



## Full wwPDB EM Validation Report ⓘ

Jul 10, 2025 – 12:53 PM EDT

PDB ID : 9C9G / pdb\_00009c9g  
EMDB ID : EMD-45361  
Title : S.c INO80 in complex with S.c 0/80 nucleosome  
Authors : Wu, H.; Kaur, U.; Narlikar, G.J.; Cheng, Y.F.  
Deposited on : 2024-06-13  
Resolution : 2.91 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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

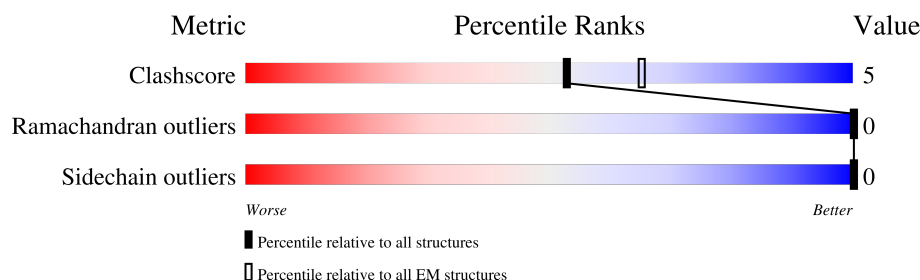
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.91 Å.

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















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	136	
1	E	136	
2	C	132	
2	G	132	
3	D	131	
3	H	131	
4	Q	1489	
5	R	755	

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Mol	Chain	Length	Quality of chain
6	S	166	
7	T	463	
7	V	463	
7	X	463	
8	U	471	
8	W	471	
8	Y	471	
9	Z	320	
10	B	103	
10	F	103	
11	J	227	
12	I	227	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 43020 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 Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	95	Total	C	N	O	0	0
			784	497	151	136		
1	E	95	Total	C	N	O	0	0
			784	497	151	136		

- Molecule 2 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	104	Total	C	N	O	0	0
			804	505	158	141		
2	G	104	Total	C	N	O	0	0
			795	496	157	142		

- Molecule 3 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	93	Total	C	N	O	S	0	0
			722	454	127	140	1		
3	H	93	Total	C	N	O	S	0	0
			726	456	127	142	1		

- Molecule 4 is a protein called Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	660	Total	C	N	O	S	0	0
			5289	3383	903	979	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	552	Total	C	N	O	S	0	0
			4097	2590	708	788	11		

- Molecule 6 is a protein called Chromatin-remodeling complex subunit IES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	125	Total	C	N	O	S	0	0
			1014	647	189	176	2		

- Molecule 7 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	435	Total	C	N	O	S	0	0
			3339	2107	575	647	10		
7	V	443	Total	C	N	O	S	0	0
			3404	2149	585	660	10		
7	X	442	Total	C	N	O	S	0	0
			3397	2144	584	659	10		

- Molecule 8 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	436	Total	C	N	O	S	0	0
			3350	2098	583	658	11		
8	W	442	Total	C	N	O	S	0	0
			3398	2123	590	673	12		
8	Y	445	Total	C	N	O	S	0	0
			3418	2136	594	677	11		

- Molecule 9 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	57	Total	C	N	O	S	0	0
			392	244	74	72	2		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	79	Total	C	N	O	S	0	0
			621	391	121	108	1		
10	F	79	Total	C	N	O	S	0	0
			620	389	120	110	1		

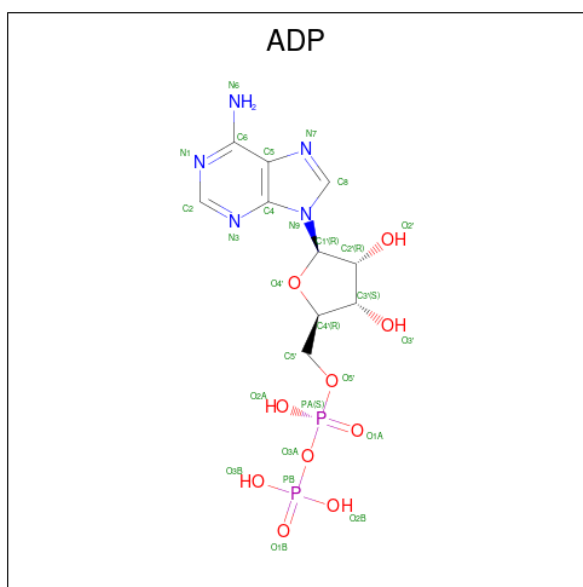
- Molecule 11 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	144	Total	C	N	O	P	0	0
			2969	1405	557	863	144		

- Molecule 12 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	144	Total	C	N	O	P	0	0
			2935	1394	532	865	144		

- Molecule 13 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>) (labeled as "Ligand of Interest" by depositor).

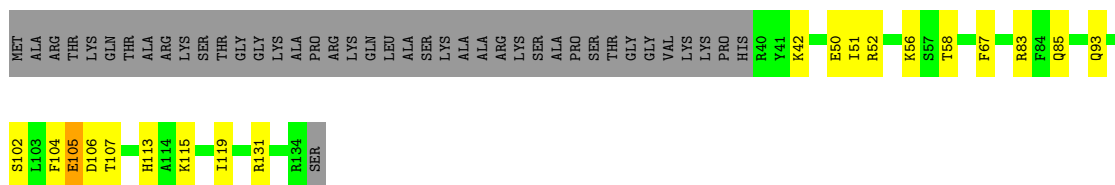


### 3 Residue-property plots [i](#)

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.

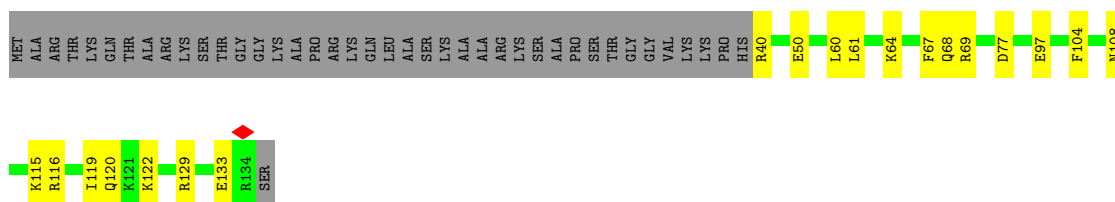
#### • Molecule 1: Histone H3

Chain A: 



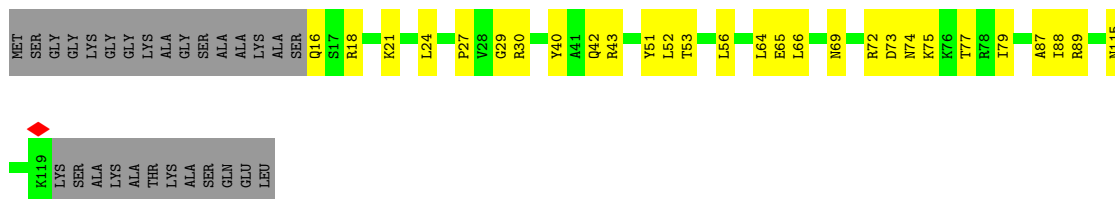
#### • Molecule 1: Histone H3

Chain E: 



#### • Molecule 2: Histone H2A.1

Chain C: 

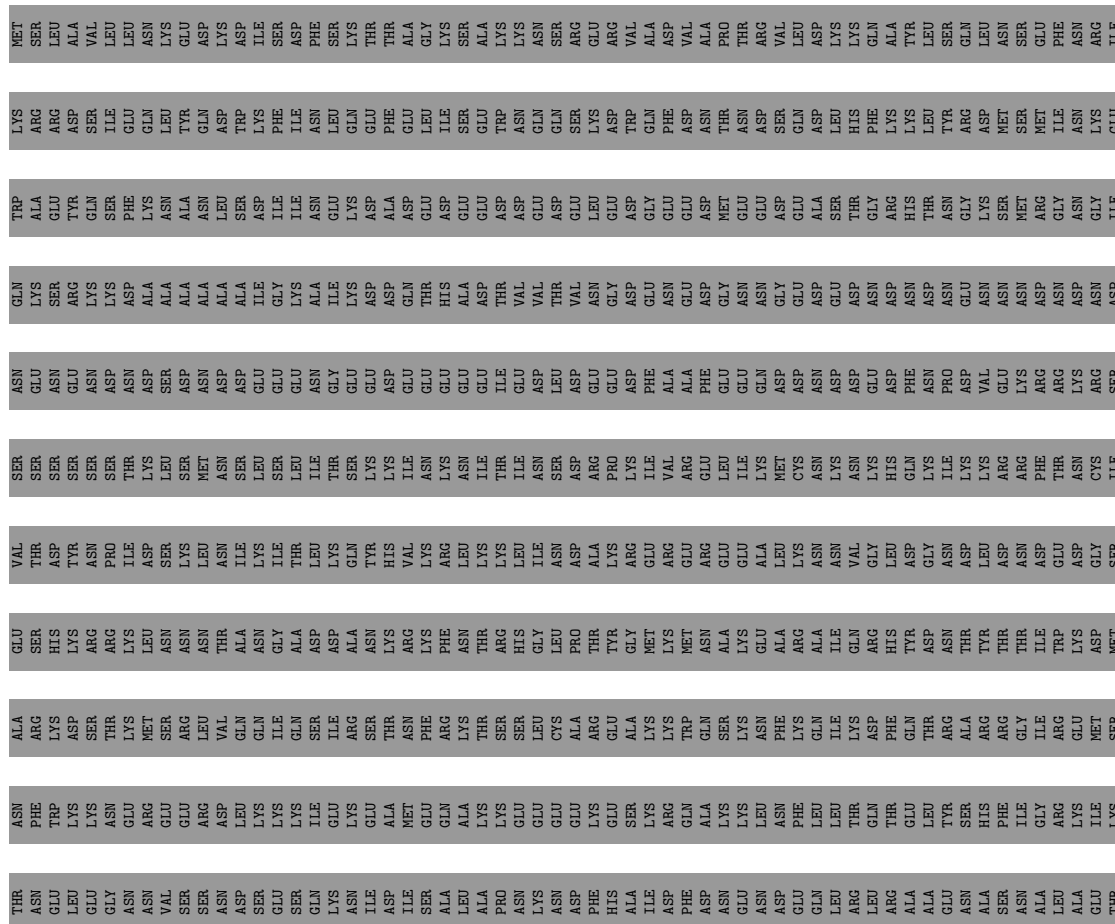
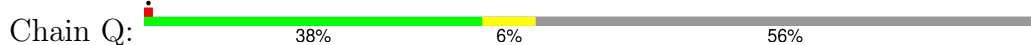
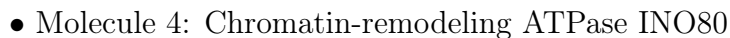


#### • Molecule 2: Histone H2A.1

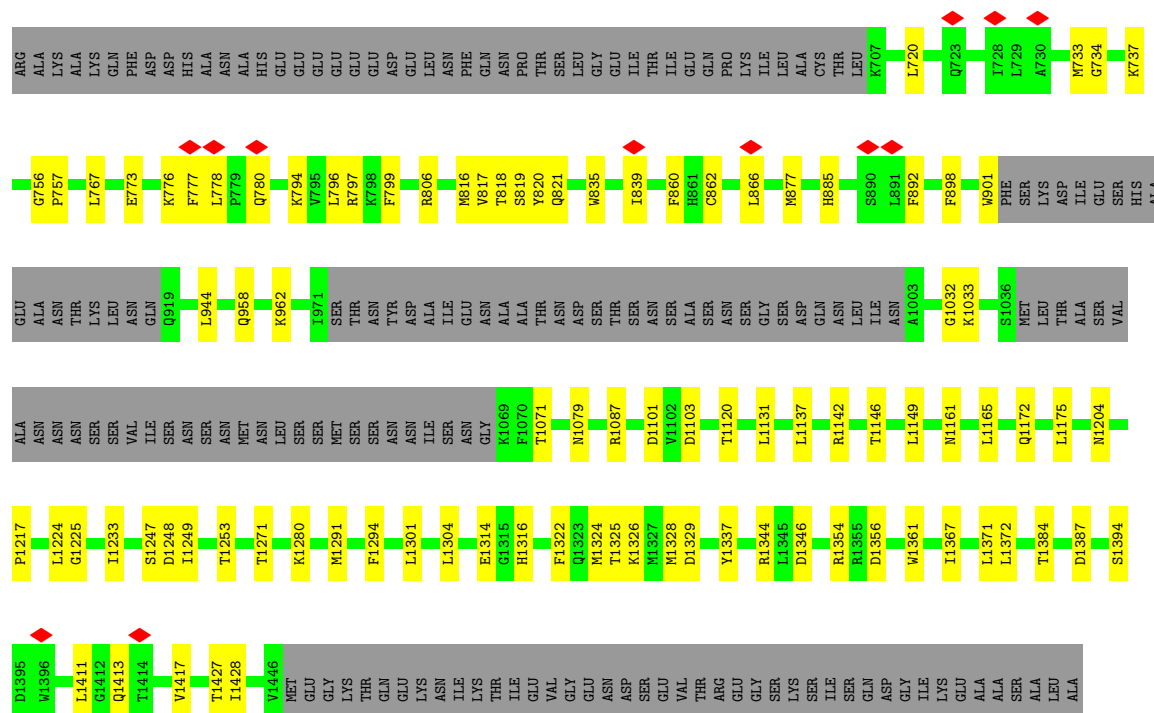
Chain G: 



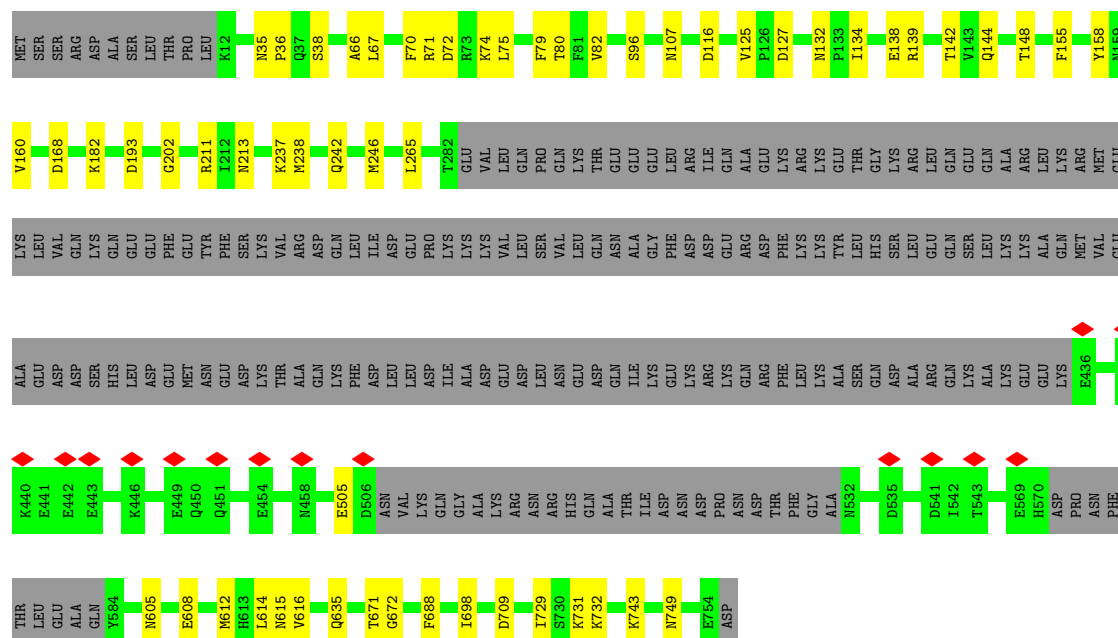
Chain D:  50% 19% . 29%





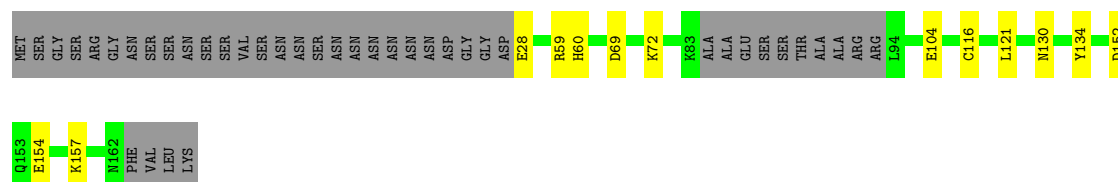


• Molecule 5: Actin-related protein 5



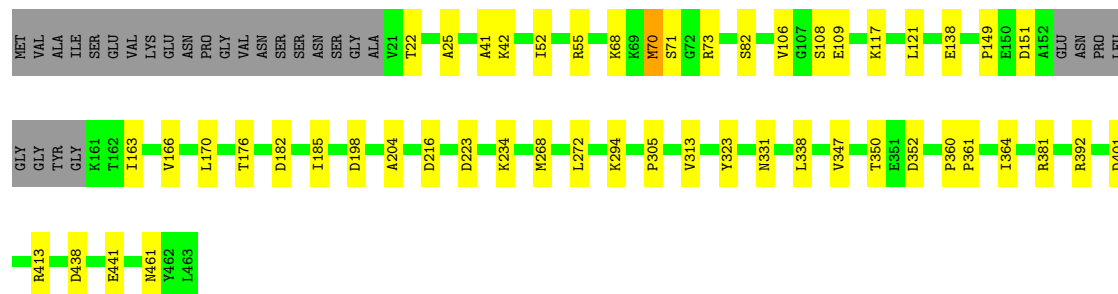
• Molecule 6: Chromatin-remodeling complex subunit IES6





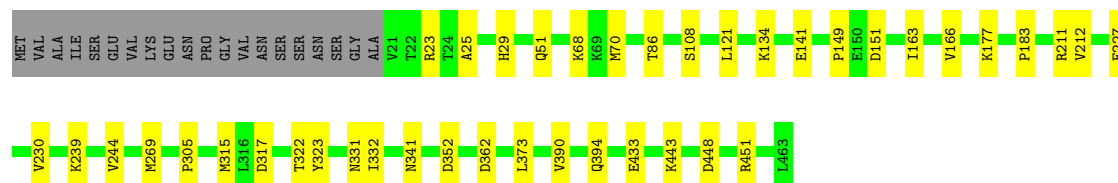
• Molecule 7: RuvB-like protein 1

Chain T: 83% 11% 6%



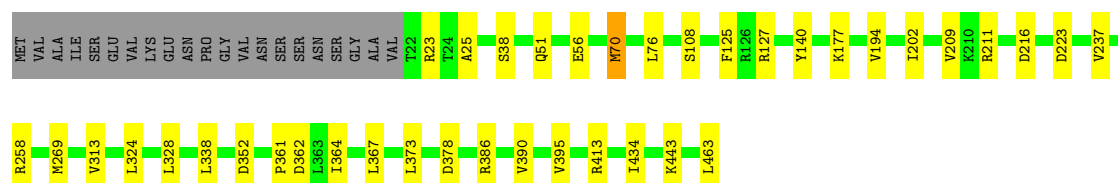
• Molecule 7: RuvB-like protein 1

Chain V: 87% 9% 4%



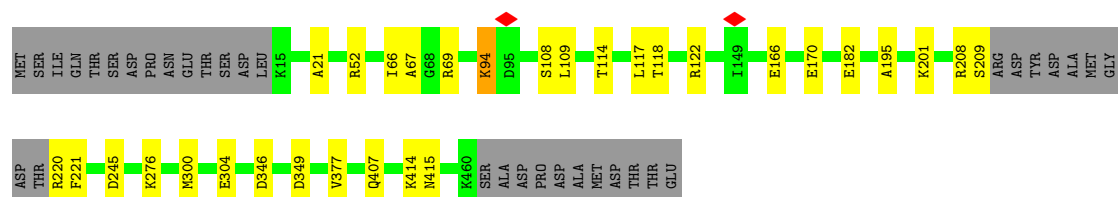
• Molecule 7: RuvB-like protein 1

Chain X: 87% 8% 5%



• Molecule 8: RuvB-like protein 2

Chain U: 86% 6% 7%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138910	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 ( $e^-/\text{\AA}^2$ )	45.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.304	Depositor
Minimum map value	-0.351	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.153	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.29	0/793	0.69	2/1060 (0.2%)
1	E	0.33	0/793	0.89	2/1060 (0.2%)
2	C	0.32	0/815	0.88	3/1102 (0.3%)
2	G	0.33	0/806	0.80	1/1091 (0.1%)
3	D	0.32	0/732	0.88	4/986 (0.4%)
3	H	0.39	0/736	0.98	2/991 (0.2%)
4	Q	0.23	0/5408	0.52	4/7340 (0.1%)
5	R	0.20	0/4186	0.39	1/5711 (0.0%)
6	S	0.27	0/1036	0.60	0/1392
7	T	0.24	0/3378	0.46	3/4569 (0.1%)
7	V	0.24	0/3446	0.45	2/4662 (0.0%)
7	X	0.24	0/3439	0.46	2/4652 (0.0%)
8	U	0.24	0/3386	0.46	1/4561 (0.0%)
8	W	0.24	0/3436	0.40	1/4632 (0.0%)
8	Y	0.24	0/3456	0.42	0/4659
9	Z	0.20	0/397	0.47	0/536
10	B	0.30	0/628	0.84	1/840 (0.1%)
10	F	0.35	0/627	0.98	2/840 (0.2%)
11	J	0.23	0/3334	0.44	0/5148
12	I	0.23	0/3288	0.43	0/5068
All	All	0.25	0/44120	0.52	31/60900 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	63	GLU	CA-CB-CG	6.90	127.90	114.10
1	A	105	GLU	CA-CB-CG	6.36	126.82	114.10
3	D	82	LYS	CA-CB-CG	6.32	126.74	114.10
8	U	94	LYS	CB-CG-CD	5.93	124.93	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	LYS	CA-CB-CG	5.92	125.94	114.10
3	D	88	LYS	CB-CG-CD	5.88	124.83	111.30
7	X	70	MET	CB-CG-SD	5.83	130.19	112.70
7	T	268	MET	CB-CG-SD	5.81	130.13	112.70
7	T	70	MET	CB-CG-SD	5.74	129.91	112.70
1	E	97	GLU	CA-CB-CG	5.73	125.56	114.10
3	D	65	LEU	CA-CB-CG	5.70	136.25	116.30
2	C	75	LYS	CA-CB-CG	5.70	125.50	114.10
10	F	67	ARG	CG-CD-NE	5.62	124.36	112.00
8	W	175	MET	CB-CG-SD	5.60	129.51	112.70
3	H	62	MET	CB-CG-SD	5.49	129.17	112.70
7	V	315	MET	CB-CG-SD	5.46	129.09	112.70
4	Q	806	ARG	CB-CA-C	-5.38	110.39	116.63
4	Q	816	MET	CB-CG-SD	5.35	128.74	112.70
3	H	37	LYS	CA-CB-CG	5.33	124.76	114.10
7	X	258	ARG	CA-CB-CG	5.28	124.66	114.10
5	R	125	VAL	CB-CA-C	5.27	117.26	111.04
10	B	90	LEU	CA-CB-CG	5.23	134.60	116.30
1	E	50	GLU	CA-CB-CG	5.21	124.51	114.10
2	G	75	LYS	CB-CG-CD	5.20	123.26	111.30
4	Q	720	LEU	CA-CB-CG	5.17	134.39	116.30
7	V	70	MET	CB-CG-SD	5.12	128.06	112.70
7	T	234	LYS	CA-CB-CG	5.11	124.33	114.10
4	Q	877	MET	CB-CG-SD	5.10	127.99	112.70
2	C	74	ASN	CA-C-N	5.05	131.19	121.54
2	C	74	ASN	C-N-CA	5.05	131.19	121.54
3	D	64	ILE	CA-CB-CG1	5.04	118.97	110.40

There are no chirality outliers.

There are no planarity outliers.

## 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	784	0	836	23	0
1	E	784	0	836	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	804	0	847	27	0
2	G	795	0	821	21	0
3	D	722	0	744	32	0
3	H	726	0	748	10	0
4	Q	5289	0	5195	77	0
5	R	4097	0	3678	36	0
6	S	1014	0	1050	11	0
7	T	3339	0	3468	37	0
7	V	3404	0	3540	30	0
7	X	3397	0	3533	30	0
8	U	3350	0	3444	25	0
8	W	3398	0	3470	32	0
8	Y	3418	0	3492	36	0
9	Z	392	0	303	3	0
10	B	621	0	652	12	0
10	F	620	0	643	22	0
11	J	2969	0	1616	29	0
12	I	2935	0	1617	17	0
13	T	27	0	12	0	0
13	U	27	0	12	0	0
13	V	27	0	12	1	0
13	W	27	0	12	4	0
13	X	27	0	12	0	0
13	Y	27	0	12	0	0
All	All	43020	0	40605	420	0

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

All (420) 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)
2:G:30:ARG:NH1	3:H:38:GLU:OE1	1.65	1.28
4:Q:767:LEU:HD22	4:Q:817:VAL:CG1	1.65	1.25
1:A:58:THR:HB	2:G:82:ARG:NH2	1.59	1.16
4:Q:1131:LEU:HD12	4:Q:1165:LEU:HD22	1.26	1.16
4:Q:767:LEU:CD2	4:Q:817:VAL:CG1	2.25	1.15
4:Q:767:LEU:HD22	4:Q:817:VAL:HG12	1.30	1.14
5:R:615:ASN:OD1	5:R:616:VAL:HG23	1.46	1.14
8:W:298:VAL:HG21	8:W:323:MET:HB3	1.21	1.12
4:Q:1131:LEU:CD1	4:Q:1165:LEU:HD22	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:ARG:NH1	3:H:38:GLU:CD	2.17	1.01
1:A:58:THR:HB	2:G:82:ARG:HH21	1.15	0.99
3:D:82:LYS:CD	3:D:86:TYR:HD2	1.85	0.90
2:G:89:ARG:NH1	2:G:95:ASN:OD1	2.05	0.90
5:R:615:ASN:OD1	5:R:616:VAL:N	2.05	0.89
2:C:79:ILE:CG2	3:D:57:ILE:HD13	2.03	0.89
7:T:313:VAL:HG21	7:T:338:LEU:HB3	1.53	0.89
3:D:82:LYS:HD3	3:D:86:TYR:CD2	2.12	0.84
8:W:298:VAL:HG21	8:W:323:MET:CB	2.06	0.83
1:E:67:PHE:HE2	10:F:62:LEU:HD11	1.43	0.83
2:C:79:ILE:HG22	3:D:57:ILE:HD13	1.61	0.82
8:Y:23:HIS:HD2	8:Y:86:MET:HG2	1.43	0.82
2:C:52:LEU:HD21	3:D:73:PHE:CE1	2.15	0.81
4:Q:1253:THR:HG23	7:V:151:ASP:OD1	1.81	0.80
7:V:86:THR:OG1	13:V:501:ADP:O1A	1.99	0.80
3:D:82:LYS:HD3	3:D:86:TYR:HD2	1.47	0.79
6:S:116:CYS:SG	6:S:134:TYR:HA	2.24	0.78
4:Q:767:LEU:HD22	4:Q:817:VAL:HG11	1.59	0.77
4:Q:767:LEU:CD2	4:Q:817:VAL:HG12	2.00	0.77
2:C:79:ILE:HG21	3:D:57:ILE:CD1	2.14	0.76
4:Q:767:LEU:CD2	4:Q:817:VAL:HG13	2.14	0.76
8:Y:23:HIS:CD2	8:Y:86:MET:HG2	2.21	0.76
1:A:58:THR:HB	2:G:82:ARG:CZ	2.16	0.75
10:F:66:ILE:O	10:F:70:VAL:HG23	1.87	0.74
3:D:83:LEU:O	3:D:87:ASN:HB2	1.86	0.74
4:Q:1322:PHE:CD2	4:Q:1328:MET:HG2	2.25	0.72
11:J:-4:DG:H1	12:I:4:DC:H42	1.38	0.71
2:C:79:ILE:CG2	3:D:57:ILE:CD1	2.69	0.71
11:J:59:DA:H61	12:I:-59:DT:H3	1.38	0.71
4:Q:1326:LYS:HA	4:Q:1329:ASP:HB2	1.73	0.69
4:Q:1280:LYS:NZ	7:V:227:GLU:OE1	2.25	0.69
3:D:82:LYS:HD2	3:D:86:TYR:HD2	1.59	0.68
1:E:108:ASN:HB2	10:F:43:VAL:HG22	1.76	0.67
5:R:615:ASN:OD1	5:R:616:VAL:CG2	2.36	0.67
1:E:67:PHE:CE2	10:F:62:LEU:HD11	2.28	0.66
8:W:298:VAL:CG2	8:W:323:MET:HB3	2.12	0.65
11:J:64:DG:H1	12:I:-64:DC:H42	1.42	0.65
6:S:154:GLU:HA	6:S:157:LYS:HB2	1.77	0.65
4:Q:1280:LYS:NZ	7:V:227:GLU:CD	2.56	0.63
4:Q:1325:THR:HG23	11:J:-61:DT:H5'	1.81	0.63
1:A:58:THR:OG1	2:G:82:ARG:NE	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:1322:PHE:CD2	4:Q:1328:MET:CG	2.82	0.62
3:D:79:GLU:O	3:D:83:LEU:HG	1.97	0.62
7:X:386:ARG:O	7:X:390:VAL:HG23	1.99	0.62
3:D:82:LYS:CD	3:D:86:TYR:CD2	2.71	0.62
1:A:52:ARG:O	1:A:56:LYS:HB2	1.99	0.62
1:E:116:ARG:HD3	11:J:-3:DA:H3'	1.82	0.61
10:F:78:ARG:HD3	12:I:28:DG:H5'	1.82	0.61
1:A:58:THR:O	1:A:58:THR:HG22	2.01	0.60
5:R:134:ILE:HG13	5:R:160:VAL:HG11	1.84	0.60
5:R:709:ASP:OD1	5:R:709:ASP:N	2.35	0.59
5:R:67:LEU:HD13	5:R:82:VAL:HG22	1.84	0.59
10:F:29:ILE:HG12	10:F:58:LEU:HD21	1.83	0.59
2:C:42:GLN:NE2	3:D:90:SER:OG	2.35	0.59
4:Q:1324:MET:HA	11:J:-61:DT:H4'	1.84	0.59
8:W:82:THR:OG1	13:W:501:ADP:O2A	2.18	0.58
2:C:52:LEU:HD21	3:D:73:PHE:CD1	2.38	0.58
4:Q:1253:THR:HG23	7:V:151:ASP:CG	2.29	0.57
2:C:40:TYR:HB3	3:D:81:SER:HB2	1.86	0.57
5:R:66:ALA:HB1	5:R:96:SER:HB2	1.87	0.57
3:D:82:LYS:HD3	3:D:86:TYR:CE2	2.40	0.57
2:G:40:TYR:HB3	3:H:81:SER:HB2	1.87	0.57
8:Y:115:GLU:OE2	8:Y:270:ARG:NH2	2.37	0.57
5:R:265:LEU:HD12	6:S:121:LEU:HD11	1.87	0.57
7:T:461:ASN:N	7:T:461:ASN:OD1	2.38	0.57
3:D:36:ARG:N	11:J:50:DG:OP1	2.39	0.56
1:E:116:ARG:NH1	1:E:120:GLN:OE1	2.38	0.56
4:Q:733:MET:HE3	4:Q:734:GLY:H	1.71	0.56
4:Q:767:LEU:HD21	4:Q:817:VAL:CG1	2.32	0.56
4:Q:1328:MET:O	4:Q:1344:ARG:NH1	2.38	0.56
2:C:73:ASP:OD1	2:C:73:ASP:N	2.36	0.56
7:X:463:LEU:HD22	8:Y:76:PRO:HD3	1.87	0.56
1:E:77:ASP:OD2	1:E:77:ASP:N	2.35	0.56
8:W:346:ASP:OD2	8:W:346:ASP:N	2.37	0.56
8:Y:23:HIS:HB2	8:Y:26:ILE:HD12	1.87	0.56
2:C:88:ILE:HD12	2:C:89:ARG:HD3	1.88	0.56
5:R:605:ASN:HB3	5:R:608:GLU:HB2	1.88	0.55
4:Q:1427:THR:OG1	4:Q:1428:ILE:N	2.39	0.55
7:T:381:ARG:NH1	7:T:401:ASP:OD1	2.40	0.55
7:V:68:LYS:HG2	7:V:305:PRO:HD2	1.87	0.55
6:S:69:ASP:HA	6:S:72:LYS:HG2	1.89	0.55
7:X:51:GLN:NE2	7:X:373:LEU:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:76:LEU:HB3	7:X:367:LEU:HD13	1.87	0.55
7:X:194:VAL:HG22	7:X:211:ARG:HG3	1.89	0.55
4:Q:958:GLN:O	4:Q:962:LYS:HB2	2.07	0.54
2:G:78:ARG:HH22	11:J:-53:DA:H5'	1.72	0.54
4:Q:1387:ASP:HB2	4:Q:1417:VAL:HA	1.88	0.54
5:R:168:ASP:OD1	5:R:168:ASP:N	2.39	0.54
10:F:24:ASP:HA	10:F:27:GLN:HB2	1.90	0.54
7:X:23:ARG:NH1	8:Y:316:GLU:O	2.41	0.54
1:A:85:GLN:NE2	12:I:-24:DG:OP1	2.40	0.54
2:C:18:ARG:NH1	12:I:-43:DT:OP2	2.40	0.54
2:C:79:ILE:HG21	3:D:57:ILE:HD12	1.89	0.54
7:V:51:GLN:NE2	7:V:373:LEU:O	2.40	0.54
10:F:30:THR:HG21	11:J:-13:DA:H5''	1.88	0.54
8:W:38:ARG:O	8:W:51:ARG:NH2	2.40	0.54
1:E:60:LEU:HD13	1:E:64:LYS:HE3	1.89	0.54
7:T:151:ASP:OD1	7:T:151:ASP:N	2.41	0.54
4:Q:821:GLN:HG3	11:J:-58:DC:H4'	1.90	0.53
10:F:30:THR:OG1	10:F:31:LYS:N	2.40	0.53
4:Q:1301:LEU:CD1	4:Q:1304:LEU:HD23	2.38	0.53
5:R:211:ARG:NH2	6:S:104:GLU:OE1	2.42	0.53
1:E:67:PHE:HZ	10:F:62:LEU:HD21	1.73	0.53
8:Y:40:THR:HG22	8:Y:45:VAL:HG22	1.90	0.53
1:A:58:THR:CB	2:G:82:ARG:NE	2.72	0.53
4:Q:778:LEU:HD22	4:Q:780:GLN:HE22	1.74	0.53
4:Q:1204:ASN:ND2	8:W:195:ALA:O	2.42	0.53
4:Q:1314:GLU:OE1	4:Q:1316:HIS:ND1	2.41	0.53
7:V:23:ARG:NH2	8:W:316:GLU:O	2.42	0.53
7:X:378:ASP:OD1	7:X:378:ASP:N	2.40	0.53
2:C:51:TYR:HE2	3:D:98:GLN:HB3	1.74	0.53
4:Q:1131:LEU:HD11	4:Q:1165:LEU:HD22	1.82	0.53
4:Q:1247:SER:OG	4:Q:1248:ASP:N	2.39	0.53
3:H:103:LEU:O	10:F:92:ARG:NH2	2.42	0.52
7:T:22:THR:OG1	7:T:392:ARG:NH1	2.42	0.52
5:R:671:THR:OG1	5:R:672:GLY:N	2.42	0.52
8:U:377:VAL:HG22	8:U:407:GLN:HG3	1.90	0.52
4:Q:860:PHE:HD1	4:Q:862:CYS:H	1.56	0.52
7:X:25:ALA:HB2	8:Y:67:ALA:HB3	1.92	0.52
2:C:43:ARG:HB2	3:D:91:THR:HG22	1.91	0.52
4:Q:1087:ARG:NH1	4:Q:1224:LEU:O	2.41	0.52
5:R:238:MET:HE3	5:R:612:MET:SD	2.50	0.52
4:Q:885:HIS:ND1	4:Q:892:PHE:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:ARG:CZ	3:H:38:GLU:OE1	2.52	0.52
4:Q:1172:GLN:HA	4:Q:1175:LEU:HB3	1.91	0.52
3:H:61:SER:HA	3:H:64:ILE:HG12	1.91	0.51
1:E:69:ARG:NH2	12:I:17:DA:OP1	2.44	0.51
4:Q:773:GLU:HA	4:Q:776:LYS:HG2	1.93	0.51
8:W:147:ARG:HG2	8:W:154:LYS:HG2	1.91	0.51
7:X:395:VAL:HG22	7:X:434:ILE:HD12	1.92	0.51
1:A:106:ASP:OD1	1:A:131:ARG:NH2	2.39	0.51
8:Y:16:SER:OG	8:Y:17:LEU:N	2.43	0.51
2:C:52:LEU:HD21	3:D:73:PHE:HE1	1.69	0.51
2:C:65:GLU:O	2:C:69:ASN:ND2	2.43	0.51
7:T:223:ASP:HB2	8:U:170:GLU:H	1.74	0.51
4:Q:1120:THR:O	7:T:294:LYS:NZ	2.43	0.51
8:W:413:ARG:NH1	8:W:422:ASP:OD1	2.43	0.51
11:J:47:DA:N6	12:I:-48:DC:N3	2.58	0.51
5:R:71:ARG:NH1	5:R:72:ASP:O	2.43	0.51
4:Q:1361:TRP:HE3	4:Q:1367:ILE:HD13	1.77	0.50
7:T:41:ALA:HB3	7:T:52:ILE:HG23	1.93	0.50
7:V:141:GLU:OE2	7:V:239:LYS:NZ	2.42	0.50
5:R:74:LYS:HD2	5:R:75:LEU:HG	1.92	0.50
5:R:138:GLU:OE2	5:R:749:ASN:ND2	2.43	0.50
10:F:91:LYS:HA	10:F:96:THR:HG22	1.93	0.50
1:A:119:ILE:O	10:B:47:SER:OG	2.29	0.50
7:V:394:GLN:NE2	7:V:433:GLU:OE1	2.45	0.50
7:T:331:ASN:OD1	8:Y:21:ALA:HB2	2.11	0.50
8:Y:432:ASP:OD1	8:Y:435:ARG:NH1	2.44	0.50
1:A:113:HIS:O	1:E:122:LYS:NZ	2.44	0.50
8:Y:23:HIS:CD2	8:Y:86:MET:CG	2.95	0.50
10:F:32:PRO:HB3	10:F:35:ARG:HH21	1.77	0.50
11:J:17:DA:H61	12:I:-17:DT:H3	1.60	0.50
4:Q:1103:ASP:N	4:Q:1103:ASP:OD1	2.39	0.50
7:T:361:PRO:HA	7:T:364:ILE:HB	1.94	0.50
7:T:413:ARG:NH1	8:U:349:ASP:OD2	2.45	0.50
2:C:16:GLN:O	2:C:21:LYS:NZ	2.44	0.50
7:T:272:LEU:HD12	7:V:269:MET:HE2	1.94	0.49
7:V:317:ASP:OD1	7:V:317:ASP:N	2.40	0.49
2:G:15:SER:OG	11:J:-42:DG:OP1	2.30	0.49
5:R:193:ASP:OD1	5:R:193:ASP:N	2.43	0.49
8:U:415:ASN:OD1	8:U:415:ASN:N	2.45	0.49
11:J:-18:DG:N2	12:I:19:DC:O2	2.45	0.49
6:S:59:ARG:NH1	12:I:34:DT:OP1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:70:VAL:HA	10:B:73:THR:HG22	1.93	0.49
2:C:77:THR:OG1	3:D:54:ASP:O	2.31	0.49
7:X:362:ASP:OD1	7:X:362:ASP:N	2.45	0.49
4:Q:1387:ASP:OD1	4:Q:1387:ASP:N	2.41	0.49
6:S:130:ASN:OD1	6:S:130:ASN:N	2.44	0.49
7:T:182:ASP:HB3	7:T:185:ILE:HG13	1.93	0.49
7:V:448:ASP:OD1	7:V:451:ARG:NH1	2.45	0.49
8:W:27:THR:HA	8:W:90:GLN:HG2	1.94	0.49
8:U:220:ARG:HG3	8:U:221:PHE:HD1	1.76	0.49
8:W:359:TYR:OH	13:W:501:ADP:N7	2.39	0.49
1:A:58:THR:CB	2:G:82:ARG:HE	2.26	0.49
4:Q:1137:LEU:HB2	8:Y:200:THR:HB	1.94	0.49
7:T:441:GLU:OE2	8:U:52:ARG:NH2	2.46	0.49
8:Y:76:PRO:O	8:Y:79:THR:OG1	2.30	0.49
8:Y:346:ASP:OD1	8:Y:346:ASP:N	2.41	0.49
1:A:58:THR:CB	2:G:82:ARG:CZ	2.89	0.48
7:T:352:ASP:N	7:T:352:ASP:OD1	2.44	0.48
8:Y:336:ASN:OD1	8:Y:336:ASN:N	2.44	0.48
7:T:70:MET:HE1	8:Y:375:GLU:HG2	1.95	0.48
7:T:82:SER:O	7:T:82:SER:OG	2.27	0.48
9:Z:303:GLU:N	9:Z:303:GLU:OE2	2.46	0.48
10:B:45:ARG:HD2	11:J:8:DG:H5'	1.95	0.48
1:E:104:PHE:HB3	10:F:41:GLY:HA3	1.94	0.48
1:A:50:GLU:OE2	10:B:39:ARG:NH1	2.47	0.48
3:H:47:VAL:HG23	3:H:50:GLN:NE2	2.28	0.48
7:T:68:LYS:HG2	7:T:305:PRO:HD2	1.96	0.48
2:G:30:ARG:HH21	12:I:48:DG:H5''	1.79	0.48
8:W:162:THR:OG1	8:W:163:THR:N	2.46	0.48
10:B:30:THR:OG1	10:B:31:LYS:N	2.46	0.48
4:Q:839:ILE:HG12	4:Q:866:LEU:HD23	1.96	0.48
4:Q:1032:GLY:HA3	8:U:182:GLU:HA	1.96	0.48
4:Q:773:GLU:HG2	4:Q:776:LYS:HE2	1.95	0.48
8:Y:240:SER:OG	8:Y:243:GLU:OE1	2.27	0.47
4:Q:1346:ASP:N	4:Q:1346:ASP:OD1	2.46	0.47
8:U:21:ALA:HB2	7:V:331:ASN:HB3	1.96	0.47
3:H:48:LEU:HG	3:H:57:ILE:HD11	1.95	0.47
4:Q:1101:ASP:OD1	4:Q:1101:ASP:N	2.47	0.47
4:Q:1384:THR:O	4:Q:1413:GLN:NE2	2.47	0.47
5:R:70:PHE:HB3	5:R:79:PHE:HB2	1.95	0.47
4:Q:796:LEU:HD23	4:Q:799:PHE:HD2	1.80	0.47
4:Q:733:MET:HE1	4:Q:737:LYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:818:THR:OG1	4:Q:819:SER:N	2.46	0.47
9:Z:319:THR:OG1	9:Z:320:PHE:N	2.48	0.47
8:U:114:THR:O	8:U:118:THR:OG1	2.31	0.47
8:W:412:LYS:HD2	7:X:38:SER:HA	1.97	0.47
1:A:102:SER:HA	1:A:105:GLU:HG2	1.96	0.46
7:T:151:ASP:HA	7:T:163:ILE:HA	1.96	0.46
5:R:237:LYS:HB2	5:R:237:LYS:HE2	1.75	0.46
10:F:47:SER:HB2	10:F:50:ILE:HG23	1.96	0.46
4:Q:835:TRP:HB2	4:Q:862:CYS:HB2	1.97	0.46
6:S:28:GLU:OE2	6:S:28:GLU:N	2.49	0.46
7:X:202:ILE:HG12	7:X:209:VAL:HG12	1.96	0.46
10:F:44:LYS:HG2	10:F:45:ARG:HG2	1.96	0.46
12:I:17:DA:H1'	12:I:18:DC:H5'	1.97	0.46
11:J:-68:DA:H2'	11:J:-67:DT:C6	2.51	0.46
4:Q:1071:THR:OG1	7:V:177:LYS:NZ	2.47	0.46
10:F:78:ARG:HD2	10:F:80:THR:H	1.79	0.46
8:W:47:GLN:HE22	8:W:356:THR:HB	1.81	0.46
8:Y:44:MET:HB3	8:Y:44:MET:HE2	1.82	0.46
6:S:60:HIS:NE2	11:J:-30:DA:OP1	2.48	0.46
11:J:55:DC:H2''	11:J:56:DG:N7	2.31	0.46
7:X:108:SER:HB3	8:Y:304:GLU:HB3	1.98	0.46
9:Z:295:LYS:HB2	9:Z:295:LYS:HE3	1.74	0.46
2:C:24:LEU:HD22	2:C:53:THR:HG23	1.97	0.46
5:R:139:ARG:O	5:R:142:THR:OG1	2.34	0.46
7:T:438:ASP:N	7:T:438:ASP:OD1	2.48	0.46
8:Y:165:MET:HE3	8:Y:229:LEU:H	1.80	0.46
8:W:81:LYS:N	13:W:501:ADP:O2B	2.43	0.45
11:J:-54:DC:H2'	11:J:-53:DA:H8	1.81	0.45
4:Q:767:LEU:CD2	4:Q:817:VAL:HG11	2.25	0.45
7:X:361:PRO:HA	7:X:364:ILE:HB	1.98	0.45
10:F:39:ARG:HE	10:F:39:ARG:HB2	1.65	0.45
7:T:121:LEU:HD23	7:T:323:TYR:HD2	1.81	0.45
7:T:198:ASP:OD1	7:T:198:ASP:N	2.49	0.45
8:U:346:ASP:OD1	8:U:346:ASP:N	2.48	0.45
8:W:262:THR:O	8:W:262:THR:OG1	2.28	0.45
10:B:68:ASP:OD2	10:B:93:GLN:NE2	2.49	0.45
7:X:313:VAL:HG11	7:X:338:LEU:HB3	1.98	0.45
1:A:83:ARG:HB2	10:B:80:THR:HA	1.98	0.45
3:D:39:THR:OG1	3:D:40:TYR:N	2.49	0.45
10:B:78:ARG:NH1	10:B:80:THR:O	2.50	0.45
1:A:104:PHE:HA	1:A:107:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:27:PRO:HB2	2:C:30:ARG:HB3	1.97	0.45
1:E:115:LYS:HB2	1:E:115:LYS:HE2	1.84	0.45
12:I:15:DT:H2''	12:I:16:DA:C8	2.52	0.45
1:A:67:PHE:HE2	1:A:93:GLN:HA	1.81	0.45
1:E:64:LYS:O	1:E:68:GLN:HB2	2.17	0.45
2:G:43:ARG:HD2	12:I:39:DA:H5'	1.99	0.45
4:Q:1131:LEU:CD1	4:Q:1165:LEU:CD2	2.79	0.45
7:T:108:SER:HB3	8:U:304:GLU:HB3	1.98	0.45
7:X:216:ASP:OD1	7:X:216:ASP:N	2.49	0.45
8:U:66:ILE:HG23	8:U:69:ARG:HH21	1.82	0.45
7:X:51:GLN:HE22	7:X:373:LEU:H	1.65	0.45
5:R:729:ILE:HD11	5:R:743:LYS:HB2	1.98	0.44
7:T:149:PRO:HB3	7:T:166:VAL:HG22	1.98	0.44
7:V:443:LYS:HB3	7:V:443:LYS:HE3	1.78	0.44
5:R:246:MET:HE3	5:R:614:LEU:HD11	1.99	0.44
2:C:115:ASN:OD1	2:C:115:ASN:N	2.50	0.44
4:Q:1249:ILE:HG13	4:Q:1271:THR:HG21	1.98	0.44
4:Q:1149:LEU:HD22	7:T:272:LEU:HD13	1.98	0.44
1:A:115:LYS:HZ1	1:E:116:ARG:HH21	1.64	0.44
7:T:117:LYS:H	7:T:117:LYS:HG2	1.54	0.44
8:W:162:THR:HG23	8:W:165:MET:H	1.82	0.44
8:Y:160:ILE:HG23	8:Y:229:LEU:HD21	1.99	0.44
3:D:37:LYS:N	11:J:50:DG:OP1	2.47	0.44
5:R:116:ASP:OD1	5:R:158:TYR:OH	2.31	0.44
4:Q:1322:PHE:HE2	4:Q:1371:LEU:HD22	1.82	0.44
5:R:144:GLN:NE2	5:R:148:THR:OG1	2.46	0.44
8:W:122:ARG:NH1	8:W:245:ASP:OD2	2.50	0.44
7:X:443:LYS:HB3	7:X:443:LYS:HE3	1.77	0.44
8:Y:259:THR:OG1	8:Y:261:ASP:OD1	2.36	0.44
4:Q:756:GLY:HA3	4:Q:757:PRO:HD3	1.83	0.43
4:Q:1356:ASP:OD1	4:Q:1356:ASP:N	2.40	0.43
7:X:140:TYR:HB2	7:X:202:ILE:HB	1.99	0.43
11:J:-66:DG:H1'	11:J:-65:DT:H5'	2.00	0.43
2:C:72:ARG:HH22	2:C:77:THR:HA	1.83	0.43
3:D:57:ILE:HG22	3:D:58:SER:O	2.19	0.43
4:Q:1079:ASN:ND2	4:Q:1217:PRO:O	2.49	0.43
4:Q:1372:LEU:HD23	4:Q:1372:LEU:HA	1.88	0.43
4:Q:1394:SER:O	4:Q:1394:SER:OG	2.30	0.43
7:T:25:ALA:HB2	8:U:67:ALA:HB3	1.99	0.43
8:U:122:ARG:NE	8:U:245:ASP:OD2	2.48	0.43
8:U:208:ARG:HH11	8:U:209:SER:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:362:ASP:OD1	7:V:362:ASP:N	2.44	0.43
7:X:223:ASP:OD1	7:X:223:ASP:N	2.42	0.43
11:J:-60:DA:H2'	11:J:-59:DT:C6	2.52	0.43
4:Q:794:LYS:HD3	4:Q:797:ARG:HE	1.83	0.43
4:Q:1142:ARG:O	4:Q:1146:THR:OG1	2.32	0.43
7:V:163:ILE:HG13	7:V:183:PRO:HG3	1.99	0.43
7:T:71:SER:HB3	8:Y:19:LEU:HB2	2.00	0.43
2:C:29:GLY:HA3	12:I:-44:DA:H3'	2.00	0.43
2:C:66:LEU:HB3	2:C:87:ALA:HB1	2.00	0.43
1:E:129:ARG:O	1:E:129:ARG:NH1	2.52	0.43
4:Q:944:LEU:HD21	4:Q:1411:LEU:HD12	1.99	0.43
5:R:127:ASP:OD1	5:R:127:ASP:N	2.52	0.43
10:F:73:THR:OG1	10:F:78:ARG:O	2.36	0.43
3:D:61:SER:HA	3:D:64:ILE:HG13	2.01	0.43
1:E:119:ILE:H	1:E:119:ILE:HG13	1.62	0.43
7:V:134:LYS:HG2	7:V:244:VAL:HG22	2.00	0.43
4:Q:1291:MET:HG2	4:Q:1337:TYR:CG	2.54	0.43
7:V:108:SER:HB3	8:W:304:GLU:HB3	2.01	0.43
7:V:211:ARG:NH2	7:V:227:GLU:OE2	2.45	0.43
8:W:94:LYS:HA	8:W:94:LYS:HD3	1.70	0.43
8:W:114:THR:O	8:W:118:THR:OG1	2.35	0.43
7:X:127:ARG:NH1	8:Y:268:GLU:OE2	2.52	0.43
4:Q:1161:ASN:OD1	4:Q:1161:ASN:N	2.51	0.43
5:R:107:ASN:OD1	5:R:107:ASN:N	2.43	0.43
7:T:170:LEU:O	7:T:176:THR:OG1	2.33	0.43
11:J:-54:DC:H2'	11:J:-53:DA:C8	2.53	0.43
2:C:56:LEU:HD22	3:D:69:VAL:HG23	2.00	0.42
3:H:47:VAL:HG23	3:H:50:GLN:HE21	1.83	0.42
4:Q:1033:LYS:O	8:U:201:LYS:NZ	2.52	0.42
5:R:732:LYS:HE2	5:R:732:LYS:HB2	1.81	0.42
7:T:42:LYS:O	7:T:55:ARG:NH2	2.46	0.42
7:V:212:VAL:HG12	7:V:230:VAL:HG21	2.01	0.42
10:F:51:TYR:O	10:F:54:THR:OG1	2.33	0.42
10:F:62:LEU:O	10:F:66:ILE:HG13	2.19	0.42
4:Q:1354:ARG:NH2	11:J:-58:DC:OP2	2.39	0.42
6:S:152:ASP:OD1	6:S:152:ASP:N	2.49	0.42
8:U:276:LYS:HA	8:U:276:LYS:HD3	1.76	0.42
3:D:49:LYS:HD2	3:D:49:LYS:HA	1.81	0.42
4:Q:1301:LEU:HD12	4:Q:1304:LEU:HD23	2.01	0.42
5:R:182:LYS:O	5:R:202:GLY:N	2.51	0.42
6:S:134:TYR:OH	8:U:166:GLU:O	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:216:ASP:OD1	7:T:216:ASP:N	2.52	0.42
8:U:108:SER:OG	8:U:109:LEU:N	2.53	0.42
7:V:121:LEU:HD23	7:V:323:TYR:HD2	1.85	0.42
7:V:352:ASP:OD1	7:V:352:ASP:N	2.42	0.42
11:J:-50:DT:H2''	11:J:-49:DG:C8	2.55	0.42
1:A:56:LYS:HZ2	5:R:505:GLU:N	2.18	0.42
2:C:64:LEU:HD21	3:D:48:LEU:HA	2.00	0.42
8:W:44:MET:HE2	8:W:44:MET:HB3	1.82	0.42
8:Y:110:GLU:OE1	8:Y:110:GLU:N	2.52	0.42
4:Q:1225:GLY:HA2	8:U:195:ALA:HB3	2.01	0.42
8:W:40:THR:HG23	8:W:45:VAL:HG12	2.02	0.42
8:Y:165:MET:HE3	8:Y:229:LEU:HB2	2.02	0.42
12:I:71:DT:H2''	12:I:72:DG:C8	2.55	0.42
2:G:117:LEU:HD22	2:G:117:LEU:HA	1.88	0.42
5:R:35:ASN:HA	5:R:36:PRO:HD3	1.90	0.42
7:T:347:VAL:HG11	7:T:360:PRO:HG3	2.02	0.42
7:V:25:ALA:HB2	8:W:67:ALA:HB3	2.01	0.42
3:D:37:LYS:HE3	3:D:37:LYS:HB3	1.92	0.42
8:U:300:MET:HG3	7:V:322:THR:HG21	2.01	0.42
8:Y:432:ASP:OD1	8:Y:432:ASP:N	2.35	0.42
4:Q:1291:MET:O	4:Q:1294:PHE:HB3	2.20	0.42
10:B:59:LYS:HE3	10:B:59:LYS:HB3	1.93	0.42
11:J:16:DA:H1'	11:J:17:DA:C8	2.54	0.42
8:W:233:LYS:HA	8:W:233:LYS:HD3	1.89	0.42
7:V:29:HIS:HB3	7:V:390:VAL:HG21	2.02	0.41
4:Q:898:PHE:HA	4:Q:901:TRP:HE3	1.84	0.41
8:Y:94:LYS:HD2	8:Y:94:LYS:HA	1.88	0.41
8:Y:129:ILE:HD13	8:Y:129:ILE:HA	1.95	0.41
1:A:51:ILE:HD11	10:B:42:GLY:HA2	2.02	0.41
5:R:155:PHE:O	5:R:731:LYS:NZ	2.51	0.41
7:V:341:ASN:OD1	7:V:341:ASN:N	2.54	0.41
8:W:375:GLU:HG2	7:X:70:MET:HE1	2.01	0.41
8:Y:146:ASP:HB2	8:Y:155:GLN:HG2	2.02	0.41
4:Q:773:GLU:O	4:Q:777:PHE:HB2	2.20	0.41
4:Q:819:SER:OG	4:Q:820:TYR:N	2.53	0.41
5:R:67:LEU:HD11	5:R:80:THR:HG23	2.02	0.41
5:R:242:GLN:O	5:R:246:MET:HG3	2.20	0.41
7:T:138:GLU:HB3	7:T:204:ALA:HB3	2.01	0.41
8:U:208:ARG:H	8:U:208:ARG:HG3	1.67	0.41
8:W:425:ARG:NH2	7:X:56:GLU:OE1	2.53	0.41
8:Y:325:THR:HG22	8:Y:327:ARG:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:LEU:HD13	3:D:47:VAL:HG12	2.01	0.41
2:G:77:THR:O	2:G:77:THR:OG1	2.38	0.41
2:G:117:LEU:HA	2:G:118:PRO:HD3	1.89	0.41
4:Q:1233:ILE:HD13	4:Q:1233:ILE:HA	1.91	0.41
5:R:38:SER:O	5:R:132:ASN:ND2	2.52	0.41
11:J:-72:DC:H2"	11:J:-71:DA:C8	2.56	0.41
8:W:179:LEU:HD22	8:W:184:VAL:HG21	2.02	0.41
7:X:177:LYS:HB3	7:X:237:VAL:HG21	2.03	0.41
1:E:61:LEU:O	10:F:36:ARG:NH1	2.54	0.41
1:E:133:GLU:N	1:E:133:GLU:OE1	2.53	0.41
4:Q:767:LEU:HD21	4:Q:817:VAL:HG13	1.96	0.41
7:T:106:VAL:HB	7:T:109:GLU:HG3	2.02	0.41
7:X:352:ASP:N	7:X:352:ASP:OD1	2.53	0.41
1:A:58:THR:O	1:A:58:THR:CG2	2.69	0.41
5:R:213:ASN:OD1	5:R:635:GLN:NE2	2.52	0.41
7:T:73:ARG:HH22	8:Y:401:ASN:HA	1.86	0.41
7:T:347:VAL:O	7:T:350:THR:OG1	2.37	0.41
7:T:272:LEU:HD11	7:X:269:MET:HE1	2.03	0.41
7:X:125:PHE:HZ	7:X:324:LEU:CD1	2.34	0.41
7:X:413:ARG:NH1	8:Y:349:ASP:OD2	2.53	0.41
8:Y:23:HIS:NE2	8:Y:86:MET:HB2	2.36	0.41
8:Y:311:ARG:HD2	8:Y:311:ARG:HA	1.87	0.41
5:R:688:PHE:HB3	5:R:698:ILE:HD13	2.03	0.41
8:U:117:LEU:HD23	8:U:117:LEU:HA	1.96	0.41
7:X:328:LEU:HD23	7:X:328:LEU:HA	1.95	0.41
11:J:37:DC:H2"	11:J:38:DG:C8	2.56	0.41
3:H:44:ILE:HA	3:H:47:VAL:HG12	2.02	0.40
8:W:295:ILE:O	8:W:298:VAL:HG23	2.21	0.40
1:A:58:THR:HB	2:G:82:ARG:NE	2.33	0.40
8:U:414:LYS:HB2	8:U:414:LYS:HE2	1.76	0.40
7:V:149:PRO:HB3	7:V:166:VAL:HG22	2.04	0.40
7:X:269:MET:HE3	7:X:269:MET:HB2	1.87	0.40
10:B:47:SER:HA	11:J:7:DC:H5"	2.02	0.40
3:D:118:THR:HA	3:D:121:VAL:HG12	2.04	0.40
4:Q:794:LYS:HD3	4:Q:794:LYS:HA	1.89	0.40
8:U:94:LYS:HA	8:U:94:LYS:HE2	2.04	0.40
7:V:332:ILE:HD12	7:V:332:ILE:HA	1.92	0.40
10:B:87:VAL:HA	10:B:90:LEU:HD23	2.02	0.40
1:E:40:ARG:HD2	1:E:40:ARG:HA	1.89	0.40
2:G:85:GLN:HE21	2:G:103:ILE:HG21	1.85	0.40
8:W:81:LYS:NZ	13:W:501:ADP:O1B	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:395:SER:OG	8:W:396:LEU:N	2.55	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	93/136 (68%)	93 (100%)	0	0	100	100
1	E	93/136 (68%)	91 (98%)	2 (2%)	0	100	100
2	C	102/132 (77%)	96 (94%)	6 (6%)	0	100	100
2	G	102/132 (77%)	99 (97%)	3 (3%)	0	100	100
3	D	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
3	H	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
4	Q	652/1489 (44%)	615 (94%)	37 (6%)	0	100	100
5	R	544/755 (72%)	535 (98%)	9 (2%)	0	100	100
6	S	121/166 (73%)	112 (93%)	9 (7%)	0	100	100
7	T	431/463 (93%)	422 (98%)	9 (2%)	0	100	100
7	V	441/463 (95%)	424 (96%)	17 (4%)	0	100	100
7	X	440/463 (95%)	423 (96%)	17 (4%)	0	100	100
8	U	432/471 (92%)	416 (96%)	16 (4%)	0	100	100
8	W	440/471 (93%)	425 (97%)	15 (3%)	0	100	100
8	Y	443/471 (94%)	422 (95%)	21 (5%)	0	100	100
9	Z	53/320 (17%)	52 (98%)	1 (2%)	0	100	100
10	B	77/103 (75%)	74 (96%)	3 (4%)	0	100	100
10	F	77/103 (75%)	72 (94%)	5 (6%)	0	100	100
All	All	4723/6536 (72%)	4551 (96%)	172 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	83/113 (74%)	83 (100%)	0	100	100
1	E	83/113 (74%)	83 (100%)	0	100	100
2	C	83/99 (84%)	83 (100%)	0	100	100
2	G	81/99 (82%)	81 (100%)	0	100	100
3	D	80/109 (73%)	80 (100%)	0	100	100
3	H	81/109 (74%)	81 (100%)	0	100	100
4	Q	583/1350 (43%)	583 (100%)	0	100	100
5	R	394/682 (58%)	394 (100%)	0	100	100
6	S	109/142 (77%)	109 (100%)	0	100	100
7	T	367/391 (94%)	367 (100%)	0	100	100
7	V	375/391 (96%)	375 (100%)	0	100	100
7	X	374/391 (96%)	374 (100%)	0	100	100
8	U	371/403 (92%)	371 (100%)	0	100	100
8	W	375/403 (93%)	375 (100%)	0	100	100
8	Y	377/403 (94%)	377 (100%)	0	100	100
9	Z	27/285 (10%)	27 (100%)	0	100	100
10	B	62/79 (78%)	62 (100%)	0	100	100
10	F	62/79 (78%)	62 (100%)	0	100	100
All	All	3967/5641 (70%)	3967 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	69	ASN

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Mol	Chain	Res	Type
2	C	95	ASN
2	C	111	ASN
1	E	76	GLN
4	Q	769	ASN
4	Q	875	ASN
4	Q	1279	ASN
4	Q	1362	GLN
4	Q	1382	ASN
4	Q	1438	GLN
5	R	23	GLN
5	R	78	ASN
5	R	109	ASN
5	R	191	HIS
5	R	607	HIS
5	R	701	ASN
8	U	373	GLN
8	U	453	ASN
7	V	190	GLN
7	V	440	ASN
8	W	34	ASN
8	W	237	HIS
8	W	242	HIS
8	W	310	ASN
8	W	441	GLN
7	X	51	GLN
7	X	263	GLN
7	X	286	GLN
8	Y	34	ASN
8	Y	144	GLN
8	Y	230	GLN
10	B	25	ASN
10	B	93	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	V	501	-	24,29,29	0.89	0	29,45,45	1.27	3 (10%)
13	ADP	W	501	-	24,29,29	0.83	0	29,45,45	1.26	2 (6%)
13	ADP	Y	501	-	24,29,29	0.85	0	29,45,45	1.23	2 (6%)
13	ADP	U	501	-	24,29,29	0.88	0	29,45,45	1.20	2 (6%)
13	ADP	X	501	-	24,29,29	0.82	0	29,45,45	1.20	2 (6%)
13	ADP	T	501	-	24,29,29	0.85	0	29,45,45	1.25	3 (10%)

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	V	501	-	-	4/12/32/32	0/3/3/3
13	ADP	W	501	-	-	3/12/32/32	0/3/3/3
13	ADP	Y	501	-	-	6/12/32/32	0/3/3/3
13	ADP	U	501	-	-	2/12/32/32	0/3/3/3
13	ADP	X	501	-	-	3/12/32/32	0/3/3/3
13	ADP	T	501	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	W	501	ADP	N3-C2-N1	-3.89	123.39	128.67
13	Y	501	ADP	N3-C2-N1	-3.73	123.61	128.67
13	T	501	ADP	N3-C2-N1	-3.68	123.67	128.67
13	X	501	ADP	N3-C2-N1	-3.59	123.80	128.67
13	U	501	ADP	N3-C2-N1	-3.55	123.85	128.67
13	V	501	ADP	N3-C2-N1	-3.51	123.91	128.67
13	Y	501	ADP	C4-C5-N7	-2.51	106.68	109.34
13	X	501	ADP	C4-C5-N7	-2.43	106.77	109.34
13	V	501	ADP	C4-C5-N7	-2.42	106.78	109.34
13	U	501	ADP	C4-C5-N7	-2.38	106.83	109.34
13	T	501	ADP	C4-C5-N7	-2.34	106.87	109.34
13	W	501	ADP	C4-C5-N7	-2.20	107.01	109.34
13	T	501	ADP	O3B-PB-O2B	2.12	115.73	107.80
13	V	501	ADP	C4'-O4'-C1'	2.05	111.81	109.92

There are no chirality outliers.

All (21) torsion outliers are listed below:

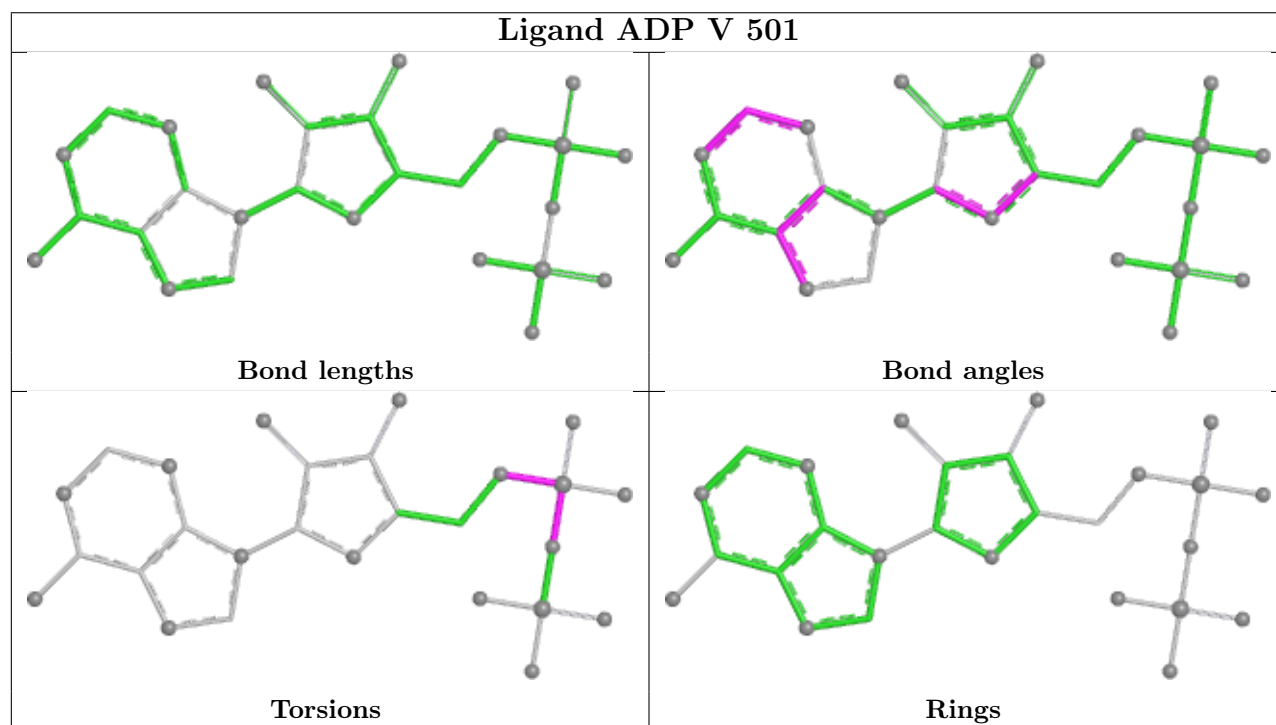
Mol	Chain	Res	Type	Atoms
13	V	501	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	C5'-O5'-PA-O2A
13	V	501	ADP	C5'-O5'-PA-O3A
13	W	501	ADP	C5'-O5'-PA-O2A
13	X	501	ADP	C5'-O5'-PA-O2A
13	X	501	ADP	C5'-O5'-PA-O3A
13	Y	501	ADP	C5'-O5'-PA-O1A
13	Y	501	ADP	C5'-O5'-PA-O2A
13	Y	501	ADP	C5'-O5'-PA-O3A
13	Y	501	ADP	O4'-C4'-C5'-O5'
13	T	501	ADP	PB-O3A-PA-O1A
13	V	501	ADP	PB-O3A-PA-O5'
13	U	501	ADP	PB-O3A-PA-O2A
13	W	501	ADP	C3'-C4'-C5'-O5'
13	T	501	ADP	C5'-O5'-PA-O1A
13	W	501	ADP	C5'-O5'-PA-O3A
13	X	501	ADP	C5'-O5'-PA-O1A
13	T	501	ADP	PB-O3A-PA-O2A
13	U	501	ADP	PB-O3A-PA-O1A
13	Y	501	ADP	PB-O3A-PA-O1A
13	Y	501	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

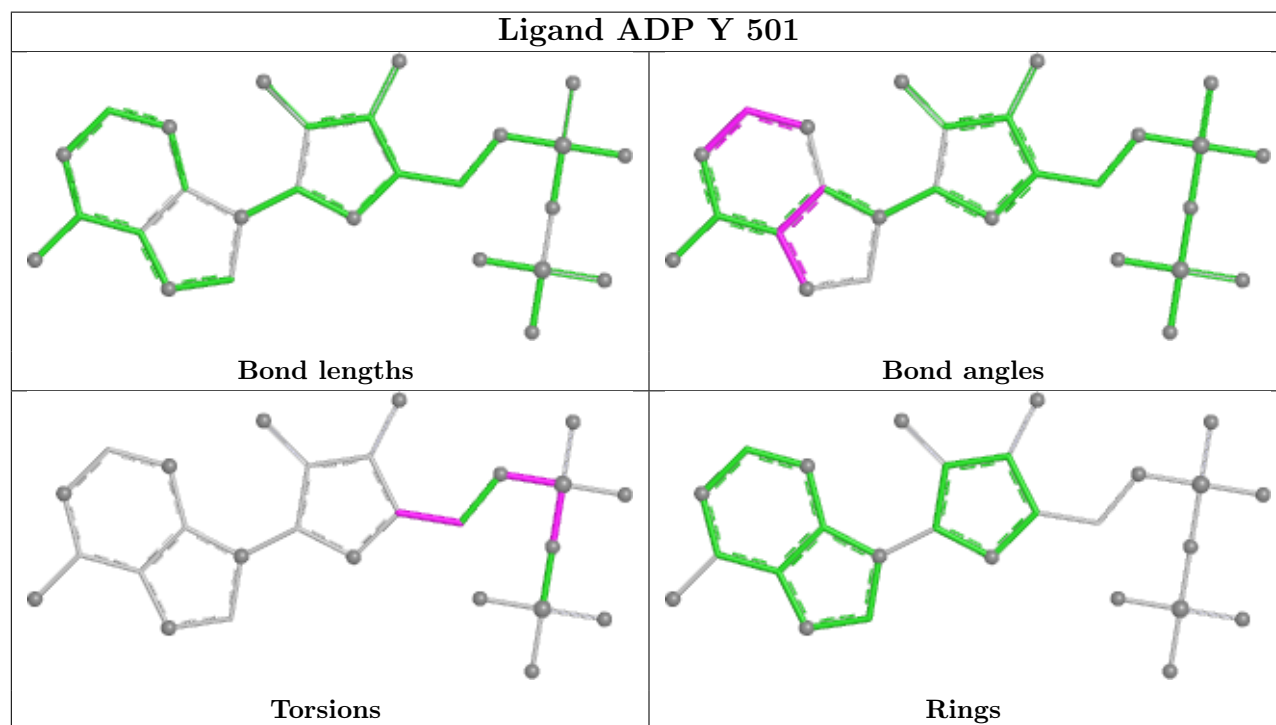
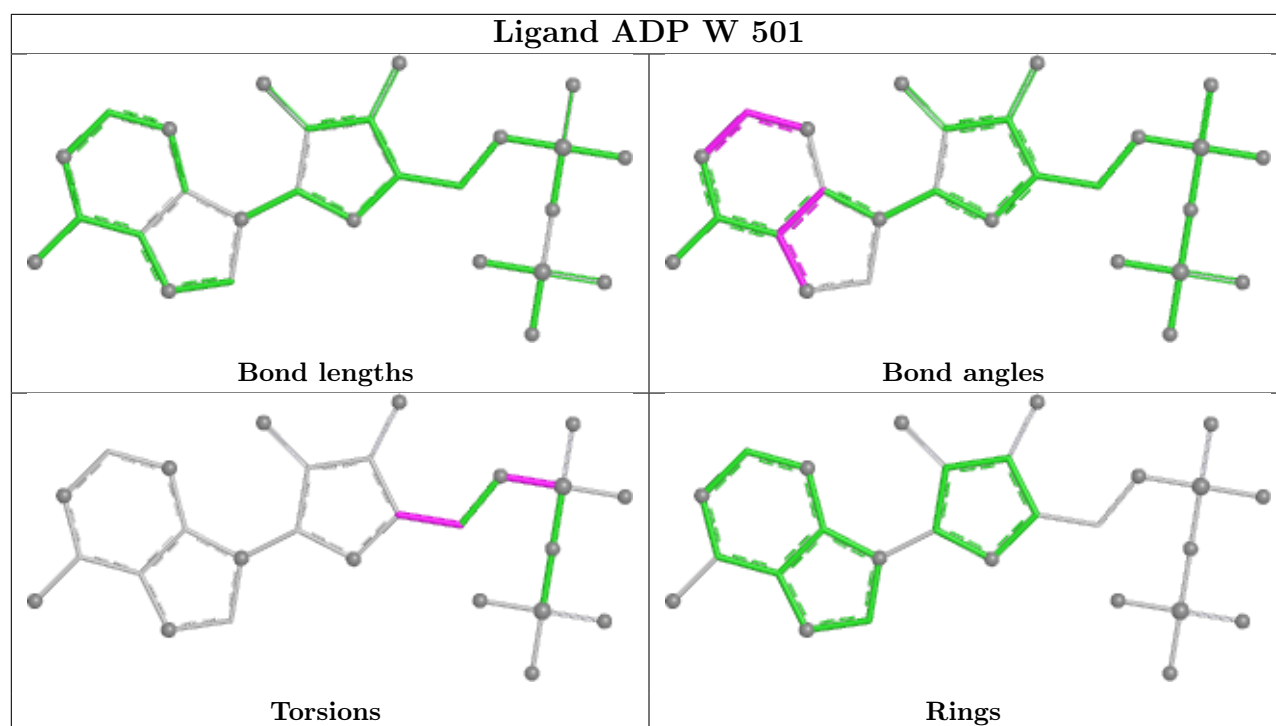
2 monomers are involved in 5 short contacts:

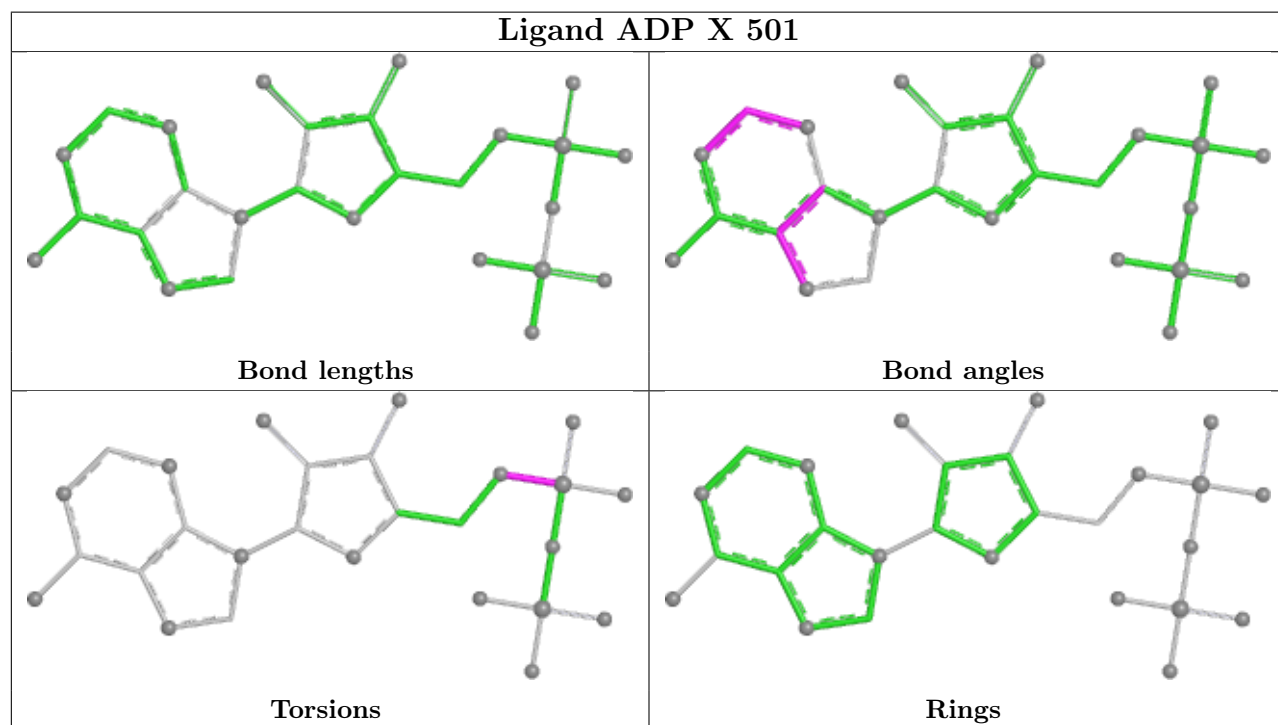
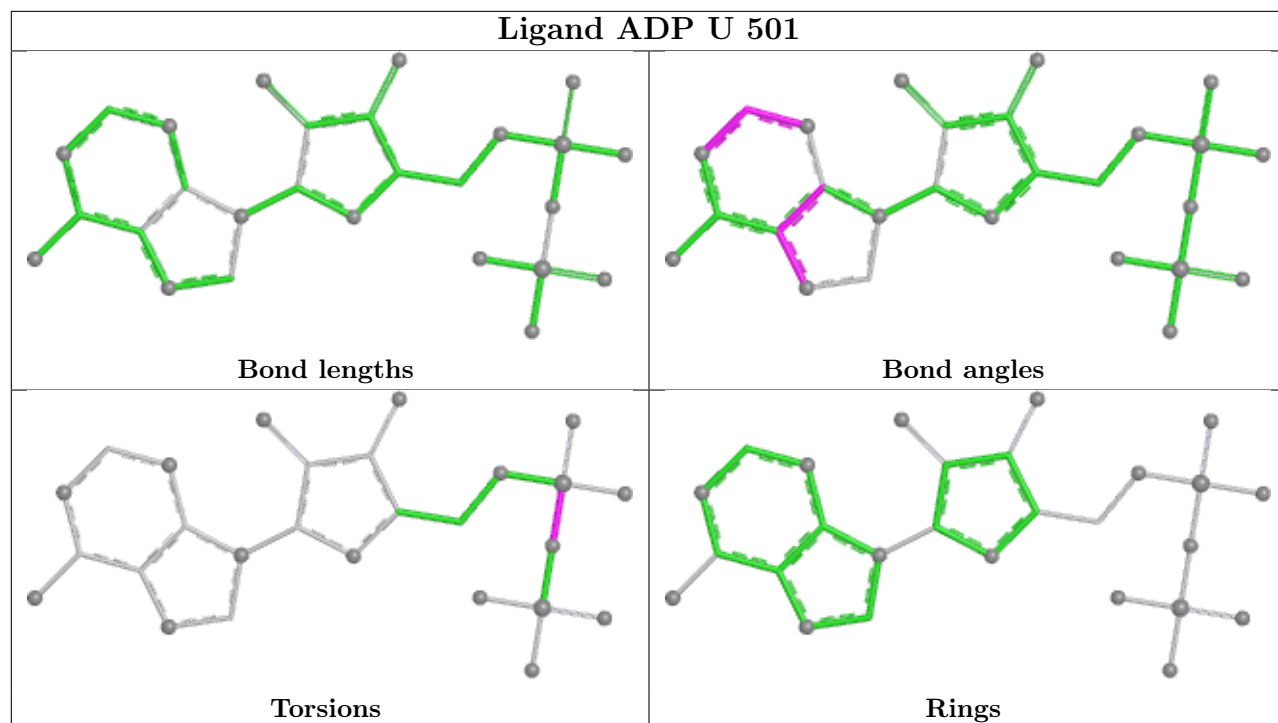
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	V	501	ADP	1	0
13	W	501	ADP	4	0

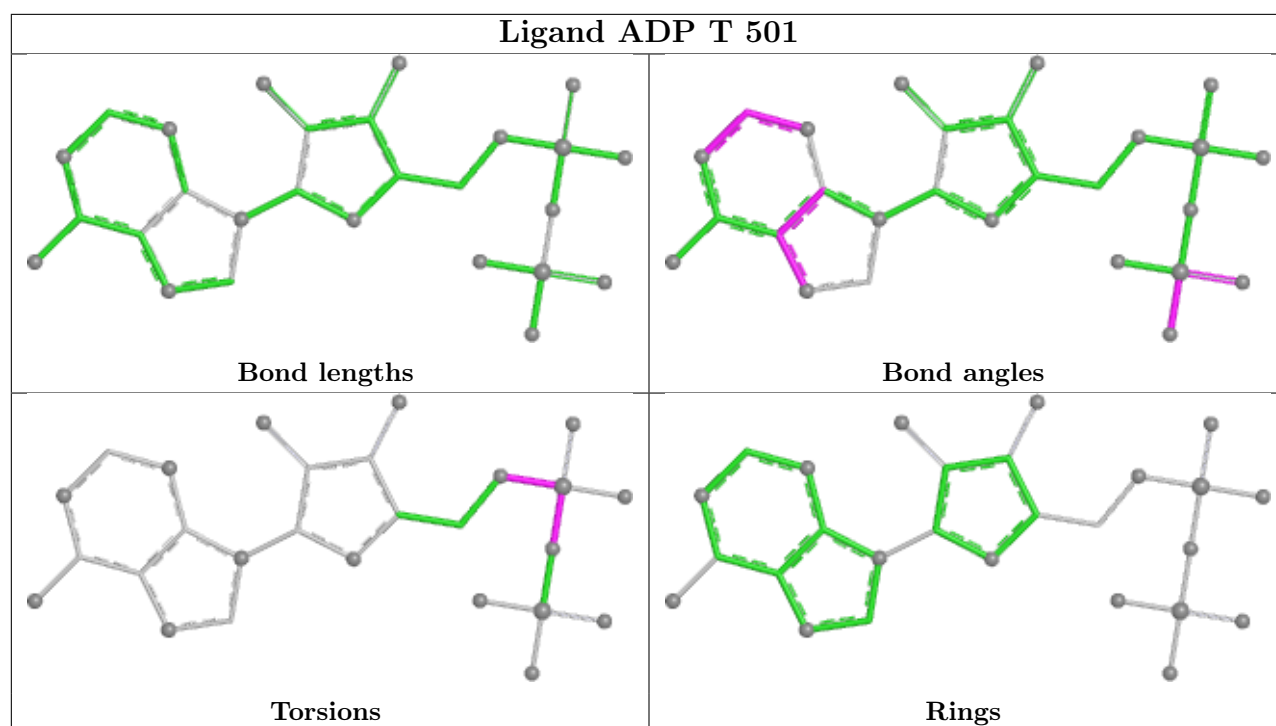
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

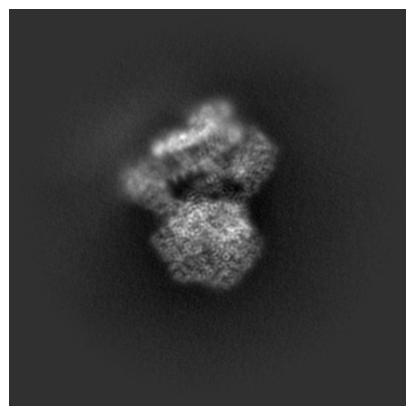
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45361. These allow visual inspection of the internal detail of the map and identification of artifacts.

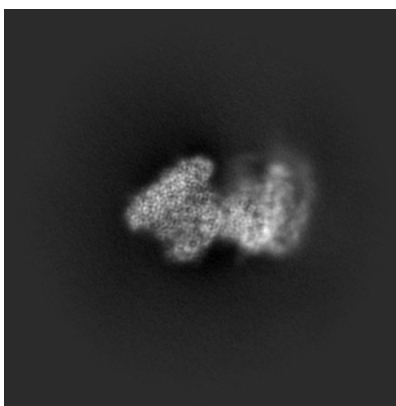
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

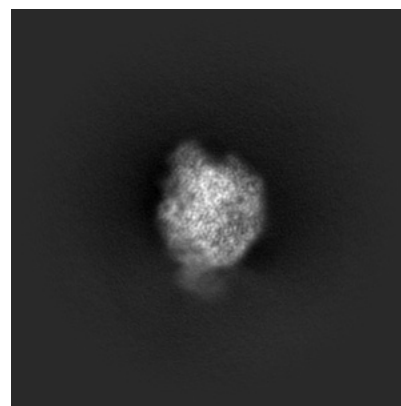
#### 6.1.1 Primary map



X

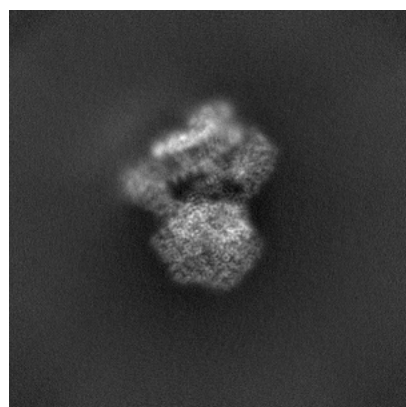


Y

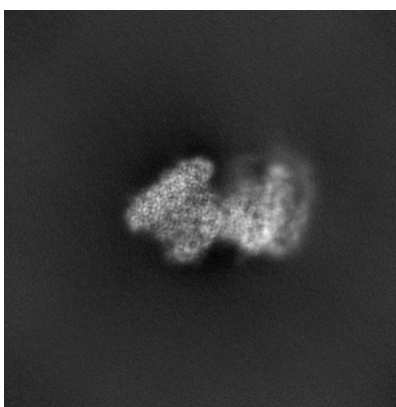


Z

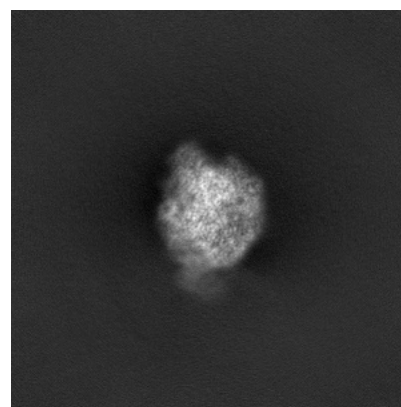
#### 6.1.2 Raw map



X



Y

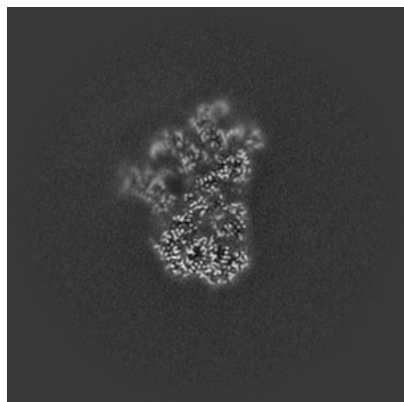


Z

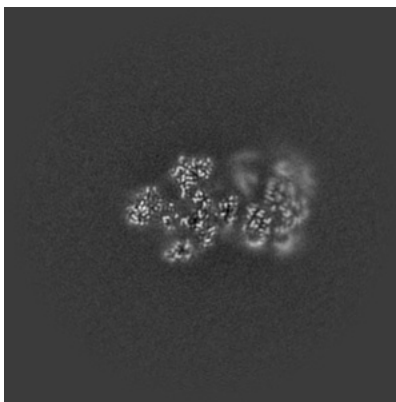
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

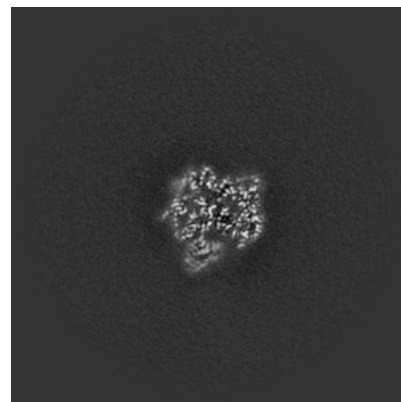
### 6.2.1 Primary map



X Index: 256

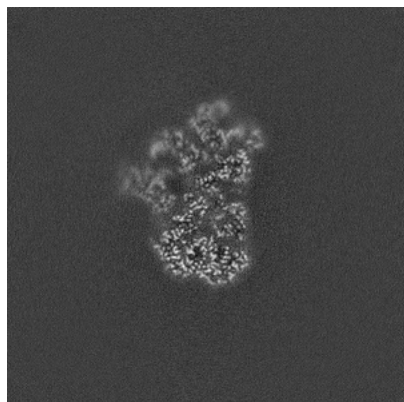


Y Index: 256

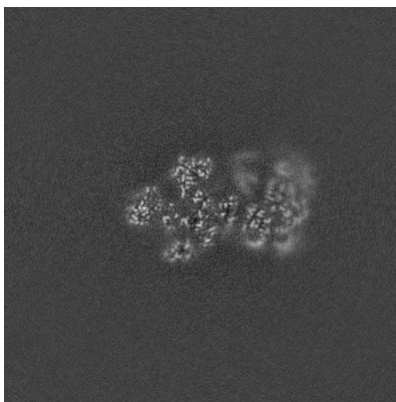


Z Index: 256

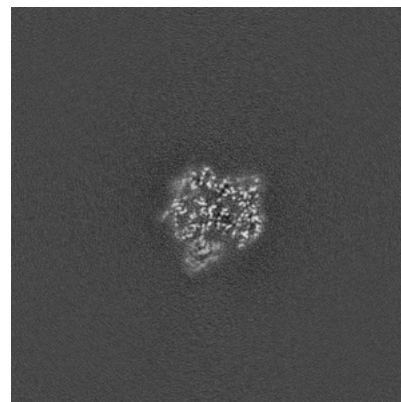
### 6.2.2 Raw map



X Index: 256



Y Index: 256

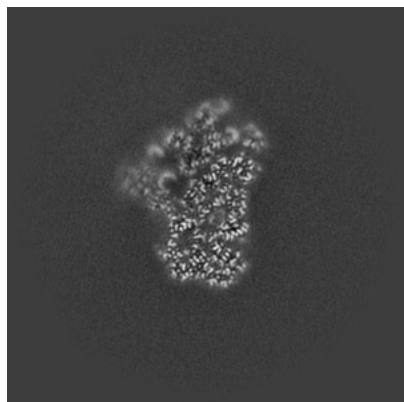


Z Index: 256

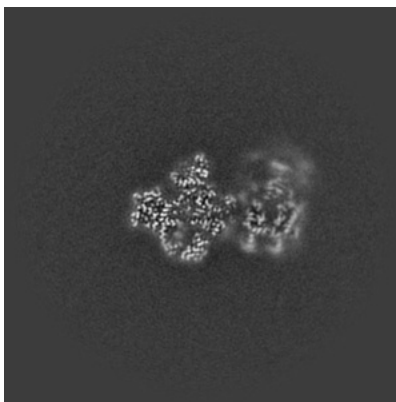
The images above show central slices of the map in three orthogonal directions.

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

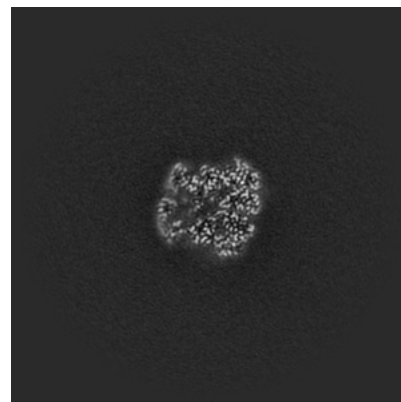
### 6.3.1 Primary map



X Index: 249

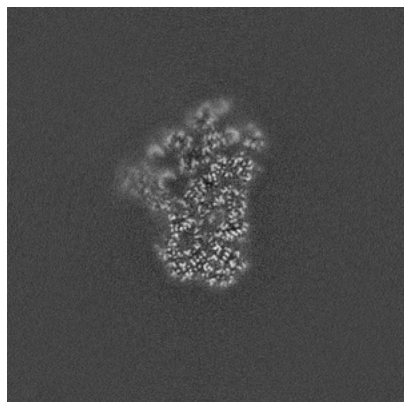


Y Index: 245

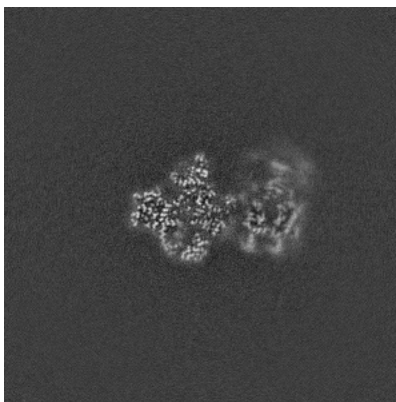


Z Index: 230

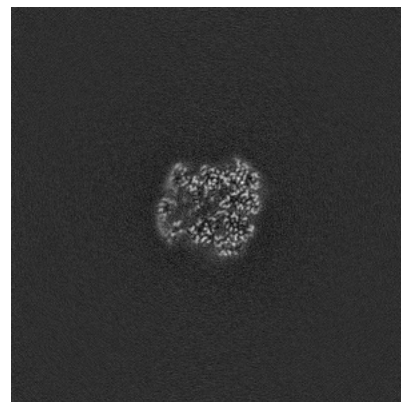
### 6.3.2 Raw map



X Index: 250



Y Index: 245



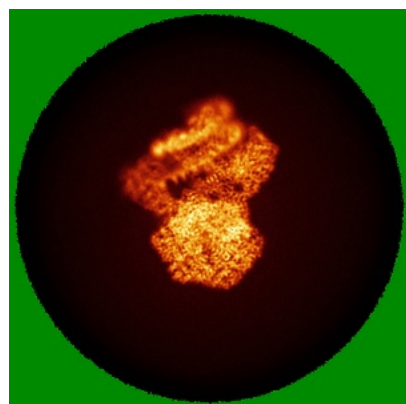
Z Index: 230

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

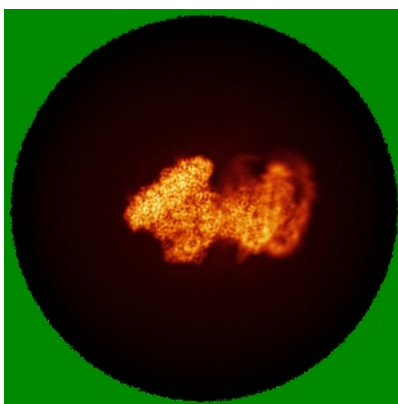


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

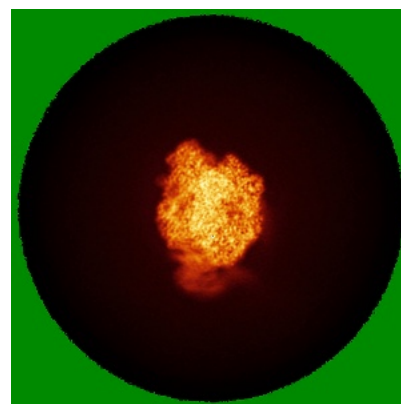
### 6.4.1 Primary map



X

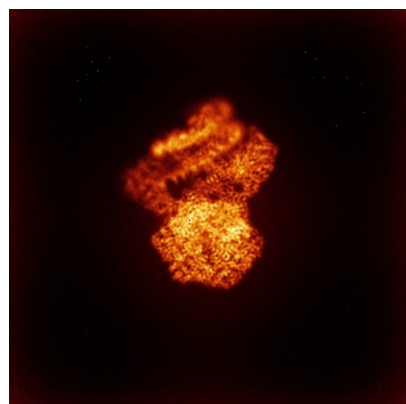


Y

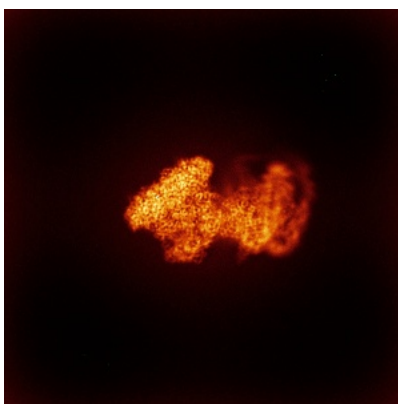


Z

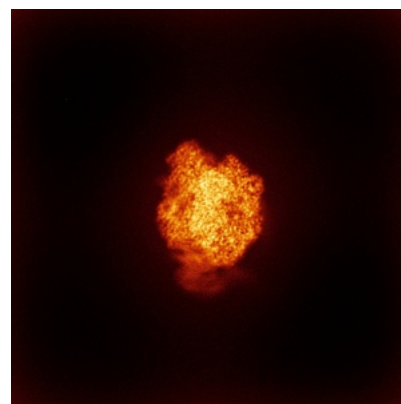
### 6.4.2 Raw map



X



Y



Z

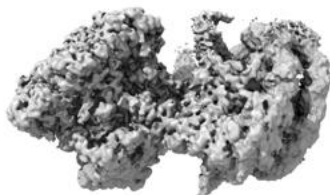
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 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 0.153. 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](#)

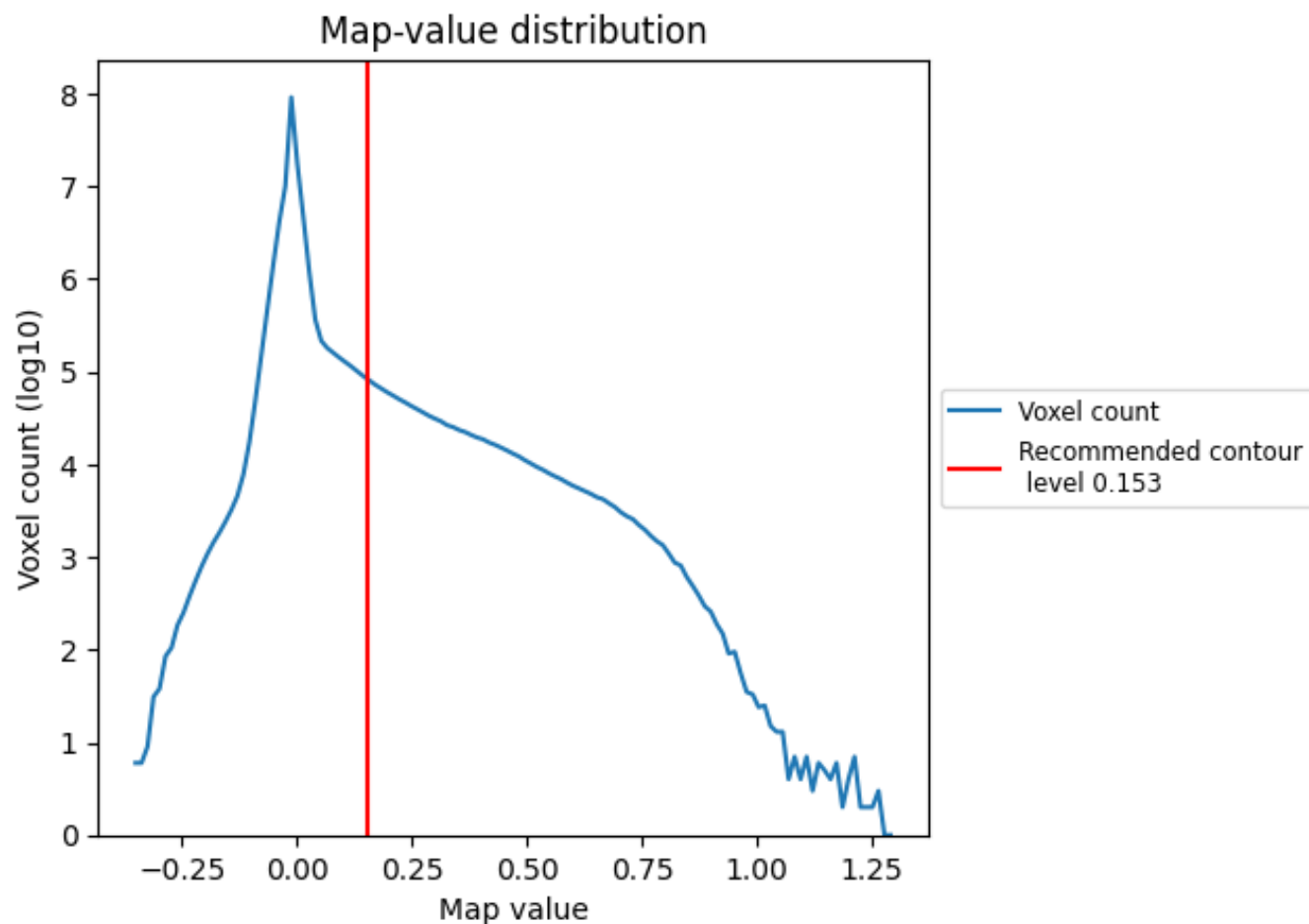
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

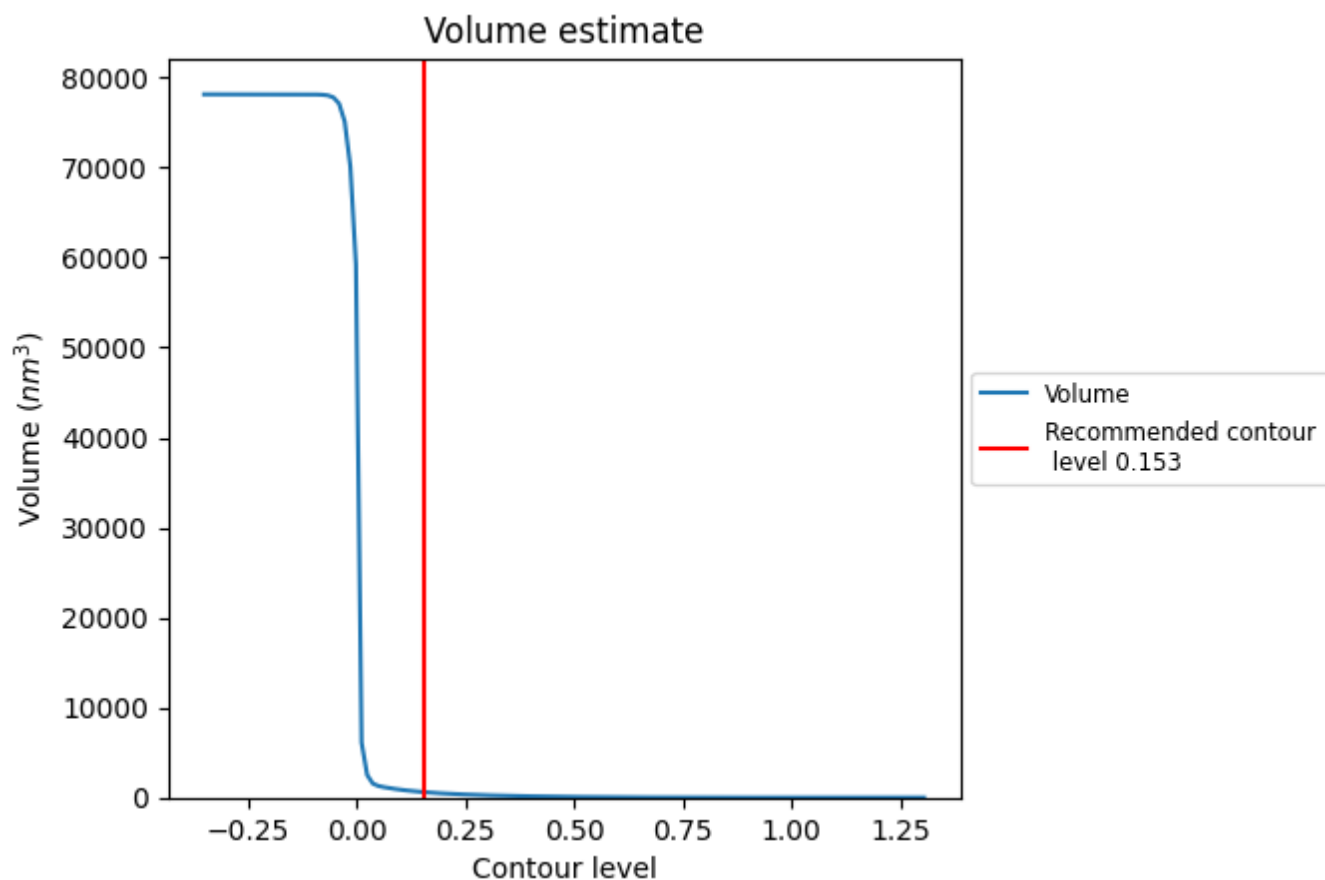
This section contains the results of statistical analysis of the map.

### 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.

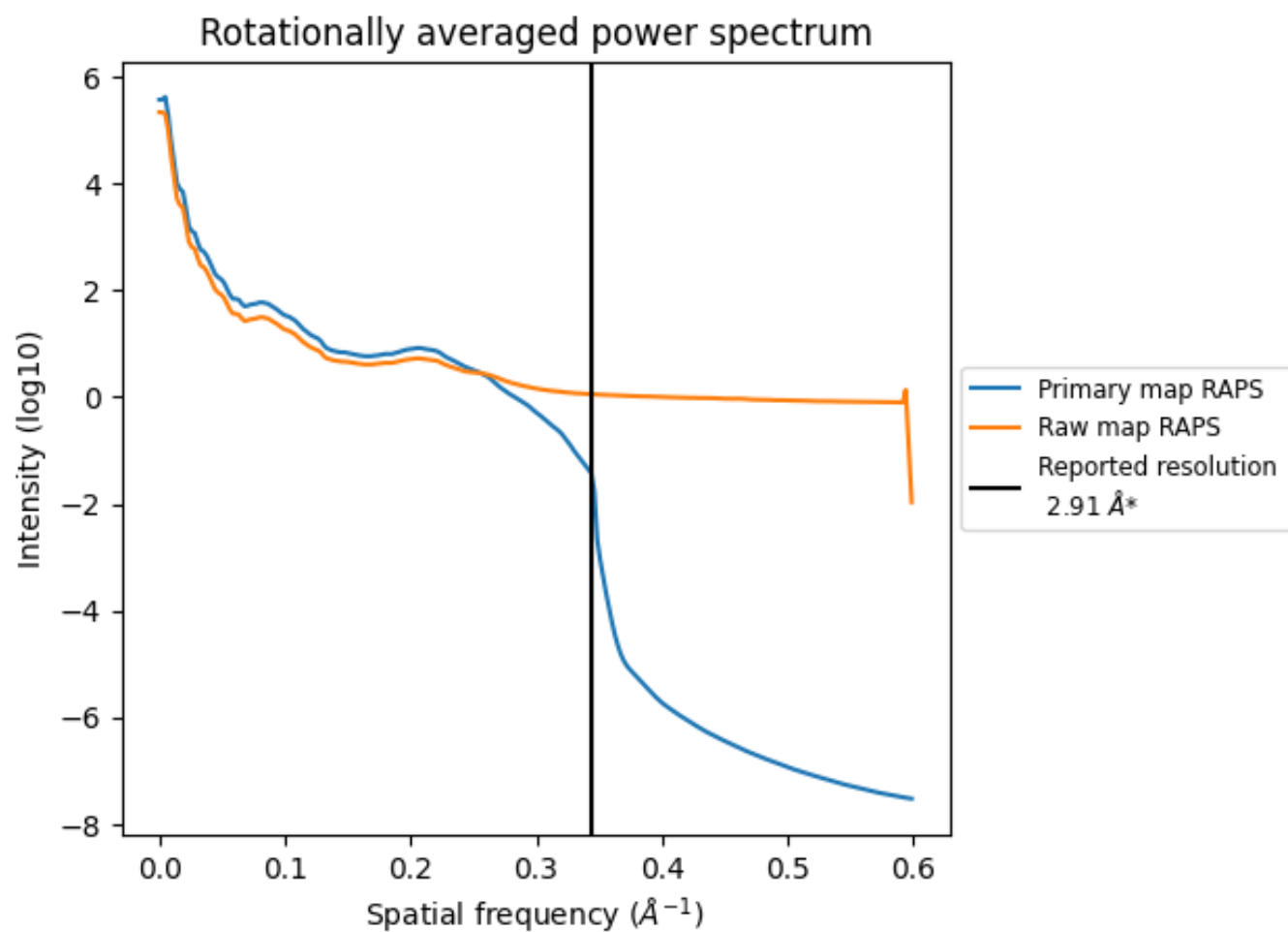
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 608  $\text{nm}^3$ ; this corresponds to an approximate mass of 549 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 ⓘ

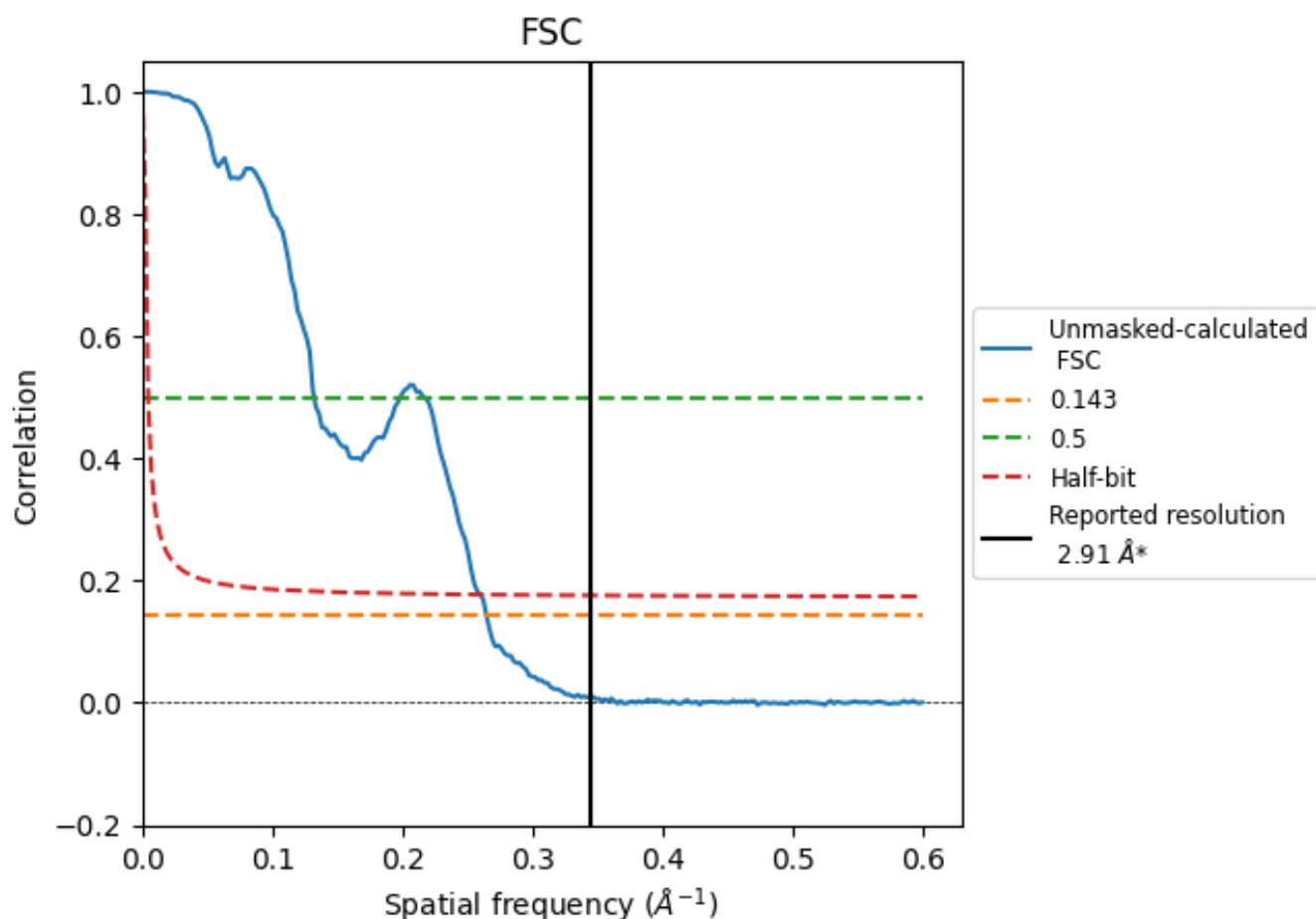


\*Reported resolution corresponds to spatial frequency of 0.344 Å<sup>-1</sup>

## 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  $0.344 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

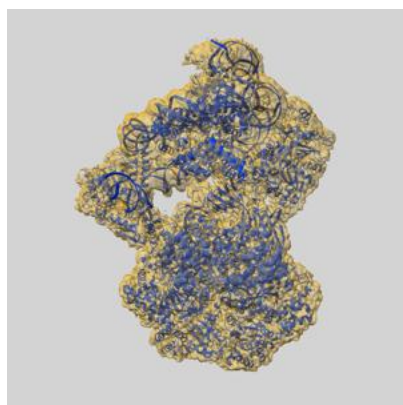
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	7.58	3.85

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 2.91 by more than 10 %

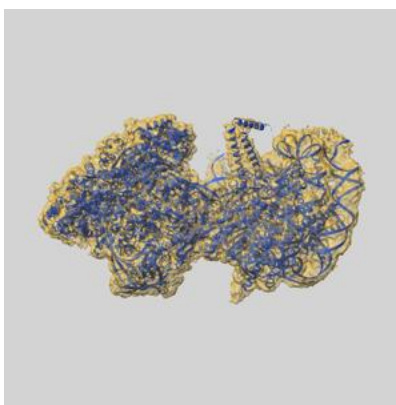
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45361 and PDB model 9C9G. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

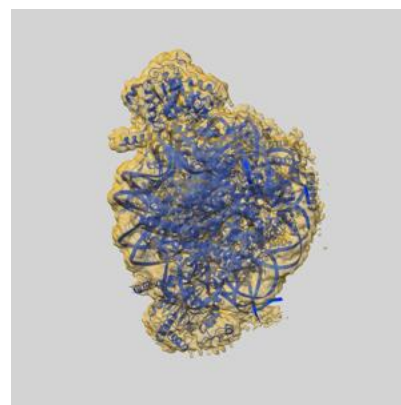
### 9.1 Map-model overlay [i](#)



X



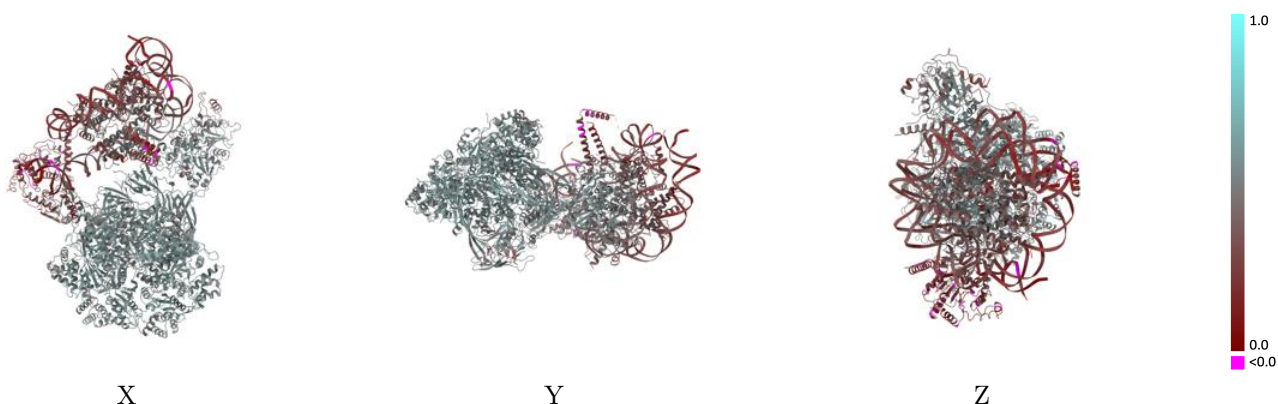
Y



Z

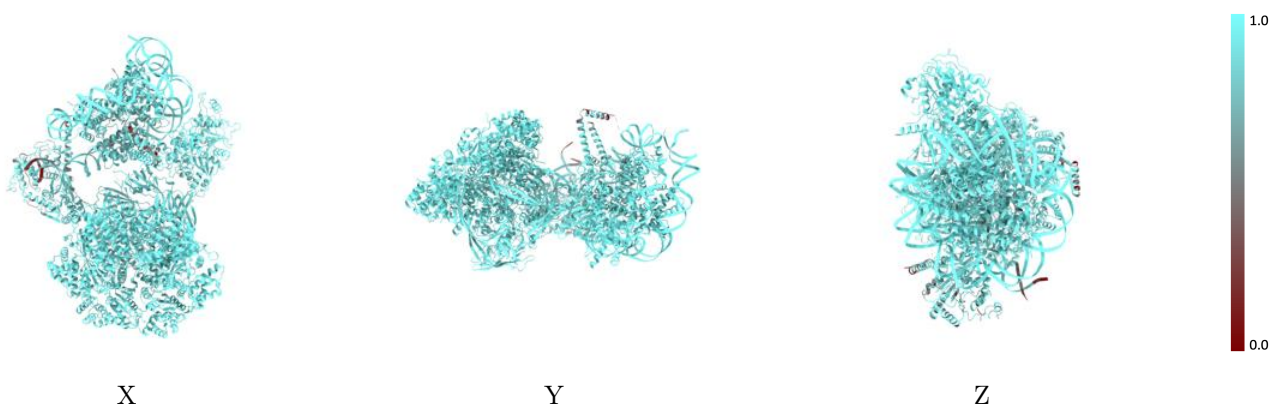
The images above show the 3D surface view of the map at the recommended contour level 0.153 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



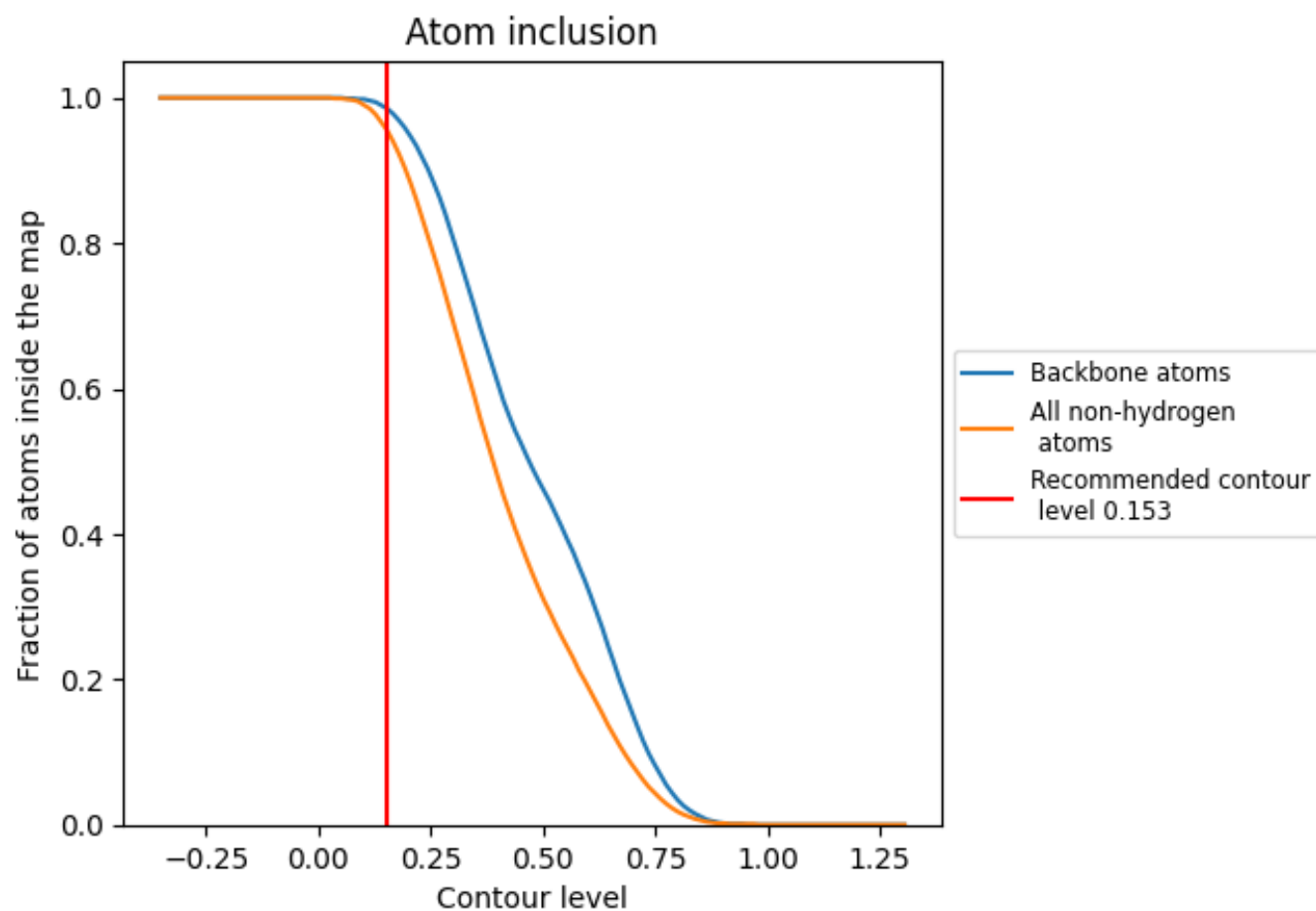
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.153).

## 9.4 Atom inclusion [i](#)













































At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.153) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.4450
A	 0.9700	 0.3640
B	 0.9720	 0.3810
C	 0.9600	 0.3420
D	 0.9560	 0.3580
E	 0.9250	 0.3400
F	 0.9130	 0.3770
G	 0.9200	 0.4510
H	 0.9280	 0.4570
I	 0.9540	 0.2560
J	 0.9570	 0.2580
Q	 0.8990	 0.3630
R	 0.9580	 0.4590
S	 0.9810	 0.4700
T	 0.9690	 0.5380
U	 0.9620	 0.5390
V	 0.9720	 0.5450
W	 0.9780	 0.5380
X	 0.9760	 0.5210
Y	 0.9790	 0.5300
Z	 0.8630	 0.3870

