



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 09:23 PM UTC

PDB ID : 9OB1 / pdb\_00009ob1  
EMDB ID : EMD-70289  
Title : S.c INO80 in complex with Yeast 0/80 nucleosome, Apo State  
Authors : Wu, H.; Kaur, U.; Narlikar, G.J.; Cheng, Y.F.  
Deposited on : 2025-04-21  
Resolution : 3.20 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

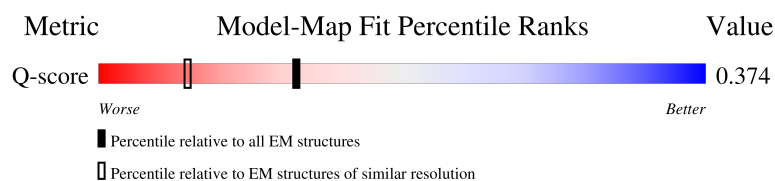
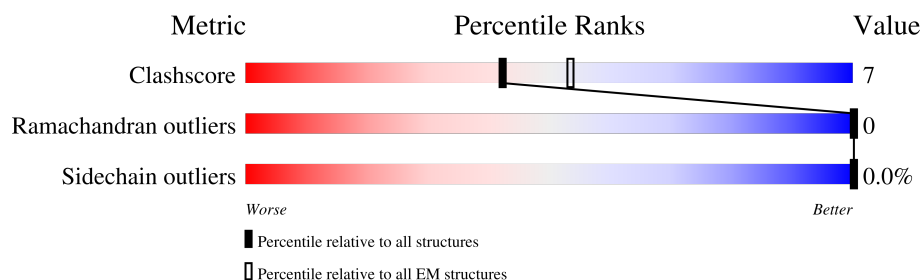
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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.



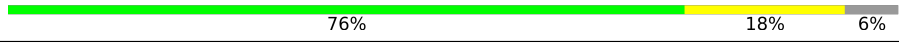



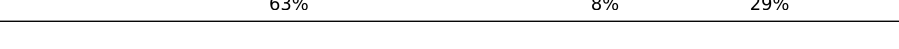







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

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	I	227	
2	J	227	
3	Q	1489	
4	R	755	

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Mol	Chain	Length	Quality of chain
5	S	166	
6	T	463	
6	V	463	
6	X	463	
7	U	471	
7	W	471	
7	Y	471	
8	Z	320	
9	A	136	
9	E	136	
10	B	103	
10	F	103	
11	C	132	
11	G	132	
12	D	131	
12	H	131	

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 40498 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 DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	145	Total	C	N	O	P	0	0
			2954	1404	537	869	144		

- Molecule 2 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	145	Total	C	N	O	P	0	0
			2985	1414	560	867	144		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	419	Total	C	N	O	S	0	0
			3372	2143	565	649	15		

- Molecule 4 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	442	Total	C	N	O	S	0	0
			3512	2235	591	675	11		

- Molecule 5 is a protein called Chromatin-remodeling complex subunit IES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	128	Total	C	N	O	S	0	0
			1015	652	184	177	2		

- Molecule 6 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	437	Total	C	N	O	S	0	0
			3351	2111	578	652	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	442	Total	C	N	O	S	0	0
			3394	2141	584	659	10		
6	X	443	Total	C	N	O	S	0	0
			3404	2149	585	660	10		

- Molecule 7 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	445	Total	C	N	O	S	0	0
			3421	2138	594	677	12		
7	W	442	Total	C	N	O	S	0	0
			3398	2123	590	673	12		
7	Y	436	Total	C	N	O	S	0	0
			3351	2097	583	660	11		

- Molecule 8 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	28	Total	C	N	O	S	0	0
			245	155	45	43	2		

- Molecule 9 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	97	Total	C	N	O		0	0
			801	508	155	138			
9	E	97	Total	C	N	O		0	0
			794	502	155	137			

- 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	389	121	110	1		
10	F	79	Total	C	N	O	S	0	0
			620	389	120	110	1		

- Molecule 11 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	106	Total	C	N	O		0	0
			819	514	161	144			

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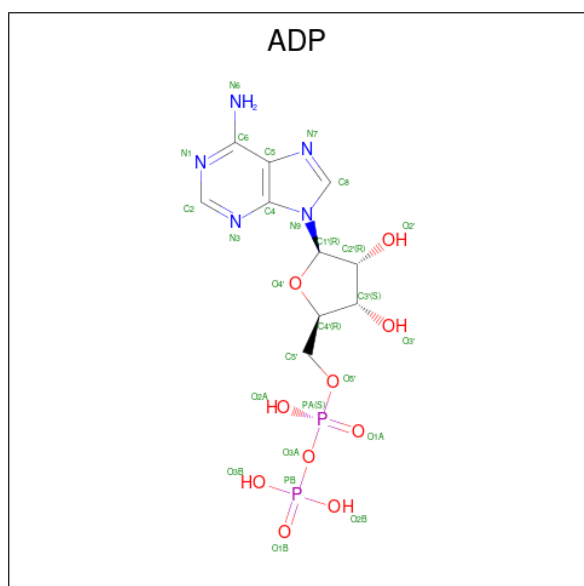
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Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	108	Total	C	N	O	0	0
			827	517	164	146		

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

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

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



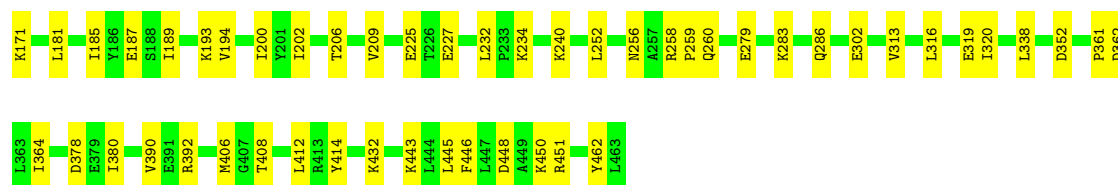
Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	



- Molecule 4: Actin-related protein 5

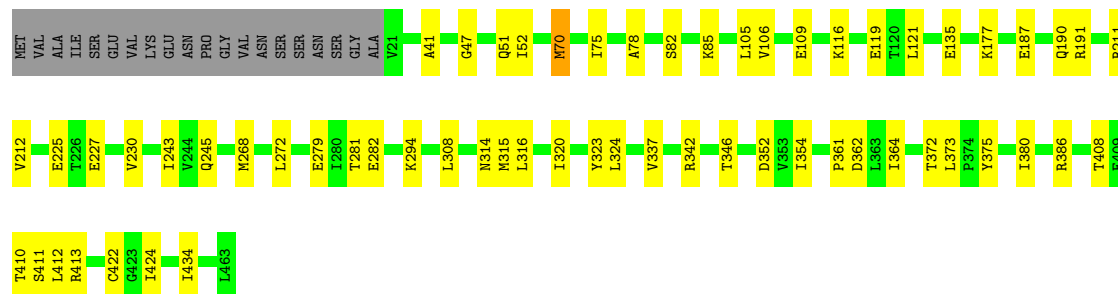






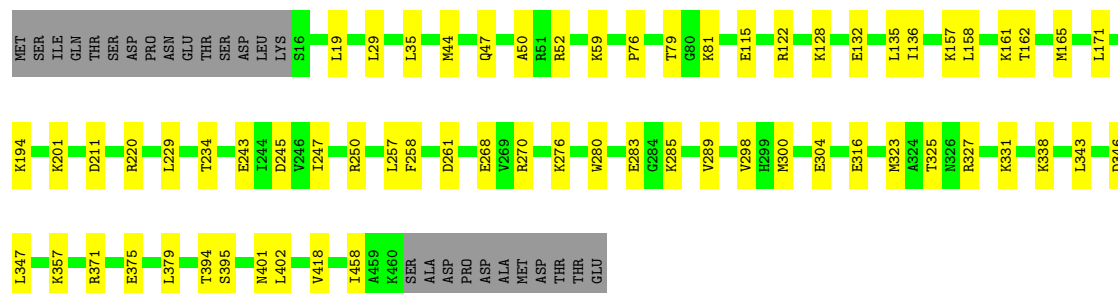
• Molecule 6: RuvB-like protein 1

Chain X: 83% 13% .



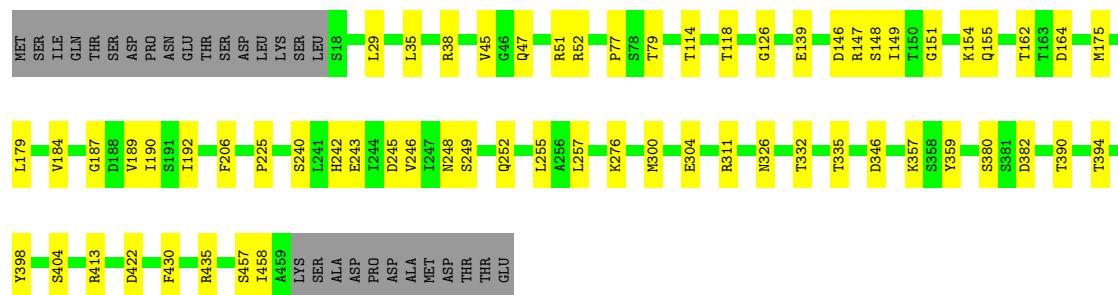
• Molecule 7: RuvB-like protein 2

Chain U: 81% 14% 6%



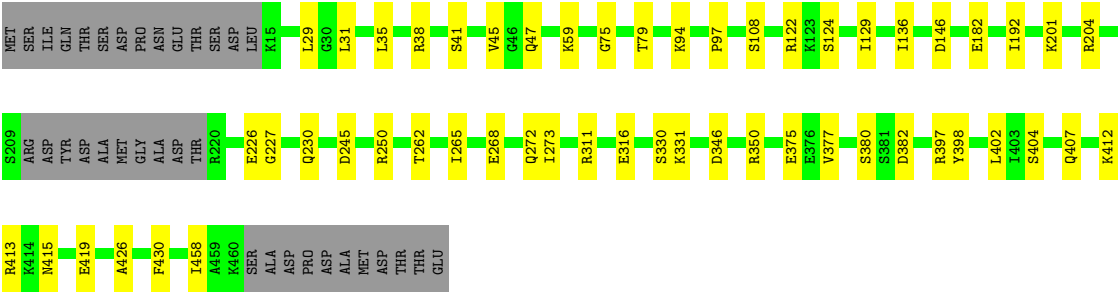
• Molecule 7: RuvB-like protein 2

Chain W: 80% 13% 6%



• Molecule 7: RuvB-like protein 2

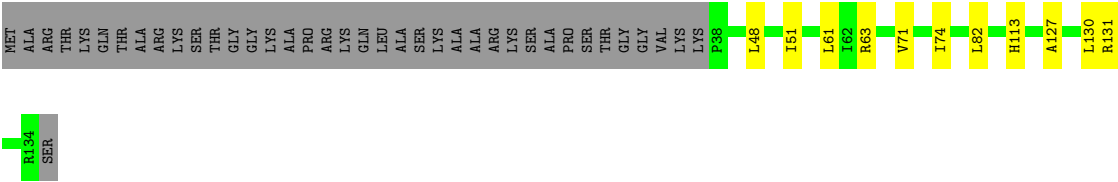
Chain Y: 81% 11% 7%



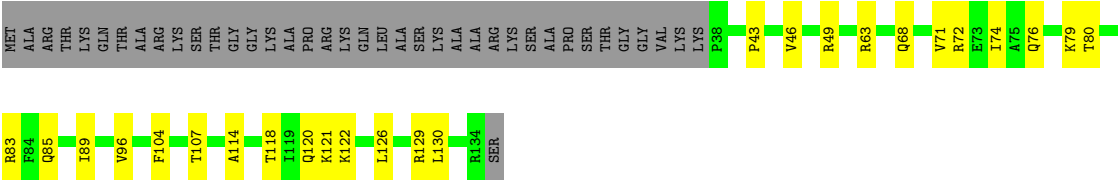
• Molecule 8: Ino eighty subunit 2



• Molecule 9: Histone H3



• Molecule 9: Histone H3



• Molecule 10: Histone H4

Chain B: 



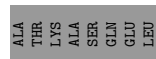
- Molecule 10: Histone H4

Chain F: 



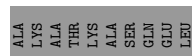
- Molecule 11: Histone H2A.1

Chain C: 



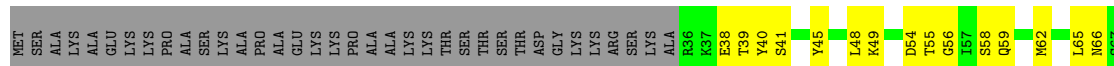
- Molecule 11: Histone H2A.1

Chain G: 



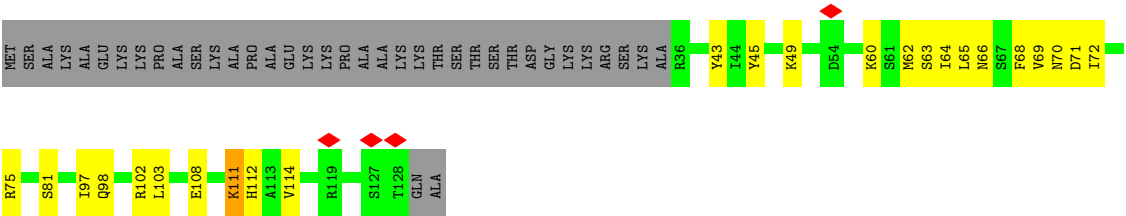
- Molecule 12: Histone H2B.1

Chain D: 



- Molecule 12: Histone H2B.1

Chain H: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17836	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47.7	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	0.929	Depositor
Minimum map value	-0.412	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.08	Depositor
Map size ( $\text{\AA}$ )	366.8672, 366.8672, 366.8672	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8189, 0.8189, 0.8189	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

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	I	0.20	0/3310	0.41	0/5103
2	J	0.19	0/3352	0.40	0/5176
3	Q	0.24	0/3436	0.54	1/4660 (0.0%)
4	R	0.22	0/3602	0.56	5/4903 (0.1%)
5	S	0.26	0/1037	0.63	1/1397 (0.1%)
6	T	0.22	0/3390	0.46	1/4585 (0.0%)
6	V	0.22	0/3436	0.49	0/4648
6	X	0.25	0/3446	0.53	2/4662 (0.0%)
7	U	0.21	0/3459	0.42	0/4662
7	W	0.21	0/3436	0.43	2/4632 (0.0%)
7	Y	0.20	0/3387	0.44	0/4562
8	Z	0.22	0/251	0.43	0/334
9	A	0.21	0/812	0.50	0/1086
9	E	0.18	0/804	0.43	0/1075
10	B	0.25	0/628	0.68	2/840 (0.2%)
10	F	0.29	0/627	0.70	1/840 (0.1%)
11	C	0.21	0/830	0.54	0/1121
11	G	0.26	0/838	0.64	0/1131
12	D	0.25	0/736	0.72	0/991
12	H	0.28	0/736	0.70	1/991 (0.1%)
All	All	0.22	0/41553	0.50	16/57399 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	45	PRO	CA-N-CD	-6.56	102.81	112.00
6	T	70	MET	CB-CG-SD	6.18	131.23	112.70
12	H	111	LYS	CA-CB-CG	6.14	126.38	114.10
10	F	41	ARG	CA-CB-CG	5.95	126.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	89	TYR	CA-CB-CG	5.93	124.57	113.90
4	R	83	GLY	N-CA-C	5.77	117.21	111.21
4	R	19	PRO	N-CA-C	5.76	117.72	110.70
6	X	294	LYS	CB-CG-CD	5.71	124.42	111.30
4	R	87	LEU	CA-CB-CG	5.53	135.65	116.30
7	W	300	MET	CB-CG-SD	5.38	128.83	112.70
4	R	614	LEU	CA-CB-CG	5.30	134.86	116.30
4	R	126	PRO	CA-N-CD	-5.29	104.59	112.00
3	Q	1293	ARG	CA-CB-CG	5.25	124.61	114.10
6	X	70	MET	CB-CG-SD	5.20	128.28	112.70
10	B	96	ARG	CG-CD-NE	5.11	123.24	112.00
7	W	175	MET	CB-CG-SD	5.05	127.86	112.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	I	2954	0	1629	23	0
2	J	2985	0	1628	16	0
3	Q	3372	0	3339	62	0
4	R	3512	0	3374	43	0
5	S	1015	0	1033	9	0
6	T	3351	0	3464	59	0
6	V	3394	0	3524	52	0
6	X	3404	0	3542	42	0
7	U	3421	0	3499	46	0
7	W	3398	0	3470	43	0
7	Y	3351	0	3439	41	0
8	Z	245	0	233	3	0
9	A	801	0	851	16	0
9	E	794	0	844	34	0
10	B	621	0	645	22	0
10	F	620	0	643	21	0
11	C	819	0	865	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	827	0	865	16	0
12	D	726	0	748	29	0
12	H	726	0	748	16	0
13	T	27	0	12	3	0
13	U	27	0	12	0	0
13	V	27	0	12	2	0
13	W	27	0	12	2	0
13	X	27	0	12	2	0
13	Y	27	0	12	2	0
All	All	40498	0	38455	498	0

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

All (498) 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)
9:E:96:VAL:CG1	10:F:63:LEU:HD21	1.59	1.29
9:E:96:VAL:HG12	10:F:63:LEU:HD21	1.10	1.06
9:A:113:HIS:HB2	9:E:126:LEU:HD22	1.37	1.02
6:V:35:LEU:CD2	6:V:41:ALA:HB2	1.89	1.01
9:A:113:HIS:CB	9:E:126:LEU:HD22	1.91	0.99
6:V:35:LEU:HD23	6:V:41:ALA:HB2	1.47	0.97
3:Q:1183:SER:O	3:Q:1184:GLU:HG2	1.67	0.95
11:C:59:LEU:HG	12:D:68:PHE:HZ	1.32	0.93
9:E:96:VAL:HG11	10:F:63:LEU:HD11	1.51	0.93
6:T:111:TYR:CD1	6:T:117:LYS:HD3	2.04	0.91
9:E:96:VAL:HG12	10:F:63:LEU:CD2	1.99	0.91
9:E:96:VAL:CG1	10:F:63:LEU:CD2	2.50	0.87
11:C:59:LEU:HD21	12:D:68:PHE:CE1	2.12	0.85
6:X:191:ARG:NH1	6:X:268:MET:HE1	1.92	0.85
9:A:113:HIS:CG	9:E:126:LEU:CD2	2.62	0.82
9:A:113:HIS:CG	9:E:126:LEU:HD22	2.16	0.81
6:V:35:LEU:HD23	6:V:41:ALA:CB	2.11	0.79
6:X:191:ARG:CZ	6:X:268:MET:HE1	2.14	0.78
9:E:96:VAL:HG13	10:F:63:LEU:HD21	1.63	0.76
4:R:134:ILE:HG22	4:R:160:VAL:HG11	1.70	0.74
6:T:117:LYS:HD2	6:T:320:ILE:HD11	1.72	0.72
9:A:113:HIS:CB	9:E:126:LEU:CD2	2.66	0.71
11:C:59:LEU:HD21	12:D:68:PHE:HE1	1.53	0.70
11:C:59:LEU:CG	12:D:68:PHE:HZ	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:35:LEU:HD21	6:V:41:ALA:HB2	1.76	0.68
11:G:56:LEU:HD11	12:H:69:VAL:HG23	1.75	0.67
11:C:59:LEU:CD2	12:D:68:PHE:CZ	2.77	0.67
6:T:111:TYR:CD1	6:T:117:LYS:CD	2.76	0.66
7:Y:136:ILE:HB	7:Y:192:ILE:HB	1.75	0.66
3:Q:1183:SER:O	3:Q:1184:GLU:CG	2.44	0.65
5:S:49:LYS:HG3	5:S:51:ALA:H	1.62	0.64
6:T:130:GLY:HA2	6:T:248:THR:HA	1.79	0.64
6:T:284:LEU:HD12	7:U:258:PHE:HB3	1.80	0.63
6:T:260:GLN:HE21	6:T:273:LEU:HG	1.64	0.63
4:R:143:VAL:HB	4:R:146:GLN:HG3	1.79	0.63
9:E:79:LYS:HZ1	10:F:71:VAL:HB	1.64	0.62
3:Q:1317:ARG:HH12	3:Q:1319:LEU:HB2	1.64	0.62
11:C:33:ARG:HA	11:C:37:ARG:HH21	1.65	0.61
4:R:277:VAL:HB	4:R:612:MET:HB3	1.82	0.61
7:U:250:ARG:NH2	7:U:261:ASP:O	2.34	0.61
6:V:42:LYS:O	6:V:55:ARG:NH2	2.33	0.61
12:D:49:LYS:NZ	12:D:55:THR:O	2.34	0.61
4:R:134:ILE:HG23	4:R:163:VAL:HG23	1.83	0.60
7:W:151:GLY:O	7:W:154:LYS:NZ	2.34	0.60
10:F:30:ILE:O	10:F:56:ARG:NH2	2.35	0.60
10:F:62:PHE:CE2	10:F:63:LEU:HD23	2.37	0.60
12:H:102:ARG:HE	12:H:103:LEU:HD22	1.66	0.60
2:J:-13:DA:OP2	10:F:37:ARG:NH2	2.35	0.59
5:S:64:ARG:O	5:S:64:ARG:NH1	2.35	0.59
3:Q:1427:THR:HG23	3:Q:1429:GLU:H	1.66	0.59
6:T:111:TYR:HA	6:T:117:LYS:HG2	1.82	0.59
4:R:67:LEU:HB2	4:R:82:VAL:HA	1.84	0.59
1:I:37:DC:O2	2:J:-36:DG:N2	2.35	0.59
6:T:111:TYR:HD1	6:T:117:LYS:HD3	1.62	0.58
6:X:314:ASN:HD22	6:X:342:ARG:HG2	1.68	0.58
6:V:73:ARG:NH2	7:W:404:SER:OG	2.36	0.58
6:T:364:ILE:HA	6:T:367:LEU:HD12	1.85	0.58
6:V:29:HIS:HB3	6:V:390:VAL:HG21	1.84	0.58
4:R:225:ASP:HB3	5:S:158:LEU:HD11	1.85	0.58
6:T:313:VAL:HG21	6:T:338:LEU:HD13	1.86	0.58
4:R:138:GLU:HB2	4:R:165:PHE:HB2	1.84	0.57
9:E:46:VAL:HG23	9:E:49:ARG:HH21	1.69	0.57
6:T:110:LEU:O	6:T:117:LYS:HG2	2.04	0.57
3:Q:1033:LYS:O	7:Y:201:LYS:NZ	2.37	0.57
11:C:59:LEU:HD21	12:D:68:PHE:CZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:49:DC:H5''	12:D:38:GLU:HA	1.86	0.57
3:Q:1182:PRO:HD2	6:V:206:THR:HG22	1.85	0.57
7:U:325:THR:HG22	7:U:327:ARG:H	1.70	0.57
1:I:-28:DT:O2	2:J:29:DG:N2	2.38	0.57
3:Q:1293:ARG:HH11	3:Q:1297:GLU:HG3	1.70	0.57
9:E:96:VAL:CG1	10:F:63:LEU:HD11	2.31	0.57
6:V:202:ILE:HG12	6:V:209:VAL:HG12	1.87	0.57
7:Y:29:LEU:HB3	7:Y:31:LEU:HD13	1.86	0.57
4:R:72:ASP:H	4:R:77:LYS:HA	1.69	0.56
4:R:230:LYS:NZ	4:R:613:HIS:O	2.37	0.56
4:R:624:VAL:HG23	4:R:630:MET:HB2	1.86	0.56
6:V:406:MET:SD	6:V:443:LYS:NZ	2.73	0.56
6:X:191:ARG:CZ	6:X:268:MET:CE	2.82	0.56
10:F:28:GLN:HA	10:F:56:ARG:HH22	1.70	0.56
4:R:43:ASP:OD2	4:R:50:ARG:NH1	2.39	0.56
3:Q:1301:LEU:HD21	3:Q:1333:GLU:HG3	1.86	0.56
7:W:126:GLY:HA2	7:W:240:SER:HA	1.88	0.56
9:A:113:HIS:CG	9:E:126:LEU:HD23	2.40	0.56
11:C:59:LEU:CD2	12:D:68:PHE:CE1	2.88	0.56
4:R:51:ALA:HB3	4:R:61:HIS:HB2	1.88	0.56
7:U:136:ILE:HD11	7:U:194:LYS:HG3	1.87	0.56
7:W:47:GLN:NE2	7:W:357:LYS:O	2.38	0.56
6:T:73:ARG:NH2	7:U:401:ASN:O	2.40	0.55
4:R:615:ASN:HA	4:R:618:ARG:HB3	1.88	0.55
7:U:162:THR:HG23	7:U:229:LEU:HD12	1.88	0.55
11:C:64:LEU:HD22	12:D:48:LEU:HD13	1.88	0.55
6:T:106:VAL:HG12	6:T:108:SER:H	1.71	0.55
1:I:38:DT:O2	2:J:-37:DG:N2	2.40	0.55
5:S:67:ILE:HG23	5:S:101:PHE:HE2	1.72	0.55
7:Y:382:ASP:OD1	7:Y:382:ASP:N	2.39	0.55
10:F:62:PHE:CE2	10:F:63:LEU:CD2	2.90	0.55
7:Y:413:ARG:NH2	7:Y:419:GLU:OE1	2.40	0.55
6:T:76:LEU:HD23	6:T:369:ILE:HG12	1.88	0.55
4:R:275:VAL:O	4:R:615:ASN:ND2	2.39	0.54
7:Y:136:ILE:HG12	7:Y:230:GLN:HB2	1.89	0.54
6:T:280:ILE:HB	6:T:285:ARG:HH21	1.72	0.54
11:C:85:GLN:NE2	11:C:107:GLY:O	2.41	0.54
1:I:-54:DA:H5'	12:D:58:SER:HA	1.89	0.54
6:T:325:ASN:OD1	6:T:366:ARG:NH1	2.40	0.54
6:V:225:GLU:HG3	6:V:227:GLU:H	1.72	0.54
6:T:182:ASP:N	6:T:182:ASP:OD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:18:ARG:HA	11:G:21:LYS:HG2	1.89	0.54
3:Q:1280:LYS:NZ	6:X:225:GLU:O	2.37	0.54
6:X:51:GLN:NE2	6:X:373:LEU:O	2.41	0.54
7:W:155:GLN:NE2	8:Z:301:ASN:O	2.39	0.54
3:Q:1103:ASP:HB2	6:T:206:THR:HG21	1.89	0.54
6:V:283:LYS:O	6:V:286:GLN:NE2	2.41	0.54
3:Q:1210:TYR:HB3	7:W:248:ASN:HB3	1.90	0.54
6:V:408:THR:HG22	7:W:458:ILE:HD11	1.89	0.53
1:I:26:DG:N2	2:J:-25:DC:O2	2.41	0.53
4:R:29:ASP:OD1	4:R:29:ASP:N	2.42	0.53
11:C:113:HIS:HB2	11:C:116:LEU:HG	1.90	0.53
4:R:168:ASP:OD1	4:R:168:ASP:N	2.39	0.53
6:T:151:ASP:HA	6:T:163:ILE:HA	1.91	0.53
6:T:211:ARG:NH2	6:T:227:GLU:OE2	2.41	0.53
7:W:243:GLU:HA	7:W:257:LEU:HD21	1.90	0.53
9:E:96:VAL:HG12	10:F:62:PHE:HE2	1.74	0.53
1:I:26:DG:H4'	9:E:83:ARG:HH12	1.73	0.53
6:X:75:ILE:HG12	6:X:337:VAL:HG12	1.91	0.53
7:U:115:GLU:OE2	7:U:270:ARG:NH2	2.42	0.53
3:Q:1023:ASP:HB3	3:Q:1287:SER:HB2	1.91	0.53
7:W:359:TYR:OH	13:W:501:ADP:N7	2.41	0.53
1:I:-13:DA:OP2	10:B:37:ARG:NH1	2.41	0.53
2:J:68:DC:H2''	2:J:69:DT:C5	2.44	0.53
6:X:135:GLU:N	6:X:243:ILE:O	2.40	0.53
1:I:29:DA:OP2	10:F:79:ARG:NH1	2.42	0.53
6:T:62:VAL:HA	6:T:65:ILE:HD12	1.91	0.53
1:I:-14:DA:O3'	9:A:63:ARG:NH1	2.41	0.53
3:Q:1121:ASN:OD1	6:T:290:LYS:NZ	2.41	0.53
6:V:26:ALA:O	13:V:501:ADP:O3'	2.27	0.53
6:T:29:HIS:NE2	13:T:501:ADP:O2'	2.33	0.52
6:T:408:THR:HG22	7:U:458:ILE:HD11	1.90	0.52
7:W:77:PRO:HG3	7:W:326:ASN:HD22	1.75	0.52
3:Q:1394:SER:HB3	3:Q:1432:MET:HE1	1.91	0.52
3:Q:1035:THR:OG1	7:Y:204:ARG:NH1	2.42	0.52
7:U:280:TRP:HA	7:U:283:GLU:HG2	1.91	0.52
1:I:-54:DA:OP2	12:D:59:GLN:NE2	2.38	0.52
6:T:315:MET:HA	6:T:348:ARG:HD3	1.91	0.52
6:T:463:LEU:HD22	7:Y:75:GLY:HA2	1.91	0.52
7:Y:380:SER:OG	7:Y:382:ASP:OD1	2.27	0.52
6:V:132:ARG:HB3	6:V:302:GLU:HB3	1.92	0.52
6:V:352:ASP:N	6:V:352:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:61:LEU:HD12	10:B:41:ARG:HD3	1.92	0.52
6:T:23:ARG:NH1	7:Y:316:GLU:O	2.43	0.51
7:W:162:THR:OG1	7:W:225:PRO:O	2.26	0.51
10:B:32:LYS:HD2	10:B:56:ARG:HH22	1.75	0.51
4:R:29:ASP:H	4:R:121:HIS:HE1	1.59	0.51
7:U:29:LEU:HD23	7:U:44:MET:HE1	1.93	0.51
11:C:36:ARG:HE	11:C:37:ARG:HH22	1.56	0.51
6:X:362:ASP:OD1	6:X:362:ASP:N	2.43	0.51
11:G:91:ASP:HB3	11:G:94:LEU:HB2	1.92	0.51
3:Q:1078:ARG:NH1	7:Y:182:GLU:OE2	2.44	0.51
12:H:108:GLU:O	12:H:112:HIS:ND1	2.43	0.51
6:T:424:ILE:HD13	7:Y:59:LYS:HB3	1.93	0.51
11:C:59:LEU:HG	12:D:68:PHE:CZ	2.25	0.51
6:T:449:ALA:O	6:T:453:THR:OG1	2.28	0.51
7:U:47:GLN:HB3	7:U:50:ALA:HB3	1.93	0.51
10:B:30:ILE:HG23	10:B:56:ARG:HE	1.76	0.51
10:B:85:MET:SD	10:B:85:MET:N	2.84	0.51
7:W:398:TYR:OH	7:W:435:ARG:NH2	2.44	0.51
6:X:413:ARG:NH2	13:X:501:ADP:O3A	2.44	0.51
3:Q:1086:PRO:HG2	7:Y:129:ILE:HD12	1.92	0.50
3:Q:976:ASP:N	3:Q:976:ASP:OD1	2.40	0.50
6:V:22:THR:OG1	6:V:392:ARG:NH2	2.44	0.50
6:X:212:VAL:HG12	6:X:230:VAL:HG11	1.92	0.50
9:E:129:ARG:O	9:E:129:ARG:NH1	2.42	0.50
3:Q:1087:ARG:NH1	3:Q:1224:LEU:O	2.41	0.50
6:V:138:GLU:HB2	6:V:240:LYS:HD3	1.92	0.50
3:Q:1254:GLN:OE1	7:W:148:SER:OG	2.29	0.50
7:Y:122:ARG:NE	7:Y:245:ASP:OD2	2.43	0.50
11:G:66:LEU:HB3	11:G:87:ALA:HB1	1.93	0.50
3:Q:1207:GLN:N	3:Q:1207:GLN:OE1	2.45	0.50
6:V:450:LYS:NZ	7:W:457:SER:OG	2.44	0.50
11:G:89:ARG:NH1	11:G:95:ASN:OD1	2.45	0.50
3:Q:1324:MET:HE3	3:Q:1325:THR:H	1.77	0.50
6:T:154:ASN:OD1	6:T:154:ASN:N	2.43	0.50
7:W:179:LEU:HD22	7:W:184:VAL:HG21	1.93	0.50
9:A:61:LEU:HD13	10:B:37:ARG:HB3	1.94	0.50
6:V:117:LYS:NZ	6:V:319:GLU:OE1	2.40	0.49
6:V:362:ASP:OD1	6:V:362:ASP:N	2.45	0.49
10:B:76:HIS:HB2	12:D:99:THR:HG21	1.94	0.49
6:V:252:LEU:O	6:V:256:ASN:ND2	2.45	0.49
7:W:380:SER:OG	7:W:382:ASP:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:118:THR:O	9:E:120:GLN:NE2	2.44	0.49
7:U:268:GLU:OE1	6:V:127:ARG:NH1	2.45	0.49
3:Q:960:GLN:NE2	3:Q:1010:VAL:O	2.46	0.49
6:T:82:SER:O	6:T:82:SER:OG	2.30	0.49
6:T:127:ARG:NH1	7:Y:268:GLU:OE1	2.45	0.49
7:U:122:ARG:NE	7:U:245:ASP:OD2	2.46	0.49
6:V:316:LEU:HD22	6:V:320:ILE:HG21	1.94	0.49
6:X:211:ARG:NH2	6:X:227:GLU:OE2	2.46	0.49
1:I:-13:DA:OP1	10:B:37:ARG:NH2	2.44	0.49
3:Q:1103:ASP:N	3:Q:1103:ASP:OD1	2.43	0.49
6:V:181:LEU:HB3	6:V:185:ILE:HD13	1.94	0.49
3:Q:1198:TYR:OH	3:Q:1278:LEU:O	2.31	0.49
6:T:85:LYS:N	13:T:501:ADP:O1B	2.41	0.49
7:Y:402:LEU:HD22	7:Y:426:ALA:HB1	1.95	0.49
3:Q:1249:ILE:HG13	3:Q:1271:THR:HG21	1.95	0.49
11:G:89:ARG:HH22	11:G:98:LEU:HB2	1.78	0.49
4:R:277:VAL:O	4:R:612:MET:N	2.46	0.49
3:Q:1300:LYS:HG3	3:Q:1422:LEU:HD12	1.94	0.48
7:Y:375:GLU:OE1	7:Y:404:SER:OG	2.30	0.48
6:T:355:SER:OG	6:T:359:VAL:O	2.28	0.48
7:U:346:ASP:OD1	7:U:346:ASP:N	2.45	0.48
6:V:187:GLU:OE1	7:W:147:ARG:NH2	2.43	0.48
6:V:189:ILE:HG23	6:V:194:VAL:HB	1.94	0.48
6:X:352:ASP:N	6:X:352:ASP:OD1	2.44	0.48
1:I:-45:DA:H4'	11:C:30:ARG:HH21	1.78	0.48
4:R:135:LEU:HD11	4:R:718:ALA:HB2	1.95	0.48
7:U:128:LYS:HG3	7:U:289:VAL:HG21	1.94	0.48
7:U:158:LEU:HB2	7:U:171:LEU:HD21	1.95	0.48
7:U:316:GLU:O	6:V:23:ARG:NH2	2.46	0.48
6:X:119:GLU:HG2	6:X:279:GLU:HA	1.96	0.48
3:Q:1175:LEU:HD11	6:V:258:ARG:HD3	1.96	0.48
3:Q:1191:LEU:O	6:V:260:GLN:NE2	2.45	0.48
5:S:130:ASN:OD1	5:S:130:ASN:N	2.40	0.48
10:F:72:THR:HA	10:F:75:GLU:HG3	1.96	0.48
3:Q:1151:ARG:O	3:Q:1155:ARG:NE	2.45	0.48
7:U:343:LEU:HB3	7:U:347:LEU:HD23	1.96	0.48
7:U:371:ARG:NH2	7:U:375:GLU:OE2	2.44	0.48
6:X:187:GLU:HA	6:X:190:GLN:HG3	1.96	0.48
10:B:61:VAL:O	10:B:65:ASN:ND2	2.46	0.48
1:I:-63:DC:O2	2:J:64:DG:N2	2.47	0.48
10:B:92:LYS:HA	10:B:97:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:121:LEU:HD23	6:X:323:TYR:HD2	1.79	0.47
1:I:9:DG:H5"	9:E:43:PRO:HA	1.96	0.47
5:S:67:ILE:HG23	5:S:101:PHE:CE2	2.49	0.47
6:X:316:LEU:HD22	6:X:320:ILE:HG21	1.96	0.47
11:C:97:LEU:HD13	12:D:106:PRO:HD3	1.96	0.47
4:R:187:ILE:HB	4:R:670:ILE:HG22	1.95	0.47
10:B:58:VAL:HA	10:B:61:VAL:HG22	1.96	0.47
7:W:187:GLY:HA3	7:W:206:PHE:HB2	1.95	0.47
11:G:51:TYR:HB3	12:H:97:ILE:HD11	1.97	0.47
3:Q:1143:VAL:O	3:Q:1151:ARG:NH1	2.47	0.47
6:X:135:GLU:OE1	6:X:245:GLN:NE2	2.47	0.47
9:A:127:ALA:O	9:A:131:ARG:HB2	2.14	0.47
11:G:80:ILE:HG21	11:G:82:ARG:HE	1.80	0.47
4:R:643:GLU:OE2	4:R:648:LYS:NZ	2.47	0.47
6:V:232:LEU:O	6:V:234:LYS:NZ	2.43	0.47
11:C:35:LEU:HB3	11:C:44:ILE:HD11	1.95	0.47
3:Q:1317:ARG:NH2	3:Q:1318:VAL:O	2.48	0.47
4:R:139:ARG:O	4:R:142:THR:OG1	2.32	0.47
6:V:49:VAL:O	13:V:501:ADP:N6	2.40	0.47
6:X:116:LYS:HE3	6:X:279:GLU:HG2	1.97	0.47
6:X:281:THR:OG1	6:X:282:GLU:OE1	2.33	0.47
3:Q:1071:THR:OG1	6:X:177:LYS:NZ	2.48	0.47
3:Q:1208:ARG:O	7:W:276:LYS:NZ	2.47	0.47
3:Q:1328:MET:SD	3:Q:1328:MET:N	2.83	0.47
6:T:380:ILE:HG12	6:T:412:LEU:HD13	1.95	0.47
10:B:83:THR:OG1	10:B:84:ALA:N	2.48	0.47
6:T:413:ARG:NH2	13:T:501:ADP:O2A	2.48	0.47
7:U:243:GLU:HA	7:U:257:LEU:HD21	1.97	0.47
7:W:148:SER:OG	7:W:149:ILE:N	2.48	0.47
6:T:83:THR:O	6:T:375:TYR:OH	2.32	0.47
6:V:119:GLU:HG2	6:V:279:GLU:HA	1.96	0.47
1:I:-26:DT:O2	2:J:27:DG:N2	2.49	0.46
7:U:201:LYS:O	7:U:220:ARG:NH2	2.48	0.46
7:U:298:VAL:HG11	7:U:323:MET:HB3	1.98	0.46
11:G:51:TYR:HE2	12:H:98:GLN:HB2	1.80	0.46
1:I:-4:DC:OP1	10:B:45:LYS:NZ	2.48	0.46
3:Q:959:ARG:NH2	3:Q:1018:GLU:OE2	2.47	0.46
4:R:71:ARG:HD2	4:R:77:LYS:HG2	1.97	0.46
7:Y:415:ASN:ND2	7:Y:419:GLU:OE2	2.48	0.46
3:Q:1100:ASN:OD1	3:Q:1101:ASP:N	2.48	0.46
7:Y:397:ARG:NH1	13:Y:501:ADP:O2A	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:91:LEU:HB3	10:F:96:ARG:HG3	1.97	0.46
7:W:398:TYR:OH	7:W:430:PHE:O	2.34	0.46
7:Y:262:THR:HB	7:Y:265:ILE:HD11	1.96	0.46
6:T:71:SER:HB2	7:U:19:LEU:HB2	1.97	0.46
6:X:41:ALA:HB3	6:X:52:ILE:HG23	1.98	0.46
12:H:60:LYS:O	12:H:64:ILE:HG13	2.16	0.46
3:Q:1317:ARG:HH21	3:Q:1370:PHE:HB3	1.80	0.46
9:E:104:PHE:HA	9:E:107:THR:HG22	1.98	0.46
3:Q:1266:GLU:OE2	6:V:193:LYS:NZ	2.46	0.46
9:A:130:LEU:HD12	9:E:130:LEU:HD12	1.97	0.46
11:C:77:THR:OG1	12:D:54:ASP:O	2.34	0.46
4:R:67:LEU:HD22	4:R:114:ILE:HD11	1.98	0.46
6:T:352:ASP:N	6:T:352:ASP:OD1	2.47	0.46
7:Y:146:ASP:OD1	7:Y:146:ASP:N	2.42	0.46
12:D:54:ASP:N	12:D:54:ASP:OD1	2.49	0.46
3:Q:1076:SER:HG	3:Q:1078:ARG:HH12	1.62	0.46
7:W:245:ASP:O	7:W:249:SER:HB3	2.16	0.46
7:U:157:LYS:HA	7:U:157:LYS:HD3	1.77	0.46
10:F:41:ARG:O	10:F:41:ARG:NE	2.47	0.46
7:W:413:ARG:NE	7:W:422:ASP:OD1	2.48	0.45
11:C:85:GLN:HA	11:C:88:ILE:HG22	1.97	0.45
3:Q:1104:ILE:HG21	6:T:243:ILE:HD11	1.98	0.45
6:T:119:GLU:HG2	6:T:279:GLU:HA	1.97	0.45
6:T:191:ARG:NH2	6:T:192:GLU:OE2	2.50	0.45
6:X:106:VAL:HB	6:X:109:GLU:HG3	1.98	0.45
12:D:116:GLU:HB3	12:D:119:ARG:HH21	1.80	0.45
12:D:118:THR:HA	12:D:121:VAL:HG12	1.97	0.45
1:I:47:DT:O2	2:J:48:DG:N2	2.50	0.45
4:R:210:LYS:HD2	5:S:106:PRO:HD3	1.97	0.45
12:D:65:LEU:HA	12:D:68:PHE:HB3	1.97	0.45
1:I:26:DT:H3	2:J:26:DA:H61	1.63	0.45
6:V:414:TYR:OH	6:V:446:PHE:O	2.35	0.45
7:U:276:LYS:HB2	7:U:276:LYS:HE2	1.76	0.45
7:W:332:THR:O	7:W:335:THR:OG1	2.33	0.45
1:I:38:DT:OP2	11:G:46:SER:OG	2.35	0.45
4:R:210:LYS:HG3	4:R:641:LEU:HD22	1.99	0.45
6:T:109:GLU:OE1	6:T:109:GLU:N	2.44	0.45
6:V:448:ASP:HB3	6:V:451:ARG:HG3	1.97	0.45
4:R:676:LYS:HA	4:R:702:MET:HE1	1.99	0.45
6:T:120:THR:O	6:T:124:ASN:ND2	2.48	0.45
7:U:76:PRO:HG2	7:U:79:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:285:LYS:O	7:U:285:LYS:NZ	2.45	0.45
7:U:394:THR:OG1	7:U:395:SER:N	2.50	0.45
7:W:45:VAL:O	13:W:501:ADP:N6	2.49	0.45
6:X:361:PRO:HA	6:X:364:ILE:HB	1.98	0.45
7:Y:346:ASP:OD1	7:Y:346:ASP:N	2.48	0.45
7:Y:377:VAL:HG13	7:Y:407:GLN:HG3	1.99	0.45
9:A:82:LEU:HD22	10:B:82:VAL:HG13	1.99	0.45
2:J:-22:DG:OP2	9:E:72:ARG:NH1	2.49	0.45
11:G:16:GLN:HE22	11:G:20:ALA:HB3	1.82	0.45
3:Q:1249:ILE:HD11	3:Q:1269:PRO:HG2	1.98	0.45
10:B:99:TYR:OH	12:H:71:ASP:OD1	2.29	0.45
11:C:44:ILE:HG13	12:D:92:ILE:HD11	1.99	0.45
11:G:24:LEU:HD22	11:G:57:GLU:HG3	1.99	0.45
3:Q:1320:ILE:CD1	3:Q:1371:LEU:HD22	2.46	0.45
6:V:143:GLU:N	6:V:171:LYS:O	2.50	0.45
6:V:361:PRO:HA	6:V:364:ILE:HB	1.98	0.45
12:D:62:MET:O	12:D:66:ASN:HB2	2.17	0.45
9:E:68:GLN:HG3	9:E:89:ILE:HG12	1.98	0.45
6:V:380:ILE:HG12	6:V:412:LEU:HD13	1.98	0.44
9:E:89:ILE:HD12	9:E:89:ILE:HA	1.83	0.44
3:Q:1398:PRO:HA	3:Q:1401:ASP:HB3	1.99	0.44
4:R:145:SER:O	4:R:149:ASN:ND2	2.50	0.44
4:R:733:GLU:O	4:R:737:TYR:HB2	2.18	0.44
7:W:38:ARG:O	7:W:51:ARG:NH2	2.43	0.44
10:F:27:ILE:HD11	10:F:60:LYS:HE3	1.98	0.44
7:U:331:LYS:HA	7:U:338:LYS:HA	1.98	0.44
11:G:30:ARG:NH1	12:H:43:TYR:OH	2.50	0.44
4:R:210:LYS:HD3	4:R:210:LYS:HA	1.78	0.44
7:U:304:GLU:HB3	6:V:108:SER:HB3	1.98	0.44
6:T:198:ASP:OD1	6:T:198:ASP:N	2.50	0.44
6:T:378:ASP:OD1	6:T:378:ASP:N	2.50	0.44
9:E:85:GLN:HG3	10:F:83:THR:HA	2.00	0.44
4:R:263:LYS:O	4:R:269:ASN:ND2	2.44	0.44
6:X:82:SER:O	6:X:82:SER:OG	2.30	0.44
6:X:408:THR:HG22	7:Y:458:ILE:HD11	1.99	0.44
12:D:39:THR:OG1	12:D:40:TYR:N	2.51	0.44
7:W:139:GLU:HG3	7:W:189:VAL:HG22	2.00	0.44
9:A:71:VAL:HA	9:A:74:ILE:HG12	2.00	0.44
10:B:79:ARG:NH2	10:B:86:ASP:OD2	2.44	0.44
6:V:152:ALA:HB2	6:V:164:SER:HB2	1.99	0.44
7:Y:330:SER:OG	7:Y:331:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:1316:HIS:HB3	3:Q:1388:THR:HB	2.00	0.44
6:T:428:THR:HG21	7:Y:35:LEU:HD11	2.00	0.44
1:I:39:DA:OP1	11:G:36:ARG:NH1	2.51	0.43
3:Q:1125:CYS:HB3	3:Q:1137:LEU:HD22	2.00	0.43
4:R:81:PHE:HB3	4:R:82:VAL:HG23	2.00	0.43
6:T:435:VAL:HG12	6:T:437:ASN:H	1.83	0.43
3:Q:1120:THR:O	6:T:294:LYS:NZ	2.48	0.43
7:W:35:LEU:O	7:W:52:ARG:NH1	2.50	0.43
7:Y:412:LYS:HA	7:Y:412:LYS:HD3	1.76	0.43
9:E:71:VAL:HA	9:E:74:ILE:HG12	1.99	0.43
6:V:117:LYS:HG3	6:V:320:ILE:HD11	1.99	0.43
11:C:78:ARG:HD2	12:D:56:GLY:HA3	2.00	0.43
12:H:66:ASN:O	12:H:70:ASN:OD1	2.37	0.43
7:W:346:ASP:OD1	7:W:346:ASP:N	2.51	0.43
6:X:375:TYR:OH	13:X:501:ADP:N7	2.44	0.43
7:U:247:ILE:HD13	7:U:247:ILE:HA	1.88	0.43
7:W:79:THR:O	7:W:359:TYR:OH	2.34	0.43
6:T:79:GLY:HA3	6:T:372:THR:HB	2.00	0.43
6:T:414:TYR:OH	6:T:446:PHE:O	2.37	0.43
7:U:379:LEU:HA	7:U:418:VAL:HG22	2.01	0.43
6:X:410:THR:OG1	6:X:411:SER:N	2.52	0.43
7:Y:346:ASP:HB2	7:Y:350:ARG:HH12	1.84	0.43
3:Q:983:THR:HG23	3:Q:1435:ARG:HE	1.81	0.43
7:Y:250:ARG:HH11	7:Y:250:ARG:HA	1.83	0.43
4:R:75:LEU:O	4:R:76:ASN:ND2	2.51	0.43
4:R:177:ASN:HB3	4:R:182:LYS:HG3	2.01	0.43
10:B:93:ARG:HD2	10:B:94:GLN:HB3	2.01	0.43
3:Q:1383:LEU:HD23	3:Q:1383:LEU:HA	1.91	0.43
4:R:604:GLU:OE1	4:R:604:GLU:N	2.48	0.43
7:U:161:LYS:HE3	7:U:161:LYS:HB3	1.92	0.43
7:U:327:ARG:NH1	6:V:462:TYR:OH	2.51	0.43
7:W:162:THR:HG23	7:W:164:ASP:H	1.83	0.43
7:Y:226:GLU:OE1	7:Y:227:GLY:N	2.50	0.43
12:H:68:PHE:O	12:H:72:ILE:HG12	2.19	0.43
3:Q:954:CYS:SG	3:Q:1303:LYS:NZ	2.76	0.42
6:T:347:VAL:HG11	6:T:360:PRO:HG3	2.01	0.42
2:J:-67:DT:H2"	2:J:-66:DG:C8	2.54	0.42
3:Q:1185:GLY:O	3:Q:1186:VAL:C	2.62	0.42
4:R:605:ASN:O	4:R:609:GLN:NE2	2.52	0.42
7:U:132:GLU:OE1	7:U:234:THR:OG1	2.32	0.42
6:X:70:MET:HE1	7:Y:375:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:45:VAL:O	13:Y:501:ADP:N6	2.53	0.42
6:V:378:ASP:OD1	6:V:378:ASP:N	2.49	0.42
7:W:114:THR:O	7:W:118:THR:OG1	2.31	0.42
7:W:413:ARG:NH2	7:W:422:ASP:OD2	2.51	0.42
2:J:-23:DT:H3'	9:E:72:ARG:HH22	1.85	0.42
4:R:189:CYS:HB2	4:R:194:THR:HG22	2.00	0.42
9:A:48:LEU:HA	9:A:51:ILE:HG22	2.01	0.42
10:B:52:TYR:HB3	10:B:56:ARG:HH12	1.82	0.42
11:C:33:ARG:HG2	11:C:37:ARG:HE	1.83	0.42
9:E:46:VAL:HA	9:E:49:ARG:HE	1.85	0.42
4:R:55:ASN:OD1	4:R:55:ASN:N	2.49	0.42
6:T:319:GLU:HG3	7:U:300:MET:HE2	2.01	0.42
10:B:89:TYR:HA	10:B:92:LYS:HE3	2.02	0.42
10:B:100:GLY:O	12:H:63:SER:OG	2.32	0.42
6:T:128:ALA:HB3	6:T:334:PRO:HG3	2.02	0.42
7:U:35:LEU:O	7:U:52:ARG:NH1	2.46	0.42
7:U:59:LYS:HB2	7:U:59:LYS:HE2	1.84	0.42
7:W:242:HIS:O	7:W:246:VAL:HG23	2.19	0.42
6:X:47:GLY:HA2	6:X:386:ARG:HE	1.85	0.42
3:Q:1324:MET:HE1	3:Q:1327:MET:HG2	2.01	0.42
4:R:623:GLU:OE2	4:R:627:GLN:NE2	2.42	0.42
11:C:80:ILE:HG22	11:C:82:ARG:H	1.85	0.42
12:H:111:LYS:HA	12:H:114:VAL:HG22	2.02	0.42
3:Q:1195:LYS:HA	3:Q:1195:LYS:HD2	1.77	0.42
7:W:304:GLU:HG2	6:X:315:MET:HE2	2.02	0.42
6:X:78:ALA:O	6:X:372:THR:OG1	2.35	0.42
7:Y:94:LYS:HB2	7:Y:94:LYS:HE2	1.90	0.42
7:Y:273:ILE:HD13	7:Y:273:ILE:HA	1.83	0.42
6:V:50:GLY:O	6:V:55:ARG:NH1	2.53	0.42
6:V:121:LEU:HD22	6:V:320:ILE:HG23	2.01	0.42
7:W:382:ASP:OD1	7:W:382:ASP:N	2.52	0.42
12:H:62:MET:HA	12:H:65:LEU:HG	2.01	0.42
3:Q:1160:LYS:HD3	3:Q:1160:LYS:HA	1.80	0.41
4:R:261:ILE:H	4:R:261:ILE:HG13	1.71	0.41
8:Z:310:ARG:NH1	8:Z:315:ASP:OD2	2.53	0.41
11:C:22:ALA:O	12:D:123:LYS:NZ	2.41	0.41
7:U:47:GLN:NE2	7:U:357:LYS:O	2.53	0.41
6:V:200:ILE:HD13	6:V:200:ILE:HA	1.87	0.41
11:G:40:TYR:HB3	12:H:81:SER:HB2	2.01	0.41
1:I:-54:DA:OP1	12:D:58:SER:OG	2.30	0.41
2:J:-14:DA:O3'	9:E:63:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:1317:ARG:HH11	3:Q:1389:VAL:HG23	1.85	0.41
4:R:705:ASP:OD1	4:R:707:SER:OG	2.35	0.41
7:W:252:GLN:NE2	6:X:272:LEU:O	2.54	0.41
6:X:121:LEU:HD21	6:X:324:LEU:HD13	2.02	0.41
7:Y:47:GLN:NE2	7:Y:79:THR:O	2.53	0.41
7:Y:398:TYR:OH	7:Y:430:PHE:O	2.32	0.41
3:Q:999:ASN:HB3	3:Q:1000:LEU:H	1.67	0.41
6:T:132:ARG:HH21	6:T:244:VAL:HG11	1.85	0.41
7:U:402:LEU:HD23	7:U:402:LEU:HA	1.95	0.41
12:H:45:TYR:O	12:H:49:LYS:HB2	2.21	0.41
3:Q:1131:LEU:HD12	7:U:247:ILE:HG13	2.01	0.41
6:V:283:LYS:HA	6:V:286:GLN:HE21	1.85	0.41
7:Y:38:ARG:HD2	7:Y:41:SER:HB2	2.03	0.41
12:D:41:SER:O	12:D:45:TYR:HB2	2.21	0.41
1:I:58:DG:H5'	11:G:78:ARG:HG3	2.02	0.41
2:J:-61:DT:H2''	2:J:-60:DA:C8	2.56	0.41
6:T:152:ALA:HB3	6:T:164:SER:HB3	2.02	0.41
6:V:432:LYS:HD2	6:V:432:LYS:HA	1.92	0.41
7:W:190:ILE:HD12	7:W:192:ILE:HD11	2.03	0.41
12:H:71:ASP:OD2	12:H:75:ARG:NH2	2.53	0.41
3:Q:953:LEU:HD13	3:Q:1423:LEU:HG	2.02	0.41
3:Q:1280:LYS:H	3:Q:1280:LYS:HG2	1.46	0.41
4:R:241:LEU:O	4:R:245:THR:HG23	2.20	0.41
6:X:346:THR:HB	6:X:354:ILE:HD13	2.02	0.41
6:X:422:CYS:HB3	6:X:434:ILE:HD13	2.03	0.41
3:Q:967:LEU:HD12	3:Q:967:LEU:HA	1.92	0.41
5:S:59:ARG:H	5:S:59:ARG:HG3	1.64	0.41
7:U:52:ARG:HG2	6:V:445:LEU:HD11	2.03	0.41
7:U:162:THR:OG1	7:U:165:MET:O	2.37	0.41
6:X:85:LYS:HB2	6:X:85:LYS:HE2	1.89	0.41
6:V:259:PRO:HB3	7:W:255:LEU:HD11	2.02	0.41
7:Y:311:ARG:HA	7:Y:311:ARG:HD3	1.87	0.41
1:I:28:DG:H3'	10:F:79:ARG:HH11	1.86	0.40
3:Q:1317:ARG:HB2	3:Q:1370:PHE:HB2	2.03	0.40
6:T:431:ARG:HE	6:T:431:ARG:HB2	1.51	0.40
7:W:29:LEU:HD12	7:W:29:LEU:HA	1.90	0.40
7:W:311:ARG:O	7:W:311:ARG:NH1	2.46	0.40
7:Y:97:PRO:HB2	7:Y:124:SER:HA	2.02	0.40
9:A:113:HIS:O	9:E:122:LYS:NZ	2.41	0.40
10:B:78:LYS:HE2	10:B:78:LYS:HB2	1.84	0.40
5:S:49:LYS:HE3	5:S:49:LYS:HB2	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:81:LYS:HB2	7:U:81:LYS:HE2	1.94	0.40
7:U:211:ASP:OD1	7:U:211:ASP:N	2.51	0.40
6:X:116:LYS:HE2	7:Y:108:SER:HB2	2.03	0.40
4:R:49:LEU:HD23	4:R:63:PHE:HB2	2.02	0.40
6:T:375:TYR:HB3	6:T:379:GLU:HG3	2.03	0.40
7:U:135:LEU:HD23	7:U:135:LEU:HA	1.92	0.40
7:W:146:ASP:OD2	8:Z:300:TYR:OH	2.32	0.40
7:W:390:THR:O	7:W:394:THR:OG1	2.37	0.40
7:Y:268:GLU:O	7:Y:272:GLN:HG3	2.21	0.40
9:A:113:HIS:CE1	9:E:114:ALA:HB2	2.56	0.40
10:B:93:ARG:HH12	12:D:103:LEU:C	2.29	0.40
11:C:114:GLN:OE1	11:C:114:GLN:N	2.51	0.40
9:E:76:GLN:HG2	9:E:80:THR:HG22	2.02	0.40
6:T:216:ASP:OD1	6:T:216:ASP:N	2.54	0.40
6:X:424:ILE:HD13	6:X:424:ILE:HA	1.93	0.40
12:D:82:LYS:HG2	12:D:86:TYR:CE1	2.56	0.40
9:E:121:LYS:HE3	9:E:121:LYS:HB3	1.88	0.40
3:Q:1291:MET:HE1	3:Q:1332:GLU:HG3	2.03	0.40
6:V:313:VAL:HG11	6:V:338:LEU:HD22	2.04	0.40
6:X:105:LEU:HD22	6:X:308:LEU:HD11	2.03	0.40
6:X:281:THR:OG1	6:X:282:GLU:N	2.55	0.40
6:X:380:ILE:HG12	6:X:412:LEU:HD13	2.02	0.40
11:C:16:GLN:HE22	11:C:21:LYS:HB3	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	
3	Q	407/1489 (27%)	386 (95%)	21 (5%)	0	100	100
4	R	438/755 (58%)	418 (95%)	20 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	124/166 (75%)	117 (94%)	7 (6%)	0	100	100
6	T	433/463 (94%)	421 (97%)	12 (3%)	0	100	100
6	V	440/463 (95%)	421 (96%)	19 (4%)	0	100	100
6	X	441/463 (95%)	425 (96%)	16 (4%)	0	100	100
7	U	443/471 (94%)	430 (97%)	13 (3%)	0	100	100
7	W	440/471 (93%)	426 (97%)	14 (3%)	0	100	100
7	Y	432/471 (92%)	412 (95%)	20 (5%)	0	100	100
8	Z	26/320 (8%)	26 (100%)	0	0	100	100
9	A	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
9	E	95/136 (70%)	95 (100%)	0	0	100	100
10	B	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
10	F	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
11	C	104/132 (79%)	100 (96%)	4 (4%)	0	100	100
11	G	106/132 (80%)	102 (96%)	4 (4%)	0	100	100
12	D	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
12	H	91/131 (70%)	86 (94%)	5 (6%)	0	100	100
All	All	4360/6536 (67%)	4200 (96%)	160 (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	
3	Q	387/1350 (29%)	387 (100%)	0	100	100
4	R	386/682 (57%)	386 (100%)	0	100	100
5	S	106/142 (75%)	105 (99%)	1 (1%)	70	81
6	T	367/391 (94%)	367 (100%)	0	100	100
6	V	373/391 (95%)	373 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	X	375/391 (96%)	375 (100%)	0	100	100
7	U	378/403 (94%)	378 (100%)	0	100	100
7	W	375/403 (93%)	375 (100%)	0	100	100
7	Y	371/403 (92%)	371 (100%)	0	100	100
8	Z	26/285 (9%)	26 (100%)	0	100	100
9	A	85/113 (75%)	85 (100%)	0	100	100
9	E	84/113 (74%)	84 (100%)	0	100	100
10	B	62/79 (78%)	62 (100%)	0	100	100
10	F	62/79 (78%)	62 (100%)	0	100	100
11	C	85/99 (86%)	85 (100%)	0	100	100
11	G	84/99 (85%)	84 (100%)	0	100	100
12	D	81/109 (74%)	81 (100%)	0	100	100
12	H	81/109 (74%)	81 (100%)	0	100	100
All	All	3768/5641 (67%)	3767 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	125	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	980	ASN
3	Q	1002	ASN
3	Q	1231	ASN
3	Q	1339	GLN
3	Q	1359	HIS
4	R	31	GLN
4	R	37	GLN
4	R	65	ASN
4	R	76	ASN
4	R	90	GLN
4	R	132	ASN
4	R	609	GLN
4	R	659	GLN

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Mol	Chain	Res	Type
5	S	75	ASN
5	S	82	ASN
5	S	135	HIS
6	T	205	ASN
6	T	245	GLN
6	T	256	ASN
6	T	286	GLN
6	T	417	GLN
6	T	437	ASN
6	T	440	ASN
7	U	223	GLN
7	U	230	GLN
7	U	272	GLN
6	V	124	ASN
6	V	154	ASN
6	V	190	GLN
6	V	256	ASN
6	V	263	GLN
6	V	286	GLN
6	V	417	GLN
7	W	49	GLN
7	W	408	GLN
7	W	441	GLN
6	X	286	GLN
7	Y	362	GLN
7	Y	408	GLN
7	Y	451	GLN
11	C	42	GLN
11	C	74	ASN
11	C	83	HIS
11	C	115	ASN
12	D	98	GLN
9	E	39	HIS
9	E	55	GLN
11	G	39	ASN
11	G	90	ASN
12	H	52	HIS

### 5.3.3 RNA ⓘ

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](#)

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	W	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	8 (18%)
13	ADP	Y	501	-	28,29,29	1.37	5 (17%)	43,45,45	1.82	8 (18%)
13	ADP	T	501	-	28,29,29	1.34	5 (17%)	43,45,45	1.87	9 (20%)
13	ADP	V	501	-	28,29,29	1.39	5 (17%)	43,45,45	1.83	10 (23%)
13	ADP	U	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.89	8 (18%)
13	ADP	X	501	-	28,29,29	1.37	5 (17%)	43,45,45	1.84	8 (18%)

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	W	501	-	-	2/16/32/32	0/3/3/3
13	ADP	Y	501	-	-	3/16/32/32	0/3/3/3
13	ADP	T	501	-	-	3/16/32/32	0/3/3/3
13	ADP	V	501	-	-	3/16/32/32	0/3/3/3
13	ADP	U	501	-	-	3/16/32/32	0/3/3/3
13	ADP	X	501	-	-	6/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	501	ADP	C5-C4	4.54	1.47	1.39
13	U	501	ADP	C5-C4	4.48	1.47	1.39
13	X	501	ADP	C5-C4	4.37	1.46	1.39
13	V	501	ADP	C5-C4	4.35	1.46	1.39
13	Y	501	ADP	C5-C4	4.31	1.46	1.39
13	T	501	ADP	C5-C4	4.19	1.46	1.39
13	U	501	ADP	C5-N7	-2.72	1.34	1.39
13	W	501	ADP	C5-N7	-2.64	1.34	1.39
13	Y	501	ADP	C5-N7	-2.59	1.34	1.39
13	X	501	ADP	C5-N7	-2.58	1.34	1.39
13	V	501	ADP	C5-C6	2.54	1.48	1.41
13	W	501	ADP	C5-C6	2.48	1.47	1.41
13	T	501	ADP	C5-C6	2.48	1.47	1.41
13	V	501	ADP	C5-N7	-2.46	1.34	1.39
13	T	501	ADP	C5-N7	-2.45	1.34	1.39
13	Y	501	ADP	C5-C6	2.41	1.47	1.41
13	X	501	ADP	C5-C6	2.40	1.47	1.41
13	U	501	ADP	C5-C6	2.35	1.47	1.41
13	V	501	ADP	C4-N9	-2.33	1.32	1.37
13	T	501	ADP	C8-N7	2.22	1.35	1.31
13	Y	501	ADP	C4-N9	-2.22	1.33	1.37
13	V	501	ADP	C8-N7	2.20	1.35	1.31
13	W	501	ADP	C8-N7	2.18	1.35	1.31
13	Y	501	ADP	C8-N7	2.15	1.35	1.31
13	X	501	ADP	C8-N7	2.13	1.35	1.31
13	U	501	ADP	C8-N7	2.07	1.35	1.31
13	T	501	ADP	C4-N9	-2.05	1.33	1.37
13	X	501	ADP	C4-N9	-2.05	1.33	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	501	ADP	C5-C4-N3	-6.14	118.27	126.72
13	T	501	ADP	C5-C4-N3	-5.97	118.49	126.72
13	W	501	ADP	C5-C4-N3	-5.92	118.57	126.72
13	U	501	ADP	C5-C4-N3	-5.90	118.59	126.72
13	Y	501	ADP	C5-C4-N3	-5.64	118.96	126.72
13	V	501	ADP	C5-C4-N3	-5.42	119.26	126.72
13	X	501	ADP	N3-C4-N9	4.92	135.53	127.17
13	U	501	ADP	N3-C4-N9	4.92	135.53	127.17
13	T	501	ADP	N3-C4-N9	4.73	135.21	127.17
13	W	501	ADP	N3-C4-N9	4.61	135.00	127.17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Y	501	ADP	N3-C4-N9	4.57	134.94	127.17
13	V	501	ADP	N3-C4-N9	4.40	134.65	127.17
13	X	501	ADP	C2-N3-C4	3.80	121.10	111.83
13	T	501	ADP	C2-N3-C4	3.77	121.04	111.83
13	Y	501	ADP	C2-N3-C4	3.66	120.76	111.83
13	W	501	ADP	C2-N3-C4	3.62	120.67	111.83
13	U	501	ADP	C2-N3-C4	3.60	120.62	111.83
13	V	501	ADP	C2-N3-C4	3.59	120.60	111.83
13	V	501	ADP	C4-C5-N7	-3.47	106.61	110.58
13	W	501	ADP	C4-C5-N7	-3.43	106.66	110.58
13	Y	501	ADP	N3-C2-N1	-3.42	123.41	128.58
13	T	501	ADP	C4-C5-N7	-3.31	106.80	110.58
13	V	501	ADP	N3-C2-N1	-3.29	123.61	128.58
13	V	501	ADP	C4-N9-C8	3.26	109.16	105.74
13	T	501	ADP	N3-C2-N1	-3.24	123.68	128.58
13	Y	501	ADP	C4-C5-N7	-3.24	106.88	110.58
13	X	501	ADP	N3-C2-N1	-3.18	123.77	128.58
13	U	501	ADP	N3-C2-N1	-3.18	123.77	128.58
13	X	501	ADP	C4-C5-N7	-3.17	106.95	110.58
13	U	501	ADP	C4-C5-N7	-3.11	107.03	110.58
13	W	501	ADP	N3-C2-N1	-3.06	123.95	128.58
13	Y	501	ADP	C4-N9-C8	2.87	108.75	105.74
13	T	501	ADP	C4-N9-C8	2.74	108.62	105.74
13	U	501	ADP	C4-N9-C8	2.74	108.62	105.74
13	V	501	ADP	C5-N7-C8	2.55	107.45	103.45
13	X	501	ADP	C4-N9-C8	2.50	108.36	105.74
13	T	501	ADP	C5-N7-C8	2.45	107.30	103.45
13	U	501	ADP	C5-N7-C8	2.38	107.19	103.45
13	Y	501	ADP	C5-N7-C8	2.38	107.19	103.45
13	U	501	ADP	C3'-C2'-C1'	2.37	105.94	101.46
13	W	501	ADP	C5-N7-C8	2.35	107.14	103.45
13	V	501	ADP	N9-C8-N7	-2.30	110.67	113.94
13	X	501	ADP	C5-N7-C8	2.27	107.02	103.45
13	W	501	ADP	C4-N9-C8	2.24	108.09	105.74
13	V	501	ADP	C6-C5-N7	2.21	136.34	132.09
13	T	501	ADP	C3'-C2'-C1'	2.18	105.59	101.46
13	X	501	ADP	C3'-C2'-C1'	2.11	105.45	101.46
13	T	501	ADP	N9-C8-N7	-2.08	110.98	113.94
13	W	501	ADP	O3B-PB-O2B	2.03	115.43	107.80
13	Y	501	ADP	N9-C8-N7	-2.02	111.07	113.94
13	V	501	ADP	C2'-C1'-N9	-2.02	108.29	113.30

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	501	ADP	C5'-O5'-PA-O1A
13	T	501	ADP	C5'-O5'-PA-O2A
13	T	501	ADP	C5'-O5'-PA-O3A
13	U	501	ADP	C5'-O5'-PA-O2A
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	X	501	ADP	C5'-O5'-PA-O1A
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	X	501	ADP	PB-O3A-PA-O2A
13	U	501	ADP	C5'-O5'-PA-O1A
13	U	501	ADP	C5'-O5'-PA-O3A
13	W	501	ADP	C5'-O5'-PA-O1A
13	X	501	ADP	O4'-C4'-C5'-O5'
13	X	501	ADP	C3'-C4'-C5'-O5'
13	W	501	ADP	PA-O3A-PB-O1B
13	X	501	ADP	PB-O3A-PA-O1A

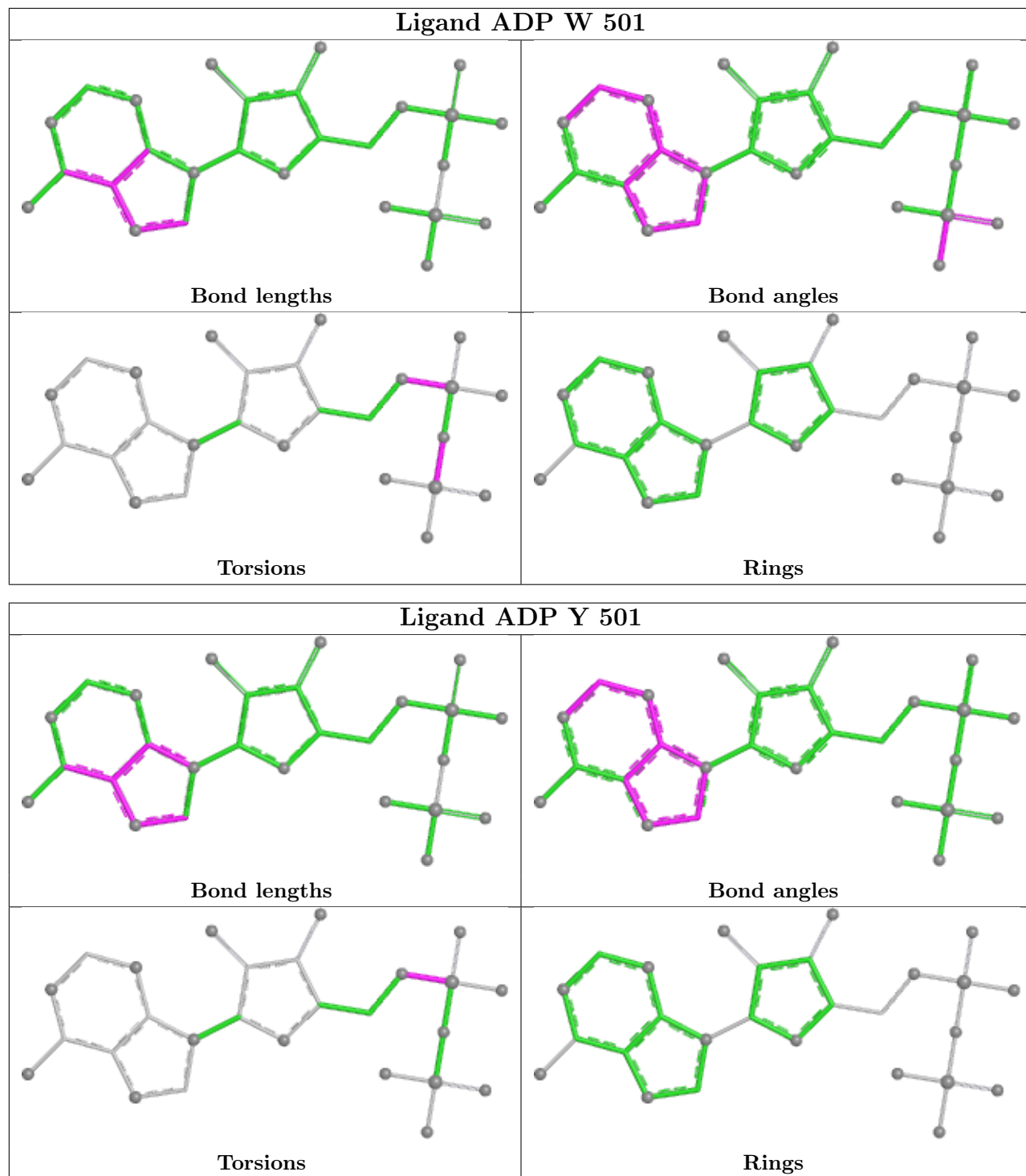
There are no ring outliers.

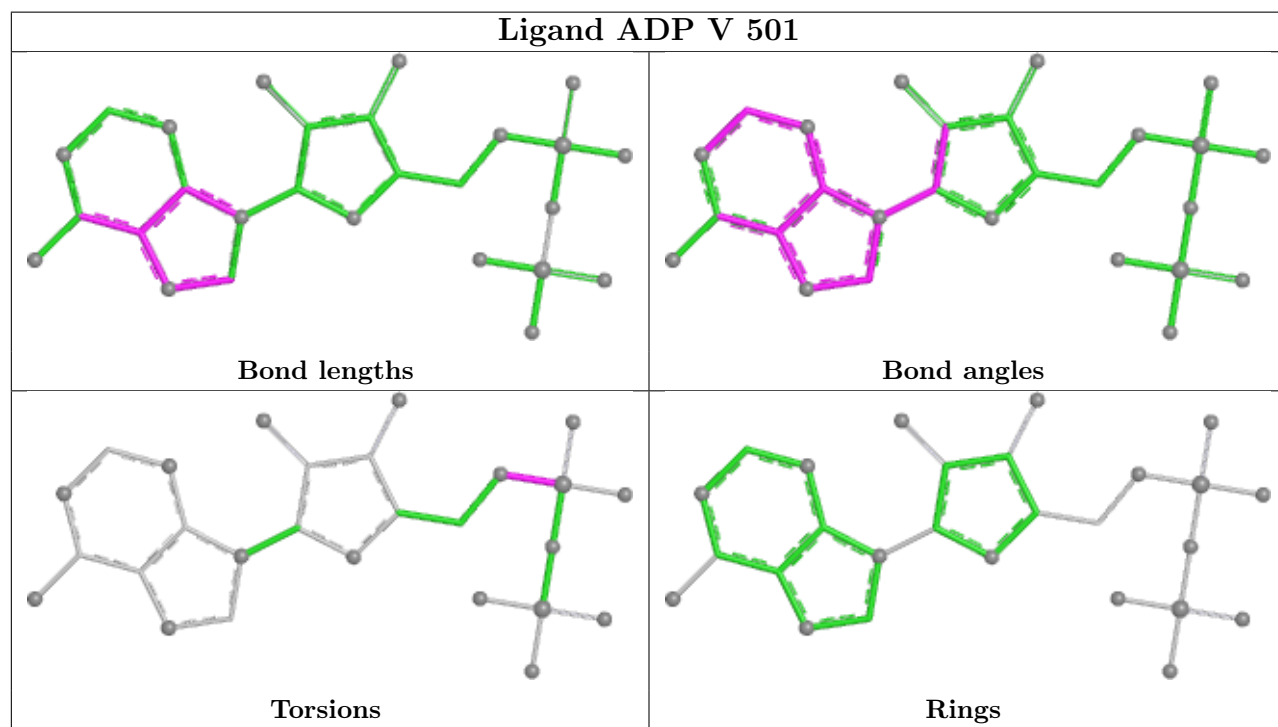
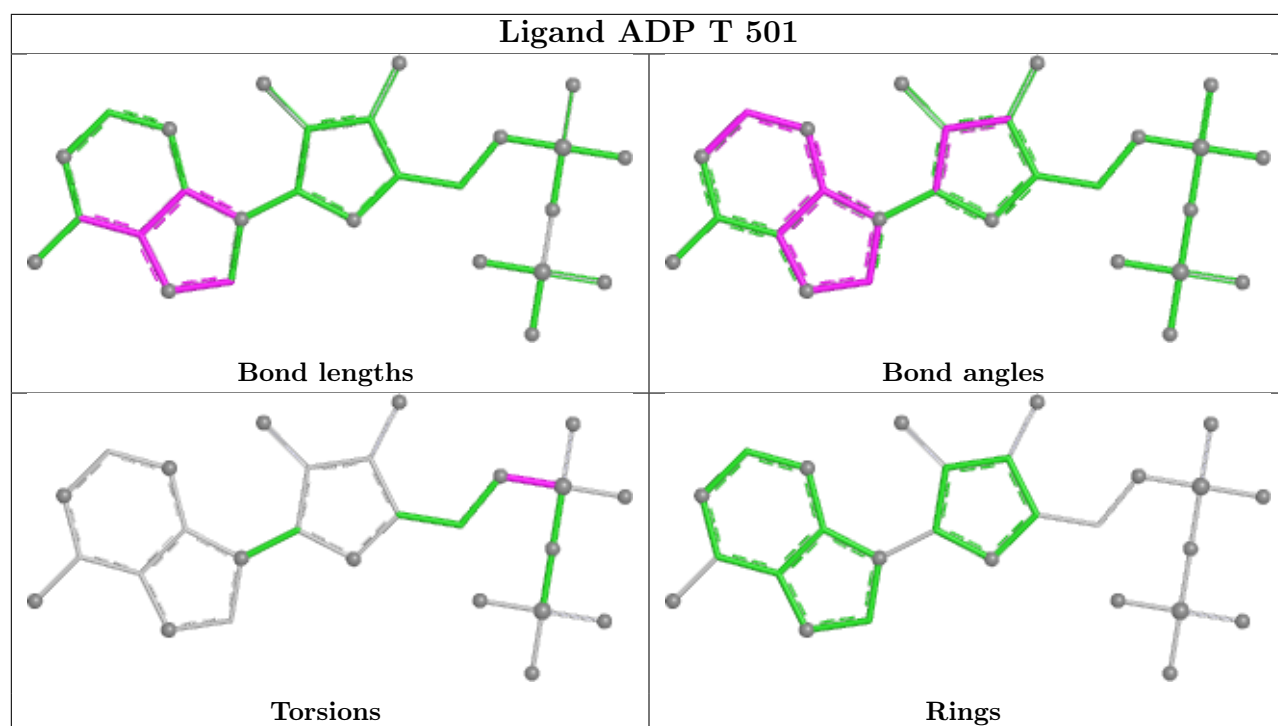
5 monomers are involved in 11 short contacts:

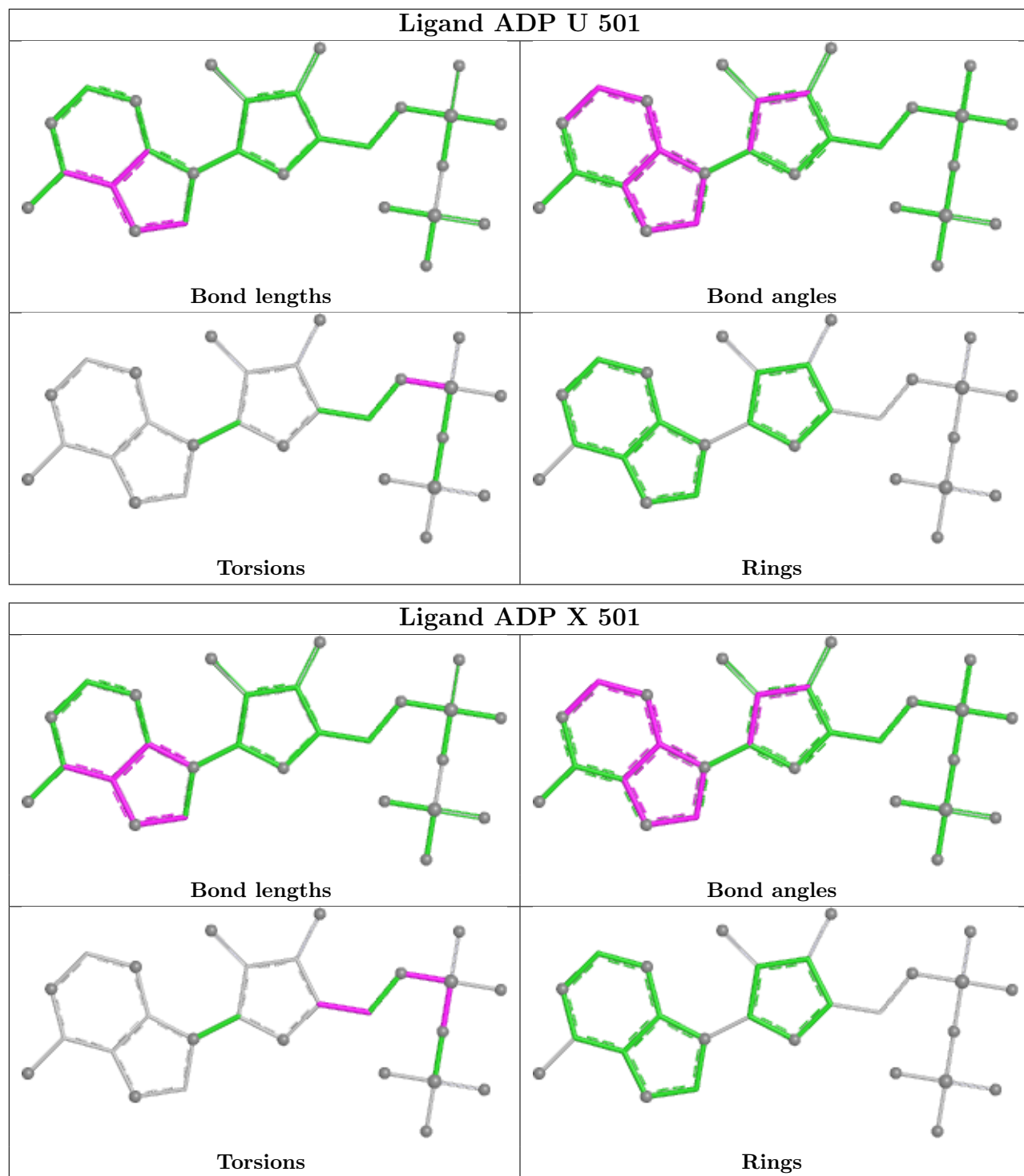
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	W	501	ADP	2	0
13	Y	501	ADP	2	0
13	T	501	ADP	3	0
13	V	501	ADP	2	0
13	X	501	ADP	2	0

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

equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



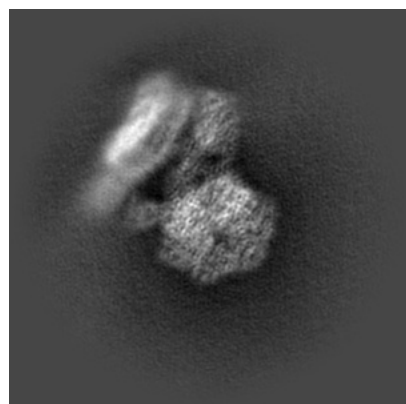
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70289. These allow visual inspection of the internal detail of the map and identification of artifacts.

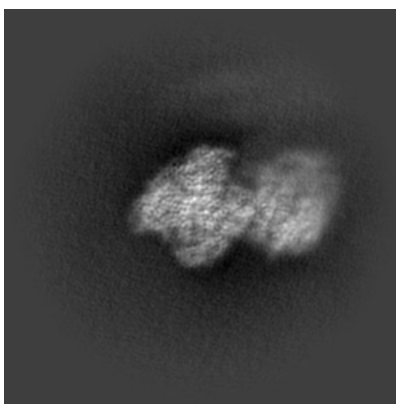
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

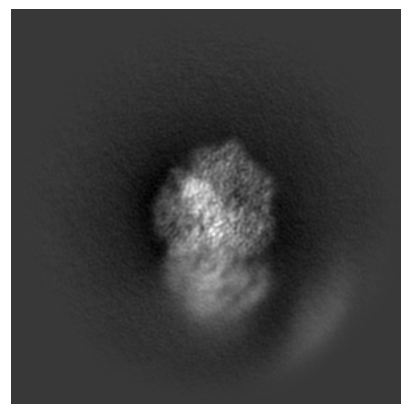
#### 6.1.1 Primary map



X

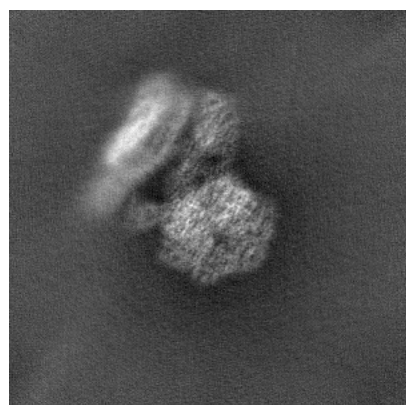


Y

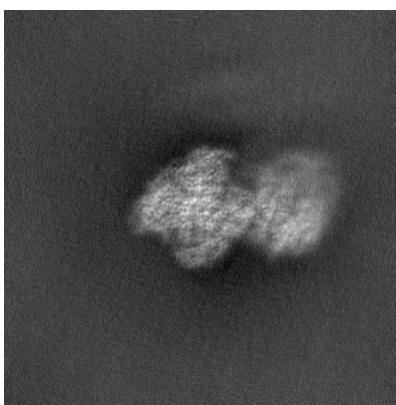


Z

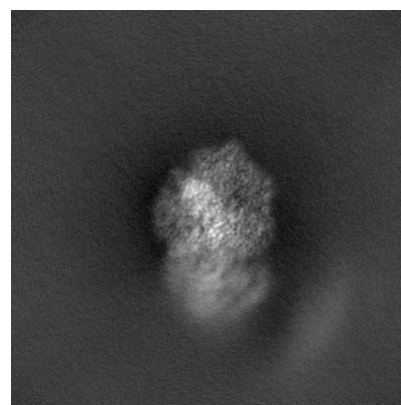
#### 6.1.2 Raw map



X



Y

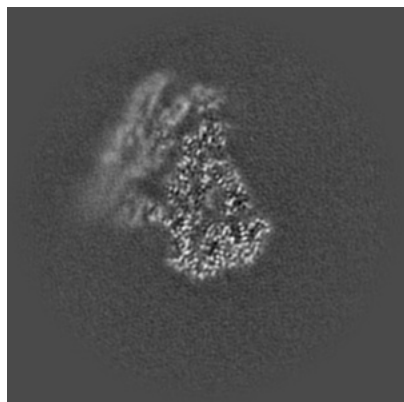


Z

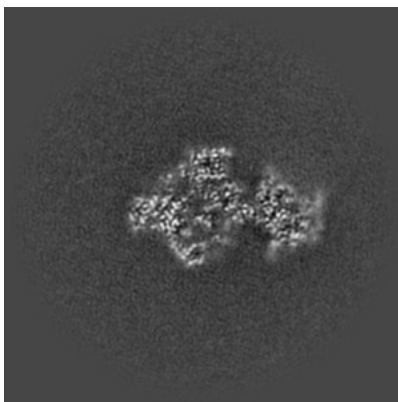
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

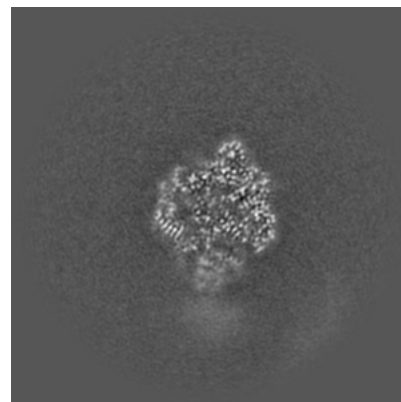
### 6.2.1 Primary map



X Index: 224

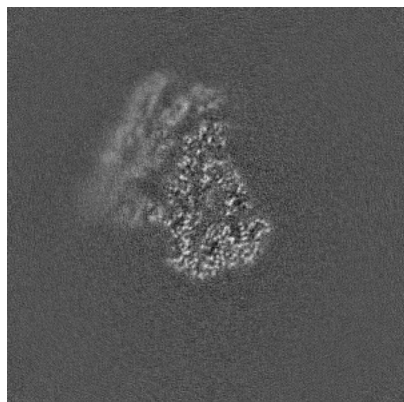


Y Index: 224

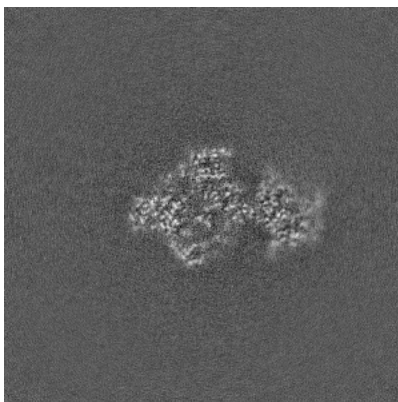


Z Index: 224

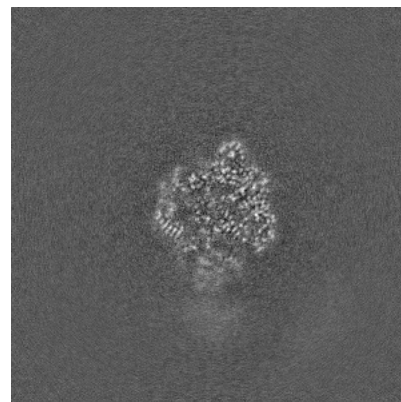
### 6.2.2 Raw map



X Index: 224



Y Index: 224

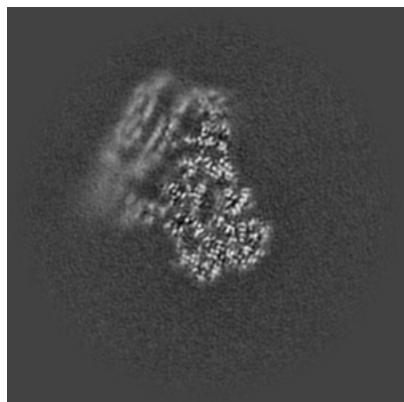


Z Index: 224

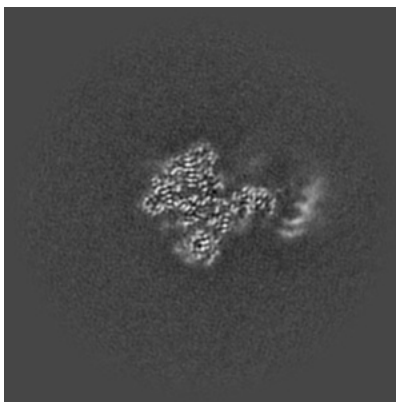
The images above show central slices of the map in three orthogonal directions.

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

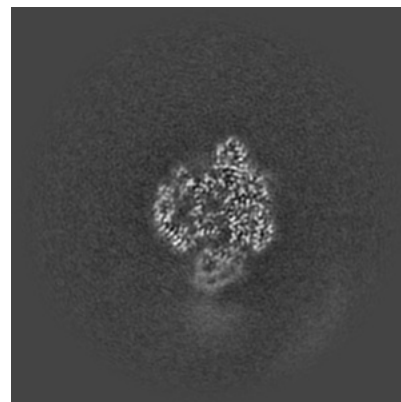
### 6.3.1 Primary map



X Index: 218

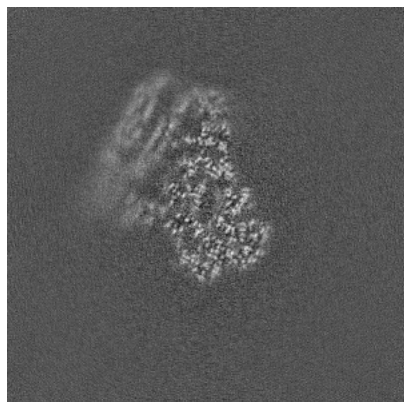


Y Index: 199

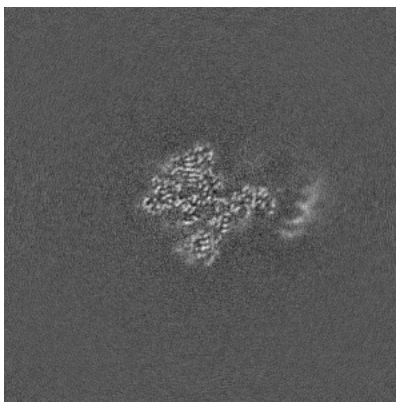


Z Index: 219

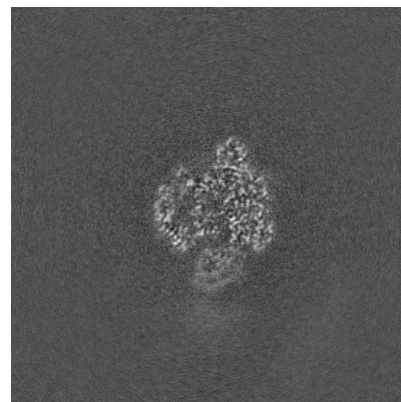
### 6.3.2 Raw map



X Index: 218



Y Index: 200

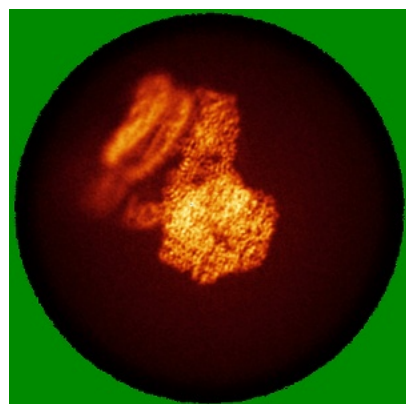


Z Index: 219

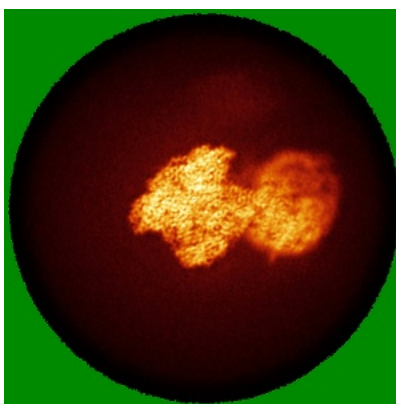
The images above show the largest variance slices of the map in three orthogonal directions.

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

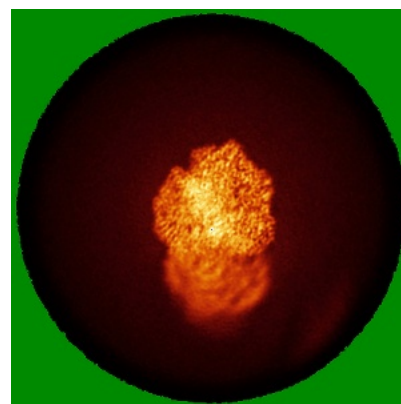
### 6.4.1 Primary map



X

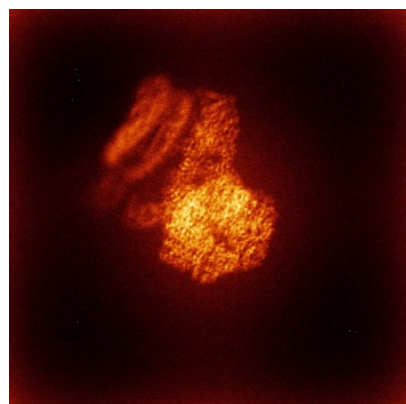


Y

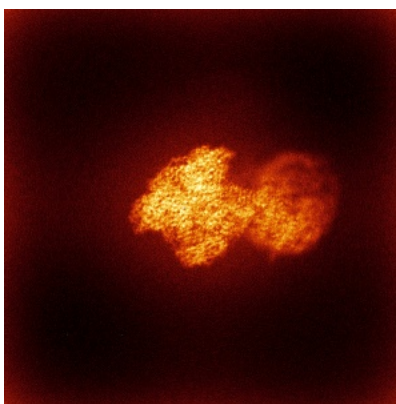


Z

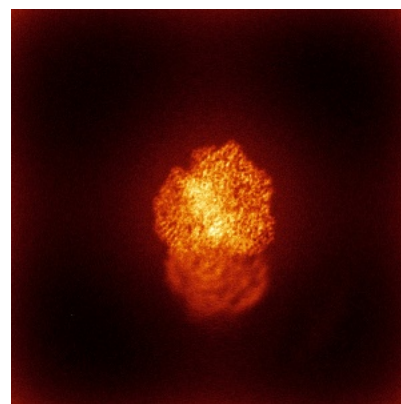
### 6.4.2 Raw map



X



Y



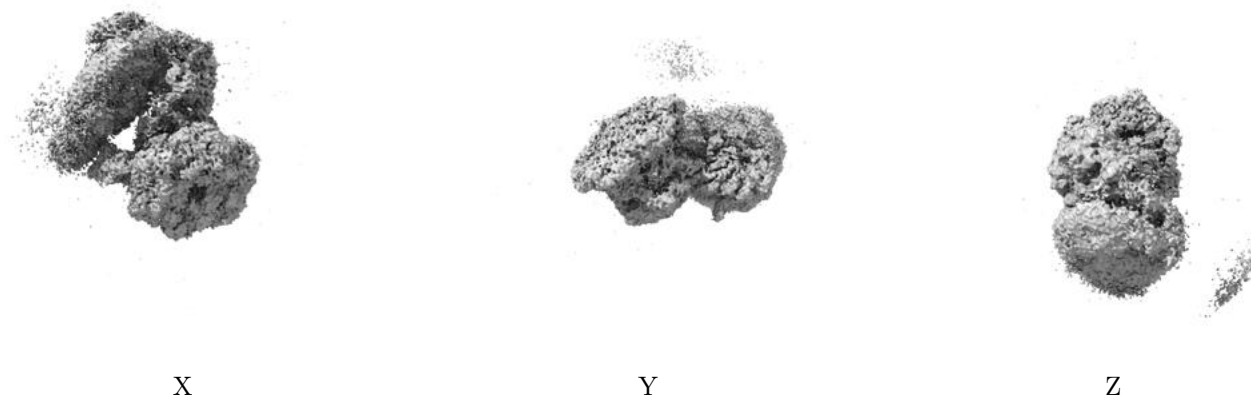
Z

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



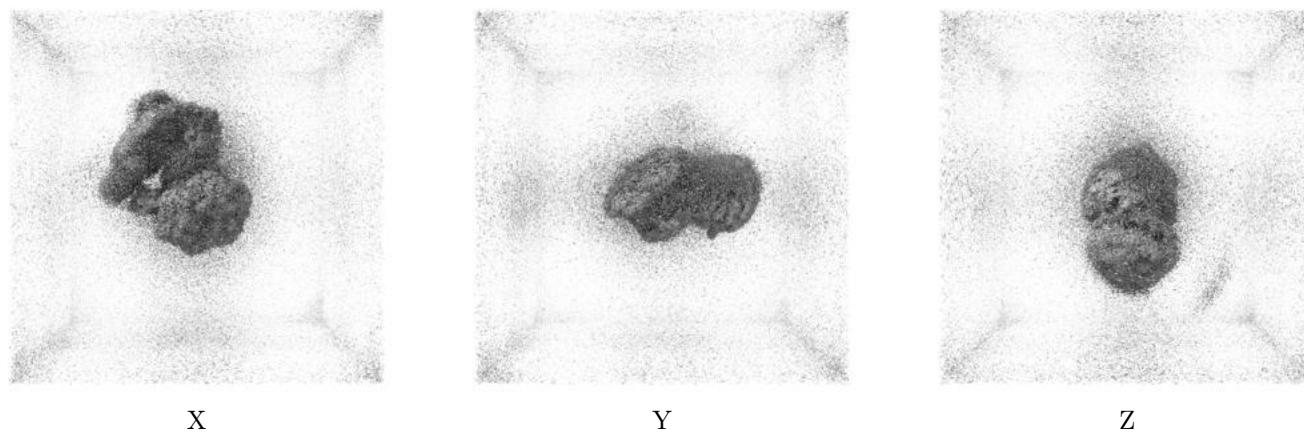
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

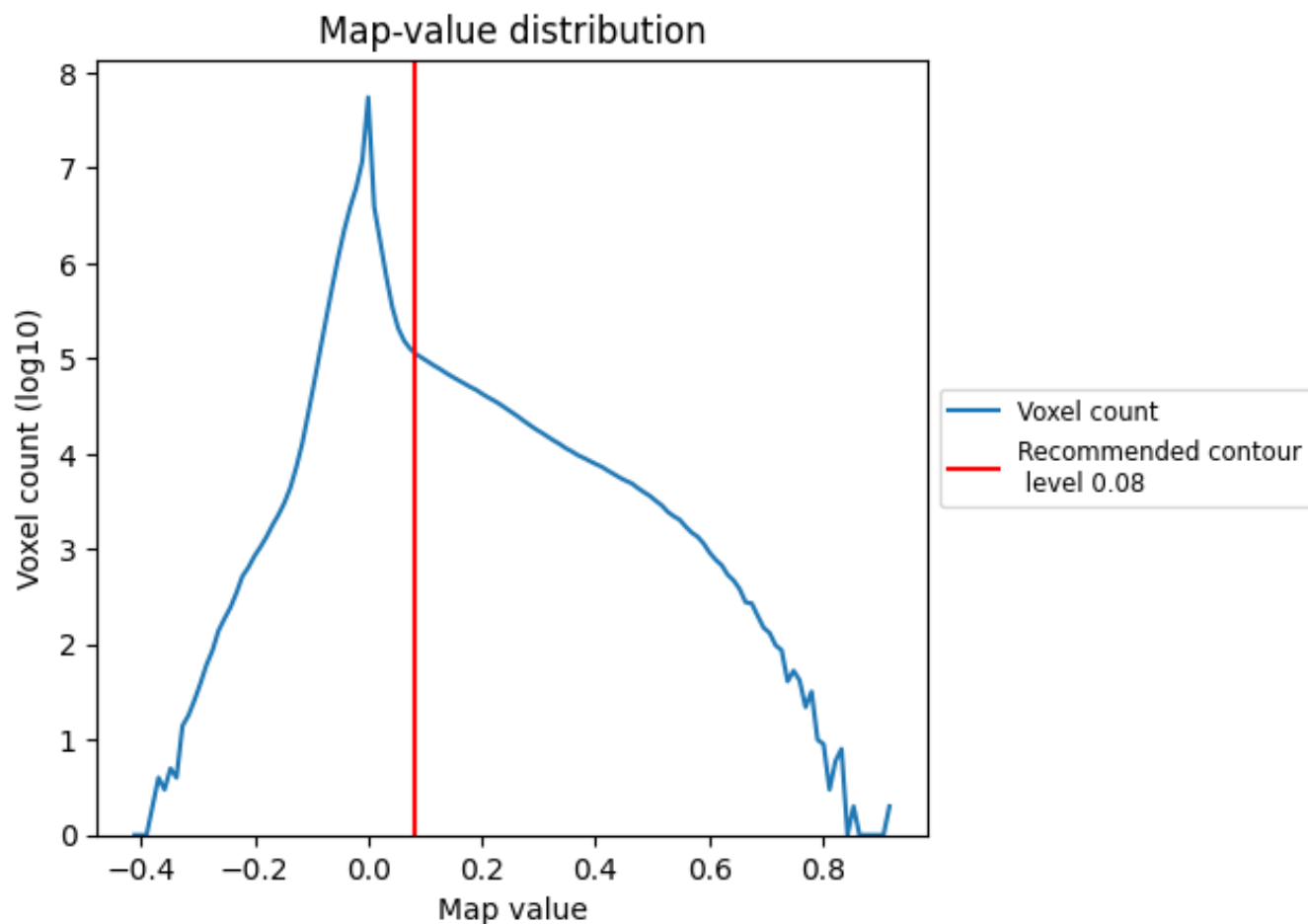
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

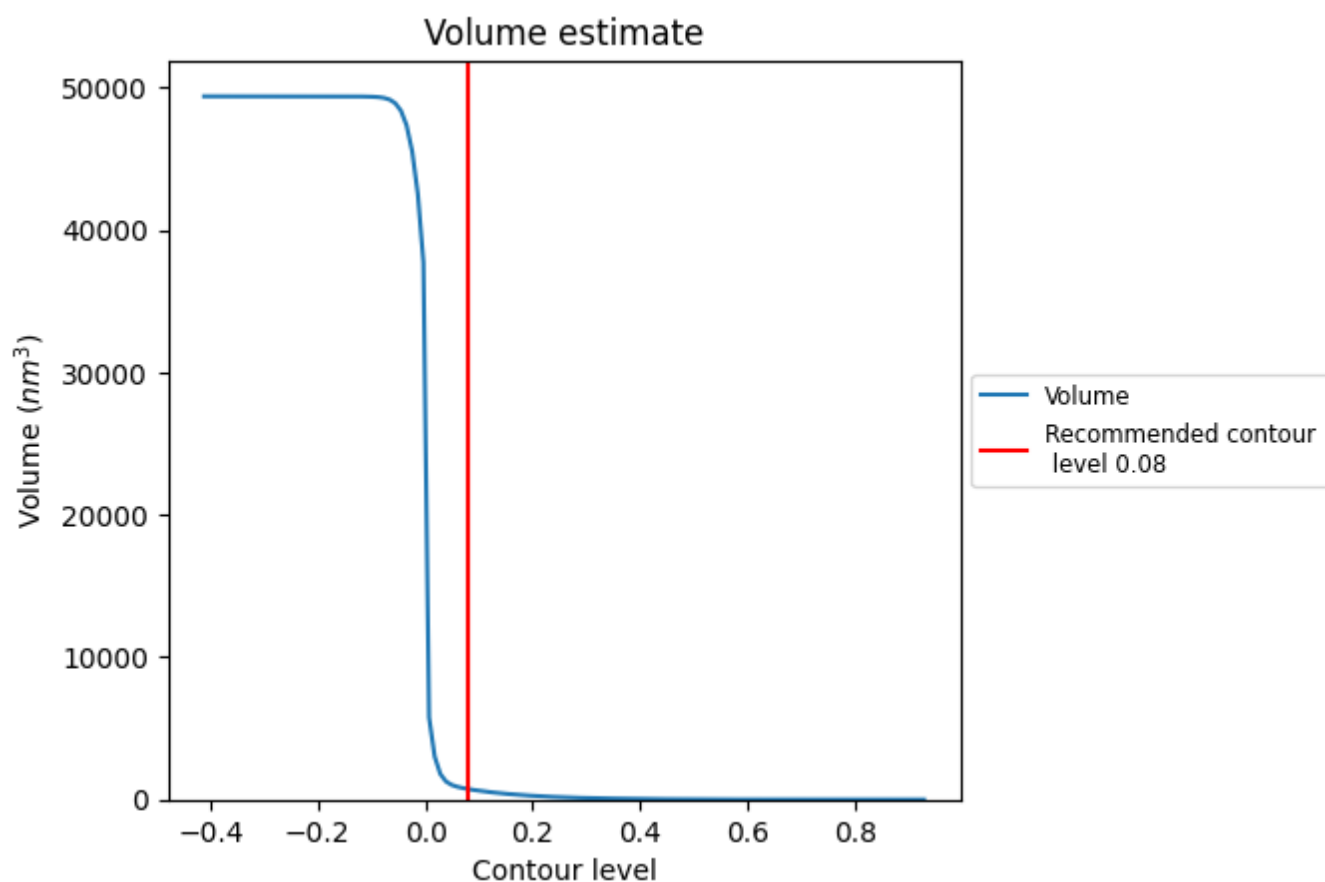
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

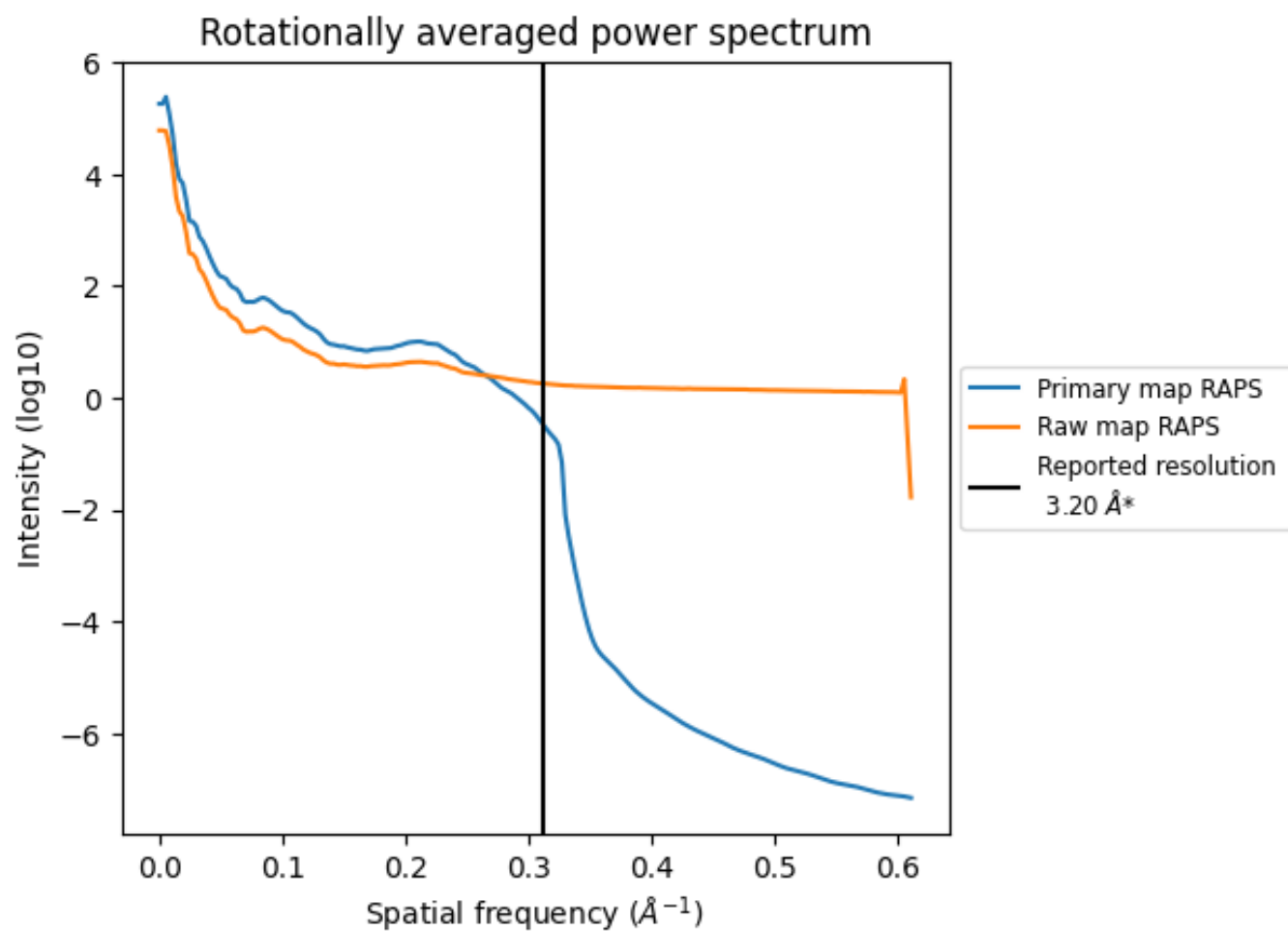
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 738 nm<sup>3</sup>; this corresponds to an approximate mass of 667 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 ⓘ



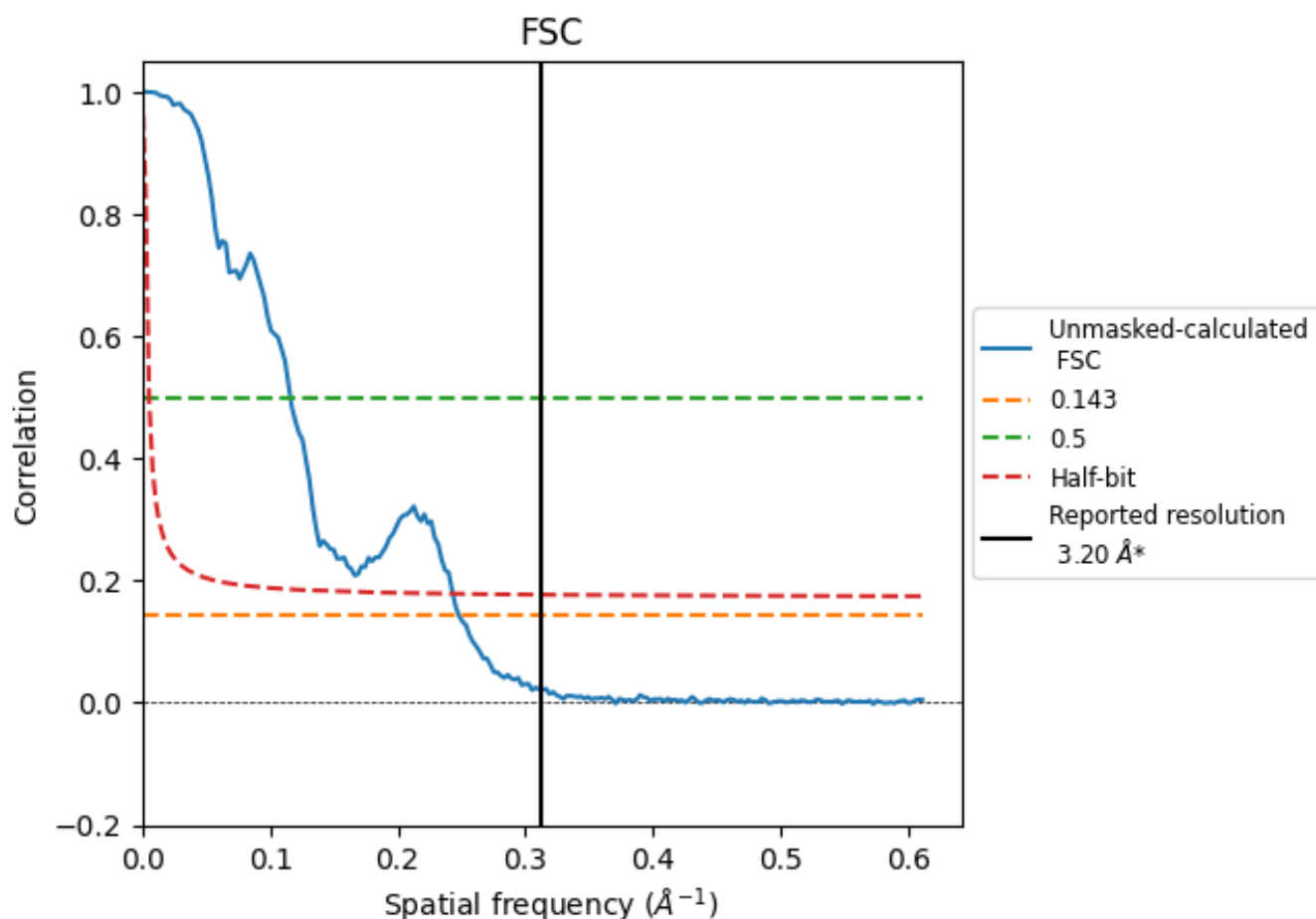
\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



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

## 8.2 Resolution estimates [i](#)

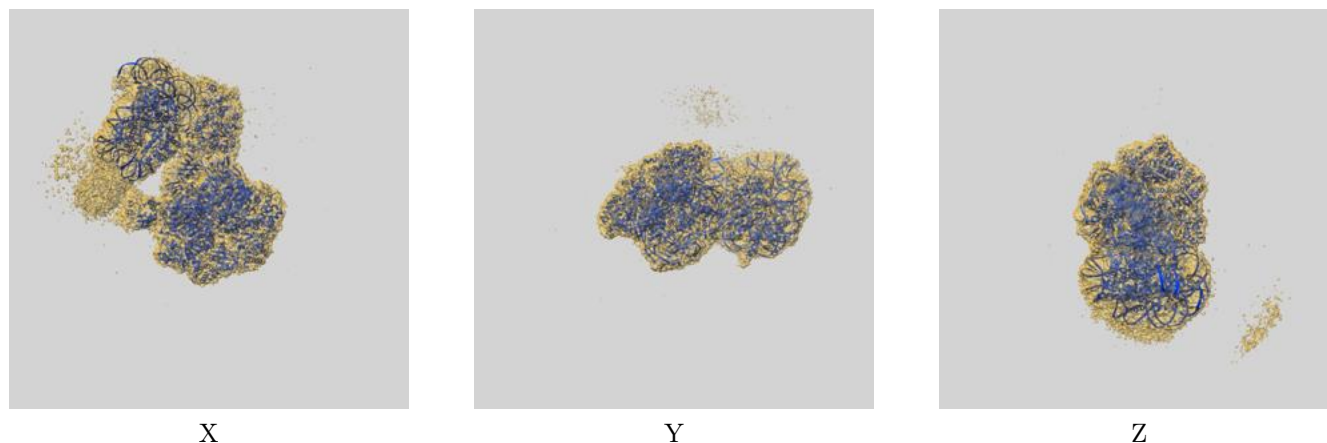
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	8.62	4.11

\*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 4.03 differs from the reported value 3.2 by more than 10 %

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

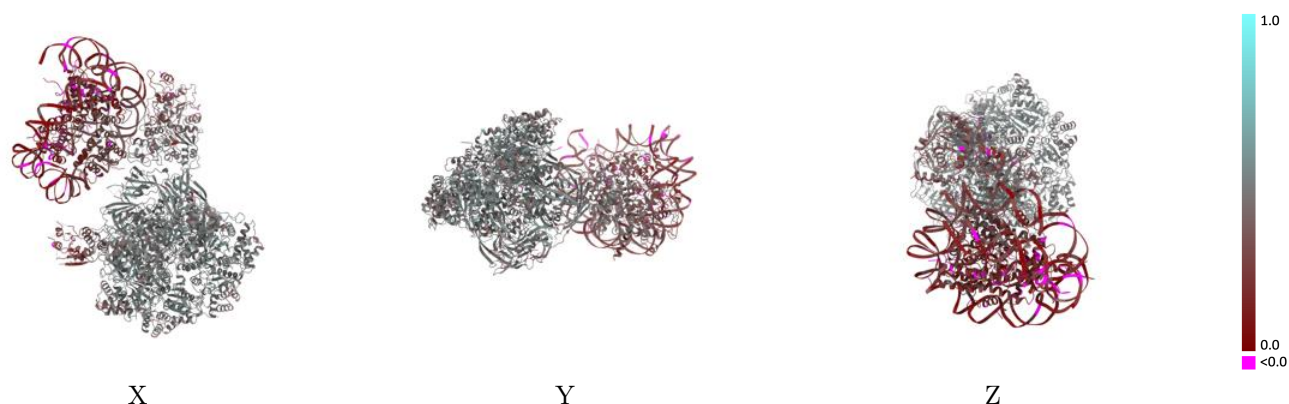
This section contains information regarding the fit between EMDB map EMD-70289 and PDB model 9OB1. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



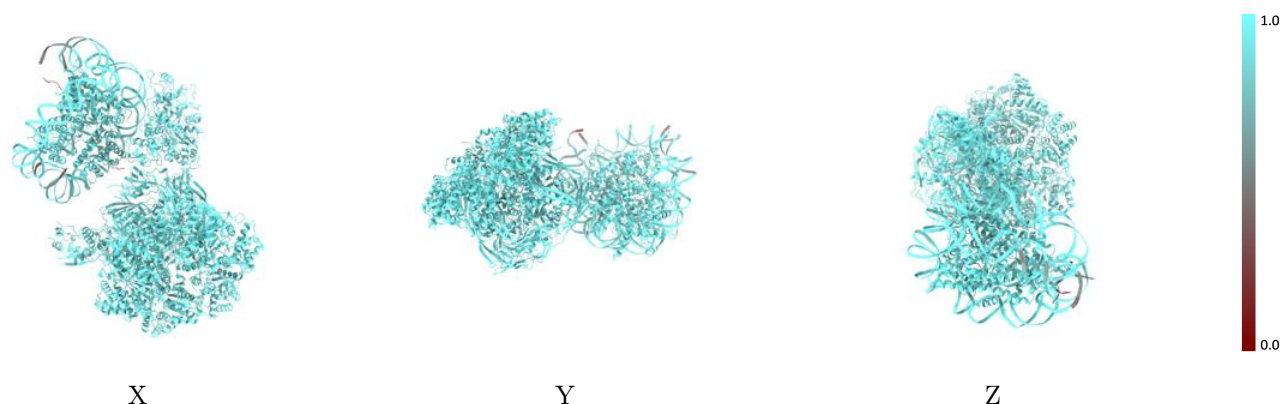
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



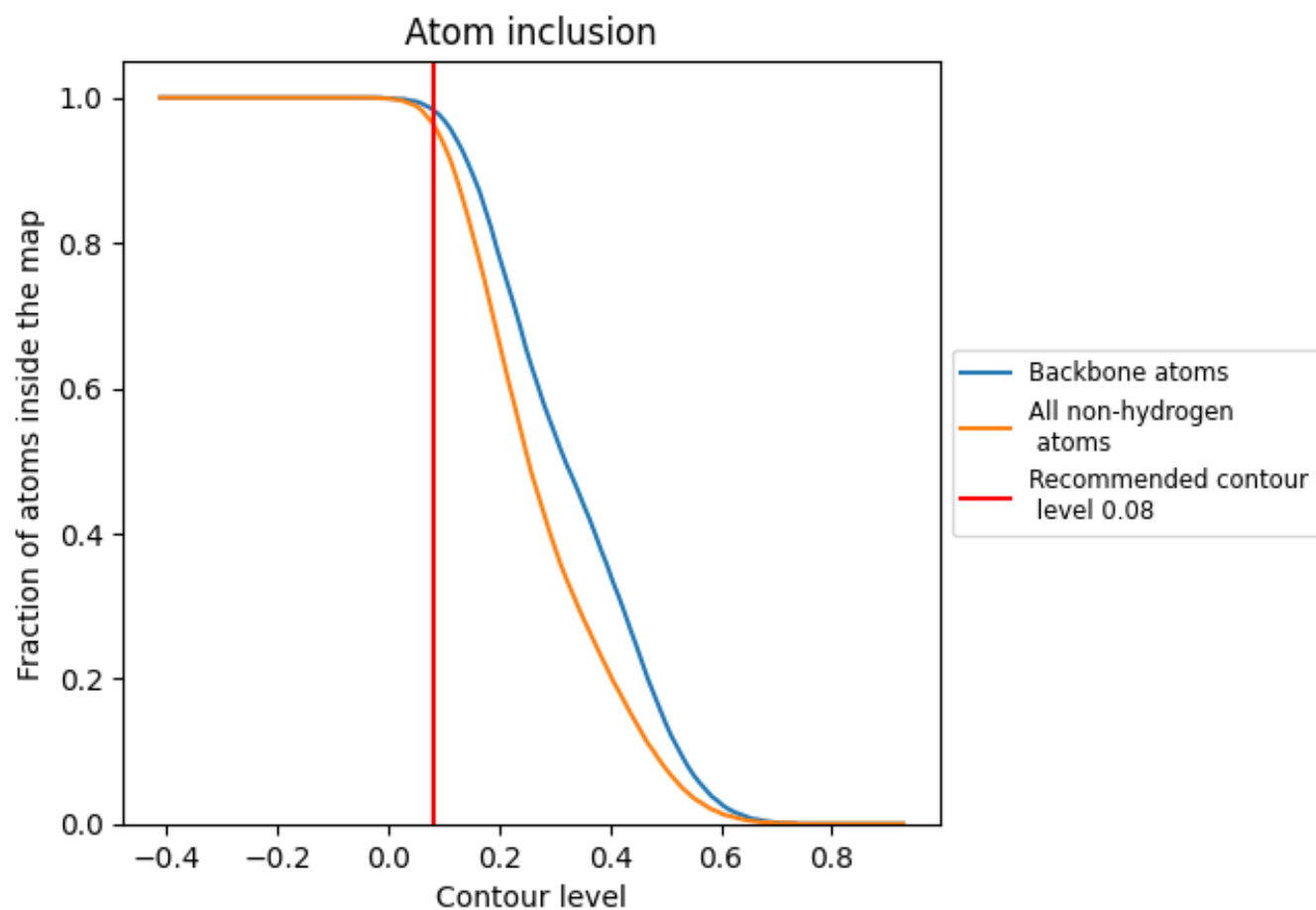
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).











































## 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.3740
A	 0.9860	 0.1490
B	 0.9750	 0.1590
C	 0.9280	 0.1630
D	 0.9730	 0.1810
E	 0.9350	 0.1530
F	 0.9530	 0.2400
G	 0.8980	 0.2400
H	 0.9010	 0.2520
I	 0.9330	 0.1700
J	 0.9390	 0.1620
Q	 0.9460	 0.4000
R	 0.9530	 0.3760
S	 0.9720	 0.3850
T	 0.9830	 0.4840
U	 0.9890	 0.4810
V	 0.9880	 0.4640
W	 0.9880	 0.4820
X	 0.9780	 0.4910
Y	 0.9710	 0.4790
Z	 1.0000	 0.4860

