wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Sep 16, 2018 – 02:11 PM EDT

PDB ID	:	6MDP
EMDB ID:	:	EMD-9103
Title	:	The D1 and D2 domain rings of NSF engaging the SNAP-25 N-terminus within the 20S supercomplex (focused refinement on D1/D2 rings, class 2)
Authors	:	White, K.I.; Zhao, M.; Brunger, A.T.
Deposited on	:	2018-09-04
Resolution	:	3.80 Å(reported)
Based on PDB ID	:	3J96

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB 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 (i) symbol.

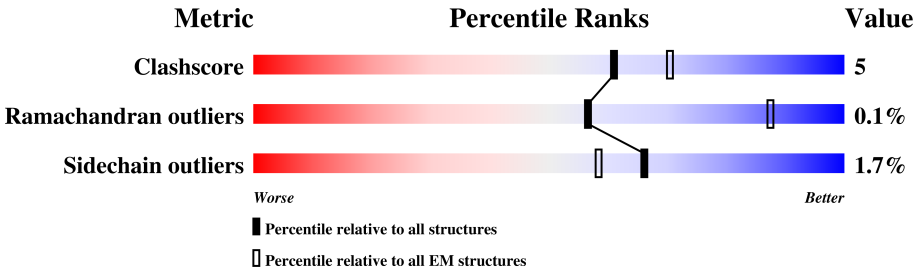
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031172

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	768	55% 11% • 33%
1	B	768	56% 10% • 33%
1	C	768	59% 9% 31%
1	D	768	59% 9% 32%
1	E	768	54% 10% 36%
1	F	768	27% 5% 68%
2	H	207	7% • 92%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 45342 atoms, of which 22909 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
			8088	2526	4103	696	741	22		
1	B	516	Total	C	H	N	O	S	0	0
			8167	2550	4145	702	748	22		
1	C	527	Total	C	H	N	O	S	0	0
			8337	2604	4227	715	768	23		
1	D	526	Total	C	H	N	O	S	0	0
			8314	2596	4214	714	767	23		
1	E	492	Total	C	H	N	O	S	0	0
			7788	2425	3958	671	714	20		
1	F	243	Total	C	H	N	O	S	0	0
			3906	1224	1997	320	354	11		

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

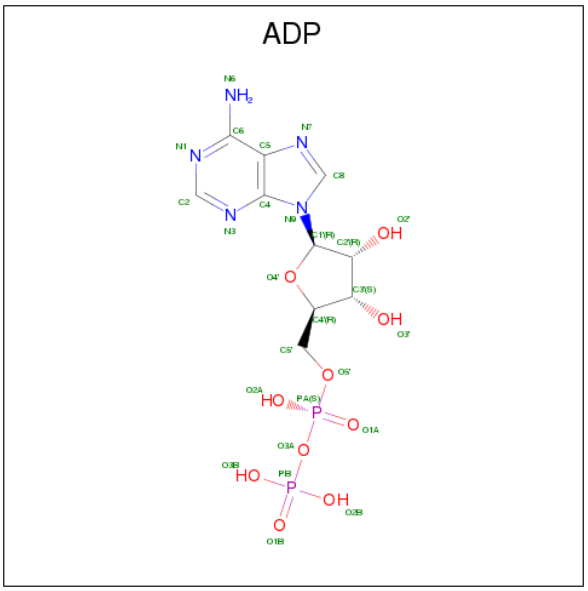
- Molecule 2 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	17	Total	C	H	N	O	S	0	0
			277	82	133	28	31	3		

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



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

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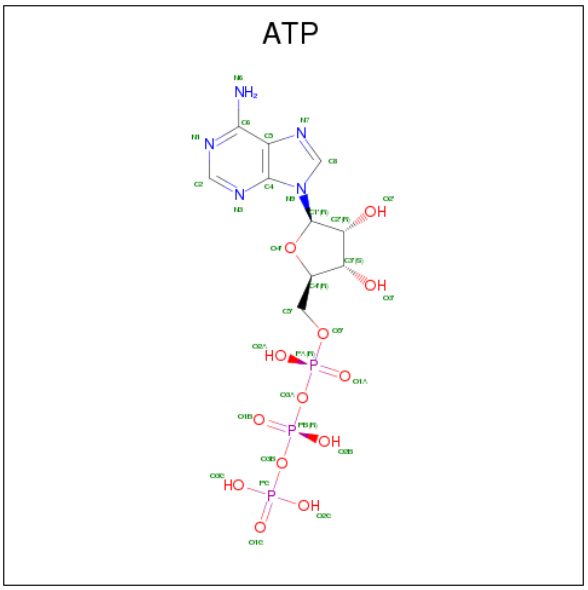
Mol	Chain	Residues	Atoms						AltConf
3	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



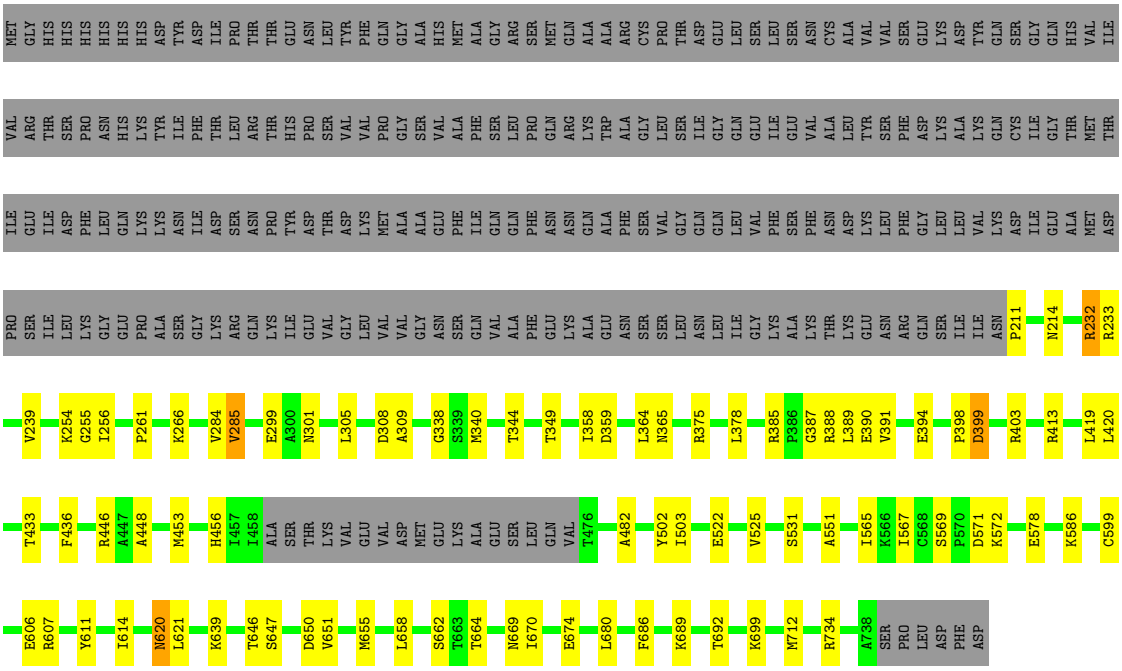
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	B	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
4	B	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
4	C	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
4	C	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
4	D	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
4	D	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
4	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

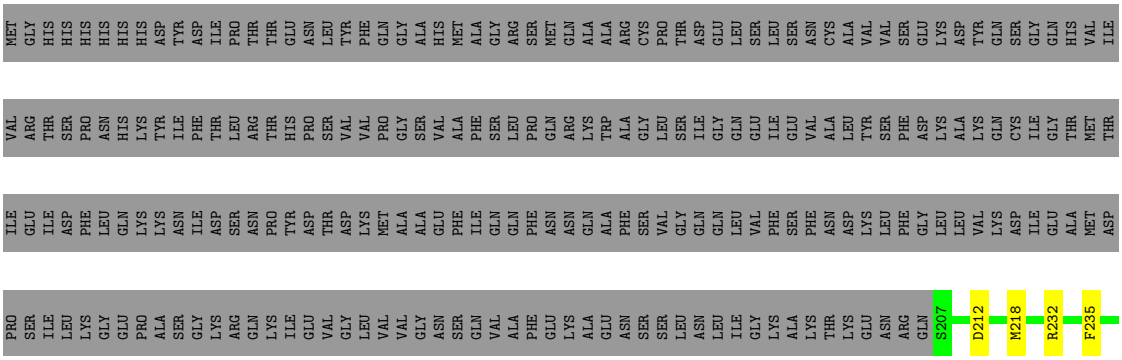
• Molecule 1: Vesicle-fusing ATPase

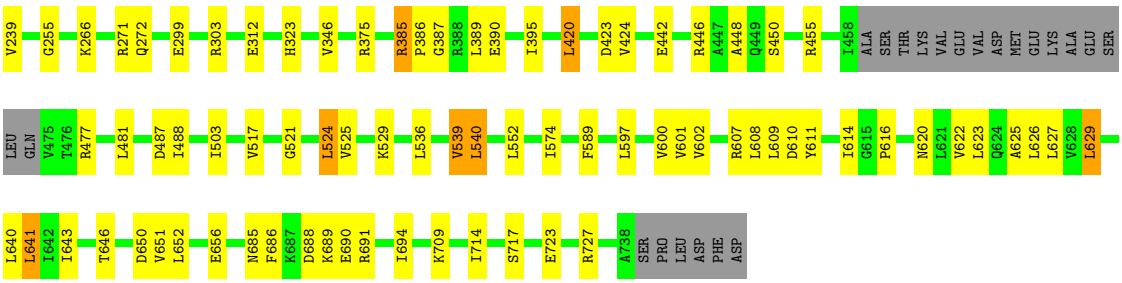
Chain A:



• Molecule 1: Vesicle-fusing ATPase

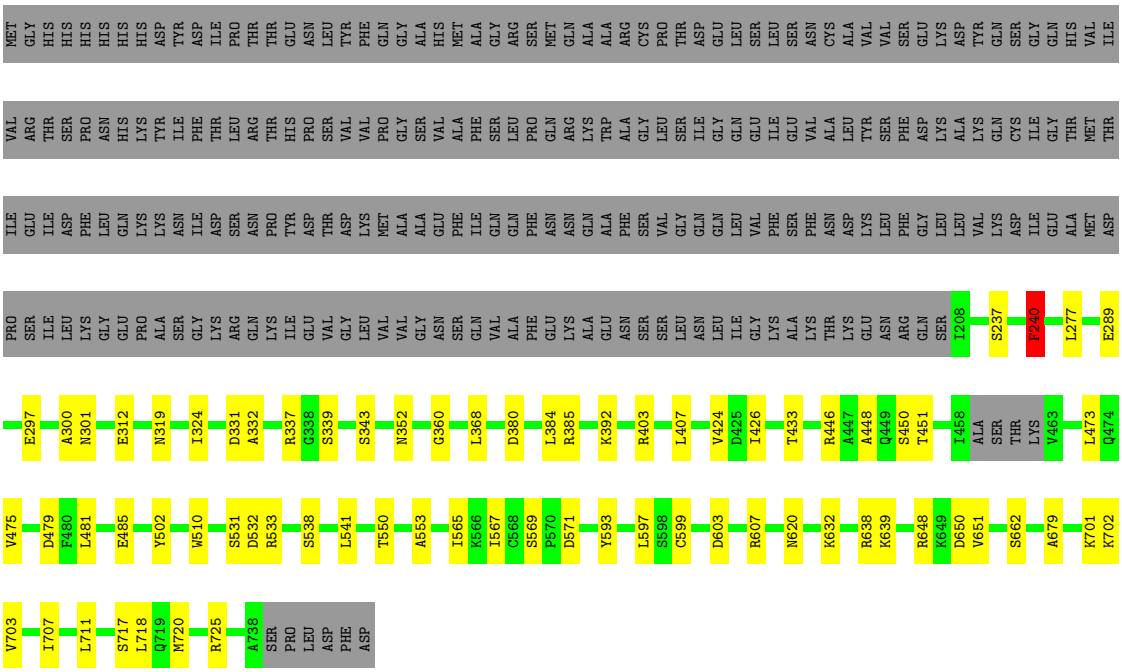
Chain B:





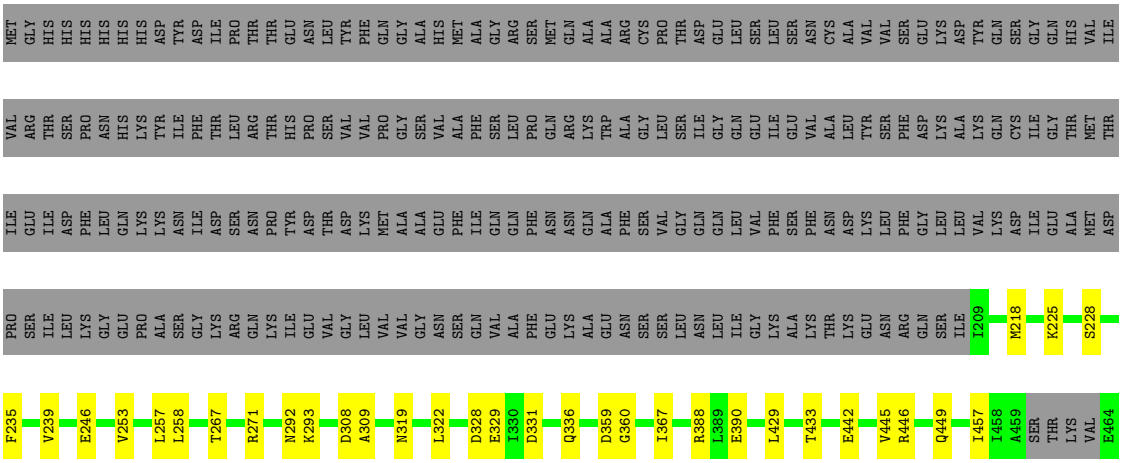
• Molecule 1: Vesicle-fusing ATPase

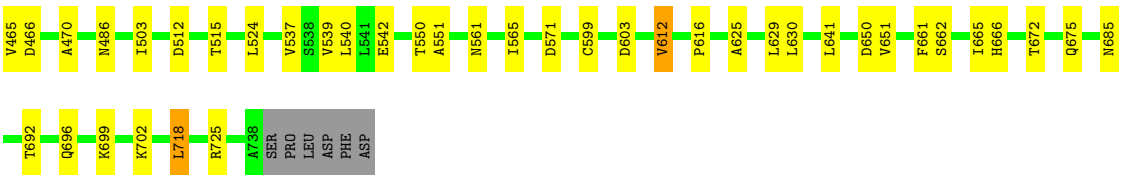
Chain C:



• Molecule 1: Vesicle-fusing ATPase

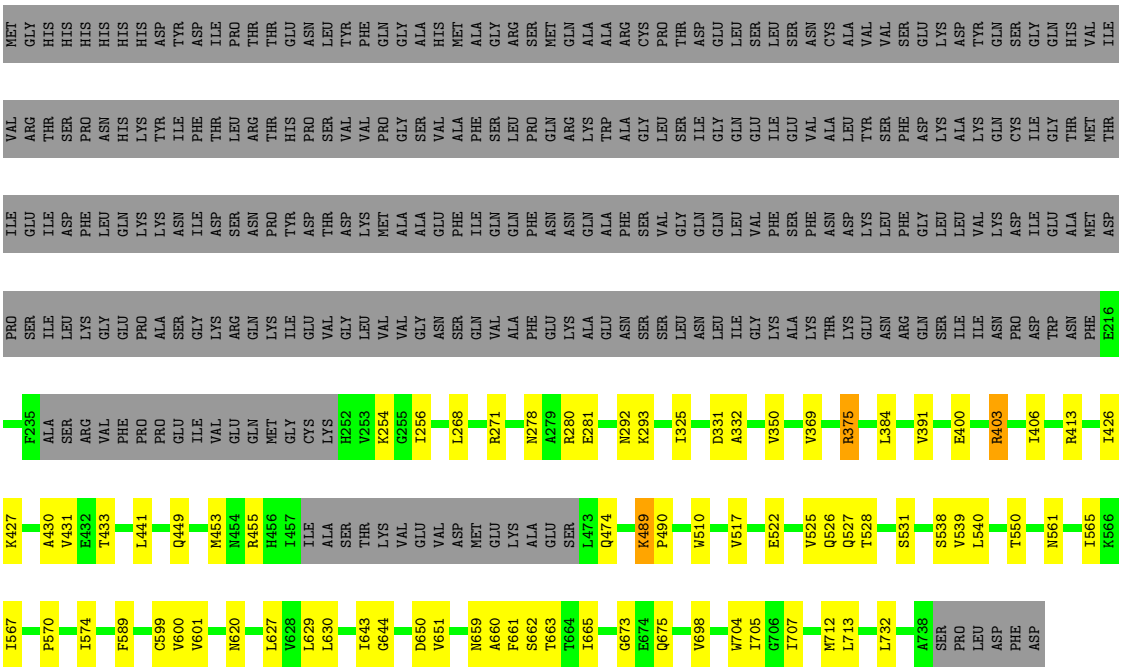
Chain D:





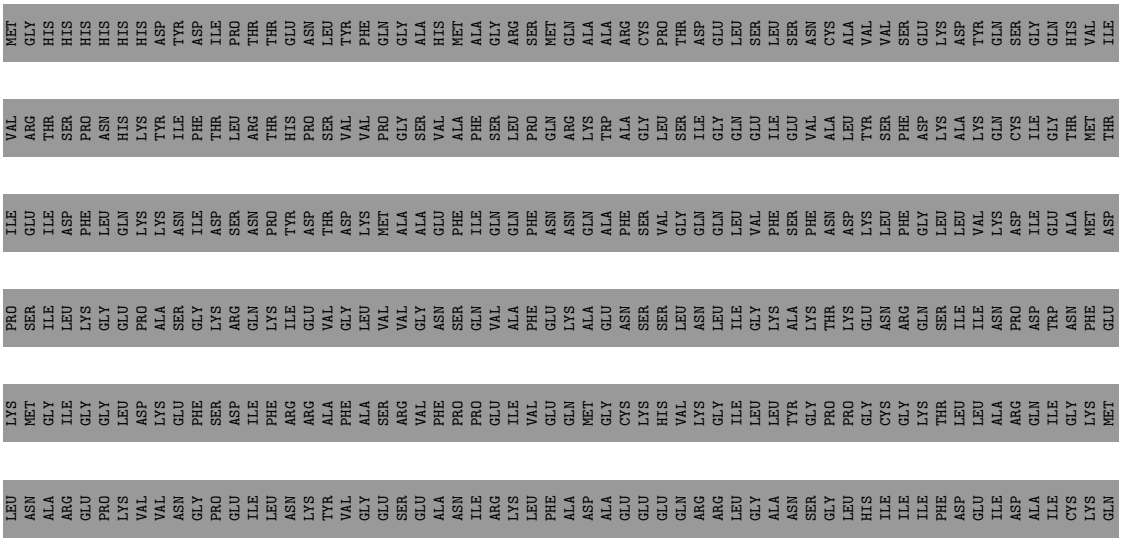
• Molecule 1: Vesicle-fusing ATPase

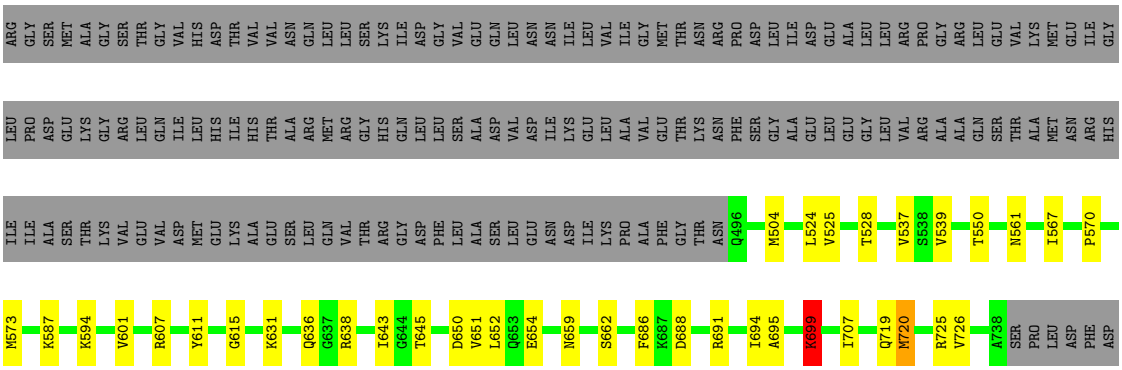
Chain E:



• Molecule 1: Vesicle-fusing ATPase

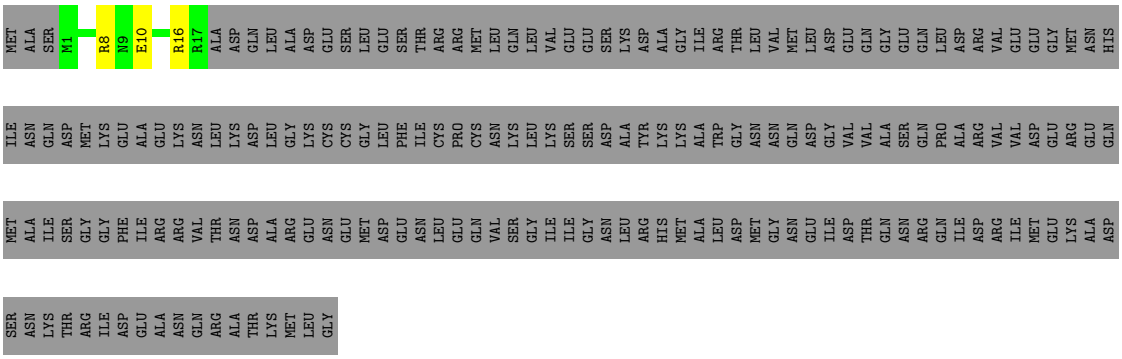
Chain F:





• Molecule 2: Synaptosomal-associated protein 25

Chain H: 7% 92%



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	184555	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	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.41	0/4046	0.74	6/5450 (0.1%)
1	B	0.41	0/4083	0.85	22/5502 (0.4%)
1	C	0.39	0/4171	0.72	9/5620 (0.2%)
1	D	0.37	0/4161	0.73	4/5606 (0.1%)
1	E	0.36	0/3883	0.67	1/5227 (0.0%)
1	F	0.38	0/1939	0.71	4/2616 (0.2%)
2	H	0.35	0/143	0.72	0/187
All	All	0.39	0/22426	0.74	46/30208 (0.2%)

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	702	LYS	CD-CE-NZ	11.46	138.07	111.70
1	B	623	LEU	CB-CG-CD2	7.77	124.21	111.00
1	B	641	LEU	CB-CG-CD2	7.62	123.95	111.00
1	B	517	VAL	CG1-CB-CG2	7.48	122.87	110.90
1	A	284	VAL	CG1-CB-CG2	7.44	122.80	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3985	4103	4111	51	0
1	B	4022	4145	4152	46	0
1	C	4110	4227	4238	41	0
1	D	4100	4214	4223	40	0
1	E	3830	3958	3965	46	0
1	F	1909	1997	1998	21	0
2	H	144	133	135	1	0
3	A	27	12	12	0	0
3	E	27	12	12	1	0
4	A	31	12	12	0	0
4	B	62	24	24	3	0
4	C	62	24	24	1	0
4	D	62	24	24	3	0
4	E	31	12	12	3	0
4	F	31	12	12	1	0
All	All	22433	22909	22954	226	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 226 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:A:448:ALA:HB1	1:A:482:ALA:HB1	1.46	0.97
1:D:246:GLU:O	1:E:413:ARG:NH2	2.16	0.79
1:B:232:ARG:O	1:C:450:SER:OG	2.02	0.77
1:B:385:ARG:NH1	1:B:386:PRO:O	2.18	0.76
1:A:620:ASN:ND2	1:B:610:ASP:OD2	2.19	0.76

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%)	493 (97%)	13 (3%)	1 (0%)	49 83
1	B	512/768 (67%)	495 (97%)	16 (3%)	1 (0%)	49 83
1	C	523/768 (68%)	511 (98%)	12 (2%)	0	100 100
1	D	522/768 (68%)	510 (98%)	11 (2%)	1 (0%)	49 83
1	E	486/768 (63%)	475 (98%)	10 (2%)	1 (0%)	49 83
1	F	241/768 (31%)	237 (98%)	4 (2%)	0	100 100
2	H	15/207 (7%)	15 (100%)	0	0	100 100
All	All	2806/4815 (58%)	2736 (98%)	66 (2%)	4 (0%)	56 87

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	ASP
1	B	616	PRO
1	E	489	LYS
1	D	616	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	435/658 (66%)	425 (98%)	10 (2%)	53 78
1	B	440/658 (67%)	437 (99%)	3 (1%)	85 93
1	C	450/658 (68%)	443 (98%)	7 (2%)	65 85
1	D	448/658 (68%)	441 (98%)	7 (2%)	65 85
1	E	418/658 (64%)	412 (99%)	6 (1%)	69 86
1	F	213/658 (32%)	206 (97%)	7 (3%)	41 72
2	H	15/177 (8%)	13 (87%)	2 (13%)	4 26
All	All	2419/4125 (59%)	2377 (98%)	42 (2%)	66 84

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	701	LYS
1	D	561	ASN
1	F	699	LYS
1	C	702	LYS
1	D	319	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	278	ASN
1	D	408	HIS
1	F	561	ASN
1	D	374	ASN
1	D	561	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 carbohydrates 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	$\#\|Z\|>2$
3	ADP	A	801	-	25,29,29	1.01	2 (8%)	25,45,45	1.88	4 (16%)
4	ATP	A	802	-	27,33,33	1.07	2 (7%)	27,52,52	1.98	6 (22%)
4	ATP	B	801	-	27,33,33	1.08	2 (7%)	27,52,52	2.15	6 (22%)
4	ATP	B	802	-	27,33,33	1.09	2 (7%)	27,52,52	2.13	6 (22%)
4	ATP	C	801	-	27,33,33	0.98	2 (7%)	27,52,52	2.28	5 (18%)
4	ATP	C	802	-	27,33,33	0.97	1 (3%)	27,52,52	2.14	4 (14%)
4	ATP	D	801	-	27,33,33	1.09	2 (7%)	27,52,52	1.90	4 (14%)
4	ATP	D	802	-	27,33,33	0.99	2 (7%)	27,52,52	1.86	4 (14%)
4	ATP	E	801	-	27,33,33	0.98	2 (7%)	27,52,52	1.98	4 (14%)
3	ADP	E	802	-	25,29,29	0.89	1 (4%)	25,45,45	1.87	5 (20%)
4	ATP	F	801	-	27,33,33	1.07	2 (7%)	27,52,52	2.44	8 (29%)

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
3	ADP	A	801	-	-	0/12/32/32	0/3/3/3
4	ATP	A	802	-	-	0/18/38/38	0/3/3/3
4	ATP	B	801	-	-	0/18/38/38	0/3/3/3
4	ATP	B	802	-	-	0/18/38/38	0/3/3/3
4	ATP	C	801	-	-	0/18/38/38	0/3/3/3
4	ATP	C	802	-	-	0/18/38/38	0/3/3/3
4	ATP	D	801	-	-	0/18/38/38	0/3/3/3
4	ATP	D	802	-	-	0/18/38/38	0/3/3/3
4	ATP	E	801	-	-	0/18/38/38	0/3/3/3
3	ADP	E	802	-	-	0/12/32/32	0/3/3/3
4	ATP	F	801	-	-	0/18/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	801	ATP	C8-N9	-3.29	1.33	1.36
4	B	801	ATP	C8-N9	-3.28	1.33	1.36
4	B	802	ATP	C8-N9	-3.17	1.33	1.36
4	A	802	ATP	C8-N9	-2.80	1.33	1.36
3	A	801	ADP	C8-N9	-2.14	1.34	1.36

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	802	ATP	N3-C2-N1	-7.08	122.81	128.86
4	C	801	ATP	N3-C2-N1	-7.01	122.87	128.86
4	F	801	ATP	N3-C2-N1	-6.94	122.92	128.86
4	B	801	ATP	N3-C2-N1	-6.73	123.11	128.86
3	E	802	ADP	N3-C2-N1	-6.48	123.32	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

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

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.