



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:29 AM UTC

PDB ID : 9C9Z / pdb_00009c9z
EMDB ID : EMD-45377
Title : S.c INO80 in complex with Xenopus 0/80 nucleosome, INO80 Core
Authors : Wu, H.; Kaur, U.; Narlikar, G.J.; Cheng, Y.F.
Deposited on : 2024-06-16
Resolution : 2.55 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

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>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

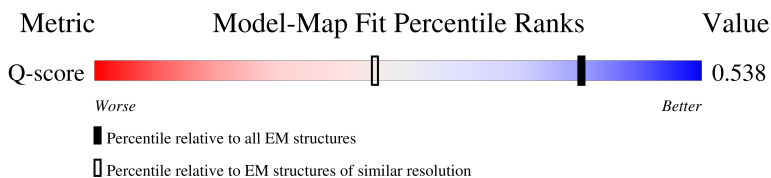
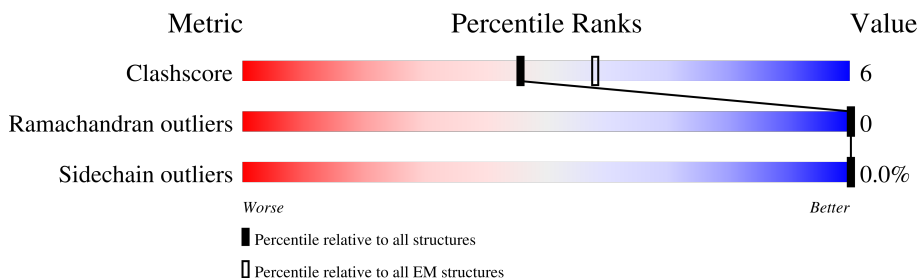
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 Å.

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









Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7475 (2.05 - 3.05)

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 ≥ 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	 22% 6% 72%
2	R	755	 47% 12% 41%
3	S	166	 66% 10% 23%
4	T	463	 81% 13% 6%

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Mol	Chain	Length	Quality of chain
4	V	463	 79%16%5%
4	X	463	 83%13%•
5	U	460	 83%13%•
5	W	460	 84%12%•
5	Y	460	 85%10%5%
6	Z	320	 7%•91%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 28632 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	419	Total	C	N	O	S	0	0
			3372	2143	565	649	15		

- 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
			3519	2241	591	676	11		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	437	Total	C	N	O	S	0	0
			3351	2111	578	652	10		
4	V	442	Total	C	N	O	S	0	0
			3394	2141	584	659	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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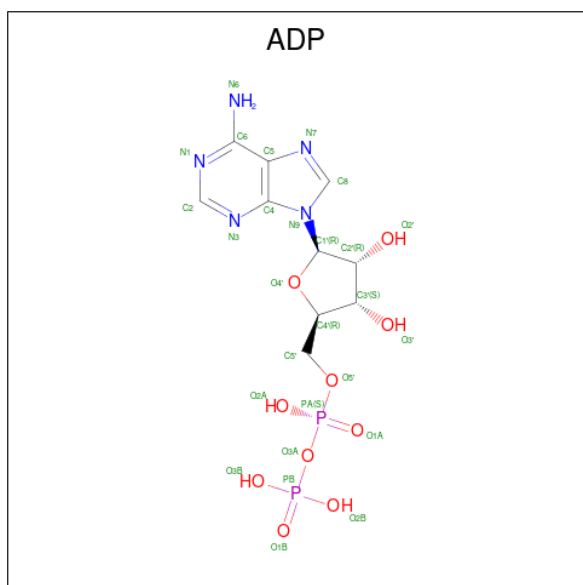
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	436	Total	C	N	O	S	0	0
			3351	2097	583	660	11		

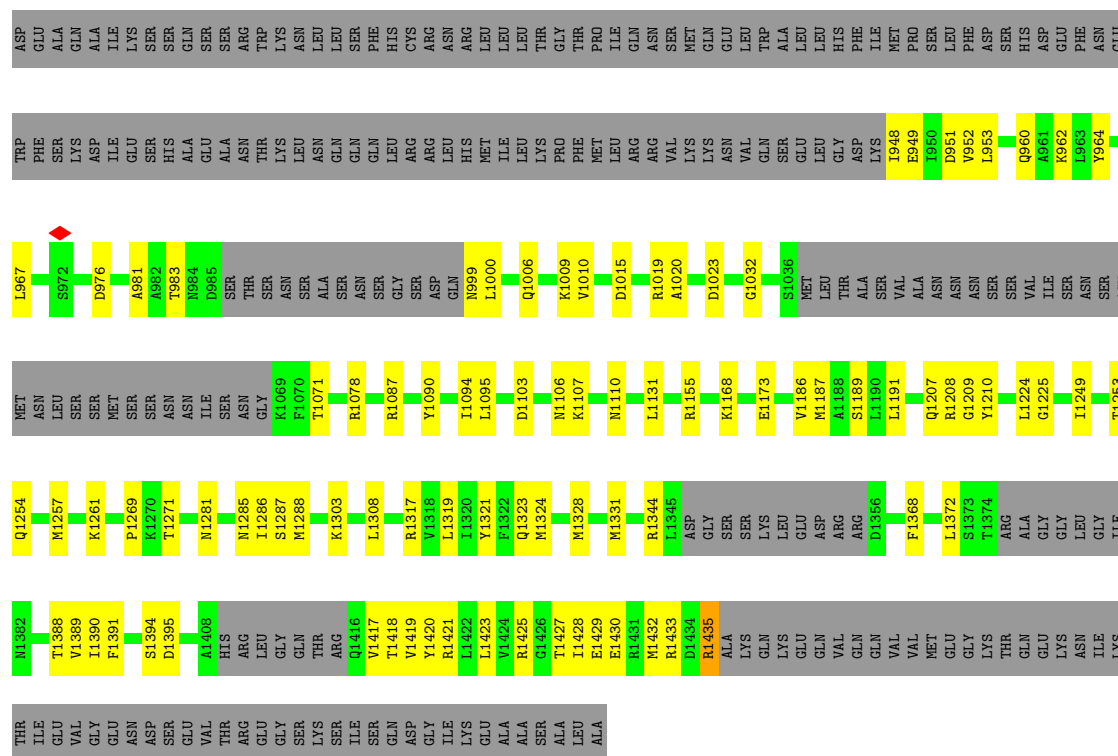
- Molecule 6 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	28	Total	C	N	O	S	0	0
			245	155	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).

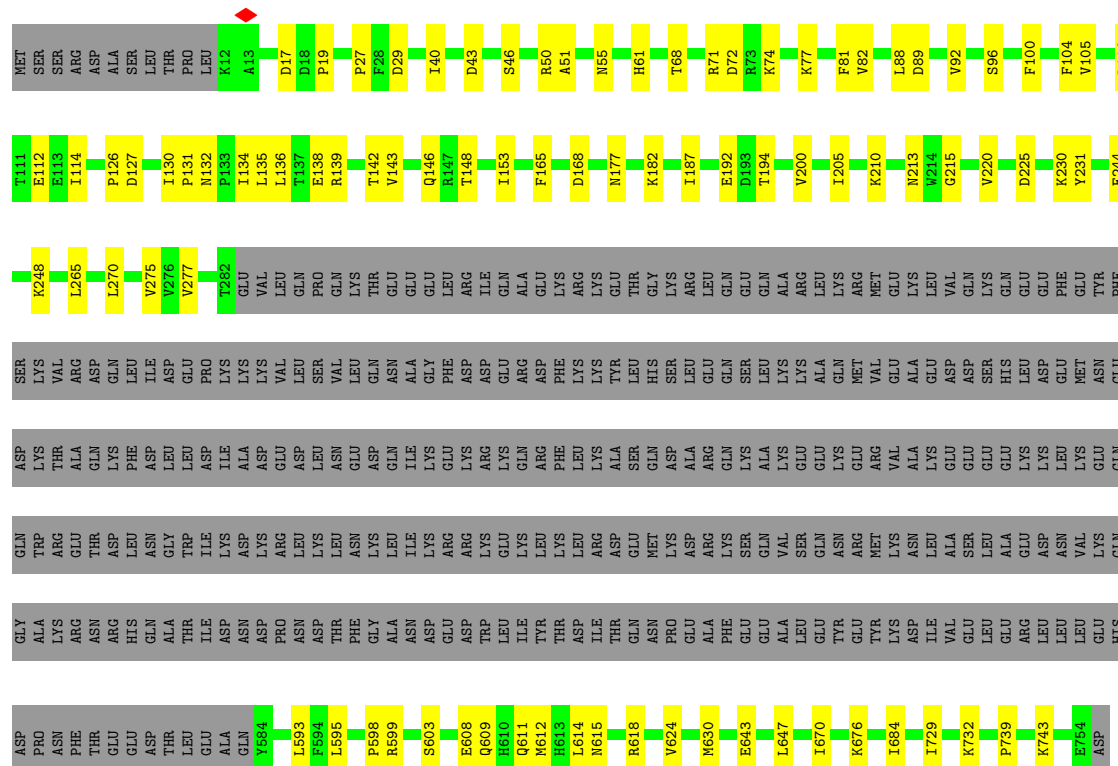


Mol	Chain	Residues	Atoms					AltConf
7	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	



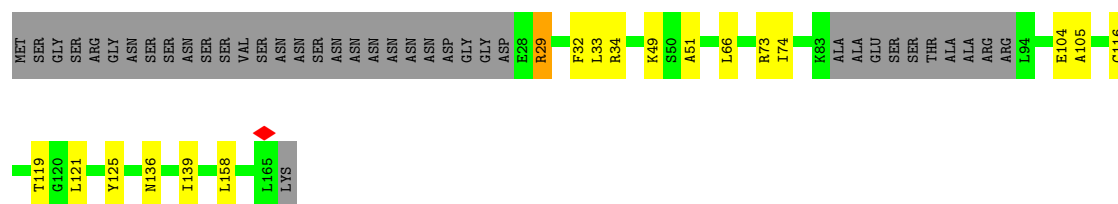
• Molecule 2: Actin-related protein 5

Chain R: 47% 12% 41%




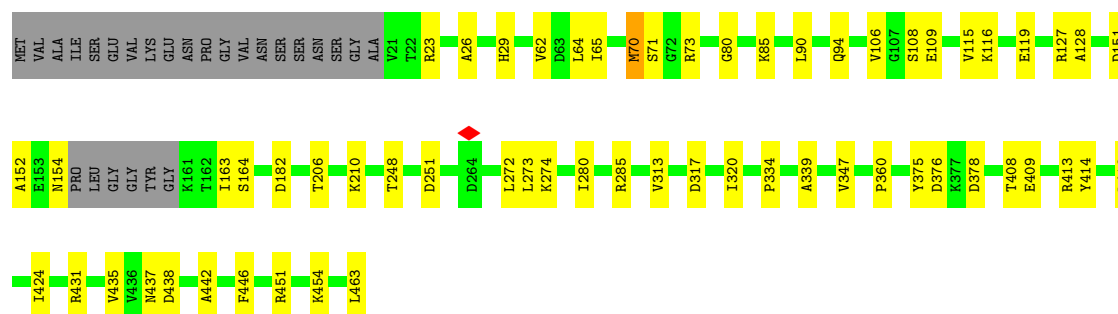
• Molecule 3: Chromatin-remodeling complex subunit IES6

Chain S: 




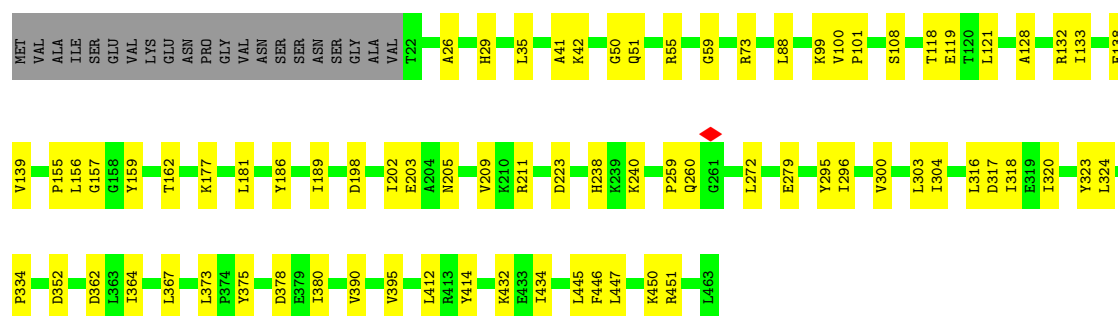
- Molecule 4: RuvB-like protein 1

Chain T: 




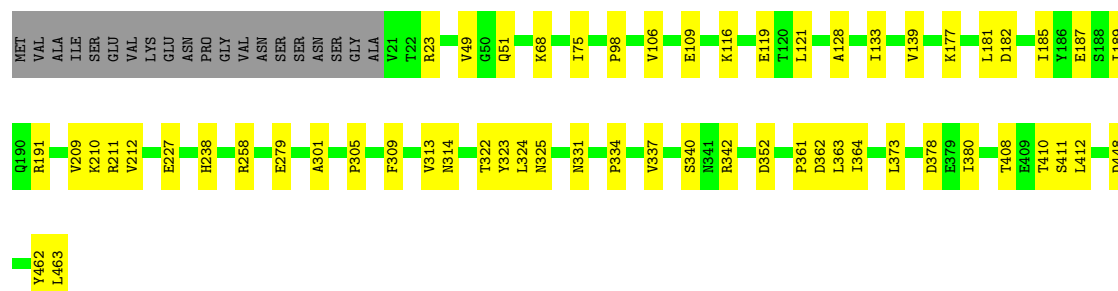
- Molecule 4: RuvB-like protein 1

Chain V: 



- Molecule 4: RuvB-like protein 1

Chain X: 



ARG	ARG	ALA	GLU	ASN	ALA	ARG	LYS	ARG	LYS	ASN	LEU	SER	GLU	LYS	ARG	LEU	GLU	GLU	LYS	GLN	ASP	THR	ILE	ASN	LYS	LEU	LEU	LYS	LYS	ARG	ALA	GLY	LYS	SER	SER	ARG	SER	HIS	LEU	PRO	ASN	ASP	ASP	GLU	LYS	ASN	ASP	GLY	SER	SER	SER	F293	N301	S302	M305	T306	R307
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R311	E314	F320
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109876	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	1.371	Depositor
Minimum map value	-0.358	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.13	Depositor
Map size (\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 (\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	0.28	0/3436	0.58	2/4660 (0.0%)
2	R	0.27	0/3610	0.60	4/4914 (0.1%)
3	S	0.34	0/1037	0.75	1/1397 (0.1%)
4	T	0.19	0/3390	0.43	1/4585 (0.0%)
4	V	0.19	0/3436	0.49	0/4648
4	X	0.19	0/3446	0.45	1/4662 (0.0%)
5	U	0.19	0/3459	0.44	1/4662 (0.0%)
5	W	0.17	0/3436	0.40	0/4632
5	Y	0.19	0/3387	0.40	1/4562 (0.0%)
6	Z	0.35	0/251	0.62	0/334
All	All	0.22	0/28888	0.49	11/39056 (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
6	Z	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	126	PRO	CA-N-CD	-11.44	95.99	112.00
1	Q	1372	LEU	CA-CB-CG	5.99	137.27	116.30
2	R	74	LYS	CA-CB-CG	5.81	125.72	114.10
5	U	165	MET	CB-CG-SD	5.75	129.94	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	70	MET	CB-CG-SD	5.66	129.69	112.70
2	R	19	PRO	N-CA-C	5.66	117.61	110.70
5	Y	175	MET	CB-CG-SD	5.34	128.73	112.70
4	X	462	TYR	CA-CB-CG	5.27	123.38	113.90
1	Q	1324	MET	CB-CG-SD	5.19	128.27	112.70
2	R	126	PRO	N-CD-CG	-5.19	95.42	103.20
3	S	29	ARG	CB-CG-CD	5.01	122.82	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Q	1421	ARG	Sidechain
6	Z	311	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	3372	0	3339	79	0
2	R	3519	0	3381	58	0
3	S	1015	0	1033	15	0
4	T	3351	0	3464	44	0
4	V	3394	0	3524	59	0
4	X	3404	0	3542	40	0
5	U	3421	0	3499	40	0
5	W	3398	0	3470	38	0
5	Y	3351	0	3439	31	0
6	Z	245	0	233	4	0
7	T	27	0	12	3	0
7	U	27	0	12	0	0
7	V	27	0	12	2	0
7	W	27	0	12	1	0
7	X	27	0	12	1	0
7	Y	27	0	12	2	0
All	All	28632	0	28996	358	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 (358) 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:1395:ASP:HB2	1:Q:1433:ARG:HH11	1.35	0.91
4:V:35:LEU:HD23	4:V:41:ALA:HB2	1.66	0.78
1:Q:1388:THR:HG23	1:Q:1418:THR:HB	1.64	0.78
1:Q:1432:MET:O	1:Q:1435:ARG:HG3	1.87	0.74
1:Q:1423:LEU:HD22	1:Q:1433:ARG:HG2	1.68	0.74
5:W:47:GLN:NE2	5:W:357:LYS:O	2.20	0.74
4:X:325:ASN:HD21	4:X:362:ASP:CG	1.98	0.71
3:S:29:ARG:O	3:S:33:LEU:HD13	1.92	0.70
1:Q:1186:VAL:HG21	4:V:300:VAL:HG21	1.73	0.69
1:Q:949:GLU:HA	1:Q:1419:VAL:HB	1.75	0.69
4:X:362:ASP:OD1	4:X:363:LEU:N	2.26	0.69
5:W:40:THR:OG1	5:W:45:VAL:HG23	1.92	0.68
4:V:186:TYR:O	4:V:189:ILE:HB	1.96	0.65
1:Q:983:THR:HG23	1:Q:1435:ARG:HG2	1.78	0.65
4:X:314:ASN:HD22	4:X:342:ARG:HG2	1.61	0.65
1:Q:1308:LEU:HD22	1:Q:1368:PHE:HE2	1.64	0.63
1:Q:951:ASP:HB2	1:Q:1433:ARG:HH21	1.63	0.63
1:Q:1429:GLU:O	1:Q:1432:MET:HG3	1.98	0.63
4:T:115:VAL:HG21	4:T:119:GLU:HG2	1.80	0.62
1:Q:948:ILE:HG13	1:Q:1417:VAL:HG12	1.80	0.62
1:Q:1423:LEU:CD2	1:Q:1433:ARG:HG2	2.29	0.61
2:R:143:VAL:HB	2:R:146:GLN:HG3	1.80	0.61
5:W:132:GLU:HB3	5:W:232:ARG:HH22	1.65	0.61
1:Q:1435:ARG:C	1:Q:1435:ARG:HH11	2.09	0.60
5:U:136:ILE:O	5:U:191:SER:HA	2.01	0.60
4:T:151:ASP:HA	4:T:163:ILE:HA	1.84	0.60
3:S:49:LYS:HG3	3:S:51:ALA:H	1.67	0.59
5:U:162:THR:HG23	5:U:229:LEU:HD12	1.83	0.59
4:V:35:LEU:CD2	4:V:41:ALA:HB2	2.33	0.59
5:W:361:GLU:HG2	5:W:392:VAL:HG21	1.85	0.59
5:U:361:GLU:HG2	5:U:392:VAL:HG21	1.83	0.59
4:V:155:PRO:HB2	4:V:162:THR:CG2	2.32	0.59
4:V:155:PRO:HB2	4:V:162:THR:HG22	1.83	0.59
4:V:101:PRO:HD3	4:V:304:ILE:CD1	2.33	0.58
1:Q:948:ILE:HG23	1:Q:949:GLU:H	1.69	0.57
2:R:277:VAL:HB	2:R:612:MET:HB3	1.86	0.57
2:R:732:LYS:HE2	2:R:732:LYS:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:106:VAL:HG12	4:T:108:SER:H	1.70	0.57
2:R:225:ASP:HB3	3:S:158:LEU:HD11	1.85	0.57
4:V:42:LYS:O	4:V:55:ARG:NH2	2.37	0.57
4:V:101:PRO:HD3	4:V:304:ILE:HD12	1.87	0.57
4:V:447:LEU:HD12	4:V:451:ARG:HH21	1.70	0.57
1:Q:1249:ILE:HG13	1:Q:1271:THR:HG21	1.87	0.56
1:Q:1391:PHE:CE2	1:Q:1419:VAL:HG13	2.40	0.56
2:R:100:PHE:HA	2:R:105:VAL:HA	1.86	0.56
1:Q:1155:ARG:HD2	5:U:252:GLN:HE21	1.70	0.56
4:T:280:ILE:HB	4:T:285:ARG:HH21	1.70	0.56
1:Q:1395:ASP:HB2	1:Q:1433:ARG:NH1	2.12	0.56
4:V:29:HIS:HB3	4:V:390:VAL:HG21	1.88	0.56
2:R:200:VAL:HB	2:R:205:ILE:HD11	1.88	0.56
4:X:106:VAL:HB	4:X:109:GLU:HG3	1.88	0.56
4:V:362:ASP:OD1	4:V:362:ASP:N	2.37	0.56
2:R:265:LEU:HD12	3:S:121:LEU:HD11	1.88	0.56
5:U:250:ARG:NH2	5:U:261:ASP:O	2.37	0.56
2:R:248:LYS:HE2	2:R:676:LYS:HE2	1.89	0.56
4:V:316:LEU:HD22	4:V:320:ILE:HG21	1.88	0.56
4:V:352:ASP:OD2	4:V:352:ASP:N	2.39	0.56
4:V:259:PRO:HB3	5:W:255:LEU:HD21	1.88	0.55
2:R:230:LYS:HE2	2:R:595:LEU:HD13	1.88	0.55
4:X:121:LEU:HD21	4:X:324:LEU:HD13	1.88	0.55
1:Q:976:ASP:N	1:Q:976:ASP:OD1	2.36	0.55
1:Q:1435:ARG:C	1:Q:1435:ARG:HD2	2.32	0.55
2:R:29:ASP:OD1	2:R:29:ASP:N	2.40	0.55
4:T:106:VAL:HB	4:T:109:GLU:HG3	1.89	0.55
2:R:275:VAL:O	2:R:615:ASN:ND2	2.40	0.54
5:U:325:THR:HG22	5:U:327:ARG:H	1.72	0.54
4:T:272:LEU:HG	4:T:273:LEU:HG	1.89	0.54
4:V:73:ARG:NH2	5:W:404:SER:OG	2.41	0.54
4:V:118:THR:HG21	5:W:105:GLU:HG3	1.90	0.54
3:S:136:ASN:OD1	3:S:139:ILE:HD12	2.07	0.54
2:R:43:ASP:HB3	2:R:50:ARG:HB2	1.90	0.53
5:Y:29:LEU:HB3	5:Y:31:LEU:HD13	1.89	0.53
1:Q:948:ILE:HA	1:Q:1417:VAL:O	2.08	0.53
1:Q:1210:TYR:HB3	5:W:248:ASN:HB3	1.91	0.53
4:T:313:VAL:HG12	4:T:339:ALA:O	2.09	0.53
5:U:47:GLN:NE2	5:U:357:LYS:O	2.41	0.53
5:U:346:ASP:OD1	5:U:346:ASP:N	2.41	0.53
5:Y:45:VAL:O	7:Y:501:ADP:N6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1090:TYR:HA	1:Q:1094:ILE:HD12	1.91	0.53
4:X:75:ILE:HG12	4:X:337:VAL:HG12	1.89	0.53
2:R:138:GLU:HB2	2:R:165:PHE:HB2	1.90	0.53
1:Q:1078:ARG:NH1	5:Y:182:GLU:OE2	2.42	0.53
2:R:603:SER:O	2:R:609:GLN:NE2	2.42	0.53
5:W:223:GLN:NE2	5:W:224:CYS:SG	2.81	0.53
4:T:378:ASP:OD1	4:T:378:ASP:N	2.42	0.53
5:U:343:LEU:HB3	5:U:347:LEU:HD23	1.91	0.53
5:W:415:ASN:ND2	5:W:417:THR:O	2.42	0.53
4:T:152:ALA:HB3	4:T:164:SER:HB3	1.90	0.52
5:W:155:GLN:NE2	6:Z:301:ASN:O	2.41	0.52
1:Q:1155:ARG:HD3	4:V:272:LEU:HD11	1.91	0.52
4:V:155:PRO:CB	4:V:162:THR:CG2	2.86	0.52
4:X:68:LYS:HG2	4:X:305:PRO:HD2	1.92	0.52
2:R:270:LEU:HD12	2:R:598:PRO:HD3	1.92	0.52
2:R:43:ASP:OD2	2:R:50:ARG:NH1	2.43	0.52
4:V:162:THR:HG23	4:V:162:THR:O	2.08	0.52
1:Q:1308:LEU:HD22	1:Q:1368:PHE:CE2	2.44	0.52
5:U:171:LEU:HG	5:U:175:MET:HG3	1.91	0.52
5:W:243:GLU:HA	5:W:257:LEU:HD21	1.91	0.52
4:X:380:ILE:HG12	4:X:412:LEU:HD13	1.91	0.52
4:X:139:VAL:O	4:X:238:HIS:HA	2.10	0.51
4:V:50:GLY:O	4:V:55:ARG:NH1	2.44	0.51
5:Y:40:THR:OG1	5:Y:45:VAL:HG12	2.09	0.51
1:Q:964:TYR:OH	1:Q:1428:ILE:HG23	2.11	0.51
4:V:317:ASP:OD1	4:V:318:ILE:N	2.44	0.51
2:R:168:ASP:OD1	2:R:168:ASP:N	2.43	0.51
4:V:375:TYR:OH	7:V:501:ADP:N7	2.42	0.51
4:V:380:ILE:HG12	4:V:412:LEU:HD13	1.91	0.51
3:S:125:TYR:OH	5:Y:229:LEU:O	2.26	0.51
2:R:112:GLU:HG3	2:R:153:ILE:HD11	1.93	0.50
1:Q:949:GLU:HG2	1:Q:1419:VAL:HG11	1.94	0.50
5:Y:191:SER:HG	5:Y:200:THR:HG1	1.60	0.50
5:Y:298:VAL:HG13	5:Y:343:LEU:HD21	1.93	0.50
1:Q:981:ALA:HB1	1:Q:1000:LEU:HD11	1.93	0.50
1:Q:1187:MET:HE1	4:V:133:ILE:HD13	1.94	0.50
4:T:182:ASP:OD1	4:T:182:ASP:N	2.38	0.50
4:T:413:ARG:NH2	7:T:501:ADP:O2A	2.45	0.50
4:X:322:THR:HG21	5:Y:300:MET:HG3	1.93	0.50
2:R:624:VAL:HG23	2:R:630:MET:HB2	1.92	0.50
1:Q:1071:THR:OG1	4:X:177:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:26:ALA:HB3	5:Y:314:GLU:HG3	1.94	0.50
5:Y:130:LYS:HG2	5:Y:236:VAL:HG22	1.94	0.50
4:T:424:ILE:HD13	5:Y:59:LYS:HB3	1.94	0.49
4:V:138:GLU:HB2	4:V:240:LYS:HD3	1.94	0.49
1:Q:1191:LEU:O	4:V:260:GLN:NE2	2.40	0.49
4:V:26:ALA:O	7:V:501:ADP:O3'	2.30	0.49
5:U:169:TYR:HD1	4:V:223:ASP:HB3	1.77	0.49
5:Y:122:ARG:NE	5:Y:245:ASP:OD2	2.43	0.49
5:W:298:VAL:HG13	5:W:343:LEU:HD21	1.94	0.49
5:W:359:TYR:OH	7:W:501:ADP:N7	2.45	0.49
5:W:398:TYR:OH	5:W:435:ARG:NH2	2.45	0.49
3:S:136:ASN:OD1	3:S:139:ILE:CD1	2.60	0.49
4:T:408:THR:HG22	5:U:458:ILE:HD11	1.94	0.49
5:U:38:ARG:O	5:U:51:ARG:NH2	2.43	0.49
4:V:159:TYR:OH	6:Z:307:ARG:NH1	2.46	0.49
3:S:73:ARG:HG2	3:S:74:ILE:HD13	1.93	0.49
1:Q:1087:ARG:NH1	1:Q:1224:LEU:O	2.43	0.49
2:R:27:PRO:HG3	2:R:88:LEU:HD21	1.95	0.49
2:R:615:ASN:HA	2:R:618:ARG:HB3	1.95	0.49
4:T:154:ASN:OD1	4:T:154:ASN:N	2.46	0.48
5:W:407:GLN:NE2	5:W:411:MET:SD	2.86	0.48
4:X:410:THR:OG1	4:X:411:SER:N	2.46	0.48
2:R:51:ALA:HB3	2:R:61:HIS:HB2	1.95	0.48
4:X:352:ASP:N	4:X:352:ASP:OD1	2.44	0.48
1:Q:1131:LEU:HD22	5:U:247:ILE:HG13	1.95	0.48
2:R:17:ASP:HB2	2:R:277:VAL:HA	1.95	0.48
5:W:316:GLU:O	4:X:23:ARG:NH1	2.46	0.48
4:T:62:VAL:HA	4:T:65:ILE:HD12	1.95	0.48
4:T:73:ARG:NH2	5:U:401:ASN:O	2.46	0.48
4:X:182:ASP:OD1	4:X:182:ASP:N	2.42	0.48
4:T:347:VAL:HG11	4:T:360:PRO:HG3	1.96	0.48
1:Q:1095:LEU:HD13	4:T:210:LYS:HD2	1.96	0.48
5:U:304:GLU:HB3	4:V:108:SER:HB3	1.96	0.48
5:U:394:THR:OG1	5:U:395:SER:N	2.47	0.48
5:W:128:LYS:HB3	5:W:287:GLU:HG2	1.95	0.48
5:Y:71:VAL:HG12	5:Y:352:ILE:HG13	1.96	0.48
2:R:177:ASN:HB3	2:R:182:LYS:HG3	1.95	0.48
4:T:414:TYR:OH	4:T:451:ARG:NH2	2.47	0.48
4:X:378:ASP:N	4:X:378:ASP:OD1	2.42	0.48
1:Q:1394:SER:OG	1:Q:1433:ARG:HB2	2.13	0.48
5:W:38:ARG:O	5:W:51:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:119:GLU:HG2	4:X:279:GLU:HA	1.95	0.48
4:X:211:ARG:NH2	4:X:227:GLU:OE1	2.47	0.47
4:T:80:GLY:O	4:T:85:LYS:NZ	2.47	0.47
5:U:160:ILE:HG23	5:U:229:LEU:HD11	1.95	0.47
4:V:121:LEU:HD21	4:V:324:LEU:HD13	1.95	0.47
1:Q:1394:SER:HB3	1:Q:1432:MET:SD	2.54	0.47
2:R:72:ASP:HB3	3:S:34:ARG:HH21	1.79	0.47
4:T:463:LEU:HD22	5:Y:75:GLY:HA2	1.94	0.47
4:V:100:VAL:HA	4:V:304:ILE:HD12	1.96	0.47
5:W:139:GLU:HG3	5:W:189:VAL:HG22	1.95	0.47
4:X:49:VAL:O	7:X:501:ADP:N6	2.47	0.47
2:R:187:ILE:HB	2:R:670:ILE:HG22	1.96	0.47
1:Q:1168:LYS:HG3	1:Q:1173:GLU:HG3	1.97	0.47
1:Q:1427:THR:O	1:Q:1430:GLU:HG3	2.15	0.47
4:X:51:GLN:NE2	4:X:373:LEU:O	2.47	0.47
1:Q:948:ILE:HG12	1:Q:949:GLU:N	2.30	0.47
5:U:146:ASP:HB2	5:U:155:GLN:HB2	1.96	0.47
5:Y:359:TYR:OH	7:Y:501:ADP:N7	2.46	0.47
1:Q:960:GLN:NE2	1:Q:1010:VAL:O	2.48	0.47
5:U:190:ILE:HD12	5:U:192:ILE:HD11	1.96	0.47
1:Q:1106:ASN:O	1:Q:1110:ASN:HB2	2.15	0.47
4:T:71:SER:HB2	5:U:19:LEU:HB2	1.97	0.46
1:Q:1023:ASP:HB3	1:Q:1287:SER:HB3	1.96	0.46
1:Q:1103:ASP:N	1:Q:1103:ASP:OD1	2.44	0.46
5:W:190:ILE:HG22	5:W:201:LYS:HA	1.96	0.46
4:T:64:LEU:HD21	4:T:73:ARG:HG3	1.96	0.46
2:R:81:PHE:HB3	2:R:82:VAL:HG23	1.96	0.46
3:S:116:CYS:SG	3:S:119:THR:OG1	2.72	0.46
4:X:361:PRO:HA	4:X:364:ILE:HB	1.98	0.46
1:Q:1328:MET:SD	1:Q:1328:MET:N	2.71	0.46
2:R:46:SER:OG	2:R:192:GLU:OE1	2.34	0.46
2:R:729:ILE:HG12	2:R:743:LYS:CD	2.45	0.46
1:Q:1317:ARG:NH2	1:Q:1319:LEU:HD23	2.31	0.46
2:R:270:LEU:HG	2:R:593:LEU:HD12	1.97	0.46
5:U:122:ARG:NE	5:U:245:ASP:OD2	2.49	0.46
2:R:71:ARG:HD2	2:R:77:LYS:HG2	1.98	0.45
2:R:210:LYS:HD2	3:S:105:ALA:HA	1.98	0.45
5:W:162:THR:OG1	5:W:225:PRO:O	2.32	0.45
1:Q:1286:ILE:HB	4:X:210:LYS:HB2	1.97	0.45
1:Q:967:LEU:HD21	1:Q:1006:GLN:HG3	1.99	0.45
4:T:431:ARG:NH2	4:T:438:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:35:LEU:HD23	4:V:41:ALA:CB	2.43	0.45
4:V:155:PRO:CB	4:V:162:THR:HG21	2.45	0.45
4:V:181:LEU:HA	5:W:214:ALA:HB2	1.98	0.45
4:T:414:TYR:OH	4:T:446:PHE:O	2.34	0.45
4:V:121:LEU:HD23	4:V:323:TYR:HD2	1.81	0.45
5:W:136:ILE:HB	5:W:192:ILE:HB	1.99	0.45
1:Q:1107:LYS:HD2	4:T:206:THR:HA	1.97	0.45
5:U:52:ARG:HG2	4:V:445:LEU:HD11	1.99	0.45
5:U:108:SER:OG	5:U:111:LEU:O	2.34	0.45
4:X:408:THR:HG22	5:Y:458:ILE:HD11	1.99	0.45
5:Y:140:VAL:HA	5:Y:160:ILE:HG13	1.99	0.45
4:X:331:ASN:OD1	4:X:331:ASN:N	2.46	0.45
2:R:55:ASN:OD1	2:R:55:ASN:N	2.49	0.45
5:U:154:LYS:H	5:U:173:ASN:HB3	1.82	0.45
5:W:416:ASN:OD1	5:W:416:ASN:N	2.45	0.45
2:R:210:LYS:HD3	2:R:210:LYS:HA	1.74	0.45
2:R:220:VAL:HG21	2:R:244:GLU:HG3	1.98	0.45
4:V:55:ARG:HG2	4:V:88:LEU:HD21	1.99	0.45
4:T:375:TYR:OH	7:T:501:ADP:N7	2.44	0.44
4:V:414:TYR:OH	4:V:446:PHE:O	2.35	0.44
4:X:258:ARG:HA	4:X:258:ARG:HD3	1.81	0.44
1:Q:1319:LEU:HD13	1:Q:1321:TYR:H	1.82	0.44
2:R:139:ARG:O	2:R:142:THR:OG1	2.34	0.44
5:U:76:PRO:O	5:U:79:THR:OG1	2.30	0.44
4:V:395:VAL:HG22	4:V:434:ILE:HD12	1.99	0.44
5:Y:164:ASP:HB2	5:Y:227:GLY:HA3	1.98	0.44
6:Z:302:SER:HA	6:Z:305:MET:HE2	1.99	0.44
1:Q:1423:LEU:HD11	1:Q:1430:GLU:HA	1.99	0.44
3:S:66:LEU:HD12	3:S:66:LEU:HA	1.84	0.44
4:T:274:LYS:HD2	4:T:274:LYS:HA	1.84	0.44
5:U:243:GLU:HA	5:U:257:LEU:HD21	1.99	0.44
4:X:121:LEU:HD23	4:X:323:TYR:HD2	1.83	0.44
4:T:376:ASP:OD1	4:T:376:ASP:N	2.46	0.44
5:U:35:LEU:HD11	5:U:59:LYS:HG3	2.00	0.44
4:V:205:ASN:OD1	4:V:205:ASN:N	2.51	0.44
1:Q:1331:MET:HE1	1:Q:1344:ARG:HD3	2.00	0.43
5:U:179:LEU:HD22	5:U:184:VAL:HG11	1.99	0.43
1:Q:1032:GLY:HA3	5:Y:182:GLU:HA	2.00	0.43
1:Q:1249:ILE:HB	1:Q:1254:GLN:HE21	1.82	0.43
1:Q:1389:VAL:HG12	1:Q:1418:THR:O	2.18	0.43
5:U:211:ASP:OD1	5:U:211:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:262:THR:HB	5:Y:265:ILE:HD11	2.00	0.43
1:Q:1208:ARG:NH1	1:Q:1285:ASN:OD1	2.48	0.43
4:V:364:ILE:HD13	4:V:367:LEU:HD11	1.99	0.43
1:Q:952:VAL:HG22	1:Q:1303:LYS:NZ	2.33	0.43
5:W:76:PRO:HD3	4:X:463:LEU:HD22	1.99	0.43
2:R:82:VAL:HG11	2:R:114:ILE:HA	2.00	0.43
5:Y:273:ILE:HD13	5:Y:273:ILE:HA	1.87	0.43
2:R:68:THR:HB	2:R:96:SER:HA	2.00	0.43
2:R:194:THR:HG23	2:R:215:GLY:H	1.83	0.43
1:Q:999:ASN:HB3	1:Q:1000:LEU:H	1.56	0.43
4:T:418:LEU:HD22	4:T:442:ALA:HB1	2.01	0.43
4:V:450:LYS:NZ	5:W:457:SER:OG	2.52	0.43
5:Y:69:ARG:HB2	5:Y:320:ILE:HG12	1.99	0.43
2:R:72:ASP:H	2:R:77:LYS:HA	1.84	0.43
4:X:187:GLU:HB3	4:X:191:ARG:HH22	1.84	0.43
5:Y:20:ILE:HG21	5:Y:375:GLU:HG2	2.01	0.43
1:Q:1209:GLY:HA2	5:W:276:LYS:HG2	2.00	0.43
4:X:189:ILE:HD13	4:X:209:VAL:HG11	2.00	0.43
1:Q:1207:GLN:HA	1:Q:1281:ASN:HD22	1.84	0.42
1:Q:1254:GLN:OE1	5:W:148:SER:OG	2.36	0.42
5:U:147:ARG:HH12	5:U:151:GLY:HA2	1.84	0.42
4:V:51:GLN:NE2	4:V:373:LEU:O	2.52	0.42
4:X:448:ASP:OD1	4:X:448:ASP:N	2.44	0.42
2:R:110:LEU:O	2:R:114:ILE:HG12	2.18	0.42
6:Z:314:GLU:OE2	6:Z:314:GLU:N	2.52	0.42
1:Q:1189:SER:HB2	4:V:295:TYR:HE2	1.83	0.42
4:T:409:GLU:O	5:U:457:SER:OG	2.37	0.42
1:Q:952:VAL:HG13	1:Q:1303:LYS:HZ1	1.84	0.42
1:Q:953:LEU:CD1	1:Q:1423:LEU:HB3	2.49	0.42
1:Q:1225:GLY:HA2	5:Y:195:ALA:HB3	2.01	0.42
2:R:231:TYR:OH	2:R:595:LEU:O	2.38	0.42
2:R:614:LEU:HD22	2:R:615:ASN:H	1.85	0.42
4:T:23:ARG:NH1	5:Y:316:GLU:O	2.53	0.42
4:T:70:MET:HE1	5:U:375:GLU:HG2	2.01	0.42
4:V:99:LYS:HD3	4:V:132:ARG:HH22	1.84	0.42
4:V:128:ALA:HB3	4:V:334:PRO:HG3	2.01	0.42
1:Q:1009:LYS:HG3	1:Q:1323:GLN:HE22	1.84	0.42
5:U:124:SER:HB2	5:U:319:PRO:HG3	2.01	0.42
4:X:116:LYS:H	4:X:116:LYS:HG2	1.62	0.42
1:Q:949:GLU:HA	1:Q:1419:VAL:CB	2.48	0.42
2:R:684:ILE:HD13	2:R:684:ILE:HA	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:161:LYS:HG3	5:U:166:GLU:HB2	2.02	0.42
2:R:599:ARG:HD3	2:R:599:ARG:HA	1.85	0.42
4:V:35:LEU:HD11	4:V:59:GLY:HA3	2.02	0.42
2:R:130:ILE:HG22	2:R:132:ASN:H	1.85	0.42
4:V:378:ASP:OD1	4:V:378:ASP:N	2.50	0.42
5:W:346:ASP:OD1	5:W:346:ASP:N	2.49	0.42
5:Y:135:LEU:O	5:Y:230:GLN:HA	2.20	0.42
5:W:47:GLN:HG2	5:W:359:TYR:CE1	2.54	0.42
2:R:127:ASP:HB3	2:R:131:PRO:HB3	2.02	0.41
4:V:139:VAL:HG12	4:V:203:GLU:HA	2.02	0.41
5:W:47:GLN:HG2	5:W:359:TYR:HE1	1.85	0.41
5:Y:400:SER:HA	5:Y:403:ILE:HD12	2.01	0.41
1:Q:1253:THR:O	1:Q:1257:MET:HG3	2.20	0.41
4:T:317:ASP:H	4:T:320:ILE:HD12	1.85	0.41
4:V:177:LYS:HE3	4:V:238:HIS:HB2	2.02	0.41
4:X:128:ALA:HB3	4:X:334:PRO:HG3	2.01	0.41
1:Q:949:GLU:HA	1:Q:1419:VAL:CG1	2.50	0.41
5:W:210:ARG:NH1	5:W:211:ASP:O	2.54	0.41
1:Q:1425:ARG:HA	1:Q:1430:GLU:HG2	2.01	0.41
2:R:135:LEU:HD12	2:R:135:LEU:HA	1.97	0.41
2:R:608:GLU:HA	2:R:611:GLN:HB2	2.03	0.41
4:T:435:VAL:HG13	4:T:437:ASN:H	1.85	0.41
4:V:198:ASP:OD2	4:V:211:ARG:NE	2.46	0.41
4:X:133:ILE:HG23	4:X:301:ALA:HB2	2.01	0.41
2:R:104:PHE:CE1	2:R:146:GLN:HG2	2.56	0.41
5:U:135:LEU:HD23	5:U:135:LEU:HA	1.95	0.41
4:V:296:ILE:HD11	4:V:303:LEU:HB2	2.02	0.41
5:W:371:ARG:HD2	5:W:371:ARG:HA	1.82	0.41
5:Y:413:ARG:HH22	5:Y:415:ASN:HD22	1.67	0.41
1:Q:1015:ASP:OD1	1:Q:1020:ALA:N	2.53	0.41
2:R:213:ASN:ND2	3:S:104:GLU:OE2	2.53	0.41
2:R:643:GLU:O	2:R:647:LEU:HB2	2.20	0.41
4:T:29:HIS:NE2	7:T:501:ADP:O2'	2.39	0.41
4:T:418:LEU:HD21	4:T:446:PHE:HB2	2.03	0.41
5:U:45:VAL:HG11	5:U:366:THR:HB	2.03	0.41
5:W:114:THR:O	5:W:118:THR:OG1	2.33	0.41
1:Q:1249:ILE:HD11	1:Q:1269:PRO:HG2	2.03	0.41
1:Q:1257:MET:HA	1:Q:1261:LYS:HB2	2.03	0.41
1:Q:1390:ILE:HG12	1:Q:1420:TYR:HB2	2.02	0.41
3:S:29:ARG:O	3:S:33:LEU:CD1	2.67	0.41
3:S:29:ARG:HH21	3:S:32:PHE:HD2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:90:LEU:O	4:T:94:GLN:HG2	2.20	0.41
4:T:248:THR:OG1	4:T:251:ASP:OD1	2.37	0.41
4:V:119:GLU:HG2	4:V:279:GLU:HA	2.02	0.41
4:X:177:LYS:HB2	4:X:177:LYS:HE2	1.88	0.41
4:X:309:PHE:HD1	4:X:337:VAL:HG23	1.86	0.41
1:Q:962:LYS:HE2	4:X:98:PRO:HB2	2.02	0.41
2:R:40:ILE:HB	2:R:134:ILE:HD12	2.03	0.41
4:T:128:ALA:HB3	4:T:334:PRO:HG3	2.03	0.41
5:U:298:VAL:HG13	5:U:343:LEU:HD21	2.03	0.41
4:V:202:ILE:HG12	4:V:209:VAL:HG12	2.02	0.41
2:R:82:VAL:HG13	2:R:114:ILE:HD13	2.02	0.40
2:R:89:ASP:HB3	2:R:92:VAL:HG12	2.03	0.40
2:R:136:LEU:HB3	2:R:165:PHE:HB3	2.02	0.40
5:U:76:PRO:HG2	5:U:79:THR:HG21	2.04	0.40
5:U:161:LYS:HE3	5:U:161:LYS:HB3	1.94	0.40
4:X:116:LYS:HD2	5:Y:108:SER:HA	2.03	0.40
4:X:181:LEU:HD13	4:X:185:ILE:HG22	2.03	0.40
4:X:313:VAL:HG12	4:X:340:SER:HB2	2.03	0.40
5:Y:69:ARG:HD3	5:Y:69:ARG:HA	1.90	0.40
1:Q:1288:MET:HG3	4:X:212:VAL:HG13	2.03	0.40
2:R:130:ILE:HD13	2:R:130:ILE:HA	2.00	0.40
4:T:127:ARG:NH1	5:Y:268:GLU:OE1	2.43	0.40
4:V:156:LEU:HB3	4:V:157:GLY:H	1.78	0.40
4:V:324:LEU:HD12	4:V:324:LEU:HA	1.94	0.40
1:Q:983:THR:HG23	1:Q:1435:ARG:CG	2.49	0.40
4:T:115:VAL:HG22	4:T:116:LYS:N	2.37	0.40
4:V:432:LYS:HD2	4:V:432:LYS:HA	1.96	0.40
5:W:79:THR:O	5:W:359:TYR:OH	2.37	0.40
5:W:273:ILE:HD13	5:W:273:ILE:HA	1.93	0.40
1:Q:948:ILE:HG13	1:Q:1417:VAL:CG1	2.47	0.40
1:Q:1019:ARG:HA	1:Q:1019:ARG:HD2	1.95	0.40
2:R:148:THR:HG22	2:R:739:PRO:HB2	2.04	0.40
4:T:454:LYS:HA	4:T:454:LYS:HD3	1.88	0.40
5:W:147:ARG:HG2	5:W:154:LYS:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	407/1489 (27%)	387 (95%)	20 (5%)	0	100	100
2	R	438/755 (58%)	416 (95%)	22 (5%)	0	100	100
3	S	124/166 (75%)	115 (93%)	9 (7%)	0	100	100
4	T	433/463 (94%)	424 (98%)	9 (2%)	0	100	100
4	V	440/463 (95%)	425 (97%)	15 (3%)	0	100	100
4	X	441/463 (95%)	432 (98%)	9 (2%)	0	100	100
5	U	443/460 (96%)	432 (98%)	11 (2%)	0	100	100
5	W	440/460 (96%)	425 (97%)	15 (3%)	0	100	100
5	Y	432/460 (94%)	417 (96%)	15 (4%)	0	100	100
6	Z	26/320 (8%)	25 (96%)	1 (4%)	0	100	100
All	All	3624/5499 (66%)	3498 (96%)	126 (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	387/1350 (29%)	386 (100%)	1 (0%)	86	92
2	R	387/682 (57%)	387 (100%)	0	100	100
3	S	106/142 (75%)	106 (100%)	0	100	100
4	T	367/391 (94%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	V	373/391 (95%)	373 (100%)	0	100	100
4	X	375/391 (96%)	375 (100%)	0	100	100
5	U	378/394 (96%)	378 (100%)	0	100	100
5	W	375/394 (95%)	375 (100%)	0	100	100
5	Y	371/394 (94%)	371 (100%)	0	100	100
6	Z	26/285 (9%)	26 (100%)	0	100	100
All	All	3145/4814 (65%)	3144 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	Q	1435	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	958	GLN
1	Q	965	GLN
1	Q	1110	ASN
1	Q	1204	ASN
1	Q	1231	ASN
1	Q	1323	GLN
1	Q	1339	GLN
1	Q	1362	GLN
2	R	23	GLN
2	R	152	GLN
2	R	177	ASN
2	R	191	HIS
2	R	609	GLN
2	R	653	GLN
2	R	659	GLN
2	R	701	ASN
2	R	720	ASN
3	S	82	ASN
4	T	27	HIS
4	T	260	GLN
4	T	427	GLN
4	T	440	ASN
5	U	407	GLN

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Mol	Chain	Res	Type
4	V	27	HIS
4	V	94	GLN
4	V	124	ASN
4	V	263	GLN
4	V	331	ASN
4	V	417	GLN
5	W	144	GLN
5	W	223	GLN
5	W	242	HIS
5	W	415	ASN
4	X	124	ASN
4	X	190	GLN
4	X	325	ASN
4	X	417	GLN
5	Y	408	GLN
5	Y	415	ASN
5	Y	451	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 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	W	501	-	28,29,29	1.39	4 (14%)	43,45,45	1.81	7 (16%)
7	ADP	T	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.83	8 (18%)
7	ADP	V	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.83	9 (20%)
7	ADP	U	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	9 (20%)
7	ADP	Y	501	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	7 (16%)
7	ADP	X	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	W	501	-	-	0/16/32/32	0/3/3/3
7	ADP	T	501	-	-	3/16/32/32	0/3/3/3
7	ADP	V	501	-	-	3/16/32/32	0/3/3/3
7	ADP	U	501	-	-	3/16/32/32	0/3/3/3
7	ADP	Y	501	-	-	3/16/32/32	0/3/3/3
7	ADP	X	501	-	-	2/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	501	ADP	C5-C4	4.60	1.47	1.39
7	Y	501	ADP	C5-C4	4.58	1.47	1.39
7	W	501	ADP	C5-C4	4.53	1.47	1.39
7	X	501	ADP	C5-C4	4.51	1.47	1.39
7	V	501	ADP	C5-C4	4.47	1.47	1.39
7	T	501	ADP	C5-C4	4.45	1.47	1.39
7	U	501	ADP	C5-C6	2.70	1.48	1.41
7	W	501	ADP	C5-C6	2.67	1.48	1.41
7	X	501	ADP	C5-C6	2.67	1.48	1.41
7	V	501	ADP	C5-C6	2.63	1.48	1.41
7	T	501	ADP	C5-C6	2.60	1.48	1.41
7	Y	501	ADP	C5-C6	2.59	1.48	1.41
7	U	501	ADP	C5-N7	-2.46	1.34	1.39
7	X	501	ADP	C5-N7	-2.39	1.34	1.39
7	T	501	ADP	C5-N7	-2.38	1.34	1.39
7	Y	501	ADP	C5-N7	-2.35	1.34	1.39
7	W	501	ADP	C5-N7	-2.33	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	501	ADP	C5-N7	-2.32	1.34	1.39
7	Y	501	ADP	C8-N7	2.25	1.36	1.31
7	T	501	ADP	C8-N7	2.24	1.36	1.31
7	W	501	ADP	C8-N7	2.20	1.35	1.31
7	U	501	ADP	C8-N7	2.19	1.35	1.31
7	X	501	ADP	C8-N7	2.19	1.35	1.31
7	V	501	ADP	C8-N7	2.18	1.35	1.31

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	501	ADP	C5-C4-N3	-5.95	118.53	126.72
7	X	501	ADP	C5-C4-N3	-5.91	118.57	126.72
7	T	501	ADP	C5-C4-N3	-5.89	118.60	126.72
7	U	501	ADP	C5-C4-N3	-5.88	118.62	126.72
7	V	501	ADP	C5-C4-N3	-5.79	118.74	126.72
7	Y	501	ADP	C5-C4-N3	-5.78	118.76	126.72
7	X	501	ADP	N3-C4-N9	4.81	135.35	127.17
7	W	501	ADP	N3-C4-N9	4.74	135.23	127.17
7	T	501	ADP	N3-C4-N9	4.71	135.18	127.17
7	Y	501	ADP	N3-C4-N9	4.68	135.12	127.17
7	V	501	ADP	N3-C4-N9	4.67	135.10	127.17
7	U	501	ADP	N3-C4-N9	4.64	135.06	127.17
7	T	501	ADP	C2-N3-C4	3.75	121.00	111.83
7	X	501	ADP	C2-N3-C4	3.75	121.00	111.83
7	W	501	ADP	C2-N3-C4	3.71	120.88	111.83
7	U	501	ADP	C2-N3-C4	3.70	120.87	111.83
7	Y	501	ADP	C2-N3-C4	3.68	120.83	111.83
7	V	501	ADP	C2-N3-C4	3.66	120.77	111.83
7	V	501	ADP	C4-C5-N7	-3.45	106.64	110.58
7	U	501	ADP	C4-C5-N7	-3.44	106.64	110.58
7	T	501	ADP	C4-C5-N7	-3.36	106.74	110.58
7	Y	501	ADP	C4-C5-N7	-3.33	106.77	110.58
7	W	501	ADP	C4-C5-N7	-3.31	106.79	110.58
7	T	501	ADP	N3-C2-N1	-3.29	123.60	128.58
7	X	501	ADP	N3-C2-N1	-3.28	123.62	128.58
7	X	501	ADP	C4-C5-N7	-3.28	106.84	110.58
7	Y	501	ADP	N3-C2-N1	-3.21	123.72	128.58
7	V	501	ADP	N3-C2-N1	-3.20	123.73	128.58
7	U	501	ADP	N3-C2-N1	-3.17	123.79	128.58
7	W	501	ADP	N3-C2-N1	-3.15	123.82	128.58
7	V	501	ADP	C4-N9-C8	2.86	108.75	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	501	ADP	C4-N9-C8	2.78	108.66	105.74
7	T	501	ADP	C4-N9-C8	2.73	108.61	105.74
7	Y	501	ADP	C4-N9-C8	2.73	108.60	105.74
7	V	501	ADP	C5-N7-C8	2.58	107.51	103.45
7	W	501	ADP	C4-N9-C8	2.57	108.44	105.74
7	U	501	ADP	C3'-C2'-C1'	2.54	106.27	101.46
7	X	501	ADP	C5-N7-C8	2.50	107.38	103.45
7	T	501	ADP	C5-N7-C8	2.49	107.36	103.45
7	U	501	ADP	C4-N9-C8	2.49	108.35	105.74
7	U	501	ADP	C5-N7-C8	2.48	107.35	103.45
7	Y	501	ADP	C5-N7-C8	2.44	107.28	103.45
7	W	501	ADP	C5-N7-C8	2.35	107.15	103.45
7	V	501	ADP	N9-C8-N7	-2.11	110.95	113.94
7	X	501	ADP	N9-C8-N7	-2.03	111.05	113.94
7	V	501	ADP	C6-C5-N7	2.02	135.98	132.09
7	T	501	ADP	N9-C8-N7	-2.02	111.07	113.94
7	U	501	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

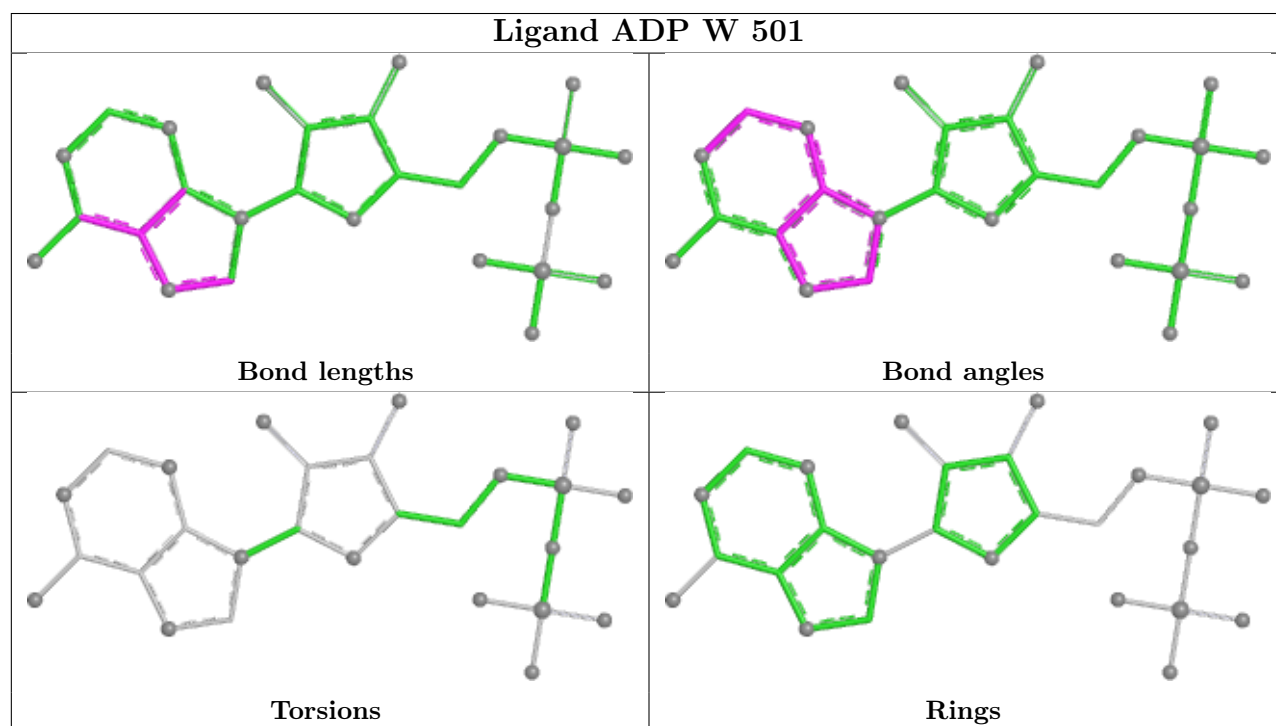
Mol	Chain	Res	Type	Atoms
7	T	501	ADP	C5'-O5'-PA-O1A
7	T	501	ADP	C5'-O5'-PA-O2A
7	T	501	ADP	C5'-O5'-PA-O3A
7	U	501	ADP	C5'-O5'-PA-O1A
7	U	501	ADP	C5'-O5'-PA-O2A
7	U	501	ADP	C5'-O5'-PA-O3A
7	V	501	ADP	C5'-O5'-PA-O2A
7	V	501	ADP	C5'-O5'-PA-O3A
7	Y	501	ADP	C5'-O5'-PA-O1A
7	Y	501	ADP	C5'-O5'-PA-O2A
7	Y	501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

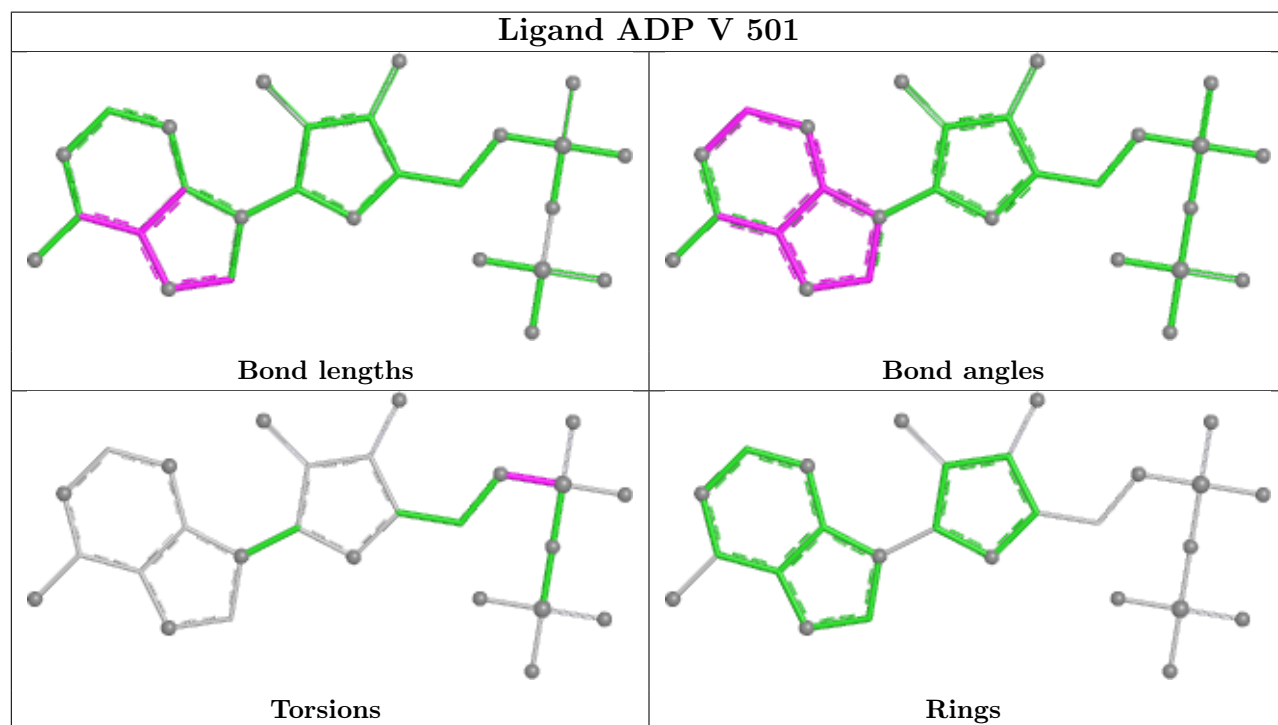
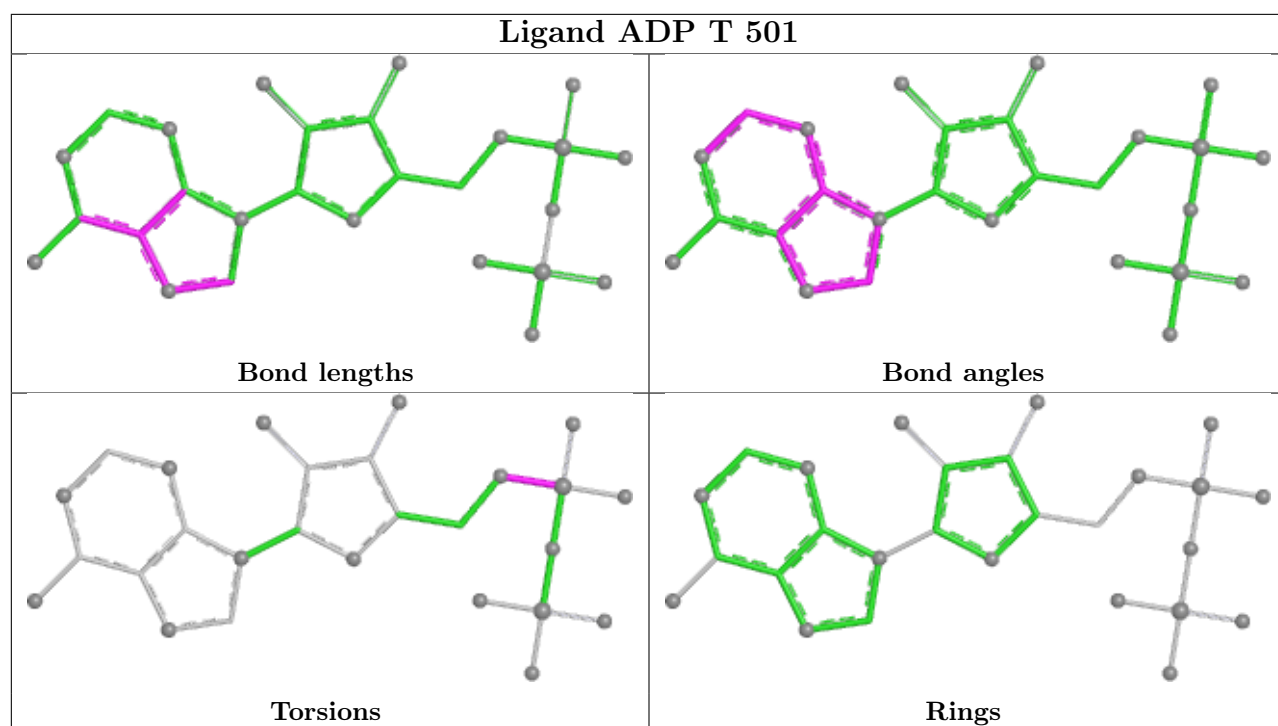
There are no ring outliers.

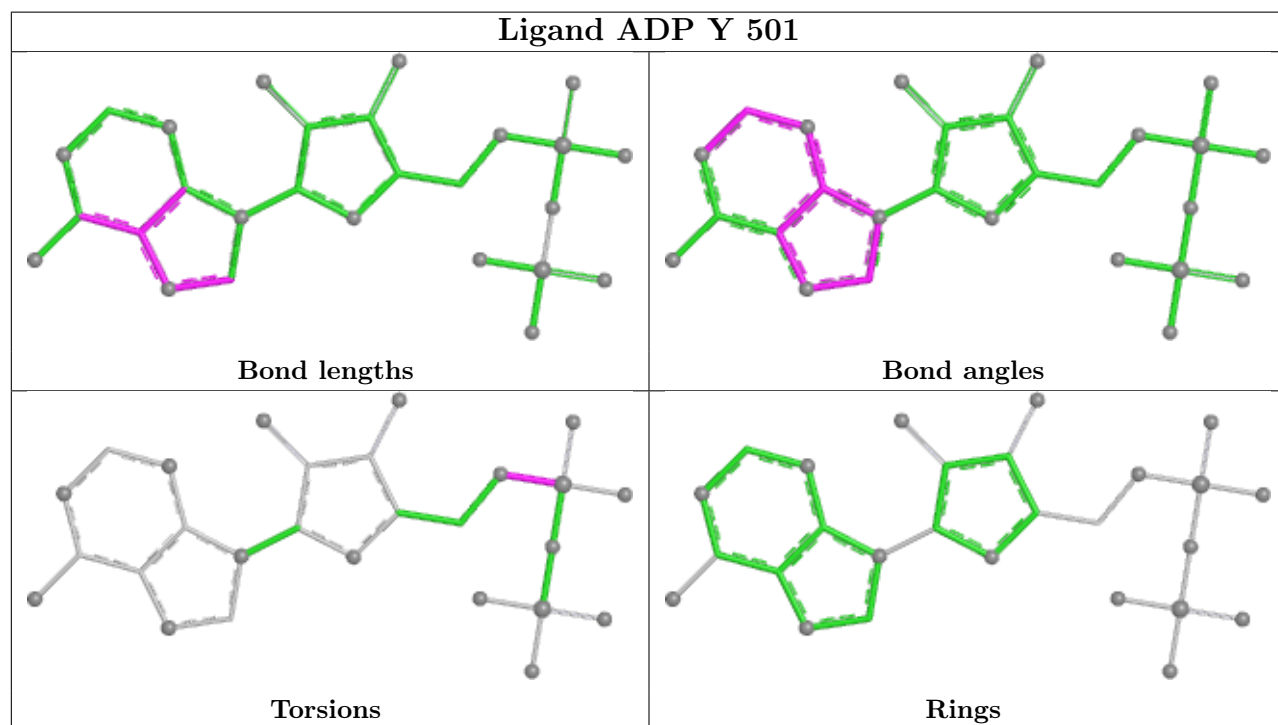
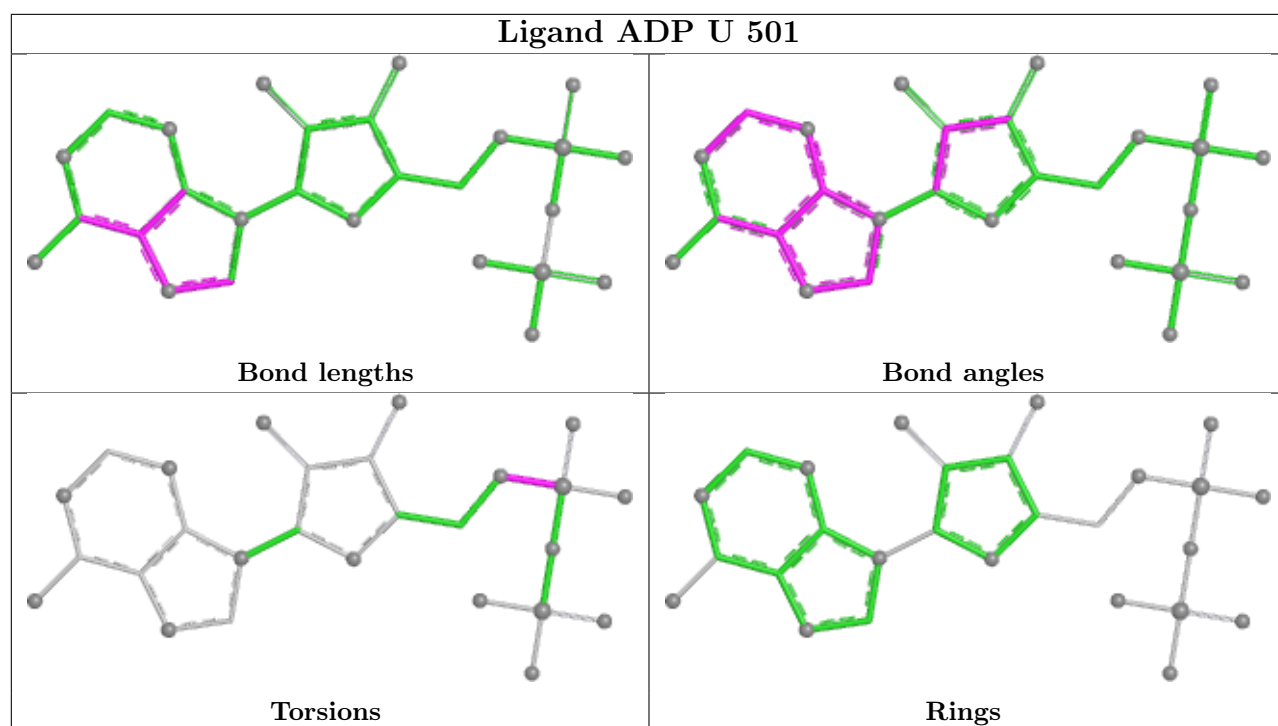
5 monomers are involved in 9 short contacts:

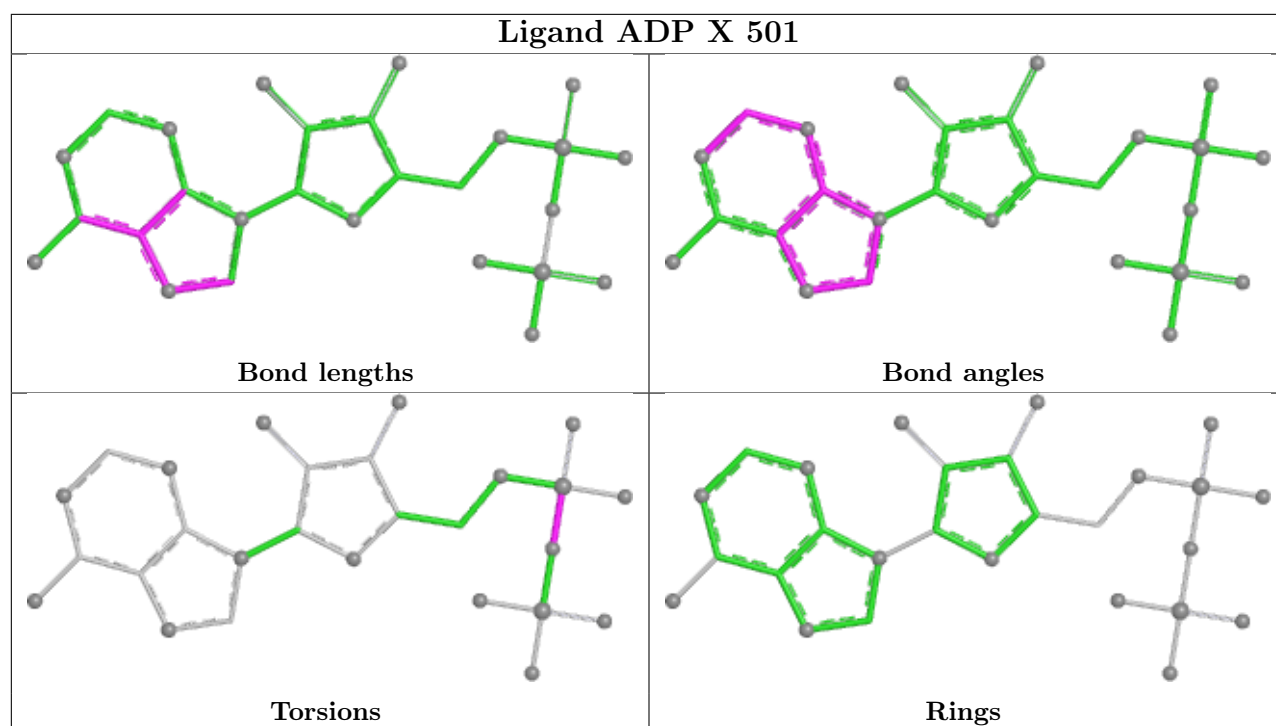
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	W	501	ADP	1	0
7	T	501	ADP	3	0
7	V	501	ADP	2	0
7	Y	501	ADP	2	0
7	X	501	ADP	1	0

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 [i](#)

There are no chain breaks in this entry.

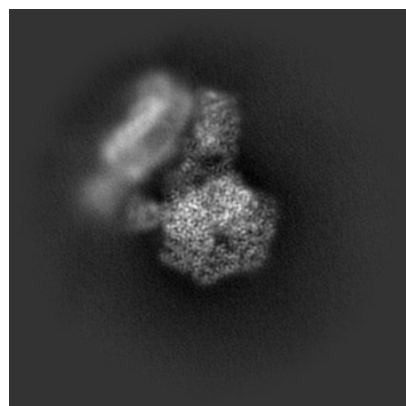
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45377. These allow visual inspection of the internal detail of the map and identification of artifacts.

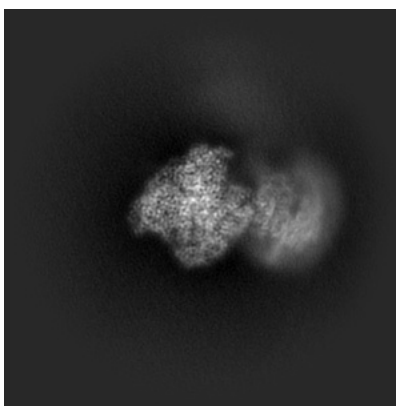
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

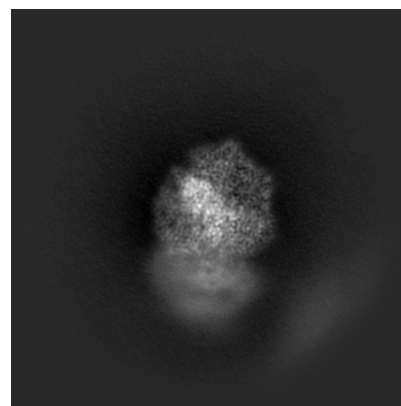
6.1.1 Primary map



X

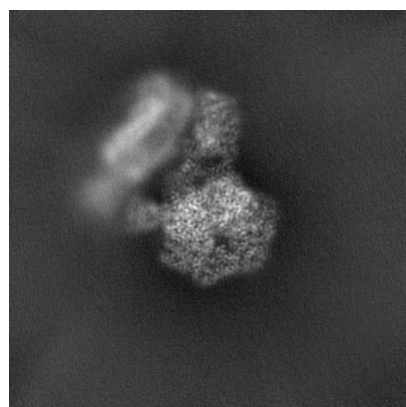


Y

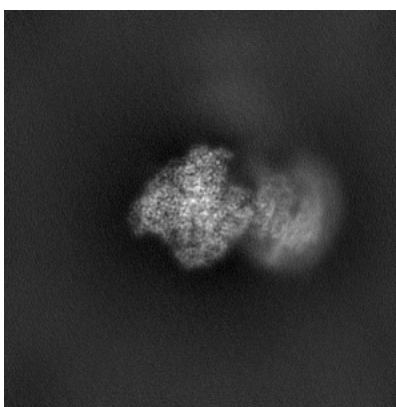


Z

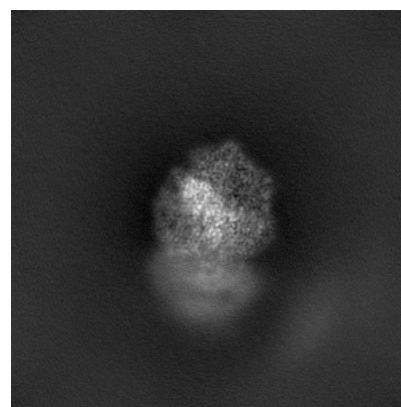
6.1.2 Raw map



X



Y

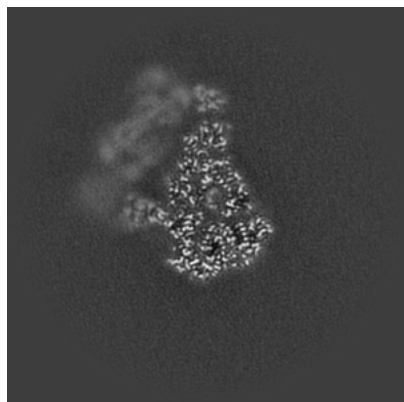


Z

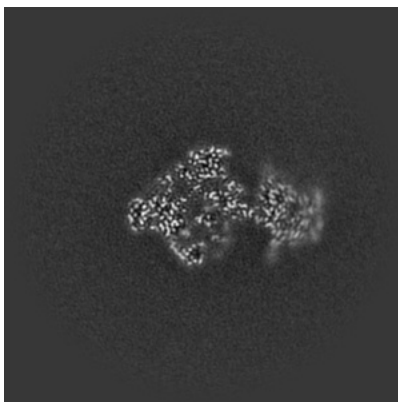
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

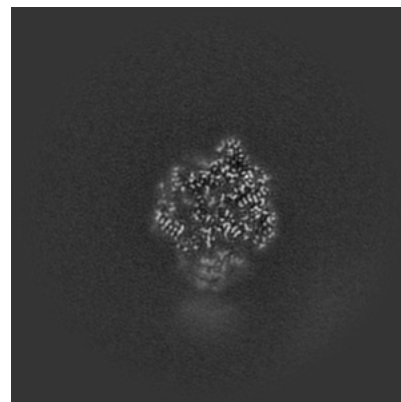
6.2.1 Primary map



X Index: 224

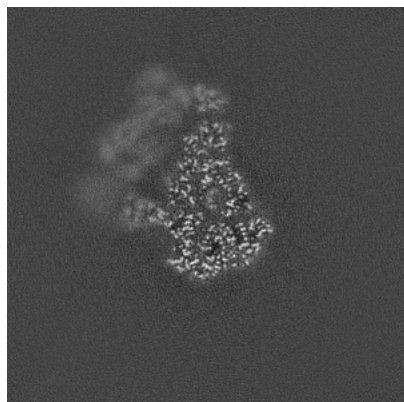


Y Index: 224

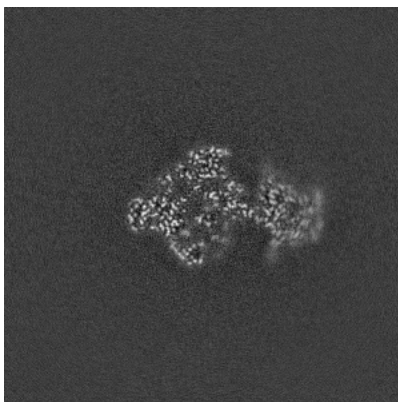


Z Index: 224

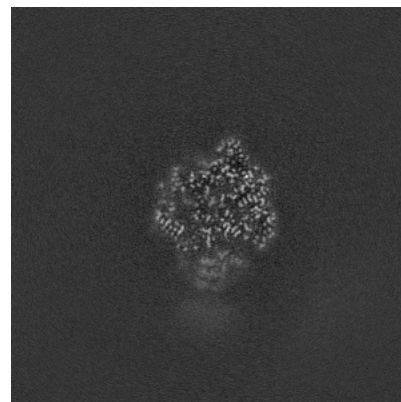
6.2.2 Raw map



X Index: 224



Y Index: 224

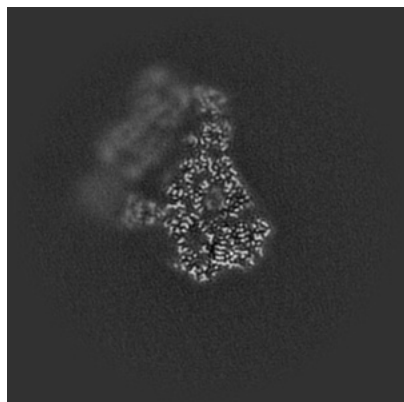


Z Index: 224

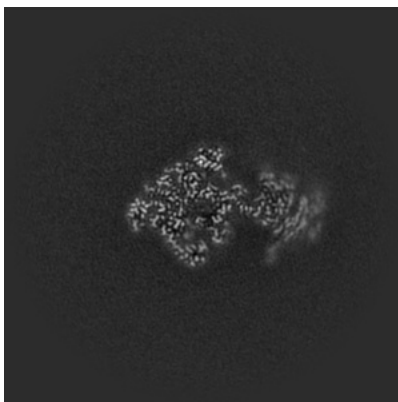
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

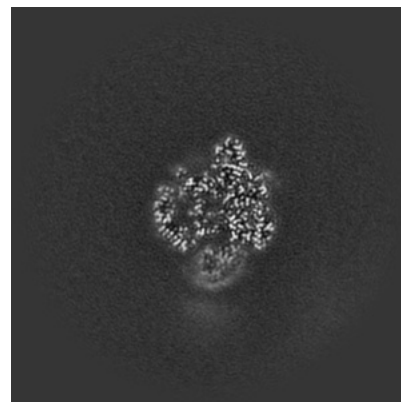
6.3.1 Primary map



X Index: 221

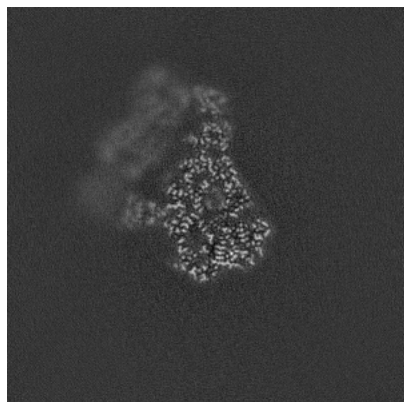


Y Index: 220

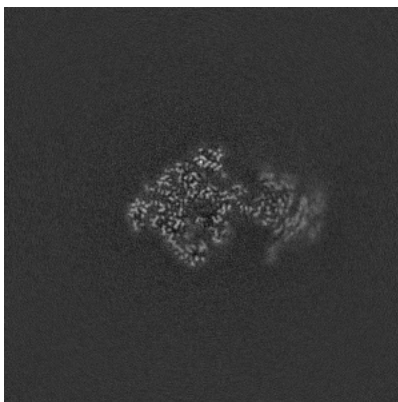


Z Index: 218

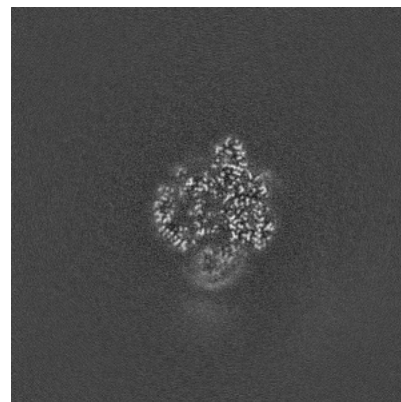
6.3.2 Raw map



X Index: 221



Y Index: 220

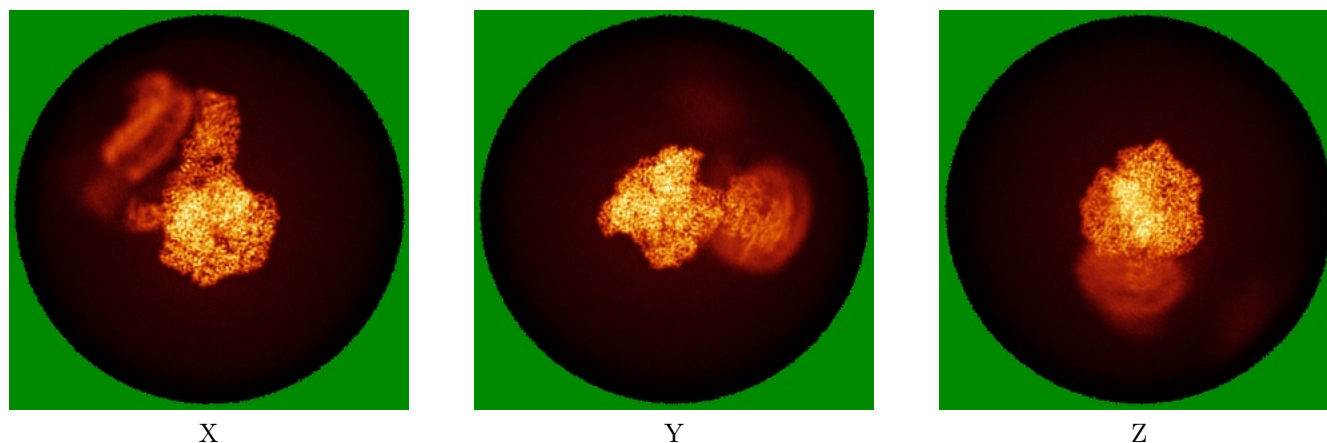


Z Index: 218

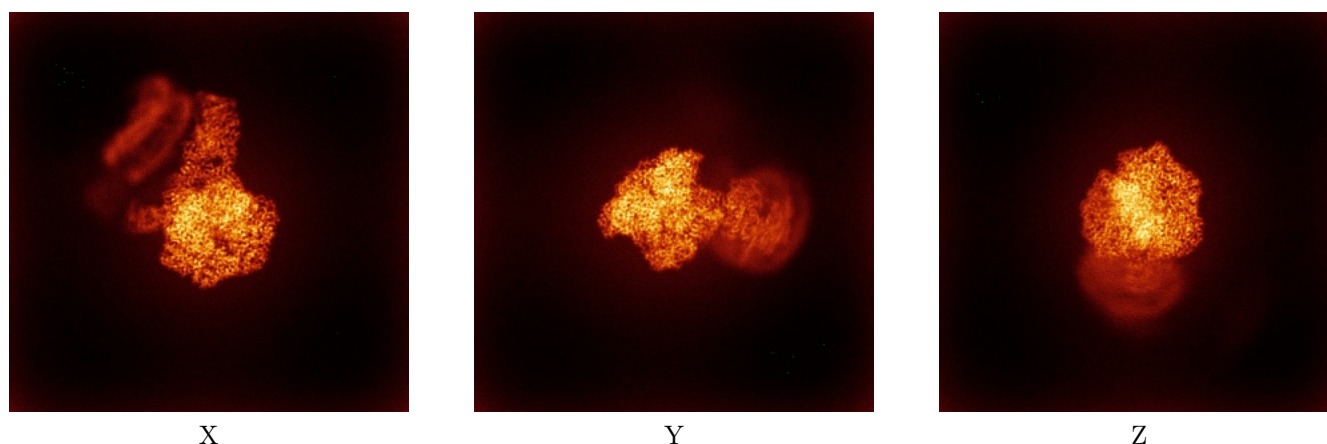
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

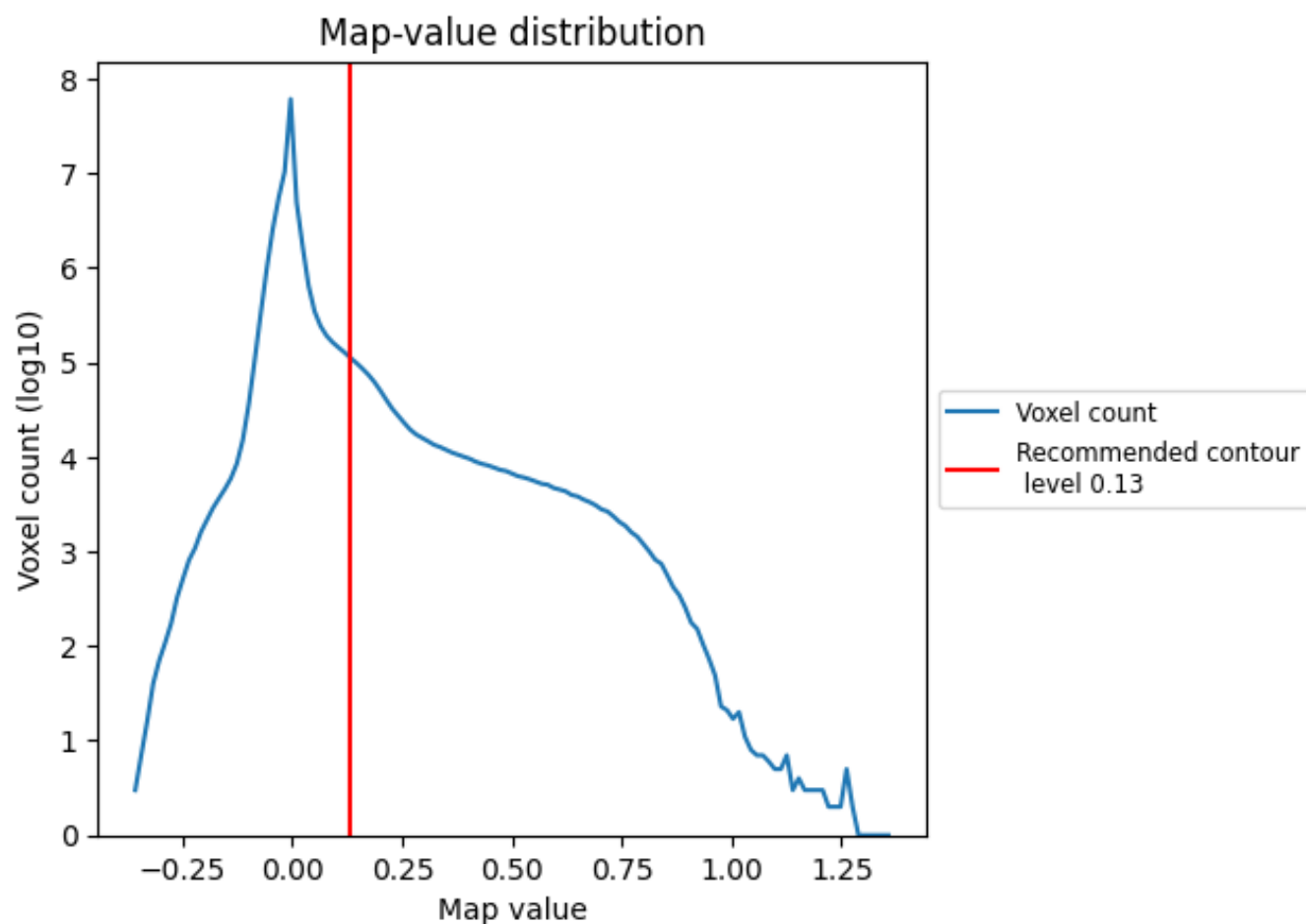
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

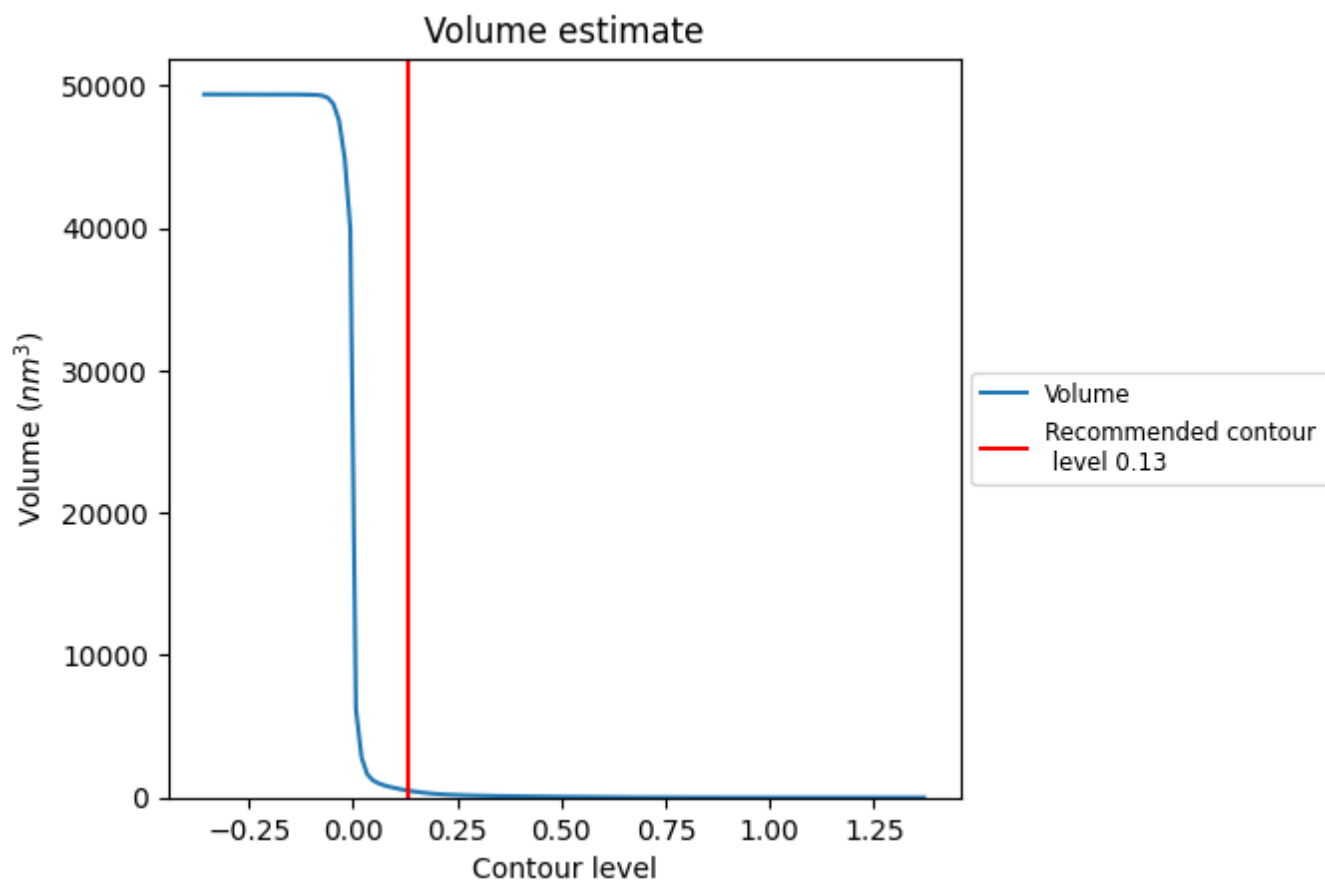
This section contains the results of statistical analysis of the map.

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.

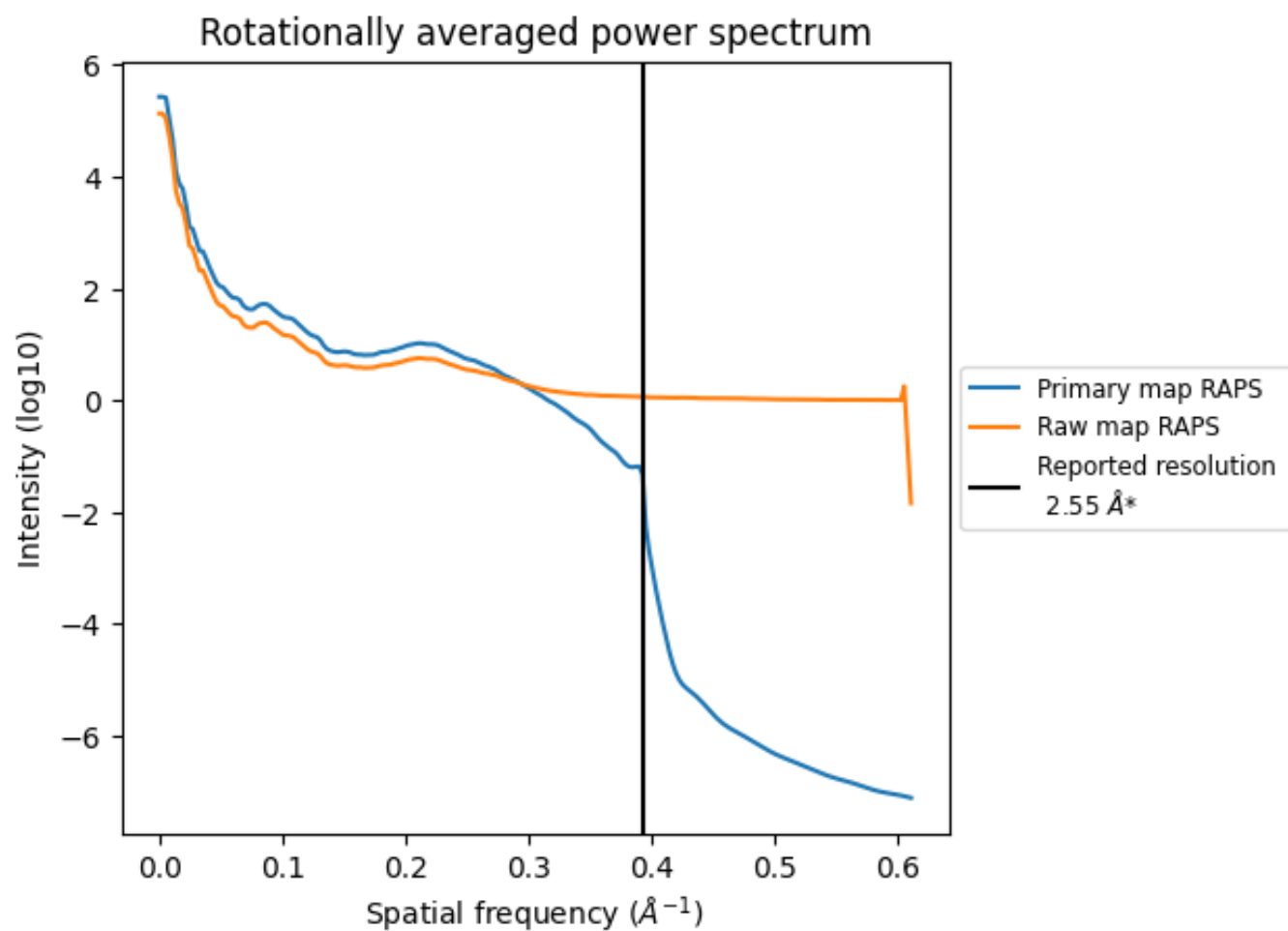
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 500 nm^3 ; this corresponds to an approximate mass of 451 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 ⓘ

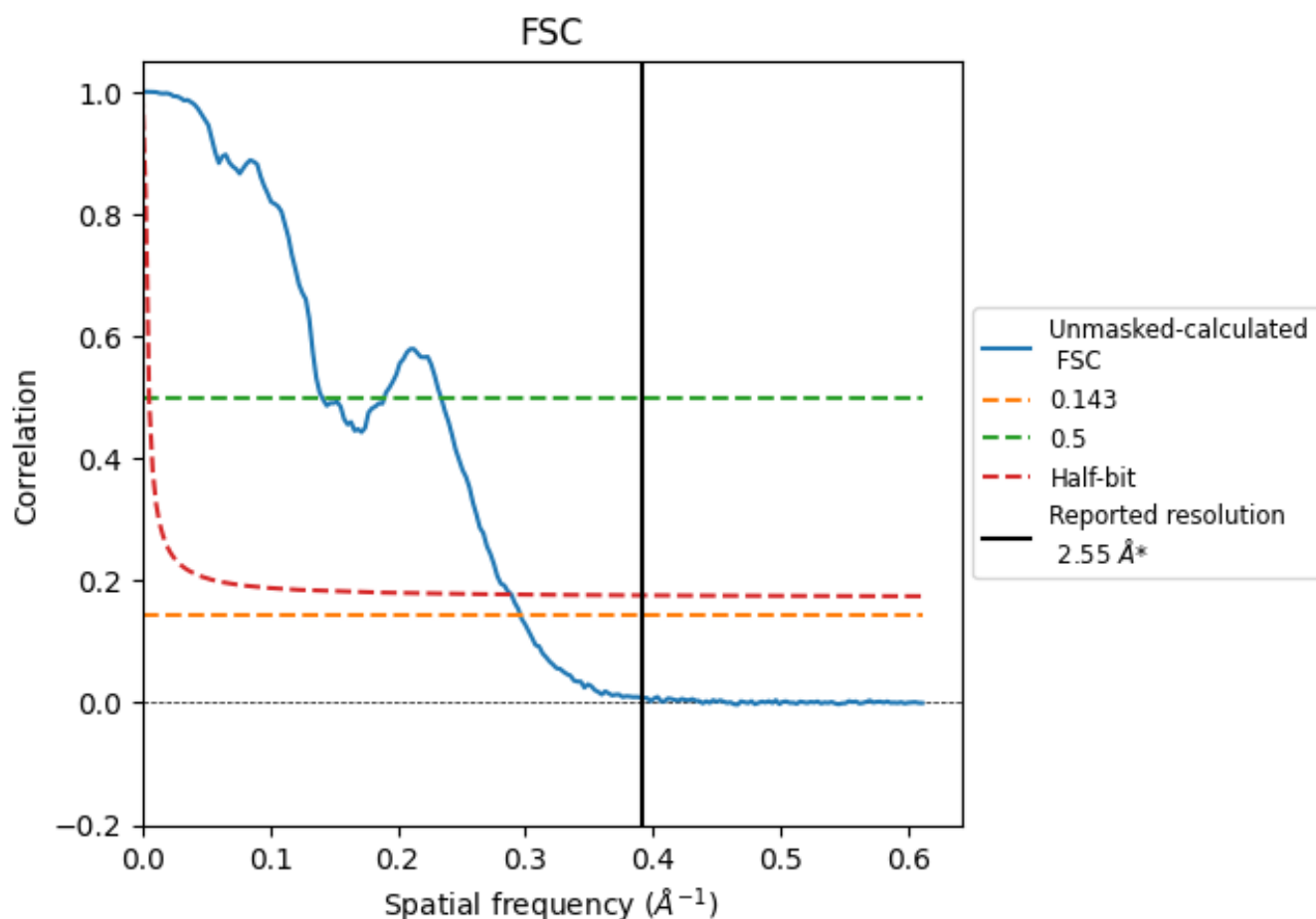


*Reported resolution corresponds to spatial frequency of 0.392 \AA^{-1}

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 0.392 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	7.11	3.46

*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 3.38 differs from the reported value 2.55 by more than 10 %

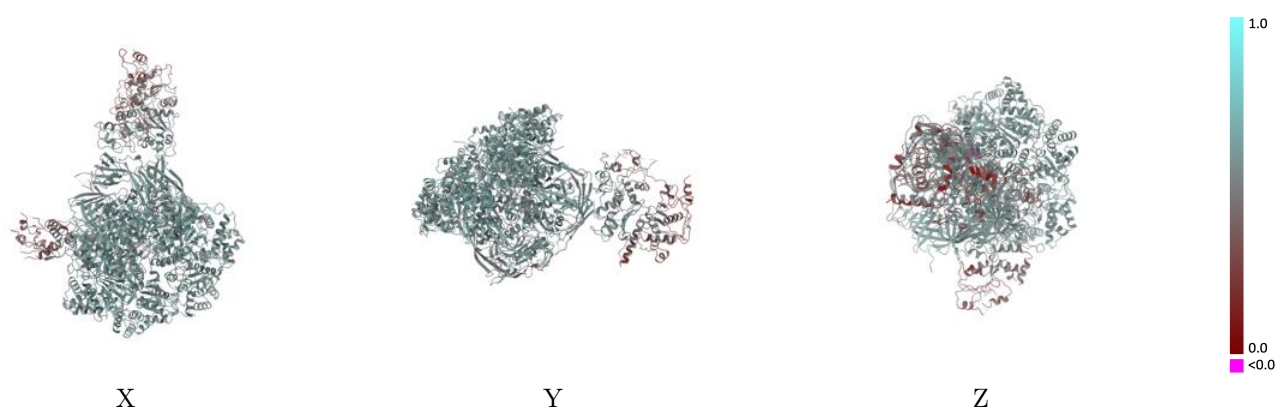
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-45377 and PDB model 9C9Z. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

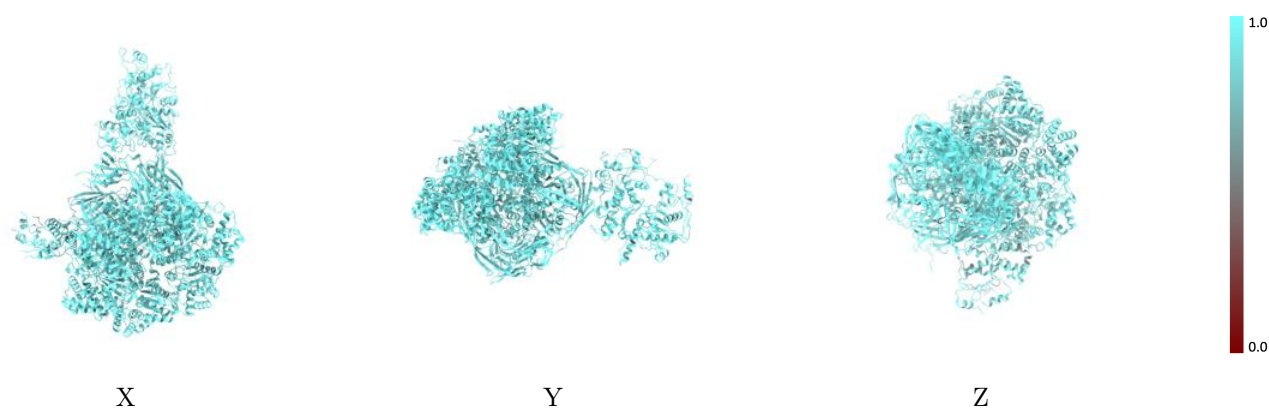
This section was not generated.

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



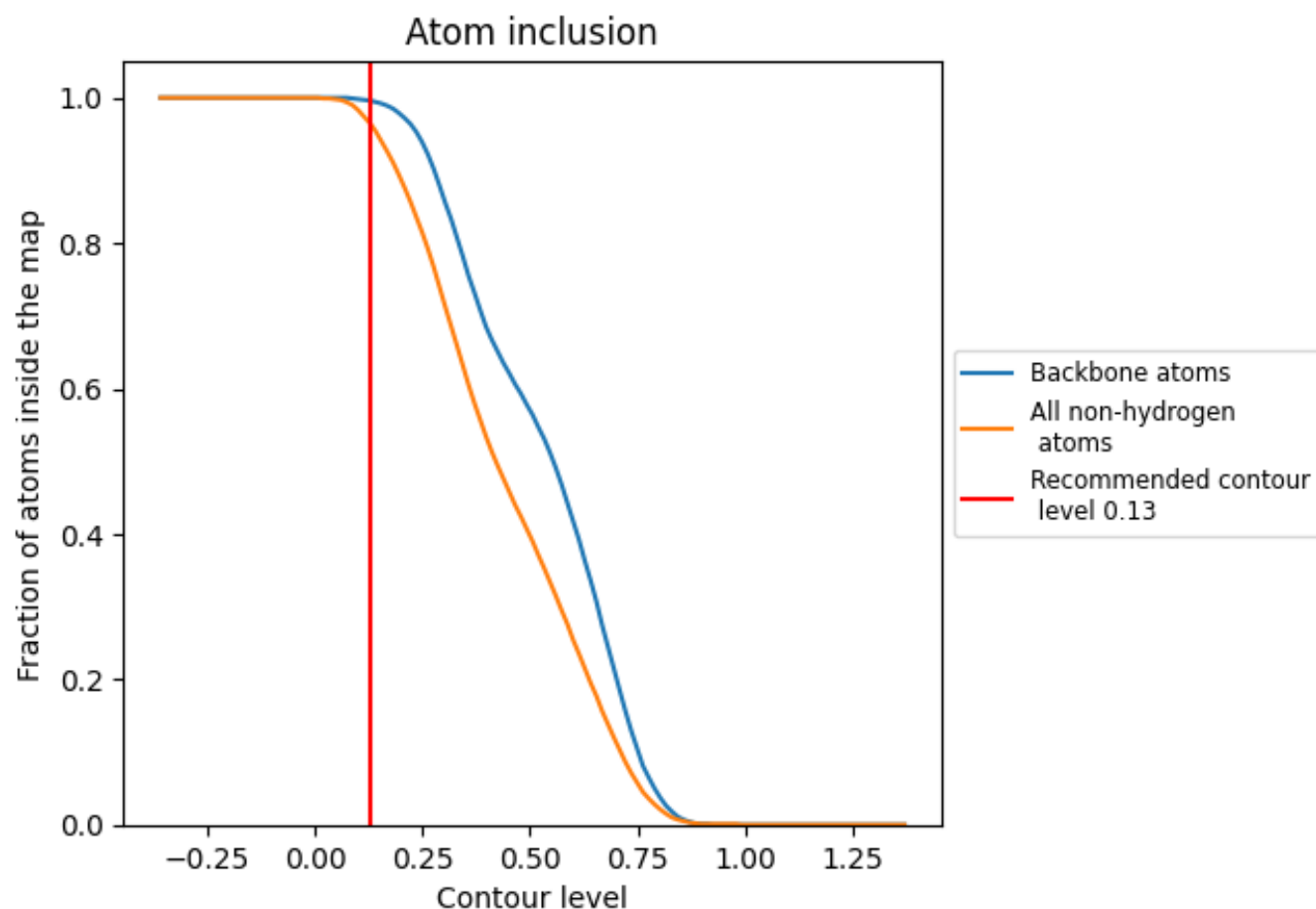
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9640	<div><div></div></div> 0.5380
Q	<div><div></div></div> 0.9280	<div><div></div></div> 0.4830
R	<div><div></div></div> 0.9470	<div><div></div></div> 0.4360
S	<div><div></div></div> 0.9380	<div><div></div></div> 0.4360
T	<div><div></div></div> 0.9740	<div><div></div></div> 0.5700
U	<div><div></div></div> 0.9780	<div><div></div></div> 0.5680
V	<div><div></div></div> 0.9710	<div><div></div></div> 0.5550
W	<div><div></div></div> 0.9760	<div><div></div></div> 0.5720
X	<div><div></div></div> 0.9740	<div><div></div></div> 0.5830
Y	<div><div></div></div> 0.9680	<div><div></div></div> 0.5680
Z	<div><div></div></div> 0.9960	<div><div></div></div> 0.5680

1.0

0.0

<0.0