



Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 02:38 PM EDT

PDB ID : 9YNE / pdb_00009yne
EMDB ID : EMD-73175
Title : Motor domain of human dynein-1 in pre-power stroke bound to dynactin-p15
0glued-CC1B-ICD and LIS1
Authors : Yang, J.; Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2025-10-10
Resolution : 8.46 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:

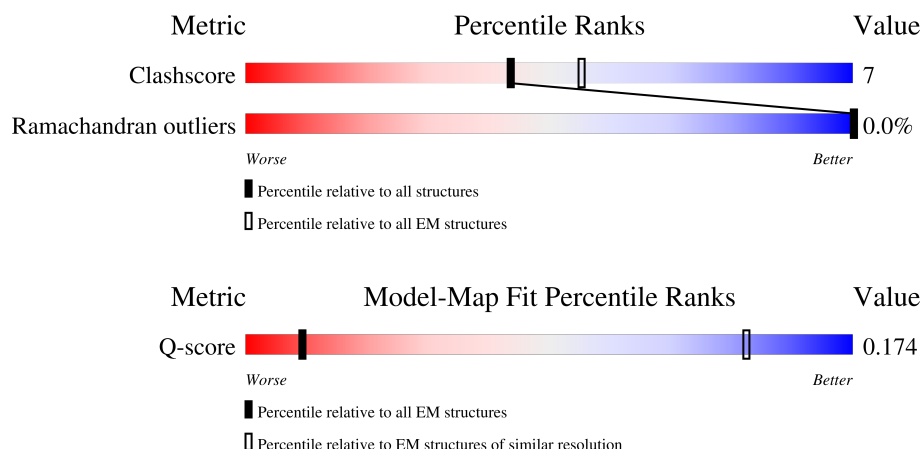
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 8.46 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	277 (7.97 - 8.96)

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 $\leq 5\%$. 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	4646	
2	B	410	
2	C	410	
3	D	638	
3	E	638	

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Mol	Chain	Length	Quality of chain
4	F	1281	38% 60%
4	G	1281	38% 60%
5	d	89	57% 91% 9%
5	i	89	93% 7%
6	k	113	9% 92% 8%
6	v	113	24% 88% 12%
7	u	492	23% 55% 43%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 29128 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	3270	Total	C	N	O	0	0
			16199	9659	3270	3270		

- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	402	Total	C	N	O	0	0
			1988	1184	402	402		
2	C	402	Total	C	N	O	0	0
			1988	1184	402	402		

- Molecule 3 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	35	Total	C	N	O	0	0
			175	105	35	35		
3	E	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 4 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	514	Total	C	N	O	0	0
			2549	1521	514	514		
4	G	516	Total	C	N	O	0	0
			2559	1527	516	516		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	118	ARG	LYS	conflict	UNP Q14203
F	124	SER	THR	conflict	UNP Q14203
F	125	ASN	THR	conflict	UNP Q14203

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Chain	Residue	Modelled	Actual	Comment	Reference
F	134	PRO	LEU	conflict	UNP Q14203
F	200	ALA	VAL	conflict	UNP Q14203
F	207	ALA	VAL	conflict	UNP Q14203
F	631	ASP	GLU	conflict	UNP Q14203
F	742	SER	CYS	conflict	UNP Q14203
F	778	SER	THR	conflict	UNP Q14203
F	821	ALA	PRO	conflict	UNP Q14203
F	862	PRO	LEU	conflict	UNP Q14203
F	1048	ILE	LEU	conflict	UNP Q14203
F	1072	GLY	ALA	conflict	UNP Q14203
F	1073	ALA	ILE	conflict	UNP Q14203
F	1080	ILE	SER	conflict	UNP Q14203
F	1113	VAL	ILE	conflict	UNP Q14203
F	1125	ALA	SER	conflict	UNP Q14203
F	1136	LEU	-	insertion	UNP Q14203
F	1137	PRO	-	insertion	UNP Q14203
F	1138	PRO	-	insertion	UNP Q14203
F	1147	ALA	PRO	conflict	UNP Q14203
F	1156	ASN	SER	conflict	UNP Q14203
F	1177	SER	THR	conflict	UNP Q14203
F	1189	LEU	MET	conflict	UNP Q14203
F	1193	THR	ALA	conflict	UNP Q14203
F	1202	ILE	VAL	conflict	UNP Q14203
F	1259	LEU	PHE	conflict	UNP Q14203
F	1277	ASP	SER	conflict	UNP Q14203
G	118	ARG	LYS	conflict	UNP Q14203
G	124	SER	THR	conflict	UNP Q14203
G	125	ASN	THR	conflict	UNP Q14203
G	134	PRO	LEU	conflict	UNP Q14203
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G	1156	ASN	SER	conflict	UNP Q14203
G	1177	SER	THR	conflict	UNP Q14203
G	1189	LEU	MET	conflict	UNP Q14203
G	1193	THR	ALA	conflict	UNP Q14203
G	1202	ILE	VAL	conflict	UNP Q14203
G	1259	LEU	PHE	conflict	UNP Q14203
G	1277	ASP	SER	conflict	UNP Q14203

- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	d	89	Total	C	N	O	0	0
			441	263	89	89		
5	i	89	Total	C	N	O	0	0
			441	263	89	89		

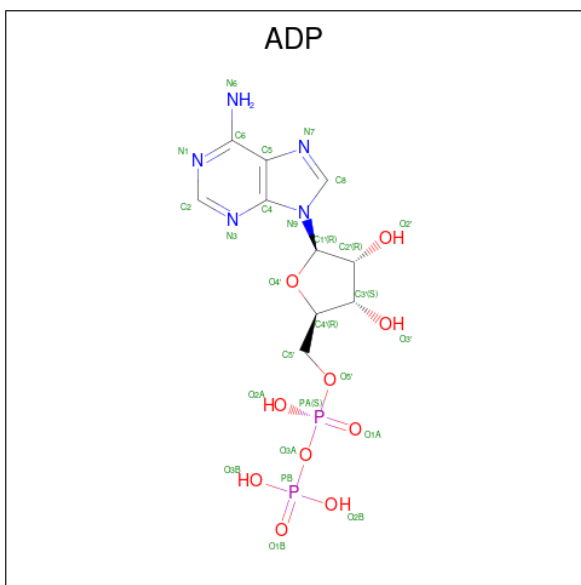
- Molecule 6 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	k	113	Total	C	N	O	0	0
			558	332	113	113		
6	v	113	Total	C	N	O	0	0
			558	332	113	113		

- Molecule 7 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	u	280	Total	C	N	O	0	0
			1383	823	280	280		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

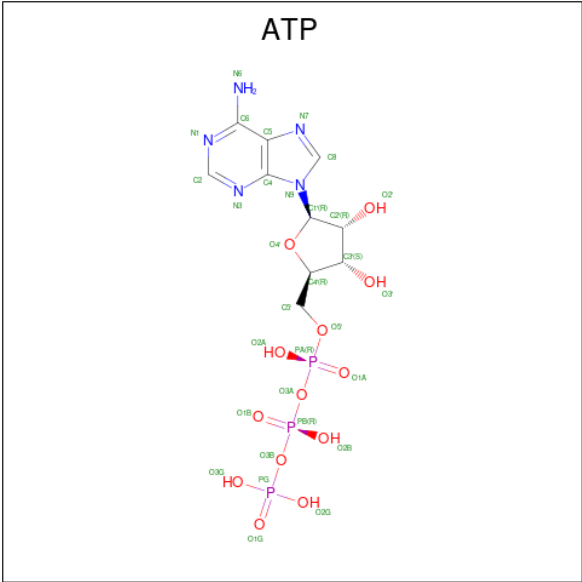


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

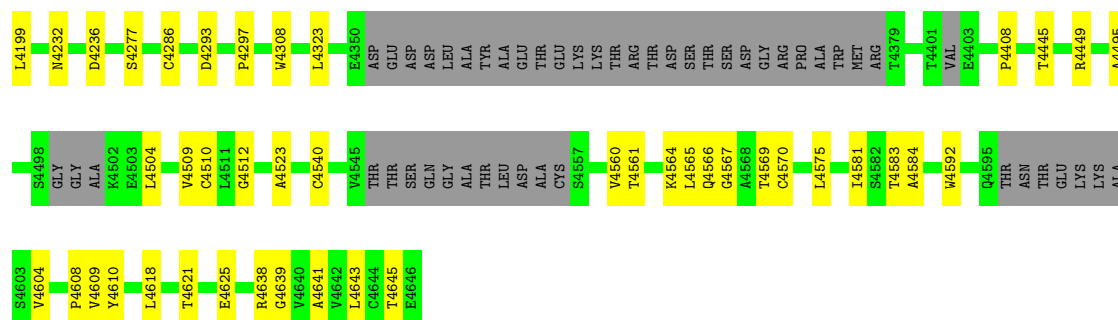
Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	Mg	0
			2	2	

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



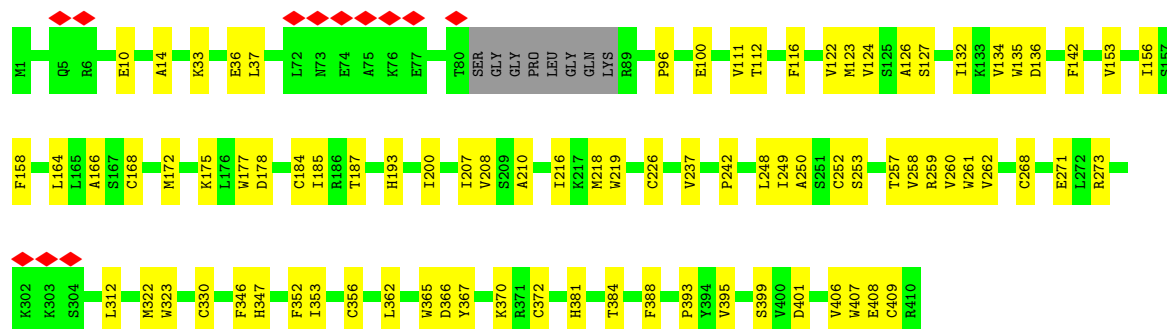
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			31	10	5	13	3	





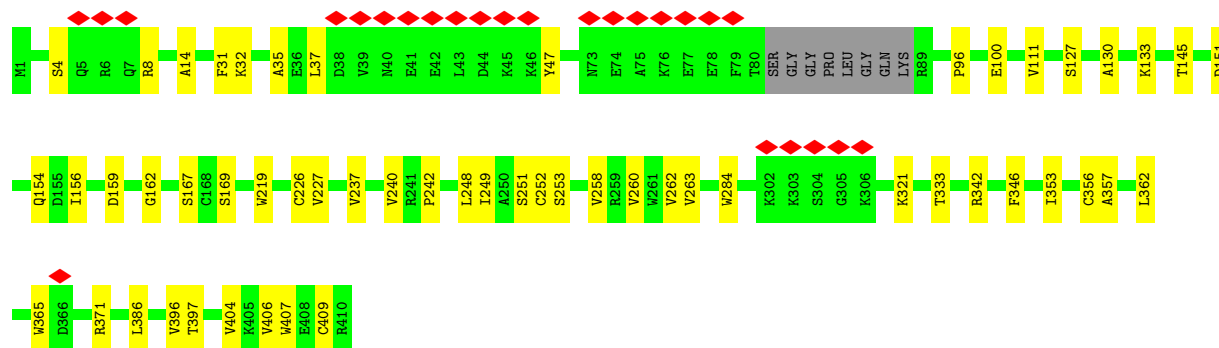
• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

Chain B: 78% 20%



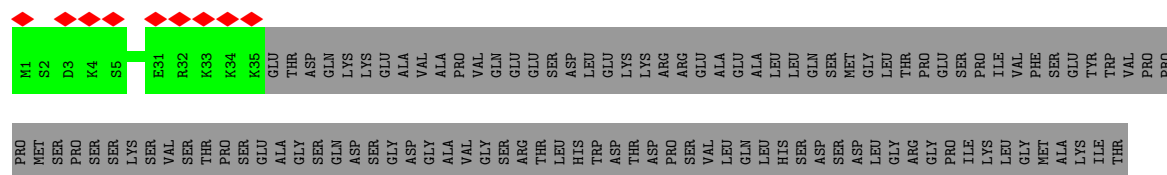
• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

Chain C: 6% 85% 13%



• Molecule 3: Cytoplasmic dynein 1 intermediate chain 2

Chain D: 5% 95%





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● Molecule 4: Dynactin subunit 1



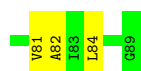
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● Molecule 4: Dynactin subunit 1

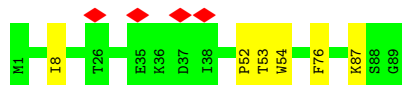
Response	Percentage
Yes	38%
No	60%

- Molecule 5: Dynein light chain 1, cytoplasmic

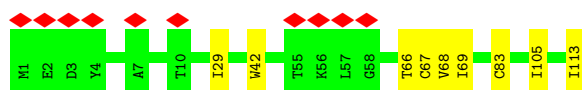
M1	C2	D3	R4	K5	A6	V7	I8	A11	D12	M13	S14	E15	E16	M17	Q18	Q19	D20	S21	V22	E23	E24	A25	T26	Q27	A28	L29	E30	K31	Y32	N33	I34	D37	I38	A39	A40	H41	I42	K43	K44	E45	F46	D47	K48	K49	Y50	N51	C56	G59	H72	F73	I74	Y75	F76	F77
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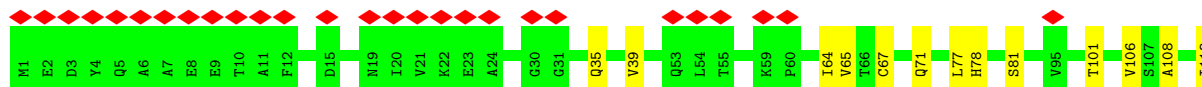
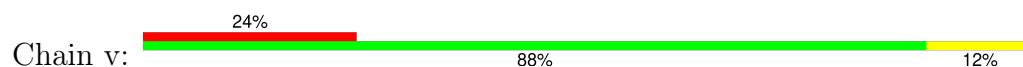
- Molecule 5: Dynein light chain 1, cytoplasmic



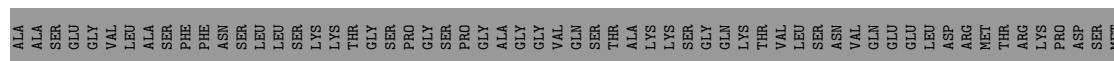
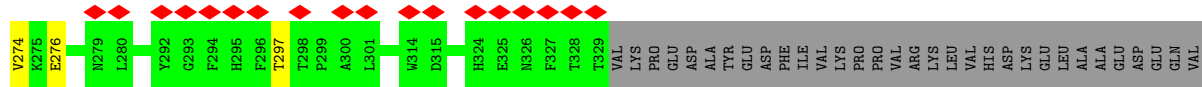
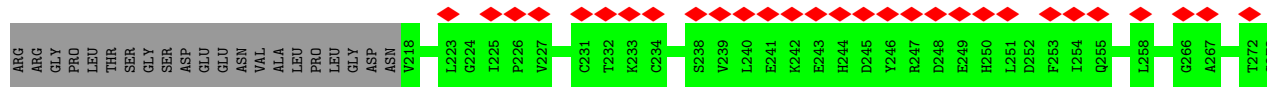
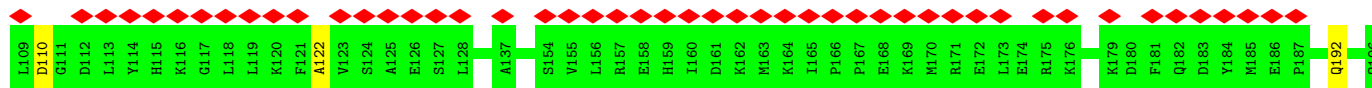
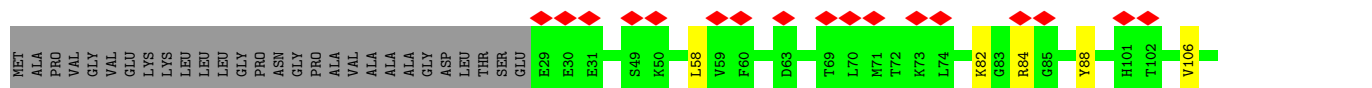
- Molecule 6: Dynein light chain Tctex-type 1



- Molecule 6: Dynein light chain Tctex-type 1



- Molecule 7: Cytoplasmic dynein 1 light intermediate chain 2



VAL
THR
ASN
SER
SER
THR
GLU
ASN
GLU
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52203	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.101	Depositor
Minimum map value	-0.524	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	520.80005, 520.80005, 520.80005	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.6040003, 2.6040003, 2.6040003	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/16185	0.55	0/22546
2	B	0.25	0/1986	0.61	0/2764
2	C	0.24	0/1986	0.64	2/2764 (0.1%)
3	D	0.21	0/174	0.44	0/242
3	E	0.17	0/174	0.47	0/242
4	F	0.24	0/2547	0.55	0/3550
4	G	0.21	0/2557	0.47	0/3564
5	d	0.24	0/440	0.61	1/612 (0.2%)
5	i	0.24	0/440	0.58	0/612
6	k	0.19	0/557	0.47	0/774
6	v	0.23	0/557	0.53	0/774
7	u	0.25	0/1381	0.66	0/1920
All	All	0.23	0/28984	0.56	3/40364 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	1
4	F	0	1
5	d	0	1
7	u	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	284	TRP	CA-C-N	-9.72	106.66	121.83
2	C	284	TRP	C-N-CA	-9.72	106.66	121.83
5	d	50	TYR	N-CA-C	5.59	117.15	110.44

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1729	LYS	Peptide
2	C	262	VAL	Peptide
4	F	810	ALA	Peptide
5	d	49	LYS	Peptide
7	u	82	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16199	0	7147	149	0
2	B	1988	0	878	47	0
2	C	1988	0	878	28	0
3	D	175	0	78	0	0
3	E	175	0	78	0	0
4	F	2549	0	1211	18	0
4	G	2559	0	1215	15	0
5	d	441	0	204	3	0
5	i	441	0	204	3	0
6	k	558	0	261	7	0
6	v	558	0	261	9	0
7	u	1383	0	604	6	0
8	A	81	0	36	6	0
9	A	2	0	0	0	0
10	A	31	0	12	2	0
All	All	29128	0	13067	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (275) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3928:THR:O	1:A:3932:ALA:HB2	1.63	0.99
1:A:1840:SER:HA	1:A:1862:ALA:HB2	1.57	0.87
1:A:4610:TYR:HA	1:A:4618:LEU:HA	1.57	0.87
1:A:1549:GLY:HA3	1:A:1642:GLY:HA2	1.55	0.86
1:A:4565:LEU:H	1:A:4583:THR:H	1.22	0.86
4:G:605:CYS:HA	4:G:686:GLY:HA3	1.59	0.84
2:B:237:VAL:HA	2:B:253:SER:HA	1.60	0.84
1:A:1350:PRO:HA	1:A:1430:THR:HA	1.61	0.81
1:A:2500:TRP:HA	1:A:2504:GLY:HA3	1.63	0.81
1:A:2616:GLU:H	1:A:2659:LEU:HA	1.46	0.81
2:B:248:LEU:HA	2:B:262:VAL:HA	1.62	0.80
1:A:4567:GLY:H	1:A:4581:ILE:HA	1.47	0.80
2:B:388:PHE:HA	2:B:395:VAL:HA	1.63	0.80
1:A:2473:ASN:HA	1:A:2481:MET:H	1.45	0.79
2:B:135:TRP:HA	2:B:142:PHE:HA	1.64	0.79
2:B:323:TRP:HA	2:B:330:CYS:HA	1.65	0.79
1:A:2252:HIS:H	1:A:2301:ILE:HA	1.48	0.77
4:G:816:ALA:HB3	4:G:914:ALA:HB3	1.66	0.77
2:B:208:VAL:HA	2:B:218:MET:HA	1.67	0.76
1:A:2537:TYR:HA	1:A:2547:PRO:HA	1.68	0.75
1:A:2639:CYS:HA	1:A:2653:VAL:H	1.52	0.75
1:A:2326:THR:HA	1:A:2332:ARG:HA	1.69	0.74
1:A:3928:THR:O	1:A:3932:ALA:CB	2.34	0.74
2:B:200:ILE:HA	2:B:207:ILE:HA	1.70	0.73
2:C:321:LYS:HA	2:C:333:THR:HA	1.71	0.73
1:A:1546:TYR:HA	1:A:1642:GLY:HA3	1.71	0.72
2:C:31:PHE:O	2:C:35:ALA:HB3	1.89	0.72
4:G:642:LEU:HA	4:G:647:GLY:HA3	1.69	0.72
1:A:1767:SER:HA	1:A:1832:ASN:HA	1.71	0.72
1:A:1954:TRP:HA	1:A:2013:ALA:H	1.55	0.70
5:d:77:TYR:HA	5:d:82:ALA:HA	1.74	0.70
1:A:1666:LEU:HA	1:A:1673:VAL:HA	1.73	0.70
1:A:2691:GLY:HA3	1:A:2702:LYS:HA	1.72	0.69
1:A:1763:GLU:HA	1:A:1833:ALA:HB2	1.74	0.69
2:B:177:TRP:HA	2:B:184:CYS:HA	1.74	0.69
7:u:84:ARG:HA	7:u:110:ASP:HA	1.72	0.69
1:A:1431:LEU:O	1:A:1435:TRP:CB	2.41	0.69
2:B:346:PHE:HA	2:B:353:ILE:HA	1.75	0.69
1:A:1902:GLY:HA2	1:A:2037:ARG:H	1.58	0.68
1:A:2995:ASP:HA	1:A:3067:THR:H	1.59	0.68
4:F:777:ALA:HA	4:F:781:ALA:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:v:65:VAL:HA	6:v:108:ALA:HA	1.74	0.68
7:u:58:LEU:HA	7:u:122:ALA:HB1	1.75	0.68
2:C:342:ARG:H	2:C:357:ALA:HA	1.60	0.66
1:A:1550:ILE:O	1:A:1554:SER:CB	2.44	0.66
1:A:1846:PHE:HA	1:A:1857:LEU:HA	1.76	0.66
2:C:133:LYS:HA	2:C:145:THR:HA	1.78	0.66
1:A:2582:TYR:O	1:A:2586:ALA:CB	2.44	0.65
7:u:192:GLN:HA	7:u:297:THR:HA	1.79	0.65
2:C:242:PRO:HA	2:C:249:ILE:HA	1.80	0.64
5:i:8:ILE:HA	5:i:76:PHE:HA	1.79	0.64
1:A:3505:GLY:HA3	1:A:3543:PHE:HA	1.78	0.64
1:A:3934:ALA:HB1	1:A:3995:ALA:HA	1.79	0.64
1:A:2763:ARG:HA	1:A:2766:ALA:HB2	1.78	0.64
1:A:3029:LEU:O	1:A:3033:CYS:CB	2.46	0.64
2:B:164:LEU:HA	2:B:178:ASP:HA	1.79	0.63
1:A:1765:ALA:HB1	1:A:1778:LEU:HA	1.81	0.62
4:F:654:ALA:HB1	4:F:759:CYS:HA	1.80	0.62
2:C:96:PRO:HA	2:C:409:CYS:HA	1.82	0.62
2:B:126:ALA:HA	2:B:132:ILE:HA	1.82	0.61
2:C:14:ALA:HA	2:C:47:TYR:O	1.99	0.61
1:A:2905:LEU:HA	1:A:3654:ARG:HA	1.81	0.61
1:A:3751:GLN:O	1:A:3755:GLU:CB	2.48	0.61
2:B:347:HIS:H	2:B:353:ILE:HA	1.66	0.61
2:C:396:VAL:HA	2:C:406:VAL:HA	1.82	0.61
1:A:2227:GLY:HA2	10:A:4803:ATP:H5'1	1.82	0.60
1:A:3718:LYS:HA	1:A:3722:PRO:HA	1.83	0.60
5:d:75:TYR:HA	5:d:84:LEU:HA	1.83	0.60
2:B:219:TRP:HA	2:B:226:CYS:HA	1.84	0.60
2:B:116:PHE:HA	2:B:123:MET:HA	1.84	0.59
1:A:3535:HIS:O	1:A:3539:ALA:HB3	2.02	0.59
2:C:219:TRP:HA	2:C:227:VAL:H	1.66	0.59
1:A:4174:ASN:H	1:A:4232:ASN:HA	1.67	0.59
2:B:153:VAL:HA	2:B:168:CYS:O	2.03	0.59
2:B:250:ALA:HA	2:B:260:VAL:HA	1.83	0.59
2:C:111:VAL:HA	2:C:127:SER:HA	1.83	0.58
1:A:1761:ASN:O	1:A:1765:ALA:HB2	2.02	0.58
2:C:346:PHE:HA	2:C:353:ILE:HA	1.85	0.58
1:A:2600:GLY:H	8:A:4805:ADP:H5'1	1.69	0.57
2:B:210:ALA:HA	2:B:216:ILE:HA	1.86	0.57
4:G:776:GLU:HA	4:G:781:ALA:HB3	1.86	0.57
1:A:1672:VAL:HA	1:A:1690:VAL:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2693:TYR:HA	1:A:2700:TRP:HA	1.86	0.57
1:A:4604:VAL:HA	1:A:4625:GLU:HA	1.87	0.56
1:A:2668:LEU:HA	1:A:2719:GLY:O	2.05	0.56
1:A:2582:TYR:O	1:A:2586:ALA:HB3	2.05	0.56
1:A:2651:ALA:HA	1:A:2705:ARG:H	1.69	0.56
1:A:2752:ASN:O	1:A:2756:LEU:CB	2.54	0.56
2:B:259:ARG:HA	2:B:271:GLU:HA	1.87	0.56
2:C:248:LEU:HA	2:C:263:VAL:H	1.72	0.55
6:v:67:CYS:HA	6:v:106:VAL:HA	1.89	0.55
6:k:66:THR:HA	6:v:81:SER:HA	1.89	0.55
1:A:4408:PRO:C	1:A:4523:ALA:HB1	2.31	0.55
2:B:352:PHE:HA	2:B:366:ASP:HA	1.89	0.55
2:C:100:GLU:HA	2:C:407:TRP:HA	1.88	0.55
1:A:4088:VAL:HA	1:A:4119:HIS:H	1.72	0.55
2:B:365:TRP:HA	2:B:372:CYS:HA	1.89	0.54
2:B:10:GLU:O	2:B:14:ALA:HB2	2.07	0.54
2:B:122:VAL:HA	2:B:136:ASP:HA	1.90	0.54
2:C:356:CYS:HA	2:C:362:LEU:HA	1.88	0.54
5:i:54:TRP:HA	5:i:87:LYS:HA	1.89	0.54
1:A:2426:TYR:HA	1:A:2431:GLY:HA3	1.89	0.54
1:A:2426:TYR:HA	1:A:2432:LEU:H	1.73	0.54
2:B:395:VAL:C	2:B:406:VAL:HA	2.33	0.54
2:B:172:MET:HA	2:B:193:HIS:O	2.07	0.54
4:F:423:ILE:O	4:F:427:LYS:CB	2.55	0.54
4:G:890:ARG:O	4:G:894:ASN:CB	2.55	0.54
2:B:242:PRO:HA	2:B:249:ILE:HA	1.88	0.54
1:A:2819:GLU:O	1:A:2866:ALA:HA	2.08	0.54
2:B:111:VAL:HA	2:B:127:SER:HA	1.89	0.54
1:A:1400:VAL:O	1:A:1404:LYS:CB	2.56	0.54
2:B:156:ILE:HA	2:B:166:ALA:O	2.09	0.53
2:C:386:LEU:HA	2:C:397:THR:HA	1.91	0.53
6:k:113:ILE:HA	6:v:113:ILE:HA	1.90	0.53
1:A:1673:VAL:O	1:A:1689:PRO:HA	2.08	0.53
1:A:4566:GLN:HA	1:A:4581:ILE:O	2.08	0.53
2:B:177:TRP:HA	2:B:185:ILE:H	1.73	0.53
1:A:1121:ASP:O	1:A:1125:LYS:CB	2.57	0.53
1:A:3589:ILE:HA	1:A:3699:VAL:O	2.09	0.53
2:B:175:LYS:HA	2:B:187:THR:HA	1.91	0.53
4:F:771:LEU:HA	4:F:861:LEU:O	2.10	0.53
2:C:4:SER:O	2:C:8:ARG:CB	2.57	0.52
2:C:154:GLN:H	2:C:169:SER:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:777:ALA:HA	4:F:781:ALA:CB	2.38	0.52
2:B:33:LYS:HA	2:B:37:LEU:H	1.74	0.52
2:B:312:LEU:HA	2:B:322:MET:HA	1.90	0.52
2:C:219:TRP:HA	2:C:226:CYS:HA	1.90	0.52
1:A:4608:PRO:O	1:A:4641:ALA:HB1	2.10	0.52
1:A:4297:PRO:HA	1:A:4308:TRP:CB	2.40	0.52
4:F:763:GLU:O	4:F:845:ALA:HB2	2.10	0.52
1:A:1582:VAL:O	1:A:1586:PRO:HA	2.10	0.52
1:A:4510:CYS:HA	1:A:4561:THR:C	2.35	0.52
1:A:4495:ALA:HB1	1:A:4504:LEU:HA	1.92	0.51
2:B:112:THR:H	2:B:127:SER:HA	1.75	0.51
2:B:33:LYS:C	2:B:36:GLU:H	2.17	0.51
2:B:124:VAL:HA	2:B:134:VAL:HA	1.91	0.51
4:G:771:LEU:HA	4:G:861:LEU:O	2.09	0.51
2:C:252:CYS:HA	2:C:258:VAL:HA	1.94	0.50
1:A:2930:GLN:HA	1:A:3063:HIS:HA	1.94	0.50
1:A:3613:SER:HA	1:A:3636:GLN:O	2.12	0.50
6:v:35:GLN:O	6:v:39:VAL:CB	2.60	0.50
1:A:1667:ASN:CB	1:A:1672:VAL:H	2.25	0.49
1:A:2198:GLU:C	1:A:2201:GLY:H	2.21	0.49
1:A:4510:CYS:HA	1:A:4561:THR:O	2.11	0.49
2:B:393:PRO:O	2:B:408:GLU:HA	2.12	0.49
1:A:1761:ASN:O	1:A:1765:ALA:CB	2.60	0.49
1:A:2582:TYR:O	1:A:2586:ALA:HB2	2.11	0.49
4:G:683:LYS:O	4:G:687:SER:CB	2.60	0.49
1:A:1956:CYS:HA	1:A:2015:PHE:H	1.77	0.49
4:F:928:ALA:HB1	4:G:590:ALA:HB1	1.95	0.49
1:A:2256:PRO:N	1:A:2305:GLY:HA3	2.28	0.49
1:A:3078:ARG:O	1:A:3082:SER:CB	2.60	0.49
1:A:3578:ILE:O	1:A:3582:ARG:CB	2.61	0.49
2:B:395:VAL:H	2:B:407:TRP:N	2.11	0.49
1:A:3179:PHE:O	1:A:3511:ALA:HB1	2.13	0.48
1:A:2569:VAL:N	8:A:4805:ADP:HN62	2.11	0.48
1:A:4199:LEU:HA	1:A:4639:GLY:HA3	1.95	0.48
1:A:2224:GLY:HA2	1:A:2364:PHE:O	2.13	0.48
1:A:4569:THR:O	1:A:4575:LEU:HA	2.14	0.48
2:C:130:ALA:HB2	2:C:151:ASP:C	2.38	0.48
5:i:52:PRO:HA	5:i:53:THR:HA	1.54	0.48
1:A:2539:VAL:HA	1:A:2545:TRP:HA	1.95	0.48
4:G:830:CYS:HA	4:G:896:LEU:HA	1.96	0.47
4:F:752:PHE:O	4:F:756:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:566:ALA:O	4:G:570:GLU:CB	2.61	0.47
1:A:2229:GLY:HA2	10:A:4803:ATP:H8	1.79	0.47
1:A:4323:LEU:HA	1:A:4638:ARG:HA	1.95	0.47
1:A:4564:LYS:HA	1:A:4584:ALA:HA	1.96	0.47
5:d:59:GLY:C	5:d:81:VAL:HA	2.39	0.47
2:B:261:TRP:HA	2:B:268:CYS:HA	1.96	0.47
4:F:592:MET:HA	4:G:591:PHE:O	2.14	0.47
1:A:2249:GLY:HA2	1:A:2298:ARG:O	2.13	0.47
1:A:1167:VAL:CB	1:A:1300:ALA:HA	2.45	0.47
1:A:4512:GLY:HA2	1:A:4645:THR:HA	1.97	0.46
1:A:3535:HIS:O	1:A:3539:ALA:CB	2.62	0.46
1:A:4445:THR:O	1:A:4449:ARG:CB	2.63	0.46
1:A:4570:CYS:HA	1:A:4575:LEU:HA	1.97	0.46
4:F:663:LEU:HA	4:F:724:ILE:HA	1.98	0.46
1:A:2251:ALA:HA	1:A:2300:TRP:O	2.15	0.46
1:A:2984:GLY:HA2	1:A:3057:GLN:CB	2.45	0.46
2:B:158:PHE:HA	2:B:164:LEU:O	2.15	0.46
1:A:3044:LEU:CB	1:A:3050:LEU:HA	2.45	0.46
6:k:29:ILE:HA	6:k:42:TRP:CB	2.46	0.46
7:u:84:ARG:HA	7:u:110:ASP:CA	2.42	0.46
1:A:1751:VAL:HA	1:A:1811:LEU:HA	1.98	0.46
1:A:3950:LYS:O	1:A:3954:ASP:CB	2.64	0.46
7:u:274:VAL:C	7:u:276:GLU:H	2.23	0.46
1:A:1178:ARG:HA	4:F:909:GLU:HA	1.98	0.46
1:A:2618:VAL:H	1:A:2661:LEU:HA	1.81	0.46
4:G:597:LEU:HA	4:G:603:HIS:CB	2.45	0.46
1:A:2614:ASP:O	1:A:2657:LYS:HA	2.16	0.45
1:A:2938:VAL:HA	1:A:3069:ASN:HA	1.98	0.45
1:A:2324:LEU:HA	1:A:2334:SER:HA	1.99	0.45
1:A:4509:VAL:H	1:A:4560:VAL:HA	1.82	0.45
1:A:1675:GLY:HA3	1:A:1685:MET:HA	1.98	0.45
4:F:620:GLU:O	4:F:624:LYS:CB	2.64	0.45
2:C:365:TRP:HA	2:C:371:ARG:O	2.17	0.45
1:A:2537:TYR:HA	1:A:2548:TRP:H	1.81	0.45
2:C:237:VAL:HA	2:C:253:SER:HA	1.99	0.45
6:k:69:ILE:O	6:v:77:LEU:HA	2.16	0.45
1:A:2981:ARG:O	1:A:2985:CYS:CB	2.64	0.45
2:C:159:ASP:C	2:C:162:GLY:H	2.25	0.45
1:A:2933:LEU:HA	1:A:3090:VAL:N	2.33	0.44
1:A:2228:SER:CB	1:A:2366:GLU:HA	2.47	0.44
1:A:2592:VAL:HA	1:A:2710:GLY:C	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1842:MET:HA	1:A:1861:MET:HA	1.98	0.44
1:A:4610:TYR:O	1:A:4643:LEU:HA	2.17	0.44
4:G:743:THR:HA	4:G:817:LEU:CB	2.48	0.44
1:A:1758:TRP:O	1:A:1762:VAL:CB	2.66	0.44
1:A:1911:GLY:HA3	8:A:4801:ADP:C8	2.52	0.44
1:A:4236:ASP:H	1:A:4277:SER:HA	1.82	0.44
2:B:356:CYS:HA	2:B:362:LEU:HA	1.98	0.44
4:G:871:PHE:HA	4:G:885:PRO:N	2.32	0.44
1:A:1175:SER:HA	4:F:811:PRO:O	2.17	0.44
4:F:690:PRO:O	4:F:694:ALA:HB2	2.17	0.43
1:A:1869:GLY:N	1:A:1924:GLY:HA3	2.33	0.43
1:A:2672:ASP:H	1:A:2676:THR:N	2.17	0.43
1:A:2183:LYS:HA	1:A:2193:TYR:CB	2.49	0.43
1:A:4609:VAL:H	1:A:4621:THR:HA	1.83	0.43
1:A:4236:ASP:N	1:A:4277:SER:HA	2.34	0.43
1:A:2725:HIS:O	1:A:2729:ARG:CB	2.67	0.43
4:F:830:CYS:CB	4:F:896:LEU:HA	2.49	0.43
7:u:88:TYR:HA	7:u:106:VAL:O	2.19	0.43
1:A:2942:GLY:HA2	8:A:4806:ADP:H5'2	2.00	0.43
1:A:2995:ASP:H	1:A:2998:ASN:CB	2.32	0.43
2:B:252:CYS:HA	2:B:258:VAL:HA	2.01	0.43
6:k:83:CYS:HA	6:v:64:ILE:HA	2.01	0.43
1:A:2813:LEU:C	1:A:2815:THR:H	2.26	0.42
1:A:2951:ALA:HB1	1:A:2956:LEU:O	2.19	0.42
1:A:2264:LEU:HA	1:A:2280:PHE:H	1.84	0.42
2:B:100:GLU:HA	2:B:407:TRP:HA	2.01	0.42
4:F:436:ALA:HB1	4:G:436:ALA:HB3	2.00	0.42
4:F:852:ILE:HA	4:F:855:LEU:CB	2.50	0.42
1:A:1858:SER:HA	1:A:1867:ASN:HA	2.00	0.42
1:A:3947:LEU:O	1:A:3951:VAL:CB	2.67	0.42
2:C:156:ILE:HA	2:C:167:SER:HA	2.00	0.42
1:A:1675:GLY:HA2	1:A:1686:PHE:H	1.84	0.42
1:A:4112:LYS:O	1:A:4116:LEU:CB	2.67	0.42
2:B:384:THR:H	2:B:399:SER:HA	1.83	0.42
1:A:1416:LEU:O	1:A:1420:LEU:CB	2.68	0.42
1:A:3939:SER:HA	1:A:3945:LYS:HA	2.00	0.42
1:A:4540:CYS:O	1:A:4592:TRP:HA	2.19	0.42
1:A:4565:LEU:N	1:A:4583:THR:H	2.04	0.42
1:A:1950:GLN:HA	1:A:2007:LYS:O	2.19	0.42
1:A:2266:GLY:HA2	1:A:2278:GLY:N	2.34	0.42
1:A:2430:ASN:HA	1:A:2434:THR:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1167:VAL:HA	1:A:1303:ALA:HB3	2.01	0.41
1:A:1473:TYR:C	1:A:1588:VAL:H	2.28	0.41
1:A:1762:VAL:HA	1:A:1765:ALA:HB3	2.02	0.41
2:B:381:HIS:H	2:B:401:ASP:CB	2.34	0.41
6:k:68:VAL:HA	6:v:78:HIS:O	2.20	0.41
1:A:2000:GLU:HA	1:A:2005:GLN:HA	2.00	0.41
1:A:2780:SER:O	1:A:2784:PHE:CB	2.69	0.41
6:v:71:GLN:HA	6:v:101:THR:O	2.20	0.41
6:k:67:CYS:HA	6:k:105:ILE:O	2.20	0.41
1:A:4286:CYS:HA	1:A:4293:ASP:HA	2.02	0.41
2:C:397:THR:O	2:C:404:VAL:HA	2.21	0.41
1:A:3563:GLN:HA	1:A:3567:LEU:O	2.21	0.41
1:A:4569:THR:HA	1:A:4583:THR:CB	2.51	0.41
1:A:1677:SER:HA	1:A:1683:GLU:HA	2.03	0.41
1:A:1909:GLY:HA2	8:A:4801:ADP:H5'1	2.01	0.41
1:A:2266:GLY:HA2	1:A:2278:GLY:H	1.86	0.41
1:A:2318:VAL:O	1:A:2323:LYS:HA	2.21	0.41
2:C:240:VAL:HA	2:C:251:SER:HA	2.03	0.41
2:C:251:SER:H	2:C:260:VAL:HA	1.86	0.41
4:F:819:PHE:CB	4:F:912:TYR:HA	2.51	0.41
2:B:96:PRO:HA	2:B:409:CYS:HA	2.03	0.40
2:C:32:LYS:HA	2:C:37:LEU:CB	2.51	0.40
1:A:1233:GLN:HA	1:A:1236:VAL:CB	2.51	0.40
2:B:257:THR:HA	2:B:273:ARG:HA	2.03	0.40
1:A:2872:LEU:O	1:A:2883:PRO:HA	2.22	0.40
1:A:2600:GLY:N	8:A:4805:ADP:H5'1	2.35	0.40
1:A:3022:GLU:C	1:A:3026:TYR:H	2.29	0.40
2:B:10:GLU:O	2:B:14:ALA:CB	2.69	0.40
2:B:367:TYR:C	2:B:370:LYS:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	3242/4646 (70%)	3023 (93%)	218 (7%)	1 (0%)	100	100
2	B	398/410 (97%)	339 (85%)	59 (15%)	0	100	100
2	C	398/410 (97%)	364 (92%)	34 (8%)	0	100	100
3	D	33/638 (5%)	33 (100%)	0	0	100	100
3	E	33/638 (5%)	33 (100%)	0	0	100	100
4	F	510/1281 (40%)	485 (95%)	25 (5%)	0	100	100
4	G	512/1281 (40%)	494 (96%)	18 (4%)	0	100	100
5	d	87/89 (98%)	78 (90%)	9 (10%)	0	100	100
5	i	87/89 (98%)	76 (87%)	11 (13%)	0	100	100
6	k	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
6	v	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
7	u	276/492 (56%)	249 (90%)	27 (10%)	0	100	100
All	All	5798/10200 (57%)	5379 (93%)	418 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1647	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
8	ADP	A	4801	9	28,29,29	1.42	4 (14%)	43,45,45	1.91	9 (20%)
10	ATP	A	4803	9	32,33,33	0.39	0	48,52,52	0.52	1 (2%)
8	ADP	A	4806	-	28,29,29	1.46	5 (17%)	43,45,45	1.85	8 (18%)
8	ADP	A	4805	-	28,29,29	1.41	4 (14%)	43,45,45	1.89	11 (25%)

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
8	ADP	A	4801	9	-	5/16/32/32	0/3/3/3
10	ATP	A	4803	9	-	6/22/38/38	0/3/3/3
8	ADP	A	4806	-	-	5/16/32/32	0/3/3/3
8	ADP	A	4805	-	-	4/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	4806	ADP	C5-C4	4.97	1.47	1.39
8	A	4801	ADP	C5-C4	4.86	1.47	1.39
8	A	4805	ADP	C5-C4	4.75	1.47	1.39
8	A	4805	ADP	C5-C6	2.81	1.48	1.41
8	A	4806	ADP	C5-C6	2.73	1.48	1.41
8	A	4801	ADP	C5-C6	2.57	1.48	1.41
8	A	4801	ADP	C5-N7	-2.49	1.34	1.39
8	A	4806	ADP	C5-N7	-2.40	1.34	1.39
8	A	4805	ADP	C8-N7	2.30	1.36	1.31
8	A	4806	ADP	C8-N7	2.23	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	4805	ADP	C5-N7	-2.19	1.35	1.39
8	A	4801	ADP	C8-N7	2.11	1.35	1.31
8	A	4806	ADP	PA-O3A	2.01	1.61	1.59

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	4801	ADP	C5-C4-N3	-6.33	118.00	126.72
8	A	4806	ADP	C5-C4-N3	-6.19	118.20	126.72
8	A	4805	ADP	C5-C4-N3	-5.89	118.60	126.72
8	A	4801	ADP	N3-C4-N9	5.26	136.12	127.17
8	A	4806	ADP	N3-C4-N9	4.88	135.47	127.17
8	A	4805	ADP	N3-C4-N9	4.79	135.32	127.17
8	A	4801	ADP	C2-N3-C4	3.84	121.22	111.83
8	A	4805	ADP	C2-N3-C4	3.72	120.91	111.83
8	A	4806	ADP	C2-N3-C4	3.71	120.89	111.83
8	A	4801	ADP	N3-C2-N1	-3.47	123.33	128.58
8	A	4805	ADP	C4-C5-N7	-3.46	106.63	110.58
8	A	4806	ADP	C4-C5-N7	-3.37	106.73	110.58
8	A	4805	ADP	N3-C2-N1	-3.17	123.78	128.58
8	A	4801	ADP	C4-C5-N7	-3.12	107.01	110.58
8	A	4806	ADP	N3-C2-N1	-3.06	123.96	128.58
8	A	4805	ADP	C4-N9-C8	2.81	108.69	105.74
8	A	4806	ADP	C3'-C2'-C1'	2.74	106.64	101.46
8	A	4805	ADP	C5-N7-C8	2.60	107.54	103.45
8	A	4801	ADP	C3'-C2'-C1'	2.47	106.13	101.46
8	A	4805	ADP	C3'-C2'-C1'	2.45	106.10	101.46
8	A	4801	ADP	C5-N7-C8	2.40	107.22	103.45
8	A	4801	ADP	C4-N9-C8	2.33	108.18	105.74
8	A	4806	ADP	C5-N7-C8	2.26	107.00	103.45
8	A	4805	ADP	C2'-C1'-N9	-2.19	107.87	113.30
8	A	4801	ADP	C2-N1-C6	2.17	122.30	118.73
10	A	4803	ATP	C4'-O4'-C1'	-2.08	104.86	109.47
8	A	4805	ADP	C6-C5-N7	2.07	136.08	132.09
8	A	4805	ADP	N9-C8-N7	-2.02	111.06	113.94
8	A	4806	ADP	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	4801	ADP	PA-O3A-PB-O3B

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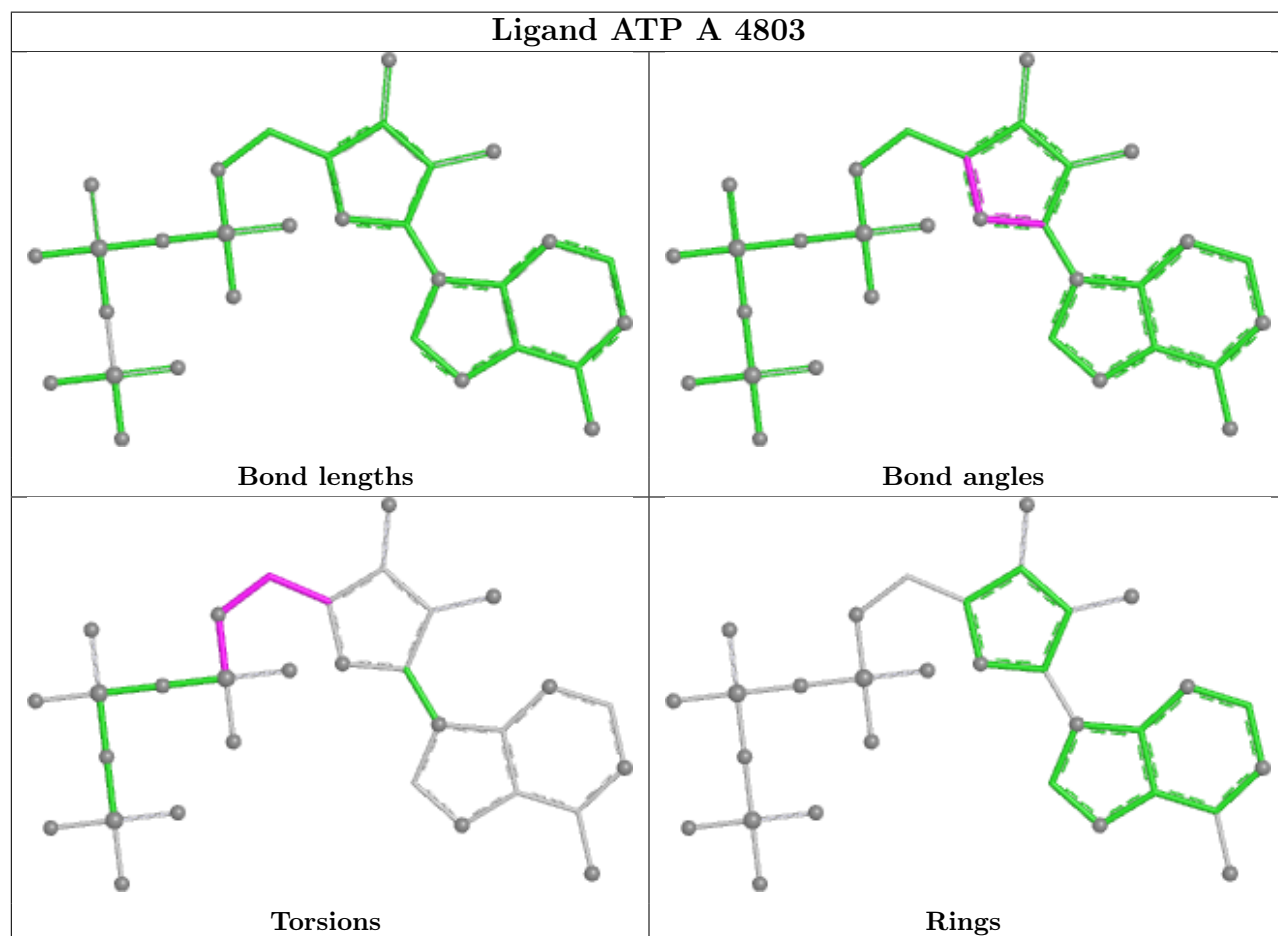
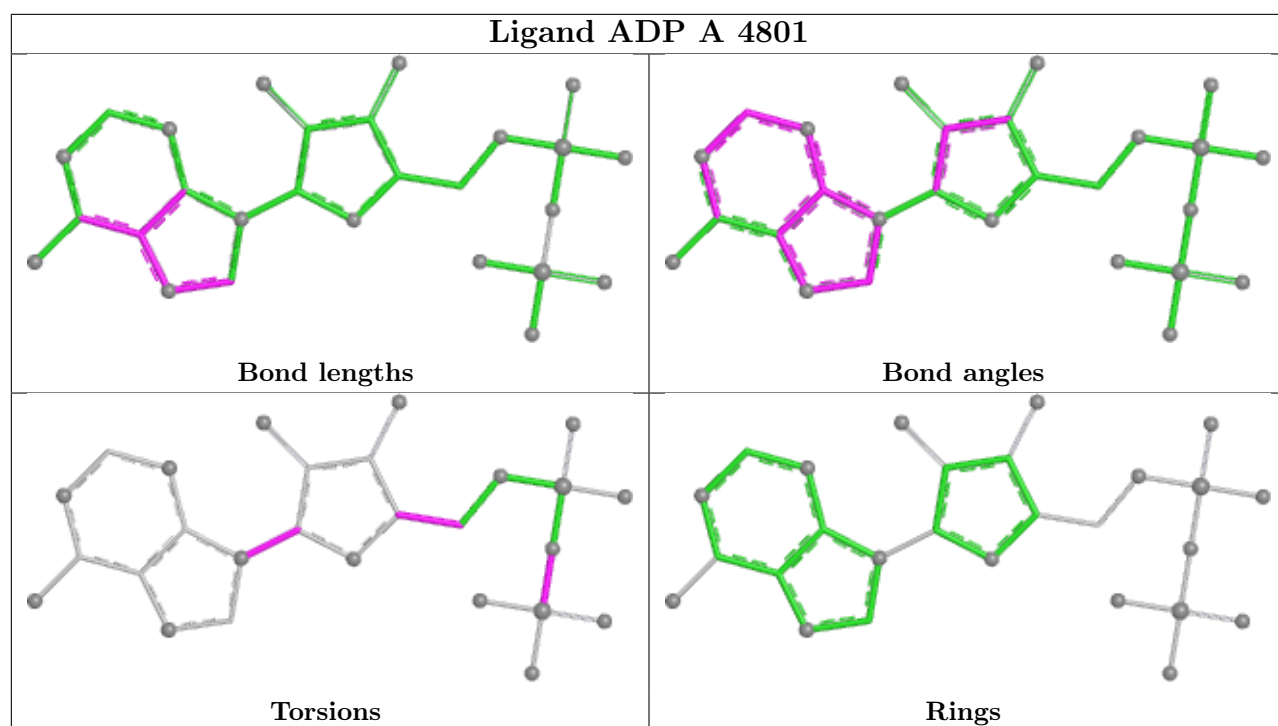
Mol	Chain	Res	Type	Atoms
8	A	4805	ADP	C5'-O5'-PA-O3A
8	A	4806	ADP	C5'-O5'-PA-O2A
10	A	4803	ATP	C5'-O5'-PA-O2A
8	A	4806	ADP	C3'-C4'-C5'-O5'
10	A	4803	ATP	O4'-C4'-C5'-O5'
8	A	4805	ADP	O4'-C4'-C5'-O5'
8	A	4806	ADP	O4'-C4'-C5'-O5'
10	A	4803	ATP	C3'-C4'-C5'-O5'
8	A	4805	ADP	C3'-C4'-C5'-O5'
8	A	4801	ADP	PA-O3A-PB-O2B
10	A	4803	ATP	C4'-C5'-O5'-PA
8	A	4805	ADP	C5'-O5'-PA-O1A
8	A	4806	ADP	C5'-O5'-PA-O1A
8	A	4806	ADP	C5'-O5'-PA-O3A
10	A	4803	ATP	C5'-O5'-PA-O1A
10	A	4803	ATP	C5'-O5'-PA-O3A
8	A	4801	ADP	PA-O3A-PB-O1B
8	A	4801	ADP	C2'-C1'-N9-C8
8	A	4801	ADP	O4'-C4'-C5'-O5'

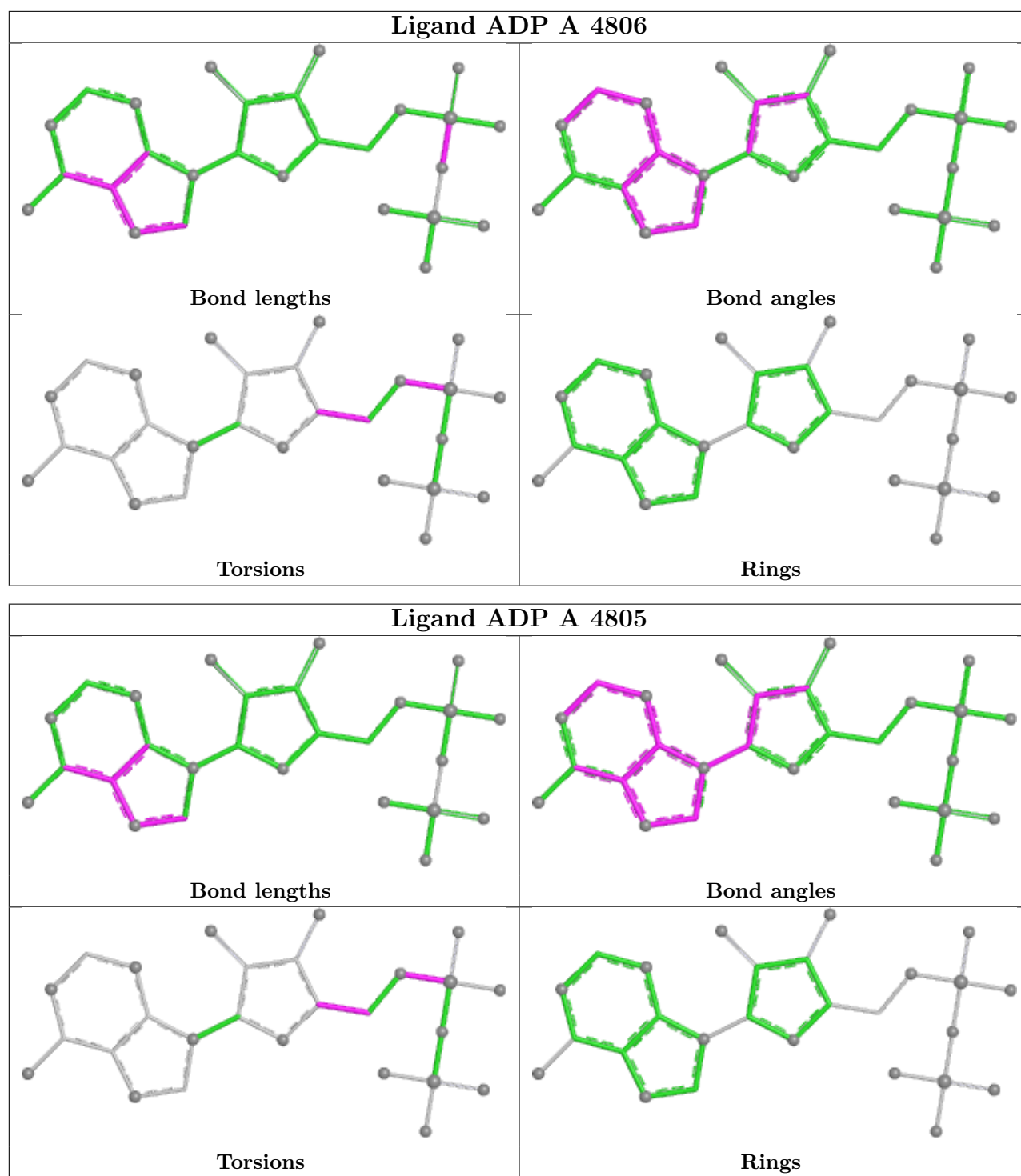
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	4801	ADP	2	0
10	A	4803	ATP	2	0
8	A	4806	ADP	1	0
8	A	4805	ADP	3	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 than 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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

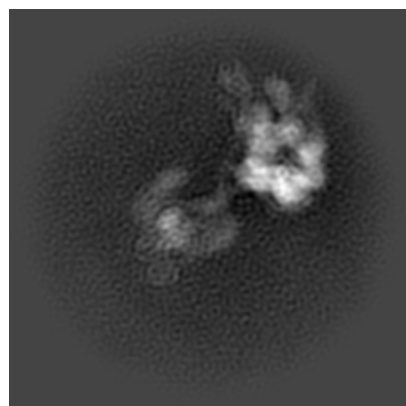
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73175. These allow visual inspection of the internal detail of the map and identification of artifacts.

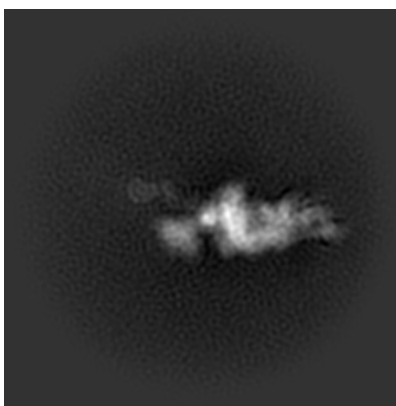
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

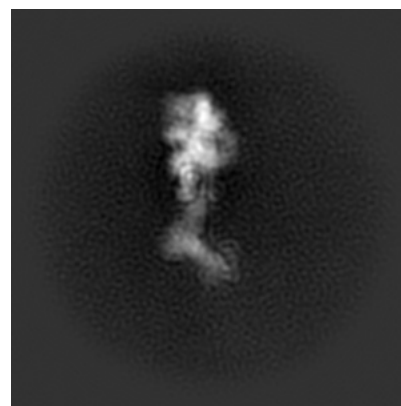
6.1.1 Primary map



X

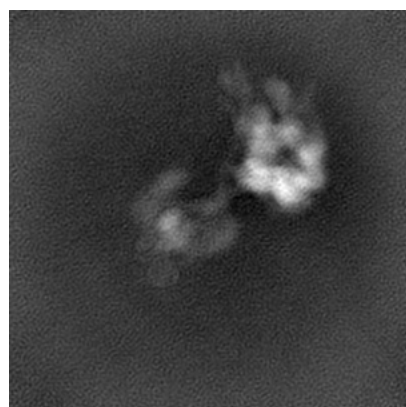


Y

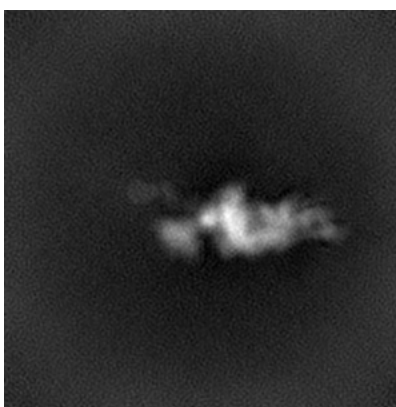


Z

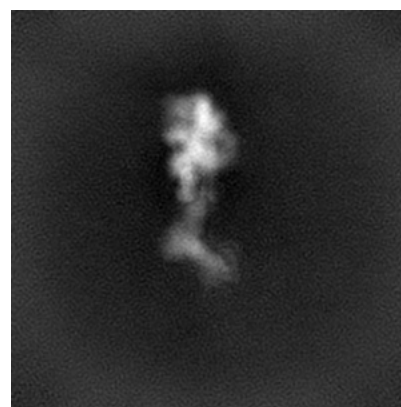
6.1.2 Raw map



X



Y

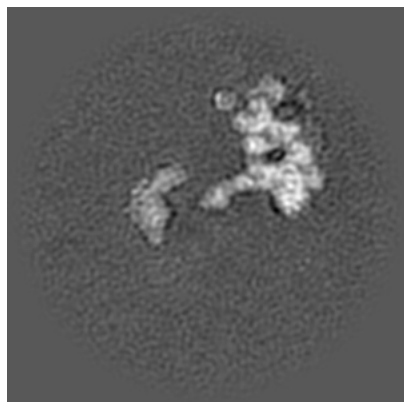


Z

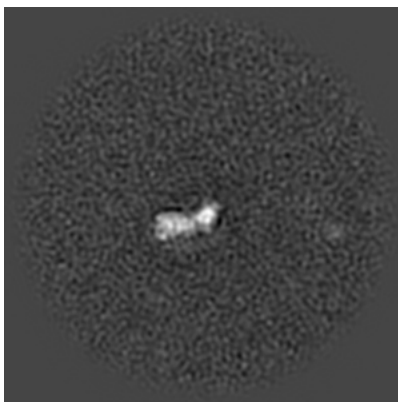
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

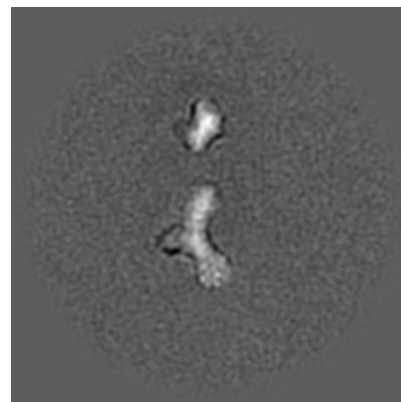
6.2.1 Primary map



X Index: 100

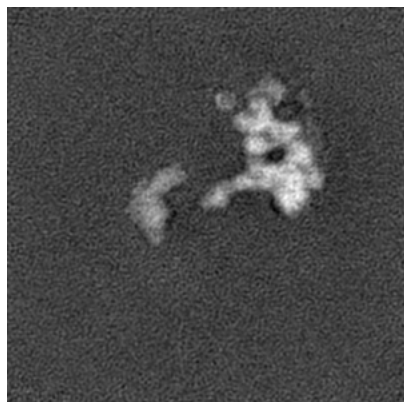


Y Index: 100



Z Index: 100

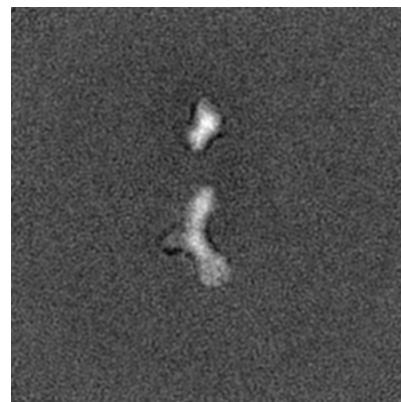
6.2.2 Raw map



X Index: 100



Y Index: 100

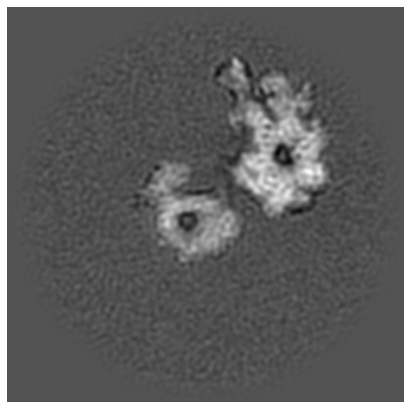


Z Index: 100

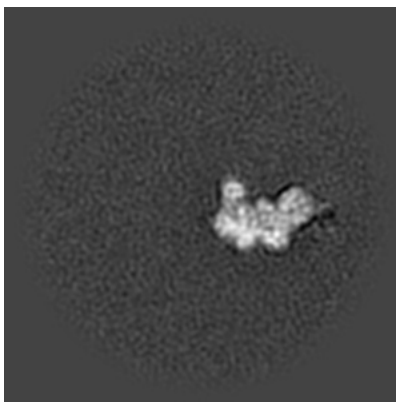
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

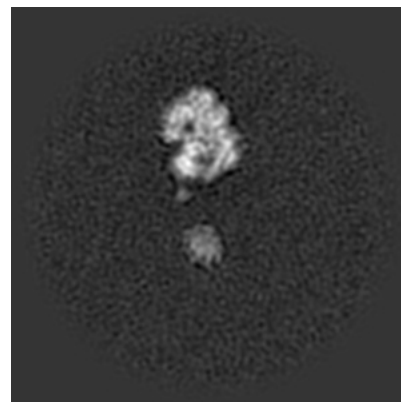
6.3.1 Primary map



X Index: 92

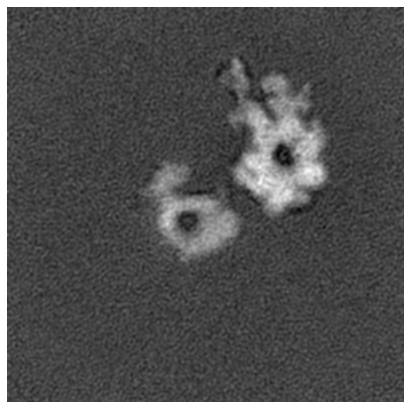


Y Index: 126



Z Index: 114

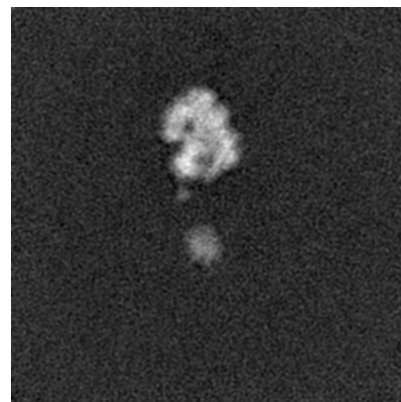
6.3.2 Raw map



X Index: 92



Y Index: 125

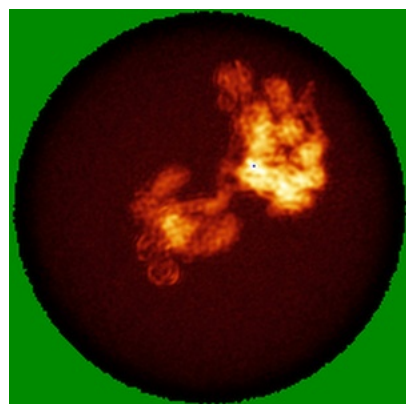


Z Index: 114

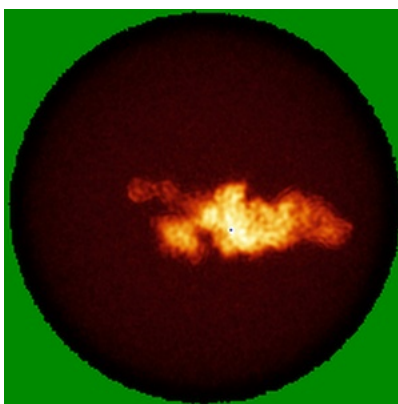
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

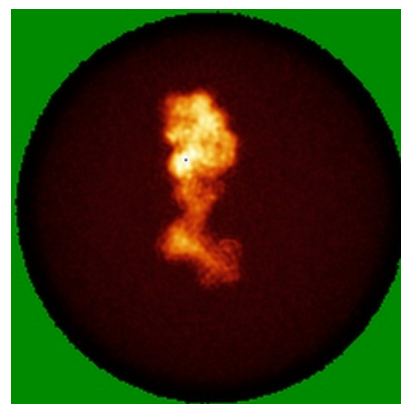
6.4.1 Primary map



X

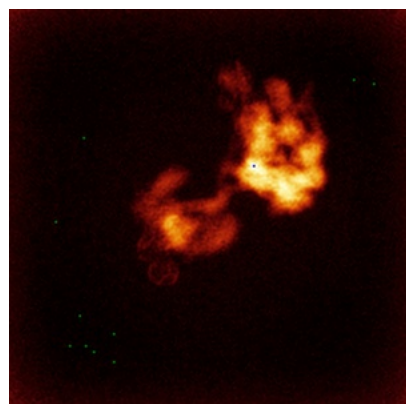


Y

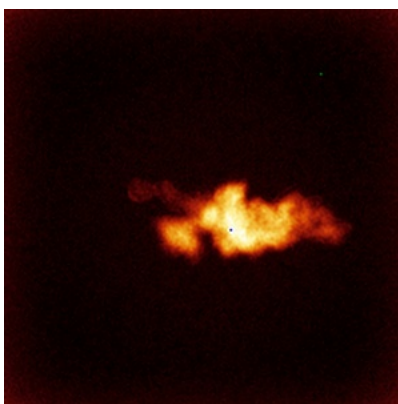


Z

6.4.2 Raw map



X



Y

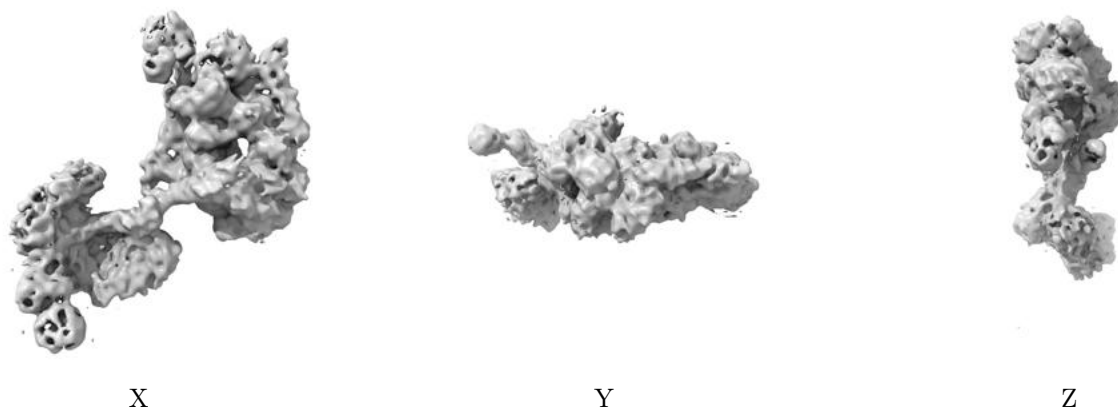


Z

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.

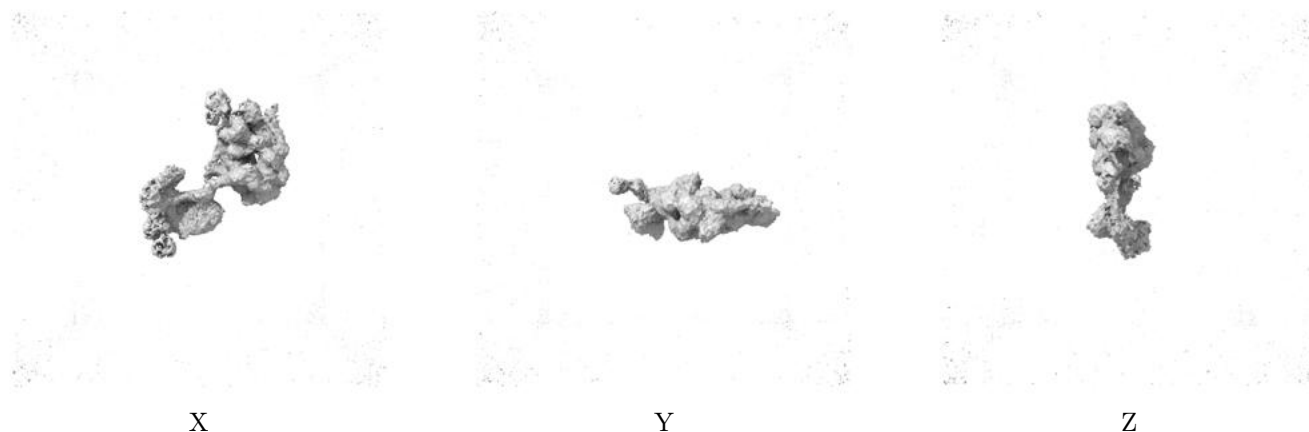
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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



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.

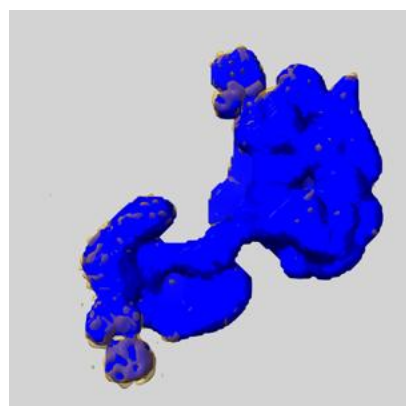
6.6 Mask visualisation [i](#)

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

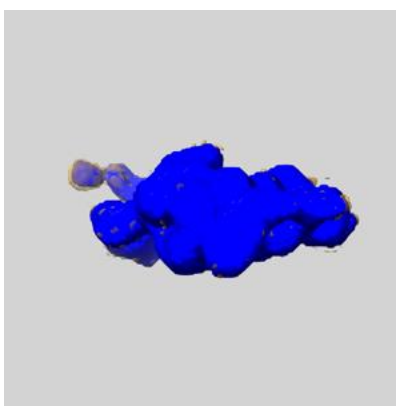
A mask typically either:

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

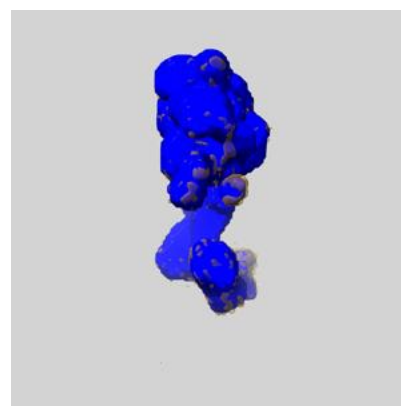
6.6.1 emd_73175_msk_1.map [i](#)



X



Y

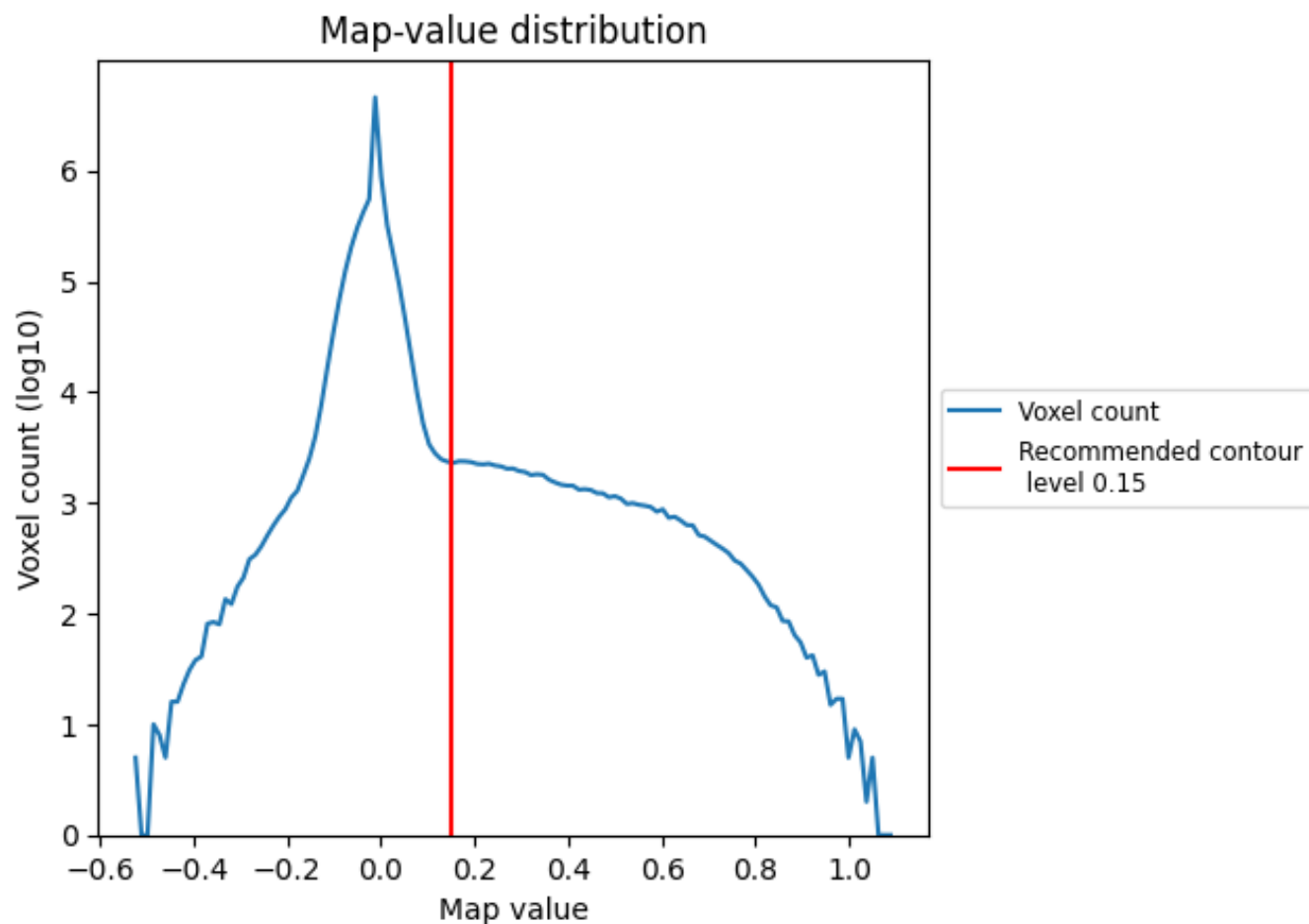


Z

7 Map analysis [i](#)

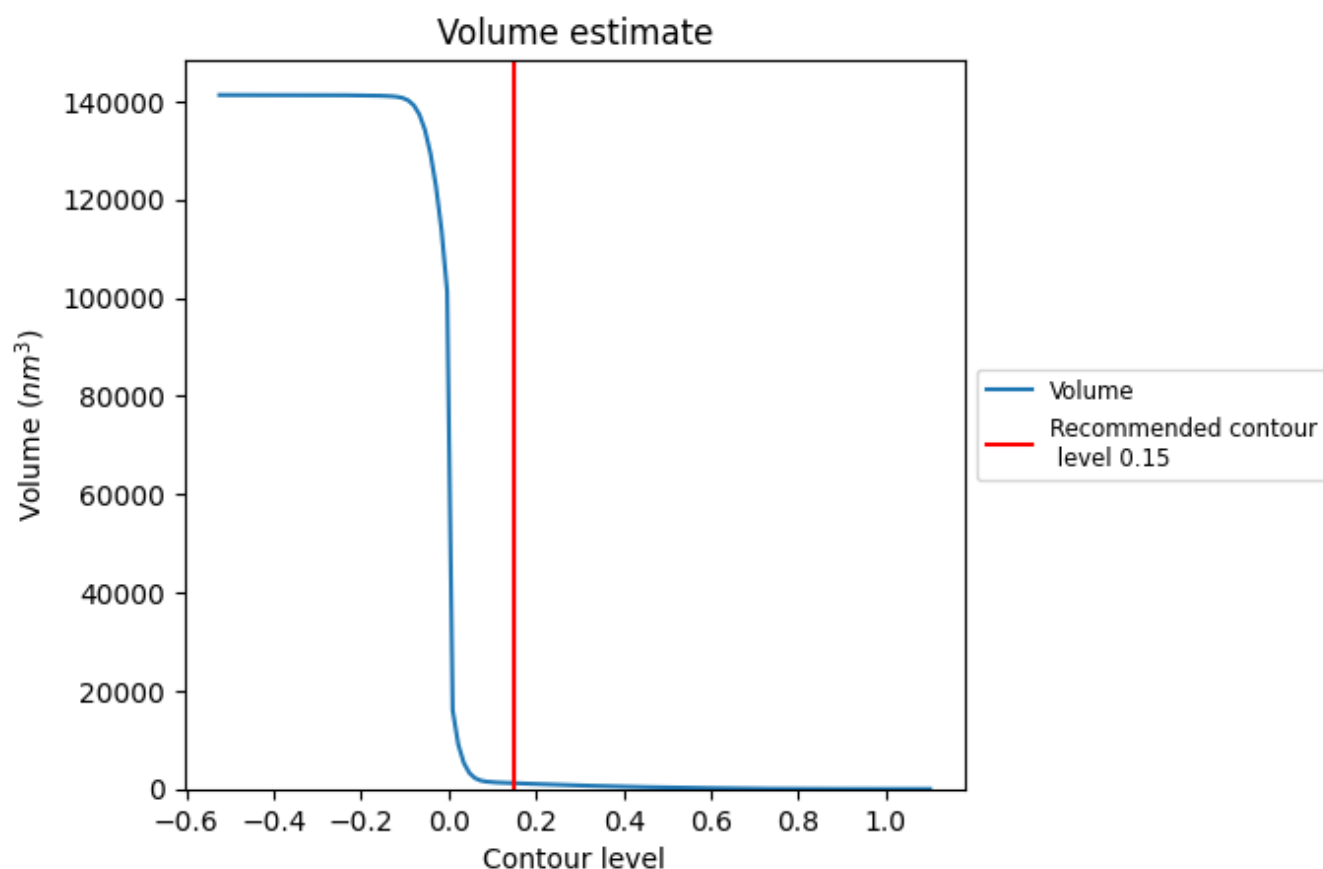
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

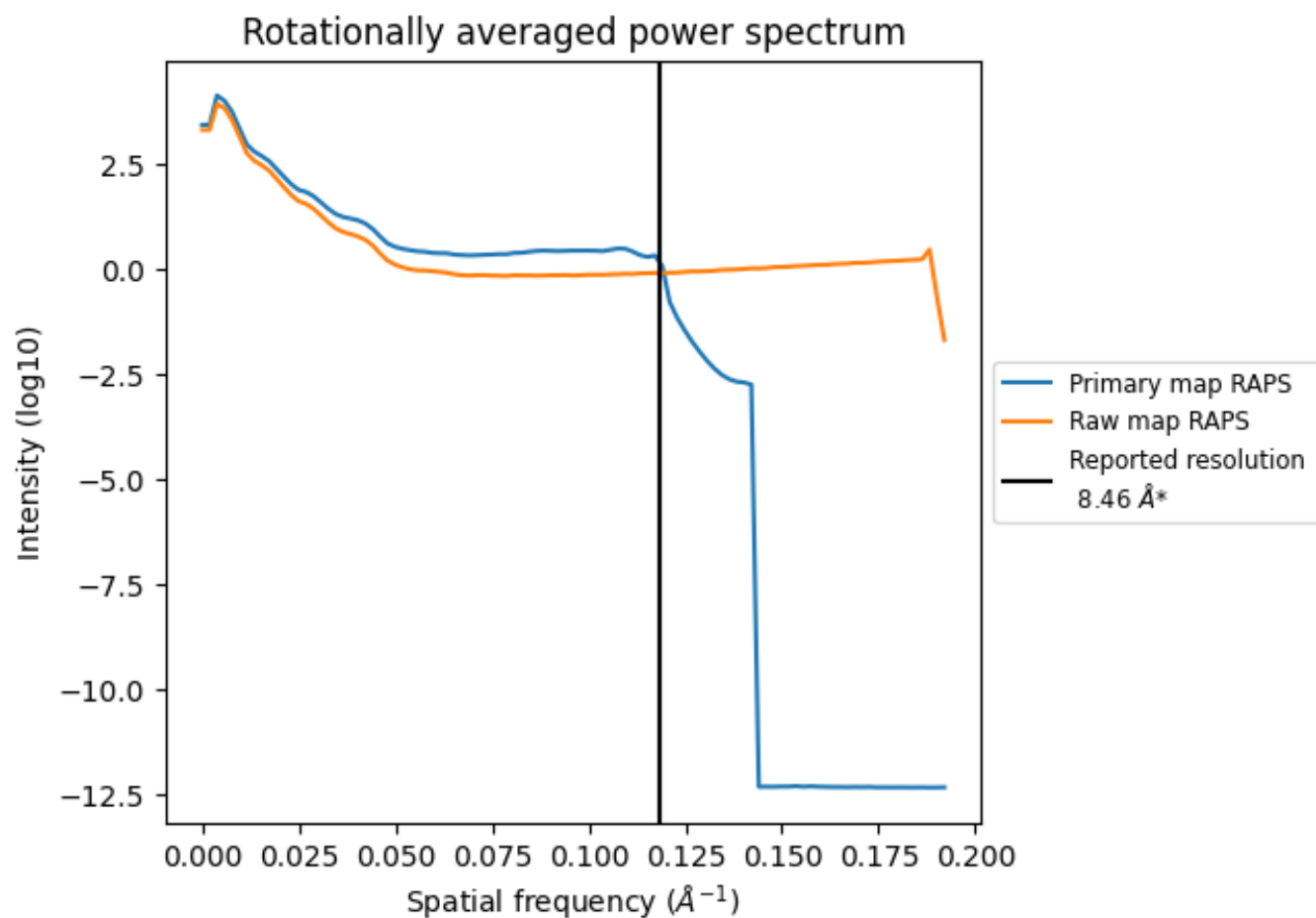
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1173 nm^3 ; this corresponds to an approximate mass of 1059 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 ⓘ

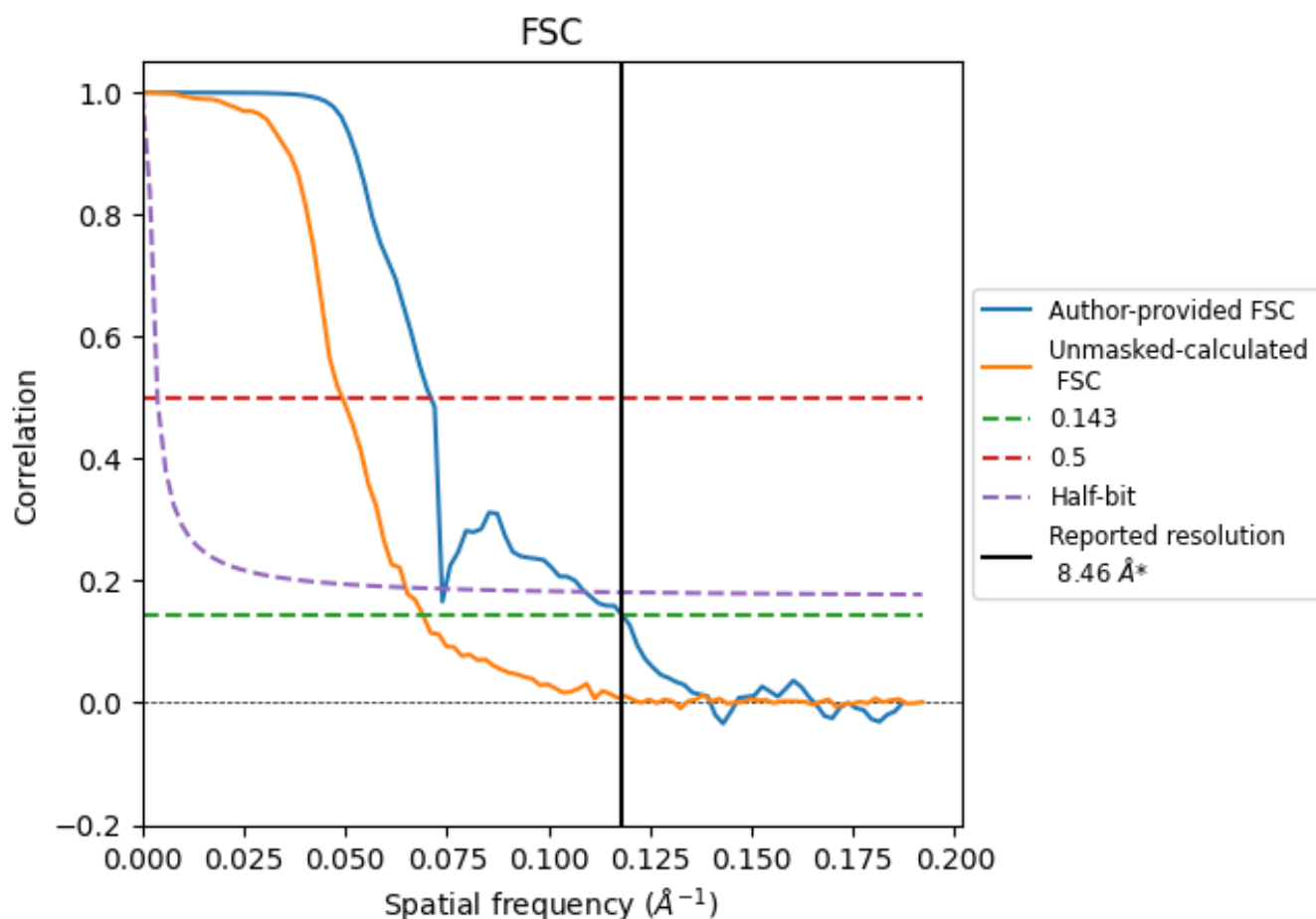


*Reported resolution corresponds to spatial frequency of 0.118 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.118 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

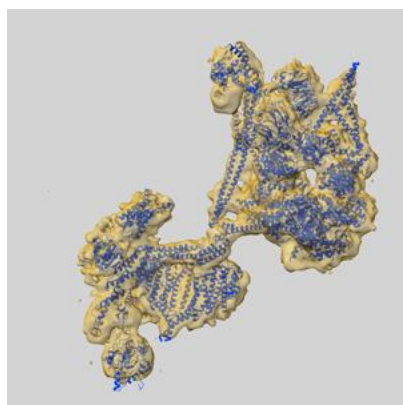
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.46	-	-
Author-provided FSC curve	8.46	14.08	13.55
Unmasked-calculated*	14.45	20.33	15.43

*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 14.45 differs from the reported value 8.46 by more than 10 %

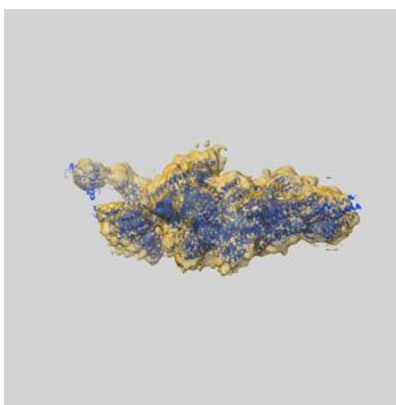
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73175 and PDB model 9YNE. Per-residue inclusion information can be found in section [3](#) on page [9](#).

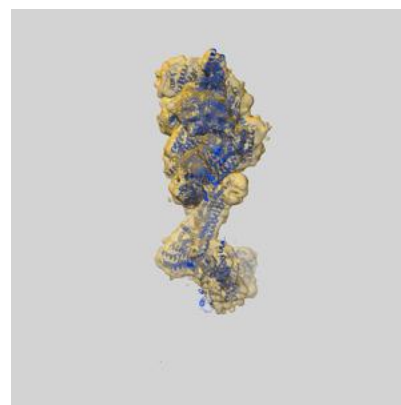
9.1 Map-model overlay [i](#)



X



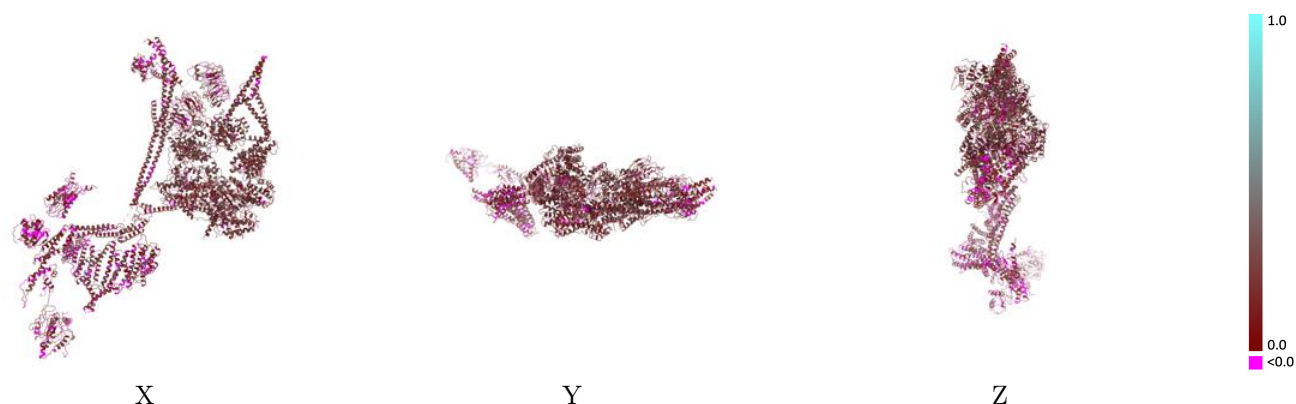
Y



Z

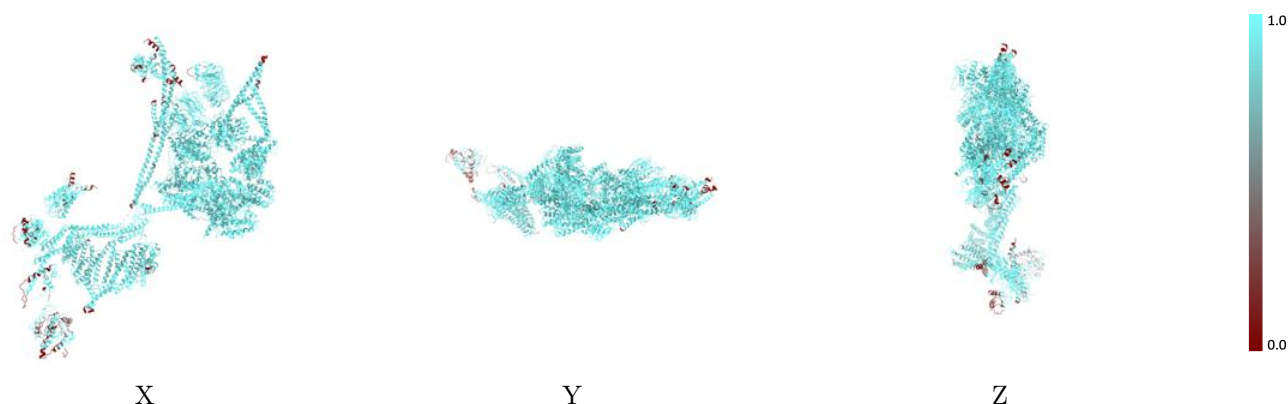
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



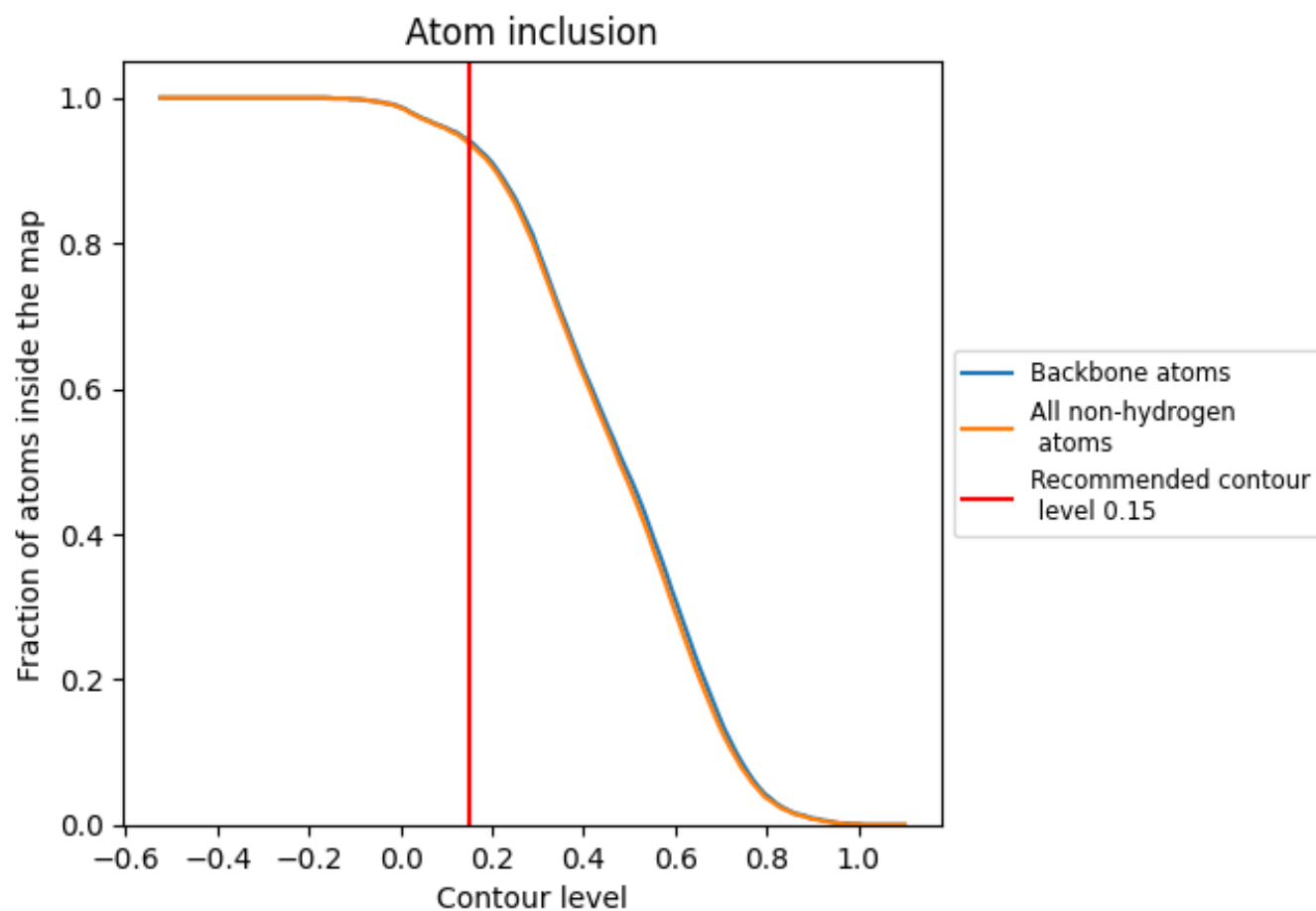
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9370	0.1740
A	0.9860	0.2050
B	0.9660	0.1600
C	0.9240	0.1600
D	0.7260	0.2290
E	0.8460	0.1840
F	0.9610	0.1200
G	0.9310	0.1180
d	0.4170	0.1100
i	0.9320	0.0530
k	0.9160	0.1060
u	0.5990	0.1350
v	0.7560	0.1340

1.0

0.0

<0.0