



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 10:01 PM JST

PDB ID : 22ET / pdb_000022et
EMDB ID : EMD-68219
Title : Cryo-EM structure of Retron Ec78 complex (cis)
Authors : Lin, Z.; Guo, M.; Zhu, Y.; Lu, Z.; Huang, Z.
Deposited on : 2026-01-08
Resolution : 2.69 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

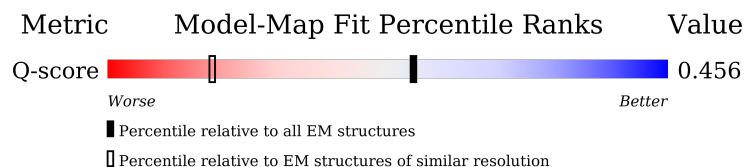
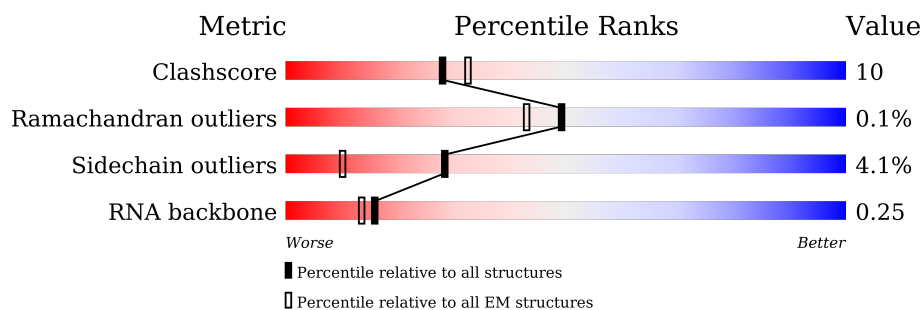
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9309 (2.19 - 3.19)

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	B	551	5% 85% 14% .
1	C	551	11% 81% 18% .
1	D	551	9% 75% 24% .

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Mol	Chain	Length	Quality of chain
1	E	551	9% 75% 24% .
2	M	74	26% 72% ..
3	N	66	18% 15% 24% 42%
4	A	310	85% 15%
5	F	215	68% 28% ..
5	H	215	45% 67% 30% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26167 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 PtuaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	551	Total	C	N	O	S	0	0
			4439	2796	781	849	13		
1	D	551	Total	C	N	O	S	0	0
			4439	2796	781	849	13		
1	B	551	Total	C	N	O	S	0	0
			4439	2796	781	849	13		
1	C	551	Total	C	N	O	S	0	0
			4439	2796	781	849	13		

- Molecule 2 is a DNA chain called DNA (74-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	73	Total	C	N	O	P	0	0
			1511	714	294	430	73		

- Molecule 3 is a RNA chain called RNA (66-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	38	Total	C	N	O	P	0	0
			799	357	138	266	38		

- Molecule 4 is a protein called Retron.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	310	Total	C	N	O	S	0	0
			2550	1630	455	454	11		

- Molecule 5 is a protein called Ptub.

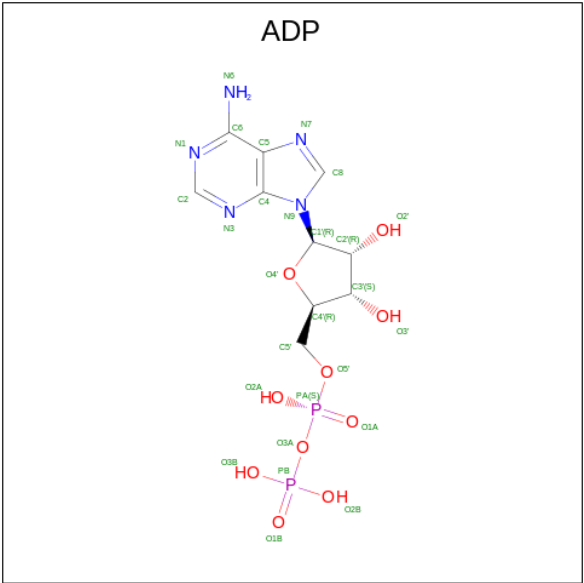
Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	215	Total	C	N	O	S	0	0
			1730	1095	305	320	10		

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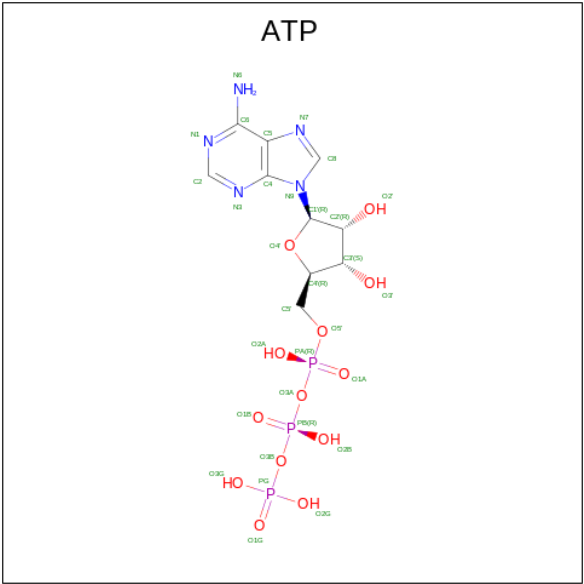
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	215	1730	1095	305	320	10	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

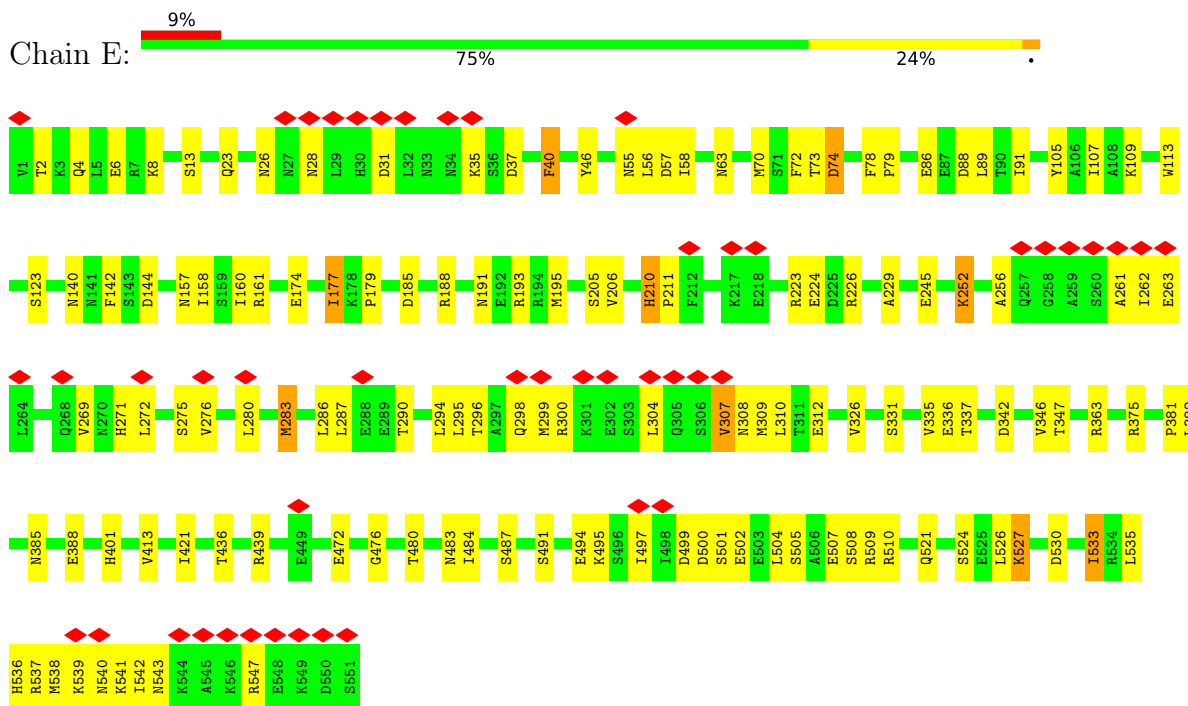
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	H	1	Total	Zn	0
			1	1	
8	F	1	Total	Zn	0
			1	1	

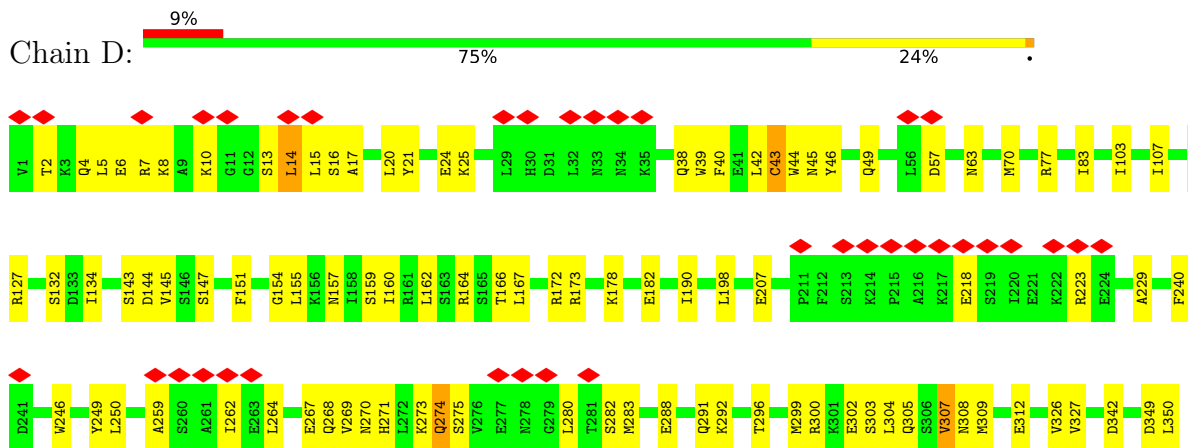
3 Residue-property plots

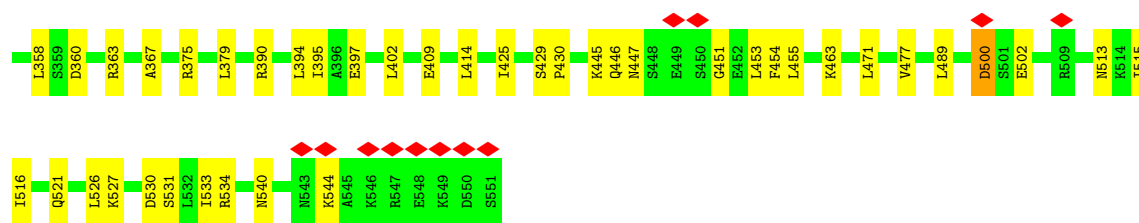
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

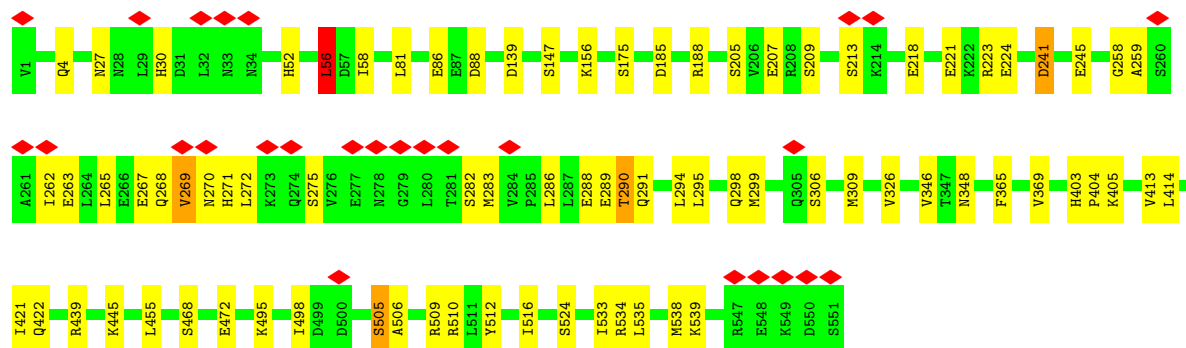
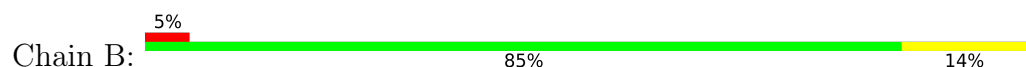


• Molecule 1: PtuA

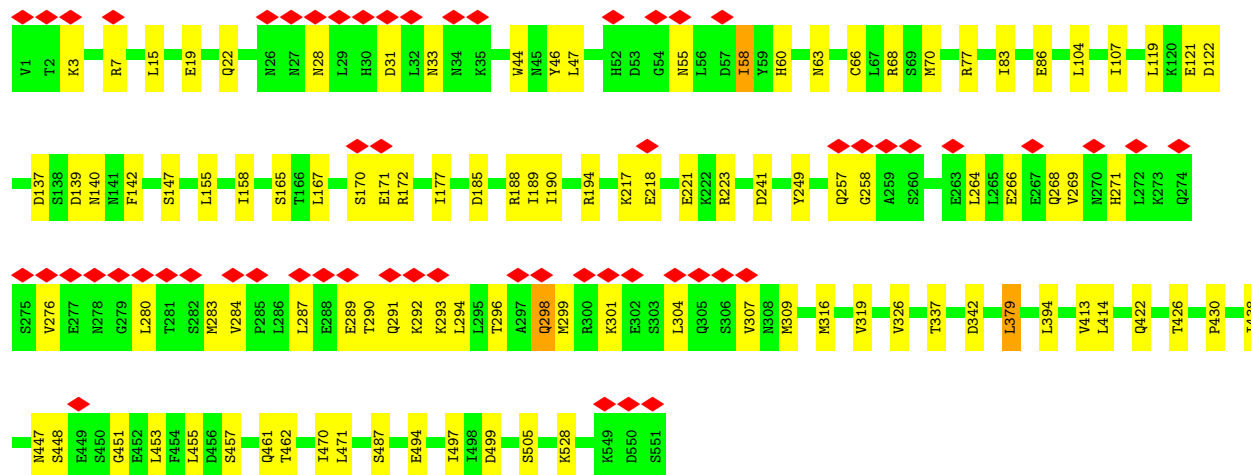
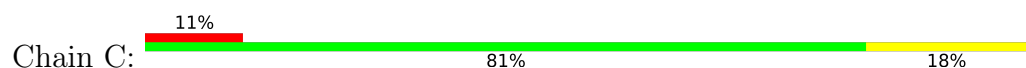




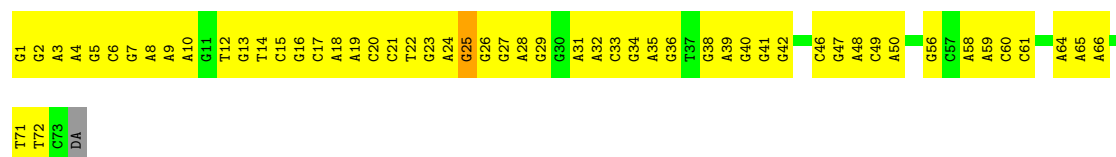
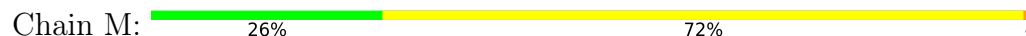
• Molecule 1: PtuA



• Molecule 1: PtuA

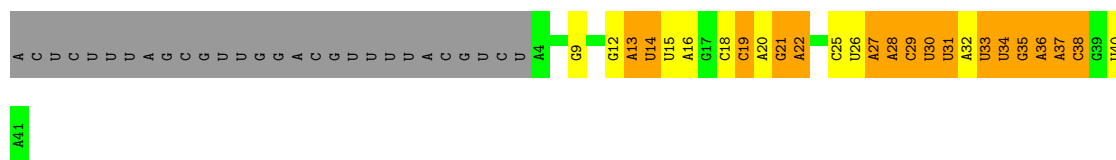


• Molecule 2: DNA (74-MER)



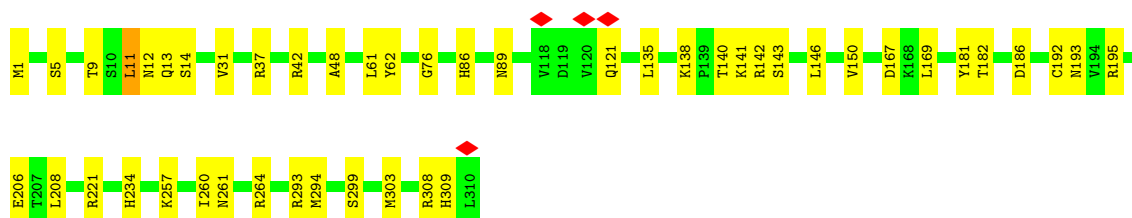
- Molecule 3: RNA (66-MER)

Chain N: 



- Molecule 4: Retron

Chain A: 



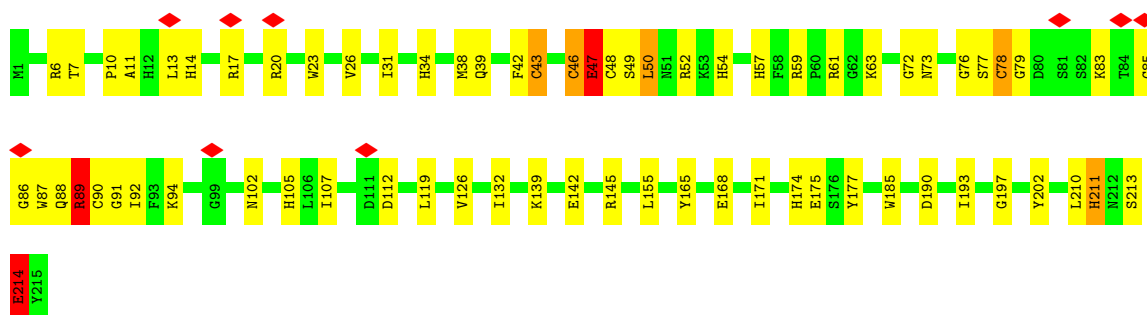
- Molecule 5: PtuB

Chain H: 



- Molecule 5: PtuB

Chain F: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	272348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.540	Depositor
Minimum map value	-0.469	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	288.0, 288.0, 288.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.21	0/4519	0.35	1/6100 (0.0%)
1	C	0.13	0/4519	0.28	0/6100
1	D	0.15	0/4519	0.34	0/6100
1	E	0.18	0/4519	0.37	1/6100 (0.0%)
2	M	0.27	0/1700	0.67	5/2624 (0.2%)
3	N	0.24	0/892	0.68	2/1387 (0.1%)
4	A	0.20	0/2603	0.40	3/3507 (0.1%)
5	F	0.78	0/1779	0.98	7/2405 (0.3%)
5	H	0.78	0/1779	0.78	1/2405 (0.0%)
All	All	0.33	0/26829	0.49	20/36728 (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
5	F	0	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	78	CYS	CB-CA-C	-15.38	82.89	109.65
3	N	40	U	OP1-P-O3'	-11.12	74.66	108.00
2	M	25	DG	OP1-P-O3'	-11.01	74.97	108.00
2	M	66	DA	OP1-P-O3'	-10.76	75.72	108.00
5	F	43	CYS	CB-CA-C	-9.71	94.35	109.89
2	M	66	DA	OP2-P-O3'	-9.68	78.96	108.00
3	N	40	U	OP2-P-O3'	-9.59	79.22	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	25	DG	OP2-P-O3'	-9.32	80.03	108.00
5	F	214	GLU	CB-CG-CD	7.03	124.56	112.60
5	F	47	GLU	CA-C-N	-6.85	113.27	122.72
5	F	47	GLU	C-N-CA	-6.85	113.27	122.72
4	A	11	LEU	CA-C-N	6.03	136.81	126.32
4	A	11	LEU	C-N-CA	6.03	136.81	126.32
4	A	135	LEU	N-CA-C	5.73	118.73	111.69
1	E	308	ASN	N-CA-C	-5.57	104.45	111.92
5	F	49	SER	CA-C-N	-5.37	115.20	122.77
5	F	49	SER	C-N-CA	-5.37	115.20	122.77
1	B	56	LEU	N-CA-C	-5.24	106.86	113.20
2	M	71	DT	O3'-P-O5'	-5.08	96.38	104.00
5	H	121	LEU	N-CA-CB	-5.06	102.38	110.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	89	ARG	Sidechain

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	B	4439	0	4444	66	0
1	C	4439	0	4444	66	0
1	D	4439	0	4444	97	0
1	E	4439	0	4444	98	0
2	M	1511	0	817	57	0
3	N	799	0	403	19	0
4	A	2550	0	2603	32	0
5	F	1730	0	1647	53	0
5	H	1730	0	1646	53	0
6	D	27	0	12	1	0
7	B	31	0	12	0	0
7	C	31	0	12	0	0
8	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1	0	0	0	0
All	All	26167	0	24928	487	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (487) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:502:GLU:HB2	1:E:540:ASN:HB2	1.54	0.86
1:E:195:MET:HE1	1:E:307:VAL:HA	1.58	0.84
1:D:516:ILE:HG13	1:D:521:GLN:HB2	1.64	0.80
1:B:445:LYS:HB3	5:F:83:LYS:HE3	1.64	0.79
2:M:1:DG:H1	2:M:60:DC:H41	1.31	0.79
5:H:121:LEU:HD12	5:H:125:HIS:HB2	1.63	0.79
1:D:83:ILE:HD12	1:D:455:LEU:HD13	1.66	0.78
1:D:24:GLU:HG2	1:D:39:TRP:HZ3	1.50	0.77
4:A:86:HIS:HE2	4:A:182:THR:HG1	1.33	0.76
1:C:309:MET:SD	1:C:309:MET:N	2.60	0.75
1:E:500:ASP:HA	1:E:539:LYS:HE2	1.69	0.74
1:D:5:LEU:HA	1:D:8:LYS:HG2	1.70	0.74
1:D:304:LEU:O	1:D:308:ASN:N	2.21	0.73
5:F:46:CYS:HB2	5:F:48:CYS:SG	2.28	0.73
2:M:24:DA:H2''	2:M:25:DG:H2'	1.71	0.72
4:A:1:MET:HA	4:A:1:MET:HE2	1.70	0.71
2:M:22:DT:H2''	2:M:23:DG:C8	2.26	0.71
1:D:280:LEU:HD21	1:B:271:HIS:HD2	1.56	0.71
1:E:504:LEU:HD12	1:E:508:SER:HB3	1.73	0.70
5:F:79:GLY:HA3	5:F:92:ILE:HD11	1.72	0.70
3:N:9:G:H5''	4:A:293:ARG:HH12	1.56	0.70
5:H:155:LEU:HG	5:H:159:ARG:HH21	1.55	0.69
1:E:191:ASN:HA	1:E:195:MET:HA	1.73	0.69
1:E:210:HIS:ND1	1:E:211:PRO:HD2	2.08	0.68
4:A:13:GLN:N	4:A:13:GLN:OE1	2.26	0.68
1:E:223:ARG:NH1	1:E:245:GLU:OE1	2.27	0.68
1:C:185:ASP:OD1	1:C:188:ARG:NH2	2.27	0.67
1:B:445:LYS:NZ	5:F:86:GLY:HA3	2.09	0.67
1:B:268:GLN:HG3	1:B:272:LEU:HB2	1.75	0.67
3:N:32:A:OP1	4:A:42:ARG:NH2	2.27	0.67
1:B:495:LYS:HA	1:B:498:ILE:HD12	1.77	0.66
1:B:326:VAL:HG11	1:B:369:VAL:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:ILE:HD12	1:B:534:ARG:N	2.10	0.66
1:D:358:LEU:O	1:D:363:ARG:NH2	2.29	0.66
4:A:89:ASN:ND2	4:A:193:ASN:OD1	2.28	0.65
3:N:25:C:H1'	4:A:195:ARG:NH1	2.11	0.65
5:H:144:ILE:HD12	5:H:149:LEU:HD11	1.78	0.65
2:M:6:DC:H5	2:M:56:DG:H1	1.44	0.65
2:M:24:DA:H61	2:M:38:DG:H21	1.44	0.65
1:E:494:GLU:O	1:E:497:ILE:HG13	1.95	0.65
5:F:87:TRP:C	5:F:89:ARG:H	2.05	0.65
1:E:495:LYS:HE3	5:H:127:VAL:HG11	1.77	0.65
1:B:498:ILE:HD13	5:F:119:LEU:HD21	1.79	0.65
1:E:483:ASN:ND2	1:D:409:GLU:OE2	2.31	0.64
3:N:38:C:OP2	4:A:76:GLY:N	2.30	0.64
1:D:63:ASN:O	1:D:390:ARG:NH1	2.30	0.64
2:M:13:DG:H2''	2:M:14:DT:H5''	1.77	0.64
1:D:5:LEU:HG	1:D:20:LEU:HD23	1.79	0.64
1:D:15:LEU:HD12	1:D:155:LEU:HD23	1.79	0.64
1:D:268:GLN:HE21	1:B:286:LEU:HD13	1.63	0.64
1:B:241:ASP:OD1	1:B:241:ASP:N	2.30	0.63
1:E:307:VAL:HG13	1:E:381:PRO:HB2	1.80	0.63
5:H:121:LEU:HD11	5:H:127:VAL:HG13	1.80	0.63
1:C:217:LYS:N	1:C:217:LYS:HE2	2.13	0.63
1:D:14:LEU:HD23	1:D:154:GLY:N	2.13	0.63
5:H:180:LEU:HD22	5:H:184:LEU:HG	1.80	0.63
1:D:70:MET:HE1	1:D:107:ILE:HG12	1.81	0.63
1:C:221:GLU:OE1	1:C:221:GLU:N	2.28	0.63
1:D:326:VAL:HG23	1:D:327:VAL:HG23	1.81	0.62
1:C:296:THR:HA	1:C:299:MET:HE1	1.80	0.62
1:B:512:TYR:O	1:B:516:ILE:HD12	2.00	0.62
1:E:229:ALA:O	1:E:375:ARG:NH1	2.29	0.62
2:M:31:DA:H1'	2:M:32:DA:C2	2.34	0.62
2:M:35:DA:H2''	2:M:36:DG:N7	2.15	0.62
1:D:4:GLN:N	1:D:4:GLN:OE1	2.32	0.62
1:D:8:LYS:HG3	1:D:16:SER:HB3	1.82	0.62
2:M:25:DG:H2''	2:M:26:DG:C8	2.34	0.62
2:M:20:DC:H2''	2:M:21:DC:H5'	1.80	0.62
1:E:307:VAL:HG12	1:E:309:MET:N	2.15	0.62
1:B:445:LYS:HZ1	5:F:85:GLY:C	2.08	0.61
5:F:177:TYR:HB2	5:F:185:TRP:CD1	2.35	0.61
1:D:500:ASP:OD1	1:D:500:ASP:N	2.32	0.61
1:E:533:ILE:HA	1:E:536:HIS:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:GLN:NE2	1:B:286:LEU:HD13	2.16	0.61
5:F:142:GLU:OE2	5:F:145:ARG:NH1	2.34	0.61
1:C:83:ILE:HD12	1:C:455:LEU:HD13	1.83	0.60
1:E:538:MET:SD	5:H:174:HIS:HB3	2.41	0.60
1:D:430:PRO:HG3	1:D:471:LEU:HD13	1.82	0.60
1:E:74:ASP:HA	1:E:79:PRO:HA	1.84	0.60
1:E:494:GLU:OE1	5:H:121:LEU:HB3	2.01	0.60
4:A:138:LYS:HD2	4:A:146:LEU:HD11	1.84	0.60
1:D:292:LYS:O	1:D:296:THR:HG23	2.02	0.59
1:B:309:MET:HE2	1:B:309:MET:H	1.67	0.59
1:C:167:LEU:HD23	1:C:167:LEU:H	1.67	0.59
2:M:24:DA:H1'	2:M:25:DG:H8	1.67	0.59
1:E:491:SER:HB2	5:H:123:THR:HG21	1.84	0.59
1:E:185:ASP:OD1	1:E:188:ARG:NH2	2.36	0.59
1:C:70:MET:HE1	1:C:107:ILE:HG12	1.84	0.59
1:D:271:HIS:O	1:D:274:GLN:HG3	2.02	0.59
3:N:28:A:N6	4:A:234:HIS:O	2.36	0.59
1:B:265:LEU:HB2	1:B:268:GLN:HB2	1.85	0.59
1:C:447:ASN:O	1:C:451:GLY:N	2.36	0.59
2:M:40:DG:H2''	2:M:41:DG:C8	2.38	0.59
1:E:224:GLU:OE1	1:E:224:GLU:N	2.31	0.58
1:B:267:GLU:O	1:B:270:ASN:ND2	2.34	0.58
1:C:46:TYR:O	1:C:63:ASN:ND2	2.35	0.58
1:C:28:ASN:ND2	1:C:33:ASN:OD1	2.36	0.58
1:E:55:ASN:OD1	1:E:56:LEU:N	2.36	0.58
2:M:39:DA:H2''	2:M:40:DG:H5''	1.85	0.58
1:D:264:LEU:HD11	1:B:282:SER:HB2	1.85	0.58
1:B:86:GLU:OE1	1:B:439:ARG:NH1	2.37	0.58
1:C:155:LEU:HD13	1:C:158:ILE:HD11	1.86	0.57
1:E:191:ASN:OD1	1:E:226:ARG:NH1	2.37	0.57
1:E:195:MET:HE3	1:E:382:LEU:HD21	1.85	0.57
1:E:276:VAL:HG21	1:E:287:LEU:HD22	1.86	0.57
1:B:299:MET:HA	1:B:299:MET:HE2	1.86	0.57
2:M:15:DC:H5	2:M:47:DG:H1	1.52	0.57
5:H:80:ASP:HB3	5:H:83:LYS:HB2	1.85	0.57
1:D:144:ASP:OD2	1:D:173:ARG:NH2	2.37	0.57
5:H:46:CYS:SG	5:H:89:ARG:NH2	2.77	0.57
4:A:261:ASN:OD1	4:A:264:ARG:NH2	2.37	0.57
1:E:385:ASN:ND2	1:E:388:GLU:OE2	2.35	0.57
1:C:77:ARG:HH21	1:C:453:LEU:HD11	1.68	0.57
1:C:104:LEU:HD22	1:C:394:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:494:GLU:OE2	5:H:121:LEU:HD22	2.05	0.57
1:D:304:LEU:HD22	1:D:309:MET:HB2	1.87	0.57
1:C:241:ASP:OD1	1:C:241:ASP:N	2.37	0.57
4:A:192:CYS:SG	4:A:193:ASN:N	2.78	0.57
1:D:57:ASP:OD1	1:D:57:ASP:N	2.38	0.57
1:B:139:ASP:OD1	1:B:139:ASP:N	2.38	0.57
2:M:41:DG:H2''	2:M:42:DG:O5'	2.05	0.57
4:A:308:ARG:O	4:A:309:HIS:ND1	2.38	0.56
5:H:143:THR:HA	5:H:146:VAL:HG12	1.87	0.56
1:E:507:GLU:HA	1:E:510:ARG:HG2	1.88	0.56
5:H:108:LYS:HB3	5:H:111:ASP:HB2	1.87	0.56
5:H:177:TYR:HB2	5:H:185:TRP:CD1	2.40	0.56
5:F:211:HIS:C	5:F:213:SER:H	2.12	0.56
5:H:202:TYR:O	5:H:206:LYS:HB3	2.05	0.56
1:D:77:ARG:HH21	1:D:453:LEU:HD11	1.70	0.56
1:B:445:LYS:HZ1	5:F:86:GLY:HA3	1.70	0.56
5:F:48:CYS:SG	5:F:155:LEU:HD13	2.46	0.56
1:C:298:GLN:HE21	1:C:298:GLN:HA	1.69	0.56
2:M:28:DA:H1'	2:M:35:DA:H62	1.71	0.55
3:N:25:C:H2'	3:N:27:A:N7	2.21	0.55
1:D:14:LEU:HD23	1:D:154:GLY:H	1.72	0.55
1:B:271:HIS:O	1:B:271:HIS:ND1	2.38	0.55
5:F:52:ARG:NH2	5:F:79:GLY:O	2.39	0.55
5:H:81:SER:HA	5:H:92:ILE:HG23	1.87	0.55
1:B:262:ILE:HA	1:B:265:LEU:HG	1.89	0.54
5:H:124:GLY:O	5:H:159:ARG:NH1	2.39	0.54
1:D:349:ASP:O	1:D:350:LEU:HD23	2.08	0.54
5:H:121:LEU:HD11	5:H:127:VAL:CG1	2.37	0.54
1:E:86:GLU:OE1	1:E:439:ARG:NH1	2.40	0.54
1:E:499:ASP:OD2	1:E:501:SER:OG	2.24	0.54
1:C:28:ASN:ND2	1:C:31:ASP:OD2	2.40	0.54
5:F:48:CYS:SG	5:F:155:LEU:CD1	2.95	0.54
1:C:494:GLU:O	1:C:497:ILE:HG13	2.07	0.54
2:M:64:DA:H2''	4:A:48:ALA:HB2	1.89	0.54
1:B:52:HIS:HB3	1:B:56:LEU:HD23	1.90	0.54
1:E:476:GLY:C	5:H:153:PRO:HG2	2.33	0.54
1:B:286:LEU:O	1:B:289:GLU:HG3	2.07	0.54
1:C:291:GLN:O	1:C:294:LEU:HB3	2.08	0.54
2:M:24:DA:H61	2:M:38:DG:N2	2.06	0.54
5:F:87:TRP:C	5:F:89:ARG:N	2.63	0.54
5:F:213:SER:O	5:F:214:GLU:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ASP:HA	1:E:40:PHE:HD2	1.72	0.53
1:B:185:ASP:OD1	1:B:188:ARG:NH2	2.40	0.53
1:D:14:LEU:HD13	1:D:46:TYR:CZ	2.44	0.53
5:H:23:TRP:HB3	5:H:61:ARG:HH21	1.74	0.53
1:B:221:GLU:H	1:B:221:GLU:CD	2.17	0.53
3:N:31:U:H5''	4:A:37:ARG:HD2	1.90	0.53
3:N:35:G:H2'	3:N:36:A:C8	2.43	0.53
4:A:5:SER:O	4:A:9:THR:HG22	2.09	0.53
1:D:134:ILE:HD13	1:D:143:SER:HB2	1.90	0.53
1:D:172:ARG:NH1	2:M:27:DG:OP2	2.42	0.53
1:C:19:GLU:HA	1:C:22:GLN:HE21	1.72	0.53
2:M:26:DG:H1'	2:M:27:DG:H5'	1.89	0.53
5:H:98:ALA:O	5:H:145:ARG:NH1	2.35	0.53
1:E:538:MET:HA	1:E:541:LYS:HD2	1.90	0.53
1:B:288:GLU:O	1:B:291:GLN:NE2	2.41	0.53
2:M:4:DA:H4'	2:M:5:DG:OP1	2.09	0.53
4:A:1:MET:SD	4:A:5:SER:OG	2.57	0.53
5:H:56:GLU:HG2	5:H:94:LYS:HD3	1.91	0.52
1:E:269:VAL:HG21	1:E:294:LEU:HD22	1.92	0.52
1:D:489:LEU:HB3	1:D:515:ILE:HD11	1.91	0.52
1:C:304:LEU:HA	1:C:309:MET:HE1	1.90	0.52
5:F:89:ARG:HH22	5:F:90:CYS:HB2	1.72	0.52
1:E:472:GLU:OE2	5:H:157:GLY:HA3	2.10	0.52
5:F:91:GLY:O	5:F:94:LYS:HB3	2.09	0.52
1:E:494:GLU:CD	5:H:121:LEU:HB3	2.34	0.52
1:C:217:LYS:HE2	1:C:217:LYS:H	1.73	0.52
2:M:61:DC:H2''	4:A:31:VAL:HB	1.92	0.52
1:D:240:PHE:HD1	1:D:367:ALA:HB2	1.73	0.52
3:N:18:C:O2'	3:N:19:C:O2	2.25	0.52
1:D:299:MET:N	1:D:299:MET:HE2	2.25	0.52
5:F:10:PRO:HD2	5:F:13:LEU:HD12	1.90	0.51
1:E:472:GLU:HG3	5:H:153:PRO:CB	2.40	0.51
1:D:25:LYS:HD3	1:D:40:PHE:HB2	1.93	0.51
1:E:326:VAL:HA	1:E:413:VAL:HG11	1.92	0.51
1:B:258:GLY:HA3	1:B:262:ILE:HB	1.90	0.51
2:M:2:DG:H22	2:M:58:DA:H2''	1.75	0.51
1:E:73:THR:HG22	1:E:144:ASP:H	1.75	0.51
1:C:294:LEU:O	1:C:298:GLN:OE1	2.29	0.51
4:A:206:GLU:OE2	4:A:221:ARG:NH1	2.42	0.51
1:E:195:MET:CE	1:E:307:VAL:HA	2.35	0.51
5:H:6:ARG:NH2	5:H:110:ASP:OD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ASP:OD1	1:E:89:LEU:N	2.41	0.51
1:E:401:HIS:ND1	1:D:397:GLU:OE2	2.42	0.51
1:C:307:VAL:HB	1:C:309:MET:SD	2.51	0.51
3:N:37:A:O2'	3:N:38:C:O5'	2.21	0.51
1:D:527:LYS:HB3	5:H:165:TYR:CE2	2.45	0.51
1:E:56:LEU:HD22	1:E:58:ILE:H	1.76	0.50
1:D:270:ASN:HA	1:D:273:LYS:HB2	1.93	0.50
1:B:510:ARG:HH11	1:B:510:ARG:HG3	1.76	0.50
1:D:14:LEU:HD21	1:D:151:PHE:O	2.12	0.50
1:B:81:LEU:HD11	1:B:455:LEU:HD13	1.92	0.50
5:H:89:ARG:CZ	5:H:90:CYS:SG	2.99	0.50
5:H:184:LEU:O	5:H:187:GLU:HG2	2.11	0.50
1:D:14:LEU:CD2	1:D:155:LEU:H	2.24	0.50
1:B:539:LYS:NZ	5:F:211:HIS:H	2.09	0.50
4:A:167:ASP:OD1	4:A:181:TYR:OH	2.28	0.50
5:H:112:ASP:OD1	5:H:112:ASP:N	2.45	0.50
1:C:3:LYS:O	1:C:7:ARG:HG3	2.12	0.50
1:B:445:LYS:HZ3	5:F:86:GLY:HA3	1.77	0.50
1:C:121:GLU:OE2	1:C:122:ASP:N	2.45	0.50
2:M:1:DG:O3'	4:A:142:ARG:NH1	2.33	0.50
1:E:533:ILE:O	1:E:537:ARG:N	2.45	0.50
1:E:70:MET:HE1	1:E:107:ILE:HG12	1.93	0.50
1:E:535:LEU:HD11	5:H:171:ILE:HG13	1.94	0.49
5:F:43:CYS:SG	5:F:50:LEU:HD23	2.52	0.49
1:E:283:MET:SD	1:E:283:MET:N	2.86	0.49
1:C:298:GLN:HE21	1:C:298:GLN:CA	2.25	0.49
2:M:35:DA:H2'	2:M:36:DG:C8	2.47	0.49
1:E:504:LEU:CD1	1:E:508:SER:HB3	2.42	0.49
1:E:74:ASP:N	1:E:74:ASP:OD1	2.46	0.49
1:E:275:SER:OG	1:C:283:MET:HE3	2.13	0.49
2:M:48:DA:H2'	2:M:49:DC:O5'	2.13	0.49
1:B:326:VAL:HA	1:B:413:VAL:HG11	1.95	0.49
1:E:46:TYR:O	1:E:63:ASN:ND2	2.45	0.49
1:E:272:LEU:HD23	1:E:290:THR:HG21	1.95	0.49
1:C:140:ASN:HB3	1:C:142:PHE:CE2	2.47	0.49
1:D:132:SER:O	6:D:601:ADP:N6	2.43	0.48
1:D:207:GLU:N	1:D:207:GLU:OE1	2.46	0.48
5:H:22:PRO:O	5:H:25:SER:OG	2.29	0.48
5:H:24:MET:HE2	5:H:24:MET:H	1.77	0.48
1:D:534:ARG:HA	1:D:534:ARG:CZ	2.43	0.48
1:E:296:THR:HA	1:E:299:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:210:LEU:HD23	5:H:213:SER:HB2	1.96	0.48
1:E:540:ASN:HA	1:E:543:ASN:HB2	1.94	0.48
1:C:528:LYS:HE3	5:F:165:TYR:CE1	2.48	0.48
1:E:28:ASN:HA	1:E:31:ASP:O	2.13	0.48
1:C:298:GLN:CA	1:C:298:GLN:NE2	2.77	0.48
1:C:326:VAL:HA	1:C:413:VAL:HG11	1.96	0.48
4:A:294:MET:HE2	4:A:294:MET:HA	1.96	0.48
5:H:38:MET:HE3	5:H:39:GLN:HG2	1.95	0.48
1:D:198:LEU:HB2	1:D:379:LEU:HD22	1.94	0.48
2:M:17:DC:H2''	2:M:18:DA:C8	2.49	0.48
1:E:524:SER:O	1:E:527:LYS:HG3	2.14	0.48
2:M:9:DA:H2''	2:M:10:DA:C8	2.48	0.48
5:H:43:CYS:SG	5:H:46:CYS:SG	3.12	0.48
1:D:166:THR:OG1	1:D:167:LEU:N	2.46	0.48
5:H:89:ARG:HE	5:H:155:LEU:HB2	1.78	0.48
1:D:145:VAL:HG23	1:D:162:LEU:HB2	1.96	0.48
1:C:266:GLU:HA	1:C:269:VAL:HG12	1.95	0.48
4:A:257:LYS:HD3	4:A:294:MET:HE1	1.96	0.48
1:E:300:ARG:O	1:E:304:LEU:HG	2.13	0.47
2:M:1:DG:H2''	2:M:2:DG:H8	1.79	0.47
1:D:288:GLU:O	1:D:291:GLN:HG3	2.13	0.47
1:B:224:GLU:OE1	1:B:224:GLU:HA	2.14	0.47
1:E:2:THR:O	1:E:6:GLU:HG2	2.14	0.47
1:D:24:GLU:HG2	1:D:39:TRP:CZ3	2.39	0.47
1:D:303:SER:O	1:D:307:VAL:HG23	2.14	0.47
1:D:360:ASP:HA	1:D:363:ARG:NH1	2.28	0.47
1:D:447:ASN:O	1:D:451:GLY:N	2.42	0.47
1:C:461:GLN:OE1	1:C:462:THR:N	2.47	0.47
2:M:17:DC:H2''	2:M:18:DA:H8	1.80	0.47
2:M:72:DT:H71	3:N:36:A:N1	2.30	0.47
1:D:521:GLN:HA	1:D:526:LEU:HD13	1.96	0.47
2:M:49:DC:H2''	2:M:50:DA:C8	2.50	0.47
5:F:89:ARG:NH2	5:F:90:CYS:HB2	2.30	0.47
1:D:21:TYR:O	1:D:25:LYS:HB2	2.15	0.47
1:D:229:ALA:O	1:D:375:ARG:NH1	2.48	0.47
3:N:30:U:H4'	3:N:31:U:O5'	2.14	0.47
5:H:48:CYS:HB3	5:H:89:ARG:HH22	1.80	0.47
5:F:168:GLU:O	5:F:171:ILE:HG13	2.15	0.47
2:M:19:DA:H2''	2:M:20:DC:O5'	2.15	0.47
1:D:395:ILE:O	1:D:425:ILE:HA	2.15	0.47
5:F:190:ASP:O	5:F:193:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LYS:HD2	3:N:29:C:H5''	1.97	0.47
5:F:46:CYS:C	5:F:48:CYS:N	2.71	0.47
1:E:57:ASP:OD1	1:E:57:ASP:N	2.35	0.46
1:B:309:MET:H	1:B:309:MET:CE	2.28	0.46
5:F:54:HIS:ND1	5:F:79:GLY:O	2.38	0.46
1:D:159:SER:C	1:D:160:ILE:HD12	2.40	0.46
2:M:2:DG:OP1	4:A:142:ARG:NH2	2.31	0.46
1:D:6:GLU:HG2	1:D:39:TRP:CH2	2.49	0.46
1:C:430:PRO:HG3	1:C:471:LEU:HD13	1.96	0.46
1:D:38:GLN:HE22	1:D:39:TRP:NE1	2.13	0.46
1:D:530:ASP:O	1:D:533:ILE:HG22	2.16	0.46
2:M:12:DT:H1'	2:M:13:DG:H5'	1.97	0.46
1:B:538:MET:HE2	5:F:174:HIS:HB3	1.98	0.46
4:A:140:THR:HB	4:A:143:SER:HB3	1.98	0.46
1:C:447:ASN:O	1:C:451:GLY:CA	2.64	0.46
5:H:140:ALA:O	5:H:143:THR:HG22	2.15	0.46
1:E:495:LYS:CE	5:H:127:VAL:HG11	2.43	0.46
1:E:280:LEU:HD11	1:C:268:GLN:HA	1.98	0.46
2:M:31:DA:H1'	2:M:32:DA:H2	1.80	0.46
1:E:537:ARG:HH12	1:E:541:LYS:HD2	1.80	0.46
1:B:295:LEU:HA	1:B:298:GLN:HG3	1.97	0.46
2:M:3:DA:N6	2:M:59:DA:C8	2.84	0.46
1:D:302:GLU:O	1:D:305:GLN:HG3	2.16	0.45
1:E:527:LYS:HA	1:E:530:ASP:OD2	2.16	0.45
1:D:39:TRP:O	1:D:42:LEU:HG	2.16	0.45
1:D:249:TYR:HD2	1:D:250:LEU:HD23	1.81	0.45
1:D:471:LEU:HG	1:D:477:VAL:HB	1.97	0.45
1:C:379:LEU:HD12	1:C:379:LEU:HA	1.82	0.45
2:M:29:DG:C8	2:M:35:DA:C6	3.04	0.45
5:F:11:ALA:HA	5:F:14:HIS:CD2	2.51	0.45
1:E:491:SER:CB	5:H:123:THR:HG21	2.46	0.45
1:D:280:LEU:HD12	1:D:282:SER:H	1.81	0.45
1:B:283:MET:SD	1:B:283:MET:N	2.90	0.45
1:C:185:ASP:O	1:C:189:ILE:HD13	2.17	0.45
5:H:89:ARG:NH2	5:H:90:CYS:SG	2.90	0.45
2:M:21:DC:H2''	2:M:22:DT:C6	2.52	0.45
2:M:29:DG:O6	2:M:34:DG:H1'	2.17	0.45
1:E:23:GLN:HA	1:E:26:ASN:OD1	2.17	0.45
1:E:256:ALA:HB1	1:E:261:ALA:HB1	1.99	0.45
1:D:5:LEU:HD23	1:D:5:LEU:H	1.82	0.45
4:A:169:LEU:HD13	4:A:208:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:LYS:HZ1	5:F:86:GLY:CA	2.30	0.45
1:B:509:ARG:HH11	1:B:509:ARG:HG2	1.82	0.45
5:H:28:GLN:HA	5:H:31:ILE:HD12	1.99	0.44
1:B:218:GLU:O	1:B:223:ARG:NH2	2.50	0.44
3:N:12:G:O2'	3:N:13:A:O5'	2.32	0.44
5:F:197:GLY:HA2	5:F:202:TYR:CD1	2.53	0.44
1:C:316:MET:HE3	1:C:316:MET:HB3	1.85	0.44
5:H:174:HIS:HD2	5:H:185:TRP:HE1	1.64	0.44
1:D:246:TRP:CZ2	1:D:250:LEU:HD11	2.53	0.44
1:B:259:ALA:O	1:B:262:ILE:HG22	2.18	0.44
5:H:167:MET:HE3	5:H:167:MET:HB3	1.75	0.44
1:E:272:LEU:HD11	1:E:283:MET:HB3	1.98	0.44
2:M:34:DG:H2''	2:M:35:DA:H8	1.82	0.44
1:E:252:LYS:HE3	1:E:342:ASP:OD2	2.17	0.44
1:D:43:CYS:SG	1:D:44:TRP:N	2.88	0.44
1:D:166:THR:HG23	1:D:167:LEU:HG	2.00	0.44
1:D:502:GLU:OE1	1:D:540:ASN:HB3	2.18	0.44
1:B:286:LEU:O	1:B:290:THR:OG1	2.35	0.44
1:B:445:LYS:NZ	5:F:85:GLY:O	2.46	0.44
5:F:31:ILE:HD12	5:F:31:ILE:H	1.83	0.44
1:E:91:ILE:HD12	1:E:436:THR:HG21	2.00	0.44
1:C:284:VAL:O	1:C:287:LEU:HB3	2.17	0.44
1:C:292:LYS:HD3	1:C:292:LYS:HA	1.71	0.44
1:D:530:ASP:O	1:D:534:ARG:HG2	2.18	0.44
1:E:4:GLN:O	1:E:8:LYS:HG2	2.18	0.44
1:B:468:SER:O	1:B:472:GLU:HG3	2.18	0.44
2:M:9:DA:H2''	2:M:10:DA:H8	1.81	0.44
5:F:46:CYS:O	5:F:47:GLU:C	2.61	0.44
1:D:6:GLU:HG2	1:D:39:TRP:HH2	1.83	0.43
1:D:126:GLN:HA	2:M:40:DG:OP1	2.18	0.43
1:B:4:GLN:OE1	1:B:4:GLN:N	2.45	0.43
1:D:259:ALA:HA	1:D:262:ILE:HG23	2.00	0.43
2:M:1:DG:H22	2:M:60:DC:H5	1.67	0.43
3:N:21:G:O2'	3:N:22:A:O5'	2.32	0.43
4:A:11:LEU:O	4:A:12:ASN:OD1	2.36	0.43
5:F:14:HIS:HA	5:F:17:ARG:NH2	2.33	0.43
1:D:264:LEU:O	1:D:267:GLU:HG3	2.18	0.43
1:B:86:GLU:O	1:B:422:GLN:NE2	2.51	0.43
1:C:47:LEU:HD12	1:C:190:ILE:HG21	1.99	0.43
2:M:7:DG:H2''	2:M:8:DA:C8	2.53	0.43
2:M:8:DA:C8	2:M:8:DA:H5'	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:210:LEU:CD2	5:H:213:SER:HB2	2.49	0.43
1:D:15:LEU:HB2	1:D:155:LEU:HA	2.00	0.43
1:E:537:ARG:NH2	1:E:538:MET:HG2	2.33	0.43
1:C:86:GLU:O	1:C:422:GLN:NE2	2.52	0.43
1:C:171:GLU:HA	1:C:172:ARG:NH2	2.33	0.43
5:H:42:PHE:HB3	5:H:47:GLU:HA	2.00	0.43
2:M:26:DG:H2'	2:M:27:DG:C8	2.54	0.43
4:A:61:LEU:HB3	4:A:62:TYR:CD1	2.54	0.43
1:E:35:LYS:HE2	1:E:35:LYS:HB2	1.66	0.43
1:E:37:ASP:HA	1:E:40:PHE:CD2	2.53	0.43
1:E:295:LEU:HA	1:E:298:GLN:HB2	2.01	0.43
1:E:472:GLU:HG3	5:H:153:PRO:HB2	2.01	0.43
5:F:59:ARG:HG2	5:F:73:ASN:OD1	2.18	0.43
1:B:88:ASP:OD1	1:B:88:ASP:N	2.47	0.43
1:B:538:MET:CE	5:F:174:HIS:HB3	2.48	0.43
5:F:17:ARG:HB2	5:F:20:ARG:CZ	2.48	0.43
1:B:538:MET:HE1	5:F:175:GLU:HA	2.00	0.43
1:E:262:ILE:HG23	1:E:263:GLU:HG3	2.01	0.43
1:D:103:ILE:O	1:D:107:ILE:HG13	2.19	0.43
1:B:309:MET:N	1:B:309:MET:SD	2.92	0.43
1:B:505:SER:OG	1:B:506:ALA:N	2.52	0.43
1:E:105:TYR:OH	1:E:109:LYS:HE2	2.18	0.42
1:D:414:LEU:HD23	1:D:414:LEU:HA	1.82	0.42
3:N:33:U:O2'	3:N:34:U:P	2.77	0.42
4:A:141:LYS:HE2	4:A:141:LYS:HB2	1.71	0.42
5:F:43:CYS:SG	5:F:78:CYS:N	2.92	0.42
1:E:312:GLU:OE1	1:E:312:GLU:N	2.48	0.42
1:B:306:SER:OG	1:B:309:MET:HE1	2.20	0.42
1:C:44:TRP:NE1	1:C:194:ARG:HG2	2.34	0.42
1:C:218:GLU:OE1	1:C:223:ARG:NH1	2.52	0.42
1:C:257:GLN:HG2	1:C:258:GLY:N	2.32	0.42
4:A:121:GLN:H	4:A:121:GLN:HG3	1.72	0.42
5:H:121:LEU:HD12	5:H:125:HIS:CB	2.42	0.42
1:E:272:LEU:HD12	1:E:275:SER:HB2	2.00	0.42
1:E:494:GLU:OE1	5:H:121:LEU:HD13	2.19	0.42
1:D:282:SER:HB2	1:D:283:MET:HE2	2.00	0.42
2:M:15:DC:H4'	2:M:16:DG:OP1	2.18	0.42
5:F:102:ASN:HB3	5:F:105:HIS:HB2	2.00	0.42
4:A:260:ILE:HD13	4:A:303:MET:HE1	2.00	0.42
1:E:205:SER:OG	1:E:206:VAL:N	2.53	0.42
1:D:190:ILE:HD13	1:D:190:ILE:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:OD1	1:D:270:ASN:N	2.52	0.42
1:B:259:ALA:O	1:B:263:GLU:HG2	2.20	0.42
1:C:104:LEU:HD11	1:C:426:THR:HG23	2.00	0.42
5:H:89:ARG:HE	5:H:155:LEU:HD13	1.84	0.42
1:E:271:HIS:ND1	1:C:280:LEU:HD21	2.34	0.42
1:D:10:LYS:HA	1:D:10:LYS:HD2	1.70	0.42
1:C:58:ILE:HD13	1:C:60:HIS:CD2	2.54	0.42
1:C:414:LEU:HD23	1:C:414:LEU:HA	1.89	0.42
1:E:161:ARG:NH2	1:E:174:GLU:O	2.39	0.42
1:D:14:LEU:HD22	1:D:46:TYR:OH	2.18	0.42
1:B:265:LEU:HD12	1:B:294:LEU:HD23	2.00	0.42
1:C:462:THR:HG23	1:C:470:ILE:HG12	2.02	0.42
1:E:70:MET:HG2	1:E:72:PHE:CE1	2.55	0.42
1:D:45:ASN:O	1:D:49:GLN:HB2	2.20	0.42
1:D:127:ARG:HD2	1:D:164:ARG:NH2	2.35	0.42
1:C:15:LEU:H	1:C:15:LEU:HD22	1.85	0.42
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.85	0.42
1:C:337:THR:HG22	1:C:342:ASP:HA	2.01	0.42
1:E:193:ARG:HB3	1:E:193:ARG:CZ	2.50	0.42
1:E:280:LEU:HD22	1:C:271:HIS:HB2	2.02	0.42
2:M:3:DA:H62	2:M:58:DA:H8	1.67	0.42
2:M:46:DC:H2''	2:M:47:DG:C8	2.55	0.42
1:D:178:LYS:O	1:D:182:GLU:HG2	2.20	0.42
1:B:535:LEU:O	1:B:539:LYS:HB2	2.20	0.42
1:C:66:CYS:SG	1:C:68:ARG:NH1	2.93	0.42
2:M:65:DA:H5'	2:M:65:DA:C8	2.55	0.42
5:F:34:HIS:O	5:F:38:MET:HG2	2.20	0.42
5:F:87:TRP:O	5:F:89:ARG:N	2.53	0.42
1:E:140:ASN:HB3	1:E:142:PHE:CE2	2.54	0.41
4:A:186:ASP:OD1	4:A:186:ASP:C	2.62	0.41
1:E:491:SER:O	1:E:494:GLU:HB3	2.20	0.41
1:D:157:ASN:N	1:D:157:ASN:OD1	2.53	0.41
1:B:269:VAL:HA	1:B:272:LEU:HB3	2.02	0.41
2:M:1:DG:H2''	2:M:2:DG:C8	2.54	0.41
1:E:484:ILE:HG22	1:E:487:SER:H	1.86	0.41
1:D:300:ARG:NH2	1:D:312:GLU:HB2	2.35	0.41
1:B:414:LEU:HD23	1:B:414:LEU:HA	1.90	0.41
1:B:498:ILE:CD1	5:F:119:LEU:HD21	2.49	0.41
5:H:89:ARG:HH21	5:H:155:LEU:HD13	1.85	0.41
5:F:63:LYS:HD3	5:F:63:LYS:HA	1.72	0.41
1:B:403:HIS:CD2	1:B:404:PRO:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:VAL:HG22	1:C:283:MET:HB3	2.02	0.41
2:M:28:DA:H1'	2:M:35:DA:N6	2.34	0.41
1:E:158:ILE:HG23	1:E:179:PRO:HB2	2.02	0.41
1:E:211:PRO:HA	1:E:363:ARG:NH2	2.36	0.41
1:E:286:LEU:O	1:E:290:THR:HG22	2.21	0.41
1:D:7:ARG:HH12	1:D:8:LYS:HB3	1.85	0.41
1:C:264:LEU:HG	1:C:268:GLN:OE1	2.21	0.41
1:D:544:LYS:HA	1:D:544:LYS:HD3	1.76	0.41
1:C:137:ASP:OD1	1:C:137:ASP:N	2.54	0.41
1:E:331:SER:OG	1:E:347:THR:O	2.35	0.41
1:E:336:GLU:O	1:E:337:THR:HG22	2.21	0.41
1:D:13:SER:O	1:D:17:ALA:N	2.52	0.41
1:D:218:GLU:O	1:D:223:ARG:NH1	2.54	0.41
1:D:402:LEU:HD23	1:D:402:LEU:HA	1.93	0.41
1:D:447:ASN:HB2	1:D:454:PHE:HE1	1.86	0.41
1:B:298:GLN:HE22	1:B:299:MET:HE3	1.86	0.41
1:C:301:LYS:HB3	1:C:301:LYS:HE3	1.78	0.41
2:M:23:DG:H1'	2:M:24:DA:C4	2.55	0.41
3:N:9:G:H1	3:N:19:C:H5	1.69	0.41
5:F:13:LEU:HD23	5:F:13:LEU:HA	1.85	0.41
5:F:107:ILE:HA	5:F:139:LYS:HE2	2.03	0.41
1:D:445:LYS:HD3	1:D:446:GLN:N	2.36	0.41
1:C:289:GLU:HG2	1:C:293:LYS:HE3	2.02	0.41
3:N:35:G:O2'	3:N:36:A:OP1	2.31	0.41
5:F:6:ARG:CZ	5:F:72:GLY:HA2	2.51	0.41
5:F:23:TRP:O	5:F:26:VAL:HG22	2.21	0.41
1:E:113:TRP:CZ3	1:E:177:ILE:HD12	2.56	0.40
1:B:348:ASN:OD1	1:B:348:ASN:C	2.63	0.40
2:M:32:DA:H1'	2:M:33:DC:H2'	2.04	0.40
3:N:12:G:O2'	3:N:14:U:O2	2.39	0.40
1:E:195:MET:HE1	1:E:307:VAL:HG22	2.02	0.40
1:E:541:LYS:HD3	1:E:542:ILE:HG12	2.02	0.40
1:D:513:ASN:HA	1:D:516:ILE:HG22	2.04	0.40
1:C:47:LEU:HD23	1:C:47:LEU:HA	1.83	0.40
5:F:39:GLN:OE1	5:F:76:GLY:N	2.54	0.40
1:E:521:GLN:O	1:E:526:LEU:HD23	2.21	0.40
1:D:270:ASN:HA	1:D:273:LYS:HD2	2.03	0.40
1:B:445:LYS:HB3	5:F:83:LYS:CE	2.43	0.40
2:M:20:DC:H2''	2:M:21:DC:H2'	2.04	0.40
2:M:49:DC:H2''	2:M:50:DA:H5'	2.02	0.40
1:E:504:LEU:HB2	1:E:509:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:SER:OG	1:B:207:GLU:HG2	2.22	0.40
1:C:55:ASN:HB3	1:C:58:ILE:HD11	2.03	0.40
1:C:249:TYR:CD1	1:C:249:TYR:C	3.00	0.40
5:F:57:HIS:CE1	5:F:61:ARG:HD3	2.57	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	B	549/551 (100%)	532 (97%)	17 (3%)	0	100	100
1	C	549/551 (100%)	537 (98%)	12 (2%)	0	100	100
1	D	549/551 (100%)	530 (96%)	19 (4%)	0	100	100
1	E	549/551 (100%)	534 (97%)	14 (3%)	1 (0%)	43	68
4	A	308/310 (99%)	296 (96%)	12 (4%)	0	100	100
5	F	213/215 (99%)	202 (95%)	9 (4%)	2 (1%)	14	35
5	H	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
All	All	2930/2944 (100%)	2839 (97%)	88 (3%)	3 (0%)	49	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	89	ARG
5	F	214	GLU
1	E	505	SER

5.3.2 Protein sidechains ⓘ

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	B	498/498 (100%)	479 (96%)	19 (4%)	29	58
1	C	498/498 (100%)	482 (97%)	16 (3%)	34	64
1	D	498/498 (100%)	484 (97%)	14 (3%)	38	68
1	E	498/498 (100%)	478 (96%)	20 (4%)	28	56
4	A	282/282 (100%)	279 (99%)	3 (1%)	65	85
5	F	183/183 (100%)	169 (92%)	14 (8%)	12	30
5	H	183/183 (100%)	162 (88%)	21 (12%)	5	14
All	All	2640/2640 (100%)	2533 (96%)	107 (4%)	28	56

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	13	SER
1	E	40	PHE
1	E	74	ASP
1	E	78	PHE
1	E	123	SER
1	E	157	ASN
1	E	160	ILE
1	E	177	ILE
1	E	210	HIS
1	E	252	LYS
1	E	283	MET
1	E	307	VAL
1	E	310	LEU
1	E	335	VAL
1	E	346	VAL
1	E	421	ILE
1	E	480	THR
1	E	527	LYS
1	E	533	ILE
1	E	547	ARG

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Mol	Chain	Res	Type
1	D	2	THR
1	D	14	LEU
1	D	43	CYS
1	D	147	SER
1	D	269	VAL
1	D	274	GLN
1	D	275	SER
1	D	307	VAL
1	D	342	ASP
1	D	394	LEU
1	D	429	SER
1	D	463	LYS
1	D	500	ASP
1	D	531	SER
1	B	27	ASN
1	B	30	HIS
1	B	56	LEU
1	B	58	ILE
1	B	147	SER
1	B	175	SER
1	B	209	SER
1	B	213	SER
1	B	241	ASP
1	B	245	GLU
1	B	269	VAL
1	B	275	SER
1	B	290	THR
1	B	346	VAL
1	B	365	PHE
1	B	405	LYS
1	B	421	ILE
1	B	505	SER
1	B	524	SER
1	C	58	ILE
1	C	139	ASP
1	C	147	SER
1	C	165	SER
1	C	170	SER
1	C	177	ILE
1	C	290	THR
1	C	298	GLN
1	C	319	VAL

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Mol	Chain	Res	Type
1	C	379	LEU
1	C	438	ILE
1	C	448	SER
1	C	457	SER
1	C	487	SER
1	C	499	ASP
1	C	505	SER
4	A	14	SER
4	A	150	VAL
4	A	299	SER
5	H	31	ILE
5	H	45	TYR
5	H	48	CYS
5	H	50	LEU
5	H	71	TRP
5	H	82	SER
5	H	100	ASN
5	H	132	ILE
5	H	142	GLU
5	H	149	LEU
5	H	154	SER
5	H	166	ILE
5	H	167	MET
5	H	172	LEU
5	H	176	SER
5	H	178	GLU
5	H	186	HIS
5	H	206	LYS
5	H	211	HIS
5	H	212	ASN
5	H	213	SER
5	F	7	THR
5	F	42	PHE
5	F	46	CYS
5	F	47	GLU
5	F	50	LEU
5	F	77	SER
5	F	88	GLN
5	F	89	ARG
5	F	112	ASP
5	F	126	VAL
5	F	132	ILE

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Mol	Chain	Res	Type
5	F	210	LEU
5	F	211	HIS
5	F	214	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	48	GLN
1	E	80	GLN
1	E	197	ASN
1	E	257	GLN
1	E	521	GLN
1	D	63	ASN
1	D	117	ASN
1	D	140	ASN
1	D	197	ASN
1	D	483	ASN
1	D	522	HIS
1	B	48	GLN
1	B	148	ASN
1	B	157	ASN
1	B	197	ASN
1	B	351	GLN
1	C	27	ASN
1	C	84	ASN
1	C	191	ASN
1	C	380	ASN
1	C	428	HIS
1	C	513	ASN
1	C	543	ASN
4	A	82	ASN
4	A	133	GLN
4	A	232	ASN
5	H	150	ASN
5	H	174	HIS
5	H	212	ASN
5	F	15	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	N	37/66 (56%)	18 (48%)	5 (13%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	N	13	A
3	N	14	U
3	N	15	U
3	N	16	A
3	N	19	C
3	N	20	A
3	N	21	G
3	N	22	A
3	N	26	U
3	N	27	A
3	N	28	A
3	N	29	C
3	N	31	U
3	N	33	U
3	N	34	U
3	N	36	A
3	N	37	A
3	N	38	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	N	26	U
3	N	30	U
3	N	33	U
3	N	35	G
3	N	37	A

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
6	ADP	D	601	-	27,29,29	1.34	4 (14%)	42,45,45	1.94	11 (26%)
7	ATP	B	601	-	29,33,33	0.33	0	44,52,52	0.44	1 (2%)
7	ATP	C	601	-	29,33,33	0.32	0	44,52,52	0.45	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	D	601	-	-	2/16/32/32	0/3/3/3
7	ATP	B	601	-	-	5/22/38/38	0/3/3/3
7	ATP	C	601	-	-	6/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	601	ADP	C5-C4	4.40	1.47	1.39
6	D	601	ADP	C5-C6	2.62	1.48	1.41
6	D	601	ADP	C8-N7	2.27	1.35	1.31
6	D	601	ADP	C5-N7	-2.21	1.34	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	601	ADP	C5-C4-N3	-6.19	118.68	126.75
6	D	601	ADP	N3-C4-N9	4.86	135.09	127.08
6	D	601	ADP	C2-N3-C4	3.83	120.80	111.75
6	D	601	ADP	C4-C5-N7	-3.25	106.66	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	601	ADP	N3-C2-N1	-3.11	123.74	128.60
6	D	601	ADP	PA-O3A-PB	-3.02	122.46	132.83
6	D	601	ADP	C5-N7-C8	2.72	107.37	103.51
6	D	601	ADP	C4-N9-C8	2.63	108.58	105.73
6	D	601	ADP	C3'-C2'-C1'	2.28	105.76	101.43
6	D	601	ADP	C6-C5-N7	2.13	135.98	132.02
7	C	601	ATP	PB-O3B-PG	2.04	139.83	132.83
7	B	601	ATP	PB-O3B-PG	2.03	139.80	132.83
6	D	601	ADP	N9-C8-N7	-2.02	111.15	113.91

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	ATP	C5'-O5'-PA-O1A
7	B	601	ATP	C5'-O5'-PA-O2A
7	C	601	ATP	C5'-O5'-PA-O1A
7	C	601	ATP	C5'-O5'-PA-O2A
7	C	601	ATP	O4'-C4'-C5'-O5'
7	C	601	ATP	PA-O3A-PB-O1B
7	B	601	ATP	C5'-O5'-PA-O3A
7	C	601	ATP	C5'-O5'-PA-O3A
6	D	601	ADP	PB-O3A-PA-O1A
7	B	601	ATP	PB-O3B-PG-O3G
6	D	601	ADP	O4'-C4'-C5'-O5'
7	B	601	ATP	O4'-C4'-C5'-O5'
7	C	601	ATP	PA-O3A-PB-O2B

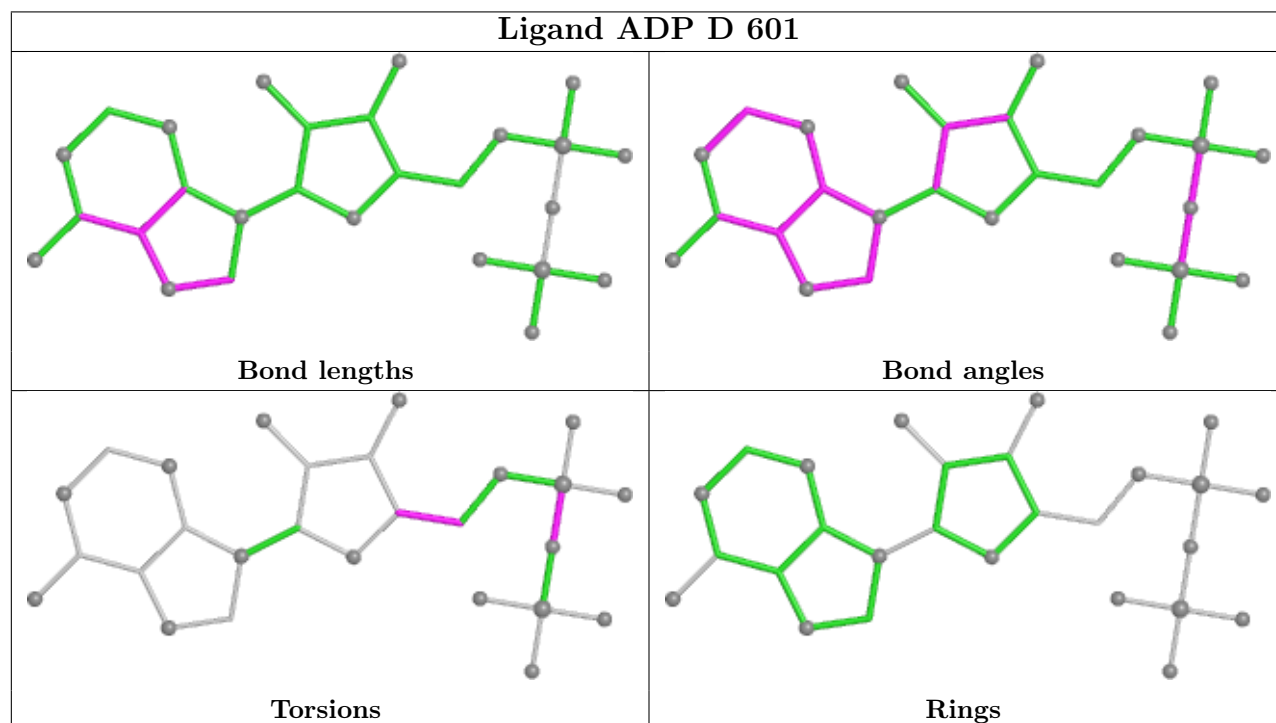
There are no ring outliers.

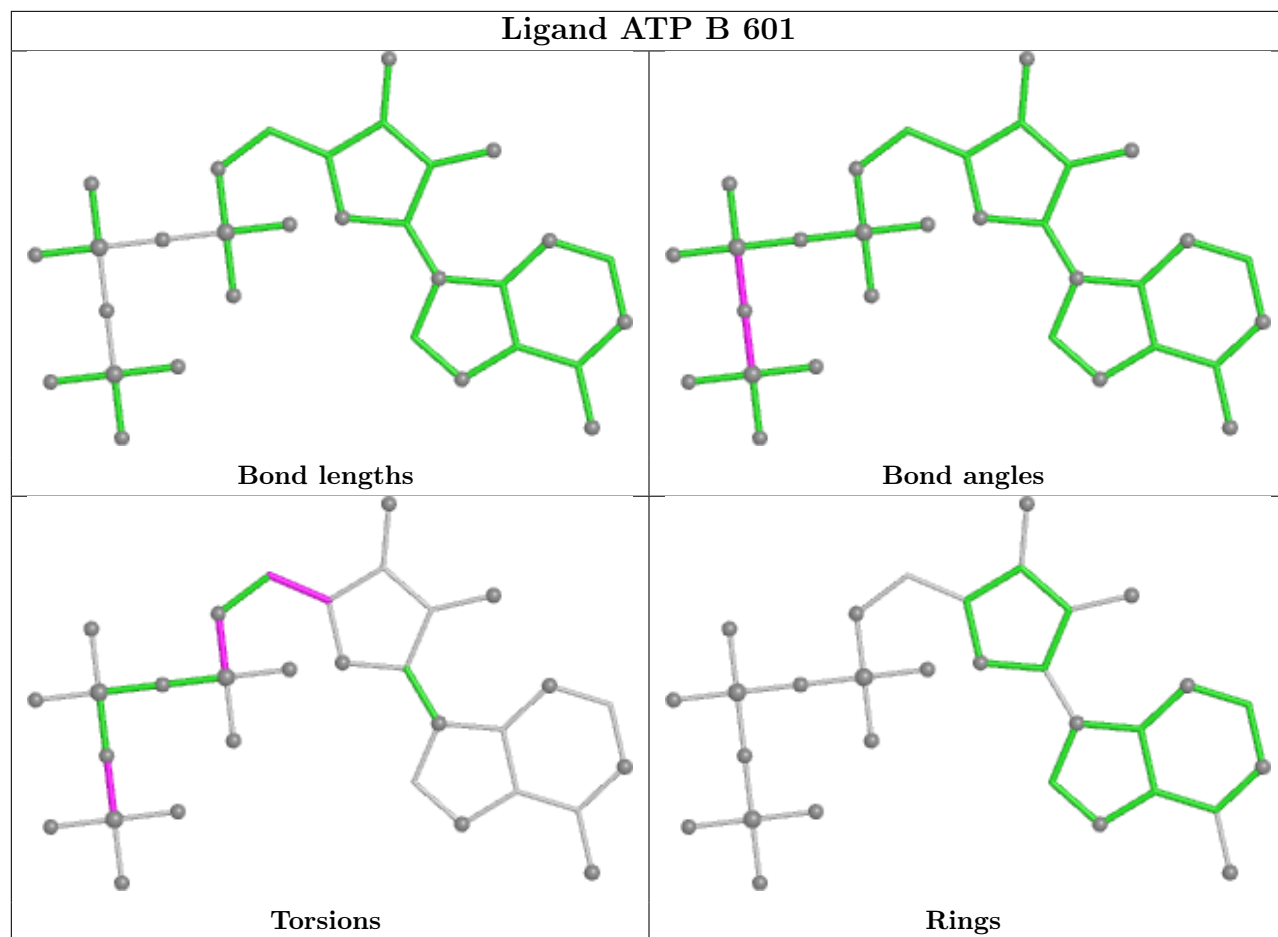
1 monomer is involved in 1 short contact:

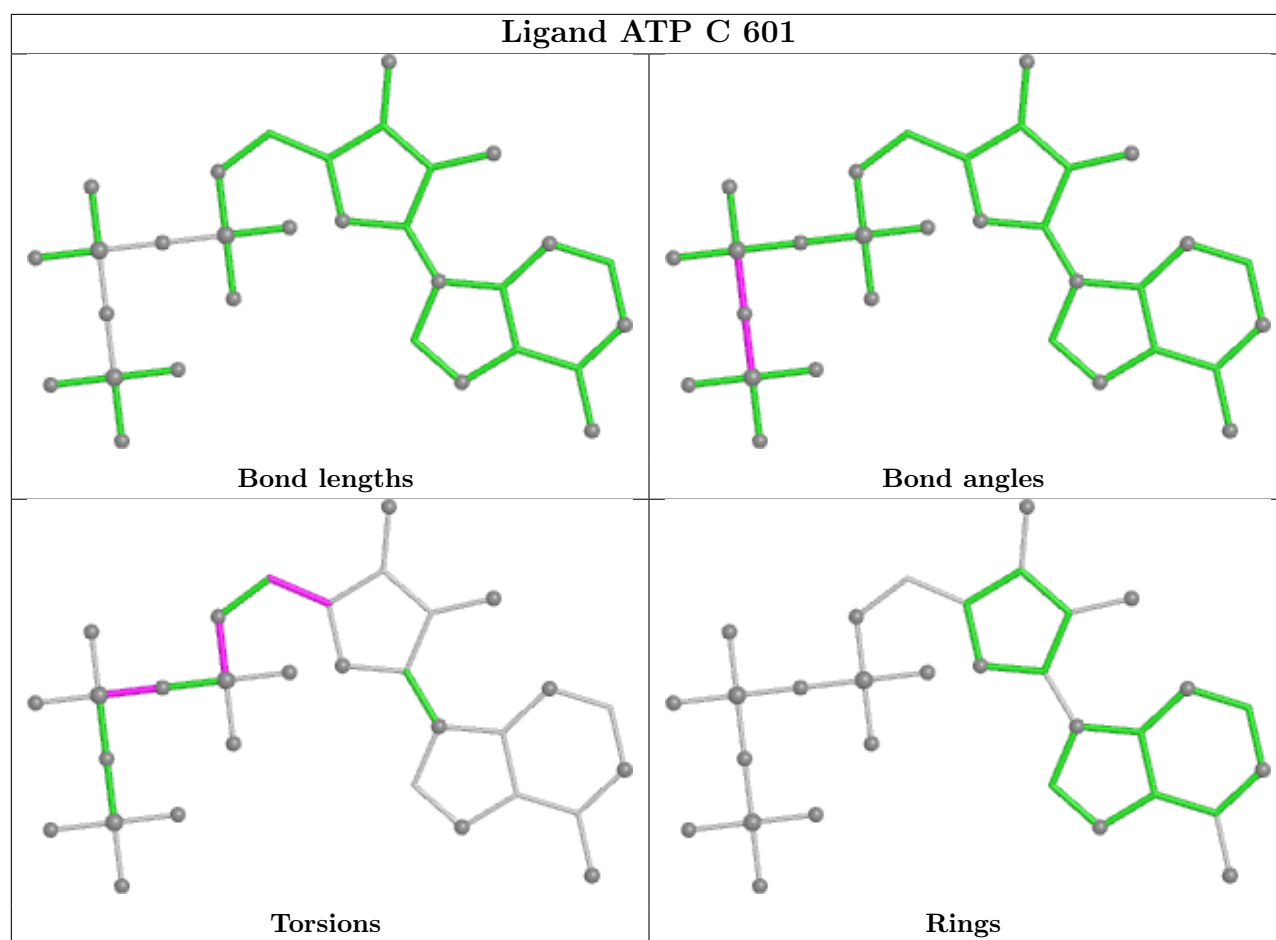
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	601	ADP	1	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

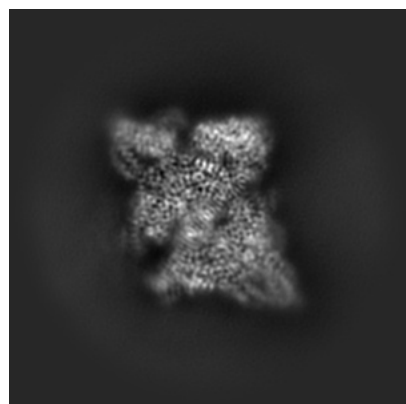
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68219. These allow visual inspection of the internal detail of the map and identification of artifacts.

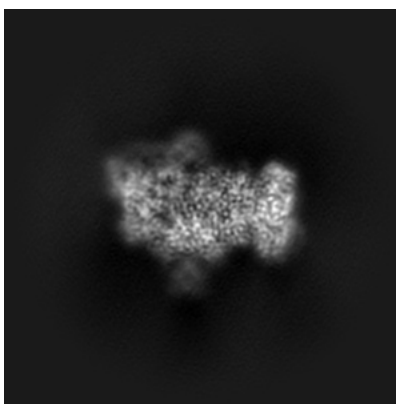
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

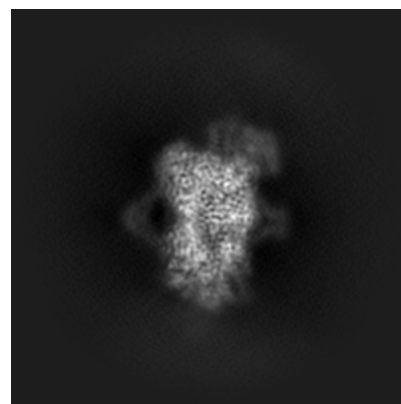
6.1.1 Primary map



X

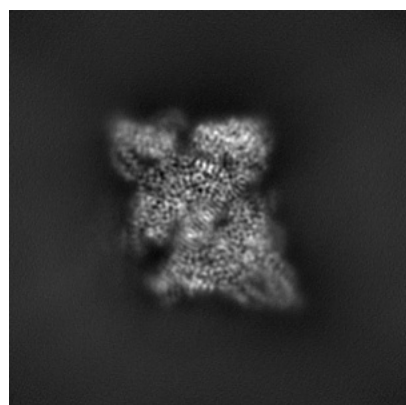


Y

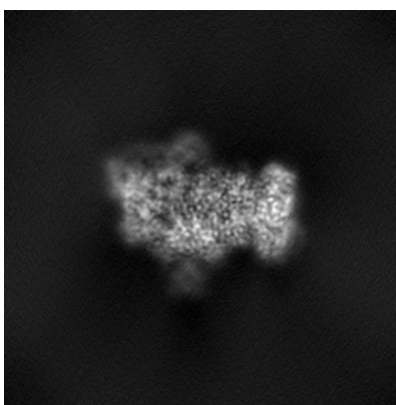


Z

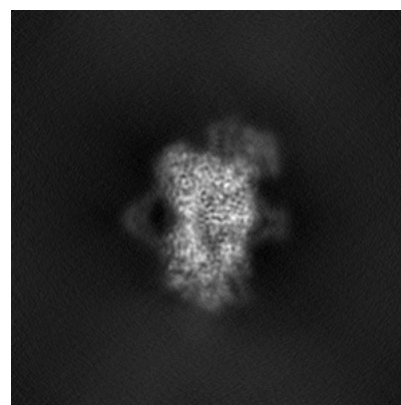
6.1.2 Raw map



X



Y

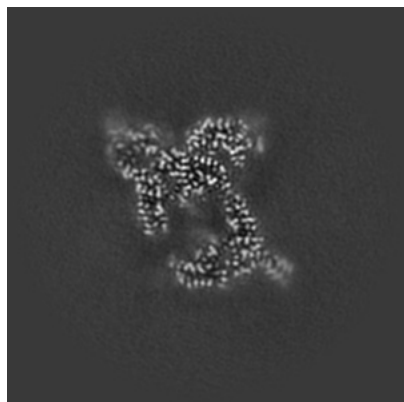


Z

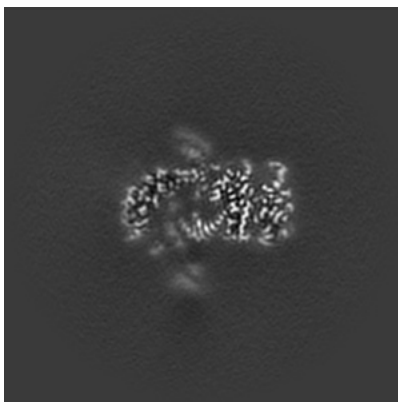
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

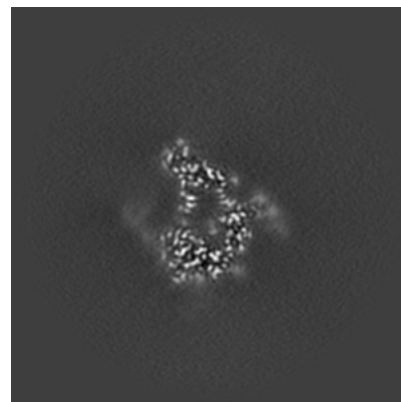
6.2.1 Primary map



X Index: 150

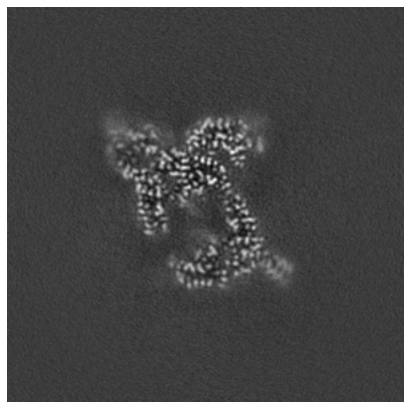


Y Index: 150

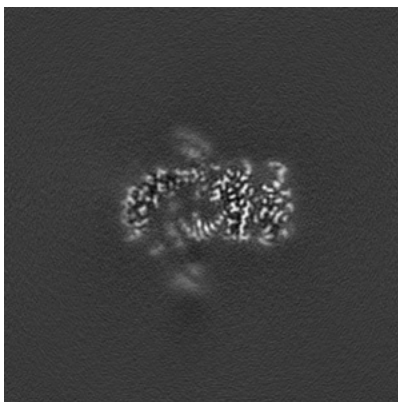


Z Index: 150

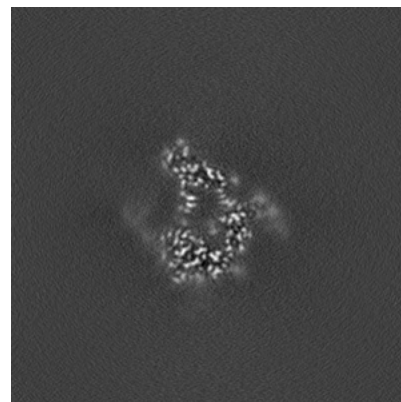
6.2.2 Raw map



X Index: 150



Y Index: 150

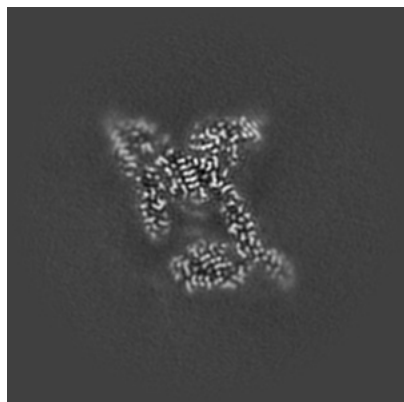


Z Index: 150

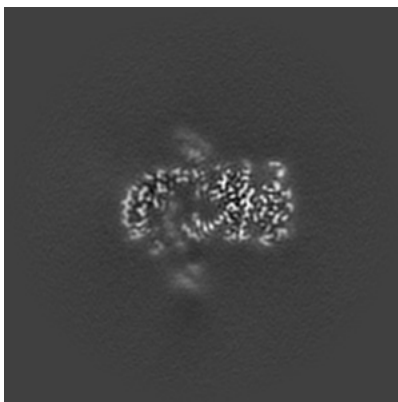
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

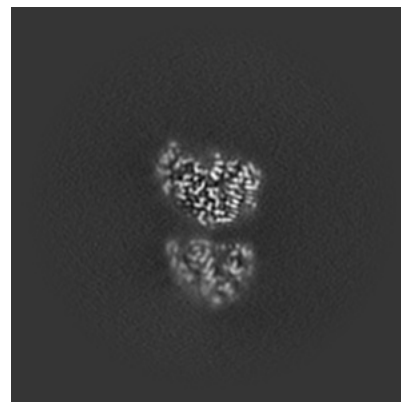
6.3.1 Primary map



X Index: 154

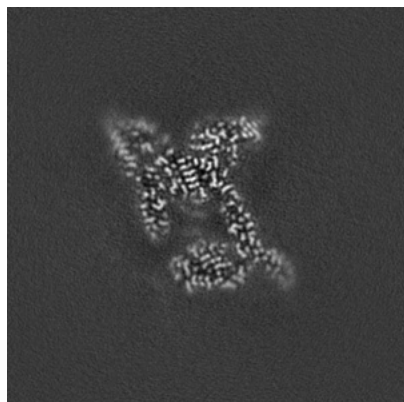


Y Index: 151

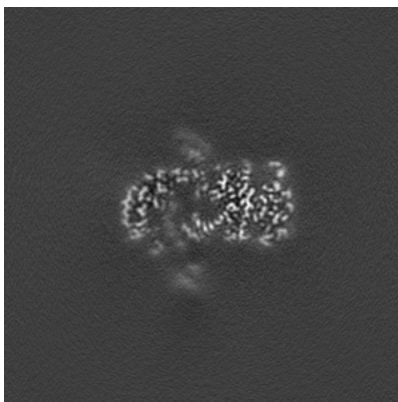


Z Index: 203

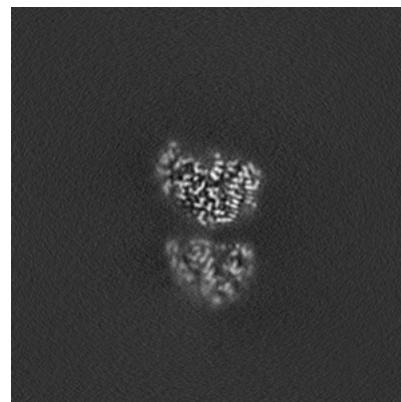
6.3.2 Raw map



X Index: 154



Y Index: 151

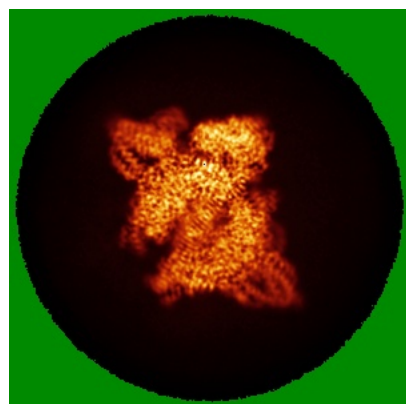


Z Index: 203

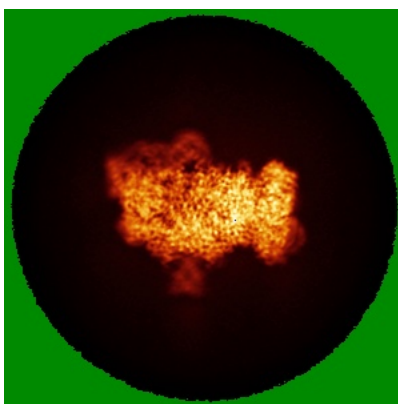
The images above show the largest variance slices of the map in three orthogonal directions.

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

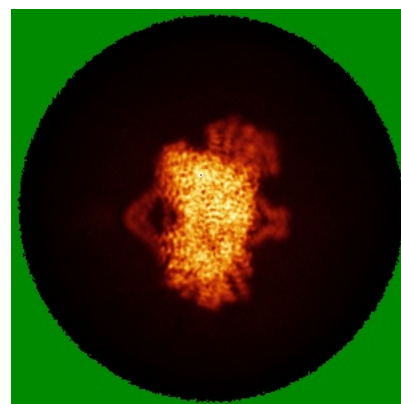
6.4.1 Primary map



X

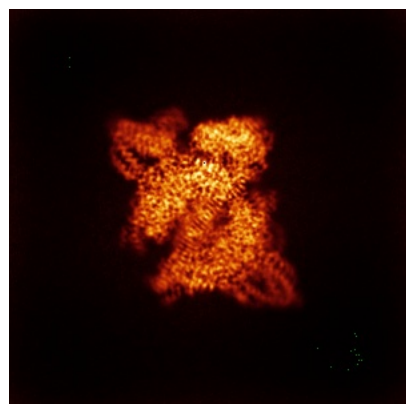


Y

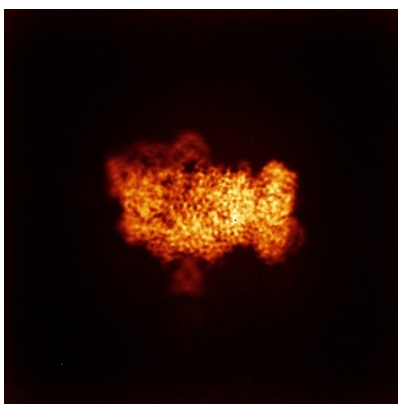


Z

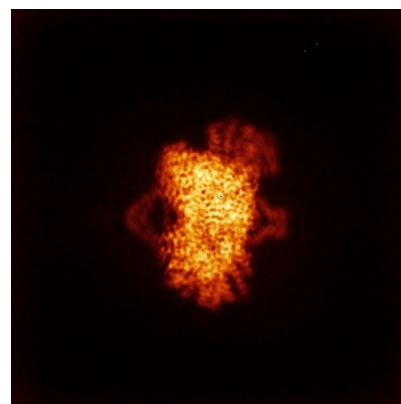
6.4.2 Raw map



X



Y

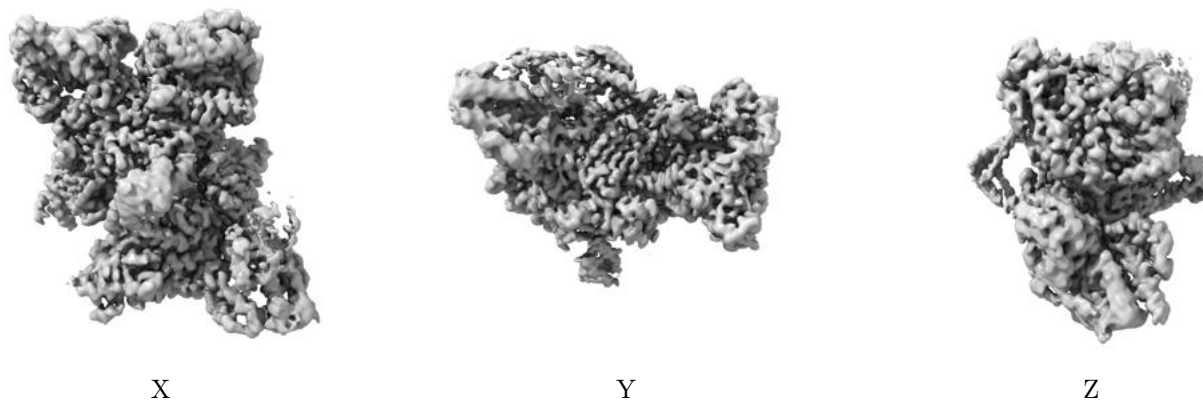


Z

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 0.2. 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.

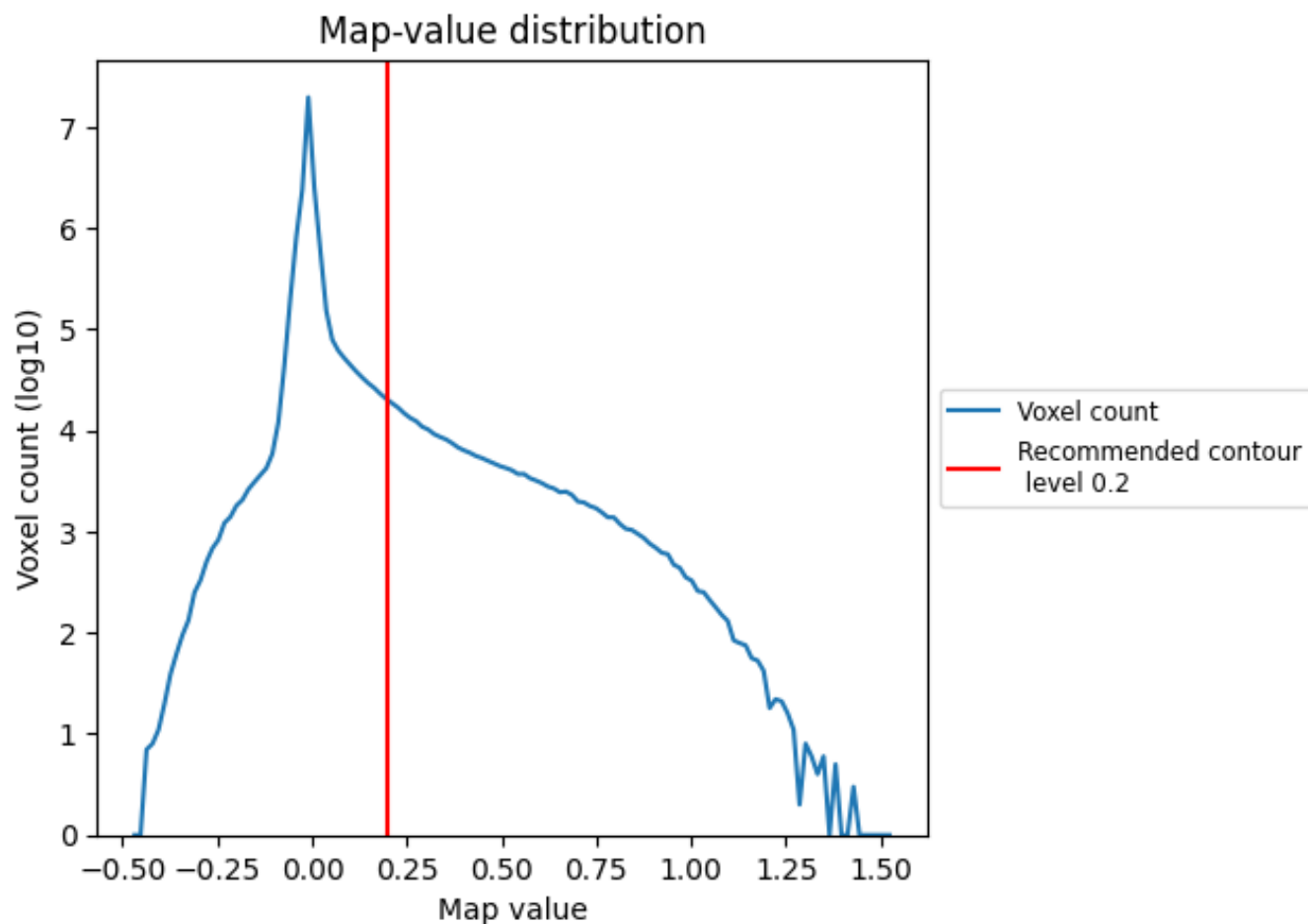
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

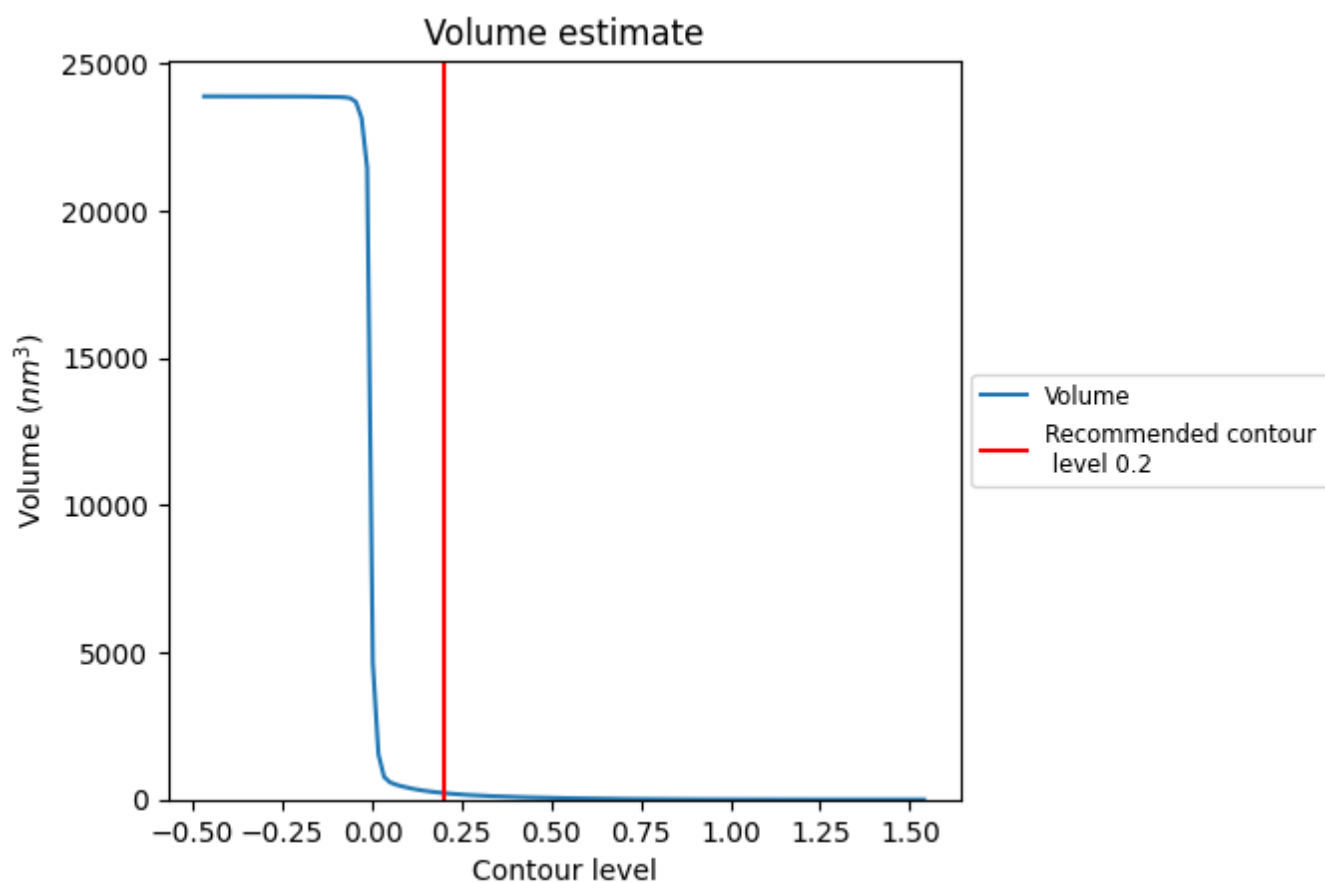
This section contains the results of statistical analysis of the map.

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.

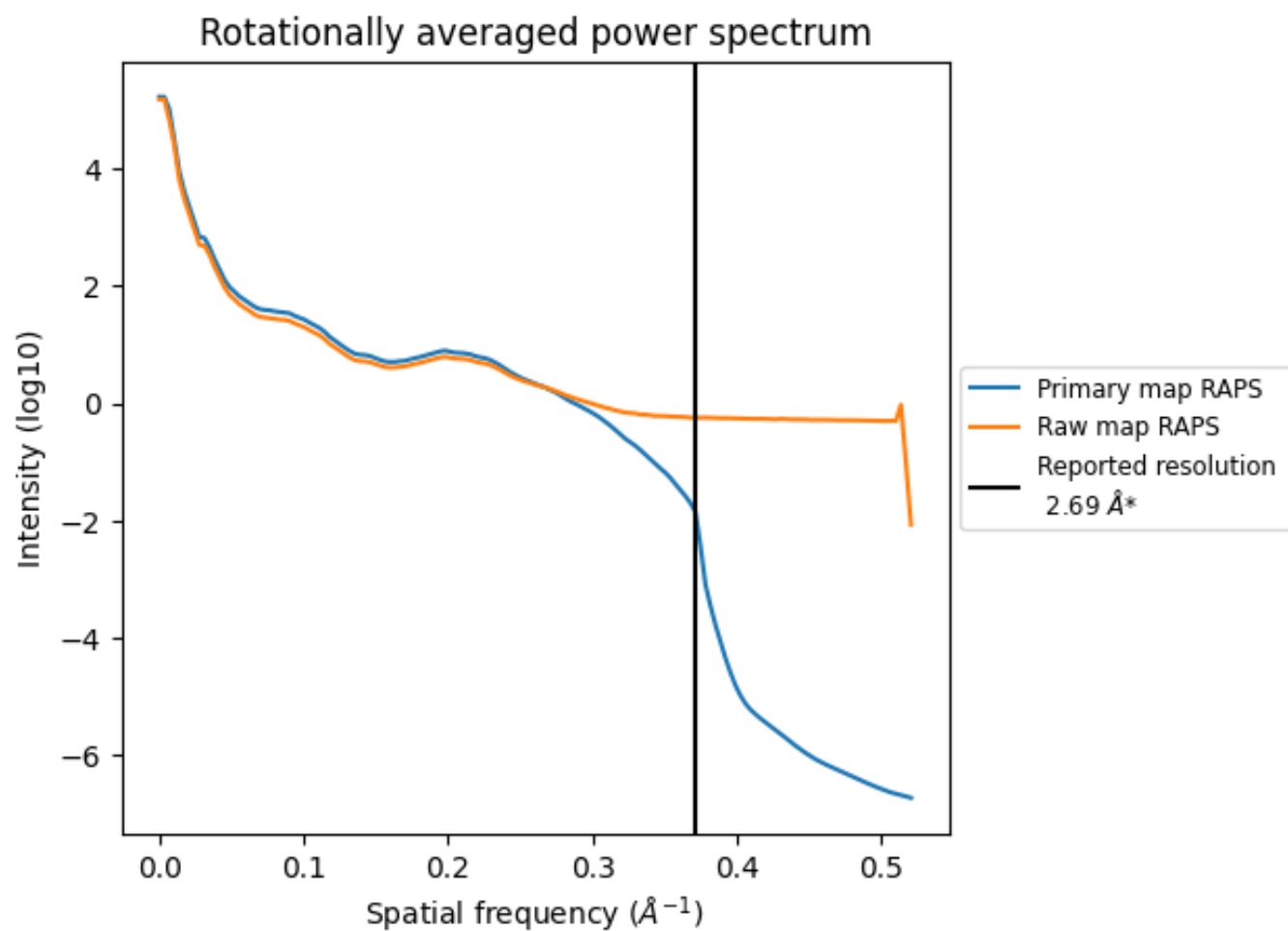
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221 nm³; this corresponds to an approximate mass of 200 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 ⓘ

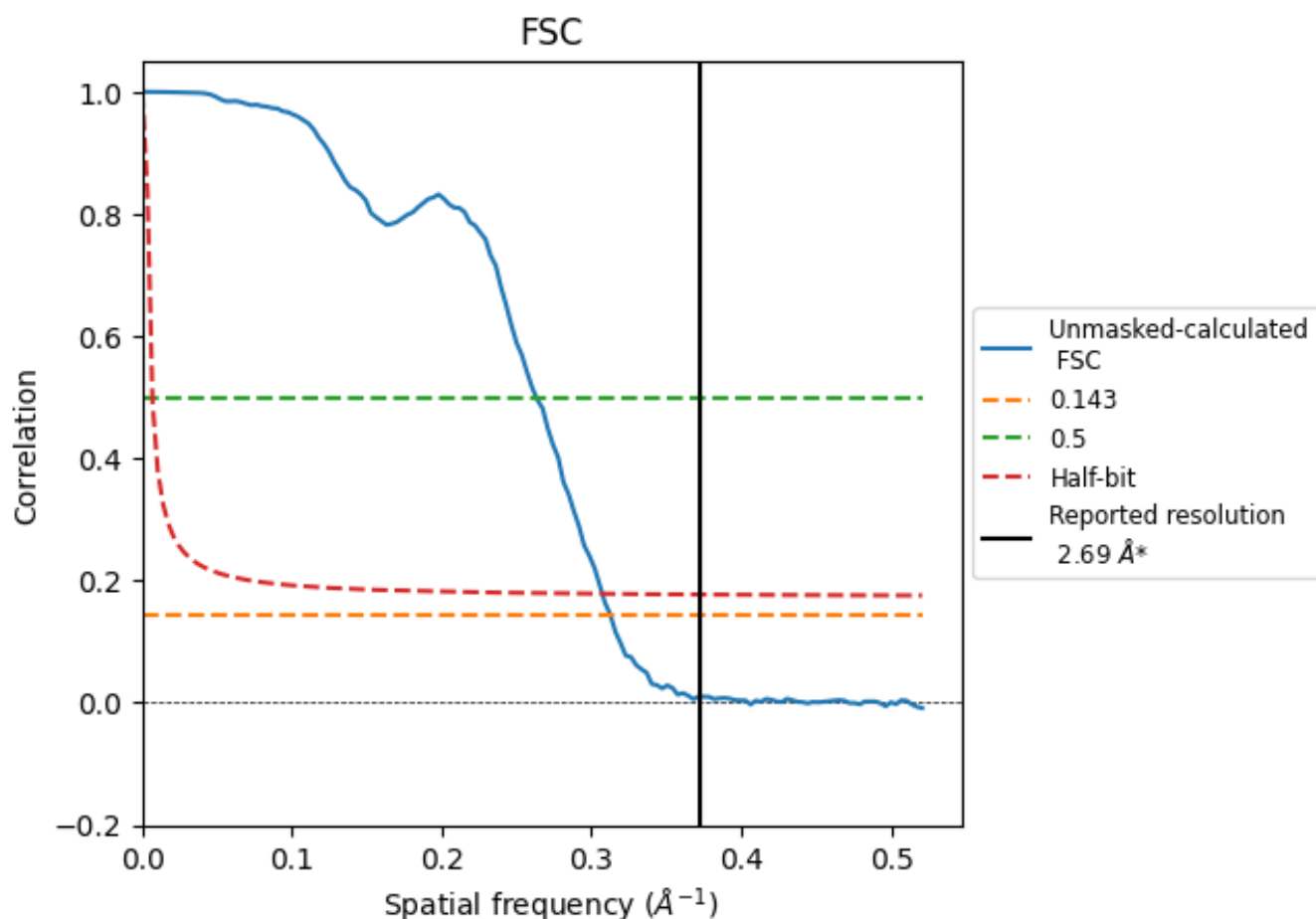


*Reported resolution corresponds to spatial frequency of $0.372 \text{ \AA}^{-1}$

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 0.372 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

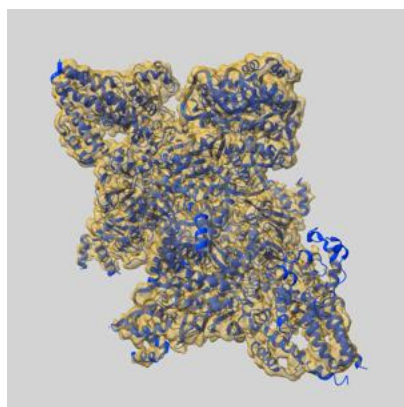
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.20	3.80	3.26

*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 3.20 differs from the reported value 2.69 by more than 10 %

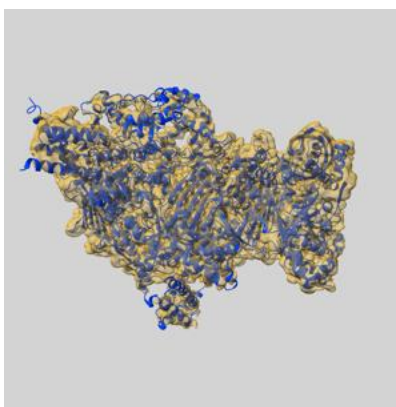
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68219 and PDB model 22ET. Per-residue inclusion information can be found in section [3](#) on page [7](#).

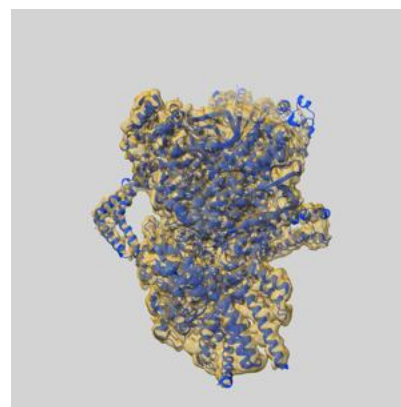
9.1 Map-model overlay [i](#)



X



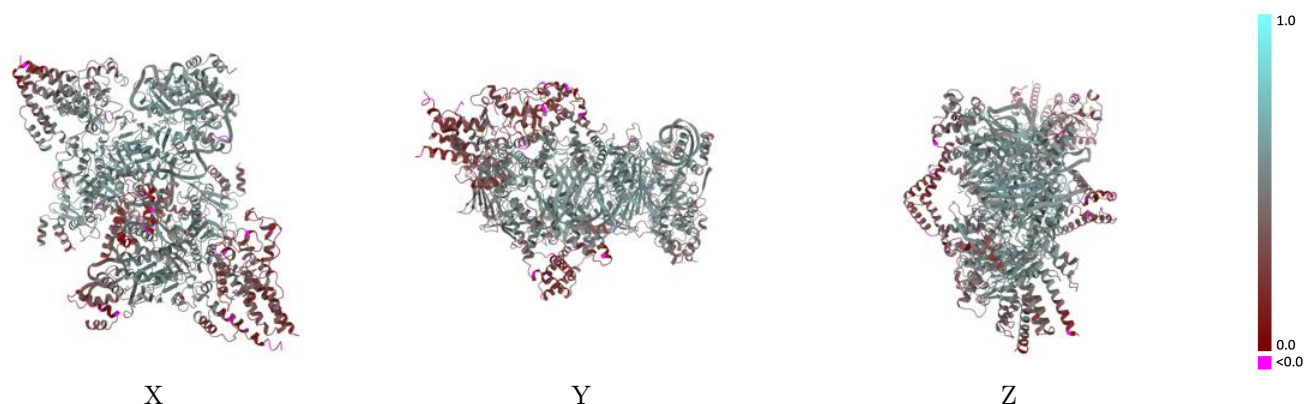
Y



Z

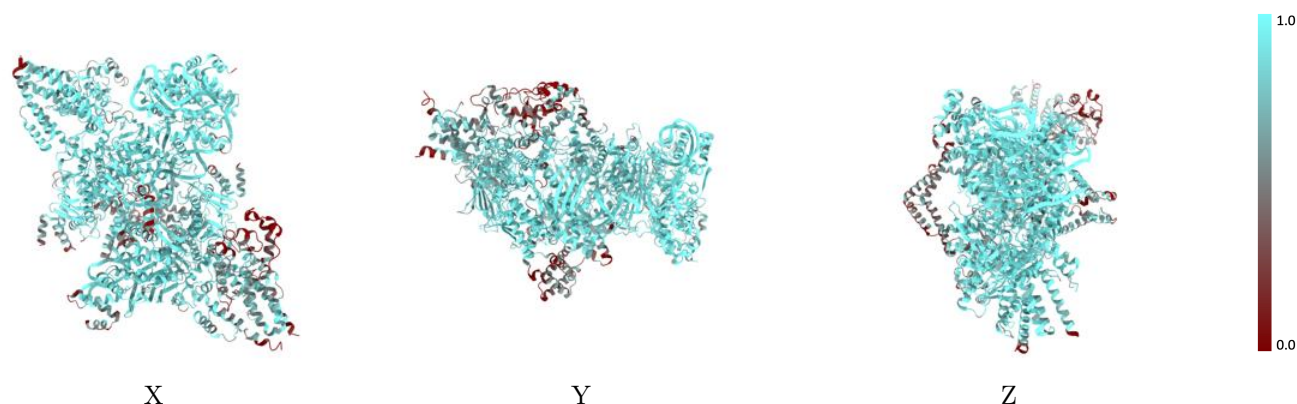
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



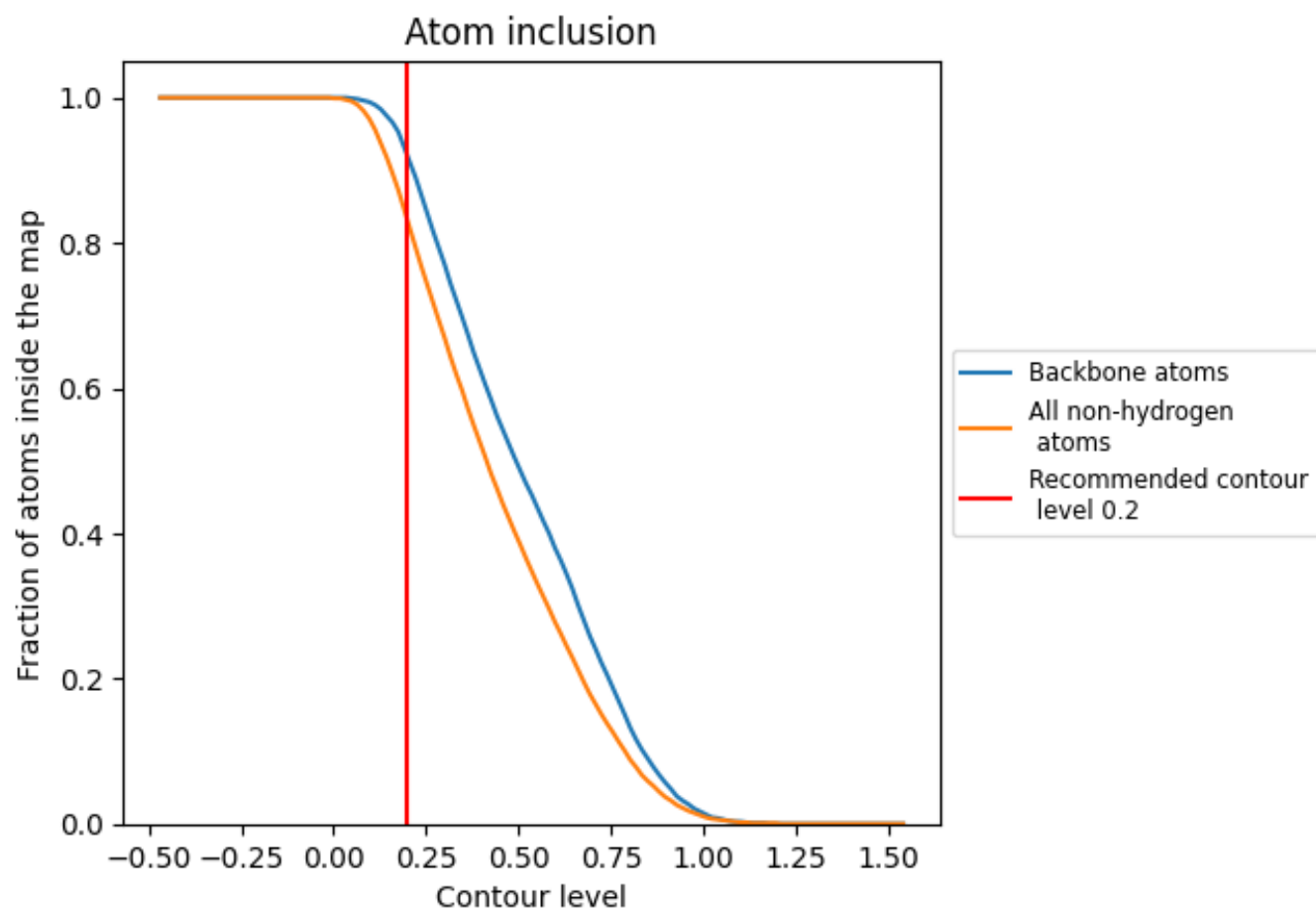
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.4560
A	0.9310	0.5190
B	0.8870	0.5140
C	0.8250	0.4760
D	0.8140	0.4230
E	0.8110	0.4410
F	0.8260	0.4020
H	0.4290	0.2660
M	0.9790	0.5080
N	0.9930	0.5300

1.0

0.0

<0.0