Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 11:29 am GMT

PDB ID	:	6Z5U
EMDB ID	:	EMD-11082
Title	:	Cryo-EM structure of the A. baumannii MlaBDEF complex bound to APPNHP
Authors	:	Mann, D.; Bergeron, J.R.C.
Deposited on	:	2020-05-27
Resolution	:	3.90 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

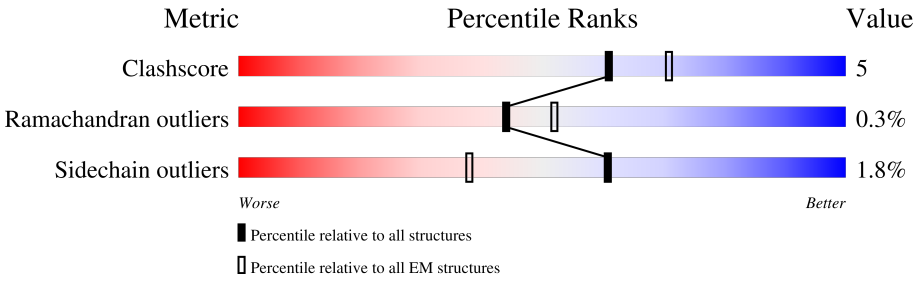
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	258	69% 92% 7% ·
1	B	258	70% 89% 9% ·
2	C	95	92% 82% 8% · 8%
2	D	95	92% 85% 5% · 8%
3	E	226	63% 77% 6% · 16%
3	F	226	70% 76% 9% · 15%
3	G	226	64% 76% 9% 15%
3	H	226	66% 75% 7% · 16%

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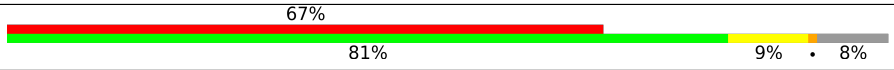
Mol	Chain	Length	Quality of chain
3	I	226	
3	J	226	
4	K	276	
4	L	276	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17880 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 ABC transporter permease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	254	Total	C	N	O	S	0	0
			1886	1235	306	330	15		
1	B	254	Total	C	N	O	S	0	0
			1886	1235	306	330	15		

- Molecule 2 is a protein called Anti-sigma factor antagonist.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	87	Total	C	N	O	S	0	0
			696	449	120	125	2		
2	D	87	Total	C	N	O	S	0	0
			696	449	120	125	2		

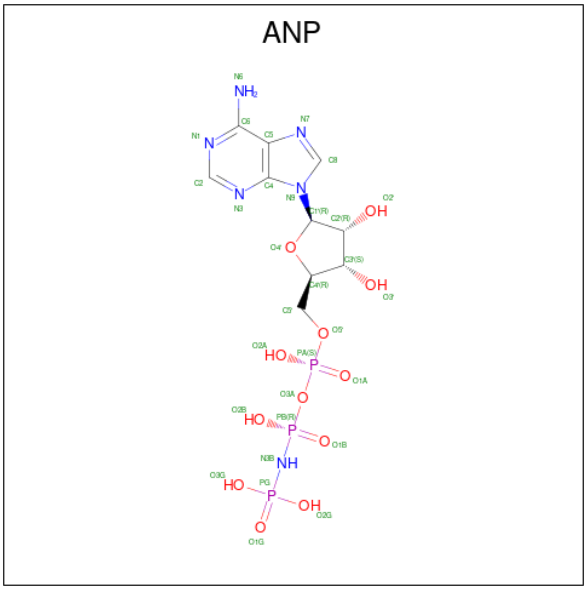
- Molecule 3 is a protein called MCE family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	190	Total	C	N	O	S	0	0
			1450	918	236	289	7		
3	G	191	Total	C	N	O	S	0	0
			1461	924	240	290	7		
3	H	189	Total	C	N	O	S	0	0
			1443	914	235	287	7		
3	I	193	Total	C	N	O	S	0	0
			1476	933	243	293	7		
3	J	190	Total	C	N	O	S	0	0
			1450	918	236	289	7		
3	F	193	Total	C	N	O	S	0	0
			1476	933	243	293	7		

- Molecule 4 is a protein called ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	253	Total	C	N	O	S	0	0
			1948	1233	335	372	8		
4	L	253	Total	C	N	O	S	0	0
			1948	1233	335	372	8		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
5	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	L	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

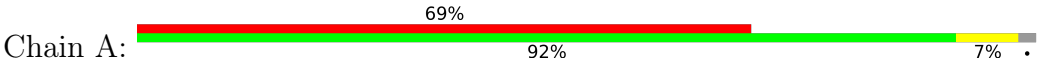
Mol	Chain	Residues	Atoms		AltConf
6	K	1	Total	Mg	0
			1	1	
6	L	1	Total	Mg	0
			1	1	

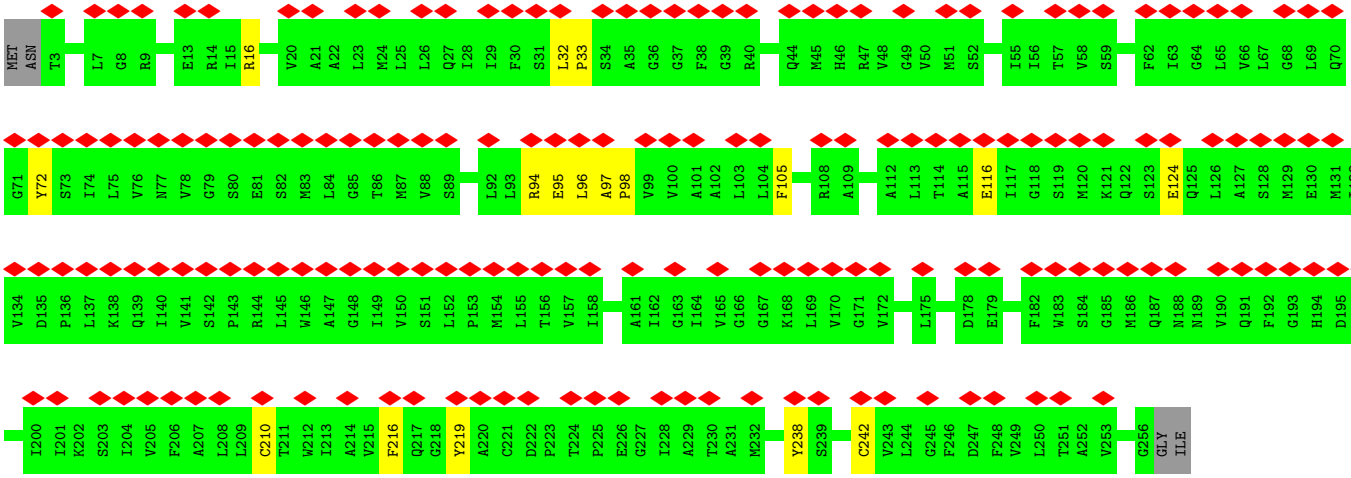
3 Residue-property plots (i)

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: ABC transporter permeable

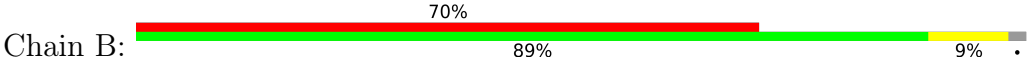
Chain A:

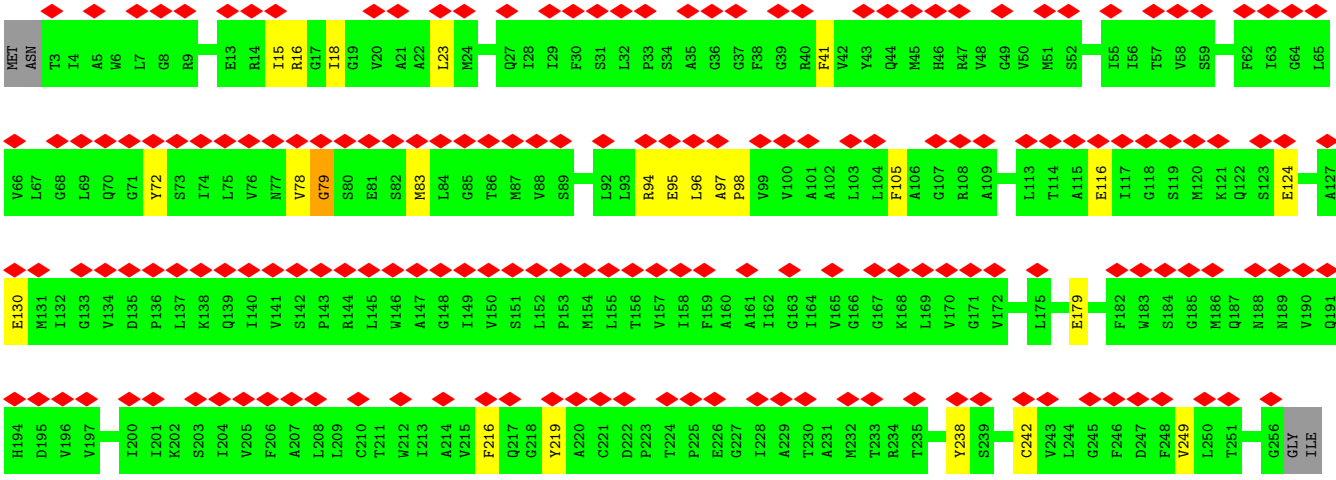




• Molecule 1: ABC transporter permeable

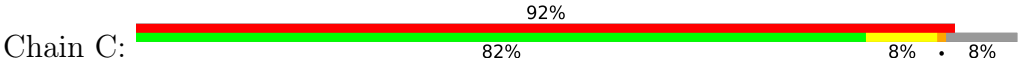
Chain B:

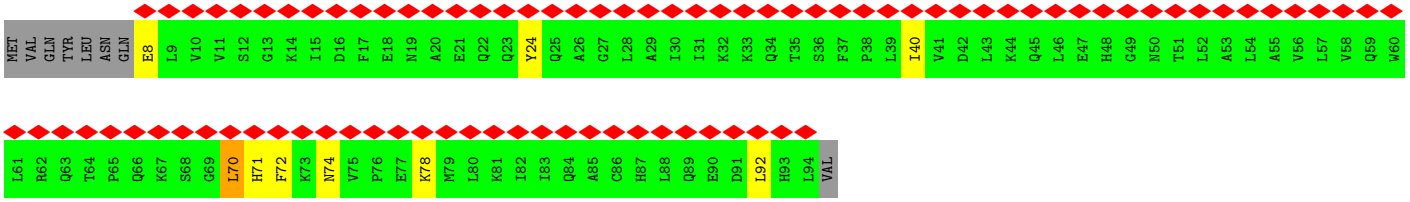




• Molecule 2: Anti-sigma factor antagonist

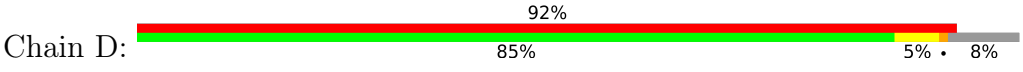
Chain C:

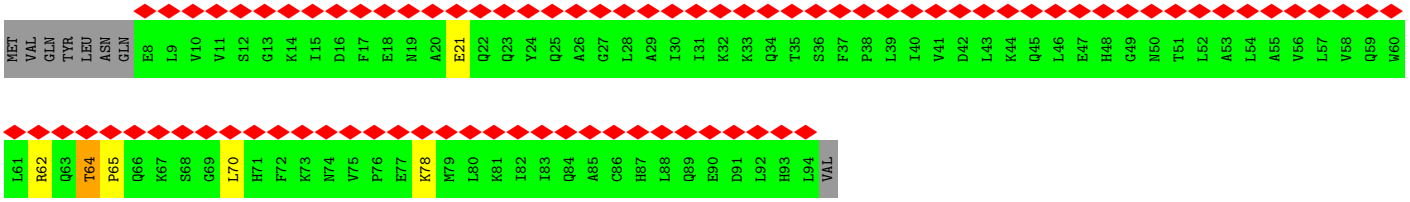




• Molecule 2: Anti-sigma factor antagonist

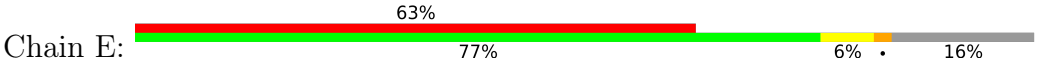
Chain D:

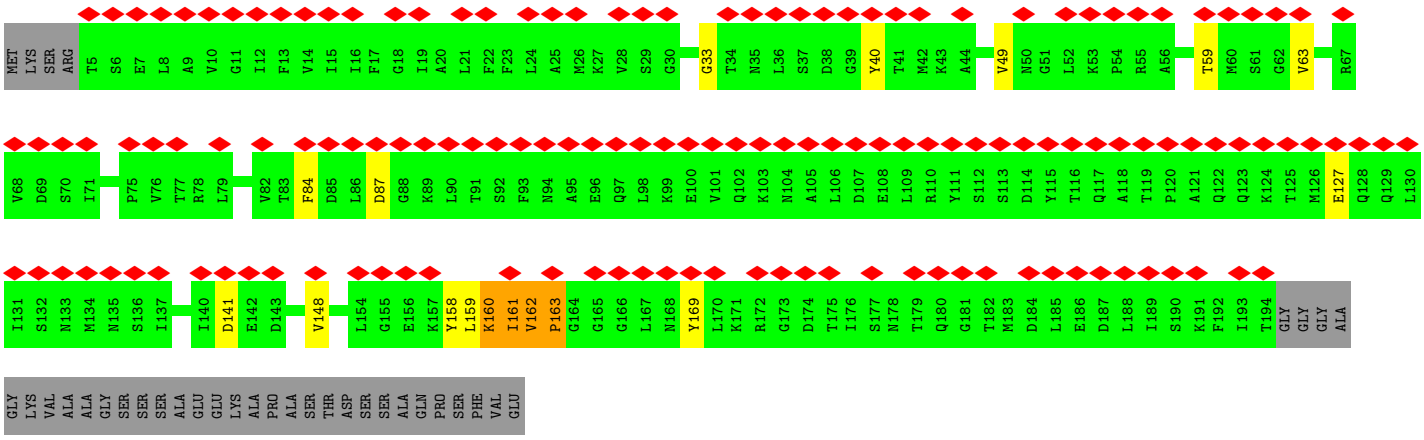




• Molecule 3: MCE family protein

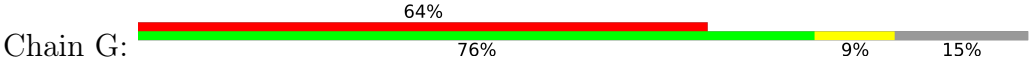
Chain E:

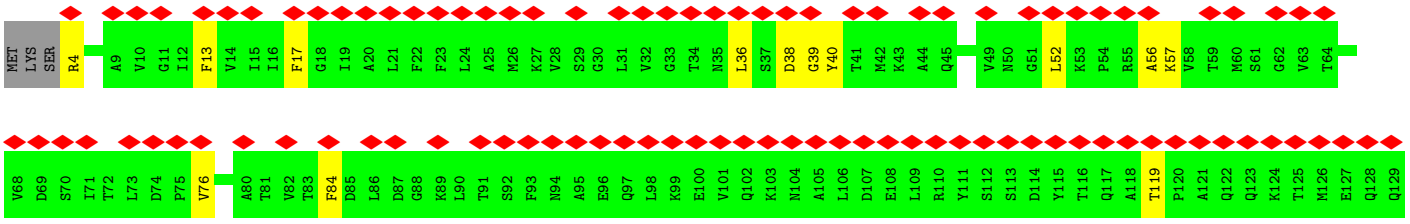


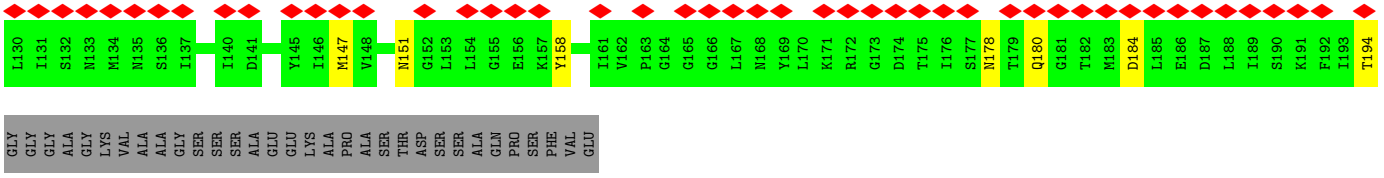


• Molecule 3: MCE family protein

Chain G:

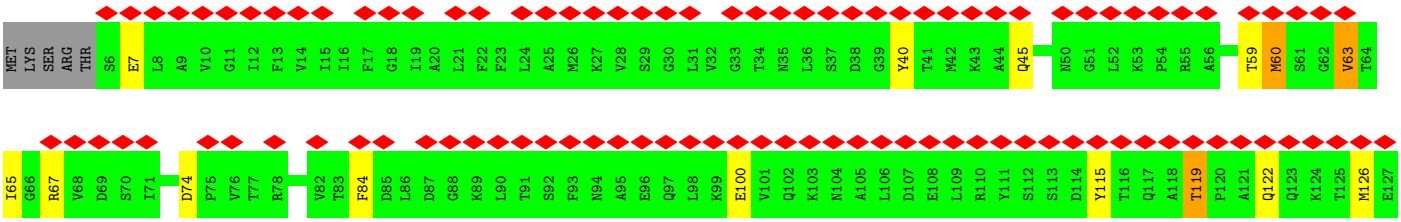






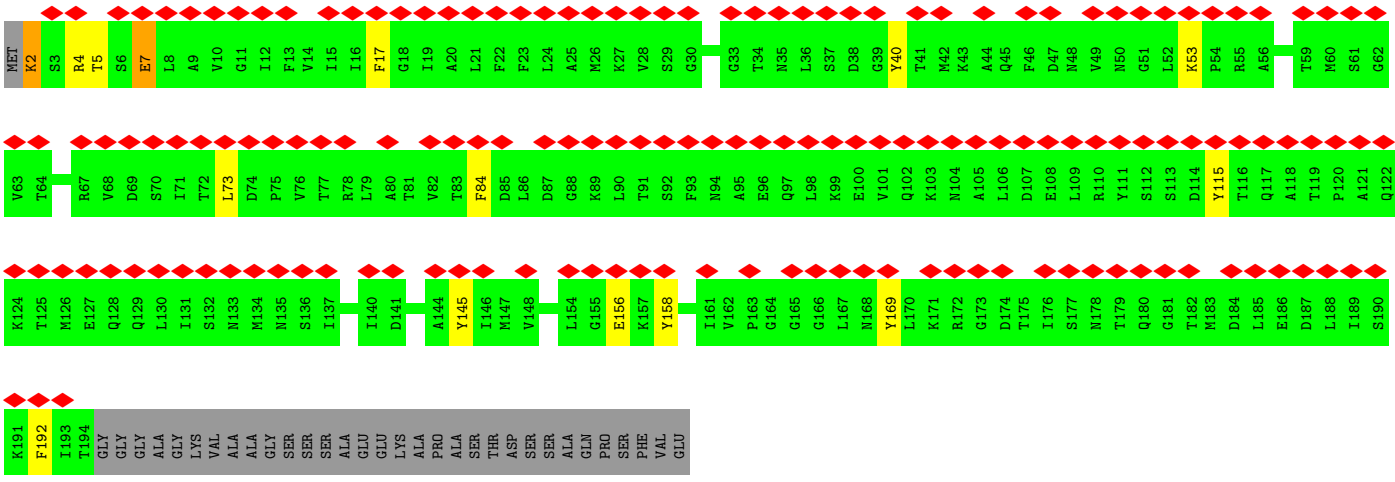
• Molecule 3: MCE family protein

Chain H:



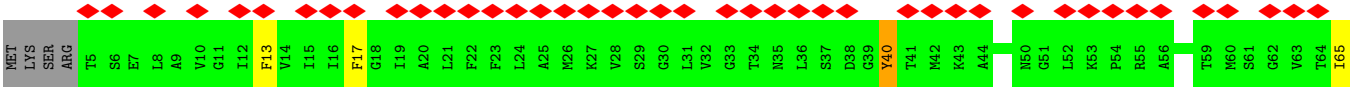
• Molecule 3: MCE family protein

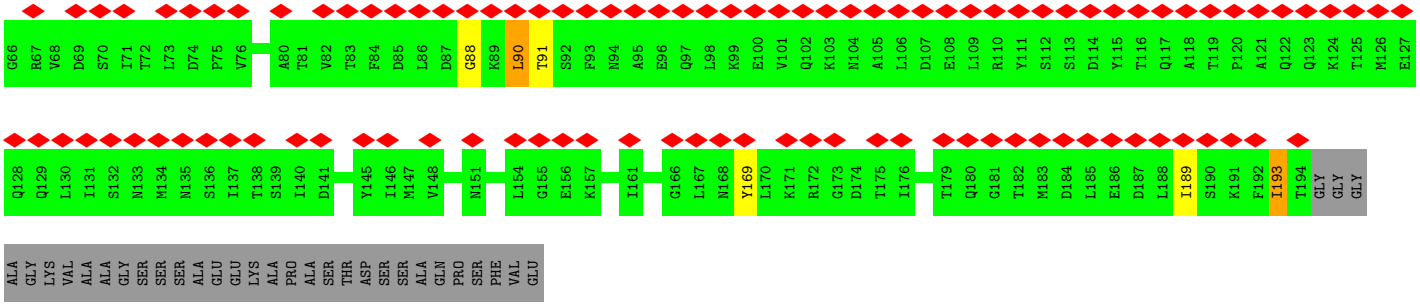
Chain I:



• Molecule 3: MCE family protein

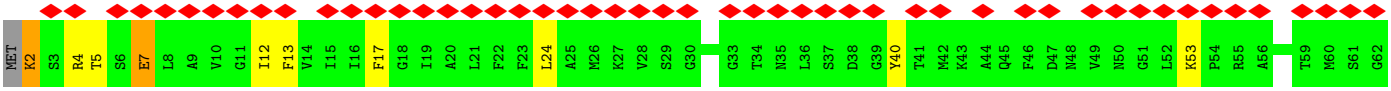
Chain J:

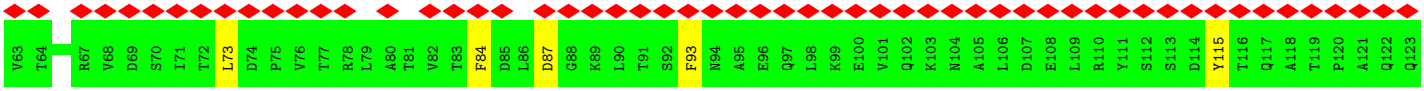


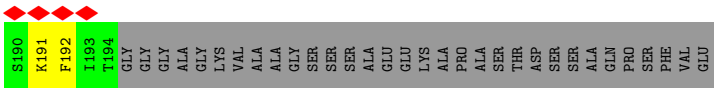


• Molecule 3: MCE family protein

Chain F:

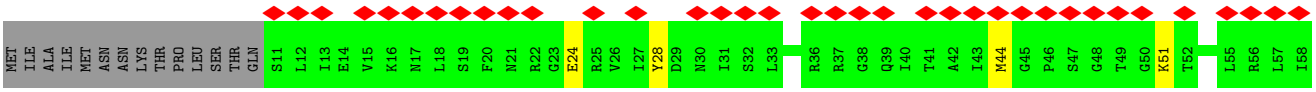


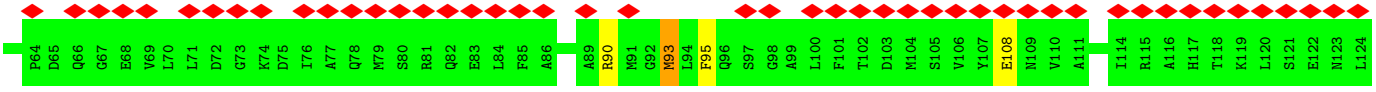


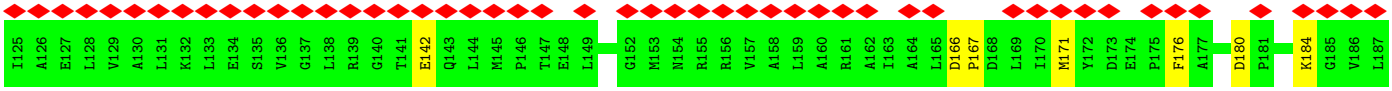


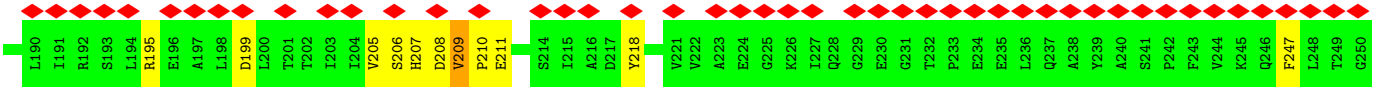
• Molecule 4: ABC transporter ATP-binding protein

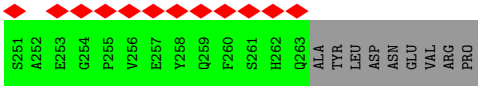
Chain K:





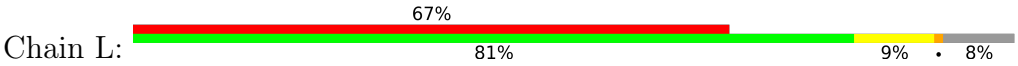


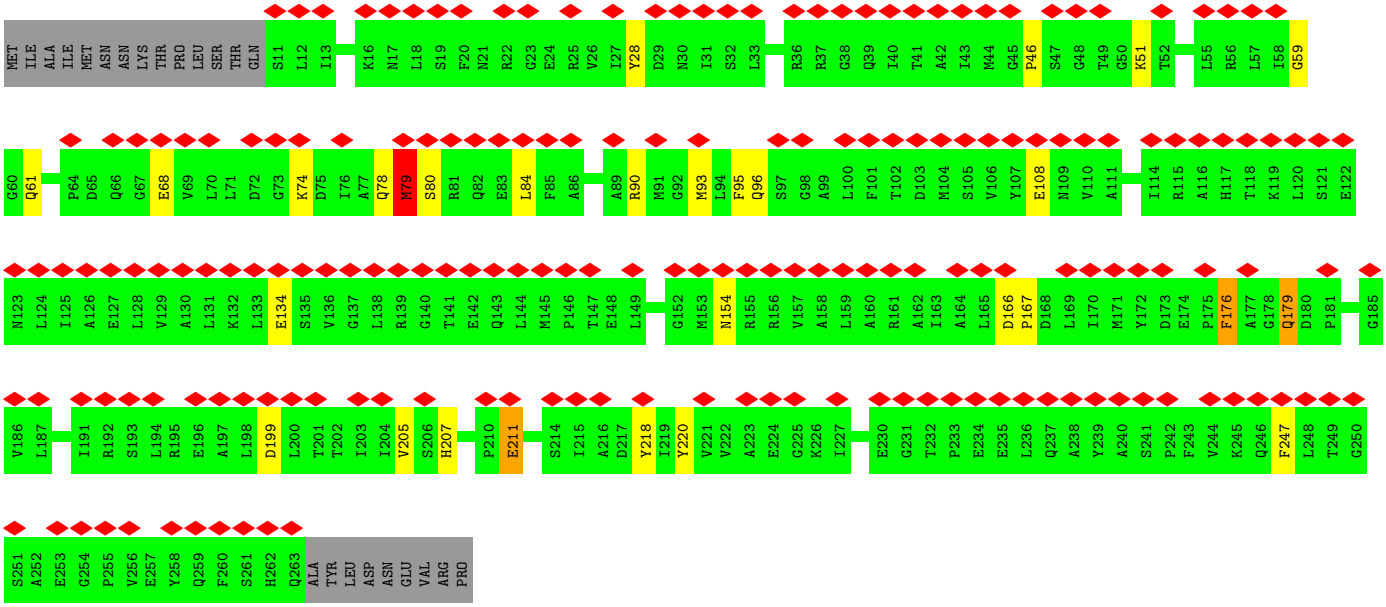




• Molecule 4: ABC transporter ATP-binding protein

Chain L:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93295	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.100	Depositor
Minimum map value	-2.040	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.458	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.21	12/1920 (0.6%)	0.96	4/2606 (0.2%)
1	B	1.23	15/1920 (0.8%)	0.97	4/2606 (0.2%)
2	C	0.94	0/708	0.79	1/956 (0.1%)
2	D	1.00	2/708 (0.3%)	0.81	1/956 (0.1%)
3	E	0.93	3/1467 (0.2%)	0.98	0/1983
3	F	0.90	2/1493 (0.1%)	0.98	3/2016 (0.1%)
3	G	0.95	4/1478 (0.3%)	0.96	1/1997 (0.1%)
3	H	1.00	5/1460 (0.3%)	0.99	4/1973 (0.2%)
3	I	0.90	2/1493 (0.1%)	0.98	3/2016 (0.1%)
3	J	0.98	2/1467 (0.1%)	0.90	2/1983 (0.1%)
4	K	1.19	9/1977 (0.5%)	0.98	5/2674 (0.2%)
4	L	1.21	10/1977 (0.5%)	0.98	5/2674 (0.2%)
All	All	1.07	66/18068 (0.4%)	0.96	33/24440 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1
3	F	0	1
3	H	0	2
3	I	0	1
4	L	0	1
All	All	0	6

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	40	TYR	CB-CG	-9.93	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	TYR	CB-CG	-8.37	1.39	1.51
1	A	238	TYR	CB-CG	-7.28	1.40	1.51
4	L	247	PHE	CB-CG	-7.04	1.39	1.51
3	H	169	TYR	CB-CG	-6.81	1.41	1.51
3	G	13	PHE	CB-CG	-6.79	1.39	1.51
1	A	95	GLU	CD-OE1	-6.77	1.18	1.25
3	H	100	GLU	CD-OE1	-6.64	1.18	1.25
1	A	116	GLU	CD-OE2	-6.62	1.18	1.25
1	A	216	PHE	CB-CG	-6.61	1.40	1.51
1	B	116	GLU	CD-OE2	-6.57	1.18	1.25
4	L	207	HIS	CB-CG	-6.48	1.38	1.50
1	B	219	TYR	CB-CG	-6.45	1.42	1.51
1	B	95	GLU	CD-OE1	-6.41	1.18	1.25
4	K	176	PHE	CB-CG	-6.36	1.40	1.51
3	H	141	ASP	CB-CG	-6.18	1.38	1.51
1	A	210	CYS	CB-SG	-6.14	1.71	1.82
1	A	219	TYR	CB-CG	-6.06	1.42	1.51
3	E	169	TYR	CB-CG	-6.00	1.42	1.51
1	B	216	PHE	CB-CG	-5.99	1.41	1.51
1	B	72	TYR	CB-CG	-5.99	1.42	1.51
1	A	116	GLU	CG-CD	-5.96	1.43	1.51
1	B	124	GLU	CD-OE2	-5.94	1.19	1.25
1	B	192	PHE	CB-CG	-5.88	1.41	1.51
1	B	116	GLU	CG-CD	-5.85	1.43	1.51
4	L	28	TYR	CD2-CE2	-5.83	1.30	1.39
4	L	154	ASN	CB-CG	-5.83	1.37	1.51
3	G	4	ARG	NE-CZ	5.79	1.40	1.33
1	A	124	GLU	CD-OE1	-5.79	1.19	1.25
4	K	142	GLU	CD-OE1	-5.68	1.19	1.25
1	B	105	PHE	CB-CG	-5.65	1.41	1.51
1	A	124	GLU	CG-CD	-5.62	1.43	1.51
1	A	72	TYR	CB-CG	-5.62	1.43	1.51
3	J	17	PHE	CB-CG	-5.60	1.41	1.51
4	K	28	TYR	CD2-CE2	-5.59	1.30	1.39
3	I	17	PHE	CB-CG	-5.59	1.41	1.51
3	F	17	PHE	CB-CG	-5.59	1.41	1.51
4	K	142	GLU	CG-CD	-5.55	1.43	1.51
2	D	21	GLU	CD-OE1	-5.54	1.19	1.25
4	L	28	TYR	CE2-CZ	-5.46	1.31	1.38
3	E	40	TYR	CB-CG	-5.33	1.43	1.51
4	L	211	GLU	CD-OE1	-5.30	1.19	1.25
4	K	205	VAL	CB-CG1	-5.29	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	40	TYR	CB-CG	-5.28	1.43	1.51
4	L	134	GLU	CD-OE1	-5.28	1.19	1.25
1	B	124	GLU	CD-OE1	-5.28	1.19	1.25
1	B	179	GLU	CD-OE2	-5.24	1.19	1.25
3	I	169	TYR	CB-CG	-5.24	1.43	1.51
3	F	169	TYR	CB-CG	-5.24	1.43	1.51
1	B	130	GLU	CD-OE1	-5.23	1.19	1.25
4	K	108	GLU	CD-OE2	-5.22	1.20	1.25
4	K	28	TYR	CE2-CZ	-5.20	1.31	1.38
4	L	108	GLU	CD-OE2	-5.20	1.20	1.25
3	G	17	PHE	CB-CG	-5.12	1.42	1.51
4	L	205	VAL	CB-CG1	-5.11	1.42	1.52
4	K	24	GLU	CD-OE2	-5.10	1.20	1.25
1	A	242	CYS	CB-SG	-5.07	1.73	1.81
4	K	247	PHE	CB-CG	-5.07	1.42	1.51
1	A	105	PHE	CB-CG	-5.06	1.42	1.51
1	B	242	CYS	CB-SG	-5.05	1.73	1.81
3	E	127	GLU	CD-OE2	-5.05	1.20	1.25
3	H	7	GLU	CD-OE2	-5.05	1.20	1.25
3	G	40	TYR	CB-CG	-5.04	1.44	1.51
4	L	68	GLU	CD-OE1	-5.04	1.20	1.25
1	B	124	GLU	CG-CD	-5.02	1.44	1.51
2	D	21	GLU	CG-CD	-5.01	1.44	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	90	ARG	NE-CZ-NH2	-9.38	115.61	120.30
4	L	28	TYR	CB-CG-CD2	-8.39	115.97	121.00
4	K	28	TYR	CB-CG-CD2	-8.32	116.01	121.00
1	A	94	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	94	ARG	NE-CZ-NH2	-7.88	116.36	120.30
4	L	218	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	A	16	ARG	NE-CZ-NH2	-6.83	116.89	120.30
4	K	218	TYR	CB-CG-CD1	-6.65	117.01	121.00
1	B	16	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	D	62	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	72	TYR	CB-CG-CD1	-5.79	117.52	121.00
3	I	115	TYR	CB-CG-CD2	-5.79	117.53	121.00
3	F	115	TYR	CB-CG-CD2	-5.79	117.53	121.00
3	I	145	TYR	CB-CG-CD2	-5.68	117.59	121.00
3	F	145	TYR	CB-CG-CD2	-5.68	117.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	93	MET	CG-SD-CE	5.60	109.17	100.20
4	K	95	PHE	CB-CG-CD1	5.60	124.72	120.80
1	B	72	TYR	CB-CG-CD1	-5.51	117.69	121.00
3	J	40	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	A	238	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	B	41	PHE	CB-CG-CD1	-5.42	117.01	120.80
2	C	24	TYR	CB-CG-CD2	-5.41	117.75	121.00
3	G	84	PHE	N-CA-CB	-5.33	101.00	110.60
4	L	220	TYR	CB-CG-CD2	-5.30	117.82	121.00
3	H	67	ARG	NE-CZ-NH1	5.27	122.93	120.30
3	I	40	TYR	CB-CG-CD2	-5.25	117.85	121.00
3	F	40	TYR	CB-CG-CD2	-5.25	117.85	121.00
3	H	115	TYR	CB-CG-CD2	-5.20	117.88	121.00
4	K	90	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	J	169	TYR	CB-CG-CD2	-5.13	117.92	121.00
3	H	169	TYR	CB-CG-CD2	-5.12	117.93	121.00
3	H	126	MET	CG-SD-CE	5.11	108.37	100.20
4	L	176	PHE	CB-CA-C	-5.07	100.26	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	84	PHE	Sidechain
3	F	84	PHE	Sidechain
3	H	158	TYR	Sidechain
3	H	84	PHE	Sidechain
3	I	84	PHE	Sidechain
4	L	79	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1886	0	1976	5	0
1	B	1886	0	1976	37	0
2	C	696	0	723	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	696	0	723	3	0
3	E	1450	0	1477	15	0
3	F	1476	0	1508	49	0
3	G	1461	0	1489	9	0
3	H	1443	0	1470	19	0
3	I	1476	0	1508	13	0
3	J	1450	0	1477	13	0
4	K	1948	0	1985	15	0
4	L	1948	0	1985	29	0
5	K	31	0	13	0	0
5	L	31	0	13	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
All	All	17880	0	18323	166	0

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

All (166) 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)
3:J:40:TYR:CE2	3:J:91:THR:HG21	1.25	1.62
3:J:40:TYR:HE2	3:J:91:THR:CG2	1.34	1.40
1:B:23:LEU:CG	3:F:12:ILE:HD13	1.68	1.23
1:B:23:LEU:HD21	3:F:12:ILE:CD1	1.67	1.22
1:B:18:ILE:CG2	3:F:13:PHE:HD1	1.55	1.19
3:G:184:ASP:OD2	3:F:160:LYS:NZ	1.74	1.19
1:B:23:LEU:HD11	3:F:12:ILE:CD1	1.75	1.16
1:B:23:LEU:HD11	3:F:12:ILE:HD12	1.22	1.14
3:H:60:MET:HB3	3:H:65:ILE:HD13	1.30	1.13
1:B:23:LEU:CG	3:F:12:ILE:CD1	2.26	1.11
1:B:23:LEU:CD2	3:F:12:ILE:CD1	2.29	1.11
1:B:23:LEU:HG	3:F:12:ILE:HD13	1.28	1.11
4:K:184:LYS:HD3	4:K:211:GLU:OE2	1.49	1.11
1:B:23:LEU:HD21	3:F:12:ILE:HD11	1.20	1.09
3:H:63:VAL:HG11	3:I:73:LEU:HB2	1.12	1.08
1:B:23:LEU:CD2	3:F:12:ILE:HD13	1.83	1.08
3:E:162:VAL:HG12	3:E:163:PRO:HD2	1.33	1.04
1:B:23:LEU:CD1	3:F:12:ILE:CD1	2.35	1.03
4:L:93:MET:CE	4:L:95:PHE:HE1	1.72	1.02
3:H:119:THR:CG2	3:H:122:GLN:HG2	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:HG12	3:F:13:PHE:CE2	1.93	1.01
3:J:40:TYR:CE2	3:J:91:THR:CG2	2.21	1.01
1:B:18:ILE:CG2	3:F:13:PHE:CD1	2.44	1.00
3:H:119:THR:HG21	3:H:122:GLN:CG	1.91	1.00
3:J:189:ILE:O	3:J:193:ILE:HG22	1.60	1.00
3:J:40:TYR:CZ	3:J:91:THR:HG21	1.98	0.98
3:J:88:GLY:HA2	3:J:91:THR:HG22	1.45	0.97
3:H:63:VAL:HG11	3:I:73:LEU:CB	1.93	0.97
1:B:23:LEU:CD1	3:F:12:ILE:HD12	1.95	0.96
3:E:59:THR:O	3:E:161:ILE:HG22	1.65	0.96
1:B:18:ILE:HG21	3:F:13:PHE:HD1	1.32	0.94
4:K:51:LYS:NZ	4:K:207:HIS:HE1	1.66	0.93
3:H:119:THR:CG2	3:H:122:GLN:CG	2.45	0.93
3:H:63:VAL:CG1	3:I:73:LEU:HB2	1.97	0.92
3:H:119:THR:HG22	3:H:122:GLN:HG2	1.50	0.92
1:B:249:VAL:CG2	3:F:24:LEU:HD13	2.01	0.90
3:J:88:GLY:O	3:J:91:THR:O	1.89	0.89
1:B:15:ILE:CG1	3:F:13:PHE:CE2	2.56	0.89
1:B:18:ILE:HG21	3:F:13:PHE:CD1	2.08	0.88
3:H:119:THR:HG21	3:H:122:GLN:HG3	1.53	0.88
4:L:93:MET:CE	4:L:95:PHE:CE1	2.57	0.87
3:F:2:LYS:O	3:F:2:LYS:NZ	2.08	0.87
4:L:176:PHE:HE2	4:L:211:GLU:HB3	1.39	0.87
3:I:2:LYS:O	3:I:2:LYS:NZ	2.08	0.85
1:B:23:LEU:CD2	3:F:12:ILE:HD11	1.98	0.84
1:B:18:ILE:HG22	3:F:13:PHE:HD1	1.43	0.83
1:B:18:ILE:HG22	3:F:13:PHE:CD1	2.14	0.83
1:B:249:VAL:CG2	3:F:24:LEU:CD1	2.57	0.83
4:L:176:PHE:CE2	4:L:211:GLU:HB3	2.15	0.82
3:J:65:ILE:HD12	3:J:90:LEU:HB2	1.61	0.82
1:B:249:VAL:HG22	3:F:24:LEU:CD1	2.10	0.82
4:L:93:MET:HE2	4:L:95:PHE:HE1	1.43	0.81
1:B:15:ILE:HG13	3:F:13:PHE:CG	2.13	0.81
1:B:249:VAL:HG21	3:F:24:LEU:HD13	1.61	0.81
4:K:51:LYS:NZ	4:K:207:HIS:CE1	2.50	0.80
3:H:60:MET:HB3	3:H:65:ILE:CD1	2.11	0.78
4:K:51:LYS:HZ3	4:K:207:HIS:HE1	1.32	0.77
4:L:93:MET:SD	4:L:95:PHE:HE1	2.08	0.76
4:K:51:LYS:HZ3	4:K:207:HIS:CE1	2.04	0.75
4:L:78:GLN:HB2	4:L:79:MET:HE3	1.66	0.75
4:K:208:ASP:OD2	4:K:210:PRO:HD2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:45:GLN:O	3:H:179:THR:HG21	1.87	0.74
4:L:74:LYS:HE2	4:L:79:MET:HB3	1.68	0.74
3:J:189:ILE:O	3:J:193:ILE:CG2	2.36	0.73
4:L:93:MET:SD	4:L:95:PHE:CE1	2.81	0.73
3:I:2:LYS:HB2	3:I:2:LYS:HZ3	1.53	0.73
3:E:160:LYS:NZ	3:E:160:LYS:HB3	2.02	0.73
4:L:79:MET:O	4:L:84:LEU:HD11	1.90	0.72
1:B:23:LEU:HG	3:F:12:ILE:CD1	2.07	0.68
4:L:93:MET:HE2	4:L:95:PHE:CE1	2.26	0.68
3:F:2:LYS:HB2	3:F:2:LYS:HZ3	1.57	0.68
3:E:162:VAL:HG12	3:E:163:PRO:CD	2.19	0.67
1:B:15:ILE:CG1	3:F:13:PHE:CD2	2.78	0.66
4:K:51:LYS:HZ1	4:K:207:HIS:HE1	1.41	0.65
3:I:192:PHE:CE2	3:J:193:ILE:O	2.50	0.65
4:L:179:GLN:HE21	4:L:179:GLN:HA	1.63	0.64
1:B:15:ILE:HG13	3:F:13:PHE:CD2	2.32	0.64
4:L:176:PHE:CE2	4:L:211:GLU:CB	2.82	0.63
3:H:60:MET:CB	3:H:65:ILE:HD13	2.20	0.62
2:D:78:LYS:NZ	4:K:199:ASP:OD2	2.32	0.61
4:L:179:GLN:HA	4:L:179:GLN:NE2	2.15	0.61
1:A:32:LEU:N	1:A:33:PRO:CD	2.64	0.60
3:E:63:VAL:HG21	3:F:73:LEU:HB2	1.82	0.60
1:B:23:LEU:HD11	3:F:12:ILE:HD11	1.76	0.59
2:C:78:LYS:NZ	4:L:199:ASP:OD2	2.34	0.59
3:E:162:VAL:CG1	3:E:163:PRO:HD2	2.21	0.59
1:B:15:ILE:CG1	3:F:13:PHE:CG	2.87	0.58
3:E:148:VAL:HA	3:E:159:LEU:HD23	1.85	0.58
3:G:147:MET:HG2	3:G:180:GLN:HG2	1.86	0.58
3:E:161:ILE:O	3:E:161:ILE:HG12	2.02	0.58
3:H:119:THR:HG22	3:H:122:GLN:CG	2.22	0.58
3:E:160:LYS:HB3	3:E:160:LYS:HZ1	1.66	0.57
3:H:119:THR:HG21	3:H:122:GLN:HG2	1.62	0.57
3:H:119:THR:HB	3:H:122:GLN:HB2	1.86	0.57
3:I:2:LYS:NZ	3:I:2:LYS:HB2	2.20	0.57
3:F:2:LYS:NZ	3:F:2:LYS:HB2	2.20	0.56
3:I:53:LYS:HE2	3:I:156:GLU:CB	2.36	0.56
2:C:72:PHE:HB2	2:C:92:LEU:O	2.06	0.55
3:E:161:ILE:O	3:E:161:ILE:HG23	2.04	0.55
3:F:53:LYS:HE2	3:F:156:GLU:CB	2.36	0.55
3:J:40:TYR:HE2	3:J:91:THR:CB	2.14	0.54
4:K:51:LYS:HZ1	4:K:207:HIS:CE1	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:53:LYS:HE2	3:F:156:GLU:HB3	1.90	0.53
3:I:53:LYS:HE2	3:I:156:GLU:HB3	1.90	0.53
1:B:249:VAL:HG22	3:F:24:LEU:HD12	1.89	0.53
4:L:176:PHE:CD2	4:L:211:GLU:CB	2.91	0.53
1:A:32:LEU:H	1:A:33:PRO:HD3	1.75	0.52
3:G:57:LYS:HE2	3:G:151:ASN:ND2	2.24	0.52
3:I:7:GLU:HA	3:I:7:GLU:OE1	2.10	0.52
4:L:74:LYS:HE2	4:L:79:MET:CB	2.39	0.52
4:L:176:PHE:CD2	4:L:211:GLU:HB2	2.45	0.51
3:F:2:LYS:NZ	3:F:2:LYS:CB	2.73	0.51
3:F:7:GLU:HA	3:F:7:GLU:OE1	2.10	0.51
1:B:23:LEU:CD1	3:F:12:ILE:HD11	2.36	0.51
4:L:176:PHE:N	4:L:176:PHE:CD1	2.79	0.50
3:I:2:LYS:NZ	3:I:2:LYS:CB	2.73	0.50
4:K:208:ASP:OD2	4:K:210:PRO:CD	2.60	0.49
3:E:160:LYS:NZ	3:E:160:LYS:CB	2.72	0.49
4:L:176:PHE:N	4:L:176:PHE:HD1	2.10	0.49
4:K:208:ASP:OD2	4:K:210:PRO:HG2	2.12	0.49
4:K:44:MET:SD	4:K:209:VAL:CG2	3.01	0.48
4:L:176:PHE:HD2	4:L:211:GLU:HB2	1.78	0.48
3:G:194:THR:CG2	3:F:191:LYS:HG2	2.44	0.48
1:B:97:ALA:N	1:B:98:PRO:CD	2.79	0.46
2:D:64:THR:HB	2:D:65:PRO:HD3	1.97	0.46
1:A:32:LEU:N	1:A:33:PRO:HD3	2.31	0.46
3:G:194:THR:HG23	3:F:192:PHE:N	2.31	0.46
4:L:80:SER:O	4:L:84:LEU:HG	2.17	0.45
3:E:160:LYS:HZ1	3:E:162:VAL:HG22	1.81	0.45
3:I:7:GLU:N	3:I:7:GLU:CD	2.71	0.45
4:L:93:MET:HE1	4:L:95:PHE:CE1	2.48	0.45
2:D:65:PRO:HB3	2:D:70:LEU:HB2	1.98	0.44
2:C:70:LEU:HD13	2:C:92:LEU:HA	1.99	0.44
3:F:7:GLU:N	3:F:7:GLU:CD	2.71	0.44
3:G:147:MET:HG2	3:G:180:GLN:CG	2.47	0.44
1:A:97:ALA:N	1:A:98:PRO:CD	2.80	0.44
1:B:15:ILE:HG12	3:F:13:PHE:CD2	2.45	0.44
3:E:162:VAL:HA	3:E:163:PRO:HD3	1.76	0.43
3:G:76:VAL:HG12	3:F:93:PHE:CE2	2.54	0.43
3:G:56:ALA:HB1	3:G:158:TYR:HA	1.99	0.43
3:H:74:ASP:OD1	3:H:74:ASP:C	2.57	0.43
3:H:119:THR:O	3:H:122:GLN:N	2.46	0.43
4:L:166:ASP:N	4:L:167:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:96:GLN:OE1	4:L:96:GLN:HA	2.19	0.42
1:B:79:GLY:O	1:B:83:MET:HB2	2.19	0.42
1:A:96:LEU:O	1:A:97:ALA:C	2.57	0.42
4:K:93:MET:HG2	4:K:171:MET:HB2	2.02	0.42
4:L:46:PRO:O	4:L:51:LYS:NZ	2.54	0.41
3:E:87:ASP:OD1	3:E:87:ASP:C	2.58	0.41
3:H:119:THR:CG2	3:H:122:GLN:CB	2.98	0.41
3:G:194:THR:HG22	3:F:191:LYS:CG	2.51	0.41
4:L:93:MET:SD	4:L:95:PHE:CZ	3.14	0.41
3:F:87:ASP:C	3:F:87:ASP:OD1	2.57	0.41
1:B:249:VAL:HG21	3:F:24:LEU:CD1	2.32	0.41
3:E:158:TYR:HE1	3:E:160:LYS:HG2	1.86	0.41
4:L:61:GLN:N	4:L:61:GLN:CD	2.75	0.41
1:B:96:LEU:O	1:B:97:ALA:C	2.56	0.41
2:C:70:LEU:HD13	2:C:92:LEU:C	2.41	0.40
2:C:8:GLU:N	2:C:40:ILE:O	2.55	0.40
4:K:180:ASP:OD1	4:K:180:ASP:C	2.59	0.40
3:J:13:PHE:CD1	3:J:13:PHE:C	2.88	0.40
4:L:79:MET:O	4:L:84:LEU:CD1	2.65	0.40
3:H:60:MET:HG3	3:H:60:MET:O	2.20	0.40
3:I:192:PHE:HE2	3:J:193:ILE:O	2.01	0.40
2:C:71:HIS:HB2	2:C:74:ASN:HD22	1.86	0.40
4:K:166:ASP:N	4:K:167:PRO:CD	2.84	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	252/258 (98%)	248 (98%)	4 (2%)	0	100	100
1	B	252/258 (98%)	248 (98%)	3 (1%)	1 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	85/95 (90%)	84 (99%)	1 (1%)	0	100	100
2	D	85/95 (90%)	83 (98%)	1 (1%)	1 (1%)	13	49
3	E	188/226 (83%)	179 (95%)	7 (4%)	2 (1%)	14	51
3	F	191/226 (84%)	188 (98%)	3 (2%)	0	100	100
3	G	189/226 (84%)	179 (95%)	8 (4%)	2 (1%)	14	51
3	H	187/226 (83%)	184 (98%)	3 (2%)	0	100	100
3	I	191/226 (84%)	188 (98%)	3 (2%)	0	100	100
3	J	188/226 (83%)	182 (97%)	6 (3%)	0	100	100
4	K	251/276 (91%)	246 (98%)	5 (2%)	0	100	100
4	L	251/276 (91%)	247 (98%)	3 (1%)	1 (0%)	34	71
All	All	2310/2614 (88%)	2256 (98%)	47 (2%)	7 (0%)	44	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	GLY
3	E	163	PRO
3	G	39	GLY
2	D	64	THR
3	E	33	GLY
3	G	119	THR
4	L	59	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	202/205 (98%)	202 (100%)	0	100	100
1	B	202/205 (98%)	201 (100%)	1 (0%)	88	93
2	C	77/85 (91%)	76 (99%)	1 (1%)	69	82
2	D	77/85 (91%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	162/186 (87%)	157 (97%)	5 (3%)	40	64
3	F	165/186 (89%)	160 (97%)	5 (3%)	41	64
3	G	163/186 (88%)	159 (98%)	4 (2%)	47	69
3	H	161/186 (87%)	154 (96%)	7 (4%)	29	57
3	I	165/186 (89%)	160 (97%)	5 (3%)	41	64
3	J	162/186 (87%)	160 (99%)	2 (1%)	71	83
4	K	210/231 (91%)	207 (99%)	3 (1%)	67	81
4	L	210/231 (91%)	208 (99%)	2 (1%)	76	86
All	All	1956/2158 (91%)	1921 (98%)	35 (2%)	61	77

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	78	VAL
2	C	70	LEU
3	E	49	VAL
3	E	141	ASP
3	E	160	LYS
3	E	161	ILE
3	E	162	VAL
3	G	36	LEU
3	G	38	ASP
3	G	52	LEU
3	G	178	ASN
3	H	59	THR
3	H	60	MET
3	H	63	VAL
3	H	119	THR
3	H	158	TYR
3	H	178	ASN
3	H	179	THR
3	I	2	LYS
3	I	4	ARG
3	I	5	THR
3	I	7	GLU
3	I	158	TYR
3	J	90	LEU
3	J	193	ILE
4	K	195	ARG

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Mol	Chain	Res	Type
4	K	206	SER
4	K	209	VAL
4	L	79	MET
4	L	179	GLN
3	F	2	LYS
3	F	4	ARG
3	F	5	THR
3	F	7	GLU
3	F	158	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	74	ASN
2	C	93	HIS
4	K	207	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ANP	L	302	6	29,33,33	2.67	10 (34%)	31,52,52	2.13	8 (25%)
5	ANP	K	301	6	29,33,33	2.42	12 (41%)	31,52,52	2.05	9 (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
5	ANP	L	302	6	-	5/14/38/38	0/3/3/3
5	ANP	K	301	6	-	5/14/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302	ANP	PB-O3A	-7.88	1.49	1.59
5	K	301	ANP	C2-N3	5.96	1.41	1.32
5	L	302	ANP	C2-N3	5.78	1.41	1.32
5	K	301	ANP	PB-O3A	-5.49	1.52	1.59
5	L	302	ANP	C4-N3	5.39	1.43	1.35
5	K	301	ANP	C4-N3	4.83	1.42	1.35
5	L	302	ANP	O4'-C1'	4.35	1.47	1.41
5	L	302	ANP	C2'-C1'	3.60	1.59	1.53
5	K	301	ANP	C2-N1	3.39	1.40	1.33
5	K	301	ANP	O4'-C1'	3.07	1.45	1.41
5	K	301	ANP	C2'-C3'	2.92	1.61	1.53
5	L	302	ANP	C2-N1	2.89	1.39	1.33
5	K	301	ANP	C8-N7	-2.59	1.30	1.34
5	L	302	ANP	PB-N3B	-2.56	1.56	1.63
5	L	302	ANP	C8-N7	-2.53	1.30	1.34
5	K	301	ANP	PG-N3B	-2.42	1.57	1.63
5	K	301	ANP	PB-O2B	2.40	1.63	1.56
5	L	302	ANP	PG-N3B	-2.36	1.57	1.63
5	K	301	ANP	PB-N3B	-2.31	1.57	1.63
5	K	301	ANP	PG-O1G	2.26	1.49	1.46
5	L	302	ANP	C2'-C3'	2.11	1.59	1.53
5	K	301	ANP	C5-C4	2.11	1.46	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	302	ANP	C1'-N9-C4	-6.10	115.92	126.64
5	L	302	ANP	N3-C2-N1	-5.18	120.58	128.68
5	K	301	ANP	N3-C2-N1	-4.68	121.36	128.68
5	K	301	ANP	O4'-C1'-C2'	-4.41	100.49	106.93
5	K	301	ANP	C1'-N9-C4	-4.31	119.07	126.64
5	K	301	ANP	O3G-PG-O1G	-4.10	103.14	113.45
5	L	302	ANP	O3A-PB-N3B	-3.97	95.58	106.59
5	K	301	ANP	O2B-PB-O3A	3.00	114.66	104.64
5	L	302	ANP	C4-C5-N7	-2.92	106.35	109.40
5	K	301	ANP	O3A-PB-N3B	-2.81	98.80	106.59
5	K	301	ANP	C4-C5-N7	-2.54	106.75	109.40
5	K	301	ANP	O5'-C5'-C4'	2.52	117.65	108.99
5	L	302	ANP	O2B-PB-O3A	2.51	113.01	104.64
5	L	302	ANP	O3G-PG-O1G	-2.25	107.79	113.45
5	L	302	ANP	PA-O5'-C5'	2.20	134.60	121.68
5	L	302	ANP	C3'-C2'-C1'	2.19	104.28	100.98
5	K	301	ANP	O4'-C4'-C3'	-2.13	100.89	105.11

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	301	ANP	PG-N3B-PB-O1B
5	K	301	ANP	PG-N3B-PB-O3A
5	L	302	ANP	PG-N3B-PB-O1B
5	L	302	ANP	PG-N3B-PB-O3A
5	L	302	ANP	C4'-C5'-O5'-PA
5	L	302	ANP	O4'-C4'-C5'-O5'
5	L	302	ANP	C3'-C4'-C5'-O5'
5	K	301	ANP	C4'-C5'-O5'-PA
5	K	301	ANP	PB-O3A-PA-O1A
5	K	301	ANP	O4'-C4'-C5'-O5'

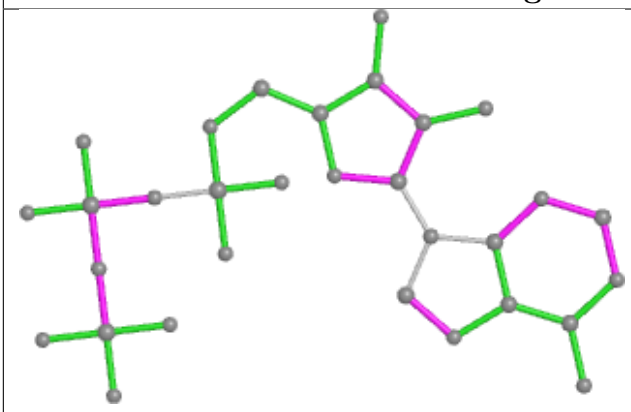
There are no ring outliers.

No monomer is involved in short contacts.

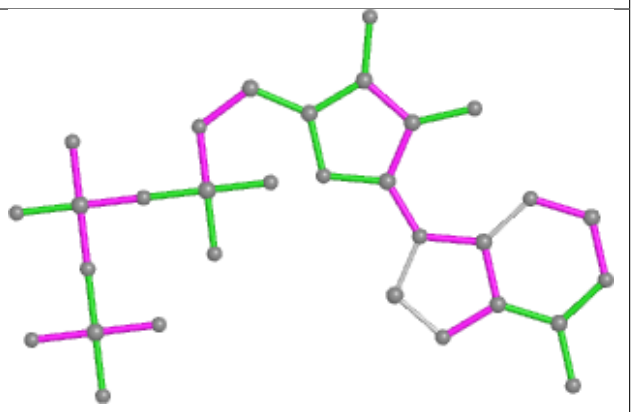
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

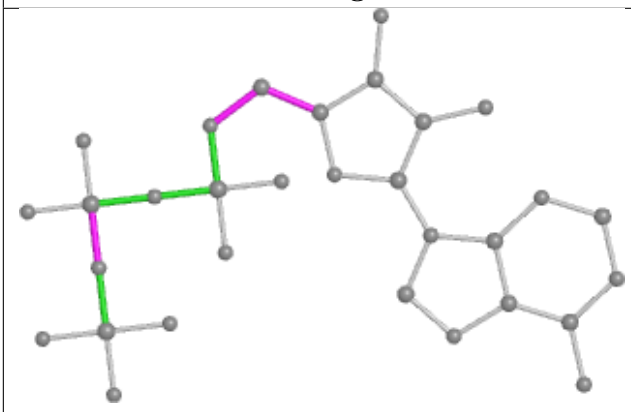
Ligand ANP L 302



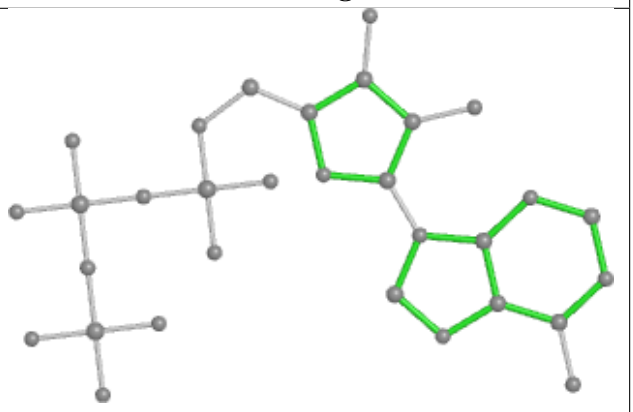
Bond lengths



Bond angles

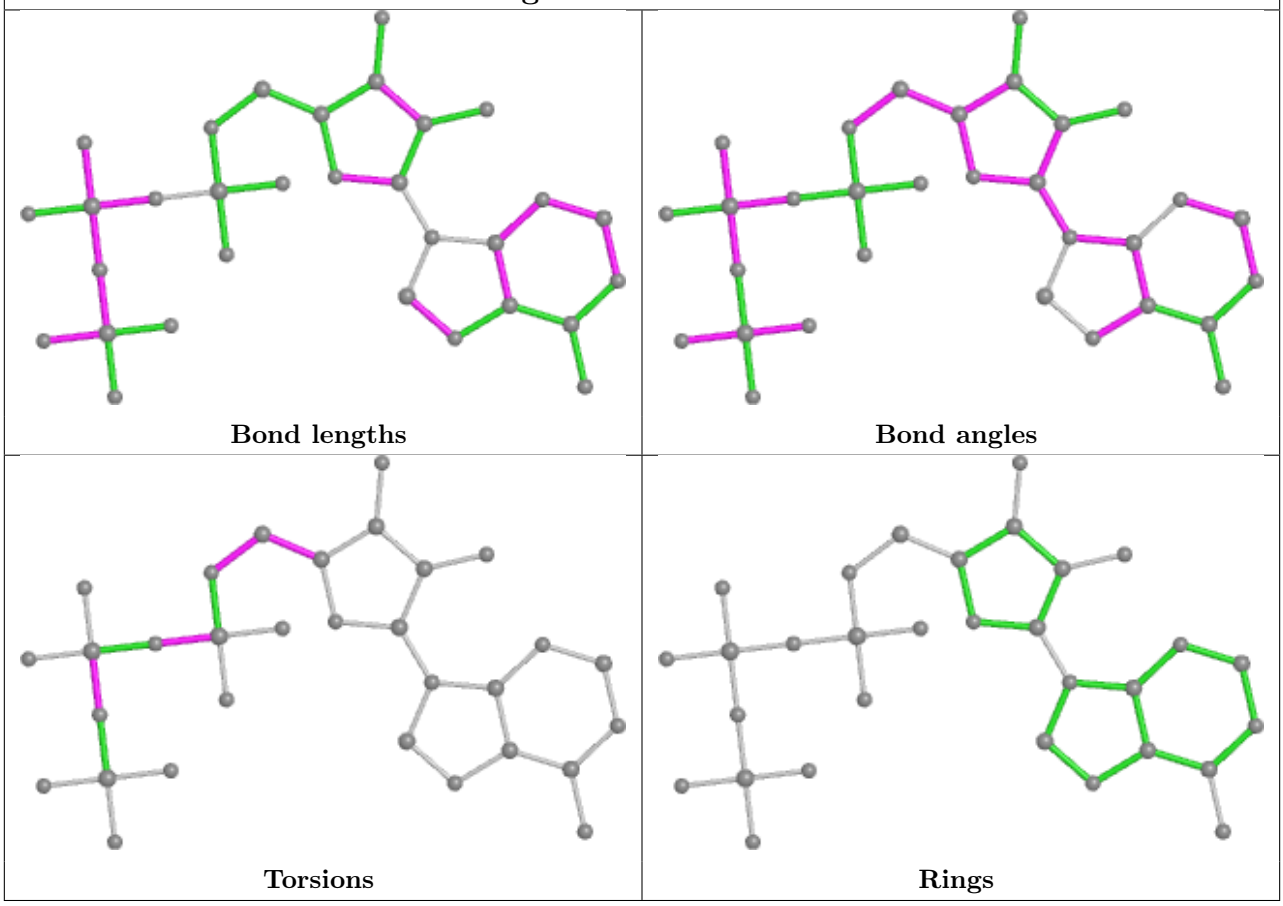


Torsions



Rings

Ligand ANP K 301



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.

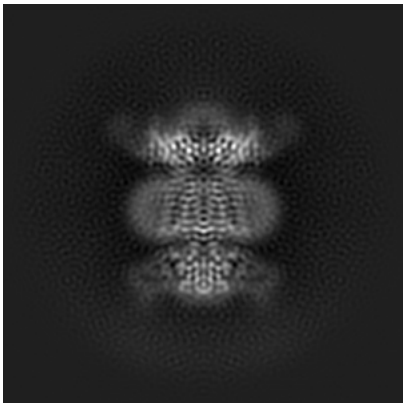
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11082. These allow visual inspection of the internal detail of the map and identification of artifacts.

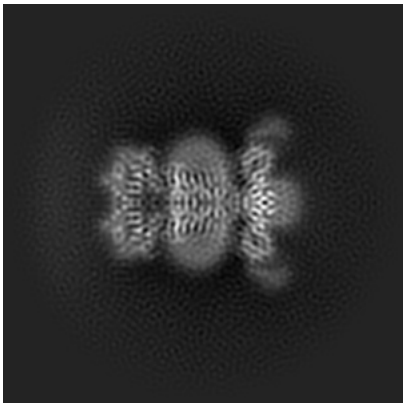
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

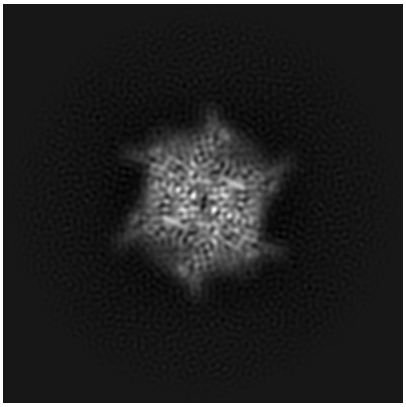
6.1.1 Primary map



X



Y

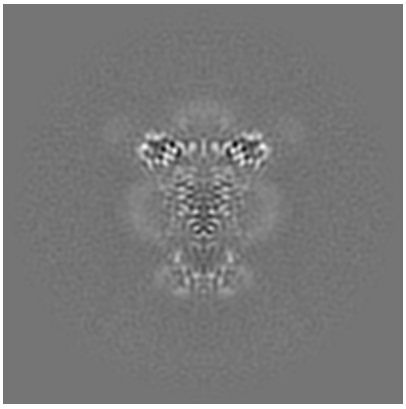


Z

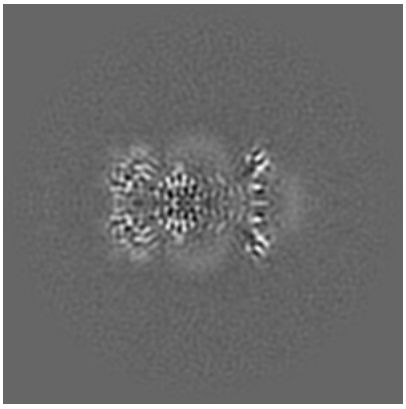
The images above show the map projected in three orthogonal directions.

6.2 Central slices

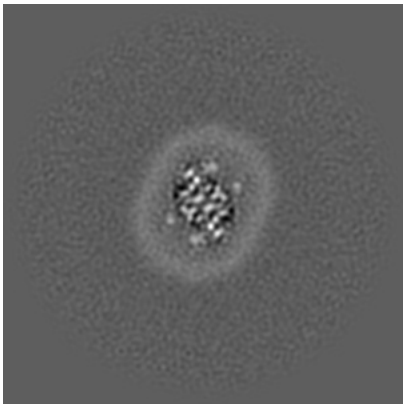
6.2.1 Primary map



X Index: 128



Y Index: 128

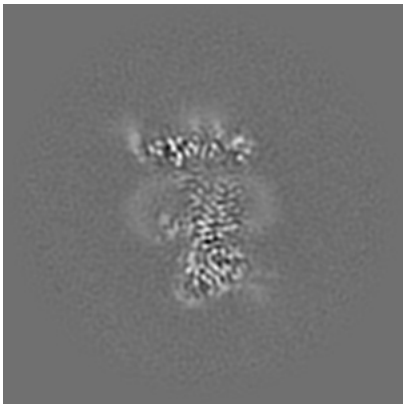


Z Index: 128

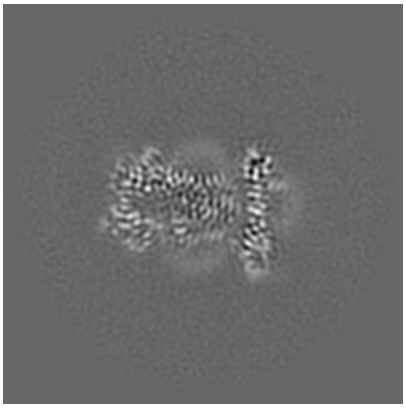
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

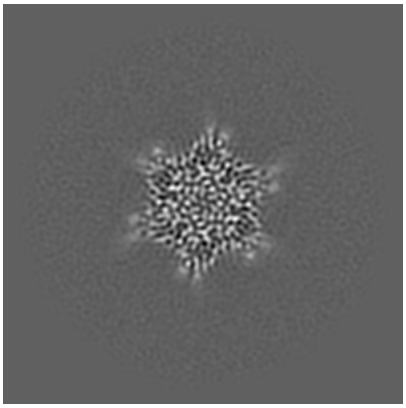
6.3.1 Primary map



X Index: 116



Y Index: 119



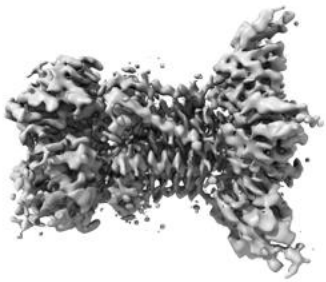
Z Index: 162

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

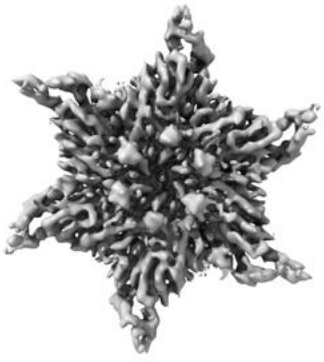
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.458. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

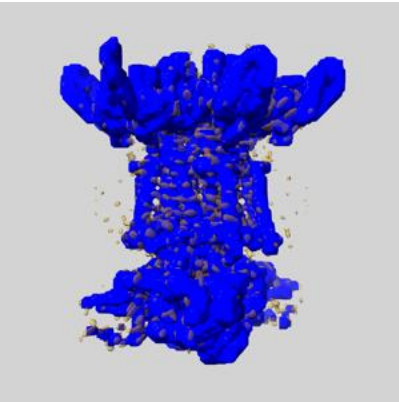
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

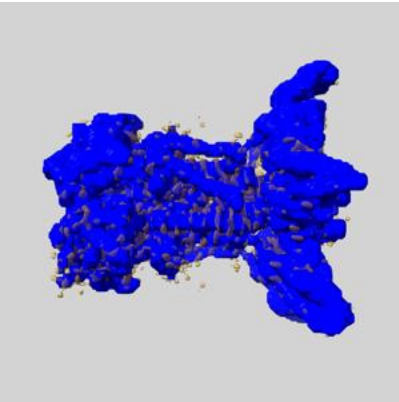
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

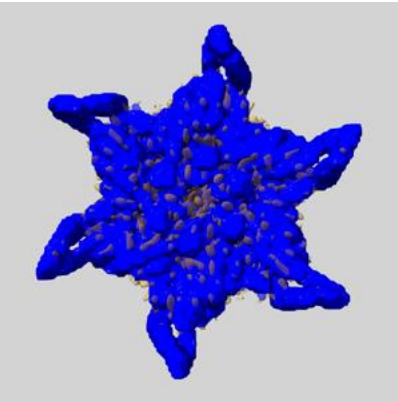
6.5.1 emd_11082_msk_1.map (i)



X



Y

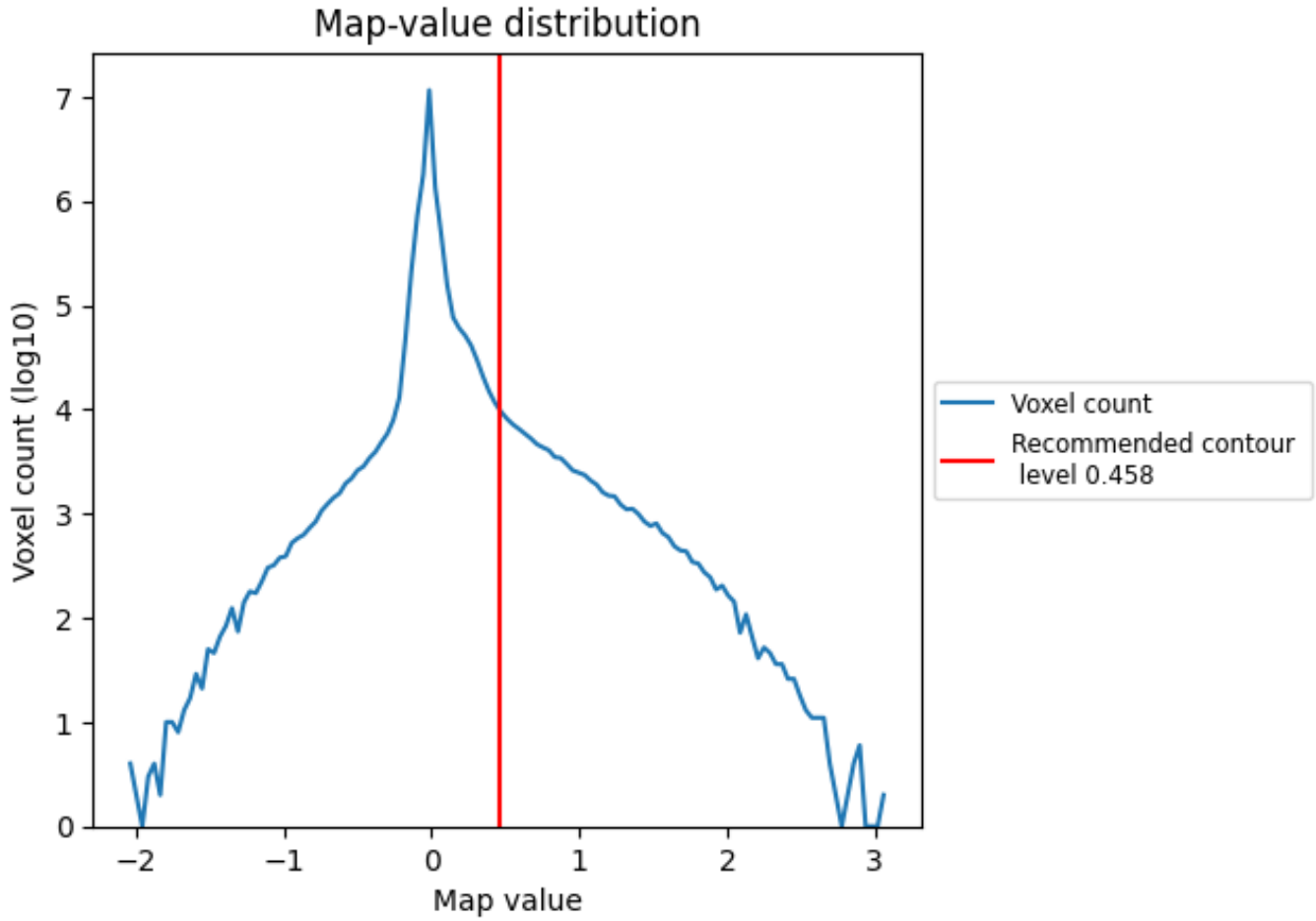


Z

7 Map analysis

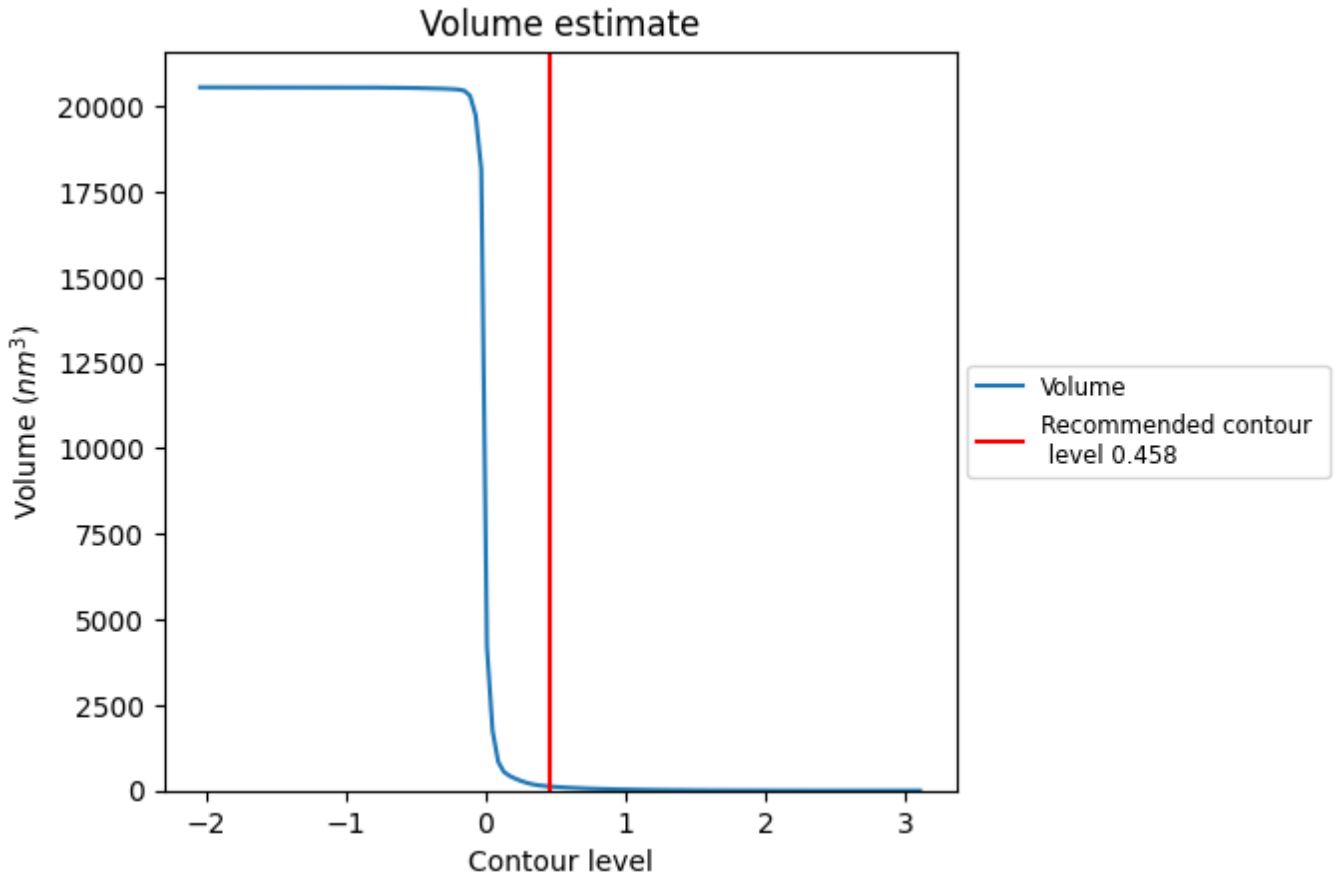
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

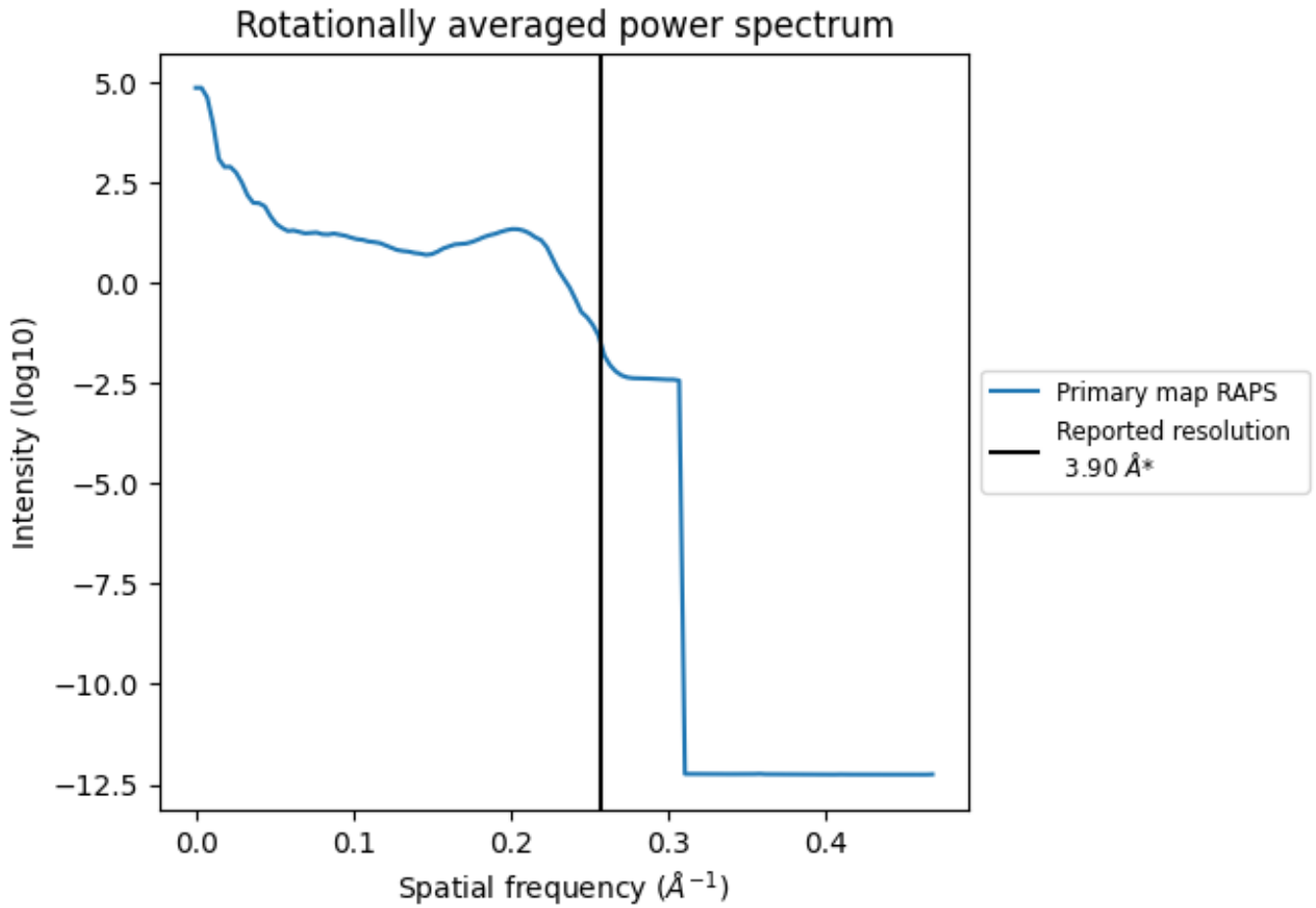
7.2 Volume estimate



The volume at the recommended contour level is 118 nm^3; this corresponds to an approximate mass of 107 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 0.256 $Å^{-1}$

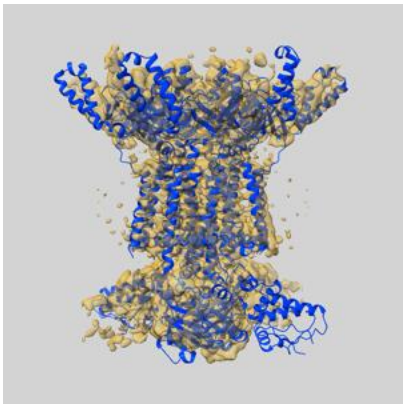
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

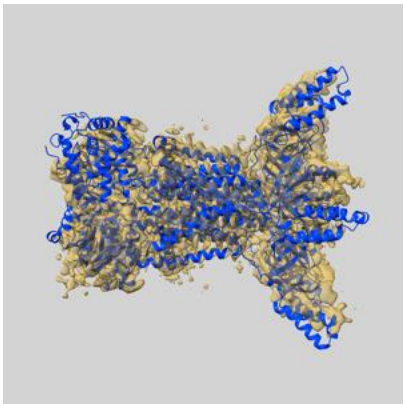
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11082 and PDB model 6Z5U. Per-residue inclusion information can be found in section 3 on page 6.

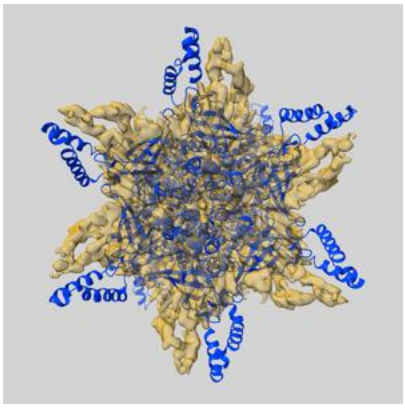
9.1 Map-model overlay



X



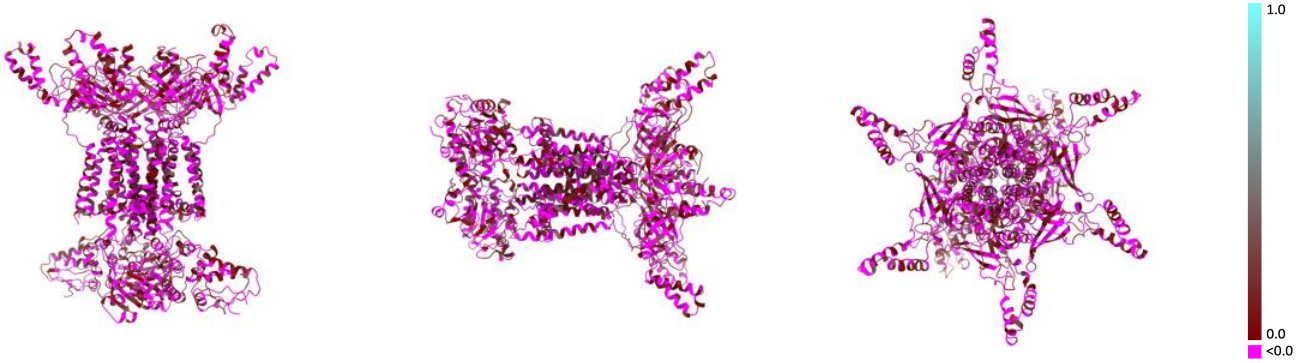
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.458 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.

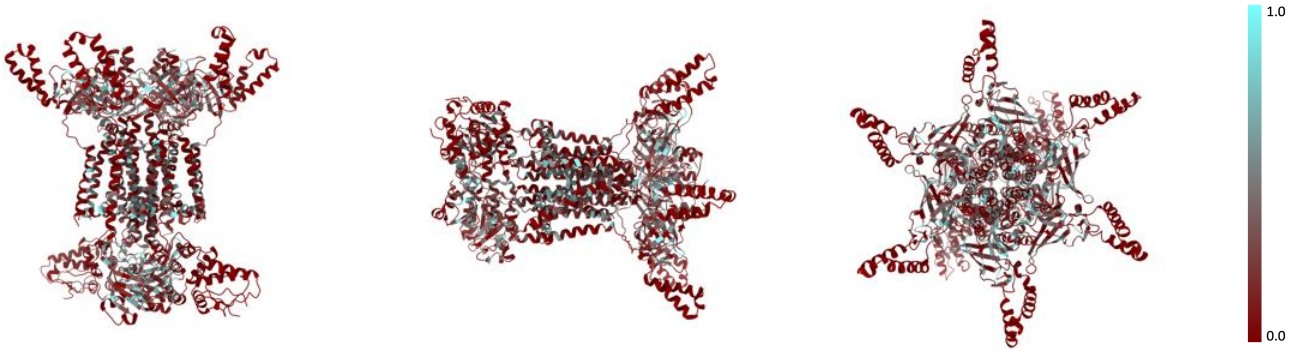
9.2 Q-score mapped to coordinate model (i)



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.

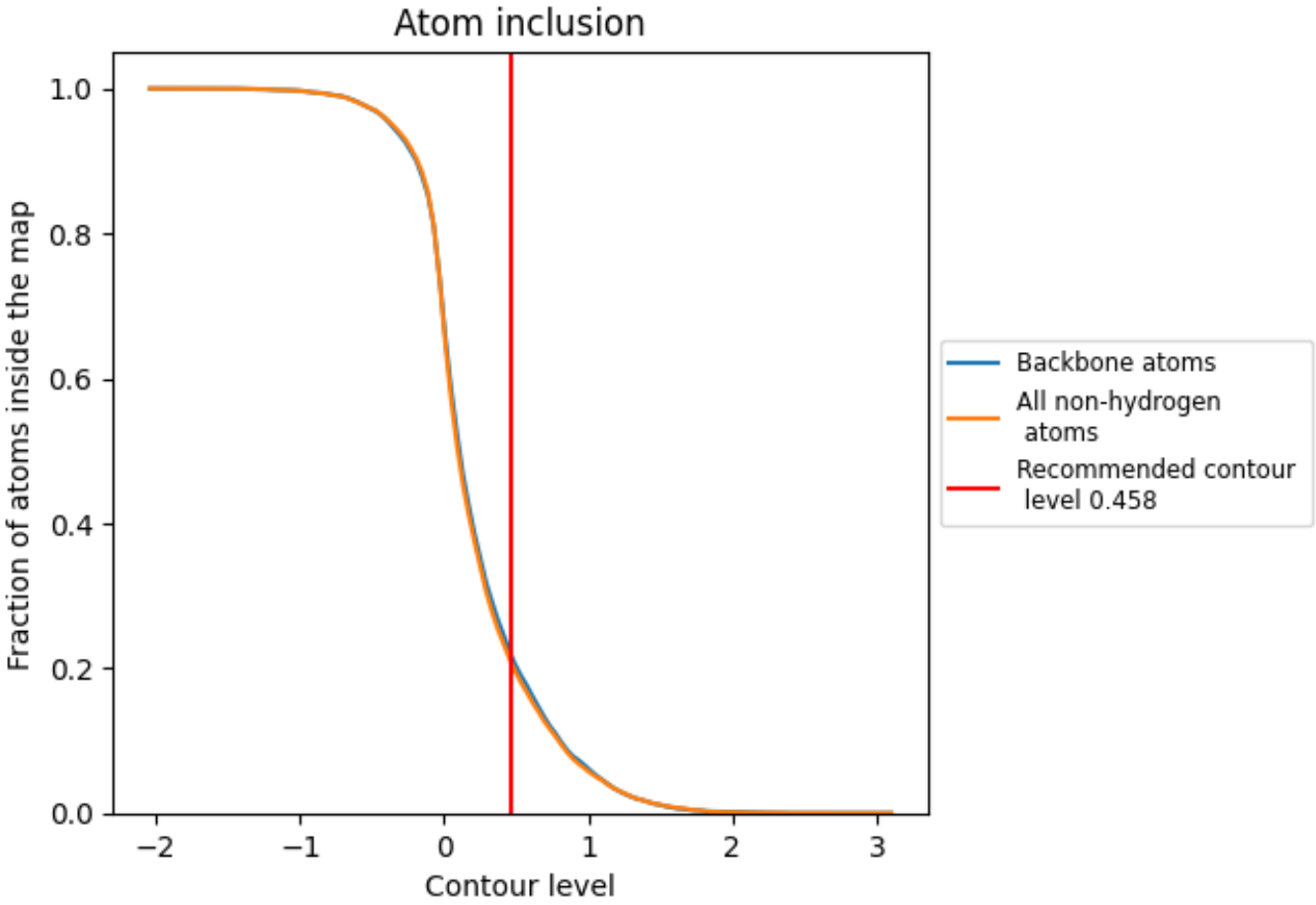
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.458).

9.4 Atom inclusion (i)



At the recommended contour level, 22% of all backbone atoms, 21% 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 (0.458) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2107	0.0030
A	0.2790	-0.0030
B	0.2806	0.0000
C	0.0000	-0.0060
D	0.0000	0.0010
E	0.2176	0.0110
F	0.1749	-0.0070
G	0.2176	0.0050
H	0.2123	0.0020
I	0.1749	-0.0060
J	0.2057	0.0100
K	0.2432	0.0080
L	0.2421	0.0120