	0.66
1:C:22:ALA:N	1:C:48:THR:O	2.29	0.66
5:L:241:CYS:SG	5:L:242:LYS:N	2.68	0.66
1:C:708:LYS:NZ	6:C:801:ATP:O3A	2.28	0.66
1:C:200:LYS:O	1:C:201:THR:CB	2.43	0.66
1:B:620:ASN:OD1	1:B:621:LEU:N	2.29	0.66
1:A:718:LEU:O	1:A:725:ARG:NH1	2.29	0.65
1:D:631:LYS:NZ	6:E:801:ATP:O1G	2.28	0.65
3:I:234:GLU:OE2	5:K:122:LYS:NZ	2.29	0.65
1:E:435:ASN:CB	1:E:495:ASN:ND2	2.57	0.65
1:B:487:ASP:O	1:B:496:GLN:NE2	2.30	0.65
1:E:266:LYS:N	7:E:802:ADP:O2A	2.29	0.65
5:L:43:GLU:OE2	5:L:47:ARG:NE	2.29	0.65
1:D:106:ASN:O	1:D:143:LYS:NZ	2.30	0.65
1:F:316:LEU:HD12	1:F:316:LEU:N	2.11	0.65
1:B:692:THR:O	1:B:696:GLN:NE2	2.30	0.64
1:C:385:ARG:NH2	6:D:802:ATP:O3A	2.31	0.64
1:C:403:ARG:NE	1:C:433:THR:O	2.30	0.64
1:E:403:ARG:NH1	1:E:433:THR:O	2.31	0.64
1:F:444:LEU:O	1:F:448:ALA:N	2.31	0.64
1:F:607:ARG:NH2	1:F:611:TYR:O	2.31	0.64
1:D:308:ASP:OD1	1:D:309:ALA:N	2.30	0.64
1:F:497:GLU:OE1	1:F:498:ASP:N	2.30	0.64
1:D:631:LYS:NZ	6:E:801:ATP:O1B	2.31	0.63
5:L:29:SER:OG	5:L:32:PHE:O	2.15	0.63
1:C:18:LEU:O	1:C:124:GLN:NE2	2.31	0.63
1:A:620:ASN:OD1	1:A:621:LEU:N	2.32	0.63
1:B:246:GLU:O	1:C:413:ARG:NH2	2.32	0.63
3:I:250:ASP:O	3:I:254:ALA:N	2.32	0.62
1:A:606:GLU:OE2	1:A:646:THR:OG1	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ASP:O	1:A:594:LYS:NZ	2.32	0.62
1:B:596:GLN:O	1:B:639:LYS:N	2.33	0.62
5:L:185:TYR:HB2	5:L:209:ALA:HB2	1.82	0.61
1:B:9:ALA:N	1:B:60:VAL:O	2.29	0.61
1:C:607:ARG:NH2	1:C:611:TYR:O	2.34	0.61
1:C:650:ASP:OD1	1:C:651:VAL:N	2.33	0.61
1:C:114:THR:HG21	1:C:200:LYS:HG2	1.83	0.61
1:F:433:THR:O	1:F:436:PHE:O	2.17	0.61
1:F:620:ASN:OD1	1:F:621:LEU:N	2.34	0.61
1:A:260:GLY:O	1:A:374:ASN:ND2	2.34	0.61
5:K:224:ALA:O	5:K:228:TYR:N	2.33	0.60
1:C:550:THR:OG1	6:C:801:ATP:O1A	2.18	0.60
1:E:692:THR:O	1:E:696:GLN:NE2	2.34	0.60
1:F:430:ALA:C	1:F:433:THR:HG23	2.26	0.60
5:K:241:CYS:O	5:K:244:MET:N	2.35	0.60
5:L:283:ILE:O	5:L:286:THR:OG1	2.17	0.60
1:E:689:LYS:O	1:E:692:THR:OG1	2.17	0.60
1:F:522:GLU:HA	1:F:525:VAL:HG12	1.84	0.59
1:E:331:ASP:OD1	1:E:332:ALA:N	2.35	0.59
1:B:688:ASP:OD1	1:B:689:LYS:N	2.36	0.59
1:D:352:ASN:ND2	1:E:331:ASP:OD2	2.36	0.59
1:E:538:SER:OG	1:E:662:SER:N	2.36	0.59
1:F:689:LYS:O	1:F:692:THR:OG1	2.08	0.59
2:H:42:ALA:HB3	3:I:216:PHE:HE2	1.67	0.58
1:E:22:ALA:N	1:E:48:THR:O	2.36	0.58
1:E:103:GLN:OE1	1:E:106:ASN:ND2	2.35	0.58
4:J:68:ASP:OD1	4:J:69:ALA:N	2.36	0.58
1:B:297:GLU:O	1:B:301:ASN:ND2	2.37	0.58
1:D:681:GLU:HB3	1:D:691:ARG:HE	1.67	0.58
1:E:466:ASP:OD1	1:E:467:MET:N	2.36	0.58
1:F:307:ALA:O	1:F:311:GLU:N	2.33	0.58
1:F:352:ASN:O	1:F:356:SER:HB3	2.03	0.58
1:B:651:VAL:O	1:B:655:MET:N	2.35	0.58
1:C:9:ALA:N	1:C:60:VAL:O	2.37	0.58
5:L:267:ASP:O	5:L:271:ARG:NH1	2.35	0.58
1:B:361:VAL:O	1:C:271:ARG:NE	2.37	0.58
1:C:292:ASN:OD1	1:C:293:LYS:N	2.37	0.58
1:C:720:MET:O	1:C:725:ARG:NH2	2.37	0.58
1:C:337:ARG:O	1:D:375:ARG:NH2	2.36	0.58
1:F:407:LEU:O	1:F:411:THR:N	2.36	0.57
1:A:525:VAL:O	1:A:528:THR:OG1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ASN:N	1:E:177:VAL:O	2.36	0.57
1:A:230:ILE:O	1:A:234:ALA:HB3	2.04	0.57
1:B:650:ASP:OD1	1:B:651:VAL:N	2.36	0.57
1:C:710:LEU:O	1:C:713:LEU:N	2.37	0.57
1:D:266:LYS:NZ	6:D:802:ATP:O3G	2.32	0.57
1:A:450:SER:OG	1:A:454:ASN:OD1	2.22	0.57
2:H:37:GLU:N	2:H:37:GLU:OE1	2.38	0.57
1:D:10:ARG:NH2	5:L:290:ASP:OD2	2.38	0.56
1:C:92:ILE:O	1:C:181:SER:OG	2.19	0.56
1:C:388:ARG:NH1	6:D:802:ATP:O1G	2.38	0.56
1:D:42:ASN:OD1	1:D:43:HIS:ND1	2.39	0.56
1:D:359:ASP:OD1	1:D:360:GLY:N	2.37	0.56
1:E:406:ILE:O	1:E:410:HIS:ND1	2.25	0.56
1:C:399:ASP:OD1	1:C:400:GLU:N	2.36	0.56
1:F:294:TYR:O	1:F:295:VAL:C	2.49	0.56
1:C:445:VAL:O	1:C:449:GLN:NE2	2.39	0.56
1:D:312:GLU:OE1	1:D:315:ARG:NH1	2.39	0.56
1:A:528:THR:O	1:A:639:LYS:NZ	2.22	0.56
1:D:224:ASP:OD1	1:D:225:LYS:N	2.38	0.56
1:E:690:GLU:O	1:E:693:THR:OG1	2.16	0.56
1:C:442:GLU:OE1	6:C:802:ATP:O2'	2.23	0.55
1:D:503:ILE:HD13	1:D:551:ALA:HB1	1.88	0.55
1:D:530:ASN:OD1	1:E:719:GLN:NE2	2.39	0.55
5:K:69:ALA:HB1	5:K:85:PHE:CD1	2.42	0.55
1:F:659:ASN:OD1	1:F:660:ALA:N	2.40	0.55
1:C:197:GLY:O	1:C:200:LYS:HE2	2.07	0.55
1:F:428:GLU:N	1:F:428:GLU:OE1	2.40	0.55
1:B:189:GLU:OE1	1:B:189:GLU:N	2.38	0.54
1:C:693:THR:O	1:C:696:GLN:NE2	2.40	0.54
1:E:530:ASN:OD1	1:E:531:SER:N	2.41	0.54
1:D:67:ARG:O	1:D:71:GLY:N	2.41	0.54
1:F:447:ALA:O	1:F:450:SER:N	2.41	0.54
1:D:365:ASN:OD1	1:D:366:ASN:N	2.39	0.54
1:F:315:ARG:C	1:F:316:LEU:CD1	2.63	0.54
1:D:278:ASN:OD1	1:D:279:ALA:N	2.41	0.54
1:C:403:ARG:NH1	1:C:434:LYS:O	2.40	0.53
1:C:340:MET:SD	1:C:347:HIS:N	2.80	0.53
4:J:86:ARG:NH1	5:K:39:GLU:OE2	2.42	0.53
1:A:263:GLY:O	1:A:437:SER:OG	2.24	0.53
1:B:100:ASP:OD1	1:B:101:PHE:N	2.41	0.53
5:L:69:ALA:HB2	5:L:84:CYS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:NH2	1:A:433:THR:O	2.41	0.53
1:C:531:SER:OG	1:C:532:ASP:N	2.41	0.53
1:D:8:ALA:O	1:D:75:GLY:N	2.40	0.53
1:E:564:PHE:HE2	1:E:592:ALA:HB2	1.74	0.53
1:C:442:GLU:O	1:C:446:ARG:N	2.41	0.53
1:F:578:GLU:OE1	1:F:578:GLU:N	2.40	0.52
5:L:131:TYR:O	5:L:137:ASP:N	2.37	0.52
1:B:442:GLU:HA	1:B:445:VAL:HG12	1.92	0.52
1:D:654:GLU:OE1	1:D:654:GLU:N	2.42	0.52
5:K:131:TYR:O	5:K:137:ASP:N	2.42	0.52
5:L:128:ALA:HB2	5:L:144:HIS:HB2	1.90	0.52
1:D:22:ALA:HB2	1:D:47:PHE:HB3	1.92	0.52
1:D:423:ASP:OD1	1:D:424:VAL:N	2.42	0.52
1:A:360:GLY:O	1:B:271:ARG:NH2	2.42	0.52
1:C:448:ALA:HB2	1:C:481:LEU:HB2	1.92	0.52
1:A:359:ASP:OD2	1:A:385:ARG:NH2	2.42	0.52
1:D:399:ASP:OD1	1:D:400:GLU:N	2.43	0.52
2:H:7:MET:SD	2:H:7:MET:N	2.83	0.52
1:C:538:SER:OG	1:C:662:SER:N	2.36	0.52
1:E:100:ASP:O	1:E:146:GLY:N	2.42	0.52
1:F:688:ASP:OD1	1:F:689:LYS:N	2.43	0.52
5:L:170:GLY:O	5:L:275:TRP:NE1	2.42	0.52
1:A:528:THR:OG1	1:A:529:LYS:N	2.43	0.52
1:B:452:ALA:HA	1:B:455:ARG:HE	1.75	0.52
1:C:591:ASP:OD1	1:C:592:ALA:N	2.43	0.52
1:D:620:ASN:OD1	1:D:621:LEU:N	2.43	0.52
1:F:315:ARG:CG	1:F:316:LEU:HD12	2.27	0.52
1:B:24:VAL:O	1:B:52:HIS:N	2.43	0.51
1:F:610:ASP:OD1	1:F:619:SER:N	2.36	0.51
1:A:578:GLU:OE1	1:A:578:GLU:N	2.42	0.51
1:B:267:THR:OG1	6:B:801:ATP:O1A	2.16	0.51
1:A:321:GLY:O	1:A:366:ASN:ND2	2.40	0.51
1:B:127:ASN:N	1:B:177:VAL:O	2.42	0.51
1:E:236:ALA:HB2	1:F:450:SER:HB2	1.93	0.51
1:C:713:LEU:HA	1:C:716:MET:HG2	1.93	0.51
1:E:200:LYS:O	1:E:201:THR:OG1	2.22	0.51
1:F:355:LEU:O	1:F:358:ILE:HG13	2.11	0.51
1:D:282:PRO:HB3	1:D:324:ILE:HD11	1.93	0.51
1:E:435:ASN:HB3	1:E:495:ASN:ND2	2.25	0.51
5:L:137:ASP:O	5:L:140:LYS:N	2.44	0.51
1:B:605:ILE:O	1:B:608:LEU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:GLY:O	1:C:566:LYS:NZ	2.23	0.50
2:H:23:ASP:OD1	2:H:24:GLU:N	2.44	0.50
1:B:445:VAL:O	1:B:449:GLN:NE2	2.44	0.50
1:A:487:ASP:OD1	1:A:488:ILE:N	2.44	0.50
1:D:538:SER:OG	1:D:662:SER:N	2.38	0.50
1:B:22:ALA:N	1:B:48:THR:O	2.43	0.49
1:B:216:GLU:HG2	1:B:218:MET:HG2	1.93	0.49
1:F:300:ALA:O	1:F:304:LYS:N	2.44	0.49
1:F:315:ARG:HE	1:F:316:LEU:HD13	1.77	0.49
1:B:687:LYS:N	1:B:690:GLU:OE2	2.36	0.49
1:F:708:LYS:NZ	6:F:801:ATP:O3B	2.44	0.49
1:C:455:ARG:NH1	1:C:477:ARG:O	2.41	0.49
1:D:496:GLN:O	1:D:498:ASP:N	2.45	0.49
1:B:232:ARG:O	1:C:450:SER:OG	2.29	0.49
1:E:538:SER:O	1:E:662:SER:N	2.45	0.49
1:F:570:PRO:HA	1:F:573:MET:HG2	1.95	0.49
5:K:69:ALA:HB2	5:K:84:CYS:HB3	1.94	0.49
1:B:23:VAL:HB	1:B:61:ALA:HB3	1.94	0.49
1:C:480:PHE:O	1:C:484:LEU:HG	2.13	0.49
1:D:590:ASP:OD1	1:D:591:ASP:N	2.46	0.49
1:B:722:PRO:HA	1:B:725:ARG:HE	1.78	0.49
1:B:662:SER:OG	1:B:663:THR:N	2.46	0.48
1:F:297:GLU:O	1:F:301:ASN:N	2.34	0.48
1:F:316:LEU:CD1	1:F:316:LEU:N	2.75	0.48
1:D:681:GLU:CB	1:D:691:ARG:HE	2.26	0.48
1:B:437:SER:O	1:B:440:GLU:N	2.45	0.48
1:D:707:ILE:O	1:D:710:LEU:N	2.46	0.48
1:A:267:THR:OG1	7:A:802:ADP:O2A	2.24	0.48
1:F:435:ASN:ND2	1:F:435:ASN:O	2.46	0.48
1:E:686:PHE:O	1:E:691:ARG:NE	2.47	0.48
1:D:447:ALA:O	1:D:450:SER:OG	2.20	0.48
1:A:548:GLY:N	6:A:801:ATP:O2A	2.44	0.48
1:B:538:SER:OG	1:B:662:SER:N	2.42	0.48
1:D:355:LEU:O	1:D:388:ARG:NH1	2.46	0.48
1:D:723:GLU:OE2	1:D:727:ARG:NH2	2.46	0.48
1:E:136:LEU:O	1:E:147:LEU:N	2.43	0.48
1:B:238:ARG:NH2	1:B:252:HIS:HB3	2.29	0.48
1:A:388:ARG:NH1	6:B:801:ATP:O3G	2.43	0.47
1:A:489:LYS:HE2	1:A:489:LYS:HA	1.96	0.47
1:B:292:ASN:OD1	1:B:293:LYS:N	2.47	0.47
1:C:355:LEU:O	1:C:388:ARG:NH2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:ASN:HB2	1:D:705:ILE:O	2.14	0.47
1:D:611:TYR:CE2	1:D:613:PRO:HD3	2.49	0.47
1:C:688:ASP:OD1	1:C:689:LYS:N	2.47	0.47
1:F:614:ILE:HD12	1:F:615:GLY:N	2.30	0.47
2:H:19:ASP:OD1	2:H:20:GLN:N	2.46	0.47
1:B:671:ALA:O	1:B:703:VAL:N	2.41	0.47
1:C:598:SER:OG	1:C:599:CYS:N	2.47	0.47
1:D:528:THR:OG1	1:D:529:LYS:N	2.46	0.47
2:H:23:ASP:O	2:H:27:GLU:N	2.44	0.47
1:A:306:PHE:HB2	1:A:357:LYS:HE2	1.95	0.47
1:B:455:ARG:NH2	1:B:478:GLY:O	2.45	0.47
1:C:315:ARG:HD2	1:C:316:LEU:HD12	1.97	0.47
1:C:487:ASP:OD1	1:C:488:ILE:N	2.46	0.47
1:D:648:ARG:HE	1:D:651:VAL:HB	1.80	0.47
1:E:271:ARG:O	1:E:275:LYS:N	2.43	0.47
1:E:564:PHE:CE2	1:E:592:ALA:HB2	2.50	0.47
1:C:64:LEU:HB3	1:C:65:PRO:HD3	1.97	0.47
1:C:266:LYS:N	6:C:802:ATP:O2A	2.48	0.47
1:D:247:GLN:O	1:E:413:ARG:NE	2.48	0.47
1:F:435:ASN:ND2	1:F:435:ASN:C	2.73	0.47
1:B:266:LYS:NZ	6:B:801:ATP:O2B	2.47	0.46
1:D:465:VAL:N	1:D:468:GLU:OE2	2.49	0.46
1:F:297:GLU:CB	1:F:301:ASN:ND2	2.78	0.46
1:E:614:ILE:HD12	1:E:615:GLY:N	2.30	0.46
5:K:219:LEU:O	5:K:222:LYS:N	2.48	0.46
1:A:662:SER:OG	1:A:663:THR:N	2.49	0.46
1:A:244:ILE:O	1:A:247:GLN:NE2	2.49	0.46
1:B:290:ILE:HD12	1:B:290:ILE:H	1.81	0.46
5:K:128:ALA:HB1	5:K:145:TYR:CE2	2.50	0.46
5:L:78:LYS:O	5:L:82:ALA:N	2.48	0.46
1:C:571:ASP:OD1	1:C:572:LYS:N	2.48	0.46
1:B:331:ASP:OD1	1:B:332:ALA:N	2.48	0.46
1:C:353:GLN:HB2	1:D:288:PRO:HG3	1.99	0.46
1:E:499:TYR:N	1:E:499:TYR:CD2	2.84	0.45
1:F:358:ILE:O	1:F:364:LEU:CB	2.64	0.45
3:I:238:GLU:O	3:I:242:ASP:N	2.45	0.45
5:K:251:HIS:ND1	5:K:287:ILE:HG12	2.31	0.45
1:A:631:LYS:NZ	6:B:802:ATP:O2G	2.34	0.45
1:B:100:ASP:O	1:B:146:GLY:N	2.45	0.45
1:C:11:CYS:N	1:C:62:PHE:O	2.50	0.45
1:D:503:ILE:CD1	1:D:551:ALA:HB1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ASN:O	1:B:365:ASN:ND2	2.45	0.45
1:C:309:ALA:HB2	1:C:323:HIS:CG	2.51	0.45
1:D:185:PHE:H	1:D:200:LYS:HA	1.82	0.45
1:D:387:GLY:N	1:D:390:GLU:OE2	2.49	0.45
1:A:570:PRO:HA	1:A:573:MET:HG2	1.98	0.45
5:L:70:GLN:O	5:L:74:GLN:NE2	2.42	0.45
1:A:230:ILE:HD12	1:A:231:PHE:N	2.32	0.45
1:C:597:LEU:HA	1:C:639:LYS:O	2.16	0.45
1:E:707:ILE:HG13	1:E:708:LYS:N	2.31	0.45
4:J:50:VAL:O	4:J:53:VAL:HG12	2.15	0.45
5:K:192:ALA:HB3	5:K:202:ALA:HB2	1.99	0.45
1:C:501:SER:OG	1:C:502:TYR:N	2.50	0.45
1:C:437:SER:HB2	1:C:440:GLU:OE1	2.17	0.45
1:B:503:ILE:O	1:B:503:ILE:HG13	2.17	0.45
1:E:306:PHE:CB	1:E:357:LYS:HE2	2.47	0.45
1:E:606:GLU:CD	1:E:607:ARG:HE	2.25	0.45
1:F:355:LEU:C	1:F:358:ILE:HG12	2.39	0.45
1:A:290:ILE:HG13	1:A:290:ILE:O	2.17	0.45
4:J:82:ALA:HB1	4:J:86:ARG:HH12	1.81	0.44
5:K:271:ARG:NH1	5:K:272:LEU:O	2.51	0.44
1:B:216:GLU:OE1	1:B:216:GLU:N	2.50	0.44
1:C:486:ASN:OD1	1:C:487:ASP:N	2.50	0.44
1:E:98:GLU:O	1:E:148:LEU:N	2.50	0.44
1:A:400:GLU:HA	1:A:403:ARG:HE	1.81	0.44
1:F:224:ASP:O	1:F:228:SER:N	2.50	0.44
1:A:385:ARG:NH2	6:B:801:ATP:O2A	2.51	0.44
1:C:97:ILE:HG21	1:C:147:LEU:HD22	1.98	0.44
1:D:499:TYR:O	1:D:503:ILE:N	2.44	0.44
1:D:604:ASP:O	1:D:607:ARG:N	2.49	0.44
2:H:20:GLN:O	2:H:22:ALA:N	2.50	0.44
1:B:222:GLY:N	1:B:405:GLN:OE1	2.41	0.44
1:B:414:MET:HE3	1:B:420:LEU:HD21	2.00	0.44
1:C:267:THR:N	6:C:802:ATP:O2A	2.50	0.44
5:L:138:VAL:HA	5:L:141:ALA:HB3	2.00	0.44
1:C:22:ALA:HB2	1:C:47:PHE:HB3	1.99	0.44
1:E:496:GLN:HG3	1:E:496:GLN:O	2.17	0.44
1:E:614:ILE:HD12	1:E:615:GLY:H	1.82	0.44
1:B:480:PHE:O	1:B:484:LEU:HD13	2.18	0.44
1:C:625:ALA:O	1:C:629:LEU:HG	2.18	0.44
1:F:453:MET:O	1:F:455:ARG:N	2.50	0.44
1:C:659:ASN:OD1	1:C:660:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:10:ALA:HB2	5:L:51:MET:HG3	2.00	0.44
1:D:246:GLU:O	1:E:413:ARG:NH2	2.50	0.43
1:E:292:ASN:OD1	1:E:293:LYS:N	2.49	0.43
1:F:625:ALA:O	1:F:628:VAL:HG12	2.18	0.43
1:D:331:ASP:OD1	1:D:332:ALA:N	2.51	0.43
1:D:496:GLN:O	1:D:496:GLN:NE2	2.51	0.43
5:K:111:TYR:CZ	5:K:116:ARG:HB3	2.52	0.43
5:L:149:ALA:HB2	5:L:164:CYS:HB2	1.99	0.43
1:C:222:GLY:N	1:C:405:GLN:OE1	2.48	0.43
1:E:503:ILE:CD1	1:E:551:ALA:HB1	2.48	0.43
1:E:549:LYS:N	6:E:801:ATP:O2A	2.52	0.43
1:C:484:LEU:HG	1:C:484:LEU:H	1.71	0.43
1:C:669:ASN:OD1	1:C:670:ILE:N	2.48	0.43
1:D:237:SER:HB3	1:D:252:HIS:ND1	2.34	0.43
1:F:315:ARG:CB	1:F:316:LEU:HD12	2.48	0.43
1:A:339:SER:CB	1:B:375:ARG:HB3	2.48	0.43
1:C:503:ILE:HD12	1:C:503:ILE:O	2.19	0.43
1:E:290:ILE:H	1:E:290:ILE:HD12	1.84	0.43
1:F:528:THR:O	1:F:639:LYS:NZ	2.52	0.43
5:L:128:ALA:HB1	5:L:145:TYR:CE2	2.53	0.43
1:B:74:ILE:HG13	5:K:218:MET:HE3	2.01	0.43
1:B:553:ALA:HB1	1:B:643:ILE:HD12	2.01	0.43
1:E:330:ILE:H	1:E:330:ILE:HD12	1.82	0.43
1:A:344:THR:OG1	1:A:345:GLY:N	2.50	0.43
1:B:549:LYS:NZ	6:B:802:ATP:O3G	2.44	0.43
1:B:519:ASP:OD1	1:B:520:ASP:N	2.52	0.43
1:C:331:ASP:OD1	1:C:332:ALA:N	2.51	0.43
1:D:300:ALA:O	1:D:304:LYS:HG2	2.19	0.43
3:I:210:ARG:NH1	5:L:268:SER:O	2.46	0.43
1:B:215:PHE:CE2	1:B:217:LYS:HD2	2.54	0.43
1:C:544:PRO:O	1:C:547:SER:OG	2.37	0.43
1:B:448:ALA:HB2	1:B:481:LEU:HB2	2.01	0.42
1:E:23:VAL:HB	1:E:61:ALA:HB3	2.01	0.42
1:B:530:ASN:OD1	1:C:719:GLN:NE2	2.46	0.42
1:C:385:ARG:NH2	6:D:802:ATP:O3B	2.52	0.42
1:D:31:SER:OG	1:D:51:THR:N	2.50	0.42
1:F:519:ASP:HA	1:F:522:GLU:HG3	2.00	0.42
1:B:307:ALA:HA	1:B:310:GLU:OE1	2.20	0.42
1:C:273:ILE:HG13	1:C:274:GLY:N	2.34	0.42
1:D:500:ALA:O	1:D:504:MET:HE2	2.18	0.42
5:K:158:ASN:HA	5:K:161:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:582:CYS:SG	1:F:583:GLN:N	2.92	0.42
1:B:282:PRO:HB3	1:B:324:ILE:HD11	2.01	0.42
1:C:266:LYS:NZ	1:C:373:THR:O	2.53	0.42
1:C:302:ILE:O	1:C:305:LEU:HB2	2.18	0.42
1:D:717:SER:OG	1:D:725:ARG:O	2.36	0.42
1:E:358:ILE:HG13	1:E:359:ASP:N	2.34	0.42
5:K:216:ILE:HG12	5:K:218:MET:HB2	2.01	0.42
1:A:714:ILE:O	1:A:718:LEU:N	2.49	0.42
1:C:267:THR:HG22	6:C:802:ATP:PA	2.59	0.42
1:D:521:GLY:HA3	1:D:556:ILE:CD1	2.49	0.42
1:E:690:GLU:O	1:E:694:ILE:HG13	2.20	0.42
1:D:415:ARG:O	1:D:418:GLN:NE2	2.53	0.42
1:D:488:ILE:HB	1:D:489:LYS:HD2	2.02	0.42
1:A:401:LYS:O	1:A:404:LEU:HG	2.20	0.42
1:C:456:HIS:NE2	1:C:474:GLN:O	2.53	0.42
2:H:29:THR:HA	2:H:32:MET:HG3	2.01	0.42
2:H:61:GLU:OE2	2:H:65:ASN:ND2	2.46	0.42
1:B:670:ILE:HD12	1:B:670:ILE:O	2.20	0.42
1:B:708:LYS:HZ2	6:B:802:ATP:PA	2.43	0.42
1:C:22:ALA:HB3	1:C:49:LEU:HD23	2.01	0.42
1:D:492:PHE:CZ	1:D:497:GLU:HB2	2.55	0.42
5:K:241:CYS:O	5:K:245:LYS:N	2.37	0.42
1:A:242:PRO:O	1:A:246:GLU:HG2	2.19	0.42
1:E:627:LEU:O	1:E:630:LEU:HB3	2.20	0.42
1:D:22:ALA:HB1	1:D:62:PHE:HE1	1.85	0.41
1:D:238:ARG:HH12	1:D:252:HIS:HB3	1.86	0.41
1:B:480:PHE:O	1:B:484:LEU:HD22	2.20	0.41
5:L:186:GLU:OE2	5:L:209:ALA:HB1	2.20	0.41
1:C:313:GLN:O	1:C:317:GLY:N	2.54	0.41
1:D:245:VAL:HA	1:D:248:MET:HE2	2.03	0.41
2:H:55:GLU:HB3	5:K:159:SER:OG	2.21	0.41
1:B:714:ILE:HD12	1:B:715:GLU:N	2.35	0.41
1:E:140:PHE:HB3	1:E:145:PHE:CE2	2.56	0.41
1:C:218:MET:O	1:C:220:ILE:HG12	2.21	0.41
1:D:108:ASP:OD2	1:D:110:ASN:ND2	2.53	0.41
1:E:402:GLY:O	1:E:405:GLN:HG2	2.20	0.41
1:B:4:ARG:NE	1:B:6:MET:SD	2.94	0.41
1:F:598:SER:O	1:F:640:LEU:HB2	2.21	0.41
5:L:104:LEU:HB3	5:L:127:ILE:HD11	2.02	0.41
1:B:522:GLU:HA	1:B:525:VAL:HG12	2.02	0.41
1:D:705:ILE:HG13	1:D:706:GLY:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:PHE:HB2	1:E:357:LYS:HE2	2.02	0.41
1:E:457:ILE:HD12	1:E:458:ILE:HG12	2.02	0.41
1:E:708:LYS:NZ	6:E:801:ATP:O1B	2.53	0.41
1:F:430:ALA:O	1:F:433:THR:HG21	2.15	0.41
5:K:108:ILE:HD12	5:K:127:ILE:HD12	2.03	0.41
1:A:567:ILE:HD13	1:A:601:VAL:CG1	2.51	0.41
1:C:233:ARG:NH2	1:C:390:GLU:OE1	2.47	0.41
1:C:612:VAL:HG12	1:C:614:ILE:H	1.86	0.41
1:D:429:LEU:O	1:D:432:GLU:N	2.53	0.41
1:E:288:PRO:O	1:E:290:ILE:N	2.54	0.41
1:E:300:ALA:O	1:E:303:ARG:HG2	2.21	0.41
5:K:10:ALA:N	5:K:51:MET:SD	2.93	0.41
1:C:440:GLU:OE1	1:C:440:GLU:N	2.43	0.41
1:A:361:VAL:O	1:A:362:GLU:HG3	2.20	0.40
1:B:222:GLY:C	1:B:223:LEU:HG	2.45	0.40
1:C:10:ARG:O	1:C:61:ALA:HB1	2.21	0.40
1:C:336:GLN:HA	1:C:380:ASP:OD1	2.20	0.40
1:C:687:LYS:HE2	1:C:687:LYS:HA	2.01	0.40
1:D:548:GLY:H	6:D:801:ATP:PB	2.44	0.40
1:F:649:LYS:HA	1:F:652:LEU:HD21	2.03	0.40
2:H:16:ARG:O	2:H:18:ALA:N	2.50	0.40
5:K:21:VAL:HA	5:K:38:ILE:HD13	2.03	0.40
1:C:445:VAL:O	1:C:448:ALA:HB3	2.21	0.40
1:F:643:ILE:HD12	1:F:643:ILE:C	2.46	0.40
2:H:156:ILE:O	2:H:159:ASN:N	2.55	0.40
1:A:499:TYR:O	1:A:502:TYR:N	2.55	0.40
1:C:117:MET:HB3	1:C:185:PHE:HE2	1.87	0.40
1:C:681:GLU:HG2	1:C:691:ARG:HH22	1.85	0.40
1:D:151:ASP:OD1	1:D:152:ILE:N	2.54	0.40
1:F:297:GLU:O	1:F:300:ALA:N	2.54	0.40
1:F:601:VAL:HG12	1:F:643:ILE:HD11	2.02	0.40
1:A:437:SER:O	1:A:440:GLU:HG2	2.21	0.40
1:B:441:LEU:H	1:B:441:LEU:HD23	1.86	0.40
1:C:615:GLY:O	1:C:617:ARG:HG3	2.21	0.40
1:C:687:LYS:N	1:C:690:GLU:OE2	2.54	0.40
1:D:185:PHE:O	1:D:201:THR:N	2.55	0.40
5:L:116:ARG:HB3	5:L:119:ILE:HG22	2.03	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	507/768 (66%)	504 (99%)	3 (1%)	0	100 100
1	B	699/768 (91%)	692 (99%)	7 (1%)	0	100 100
1	C	701/768 (91%)	688 (98%)	13 (2%)	0	100 100
1	D	705/768 (92%)	689 (98%)	15 (2%)	1 (0%)	48 83
1	E	687/768 (90%)	676 (98%)	11 (2%)	0	100 100
1	F	437/768 (57%)	408 (93%)	23 (5%)	6 (1%)	9 39
2	H	143/207 (69%)	139 (97%)	1 (1%)	3 (2%)	5 29
3	I	64/256 (25%)	63 (98%)	1 (2%)	0	100 100
4	J	59/117 (50%)	58 (98%)	1 (2%)	0	100 100
5	K	284/313 (91%)	253 (89%)	30 (11%)	1 (0%)	30 66
5	L	284/313 (91%)	260 (92%)	24 (8%)	0	100 100
All	All	4570/5814 (79%)	4430 (97%)	129 (3%)	11 (0%)	44 77

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	361	VAL
1	F	497	GLU
2	H	21	LEU
1	D	497	GLU
1	F	635	PRO
2	H	15	GLN
1	F	320	SER
1	F	496	GLN
2	H	17	ARG
1	F	296	GLY
5	K	136	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	231/658 (35%)	230 (100%)	1 (0%)	84 82
1	B	573/658 (87%)	573 (100%)	0	100 100
1	C	475/658 (72%)	475 (100%)	0	100 100
1	D	420/658 (64%)	418 (100%)	2 (0%)	81 81
1	E	560/658 (85%)	558 (100%)	2 (0%)	84 82
1	F	296/658 (45%)	291 (98%)	5 (2%)	53 67
2	H	127/177 (72%)	127 (100%)	0	100 100
3	I	60/235 (26%)	60 (100%)	0	100 100
4	J	52/96 (54%)	52 (100%)	0	100 100
5	K	229/260 (88%)	229 (100%)	0	100 100
5	L	195/260 (75%)	195 (100%)	0	100 100
All	All	3218/4976 (65%)	3208 (100%)	10 (0%)	84 84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	504	MET
1	D	246	GLU
1	D	397	LEU
1	E	499	TYR
1	E	630	LEU
1	F	354	LEU
1	F	355	LEU
1	F	356	SER
1	F	428	GLU
1	F	434	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	HIS
1	A	527	GLN
1	B	7	GLN
1	B	76	GLN
1	B	128	GLN
1	B	252	HIS
1	B	278	ASN
1	B	301	ASN
1	B	365	ASN
1	B	410	HIS
1	B	449	GLN
1	B	505	ASN
1	B	546	HIS
1	B	561	ASN
1	C	124	GLN
1	C	313	GLN
1	C	336	GLN
1	C	347	HIS
1	C	696	GLN
1	D	374	ASN
1	D	405	GLN
1	D	410	HIS
1	D	418	GLN
1	D	454	ASN
1	D	456	HIS
1	D	496	GLN
1	D	719	GLN
1	E	134	GLN
1	E	286	ASN
1	E	365	ASN
1	E	408	HIS
1	E	435	ASN
1	E	456	HIS
1	E	486	ASN
1	E	505	ASN
1	E	596	GLN
1	E	620	ASN
1	F	410	HIS
2	H	144	ASN
3	I	199	HIS
3	I	213	HIS
4	J	33	GLN
5	K	123	HIS

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Mol	Chain	Res	Type
5	L	220	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	-	32,33,33	1.32	4 (12%)	48,52,52	2.00	15 (31%)
6	ATP	D	802	-	32,33,33	1.27	4 (12%)	48,52,52	1.99	13 (27%)
7	ADP	E	802	-	28,29,29	1.38	3 (10%)	43,45,45	1.90	9 (20%)
6	ATP	C	802	-	32,33,33	1.33	4 (12%)	48,52,52	1.79	7 (14%)
6	ATP	B	802	-	32,33,33	1.39	4 (12%)	48,52,52	1.78	11 (22%)
6	ATP	A	801	-	32,33,33	1.33	4 (12%)	48,52,52	1.81	9 (18%)
6	ATP	B	801	-	32,33,33	1.30	4 (12%)	48,52,52	1.79	10 (20%)
6	ATP	E	801	-	32,33,33	1.34	6 (18%)	48,52,52	1.91	15 (31%)
7	ADP	A	802	-	28,29,29	1.42	5 (17%)	43,45,45	1.88	11 (25%)
6	ATP	D	801	-	32,33,33	1.36	4 (12%)	48,52,52	1.84	12 (25%)
6	ATP	F	801	-	32,33,33	1.26	5 (15%)	48,52,52	1.98	13 (27%)

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	-	-	7/22/38/38	0/3/3/3
6	ATP	D	802	-	-	6/22/38/38	0/3/3/3
7	ADP	E	802	-	-	5/16/32/32	0/3/3/3
6	ATP	C	802	-	-	4/22/38/38	0/3/3/3
6	ATP	B	802	-	-	0/22/38/38	0/3/3/3
6	ATP	A	801	-	-	6/22/38/38	0/3/3/3
6	ATP	B	801	-	-	3/22/38/38	0/3/3/3
6	ATP	E	801	-	-	2/22/38/38	0/3/3/3
7	ADP	A	802	-	-	8/16/32/32	0/3/3/3
6	ATP	D	801	-	-	4/22/38/38	0/3/3/3
6	ATP	F	801	-	-	5/22/38/38	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	802	ATP	C4-N9	-4.06	1.29	1.37
7	E	802	ADP	C5-C4	4.02	1.46	1.39
6	D	802	ATP	C5-N7	-4.00	1.31	1.39
6	D	801	ATP	C5-C4	3.82	1.45	1.39
6	E	801	ATP	C5-C4	3.81	1.45	1.39
7	A	802	ADP	C5-C4	3.75	1.45	1.39
6	A	801	ATP	C5-N7	-3.73	1.32	1.39
6	F	801	ATP	C5-C4	3.70	1.45	1.39
6	C	802	ATP	C5-C4	3.60	1.45	1.39
6	A	801	ATP	C5-C4	3.57	1.45	1.39
6	D	802	ATP	C5-C4	3.54	1.45	1.39
7	E	802	ADP	C5-N7	-3.41	1.32	1.39
6	B	802	ATP	C5-C4	3.39	1.45	1.39
6	B	801	ATP	C4-N9	-3.33	1.30	1.37
6	C	802	ATP	C5-N7	-3.33	1.33	1.39
6	C	801	ATP	C5-N7	-3.33	1.33	1.39
6	B	801	ATP	C5-C4	3.32	1.45	1.39
6	D	801	ATP	C4-N9	-3.29	1.30	1.37
6	B	801	ATP	C5-N7	-3.26	1.33	1.39
6	C	801	ATP	C8-N9	-3.24	1.32	1.37
6	C	801	ATP	C4-N9	-3.23	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	802	ATP	C5-N7	-3.15	1.33	1.39
7	A	802	ADP	C4-N9	-3.12	1.31	1.37
7	A	802	ADP	C5-N7	-3.02	1.33	1.39
6	A	801	ATP	C4-N9	-2.99	1.31	1.37
6	F	801	ATP	C5-N7	-2.98	1.33	1.39
6	D	801	ATP	C5-N7	-2.93	1.33	1.39
6	C	802	ATP	C4-N9	-2.80	1.31	1.37
6	E	801	ATP	C4-N9	-2.75	1.32	1.37
6	C	801	ATP	C5-C4	2.72	1.43	1.39
6	B	802	ATP	C8-N9	-2.71	1.32	1.37
6	E	801	ATP	C8-N9	-2.70	1.33	1.37
6	F	801	ATP	C4-N9	-2.69	1.32	1.37
6	E	801	ATP	C5-N7	-2.67	1.34	1.39
6	D	801	ATP	C8-N9	-2.65	1.33	1.37
7	E	802	ADP	C4-N9	-2.47	1.32	1.37
7	A	802	ADP	C8-N9	-2.31	1.33	1.37
6	D	802	ATP	C8-N9	-2.30	1.33	1.37
6	F	801	ATP	C8-N9	-2.23	1.33	1.37
6	E	801	ATP	C5-C6	2.22	1.47	1.41
7	A	802	ADP	C5-C6	2.19	1.47	1.41
6	D	802	ATP	C4-N9	-2.16	1.33	1.37
6	E	801	ATP	C8-N7	2.16	1.35	1.31
6	B	801	ATP	C8-N9	-2.11	1.34	1.37
6	C	802	ATP	C8-N9	-2.06	1.34	1.37
6	A	801	ATP	C8-N9	-2.04	1.34	1.37
6	F	801	ATP	C5-C6	2.03	1.46	1.41

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	802	ATP	C5-C4-N3	-6.90	117.22	126.72
6	C	802	ATP	C5-C4-N3	-6.08	118.34	126.72
6	D	802	ATP	N3-C4-N9	6.01	137.39	127.17
7	E	802	ADP	C5-C4-N3	-5.95	118.52	126.72
6	A	801	ATP	C5-C4-N3	-5.89	118.61	126.72
6	F	801	ATP	C5-C4-N3	-5.81	118.72	126.72
7	A	802	ADP	C5-C4-N3	-5.63	118.96	126.72
6	B	801	ATP	C5-C4-N3	-5.30	119.42	126.72
7	E	802	ADP	N3-C4-N9	5.18	135.97	127.17
6	E	801	ATP	C5-C4-N3	-5.16	119.61	126.72
6	C	801	ATP	C5-C4-N3	-5.09	119.71	126.72
6	D	801	ATP	C5-C4-N3	-4.94	119.92	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	801	ATP	N3-C4-N9	4.83	135.38	127.17
6	C	802	ATP	N3-C4-N9	4.79	135.31	127.17
6	C	801	ATP	N3-C4-N9	4.62	135.03	127.17
6	A	801	ATP	O4'-C1'-N9	4.56	116.84	108.09
6	A	801	ATP	N3-C4-N9	4.47	134.76	127.17
6	B	801	ATP	N3-C4-N9	4.37	134.60	127.17
6	B	802	ATP	C5-C4-N3	-4.09	121.08	126.72
6	C	801	ATP	C4-N9-C8	4.07	110.01	105.74
6	D	801	ATP	N3-C4-N9	4.05	134.05	127.17
6	E	801	ATP	N3-C4-N9	4.00	133.97	127.17
7	A	802	ADP	C4-C5-N7	-3.92	106.10	110.58
6	D	802	ATP	C2-N3-C4	3.90	121.36	111.83
6	C	801	ATP	N3-C2-N1	-3.79	122.84	128.58
6	C	801	ATP	C2-N3-C4	3.79	121.08	111.83
6	D	801	ATP	O4'-C1'-N9	3.77	115.33	108.09
6	F	801	ATP	C2-N3-C4	3.76	121.02	111.83
6	B	802	ATP	N3-C4-N9	3.74	133.53	127.17
7	A	802	ADP	N3-C4-N9	3.74	133.53	127.17
6	E	801	ATP	C4-N9-C8	3.72	109.64	105.74
6	F	801	ATP	C4-N9-C8	3.66	109.58	105.74
6	E	801	ATP	C4-C5-N7	-3.65	106.41	110.58
7	A	802	ADP	C3'-C2'-C1'	3.65	108.36	101.46
7	E	802	ADP	C3'-C2'-C1'	3.63	108.33	101.46
7	A	802	ADP	C2-N3-C4	3.57	120.56	111.83
6	C	802	ATP	C2-N3-C4	3.55	120.49	111.83
6	B	802	ATP	C4-N9-C8	3.48	109.40	105.74
6	F	801	ATP	N3-C2-N1	-3.44	123.38	128.58
6	B	801	ATP	C2-N3-C4	3.43	120.21	111.83
6	A	801	ATP	C2-N3-C4	3.41	120.16	111.83
6	B	801	ATP	N3-C2-N1	-3.37	123.48	128.58
6	B	802	ATP	N3-C2-N1	-3.37	123.49	128.58
6	F	801	ATP	C4-C5-N7	-3.35	106.75	110.58
6	D	801	ATP	C4-N9-C8	3.28	109.19	105.74
6	D	801	ATP	C2-N3-C4	3.26	119.78	111.83
6	B	801	ATP	C4-N9-C8	3.25	109.15	105.74
7	E	802	ADP	C2-N3-C4	3.25	119.76	111.83
6	E	801	ATP	C2-N3-C4	3.24	119.73	111.83
6	D	802	ATP	N3-C2-N1	-3.23	123.69	128.58
6	B	802	ATP	C2'-C1'-N9	-3.21	105.32	113.30
6	C	801	ATP	C2'-C1'-N9	-3.17	105.43	113.30
6	B	802	ATP	C2-N3-C4	3.12	119.45	111.83
7	A	802	ADP	N3-C2-N1	-3.12	123.86	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	801	ATP	N3-C2-N1	-3.02	124.01	128.58
6	E	801	ATP	N3-C2-N1	-2.99	124.05	128.58
6	E	801	ATP	O3G-PG-O2G	2.95	118.86	107.80
6	D	801	ATP	C4-C5-N7	-2.94	107.22	110.58
6	D	802	ATP	O4'-C1'-N9	-2.89	102.55	108.09
6	E	801	ATP	O5'-C5'-C4'	2.87	118.75	108.99
6	C	802	ATP	N3-C2-N1	-2.83	124.30	128.58
6	F	801	ATP	N9-C8-N7	-2.77	110.00	113.94
6	B	802	ATP	N6-C6-N1	2.76	124.52	118.38
6	F	801	ATP	C5-N7-C8	2.74	107.75	103.45
6	C	801	ATP	C4-C5-N7	-2.71	107.48	110.58
6	F	801	ATP	O4'-C1'-N9	2.69	113.26	108.09
6	A	801	ATP	C4-C5-N7	-2.68	107.52	110.58
6	D	801	ATP	O3A-PA-O1A	-2.66	102.69	110.70
6	F	801	ATP	O2A-PA-O1A	2.66	124.81	112.44
6	D	802	ATP	C4-C5-N7	-2.64	107.56	110.58
6	F	801	ATP	O2A-PA-O3A	-2.64	100.14	107.27
6	D	802	ATP	O3G-PG-O2G	2.62	117.62	107.80
6	E	801	ATP	C6-C5-N7	2.61	137.12	132.09
6	A	801	ATP	O3A-PA-O1A	-2.61	102.86	110.70
6	B	801	ATP	C4-C5-N7	-2.61	107.60	110.58
6	C	802	ATP	C4-C5-N7	-2.59	107.62	110.58
6	B	802	ATP	O2B-PB-O1B	2.59	124.48	112.44
6	E	801	ATP	C2'-C3'-C4'	2.58	107.60	102.61
6	E	801	ATP	N9-C8-N7	-2.58	110.27	113.94
6	D	802	ATP	C5-N7-C8	2.56	107.48	103.45
6	E	801	ATP	C5-N7-C8	2.56	107.47	103.45
6	C	801	ATP	O4'-C1'-N9	2.55	113.00	108.09
6	A	801	ATP	N3-C2-N1	-2.55	124.73	128.58
6	C	801	ATP	N9-C8-N7	-2.54	110.33	113.94
6	B	802	ATP	O2A-PA-O1A	2.52	124.17	112.44
6	C	801	ATP	C6-C5-N7	2.51	136.93	132.09
7	E	802	ADP	C4-N9-C8	2.51	108.38	105.74
7	E	802	ADP	N3-C2-N1	-2.51	124.79	128.58
6	D	802	ATP	N6-C6-N1	2.50	123.94	118.38
7	E	802	ADP	C4-C5-N7	-2.49	107.73	110.58
6	C	801	ATP	O2A-PA-O1A	2.45	123.83	112.44
6	C	801	ATP	O2A-PA-O3A	-2.44	100.67	107.27
6	C	802	ATP	O3G-PG-O2G	2.43	116.92	107.80
6	A	801	ATP	O4'-C1'-C2'	-2.42	101.44	106.62
6	B	802	ATP	C5-C6-N6	-2.40	117.34	123.29
6	A	801	ATP	O3G-PG-O2G	2.40	116.79	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	802	ATP	C1'-N9-C8	-2.37	121.82	127.09
6	D	801	ATP	O2A-PA-O1A	2.36	123.44	112.44
6	D	802	ATP	C4-N9-C8	2.32	108.17	105.74
7	A	802	ADP	C6-C5-N7	2.30	136.53	132.09
7	A	802	ADP	C5-N7-C8	2.30	107.07	103.45
6	E	801	ATP	C3'-C2'-C1'	2.30	105.82	101.46
6	B	801	ATP	N9-C8-N7	-2.29	110.69	113.94
6	C	801	ATP	C5-C6-N6	-2.21	117.82	123.29
6	E	801	ATP	O3B-PG-O1G	-2.21	99.42	111.04
6	E	801	ATP	O2B-PB-O1B	2.20	122.69	112.44
6	C	801	ATP	C5-N7-C8	2.20	106.91	103.45
6	D	802	ATP	C5-C6-N6	-2.18	117.90	123.29
6	D	801	ATP	C6-C5-N7	2.16	136.25	132.09
7	A	802	ADP	O4'-C1'-C2'	-2.16	102.00	106.62
6	D	801	ATP	O3G-PG-O2G	2.15	115.85	107.80
6	B	801	ATP	C4'-O4'-C1'	-2.14	104.73	109.47
7	E	802	ADP	C5-N7-C8	2.14	106.81	103.45
6	B	801	ATP	O3A-PA-O1A	-2.14	104.28	110.70
6	B	802	ATP	O5'-C5'-C4'	2.12	116.20	108.99
7	E	802	ADP	O3B-PB-O2B	2.11	115.70	107.80
6	B	801	ATP	O4'-C1'-N9	2.10	112.12	108.09
6	C	802	ATP	C3'-C2'-C1'	2.09	105.41	101.46
6	D	801	ATP	C4'-O4'-C1'	-2.08	104.87	109.47
7	A	802	ADP	O3B-PB-O2B	2.06	115.54	107.80
6	C	801	ATP	O3G-PG-O2G	2.05	115.48	107.80
6	F	801	ATP	O2B-PB-O1B	2.03	121.88	112.44
6	F	801	ATP	C2'-C3'-C4'	2.02	106.51	102.61
6	D	802	ATP	O2B-PB-O1B	2.01	121.81	112.44
7	A	802	ADP	C4-N9-C8	2.01	107.84	105.74

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	ATP	C5'-O5'-PA-O2A
6	A	801	ATP	C5'-O5'-PA-O3A
6	A	801	ATP	C2'-C1'-N9-C8
6	C	801	ATP	C5'-O5'-PA-O3A
6	C	801	ATP	O4'-C1'-N9-C8
6	C	801	ATP	O4'-C1'-N9-C4
6	C	802	ATP	PB-O3A-PA-O5'
6	D	801	ATP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	D	801	ATP	C5'-O5'-PA-O3A
6	D	801	ATP	O4'-C1'-N9-C8
6	D	801	ATP	O4'-C1'-N9-C4
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
6	F	801	ATP	O4'-C1'-N9-C8
6	F	801	ATP	O4'-C1'-N9-C4
7	A	802	ADP	C5'-O5'-PA-O1A
7	A	802	ADP	C5'-O5'-PA-O2A
7	A	802	ADP	C5'-O5'-PA-O3A
7	E	802	ADP	C5'-O5'-PA-O2A
7	E	802	ADP	C5'-O5'-PA-O3A
7	E	802	ADP	O4'-C1'-N9-C4
6	A	801	ATP	C3'-C4'-C5'-O5'
7	E	802	ADP	O4'-C1'-N9-C8
6	A	801	ATP	O4'-C4'-C5'-O5'
6	C	802	ATP	O4'-C1'-N9-C4
6	C	801	ATP	O4'-C4'-C5'-O5'
6	C	801	ATP	C3'-C4'-C5'-O5'
6	C	802	ATP	O4'-C1'-N9-C8
7	A	802	ADP	C2'-C1'-N9-C8
6	A	801	ATP	C2'-C1'-N9-C4
6	B	801	ATP	O4'-C1'-N9-C8
7	E	802	ADP	C3'-C4'-C5'-O5'
6	C	801	ATP	C5'-O5'-PA-O1A
7	A	802	ADP	PB-O3A-PA-O1A
6	D	802	ATP	C2'-C1'-N9-C8
6	B	801	ATP	O4'-C1'-N9-C4
6	D	802	ATP	C2'-C1'-N9-C4
7	A	802	ADP	C2'-C1'-N9-C4
6	B	801	ATP	C2'-C1'-N9-C8
6	C	801	ATP	PB-O3A-PA-O2A
6	D	802	ATP	PA-O3A-PB-O2B
6	F	801	ATP	PB-O3A-PA-O1A
7	A	802	ADP	PB-O3A-PA-O2A
7	A	802	ADP	O4'-C1'-N9-C8
6	F	801	ATP	O4'-C4'-C5'-O5'
6	C	802	ATP	C2'-C1'-N9-C8
6	D	802	ATP	PA-O3A-PB-O1B

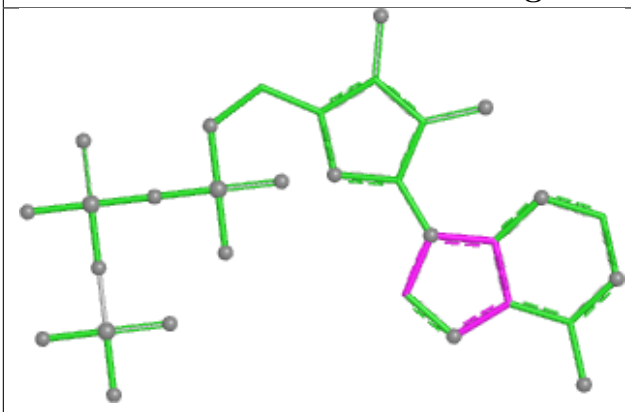
There are no ring outliers.

11 monomers are involved in 32 short contacts:

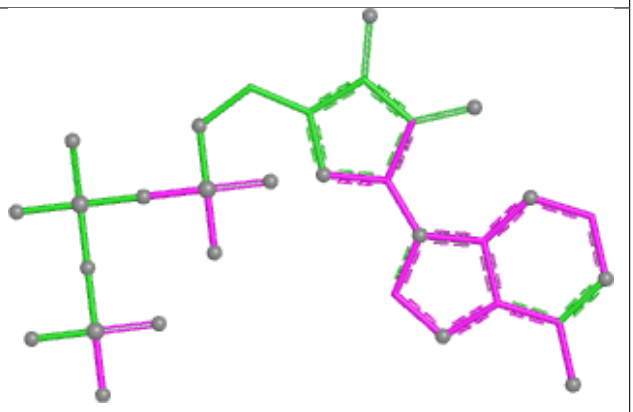
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	801	ATP	3	0
6	D	802	ATP	4	0
7	E	802	ADP	2	0
6	C	802	ATP	5	0
6	B	802	ATP	4	0
6	A	801	ATP	1	0
6	B	801	ATP	6	0
6	E	801	ATP	4	0
7	A	802	ADP	1	0
6	D	801	ATP	1	0
6	F	801	ATP	1	0

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.

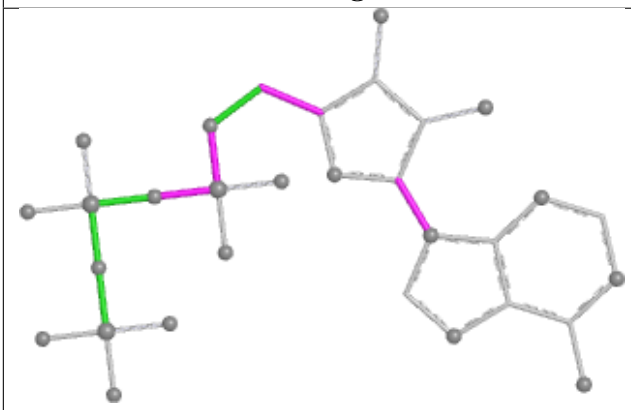
Ligand ATP C 801



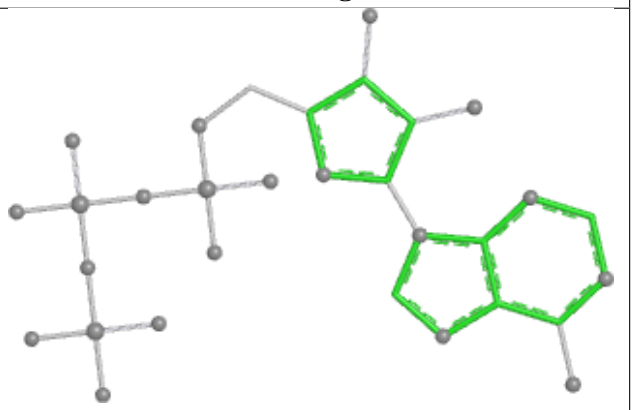
Bond lengths



Bond angles

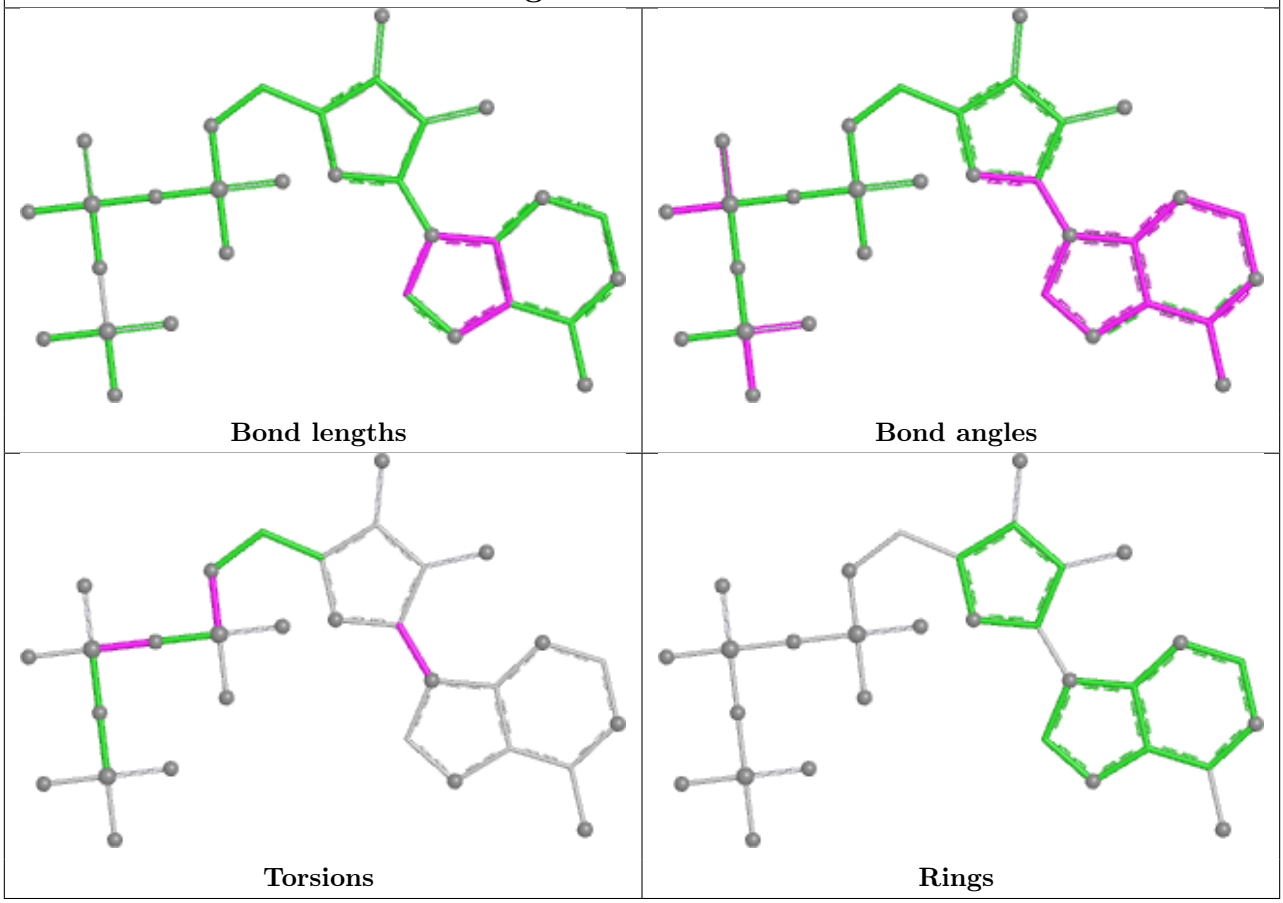


Torsions

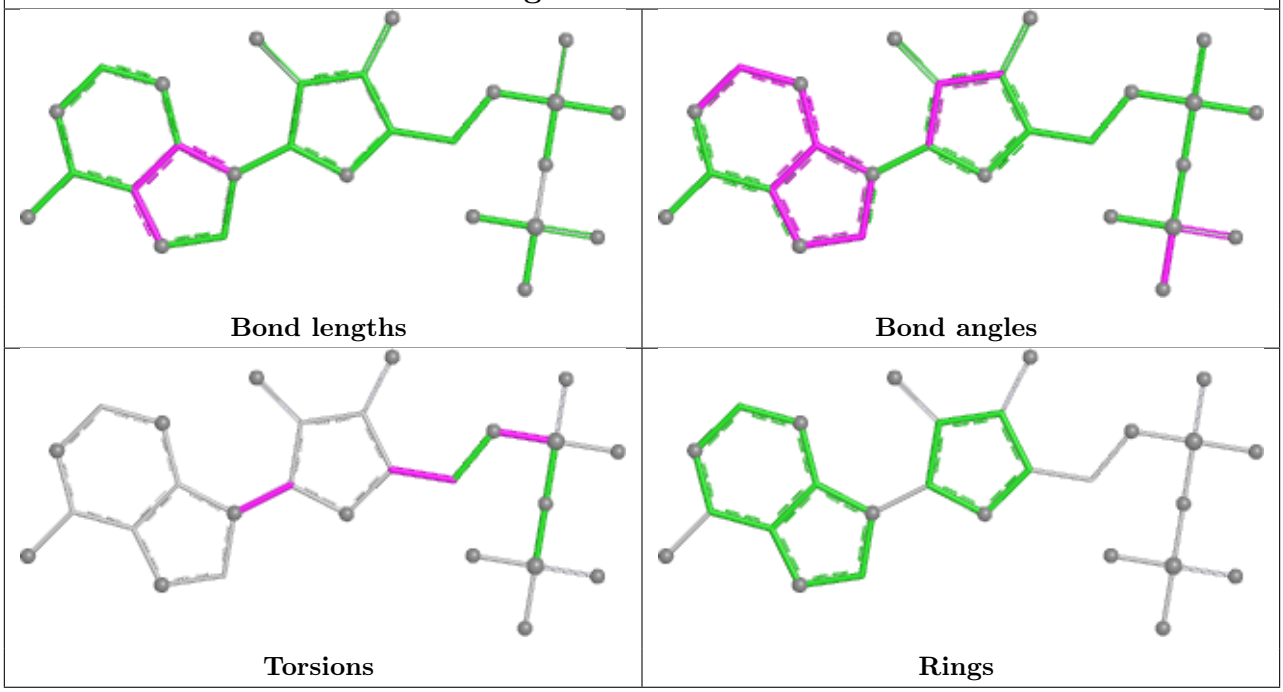


Rings

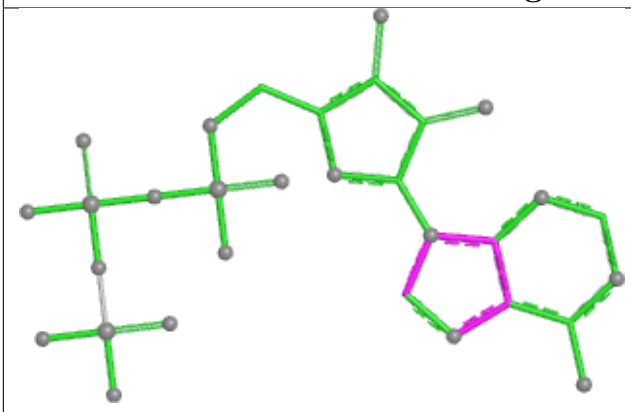
Ligand ATP D 802



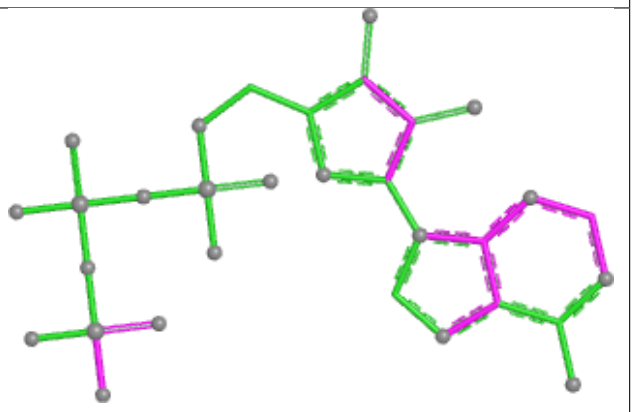
Ligand ADP E 802



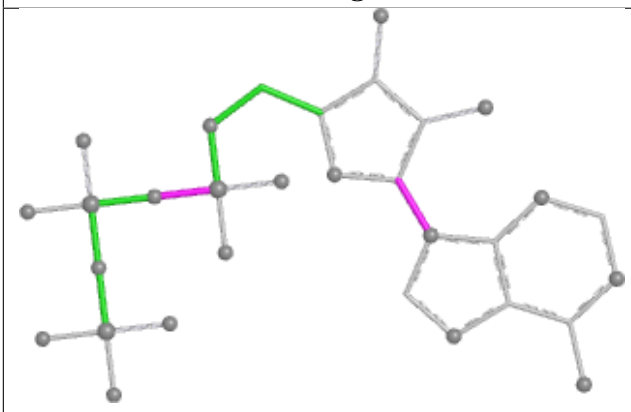
Ligand ATP C 802



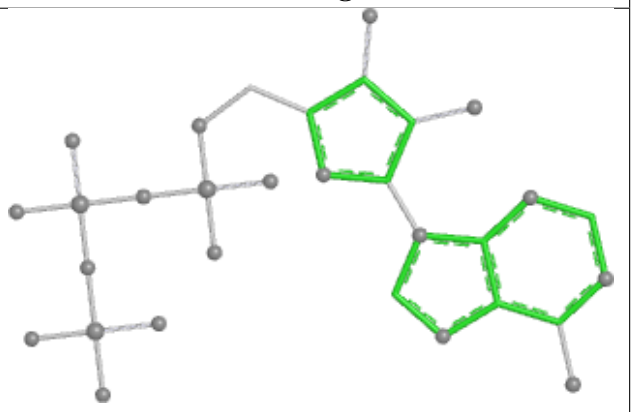
Bond lengths



Bond angles

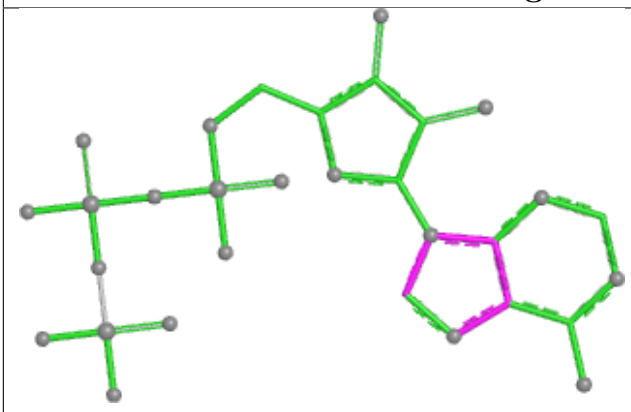


Torsions

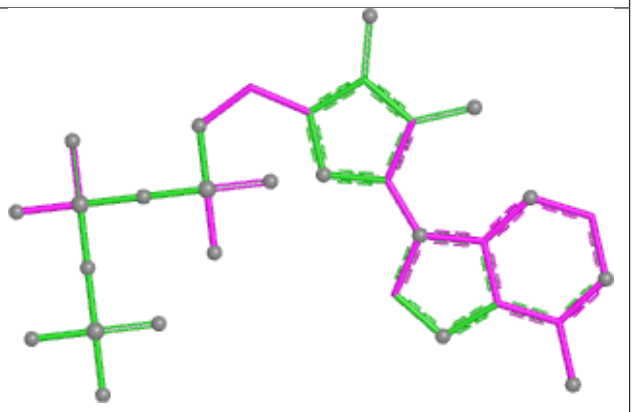


Rings

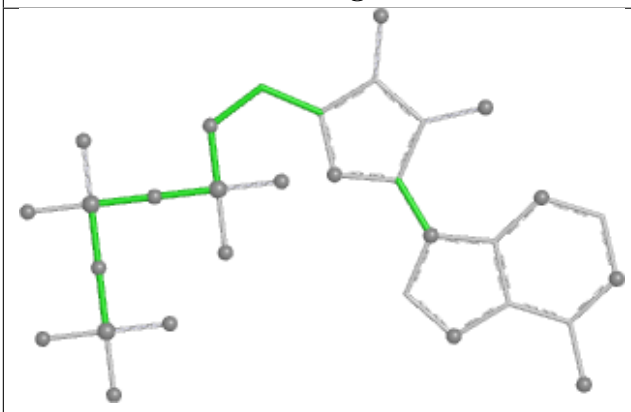
Ligand ATP B 802



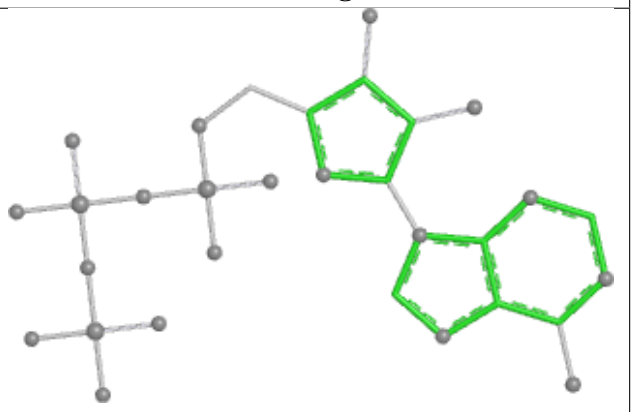
Bond lengths



Bond angles

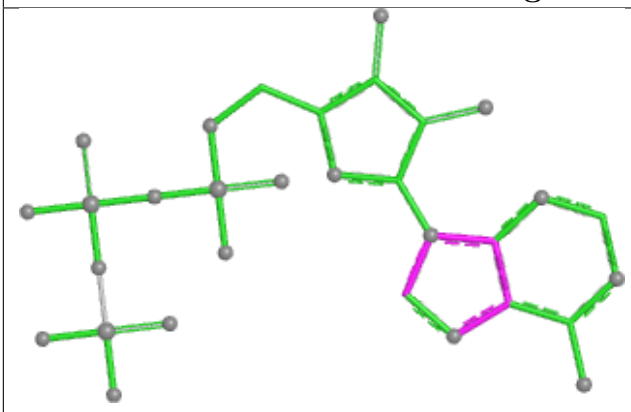


Torsions

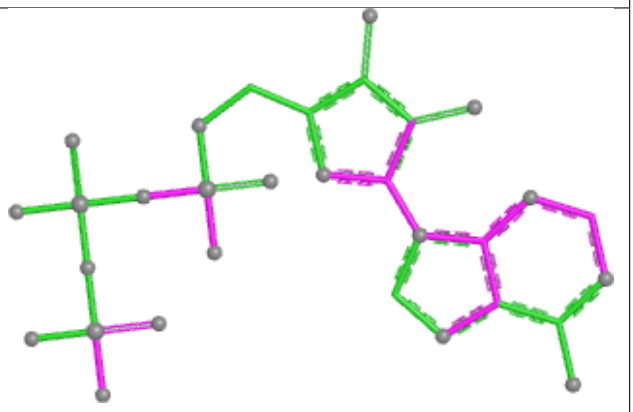


Rings

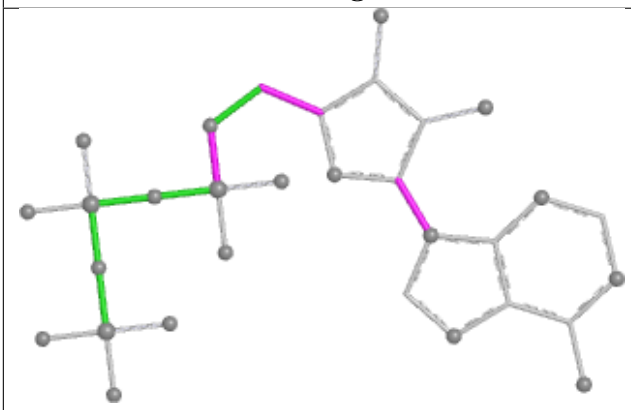
Ligand ATP A 801



Bond lengths



Bond angles



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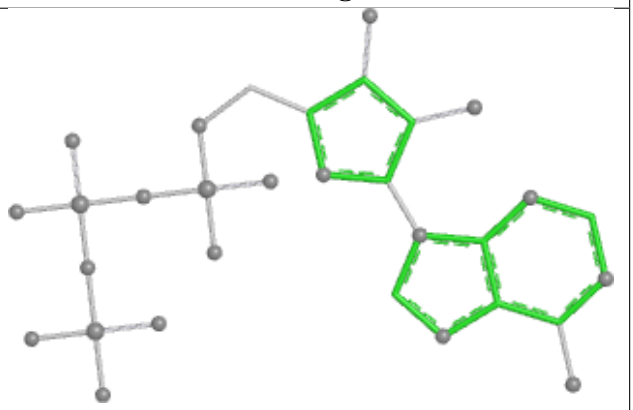
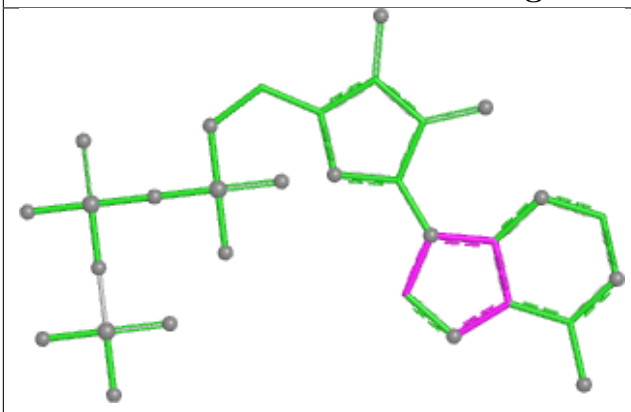
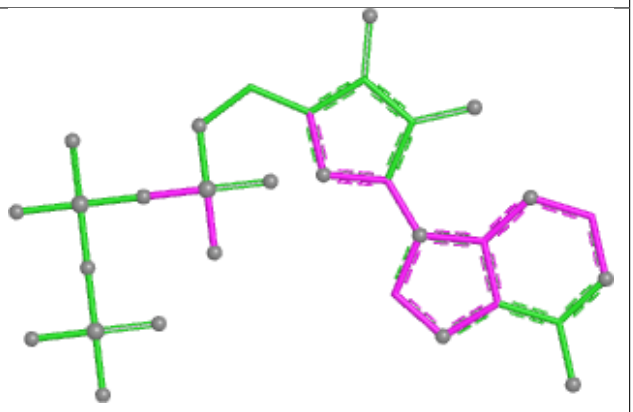


Rings

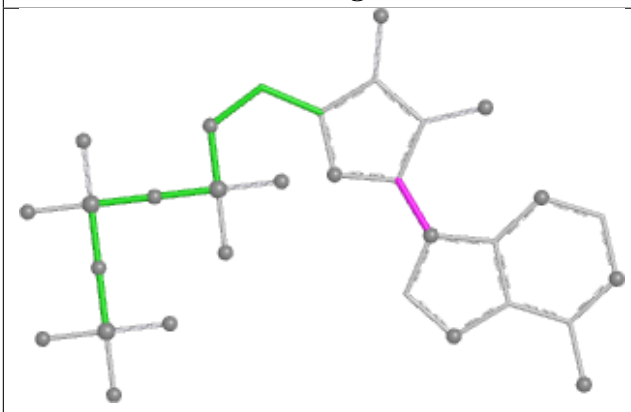
Ligand ATP B 801



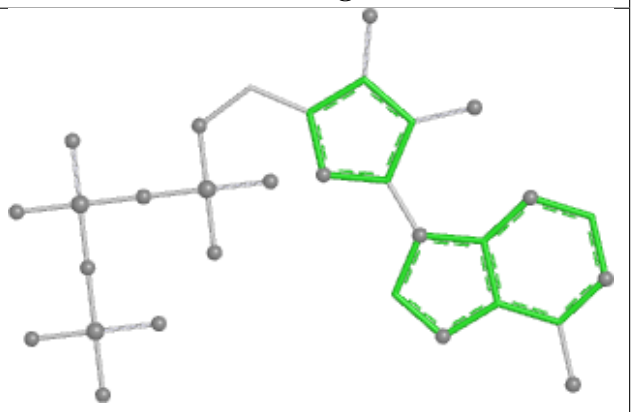
Bond lengths



Bond angles

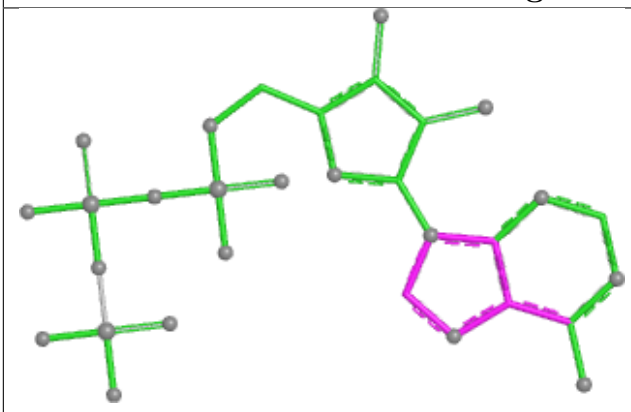


Torsions



Rings

Ligand ATP E 801



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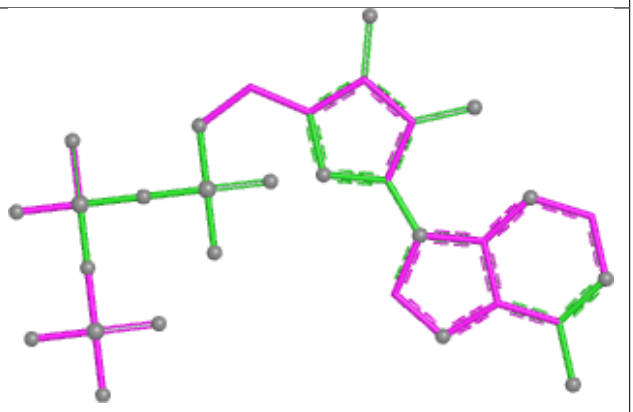
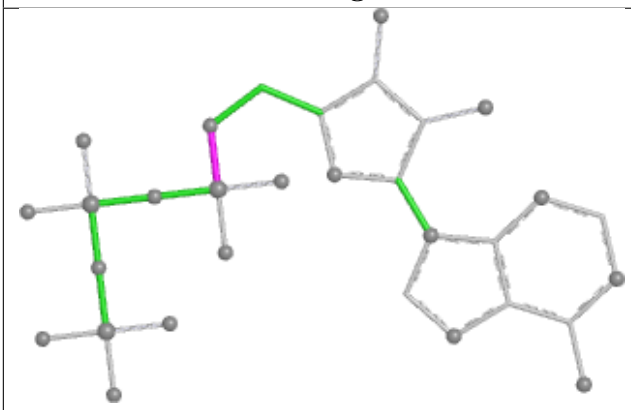


Bond angles



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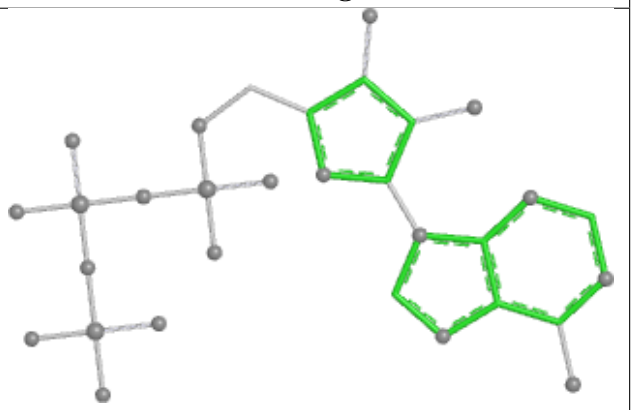
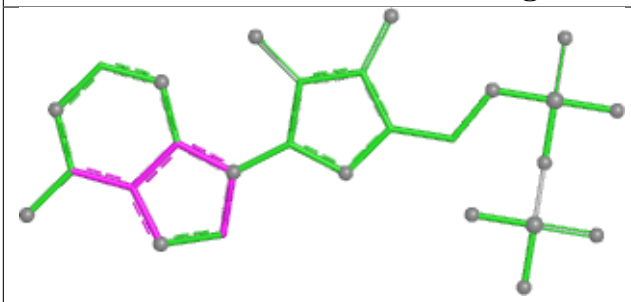


Rings

Ligand ADP A 802



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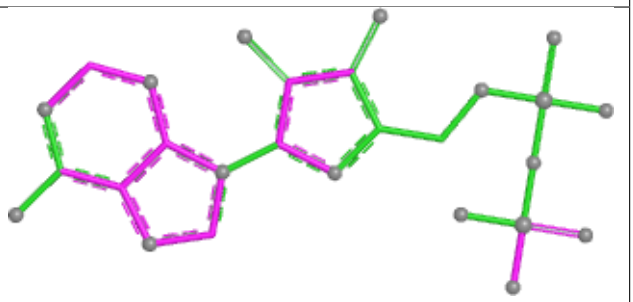
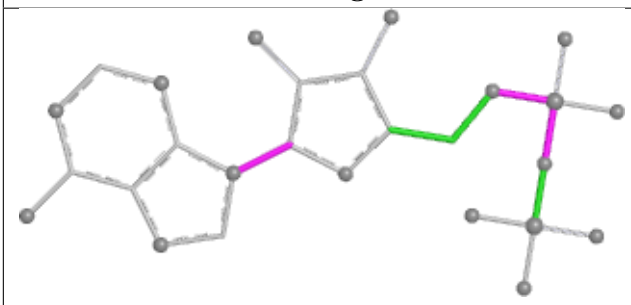


Bond angles



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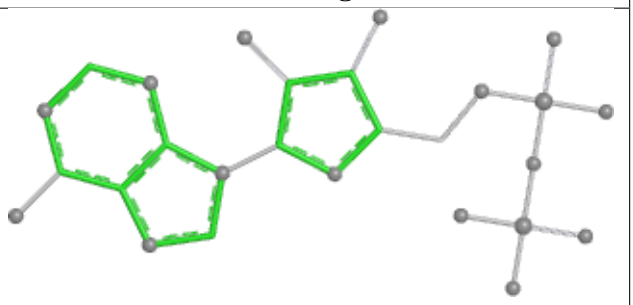
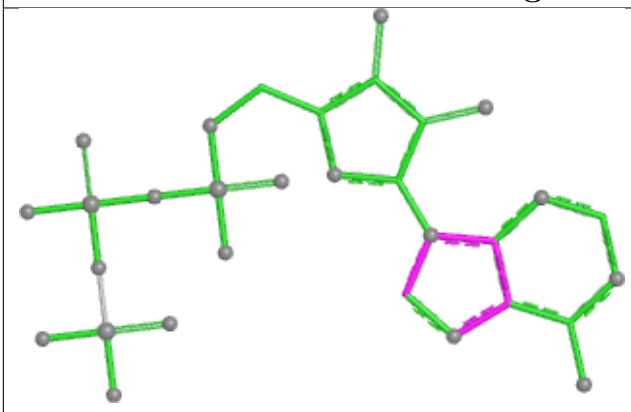
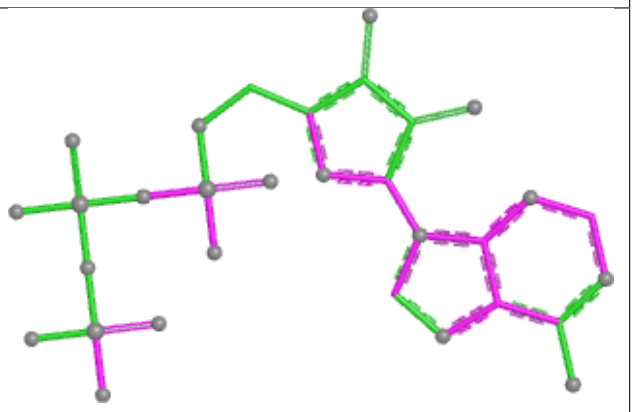


Rings

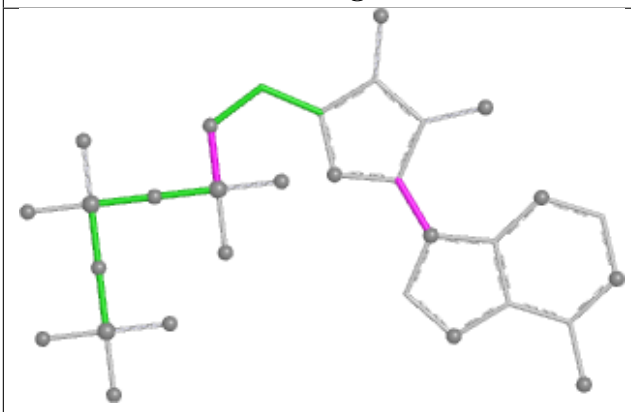
Ligand ATP D 801



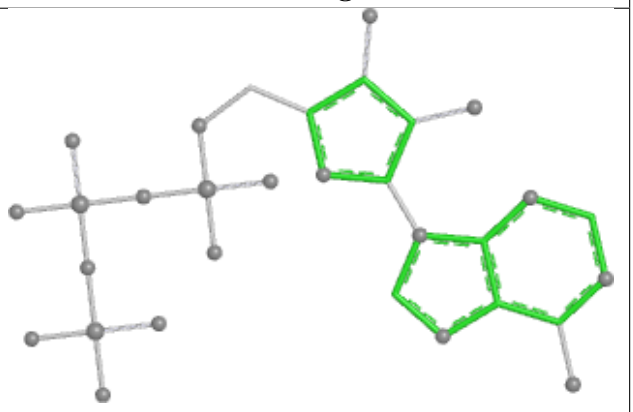
Bond lengths



Bond angles

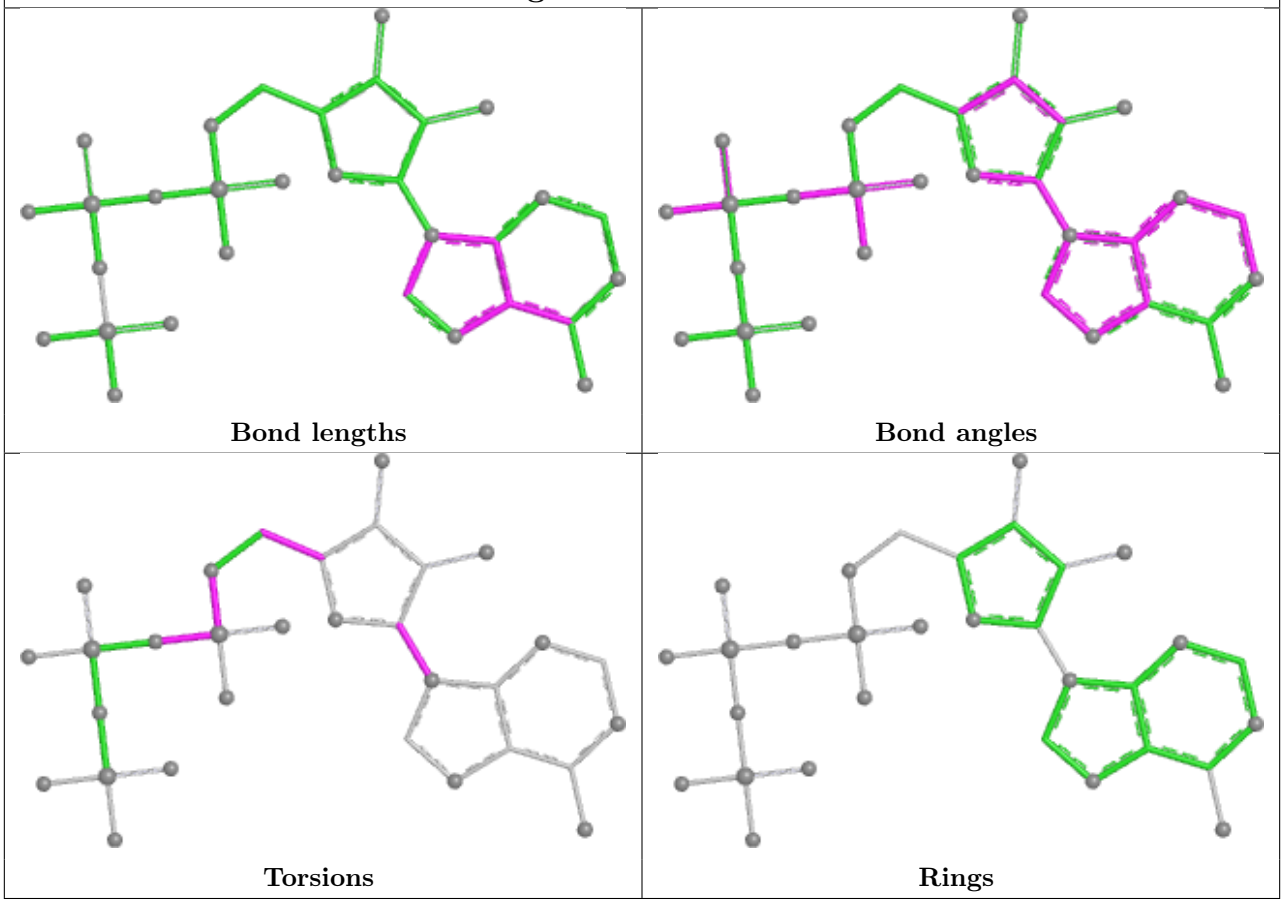


Torsions



Rings

Ligand ATP F 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.

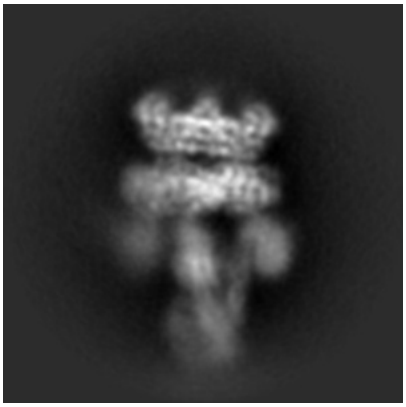
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9101. These allow visual inspection of the internal detail of the map and identification of artifacts.

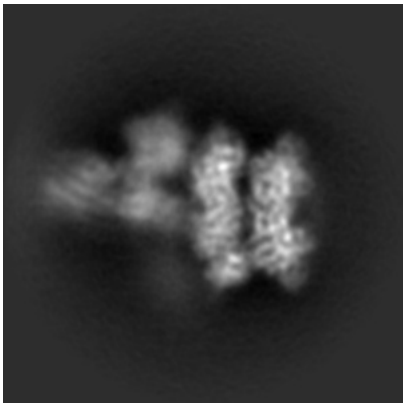
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

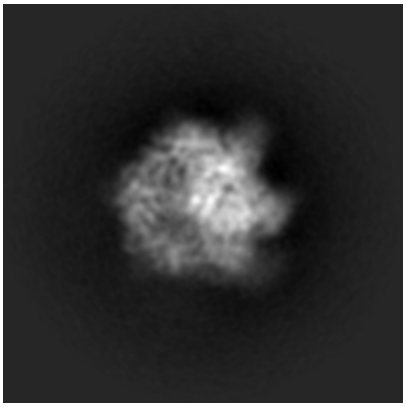
6.1.1 Primary map



X



Y

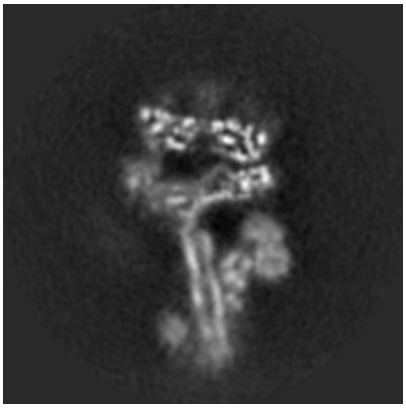


Z

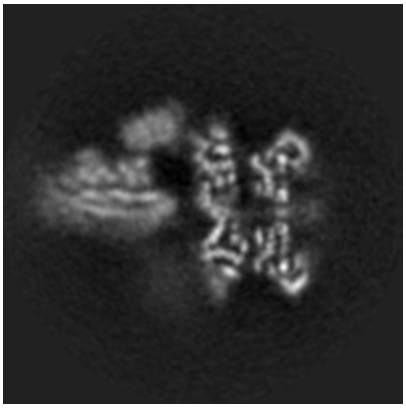
The images above show the map projected in three orthogonal directions.

6.2 Central slices

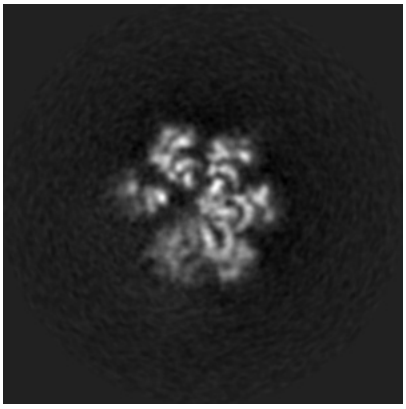
6.2.1 Primary map



X Index: 115



Y Index: 115

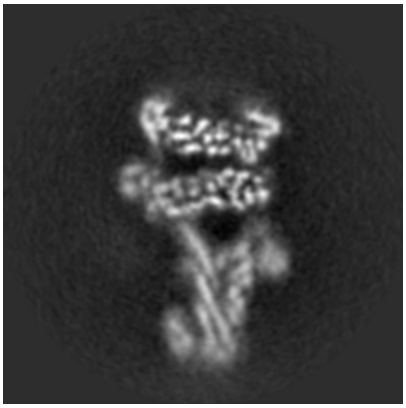


Z Index: 115

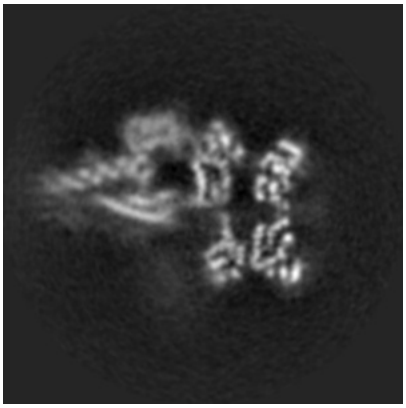
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

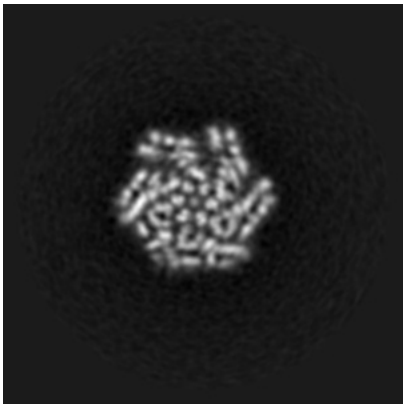
6.3.1 Primary map



X Index: 120



Y Index: 110



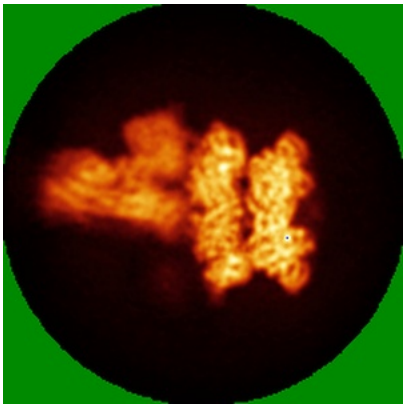
Z Index: 161

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

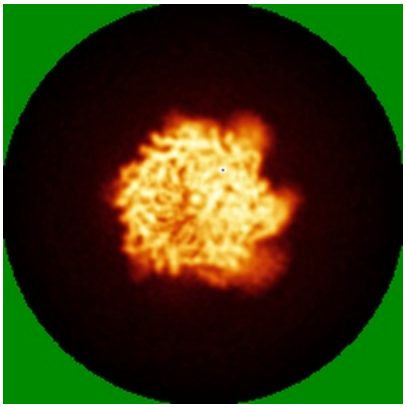
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

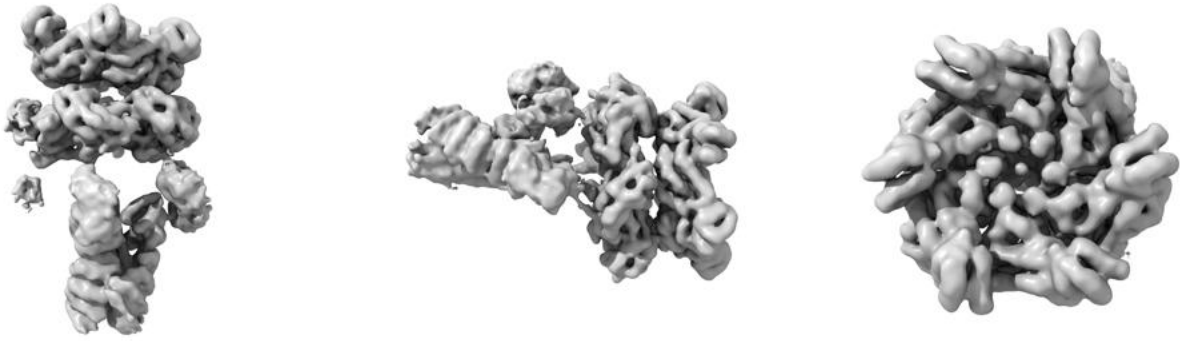


Z

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.

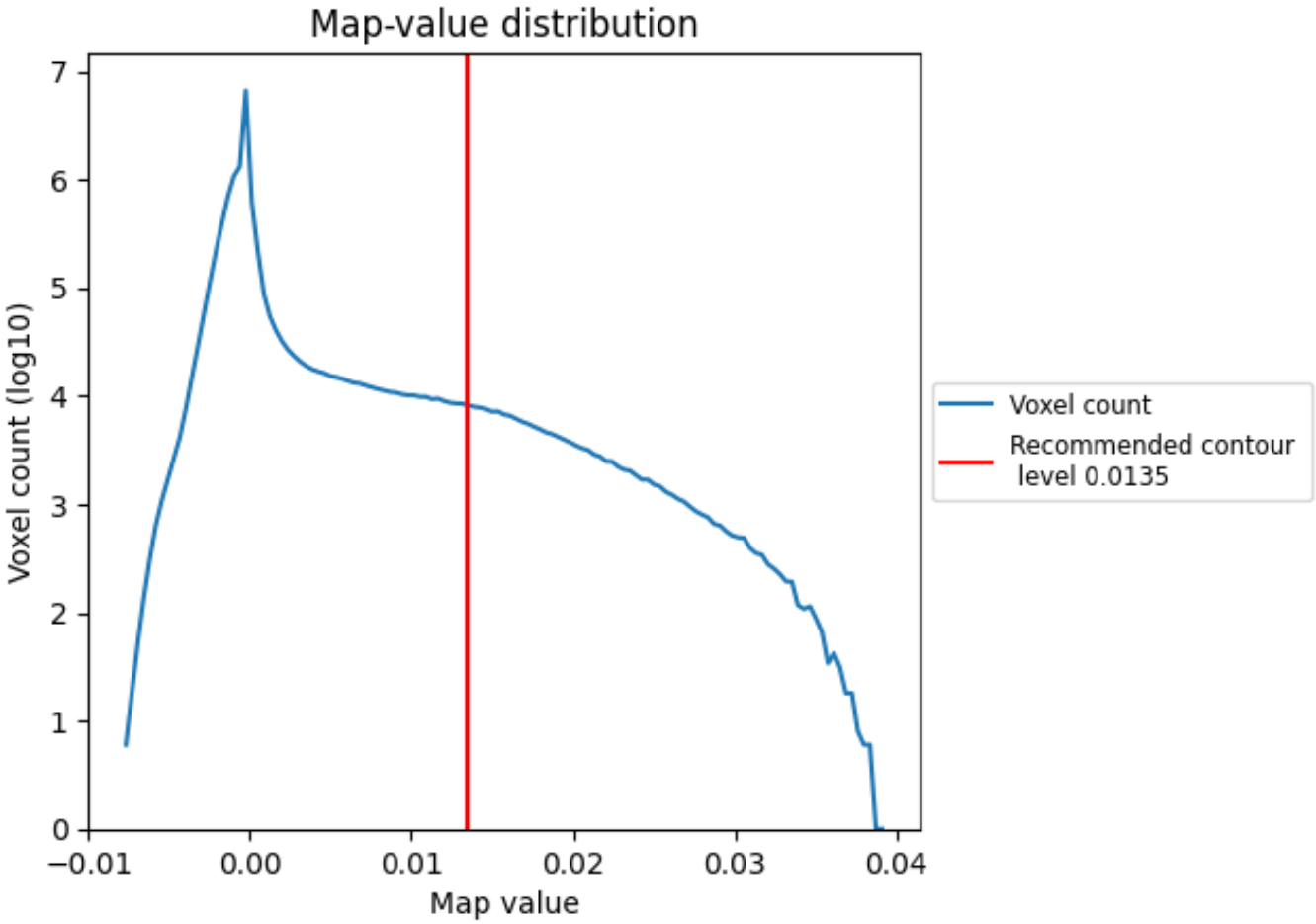
6.6 Mask visualisation (i)

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

7 Map analysis

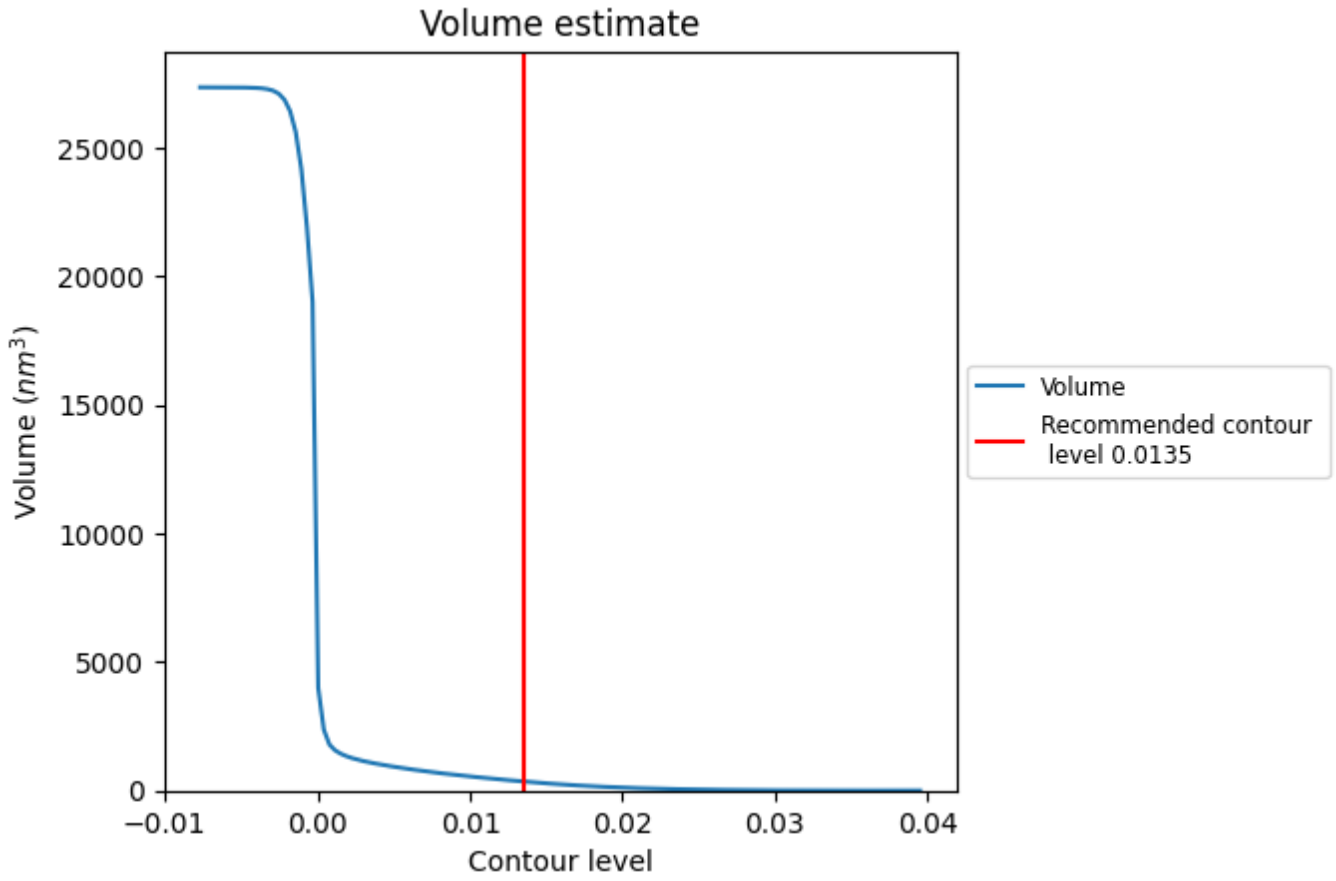
This section contains the results of statistical analysis of the map.

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.

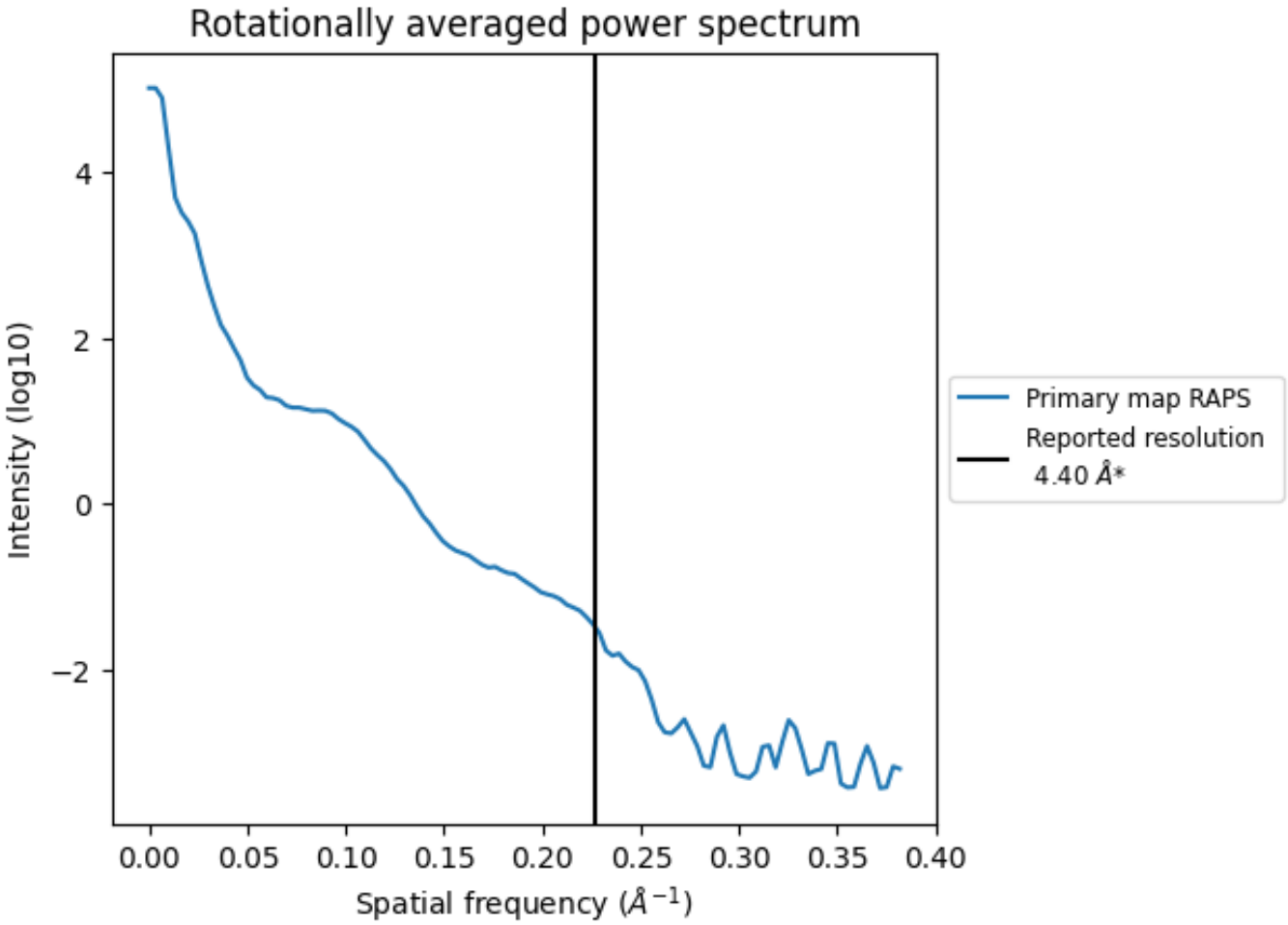
7.2 Volume estimate



The volume at the recommended contour level is 353 nm^3; this corresponds to an approximate mass of 319 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)

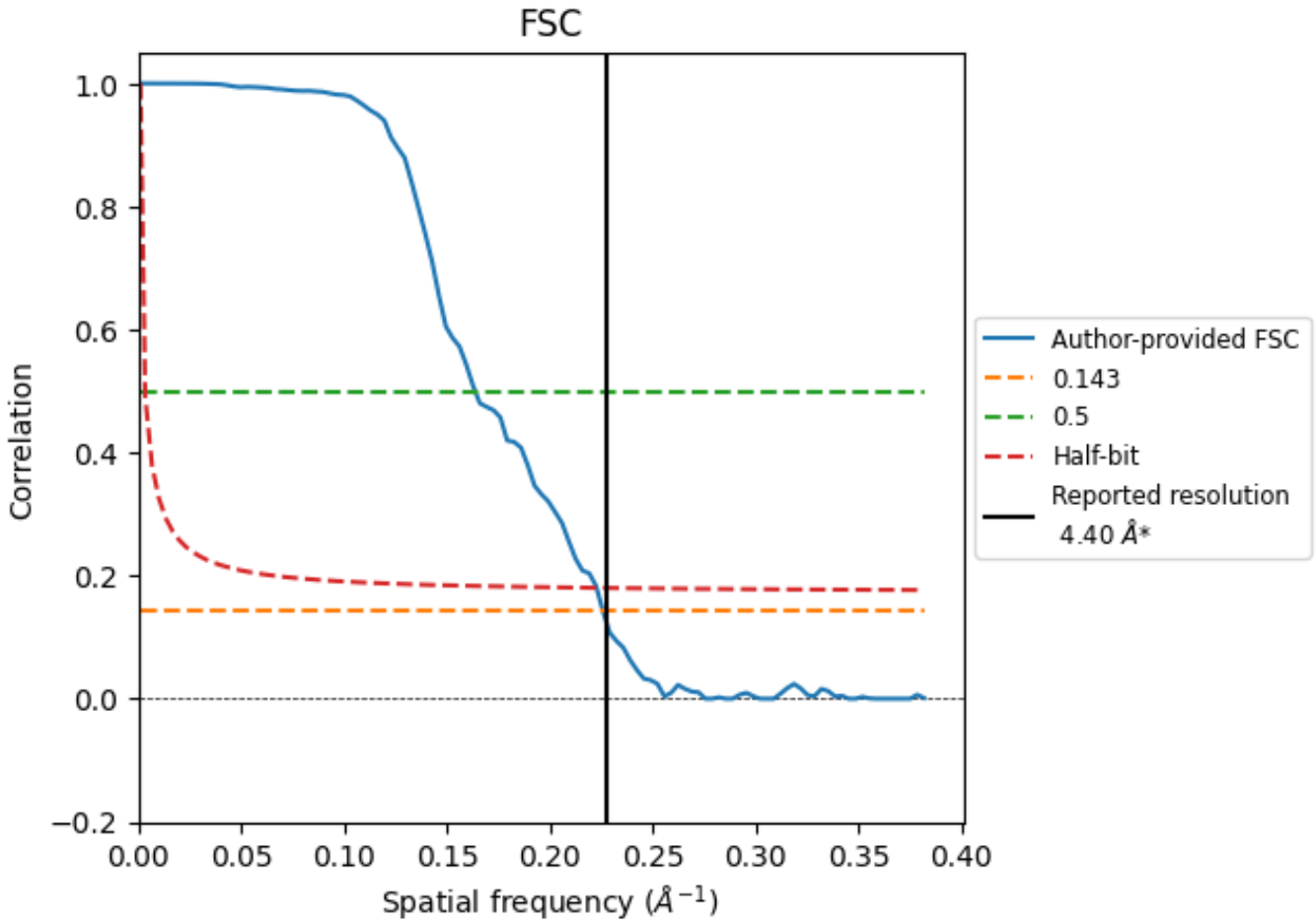


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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)

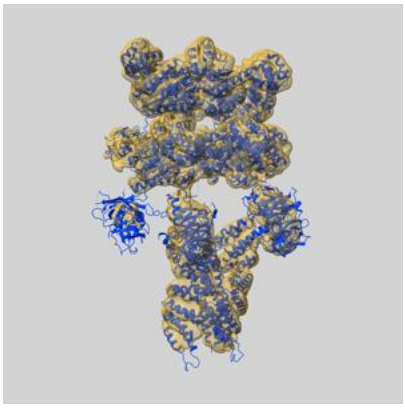
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.43	6.11	4.49
Unmasked-calculated*	-	-	-

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

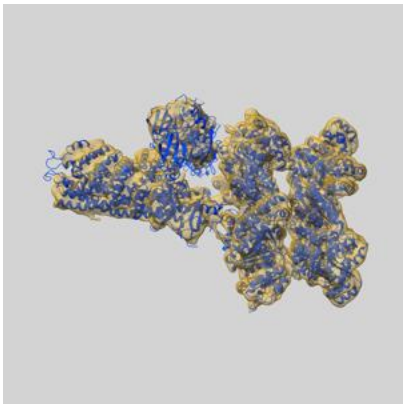
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9101 and PDB model 6MDN. Per-residue inclusion information can be found in section 3 on page 17.

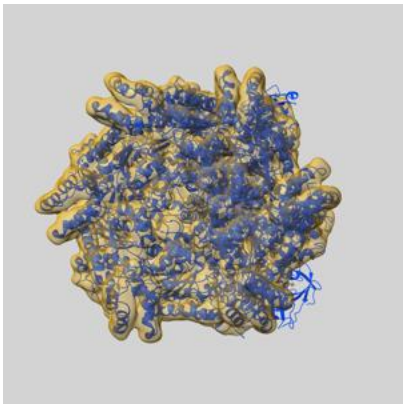
9.1 Map-model overlay



X



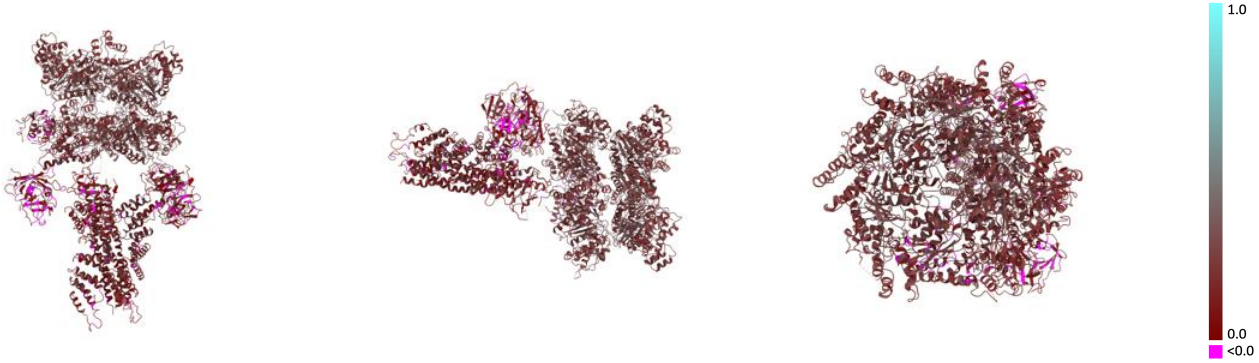
Y



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.

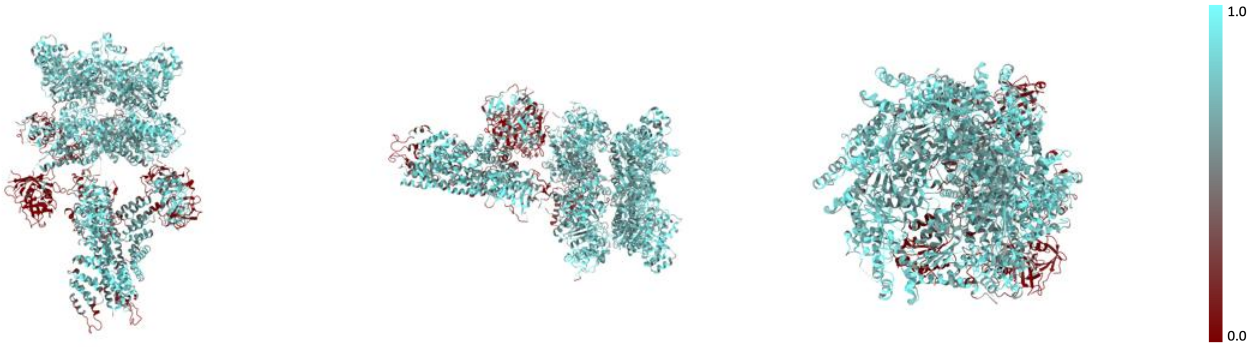
9.2 Q-score mapped to coordinate model (i)



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.

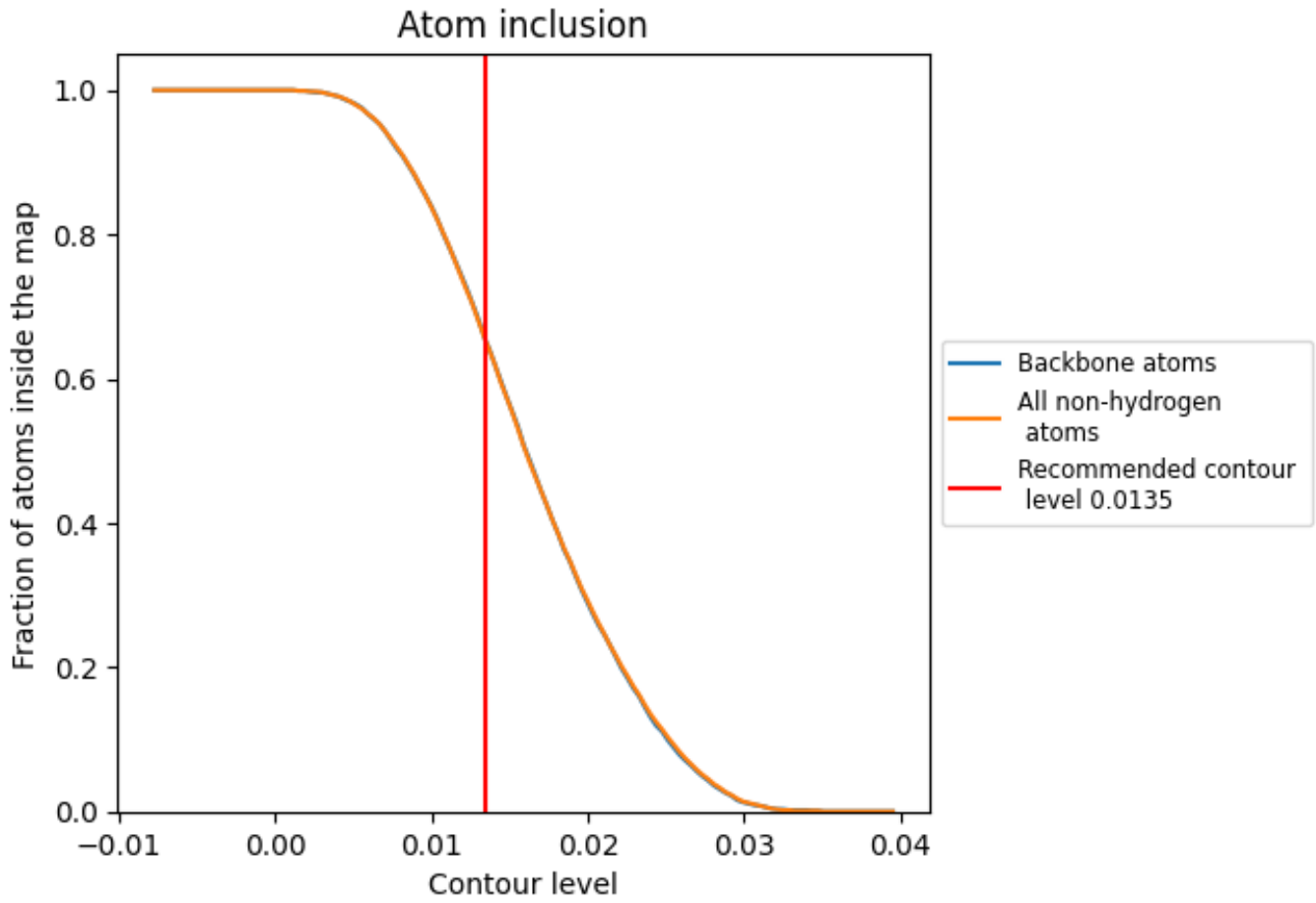
9.3 Atom inclusion mapped to coordinate model (i)



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	0.6510	0.2130
A	0.7720	0.2540
B	0.7120	0.2340
C	0.6440	0.2220
D	0.7050	0.2230
E	0.5580	0.1960
F	0.5160	0.2070
H	0.7250	0.1810
I	0.7450	0.1680
J	0.7560	0.1760
K	0.6250	0.1660
L	0.6400	0.1680