



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 10:25 AM UTC

PDB ID : 9GE5 / pdb\_00009ge5  
EMDB ID : EMD-51290  
Title : CryoEM structure of the human INO80-Hexasome complex  
Authors : Sharma, M.; Aggarwal, P.; Hopfner, K.P.  
Deposited on : 2024-08-07  
Resolution : 3.35 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](mailto: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>.

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

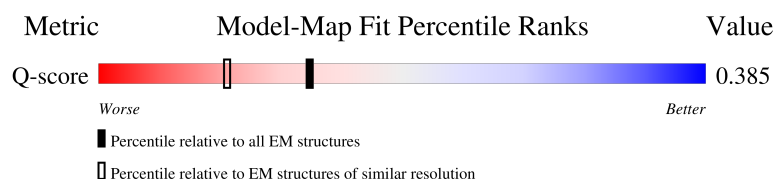
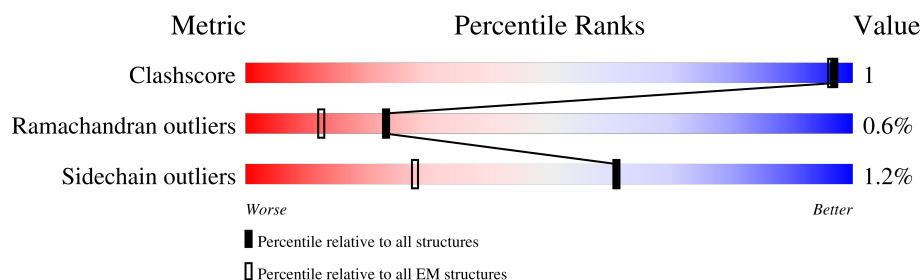
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

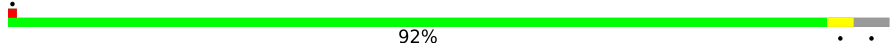
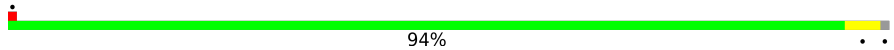
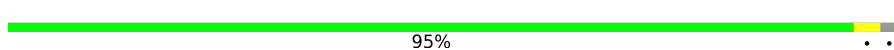
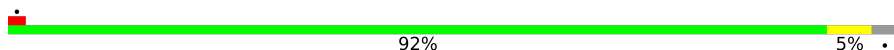
The reported resolution of this entry is 3.35 Å.

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	14390 ( 2.85 - 3.85 )

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  $\geq 3$ , 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	453	
1	B	453	
1	C	453	
2	D	439	

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Mol	Chain	Length	Quality of chain
2	E	439	
2	F	439	
3	G	733	
4	H	135	
5	I	107	
6	J	576	
7	K	113	
8	L	113	
9	M	94	
9	Q	94	
10	N	81	
10	R	81	
11	S	108	
12	T	92	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 40017 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	A	434	Total	C	N	O	S	0	0
			3345	2107	575	647	16		
1	B	447	Total	C	N	O	S	0	0
			3454	2173	592	673	16		
1	C	443	Total	C	N	O	S	0	0
			3413	2148	585	663	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	426	Total	C	N	O	S	0	0
			3318	2074	583	646	15		
2	E	439	Total	C	N	O	S	0	0
			3404	2125	597	666	16		
2	F	434	Total	C	N	O	S	0	0
			3377	2110	592	659	16		

- Molecule 3 is a protein called Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	682	Total	C	N	O	S	0	0
			5609	3599	1004	976	30		

- Molecule 4 is a protein called INO80 complex subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	101	Total	C	N	O	S	0	0
			786	478	161	138	9		

- Molecule 5 is a protein called INO80 complex subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	107	Total	C	N	O	0	0
			851	545	150	156		

- Molecule 6 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	412	Total	C	N	O	S	0	0
			3278	2088	572	597	21		

- Molecule 7 is a DNA chain called Hexasomal DNA Strand 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	113	Total	C	N	O	P	0	0
			2334	1104	441	676	113		

- Molecule 8 is a DNA chain called Hexasomal DNA strand 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	113	Total	C	N	O	P	0	0
			2299	1093	413	680	113		

- Molecule 9 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	91	Total	C	N	O	S	0	0
			739	467	138	130	4		
9	Q	94	Total	C	N	O	S	0	0
			767	482	147	134	4		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
10	R	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

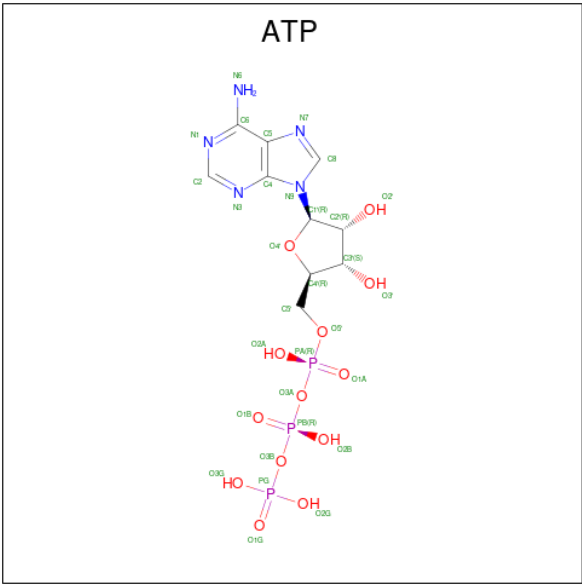
- Molecule 11 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	S	108	Total	C	N	O	0	0
			836	526	165	145		

- Molecule 12 is a protein called Histone H2B type 1-B.

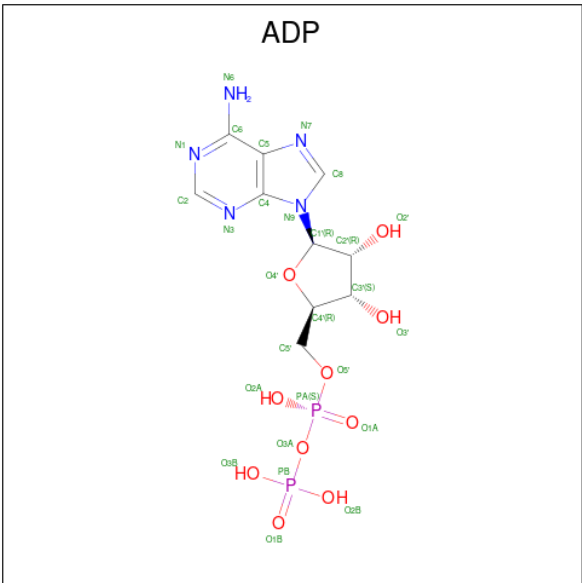
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	92	721	453	129	137	2	0	0

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

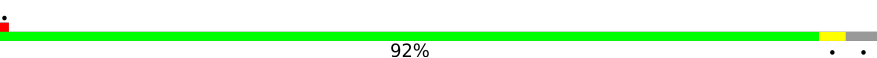
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	H	1	Total	Zn	0
			1	1	

### 3 Residue-property plots [i](#)

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

- Molecule 1: RuvB-like 1

Chain A:  92%



- Molecule 1: RuvB-like 1

Chain B:  94%



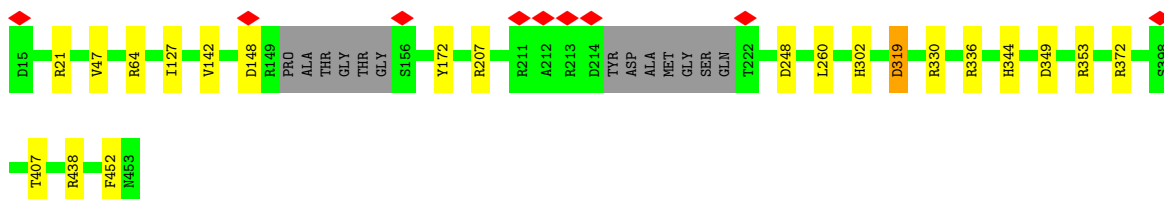
- Molecule 1: RuvB-like 1

Chain C:  95%



- Molecule 2: RuvB-like 2

Chain D:  92%

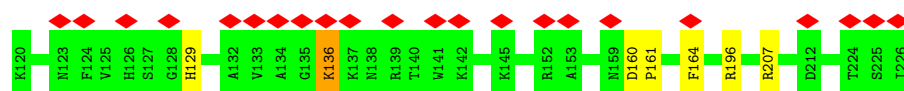
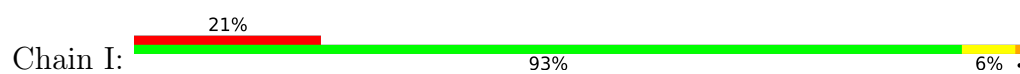


- Molecule 2: RuvB-like 2

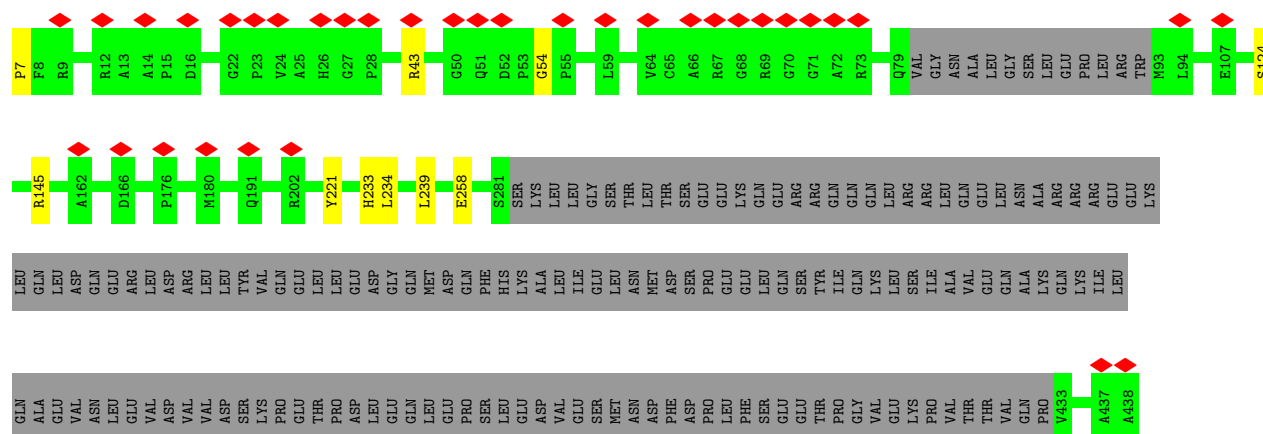
Chain E:  97%







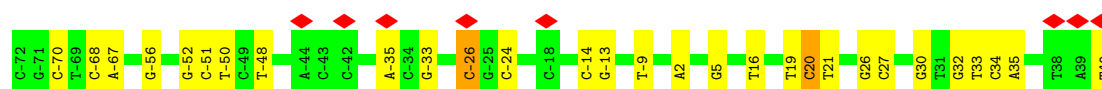
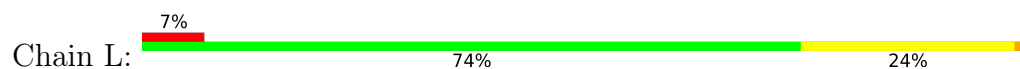
• Molecule 6: Actin-related protein 5



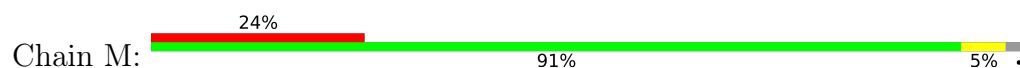
• Molecule 7: Hexasomal DNA Strand 1

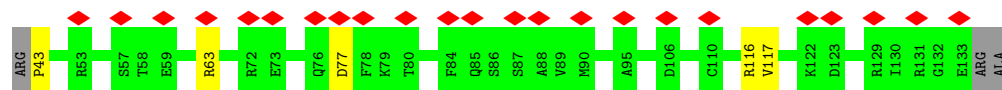


• Molecule 8: Hexasomal DNA strand 2

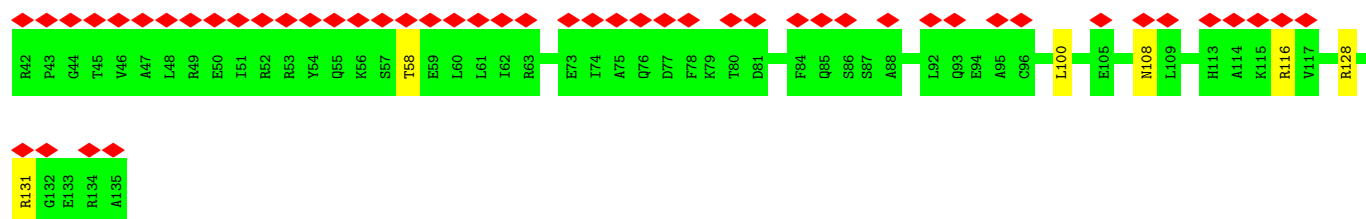


• Molecule 9: Histone H3.1

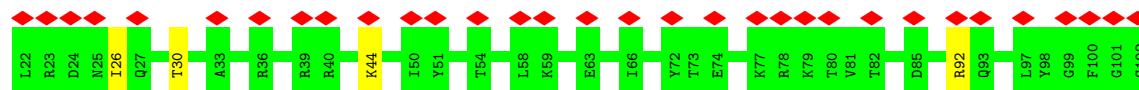
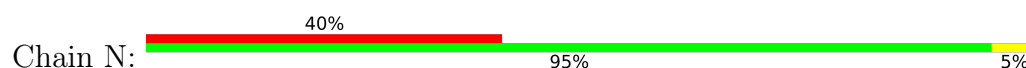




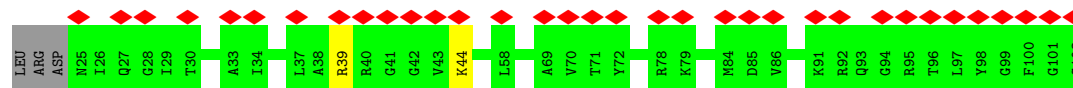
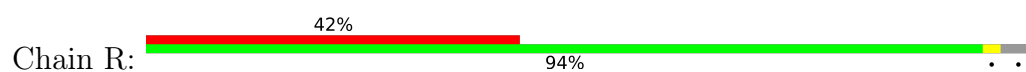
• Molecule 9: Histone H3.1



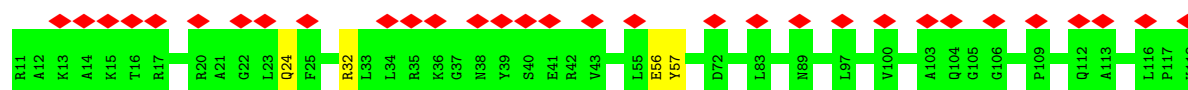
• Molecule 10: Histone H4



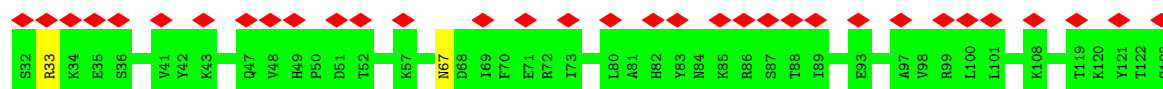
• Molecule 10: Histone H4



• Molecule 11: Histone H2A type 1-B/E



• Molecule 12: Histone H2B type 1-B



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34444	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.156	Depositor
Minimum map value	-0.676	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	290.8, 290.8, 290.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ZN, 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	A	0.68	0/3388	1.24	6/4564 (0.1%)
1	B	0.69	0/3497	1.24	9/4710 (0.2%)
1	C	0.69	0/3459	1.22	8/4662 (0.2%)
2	D	0.70	0/3354	1.25	13/4510 (0.3%)
2	E	0.71	0/3444	1.25	4/4636 (0.1%)
2	F	0.70	0/3416	1.26	11/4596 (0.2%)
3	G	0.78	0/5745	1.31	16/7759 (0.2%)
4	H	0.85	0/803	1.45	3/1080 (0.3%)
5	I	3.15	3/874 (0.3%)	1.54	10/1183 (0.8%)
6	J	0.79	0/3363	1.33	6/4558 (0.1%)
7	K	1.27	5/2622 (0.2%)	1.33	7/4049 (0.2%)
8	L	0.67	0/2574	1.34	5/3966 (0.1%)
9	M	0.80	0/748	1.37	4/1003 (0.4%)
9	Q	0.86	0/776	1.37	2/1039 (0.2%)
10	N	0.87	0/653	1.36	1/873 (0.1%)
10	R	0.86	0/626	1.40	1/837 (0.1%)
11	S	0.82	0/846	1.39	1/1139 (0.1%)
12	T	0.82	0/732	1.31	0/983
All	All	0.90	8/40920 (0.0%)	1.30	107/56147 (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	B	0	2
2	D	0	1
2	E	0	4
2	F	0	4
3	G	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	J	0	2
7	K	0	44
8	L	0	26
9	Q	0	1
11	S	0	1
All	All	0	88

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	136	LYS	CA-CB	89.44	3.03	1.53
7	K	3	DG	O4'-C1'	26.23	1.94	1.41
7	K	3	DG	C2'-C1'	24.93	2.02	1.52
7	K	3	DG	C4'-C3'	24.76	2.02	1.52
7	K	3	DG	C3'-C2'	23.67	2.00	1.52
7	K	3	DG	C4'-O4'	23.48	1.92	1.45
5	I	136	LYS	CA-C	9.99	1.66	1.52
5	I	136	LYS	N-CA	7.09	1.55	1.46

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	136	LYS	N-CA-C	-14.11	95.39	112.89
5	I	136	LYS	N-CA-CB	10.31	127.20	110.40
5	I	136	LYS	CA-CB-CG	10.19	134.49	114.10
7	K	3	DG	O4'-C1'-N9	9.96	123.34	108.40
8	L	-26	DC	C4'-C3'-O3'	7.01	120.52	110.00
7	K	48	DA	C2'-C3'-O3'	6.97	121.96	111.50
3	G	757	ASP	CA-CB-CG	6.95	119.55	112.60
2	D	248	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	333	ARG	NE-CZ-NH2	6.93	125.44	119.20
5	I	196	ARG	NE-CZ-NH2	6.86	125.38	119.20
5	I	136	LYS	CB-CA-C	6.78	124.16	109.99
8	L	34	DC	O5'-C5'-C4'	6.77	120.96	110.80
7	K	25	DC	C4'-C3'-O3'	6.68	120.02	110.00
4	H	271	PRO	CA-N-CD	-6.59	102.77	112.00
1	B	357	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	C	46	ARG	NE-CZ-NH2	6.28	124.85	119.20
7	K	57	DT	O5'-C5'-C4'	6.26	120.20	110.80
2	F	54	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	B	173	ASP	CA-CB-CG	6.20	118.80	112.60
3	G	1212	ARG	NE-CZ-NH2	6.13	124.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	-52	DG	C5'-C4'-C3'	-6.11	105.74	114.90
4	H	223	ARG	NE-CZ-NH2	6.11	124.70	119.20
2	F	438	ARG	NE-CZ-NH2	6.07	124.66	119.20
9	Q	131	ARG	NE-CZ-NH2	6.02	124.62	119.20
2	E	273	ARG	NE-CZ-NH2	6.01	124.61	119.20
2	F	29	ARG	NE-CZ-NH2	5.81	124.42	119.20
1	A	357	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	C	276	ARG	NE-CZ-NH2	5.79	124.41	119.20
5	I	207	ARG	NE-CZ-NH2	5.78	124.40	119.20
8	L	20	DC	C4'-C3'-O3'	5.78	118.67	110.00
1	C	184	ARG	NE-CZ-NH2	5.75	124.38	119.20
1	C	339	ARG	NE-CZ-NH2	5.74	124.37	119.20
4	H	336	ARG	NE-CZ-NH2	5.74	124.36	119.20
2	D	64	ARG	NE-CZ-NH2	5.71	124.34	119.20
3	G	746	ARG	NE-CZ-NH2	5.70	124.33	119.20
7	K	57	DT	C5'-C4'-O4'	5.70	117.95	109.40
1	B	46	ARG	NE-CZ-NH2	5.68	124.31	119.20
2	F	207	ARG	NE-CZ-NH2	5.67	124.31	119.20
5	I	164	PHE	CA-CB-CG	5.67	119.47	113.80
2	D	336	ARG	NE-CZ-NH2	5.66	124.29	119.20
3	G	1069	PHE	CA-CB-CG	5.65	119.45	113.80
2	F	336	ARG	NE-CZ-NH2	5.63	124.27	119.20
2	F	273	ARG	NE-CZ-NH2	5.62	124.26	119.20
3	G	862	ARG	NE-CZ-NH2	5.62	124.26	119.20
9	M	43	PRO	CA-N-CD	-5.61	104.14	112.00
3	G	1146	ARG	NE-CZ-NH2	5.60	124.24	119.20
6	J	7	PRO	CA-N-CD	-5.59	104.17	112.00
2	F	392	ARG	NE-CZ-NH2	5.57	124.22	119.20
3	G	1212	ARG	CA-C-N	5.57	128.02	120.38
3	G	1212	ARG	C-N-CA	5.57	128.02	120.38
2	E	400	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	B	348	HIS	CB-CG-CD2	-5.56	123.97	131.20
3	G	1203	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	123	ARG	NE-CZ-NH2	5.55	124.20	119.20
2	D	353	ARG	NE-CZ-NH2	5.55	124.19	119.20
2	E	21	ARG	NE-CZ-NH2	5.53	124.17	119.20
2	D	349	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	20	HIS	CB-CG-CD2	-5.51	124.03	131.20
9	Q	116	ARG	NE-CZ-NH2	5.51	124.16	119.20
3	G	1156	ARG	NE-CZ-NH2	5.48	124.13	119.20
5	I	160	ASP	CA-C-N	5.48	126.69	119.84
5	I	160	ASP	C-N-CA	5.48	126.69	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	145	ARG	NE-CZ-NH2	5.47	124.13	119.20
9	M	116	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	B	378	ARG	NE-CZ-NH2	5.44	124.10	119.20
3	G	1065	ARG	NE-CZ-NH2	5.44	124.09	119.20
11	S	32	ARG	NE-CZ-NH2	5.43	124.09	119.20
3	G	581	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	276	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	244	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	241	HIS	CB-CG-CD2	-5.36	124.23	131.20
10	N	92	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	C	357	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	E	18	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	F	248	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	276	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	D	372	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	173	ASP	CA-CB-CG	5.25	117.85	112.60
2	D	330	ARG	NE-CZ-NH2	5.21	123.89	119.20
3	G	745	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	F	130	ARG	NE-CZ-NH2	5.21	123.88	119.20
3	G	818	HIS	CB-CG-CD2	-5.20	124.44	131.20
2	D	207	ARG	NE-CZ-NH2	5.19	123.87	119.20
2	D	148	ASP	CA-CB-CG	5.19	117.79	112.60
2	D	319	ASP	CA-CB-CG	5.17	117.77	112.60
2	D	438	ARG	NE-CZ-NH2	5.15	123.83	119.20
6	J	477	ASP	CA-CB-CG	5.14	117.74	112.60
7	K	56	DC	C4'-C3'-O3'	5.14	117.71	110.00
6	J	448	ARG	NE-CZ-NH2	5.13	123.82	119.20
8	L	-14	DC	C2'-C3'-O3'	5.13	119.19	111.50
9	M	77	ASP	CA-CB-CG	5.13	117.73	112.60
10	R	39	ARG	NE-CZ-NH2	5.13	123.81	119.20
3	G	930	ARG	NE-CZ-NH2	5.12	123.80	119.20
9	M	63	ARG	NE-CZ-NH2	5.11	123.80	119.20
5	I	129	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	D	302	HIS	CB-CG-CD2	-5.09	124.59	131.20
3	G	1236	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	F	329	ASN	N-CA-CB	-5.06	103.09	111.49
7	K	45	DG	C2'-C3'-O3'	5.05	119.08	111.50
2	F	25	HIS	CB-CG-CD2	-5.05	124.64	131.20
6	J	233	HIS	CB-CG-CD2	-5.05	124.64	131.20
2	D	21	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	C	404	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	B	172	LEU	CA-C-N	5.01	127.36	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	LEU	C-N-CA	5.01	127.36	120.39
6	J	538	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	305	HIS	CB-CG-CD2	-5.01	124.69	131.20

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	192	TYR	Sidechain
1	B	202	ARG	Sidechain
2	D	172	TYR	Sidechain
2	E	18	ARG	Sidechain
2	E	207	ARG	Sidechain
2	E	211	ARG	Sidechain
2	E	71	ARG	Sidechain
2	F	207	ARG	Sidechain
2	F	21	ARG	Sidechain
2	F	438	ARG	Sidechain
2	F	54	ARG	Sidechain
3	G	640	TYR	Sidechain
3	G	746	ARG	Sidechain
3	G	845	TYR	Sidechain
6	J	221	TYR	Sidechain
6	J	43	ARG	Sidechain
7	K	-13	DG	Sidechain
7	K	-15	DG	Sidechain
7	K	-17	DT	Sidechain
7	K	-20	DG	Sidechain
7	K	-24	DT	Sidechain
7	K	-27	DG	Sidechain
7	K	-28	DT	Sidechain
7	K	-29	DG	Sidechain
7	K	-3	DC	Sidechain
7	K	-30	DC	Sidechain
7	K	-31	DA	Sidechain
7	K	-32	DC	Sidechain
7	K	-34	DG	Sidechain
7	K	-35	DT	Sidechain
7	K	-36	DC	Sidechain
7	K	-5	DC	Sidechain
7	K	-6	DC	Sidechain
7	K	-8	DA	Sidechain

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Mol	Chain	Res	Type	Group
7	K	11	DC	Sidechain
7	K	14	DG	Sidechain
7	K	19	DA	Sidechain
7	K	20	DC	Sidechain
7	K	23	DC	Sidechain
7	K	25	DC	Sidechain
7	K	27	DT	Sidechain
7	K	28	DA	Sidechain
7	K	3	DG	Sidechain
7	K	32	DG	Sidechain
7	K	33	DC	Sidechain
7	K	37	DT	Sidechain
7	K	4	DG	Sidechain
7	K	40	DG	Sidechain
7	K	42	DG	Sidechain
7	K	43	DG	Sidechain
7	K	46	DC	Sidechain
7	K	47	DT	Sidechain
7	K	49	DG	Sidechain
7	K	5	DT	Sidechain
7	K	53	DT	Sidechain
7	K	55	DT	Sidechain
7	K	57	DT	Sidechain
7	K	63	DC	Sidechain
7	K	65	DA	Sidechain
7	K	71	DC	Sidechain
8	L	-13	DG	Sidechain
8	L	-24	DC	Sidechain
8	L	-26	DC	Sidechain
8	L	-33	DG	Sidechain
8	L	-35	DA	Sidechain
8	L	-48	DT	Sidechain
8	L	-50	DT	Sidechain
8	L	-51	DC	Sidechain
8	L	-56	DG	Sidechain
8	L	-67	DA	Sidechain
8	L	-68	DC	Sidechain
8	L	-70	DC	Sidechain
8	L	-9	DT	Sidechain
8	L	16	DT	Sidechain
8	L	19	DT	Sidechain
8	L	2	DA	Sidechain

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Mol	Chain	Res	Type	Group
8	L	20	DC	Sidechain
8	L	21	DT	Sidechain
8	L	26	DG	Sidechain
8	L	27	DC	Sidechain
8	L	30	DG	Sidechain
8	L	32	DG	Sidechain
8	L	33	DT	Sidechain
8	L	35	DA	Sidechain
8	L	40	DT	Sidechain
8	L	5	DG	Sidechain
9	Q	128	ARG	Sidechain
11	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	3345	0	3451	2	0
1	B	3454	0	3563	1	0
1	C	3413	0	3508	3	0
2	D	3318	0	3395	0	0
2	E	3404	0	3472	2	0
2	F	3377	0	3446	1	0
3	G	5609	0	5651	4	0
4	H	786	0	798	1	0
5	I	851	0	852	30	0
6	J	3278	0	3215	2	0
7	K	2334	0	1268	36	0
8	L	2299	0	1270	0	0
9	M	739	0	777	0	0
9	Q	767	0	807	0	0
10	N	646	0	687	1	0
10	R	619	0	659	0	0
11	S	836	0	897	1	0
12	T	721	0	740	0	0
13	A	31	0	12	0	0
14	B	27	0	12	0	0
14	C	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	D	27	0	12	0	0
14	E	27	0	12	0	0
14	F	27	0	12	0	0
14	G	27	0	12	0	0
14	J	27	0	12	0	0
15	H	1	0	0	0	0
All	All	40017	0	38552	51	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 1.

All (51) 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)
7:K:3:DG:C3'	7:K:3:DG:C2'	2.00	1.39
7:K:3:DG:C2'	7:K:3:DG:C1'	2.02	1.37
7:K:3:DG:C3'	7:K:3:DG:C4'	2.02	1.35
5:I:136:LYS:HA	7:K:3:DG:C2'	1.63	1.28
5:I:136:LYS:HA	7:K:3:DG:C1'	1.73	1.19
7:K:3:DG:C1'	7:K:3:DG:O4'	1.94	1.16
7:K:3:DG:C4'	7:K:3:DG:O4'	1.92	1.16
5:I:136:LYS:CA	7:K:3:DG:C1'	2.26	1.13
5:I:136:LYS:CA	7:K:3:DG:C2'	2.27	1.12
5:I:136:LYS:CB	7:K:3:DG:C1'	2.27	1.12
5:I:136:LYS:CB	7:K:3:DG:C4'	2.29	1.11
5:I:136:LYS:CA	7:K:3:DG:C4'	2.28	1.11
5:I:136:LYS:CB	7:K:3:DG:C3'	2.30	1.08
5:I:136:LYS:CB	7:K:3:DG:C2'	2.31	1.07
5:I:136:LYS:CA	7:K:3:DG:C3'	2.32	1.06
5:I:136:LYS:CA	7:K:3:DG:O4'	2.17	0.92
5:I:136:LYS:CB	7:K:3:DG:O4'	2.19	0.90
5:I:136:LYS:HB2	7:K:3:DG:C3'	2.06	0.85
5:I:136:LYS:HB2	7:K:3:DG:C4'	2.05	0.85
5:I:136:LYS:HA	7:K:3:DG:H2'	1.61	0.82
5:I:136:LYS:HB3	7:K:3:DG:O4'	1.87	0.74
5:I:136:LYS:N	7:K:3:DG:H3'	2.03	0.73
5:I:136:LYS:N	7:K:3:DG:C3'	2.54	0.69
5:I:136:LYS:CG	7:K:3:DG:C2'	2.76	0.63
5:I:136:LYS:CG	7:K:3:DG:H2''	2.29	0.63
5:I:136:LYS:C	7:K:3:DG:O4'	2.44	0.60
3:G:821:LEU:HD11	3:G:1129:MET:HE2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:136:LYS:HB2	7:K:3:DG:H4'	1.83	0.58
2:E:50:LEU:H	2:E:50:LEU:HD22	1.71	0.55
1:C:256:ILE:HD13	3:G:1075:GLY:HA2	1.90	0.54
1:A:272:THR:HG23	1:A:275:LEU:H	1.73	0.54
5:I:136:LYS:H	7:K:3:DG:H5'	1.74	0.53
3:G:818:HIS:HB2	3:G:1129:MET:HE1	1.91	0.52
5:I:136:LYS:CB	7:K:3:DG:H1'	2.34	0.51
5:I:136:LYS:HB2	7:K:3:DG:O3'	2.11	0.50
5:I:136:LYS:HB3	7:K:3:DG:C1'	2.37	0.49
7:K:-13:DG:H5''	10:N:30:THR:HG21	1.95	0.49
5:I:136:LYS:H	7:K:3:DG:H3'	1.74	0.49
1:C:20:HIS:H	1:C:20:HIS:CD2	2.33	0.47
1:C:153:THR:HG22	4:H:285:SER:CB	2.46	0.46
5:I:136:LYS:N	7:K:3:DG:H5'	2.33	0.44
2:E:246:GLU:HB2	2:E:260:LEU:HD22	2.01	0.43
11:S:24:GLN:H	11:S:56:GLU:CD	2.27	0.43
3:G:817:ASN:CG	3:G:1129:MET:HE3	2.45	0.41
5:I:136:LYS:CB	7:K:3:DG:H4'	2.37	0.41
1:B:272:THR:HG22	1:B:274:LYS:H	1.86	0.41
1:A:42:GLN:HE22	1:A:363:THR:HG23	1.86	0.41
5:I:136:LYS:CA	7:K:3:DG:C5'	2.95	0.40
2:F:174:LEU:H	2:F:174:LEU:HD23	1.86	0.40
6:J:239:LEU:HD22	6:J:239:LEU:H	1.87	0.40
6:J:461:ILE:HG22	6:J:462:GLY:H	1.86	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	430/453 (95%)	413 (96%)	15 (4%)	2 (0%)	24 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	443/453 (98%)	430 (97%)	11 (2%)	2 (0%)	24	52
1	C	441/453 (97%)	421 (96%)	19 (4%)	1 (0%)	43	70
2	D	420/439 (96%)	408 (97%)	10 (2%)	2 (0%)	24	52
2	E	437/439 (100%)	427 (98%)	10 (2%)	0	100	100
2	F	430/439 (98%)	414 (96%)	15 (4%)	1 (0%)	43	70
3	G	674/733 (92%)	634 (94%)	32 (5%)	8 (1%)	10	33
4	H	97/135 (72%)	93 (96%)	3 (3%)	1 (1%)	12	38
5	I	105/107 (98%)	97 (92%)	7 (7%)	1 (1%)	12	38
6	J	406/576 (70%)	373 (92%)	30 (7%)	3 (1%)	18	46
9	M	89/94 (95%)	86 (97%)	3 (3%)	0	100	100
9	Q	92/94 (98%)	87 (95%)	4 (4%)	1 (1%)	11	36
10	N	79/81 (98%)	73 (92%)	4 (5%)	2 (2%)	4	20
10	R	76/81 (94%)	73 (96%)	2 (3%)	1 (1%)	9	32
11	S	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
12	T	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	4415/4777 (92%)	4219 (96%)	171 (4%)	25 (1%)	23	49

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	LEU
10	N	26	ILE
1	B	59	LYS
1	B	342	GLU
2	F	452	PHE
3	G	747	ILE
3	G	684	ILE
3	G	1001	CYS
3	G	1230	ILE
4	H	272	MET
1	C	210	ALA
2	D	452	PHE
3	G	682	THR
3	G	943	TYR
3	G	1143	THR
6	J	445	GLY
5	I	161	PRO

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Mol	Chain	Res	Type
10	N	44	LYS
9	Q	58	THR
10	R	44	LYS
1	A	59	LYS
2	D	344	HIS
3	G	1201	THR
6	J	124	SER
6	J	54	GLY

### 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	367/384 (96%)	364 (99%)	3 (1%)	73	76
1	B	381/384 (99%)	376 (99%)	5 (1%)	61	70
1	C	374/384 (97%)	370 (99%)	4 (1%)	65	73
2	D	361/369 (98%)	355 (98%)	6 (2%)	53	67
2	E	369/369 (100%)	367 (100%)	2 (0%)	81	80
2	F	367/369 (100%)	357 (97%)	10 (3%)	39	60
3	G	613/660 (93%)	609 (99%)	4 (1%)	76	77
4	H	86/105 (82%)	84 (98%)	2 (2%)	44	62
5	I	92/92 (100%)	92 (100%)	0	100	100
6	J	351/504 (70%)	348 (99%)	3 (1%)	70	75
9	M	79/81 (98%)	78 (99%)	1 (1%)	61	70
9	Q	81/81 (100%)	79 (98%)	2 (2%)	42	61
10	N	66/66 (100%)	66 (100%)	0	100	100
10	R	63/66 (96%)	63 (100%)	0	100	100
11	S	85/85 (100%)	85 (100%)	0	100	100
12	T	79/79 (100%)	77 (98%)	2 (2%)	42	61
All	All	3814/4078 (94%)	3770 (99%)	44 (1%)	61	72

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	167	THR
1	A	295	VAL
1	B	40	VAL
1	B	97	VAL
1	B	335	ASN
1	B	415	LEU
1	B	439	ASP
1	C	173	ASP
1	C	190	VAL
1	C	256	ILE
1	C	439	ASP
2	D	47	VAL
2	D	127	ILE
2	D	142	VAL
2	D	260	LEU
2	D	319	ASP
2	D	407	THR
2	E	270	SER
2	E	328	THR
2	F	28	ILE
2	F	116	THR
2	F	138	ILE
2	F	163	LEU
2	F	165	THR
2	F	187	VAL
2	F	231	GLU
2	F	323	VAL
2	F	328	THR
2	F	421	VAL
3	G	541	LEU
3	G	757	ASP
3	G	1148	ASP
3	G	1220	THR
4	H	215	LYS
4	H	296	VAL
6	J	234	LEU
6	J	258	GLU
6	J	487	LEU
9	M	117	VAL
9	Q	100	LEU
9	Q	108	ASN

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Mol	Chain	Res	Type
12	T	33	ARG
12	T	67	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	241	HIS
1	A	247	ASN
1	A	408	GLN
1	B	44	ASN
1	B	115	ASN
1	B	145	ASN
1	B	247	ASN
1	B	262	GLN
1	B	348	HIS
1	C	251	GLN
1	C	262	GLN
1	C	408	GLN
1	C	451	GLN
2	D	41	GLN
2	D	78	GLN
2	D	369	GLN
2	D	404	GLN
2	E	78	GLN
2	E	240	HIS
2	E	341	GLN
2	E	404	GLN
2	F	25	HIS
2	F	78	GLN
2	F	92	GLN
2	F	240	HIS
2	F	404	GLN
3	G	552	GLN
3	G	580	ASN
3	G	581	ASN
3	G	710	ASN
3	G	776	GLN
3	G	811	GLN
3	G	832	HIS
3	G	839	HIS
3	G	855	HIS

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Mol	Chain	Res	Type
3	G	903	ASN
3	G	907	GLN
3	G	1165	ASN
3	G	1205	GLN
5	I	126	HIS
5	I	146	GLN
6	J	60	GLN
6	J	125	GLN
6	J	223	GLN
6	J	441	GLN
6	J	457	GLN
9	M	93	GLN
10	N	64	ASN
11	S	24	GLN
11	S	110	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
13	ATP	A	501	-	32,33,33	1.36	4 (12%)	48,52,52	1.33	8 (16%)
14	ADP	D	501	-	28,29,29	1.06	1 (3%)	43,45,45	1.24	7 (16%)
14	ADP	C	501	-	28,29,29	1.03	1 (3%)	43,45,45	1.26	7 (16%)
14	ADP	G	1601	-	28,29,29	0.99	0	43,45,45	1.34	8 (18%)
14	ADP	F	501	-	28,29,29	1.06	2 (7%)	43,45,45	1.32	6 (13%)
14	ADP	B	501	-	28,29,29	1.08	1 (3%)	43,45,45	1.24	5 (11%)
14	ADP	E	501	-	28,29,29	1.00	1 (3%)	43,45,45	1.28	9 (20%)
14	ADP	J	701	-	28,29,29	0.96	1 (3%)	43,45,45	1.38	5 (11%)

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	ATP	A	501	-	-	1/22/38/38	0/3/3/3
14	ADP	D	501	-	-	3/16/32/32	0/3/3/3
14	ADP	C	501	-	-	1/16/32/32	0/3/3/3
14	ADP	G	1601	-	-	3/16/32/32	0/3/3/3
14	ADP	F	501	-	-	0/16/32/32	0/3/3/3
14	ADP	B	501	-	-	1/16/32/32	0/3/3/3
14	ADP	E	501	-	-	2/16/32/32	0/3/3/3
14	ADP	J	701	-	-	3/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	501	ATP	PA-O3A	-3.66	1.55	1.59
13	A	501	ATP	PB-O3B	-3.01	1.56	1.59
13	A	501	ATP	PB-O3A	-2.91	1.56	1.59
14	D	501	ADP	C5-C4	-2.41	1.34	1.39
14	B	501	ADP	C5-C4	-2.36	1.34	1.39
14	F	501	ADP	C5-C4	-2.30	1.35	1.39
13	A	501	ATP	C5-C4	-2.28	1.35	1.39
14	C	501	ADP	C5-C4	-2.26	1.35	1.39
14	E	501	ADP	C5-C4	-2.22	1.35	1.39
14	J	701	ADP	C5-C4	-2.15	1.35	1.39
14	F	501	ADP	PA-O3A	-2.06	1.57	1.59

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	501	ADP	C5-C4-N3	-3.46	121.95	126.72
13	A	501	ATP	O2B-PB-O3A	3.44	116.58	107.27
14	J	701	ADP	C4'-O4'-C1'	-3.27	102.24	109.47
14	C	501	ADP	C4-C5-N7	3.21	114.25	110.58
14	E	501	ADP	C5-C4-N3	-3.15	122.38	126.72
13	A	501	ATP	C5-C4-N3	-3.10	122.45	126.72
14	C	501	ADP	O2A-PA-O3A	3.09	115.62	107.27
13	A	501	ATP	C4-C5-N7	3.08	114.11	110.58
14	G	1601	ADP	C4-C5-N7	2.96	113.96	110.58
14	B	501	ADP	O2A-PA-O3A	2.93	115.19	107.27
14	F	501	ADP	O2A-PA-O3A	2.87	115.04	107.27
14	B	501	ADP	C4-C5-N7	2.86	113.86	110.58
14	G	1601	ADP	O2A-PA-O3A	2.84	114.94	107.27
14	C	501	ADP	C5-C4-N3	-2.83	122.82	126.72
14	D	501	ADP	C5-C4-N3	-2.83	122.82	126.72
14	G	1601	ADP	C5-C4-N3	-2.81	122.85	126.72
14	J	701	ADP	O4'-C1'-N9	2.80	113.47	108.09
14	E	501	ADP	C4-C5-N7	2.79	113.77	110.58
14	D	501	ADP	O3B-PB-O3A	2.76	113.89	104.64
14	D	501	ADP	C4-C5-N7	2.76	113.73	110.58
14	D	501	ADP	O2A-PA-O3A	2.76	114.72	107.27
14	G	1601	ADP	O3B-PB-O3A	2.64	113.50	104.64
14	F	501	ADP	C2-N1-C6	-2.61	114.45	118.73
13	A	501	ATP	N3-C4-N9	2.56	131.52	127.17
14	F	501	ADP	C4-C5-N7	2.55	113.50	110.58
14	B	501	ADP	C5-C4-N3	-2.47	123.31	126.72
14	J	701	ADP	C5-C4-N3	-2.47	123.31	126.72
14	F	501	ADP	N3-C4-N9	2.46	131.35	127.17
14	C	501	ADP	N3-C4-N9	2.43	131.30	127.17
14	D	501	ADP	C2-N1-C6	-2.38	114.83	118.73
13	A	501	ATP	C2-N1-C6	-2.35	114.87	118.73
14	J	701	ADP	C4-C5-N7	2.32	113.23	110.58
14	C	501	ADP	C2-N1-C6	-2.27	115.00	118.73
14	E	501	ADP	C5-C6-N1	2.27	123.27	117.51
13	A	501	ATP	O3G-PG-O3B	2.27	112.23	104.64
14	E	501	ADP	C2-N1-C6	-2.26	115.02	118.73
14	E	501	ADP	N3-C4-N9	2.25	131.00	127.17
14	J	701	ADP	O3A-PA-O1A	2.23	117.43	110.70
14	B	501	ADP	C2-N1-C6	-2.23	115.07	118.73
14	G	1601	ADP	O4'-C1'-C2'	-2.23	101.85	106.62
14	E	501	ADP	O2A-PA-O3A	2.22	113.29	107.27
14	G	1601	ADP	C5-C6-N1	2.19	123.08	117.51
14	F	501	ADP	C5-C6-N1	2.18	123.05	117.51

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	501	ADP	N6-C6-N1	-2.14	113.61	118.38
14	E	501	ADP	O3B-PB-O3A	2.14	111.80	104.64
14	D	501	ADP	C5-C6-N1	2.11	122.88	117.51
14	D	501	ADP	N3-C4-N9	2.11	130.75	127.17
14	G	1601	ADP	C2-N1-C6	-2.10	115.28	118.73
14	C	501	ADP	C5-C6-N1	2.07	122.78	117.51
13	A	501	ATP	C6-C5-N7	-2.07	128.10	132.09
14	G	1601	ADP	N3-C4-N9	2.07	130.68	127.17
14	C	501	ADP	C6-C5-N7	-2.06	128.12	132.09
14	B	501	ADP	C5-C6-N1	2.05	122.71	117.51
13	A	501	ATP	C5-C6-N1	2.03	122.68	117.51
14	E	501	ADP	O3A-PA-O1A	2.01	116.75	110.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

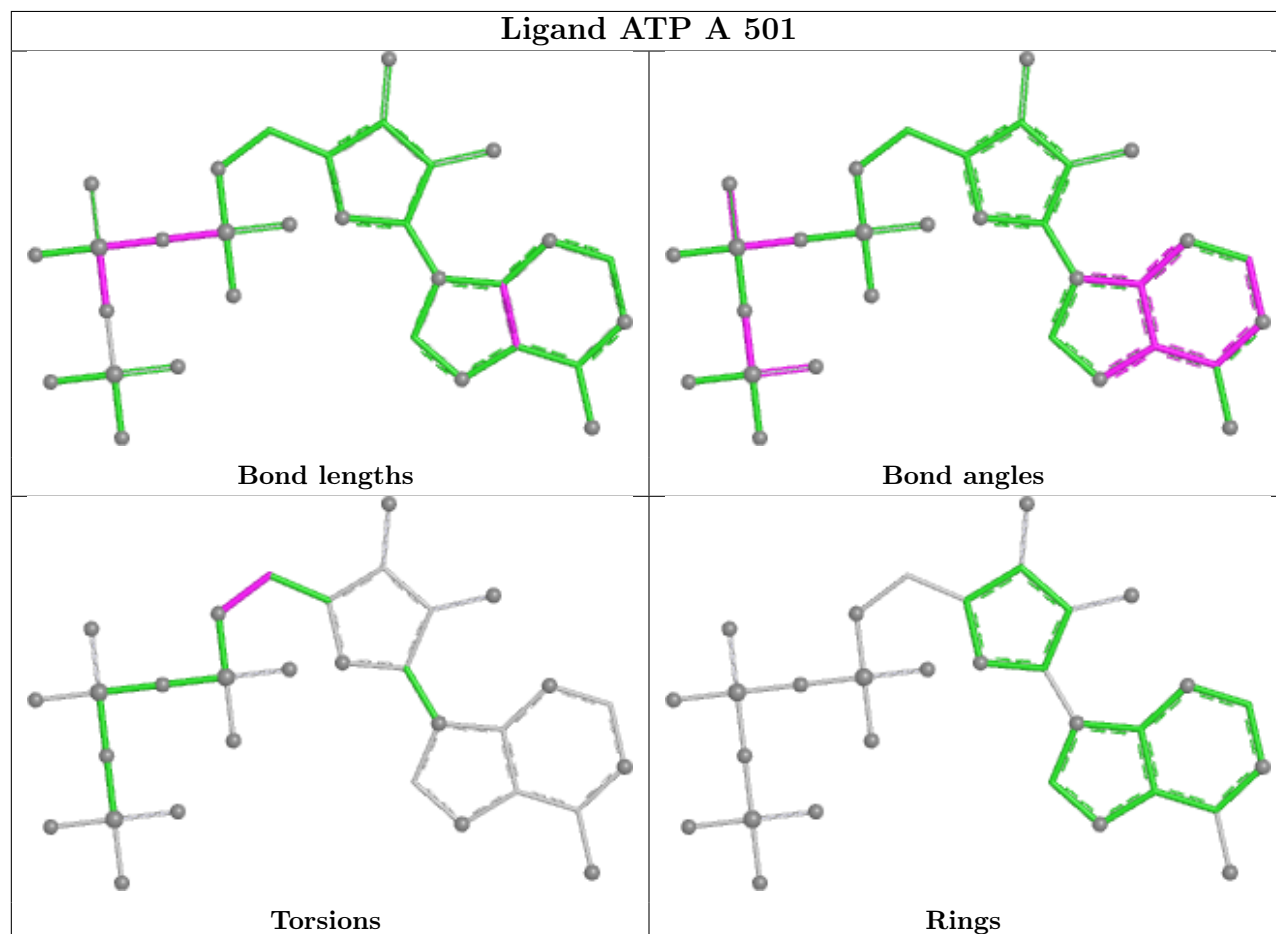
Mol	Chain	Res	Type	Atoms
14	G	1601	ADP	C5'-O5'-PA-O1A
14	J	701	ADP	O4'-C4'-C5'-O5'
14	J	701	ADP	C4'-C5'-O5'-PA
14	J	701	ADP	C3'-C4'-C5'-O5'
14	D	501	ADP	O4'-C4'-C5'-O5'
14	D	501	ADP	C3'-C4'-C5'-O5'
14	G	1601	ADP	PA-O3A-PB-O2B
14	G	1601	ADP	PA-O3A-PB-O3B
14	D	501	ADP	C4'-C5'-O5'-PA
13	A	501	ATP	C4'-C5'-O5'-PA
14	E	501	ADP	PA-O3A-PB-O2B
14	E	501	ADP	PA-O3A-PB-O3B
14	B	501	ADP	C4'-C5'-O5'-PA
14	C	501	ADP	PB-O3A-PA-O1A

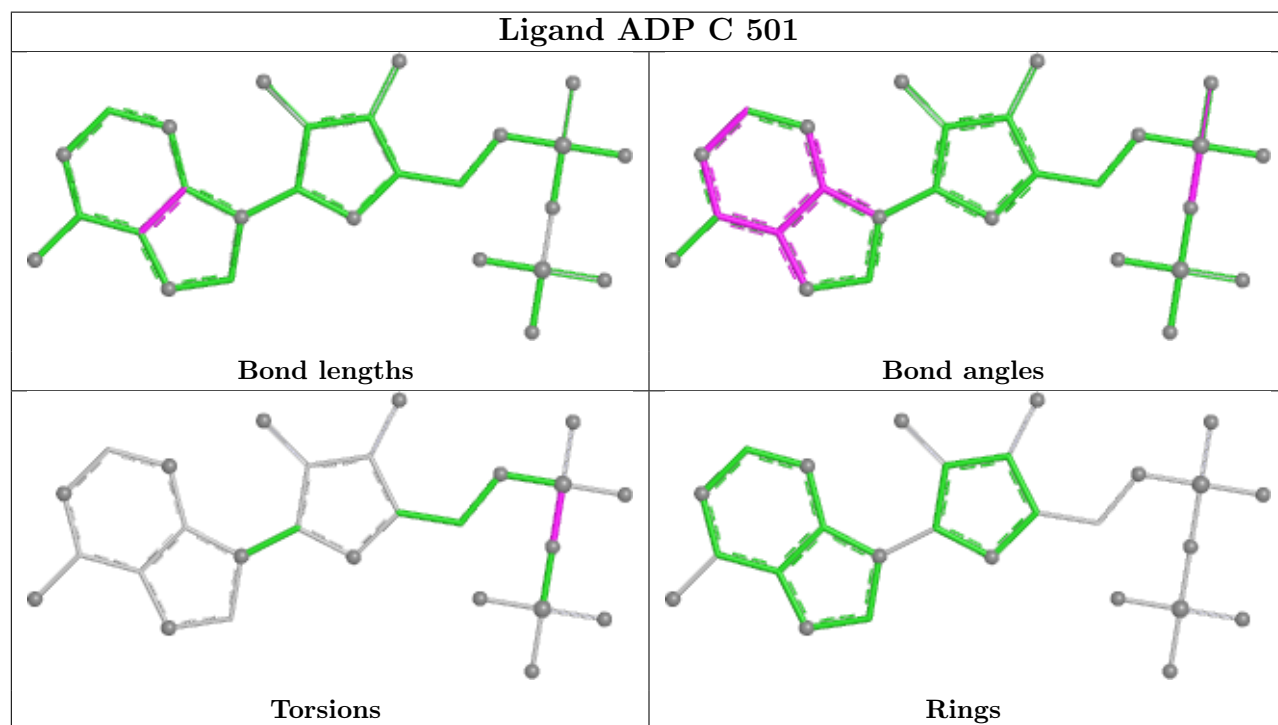
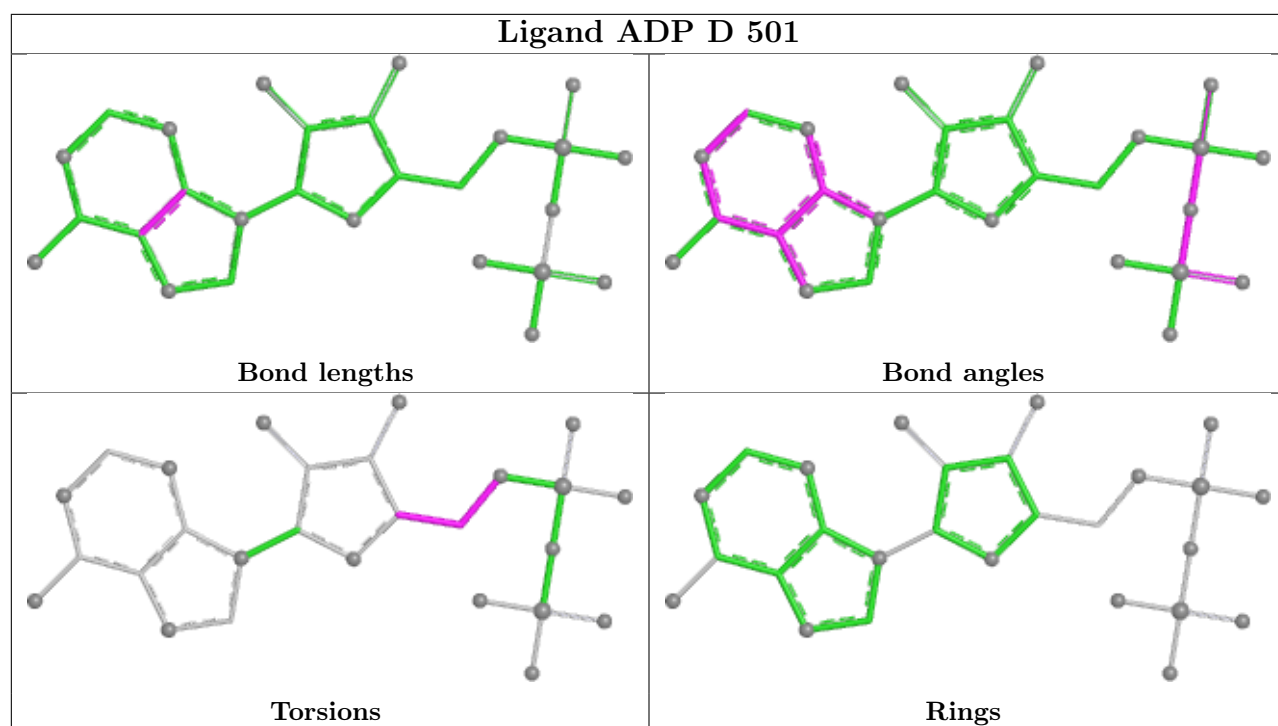
There are no ring outliers.

No monomer is involved in short contacts.

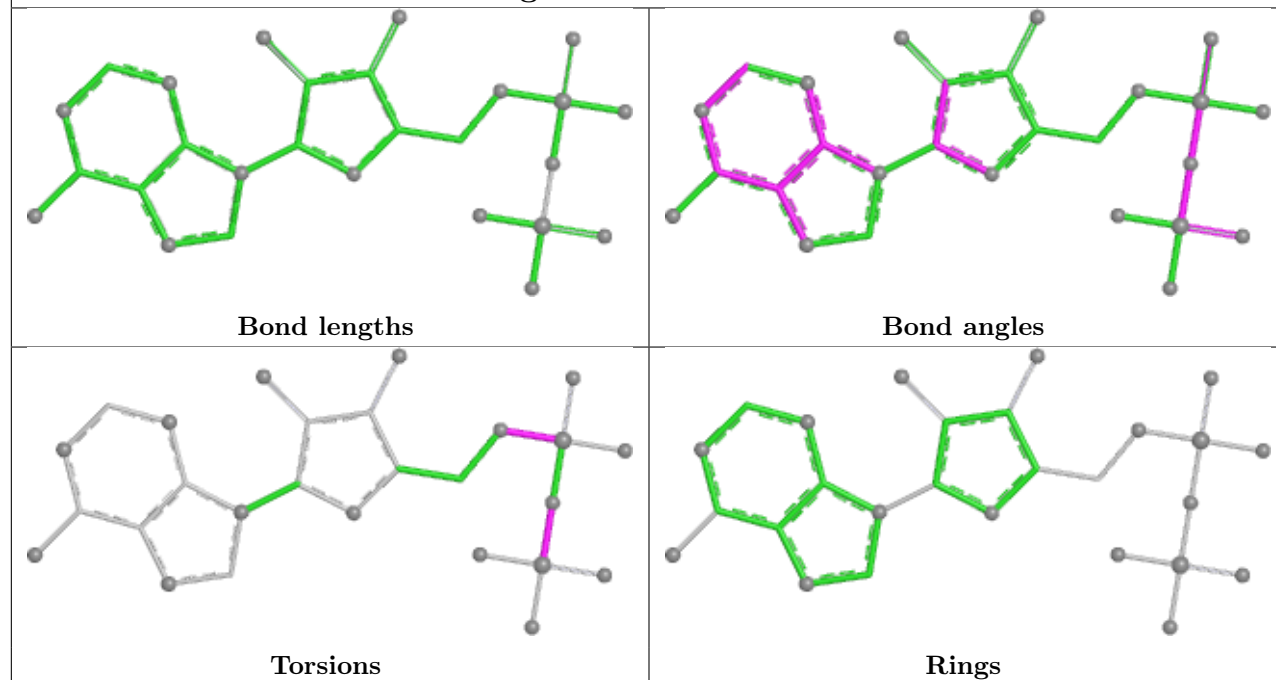
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

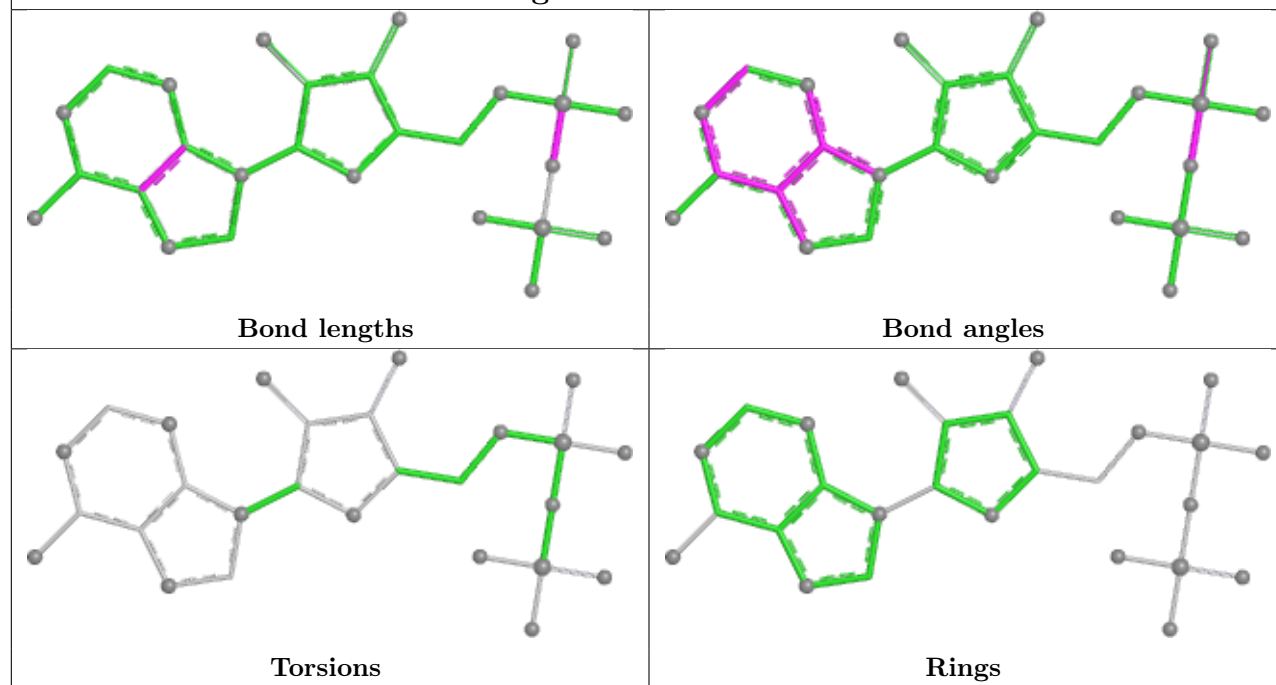




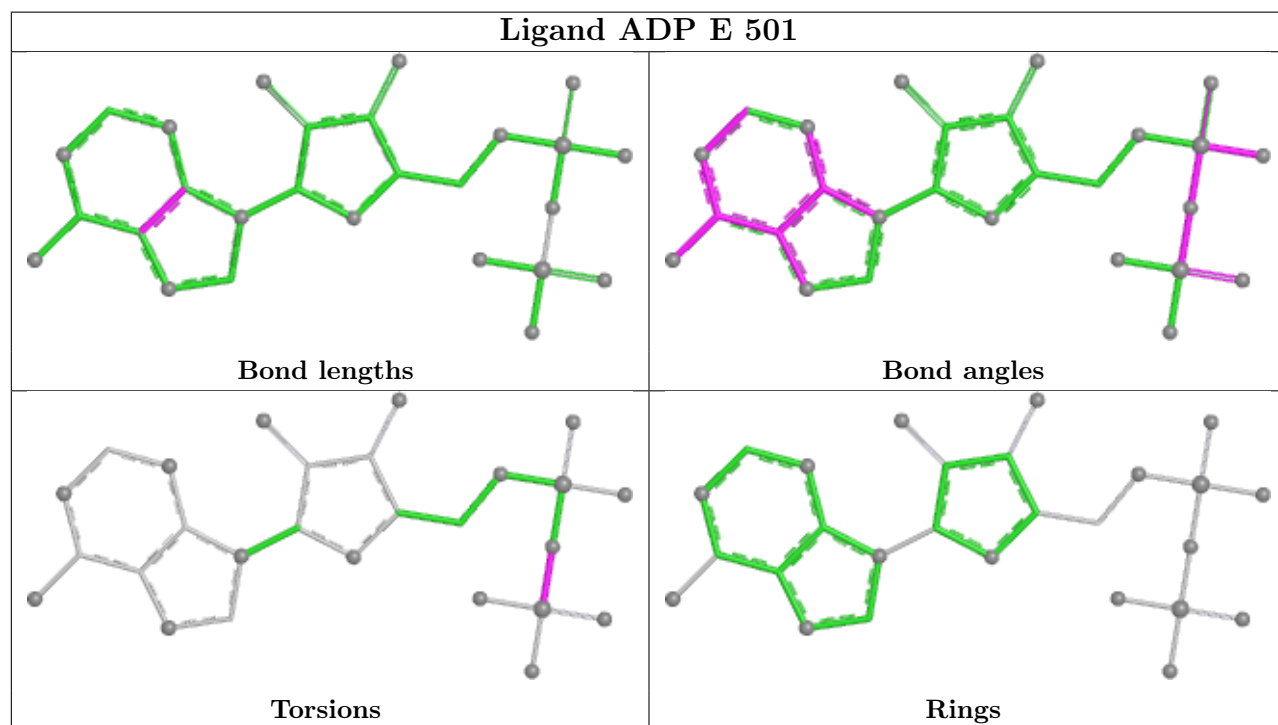
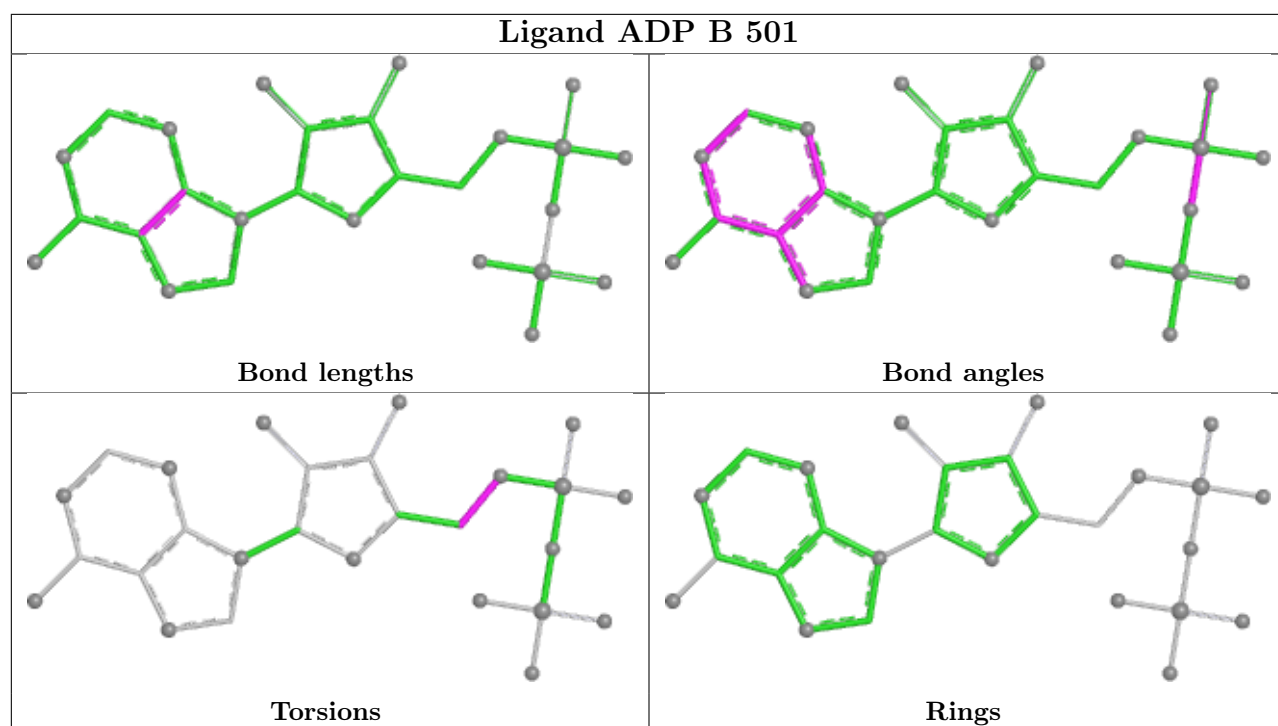
## Ligand ADP G 1601

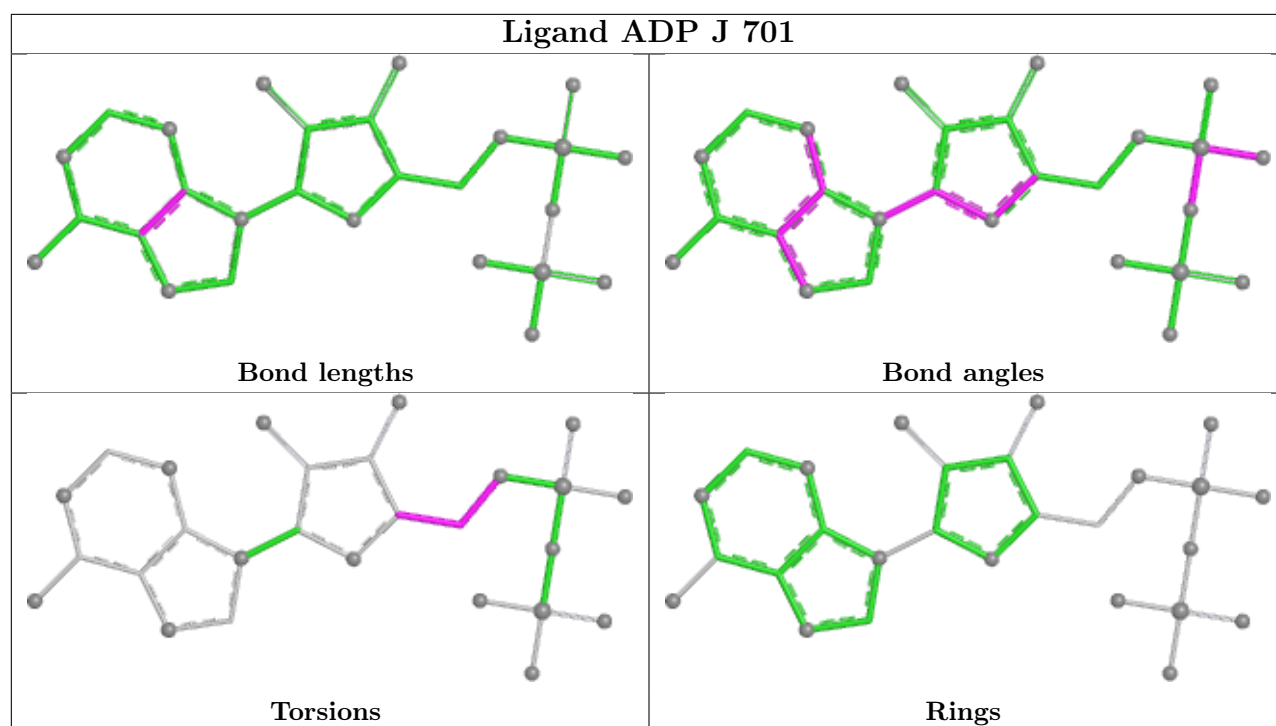


## Ligand ADP F 501









## 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.

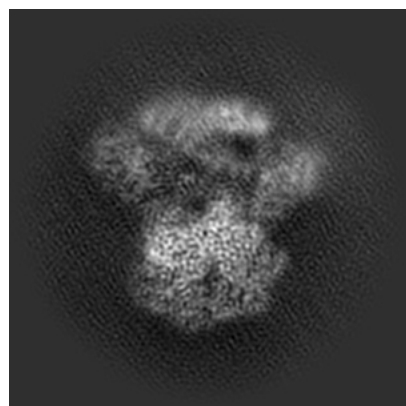
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51290. These allow visual inspection of the internal detail of the map and identification of artifacts.

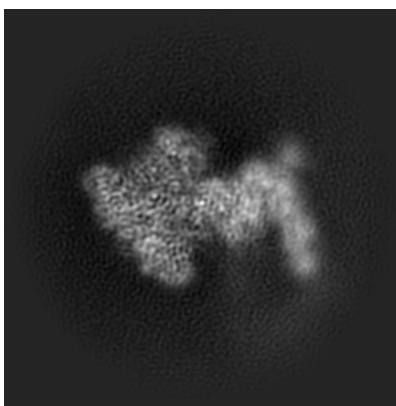
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

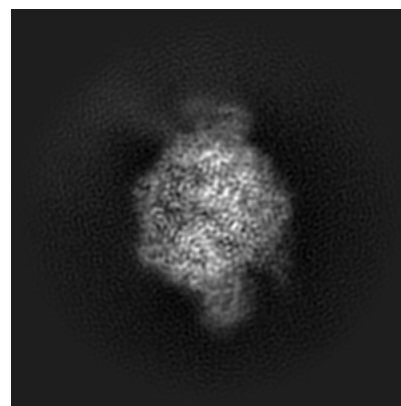
#### 6.1.1 Primary map



X

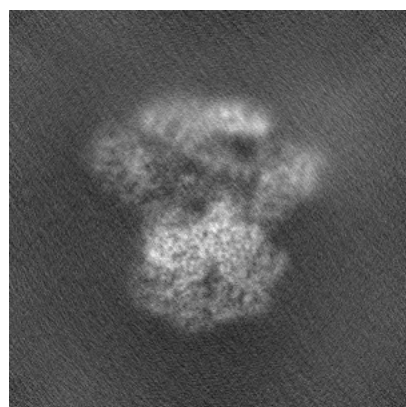


Y

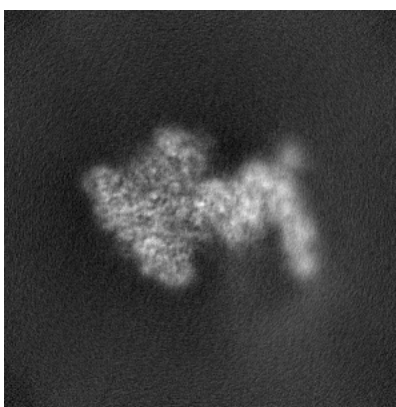


Z

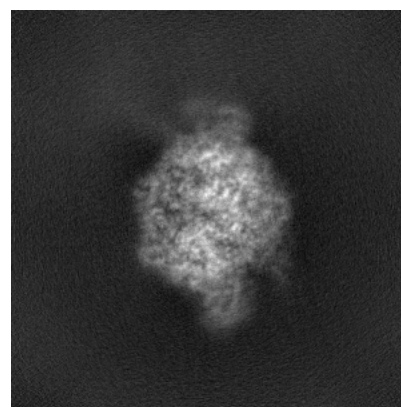
#### 6.1.2 Raw map



X



Y

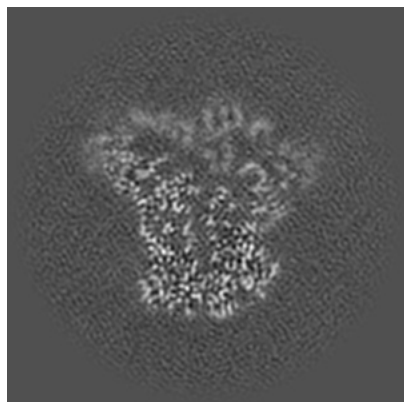


Z

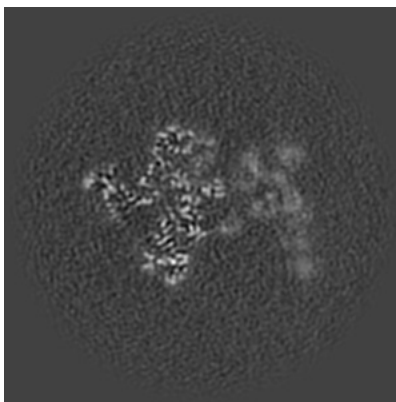
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

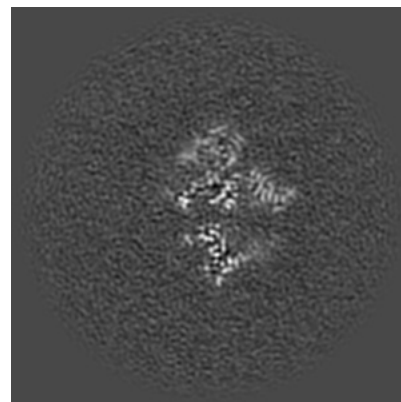
### 6.2.1 Primary map



X Index: 200

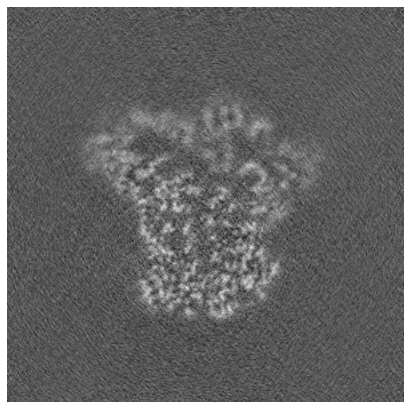


Y Index: 200

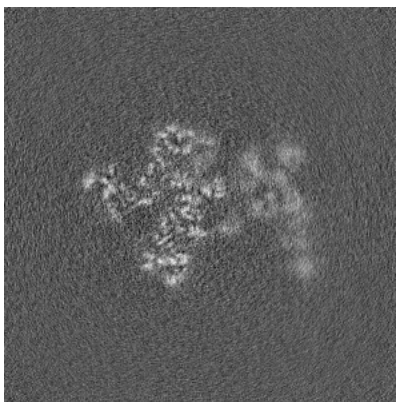


Z Index: 200

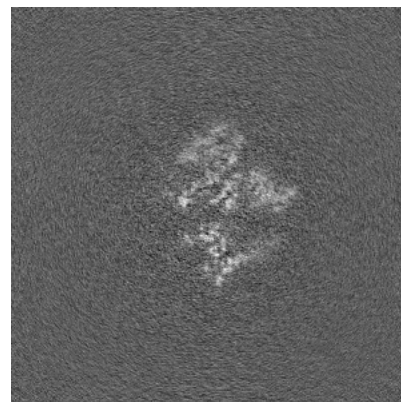
### 6.2.2 Raw map



X Index: 200



Y Index: 200

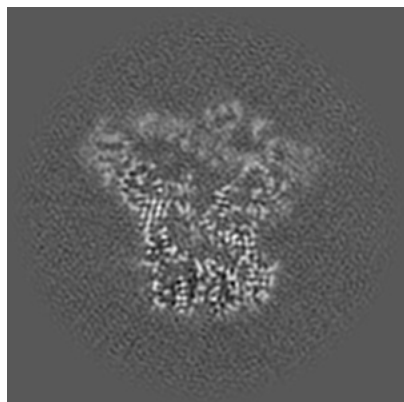


Z Index: 200

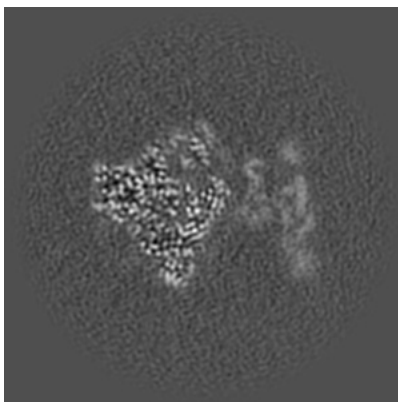
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

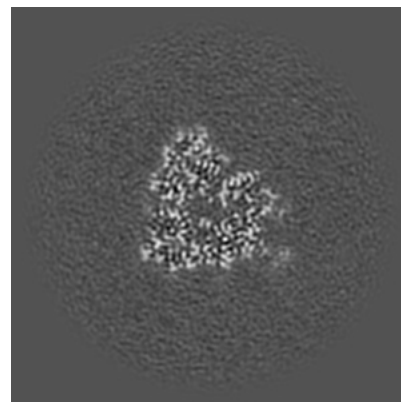
### 6.3.1 Primary map



X Index: 206

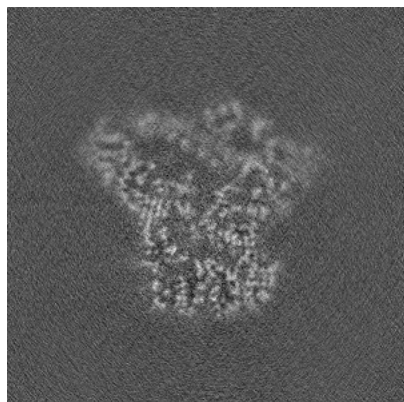


Y Index: 215

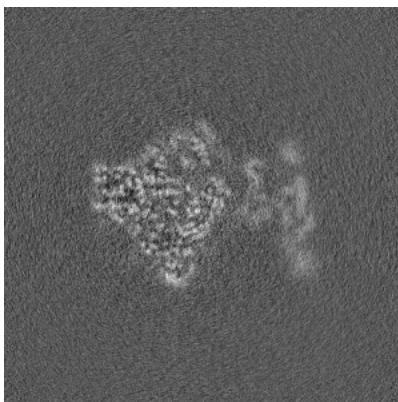


Z Index: 150

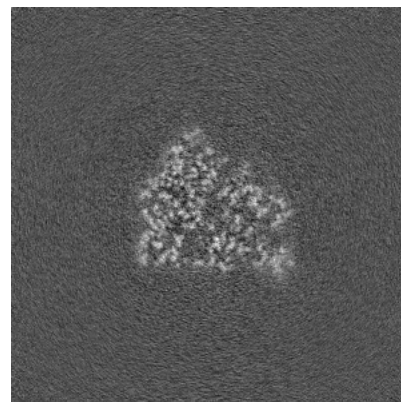
### 6.3.2 Raw map



X Index: 206



Y Index: 215



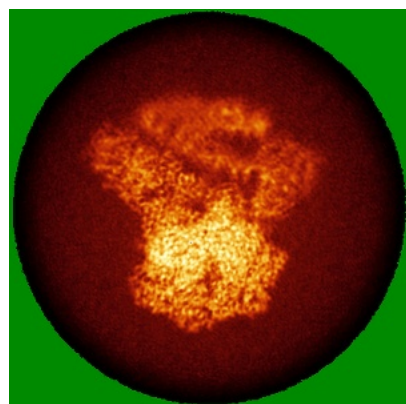
Z Index: 157

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

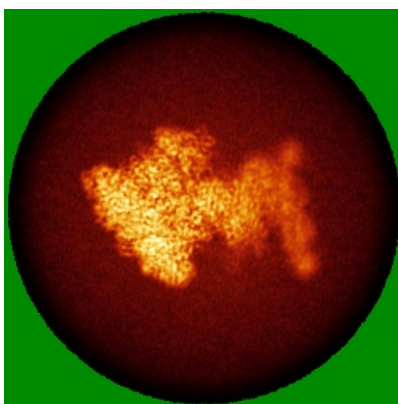


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

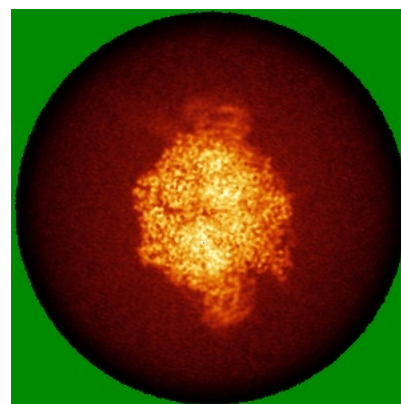
### 6.4.1 Primary map



X

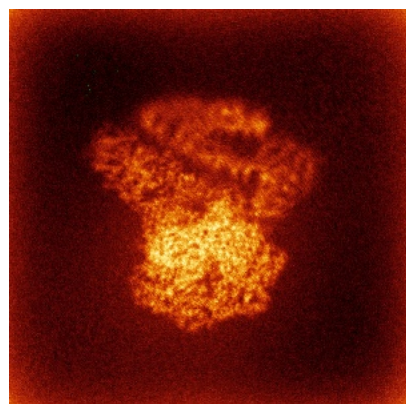


Y

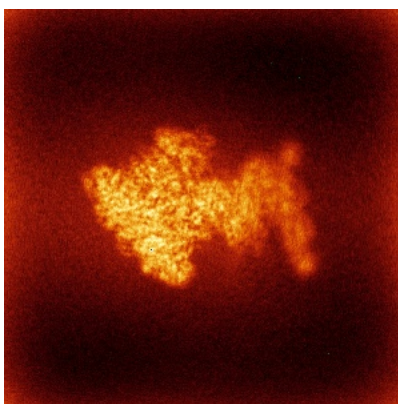


Z

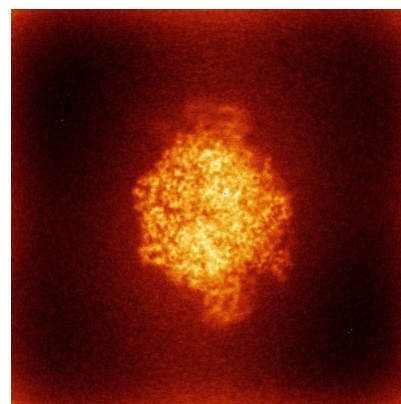
### 6.4.2 Raw map



X



Y

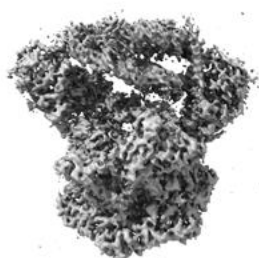


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



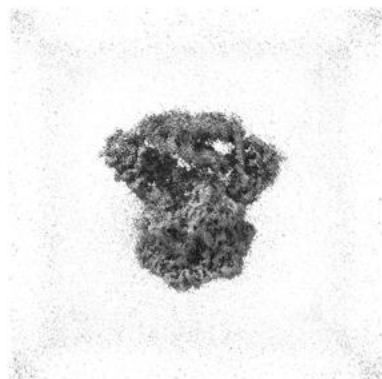
Y



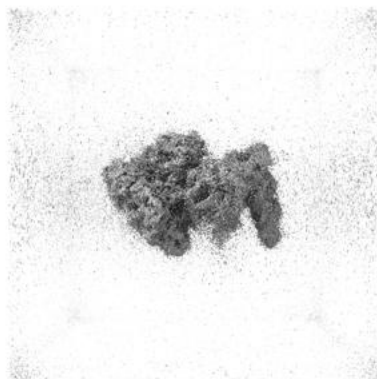
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

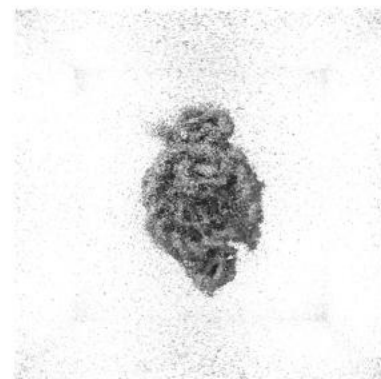
### 6.5.2 Raw map



X



Y



Z

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

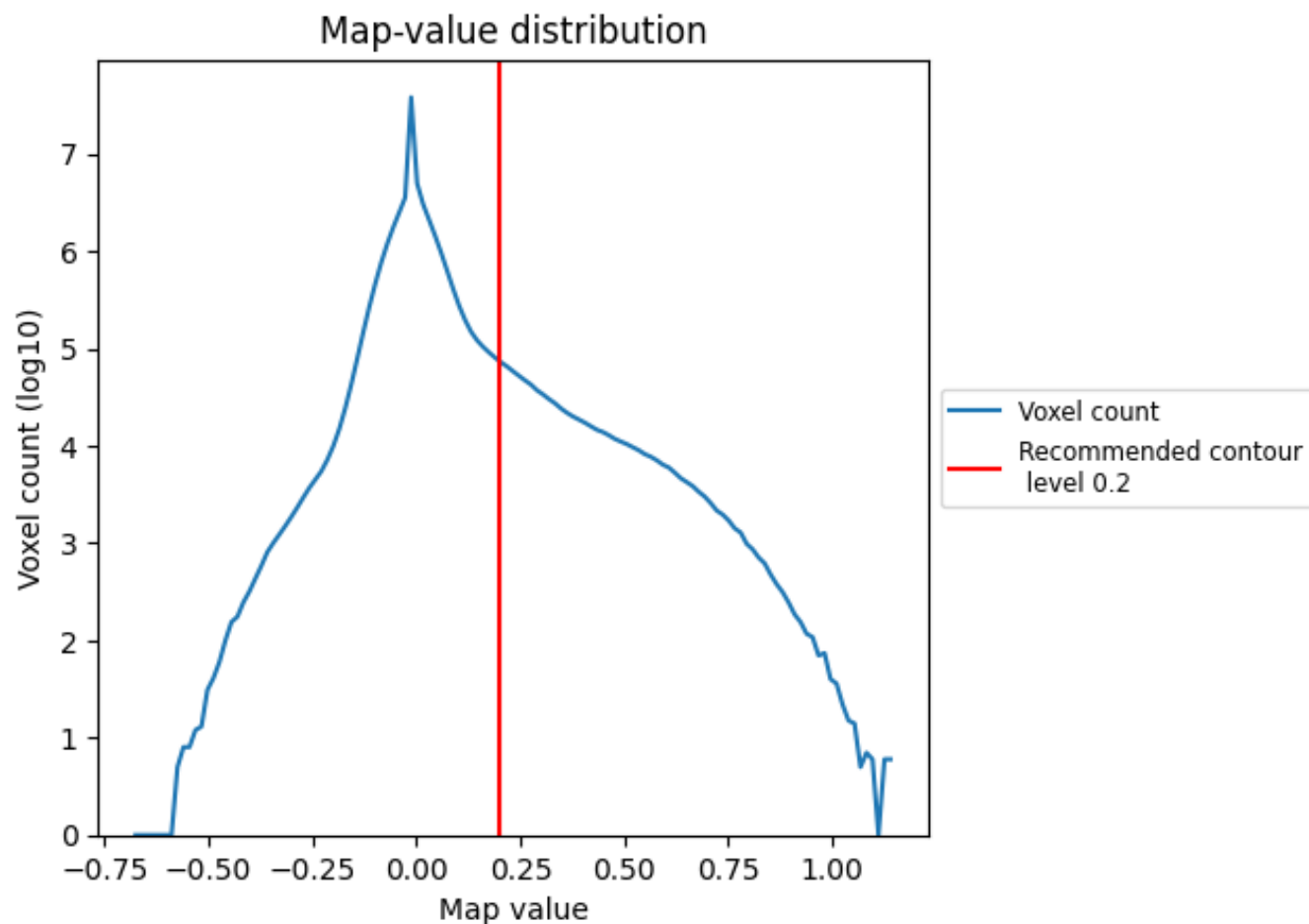
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

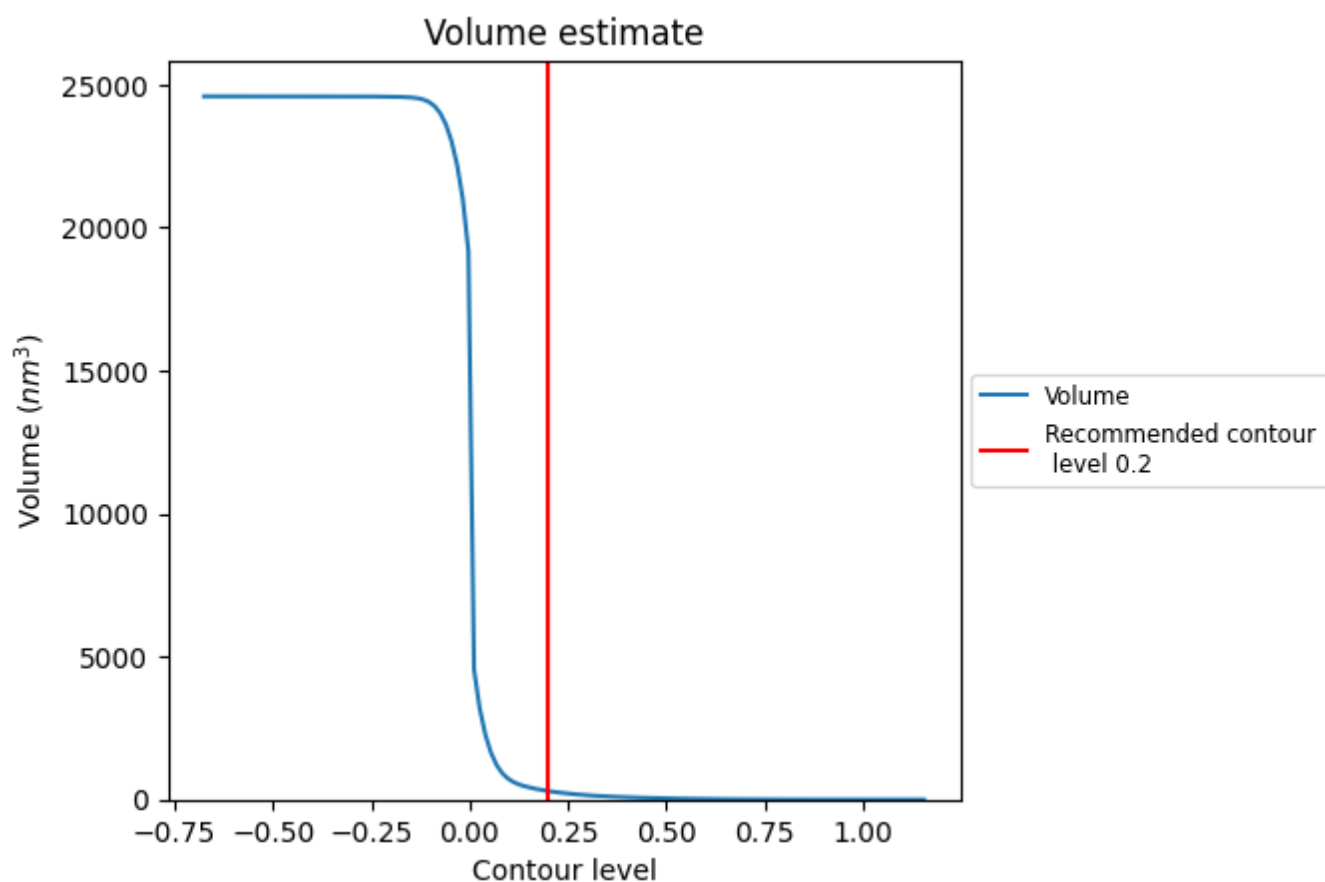
### 7.1 Map-value distribution [i](#)



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.



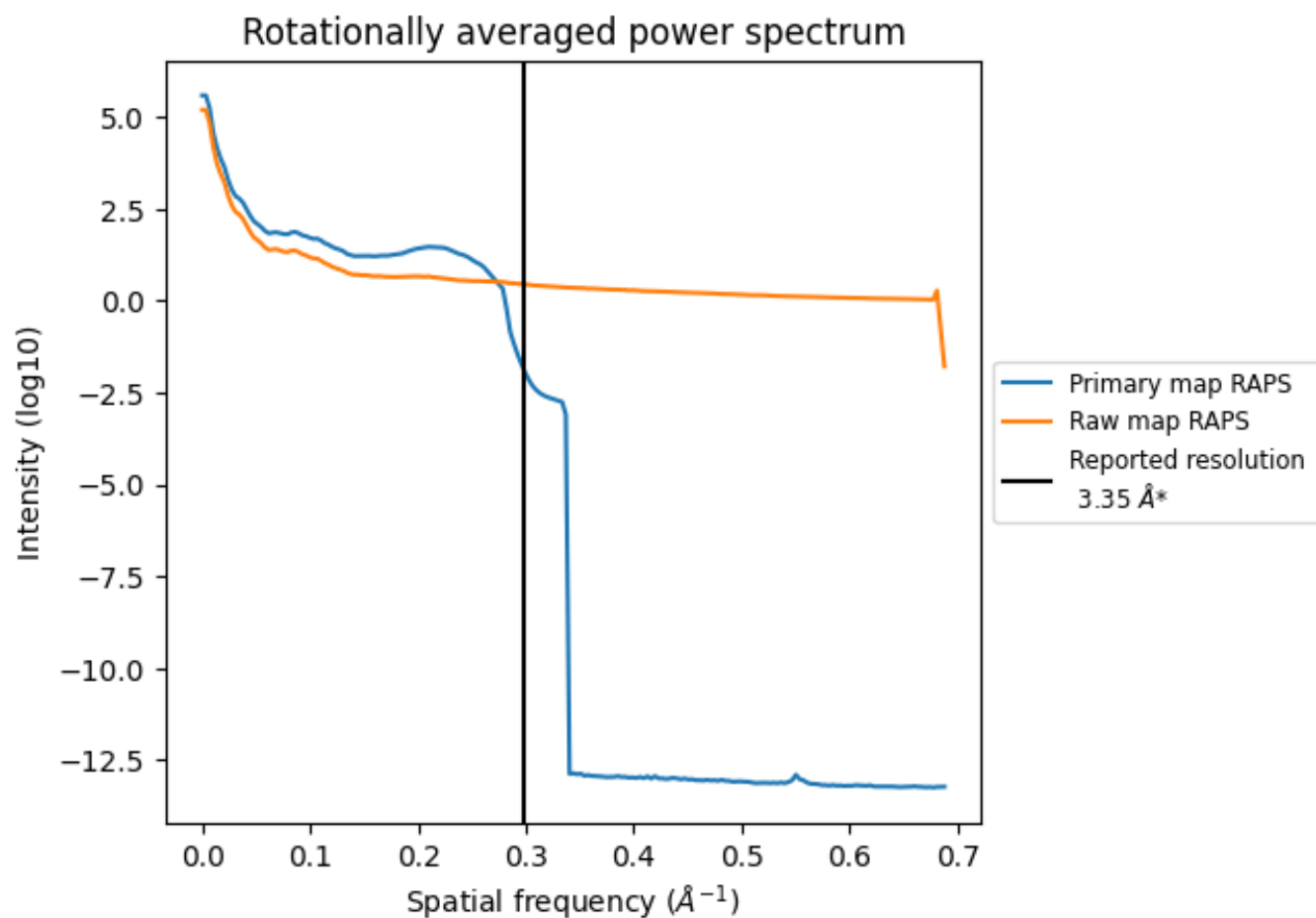
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm<sup>3</sup>; this corresponds to an approximate mass of 268 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 ⓘ

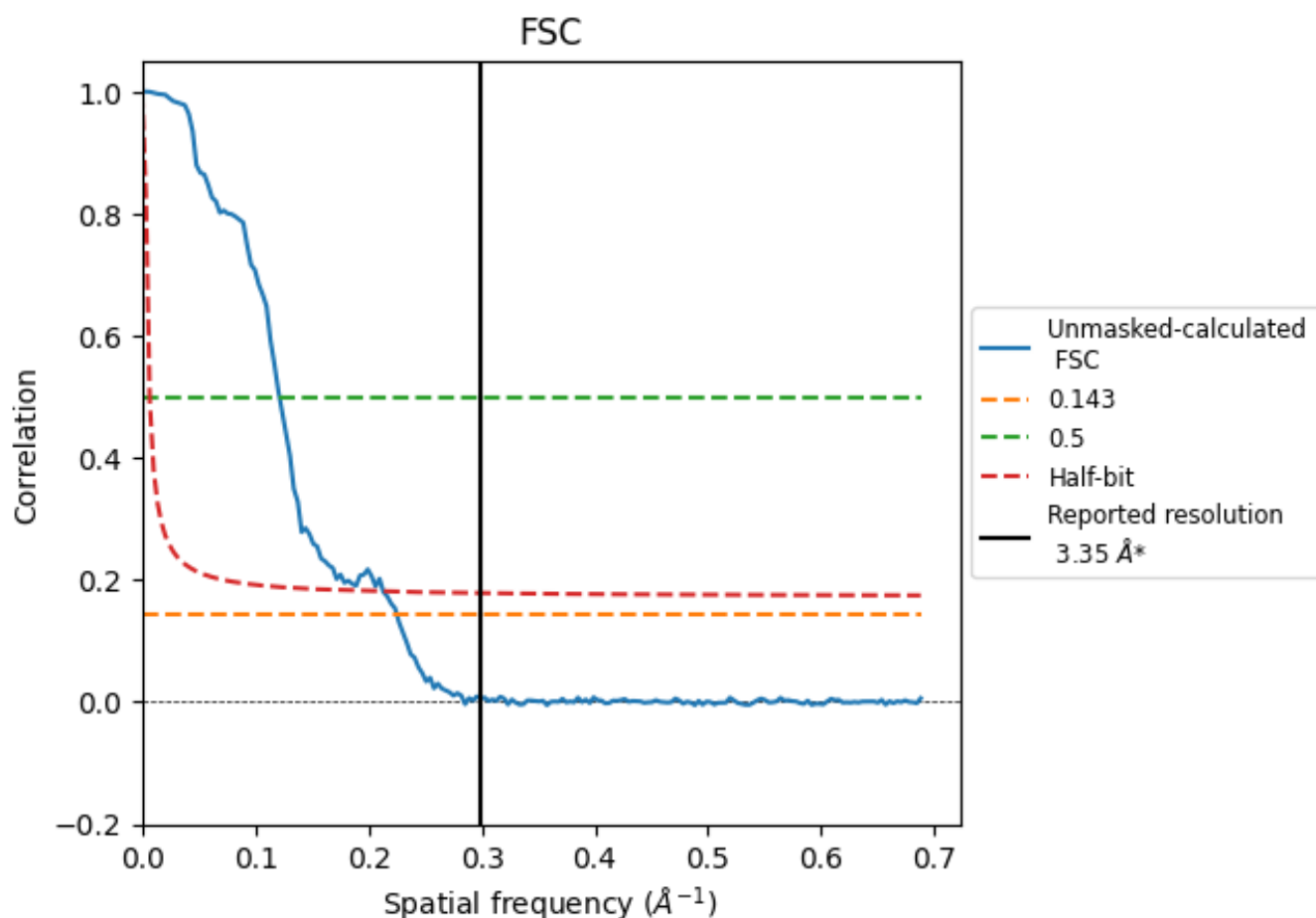


\*Reported resolution corresponds to spatial frequency of 0.299  $\text{\AA}^{-1}$

## 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 0.299  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

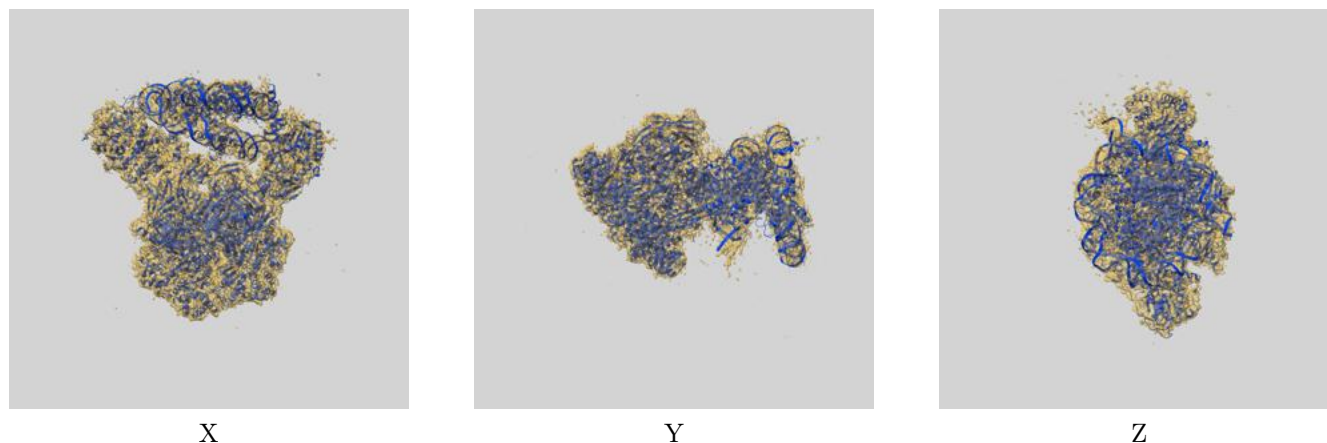
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	8.24	4.69

\*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 4.44 differs from the reported value 3.35 by more than 10 %

## 9 Map-model fit [i](#)

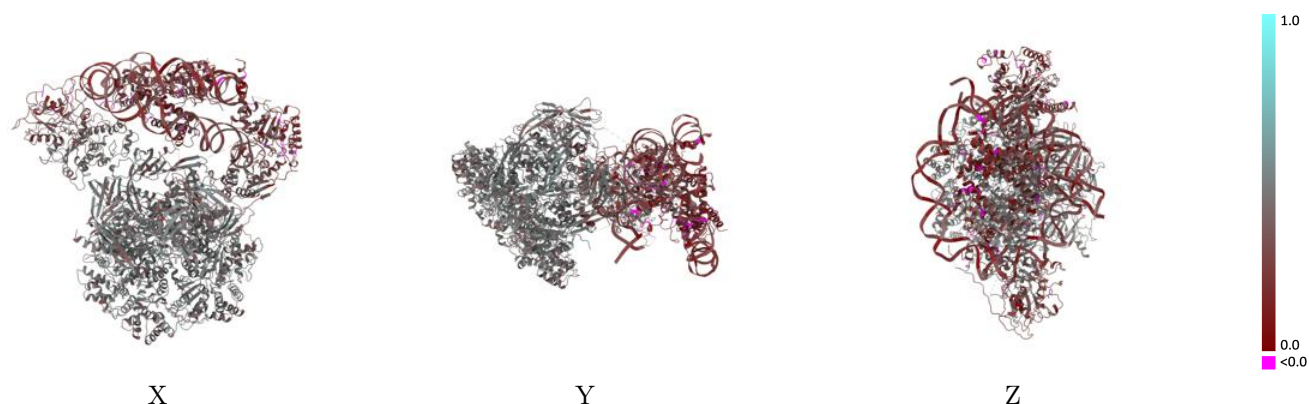
This section contains information regarding the fit between EMDB map EMD-51290 and PDB model 9GE5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



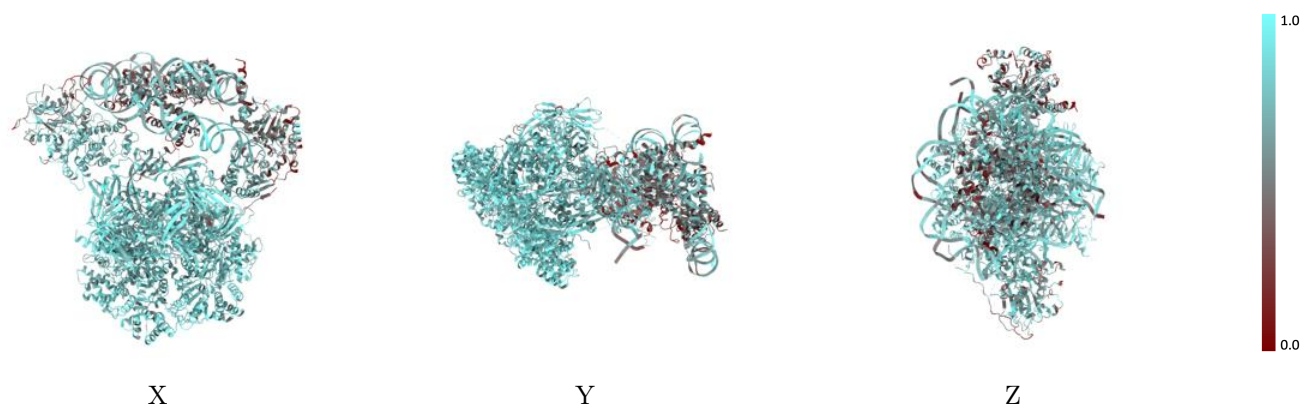
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



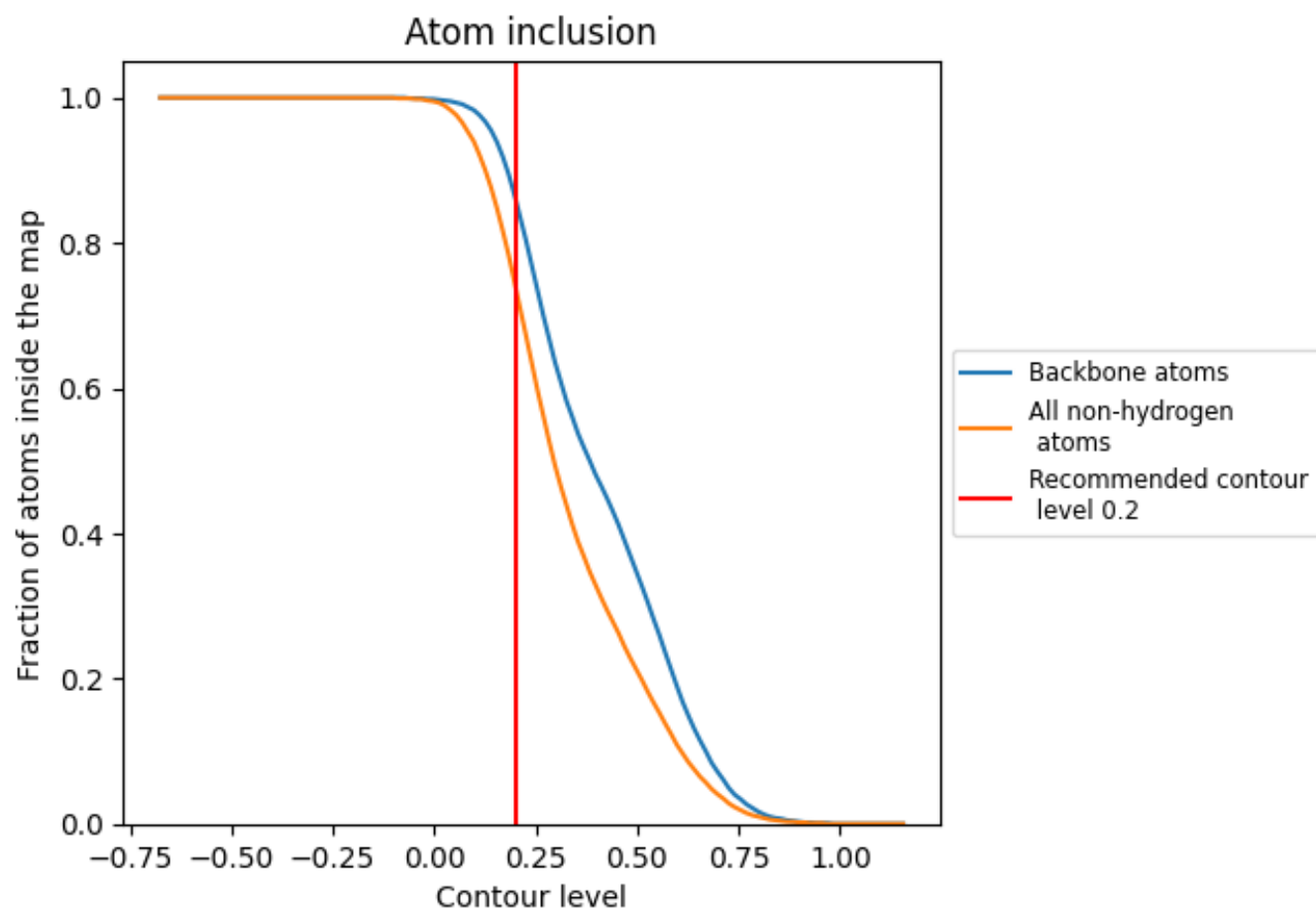
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 74% 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	 0.7400	 0.3850
A	 0.8550	 0.4740
B	 0.8280	 0.4630
C	 0.8250	 0.4580
D	 0.8350	 0.4660
E	 0.8280	 0.4590
F	 0.8350	 0.4670
G	 0.6800	 0.3660
H	 0.7220	 0.3600
I	 0.6660	 0.3710
J	 0.7020	 0.3610
K	 0.7110	 0.2440
L	 0.6820	 0.2360
M	 0.5240	 0.2440
N	 0.4680	 0.2530
Q	 0.3750	 0.1990
R	 0.4320	 0.2090
S	 0.4970	 0.2110
T	 0.4770	 0.2020

