Full wwPDB EM Validation Report

Sep 25, 2025 – 05:20 PM EDT

PDB ID	:	9CRU / pdb_00009cru
EMDB ID	:	EMD-45883
Title	:	Y20S (Sec18-Sec17-Sec9-Sso1-Snc1) EDTA - Class 1
Authors	:	Khan, Y.A.; Brunger, A.T.
Deposited on	:	2024-07-22
Resolution	:	3.89 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

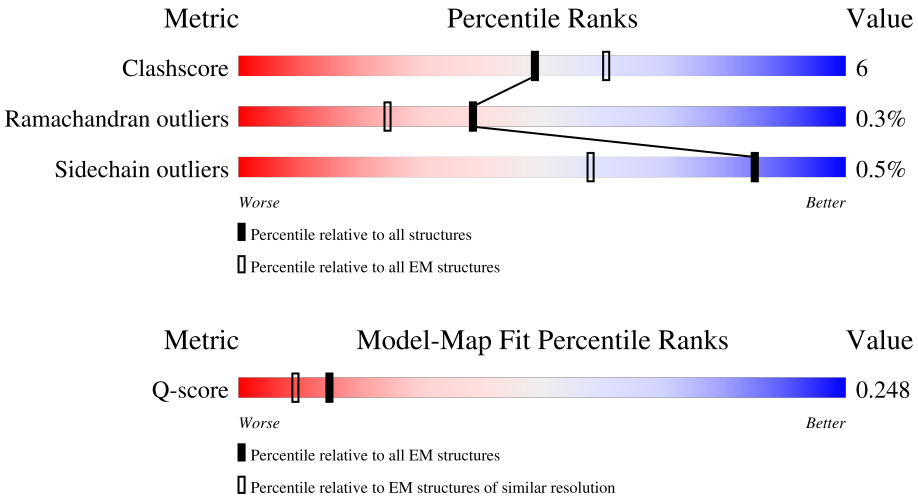
EMDB validation analysis	:	0.0.1.dev129
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive 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)	:	2.46

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 3.89 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	8712 (3.39 - 4.39)

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	761	58% 9% 34%
1	B	761	87% 9%
1	C	761	89% 9%
1	D	761	87% 11%

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Mol	Chain	Length	Quality of chain
1	E	761	59% 10% 31%
1	F	761	56% 9% 35%
2	G	293	13% 95% 5%
2	H	293	8% 92% 8%
3	J	97	60% 38%
4	K	269	6% 57% 20% 6% 17%
5	L	222	5% 50% 8% 42%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ATP	A	802	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 37375 atoms, of which 0 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 Vesicular-fusion protein SEC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	505	Total	C	N	O	S	0	0
			3928	2478	678	754	18		
1	B	728	Total	C	N	O	S	0	0
			5688	3589	985	1091	23		
1	C	741	Total	C	N	O	S	0	0
			5785	3647	1008	1107	23		
1	D	741	Total	C	N	O	S	0	0
			5785	3647	1008	1107	23		
1	E	527	Total	C	N	O	S	0	0
			4089	2576	709	786	18		
1	F	496	Total	C	N	O	S	0	0
			3867	2439	668	742	18		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P18759
A	-1	ALA	-	expression tag	UNP P18759
A	0	HIS	-	expression tag	UNP P18759
B	-2	GLY	-	expression tag	UNP P18759
B	-1	ALA	-	expression tag	UNP P18759
B	0	HIS	-	expression tag	UNP P18759
C	-2	GLY	-	expression tag	UNP P18759
C	-1	ALA	-	expression tag	UNP P18759
C	0	HIS	-	expression tag	UNP P18759
D	-2	GLY	-	expression tag	UNP P18759
D	-1	ALA	-	expression tag	UNP P18759
D	0	HIS	-	expression tag	UNP P18759
E	-2	GLY	-	expression tag	UNP P18759
E	-1	ALA	-	expression tag	UNP P18759
E	0	HIS	-	expression tag	UNP P18759
F	-2	GLY	-	expression tag	UNP P18759
F	-1	ALA	-	expression tag	UNP P18759
F	0	HIS	-	expression tag	UNP P18759

- Molecule 2 is a protein called Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	292	Total	C	N	O	S	0	0
			2306	1446	388	461	11		
2	H	292	Total	C	N	O	S	0	0
			2306	1446	388	461	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP P32602
H	0	GLY	-	expression tag	UNP P32602

- Molecule 3 is a protein called Synaptobrevin homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	60	Total	C	N	O	S	0	0
			468	282	92	92	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	GLY	-	expression tag	UNP P31109
J	-2	ALA	-	expression tag	UNP P31109
J	-1	SER	-	expression tag	UNP P31109
J	0	HIS	-	expression tag	UNP P31109

- Molecule 4 is a protein called Protein SSO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	224	Total	C	N	O	S	0	0
			1805	1105	329	367	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	GLY	-	expression tag	UNP P32867
K	-2	ALA	-	expression tag	UNP P32867
K	-1	SER	-	expression tag	UNP P32867
K	0	HIS	-	expression tag	UNP P32867

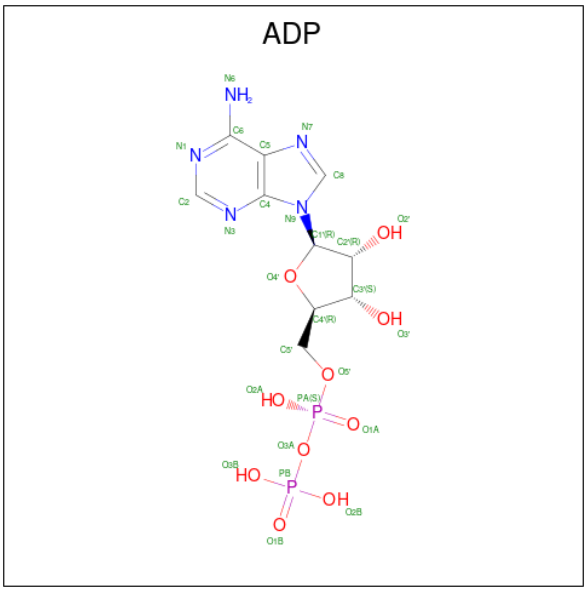
- Molecule 5 is a protein called Protein transport protein SEC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	129	Total	C	N	O	S	0	0
			1015	614	186	208	7		

There are 4 discrepancies between the modelled and reference sequences:

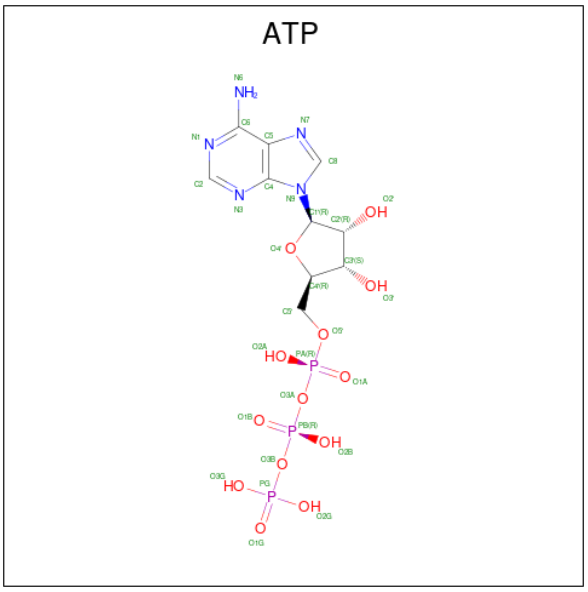
Chain	Residue	Modelled	Actual	Comment	Reference
L	429	GLY	-	expression tag	UNP P40357
L	430	ALA	-	expression tag	UNP P40357
L	431	SER	-	expression tag	UNP P40357
L	432	HIS	-	expression tag	UNP P40357

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



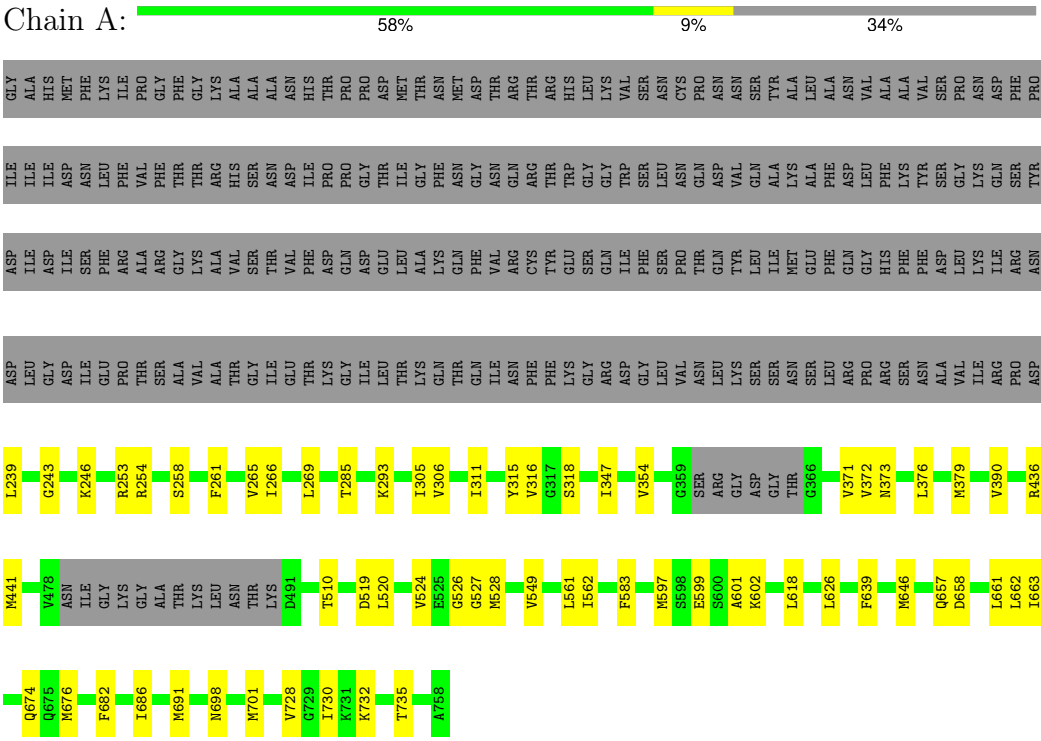
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

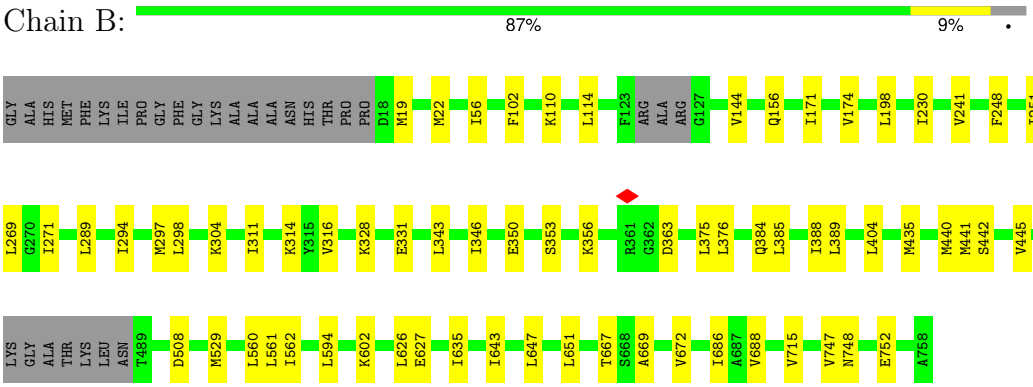
• Molecule 1: Vesicular-fusion protein SEC18

Chain A:



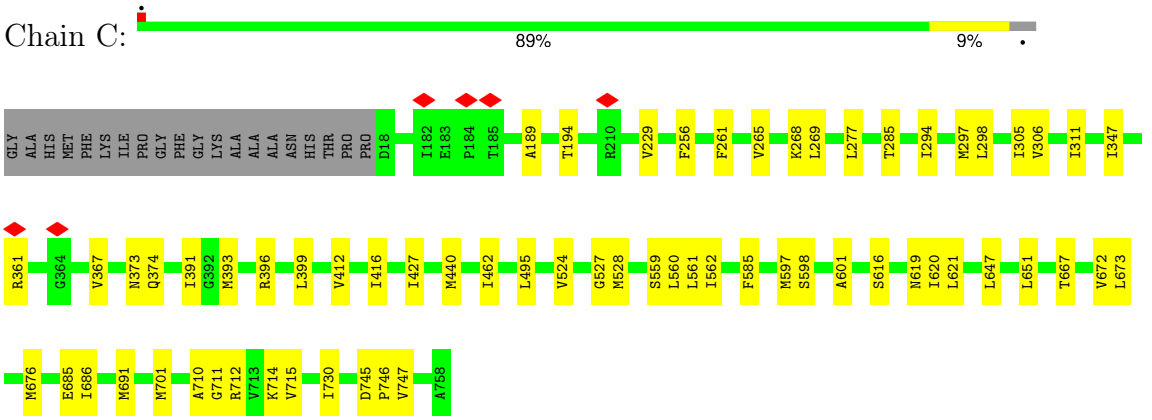
• Molecule 1: Vesicular-fusion protein SEC18

Chain B:



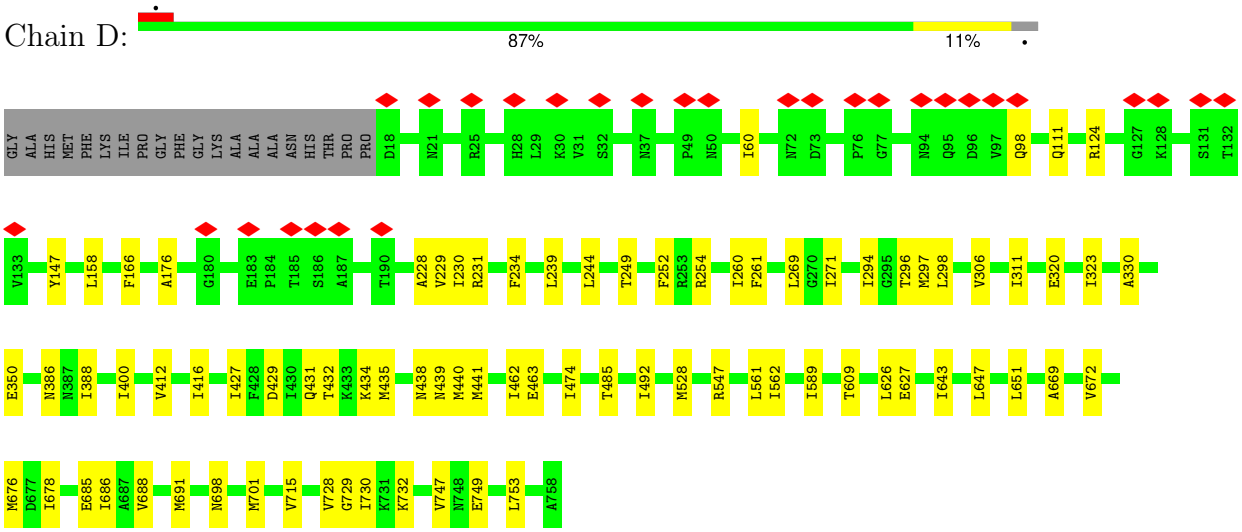
• Molecule 1: Vesicular-fusion protein SEC18

Chain C:



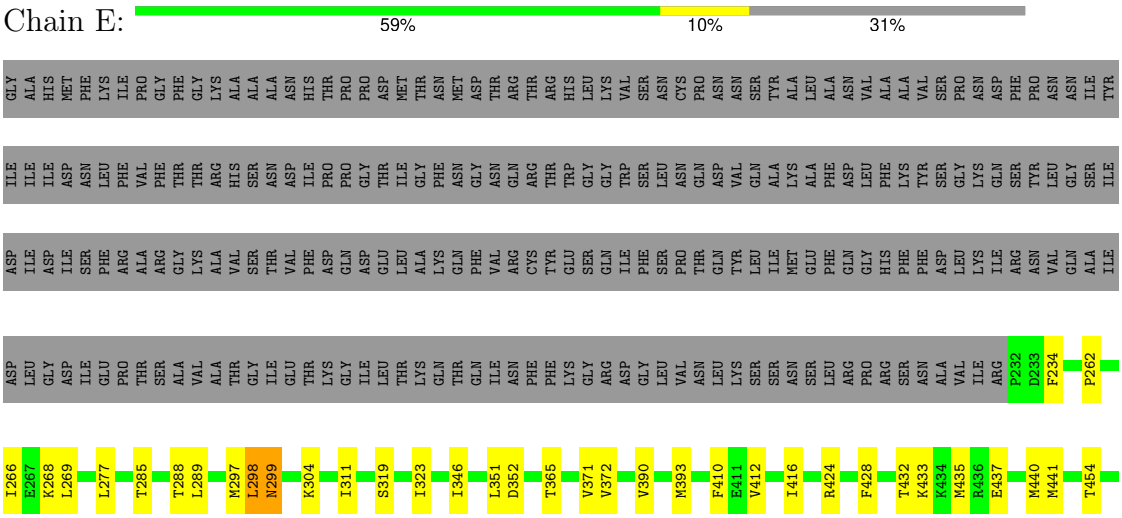
• Molecule 1: Vesicular-fusion protein SEC18

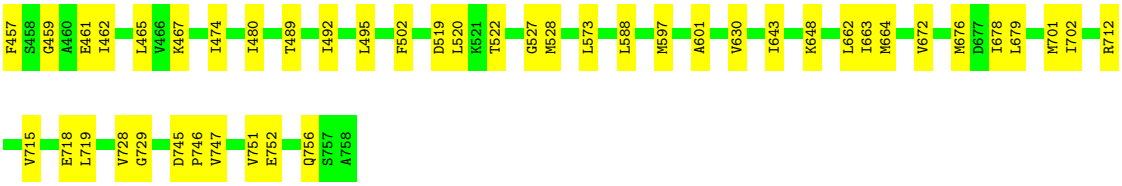
Chain D:



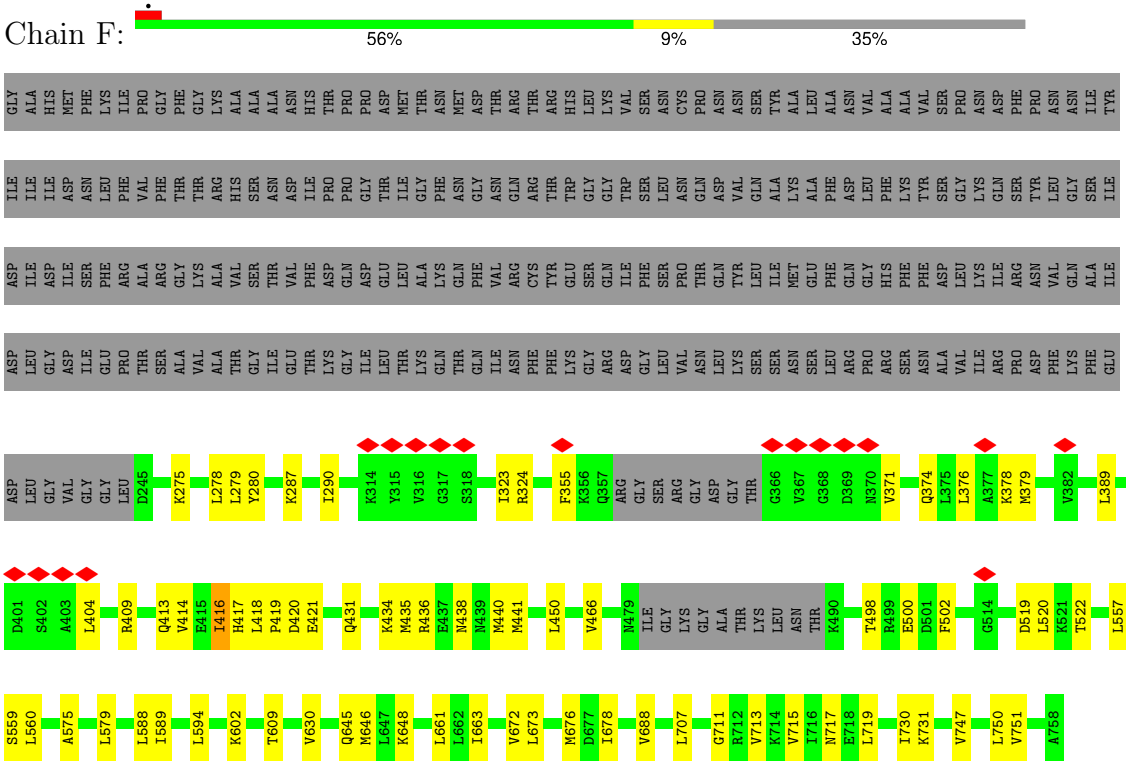
• Molecule 1: Vesicular-fusion protein SEC18

Chain E:

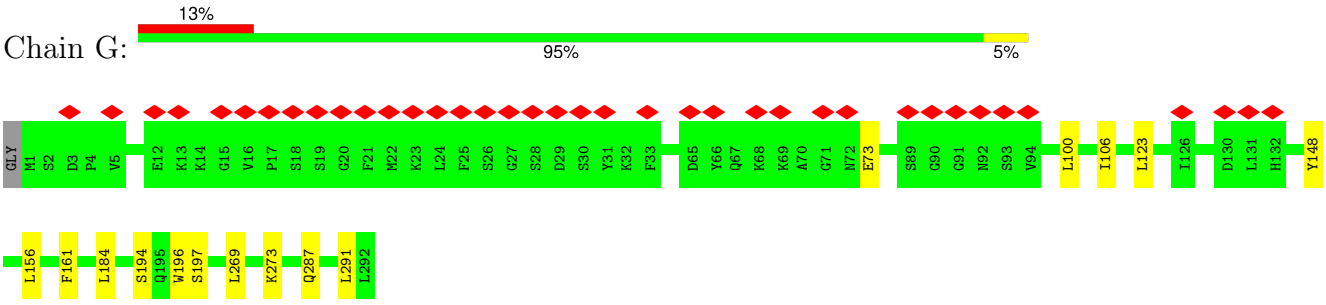




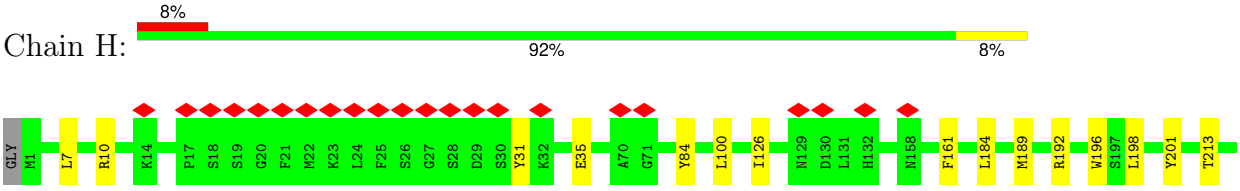
• Molecule 1: Vesicular-fusion protein SEC18



• Molecule 2: Alpha-soluble NSF attachment protein

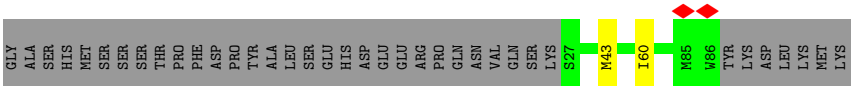


• Molecule 2: Alpha-soluble NSF attachment protein



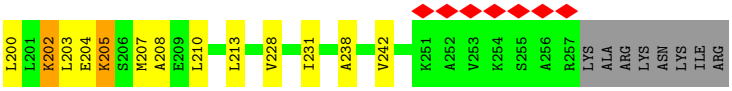
• Molecule 3: Synaptobrevin homolog 1

Chain J:



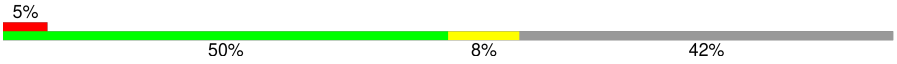
• Molecule 4: Protein SSO1

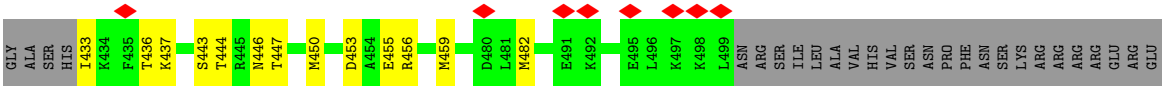
Chain K:



• Molecule 5: Protein transport protein SEC9

Chain L:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41159	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.012	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	322.224, 322.224, 322.224	wwPDB
Map dimensions	294, 294, 294	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.096, 1.096, 1.096	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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	2/3981 (0.1%)	0.60	0/5367
1	B	0.37	0/5779	0.58	0/7802
1	C	0.37	1/5878 (0.0%)	0.56	0/7936
1	D	0.37	3/5878 (0.1%)	0.55	0/7936
1	E	0.38	1/4146 (0.0%)	0.67	2/5589 (0.0%)
1	F	0.34	0/3919	0.60	1/5284 (0.0%)
2	G	0.25	0/2343	0.48	0/3144
2	H	0.25	0/2343	0.49	0/3144
3	J	0.25	0/470	0.46	0/628
4	K	0.57	0/1822	0.93	2/2448 (0.1%)
5	L	0.28	0/1016	0.53	0/1355
All	All	0.37	7/37575 (0.0%)	0.59	5/50633 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	GLY	C-N	-8.91	1.21	1.33
1	D	429	ASP	C-N	7.98	1.43	1.33
1	A	261	PHE	C-N	7.52	1.42	1.33
1	E	262	PRO	CA-C	-5.74	1.48	1.51
1	D	439	ASN	C-N	-5.57	1.25	1.33
1	D	249	THR	C-N	5.50	1.40	1.33
1	C	374	GLN	C-N	-5.42	1.26	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	155	ALA	N-CA-C	7.84	120.44	110.24
1	E	298	LEU	CA-C-N	5.82	132.66	121.54
1	E	298	LEU	C-N-CA	5.82	132.66	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	183	ARG	CB-CA-C	-5.30	109.48	115.79
1	F	416	ILE	CA-C-O	-5.02	117.72	121.68

There are no chirality outliers.

There are no planarity outliers.

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	3928	0	4019	55	0
1	B	5688	0	5742	62	0
1	C	5785	0	5853	44	0
1	D	5785	0	5853	69	0
1	E	4089	0	4188	60	0
1	F	3867	0	3963	52	0
2	G	2306	0	2243	9	0
2	H	2306	0	2243	17	0
3	J	468	0	470	4	0
4	K	1805	0	1772	80	0
5	L	1015	0	1034	27	0
6	A	27	0	12	0	0
6	E	27	0	12	0	0
7	A	31	0	12	9	0
7	B	62	0	24	2	0
7	C	62	0	24	1	0
7	D	62	0	24	1	0
7	E	31	0	12	2	0
7	F	31	0	12	1	0
All	All	37375	0	37512	422	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 6.

All (422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:200:LEU:HD11	5:L:444:THR:CG2	1.82	1.08
4:K:178:LEU:HD22	4:K:182:ARG:HH11	1.19	1.07
4:K:186:ALA:HB1	4:K:191:ALA:HB2	1.44	0.99
4:K:200:LEU:HD11	5:L:444:THR:HG23	1.42	0.98
1:E:672:VAL:HG12	1:E:676:MET:HE1	1.43	0.97
1:C:672:VAL:HG12	1:C:676:MET:HE1	1.47	0.97
5:L:455:GLU:O	5:L:459:MET:HG2	1.66	0.94
4:K:183:ARG:HA	4:K:183:ARG:NE	1.80	0.93
1:F:672:VAL:HG12	1:F:676:MET:HE1	1.51	0.92
1:A:676:MET:HE1	1:B:635:ILE:HD13	1.51	0.90
1:E:435:MET:HE1	1:E:441:MET:HE3	1.54	0.87
1:D:672:VAL:HG12	1:D:676:MET:HE1	1.57	0.85
4:K:186:ALA:HB2	5:L:433:ILE:HD11	1.64	0.80
1:C:440:MET:HE2	1:C:495:LEU:HD11	1.66	0.78
1:E:702:ILE:HG22	1:E:712:ARG:HE	1.48	0.77
4:K:200:LEU:HA	4:K:203:LEU:HD12	1.64	0.77
4:K:183:ARG:NE	4:K:183:ARG:CA	2.46	0.77
4:K:178:LEU:CD2	4:K:182:ARG:HH11	1.96	0.76
1:D:435:MET:SD	1:D:441:MET:CE	2.73	0.76
1:C:597:MET:HE2	1:C:601:ALA:HB1	1.67	0.76
4:K:65:LEU:HD22	4:K:139:GLU:OE2	1.86	0.76
4:K:186:ALA:HA	4:K:190:LEU:HB3	1.68	0.75
1:A:269:LEU:HA	1:B:435:MET:HE2	1.68	0.75
1:A:316:VAL:HG13	4:K:169:GLY:HA2	1.69	0.75
2:G:196:TRP:HZ3	5:L:607:ARG:HD2	1.53	0.74
4:K:190:LEU:HD23	5:L:433:ILE:HG21	1.69	0.74
1:F:418:LEU:HB3	1:F:419:PRO:HD2	1.67	0.74
1:D:435:MET:SD	1:D:441:MET:HE1	2.31	0.71
1:C:527:GLY:O	1:C:528:MET:HE2	1.91	0.70
1:A:562:ILE:HG22	1:A:686:ILE:HB	1.74	0.70
1:E:718:GLU:OE1	1:E:747:VAL:HG21	1.92	0.70
1:A:316:VAL:CG1	4:K:169:GLY:HA2	2.22	0.69
1:D:330:ALA:HB1	1:D:388:ILE:HD11	1.75	0.69
1:E:663:ILE:O	1:E:664:MET:HE2	1.91	0.69
1:E:268:LYS:O	1:F:435:MET:HE1	1.94	0.68
2:H:236:ARG:NH1	2:H:267:MET:HE2	2.10	0.66
4:K:183:ARG:HA	4:K:183:ARG:CZ	2.25	0.66
4:K:178:LEU:HD22	4:K:182:ARG:NH1	2.03	0.66
4:K:178:LEU:HD22	4:K:182:ARG:HD2	1.77	0.66
1:D:269:LEU:HD22	1:E:440:MET:HE1	1.77	0.65
1:A:639:PHE:HE1	1:B:635:ILE:HD11	1.61	0.65
1:E:234:PHE:CZ	1:E:297:MET:SD	2.90	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:VAL:HG21	1:C:311:ILE:HD11	1.79	0.64
3:J:60:ILE:HG22	4:K:231:ILE:HD13	1.80	0.64
1:B:294:ILE:O	1:B:298:LEU:HD23	1.98	0.63
4:K:181:ASN:O	4:K:182:ARG:C	2.41	0.63
2:G:287:GLN:NE2	2:G:291:LEU:HD21	2.13	0.63
4:K:165:SER:O	4:K:166:ASP:HB2	1.98	0.63
1:E:702:ILE:HG22	1:E:712:ARG:NE	2.14	0.62
4:K:179:ASN:ND2	4:K:182:ARG:HB2	2.14	0.62
2:G:148:TYR:CE1	2:G:156:LEU:HD13	2.35	0.62
1:A:730:ILE:HG21	7:A:802:ATP:C2	2.34	0.62
1:B:594:LEU:HD12	1:B:602:LYS:HD3	1.82	0.62
1:F:594:LEU:HD12	1:F:602:LYS:HG2	1.82	0.61
1:C:561:LEU:HD23	1:C:562:ILE:N	2.15	0.61
1:F:589:ILE:HD11	1:F:609:THR:HG21	1.82	0.61
4:K:180:ALA:O	4:K:181:ASN:C	2.43	0.61
1:A:269:LEU:HD13	1:B:435:MET:HE3	1.83	0.60
2:H:161:PHE:HB2	2:H:184:LEU:HD21	1.83	0.60
1:B:230:ILE:HD12	1:B:260:ILE:HD11	1.84	0.60
1:E:435:MET:CE	1:E:441:MET:HE3	2.29	0.60
1:F:279:LEU:HD13	1:F:414:VAL:HB	1.84	0.60
4:K:122:PHE:CE2	4:K:126:ILE:HD11	2.37	0.59
1:D:627:GLU:OE2	1:D:669:ALA:HB3	2.02	0.59
1:D:589:ILE:HD11	1:D:609:THR:HG21	1.84	0.59
1:D:271:ILE:HD11	1:E:467:LYS:HB2	1.84	0.59
1:E:285:THR:HG21	1:E:416:ILE:HG22	1.83	0.59
4:K:204:GLU:OE2	5:L:446:ASN:HB3	2.03	0.59
1:A:254:ARG:NH2	1:B:508:ASP:OD2	2.36	0.58
2:G:73:GLU:HG2	2:G:106:ILE:HG23	1.85	0.58
2:H:84:TYR:OH	2:H:126:ILE:HD11	2.03	0.58
1:E:365:THR:HG21	4:K:177:LEU:HD21	1.86	0.57
1:B:114:LEU:HD22	1:B:174:VAL:HG13	1.86	0.57
2:H:7:LEU:HD23	2:H:10:ARG:NH2	2.19	0.57
1:E:288:THR:HA	1:E:393:MET:HE1	1.86	0.57
1:E:520:LEU:HD22	1:E:588:LEU:HD23	1.86	0.57
4:K:180:ALA:O	4:K:183:ARG:N	2.37	0.57
1:F:418:LEU:HB3	1:F:419:PRO:CD	2.34	0.57
1:E:719:LEU:HD21	1:E:751:VAL:HG13	1.85	0.56
1:A:528:MET:HE1	7:A:802:ATP:HN61	1.70	0.56
1:E:461:GLU:O	1:E:465:LEU:HD23	2.05	0.56
4:K:181:ASN:O	4:K:183:ARG:HB2	2.06	0.56
5:L:455:GLU:HG2	5:L:459:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:238:ALA:HB1	5:L:482:MET:HE1	1.87	0.56
1:B:304:LYS:HB3	1:B:346:ILE:HG22	1.88	0.56
1:D:435:MET:SD	1:D:441:MET:HE3	2.45	0.56
1:C:528:MET:HE1	7:C:802:ATP:H2'	1.87	0.56
4:K:178:LEU:CD2	4:K:182:ARG:HD2	2.36	0.56
4:K:64:LEU:O	4:K:64:LEU:HD23	2.05	0.56
4:K:185:GLU:O	4:K:187:LYS:HG3	2.05	0.56
1:A:269:LEU:HD13	1:B:435:MET:CE	2.35	0.55
1:E:701:MET:HE1	1:E:715:VAL:HG21	1.87	0.55
1:F:575:ALA:O	1:F:579:LEU:HD23	2.07	0.55
1:B:22:MET:HE1	1:B:56:ILE:CD1	2.37	0.55
2:G:196:TRP:CZ3	5:L:607:ARG:HD2	2.38	0.55
1:B:297:MET:C	1:B:298:LEU:HD22	2.31	0.55
1:A:528:MET:CE	7:A:802:ATP:HN61	2.20	0.55
1:F:661:LEU:HD13	1:F:663:ILE:HG23	1.89	0.55
1:C:305:ILE:H	1:C:305:ILE:HD12	1.72	0.54
1:E:662:LEU:HG	1:E:664:MET:HE3	1.88	0.54
1:C:524:VAL:O	1:C:524:VAL:HG12	2.07	0.54
1:E:643:ILE:HD12	1:E:643:ILE:H	1.72	0.54
1:E:719:LEU:CD2	1:E:751:VAL:HG13	2.38	0.54
4:K:60:LEU:HD13	4:K:63:ARG:NH2	2.23	0.54
1:D:647:LEU:O	1:D:651:LEU:HD23	2.08	0.54
1:C:373:ASN:ND2	1:D:350:GLU:OE2	2.35	0.54
4:K:200:LEU:HD22	5:L:443:SER:HB3	1.90	0.54
1:D:715:VAL:HG12	1:D:747:VAL:HG22	1.89	0.54
1:F:323:ILE:HG13	1:F:371:VAL:HG23	1.89	0.54
1:F:376:LEU:HD23	1:F:379:MET:CE	2.38	0.54
1:F:730:ILE:HG23	1:F:731:LYS:HD3	1.88	0.54
1:B:529:MET:SD	7:B:802:ATP:C8	3.01	0.53
1:C:396:ARG:HE	1:C:399:LEU:HD13	1.73	0.53
1:D:715:VAL:CG1	1:D:747:VAL:HG22	2.38	0.53
1:B:241:VAL:HG22	1:B:289:LEU:HD23	1.90	0.53
1:C:265:VAL:O	1:C:269:LEU:HD23	2.08	0.53
1:D:435:MET:HB3	1:D:441:MET:HE3	1.89	0.53
1:D:306:VAL:HG21	1:D:311:ILE:HD11	1.91	0.53
1:E:527:GLY:O	7:E:802:ATP:C8	2.62	0.53
4:K:163:ALA:O	4:K:164:ILE:HB	2.09	0.53
1:D:269:LEU:HD22	1:E:440:MET:CE	2.37	0.53
1:B:297:MET:O	1:B:298:LEU:HD22	2.09	0.53
1:B:626:LEU:O	1:B:627:GLU:HG3	2.08	0.53
1:B:440:MET:HE3	1:B:440:MET:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ARG:CA	1:A:441:MET:HE3	2.40	0.53
1:E:597:MET:HB3	1:E:601:ALA:HB3	1.90	0.53
1:C:277:LEU:HB3	1:C:391:ILE:HG22	1.90	0.52
1:E:454:THR:O	1:E:454:THR:HG23	2.09	0.52
1:E:679:LEU:HD23	1:E:679:LEU:O	2.09	0.52
1:D:435:MET:CG	1:D:441:MET:HE3	2.39	0.52
1:A:373:ASN:HB3	1:B:350:GLU:OE1	2.09	0.52
1:D:698:ASN:HA	1:D:701:MET:HE3	1.91	0.52
4:K:65:LEU:CD1	4:K:139:GLU:HG3	2.40	0.52
1:D:244:LEU:HD21	1:D:416:ILE:HG23	1.92	0.52
4:K:178:LEU:HD22	4:K:182:ARG:CD	2.40	0.52
1:A:528:MET:SD	7:A:802:ATP:N7	2.83	0.52
1:D:485:THR:HG22	1:D:485:THR:O	2.09	0.52
1:E:424:ARG:HD3	1:E:454:THR:HG23	1.91	0.52
4:K:61:HIS:ND1	4:K:136:TYR:CG	2.78	0.52
4:K:121:ARG:O	4:K:125:LEU:HD23	2.09	0.52
1:C:561:LEU:HD21	1:C:667:THR:HG22	1.92	0.52
1:A:528:MET:HE1	7:A:802:ATP:N6	2.25	0.52
1:E:719:LEU:HD21	1:E:751:VAL:HG22	1.90	0.51
1:A:528:MET:HE3	1:A:528:MET:HA	1.91	0.51
1:C:277:LEU:HD12	1:C:412:VAL:HG23	1.91	0.51
1:D:691:MET:HE1	1:D:730:ILE:CA	2.40	0.51
2:H:213:THR:O	2:H:213:THR:HG22	2.10	0.51
4:K:65:LEU:HD11	4:K:139:GLU:HG3	1.92	0.51
1:F:275:LYS:O	1:F:389:LEU:HD12	2.11	0.51
4:K:200:LEU:CD1	5:L:444:THR:HG23	2.29	0.51
1:B:22:MET:HE1	1:B:56:ILE:HD12	1.93	0.51
1:B:669:ALA:O	1:B:672:VAL:HG12	2.11	0.51
2:H:184:LEU:HD13	2:H:201:TYR:CE1	2.46	0.51
4:K:166:ASP:O	4:K:167:VAL:HB	2.11	0.51
1:B:388:ILE:C	1:B:389:LEU:HD22	2.35	0.50
1:B:560:LEU:HD12	1:B:686:ILE:HD11	1.93	0.50
3:J:43:MET:HE1	4:K:213:LEU:HB2	1.93	0.50
1:C:229:VAL:HG12	1:C:298:LEU:HD12	1.94	0.50
1:A:583:PHE:CE2	1:A:618:LEU:HD11	2.46	0.50
1:E:311:ILE:CG2	1:E:323:ILE:HD11	2.41	0.50
1:D:230:ILE:HG22	1:D:230:ILE:O	2.12	0.50
1:D:528:MET:HE1	7:D:802:ATP:C5	2.47	0.50
1:E:519:ASP:O	1:E:522:THR:HG22	2.12	0.50
4:K:152:GLN:HG3	4:K:153:PRO:HD2	1.93	0.50
1:D:427:ILE:HG21	1:D:462:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:LEU:HD12	1:F:435:MET:SD	2.52	0.49
1:F:673:LEU:CD1	1:F:678:ILE:HD11	2.41	0.49
1:C:297:MET:C	1:C:298:LEU:HD22	2.37	0.49
1:E:266:ILE:HD12	1:E:266:ILE:H	1.76	0.49
1:A:436:ARG:HA	1:A:441:MET:HE3	1.95	0.49
1:D:431:GLN:NE2	1:D:463:GLU:HG3	2.27	0.49
1:A:372:VAL:O	1:A:376:LEU:HD23	2.12	0.49
1:F:431:GLN:CD	1:F:466:VAL:HG21	2.38	0.49
1:F:520:LEU:HD11	1:F:588:LEU:HB2	1.94	0.49
2:H:184:LEU:HD13	2:H:201:TYR:HE1	1.76	0.49
1:F:278:LEU:HD12	1:F:413:GLN:HE21	1.77	0.49
1:F:498:THR:HG23	1:F:500:GLU:HG3	1.94	0.49
1:F:520:LEU:HD11	1:F:588:LEU:CB	2.42	0.49
1:E:428:PHE:O	1:E:432:THR:HG23	2.12	0.48
1:F:519:ASP:OD1	1:F:520:LEU:HD12	2.12	0.48
1:A:657:GLN:HG3	1:A:658:ASP:H	1.78	0.48
1:B:647:LEU:O	1:B:651:LEU:HD23	2.14	0.48
1:F:434:LYS:C	1:F:435:MET:HE2	2.38	0.48
2:H:196:TRP:CZ2	5:L:453:ASP:HB3	2.48	0.48
4:K:199:GLU:HA	4:K:202:LYS:NZ	2.28	0.48
1:C:189:ALA:CB	1:C:194:THR:HG21	2.43	0.48
4:K:179:ASN:HD21	4:K:182:ARG:HB2	1.77	0.48
4:K:204:GLU:HG3	5:L:447:THR:OG1	2.13	0.48
4:K:242:VAL:HG21	5:L:482:MET:HE3	1.95	0.48
1:D:715:VAL:HG12	1:D:747:VAL:HG13	1.95	0.48
4:K:180:ALA:O	4:K:182:ARG:N	2.47	0.48
1:D:688:VAL:HG13	1:D:688:VAL:O	2.14	0.48
1:D:562:ILE:HD13	1:D:686:ILE:HB	1.95	0.48
1:E:311:ILE:HG21	1:E:323:ILE:HD11	1.96	0.48
4:K:200:LEU:HD22	5:L:443:SER:CB	2.43	0.48
1:E:648:LYS:HD2	1:E:678:ILE:HG22	1.96	0.48
1:A:438:ASN:HB3	1:A:440:MET:HE1	1.95	0.48
1:A:519:ASP:OD1	1:A:520:LEU:HD12	2.14	0.48
1:B:388:ILE:O	1:B:389:LEU:HD22	2.14	0.48
1:C:559:SER:C	1:C:560:LEU:HD22	2.39	0.47
1:E:323:ILE:HD12	1:E:323:ILE:H	1.79	0.47
1:F:719:LEU:CD2	1:F:751:VAL:HG23	2.43	0.47
1:F:376:LEU:HD23	1:F:379:MET:HE1	1.96	0.47
4:K:86:GLN:O	4:K:90:LEU:HD13	2.13	0.47
1:B:384:GLN:C	1:B:385:LEU:HD22	2.39	0.47
1:D:111:GLN:HB3	1:D:176:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:ASN:HB2	1:D:440:MET:HE2	1.97	0.47
1:F:420:ASP:CG	1:F:421:GLU:H	2.22	0.47
1:B:376:LEU:HD21	1:B:404:LEU:HD11	1.97	0.47
1:E:298:LEU:O	1:E:299:ASN:O	2.32	0.47
1:E:371:VAL:HG13	1:E:372:VAL:N	2.30	0.47
1:E:528:MET:HE3	1:E:528:MET:HA	1.95	0.47
1:C:691:MET:HE1	1:C:730:ILE:N	2.29	0.47
1:D:294:ILE:O	1:D:298:LEU:HD23	2.14	0.47
1:E:715:VAL:HG12	1:E:747:VAL:HG22	1.96	0.47
1:D:434:LYS:O	1:D:438:ASN:ND2	2.47	0.47
1:F:420:ASP:CG	1:F:421:GLU:N	2.72	0.47
1:F:661:LEU:HD12	1:F:661:LEU:C	2.39	0.47
2:G:100:LEU:HD13	2:G:123:LEU:HB2	1.95	0.47
1:A:661:LEU:HD21	1:A:663:ILE:HD11	1.97	0.47
1:F:324:ARG:HA	1:F:324:ARG:NE	2.30	0.47
1:F:646:MET:HE2	1:F:646:MET:HA	1.97	0.47
4:K:56:GLN:O	4:K:60:LEU:HD23	2.14	0.47
1:A:318:SER:N	1:B:314:LYS:HZ1	2.13	0.47
1:A:526:GLY:HA3	7:A:802:ATP:O2'	2.14	0.47
1:C:620:ILE:C	1:C:621:LEU:HD22	2.40	0.47
1:D:643:ILE:H	1:D:643:ILE:HD12	1.79	0.47
1:F:450:LEU:HD22	1:F:502:PHE:CD1	2.50	0.47
1:A:561:LEU:HD22	1:A:682:PHE:CD2	2.50	0.47
1:D:400:ILE:H	1:D:400:ILE:HD12	1.81	0.46
1:A:528:MET:CE	7:A:802:ATP:N7	2.78	0.46
3:J:43:MET:HE2	4:K:210:LEU:HD12	1.96	0.46
1:C:256:PHE:CE2	1:C:294:ILE:HD11	2.50	0.46
1:F:707:LEU:HD23	1:F:711:GLY:HA3	1.96	0.46
1:C:710:ALA:HB1	1:C:714:LYS:NZ	2.30	0.46
1:E:630:VAL:HG12	1:E:630:VAL:O	2.14	0.46
1:F:436:ARG:HB3	1:F:441:MET:HE2	1.96	0.46
1:B:110:LYS:HE3	1:B:110:LYS:HA	1.96	0.46
1:E:285:THR:CG2	1:E:416:ILE:HG22	2.45	0.46
4:K:185:GLU:O	4:K:190:LEU:HD13	2.16	0.46
1:B:248:PHE:HA	1:B:251:ILE:HG12	1.98	0.46
1:B:643:ILE:HD12	1:B:643:ILE:H	1.80	0.46
1:C:685:GLU:O	1:C:686:ILE:HD13	2.15	0.46
1:D:440:MET:O	1:D:441:MET:HE2	2.15	0.46
4:K:90:LEU:O	4:K:94:LEU:HD23	2.16	0.46
1:B:311:ILE:N	1:B:311:ILE:HD12	2.31	0.46
1:B:356:LYS:HA	1:B:356:LYS:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:ILE:N	1:B:686:ILE:HD12	2.31	0.46
1:C:495:LEU:C	1:C:495:LEU:HD12	2.41	0.46
1:C:745:ASP:OD1	1:C:746:PRO:HD3	2.15	0.46
1:D:60:ILE:HG23	1:D:98:GLN:O	2.16	0.46
1:E:573:LEU:HD21	7:E:802:ATP:C2	2.51	0.46
4:K:205:LYS:O	4:K:208:ALA:N	2.48	0.46
1:D:254:ARG:CZ	1:D:412:VAL:HG12	2.46	0.46
1:D:320:GLU:O	1:D:323:ILE:HG22	2.14	0.46
2:H:189:MET:HE1	2:H:198:LEU:HD21	1.97	0.46
1:A:626:LEU:HD21	1:A:665:THR:OG1	2.16	0.45
1:A:691:MET:HE3	1:A:728:VAL:O	2.15	0.45
1:E:390:VAL:HG23	1:E:410:PHE:HE1	1.81	0.45
3:J:43:MET:CE	4:K:210:LEU:HD12	2.46	0.45
4:K:71:GLU:HG2	4:K:72:GLN:N	2.31	0.45
4:K:183:ARG:CA	4:K:183:ARG:HE	2.27	0.45
1:E:351:LEU:HD12	1:E:352:ASP:N	2.31	0.45
1:B:688:VAL:HG13	1:B:688:VAL:O	2.16	0.45
2:H:192:ARG:HE	5:L:456:ARG:HD3	1.81	0.45
1:D:386:ASN:OD1	1:D:386:ASN:O	2.34	0.45
1:D:728:VAL:HG23	1:D:729:GLY:N	2.31	0.45
4:K:180:ALA:C	4:K:182:ARG:N	2.75	0.45
1:A:510:THR:HG23	1:A:510:THR:O	2.16	0.45
1:A:698:ASN:HA	1:A:701:MET:HE2	1.98	0.45
2:G:194:SER:O	2:G:197:SER:OG	2.20	0.45
1:A:265:VAL:O	1:A:269:LEU:HD23	2.16	0.45
1:A:732:LYS:HA	1:A:735:THR:HG22	1.99	0.45
1:B:343:LEU:HD12	1:B:389:LEU:HD23	1.99	0.45
1:D:228:ALA:HB1	1:D:260:ILE:HD12	1.99	0.45
2:H:222:LEU:HD21	2:H:242:LYS:HE2	1.97	0.45
4:K:145:LYS:C	4:K:149:MET:HE3	2.42	0.45
1:E:489:THR:HA	1:E:492:ILE:HD12	1.98	0.45
4:K:161:GLU:HB3	4:K:162:ALA:H	1.69	0.45
1:A:549:VAL:HG21	1:A:662:LEU:HD12	1.99	0.45
1:A:561:LEU:HD22	1:A:682:PHE:HD2	1.82	0.45
4:K:61:HIS:HB3	4:K:136:TYR:CD1	2.51	0.45
1:D:124:ARG:HD2	1:D:166:PHE:CB	2.48	0.44
1:E:728:VAL:HG13	1:E:729:GLY:N	2.31	0.44
1:B:144:VAL:HG22	1:B:198:LEU:HD21	1.98	0.44
1:D:124:ARG:HE	2:H:292:LEU:HB3	1.82	0.44
1:B:19:MET:HE1	1:B:102:PHE:O	2.17	0.44
1:B:561:LEU:HD21	1:B:667:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:713:VAL:HG12	1:F:717:ASN:OD1	2.17	0.44
1:C:585:PHE:CD2	1:C:619:ASN:ND2	2.85	0.44
1:D:252:PHE:HB3	1:E:480:ILE:HG21	1.99	0.44
1:F:324:ARG:NE	1:F:378:LYS:HG3	2.32	0.44
4:K:193:VAL:HG11	5:L:437:LYS:HG2	1.99	0.44
4:K:194:GLN:HA	5:L:436:THR:HG21	1.99	0.44
4:K:207:MET:HG2	4:K:210:LEU:HD23	1.98	0.44
1:C:261:PHE:HE2	1:D:492:ILE:HG22	1.81	0.44
1:E:459:GLY:HA2	1:E:462:ILE:HD12	1.99	0.44
1:F:355:PHE:CZ	1:F:371:VAL:HG22	2.53	0.44
1:D:147:TYR:CE2	1:D:158:LEU:HD21	2.53	0.44
1:F:673:LEU:HD13	1:F:678:ILE:HD11	2.00	0.44
1:A:670:TYR:O	1:A:674:GLN:OE1	2.35	0.44
1:B:350:GLU:O	1:B:350:GLU:HG2	2.18	0.44
1:F:557:LEU:HG	1:F:661:LEU:HD11	1.99	0.44
1:C:367:VAL:HG13	4:K:173:PHE:HZ	1.82	0.44
1:F:376:LEU:HD21	1:F:404:LEU:HD12	1.98	0.44
1:D:528:MET:HE2	1:D:528:MET:HA	2.00	0.43
1:F:715:VAL:HG12	1:F:747:VAL:HG13	2.00	0.43
1:D:229:VAL:CG2	1:D:230:ILE:HD12	2.48	0.43
1:D:435:MET:CB	1:D:441:MET:HE3	2.48	0.43
1:F:648:LYS:NZ	1:F:678:ILE:HG22	2.33	0.43
1:A:524:VAL:O	1:A:524:VAL:HG13	2.17	0.43
1:B:594:LEU:HD12	1:B:602:LYS:CD	2.48	0.43
1:D:678:ILE:HG22	1:D:678:ILE:O	2.18	0.43
1:E:441:MET:HE2	1:E:502:PHE:CE2	2.53	0.43
1:F:287:LYS:HB3	1:F:416:ILE:HD13	2.01	0.43
4:K:60:LEU:HD13	4:K:63:ARG:HH21	1.82	0.43
1:B:715:VAL:HB	1:B:747:VAL:HG13	2.01	0.43
1:D:435:MET:HA	1:D:440:MET:HE3	2.00	0.43
1:E:457:PHE:HE2	1:E:465:LEU:HD21	1.83	0.43
1:F:379:MET:HE3	1:F:409:ARG:HE	1.83	0.43
4:K:207:MET:HE1	5:L:450:MET:HG3	2.00	0.43
1:B:529:MET:SD	7:B:802:ATP:N7	2.92	0.43
1:D:432:THR:HG23	1:D:435:MET:HE3	1.99	0.43
1:A:315:TYR:HB3	1:B:314:LYS:HD2	2.01	0.43
1:B:156:GLN:HB3	1:B:171:ILE:HD12	2.01	0.43
1:C:715:VAL:HG12	1:C:747:VAL:HG22	2.01	0.43
5:L:437:LYS:HB3	5:L:590:MET:HE3	2.01	0.43
1:E:745:ASP:OD1	1:E:746:PRO:HD3	2.19	0.43
1:A:258:SER:O	1:A:266:ILE:HD13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:MET:SD	1:B:440:MET:HB2	2.58	0.43
2:G:161:PHE:HB2	2:G:184:LEU:HD21	2.01	0.43
1:C:373:ASN:HA	1:D:350:GLU:OE2	2.19	0.42
1:C:598:SER:O	1:C:601:ALA:HB3	2.19	0.42
1:D:732:LYS:HE2	1:D:732:LYS:HA	1.99	0.42
1:F:750:LEU:C	1:F:750:LEU:HD23	2.44	0.42
4:K:178:LEU:CD2	4:K:182:ARG:NH1	2.71	0.42
4:K:202:LYS:HE2	4:K:202:LYS:HB3	1.69	0.42
1:D:297:MET:C	1:D:298:LEU:HD22	2.44	0.42
1:D:330:ALA:CB	1:D:388:ILE:HD11	2.46	0.42
4:K:200:LEU:HD21	5:L:444:THR:N	2.34	0.42
1:C:427:ILE:HG21	1:C:462:ILE:HD12	2.01	0.42
1:B:748:ASN:O	1:B:752:GLU:OE1	2.37	0.42
1:A:305:ILE:HD12	1:A:347:ILE:HB	2.01	0.42
1:A:306:VAL:HG21	1:A:311:ILE:HD11	2.01	0.42
1:C:711:GLY:O	1:C:715:VAL:HG13	2.20	0.42
4:K:205:LYS:NZ	4:K:208:ALA:HB3	2.35	0.42
1:B:441:MET:HE3	1:B:442:SER:N	2.35	0.42
1:B:561:LEU:HD23	1:B:562:ILE:N	2.35	0.42
1:E:492:ILE:O	1:E:495:LEU:HD23	2.19	0.42
1:F:519:ASP:HA	1:F:522:THR:HG22	2.01	0.42
1:F:559:SER:C	1:F:560:LEU:HD22	2.43	0.42
2:H:84:TYR:CD1	2:H:100:LEU:HG	2.55	0.42
4:K:228:VAL:HA	4:K:231:ILE:HG22	2.02	0.42
1:A:379:MET:HE1	1:A:390:VAL:CG1	2.50	0.42
4:K:162:ALA:O	4:K:163:ALA:HB2	2.20	0.42
1:A:639:PHE:CE1	1:B:635:ILE:HD11	2.47	0.42
4:K:210:LEU:HD21	5:L:608:LEU:HD13	2.02	0.42
1:C:347:ILE:CG2	1:C:393:MET:HE1	2.50	0.42
1:D:254:ARG:NH1	1:D:412:VAL:HG12	2.35	0.42
1:D:561:LEU:HD22	1:D:685:GLU:OE1	2.20	0.42
1:F:688:VAL:HG23	1:F:688:VAL:O	2.20	0.42
1:C:440:MET:CE	1:C:495:LEU:HD11	2.43	0.42
1:D:691:MET:HE1	1:D:730:ILE:N	2.35	0.42
1:F:731:LYS:HE3	7:F:801:ATP:O3A	2.20	0.42
4:K:200:LEU:HD11	5:L:444:THR:HG22	1.87	0.42
1:A:527:GLY:O	7:A:802:ATP:C8	2.73	0.41
1:F:324:ARG:NH1	1:F:374:GLN:HG3	2.35	0.41
2:G:269:LEU:HD11	2:G:273:LYS:CB	2.50	0.41
4:K:183:ARG:HG3	4:K:184:GLY:H	1.85	0.41
1:B:363:ASP:OD1	1:C:361:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:701:MET:SD	1:C:712:ARG:HG2	2.60	0.41
1:D:547:ARG:C	1:D:547:ARG:HD2	2.45	0.41
1:D:749:GLU:O	1:D:753:LEU:HD23	2.20	0.41
1:F:280:TYR:O	1:F:416:ILE:HG13	2.20	0.41
1:A:285:THR:O	1:A:285:THR:HG22	2.20	0.41
1:B:316:VAL:HG13	1:B:316:VAL:O	2.21	0.41
1:A:354:VAL:HG11	1:A:371:VAL:HG11	2.02	0.41
1:B:328:LYS:O	1:B:331:GLU:HG3	2.20	0.41
1:C:647:LEU:O	1:C:651:LEU:HD13	2.19	0.41
1:E:319:SER:O	1:E:323:ILE:HD12	2.20	0.41
1:A:246:LYS:HE2	1:A:246:LYS:HA	2.03	0.41
1:B:230:ILE:CD1	1:B:260:ILE:HD11	2.50	0.41
1:B:269:LEU:HB3	1:B:271:ILE:HG12	2.02	0.41
1:B:375:LEU:O	1:B:375:LEU:HD23	2.20	0.41
2:H:31:TYR:O	2:H:35:GLU:OE1	2.39	0.41
5:L:455:GLU:HA	5:L:611:MET:HE1	2.02	0.41
1:A:253:ARG:NH1	1:A:254:ARG:HE	2.19	0.41
1:D:124:ARG:HH21	2:H:292:LEU:HB3	1.86	0.41
1:E:277:LEU:HD12	1:E:412:VAL:HG23	2.02	0.41
1:A:646:MET:HE2	1:A:646:MET:HA	2.03	0.41
1:D:261:PHE:CE1	1:E:474:ILE:HD11	2.56	0.41
1:B:350:GLU:OE1	1:B:353:SER:HB2	2.21	0.41
1:B:441:MET:HE2	1:B:445:VAL:HB	2.03	0.41
1:C:673:LEU:HA	1:C:676:MET:HE2	2.02	0.41
1:D:626:LEU:HD23	1:D:626:LEU:C	2.46	0.41
1:E:433:LYS:O	1:E:437:GLU:OE1	2.39	0.41
4:K:94:LEU:O	4:K:98:ILE:HG22	2.21	0.41
1:A:599:GLU:HA	1:A:602:LYS:HD2	2.03	0.41
1:B:635:ILE:O	1:B:635:ILE:HG13	2.21	0.41
1:C:285:THR:CG2	1:C:416:ILE:HG22	2.51	0.41
1:E:304:LYS:HB2	1:E:346:ILE:HD12	2.02	0.41
1:F:287:LYS:O	1:F:290:ILE:HG22	2.20	0.41
2:H:236:ARG:HH11	2:H:267:MET:HE2	1.83	0.41
4:K:242:VAL:CG2	5:L:482:MET:HE3	2.51	0.41
1:A:318:SER:HB2	1:B:314:LYS:HE2	2.01	0.41
1:B:686:ILE:HD12	1:B:686:ILE:H	1.86	0.41
1:C:268:LYS:O	1:D:440:MET:HE1	2.20	0.41
1:C:616:SER:O	1:C:619:ASN:ND2	2.53	0.41
1:D:296:THR:HG22	1:D:297:MET:HE2	2.03	0.41
1:E:289:LEU:HD23	1:E:289:LEU:C	2.46	0.41
2:H:284:ILE:O	2:H:288:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:HD21	1:A:293:LYS:HB3	2.03	0.40
1:D:234:PHE:CZ	1:D:239:LEU:HD21	2.56	0.40
1:E:752:GLU:O	1:E:756:GLN:HG3	2.20	0.40
1:F:630:VAL:HG12	1:F:630:VAL:O	2.22	0.40
1:A:730:ILE:HD13	7:A:802:ATP:H2	1.86	0.40
1:B:268:LYS:O	1:B:268:LYS:HG2	2.21	0.40
4:K:200:LEU:CD2	5:L:443:SER:OG	2.69	0.40
1:A:597:MET:CE	1:A:601:ALA:HB1	2.52	0.40
1:C:261:PHE:CE2	1:D:474:ILE:HD11	2.57	0.40
1:D:431:GLN:NE2	1:D:463:GLU:CG	2.85	0.40
1:F:438:ASN:HB3	1:F:440:MET:HE2	2.04	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	499/761 (66%)	472 (95%)	27 (5%)	0	100 100
1	B	722/761 (95%)	680 (94%)	42 (6%)	0	100 100
1	C	739/761 (97%)	694 (94%)	45 (6%)	0	100 100
1	D	739/761 (97%)	699 (95%)	39 (5%)	1 (0%)	48 80
1	E	525/761 (69%)	498 (95%)	26 (5%)	1 (0%)	44 75
1	F	490/761 (64%)	471 (96%)	19 (4%)	0	100 100
2	G	290/293 (99%)	289 (100%)	1 (0%)	0	100 100
2	H	290/293 (99%)	289 (100%)	1 (0%)	0	100 100
3	J	58/97 (60%)	58 (100%)	0	0	100 100
4	K	222/269 (82%)	197 (89%)	14 (6%)	11 (5%)	1 19
5	L	125/222 (56%)	125 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4699/5740 (82%)	4472 (95%)	214 (5%)	13 (0%)	38 70

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	299	ASN
4	K	163	ALA
4	K	166	ASP
4	K	167	VAL
4	K	158	ASP
4	K	159	GLU
4	K	161	GLU
4	K	157	GLU
4	K	164	ILE
4	K	181	ASN
4	K	188	THR
1	D	231	ARG
4	K	168	GLY

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	439/656 (67%)	439 (100%)	0	100 100
1	B	634/656 (97%)	634 (100%)	0	100 100
1	C	643/656 (98%)	643 (100%)	0	100 100
1	D	643/656 (98%)	643 (100%)	0	100 100
1	E	456/656 (70%)	456 (100%)	0	100 100
1	F	434/656 (66%)	432 (100%)	2 (0%)	86 90
2	G	245/245 (100%)	245 (100%)	0	100 100
2	H	245/245 (100%)	245 (100%)	0	100 100
3	J	48/82 (58%)	48 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	K	197/234 (84%)	178 (90%)	19 (10%)	7 25
5	L	115/201 (57%)	115 (100%)	0	100 100
All	All	4099/4943 (83%)	4078 (100%)	21 (0%)	85 90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	417	HIS
1	F	645	GLN
4	K	130	ARG
4	K	137	LYS
4	K	139	GLU
4	K	158	ASP
4	K	160	VAL
4	K	161	GLU
4	K	165	SER
4	K	166	ASP
4	K	170	GLN
4	K	175	GLN
4	K	177	LEU
4	K	178	LEU
4	K	179	ASN
4	K	183	ARG
4	K	185	GLU
4	K	187	LYS
4	K	190	LEU
4	K	202	LYS
4	K	205	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	ASN
1	A	608	ASN
1	A	684	ASN
1	A	699	ASN
1	A	727	ASN
1	B	28	HIS
1	B	563	HIS
1	B	742	HIS

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Mol	Chain	Res	Type
1	C	62	ASN
1	C	413	GLN
1	C	475	ASN
1	C	479	ASN
1	C	705	ASN
1	D	165	HIS
1	D	373	ASN
1	D	386	ASN
1	D	417	HIS
1	F	344	HIS
2	G	259	HIS
2	H	109	HIS
2	H	132	HIS
2	H	285	GLN
4	K	55	ASN
4	K	170	GLN
4	K	171	GLN
4	K	175	GLN
5	L	446	ASN
5	L	467	HIS
5	L	600	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	ADP	A	801	-	24,29,29	0.84	0	29,45,45	1.36	3 (10%)
7	ATP	D	802	-	28,33,33	0.79	0	34,52,52	1.32	4 (11%)
7	ATP	D	801	-	28,33,33	0.76	0	34,52,52	1.25	3 (8%)
7	ATP	A	802	-	28,33,33	0.96	1 (3%)	34,52,52	1.09	4 (11%)
6	ADP	E	801	-	24,29,29	0.84	0	29,45,45	1.39	3 (10%)
7	ATP	E	802	-	28,33,33	0.80	0	34,52,52	0.83	1 (2%)
7	ATP	C	801	-	28,33,33	0.84	0	34,52,52	1.23	1 (2%)
7	ATP	B	801	-	28,33,33	0.82	0	34,52,52	1.40	5 (14%)
7	ATP	F	801	-	28,33,33	0.84	1 (3%)	34,52,52	1.41	2 (5%)
7	ATP	B	802	-	28,33,33	0.84	1 (3%)	34,52,52	0.78	1 (2%)
7	ATP	C	802	-	28,33,33	0.81	1 (3%)	34,52,52	0.96	2 (5%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	802	ATP	C1'-N9	-2.94	1.42	1.49
7	F	801	ATP	C1'-N9	-2.35	1.44	1.49
7	B	802	ATP	C1'-N9	-2.32	1.44	1.49
7	C	802	ATP	C1'-N9	-2.18	1.44	1.49

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	801	ATP	C4'-O4'-C1'	-6.61	103.88	109.92
6	A	801	ADP	N3-C2-N1	-4.41	122.68	128.67
7	C	801	ATP	N3-C2-N1	-4.19	122.99	128.67
7	B	801	ATP	N3-C2-N1	-4.18	123.00	128.67
7	D	801	ATP	N3-C2-N1	-4.11	123.10	128.67
6	E	801	ADP	N3-C2-N1	-4.09	123.12	128.67
7	D	802	ATP	N3-C2-N1	-3.51	123.91	128.67
7	B	801	ATP	C1'-N9-C4	-3.11	121.18	126.64
7	C	802	ATP	C4'-O4'-C1'	-2.84	107.32	109.92
7	A	802	ATP	C5-C6-N6	2.80	124.57	120.31
7	D	802	ATP	C1'-N9-C4	-2.59	122.10	126.64
7	D	802	ATP	C4-C5-N7	-2.56	106.63	109.34
6	E	801	ADP	O4'-C1'-N9	2.54	112.12	108.75
7	B	801	ATP	O4'-C1'-N9	2.47	112.02	108.75
7	B	801	ATP	C4-C5-N7	-2.38	106.82	109.34
7	E	802	ATP	C5-C6-N6	2.35	123.89	120.31
6	E	801	ADP	C4-C5-N7	-2.32	106.89	109.34
7	B	802	ATP	C5-C6-N6	2.29	123.81	120.31
7	C	802	ATP	C5-C6-N6	2.26	123.75	120.31
7	D	801	ATP	O3G-PG-O2G	2.16	115.91	107.80
6	A	801	ADP	C1'-N9-C4	-2.16	122.85	126.64
7	D	801	ATP	C4-C5-N7	-2.16	107.06	109.34
7	D	802	ATP	O2B-PB-O1B	2.14	122.39	112.44
7	F	801	ATP	C5-C6-N6	2.10	123.51	120.31
6	A	801	ADP	O2A-PA-O1A	2.10	122.21	112.44
7	A	802	ATP	O2'-C2'-C3'	2.09	118.52	111.82
7	A	802	ATP	O4'-C1'-N9	2.07	111.49	108.75
7	A	802	ATP	C4'-O4'-C1'	-2.03	108.07	109.92
7	B	801	ATP	O3G-PG-O2G	2.00	115.30	107.80

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	ADP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

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

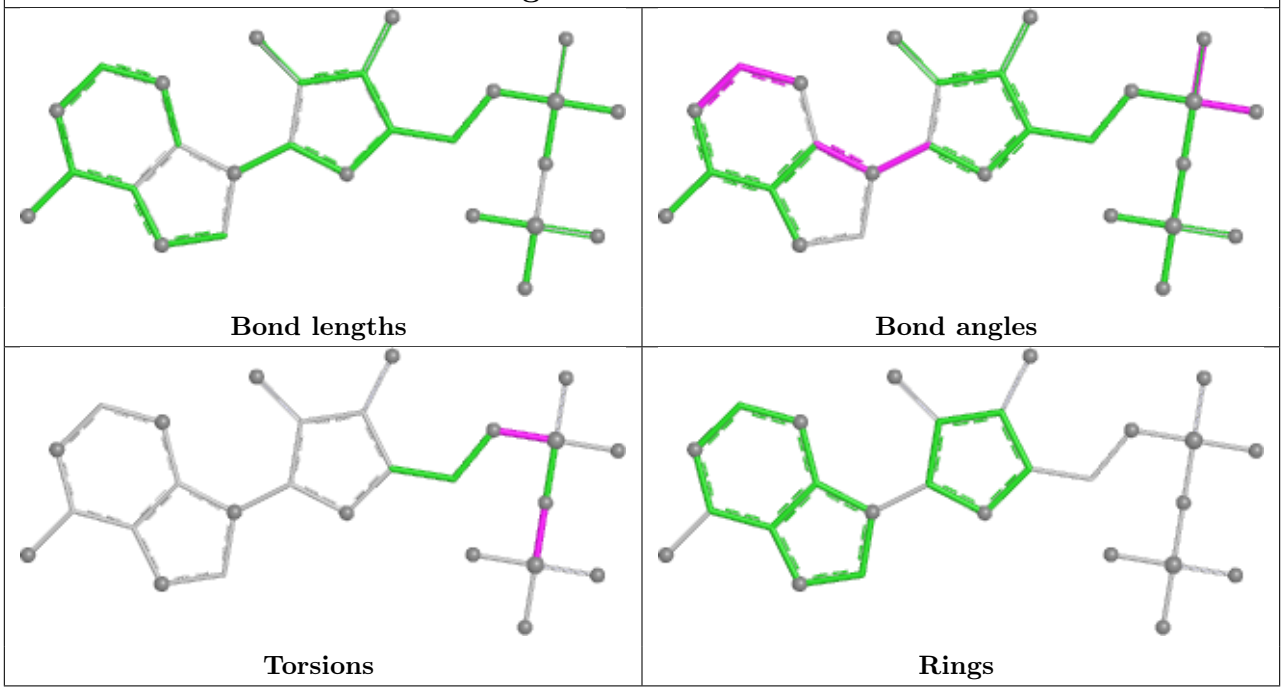
There are no ring outliers.

6 monomers are involved in 16 short contacts:

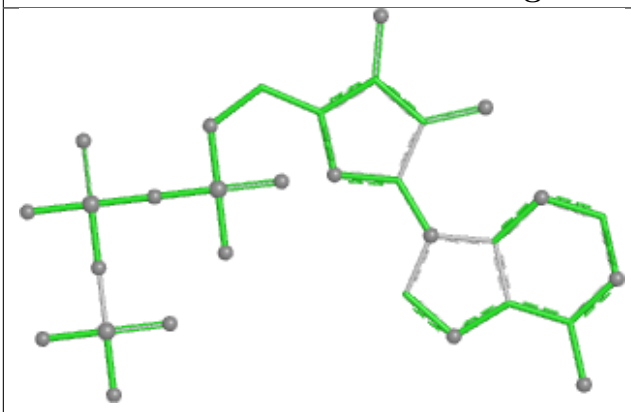
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	802	ATP	1	0
7	A	802	ATP	9	0
7	E	802	ATP	2	0
7	F	801	ATP	1	0
7	B	802	ATP	2	0
7	C	802	ATP	1	0

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.

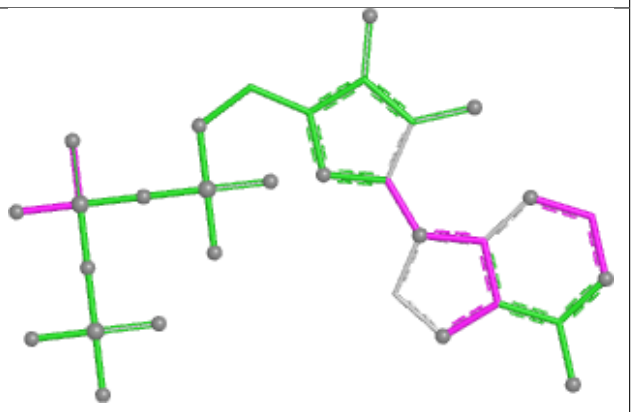
Ligand ADP A 801



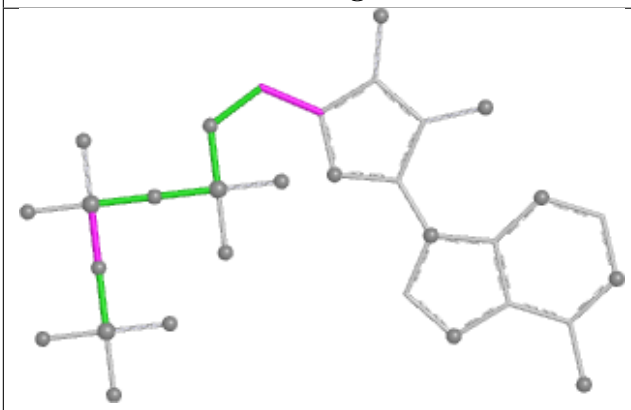
Ligand ATP D 802



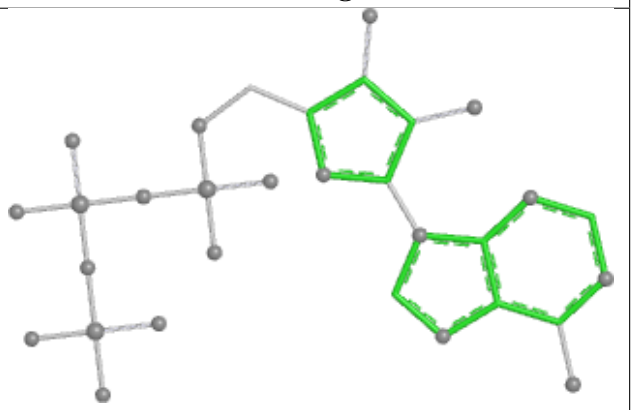
Bond lengths



Bond angles

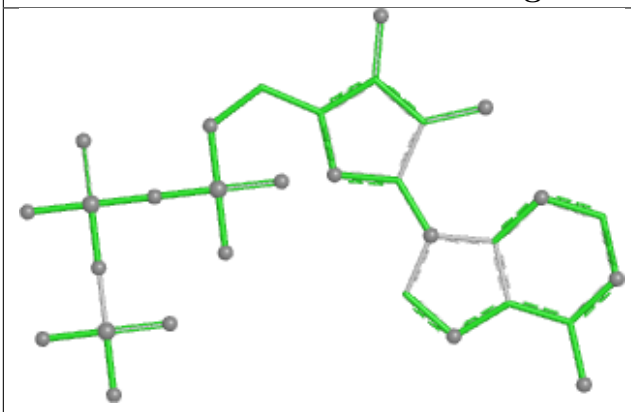


Torsions

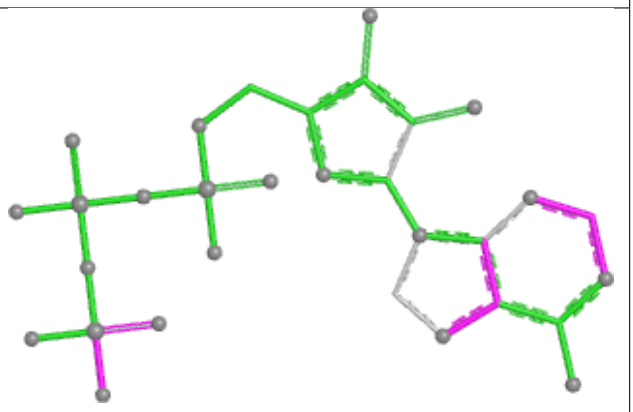


Rings

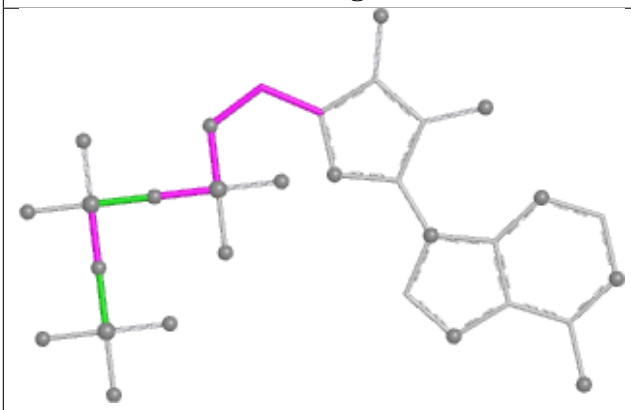
Ligand ATP D 801



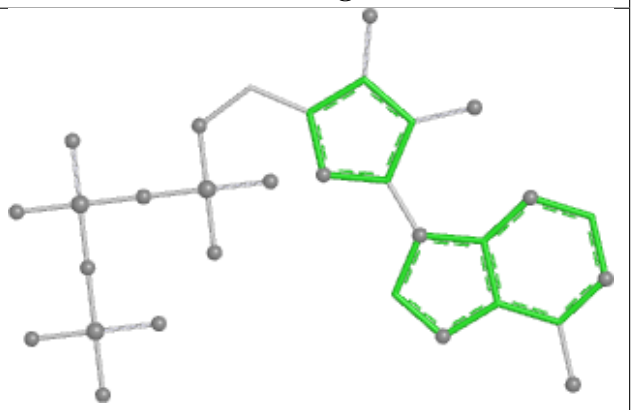
Bond lengths



Bond angles

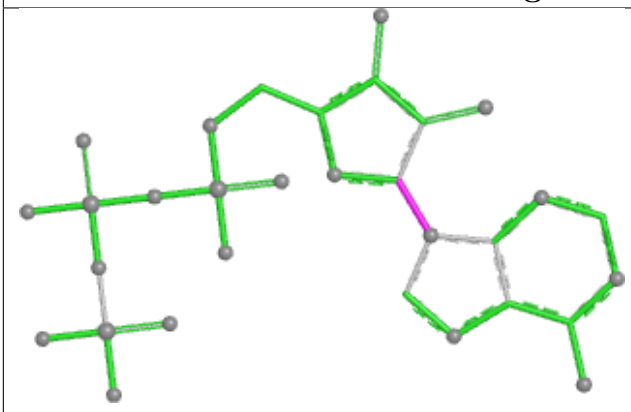


Torsions



Rings

Ligand ATP A 802



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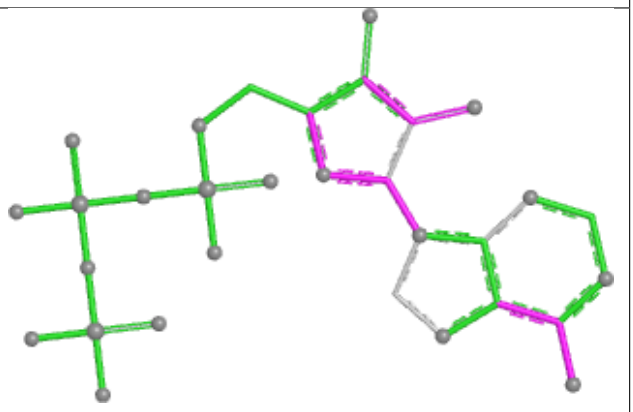
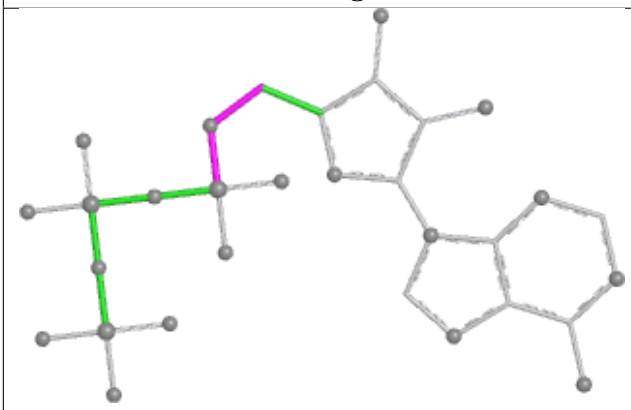


Bond angles



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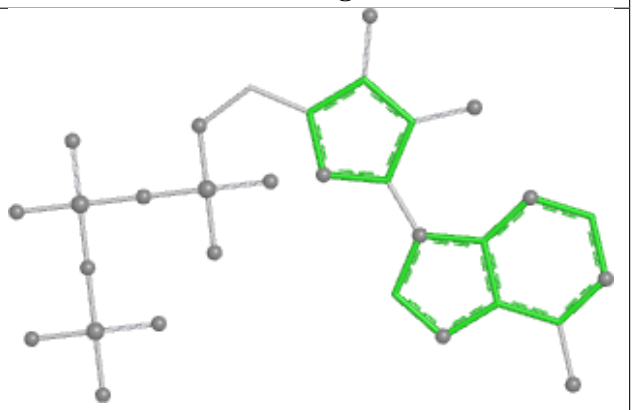
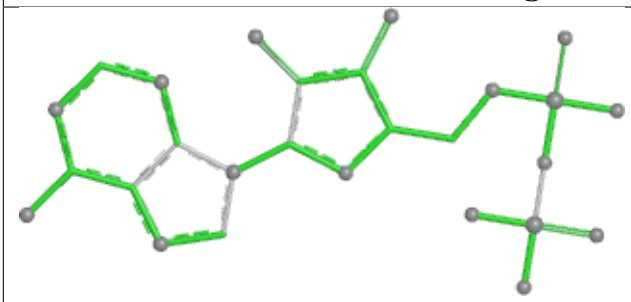


Rings

Ligand ADP E 801



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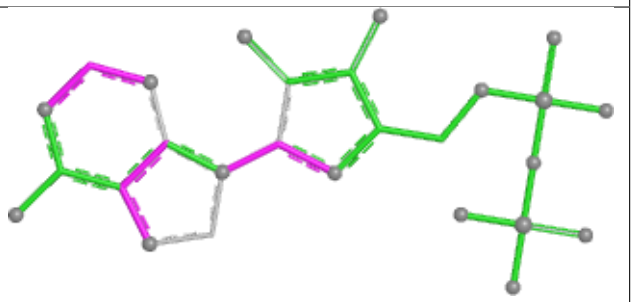
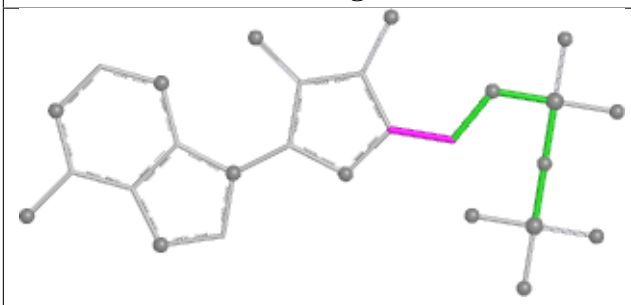


Bond angles



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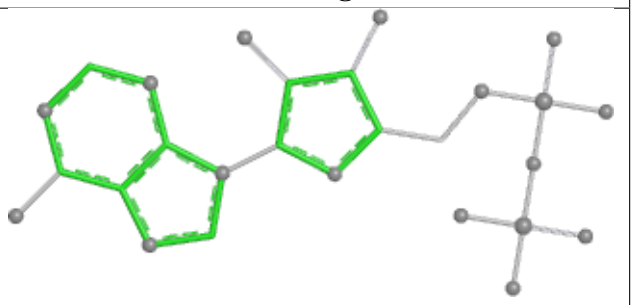
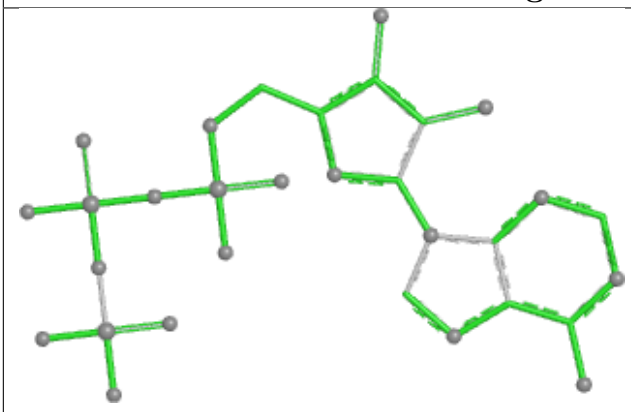


Rings

Ligand ATP E 802



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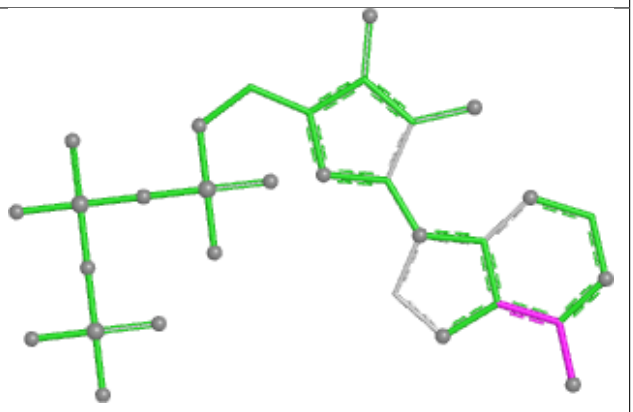

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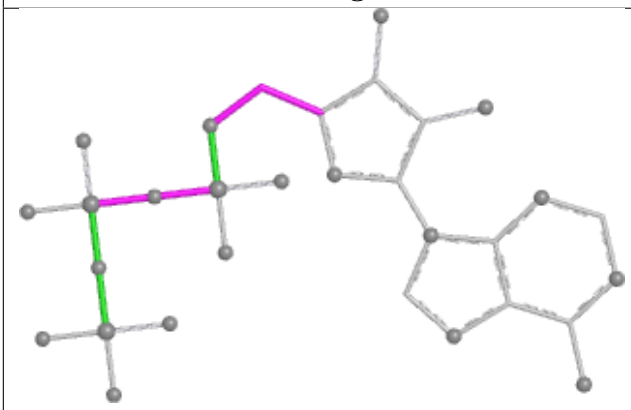

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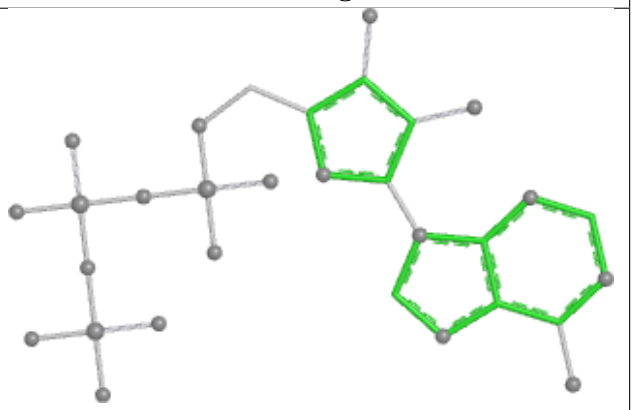
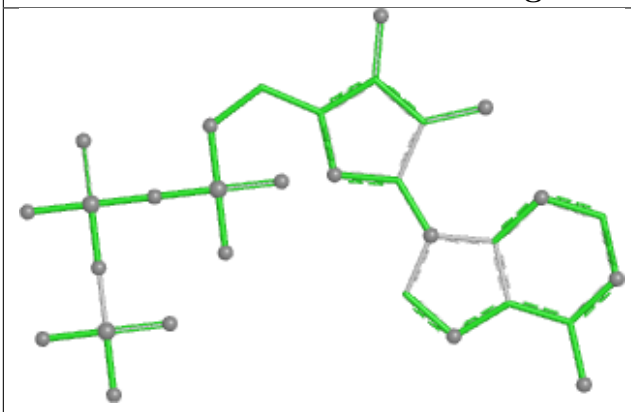


Rings

Ligand ATP C 801



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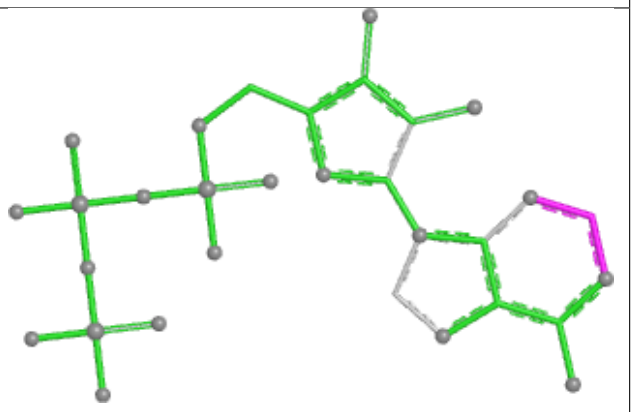

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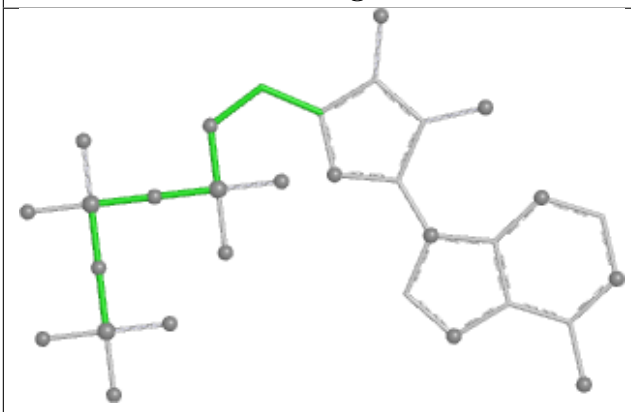

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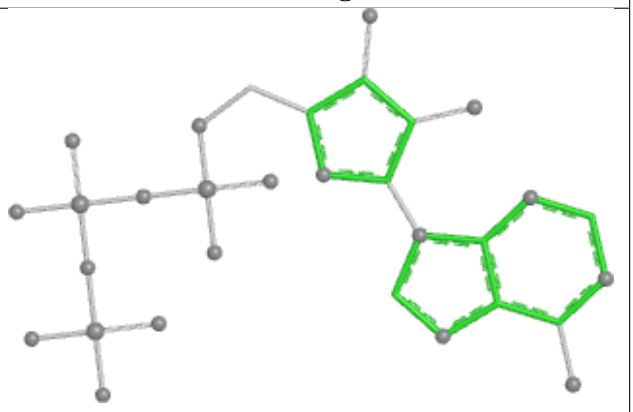
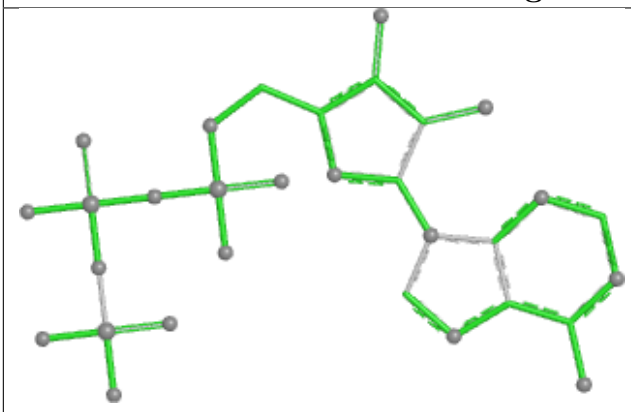


Rings

Ligand ATP B 801



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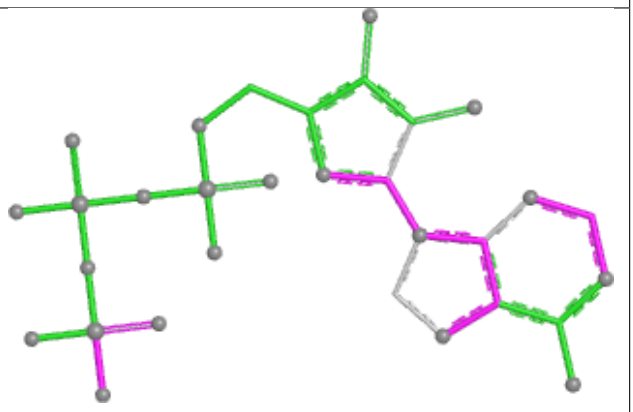

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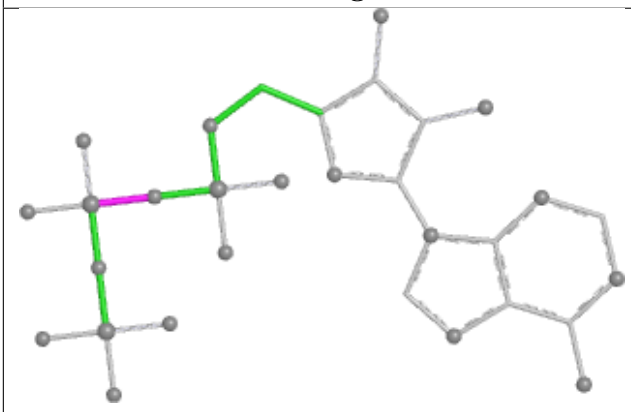

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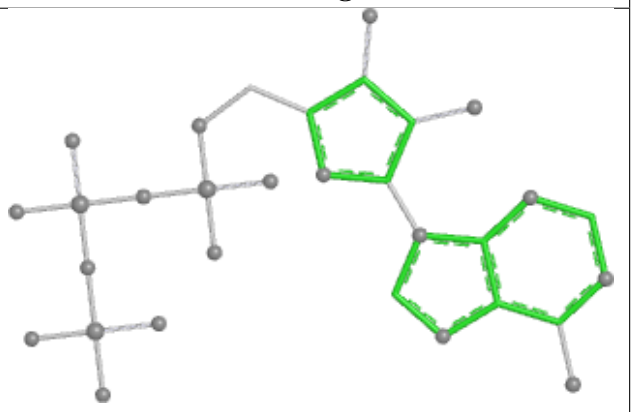
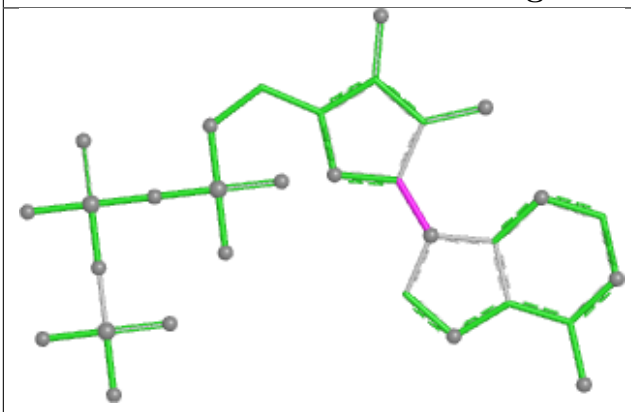


Rings

Ligand ATP F 801



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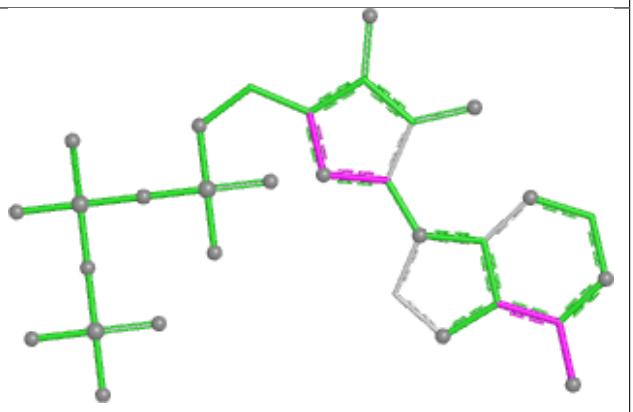
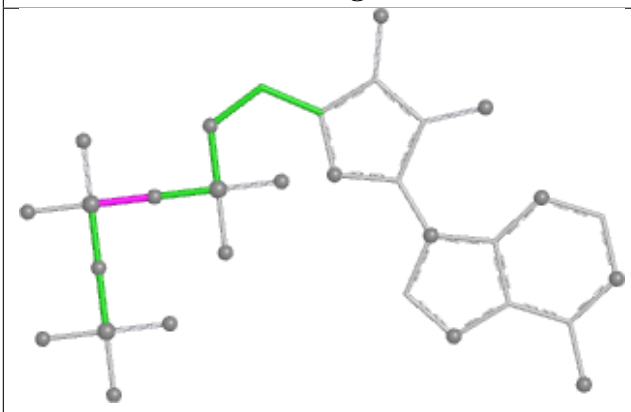
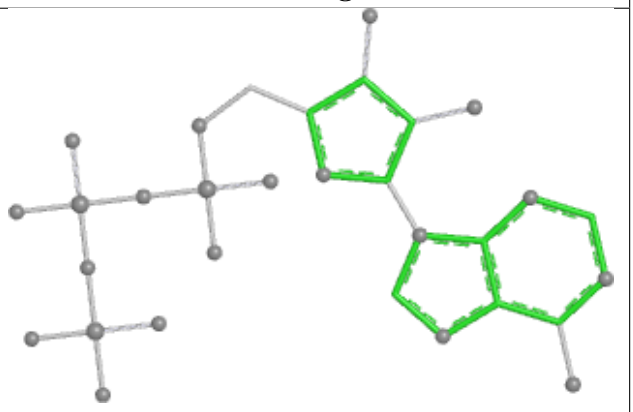


Bond angles

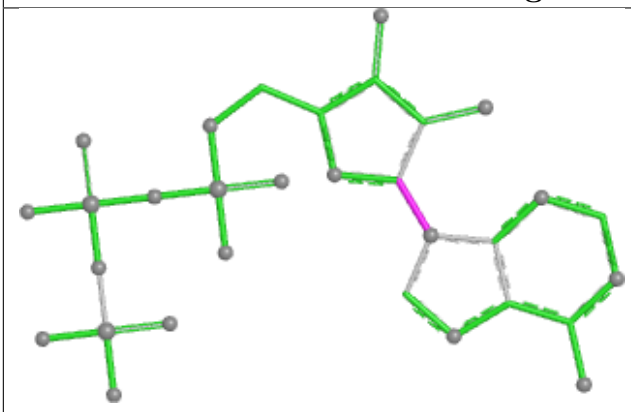


Torsions



Rings

Ligand ATP B 802



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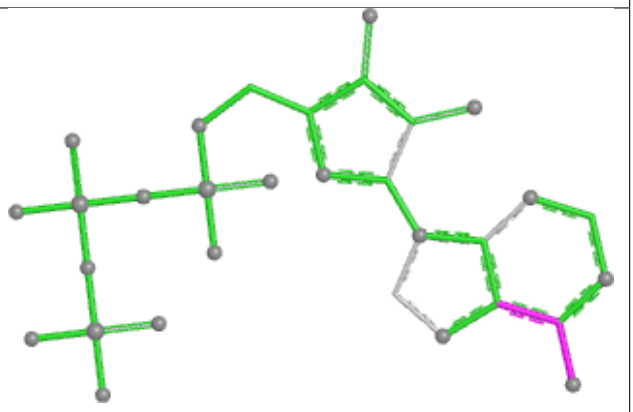
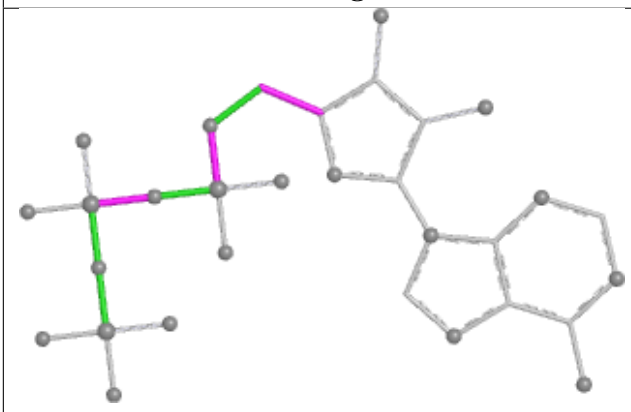


Bond angles



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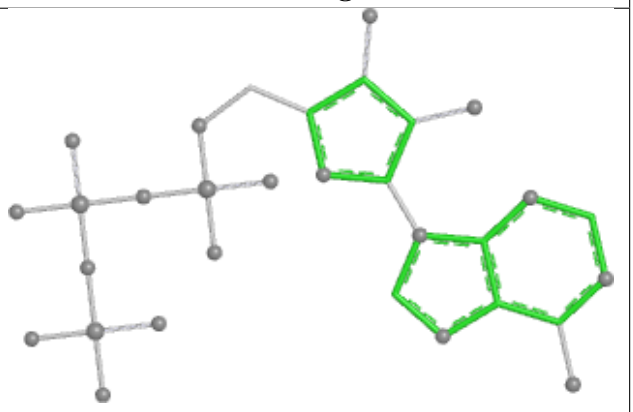
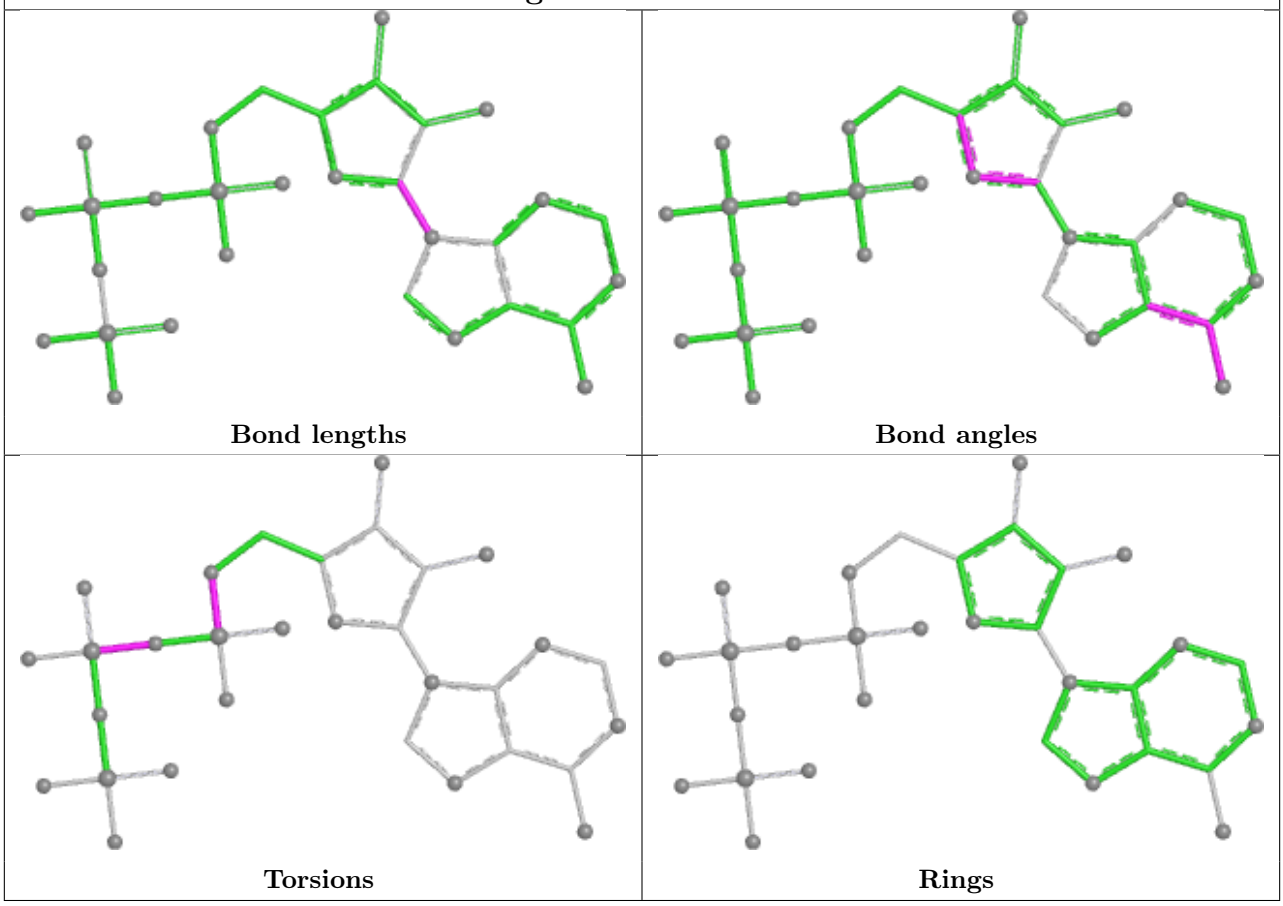


Rings

Ligand ATP C 802



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.

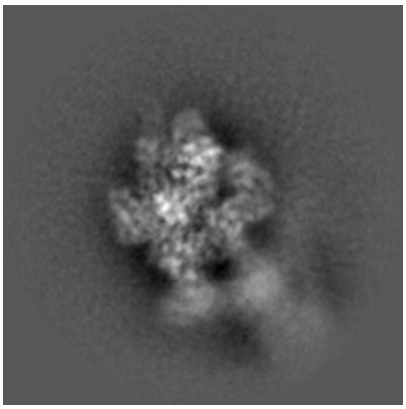
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45883. These allow visual inspection of the internal detail of the map and identification of artifacts.

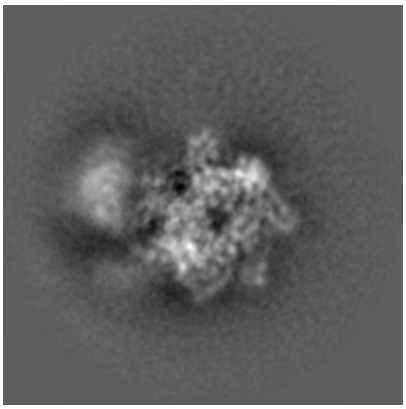
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

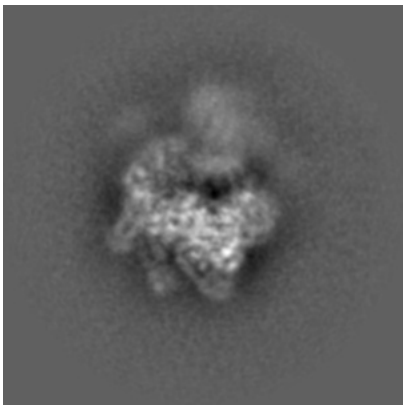
6.1.1 Primary map



X

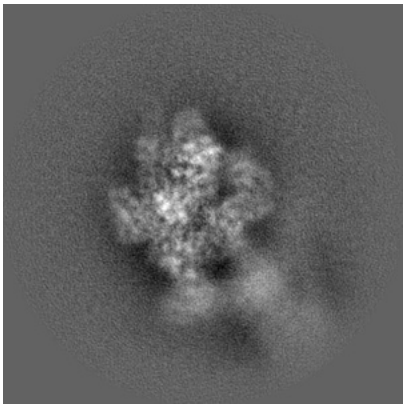


Y

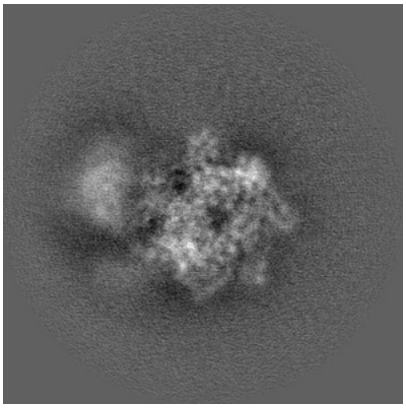


Z

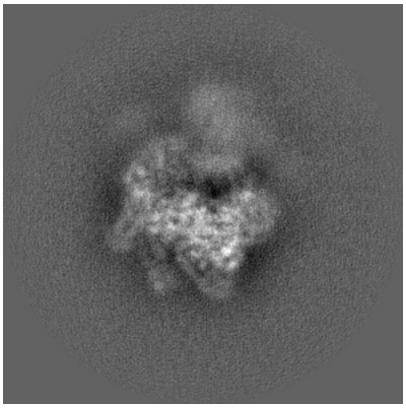
6.1.2 Raw map



X



Y

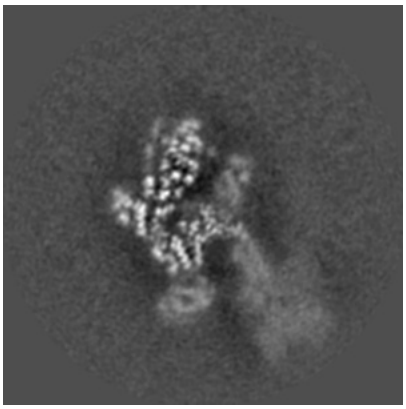


Z

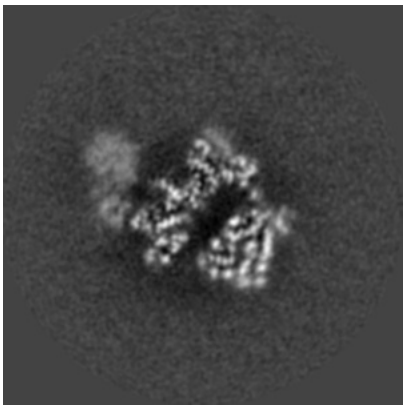
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

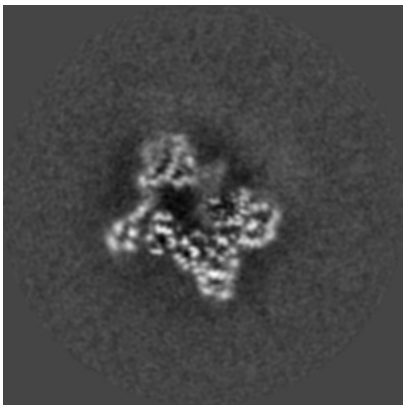
6.2.1 Primary map



X Index: 147

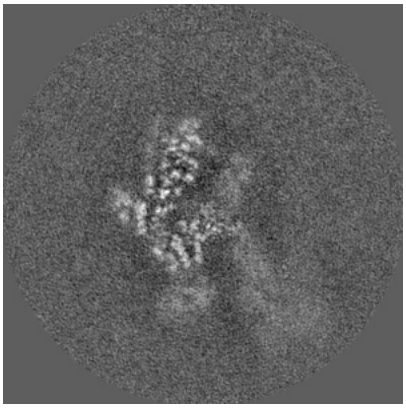


Y Index: 147

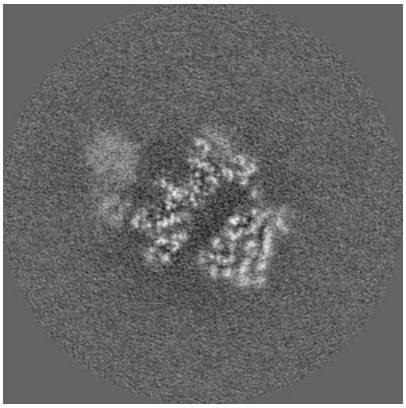


Z Index: 147

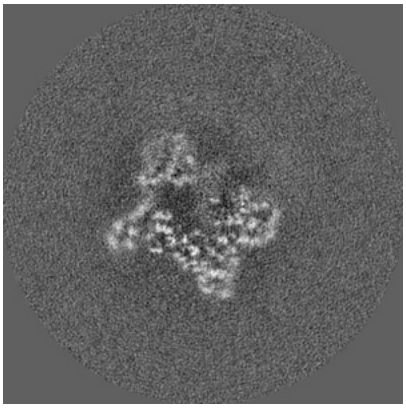
6.2.2 Raw map



X Index: 147



Y Index: 147

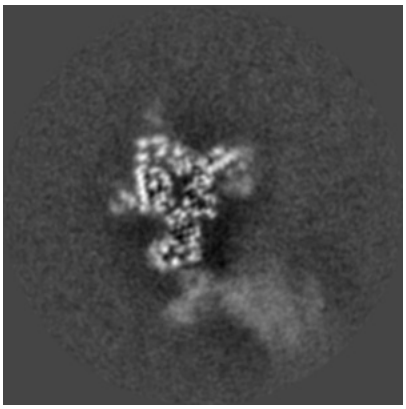


Z Index: 147

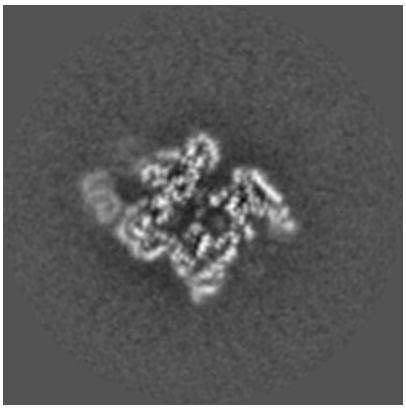
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

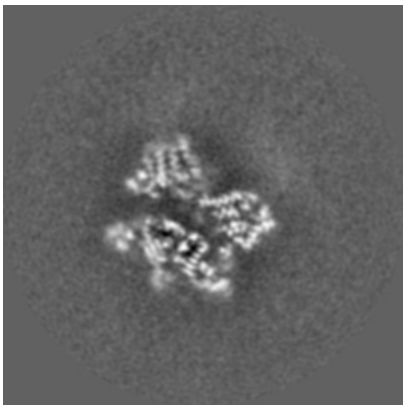
6.3.1 Primary map



X Index: 168

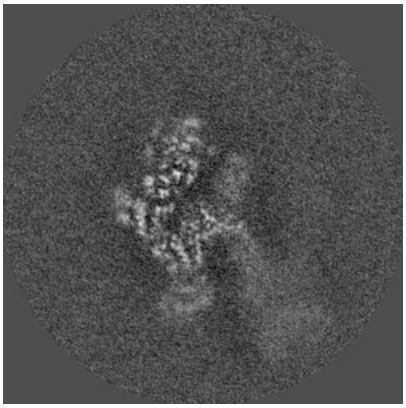


Y Index: 128

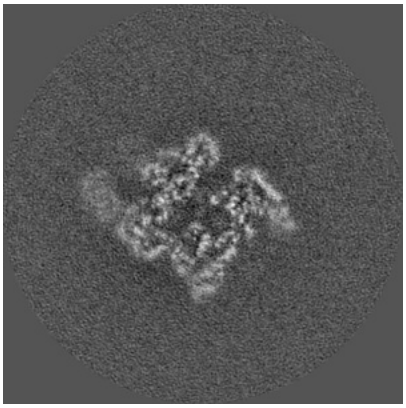


Z Index: 140

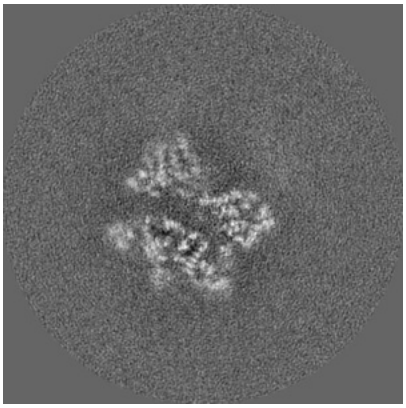
6.3.2 Raw map



X Index: 146



Y Index: 128

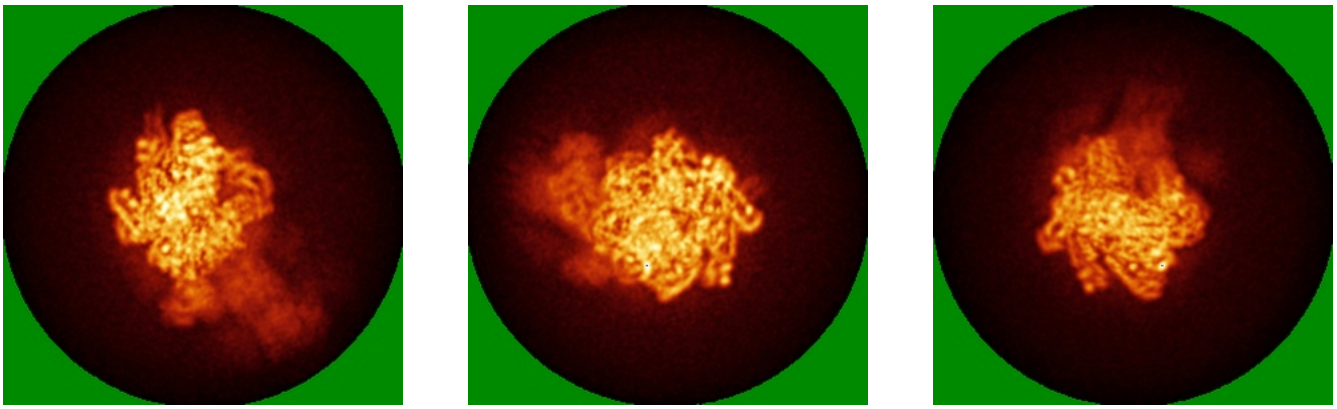


Z Index: 140

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

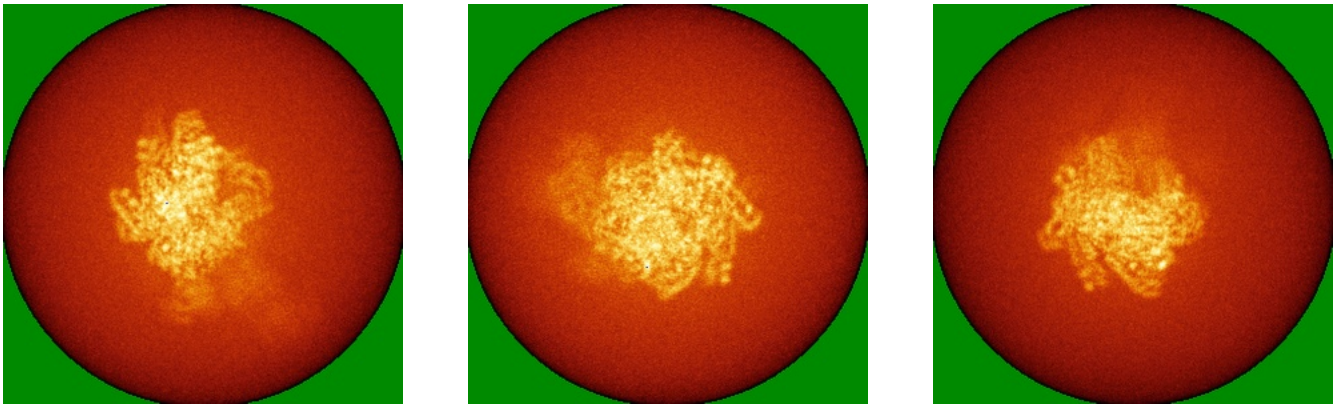
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

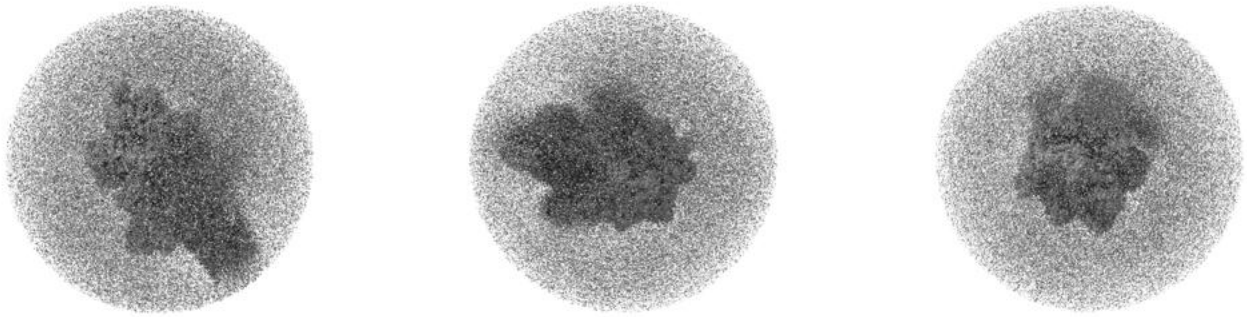
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.002. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

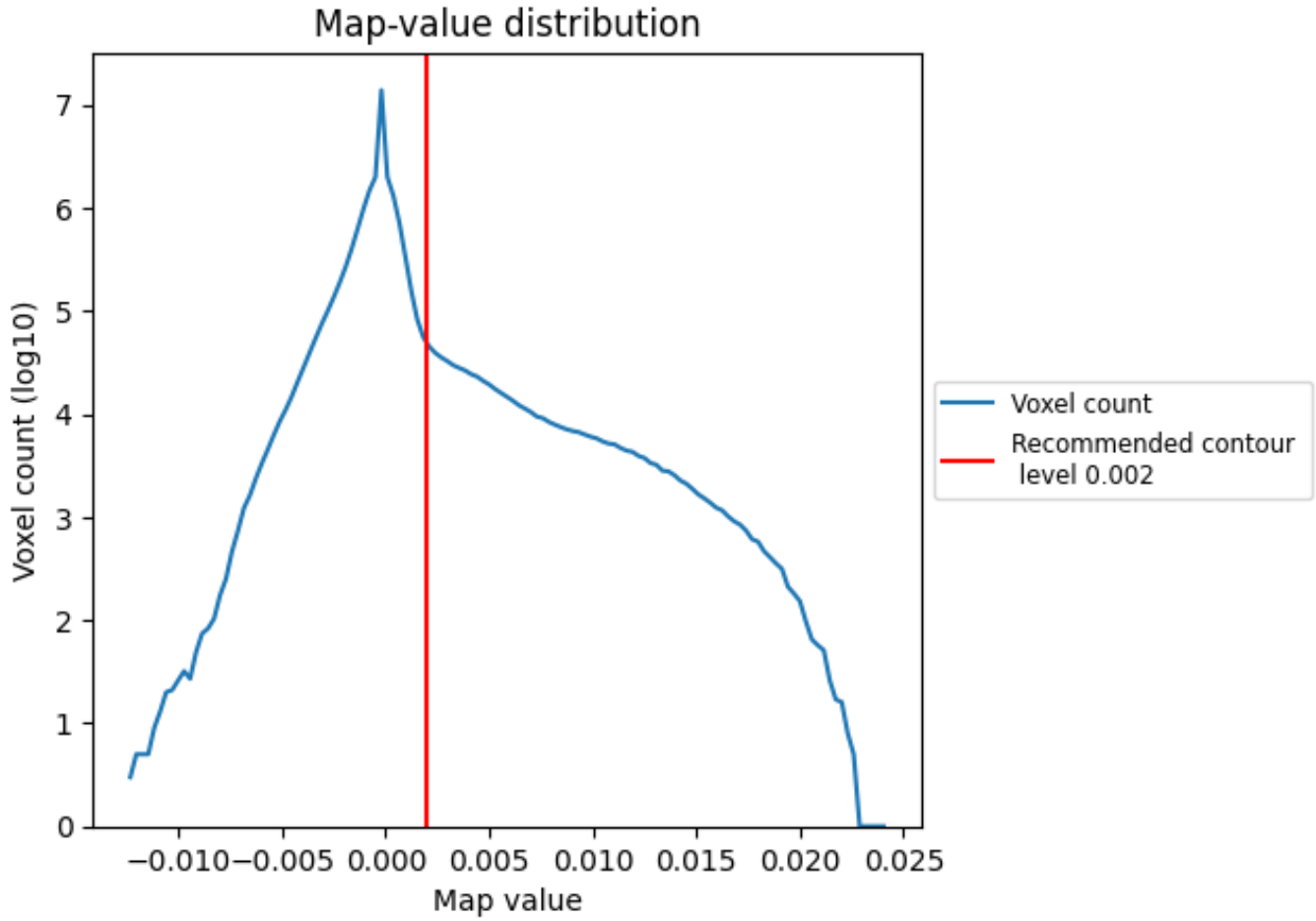
6.6 Mask visualisation (i)

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

7 Map analysis

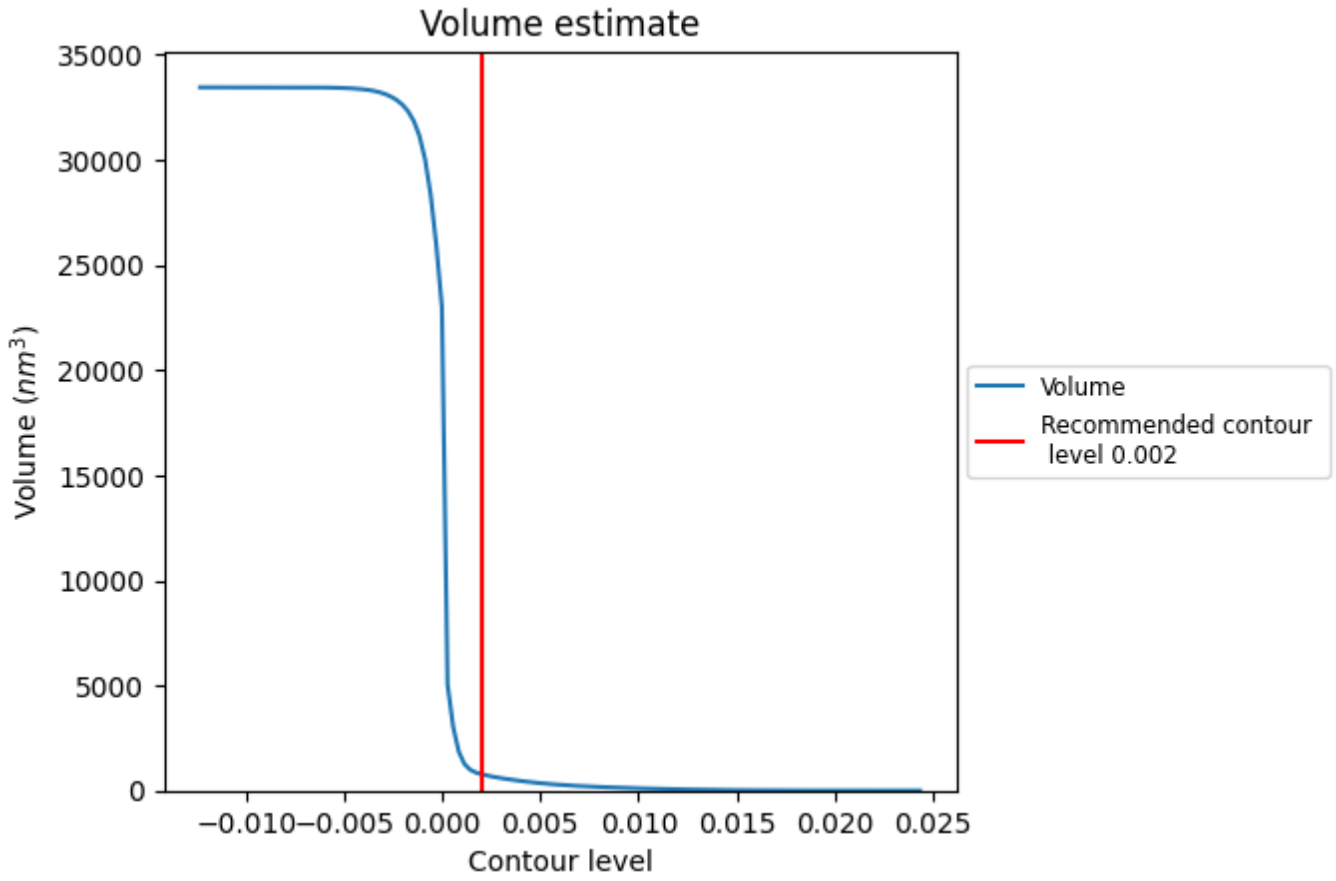
This section contains the results of statistical analysis of the map.

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.

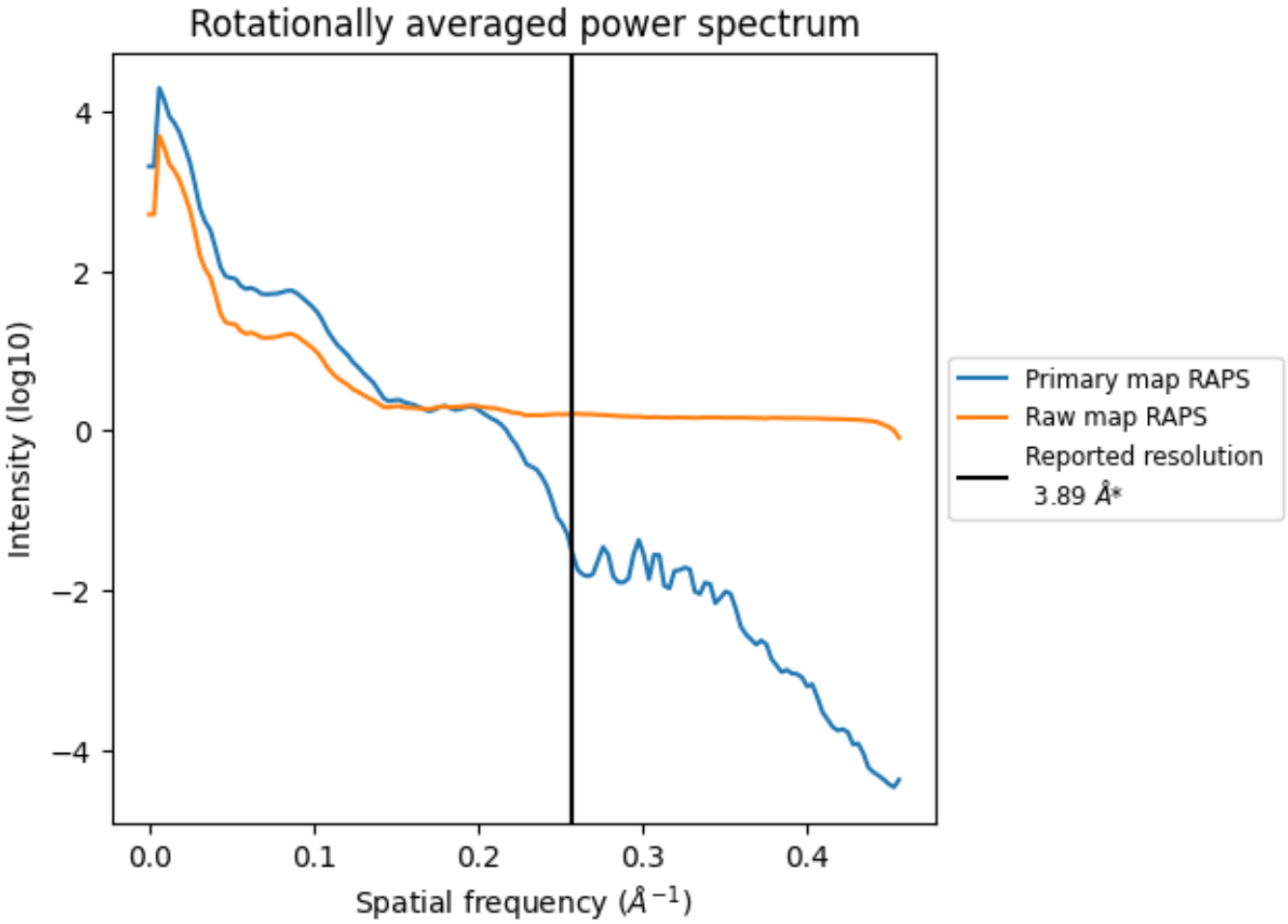
7.2 Volume estimate (i)



The volume at the recommended contour level is 779 nm^3; this corresponds to an approximate mass of 704 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)

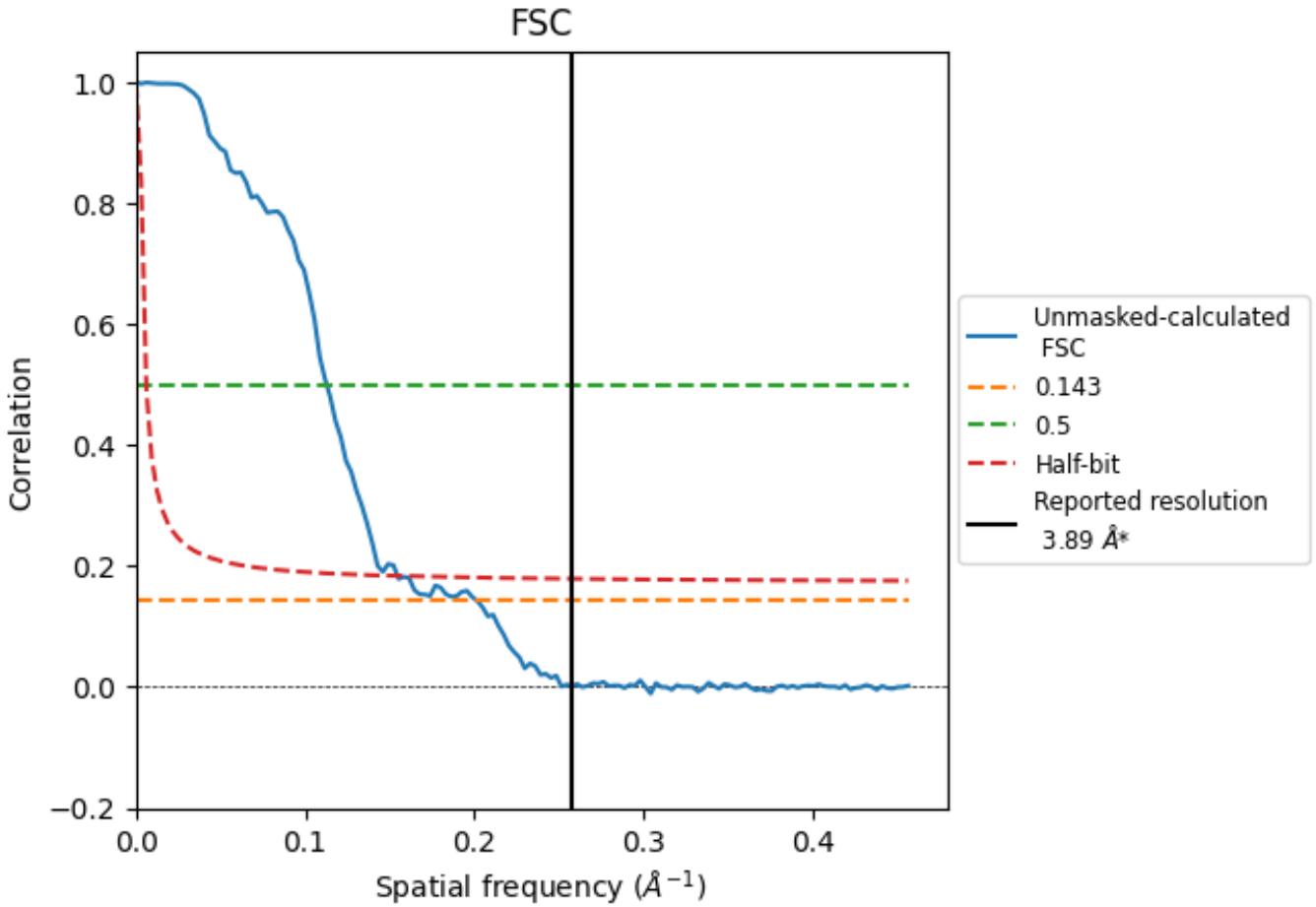


*Reported resolution corresponds to spatial frequency of 0.257 Å^{-1}

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 0.257 Å^{-1}

8.2 Resolution estimates (i)

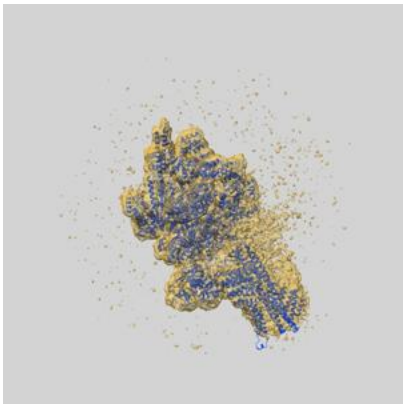
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.97	8.87	6.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.97 differs from the reported value 3.89 by more than 10 %

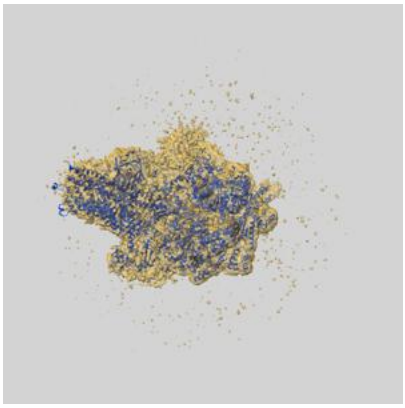
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45883 and PDB model 9CRU. Per-residue inclusion information can be found in section 3 on page 8.

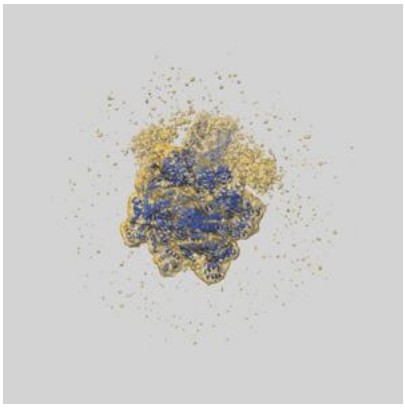
9.1 Map-model overlay



X



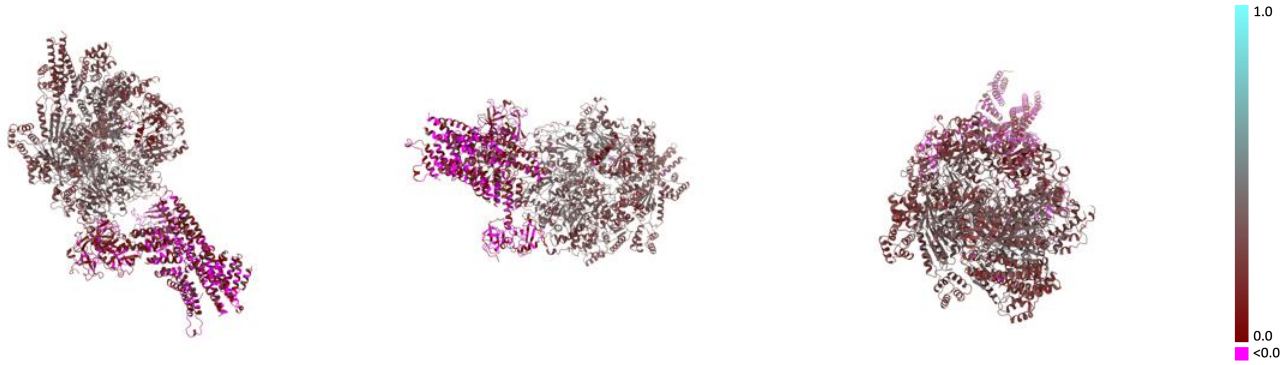
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.002 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.

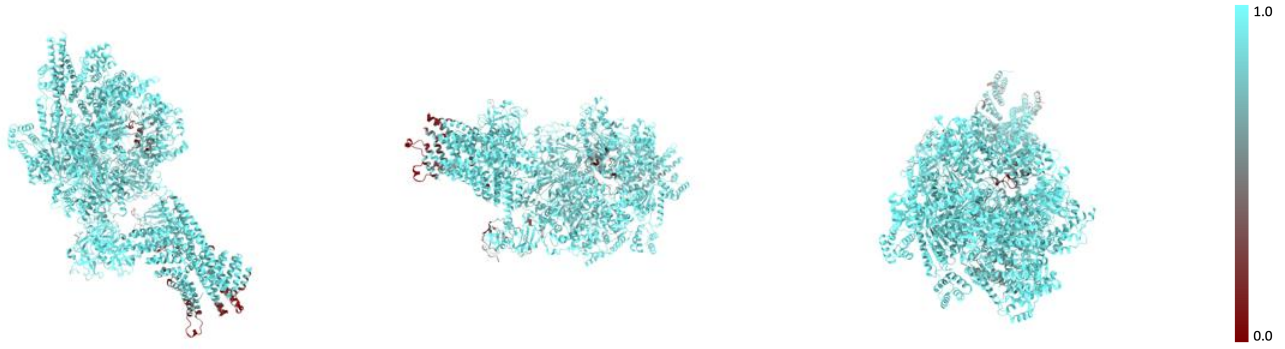
9.2 Q-score mapped to coordinate model (i)



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.

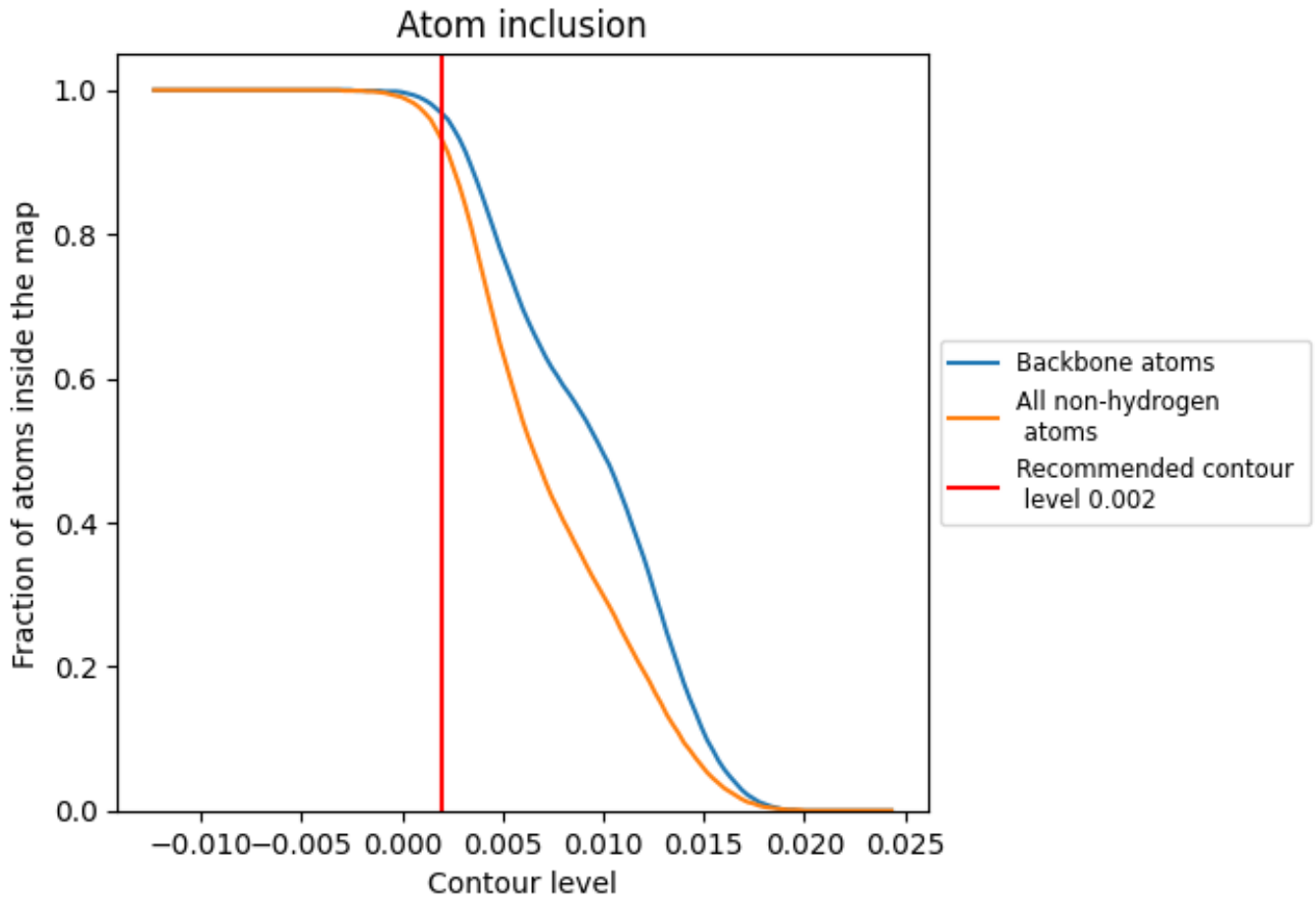
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.002).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9300	0.2480
A	0.9690	0.3380
B	0.9660	0.2840
C	0.9570	0.2900
D	0.9200	0.2540
E	0.9730	0.3060
F	0.9140	0.2630
G	0.8290	0.0870
H	0.8840	0.0670
J	0.9320	0.1110
K	0.8220	0.1800
L	0.8990	0.0770