



## Full wwPDB EM Validation Report ⓘ

Jul 10, 2025 – 12:52 PM EDT

PDB ID : 9CAT / pdb\_00009cat  
EMDB ID : EMD-45403  
Title : DeltaArp8 INO80 bound to S.c 0/40 nucleosome, INO80 Core Module  
Authors : Wu, H.; Kaur, U.; Narlikar, G.J.; Cheng, Y.F.  
Deposited on : 2024-06-17  
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

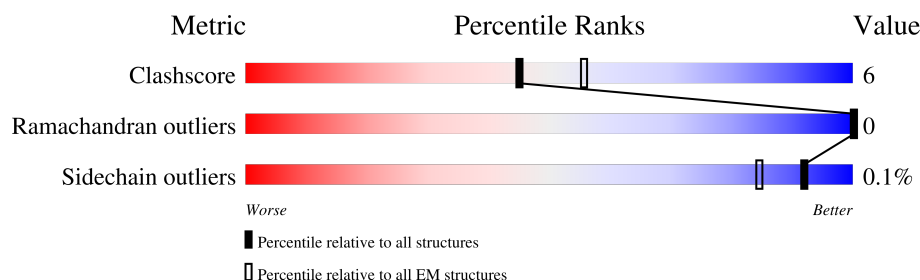
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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

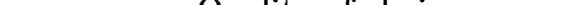



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Q	1489	
2	R	755	
3	S	166	
4	T	463	
4	V	463	
4	X	463	
5	U	460	
5	W	460	

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Mol	Chain	Length	Quality of chain
5	Y	460	
6	Z	320	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 30518 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	660	Total	C	N	O	S	0	0
			5275	3371	905	976	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	442	Total	C	N	O	S	0	0
			3535	2250	597	678	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	124	Total	C	N	O	S	0	0
			1005	642	188	173	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	435	Total	C	N	O	S	0	0
			3336	2104	575	647	10		
4	V	441	Total	C	N	O	S	0	0
			3384	2134	583	657	10		
4	X	443	Total	C	N	O	S	0	0
			3404	2149	585	660	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	445	Total	C	N	O	S	0	0
			3421	2138	594	677	12		
5	W	442	Total	C	N	O	S	0	0
			3398	2123	590	673	12		

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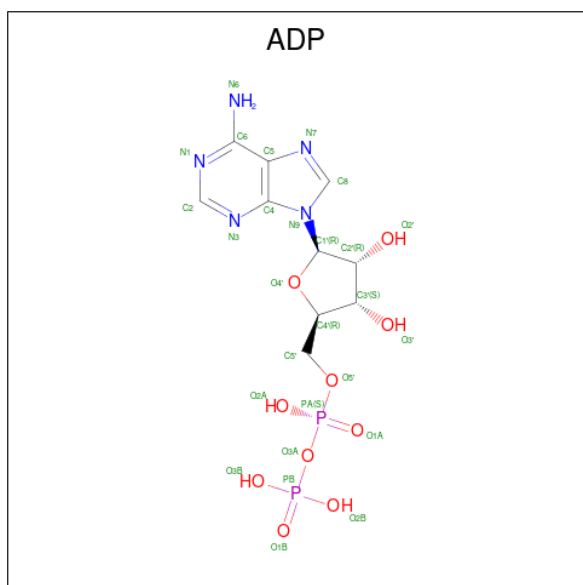
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	436	Total	C	N	O	S	0	0
			3350	2098	583	658	11		

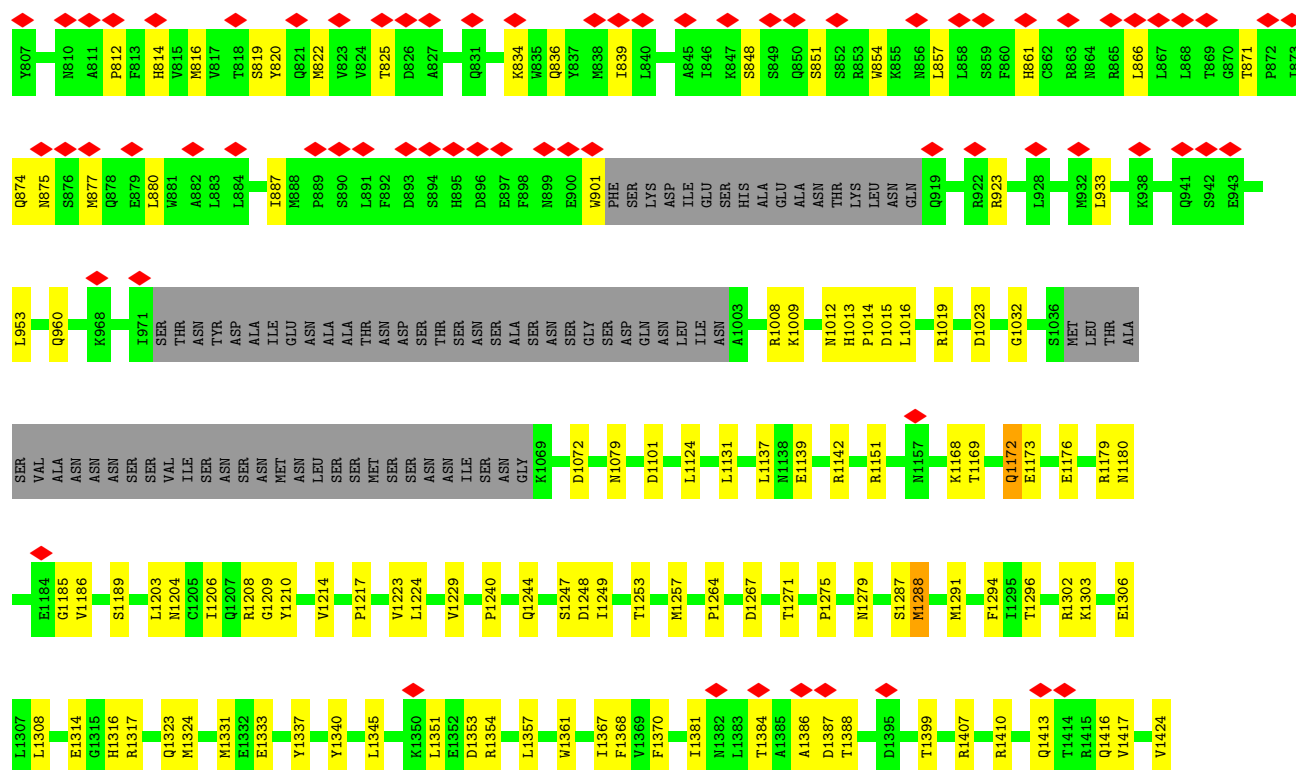
- Molecule 6 is a protein called Ino eighty subunit 2.

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 (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

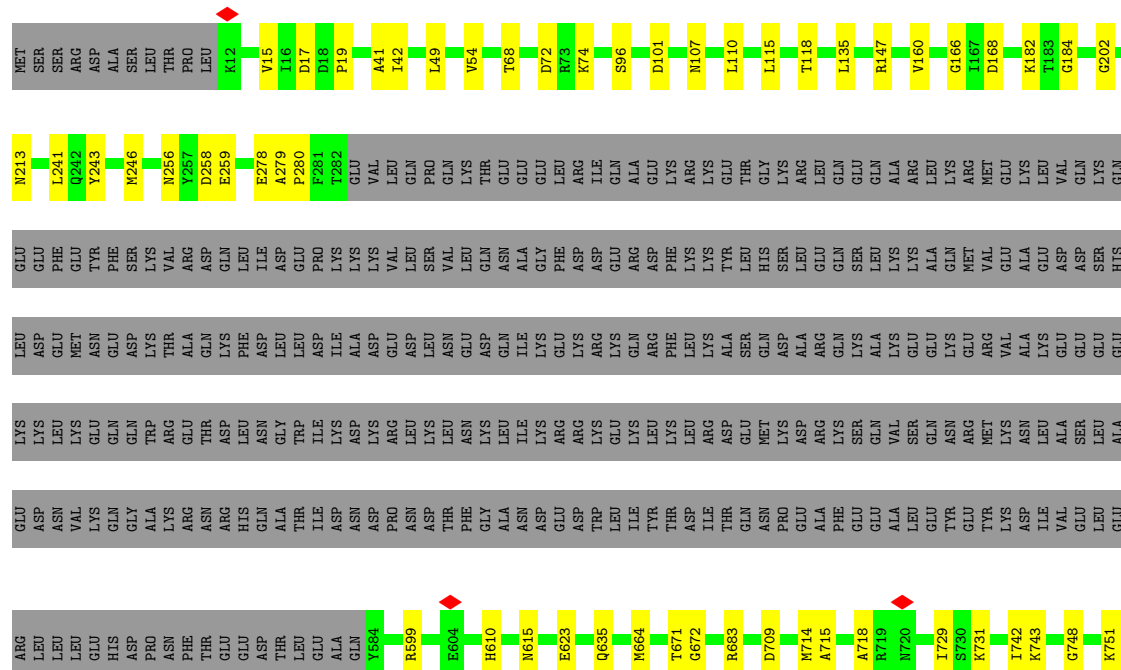






### • Molecule 2: Actin-related protein 5

Chain R: 51% 7% 41%

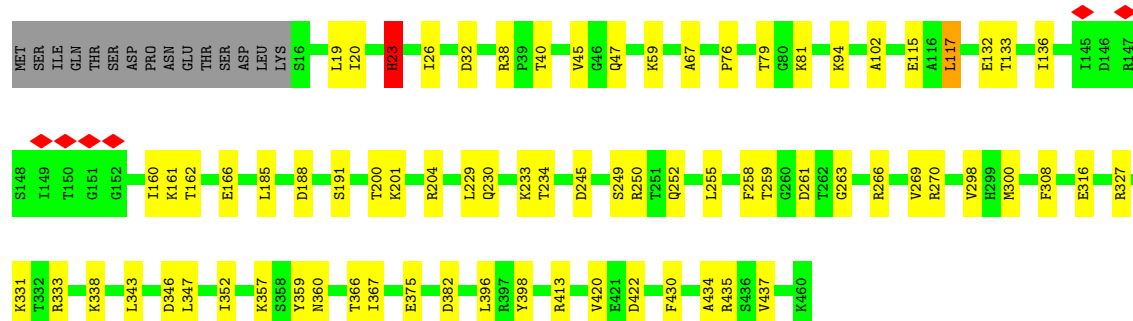
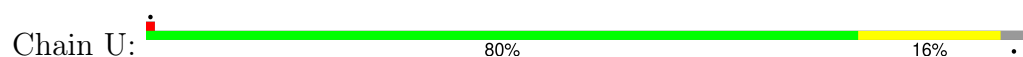




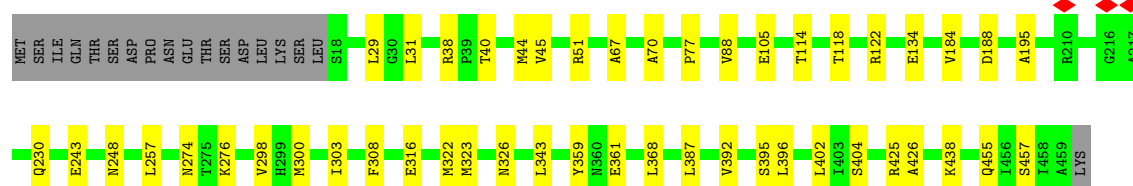
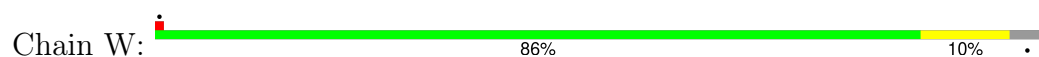




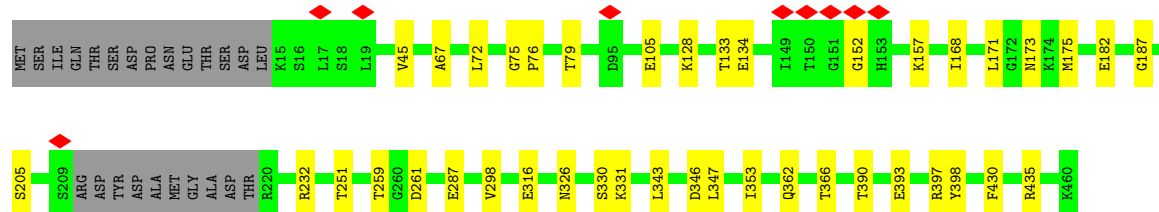
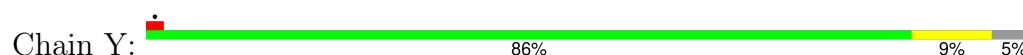
• Molecule 5: RuvB-like protein 2



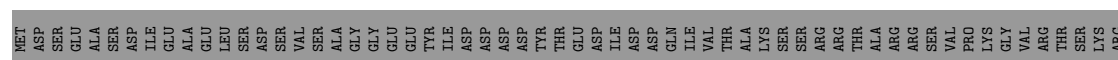
• Molecule 5: RuvB-like protein 2



• Molecule 5: RuvB-like protein 2



• Molecule 6: Ino eighty subunit 2



E314	ARG	SER	ASP	ILE
D315	ARG	ASP	GLY	ARG
L316	ALA	GLU	ILE	ASP
F317	GLU	LEU	LEU	LYS
T318	ASN	VAL	GLU	GLU
F320	ALA	SER	GLU	LEU
	ARG	VAL	GLU	SER
	LYS	VAL	GLU	VAL
	ARG	ASN	SER	GLU
	LYS	GLY	LEU	VAL
	ASN	ASN	GLU	ASP
	LEU	GLY	LYS	GLU
	SER	ASN	GLU	ASP
	GLU	GLU	LEU	TYR
	LYS	GLU	ASN	ASP
	ARG	ASP	GLY	GLU
	LEU	ASP	GLY	GLU
	GLU	GLU	GLY	GLU
	GLU	VAL	GLY	ASP
	GLU	GLU	LYS	VAL
	LYS	ALA	GLU	LEU
	GLN	THR	VAL	SER
	ASP	LYS	GLU	PRO
	THR	GLU	LYS	SER
	ILE	ASN	SER	LYS
	ASN	THR	GLU	LYS
	LYS	THR	GLU	ARG
	LEU	ASP	SER	HIS
	LEU	SER	TYR	LEU
	LYS	THR	TYR	HIS
	LYS	ARG	ALA	THR
	ARG	SER	GLN	ARG
	ALA	THR	ASN	SER
	GLY	THR	VAL	MET
	LYS	THR	GLY	ASP
	SER	ARG	GLY	ASP
	ARG	SER	GLN	LYS
	SER	LYS	LYS	ARG
	HIS	MET	GLY	VAL
	LEU	LEU	GLU	ALA
	PRO	LEU	GLU	ALA
	ASN	ASP	GLU	THR
	ASP	LEU	GLU	ALA
	ASP	LEU	ASN	SER
	GLU	GLU	GLY	GLU
	LYS	ASP	GLU	LYS
	ASN	GLY	SER	SER
	ASP	GLY	GLY	ASP
	GLY	SER	TYR	ILE
	SER	LYS	GLU	GLY
	SER	LYS	ASP	SER
	SER	LEU	ASN	LYS
	F293	THR	GLU	GLY
		ASP	PRO	ASN
	R307	GLU	SER	ASP
	T308	GLU	ILE	GLY
	L309	ILE	SER	GLU
	R310	GLN	LYS	ILE
	F312	LEU	GLU	THR

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36091	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 ( $e^-/\text{\AA}^2$ )	47.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.318	Depositor
Minimum map value	-0.428	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.198	Depositor
Map size ( $\text{\AA}$ )	366.8672, 366.8672, 366.8672	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8189, 0.8189, 0.8189	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Q	0.23	0/5393	0.57	4/7320 (0.1%)
2	R	0.19	0/3625	0.43	0/4933
3	S	0.24	0/1027	0.64	0/1380
4	T	0.20	0/3375	0.45	1/4565 (0.0%)
4	V	0.18	0/3426	0.44	0/4634
4	X	0.19	0/3446	0.44	1/4662 (0.0%)
5	U	0.19	0/3459	0.47	2/4662 (0.0%)
5	W	0.18	0/3436	0.39	0/4632
5	Y	0.18	0/3386	0.42	0/4561
6	Z	0.25	0/254	0.56	0/338
All	All	0.20	0/30827	0.47	8/41687 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Q	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	23	HIS	CB-CA-C	-8.80	98.91	111.85
5	U	23	HIS	CA-CB-CG	7.52	121.32	113.80
4	T	463	LEU	N-CA-CB	6.86	122.17	110.50
1	Q	1288	MET	CB-CG-SD	6.04	130.82	112.70
1	Q	1172	GLN	N-CA-C	-5.49	105.30	111.28
4	X	190	GLN	CB-CG-CD	5.41	121.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	776	LYS	CA-CB-CG	5.10	124.30	114.10
1	Q	877	MET	CA-CB-CG	5.03	124.15	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Q	1425	ARG	Sidechain

## 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	5275	0	5167	110	0
2	R	3535	0	3420	33	0
3	S	1005	0	1044	16	0
4	T	3336	0	3459	50	0
4	V	3384	0	3508	44	0
4	X	3404	0	3542	44	0
5	U	3421	0	3499	56	0
5	W	3398	0	3470	31	0
5	Y	3350	0	3444	31	0
6	Z	248	0	242	6	0
7	T	27	0	12	4	0
7	U	27	0	12	3	0
7	V	27	0	12	5	0
7	W	27	0	12	1	0
7	X	27	0	12	3	0
7	Y	27	0	12	2	0
All	All	30518	0	30867	376	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 (376) 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)
4:X:331:ASN:OD1	4:X:332:ILE:HG13	1.87	0.75
5:U:352:ILE:HD12	4:V:446:PHE:CD1	2.26	0.71
5:U:185:LEU:HG	5:U:185:LEU:O	1.94	0.68
1:Q:1169:THR:HG21	5:U:269:VAL:HG22	1.77	0.67
1:Q:1223:VAL:HB	1:Q:1229:VAL:HG11	1.77	0.66
4:T:387:ARG:HA	4:T:390:VAL:HG12	1.76	0.66
1:Q:834:LYS:HE2	1:Q:861:HIS:H	1.61	0.65
1:Q:1357:LEU:HD13	1:Q:1370:PHE:CZ	2.31	0.65
4:X:68:LYS:HG2	4:X:305:PRO:HD2	1.78	0.65
1:Q:1288:MET:HG3	4:X:212:VAL:HG13	1.79	0.64
5:W:77:PRO:HG3	5:W:326:ASN:HD22	1.63	0.63
1:Q:773:GLU:O	1:Q:777:PHE:HB2	1.98	0.63
5:W:184:VAL:HG23	5:W:188:ASP:HB2	1.81	0.63
1:Q:1308:LEU:HD21	1:Q:1340:TYR:CE2	2.34	0.63
2:R:135:LEU:HD12	2:R:714:MET:HB3	1.81	0.61
4:T:313:VAL:HG21	4:T:338:LEU:HD13	1.81	0.61
4:T:189:ILE:HG23	4:T:194:VAL:HB	1.81	0.61
5:U:160:ILE:HG23	5:U:229:LEU:HD21	1.83	0.61
2:R:15:VAL:HA	2:R:278:GLU:HB3	1.83	0.60
2:R:729:ILE:HG12	2:R:743:LYS:HD3	1.82	0.60
4:V:212:VAL:HG13	4:V:230:VAL:HG21	1.82	0.60
4:X:289:ASN:ND2	4:X:332:ILE:CD1	2.66	0.59
1:Q:1019:ARG:NH2	1:Q:1333:GLU:OE1	2.36	0.59
1:Q:1440:GLU:HA	1:Q:1443:GLN:HE21	1.68	0.59
1:Q:1204:ASN:ND2	5:W:195:ALA:O	2.36	0.59
5:Y:45:VAL:HG21	5:Y:366:THR:OG1	2.03	0.59
5:Y:171:LEU:HD22	5:Y:175:MET:HG2	1.84	0.59
4:T:322:THR:HG21	5:U:300:MET:HG3	1.85	0.58
1:Q:1308:LEU:CD2	1:Q:1340:TYR:HE2	2.17	0.58
4:V:362:ASP:OD1	4:V:362:ASP:N	2.37	0.58
4:X:212:VAL:HG12	4:X:230:VAL:HG21	1.84	0.58
4:T:359:VAL:HB	4:T:364:ILE:HD11	1.85	0.58
1:Q:822:MET:HA	1:Q:825:THR:HG22	1.86	0.58
2:R:54:VAL:HG11	2:R:718:ALA:HB3	1.85	0.57
4:V:118:THR:HG21	5:W:105:GLU:HG2	1.86	0.57
1:Q:784:LEU:HD21	1:Q:799:PHE:HB3	1.85	0.57
1:Q:782:LYS:HD2	1:Q:812:PRO:HA	1.85	0.57
1:Q:1186:VAL:HG21	4:V:300:VAL:HG11	1.86	0.57
4:T:224:LEU:HB3	5:Y:171:LEU:HD23	1.87	0.56
4:T:359:VAL:O	4:T:364:ILE:HD11	2.04	0.56
3:S:71:ASN:OD1	3:S:75:ASN:ND2	2.37	0.56
1:Q:1387:ASP:HB2	1:Q:1417:VAL:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:764:ALA:HB1	1:Q:1351:LEU:HD21	1.88	0.56
4:T:463:LEU:HD22	5:Y:75:GLY:HA2	1.88	0.56
5:U:346:ASP:OD1	5:U:346:ASP:N	2.39	0.56
5:W:316:GLU:O	4:X:23:ARG:NH2	2.39	0.55
1:Q:1023:ASP:HB2	1:Q:1287:SER:HB3	1.87	0.55
2:R:72:ASP:OD1	2:R:72:ASP:N	2.40	0.55
4:V:73:ARG:NH2	5:W:404:SER:OG	2.39	0.55
4:V:413:ARG:NH2	7:V:1001:ADP:O3B	2.40	0.55
1:Q:759:LEU:HD22	1:Q:816:MET:HE2	1.87	0.55
6:Z:310:ARG:NH1	6:Z:315:ASP:OD1	2.40	0.55
1:Q:1032:GLY:HA3	5:Y:182:GLU:HA	1.89	0.55
5:W:122:ARG:NH2	5:W:274:ASN:OD1	2.40	0.55
5:W:303:ILE:HG23	4:X:315:MET:HE1	1.88	0.54
1:Q:1224:LEU:HB3	5:Y:133:THR:HG21	1.88	0.54
5:U:117:LEU:HD23	5:U:308:PHE:HD2	1.72	0.54
4:V:189:ILE:HG23	4:V:194:VAL:HB	1.89	0.54
4:X:332:ILE:HG22	4:X:332:ILE:O	2.08	0.54
5:Y:362:GLN:O	5:Y:366:THR:HG23	2.08	0.54
4:V:377:LYS:HD2	4:V:408:THR:HG21	1.89	0.54
4:T:166:VAL:HG21	4:T:186:TYR:HB2	1.90	0.54
4:T:319:GLU:OE2	5:U:333:ARG:NH2	2.41	0.54
1:Q:1345:LEU:HD23	1:Q:1357:LEU:HD21	1.90	0.54
5:Y:45:VAL:O	7:Y:1001:ADP:N6	2.41	0.54
4:V:119:GLU:OE2	4:V:285:ARG:NH2	2.40	0.53
4:X:413:ARG:NH2	7:X:1001:ADP:O3A	2.41	0.53
1:Q:819:SER:HB3	1:Q:822:MET:HE1	1.89	0.53
1:Q:1357:LEU:CD1	1:Q:1370:PHE:HZ	2.22	0.53
5:U:40:THR:HG21	5:U:366:THR:HG21	1.89	0.53
1:Q:1151:ARG:NH1	5:U:252:GLN:OE1	2.40	0.53
4:T:71:SER:HB3	5:U:19:LEU:HB2	1.89	0.53
2:R:166:GLY:HA2	2:R:748:GLY:HA2	1.91	0.53
2:R:168:ASP:OD1	2:R:168:ASP:N	2.41	0.53
4:T:359:VAL:O	4:T:364:ILE:CD1	2.57	0.53
5:U:23:HIS:CE1	7:U:1001:ADP:H3'	2.44	0.52
4:X:130:GLY:HA2	4:X:248:THR:HA	1.91	0.52
5:U:40:THR:HG22	5:U:45:VAL:HG13	1.91	0.52
4:X:119:GLU:OE2	4:X:285:ARG:NH2	2.42	0.52
1:Q:1013:HIS:ND1	1:Q:1015:ASP:OD1	2.43	0.52
2:R:41:ALA:HA	2:R:135:LEU:HB2	1.89	0.52
2:R:107:ASN:HD21	2:R:110:LEU:HD22	1.74	0.52
3:S:114:LYS:NZ	4:T:223:ASP:OD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1206:ILE:O	1:Q:1279:ASN:ND2	2.42	0.52
2:R:671:THR:OG1	2:R:672:GLY:N	2.42	0.52
5:U:67:ALA:HB3	4:V:25:ALA:HB2	1.90	0.52
1:Q:1139:GLU:OE1	1:Q:1142:ARG:NH2	2.43	0.52
5:Y:390:THR:HA	5:Y:393:GLU:HG2	1.92	0.52
5:Y:171:LEU:HD22	5:Y:175:MET:CG	2.39	0.52
5:U:115:GLU:OE2	5:U:270:ARG:NH2	2.43	0.51
2:R:279:ALA:HB3	2:R:610:HIS:HB3	1.91	0.51
4:X:431:ARG:NH2	4:X:438:ASP:OD2	2.38	0.51
1:Q:1240:PRO:O	1:Q:1244:GLN:HB2	2.10	0.51
4:T:275:PRO:HG2	5:Y:251:THR:HB	1.91	0.51
4:X:173:ALA:HB3	4:X:234:LYS:HA	1.91	0.51
1:Q:1137:LEU:HB2	5:U:200:THR:HB	1.92	0.51
4:T:368:LEU:HB3	5:U:430:PHE:HB3	1.93	0.51
1:Q:1361:TRP:HA	1:Q:1367:ILE:HG21	1.93	0.51
4:V:361:PRO:HA	4:V:364:ILE:HB	1.93	0.51
5:W:359:TYR:OH	7:W:1001:ADP:N7	2.42	0.51
5:Y:128:LYS:HB3	5:Y:287:GLU:HB2	1.93	0.51
6:Z:313:GLU:HG2	6:Z:314:GLU:HG3	1.92	0.51
4:T:21:VAL:HB	4:T:392:ARG:HH22	1.75	0.51
4:T:461:ASN:OD1	4:T:461:ASN:N	2.44	0.51
5:W:38:ARG:O	5:W:51:ARG:NH2	2.39	0.51
4:T:166:VAL:HB	4:T:181:LEU:HB2	1.93	0.51
1:Q:1009:LYS:HB3	1:Q:1324:MET:HE1	1.94	0.50
1:Q:1168:LYS:CG	1:Q:1173:GLU:HG2	2.40	0.50
3:S:134:TYR:HB3	3:S:144:VAL:HG21	1.93	0.50
4:V:375:TYR:OH	7:V:1001:ADP:N7	2.38	0.50
6:Z:319:THR:OG1	6:Z:320:PHE:N	2.43	0.50
1:Q:1314:GLU:OE1	1:Q:1316:HIS:ND1	2.36	0.50
4:T:362:ASP:OD1	4:T:362:ASP:N	2.43	0.50
5:Y:346:ASP:OD1	5:Y:346:ASP:N	2.43	0.50
1:Q:1264:PRO:HG2	1:Q:1267:ASP:HB2	1.94	0.50
1:Q:1353:ASP:N	1:Q:1353:ASP:OD2	2.37	0.50
5:U:47:GLN:NE2	5:U:357:LYS:O	2.44	0.50
5:U:162:THR:HG23	5:U:229:LEU:HD13	1.94	0.50
4:X:49:VAL:O	7:X:1001:ADP:N6	2.45	0.50
4:T:42:LYS:O	4:T:55:ARG:NH2	2.41	0.50
1:Q:1303:LYS:HA	1:Q:1306:GLU:HG2	1.92	0.50
2:R:623:GLU:OE2	2:R:683:ARG:NH1	2.44	0.50
4:V:216:ASP:N	4:V:216:ASP:OD1	2.43	0.50
1:Q:765:SER:HB3	1:Q:1381:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1308:LEU:HD21	1:Q:1340:TYR:CD2	2.46	0.50
2:R:256:ASN:HB3	2:R:259:GLU:HG3	1.93	0.50
4:V:140:TYR:HB2	4:V:202:ILE:HB	1.92	0.50
1:Q:819:SER:OG	1:Q:820:TYR:N	2.42	0.50
5:W:134:GLU:OE1	5:W:230:GLN:NE2	2.44	0.50
5:Y:398:TYR:OH	5:Y:435:ARG:NH2	2.44	0.50
1:Q:757:PRO:HD2	1:Q:836:GLN:HE22	1.76	0.50
1:Q:1386:ALA:O	1:Q:1413:GLN:NE2	2.44	0.50
3:S:47:ARG:H	3:S:47:ARG:HE	1.59	0.50
4:V:49:VAL:O	7:V:1001:ADP:N6	2.45	0.50
5:Y:343:LEU:HB3	5:Y:347:LEU:HD23	1.94	0.50
1:Q:1185:GLY:O	1:Q:1189:SER:OG	2.28	0.49
5:U:263:GLY:HA3	4:V:274:LYS:HD3	1.93	0.49
3:S:46:SER:HB2	3:S:49:LYS:HG2	1.93	0.49
3:S:154:GLU:HA	3:S:157:LYS:HB2	1.94	0.49
4:V:26:ALA:O	7:V:1001:ADP:O3'	2.29	0.49
1:Q:726:ASN:ND2	1:Q:887:ILE:O	2.42	0.49
1:Q:1210:TYR:HB3	5:W:248:ASN:HB3	1.94	0.49
2:R:213:ASN:OD1	2:R:635:GLN:NE2	2.40	0.49
4:V:83:THR:O	4:V:375:TYR:OH	2.30	0.49
6:Z:313:GLU:OE2	6:Z:313:GLU:N	2.42	0.49
1:Q:901:TRP:HE3	1:Q:923:ARG:HH12	1.61	0.49
4:T:23:ARG:NH2	5:Y:316:GLU:O	2.45	0.49
4:T:317:ASP:OD2	4:T:318:ILE:N	2.46	0.49
5:U:81:LYS:NZ	7:U:1001:ADP:O3B	2.43	0.49
5:W:88:VAL:HG11	5:W:322:MET:HE1	1.95	0.49
1:Q:1079:ASN:ND2	1:Q:1217:PRO:O	2.45	0.49
1:Q:953:LEU:HD11	1:Q:1425:ARG:HB2	1.95	0.48
1:Q:1009:LYS:HB2	1:Q:1016:LEU:HD12	1.94	0.48
2:R:17:ASP:HA	2:R:280:PRO:HG3	1.95	0.48
2:R:751:LYS:H	2:R:751:LYS:HD3	1.78	0.48
2:R:742:ILE:HD12	2:R:751:LYS:HA	1.94	0.48
1:Q:1384:THR:O	1:Q:1413:GLN:NE2	2.46	0.48
4:V:313:VAL:HG12	4:V:340:SER:HB2	1.94	0.48
4:X:332:ILE:O	4:X:332:ILE:CG2	2.61	0.48
1:Q:839:ILE:HG12	1:Q:866:LEU:HD23	1.95	0.48
5:W:243:GLU:HA	5:W:257:LEU:HD21	1.96	0.48
4:T:431:ARG:NH2	4:T:438:ASP:OD2	2.46	0.48
5:U:245:ASP:OD2	5:U:270:ARG:NH1	2.46	0.48
4:V:61:ILE:HG13	4:V:75:ILE:HG12	1.96	0.48
5:U:331:LYS:HA	5:U:338:LYS:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:67:ALA:HB3	4:X:25:ALA:HB2	1.95	0.47
4:X:202:ILE:HG12	4:X:209:VAL:HG22	1.95	0.47
4:X:406:MET:HG3	4:X:443:LYS:HD2	1.95	0.47
4:T:41:ALA:HB3	4:T:52:ILE:HG23	1.97	0.47
5:U:136:ILE:HG12	5:U:230:GLN:HG2	1.96	0.47
5:W:40:THR:HG23	5:W:45:VAL:HG22	1.95	0.47
5:U:327:ARG:NH1	4:V:462:TYR:OH	2.47	0.47
5:Y:397:ARG:NH1	7:Y:1001:ADP:O1B	2.47	0.47
1:Q:875:ASN:HA	1:Q:880:LEU:HD11	1.97	0.47
4:T:225:GLU:HG3	4:T:227:GLU:H	1.80	0.47
1:Q:1247:SER:OG	1:Q:1248:ASP:N	2.47	0.47
1:Q:1308:LEU:CD2	1:Q:1340:TYR:CE2	2.96	0.47
3:S:36:VAL:O	3:S:40:ASN:ND2	2.44	0.47
5:U:23:HIS:HB3	5:U:26:ILE:HD12	1.97	0.47
1:Q:777:PHE:HB3	1:Q:778:LEU:HD22	1.97	0.47
1:Q:1180:ASN:HD21	4:V:208:ALA:HB2	1.80	0.47
1:Q:1249:ILE:HG13	1:Q:1271:THR:HG21	1.95	0.47
4:X:418:LEU:HD22	4:X:442:ALA:HB1	1.96	0.47
4:V:147:LEU:HD11	4:V:189:ILE:HD13	1.97	0.47
4:X:22:THR:OG1	4:X:392:ARG:NH2	2.48	0.47
5:U:434:ALA:HA	5:U:437:VAL:HG12	1.96	0.46
4:X:120:THR:O	4:X:124:ASN:ND2	2.47	0.46
5:Y:134:GLU:OE2	5:Y:232:ARG:NE	2.39	0.46
3:S:162:ASN:OD1	3:S:162:ASN:N	2.43	0.46
5:Y:72:LEU:HD23	5:Y:353:ILE:HG12	1.97	0.46
1:Q:1424:VAL:HG13	1:Q:1427:THR:OG1	2.16	0.46
2:R:147:ARG:NH2	2:R:752:TYR:OH	2.48	0.46
5:U:352:ILE:HG13	5:U:352:ILE:O	2.15	0.46
1:Q:1316:HIS:CD2	1:Q:1317:ARG:H	2.32	0.46
1:Q:733:MET:HG3	1:Q:1410:ARG:HH12	1.80	0.46
1:Q:1169:THR:O	1:Q:1173:GLU:HG3	2.16	0.46
1:Q:1172:GLN:O	1:Q:1176:GLU:HG2	2.15	0.46
4:T:126:ARG:NE	4:T:253:ASP:OD2	2.41	0.46
1:Q:1008:ARG:O	1:Q:1012:ASN:ND2	2.48	0.46
4:T:211:ARG:NH2	4:T:227:GLU:OE1	2.47	0.46
1:Q:737:LYS:HA	1:Q:740:GLN:HG2	1.98	0.46
4:T:131:LEU:HD22	4:T:301:ALA:HB1	1.98	0.46
4:X:461:ASN:OD1	4:X:461:ASN:O	2.34	0.46
2:R:599:ARG:HA	2:R:599:ARG:HD3	1.81	0.46
4:T:196:ILE:O	4:T:214:ARG:NH1	2.48	0.46
5:Y:259:THR:OG1	5:Y:261:ASP:OD1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:375:TYR:OH	7:T:1001:ADP:N7	2.40	0.46
1:Q:1168:LYS:HG3	1:Q:1173:GLU:HG2	1.98	0.45
4:T:138:GLU:HB3	4:T:204:ALA:HB3	1.98	0.45
4:T:342:ARG:HB3	4:T:345:THR:HG21	1.98	0.45
4:V:318:ILE:HG23	5:W:300:MET:HE1	1.98	0.45
4:X:361:PRO:HA	4:X:364:ILE:HB	1.98	0.45
4:T:432:LYS:HD3	4:T:432:LYS:HA	1.73	0.45
5:U:59:LYS:HB3	4:V:424:ILE:HD13	1.99	0.45
4:X:121:LEU:HD23	4:X:323:TYR:HD2	1.80	0.45
1:Q:1176:GLU:HA	1:Q:1179:ARG:HD3	1.97	0.45
5:U:413:ARG:NH1	5:U:422:ASP:OD2	2.50	0.45
2:R:68:THR:HG22	2:R:96:SER:HA	1.97	0.45
3:S:118:VAL:HG12	3:S:119:THR:HG23	1.98	0.45
4:X:51:GLN:NE2	4:X:373:LEU:O	2.49	0.45
1:Q:1308:LEU:HD11	1:Q:1368:PHE:CE2	2.51	0.45
2:R:17:ASP:N	2:R:17:ASP:OD1	2.48	0.45
5:U:359:TYR:OH	7:U:1001:ADP:N7	2.50	0.45
4:V:453:THR:HA	4:V:456:LEU:HD12	1.99	0.45
4:X:83:THR:N	7:X:1001:ADP:O1B	2.49	0.45
1:Q:816:MET:SD	1:Q:816:MET:N	2.90	0.45
1:Q:1101:ASP:OD1	1:Q:1101:ASP:N	2.48	0.45
1:Q:1357:LEU:CD1	1:Q:1370:PHE:CZ	2.97	0.45
2:R:101:ASP:OD1	2:R:101:ASP:N	2.45	0.45
2:R:243:TYR:HA	2:R:246:MET:HE3	1.99	0.45
4:T:49:VAL:O	7:T:1001:ADP:N6	2.49	0.45
5:U:76:PRO:O	5:U:79:THR:OG1	2.34	0.45
5:Y:331:LYS:HE2	5:Y:331:LYS:HB3	1.82	0.45
1:Q:768:HIS:HA	1:Q:771:VAL:HG22	1.99	0.45
1:Q:729:LEU:HD12	1:Q:933:LEU:HD21	1.98	0.45
3:S:140:TYR:HA	3:S:144:VAL:HB	1.98	0.45
5:U:360:ASN:OD1	5:U:360:ASN:N	2.50	0.45
5:W:114:THR:O	5:W:118:THR:OG1	2.31	0.45
1:Q:848:SER:HB3	1:Q:851:SER:HB2	1.99	0.44
5:U:161:LYS:HB2	5:U:166:GLU:HB2	1.98	0.44
4:X:42:LYS:O	4:X:55:ARG:NH2	2.47	0.44
2:R:258:ASP:OD2	3:S:113:LYS:NZ	2.50	0.44
5:U:40:THR:HG22	5:U:45:VAL:HG22	1.97	0.44
1:Q:1214:VAL:HG11	4:X:252:LEU:HD23	1.99	0.44
1:Q:1291:MET:HA	1:Q:1294:PHE:HB3	2.00	0.44
1:Q:1331:MET:HE3	1:Q:1331:MET:HB3	1.83	0.44
5:U:298:VAL:HG13	5:U:343:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:309:LEU:HB2	6:Z:316:LEU:HB2	2.00	0.44
3:S:35:SER:O	3:S:39:ARG:HB3	2.18	0.44
4:T:82:SER:O	4:T:82:SER:OG	2.30	0.44
4:T:347:VAL:O	4:T:350:THR:OG1	2.36	0.44
4:T:359:VAL:HG12	4:T:364:ILE:HG13	1.99	0.44
4:V:227:GLU:H	4:V:227:GLU:HG3	1.64	0.44
4:V:264:ASP:OD1	4:V:264:ASP:N	2.50	0.44
1:Q:1296:THR:HG22	1:Q:1302:ARG:HH11	1.82	0.44
4:X:432:LYS:HB2	4:X:432:LYS:HE2	1.72	0.44
1:Q:1317:ARG:O	1:Q:1388:THR:OG1	2.35	0.44
4:T:130:GLY:HA2	4:T:248:THR:HA	2.00	0.44
4:V:177:LYS:HB3	4:V:237:VAL:HG11	1.99	0.44
4:T:121:LEU:HD23	4:T:323:TYR:HD2	1.83	0.44
4:V:85:LYS:NZ	7:V:1001:ADP:O2B	2.44	0.44
1:Q:1209:GLY:HA2	5:W:276:LYS:HE2	1.98	0.43
1:Q:1316:HIS:HD2	1:Q:1317:ARG:H	1.66	0.43
5:U:398:TYR:OH	5:U:435:ARG:NH2	2.50	0.43
4:V:68:LYS:HE3	4:V:68:LYS:HB2	1.78	0.43
3:S:69:ASP:HA	3:S:72:LYS:HG2	1.99	0.43
4:X:289:ASN:ND2	4:X:332:ILE:HD12	2.33	0.43
5:Y:76:PRO:O	5:Y:79:THR:OG1	2.35	0.43
1:Q:960:GLN:HG3	1:Q:1014:PRO:HG3	2.01	0.43
4:T:133:ILE:HB	4:T:245:GLN:HB2	2.00	0.43
4:T:413:ARG:NH2	7:T:1001:ADP:O3A	2.51	0.43
5:U:250:ARG:NH2	5:U:261:ASP:O	2.51	0.43
5:W:395:SER:OG	5:W:396:LEU:N	2.51	0.43
1:Q:1169:THR:HB	1:Q:1172:GLN:OE1	2.18	0.43
5:U:191:SER:OG	5:U:200:THR:CG2	2.67	0.43
5:U:255:LEU:O	5:U:259:THR:OG1	2.31	0.43
5:W:361:GLU:HG3	5:W:392:VAL:HG21	1.99	0.43
5:Y:298:VAL:HG13	5:Y:343:LEU:HD21	2.01	0.43
1:Q:791:ASN:OD1	1:Q:791:ASN:N	2.50	0.43
2:R:184:GLY:HA2	2:R:664:MET:HA	1.99	0.43
4:V:42:LYS:O	4:V:55:ARG:NH2	2.49	0.43
4:V:56:GLU:OE1	5:W:425:ARG:NH2	2.43	0.43
4:T:25:ALA:HB2	5:Y:67:ALA:HB3	1.98	0.43
1:Q:1008:ARG:HH22	1:Q:1323:GLN:HG3	1.84	0.43
4:V:287:GLU:HA	4:V:290:LYS:HG2	2.01	0.43
5:W:44:MET:HE2	5:W:44:MET:HB3	1.90	0.43
4:X:362:ASP:O	4:X:366:ARG:NH1	2.50	0.43
1:Q:1275:PRO:HG2	4:X:272:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:245:ASP:O	5:U:249:SER:HB3	2.18	0.43
4:V:200:ILE:HA	4:V:211:ARG:HA	2.01	0.43
1:Q:854:TRP:HD1	1:Q:857:LEU:HD11	1.84	0.43
2:R:19:PRO:HG2	2:R:241:LEU:HB3	2.00	0.43
4:T:462:TYR:HB3	5:Y:326:ASN:O	2.19	0.43
5:U:343:LEU:HB3	5:U:347:LEU:HD23	2.00	0.43
1:Q:803:LYS:HA	1:Q:803:LYS:HD3	1.85	0.42
1:Q:1345:LEU:HD21	1:Q:1354:ARG:HG2	2.01	0.42
3:S:130:ASN:OD1	3:S:130:ASN:N	2.48	0.42
1:Q:822:MET:HE3	1:Q:822:MET:H	1.83	0.42
2:R:182:LYS:O	2:R:202:GLY:N	2.52	0.42
5:U:132:GLU:OE1	5:U:234:THR:OG1	2.31	0.42
5:U:367:ILE:HG21	5:U:396:LEU:HD21	2.01	0.42
5:W:298:VAL:HG13	5:W:343:LEU:HD21	2.00	0.42
1:Q:1224:LEU:HD23	1:Q:1224:LEU:HA	1.91	0.42
4:V:448:ASP:OD1	4:V:451:ARG:NE	2.52	0.42
1:Q:1407:ARG:HA	1:Q:1410:ARG:HH21	1.85	0.42
5:U:352:ILE:HD12	4:V:446:PHE:CE1	2.54	0.42
4:X:318:ILE:O	4:X:322:THR:OG1	2.35	0.42
1:Q:1179:ARG:HH22	4:V:260:GLN:HB3	1.83	0.42
4:T:117:LYS:H	4:T:117:LYS:HG2	1.58	0.42
5:U:94:LYS:HB2	5:U:94:LYS:HE3	1.86	0.42
5:U:188:ASP:HA	5:U:204:ARG:HA	2.00	0.42
5:Y:398:TYR:OH	5:Y:430:PHE:O	2.35	0.42
1:Q:874:GLN:HG3	1:Q:1399:THR:HG21	2.01	0.42
5:Y:157:LYS:HD2	5:Y:168:ILE:HD11	2.01	0.42
1:Q:1253:THR:O	1:Q:1257:MET:HG3	2.19	0.42
1:Q:1433:ARG:HA	1:Q:1433:ARG:HD2	1.83	0.42
4:T:199:VAL:N	4:T:213:GLY:O	2.51	0.42
5:Y:152:GLY:O	5:Y:173:ASN:ND2	2.52	0.42
1:Q:767:LEU:HB3	1:Q:787:TRP:HZ3	1.85	0.42
1:Q:1124:LEU:HD11	5:U:258:PHE:HZ	1.85	0.42
4:T:83:THR:N	7:T:1001:ADP:O1B	2.52	0.42
5:U:266:ARG:HH22	4:V:277:LYS:HG3	1.84	0.42
4:T:326:LYS:HD3	5:U:102:ALA:HB2	2.02	0.42
4:V:347:VAL:HG11	4:V:360:PRO:HG3	2.01	0.42
1:Q:1208:ARG:NH1	1:Q:1210:TYR:O	2.42	0.41
1:Q:1425:ARG:HG2	1:Q:1426:GLY:N	2.35	0.41
2:R:160:VAL:O	2:R:731:LYS:NZ	2.52	0.41
5:W:29:LEU:HB3	5:W:31:LEU:HD13	2.01	0.41
5:W:368:LEU:HD13	5:W:387:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:438:LYS:HB3	5:W:438:LYS:HE3	1.88	0.41
2:R:709:ASP:OD1	2:R:709:ASP:N	2.52	0.41
3:S:157:LYS:HE2	3:S:157:LYS:HB3	1.89	0.41
5:U:20:ILE:HD13	5:U:375:GLU:HA	2.01	0.41
4:X:418:LEU:HD23	4:X:418:LEU:HA	1.92	0.41
1:Q:1131:LEU:HA	1:Q:1131:LEU:HD12	1.87	0.41
2:R:74:LYS:HB3	2:R:74:LYS:HE2	1.81	0.41
5:U:133:THR:OG1	5:U:233:LYS:O	2.32	0.41
5:U:188:ASP:OD2	5:U:201:LYS:NZ	2.47	0.41
5:W:402:LEU:HD22	5:W:426:ALA:HB1	2.03	0.41
1:Q:1407:ARG:HA	1:Q:1410:ARG:NH2	2.35	0.41
4:T:22:THR:H	4:T:392:ARG:HH22	1.67	0.41
5:U:382:ASP:CG	5:U:420:VAL:CG2	2.94	0.41
4:X:429:SER:O	4:X:429:SER:OG	2.34	0.41
1:Q:791:ASN:HA	1:Q:794:LYS:HG2	2.02	0.41
2:R:115:LEU:HA	2:R:118:THR:HG22	2.02	0.41
5:W:308:PHE:HA	4:X:106:VAL:HG11	2.01	0.41
5:W:455:GLN:OE1	5:W:457:SER:OG	2.38	0.41
5:Y:330:SER:OG	5:Y:331:LYS:N	2.52	0.41
1:Q:1203:LEU:HD23	1:Q:1203:LEU:HA	1.89	0.41
1:Q:1291:MET:HG2	1:Q:1337:TYR:HD2	1.84	0.41
1:Q:1387:ASP:OD1	1:Q:1387:ASP:N	2.53	0.41
4:X:211:ARG:NH1	4:X:227:GLU:OE1	2.54	0.41
4:X:414:TYR:OH	4:X:446:PHE:O	2.38	0.41
6:Z:307:ARG:HB3	6:Z:318:CYS:HB2	2.02	0.41
1:Q:782:LYS:H	1:Q:814:HIS:HB2	1.85	0.41
1:Q:1291:MET:HE2	1:Q:1291:MET:HB2	1.86	0.41
4:V:386:ARG:HA	4:V:386:ARG:HD2	1.90	0.41
5:W:70:ALA:HB1	5:W:323:MET:HE2	2.03	0.41
4:X:116:LYS:NZ	5:Y:105:GLU:O	2.54	0.41
4:X:192:GLU:OE2	4:X:192:GLU:N	2.54	0.41
4:X:410:THR:OG1	4:X:411:SER:N	2.54	0.41
4:V:313:VAL:HG21	4:V:338:LEU:HD13	2.03	0.40
5:Y:187:GLY:O	5:Y:205:SER:OG	2.38	0.40
1:Q:774:ILE:HD13	1:Q:774:ILE:HA	1.88	0.40
1:Q:871:THR:O	1:Q:871:THR:OG1	2.38	0.40
5:U:316:GLU:O	4:V:23:ARG:NH1	2.54	0.40
4:X:453:THR:O	4:X:457:GLU:HG2	2.21	0.40
3:S:61:LYS:HD2	3:S:61:LYS:HA	1.92	0.40
4:T:80:GLY:O	4:T:85:LYS:NZ	2.54	0.40
1:Q:1416:GLN:NE2	1:Q:1417:VAL:O	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:42:ILE:HG23	2:R:49:LEU:HD11	2.03	0.40
2:R:54:VAL:HG13	2:R:715:ALA:HA	2.03	0.40
4:T:134:LYS:HE3	4:T:134:LYS:HB3	1.87	0.40
5:U:32:ASP:OD1	5:U:38:ARG:NE	2.54	0.40
4:X:147:LEU:HD12	4:X:147:LEU:HA	1.97	0.40
4:X:402:LEU:O	4:X:406:MET:HB2	2.21	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	652/1489 (44%)	617 (95%)	35 (5%)	0	100	100
2	R	438/755 (58%)	430 (98%)	8 (2%)	0	100	100
3	S	120/166 (72%)	115 (96%)	5 (4%)	0	100	100
4	T	431/463 (93%)	422 (98%)	9 (2%)	0	100	100
4	V	439/463 (95%)	422 (96%)	17 (4%)	0	100	100
4	X	441/463 (95%)	431 (98%)	10 (2%)	0	100	100
5	U	443/460 (96%)	425 (96%)	18 (4%)	0	100	100
5	W	440/460 (96%)	424 (96%)	16 (4%)	0	100	100
5	Y	432/460 (94%)	416 (96%)	16 (4%)	0	100	100
6	Z	26/320 (8%)	26 (100%)	0	0	100	100
All	All	3862/5499 (70%)	3728 (96%)	134 (4%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	578/1350 (43%)	577 (100%)	1 (0%)	92	98
2	R	391/682 (57%)	390 (100%)	1 (0%)	91	97
3	S	108/142 (76%)	108 (100%)	0	100	100
4	T	366/391 (94%)	366 (100%)	0	100	100
4	V	371/391 (95%)	371 (100%)	0	100	100
4	X	375/391 (96%)	375 (100%)	0	100	100
5	U	378/394 (96%)	376 (100%)	2 (0%)	86	96
5	W	375/394 (95%)	375 (100%)	0	100	100
5	Y	371/394 (94%)	371 (100%)	0	100	100
6	Z	27/285 (10%)	27 (100%)	0	100	100
All	All	3340/4814 (69%)	3336 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	1072	ASP
2	R	615	ASN
5	U	23	HIS
5	U	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	844	GLN
1	Q	856	ASN
1	Q	970	GLN
1	Q	1359	HIS
1	Q	1413	GLN
1	Q	1443	GLN
2	R	31	GLN

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Mol	Chain	Res	Type
2	R	55	ASN
2	R	56	HIS
2	R	132	ASN
2	R	152	GLN
2	R	175	ASN
2	R	195	ASN
2	R	627	GLN
2	R	659	GLN
2	R	666	ASN
3	S	82	ASN
4	T	165	HIS
4	T	205	ASN
4	T	245	GLN
4	T	417	GLN
5	U	23	HIS
5	U	173	ASN
5	U	223	GLN
5	U	443	ASN
4	V	124	ASN
4	V	154	ASN
4	V	263	GLN
4	V	286	GLN
5	W	49	GLN
5	W	223	GLN
5	W	242	HIS
5	W	362	GLN
5	W	407	GLN
5	W	408	GLN
4	X	250	HIS
5	Y	453	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	ADP	T	1001	-	24,29,29	0.89	0	29,45,45	1.29	2 (6%)
7	ADP	V	1001	-	24,29,29	0.87	0	29,45,45	1.19	2 (6%)
7	ADP	W	1001	-	24,29,29	0.93	1 (4%)	29,45,45	1.24	3 (10%)
7	ADP	Y	1001	-	24,29,29	0.89	0	29,45,45	1.21	2 (6%)
7	ADP	U	1001	-	24,29,29	0.85	0	29,45,45	1.23	2 (6%)
7	ADP	X	1001	-	24,29,29	0.88	0	29,45,45	1.26	2 (6%)

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	T	1001	-	-	2/12/32/32	0/3/3/3
7	ADP	V	1001	-	-	3/12/32/32	0/3/3/3
7	ADP	W	1001	-	-	2/12/32/32	0/3/3/3
7	ADP	Y	1001	-	-	2/12/32/32	0/3/3/3
7	ADP	U	1001	-	-	3/12/32/32	0/3/3/3
7	ADP	X	1001	-	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	1001	ADP	PA-O3A	2.18	1.61	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	1001	ADP	N3-C2-N1	-3.67	123.69	128.67
7	V	1001	ADP	N3-C2-N1	-3.64	123.73	128.67
7	U	1001	ADP	N3-C2-N1	-3.62	123.75	128.67
7	X	1001	ADP	N3-C2-N1	-3.51	123.91	128.67
7	Y	1001	ADP	N3-C2-N1	-3.49	123.94	128.67
7	W	1001	ADP	N3-C2-N1	-3.36	124.11	128.67
7	V	1001	ADP	C4-C5-N7	-2.51	106.68	109.34
7	U	1001	ADP	C4-C5-N7	-2.49	106.71	109.34
7	Y	1001	ADP	C4-C5-N7	-2.48	106.72	109.34
7	X	1001	ADP	C4-C5-N7	-2.42	106.78	109.34
7	T	1001	ADP	C4-C5-N7	-2.33	106.88	109.34
7	W	1001	ADP	C4-C5-N7	-2.27	106.94	109.34
7	W	1001	ADP	C4'-O4'-C1'	2.19	111.93	109.92

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	U	1001	ADP	C5'-O5'-PA-O1A
7	U	1001	ADP	C5'-O5'-PA-O2A
7	U	1001	ADP	C5'-O5'-PA-O3A
7	V	1001	ADP	C5'-O5'-PA-O1A
7	V	1001	ADP	C5'-O5'-PA-O2A
7	V	1001	ADP	C5'-O5'-PA-O3A
7	W	1001	ADP	O4'-C4'-C5'-O5'
7	W	1001	ADP	C3'-C4'-C5'-O5'
7	T	1001	ADP	PB-O3A-PA-O1A
7	Y	1001	ADP	PB-O3A-PA-O1A
7	T	1001	ADP	PB-O3A-PA-O2A
7	X	1001	ADP	PB-O3A-PA-O2A
7	Y	1001	ADP	PB-O3A-PA-O2A

There are no ring outliers.

6 monomers are involved in 18 short contacts:

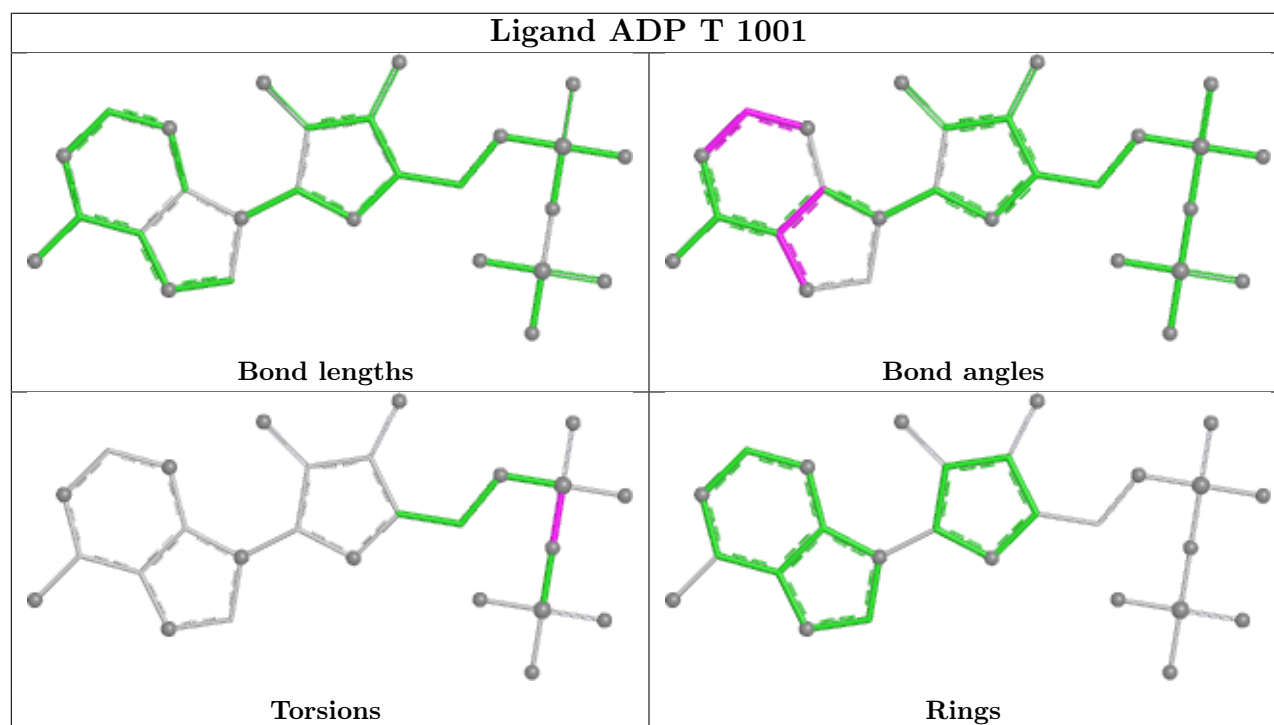
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	1001	ADP	4	0
7	V	1001	ADP	5	0
7	W	1001	ADP	1	0
7	Y	1001	ADP	2	0

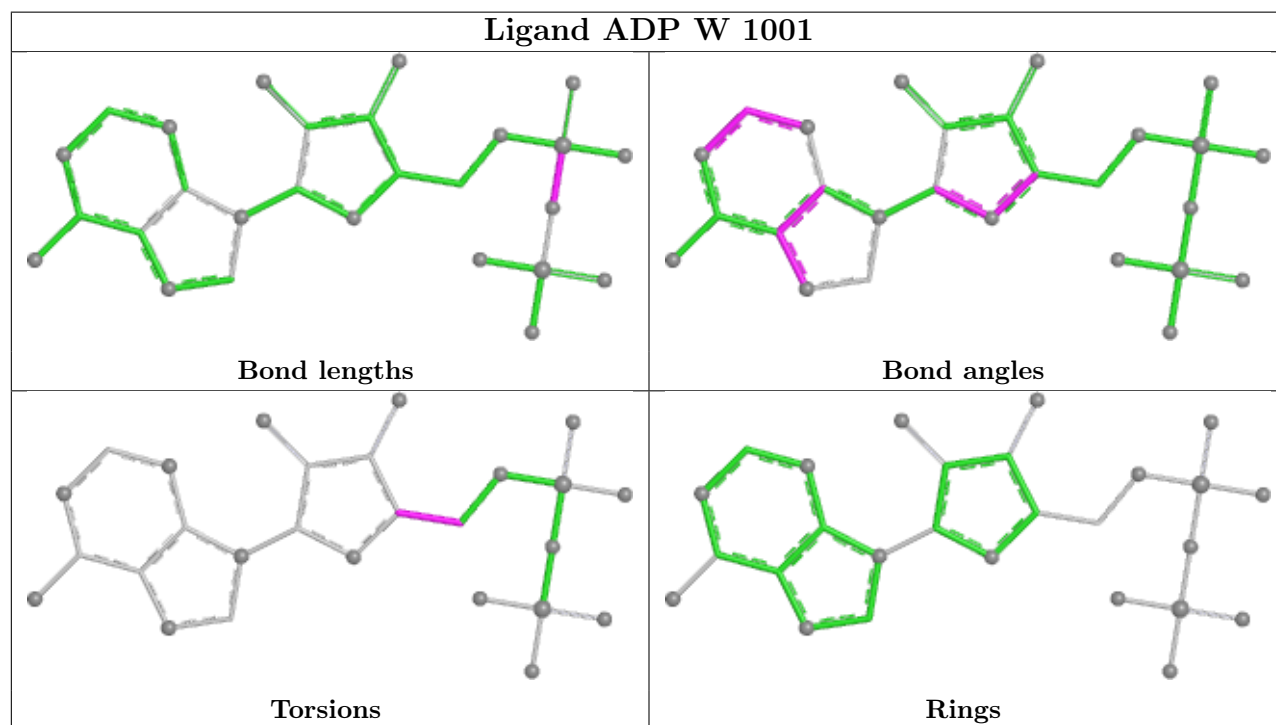
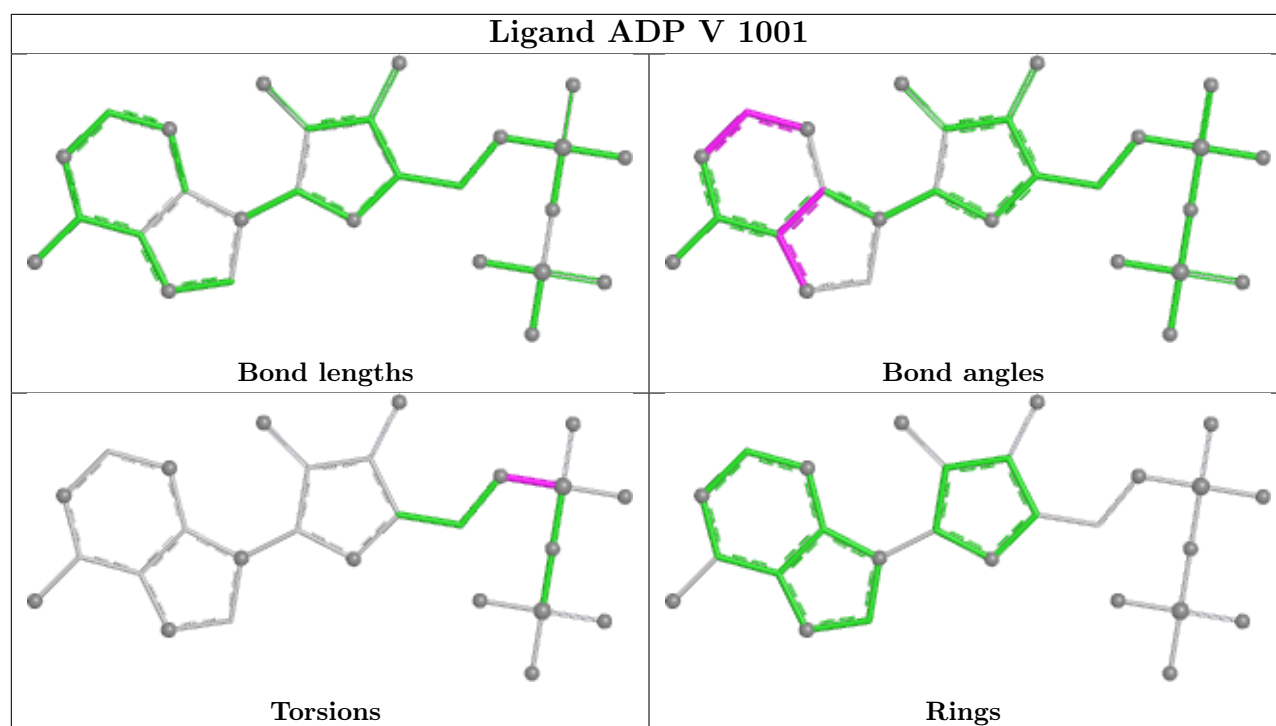
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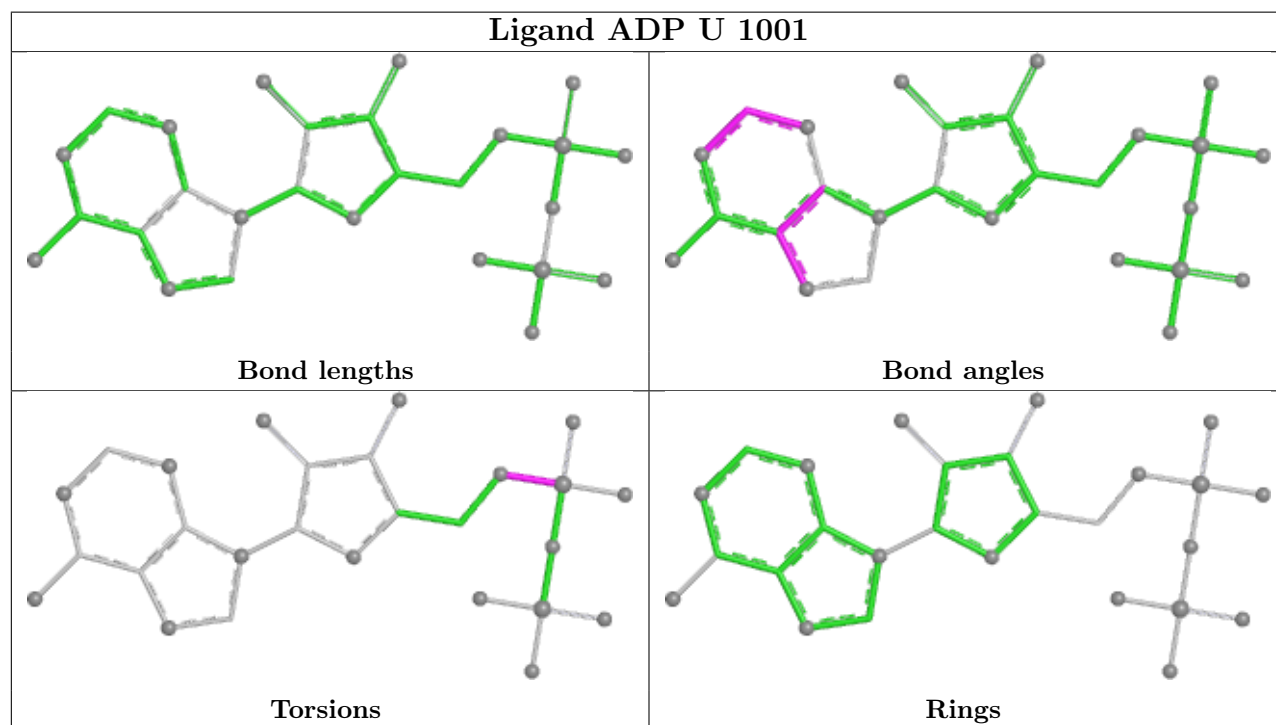
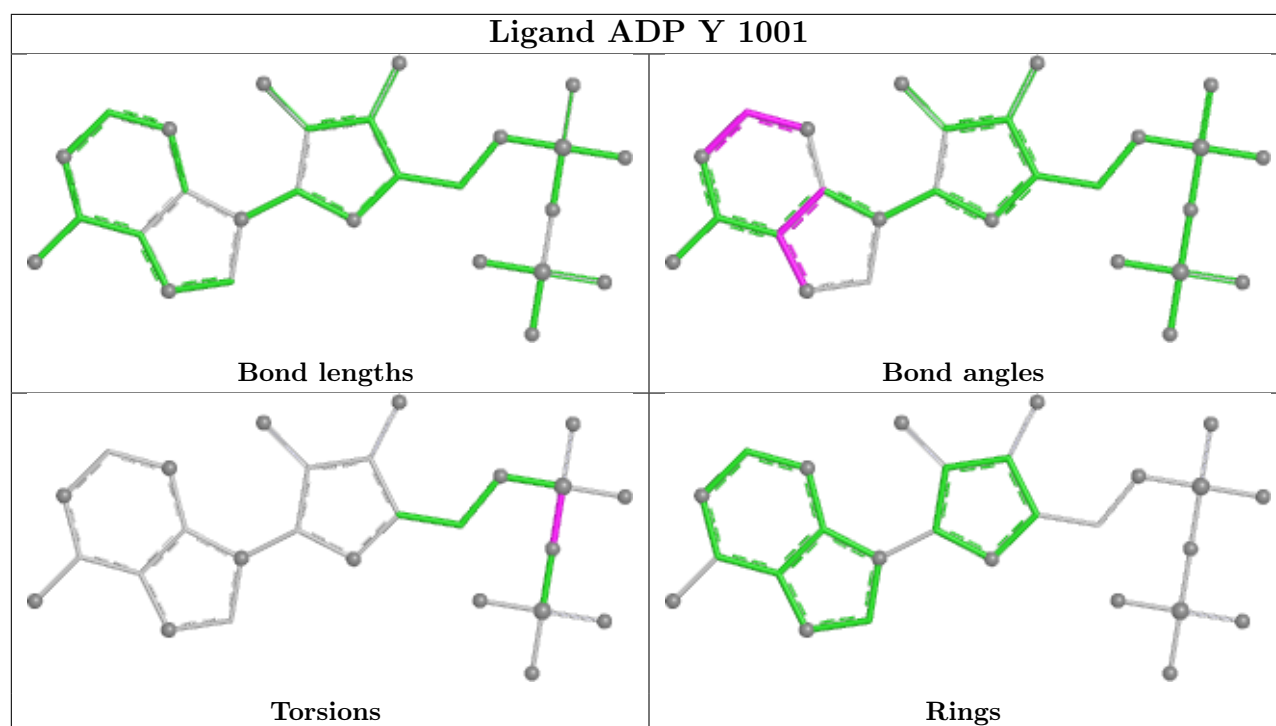
*Continued from previous page...*

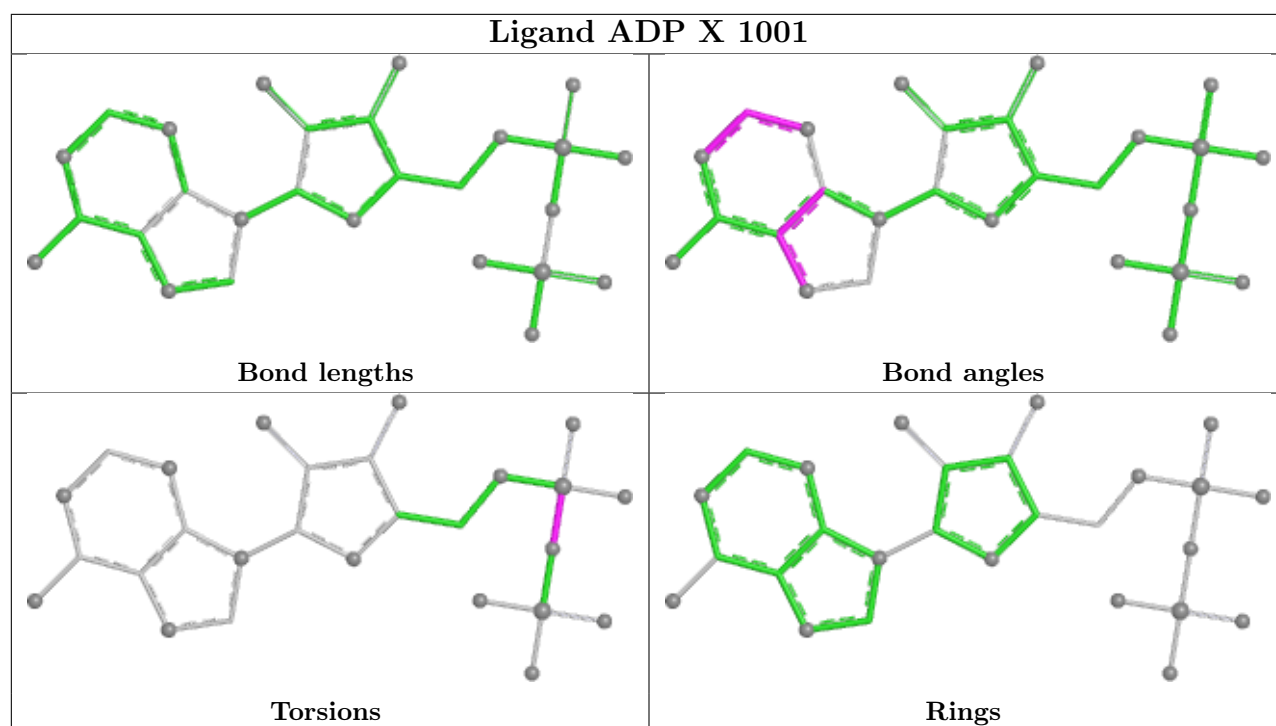
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	1001	ADP	3	0
7	X	1001	ADP	3	0

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

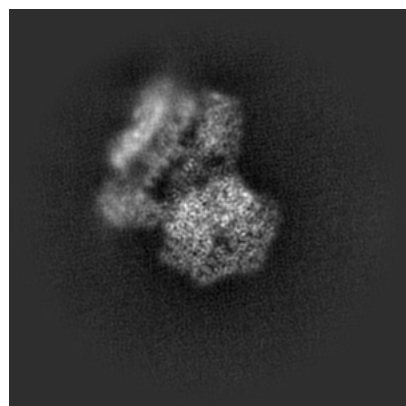
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45403. These allow visual inspection of the internal detail of the map and identification of artifacts.

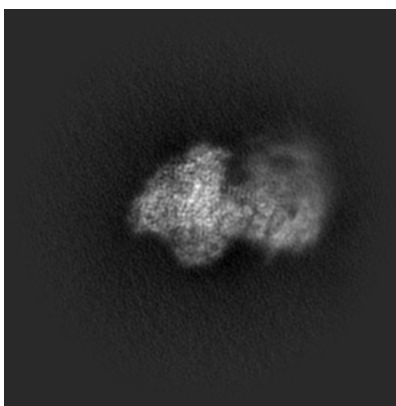
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

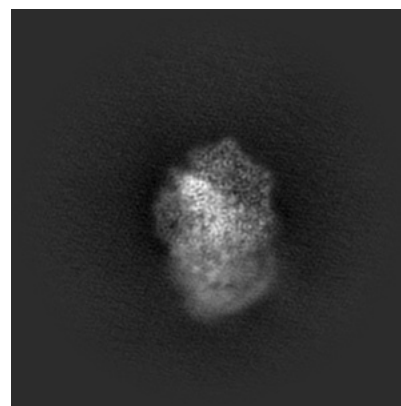
#### 6.1.1 Primary map



X

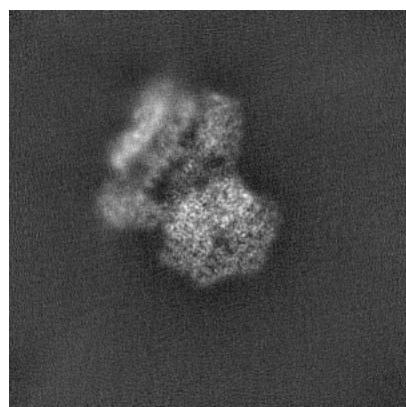


Y

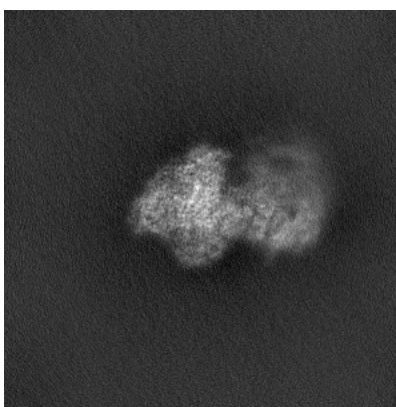


Z

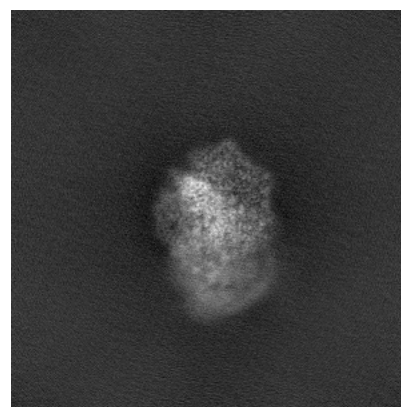
#### 6.1.2 Raw map



X



Y



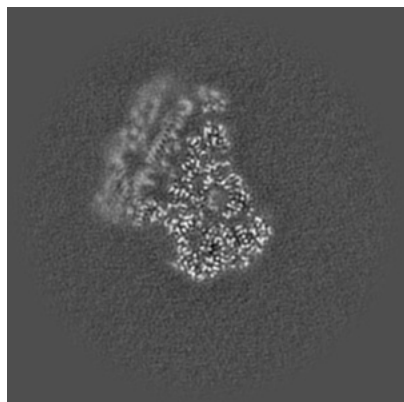
Z

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

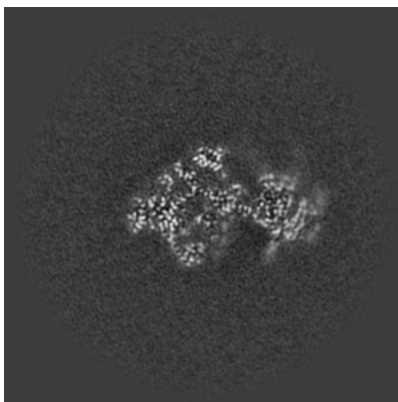


## 6.2 Central slices [i](#)

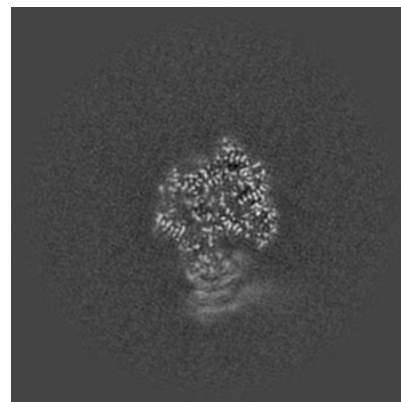
### 6.2.1 Primary map



X Index: 224

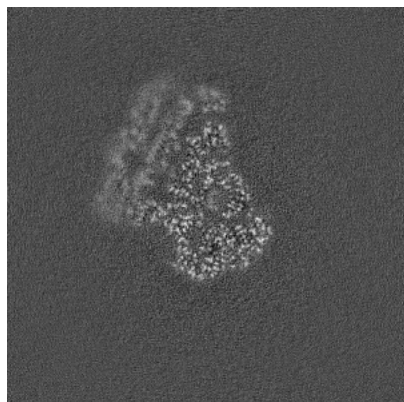


Y Index: 224

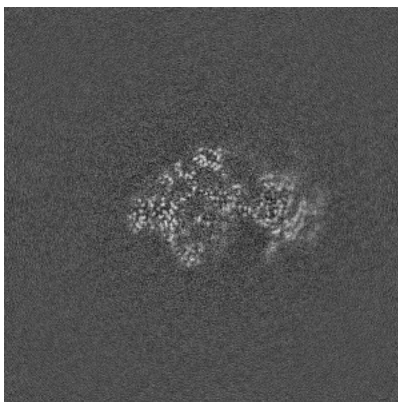


Z Index: 224

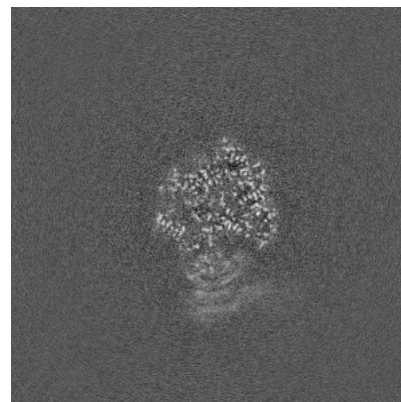
### 6.2.2 Raw map



X Index: 224



Y Index: 224

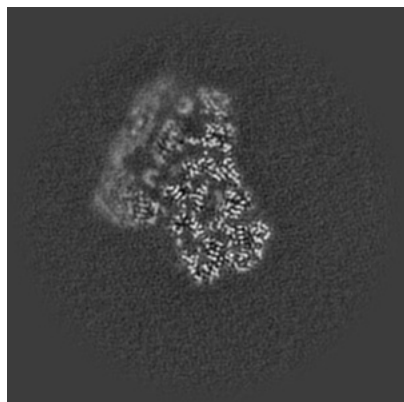


Z Index: 224

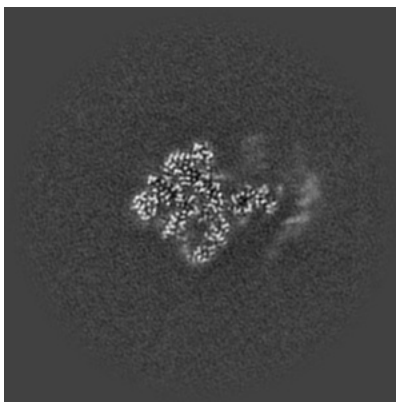
The images above show central slices of the map in three orthogonal directions.

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

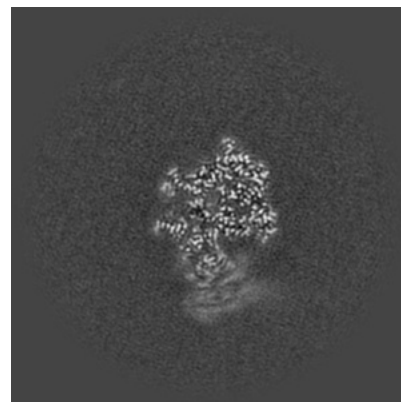
### 6.3.1 Primary map



X Index: 218

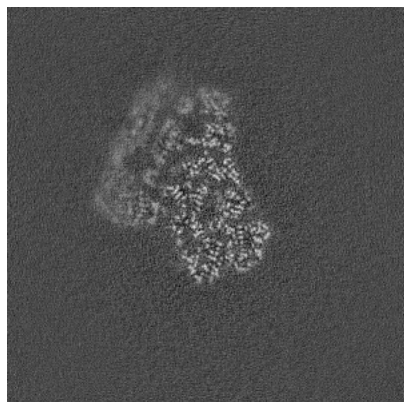


Y Index: 208

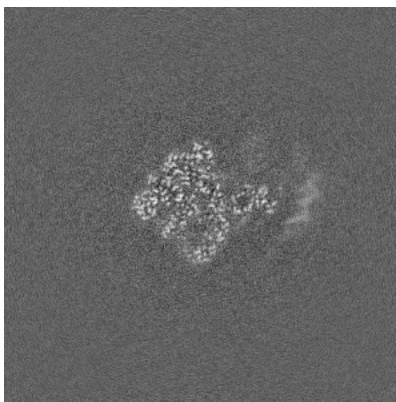


Z Index: 227

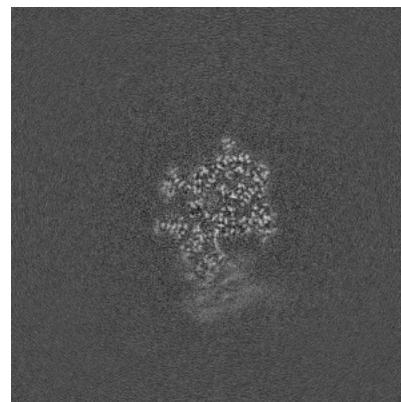
### 6.3.2 Raw map



X Index: 218



Y Index: 207

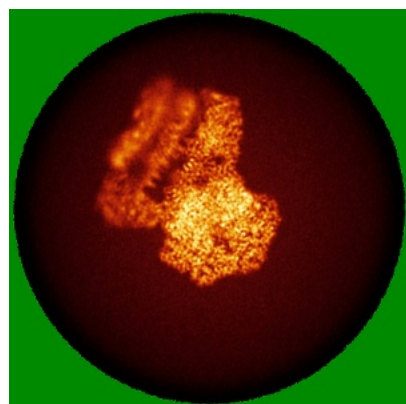


Z Index: 228

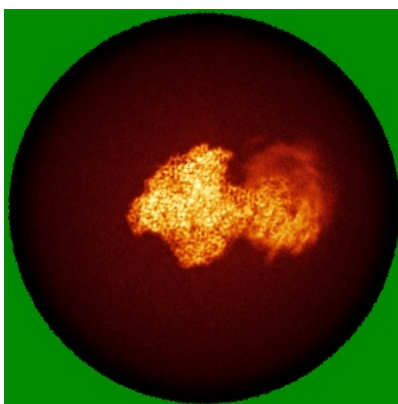
The images above show the largest variance slices of the map in three orthogonal directions.

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

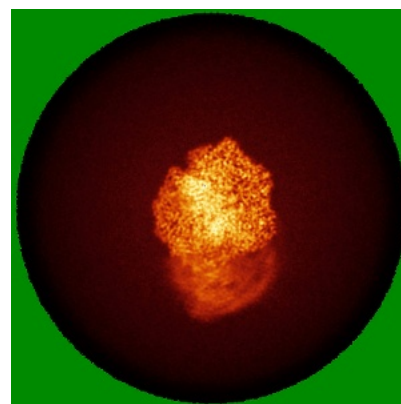
### 6.4.1 Primary map



X

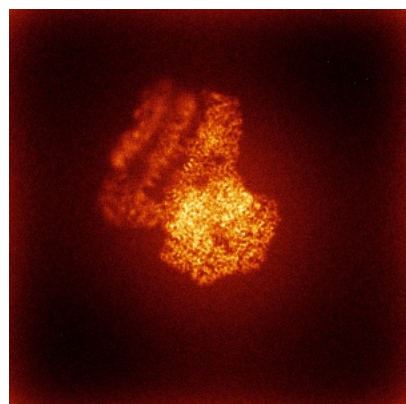


Y

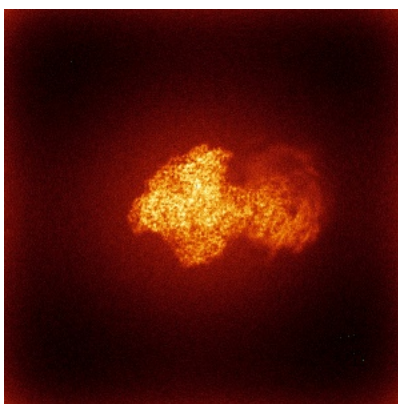


Z

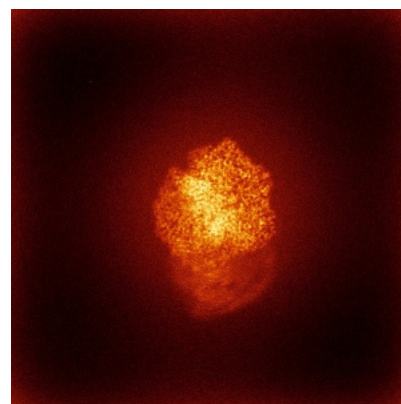
### 6.4.2 Raw map



X



Y

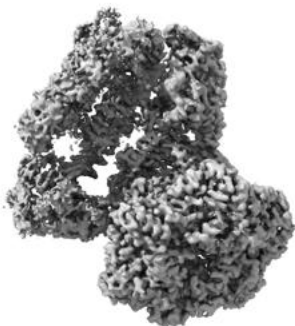


Z

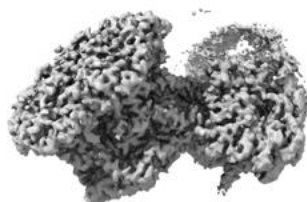
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



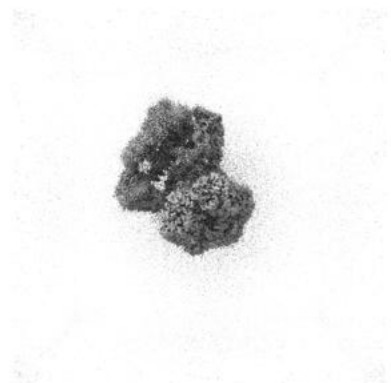
Y



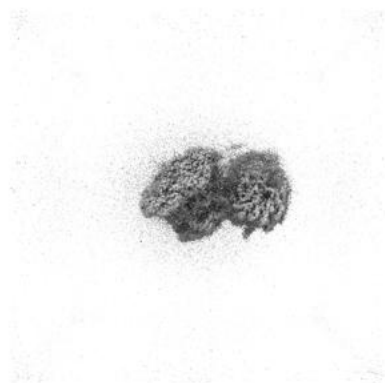
Z

The images above show the 3D surface view of the map at the recommended contour level 0.198. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

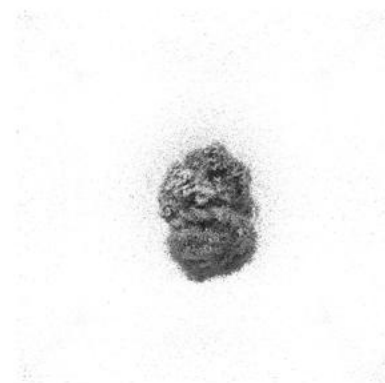
### 6.5.2 Raw map



X



Y



Z

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

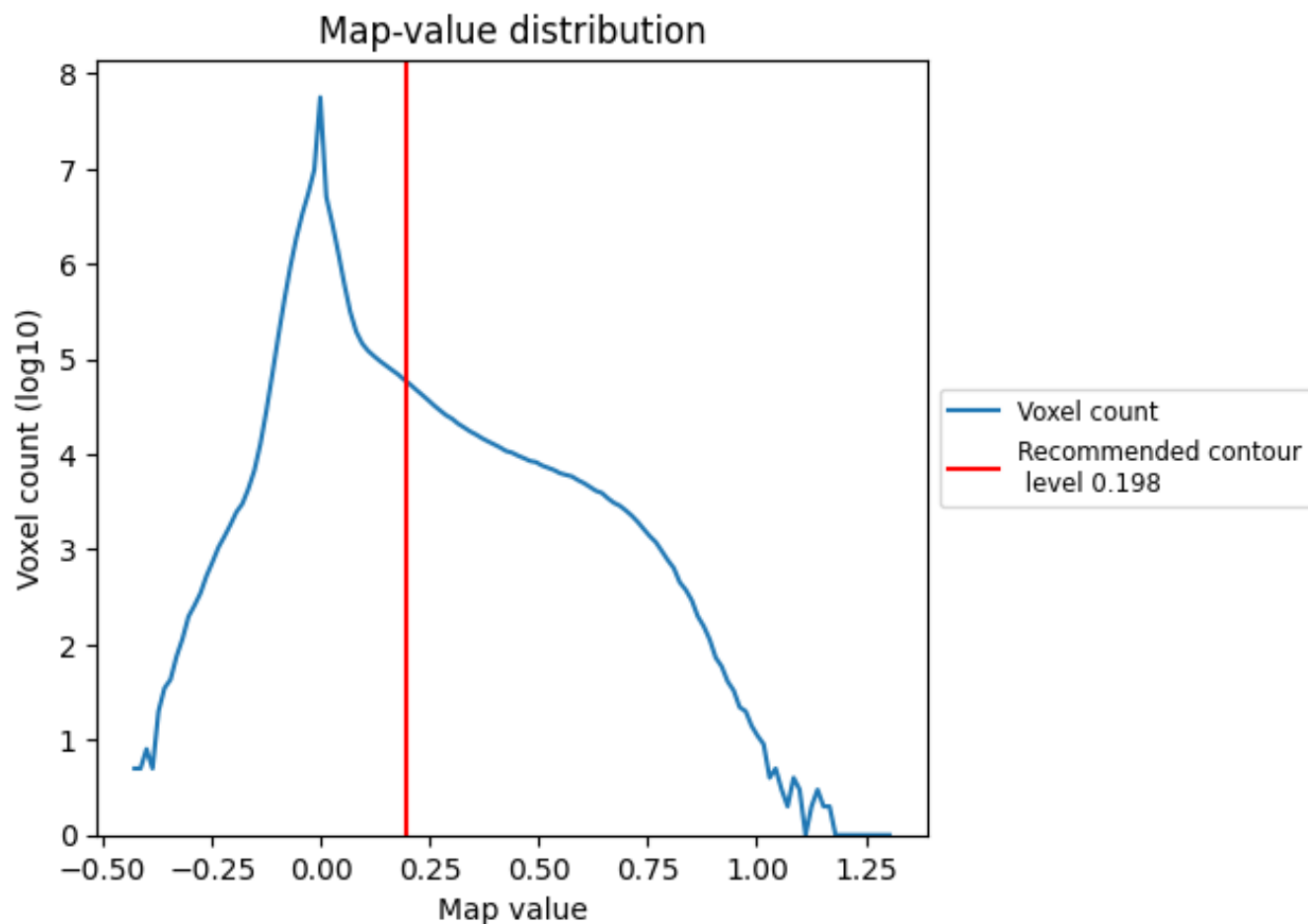
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

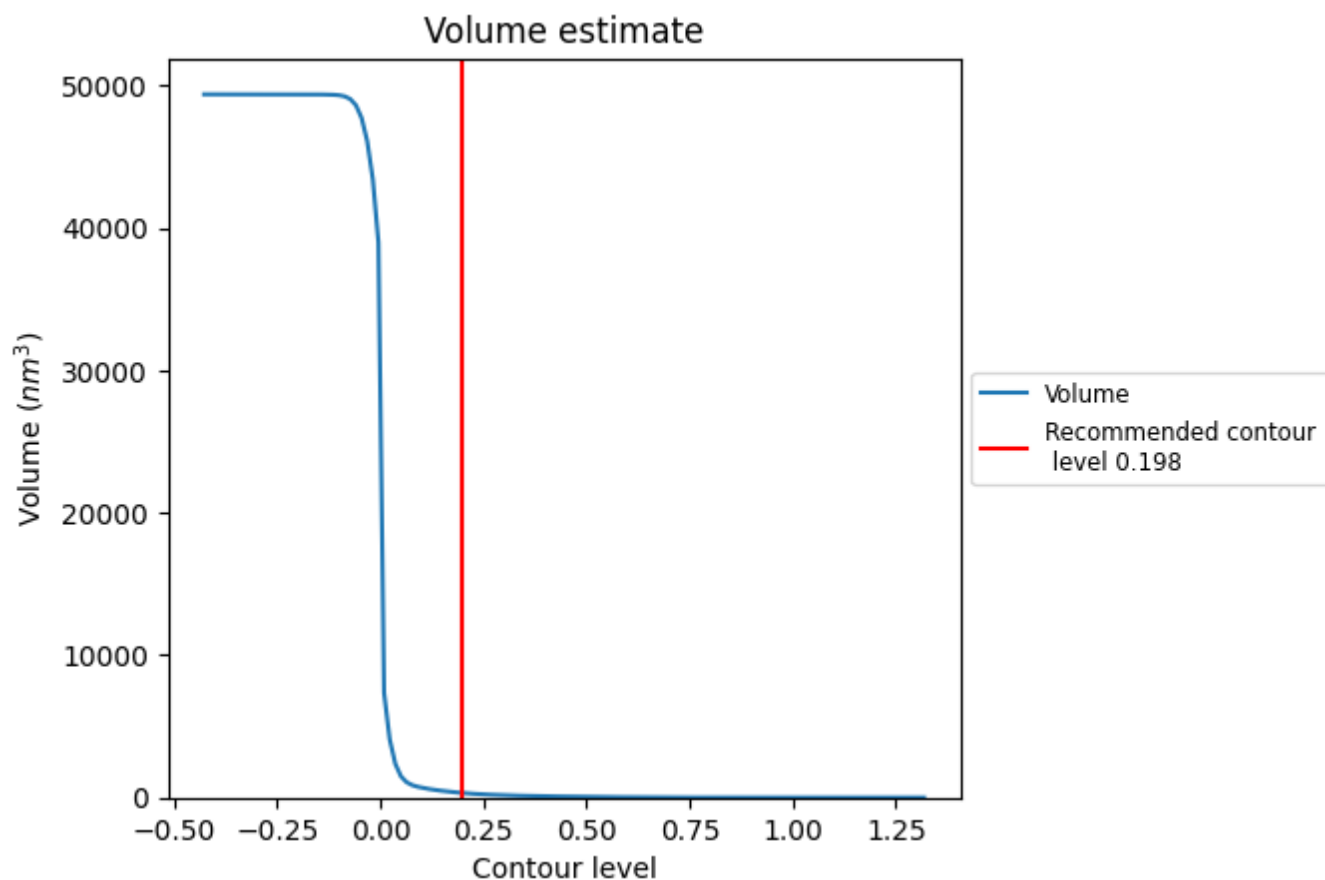
### 7.1 Map-value distribution [i](#)



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



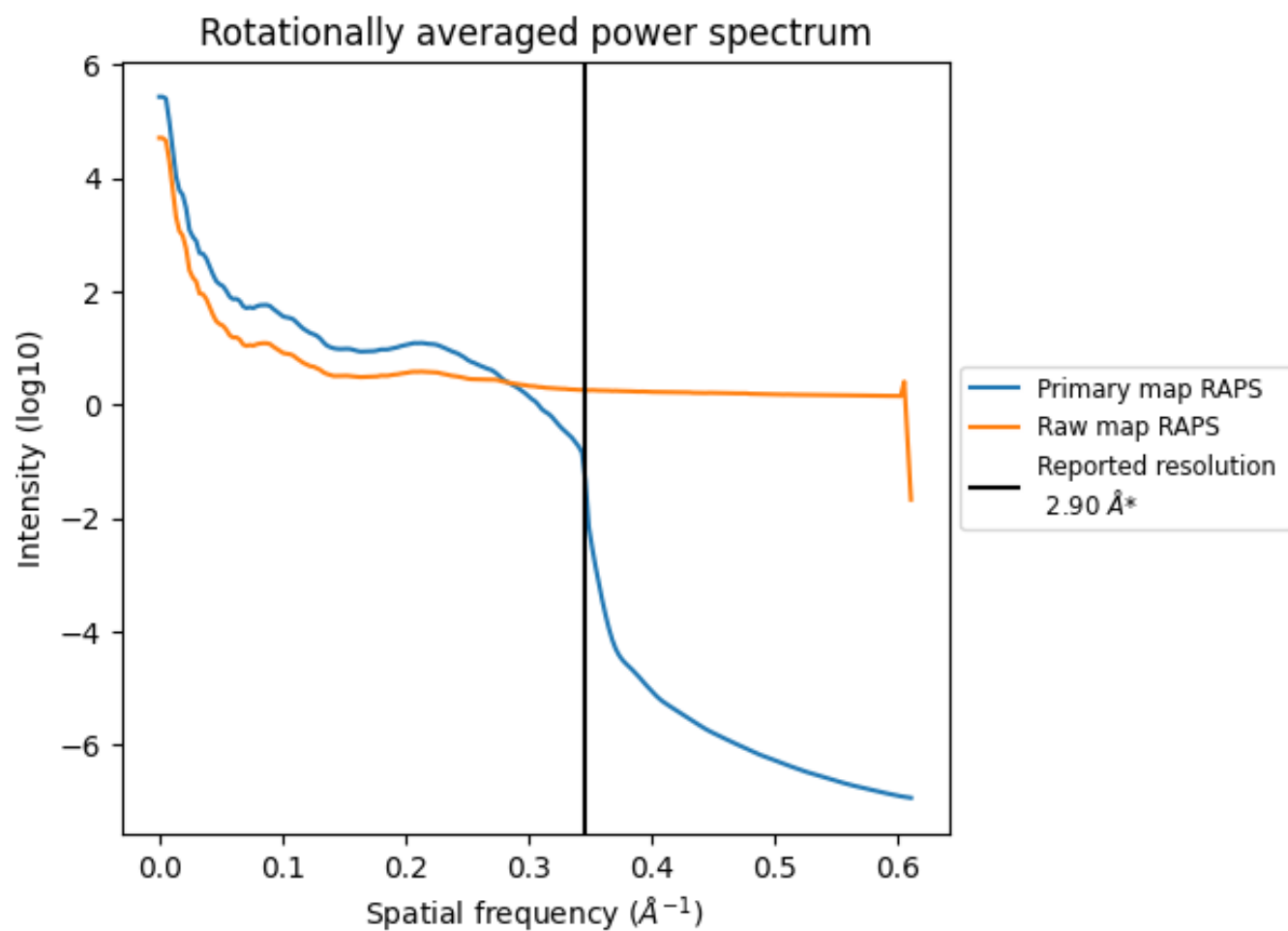
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 325 nm<sup>3</sup>; this corresponds to an approximate mass of 294 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 ⓘ

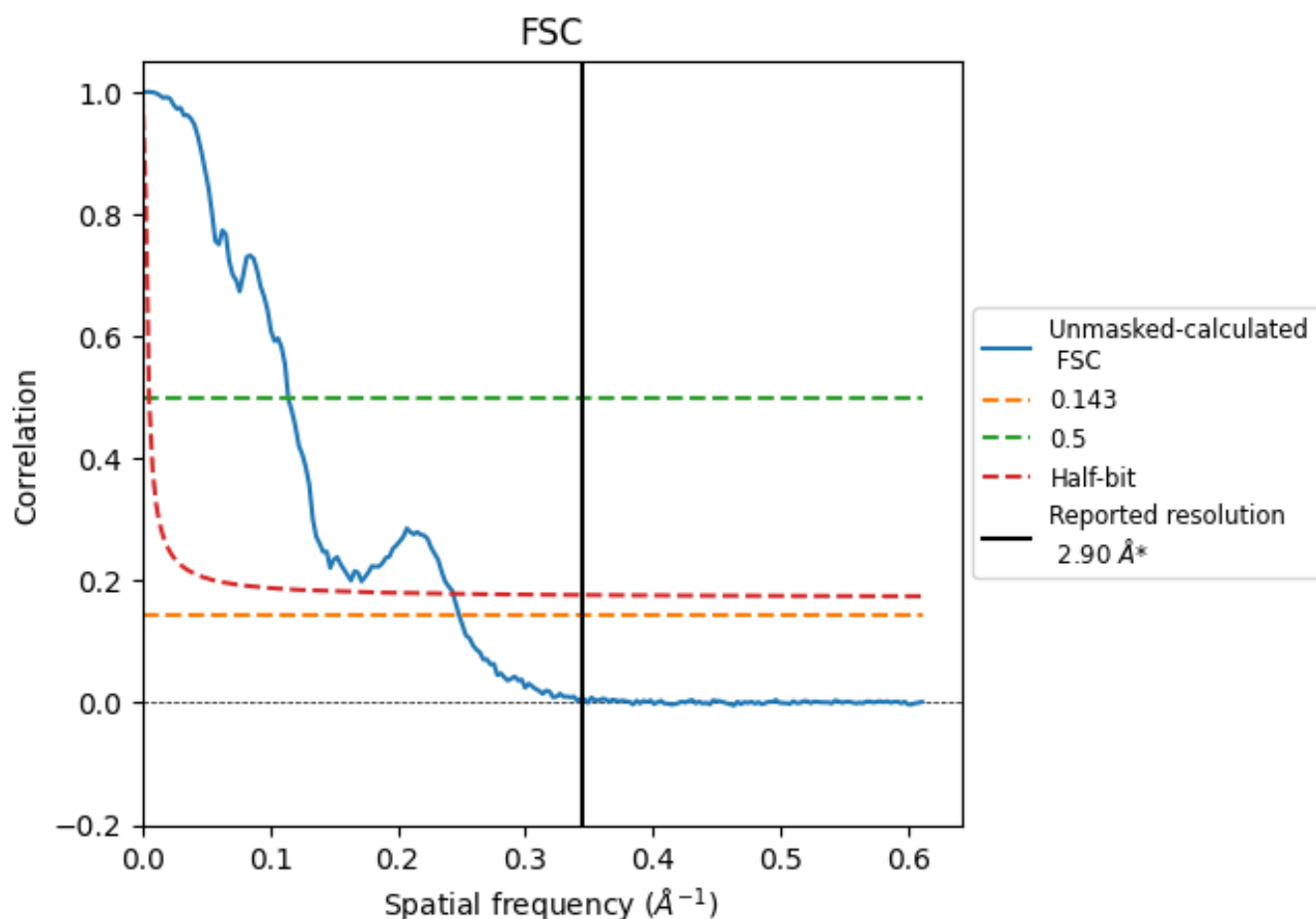


\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

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



## 8.2 Resolution estimates [i](#)

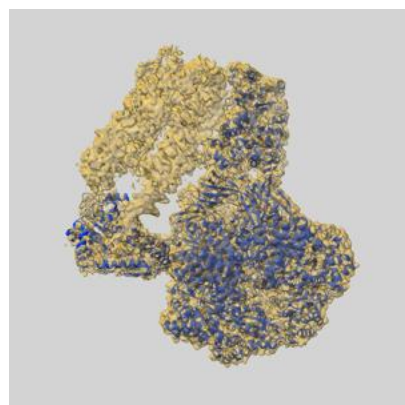
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	8.75	4.11

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 2.9 by more than 10 %

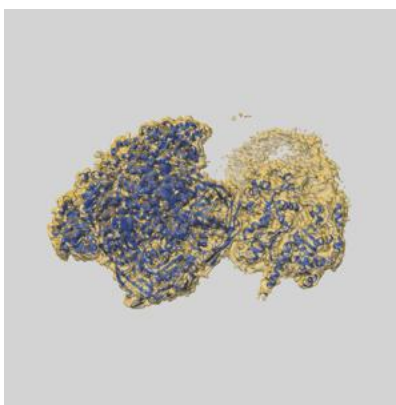
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45403 and PDB model 9CAT. Per-residue inclusion information can be found in section [3](#) on page [6](#).

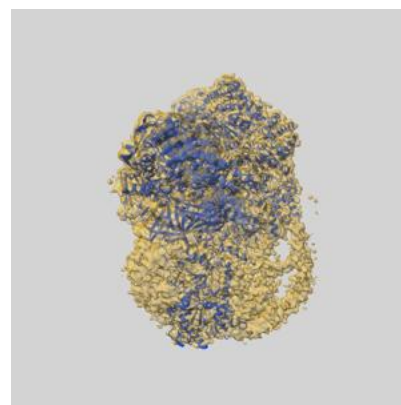
### 9.1 Map-model overlay [i](#)



X



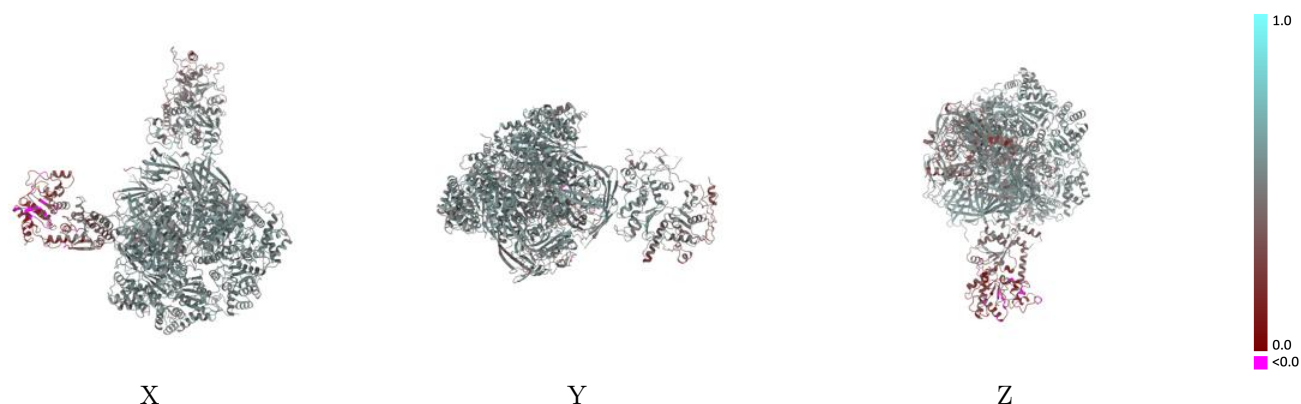
Y



Z

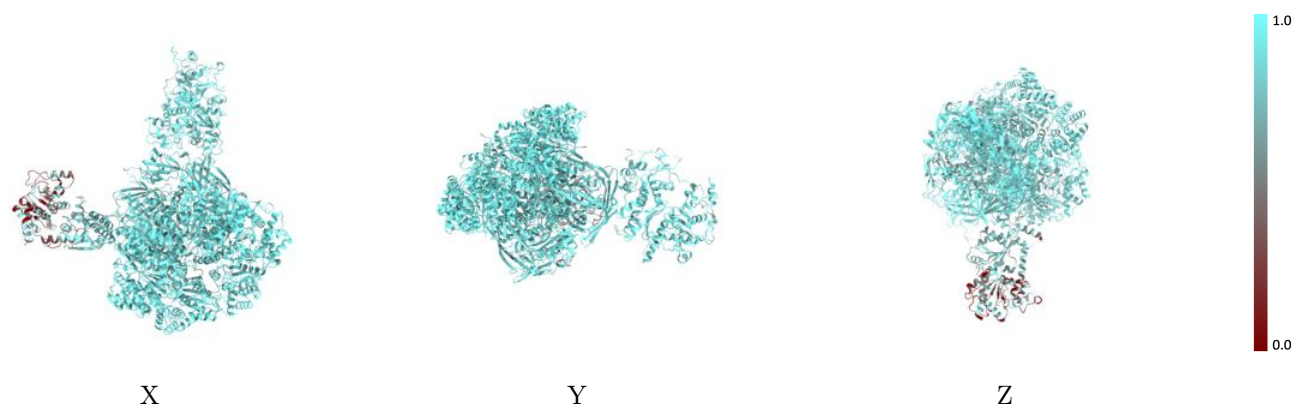
The images above show the 3D surface view of the map at the recommended contour level 0.198 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



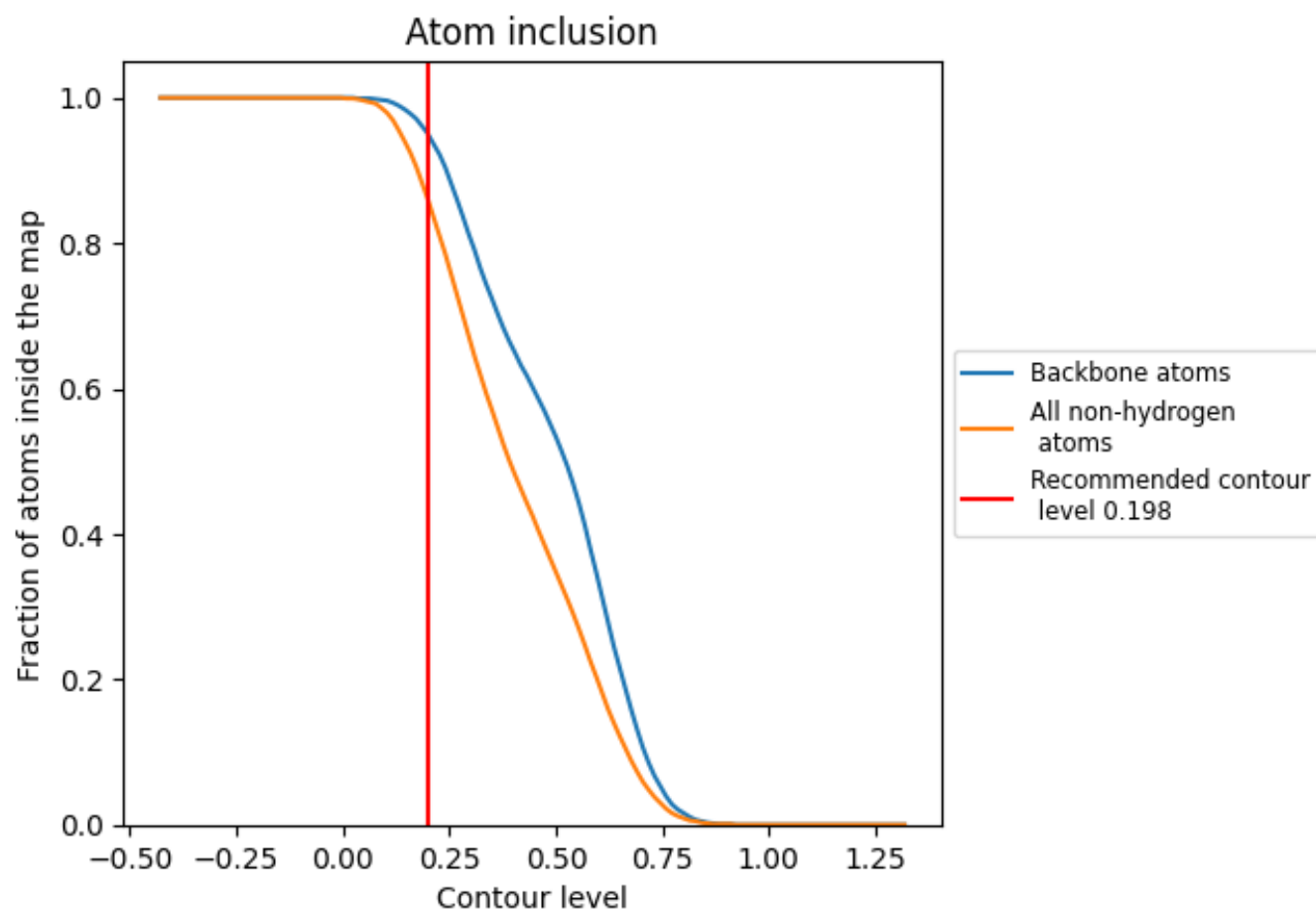
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.198).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 86% 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 (0.198) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8630	<div><div></div></div> 0.4920
Q	<div><div></div></div> 0.6920	<div><div></div></div> 0.3670
R	<div><div></div></div> 0.8770	<div><div></div></div> 0.4700
S	<div><div></div></div> 0.8560	<div><div></div></div> 0.4460
T	<div><div></div></div> 0.9000	<div><div></div></div> 0.5330
U	<div><div></div></div> 0.9080	<div><div></div></div> 0.5260
V	<div><div></div></div> 0.9060	<div><div></div></div> 0.5180
W	<div><div></div></div> 0.9180	<div><div></div></div> 0.5340
X	<div><div></div></div> 0.9020	<div><div></div></div> 0.5370
Y	<div><div></div></div> 0.8910	<div><div></div></div> 0.5300
Z	<div><div></div></div> 0.9190	<div><div></div></div> 0.5300

1.0

0.0

<0.0