



## Full wwPDB EM Validation Report ⓘ

Jun 9, 2024 – 10:47 AM EDT

PDB ID : 8EU9  
EMDB ID : EMD-28609  
Title : Class1 of the INO80-Nucleosome complex  
Authors : Wu, H.; Munoz, E.; Gourdet, M.; Cheng, Y.F.; Narlikar, G.  
Deposited on : 2022-10-18  
Resolution : 3.48 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.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

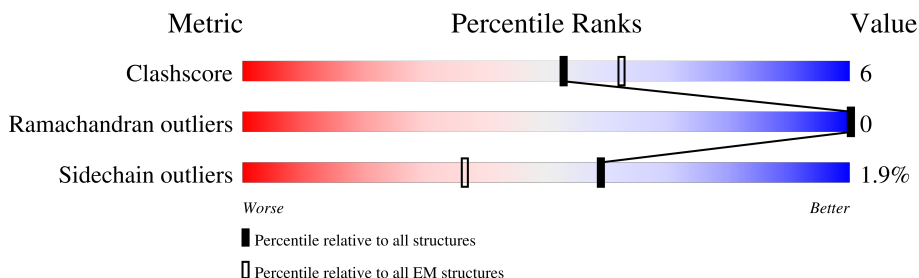
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.48 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.




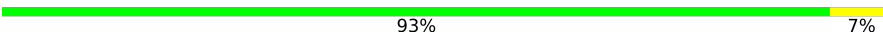
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	Q	493	<div> <div>30%</div> <div>69%</div> <div>16%</div> <div>14%</div> </div>
2	R	755	<div> <div>45%</div> <div>12%</div> <div>42%</div> </div>
3	S	135	<div> <div>6%</div> <div>73%</div> <div>16%</div> <div>10%</div> </div>
4	T	443	<div> <div>83%</div> <div>15%</div> </div>
4	V	443	<div> <div>88%</div> <div>12%</div> </div>
4	X	443	<div> <div>85%</div> <div>15%</div> </div>
5	U	446	<div> <div>82%</div> <div>15%</div> </div>
5	W	446	<div> <div>86%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
5	Y	446	 84% 15%
6	Z	28	 93% 7%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28517 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 Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	426	Total	C	N	O	S	0	0
			3413	2173	570	655	15		

- Molecule 2 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	440	Total	C	N	O	S	0	0
			3489	2215	592	671	11		

- Molecule 3 is a protein called Chromatin-remodeling complex subunit IES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	121	Total	C	N	O	S	0	0
			969	614	184	169	2		

- Molecule 4 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	437	Total	C	N	O	S	0	0
			3338	2102	575	651	10		
4	V	443	Total	C	N	O	S	0	0
			3388	2140	580	658	10		
4	X	442	Total	C	N	O	S	0	0
			3376	2131	579	656	10		

- Molecule 5 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	436	Total	C	N	O	S	0	0
			3333	2086	579	657	11		
5	W	442	Total	C	N	O	S	0	0
			3389	2119	590	668	12		

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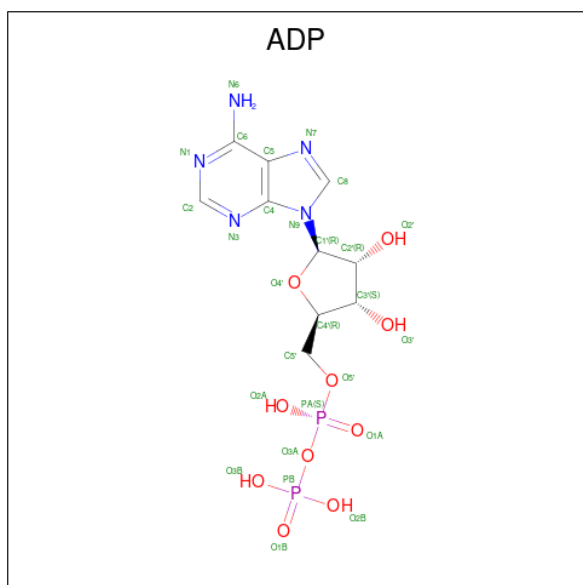
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	445	Total	C	N	O	S	0	0
			3412	2130	593	677	12		

- Molecule 6 is a protein called Ino eighty subunit 2.

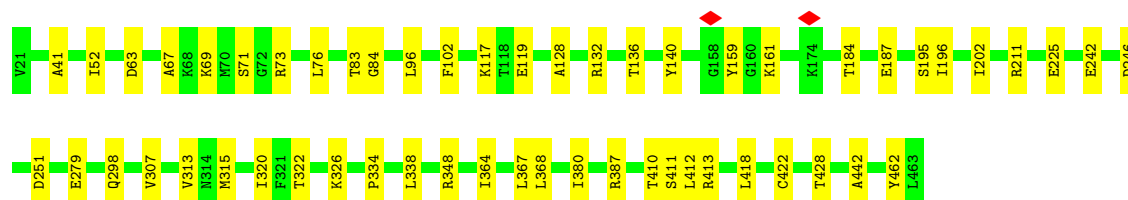
Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	28	Total	C	N	O	S	0	0
			248	158	45	43	2		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

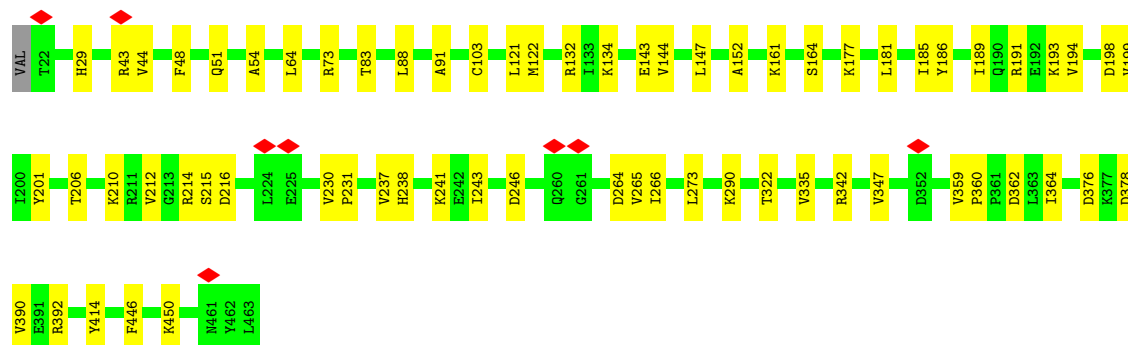
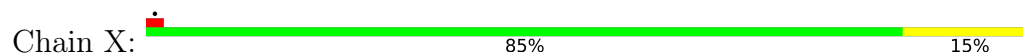




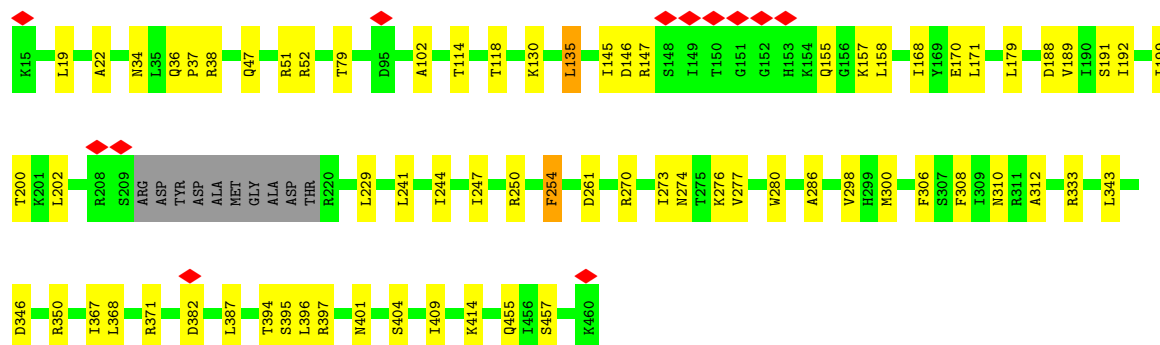
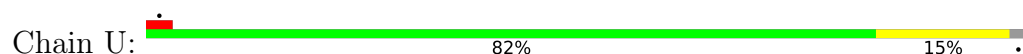




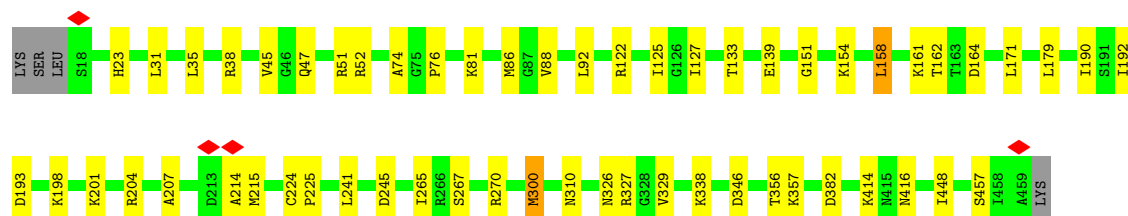
• Molecule 4: RuvB-like protein 1



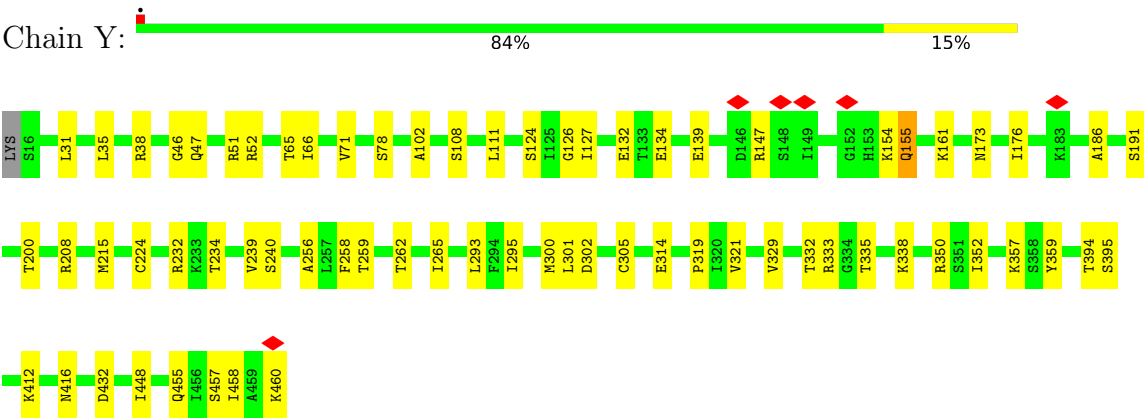
• Molecule 5: RuvB-like protein 2



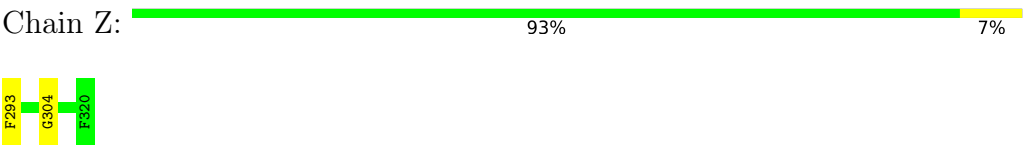
• Molecule 5: RuvB-like protein 2



• Molecule 5: RuvB-like protein 2



● Molecule 6: Ino eighty subunit 2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22054	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 ( $e^-/\text{\AA}^2$ )	43	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	1.864	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	400.8, 400.8, 400.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	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	Q	0.32	0/3478	0.68	7/4718 (0.1%)
2	R	0.34	0/3577	0.68	6/4869 (0.1%)
3	S	0.37	0/987	0.74	3/1326 (0.2%)
4	T	0.33	0/3377	0.64	1/4571 (0.0%)
4	V	0.33	0/3430	0.63	2/4643 (0.0%)
4	X	0.32	0/3418	0.64	3/4627 (0.1%)
5	U	0.32	0/3369	0.58	1/4540 (0.0%)
5	W	0.33	0/3427	0.64	5/4620 (0.1%)
5	Y	0.32	0/3450	0.60	1/4651 (0.0%)
6	Z	0.35	0/254	0.66	0/338
All	All	0.33	0/28767	0.64	29/38903 (0.1%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	245	ASP	CB-CG-OD1	10.27	127.54	118.30
1	Q	1319	LEU	CA-CB-CG	9.35	136.81	115.30
2	R	43	ASP	CB-CG-OD1	8.96	126.37	118.30
2	R	265	LEU	CA-CB-CG	8.82	135.60	115.30
4	X	376	ASP	CB-CG-OD2	8.81	126.23	118.30
1	Q	1308	LEU	CA-CB-CG	8.37	134.55	115.30
5	Y	302	ASP	CB-CG-OD2	8.10	125.59	118.30
1	Q	1288	MET	CB-CG-SD	7.20	134.01	112.40
4	V	63	ASP	CB-CG-OD2	7.07	124.67	118.30
3	S	147	MET	CB-CG-SD	6.30	131.29	112.40
1	Q	967	LEU	CA-CB-CG	6.22	129.61	115.30
4	X	122	MET	CB-CG-SD	6.20	131.00	112.40
5	W	215	MET	CB-CG-SD	5.99	130.37	112.40
1	Q	1257	MET	CA-CB-CG	5.94	123.40	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	158	LEU	CA-CB-CG	5.93	128.94	115.30
1	Q	1175	LEU	CA-CB-CG	5.65	128.31	115.30
4	T	258	ARG	CG-CD-NE	5.64	123.65	111.80
2	R	154	LEU	CA-CB-CG	5.63	128.26	115.30
5	W	215	MET	CG-SD-CE	5.55	109.08	100.20
3	S	78	LEU	CA-CB-CG	5.52	128.00	115.30
4	X	122	MET	CG-SD-CE	5.46	108.93	100.20
2	R	653	GLN	CA-CB-CG	5.36	125.19	113.40
2	R	747	LEU	CA-CB-CG	5.17	127.18	115.30
2	R	140	LEU	CA-CB-CG	5.16	127.17	115.30
5	U	135	LEU	CA-CB-CG	5.15	127.14	115.30
4	V	462	TYR	CA-CB-CG	5.10	123.09	113.40
3	S	147	MET	CA-CB-CG	5.08	121.93	113.30
1	Q	1331	MET	CA-CB-CG	5.07	121.91	113.30
5	W	414	LYS	CA-CB-CG	5.02	124.44	113.40

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	Q	3413	0	3363	45	0
2	R	3489	0	3347	53	0
3	S	969	0	994	15	0
4	T	3338	0	3434	43	0
4	V	3388	0	3506	30	0
4	X	3376	0	3491	39	0
5	U	3333	0	3401	50	0
5	W	3389	0	3459	34	0
5	Y	3412	0	3472	44	0
6	Z	248	0	242	2	0
7	T	27	0	12	3	0
7	U	27	0	12	0	0
7	V	27	0	12	3	0
7	W	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	27	0	12	0	0
7	Y	27	0	12	1	0
All	All	28517	0	28781	319	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 6.

All (319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:162:THR:HG23	5:W:164:ASP:H	1.62	0.65
2:R:647:LEU:O	2:R:652:SER:OG	2.17	0.62
5:U:300:MET:HG3	4:V:322:THR:HG21	1.82	0.61
5:W:45:VAL:O	7:W:501:ADP:N6	2.34	0.61
5:W:47:GLN:NE2	5:W:357:LYS:O	2.33	0.61
4:V:313:VAL:HG21	4:V:338:LEU:HD23	1.83	0.60
4:X:177:LYS:HB2	4:X:237:VAL:HG11	1.84	0.60
4:T:130:GLY:HA2	4:T:248:THR:HA	1.84	0.58
5:Y:31:LEU:O	5:Y:38:ARG:NH1	2.37	0.58
4:T:326:LYS:HD3	5:Y:102:ALA:HB2	1.86	0.57
5:Y:432:ASP:OD1	5:Y:432:ASP:N	2.36	0.57
2:R:607:HIS:O	2:R:611:GLN:N	2.37	0.57
2:R:139:ARG:HH22	2:R:192:GLU:HB2	1.71	0.56
5:U:191:SER:HB3	5:U:202:LEU:HD11	1.87	0.56
5:W:35:LEU:O	5:W:52:ARG:NH1	2.39	0.56
4:X:189:ILE:HG23	4:X:194:VAL:HB	1.86	0.56
4:V:41:ALA:HB3	4:V:52:ILE:HG23	1.89	0.55
5:W:204:ARG:HE	5:W:207:ALA:HA	1.71	0.55
5:Y:35:LEU:O	5:Y:52:ARG:NH1	2.39	0.55
5:U:397:ARG:O	5:U:401:ASN:ND2	2.40	0.55
1:Q:1148:LEU:HD21	4:X:273:LEU:HD21	1.89	0.55
2:R:67:LEU:HD13	2:R:110:LEU:HD23	1.88	0.55
2:R:68:THR:HG21	2:R:92:VAL:HG13	1.89	0.55
2:R:608:GLU:HA	2:R:611:GLN:HB2	1.89	0.55
5:Y:293:LEU:HG	5:Y:295:ILE:HD11	1.89	0.55
2:R:127:ASP:HB2	2:R:131:PRO:HB3	1.89	0.55
5:Y:46:GLY:O	5:Y:51:ARG:NH2	2.40	0.55
2:R:211:ARG:NH1	3:S:104:GLU:OE1	2.35	0.54
2:R:213:ASN:O	2:R:218:GLN:NE2	2.40	0.54
5:W:38:ARG:O	5:W:51:ARG:NH2	2.40	0.54
1:Q:949:GLU:HA	1:Q:1419:VAL:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1085:LEU:HB2	1:Q:1223:VAL:HG22	1.90	0.54
2:R:105:VAL:HG12	2:R:107:ASN:H	1.72	0.54
4:X:212:VAL:HG12	4:X:230:VAL:HG21	1.89	0.54
1:Q:1430:GLU:O	1:Q:1434:ASP:N	2.41	0.54
4:T:325:ASN:HD21	4:T:366:ARG:HH21	1.56	0.54
4:X:29:HIS:HB3	4:X:390:VAL:HG21	1.89	0.54
2:R:100:PHE:HA	2:R:105:VAL:HA	1.90	0.53
5:U:38:ARG:O	5:U:51:ARG:NH2	2.41	0.53
1:Q:1293:ARG:O	1:Q:1297:GLU:HB3	2.08	0.53
5:W:31:LEU:HD21	5:W:35:LEU:HD13	1.89	0.53
5:Y:295:ILE:CD1	5:Y:321:VAL:HG13	2.39	0.53
1:Q:1390:ILE:HG23	1:Q:1420:TYR:HB2	1.90	0.53
3:S:126:LYS:HD3	3:S:133:ARG:HE	1.73	0.53
5:Y:173:ASN:OD1	5:Y:173:ASN:N	2.41	0.53
5:W:151:GLY:O	5:W:154:LYS:NZ	2.41	0.53
3:S:36:VAL:HG23	3:S:39:ARG:HH21	1.73	0.53
4:T:341:ASN:OD1	4:T:342:ARG:NH1	2.41	0.53
5:U:270:ARG:O	5:U:274:ASN:ND2	2.42	0.53
1:Q:948:ILE:HB	1:Q:1418:THR:HG23	1.91	0.53
5:Y:47:GLN:HE22	5:Y:357:LYS:H	1.56	0.53
1:Q:1247:SER:OG	1:Q:1248:ASP:N	2.41	0.53
1:Q:1280:LYS:NZ	4:V:225:GLU:O	2.39	0.53
4:T:49:VAL:O	7:T:501:ADP:N6	2.40	0.53
5:U:34:ASN:O	5:U:36:GLN:NE2	2.39	0.53
5:U:145:ILE:HD12	5:U:147:ARG:HD3	1.91	0.53
2:R:148:THR:HG22	2:R:739:PRO:HB2	1.91	0.52
4:V:380:ILE:HG12	4:V:412:LEU:HD13	1.91	0.52
5:U:404:SER:OG	4:V:73:ARG:NH1	2.43	0.52
4:V:136:THR:HG22	4:V:242:GLU:HB2	1.90	0.52
4:X:43:ARG:NH2	4:X:378:ASP:OD2	2.42	0.52
4:T:116:LYS:HE3	4:T:279:GLU:HG2	1.90	0.52
5:U:300:MET:O	5:U:333:ARG:NH1	2.43	0.52
4:X:246:ASP:OD1	4:X:246:ASP:N	2.38	0.52
3:S:42:ILE:HG21	3:S:47:ARG:CZ	2.40	0.52
4:X:198:ASP:HA	4:X:214:ARG:HA	1.91	0.52
2:R:183:THR:HG22	2:R:200:VAL:HA	1.90	0.52
4:V:315:MET:O	4:V:348:ARG:NH1	2.43	0.52
2:R:143:VAL:HB	2:R:146:GLN:HG2	1.92	0.51
2:R:185:LEU:HB3	2:R:668:VAL:HG22	1.92	0.51
4:T:308:LEU:HB3	4:T:336:VAL:HG12	1.93	0.51
4:T:263:GLN:O	5:U:250:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:382:ASP:N	5:U:382:ASP:OD1	2.42	0.51
4:X:43:ARG:HG2	4:X:44:VAL:HG13	1.91	0.51
2:R:41:ALA:HA	2:R:135:LEU:HB2	1.91	0.51
2:R:670:ILE:HD11	2:R:702:MET:HB2	1.93	0.51
1:Q:1319:LEU:HG	1:Q:1391:PHE:HA	1.93	0.51
2:R:139:ARG:O	2:R:142:THR:OG1	2.29	0.51
4:T:380:ILE:HD11	5:Y:458:ILE:HD13	1.93	0.51
1:Q:1273:LEU:HB3	4:X:265:VAL:HG23	1.92	0.51
5:W:214:ALA:HB2	4:X:181:LEU:HD22	1.93	0.51
5:U:189:VAL:HG12	5:U:202:LEU:HD13	1.92	0.51
2:R:266:THR:HG23	2:R:267:LEU:HG	1.93	0.50
4:V:102:PHE:HD1	4:V:307:VAL:HG13	1.75	0.50
1:Q:1356:ASP:N	1:Q:1356:ASP:OD1	2.42	0.50
5:W:382:ASP:OD1	5:W:382:ASP:N	2.43	0.50
1:Q:1402:SER:HA	1:Q:1405:MET:HG2	1.92	0.50
4:T:313:VAL:HG21	4:T:338:LEU:HB3	1.93	0.50
2:R:619:ILE:O	2:R:622:PRO:HD2	2.12	0.50
1:Q:1106:ASN:OD1	1:Q:1110:ASN:ND2	2.44	0.50
1:Q:1257:MET:HA	1:Q:1261:LYS:HB2	1.92	0.50
1:Q:1427:THR:HG23	1:Q:1429:GLU:H	1.75	0.50
5:W:122:ARG:HH21	5:W:241:LEU:HD22	1.76	0.50
1:Q:1013:HIS:HB3	1:Q:1016:LEU:HG	1.94	0.50
5:U:241:LEU:HD21	5:U:277:VAL:HG21	1.93	0.50
4:X:181:LEU:HB3	4:X:185:ILE:HD13	1.92	0.50
2:R:717:LEU:HD13	2:R:747:LEU:HD23	1.92	0.50
4:T:151:ASP:HA	4:T:163:ILE:HA	1.93	0.50
4:T:152:ALA:HB3	4:T:164:SER:HB3	1.93	0.49
5:U:306:PHE:O	5:U:310:ASN:HB2	2.12	0.49
4:X:199:VAL:HG13	4:X:212:VAL:HB	1.94	0.49
5:U:247:ILE:HD11	5:U:254:PHE:HB3	1.94	0.49
4:T:35:LEU:HA	4:T:41:ALA:HA	1.93	0.49
4:T:361:PRO:HA	4:T:364:ILE:HG22	1.94	0.49
5:W:190:ILE:HD12	5:W:192:ILE:HD11	1.93	0.49
4:T:29:HIS:NE2	7:T:501:ADP:O2'	2.39	0.49
5:W:162:THR:OG1	5:W:225:PRO:O	2.28	0.49
5:W:300:MET:HG2	4:X:322:THR:HG21	1.94	0.49
5:U:22:ALA:O	5:U:371:ARG:NH1	2.45	0.49
4:V:140:TYR:HB2	4:V:202:ILE:HB	1.95	0.49
4:V:195:SER:OG	4:V:196:ILE:N	2.45	0.49
2:R:107:ASN:HB3	2:R:110:LEU:HD13	1.95	0.49
4:T:181:LEU:HD23	4:T:185:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:216:ASP:HB2	4:X:231:PRO:HA	1.95	0.49
5:Y:457:SER:HB3	5:Y:460:LYS:HZ2	1.78	0.49
4:X:143:GLU:HG3	4:X:215:SER:HB3	1.95	0.48
4:X:152:ALA:HB2	4:X:164:SER:HB2	1.95	0.48
2:R:639:CYS:SG	2:R:640:GLU:N	2.86	0.48
3:S:58:ARG:HH22	3:S:60:HIS:HD2	1.61	0.48
5:W:133:THR:OG1	5:W:193:ASP:OD1	2.28	0.48
4:X:144:VAL:HG21	4:X:147:LEU:HD23	1.95	0.48
5:U:191:SER:OG	5:U:200:THR:OG1	2.29	0.48
4:V:413:ARG:NH2	7:V:501:ADP:O3A	2.46	0.48
4:X:161:LYS:NZ	4:X:186:TYR:OH	2.46	0.48
1:Q:1097:ASN:HB3	1:Q:1100:ASN:HB2	1.96	0.48
3:S:118:VAL:HG21	3:S:143:ILE:HG21	1.96	0.48
5:U:308:PHE:O	5:U:312:ALA:HB2	2.13	0.48
5:Y:300:MET:HA	5:Y:333:ARG:HD3	1.95	0.48
5:U:47:GLN:NE2	5:U:79:THR:O	2.46	0.48
2:R:590:ILE:HA	2:R:593:LEU:HD12	1.95	0.48
4:T:266:ILE:HA	5:U:250:ARG:HH12	1.78	0.48
4:V:83:THR:N	7:V:501:ADP:O2B	2.47	0.48
1:Q:1103:ASP:N	1:Q:1103:ASP:OD1	2.46	0.47
5:U:135:LEU:HD21	5:U:191:SER:HB2	1.95	0.47
4:V:428:THR:HG21	5:W:35:LEU:HB2	1.96	0.47
1:Q:1131:LEU:HD21	5:Y:239:VAL:HG11	1.95	0.47
4:T:198:ASP:OD1	4:T:198:ASP:N	2.47	0.47
5:U:19:LEU:HB2	4:V:71:SER:HB3	1.96	0.47
4:V:84:GLY:N	7:V:501:ADP:O2B	2.47	0.47
5:W:76:PRO:O	5:W:81:LYS:NZ	2.46	0.47
5:W:457:SER:OG	4:X:450:LYS:NZ	2.45	0.47
5:Y:329:VAL:HG12	5:Y:338:LYS:HG3	1.96	0.47
1:Q:1344:ARG:NH1	1:Q:1345:LEU:O	2.47	0.47
4:X:73:ARG:HB2	4:X:335:VAL:HG23	1.97	0.47
1:Q:1255:TYR:HD2	6:Z:304:GLY:HA2	1.78	0.47
4:X:201:TYR:O	4:X:210:LYS:NZ	2.47	0.47
1:Q:1292:ASP:HA	1:Q:1295:ILE:HD12	1.97	0.47
2:R:683:ARG:NH1	2:R:687:GLU:OE2	2.34	0.47
2:R:189:CYS:HA	2:R:194:THR:HG22	1.97	0.47
2:R:205:ILE:HG22	2:R:208:ASP:H	1.79	0.47
4:T:116:LYS:NZ	4:T:118:THR:OG1	2.47	0.47
5:Y:71:VAL:HG12	5:Y:352:ILE:HG13	1.97	0.47
4:T:347:VAL:HG11	4:T:360:PRO:HG3	1.97	0.47
1:Q:1203:LEU:O	1:Q:1279:ASN:ND2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:191:ARG:O	4:X:193:LYS:NZ	2.44	0.47
5:Y:108:SER:OG	5:Y:111:LEU:O	2.33	0.46
1:Q:1203:LEU:HD12	1:Q:1278:LEU:HD21	1.97	0.46
4:T:355:SER:OG	4:T:359:VAL:O	2.23	0.46
4:V:364:ILE:HD12	4:V:367:LEU:HD23	1.96	0.46
5:U:241:LEU:HD23	5:U:244:ILE:HD12	1.97	0.46
4:X:392:ARG:HA	4:X:392:ARG:NH1	2.31	0.46
1:Q:1015:ASP:OD2	1:Q:1019:ARG:NH1	2.49	0.46
2:R:106:THR:OG1	3:S:61:LYS:O	2.30	0.46
2:R:277:VAL:O	2:R:612:MET:N	2.48	0.46
4:T:153:GLU:OE2	4:T:162:THR:N	2.48	0.46
5:U:102:ALA:HB2	4:V:326:LYS:HD3	1.97	0.46
5:U:280:TRP:HB3	5:U:286:ALA:HB3	1.98	0.46
5:Y:394:THR:OG1	5:Y:395:SER:N	2.49	0.46
1:Q:1364:ASN:ND2	1:Q:1366:GLU:OE2	2.49	0.45
2:R:138:GLU:N	2:R:166:GLY:O	2.45	0.45
4:T:29:HIS:HB3	4:T:390:VAL:HG11	1.98	0.45
4:V:119:GLU:HG2	4:V:279:GLU:HA	1.98	0.45
5:W:127:ILE:HD11	5:W:241:LEU:HG	1.98	0.45
5:Y:301:LEU:HB3	5:Y:305:CYS:HB2	1.97	0.45
2:R:73:ARG:H	3:S:30:LEU:HD21	1.80	0.45
4:T:26:ALA:O	7:T:501:ADP:O3'	2.34	0.45
4:T:342:ARG:HD3	5:Y:448:ILE:HB	1.99	0.45
4:X:241:LYS:HG3	4:X:243:ILE:HG12	1.98	0.45
2:R:80:THR:HB	2:R:82:VAL:HG23	1.99	0.45
4:T:140:TYR:HB2	4:T:202:ILE:HB	1.97	0.45
5:Y:186:ALA:HB1	5:Y:208:ARG:HH22	1.82	0.45
4:T:121:LEU:HD23	4:T:323:TYR:HD2	1.80	0.45
5:W:158:LEU:HB2	5:W:171:LEU:HD11	1.98	0.45
1:Q:1331:MET:HE2	1:Q:1334:TYR:HE1	1.82	0.45
4:T:408:THR:O	5:Y:457:SER:OG	2.35	0.45
2:R:66:ALA:HB1	2:R:96:SER:HB2	1.99	0.45
5:U:157:LYS:HB3	5:U:168:ILE:HD11	1.99	0.45
4:V:410:THR:OG1	4:V:411:SER:N	2.50	0.45
5:Y:78:SER:O	5:Y:78:SER:OG	2.34	0.45
4:X:132:ARG:HG2	4:X:246:ASP:HB3	1.99	0.45
4:X:414:TYR:OH	4:X:446:PHE:O	2.32	0.45
5:Y:256:ALA:HA	5:Y:259:THR:HG22	1.98	0.45
1:Q:1139:GLU:OE2	1:Q:1142:ARG:NH1	2.50	0.45
2:R:657:LEU:HD21	2:R:692:LEU:HD22	1.99	0.45
4:T:96:LEU:HD13	4:T:100:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:375:TYR:HB3	4:T:379:GLU:HB2	1.99	0.45
4:T:441:GLU:OE2	5:U:52:ARG:NH1	2.48	0.44
5:Y:65:THR:HG23	5:Y:66:ILE:HG13	1.98	0.44
5:Y:191:SER:HB3	5:Y:200:THR:HB	1.98	0.44
2:R:168:ASP:OD1	2:R:168:ASP:N	2.48	0.44
3:S:125:TYR:OH	5:U:229:LEU:O	2.32	0.44
5:W:125:ILE:HG23	5:W:241:LEU:HB2	2.00	0.44
1:Q:1240:PRO:O	1:Q:1244:GLN:HB2	2.18	0.44
5:Y:78:SER:N	7:Y:501:ADP:O1B	2.48	0.44
2:R:199:VAL:HA	2:R:204:GLY:HA2	2.00	0.44
2:R:48:LYS:HE2	2:R:48:LYS:HB2	1.88	0.44
3:S:116:CYS:SG	3:S:119:THR:OG1	2.64	0.44
5:W:329:VAL:HG12	5:W:338:LYS:HG2	1.99	0.44
5:W:346:ASP:OD1	5:W:346:ASP:N	2.49	0.44
4:T:284:LEU:HD12	5:Y:258:PHE:HB3	1.99	0.44
4:V:117:LYS:HB2	4:V:320:ILE:HD11	2.00	0.44
5:W:88:VAL:O	5:W:92:LEU:HB2	2.18	0.44
5:W:122:ARG:HE	5:W:241:LEU:HB3	1.83	0.43
4:X:54:ALA:HB1	4:X:88:LEU:HD21	2.00	0.43
4:T:395:VAL:HA	4:T:434:ILE:HB	1.99	0.43
5:U:179:LEU:HD12	5:U:199:ILE:HD13	1.99	0.43
2:R:646:LEU:HD23	2:R:646:LEU:HA	1.89	0.43
4:T:192:GLU:HB2	4:T:194:VAL:HG23	2.00	0.43
4:X:347:VAL:HG11	4:X:360:PRO:HG3	1.99	0.43
5:Y:47:GLN:HE21	5:Y:359:TYR:HE1	1.65	0.43
1:Q:1255:TYR:CD2	6:Z:304:GLY:HA2	2.52	0.43
1:Q:1332:GLU:O	1:Q:1336:THR:OG1	2.27	0.43
2:R:730:SER:N	2:R:733:GLU:OE2	2.40	0.43
5:U:310:ASN:OD1	5:U:350:ARG:NH1	2.51	0.43
2:R:126:PRO:HG3	3:S:47:ARG:HB3	2.00	0.43
3:S:70:GLU:O	3:S:74:ILE:HD12	2.18	0.43
5:U:192:ILE:HG12	5:U:199:ILE:HG22	2.01	0.43
4:X:362:ASP:OD1	4:X:362:ASP:N	2.52	0.43
5:Y:132:GLU:OE1	5:Y:234:THR:OG1	2.31	0.43
5:U:346:ASP:OD1	5:U:346:ASP:N	2.51	0.43
5:U:394:THR:OG1	5:U:395:SER:N	2.51	0.43
5:U:401:ASN:HB3	4:V:368:LEU:HD11	1.99	0.43
5:U:455:GLN:OE1	5:U:457:SER:OG	2.32	0.43
5:W:448:ILE:HB	4:X:342:ARG:HG2	2.00	0.43
1:Q:1364:ASN:OD1	1:Q:1364:ASN:N	2.52	0.43
2:R:25:PRO:HD2	2:R:88:LEU:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:617:GLU:C	2:R:619:ILE:H	2.22	0.43
1:Q:967:LEU:HD11	1:Q:1006:GLN:HB3	2.01	0.43
1:Q:1322:PHE:HD1	1:Q:1394:SER:HB2	1.82	0.43
2:R:158:TYR:CD2	3:S:49:LYS:HA	2.54	0.43
5:U:146:ASP:HB2	5:U:155:GLN:HG2	2.01	0.43
5:Y:332:THR:HG1	5:Y:335:THR:HG1	1.63	0.43
2:R:119:PHE:HA	2:R:122:LEU:HD12	2.00	0.42
3:S:143:ILE:HD13	3:S:143:ILE:HA	1.90	0.42
5:U:158:LEU:HB2	5:U:171:LEU:HD11	2.00	0.42
5:Y:147:ARG:HB3	5:Y:154:LYS:HA	2.01	0.42
1:Q:1073:LEU:HD11	4:V:140:TYR:HE2	1.83	0.42
5:U:298:VAL:HG13	5:U:343:LEU:HD21	2.00	0.42
4:V:96:LEU:HD23	4:V:96:LEU:HA	1.85	0.42
5:W:416:ASN:OD1	5:W:416:ASN:N	2.52	0.42
4:X:264:ASP:O	4:X:266:ILE:N	2.49	0.42
4:X:266:ILE:HD13	4:X:266:ILE:HA	1.86	0.42
5:Y:262:THR:HB	5:Y:265:ILE:HD11	2.00	0.42
5:Y:416:ASN:OD1	5:Y:416:ASN:N	2.52	0.42
2:R:617:GLU:C	2:R:619:ILE:N	2.72	0.42
2:R:587:ARG:HA	2:R:593:LEU:HD21	2.00	0.42
5:Y:293:LEU:HG	5:Y:295:ILE:CD1	2.50	0.42
1:Q:1198:TYR:OH	1:Q:1278:LEU:O	2.37	0.42
5:Y:134:GLU:HG2	5:Y:232:ARG:HD3	2.01	0.42
1:Q:1320:ILE:HD12	1:Q:1320:ILE:HA	1.94	0.42
1:Q:1368:PHE:HB2	1:Q:1370:PHE:CE2	2.54	0.42
2:R:49:LEU:O	2:R:63:PHE:N	2.52	0.42
5:Y:412:LYS:HA	5:Y:412:LYS:HD2	1.86	0.42
5:Y:124:SER:HB3	5:Y:319:PRO:HG3	2.01	0.42
1:Q:1182:PRO:HD3	4:X:206:THR:HG22	2.02	0.42
4:V:67:ALA:O	4:V:69:LYS:NZ	2.52	0.42
4:X:134:LYS:HE2	4:X:134:LYS:HB3	1.91	0.42
2:R:152:GLN:HA	2:R:156:GLU:HG3	2.02	0.42
4:T:256:ASN:N	4:T:256:ASN:OD1	2.51	0.42
4:T:413:ARG:HH12	5:U:350:ARG:NH2	2.17	0.42
4:V:132:ARG:NE	4:V:246:ASP:OD1	2.41	0.42
5:W:326:ASN:OD1	5:W:327:ARG:NH1	2.53	0.42
5:Y:314:GLU:OE2	5:Y:350:ARG:NH1	2.53	0.41
4:T:223:ASP:HB2	5:U:170:GLU:H	1.85	0.41
5:U:276:LYS:HD2	5:U:276:LYS:HA	1.87	0.41
5:U:367:ILE:HG21	5:U:396:LEU:HD21	2.02	0.41
5:U:409:ILE:HD12	5:U:409:ILE:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:418:LEU:HD22	4:V:442:ALA:HB1	2.02	0.41
4:T:283:LYS:O	4:T:287:GLU:HG2	2.21	0.41
4:T:168:VAL:O	4:T:179:LEU:N	2.50	0.41
5:U:368:LEU:HD13	5:U:387:LEU:HB3	2.02	0.41
5:U:414:LYS:HA	5:U:414:LYS:HD3	1.84	0.41
5:W:158:LEU:HD12	5:W:179:LEU:HD11	2.02	0.41
5:W:74:ALA:O	5:W:356:THR:OG1	2.36	0.41
4:T:272:LEU:HG	4:T:273:LEU:HD23	2.02	0.41
4:V:184:THR:HA	4:V:187:GLU:HG2	2.02	0.41
1:Q:1022:VAL:HG12	1:Q:1289:PRO:HD3	2.03	0.41
2:R:158:TYR:HD2	3:S:49:LYS:HA	1.85	0.41
4:T:170:LEU:HD21	4:T:200:ILE:HD11	2.02	0.41
5:U:241:LEU:HD23	5:U:241:LEU:HA	1.90	0.41
4:V:117:LYS:H	4:V:117:LYS:HG2	1.64	0.41
5:W:23:HIS:HB3	5:W:86:MET:HE2	2.03	0.41
5:W:190:ILE:HG22	5:W:201:LYS:HA	2.02	0.41
5:W:265:ILE:HD12	5:W:270:ARG:HH21	1.85	0.41
4:X:51:GLN:HE22	4:X:83:THR:HG22	1.85	0.41
4:X:359:VAL:HB	4:X:364:ILE:HD11	2.02	0.41
1:Q:1107:LYS:HD2	4:T:206:THR:HA	2.02	0.41
1:Q:1298:SER:HB3	1:Q:1301:LEU:HB2	2.03	0.41
5:U:273:ILE:HD13	5:U:273:ILE:HA	1.88	0.40
4:V:128:ALA:HB3	4:V:334:PRO:HG3	2.03	0.40
4:X:290:LYS:HE2	4:X:290:LYS:HB2	1.86	0.40
5:Y:147:ARG:NH2	5:Y:155:GLN:O	2.47	0.40
2:R:220:VAL:HG11	2:R:244:GLU:HG2	2.04	0.40
5:W:139:GLU:N	5:W:161:LYS:O	2.52	0.40
1:Q:1397:ASN:N	1:Q:1397:ASN:OD1	2.55	0.40
5:Y:139:GLU:N	5:Y:161:LYS:O	2.54	0.40
1:Q:981:ALA:HB1	1:Q:1000:LEU:HD12	2.02	0.40
2:R:86:THR:HA	2:R:92:VAL:HG12	2.04	0.40
2:R:193:ASP:N	2:R:193:ASP:OD1	2.55	0.40
2:R:724:TYR:O	2:R:728:VAL:HG23	2.21	0.40
4:T:359:VAL:HG13	4:T:363:LEU:HD23	2.03	0.40
5:U:36:GLN:HA	5:U:37:PRO:HD3	1.94	0.40
5:U:130:LYS:HE2	5:U:130:LYS:HB2	1.87	0.40
5:Y:35:LEU:HD13	5:Y:35:LEU:HA	1.94	0.40
5:Y:127:ILE:HG23	5:Y:239:VAL:HG23	2.04	0.40
5:U:114:THR:O	5:U:118:THR:OG1	2.30	0.40
4:X:48:PHE:HE2	4:X:91:ALA:HB2	1.87	0.40
5:Y:126:GLY:HA2	5:Y:240:SER:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:176:ILE:HD13	5:Y:176:ILE:HA	1.89	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	Q	412/493 (84%)	395 (96%)	17 (4%)	0	100	100
2	R	436/755 (58%)	413 (95%)	23 (5%)	0	100	100
3	S	115/135 (85%)	107 (93%)	8 (7%)	0	100	100
4	T	433/443 (98%)	420 (97%)	13 (3%)	0	100	100
4	V	441/443 (100%)	427 (97%)	14 (3%)	0	100	100
4	X	440/443 (99%)	425 (97%)	15 (3%)	0	100	100
5	U	432/446 (97%)	415 (96%)	17 (4%)	0	100	100
5	W	440/446 (99%)	430 (98%)	10 (2%)	0	100	100
5	Y	443/446 (99%)	428 (97%)	15 (3%)	0	100	100
6	Z	26/28 (93%)	26 (100%)	0	0	100	100
All	All	3618/4078 (89%)	3486 (96%)	132 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	Q	387/453 (85%)	372 (96%)	15 (4%)	32	63
2	R	382/682 (56%)	369 (97%)	13 (3%)	37	67
3	S	102/115 (89%)	98 (96%)	4 (4%)	32	63
4	T	364/375 (97%)	361 (99%)	3 (1%)	81	92
4	V	370/375 (99%)	362 (98%)	8 (2%)	52	77
4	X	369/375 (98%)	365 (99%)	4 (1%)	73	88
5	U	366/380 (96%)	363 (99%)	3 (1%)	81	92
5	W	372/380 (98%)	367 (99%)	5 (1%)	69	86
5	Y	375/380 (99%)	371 (99%)	4 (1%)	73	88
6	Z	27/27 (100%)	26 (96%)	1 (4%)	34	64
All	All	3114/3542 (88%)	3054 (98%)	60 (2%)	59	80

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	1007	PHE
1	Q	1011	CYS
1	Q	1070	PHE
1	Q	1092	ASP
1	Q	1122	TYR
1	Q	1161	ASN
1	Q	1198	TYR
1	Q	1215	SER
1	Q	1284	SER
1	Q	1308	LEU
1	Q	1316	HIS
1	Q	1319	LEU
1	Q	1334	TYR
1	Q	1337	TYR
1	Q	1415	ARG
2	R	44	PHE
2	R	69	LYS
2	R	73	ARG
2	R	79	PHE
2	R	189	CYS
2	R	213	ASN
2	R	225	ASP
2	R	269	ASN
2	R	273	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	R	656	LYS
2	R	701	ASN
2	R	717	LEU
2	R	744	GLU
3	S	58	ARG
3	S	83	LYS
3	S	147	MET
3	S	155	TYR
4	T	198	ASP
4	T	355	SER
4	T	378	ASP
5	U	188	ASP
5	U	254	PHE
5	U	261	ASP
4	V	76	LEU
4	V	159	TYR
4	V	161	LYS
4	V	211	ARG
4	V	251	ASP
4	V	298	GLN
4	V	387	ARG
4	V	422	CYS
5	W	198	LYS
5	W	224	CYS
5	W	267	SER
5	W	300	MET
5	W	310	ASN
4	X	64	LEU
4	X	103	CYS
4	X	121	LEU
4	X	238	HIS
5	Y	155	GLN
5	Y	215	MET
5	Y	224	CYS
5	Y	455	GLN
6	Z	293	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	121	HIS
4	V	263	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	Y	47	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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$
7	ADP	X	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.42	4 (13%)
7	ADP	V	501	-	24,29,29	0.91	1 (4%)	29,45,45	1.45	4 (13%)
7	ADP	Y	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.56	4 (13%)
7	ADP	U	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.46	3 (10%)
7	ADP	W	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	3 (10%)
7	ADP	T	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.53	4 (13%)

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
7	ADP	X	501	-	-	3/12/32/32	0/3/3/3
7	ADP	V	501	-	-	3/12/32/32	0/3/3/3
7	ADP	Y	501	-	-	4/12/32/32	0/3/3/3
7	ADP	U	501	-	-	3/12/32/32	0/3/3/3
7	ADP	W	501	-	-	3/12/32/32	0/3/3/3
7	ADP	T	501	-	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	501	ADP	C5-C4	2.32	1.47	1.40
7	Y	501	ADP	C5-C4	2.26	1.46	1.40
7	X	501	ADP	C5-C4	2.19	1.46	1.40
7	U	501	ADP	C5-C4	2.14	1.46	1.40
7	T	501	ADP	C5-C4	2.14	1.46	1.40
7	V	501	ADP	C5-C4	2.11	1.46	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	501	ADP	PA-O3A-PB	-4.29	118.12	132.83
7	T	501	ADP	PA-O3A-PB	-4.23	118.31	132.83
7	U	501	ADP	PA-O3A-PB	-3.87	119.55	132.83
7	W	501	ADP	PA-O3A-PB	-3.73	120.03	132.83
7	V	501	ADP	PA-O3A-PB	-3.66	120.27	132.83
7	X	501	ADP	PA-O3A-PB	-3.52	120.74	132.83
7	T	501	ADP	N3-C2-N1	-3.22	123.64	128.68
7	U	501	ADP	N3-C2-N1	-3.17	123.73	128.68
7	W	501	ADP	N3-C2-N1	-3.16	123.74	128.68
7	Y	501	ADP	C3'-C2'-C1'	3.11	105.66	100.98
7	X	501	ADP	N3-C2-N1	-3.06	123.89	128.68
7	Y	501	ADP	N3-C2-N1	-3.05	123.91	128.68
7	V	501	ADP	C3'-C2'-C1'	3.05	105.56	100.98
7	V	501	ADP	N3-C2-N1	-2.92	124.11	128.68
7	T	501	ADP	C4-C5-N7	-2.80	106.48	109.40
7	W	501	ADP	C3'-C2'-C1'	2.80	105.19	100.98
7	T	501	ADP	C3'-C2'-C1'	2.65	104.96	100.98
7	U	501	ADP	C4-C5-N7	-2.56	106.73	109.40
7	X	501	ADP	C4-C5-N7	-2.44	106.85	109.40
7	X	501	ADP	C3'-C2'-C1'	2.42	104.63	100.98
7	Y	501	ADP	C4-C5-N7	-2.39	106.91	109.40
7	V	501	ADP	C4-C5-N7	-2.30	107.00	109.40

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

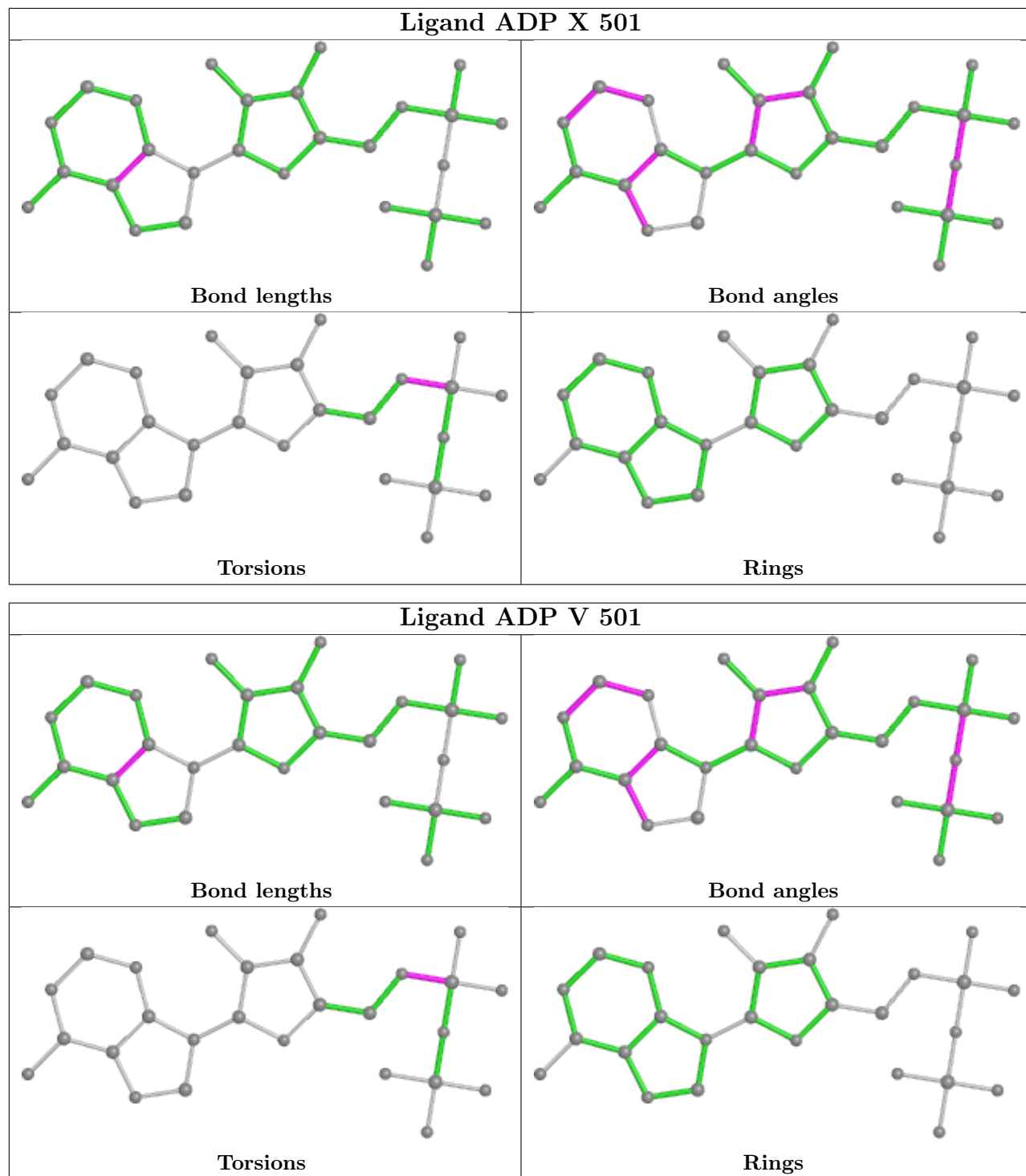
There are no ring outliers.

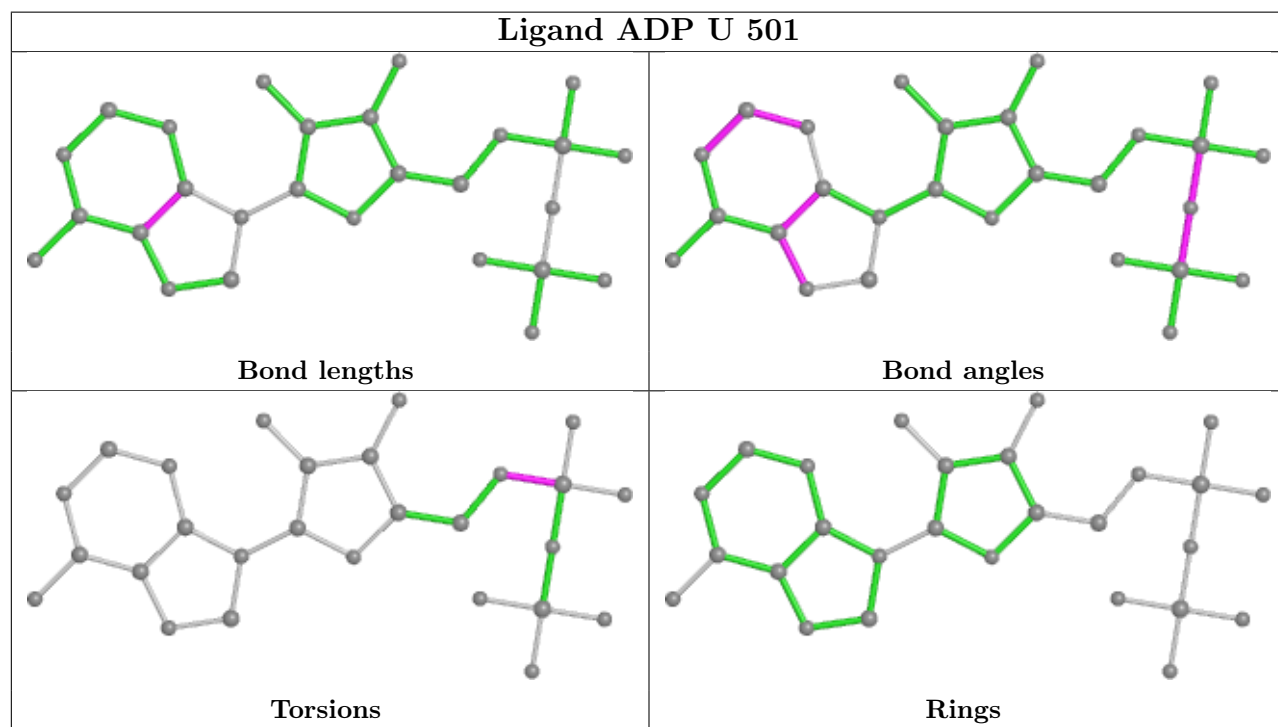
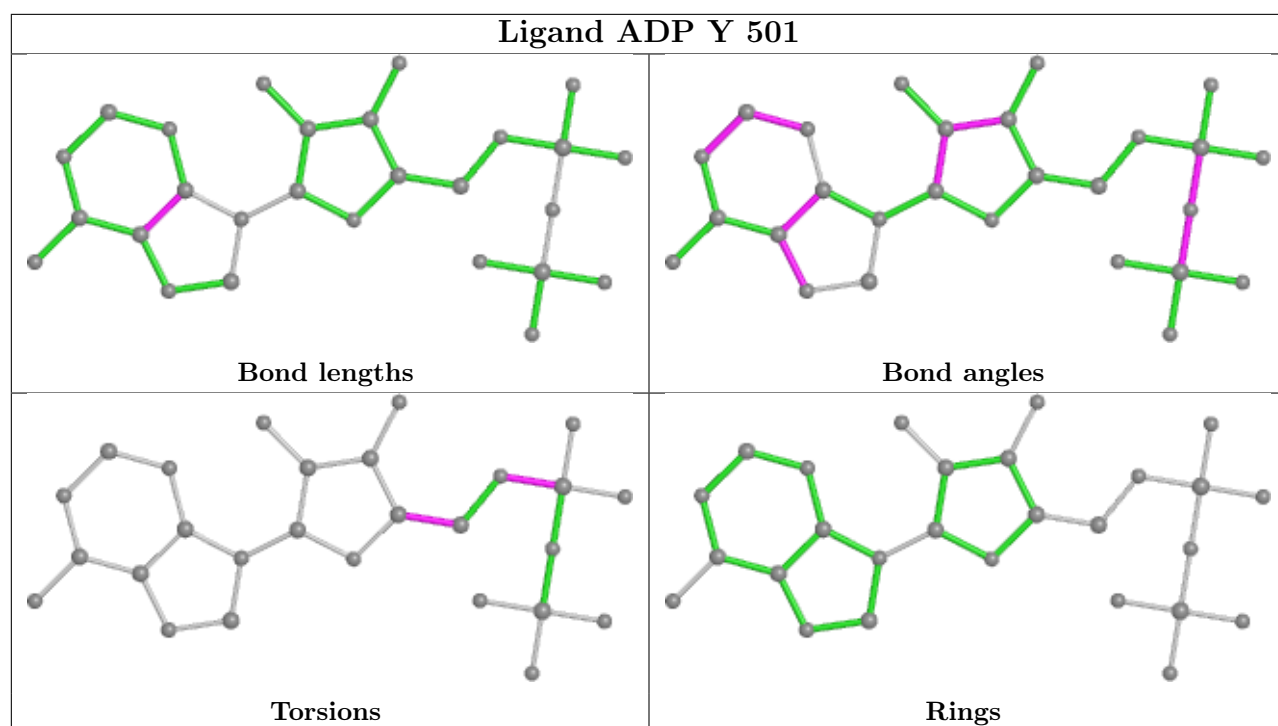
4 monomers are involved in 8 short contacts:

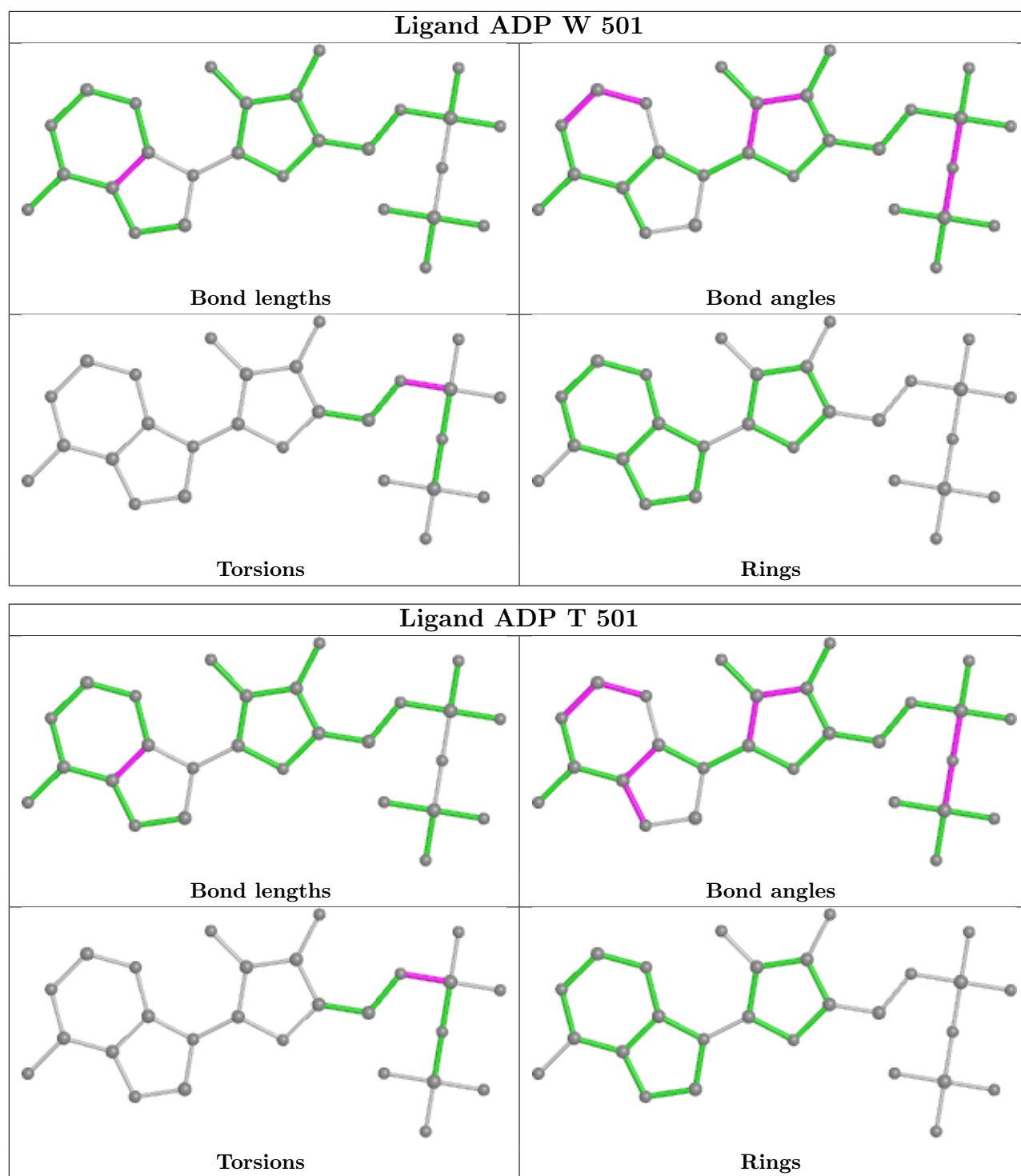
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	V	501	ADP	3	0
7	Y	501	ADP	1	0
7	W	501	ADP	1	0
7	T	501	ADP	3	0

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	1433:ARG	C	1434:ASP	N	3.26

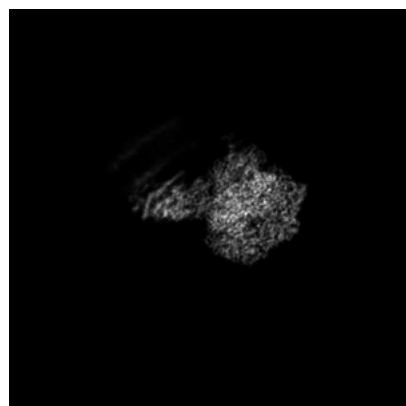
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28609. These allow visual inspection of the internal detail of the map and identification of artifacts.

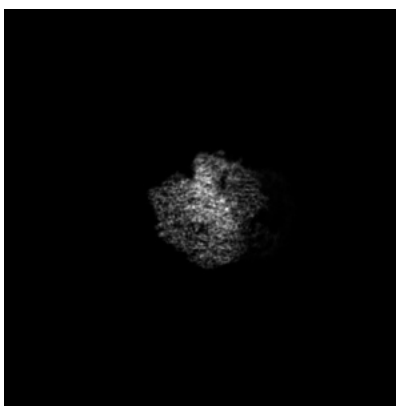
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

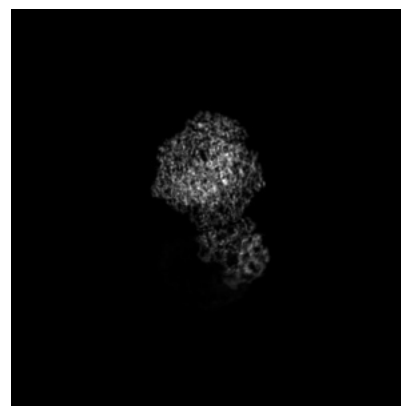
#### 6.1.1 Primary map



X

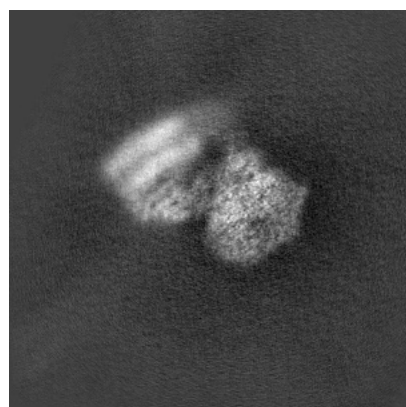


Y

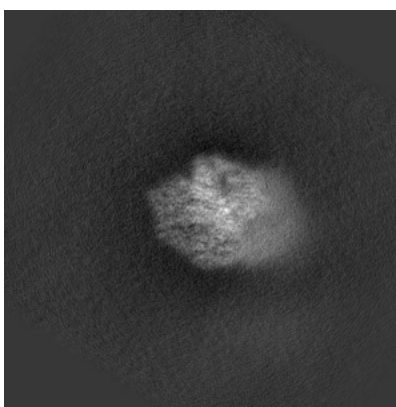


Z

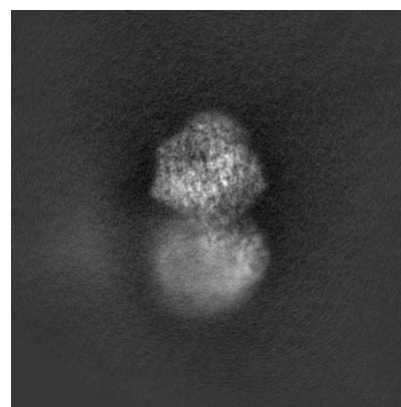
#### 6.1.2 Raw map



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: 240

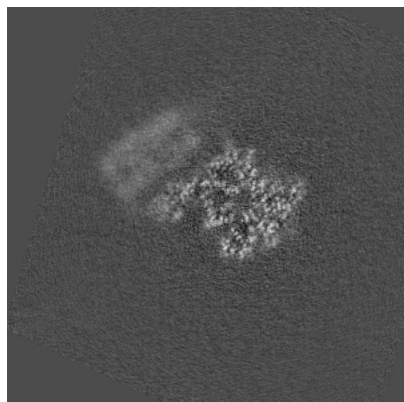


Y Index: 240

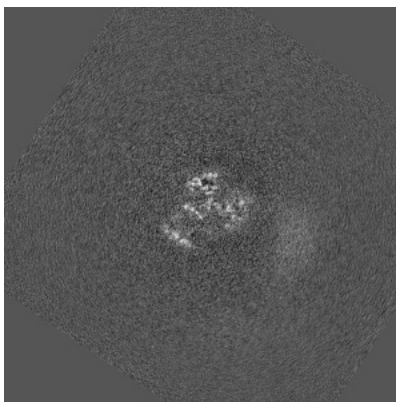


Z Index: 240

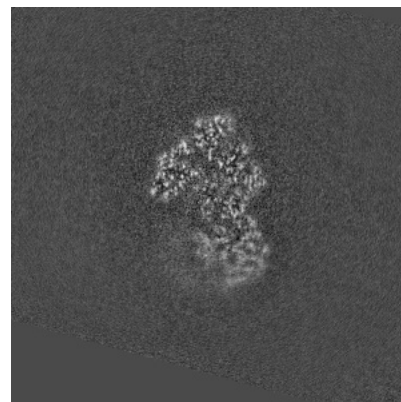
### 6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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

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

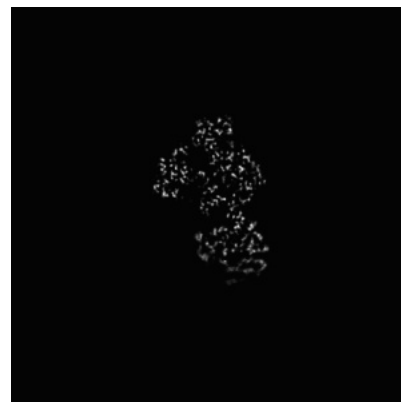
### 6.3.1 Primary map



X Index: 240

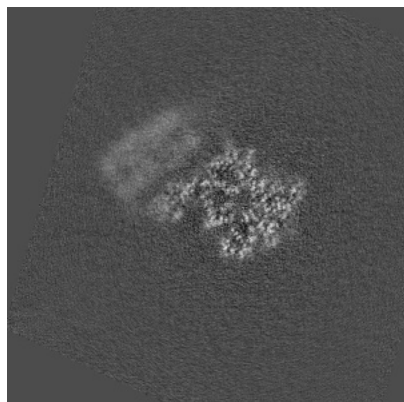


Y Index: 283

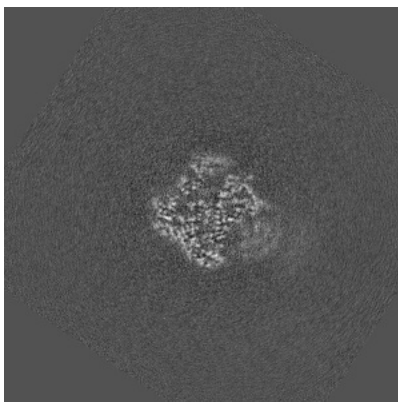


Z Index: 236

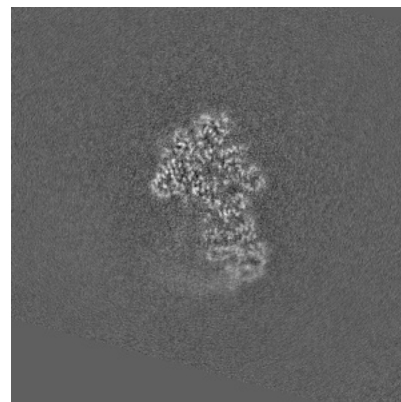
### 6.3.2 Raw map



X Index: 240



Y Index: 264

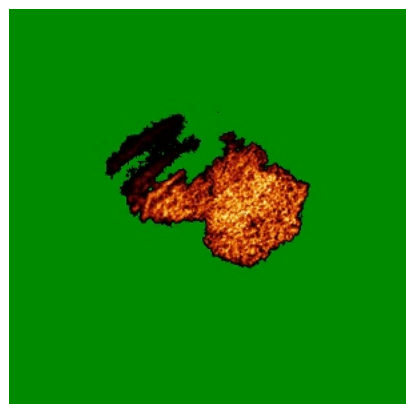


Z Index: 247

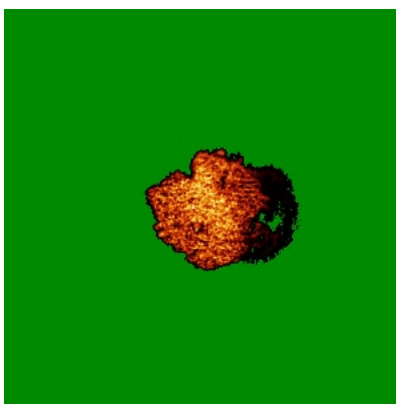
The images above show the largest variance slices of the map in three orthogonal directions.

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

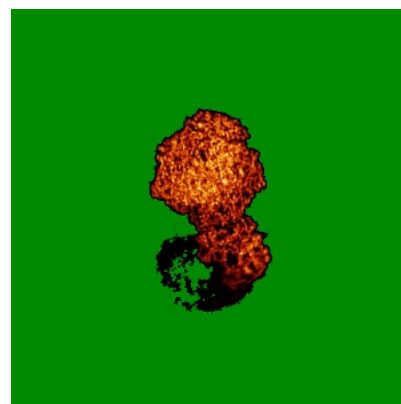
### 6.4.1 Primary map



X

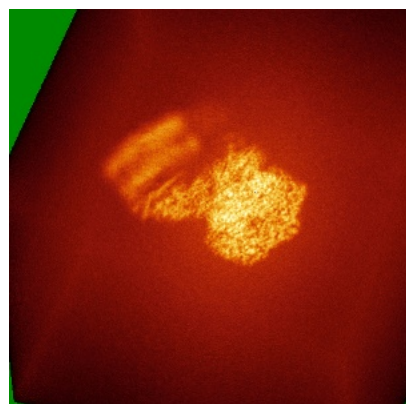


Y

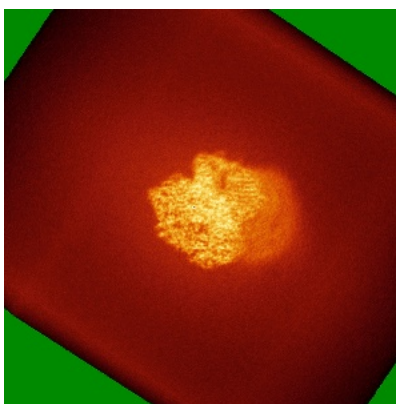


Z

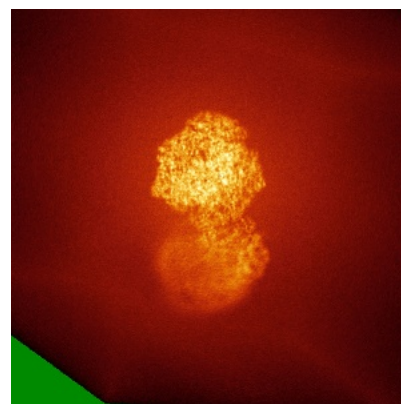
### 6.4.2 Raw map



X



Y

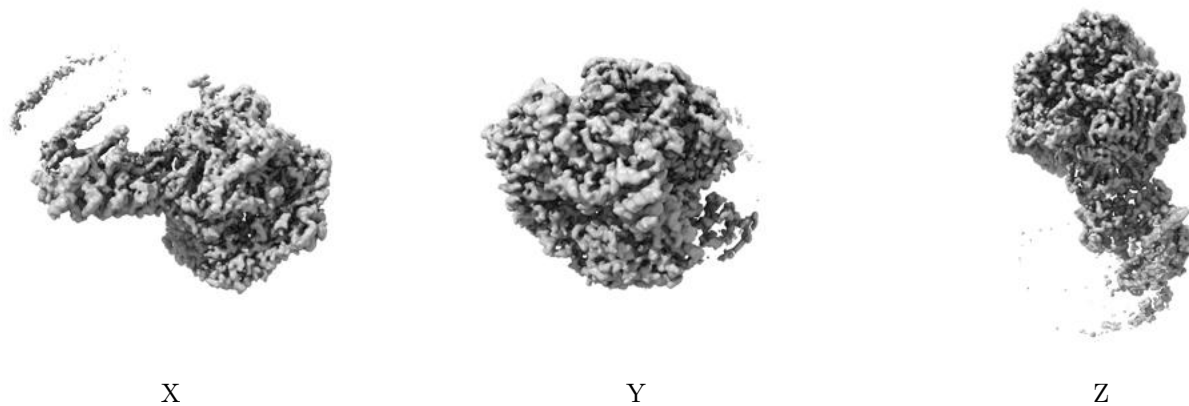


Z

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

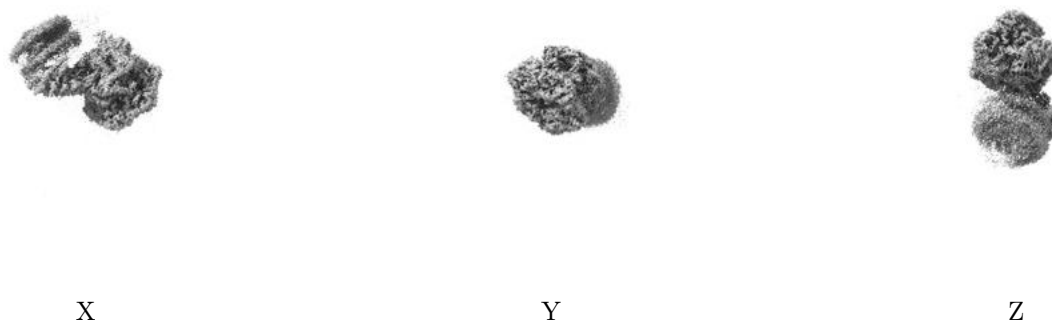
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

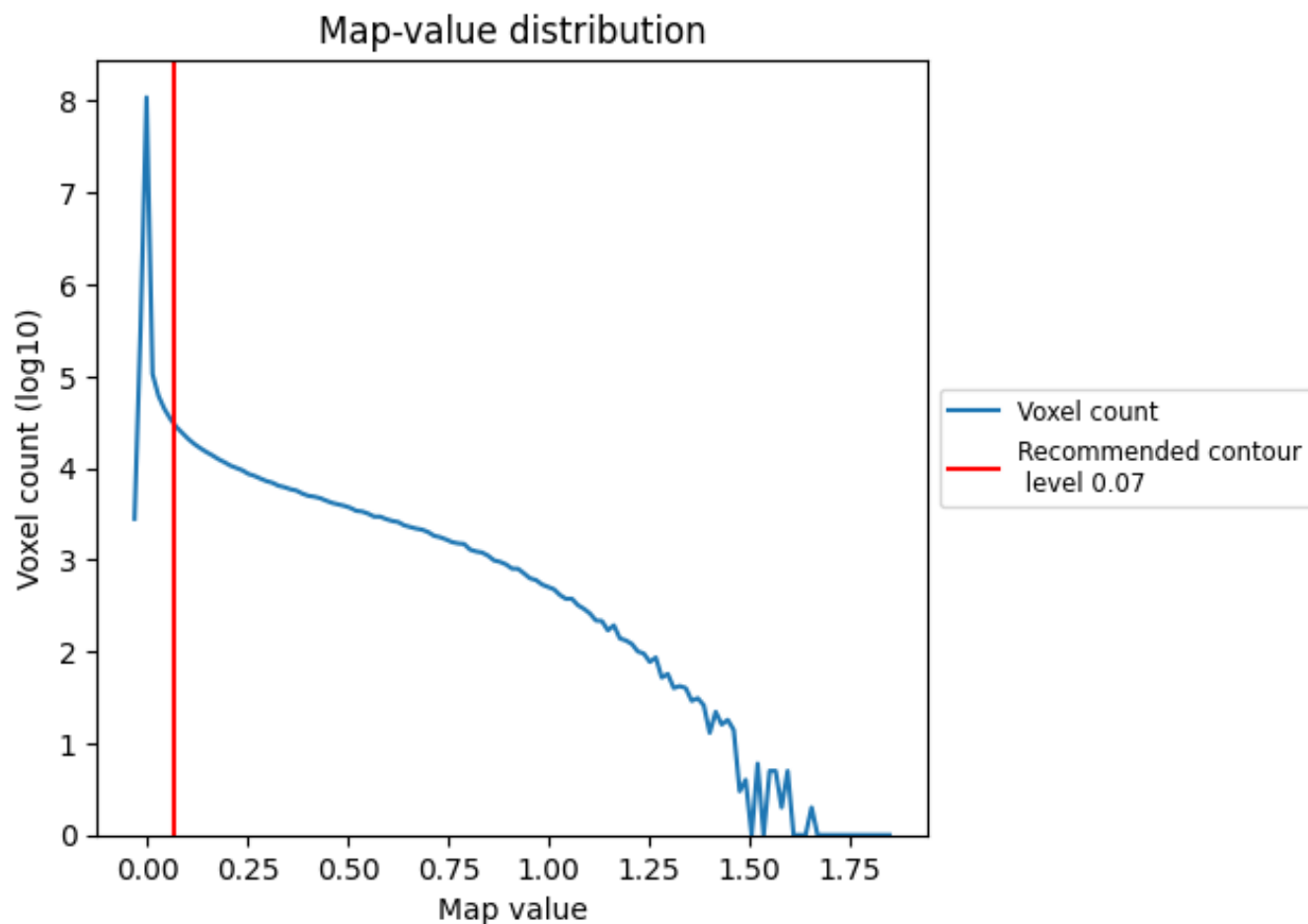
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

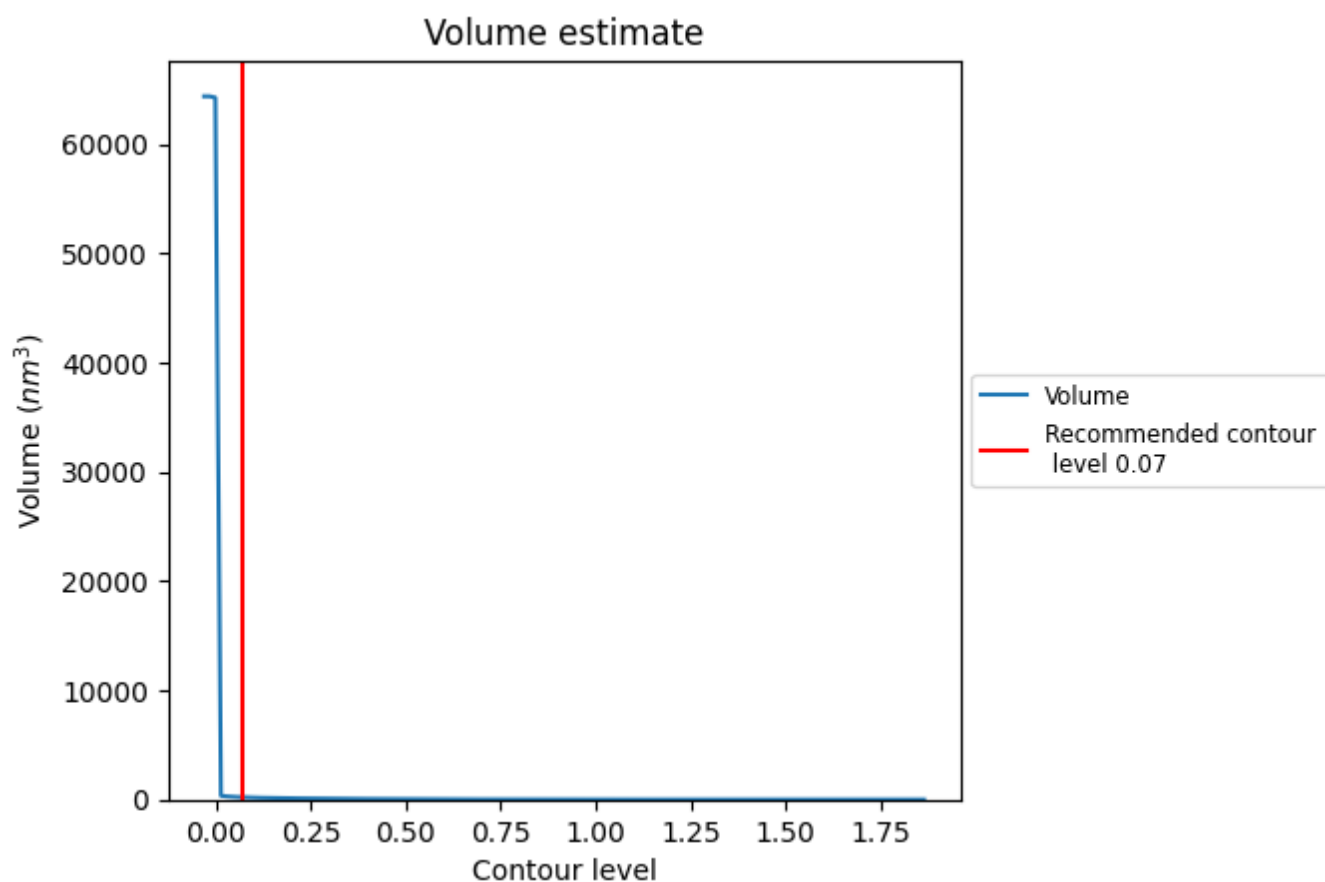
This section contains the results of statistical analysis of the map.

### 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.

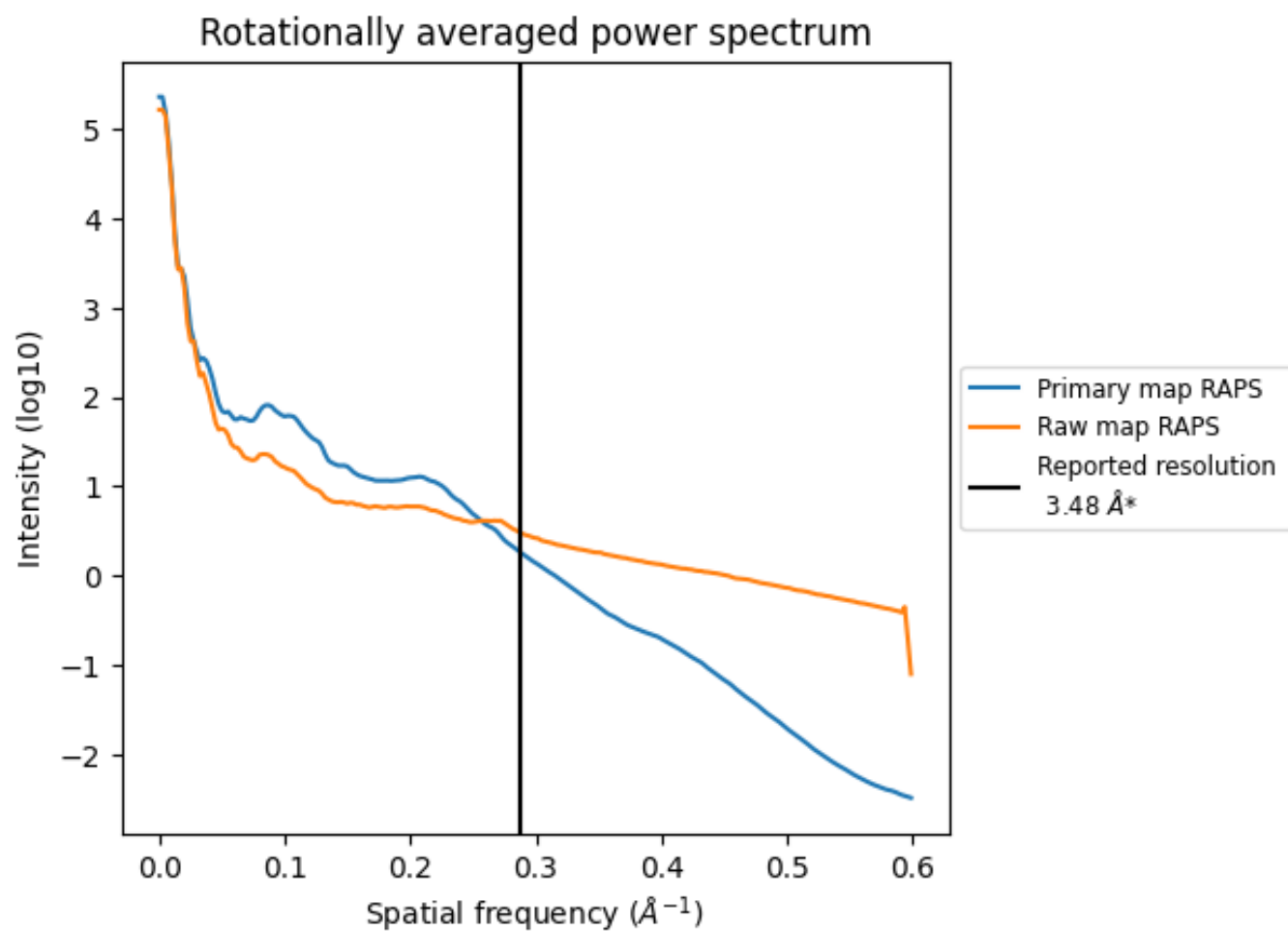
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm<sup>3</sup>; this corresponds to an approximate mass of 191 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 ⓘ

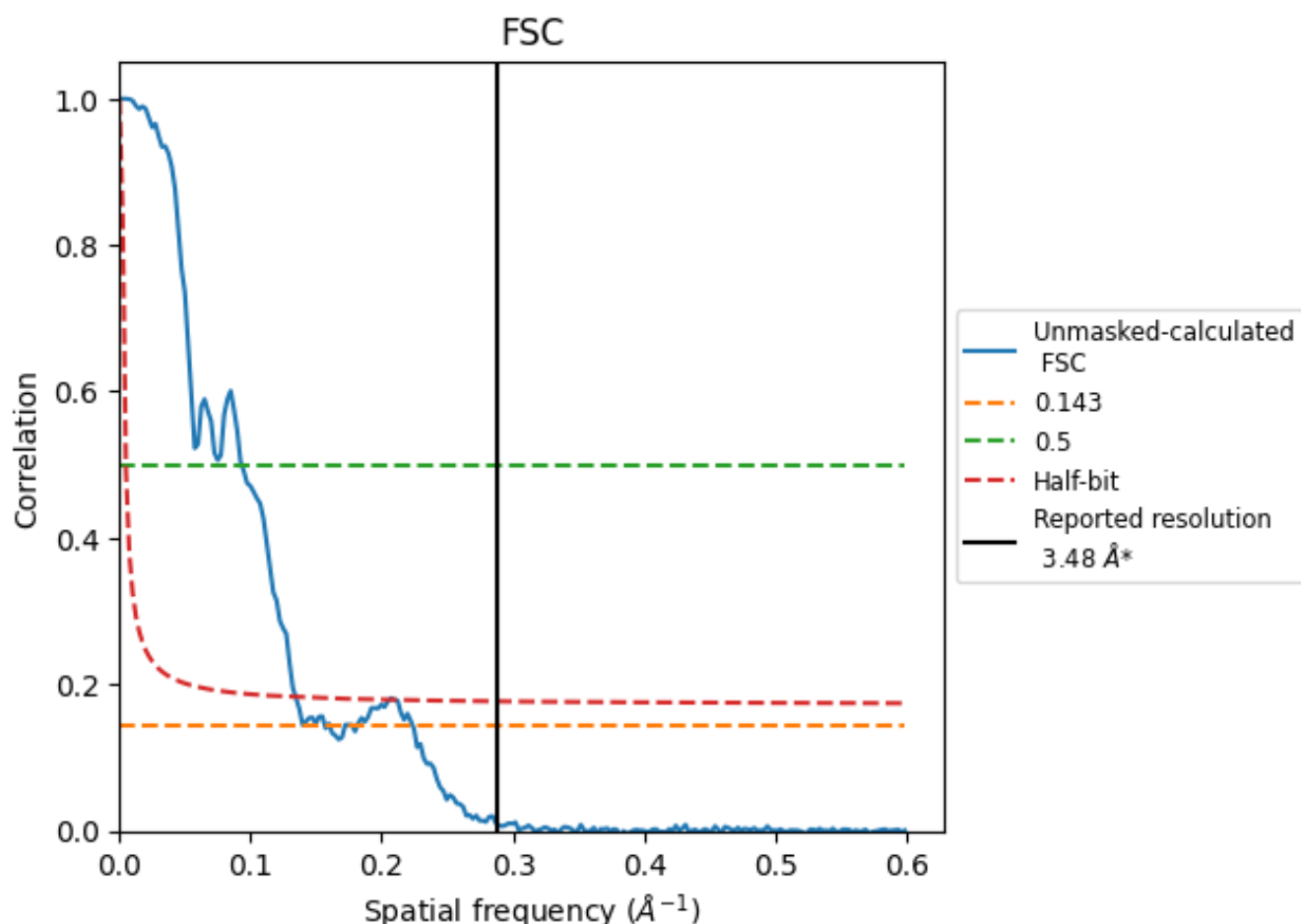


\*Reported resolution corresponds to spatial frequency of 0.287  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.287  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

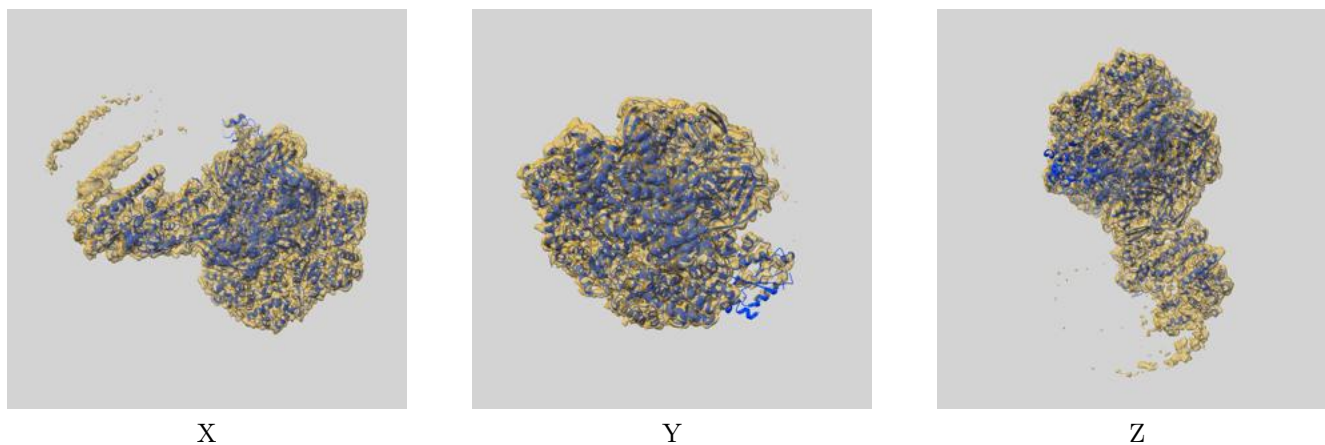
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.38	10.74	7.45

\*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 6.38 differs from the reported value 3.48 by more than 10 %

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

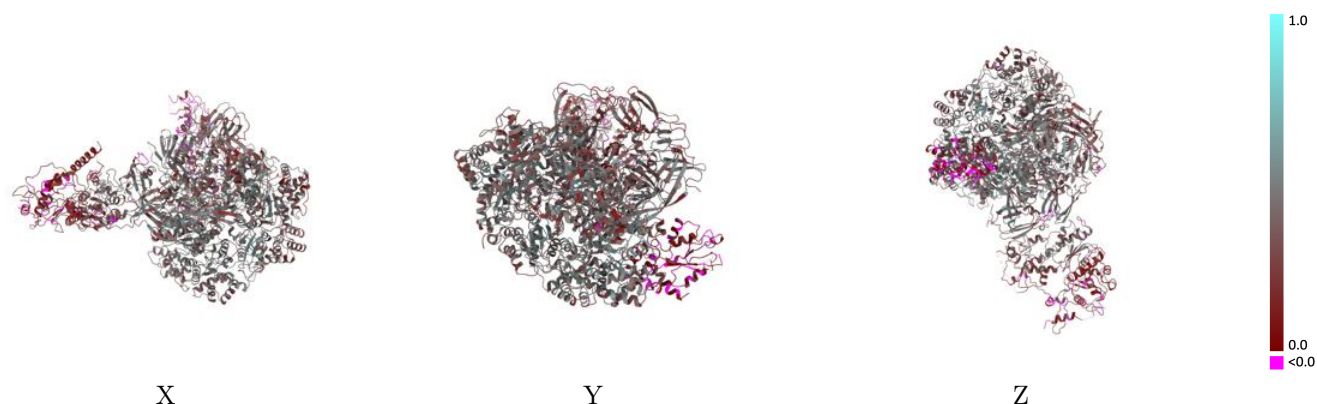
This section contains information regarding the fit between EMDB map EMD-28609 and PDB model 8EU9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



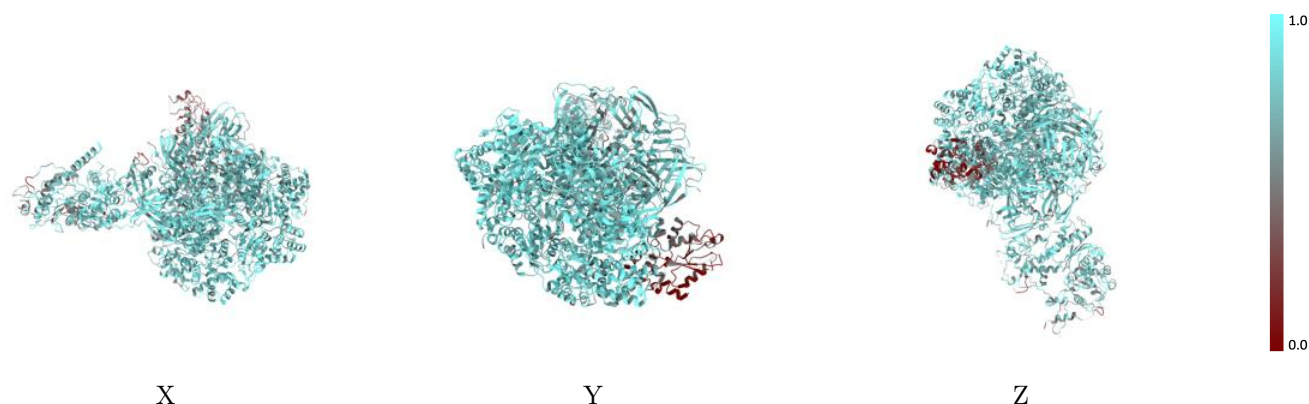
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



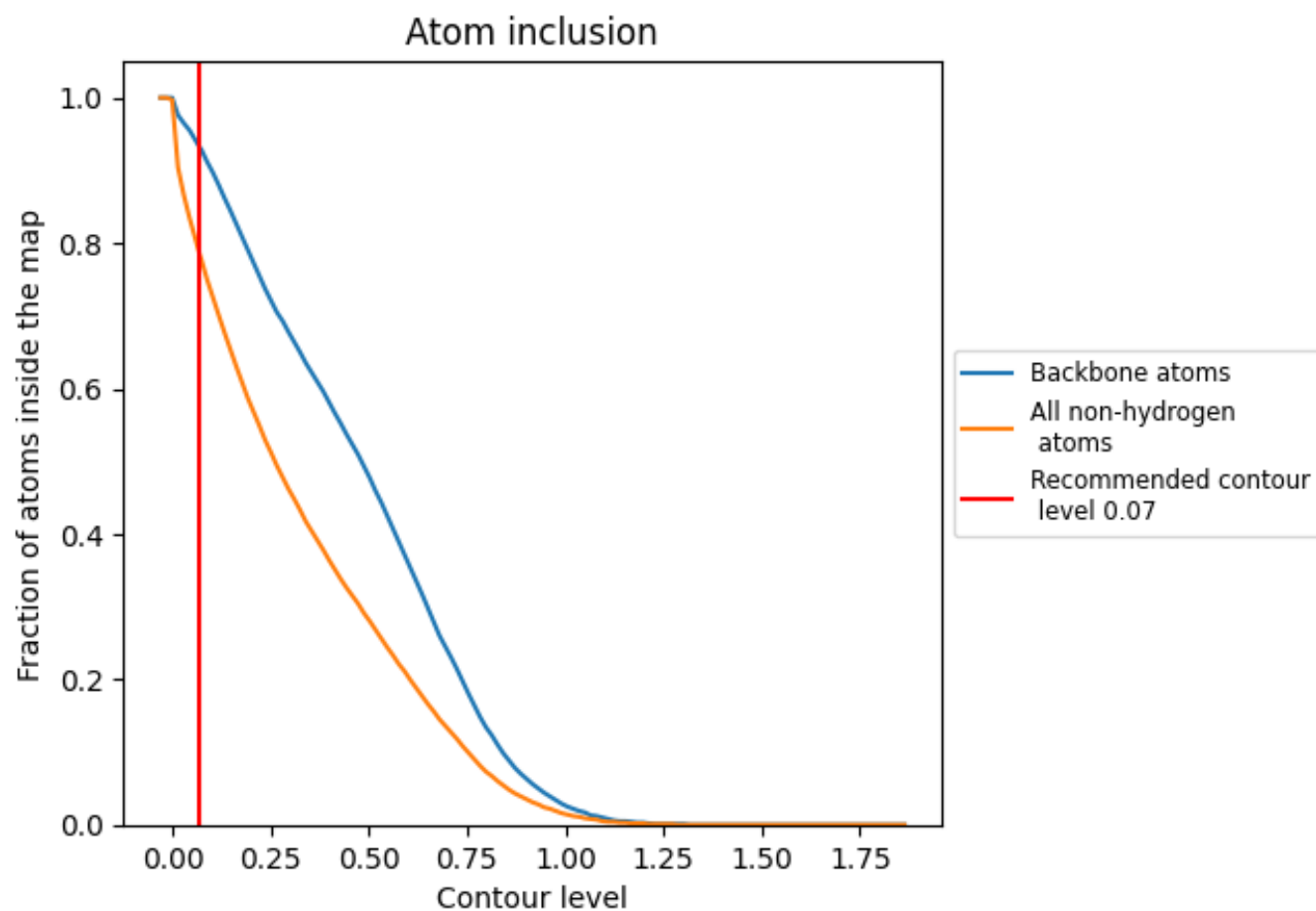
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 78% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7830	 0.3680
Q	 0.5630	 0.2600
R	 0.7170	 0.2470
S	 0.7260	 0.2770
T	 0.8390	 0.4190
U	 0.8310	 0.4260
V	 0.8450	 0.4320
W	 0.8300	 0.4060
X	 0.8130	 0.3750
Y	 0.8400	 0.4080
Z	 0.8220	 0.4190

