



## Full wwPDB EM Validation Report ⓘ

Jul 22, 2023 – 12:49 PM EDT

PDB ID : 8ETW  
EMDB ID : EMD-28601  
Title : Class3 of INO80-Hexasome complex  
Authors : Wu, H.; Munoz, E.; Gourdet, M.; Narlikar, G.; Cheng, Y.F.  
Deposited on : 2022-10-17  
Resolution : 2.64 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.dev50  
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 : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.34

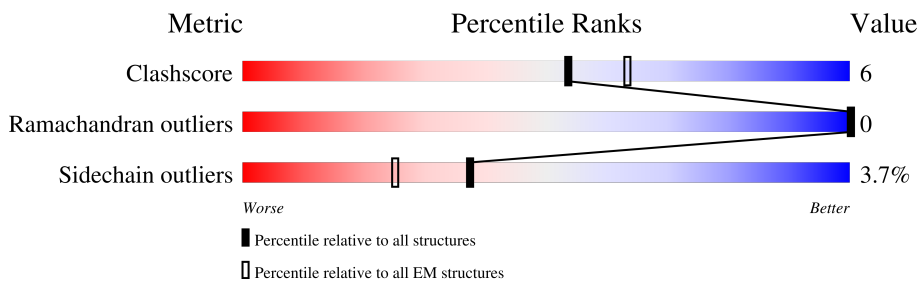
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.64 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	485	
2	R	744	
3	S	139	
4	T	443	
4	V	443	
4	X	443	
5	U	457	
5	W	457	

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Mol	Chain	Length	Quality of chain
5	Y	457	 85% 12%
6	Z	28	 64% 36%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 28666 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
			Total	C	N	O	S		
1	Q	418	3385	2154	569	647	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	442	3548	2261	598	678	11	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	U	436	3350	2098	583	658	11	0	0
5	W	442	3398	2123	590	673	12	0	0

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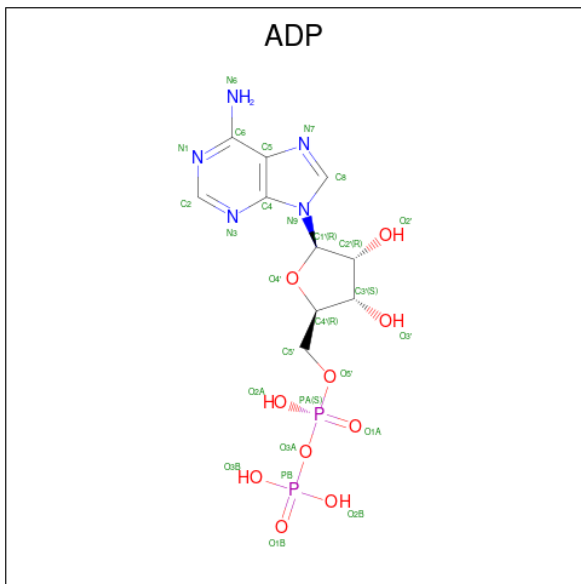
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Y	445	Total 3421	2138	594	677	12	0	0

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

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

- 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).

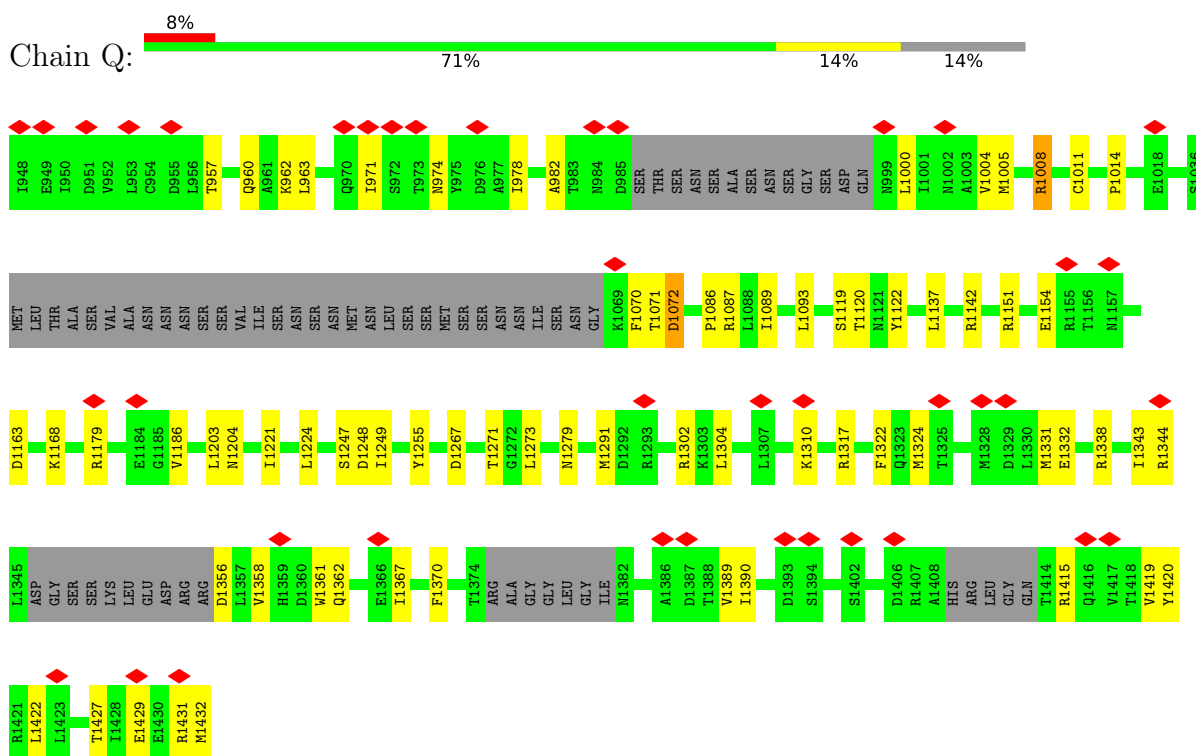


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	T	1	Total 27	10	5	10	2	0
7	U	1	Total 27	10	5	10	2	0
7	V	1	Total 27	10	5	10	2	0
7	W	1	Total 27	10	5	10	2	0
7	X	1	Total 27	10	5	10	2	0
7	Y	1	Total 27	10	5	10	2	0

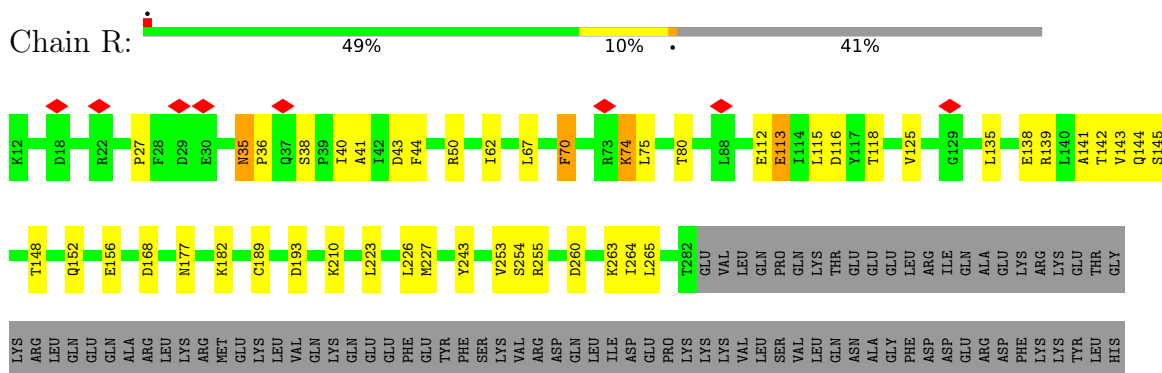
### 3 Residue-property plots

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

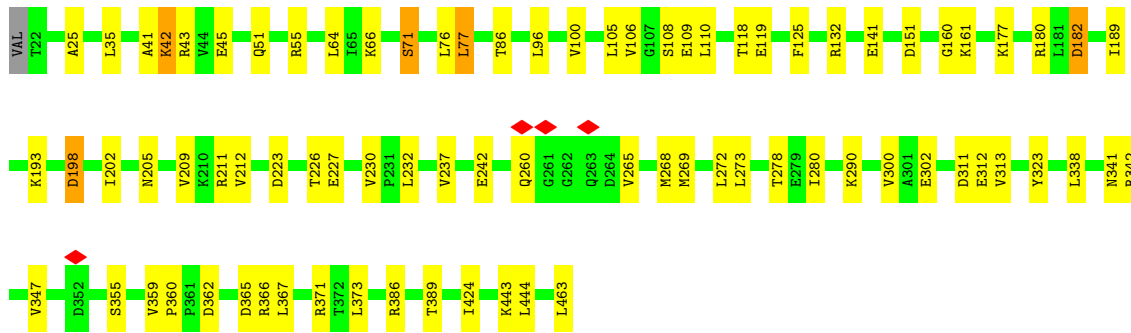
- Molecule 1: Chromatin-remodeling ATPase INO80



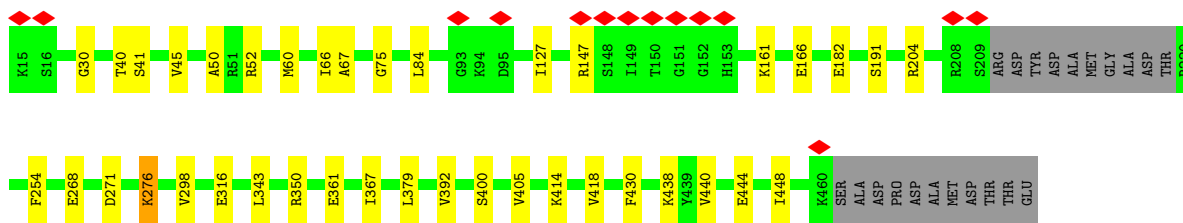
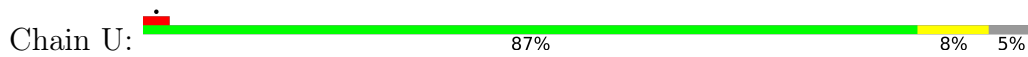
- Molecule 2: Actin-related protein 5



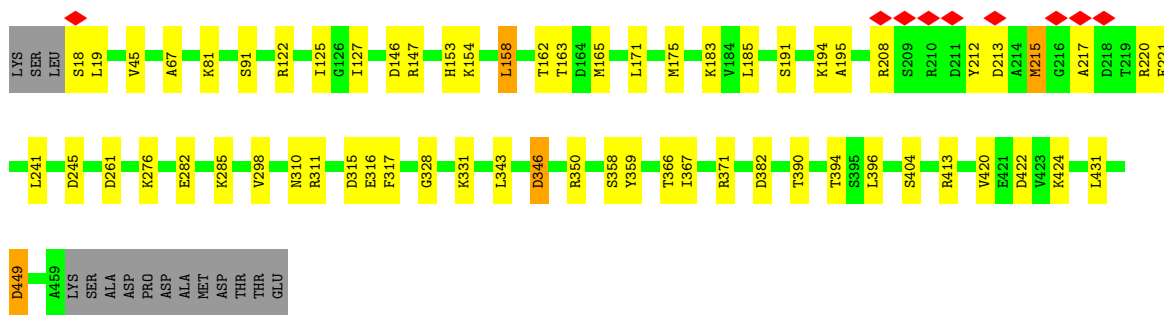
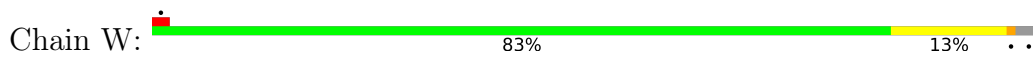




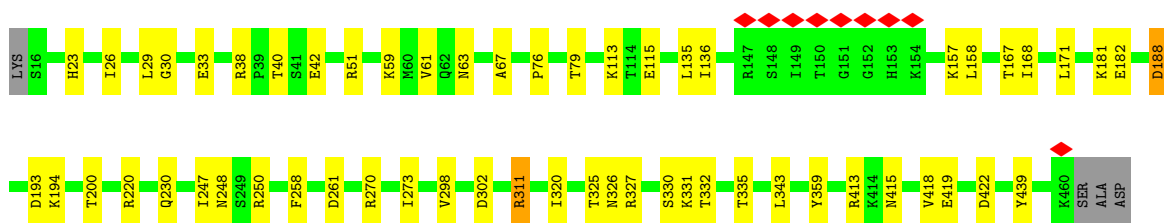
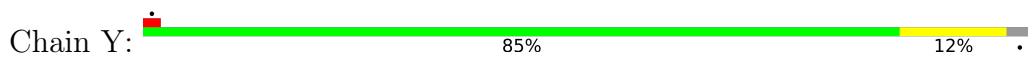
• Molecule 5: RuvB-like protein 2



• 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	233675	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 ( $e^-/\text{\AA}^2$ )	67	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	1.963	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.06	Depositor
Map size ( $\text{\AA}$ )	400.8, 400.8, 400.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.835, 0.835, 0.835	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Q	0.29	0/3451	0.56	2/4679 (0.0%)
2	R	0.31	0/3639	0.63	5/4949 (0.1%)
3	S	0.33	0/1036	0.61	0/1392
4	T	0.30	0/3378	0.57	1/4569 (0.0%)
4	V	0.32	0/3446	0.67	5/4662 (0.1%)
4	X	0.31	0/3439	0.62	1/4652 (0.0%)
5	U	0.30	0/3386	0.61	1/4561 (0.0%)
5	W	0.30	0/3436	0.57	0/4632
5	Y	0.30	0/3459	0.59	0/4662
6	Z	0.34	0/254	0.65	0/338
All	All	0.31	0/28924	0.60	15/39096 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	27	PRO	CA-N-CD	-9.82	97.75	111.50
4	V	344	MET	N-CA-CB	8.52	125.94	110.60
4	V	343	GLY	N-CA-C	8.18	133.54	113.10
2	R	602	ASP	CB-CG-OD2	8.04	125.53	118.30
4	V	182	ASP	CB-CG-OD1	7.98	125.48	118.30
4	V	344	MET	N-CA-C	-7.11	91.80	111.00
4	X	77	LEU	CA-CB-CG	6.54	130.33	115.30
2	R	70	PHE	CB-CG-CD2	6.00	125.00	120.80
1	Q	1005	MET	CB-CG-SD	5.74	129.62	112.40
4	V	268	MET	CB-CG-SD	5.64	129.32	112.40
4	T	77	LEU	CA-CB-CG	5.61	128.20	115.30
2	R	125	VAL	CG1-CB-CG2	-5.45	102.18	110.90
1	Q	963	LEU	CA-CB-CG	5.43	127.80	115.30
5	U	182	GLU	CB-CA-C	5.19	120.78	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	714	MET	CA-CB-CG	5.07	121.93	113.30

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	3385	0	3370	77	0
2	R	3548	0	3445	57	0
3	S	1014	0	1050	10	0
4	T	3339	0	3468	30	0
4	V	3404	0	3542	27	0
4	X	3397	0	3533	54	0
5	U	3350	0	3444	43	0
5	W	3398	0	3469	54	0
5	Y	3421	0	3499	47	0
6	Z	248	0	242	9	0
7	T	27	0	12	0	0
7	U	27	0	12	1	0
7	V	27	0	12	0	0
7	W	27	0	12	1	0
7	X	27	0	12	1	0
7	Y	27	0	12	0	0
All	All	28666	0	29134	318	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 (318) 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)
1:Q:1221:ILE:HD11	5:U:254:PHE:CD1	1.37	1.55
2:R:614:LEU:CD2	2:R:617:GLU:OE2	1.67	1.40
1:Q:1221:ILE:HD11	5:U:254:PHE:CE1	1.60	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1142:ARG:NH2	5:Y:182:GLU:CB	1.89	1.33
1:Q:1221:ILE:HD11	5:U:254:PHE:CG	1.66	1.28
1:Q:1142:ARG:HH22	5:Y:182:GLU:CB	1.45	1.26
1:Q:1142:ARG:NH2	5:Y:182:GLU:HB3	0.94	1.25
5:Y:113:LYS:NZ	5:Y:302:ASP:OD2	1.73	1.21
1:Q:1221:ILE:CD1	5:U:254:PHE:CE1	2.24	1.21
1:Q:1221:ILE:CD1	5:U:254:PHE:CD1	2.29	1.16
5:W:420:VAL:HG12	5:W:424:LYS:HE3	1.15	1.15
5:Y:135:LEU:HD23	5:Y:193:ASP:OD1	1.49	1.10
1:Q:1221:ILE:CG1	5:U:254:PHE:CE1	2.36	1.07
2:R:614:LEU:HD22	2:R:617:GLU:OE2	0.91	1.07
1:Q:957:THR:HB	5:W:282:GLU:OE2	1.56	1.06
5:U:448:ILE:HG21	4:V:342:ARG:NH1	1.70	1.06
1:Q:1221:ILE:CD1	5:U:254:PHE:CZ	2.40	1.03
5:W:420:VAL:CG1	5:W:424:LYS:HE3	1.88	1.03
1:Q:1186:VAL:HG21	4:X:300:VAL:HG11	1.41	1.01
5:U:448:ILE:CG2	4:V:342:ARG:NH1	2.27	0.97
1:Q:1221:ILE:HG13	5:U:254:PHE:CE1	2.01	0.96
2:R:733:GLU:OE2	2:R:741:TYR:CE2	2.19	0.96
1:Q:1221:ILE:HD11	5:U:254:PHE:CZ	2.02	0.92
5:Y:135:LEU:CD2	5:Y:193:ASP:OD1	2.17	0.91
1:Q:1221:ILE:HD11	5:U:254:PHE:CD2	2.05	0.91
4:T:44:VAL:HG22	4:T:49:VAL:HG22	1.53	0.89
1:Q:957:THR:CB	5:W:282:GLU:OE2	2.24	0.86
2:R:139:ARG:O	2:R:142:THR:HG23	1.75	0.86
5:U:448:ILE:CG2	4:V:342:ARG:HH11	1.87	0.85
2:R:733:GLU:OE2	2:R:741:TYR:HE2	1.54	0.85
1:Q:1142:ARG:HH21	5:Y:182:GLU:HB3	1.02	0.84
1:Q:1221:ILE:CD1	5:U:254:PHE:CG	2.52	0.84
3:S:99:THR:O	3:S:103:VAL:HG23	1.78	0.83
1:Q:1221:ILE:CD1	5:U:254:PHE:CE2	2.61	0.82
5:W:212:TYR:CE1	4:X:182:ASP:HA	2.15	0.81
5:U:440:VAL:HG11	4:V:343:GLY:O	1.81	0.81
5:W:45:VAL:HG11	5:W:366:THR:HG21	1.62	0.80
5:W:212:TYR:CE1	4:X:182:ASP:CA	2.64	0.79
5:U:448:ILE:HG22	4:V:342:ARG:HH11	1.47	0.79
1:Q:1221:ILE:CD1	5:U:254:PHE:CD2	2.66	0.79
1:Q:971:ILE:CG2	1:Q:974:ASN:HD21	1.95	0.78
2:R:614:LEU:HD22	2:R:617:GLU:CD	2.02	0.78
1:Q:1221:ILE:HD12	5:U:254:PHE:CE2	2.19	0.77
1:Q:1221:ILE:HD11	5:U:254:PHE:CE2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:971:ILE:HG22	1:Q:974:ASN:OD1	1.88	0.74
5:U:448:ILE:HG21	4:V:342:ARG:HH12	1.47	0.74
5:W:208:ARG:NH2	6:Z:313:GLU:O	2.22	0.72
1:Q:1142:ARG:HH22	5:Y:182:GLU:CA	2.02	0.72
1:Q:957:THR:CG2	5:W:282:GLU:OE2	2.39	0.71
6:Z:313:GLU:N	6:Z:313:GLU:OE2	2.21	0.71
2:R:254:SER:HB2	2:R:260:ASP:OD2	1.91	0.70
2:R:223:LEU:CD1	2:R:617:GLU:OE1	2.40	0.70
4:X:265:VAL:O	4:X:269:MET:HB2	1.92	0.70
1:Q:1221:ILE:HD12	5:U:254:PHE:CZ	2.27	0.69
5:W:420:VAL:HG12	5:W:424:LYS:CE	2.09	0.69
2:R:227:MET:HE3	2:R:617:GLU:OE1	1.94	0.68
1:Q:1221:ILE:HG13	5:U:254:PHE:CZ	2.27	0.68
5:W:212:TYR:CE1	4:X:182:ASP:N	2.63	0.67
1:Q:971:ILE:HG22	1:Q:971:ILE:O	1.93	0.67
1:Q:971:ILE:HG22	1:Q:974:ASN:ND2	2.10	0.66
5:W:420:VAL:O	5:W:424:LYS:HG3	1.95	0.66
1:Q:1255:TYR:HE1	6:Z:320:PHE:CE1	2.13	0.66
2:R:733:GLU:OE2	2:R:741:TYR:CZ	2.48	0.66
2:R:614:LEU:HD23	2:R:617:GLU:OE2	1.88	0.66
4:V:406:MET:SD	4:V:443:LYS:NZ	2.70	0.65
1:Q:1142:ARG:HH22	5:Y:182:GLU:HB3	0.84	0.65
5:Y:194:LYS:HD3	5:Y:230:GLN:HE22	1.62	0.65
1:Q:1142:ARG:NH2	5:Y:182:GLU:CA	2.60	0.64
2:R:729:ILE:HD13	2:R:733:GLU:OE1	1.97	0.64
4:T:251:ASP:OD1	5:U:268:GLU:OE1	2.16	0.64
5:W:212:TYR:HE1	4:X:182:ASP:CA	2.08	0.64
1:Q:971:ILE:HG22	1:Q:974:ASN:HD21	1.61	0.63
4:X:424:ILE:HD13	5:Y:59:LYS:HB3	1.79	0.63
1:Q:1137:LEU:HB2	5:Y:200:THR:HB	1.81	0.63
5:W:146:ASP:HB3	6:Z:305:MET:HE2	1.81	0.62
5:Y:30:GLY:HA2	5:Y:42:GLU:OE1	1.99	0.62
2:R:733:GLU:OE2	2:R:741:TYR:OH	2.13	0.61
5:W:208:ARG:HD3	6:Z:312:TYR:O	2.01	0.61
2:R:223:LEU:HD11	2:R:617:GLU:OE1	2.01	0.61
5:Y:418:VAL:HG13	5:Y:422:ASP:HB2	1.82	0.61
4:T:273:LEU:HD11	4:X:273:LEU:HD11	1.82	0.60
1:Q:971:ILE:HG22	1:Q:974:ASN:CG	2.23	0.60
1:Q:1089:ILE:O	1:Q:1093:LEU:HB2	2.02	0.60
5:W:122:ARG:NH1	5:W:245:ASP:OD1	2.35	0.59
1:Q:1142:ARG:HH21	5:Y:182:GLU:CB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:405:VAL:HG11	5:U:430:PHE:CE2	2.38	0.59
1:Q:1221:ILE:CG1	5:U:254:PHE:CZ	2.78	0.58
1:Q:1151:ARG:HH21	4:X:272:LEU:HD22	1.68	0.58
4:V:314:ASN:ND2	4:V:342:ARG:HE	2.01	0.58
5:W:382:ASP:OD1	5:W:382:ASP:N	2.36	0.58
1:Q:1120:THR:O	4:T:294:LYS:NZ	2.33	0.58
5:W:147:ARG:HG2	5:W:154:LYS:HG2	1.86	0.58
5:W:390:THR:O	5:W:394:THR:OG1	2.18	0.57
2:R:143:VAL:HG12	2:R:145:SER:H	1.69	0.57
4:T:132:ARG:NH1	4:T:246:ASP:OD2	2.37	0.57
2:R:138:GLU:OE1	2:R:749:ASN:ND2	2.38	0.57
5:U:448:ILE:HG22	4:V:342:ARG:NH1	2.08	0.56
5:W:212:TYR:CZ	4:X:182:ASP:HA	2.39	0.56
5:W:45:VAL:HG11	5:W:366:THR:CG2	2.32	0.56
4:V:25:ALA:HB2	5:W:67:ALA:HB3	1.86	0.56
2:R:41:ALA:HA	2:R:135:LEU:HB2	1.86	0.56
1:Q:1390:ILE:HG12	1:Q:1420:TYR:HB2	1.86	0.56
1:Q:1142:ARG:HH12	5:Y:181:LYS:HG3	1.70	0.55
4:V:189:ILE:HG12	4:V:209:VAL:HG21	1.87	0.55
2:R:43:ASP:HB3	2:R:50:ARG:HB2	1.87	0.55
4:V:41:ALA:HB3	4:V:52:ILE:HG23	1.87	0.55
1:Q:971:ILE:CG2	1:Q:974:ASN:ND2	2.65	0.55
5:W:213:ASP:OD1	5:W:213:ASP:N	2.38	0.55
5:Y:413:ARG:HH12	5:Y:415:ASN:HD22	1.54	0.55
4:X:341:ASN:OD1	4:X:342:ARG:NH1	2.40	0.54
4:T:313:VAL:HG12	4:T:339:ALA:O	2.07	0.54
4:T:381:ARG:NH1	4:T:401:ASP:OD2	2.40	0.54
5:W:127:ILE:HD11	5:W:241:LEU:HD13	1.90	0.53
2:R:144:GLN:O	2:R:148:THR:OG1	2.26	0.53
2:R:253:VAL:HG23	2:R:677:VAL:HG12	1.91	0.53
1:Q:978:ILE:HA	1:Q:1000:LEU:HD21	1.91	0.53
4:T:463:LEU:HD22	5:U:75:GLY:HA2	1.90	0.53
5:W:212:TYR:HE1	4:X:182:ASP:N	2.05	0.53
4:T:352:ASP:N	4:T:352:ASP:OD1	2.42	0.53
2:R:750:THR:OG1	2:R:751:LYS:N	2.42	0.52
5:W:346:ASP:OD1	5:W:346:ASP:N	2.42	0.52
2:R:41:ALA:HB1	2:R:714:MET:HG3	1.91	0.52
4:V:380:ILE:HD12	4:V:412:LEU:HD13	1.92	0.52
5:W:261:ASP:OD1	4:X:278:THR:OG1	2.25	0.52
4:X:51:GLN:NE2	4:X:373:LEU:O	2.43	0.52
4:X:189:ILE:HD13	4:X:209:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:362:ASP:O	4:X:366:ARG:NH1	2.43	0.52
1:Q:1203:LEU:O	1:Q:1279:ASN:ND2	2.37	0.52
2:R:223:LEU:HD12	2:R:617:GLU:OE1	2.09	0.52
5:U:50:ALA:HB1	5:U:84:LEU:HD11	1.92	0.52
4:X:226:THR:O	4:X:227:GLU:C	2.48	0.52
4:X:202:ILE:HG12	4:X:209:VAL:HG12	1.92	0.51
1:Q:1302:ARG:NH1	5:W:282:GLU:O	2.43	0.51
2:R:152:GLN:NE2	2:R:156:GLU:OE1	2.44	0.51
1:Q:971:ILE:CG2	1:Q:971:ILE:O	2.58	0.51
1:Q:1249:ILE:HG13	1:Q:1271:THR:HG21	1.92	0.51
1:Q:960:GLN:HG3	1:Q:1014:PRO:HG3	1.91	0.51
2:R:253:VAL:HG23	2:R:677:VAL:CG1	2.40	0.51
4:X:42:LYS:HE2	4:X:45:GLU:HG2	1.92	0.51
4:T:23:ARG:NH2	5:U:316:GLU:O	2.42	0.51
1:Q:957:THR:HG22	5:W:282:GLU:OE2	2.11	0.51
1:Q:1247:SER:OG	1:Q:1248:ASP:N	2.44	0.50
5:Y:38:ARG:O	5:Y:51:ARG:NH2	2.44	0.50
5:Y:115:GLU:OE2	5:Y:270:ARG:NH2	2.44	0.50
2:R:168:ASP:OD1	2:R:168:ASP:N	2.43	0.50
2:R:193:ASP:OD1	2:R:193:ASP:N	2.44	0.50
7:X:501:ADP:O3B	5:Y:311:ARG:NH2	2.45	0.50
2:R:67:LEU:HD11	2:R:113:GLU:HG2	1.94	0.50
4:V:51:GLN:NE2	4:V:373:LEU:O	2.39	0.50
1:Q:1087:ARG:NH1	1:Q:1224:LEU:O	2.42	0.50
4:V:36:ASP:OD1	4:V:42:LYS:NZ	2.38	0.50
4:X:119:GLU:OE1	4:X:280:ILE:N	2.45	0.50
1:Q:1179:ARG:HH22	4:X:260:GLN:HB3	1.76	0.50
2:R:210:LYS:HG3	2:R:641:LEU:HD22	1.94	0.50
4:X:76:LEU:HB3	4:X:367:LEU:HD13	1.93	0.50
4:T:182:ASP:N	4:T:182:ASP:OD1	2.39	0.49
1:Q:971:ILE:CG2	1:Q:974:ASN:OD1	2.60	0.49
4:X:86:THR:OG1	5:Y:311:ARG:NH2	2.44	0.49
1:Q:1332:GLU:OE1	1:Q:1344:ARG:NH1	2.42	0.49
1:Q:1356:ASP:N	1:Q:1356:ASP:OD1	2.45	0.49
1:Q:1389:VAL:HG13	1:Q:1419:VAL:HG23	1.94	0.49
2:R:112:GLU:OE2	3:S:53:TYR:OH	2.31	0.49
2:R:177:ASN:HB3	2:R:182:LYS:HG3	1.93	0.49
1:Q:1142:ARG:HH12	5:Y:181:LYS:CG	2.25	0.49
2:R:605:ASN:HB3	2:R:608:GLU:HB2	1.95	0.49
5:W:215:MET:HG2	5:W:217:ALA:H	1.77	0.49
5:Y:250:ARG:NH2	5:Y:261:ASP:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:162:THR:HG23	5:W:165:MET:H	1.78	0.48
1:Q:1322:PHE:HZ	1:Q:1331:MET:HG3	1.77	0.48
5:Y:332:THR:OG1	5:Y:335:THR:OG1	2.25	0.48
4:V:154:ASN:N	4:V:154:ASN:OD1	2.45	0.48
5:Y:325:THR:HG22	5:Y:327:ARG:H	1.78	0.48
4:X:313:VAL:HG11	4:X:338:LEU:HB3	1.95	0.48
4:X:463:LEU:HD13	5:Y:76:PRO:HD3	1.95	0.48
5:W:147:ARG:O	6:Z:305:MET:HB3	2.13	0.48
5:W:298:VAL:HG13	5:W:343:LEU:HD21	1.95	0.48
4:X:132:ARG:HB3	4:X:302:GLU:HB3	1.96	0.48
5:Y:135:LEU:HD21	5:Y:193:ASP:OD1	2.12	0.48
2:R:144:GLN:NE2	2:R:148:THR:OG1	2.37	0.47
4:X:35:LEU:HD23	4:X:41:ALA:HB2	1.96	0.47
5:W:413:ARG:NH1	5:W:422:ASP:OD1	2.48	0.47
4:X:160:GLY:O	6:Z:319:THR:O	2.32	0.47
3:S:132:ILE:HG12	3:S:156:LEU:HD21	1.95	0.47
4:T:41:ALA:HB3	4:T:52:ILE:HG23	1.95	0.47
1:Q:1204:ASN:ND2	5:W:195:ALA:O	2.46	0.47
4:X:42:LYS:O	4:X:55:ARG:NH2	2.44	0.47
5:Y:23:HIS:HB2	5:Y:26:ILE:HD12	1.97	0.47
4:T:380:ILE:HG12	4:T:412:LEU:HD13	1.96	0.47
2:R:67:LEU:HD21	2:R:80:THR:HG23	1.97	0.47
2:R:144:GLN:HB2	3:S:73:ARG:HH12	1.80	0.47
5:W:404:SER:HB3	4:X:64:LEU:HD11	1.97	0.47
4:X:177:LYS:HB3	4:X:237:VAL:HG21	1.96	0.47
5:Y:136:ILE:HD11	5:Y:194:LYS:HG3	1.96	0.47
1:Q:982:ALA:HB2	1:Q:1004:VAL:HG11	1.97	0.47
5:W:125:ILE:HD13	5:W:317:PHE:HB3	1.98	0.46
5:Y:40:THR:HG23	5:Y:40:THR:O	2.13	0.46
4:V:387:ARG:NH2	4:V:391:GLU:OE2	2.46	0.46
1:Q:1429:GLU:HA	1:Q:1432:MET:HB2	1.96	0.46
4:V:42:LYS:HE2	4:V:45:GLU:HG2	1.96	0.46
4:T:116:LYS:HE2	4:T:279:GLU:HG2	1.98	0.46
4:T:362:ASP:O	4:T:366:ARG:NH1	2.48	0.46
5:W:158:LEU:HB2	5:W:171:LEU:HD11	1.97	0.46
4:X:227:GLU:O	4:X:227:GLU:HG3	2.16	0.46
4:X:386:ARG:HA	4:X:389:THR:HG22	1.98	0.46
4:X:198:ASP:OD2	4:X:211:ARG:NH1	2.49	0.45
5:W:212:TYR:HE1	4:X:182:ASP:CB	2.28	0.45
5:W:367:ILE:HG21	5:W:396:LEU:HD21	1.97	0.45
2:R:35:ASN:HD21	2:R:38:SER:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:61:VAL:HG22	5:Y:320:ILE:HD12	1.99	0.45
4:T:51:GLN:HE22	4:T:372:THR:HG23	1.81	0.45
1:Q:1343:ILE:HG12	1:Q:1367:ILE:HG21	1.99	0.45
5:U:45:VAL:CG2	5:U:367:ILE:HG13	2.47	0.45
5:U:361:GLU:HG3	5:U:392:VAL:HG21	1.99	0.45
2:R:688:PHE:HB3	2:R:698:ILE:HD13	1.99	0.45
4:T:61:ILE:HG13	4:T:75:ILE:CD1	2.47	0.45
5:W:358:SER:OG	5:W:359:TYR:N	2.49	0.45
5:W:431:LEU:HD11	4:X:371:ARG:HD3	1.99	0.45
5:Y:29:LEU:O	5:Y:42:GLU:OE1	2.35	0.45
4:X:106:VAL:HG12	4:X:108:SER:H	1.81	0.44
1:Q:1273:LEU:HB3	4:X:265:VAL:HG13	1.99	0.44
4:T:25:ALA:HB2	5:U:67:ALA:HB3	1.98	0.44
5:Y:158:LEU:HB2	5:Y:171:LEU:HD11	1.98	0.44
5:W:81:LYS:N	7:W:501:ADP:O2B	2.37	0.44
2:R:729:ILE:HD11	2:R:743:LYS:HB2	1.99	0.44
2:R:144:GLN:HE21	2:R:148:THR:HG1	1.62	0.44
5:U:45:VAL:O	7:U:501:ADP:N6	2.45	0.44
4:X:212:VAL:HG12	4:X:230:VAL:HG21	1.98	0.44
5:Y:248:ASN:HD22	5:Y:273:ILE:HD11	1.81	0.44
1:Q:1086:PRO:HD2	1:Q:1089:ILE:HD12	2.00	0.44
4:X:105:LEU:HD21	4:X:110:LEU:HD21	1.99	0.44
4:V:149:PRO:HB3	4:V:166:VAL:HG22	2.00	0.44
5:W:185:LEU:HD23	6:Z:310:ARG:HD3	2.00	0.44
2:R:116:ASP:OD2	3:S:49:LYS:NZ	2.49	0.43
5:W:147:ARG:NH2	6:Z:308:ILE:HD11	2.33	0.43
4:X:96:LEU:HD13	4:X:100:VAL:HG11	2.00	0.43
5:U:127:ILE:HD13	5:U:127:ILE:HA	1.91	0.43
4:V:123:GLU:HG2	4:V:250:HIS:CD2	2.52	0.43
2:R:227:MET:CE	2:R:617:GLU:OE1	2.65	0.43
4:T:123:GLU:HB3	4:T:250:HIS:CD2	2.53	0.43
2:R:660:THR:O	2:R:664:MET:HG3	2.18	0.43
5:W:162:THR:OG1	5:W:163:THR:N	2.50	0.43
4:X:118:THR:HG23	4:X:323:TYR:CE2	2.53	0.43
2:R:243:TYR:HD1	2:R:243:TYR:HA	1.71	0.43
4:T:269:MET:HG2	4:V:266:ILE:HD12	2.01	0.43
4:T:461:ASN:OD1	4:T:461:ASN:N	2.52	0.43
4:V:76:LEU:HB2	4:V:367:LEU:HD13	2.00	0.43
2:R:40:ILE:HD12	2:R:41:ALA:H	1.84	0.43
5:U:298:VAL:HG13	5:U:343:LEU:HD21	2.01	0.43
4:X:189:ILE:HD13	4:X:189:ILE:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:34:ARG:H	3:S:34:ARG:HG2	1.70	0.42
4:V:80:GLY:O	4:V:85:LYS:NZ	2.51	0.42
4:X:443:LYS:HB3	4:X:443:LYS:HE3	1.82	0.42
2:R:35:ASN:HA	2:R:36:PRO:HD3	1.85	0.42
2:R:115:LEU:HA	2:R:118:THR:HG22	2.01	0.42
4:X:311:ASP:OD1	4:X:312:GLU:N	2.52	0.42
5:U:40:THR:OG1	5:U:45:VAL:HG12	2.18	0.42
1:Q:1011:CYS:SG	1:Q:1427:THR:OG1	2.76	0.42
3:S:32:PHE:O	3:S:35:SER:OG	2.33	0.42
5:W:18:SER:OG	5:W:19:LEU:N	2.50	0.42
4:T:61:ILE:HG13	4:T:75:ILE:HD12	2.01	0.42
1:Q:1204:ASN:HA	1:Q:1279:ASN:ND2	2.35	0.42
1:Q:1317:ARG:NH1	1:Q:1361:TRP:O	2.53	0.42
1:Q:962:LYS:HE3	1:Q:962:LYS:HB2	1.72	0.41
1:Q:1122:TYR:HE2	5:Y:200:THR:HG21	1.85	0.41
1:Q:1168:LYS:HD3	1:Q:1168:LYS:HA	1.79	0.41
2:R:709:ASP:OD1	2:R:709:ASP:N	2.52	0.41
5:Y:167:THR:OG1	5:Y:168:ILE:N	2.52	0.41
4:V:311:ASP:OD2	5:W:311:ARG:NE	2.53	0.41
5:W:315:ASP:OD1	5:W:316:GLU:N	2.54	0.41
4:X:106:VAL:HB	4:X:109:GLU:HG3	2.02	0.41
2:R:74:LYS:HD2	2:R:75:LEU:HG	2.02	0.41
2:R:141:ALA:HB2	3:S:103:VAL:HG21	2.03	0.41
4:T:417:GLN:HE22	5:U:350:ARG:HA	1.85	0.41
1:Q:1358:VAL:O	1:Q:1362:GLN:HG2	2.20	0.41
2:R:50:ARG:HG2	2:R:62:ILE:HG12	2.03	0.41
4:T:117:LYS:H	4:T:117:LYS:HG2	1.69	0.41
4:T:371:ARG:HH11	5:Y:439:TYR:HB3	1.86	0.41
1:Q:1071:THR:HG22	1:Q:1072:ASP:N	2.36	0.41
2:R:733:GLU:CD	2:R:741:TYR:HE2	2.19	0.41
4:X:25:ALA:HB2	5:Y:67:ALA:HB3	2.01	0.41
4:X:66:LYS:HZ3	4:X:96:LEU:HD23	1.84	0.41
5:Y:79:THR:O	5:Y:359:TYR:OH	2.38	0.41
5:Y:247:ILE:HD13	5:Y:247:ILE:HA	1.90	0.41
4:V:456:LEU:HD22	5:W:328:GLY:HA2	2.02	0.41
2:R:265:LEU:HD12	3:S:121:LEU:HD11	2.02	0.41
4:V:224:LEU:HA	5:W:194:LYS:HE2	2.03	0.41
4:X:347:VAL:HG11	4:X:360:PRO:HG3	2.02	0.41
5:Y:418:VAL:HG12	5:Y:419:GLU:N	2.35	0.41
1:Q:1004:VAL:O	1:Q:1008:ARG:HG3	2.21	0.41
3:S:69:ASP:HA	3:S:72:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:284:LEU:HD12	5:Y:258:PHE:HB3	2.03	0.41
5:U:276:LYS:HD3	5:U:276:LYS:HA	1.82	0.41
5:W:449:ASP:OD1	5:W:449:ASP:N	2.54	0.41
4:X:311:ASP:OD2	5:Y:311:ARG:CD	2.69	0.41
5:Y:298:VAL:HG13	5:Y:343:LEU:HD21	2.03	0.41
2:R:226:LEU:HD23	2:R:226:LEU:HA	1.94	0.41
2:R:264:ILE:HD13	2:R:616:VAL:HA	2.03	0.41
2:R:617:GLU:HA	2:R:620:ARG:HB3	2.01	0.41
2:R:729:ILE:CD1	2:R:733:GLU:CD	2.89	0.41
4:T:96:LEU:HD13	4:T:100:VAL:HG11	2.02	0.41
4:T:96:LEU:HD23	4:T:96:LEU:HA	1.92	0.41
5:U:379:LEU:HD23	5:U:418:VAL:HB	2.03	0.41
5:Y:135:LEU:HD23	5:Y:135:LEU:HA	1.95	0.41
1:Q:1248:ASP:HA	1:Q:1271:THR:HB	2.02	0.41
1:Q:1304:LEU:HD13	1:Q:1422:LEU:HD21	2.03	0.41
5:U:161:LYS:HB3	5:U:166:GLU:HG3	2.02	0.41
5:W:19:LEU:HD23	4:X:71:SER:HB2	2.02	0.41
4:X:161:LYS:HD2	4:X:161:LYS:HA	1.92	0.41
4:X:141:GLU:N	4:X:141:GLU:OE2	2.54	0.40
4:T:198:ASP:OD1	4:T:198:ASP:N	2.54	0.40
5:U:30:GLY:HA3	5:U:41:SER:HB3	2.03	0.40
4:V:61:ILE:HD13	4:V:61:ILE:HA	1.91	0.40
2:R:189:CYS:HB3	2:R:674:ASN:HB3	2.02	0.40
5:Y:188:ASP:OD1	5:Y:188:ASP:N	2.55	0.40
4:T:119:GLU:HG2	4:T:279:GLU:HA	2.03	0.40
5:U:60:MET:HG2	5:U:66:ILE:HD11	2.04	0.40
5:W:310:ASN:O	5:W:350:ARG:NH1	2.55	0.40
4:X:355:SER:OG	4:X:359:VAL:O	2.31	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	406/485 (84%)	393 (97%)	13 (3%)	0	100	100
2	R	438/744 (59%)	431 (98%)	7 (2%)	0	100	100
3	S	121/139 (87%)	116 (96%)	5 (4%)	0	100	100
4	T	431/443 (97%)	416 (96%)	15 (4%)	0	100	100
4	V	441/443 (100%)	422 (96%)	19 (4%)	0	100	100
4	X	440/443 (99%)	419 (95%)	21 (5%)	0	100	100
5	U	432/457 (94%)	414 (96%)	18 (4%)	0	100	100
5	W	440/457 (96%)	422 (96%)	18 (4%)	0	100	100
5	Y	443/457 (97%)	426 (96%)	17 (4%)	0	100	100
6	Z	26/28 (93%)	26 (100%)	0	0	100	100
All	All	3618/4096 (88%)	3485 (96%)	133 (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	390/446 (87%)	376 (96%)	14 (4%)	35	52
2	R	394/672 (59%)	380 (96%)	14 (4%)	35	52
3	S	109/119 (92%)	102 (94%)	7 (6%)	17	27
4	T	367/375 (98%)	352 (96%)	15 (4%)	30	47
4	V	375/375 (100%)	362 (96%)	13 (4%)	36	53
4	X	374/375 (100%)	356 (95%)	18 (5%)	25	39
5	U	371/389 (95%)	361 (97%)	10 (3%)	44	63
5	W	375/389 (96%)	360 (96%)	15 (4%)	31	47
5	Y	378/389 (97%)	369 (98%)	9 (2%)	49	67
6	Z	27/27 (100%)	24 (89%)	3 (11%)	6	8
All	All	3160/3556 (89%)	3042 (96%)	118 (4%)	37	51

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	1008	ARG
1	Q	1070	PHE
1	Q	1072	ASP
1	Q	1119	SER
1	Q	1154	GLU
1	Q	1163	ASP
1	Q	1267	ASP
1	Q	1291	MET
1	Q	1310	LYS
1	Q	1324	MET
1	Q	1338	ARG
1	Q	1370	PHE
1	Q	1415	ARG
1	Q	1431	ARG
2	R	35	ASN
2	R	44	PHE
2	R	70	PHE
2	R	74	LYS
2	R	113	GLU
2	R	255	ARG
2	R	263	LYS
2	R	585	ASP
2	R	648	LYS
2	R	663	ASP
2	R	705	ASP
2	R	719	ARG
2	R	724	TYR
2	R	725	ARG
3	S	30	LEU
3	S	44	PHE
3	S	49	LYS
3	S	58	ARG
3	S	59	ARG
3	S	127	SER
3	S	145	LYS
4	T	71	SER
4	T	198	ASP
4	T	216	ASP
4	T	224	LEU
4	T	246	ASP
4	T	290	LYS
4	T	294	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	T	297	ASP
4	T	342	ARG
4	T	348	ARG
4	T	406	MET
4	T	411	SER
4	T	431	ARG
4	T	443	LYS
4	T	454	LYS
5	U	52	ARG
5	U	147	ARG
5	U	191	SER
5	U	204	ARG
5	U	271	ASP
5	U	276	LYS
5	U	400	SER
5	U	414	LYS
5	U	438	LYS
5	U	444	GLU
4	V	69	LYS
4	V	146	GLU
4	V	172	SER
4	V	180	ARG
4	V	234	LYS
4	V	268	MET
4	V	294	LYS
4	V	297	ASP
4	V	326	LYS
4	V	386	ARG
4	V	411	SER
4	V	451	ARG
4	V	454	LYS
5	W	91	SER
5	W	153	HIS
5	W	158	LEU
5	W	175	MET
5	W	183	LYS
5	W	191	SER
5	W	215	MET
5	W	220	ARG
5	W	221	PHE
5	W	276	LYS
5	W	285	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	W	331	LYS
5	W	346	ASP
5	W	371	ARG
5	W	449	ASP
4	X	42	LYS
4	X	43	ARG
4	X	71	SER
4	X	77	LEU
4	X	125	PHE
4	X	151	ASP
4	X	180	ARG
4	X	182	ASP
4	X	193	LYS
4	X	198	ASP
4	X	205	ASN
4	X	223	ASP
4	X	232	LEU
4	X	242	GLU
4	X	268	MET
4	X	290	LYS
4	X	365	ASP
4	X	444	LEU
5	Y	33	GLU
5	Y	63	ASN
5	Y	157	LYS
5	Y	188	ASP
5	Y	220	ARG
5	Y	311	ARG
5	Y	326	ASN
5	Y	330	SER
5	Y	331	LYS
6	Z	311	ARG
6	Z	314	GLU
6	Z	315	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	314	ASN
5	W	144	GLN
5	Y	173	ASN
5	Y	230	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	0.91	1 (4%)	29,45,45	1.38	4 (13%)
7	ADP	Y	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.42	4 (13%)
7	ADP	V	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.38	4 (13%)
7	ADP	U	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.37	4 (13%)
7	ADP	T	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
7	ADP	W	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	5 (17%)

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	-	-	5/12/32/32	0/3/3/3
7	ADP	Y	501	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	V	501	-	-	2/12/32/32	0/3/3/3
7	ADP	U	501	-	-	3/12/32/32	0/3/3/3
7	ADP	T	501	-	-	5/12/32/32	0/3/3/3
7	ADP	W	501	-	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	501	ADP	C5-C4	2.36	1.47	1.40
7	W	501	ADP	C5-C4	2.32	1.47	1.40
7	T	501	ADP	C5-C4	2.31	1.47	1.40
7	X	501	ADP	C5-C4	2.20	1.46	1.40
7	Y	501	ADP	C5-C4	2.19	1.46	1.40
7	U	501	ADP	C5-C4	2.12	1.46	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	501	ADP	N3-C2-N1	-3.27	123.57	128.68
7	V	501	ADP	N3-C2-N1	-3.22	123.64	128.68
7	W	501	ADP	N3-C2-N1	-3.21	123.66	128.68
7	T	501	ADP	PA-O3A-PB	-3.19	121.88	132.83
7	T	501	ADP	N3-C2-N1	-3.18	123.71	128.68
7	W	501	ADP	C3'-C2'-C1'	3.14	105.70	100.98
7	Y	501	ADP	PA-O3A-PB	-3.12	122.12	132.83
7	U	501	ADP	N3-C2-N1	-3.11	123.83	128.68
7	U	501	ADP	PA-O3A-PB	-3.07	122.28	132.83
7	X	501	ADP	PA-O3A-PB	-3.06	122.33	132.83
7	X	501	ADP	N3-C2-N1	-3.02	123.95	128.68
7	V	501	ADP	PA-O3A-PB	-2.99	122.55	132.83
7	T	501	ADP	C3'-C2'-C1'	2.76	105.13	100.98
7	Y	501	ADP	C4-C5-N7	-2.75	106.53	109.40
7	V	501	ADP	C3'-C2'-C1'	2.64	104.95	100.98
7	W	501	ADP	PA-O3A-PB	-2.58	123.96	132.83
7	X	501	ADP	C4-C5-N7	-2.58	106.71	109.40
7	V	501	ADP	C4-C5-N7	-2.53	106.76	109.40
7	T	501	ADP	C4-C5-N7	-2.48	106.81	109.40
7	X	501	ADP	C3'-C2'-C1'	2.45	104.67	100.98
7	U	501	ADP	C3'-C2'-C1'	2.42	104.62	100.98
7	U	501	ADP	C4-C5-N7	-2.40	106.89	109.40
7	W	501	ADP	C4-C5-N7	-2.38	106.92	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	501	ADP	C3'-C2'-C1'	2.37	104.54	100.98
7	W	501	ADP	O2B-PB-O3A	2.03	111.44	104.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	501	ADP	C5'-O5'-PA-O1A
7	U	501	ADP	C5'-O5'-PA-O1A
7	X	501	ADP	PA-O3A-PB-O3B
7	X	501	ADP	C5'-O5'-PA-O1A
7	X	501	ADP	C5'-O5'-PA-O2A
7	Y	501	ADP	C5'-O5'-PA-O1A
7	Y	501	ADP	C5'-O5'-PA-O2A
7	T	501	ADP	PA-O3A-PB-O1B
7	T	501	ADP	PA-O3A-PB-O2B
7	X	501	ADP	PA-O3A-PB-O2B
7	T	501	ADP	C5'-O5'-PA-O3A
7	U	501	ADP	C5'-O5'-PA-O3A
7	W	501	ADP	O4'-C4'-C5'-O5'
7	V	501	ADP	PB-O3A-PA-O2A
7	U	501	ADP	C5'-O5'-PA-O2A
7	Y	501	ADP	O4'-C4'-C5'-O5'
7	W	501	ADP	C3'-C4'-C5'-O5'
7	X	501	ADP	C5'-O5'-PA-O3A
7	Y	501	ADP	C5'-O5'-PA-O3A
7	V	501	ADP	PB-O3A-PA-O1A
7	T	501	ADP	C5'-O5'-PA-O2A

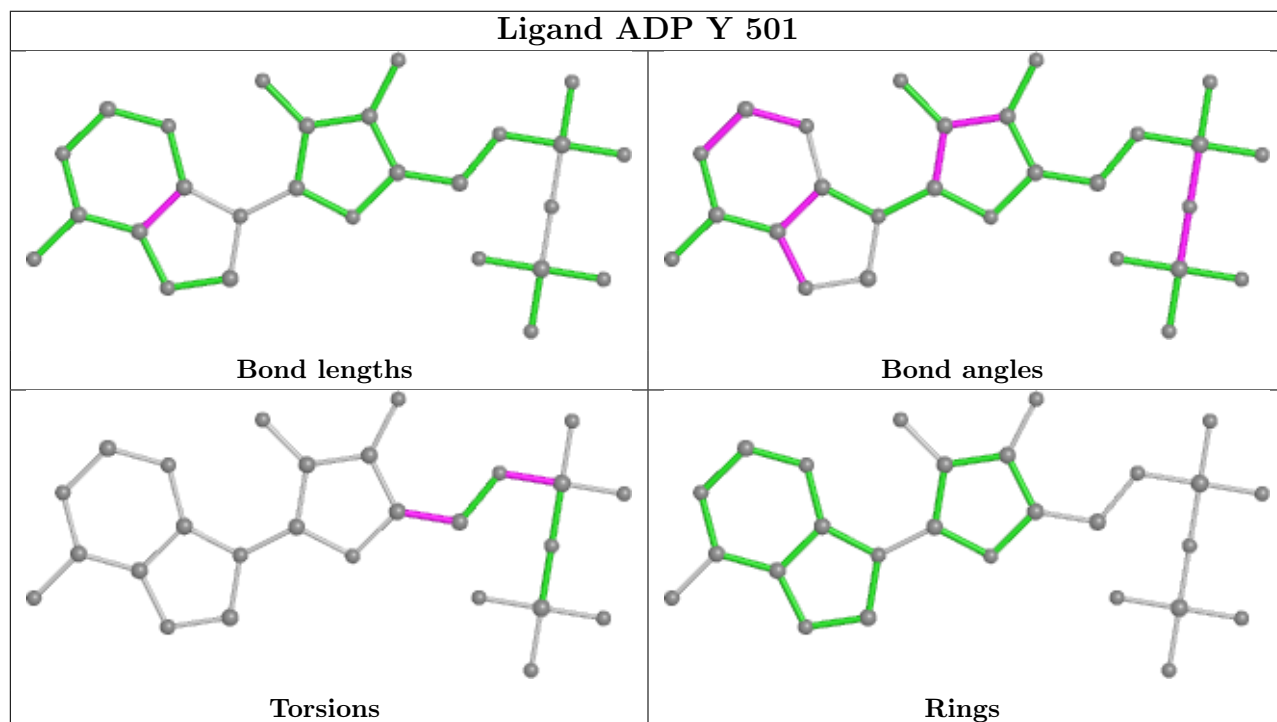
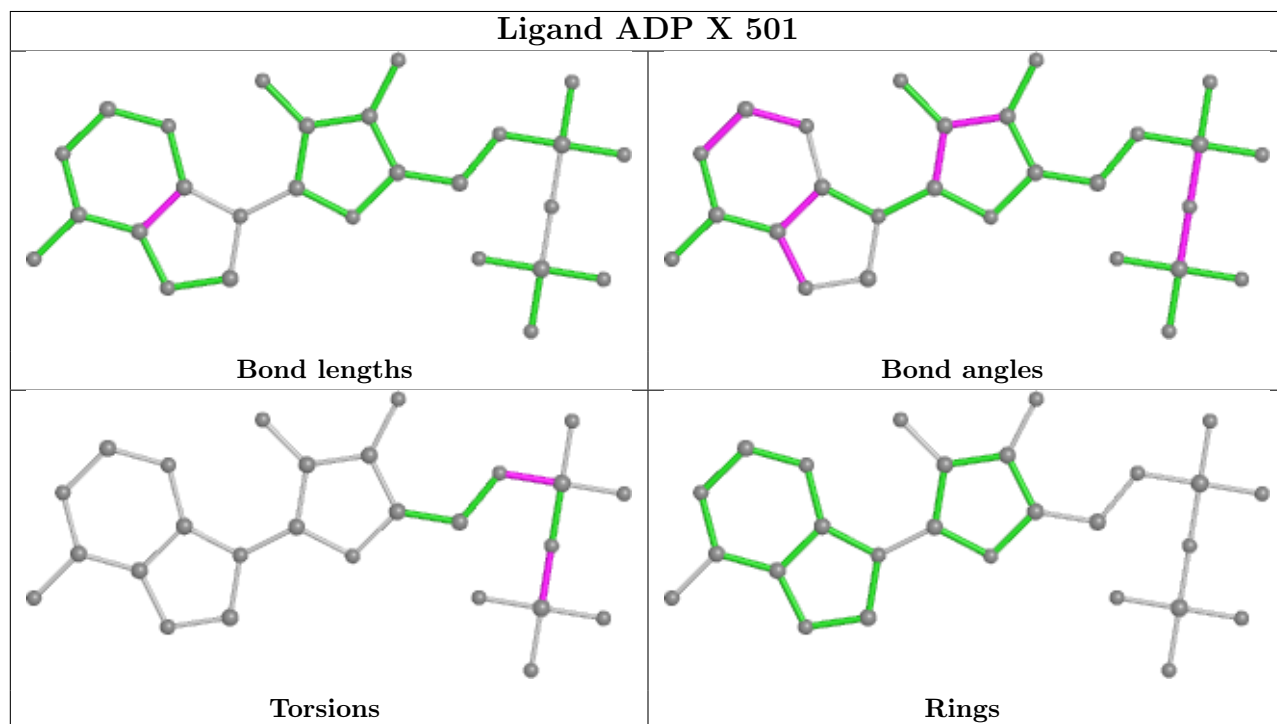
There are no ring outliers.

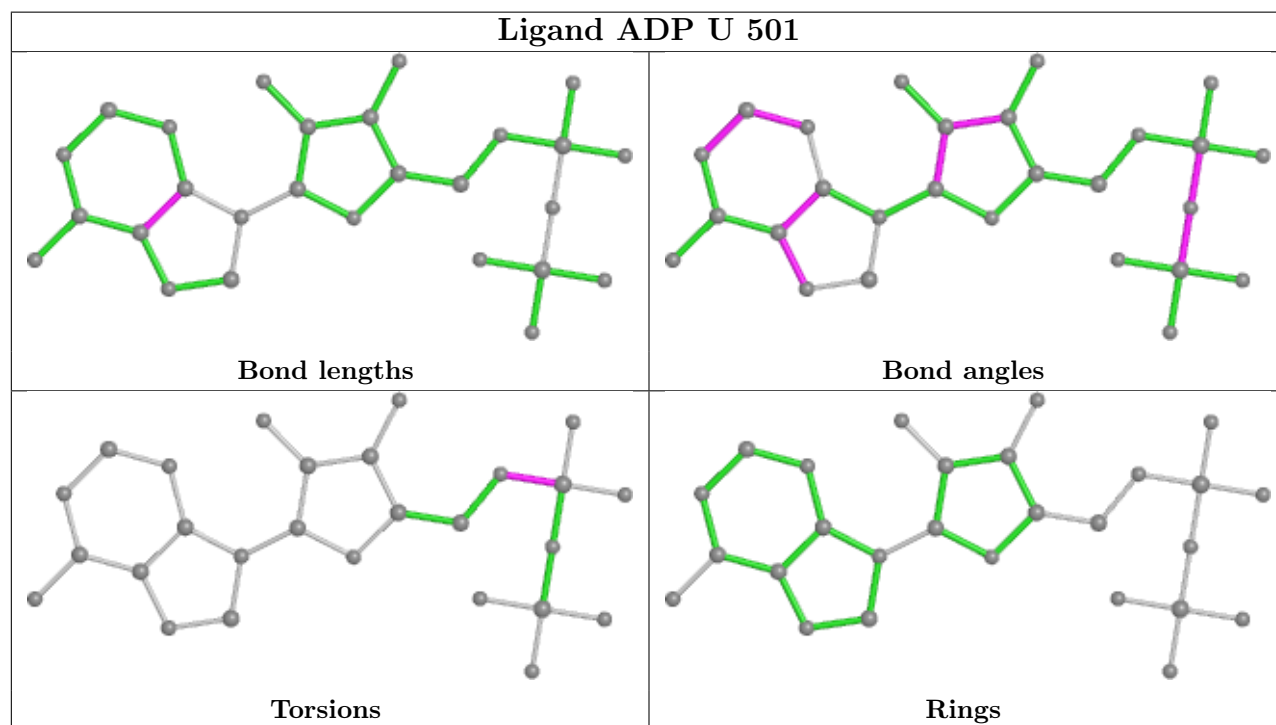
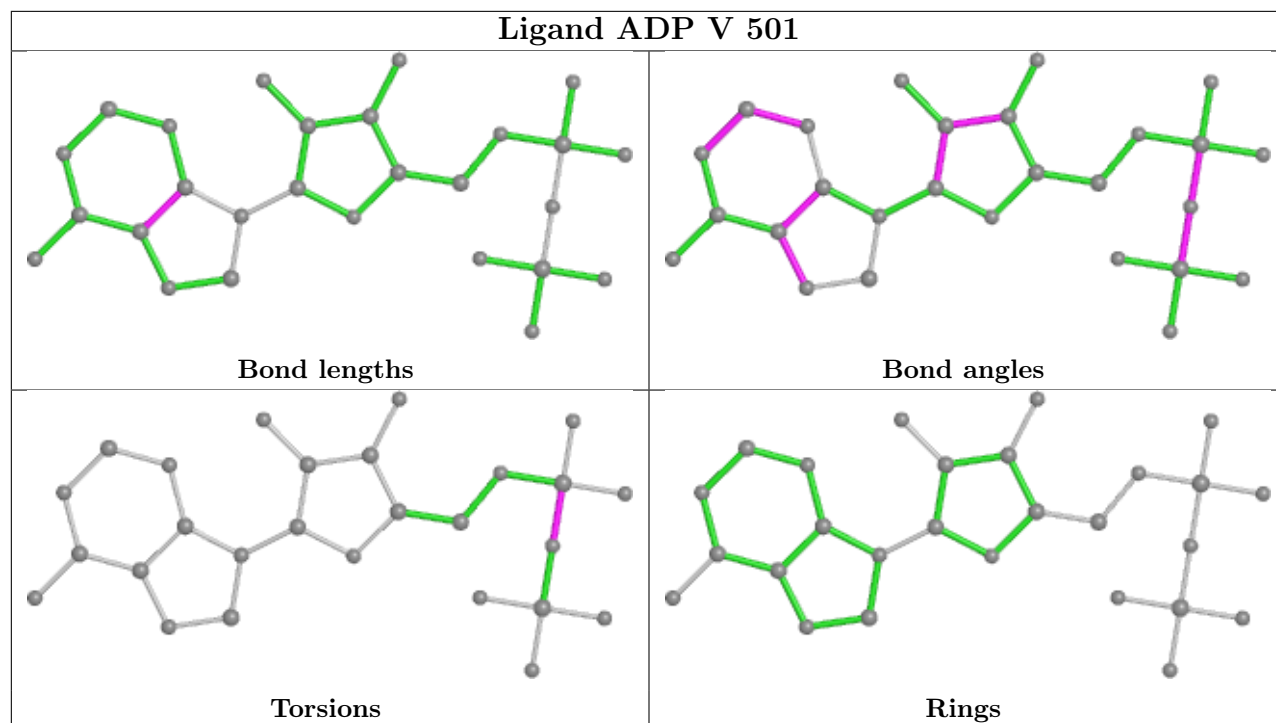
3 monomers are involved in 3 short contacts:

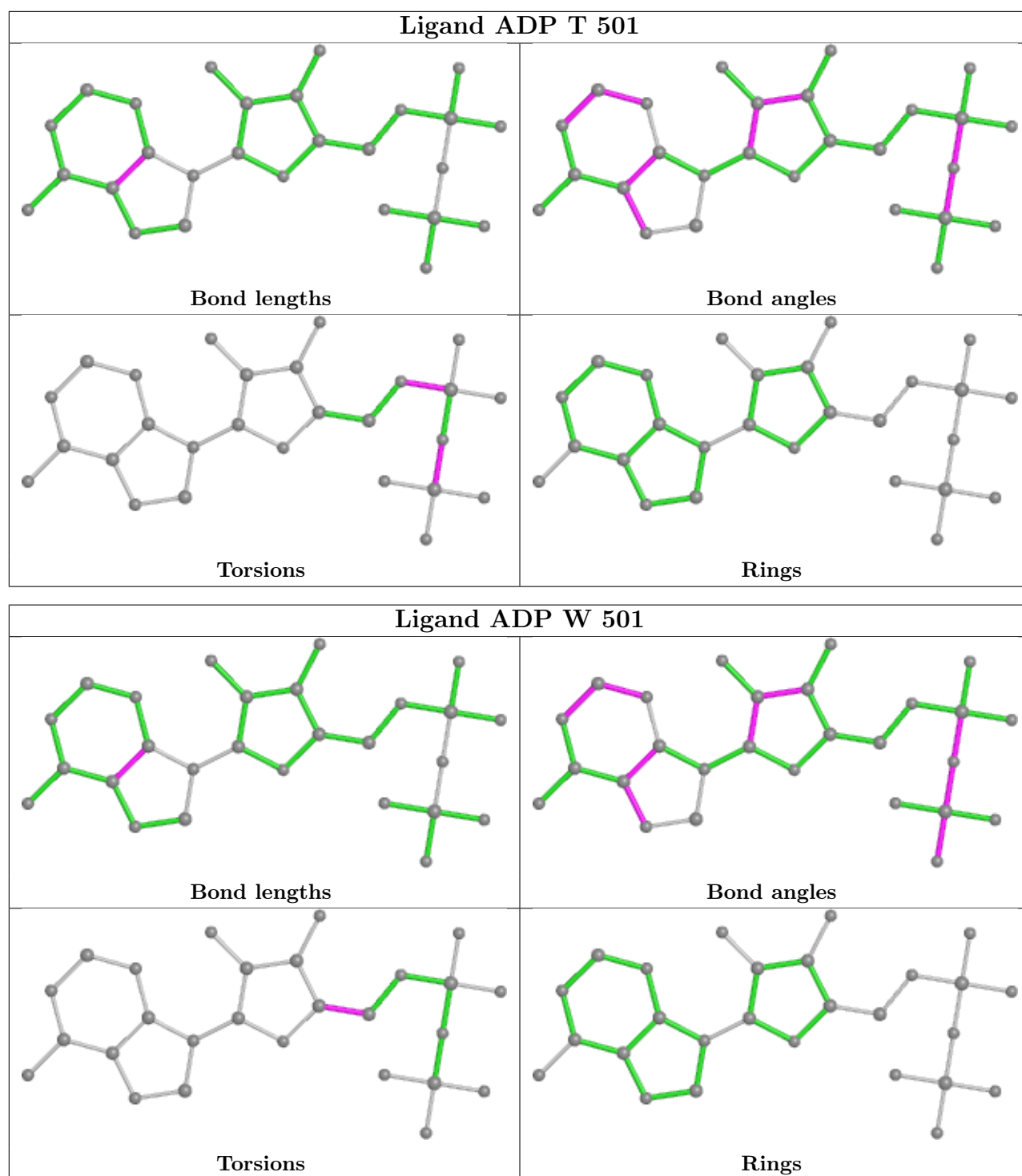
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	X	501	ADP	1	0
7	U	501	ADP	1	0
7	W	501	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

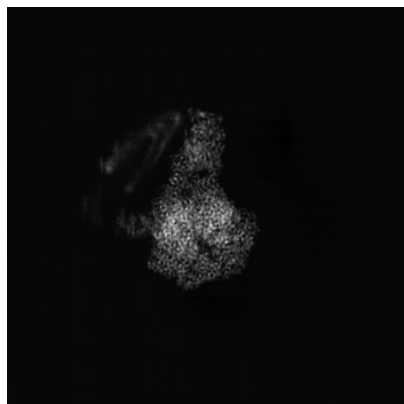
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28601. These allow visual inspection of the internal detail of the map and identification of artifacts.

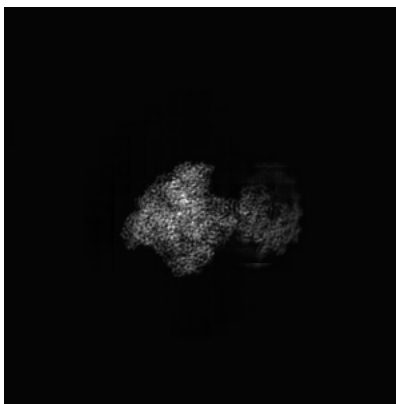
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

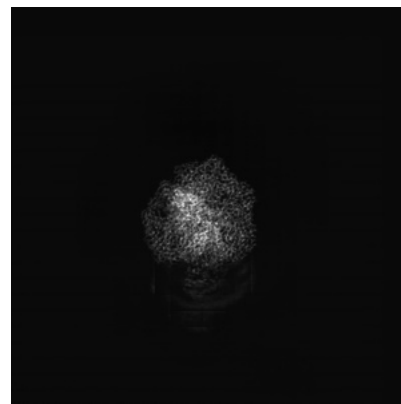
#### 6.1.1 Primary map



X

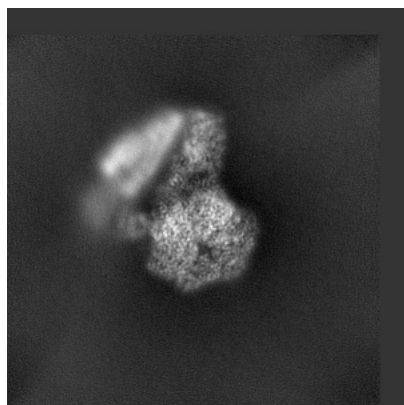


Y

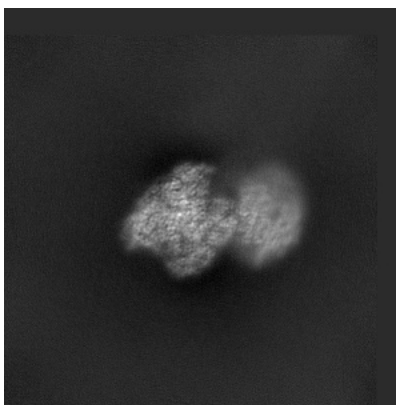


Z

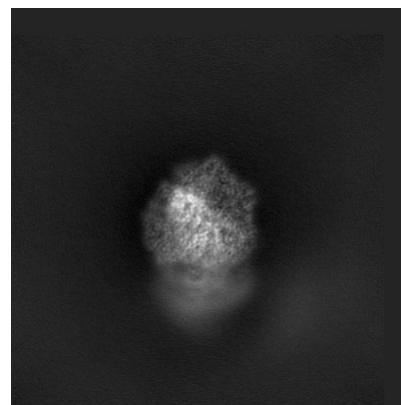
#### 6.1.2 Raw map



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

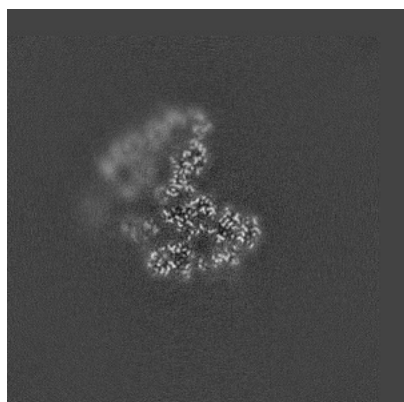


Y Index: 240

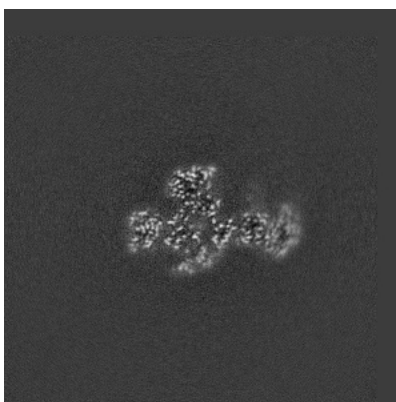


Z Index: 240

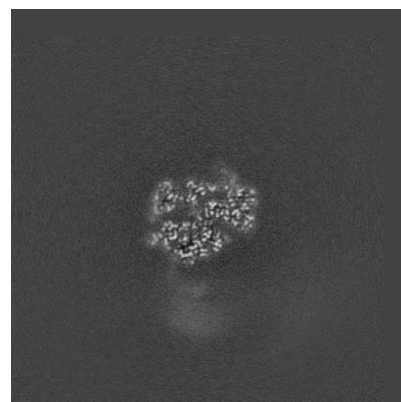
### 6.2.2 Raw map



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: 219

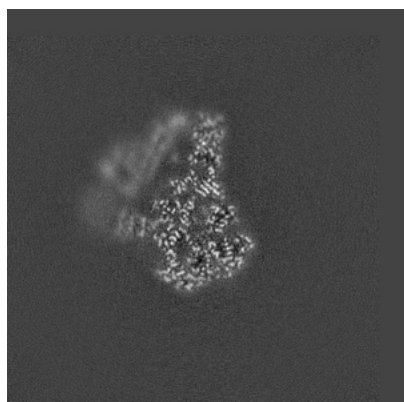


Y Index: 202

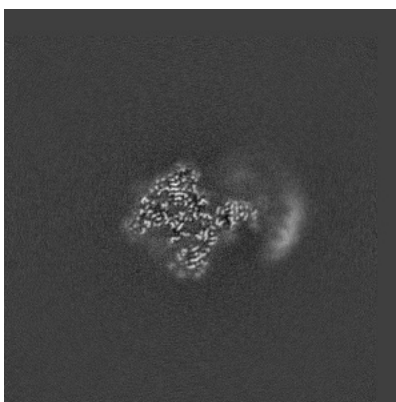


Z Index: 227

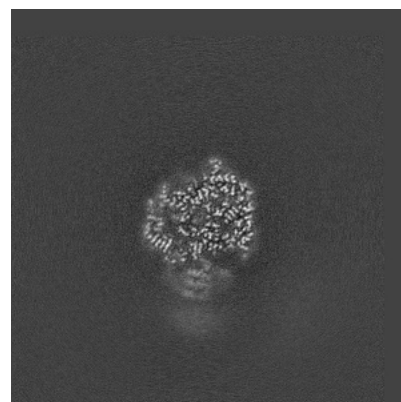
### 6.3.2 Raw map



X Index: 219



Y Index: 202

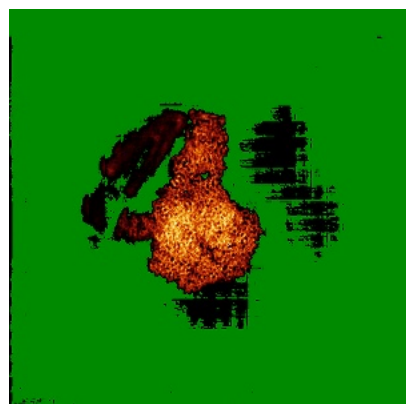


Z Index: 227

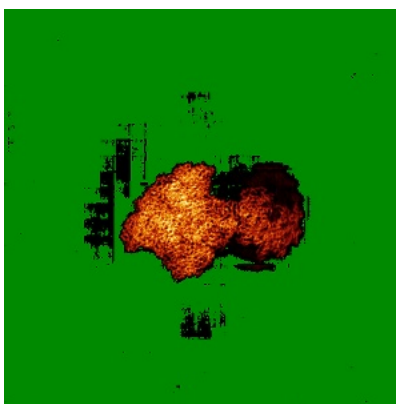
The images above show the largest variance slices of the map in three orthogonal directions.

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

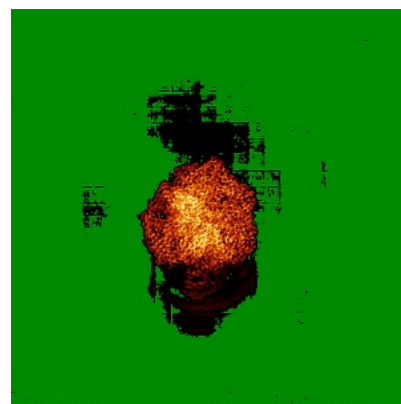
### 6.4.1 Primary map



X

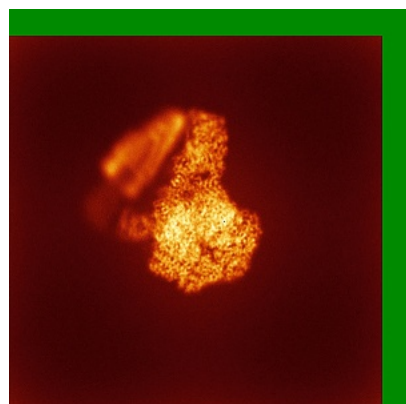


Y

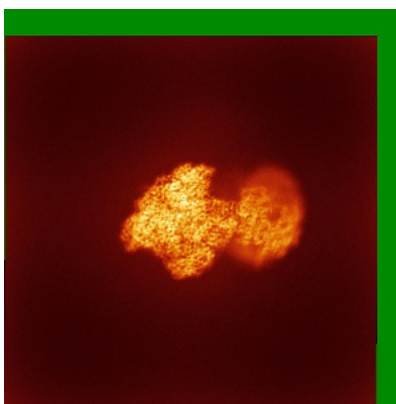


Z

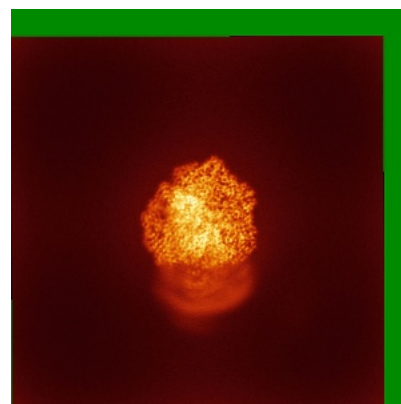
### 6.4.2 Raw map



X



Y

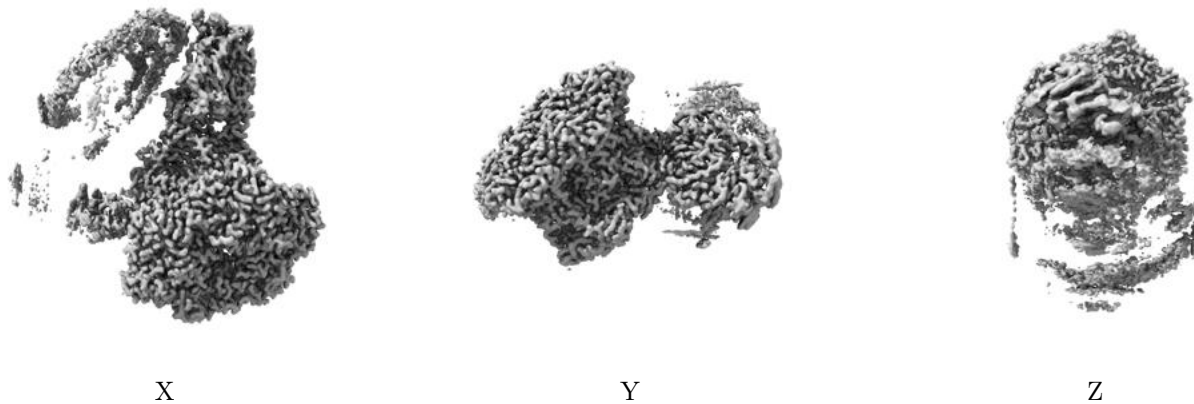


Z

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.

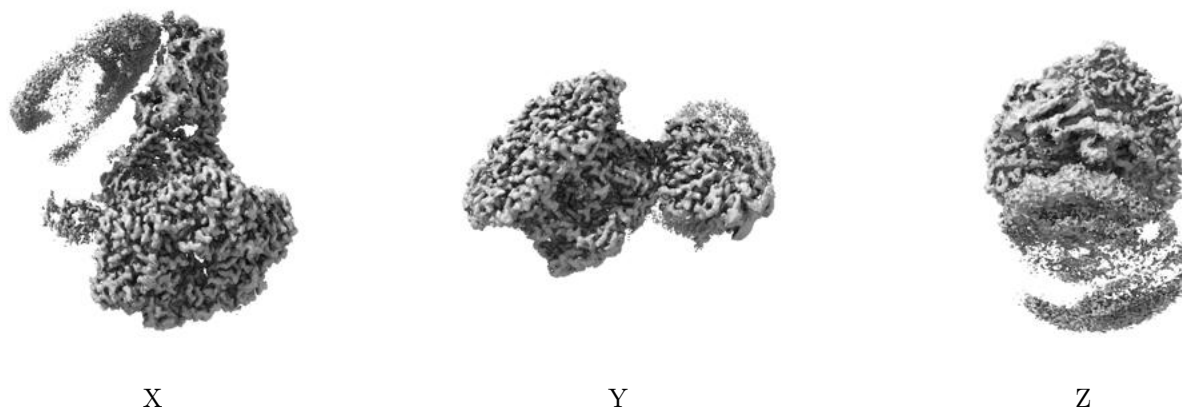
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

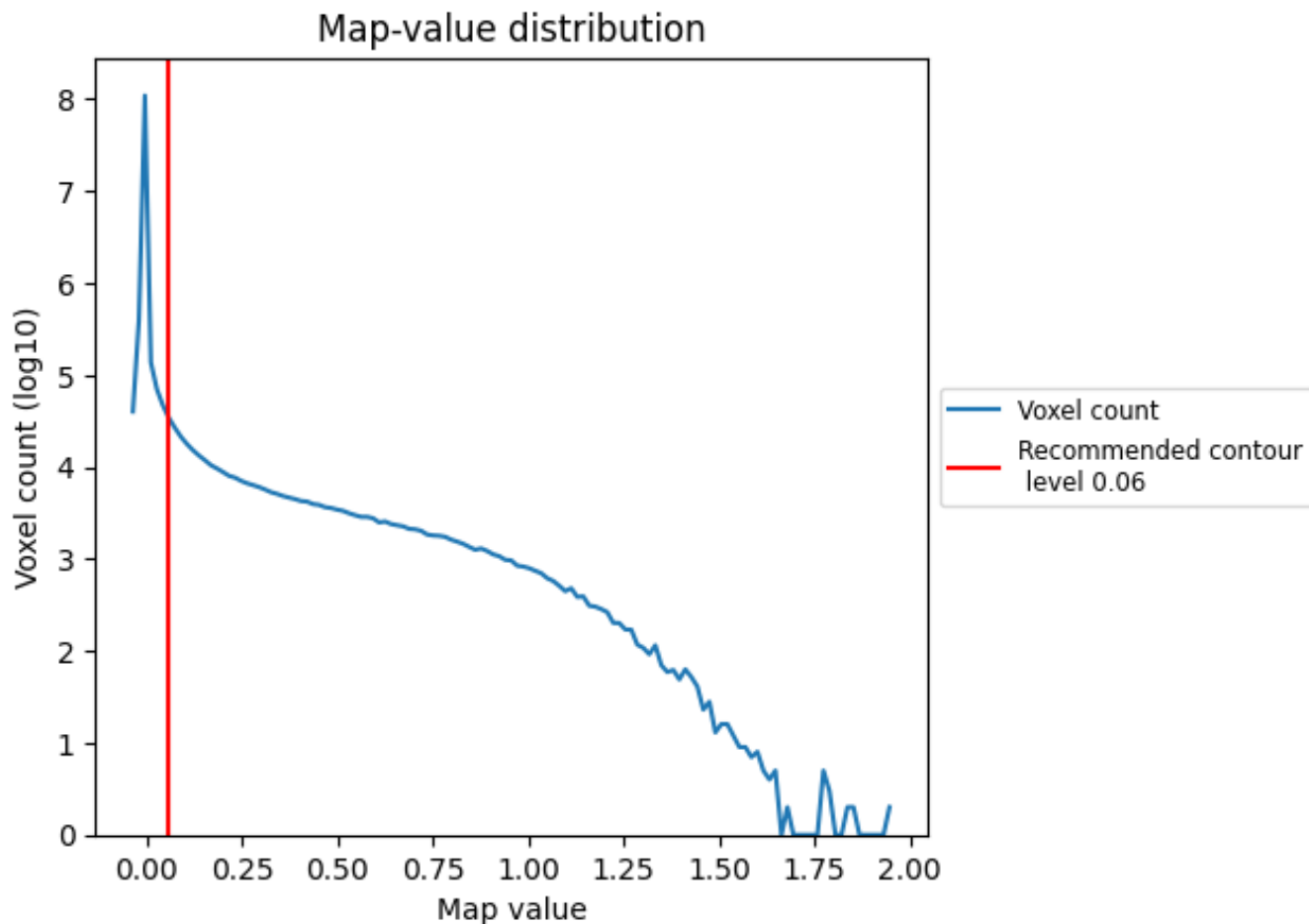
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

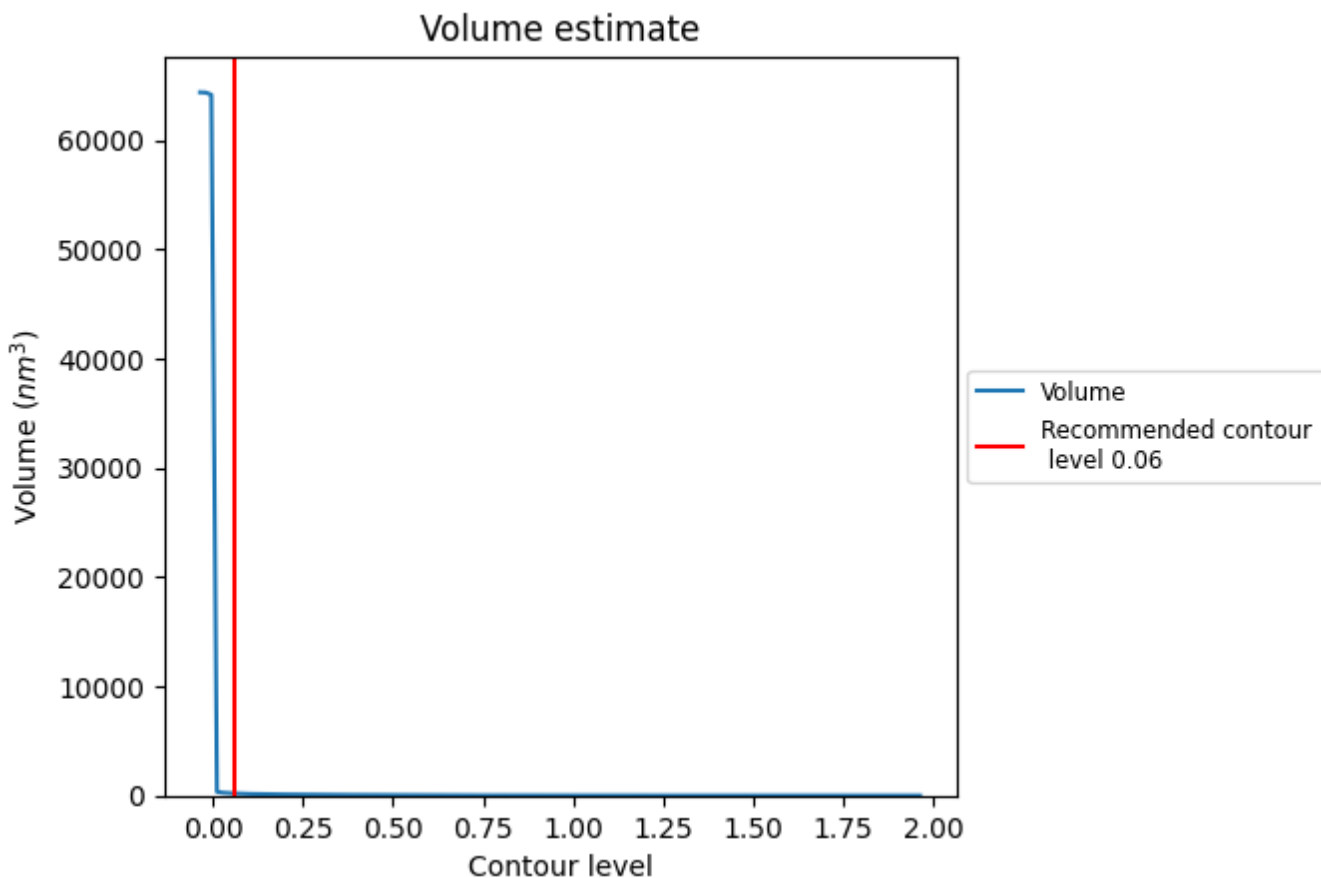
This section contains the results of statistical analysis of the map.

### 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.

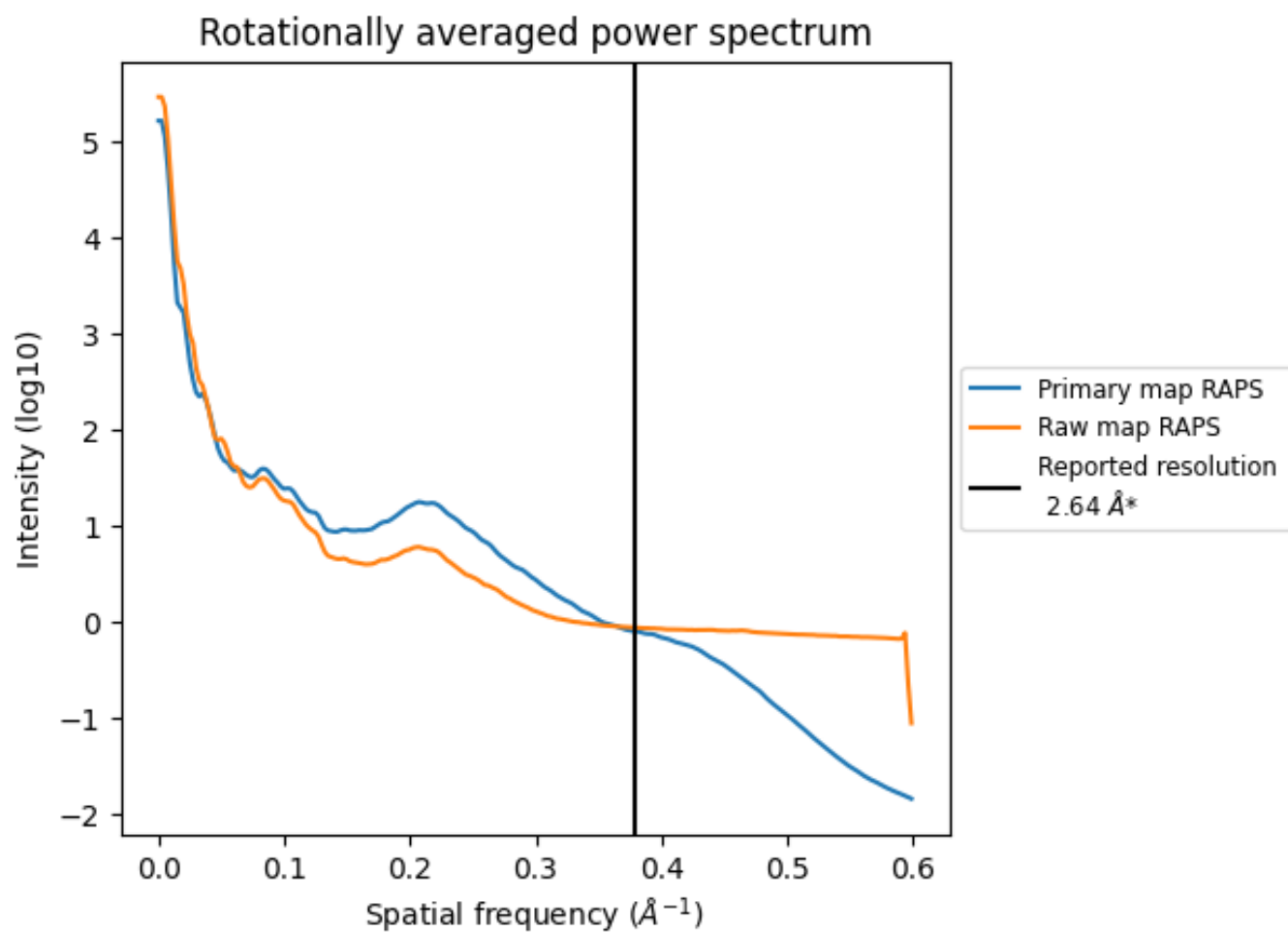
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195  $\text{nm}^3$ ; this corresponds to an approximate mass of 176 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 i

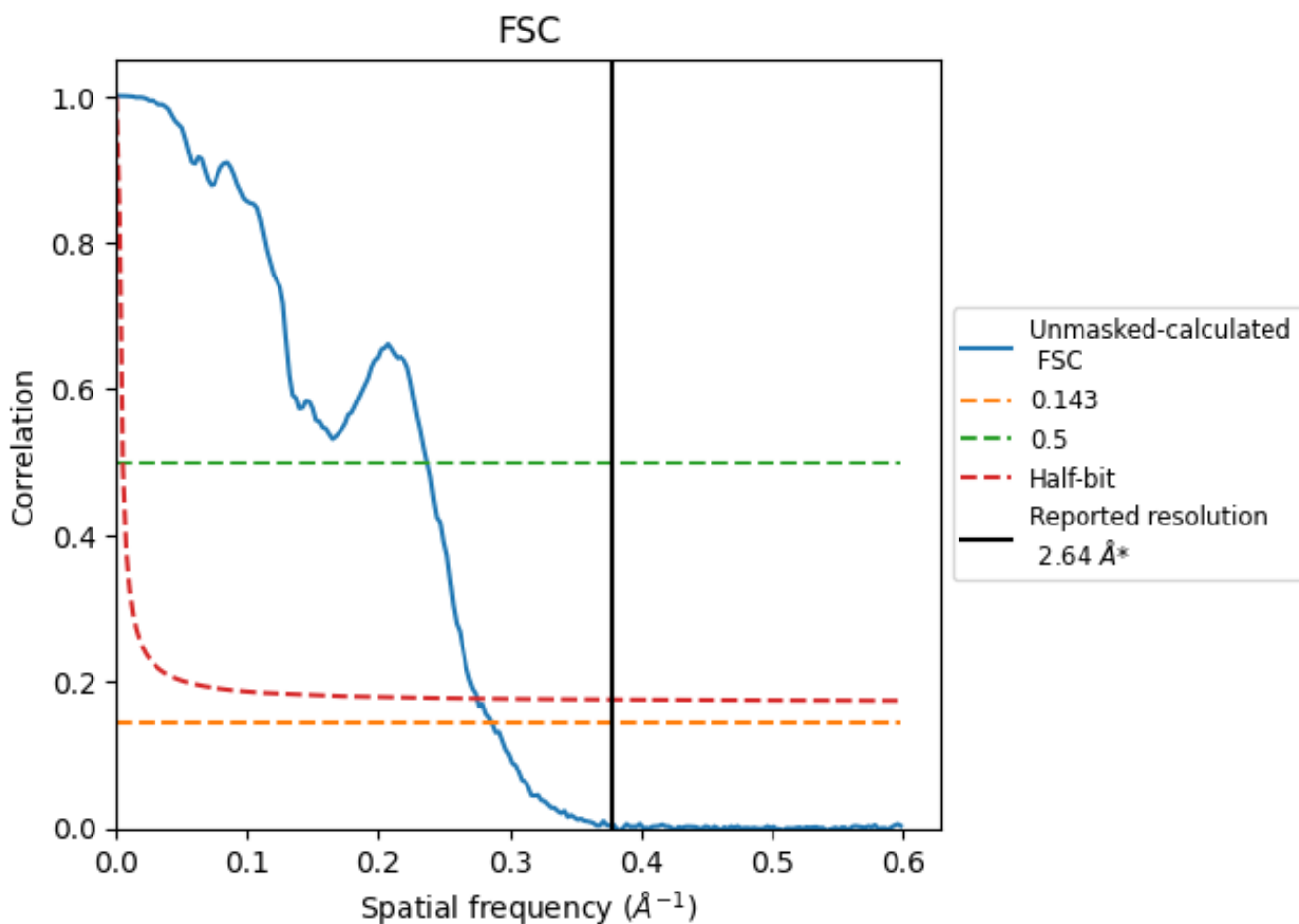


\*Reported resolution corresponds to spatial frequency of  $0.379 \text{ \AA}^{-1}$

## 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 0.379 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

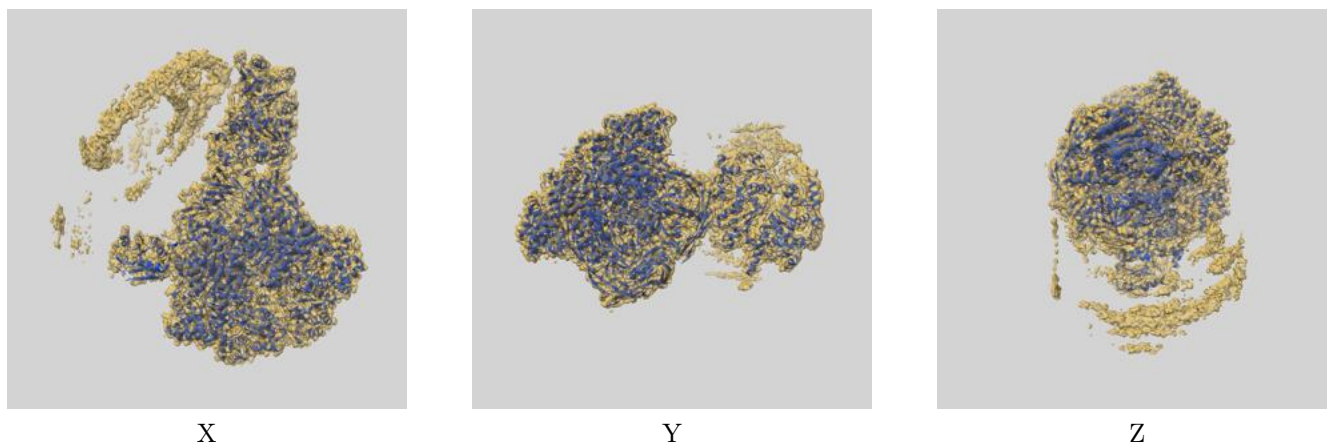
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.49	4.22	3.63

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 2.64 by more than 10 %

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

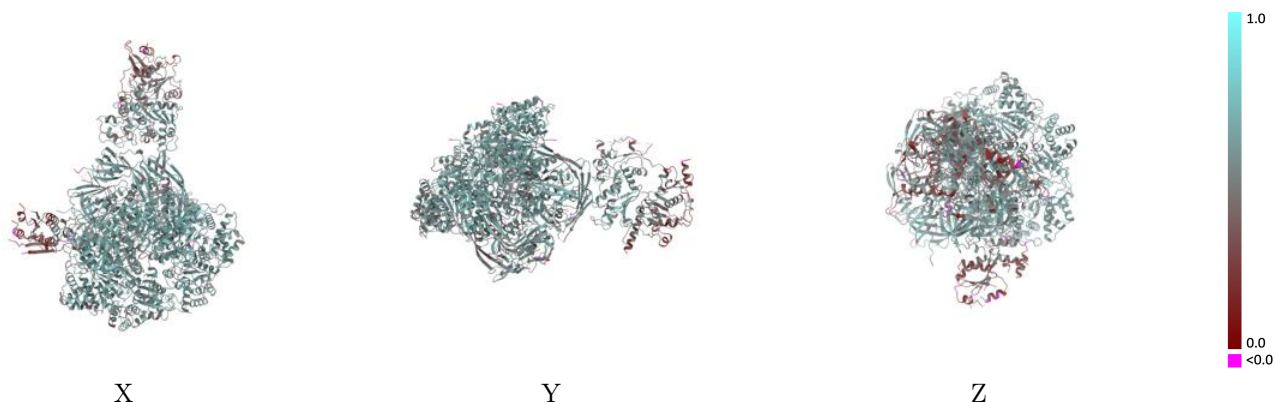
This section contains information regarding the fit between EMDB map EMD-28601 and PDB model 8ETW. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



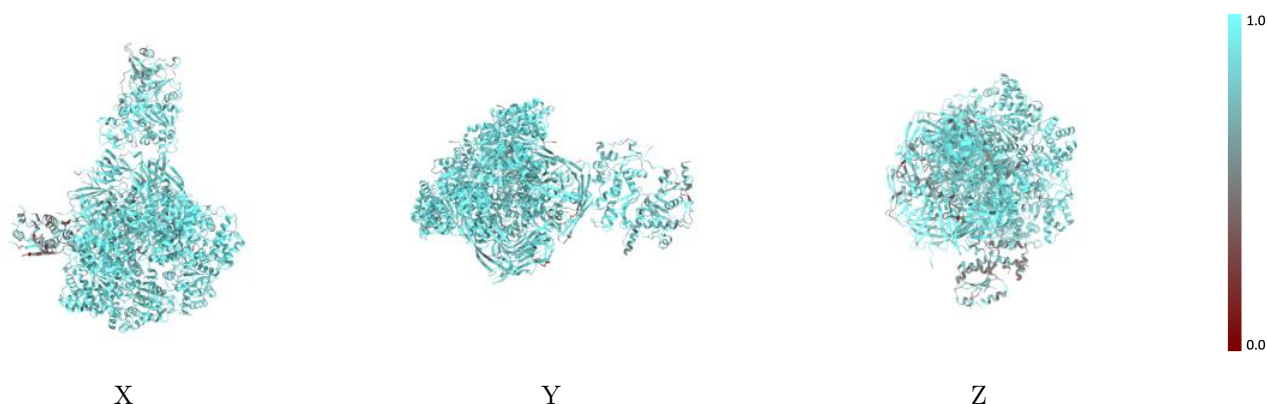
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



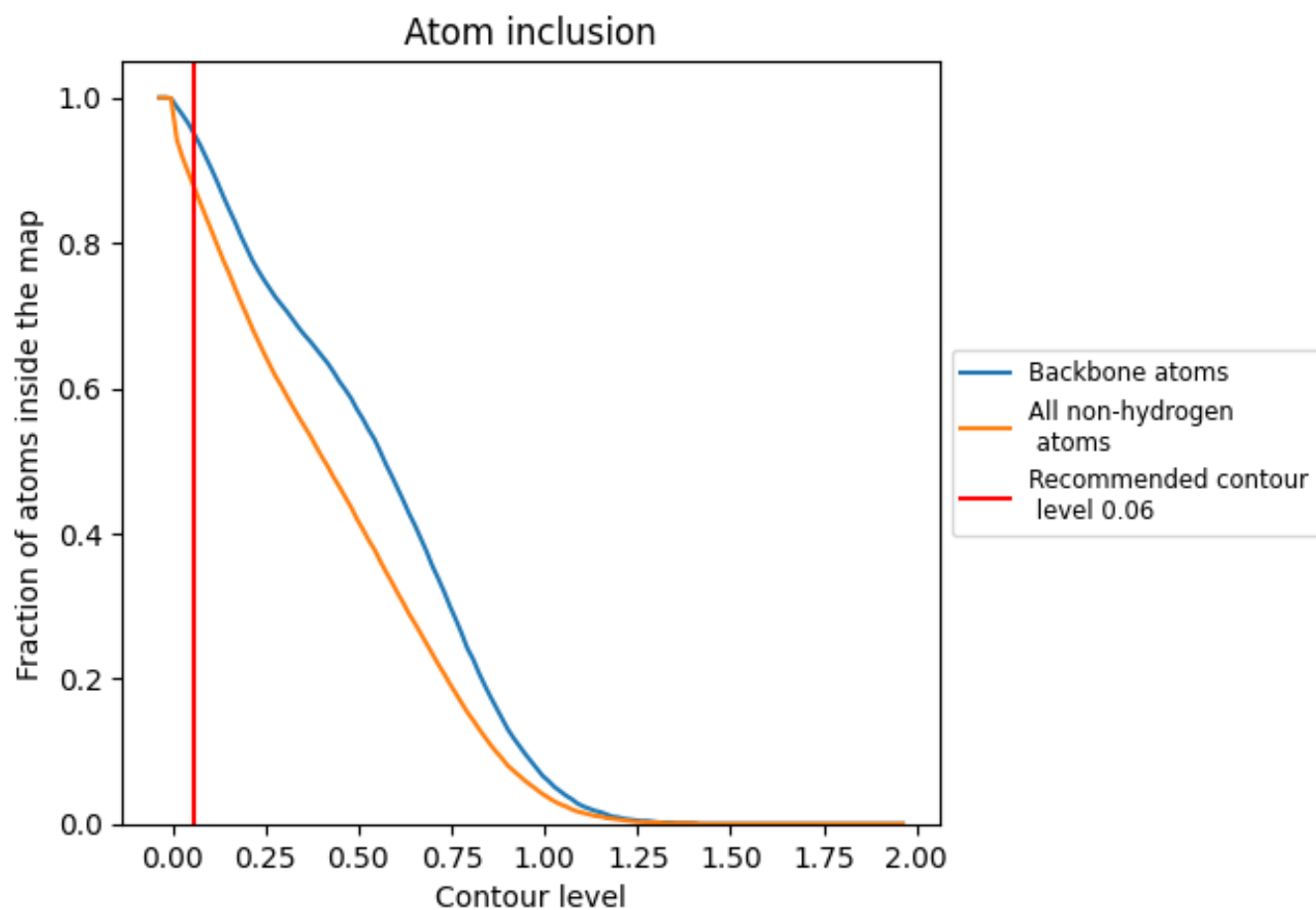
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5420
Q	 0.7750	 0.4600
R	 0.8410	 0.4740
S	 0.8030	 0.4330
T	 0.9040	 0.5850
U	 0.8970	 0.5810
V	 0.9200	 0.5920
W	 0.9040	 0.5690
X	 0.8870	 0.5450
Y	 0.8860	 0.5660
Z	 0.9150	 0.5520

