



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 07:39 pm BST

PDB ID : 9GEV / pdb_00009gev
EMDB ID : EMD-51307
Title : CryoEM structure of the human INO80 core-nucleosome complex state N-6
Authors : Sharma, M.; Aggarwal, P.; Hopfner, K.P.
Deposited on : 2024-08-07
Resolution : 3.47 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:

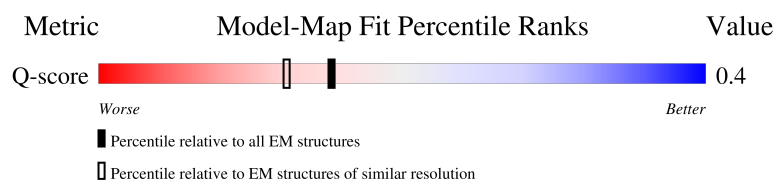
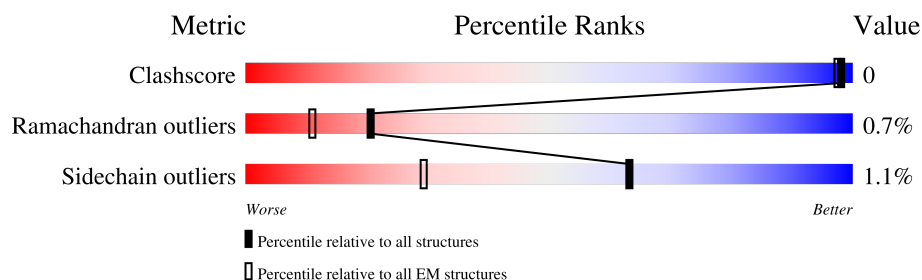
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.47 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.



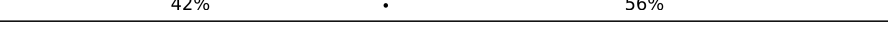
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13733 (2.97 - 3.97)

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	456	92% 5%
1	B	456	94% . .
1	C	456	94% . .
2	D	463	86% 5% . 8%

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Mol	Chain	Length	Quality of chain
2	E	463	 91% • 5%
2	F	463	 87% 6% • 6%
3	I	192	 53% •• 44%
4	K	152	 59% 28% •• 11%
5	L	152	 60% 22% 6% • 11%
6	M	136	 65% • 32%
6	Q	136	 68% • 27%
7	N	102	 76% • 22%
7	R	102	 75% • 23%
8	O	129	 79% • 18%
8	S	129	 79% •• 16%
9	P	125	 75% 25%
9	T	125	 73% • 26%
10	G	1556	 42% • 56%
11	H	356	 40% • 59%
12	J	607	 65% • 32%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 42875 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	443	Total	C	N	O	S	0	0
			3412	2148	585	662	17		
1	A	434	Total	C	N	O	S	0	0
			3344	2107	575	646	16		
1	B	447	Total	C	N	O	S	0	0
			3453	2173	592	672	16		

- Molecule 2 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	439	Total	C	N	O	S	0	0
			3403	2125	597	665	16		
2	D	426	Total	C	N	O	S	0	0
			3317	2074	583	645	15		
2	F	434	Total	C	N	O	S	0	0
			3376	2110	592	658	16		

- Molecule 3 is a protein called INO80 complex subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	107	Total	C	N	O	0	0
			842	540	148	154		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	143	TYR	ASN	conflict	UNP Q6PI98

- Molecule 4 is a DNA chain called Nucleosomal DNA Strand 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	135	Total	C	N	O	P	0	0
			2787	1319	526	807	135		

- Molecule 5 is a DNA chain called Nucleosomal DNA Strand 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	135	Total	C	N	O	P	0	0
			2748	1307	493	813	135		

- Molecule 6 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	93	Total	C	N	O	S	0	0
			761	479	146	132	4		
6	Q	99	Total	C	N	O	S	0	0
			816	514	158	140	4		

- Molecule 7 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
7	R	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

- Molecule 8 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	106	Total	C	N	O	0	0
			819	517	160	142		
8	S	108	Total	C	N	O	0	0
			835	526	165	144		

- Molecule 9 is a protein called Histone H2B type 2-E.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	94	Total	C	N	O	S	0	0
			735	462	132	139	2		
9	T	93	Total	C	N	O	S	0	0
			731	459	133	137	2		

- Molecule 10 is a protein called Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	682	Total	C	N	O	S	0	0
			5608	3599	1004	975	30		

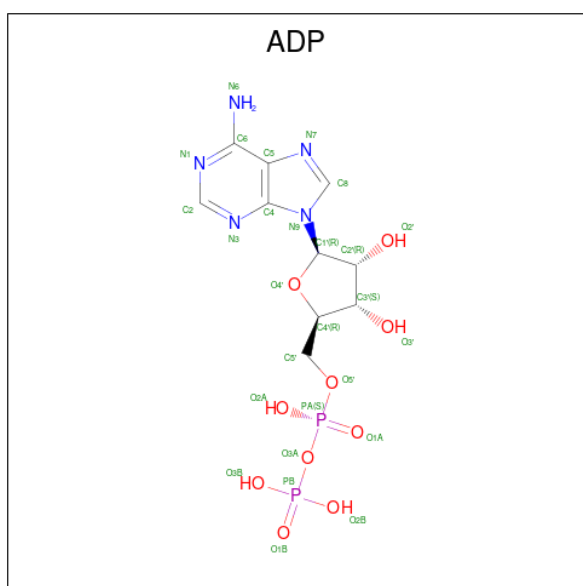
- Molecule 11 is a protein called INO80 complex subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	147	Total	C	N	O	S	0	0
			1153	698	231	215	9		

- Molecule 12 is a protein called Actin-related protein 5.

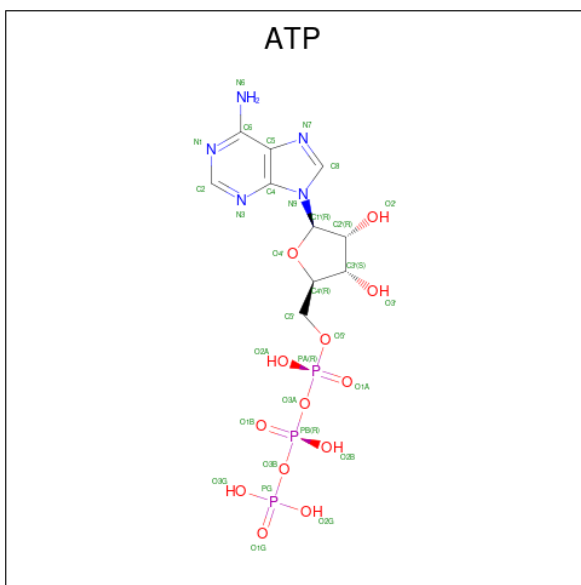
Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	412	Total	C	N	O	S	0	0
			3277	2088	572	596	21		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

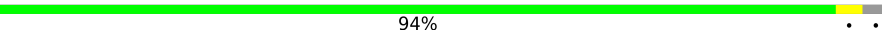


Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

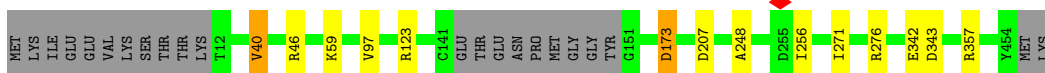
- Molecule 1: RuvB-like 1

Chain C:  94%

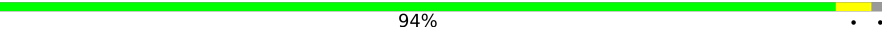


- Molecule 1: RuvB-like 1

Chain A:  92% 5%



- Molecule 1: RuvB-like 1

Chain B:  94%



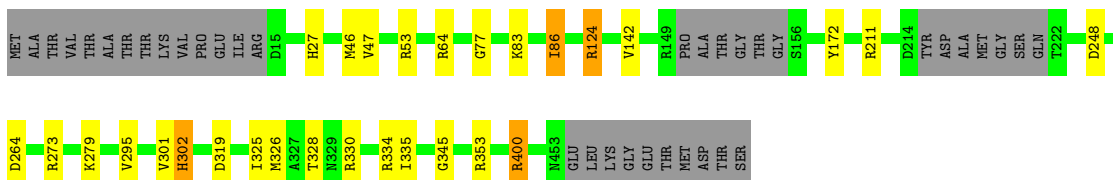
- Molecule 2: RuvB-like 2

Chain E:  91% 5%



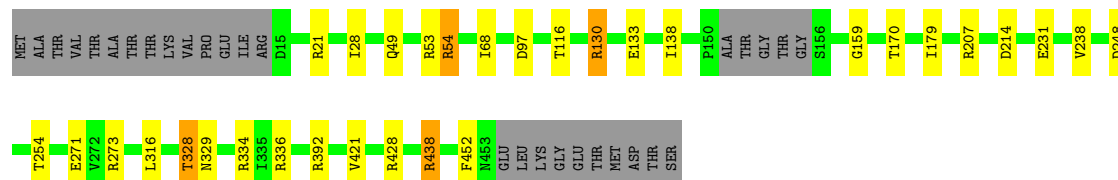
- Molecule 2: RuvB-like 2

Chain D:  86% 5% 8%



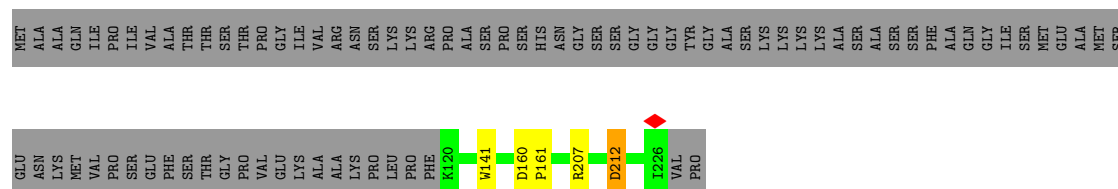
- Molecule 2: RuvB-like 2

Chain F:  87% 6% • 6%



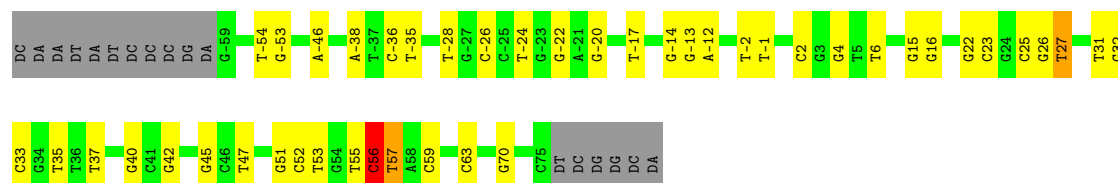
- Molecule 3: INO80 complex subunit C

Chain I:  53% 44%



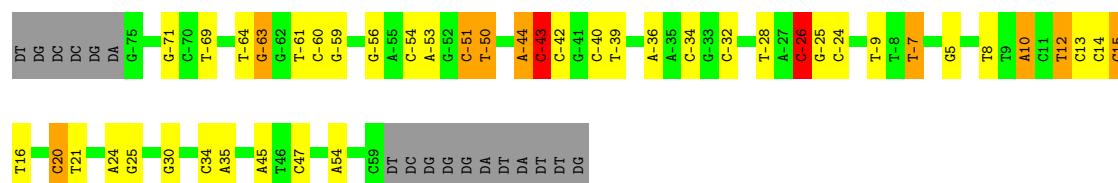
- Molecule 4: Nucleosomal DNA Strand 1

Chain K:  59% 28% • 11%



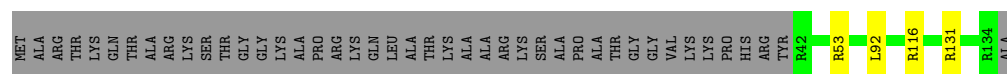
- Molecule 5: Nucleosomal DNA Strand 2

Chain L:  60% 22% 6% • 11%



- Molecule 6: Histone H3.1

Chain M:  65% 32%



- Molecule 6: Histone H3.1

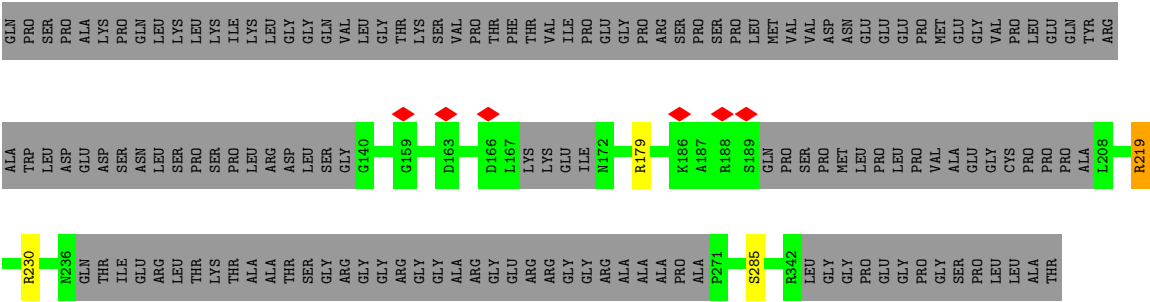
Chain Q:  68% 27%

Response	Percentage
Yes, the U.S. is a democracy	42%
No, the U.S. is not a democracy	56%

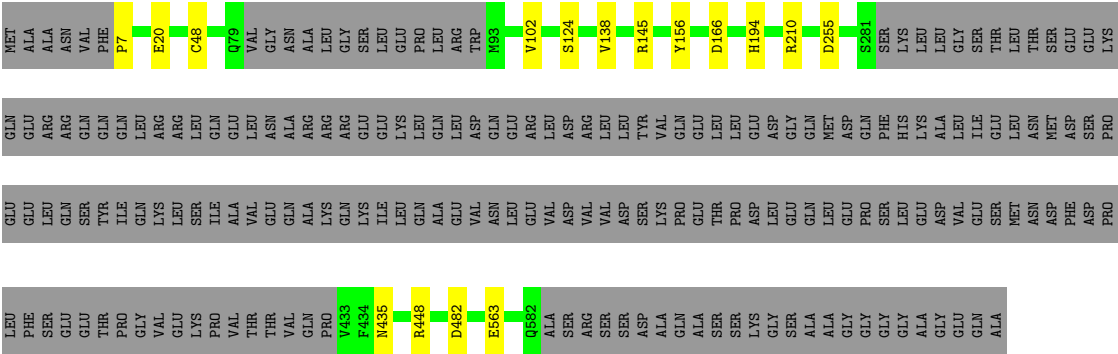
- Molecule 11: INO80 complex subunit B

Response	Percentage
Yes	40%
No	59%

MET	SER	SER	LYS	TRP	ARG	ARG	GLY	GLY	THR	SER	SER	GLY	ALA	ALA	MET	GLU	PRO	PRO	GLU	GLY	GLY	GLU	ALA	ALA	LEU	LEU	LEU	SER	SER	GLY	ALA	ALA	GLY	GLY	HIS	HIS	HIS	GLY	VAL	HIS	HIS	LYS	LYS	LYS	LYS	LYS	LYS	HIS	HIS	LYS	LYS	LYS	LYS	GLN	GLU	GLU	ASP	GLY	GLY	PRO
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● Molecule 12: Actin-related protein 5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82269	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.029	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.042	Depositor
Minimum map value	-1.491	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	419.6, 419.6, 419.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.049, 1.049, 1.049	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	0/3387	1.25	5/4564 (0.1%)
1	B	0.68	0/3496	1.24	9/4710 (0.2%)
1	C	0.68	0/3458	1.22	7/4662 (0.2%)
2	D	0.70	0/3353	1.30	13/4510 (0.3%)
2	E	0.70	0/3443	1.26	6/4636 (0.1%)
2	F	0.70	0/3415	1.27	14/4596 (0.3%)
3	I	0.78	0/865	1.35	4/1173 (0.3%)
4	K	0.67	0/3131	1.27	3/4835 (0.1%)
5	L	1.43	5/3077 (0.2%)	1.41	14/4742 (0.3%)
6	M	0.80	0/770	1.31	2/1032 (0.2%)
6	Q	0.84	0/828	1.42	3/1109 (0.3%)
7	N	0.83	0/645	1.37	2/862 (0.2%)
7	R	0.82	0/634	1.32	2/848 (0.2%)
8	O	0.82	0/829	1.38	3/1118 (0.3%)
8	S	0.82	0/845	1.41	3/1139 (0.3%)
9	P	0.79	0/746	1.33	0/1001
9	T	0.78	0/742	1.33	1/997 (0.1%)
10	G	0.76	0/5744	1.30	12/7759 (0.2%)
11	H	0.84	0/1170	1.39	3/1569 (0.2%)
12	J	0.77	0/3362	1.32	7/4558 (0.2%)
All	All	0.80	5/43940 (0.0%)	1.30	113/60420 (0.2%)

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	C	0	2
2	D	0	4
2	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	4
4	K	0	42
5	L	0	41
8	O	0	1
8	S	0	2
10	G	0	5
12	J	0	2
All	All	0	105

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	-26	DC	O4'-C1'	32.84	2.07	1.41
5	L	-26	DC	C2'-C1'	32.69	2.18	1.52
5	L	-26	DC	C3'-C2'	31.00	2.15	1.52
5	L	-26	DC	C4'-C3'	30.33	2.13	1.52
5	L	-26	DC	C4'-O4'	29.34	2.04	1.45

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	32	ARG	NE-CZ-NH2	8.23	126.61	119.20
2	E	273	ARG	NE-CZ-NH2	6.96	125.47	119.20
3	I	212	ASP	CA-CB-CG	6.93	119.53	112.60
1	C	244	ASP	CA-CB-CG	6.87	119.47	112.60
2	F	329	ASN	N-CA-CB	-6.75	103.69	111.79
2	D	353	ARG	NE-CZ-NH2	6.67	125.20	119.20
10	G	1069	PHE	CA-CB-CG	6.58	120.39	113.80
5	L	-26	DC	O4'-C1'-N1	6.57	118.26	108.40
5	L	20	DC	C4'-C3'-O3'	6.48	119.72	110.00
2	F	54	ARG	NE-CZ-NH2	6.47	125.03	119.20
2	F	438	ARG	NE-CZ-NH2	6.43	124.99	119.20
11	H	179	ARG	NE-CZ-NH2	6.31	124.88	119.20
2	E	353	ARG	NE-CZ-NH2	6.22	124.80	119.20
4	K	37	DT	C2'-C3'-O3'	6.19	120.78	111.50
10	G	1146	ARG	NE-CZ-NH2	6.18	124.76	119.20
3	I	160	ASP	CA-C-N	6.02	127.37	119.84
3	I	160	ASP	C-N-CA	6.02	127.37	119.84
3	I	207	ARG	NE-CZ-NH2	5.94	124.55	119.20
11	H	219	ARG	NE-CZ-NH2	5.89	124.51	119.20
1	B	357	ARG	NE-CZ-NH2	5.88	124.49	119.20
2	D	319	ASP	CA-CB-CG	5.86	118.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	116	ARG	NE-CZ-NH2	5.81	124.43	119.20
8	S	29	ARG	NE-CZ-NH2	5.78	124.40	119.20
12	J	482	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	276	ARG	NE-CZ-NH2	5.76	124.39	119.20
2	D	53	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	B	317	ARG	NE-CZ-NH2	5.73	124.36	119.20
2	D	264	ASP	CA-CB-CG	5.69	118.29	112.60
2	D	211	ARG	NE-CZ-NH2	5.67	124.30	119.20
12	J	166	ASP	CA-CB-CG	5.66	118.26	112.60
1	C	46	ARG	NE-CZ-NH2	5.65	124.28	119.20
2	F	428	ARG	NE-CZ-NH2	5.64	124.28	119.20
5	L	-63	DG	O3'-P-O5'	5.63	112.44	104.00
2	F	273	ARG	NE-CZ-NH2	5.63	124.26	119.20
5	L	-26	DC	C2'-C3'-O3'	5.62	119.92	111.50
1	B	276	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	F	214	ASP	CA-CB-CG	5.61	118.21	112.60
6	M	131	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	173	ASP	CA-CB-CG	5.57	118.17	112.60
8	O	29	ARG	NE-CZ-NH2	5.57	124.21	119.20
2	E	21	ARG	NE-CZ-NH2	5.56	124.21	119.20
4	K	59	DC	C5'-C4'-O4'	5.56	117.74	109.40
2	F	392	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	C	339	ARG	NE-CZ-NH2	5.54	124.19	119.20
2	D	400	ARG	NE-CZ-NH2	5.54	124.18	119.20
9	T	72	ARG	NE-CZ-NH2	5.52	124.17	119.20
2	D	248	ASP	CA-CB-CG	5.50	118.11	112.60
2	F	336	ARG	NE-CZ-NH2	5.50	124.15	119.20
2	D	273	ARG	NE-CZ-NH2	5.48	124.14	119.20
5	L	24	DA	O5'-C5'-C4'	5.47	119.00	110.80
12	J	7	PRO	CA-N-CD	-5.46	104.36	112.00
7	N	55	ARG	NE-CZ-NH2	5.46	124.11	119.20
10	G	605	ARG	NE-CZ-NH2	5.45	124.10	119.20
10	G	746	ARG	NE-CZ-NH2	5.44	124.10	119.20
5	L	10	DA	O5'-C5'-C4'	5.40	118.90	110.80
1	C	276	ARG	NE-CZ-NH2	5.39	124.06	119.20
6	Q	131	ARG	NE-CZ-NH2	5.39	124.05	119.20
12	J	448	ARG	NE-CZ-NH2	5.38	124.04	119.20
8	O	77	ARG	NE-CZ-NH2	5.38	124.04	119.20
2	F	207	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	404	ARG	NE-CZ-NH2	5.37	124.03	119.20
2	F	248	ASP	CA-CB-CG	5.36	117.96	112.60
2	F	53	ARG	NE-CZ-NH2	5.36	124.02	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	ASP	CA-CB-CG	5.35	117.95	112.60
5	L	-40	DC	O5'-C5'-C4'	5.35	118.83	110.80
2	F	328	THR	CA-CB-CG2	5.33	119.55	110.50
7	R	55	ARG	NE-CZ-NH2	5.32	123.99	119.20
5	L	-7	DT	O5'-C5'-C4'	5.32	118.77	110.80
10	G	745	ARG	NE-CZ-NH2	5.32	123.98	119.20
2	E	18	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	E	428	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	B	205	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	B	244	ASP	CA-CB-CG	5.28	117.88	112.60
6	Q	69	ARG	NE-CZ-NH2	5.27	123.94	119.20
2	D	302	HIS	CB-CG-CD2	-5.26	124.36	131.20
7	N	35	ARG	NE-CZ-NH2	5.26	123.93	119.20
5	L	15	DC	O5'-C5'-C4'	5.25	118.67	110.80
10	G	1156	ARG	NE-CZ-NH2	5.25	123.92	119.20
12	J	255	ASP	CA-CB-CG	5.24	117.84	112.60
6	Q	49	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	C	353	ASP	CA-CB-CG	5.21	117.81	112.60
5	L	-43	DC	O5'-C5'-C4'	5.21	118.61	110.80
1	A	46	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	D	334	ARG	NE-CZ-NH2	5.20	123.88	119.20
10	G	862	ARG	NE-CZ-NH2	5.20	123.88	119.20
10	G	999	ARG	NE-CZ-NH2	5.20	123.88	119.20
8	O	71	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	A	123	ARG	NE-CZ-NH2	5.19	123.87	119.20
10	G	818	HIS	CB-CG-CD2	-5.18	124.46	131.20
11	H	230	ARG	NE-CZ-NH2	5.18	123.86	119.20
5	L	-44	DA	C5'-C4'-C3'	-5.18	107.13	114.90
12	J	48	CYS	CB-CA-C	5.17	115.50	111.00
10	G	610	ARG	NE-CZ-NH2	5.14	123.83	119.20
5	L	-26	DC	C5'-C4'-O4'	5.14	117.11	109.40
1	B	324	ALA	CA-C-N	5.13	125.14	120.21
1	B	324	ALA	C-N-CA	5.13	125.14	120.21
1	B	46	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	C	205	ARG	NE-CZ-NH2	5.10	123.79	119.20
10	G	1119	ARG	NE-CZ-NH2	5.10	123.79	119.20
5	L	-26	DC	P-O3'-C3'	5.10	127.85	120.20
7	R	39	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	357	ARG	NE-CZ-NH2	5.10	123.79	119.20
2	D	27	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	D	124	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	F	334	ARG	NE-CZ-NH2	5.09	123.78	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	344	HIS	CB-CG-CD2	-5.07	124.60	131.20
10	G	879	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	D	330	ARG	NE-CZ-NH2	5.04	123.73	119.20
12	J	145	ARG	NE-CZ-NH2	5.03	123.72	119.20
4	K	56	DC	C4'-C3'-O3'	5.02	117.53	110.00
8	S	17	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	F	130	ARG	NE-CZ-NH2	5.01	123.71	119.20
5	L	12	DT	O5'-C5'-C4'	5.00	118.30	110.80

There are no chirality outliers.

All (105) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	150	TYR	Sidechain
1	C	366	TYR	Sidechain
2	D	124	ARG	Sidechain
2	D	172	TYR	Sidechain
2	D	400	ARG	Sidechain
2	D	64	ARG	Sidechain
2	E	18	ARG	Sidechain
2	E	353	ARG	Sidechain
2	F	130	ARG	Sidechain
2	F	21	ARG	Sidechain
2	F	438	ARG	Sidechain
2	F	54	ARG	Sidechain
10	G	1033	TYR	Sidechain
10	G	1139	TYR	Sidechain
10	G	1144	TYR	Sidechain
10	G	533	TYR	Sidechain
10	G	640	TYR	Sidechain
12	J	156	TYR	Sidechain
12	J	210	ARG	Sidechain
4	K	-1	DT	Sidechain
4	K	-12	DA	Sidechain
4	K	-13	DG	Sidechain
4	K	-14	DG	Sidechain
4	K	-17	DT	Sidechain
4	K	-2	DT	Sidechain
4	K	-20	DG	Sidechain
4	K	-22	DG	Sidechain
4	K	-24	DT	Sidechain
4	K	-28	DT	Sidechain

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Mol	Chain	Res	Type	Group
4	K	-35	DT	Sidechain
4	K	-36	DC	Sidechain
4	K	-38	DA	Sidechain
4	K	-46	DA	Sidechain
4	K	-53	DG	Sidechain
4	K	-54	DT	Sidechain
4	K	15	DG	Sidechain
4	K	16	DG	Sidechain
4	K	2	DC	Sidechain
4	K	22	DG	Sidechain
4	K	23	DC	Sidechain
4	K	25	DC	Sidechain
4	K	26	DG	Sidechain
4	K	27	DT	Sidechain
4	K	31	DT	Sidechain
4	K	32	DG	Sidechain
4	K	33	DC	Sidechain
4	K	35	DT	Sidechain
4	K	4	DG	Sidechain
4	K	40	DG	Sidechain
4	K	42	DG	Sidechain
4	K	45	DG	Sidechain
4	K	47	DT	Sidechain
4	K	51	DG	Sidechain
4	K	52	DC	Sidechain
4	K	53	DT	Sidechain
4	K	55	DT	Sidechain
4	K	56	DC	Sidechain
4	K	57	DT	Sidechain
4	K	6	DT	Sidechain
4	K	63	DC	Sidechain
4	K	70	DG	Sidechain
5	L	-24	DC	Sidechain
5	L	-25	DG	Sidechain
5	L	-26	DC	Sidechain
5	L	-28	DT	Sidechain
5	L	-32	DC	Sidechain
5	L	-34	DC	Sidechain
5	L	-36	DA	Sidechain
5	L	-39	DT	Sidechain
5	L	-42	DC	Sidechain
5	L	-43	DC	Sidechain

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Mol	Chain	Res	Type	Group
5	L	-50	DT	Sidechain
5	L	-51	DC	Sidechain
5	L	-53	DA	Sidechain
5	L	-54	DC	Sidechain
5	L	-56	DG	Sidechain
5	L	-59	DG	Sidechain
5	L	-60	DC	Sidechain
5	L	-61	DT	Sidechain
5	L	-63	DG	Sidechain
5	L	-64	DT	Sidechain
5	L	-69	DT	Sidechain
5	L	-7	DT	Sidechain
5	L	-71	DG	Sidechain
5	L	-9	DT	Sidechain
5	L	10	DA	Sidechain
5	L	12	DT	Sidechain
5	L	13	DC	Sidechain
5	L	14	DC	Sidechain
5	L	15	DC	Sidechain
5	L	16	DT	Sidechain
5	L	20	DC	Sidechain
5	L	21	DT	Sidechain
5	L	25	DG	Sidechain
5	L	30	DG	Sidechain
5	L	34	DC	Sidechain
5	L	35	DA	Sidechain
5	L	45	DA	Sidechain
5	L	47	DC	Sidechain
5	L	5	DG	Sidechain
5	L	54	DA	Sidechain
5	L	8	DT	Sidechain
8	O	57	TYR	Sidechain
8	S	32	ARG	Sidechain
8	S	57	TYR	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	A	3344	0	3451	2	0
1	B	3453	0	3563	2	0
1	C	3412	0	3508	1	0
2	D	3317	0	3395	6	0
2	E	3403	0	3472	4	0
2	F	3376	0	3446	1	0
3	I	842	0	836	0	0
4	K	2787	0	1515	4	0
5	L	2748	0	1518	7	0
6	M	761	0	802	0	0
6	Q	816	0	856	0	0
7	N	638	0	676	0	0
7	R	627	0	663	1	0
8	O	819	0	879	0	0
8	S	835	0	897	0	0
9	P	735	0	755	0	0
9	T	731	0	753	0	0
10	G	5608	0	5651	4	0
11	H	1153	0	1151	3	0
12	J	3277	0	3215	0	0
13	B	27	0	12	0	0
13	C	27	0	12	0	0
13	D	27	0	12	0	0
13	E	27	0	12	0	0
13	F	27	0	12	0	0
13	G	27	0	12	0	0
14	A	31	0	12	1	0
All	All	42875	0	41086	30	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 0.

All (30) 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)
5:L:-26:DC:C3'	5:L:-26:DC:C4'	2.13	1.27
5:L:-26:DC:C3'	5:L:-26:DC:C2'	2.14	1.24
5:L:-26:DC:C2'	5:L:-26:DC:C1'	2.18	1.20
5:L:-26:DC:C4'	5:L:-26:DC:O4'	2.04	1.06
5:L:-26:DC:C1'	5:L:-26:DC:O4'	2.07	1.01
2:D:46:MET:HE1	2:D:86:ILE:HG22	1.65	0.79
1:A:40:VAL:H	14:A:501:ATP:N6	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:550:THR:HG22	10:G:582:TRP:CZ2	2.44	0.53
4:K:56:DC:H1'	4:K:57:DT:C6	2.47	0.50
1:B:272:THR:HG23	1:B:275:LEU:H	1.78	0.49
2:F:159:GLY:H	2:F:179:ILE:HD11	1.77	0.48
2:D:279:LYS:HE3	10:G:853:PHE:CD1	2.50	0.46
2:D:77:GLY:O	2:D:83:LYS:HE2	2.16	0.46
10:G:550:THR:HG22	10:G:582:TRP:CH2	2.52	0.44
10:G:818:HIS:HB2	10:G:1129:MET:HE1	2.00	0.43
2:D:301:VAL:HG21	2:D:326:MET:HB3	2.00	0.43
2:E:397:THR:HG22	2:E:398:SER:N	2.34	0.42
4:K:-26:DC:H41	11:H:219:ARG:HH11	1.67	0.42
2:E:354:LEU:C	2:E:354:LEU:HD12	2.45	0.42
2:E:328:THR:HG22	2:E:330:ARG:H	1.83	0.42
2:D:295:VAL:HG13	2:D:325:ILE:HD12	2.01	0.42
5:L:-51:DC:H2'	5:L:-50:DT:C6	2.55	0.42
4:K:-26:DC:N4	11:H:219:ARG:HH11	2.19	0.41
2:E:145:ILE:CD1	2:E:187:VAL:HG13	2.51	0.41
2:D:335:ILE:HG22	2:D:345:GLY:C	2.44	0.41
1:C:153:THR:HG22	11:H:285:SER:HB3	2.02	0.41
1:B:333:ARG:HB3	1:B:336:CYS:SG	2.61	0.41
1:A:248:ALA:CB	1:A:271:ILE:HD12	2.51	0.41
4:K:27:DT:H5''	7:R:80:THR:HG22	2.02	0.40
5:L:-44:DA:H2''	5:L:-43:DC:C6	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	A	430/456 (94%)	410 (95%)	16 (4%)	4 (1%)	14 47
1	B	443/456 (97%)	431 (97%)	10 (2%)	2 (0%)	24 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	441/456 (97%)	422 (96%)	18 (4%)	1 (0%)	43	74
2	D	420/463 (91%)	402 (96%)	17 (4%)	1 (0%)	43	74
2	E	437/463 (94%)	428 (98%)	8 (2%)	1 (0%)	43	74
2	F	430/463 (93%)	413 (96%)	15 (4%)	2 (0%)	24	58
3	I	105/192 (55%)	95 (90%)	8 (8%)	2 (2%)	6	32
6	M	91/136 (67%)	89 (98%)	2 (2%)	0	100	100
6	Q	97/136 (71%)	92 (95%)	2 (2%)	3 (3%)	3	25
7	N	78/102 (76%)	74 (95%)	4 (5%)	0	100	100
7	R	77/102 (76%)	75 (97%)	2 (3%)	0	100	100
8	O	104/129 (81%)	98 (94%)	6 (6%)	0	100	100
8	S	106/129 (82%)	101 (95%)	4 (4%)	1 (1%)	14	47
9	P	92/125 (74%)	89 (97%)	3 (3%)	0	100	100
9	T	91/125 (73%)	88 (97%)	2 (2%)	1 (1%)	11	42
10	G	674/1556 (43%)	620 (92%)	42 (6%)	12 (2%)	6	33
11	H	139/356 (39%)	131 (94%)	8 (6%)	0	100	100
12	J	406/607 (67%)	375 (92%)	27 (7%)	4 (1%)	12	44
All	All	4661/6452 (72%)	4433 (95%)	194 (4%)	34 (1%)	20	51

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	T	103	PRO
1	B	342	GLU
10	G	580	ASN
10	G	747	ILE
10	G	1143	THR
1	C	183	GLU
8	S	13	LYS
1	A	59	LYS
1	A	256	ILE
1	B	59	LYS
10	G	682	THR
10	G	943	TYR
10	G	1001	CYS
10	G	1200	PRO
12	J	20	GLU

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Mol	Chain	Res	Type
12	J	124	SER
1	A	342	GLU
1	A	343	ASP
2	F	316	LEU
2	F	452	PHE
10	G	563	ARG
10	G	684	ILE
2	E	316	LEU
6	Q	40	ARG
6	Q	41	TYR
6	Q	134	ARG
2	D	302	HIS
3	I	141	TRP
10	G	936	GLU
10	G	993	SER
12	J	435	ASN
3	I	161	PRO
12	J	138	VAL
10	G	1230	ILE

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	A	367/387 (95%)	363 (99%)	4 (1%)	65	74
1	B	381/387 (98%)	375 (98%)	6 (2%)	55	70
1	C	374/387 (97%)	369 (99%)	5 (1%)	61	72
2	D	361/390 (93%)	357 (99%)	4 (1%)	65	74
2	E	369/390 (95%)	366 (99%)	3 (1%)	73	76
2	F	367/390 (94%)	353 (96%)	14 (4%)	29	56
3	I	90/158 (57%)	89 (99%)	1 (1%)	65	74
6	M	81/111 (73%)	79 (98%)	2 (2%)	42	63
6	Q	86/111 (78%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	N	65/78 (83%)	65 (100%)	0	100	100
7	R	64/78 (82%)	64 (100%)	0	100	100
8	O	84/99 (85%)	84 (100%)	0	100	100
8	S	85/99 (86%)	84 (99%)	1 (1%)	63	73
9	P	80/105 (76%)	80 (100%)	0	100	100
9	T	80/105 (76%)	80 (100%)	0	100	100
10	G	613/1359 (45%)	610 (100%)	3 (0%)	81	80
11	H	123/288 (43%)	123 (100%)	0	100	100
12	J	351/520 (68%)	348 (99%)	3 (1%)	70	75
All	All	4021/5442 (74%)	3975 (99%)	46 (1%)	63	74

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	40	VAL
1	C	153	THR
1	C	190	VAL
1	C	237	ASP
1	C	439	ASP
2	E	59	VAL
2	E	144	GLU
2	E	170	THR
3	I	212	ASP
6	M	53	ARG
6	M	92	LEU
8	S	100	VAL
1	A	40	VAL
1	A	97	VAL
1	A	173	ASP
1	A	207	ASP
1	B	40	VAL
1	B	130	VAL
1	B	165	LYS
1	B	283	VAL
1	B	304	VAL
1	B	415	LEU
2	D	47	VAL
2	D	86	ILE
2	D	142	VAL

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Mol	Chain	Res	Type
2	D	328	THR
2	F	28	ILE
2	F	49	GLN
2	F	68	ILE
2	F	97	ASP
2	F	116	THR
2	F	133	GLU
2	F	138	ILE
2	F	170	THR
2	F	231	GLU
2	F	238	VAL
2	F	254	THR
2	F	271	GLU
2	F	328	THR
2	F	421	VAL
10	G	767	LEU
10	G	901	MET
10	G	1202	VAL
12	J	102	VAL
12	J	194	HIS
12	J	563	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	115	ASN
1	C	451	GLN
2	E	41	GLN
2	E	369	GLN
3	I	162	ASN
6	M	85	GLN
7	N	25	ASN
7	N	93	GLN
8	O	31	HIS
1	A	20	HIS
1	A	181	GLN
1	A	241	HIS
1	A	373	GLN
1	A	450	GLN
1	B	115	ASN
1	B	181	GLN
1	B	251	GLN

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Mol	Chain	Res	Type
2	D	41	GLN
2	D	49	GLN
2	D	344	HIS
2	D	369	GLN
2	D	404	GLN
2	F	78	GLN
2	F	245	HIS
2	F	341	GLN
2	F	404	GLN
10	G	552	GLN
10	G	565	ASN
10	G	625	HIS
10	G	776	GLN
10	G	780	ASN
10	G	883	ASN
10	G	903	ASN
10	G	1048	GLN
10	G	1052	ASN
10	G	1116	GLN
10	G	1164	GLN
10	G	1205	GLN
11	H	298	GLN
11	H	327	GLN
11	H	338	ASN
12	J	37	ASN
12	J	125	GLN
12	J	223	GLN
12	J	441	GLN
12	J	457	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	ADP	E	501	-	27,29,29	1.01	1 (3%)	42,45,45	1.24	5 (11%)
13	ADP	B	501	-	27,29,29	1.04	1 (3%)	42,45,45	1.24	6 (14%)
13	ADP	D	501	-	27,29,29	1.01	1 (3%)	42,45,45	1.40	7 (16%)
13	ADP	F	501	-	27,29,29	1.05	1 (3%)	42,45,45	1.31	7 (16%)
13	ADP	G	1601	-	27,29,29	0.98	1 (3%)	42,45,45	1.28	7 (16%)
14	ATP	A	501	-	29,33,33	1.06	1 (3%)	44,52,52	1.69	12 (27%)
13	ADP	C	501	-	27,29,29	1.00	1 (3%)	42,45,45	1.28	6 (14%)

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
13	ADP	E	501	-	-	0/16/32/32	0/3/3/3
13	ADP	B	501	-	-	1/16/32/32	0/3/3/3
13	ADP	D	501	-	-	5/16/32/32	0/3/3/3
13	ADP	F	501	-	-	0/16/32/32	0/3/3/3
13	ADP	G	1601	-	-	7/16/32/32	0/3/3/3
14	ATP	A	501	-	-	9/22/38/38	0/3/3/3
13	ADP	C	501	-	-	3/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	501	ADP	C5-C4	-2.59	1.34	1.39
13	C	501	ADP	C5-C4	-2.42	1.34	1.39
13	B	501	ADP	C5-C4	-2.36	1.34	1.39
13	E	501	ADP	C5-C4	-2.34	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	501	ADP	C5-C4	-2.31	1.34	1.39
14	A	501	ATP	C5-C4	-2.29	1.34	1.39
13	G	1601	ADP	C8-N7	2.06	1.35	1.31

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	501	ATP	PA-O3A-PB	-4.21	118.38	132.83
14	A	501	ATP	C5-C4-N3	-3.60	122.05	126.75
13	F	501	ADP	PA-O3A-PB	-3.49	120.83	132.83
13	C	501	ADP	PA-O3A-PB	-3.43	121.06	132.83
13	E	501	ADP	PA-O3A-PB	-3.29	121.52	132.83
14	A	501	ATP	O4'-C1'-C2'	-3.28	99.49	106.64
13	D	501	ADP	PA-O3A-PB	-3.24	121.70	132.83
14	A	501	ATP	PB-O3B-PG	-3.16	121.98	132.83
13	D	501	ADP	C5-C4-N3	-3.13	122.67	126.75
13	C	501	ADP	C5-C4-N3	-3.11	122.70	126.75
13	B	501	ADP	PA-O3A-PB	-3.09	122.21	132.83
13	G	1601	ADP	C5-C4-N3	-3.05	122.77	126.75
14	A	501	ATP	N6-C6-N1	-2.96	111.87	118.35
13	D	501	ADP	C4-C5-N7	2.84	114.08	110.62
13	C	501	ADP	C4-C5-N7	2.83	114.06	110.62
13	F	501	ADP	C5-C4-N3	-2.74	123.18	126.75
14	A	501	ATP	C4-C5-N7	2.73	113.94	110.62
13	B	501	ADP	C4-C5-N7	2.73	113.94	110.62
13	B	501	ADP	C5-C4-N3	-2.72	123.20	126.75
13	E	501	ADP	C5-C4-N3	-2.70	123.23	126.75
13	G	1601	ADP	C4-C5-N7	2.68	113.89	110.62
13	D	501	ADP	C5-C6-N1	2.66	123.11	117.39
14	A	501	ATP	C5-C6-N1	2.66	123.10	117.39
13	F	501	ADP	C4-C5-N7	2.65	113.84	110.62
13	F	501	ADP	C5-C6-N1	2.64	123.06	117.39
13	G	1601	ADP	C5-C6-N1	2.59	122.95	117.39
13	E	501	ADP	C5-C6-N1	2.56	122.88	117.39
13	C	501	ADP	C5-C6-N1	2.54	122.85	117.39
13	E	501	ADP	C4-C5-N7	2.52	113.69	110.62
13	D	501	ADP	N3-C4-N9	2.51	131.22	127.08
13	B	501	ADP	C5-C6-N1	2.51	122.78	117.39
13	D	501	ADP	C2-N1-C6	-2.39	114.67	118.77
13	F	501	ADP	C2-N1-C6	-2.38	114.67	118.77
14	A	501	ATP	C4'-O4'-C1'	-2.32	104.34	109.47
13	C	501	ADP	N3-C4-N9	2.32	130.90	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	501	ATP	N3-C4-N9	2.30	130.87	127.08
13	G	1601	ADP	PA-O3A-PB	-2.28	125.00	132.83
13	D	501	ADP	O4'-C1'-C2'	-2.25	101.73	106.64
13	E	501	ADP	C2-N1-C6	-2.25	114.91	118.77
14	A	501	ATP	C2-N1-C6	-2.24	114.92	118.77
13	C	501	ADP	C2-N1-C6	-2.22	114.95	118.77
14	A	501	ATP	O3G-PG-O3B	2.20	112.02	104.64
13	G	1601	ADP	N3-C4-N9	2.19	130.70	127.08
13	G	1601	ADP	N6-C6-N1	-2.18	113.58	118.35
13	F	501	ADP	N3-C4-N9	2.18	130.67	127.08
13	B	501	ADP	N3-C4-N9	2.13	130.59	127.08
13	F	501	ADP	O3B-PB-O3A	2.12	111.76	104.64
13	B	501	ADP	C2-N1-C6	-2.11	115.14	118.77
14	A	501	ATP	O4'-C1'-N9	2.06	112.13	108.06
13	G	1601	ADP	C2-N1-C6	-2.03	115.29	118.77

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	501	ADP	C5'-O5'-PA-O3A
13	G	1601	ADP	C5'-O5'-PA-O2A
13	G	1601	ADP	C4'-C5'-O5'-PA
13	G	1601	ADP	C3'-C4'-C5'-O5'
14	A	501	ATP	C4'-C5'-O5'-PA
14	A	501	ATP	C2'-C1'-N9-C8
14	A	501	ATP	O4'-C4'-C5'-O5'
14	A	501	ATP	C3'-C4'-C5'-O5'
13	G	1601	ADP	O4'-C4'-C5'-O5'
13	D	501	ADP	C4'-C5'-O5'-PA
13	C	501	ADP	O4'-C4'-C5'-O5'
13	G	1601	ADP	C5'-O5'-PA-O3A
13	D	501	ADP	C5'-O5'-PA-O1A
13	G	1601	ADP	C5'-O5'-PA-O1A
13	D	501	ADP	C3'-C4'-C5'-O5'
13	C	501	ADP	C4'-C5'-O5'-PA
14	A	501	ATP	PA-O3A-PB-O2B
13	C	501	ADP	C3'-C4'-C5'-O5'
14	A	501	ATP	C2'-C1'-N9-C4
13	B	501	ADP	C4'-C5'-O5'-PA
14	A	501	ATP	C5'-O5'-PA-O3A
14	A	501	ATP	PA-O3A-PB-O1B

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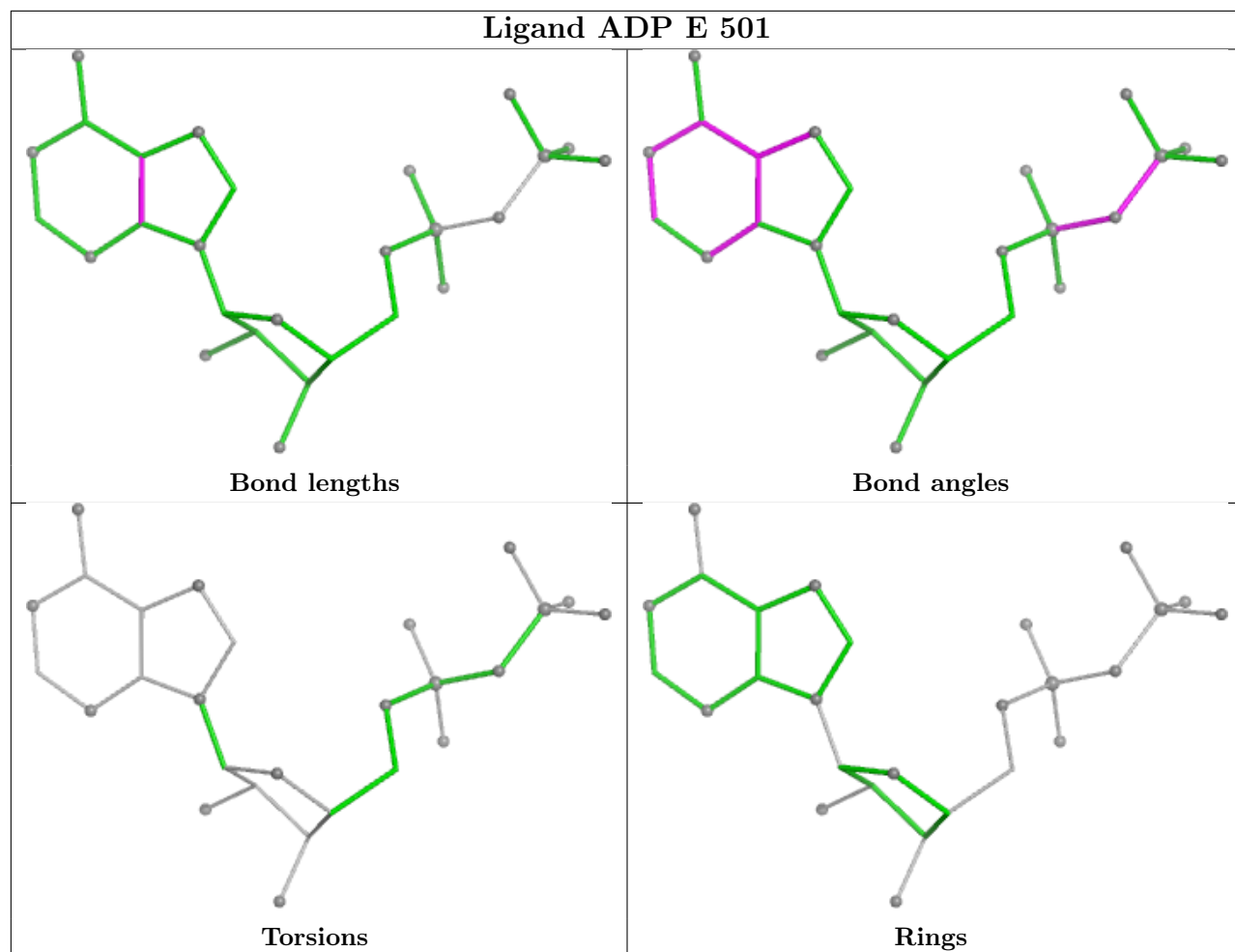
Mol	Chain	Res	Type	Atoms
13	G	1601	ADP	C2'-C1'-N9-C8
14	A	501	ATP	C5'-O5'-PA-O1A
13	D	501	ADP	O4'-C4'-C5'-O5'

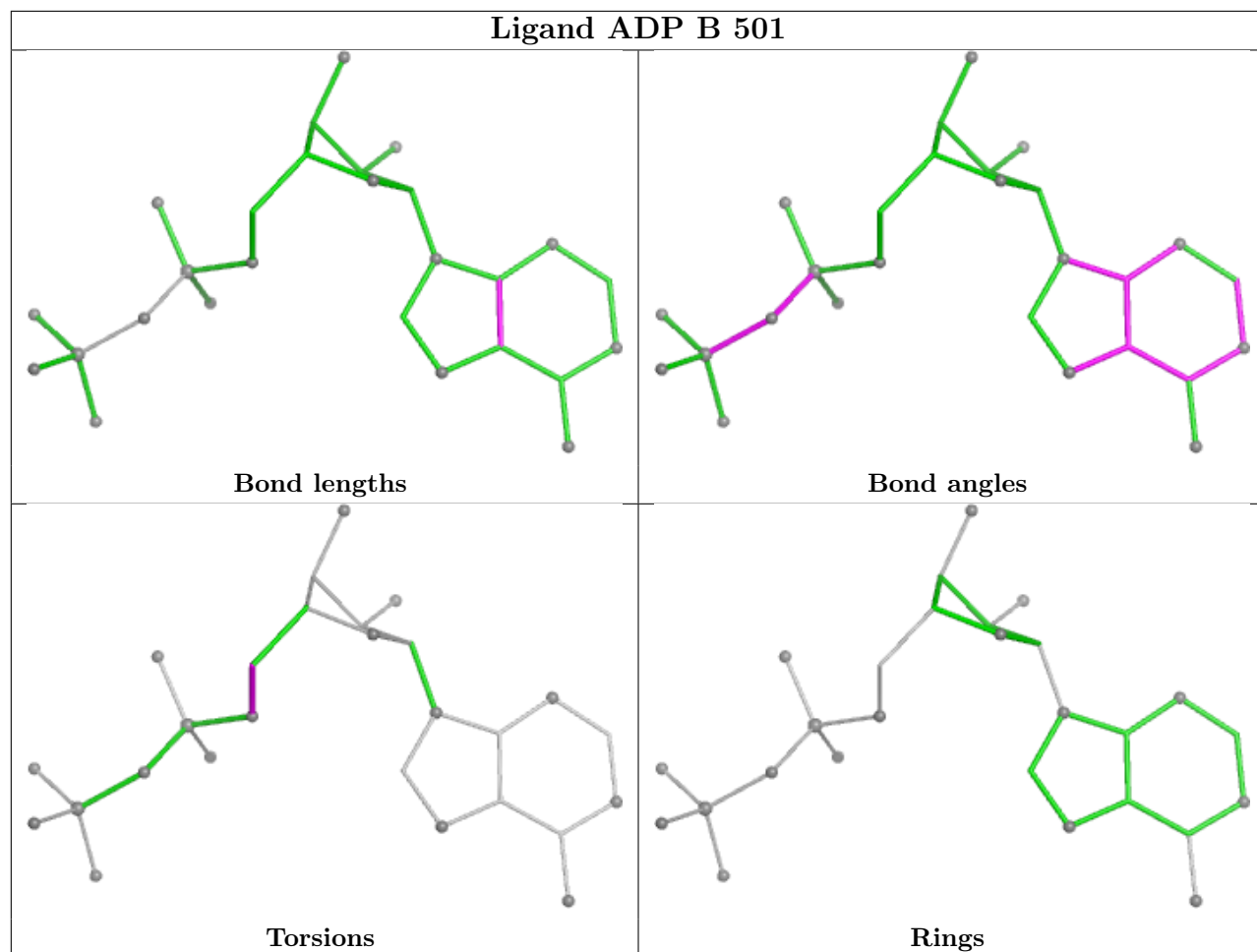
There are no ring outliers.

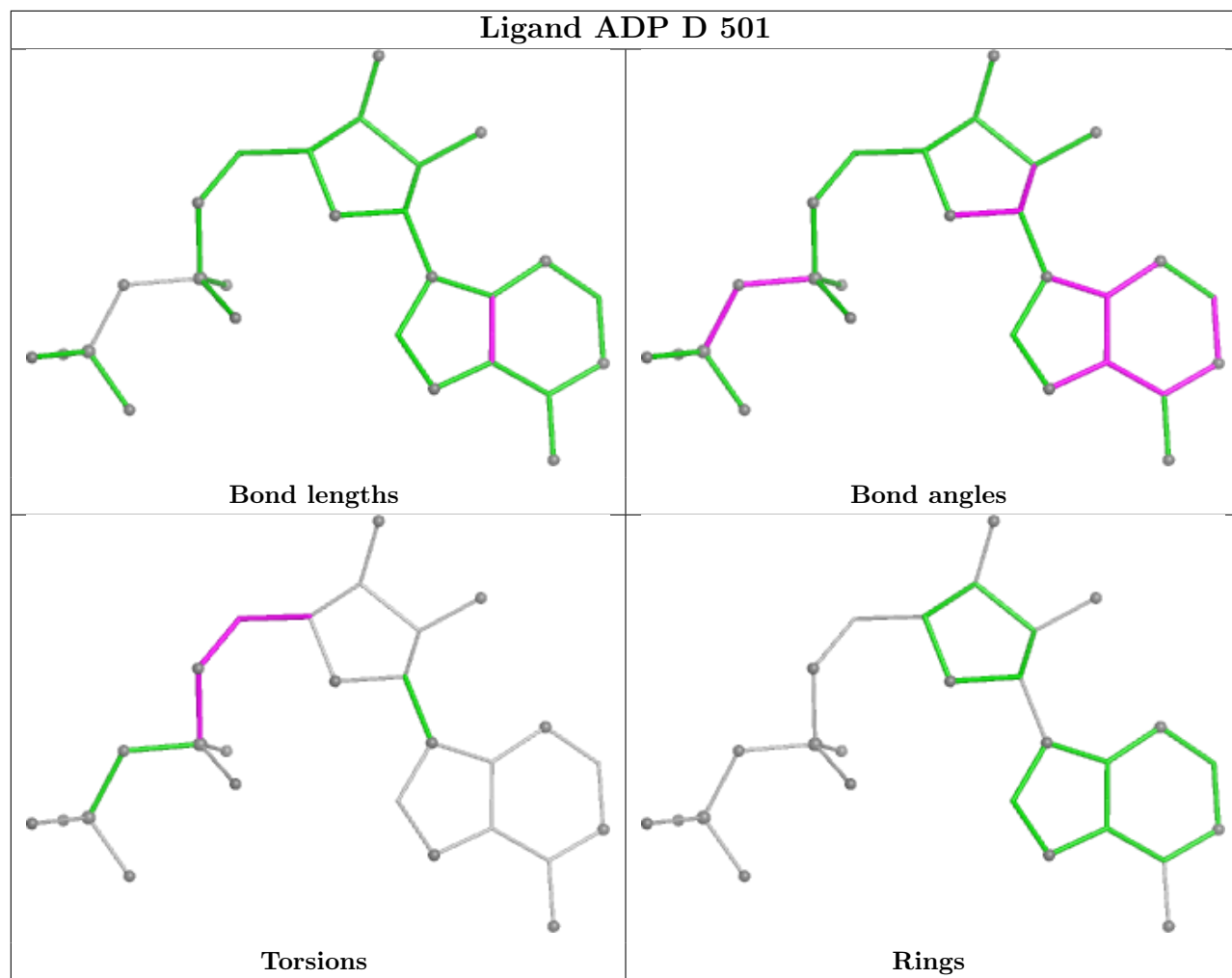
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	501	ATP	1	0

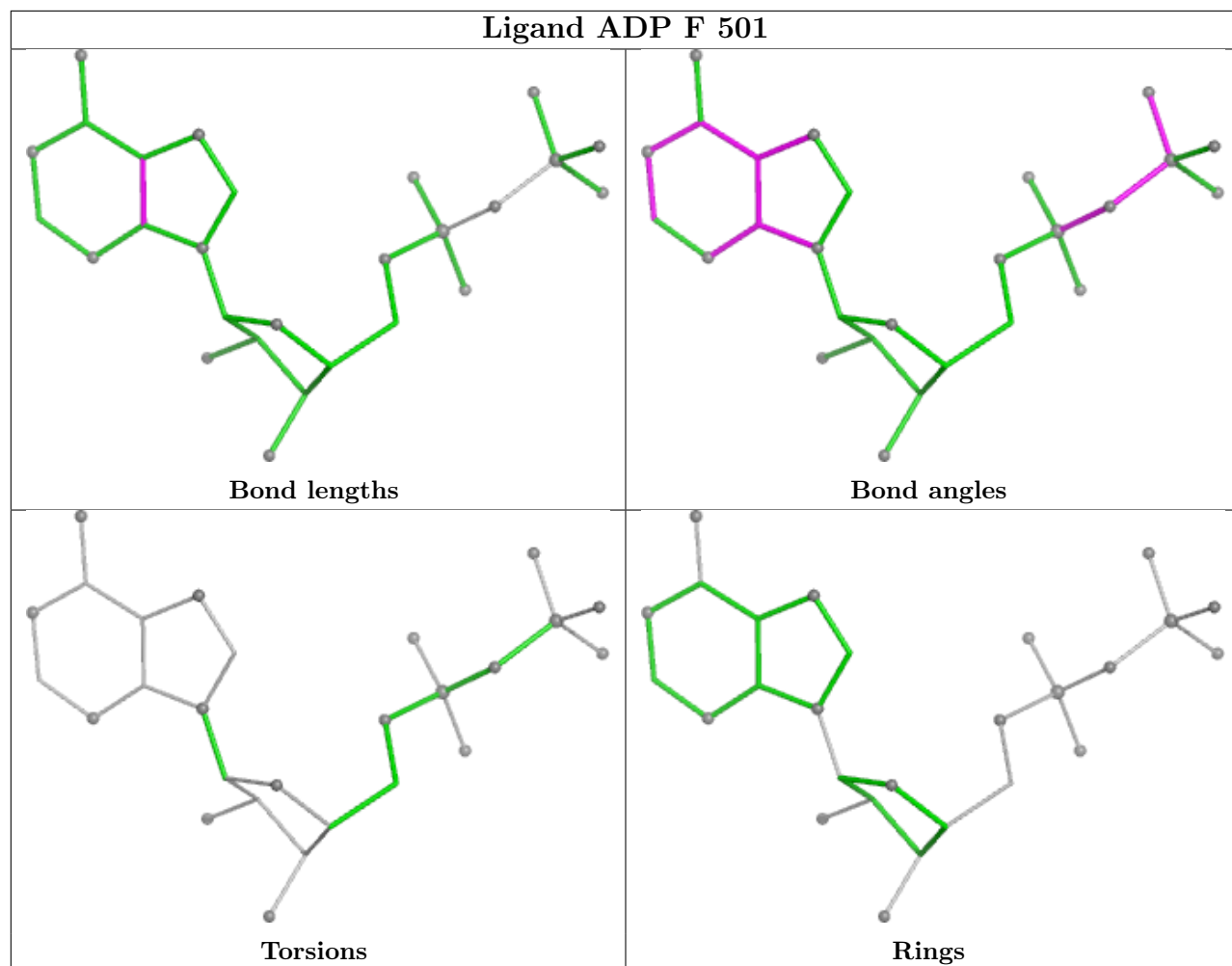
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



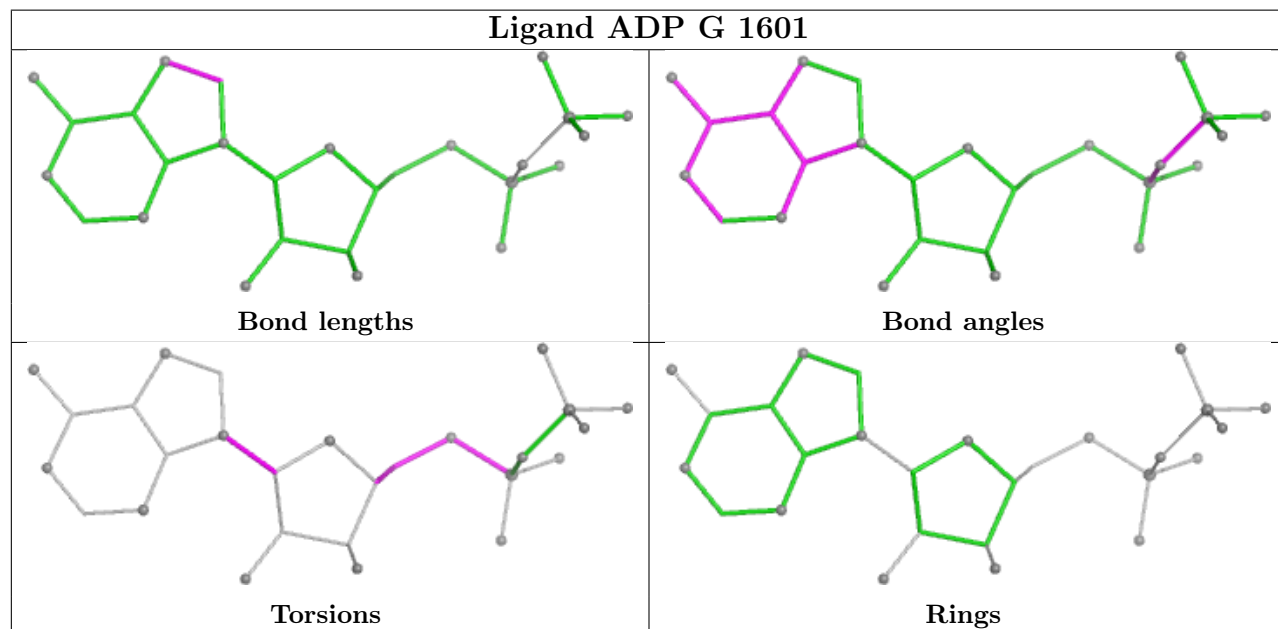


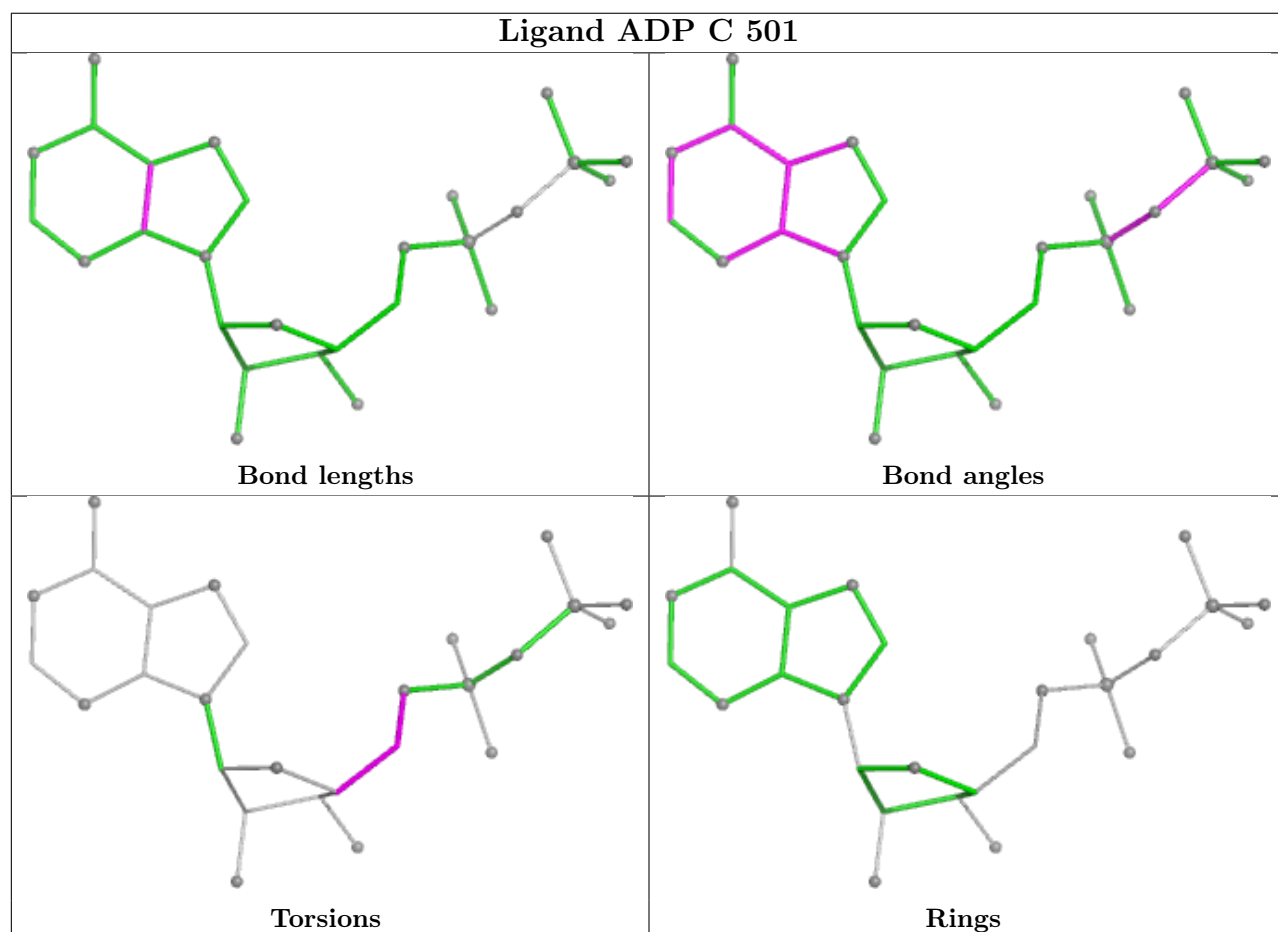
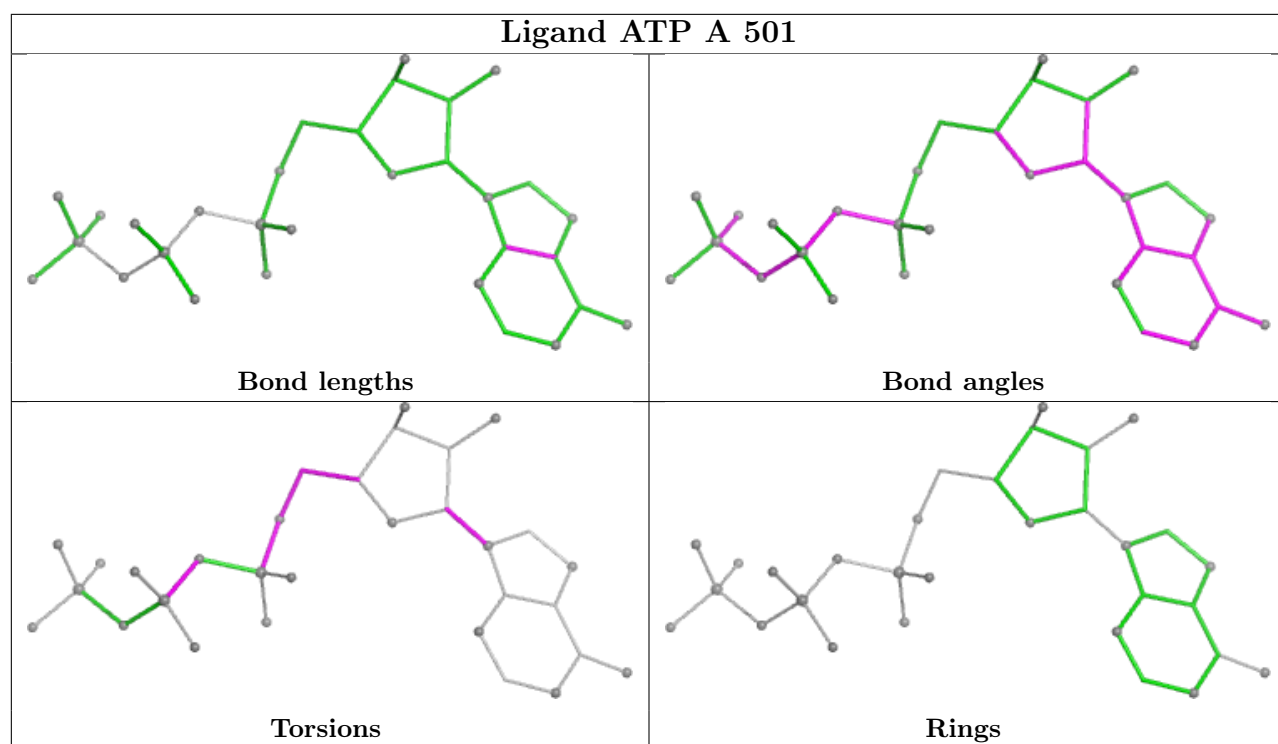


Ligand ADP F 501



Ligand ADP G 1601





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.

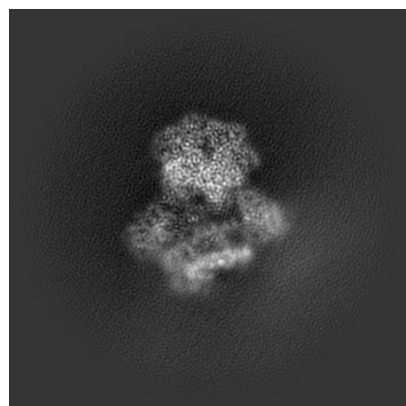
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51307. These allow visual inspection of the internal detail of the map and identification of artifacts.

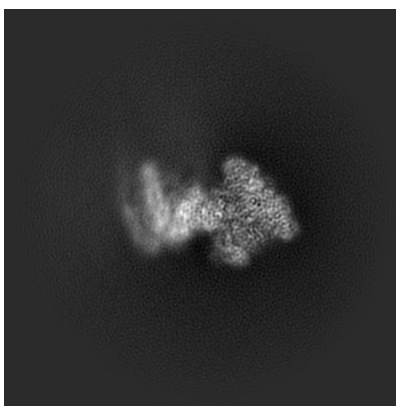
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

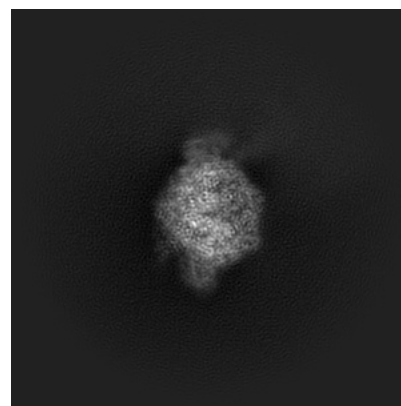
6.1.1 Primary map



X

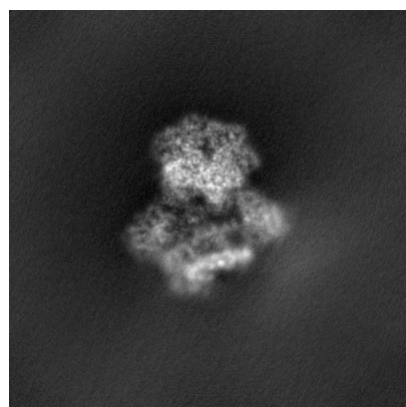


Y

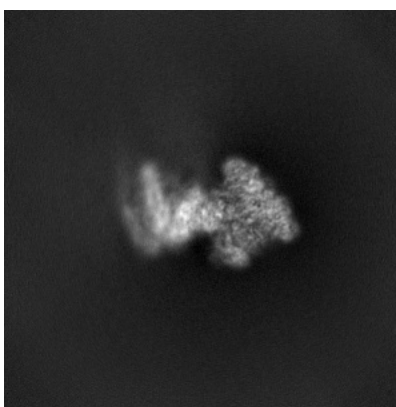


Z

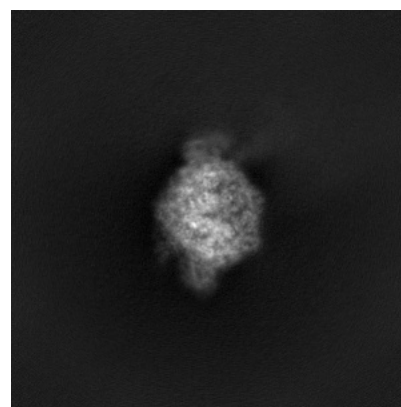
6.1.2 Raw map



X



Y

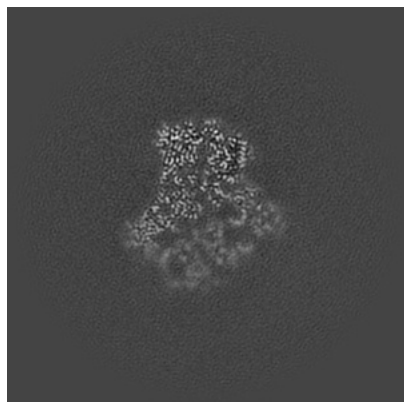


Z

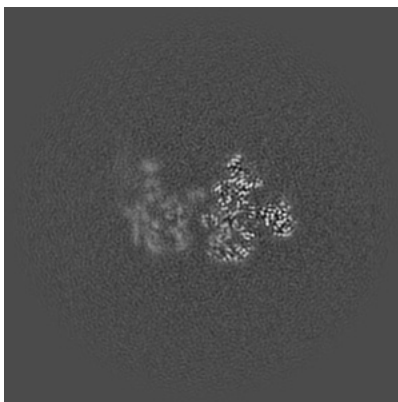
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

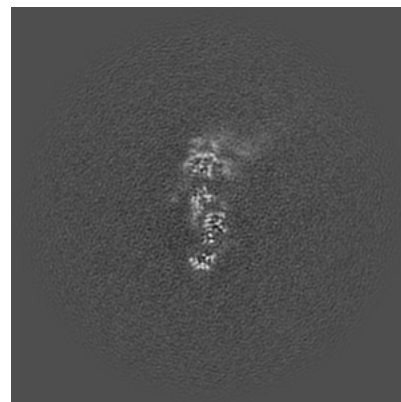
6.2.1 Primary map



X Index: 200

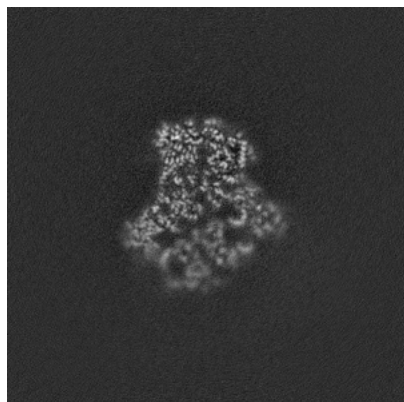


Y Index: 200

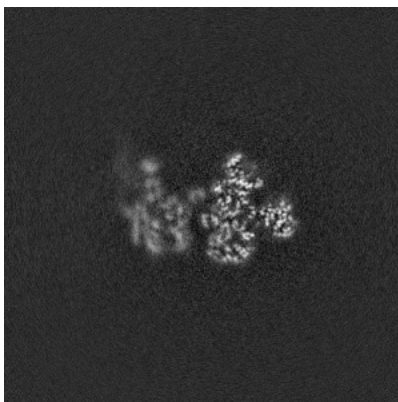


Z Index: 200

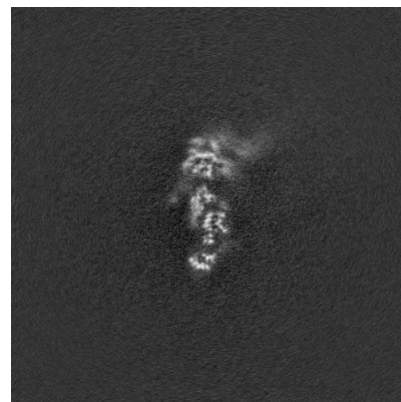
6.2.2 Raw map



X Index: 200



Y Index: 200

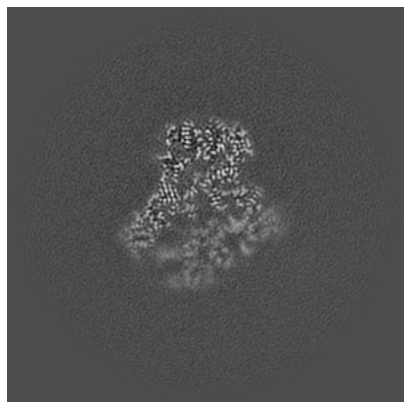


Z Index: 200

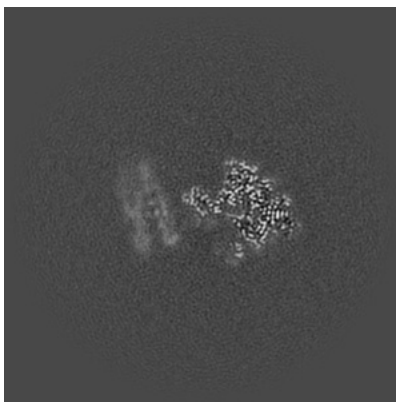
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

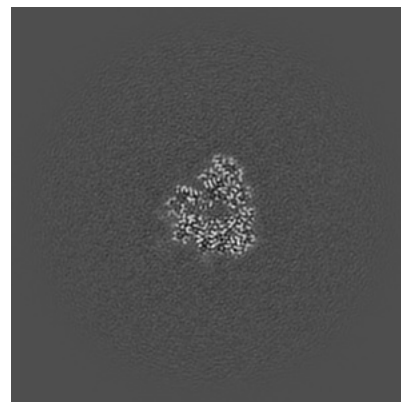
6.3.1 Primary map



X Index: 194

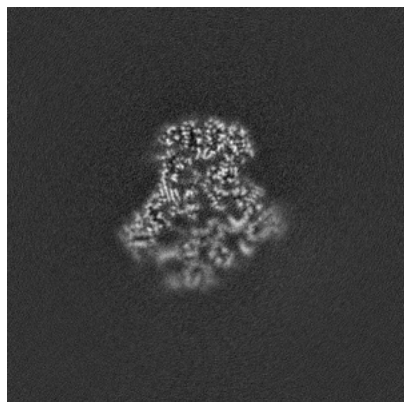


Y Index: 180

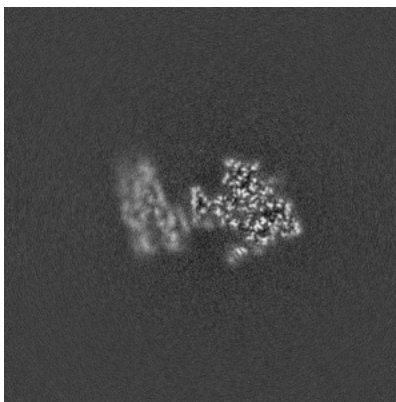


Z Index: 247

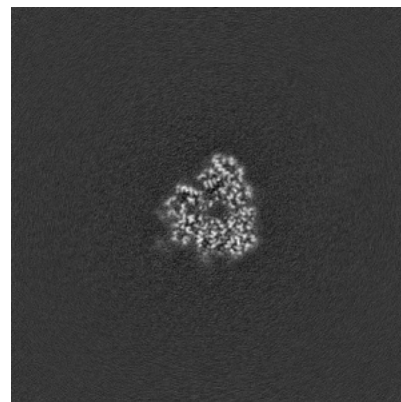
6.3.2 Raw map



X Index: 195



Y Index: 184

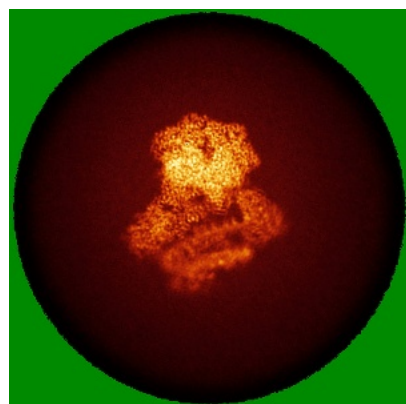


Z Index: 247

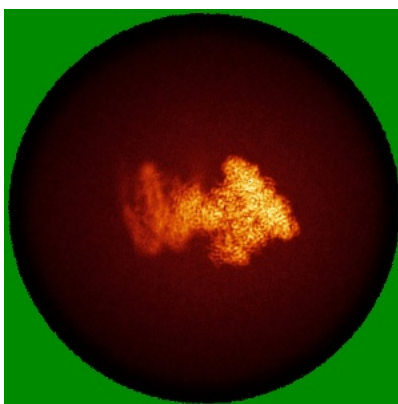
The images above show the largest variance slices of the map in three orthogonal directions.

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

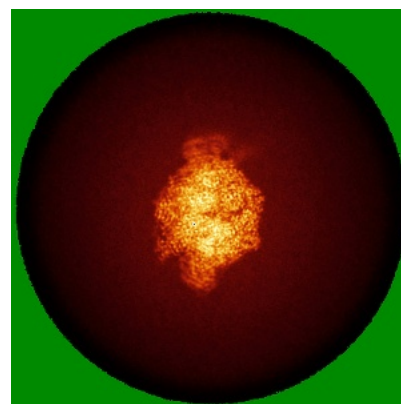
6.4.1 Primary map



X

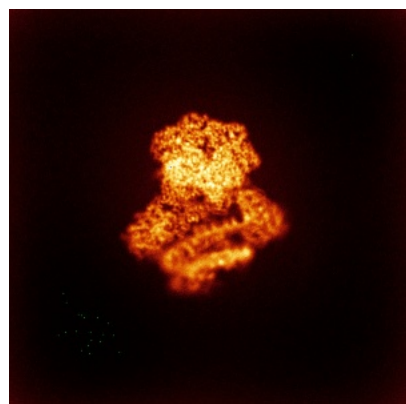


Y

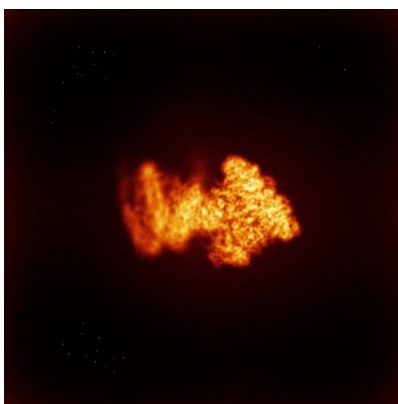


Z

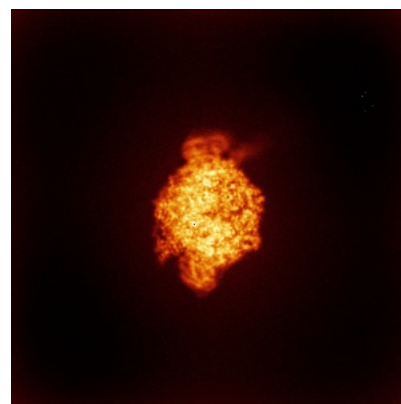
6.4.2 Raw map



X



Y

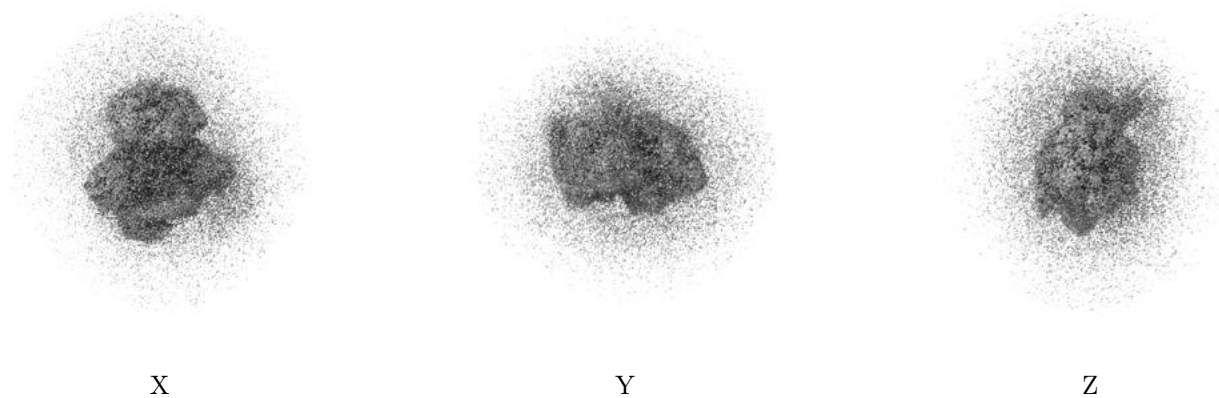


Z

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.

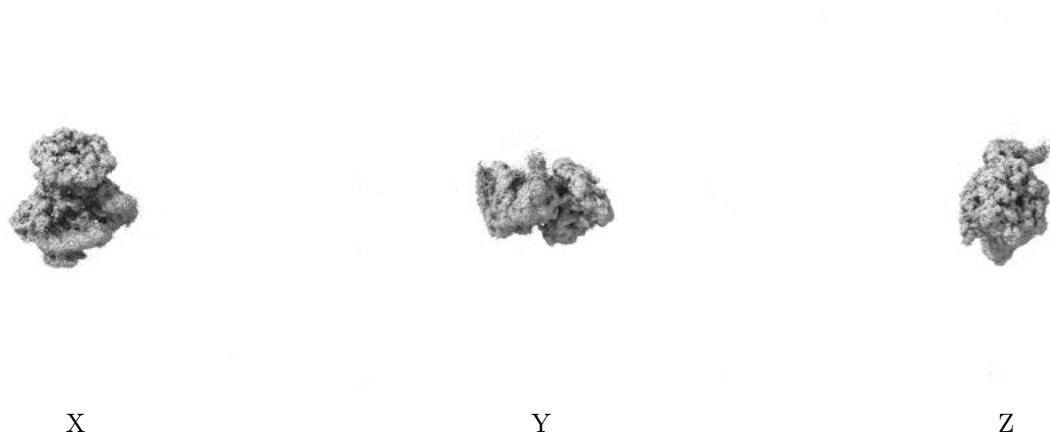
6.5 Orthogonal surface views [i](#)

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.

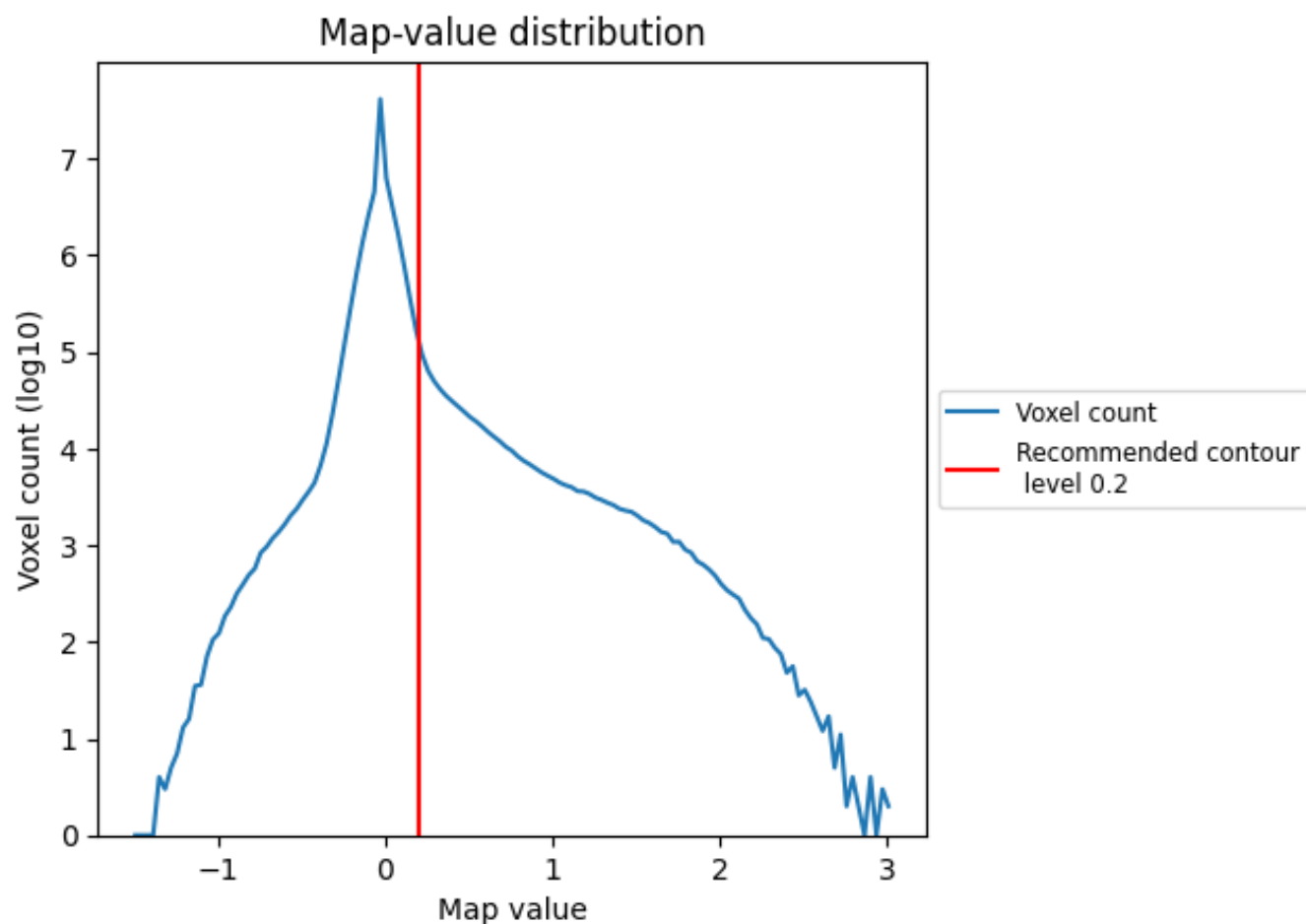
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

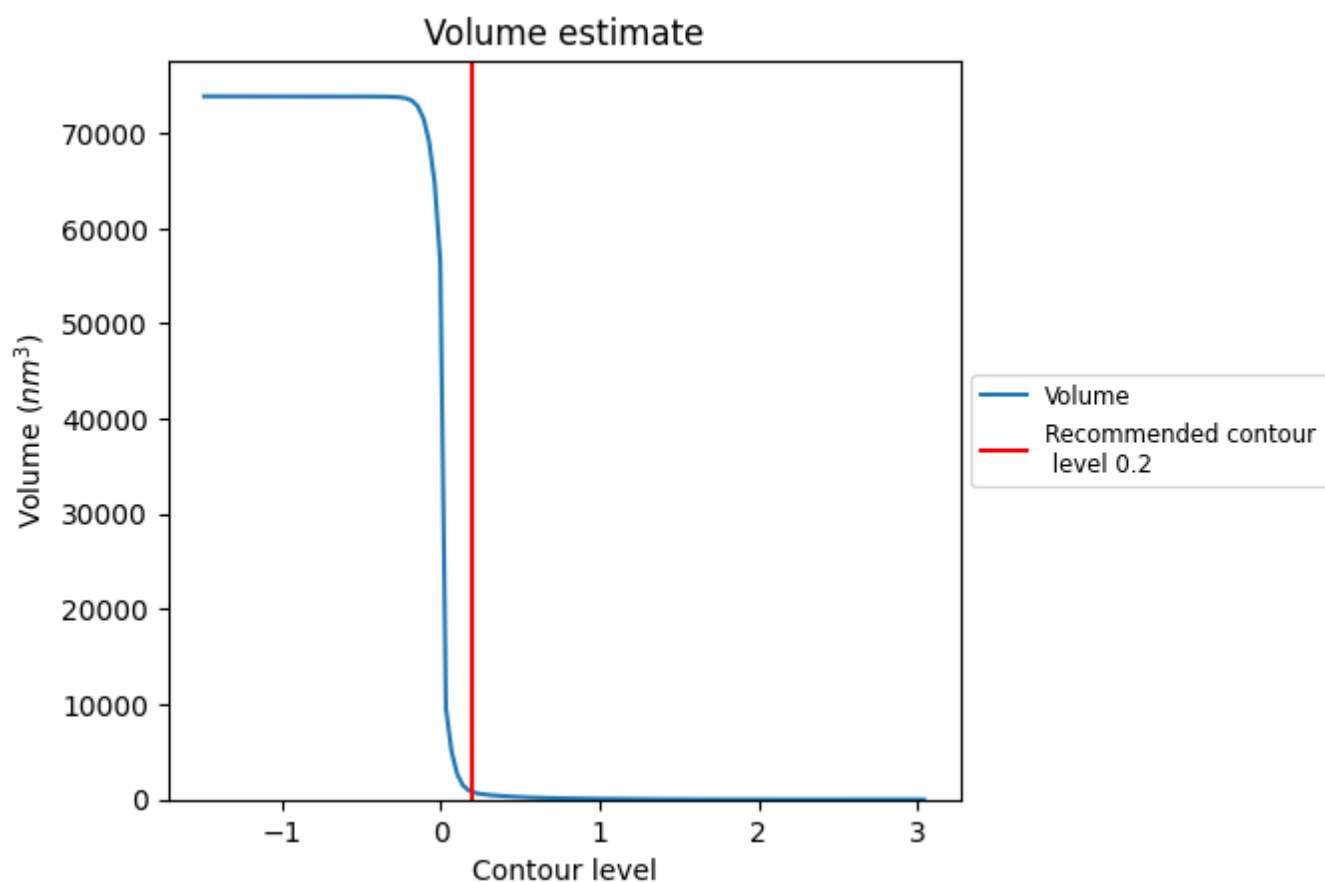
This section contains the results of statistical analysis of the map.

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.

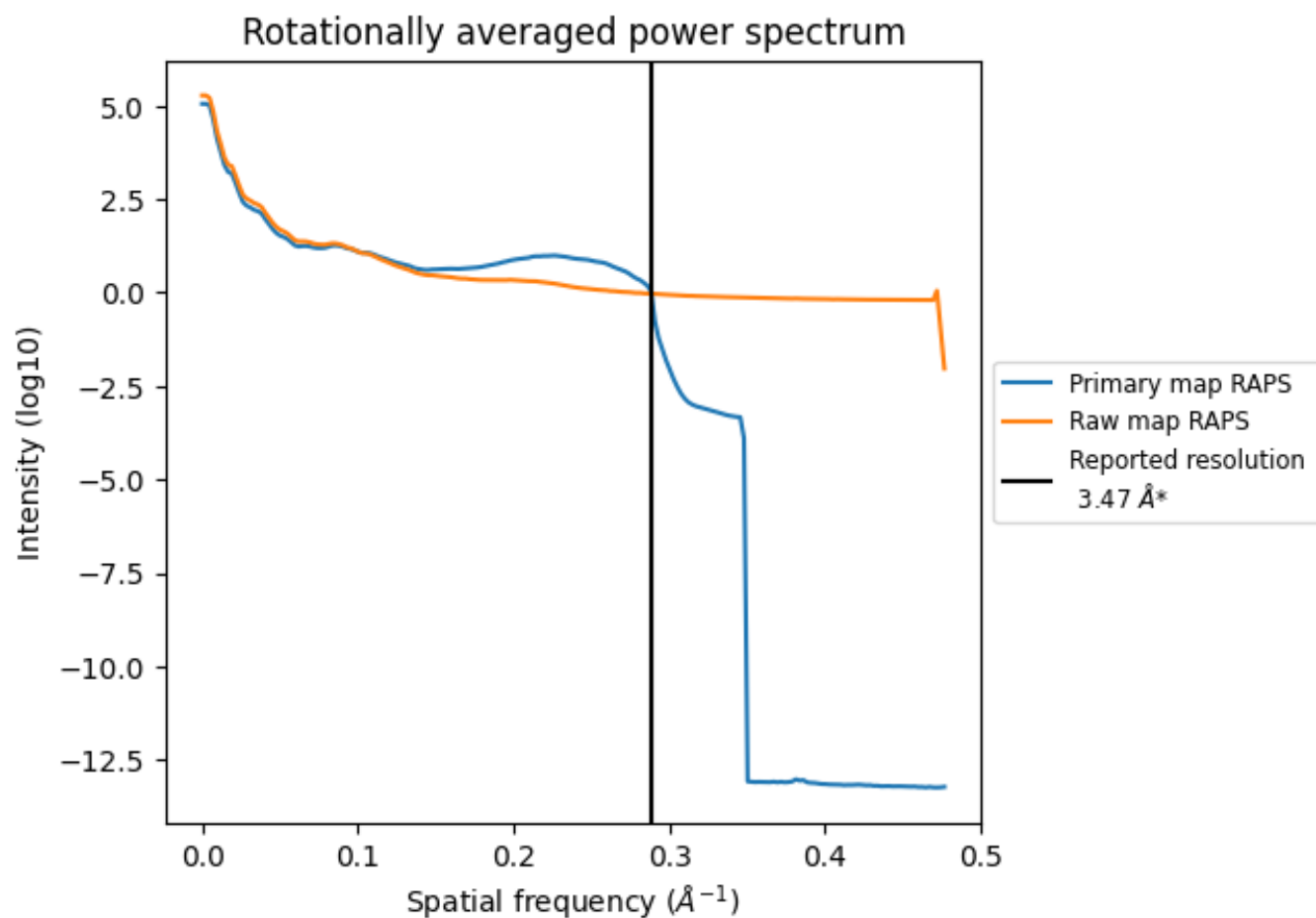
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 796 nm^3 ; this corresponds to an approximate mass of 719 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 ⓘ

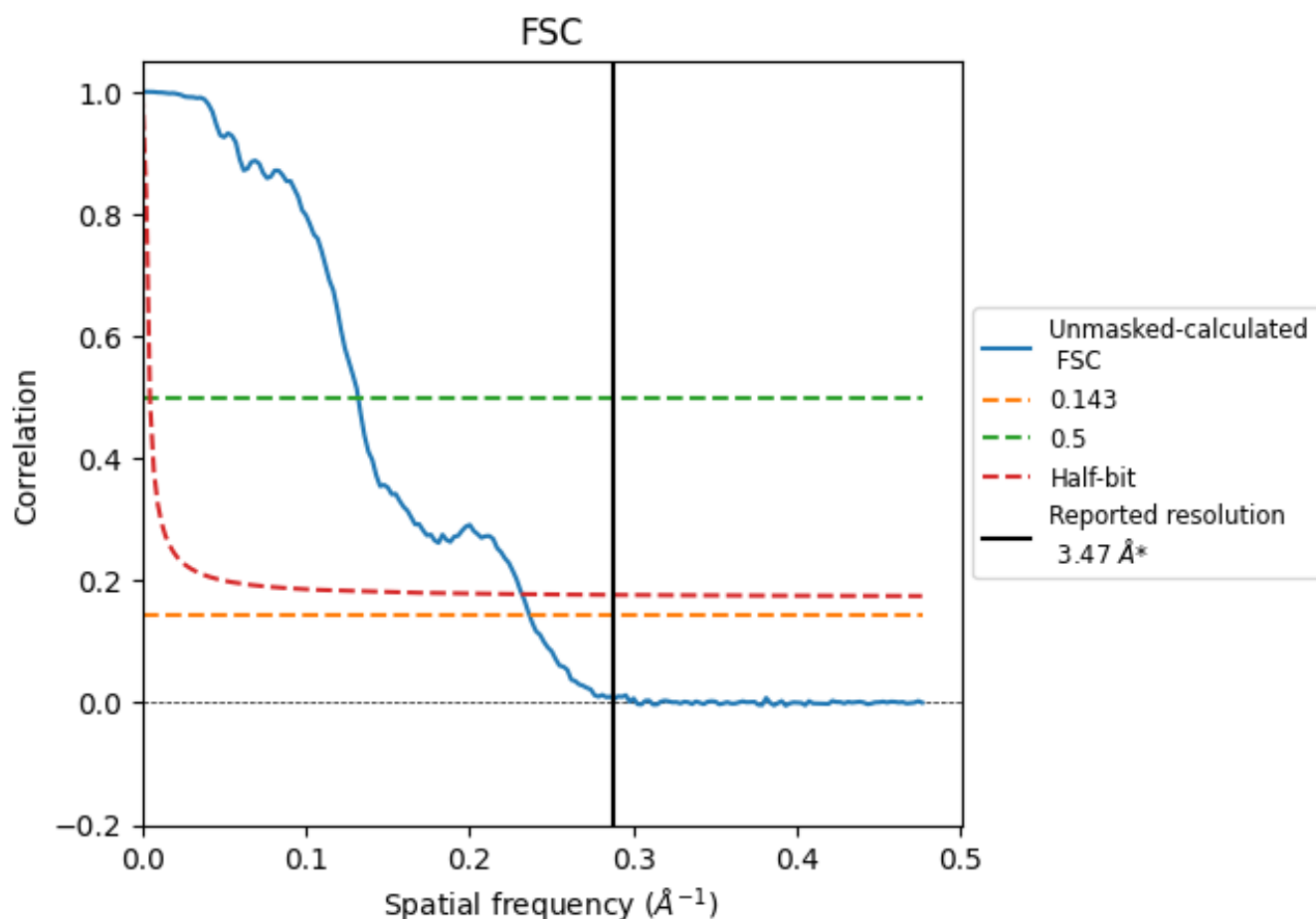


*Reported resolution corresponds to spatial frequency of 0.288 Å⁻¹

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 0.288 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

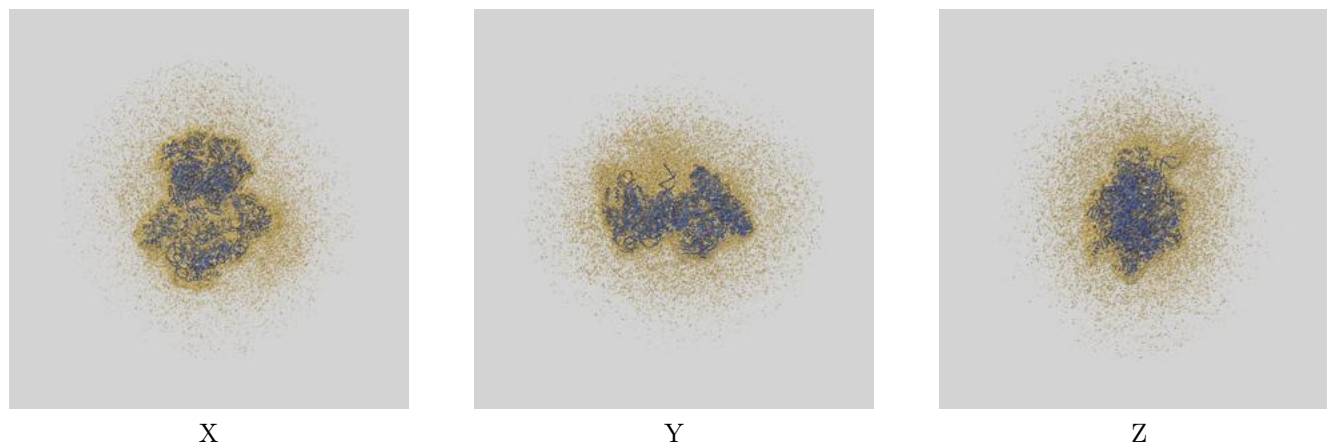
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.22	7.58	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.47 by more than 10 %

9 Map-model fit [i](#)

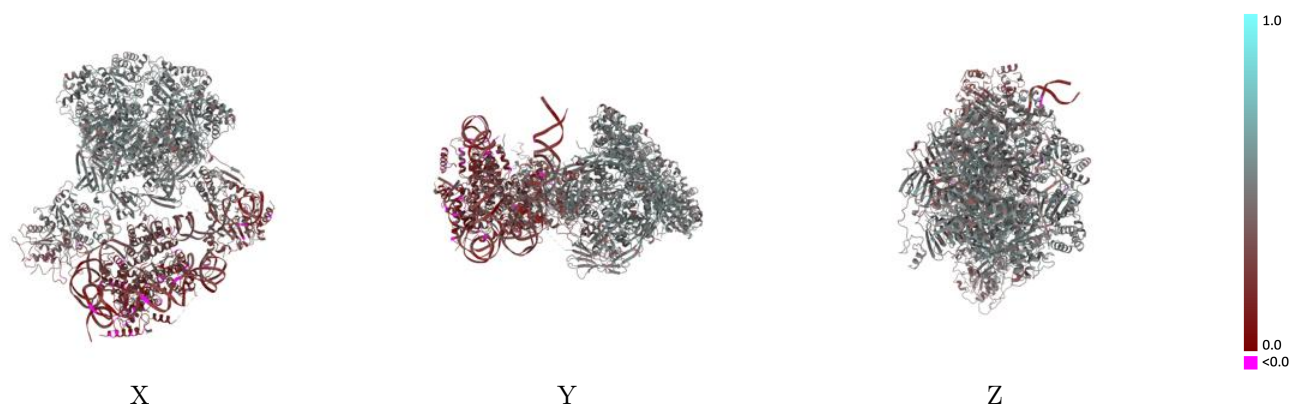
This section contains information regarding the fit between EMDB map EMD-51307 and PDB model 9GEV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



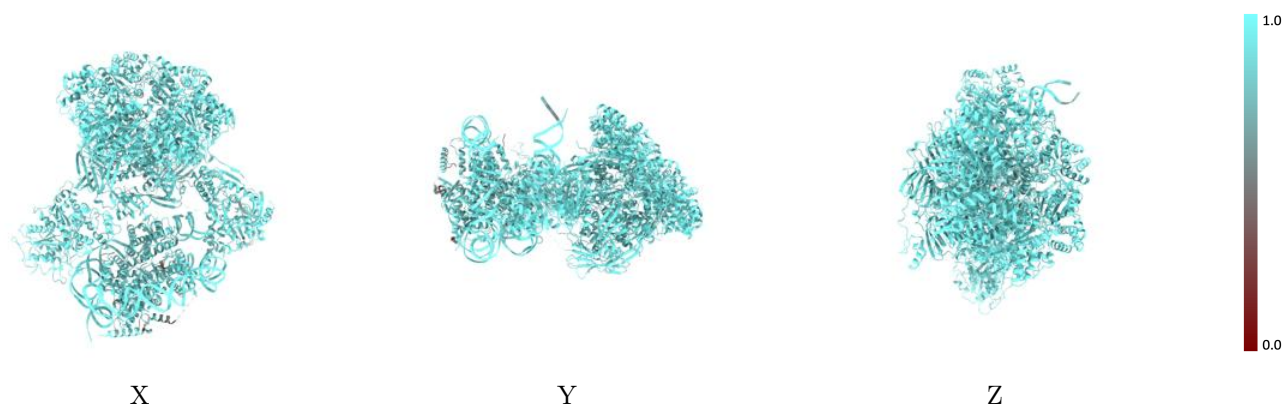
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



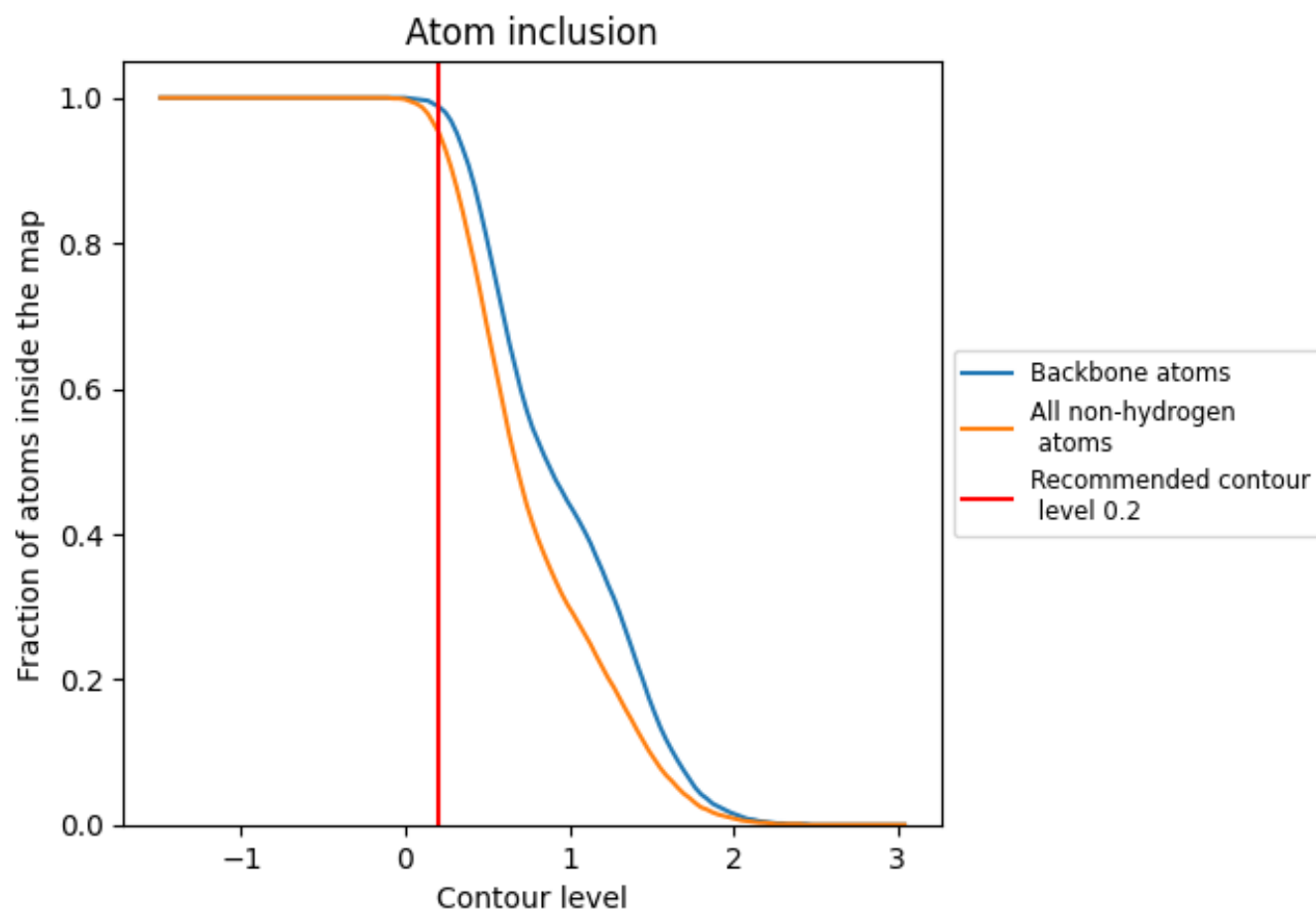
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 99% of all backbone atoms, 95% 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	 0.9540	 0.4000
A	 0.9670	 0.5040
B	 0.9700	 0.4930
C	 0.9650	 0.4930
D	 0.9660	 0.4910
E	 0.9650	 0.4880
F	 0.9680	 0.5000
G	 0.9560	 0.3980
H	 0.8850	 0.3230
I	 0.9430	 0.4080
J	 0.9600	 0.4090
K	 0.9680	 0.2160
L	 0.9730	 0.2290
M	 0.9150	 0.2380
N	 0.9230	 0.2590
O	 0.9040	 0.2380
P	 0.8930	 0.2180
Q	 0.8800	 0.2030
R	 0.9020	 0.2320
S	 0.8920	 0.2980
T	 0.9310	 0.3340

