Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:29 AM UTC

PDB ID	:	9C9T / pdb_00009c9t
EMDB ID	:	EMD-45370
Title	:	S.c INO80 in complex with S.c 0/40 nucleosome, Class 2
Authors	:	Wu, H.; Kaur, U.; Narlikar, G.J.; Cheng, Y.F.
Deposited on	:	2024-06-15
Resolution	:	3.16 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:

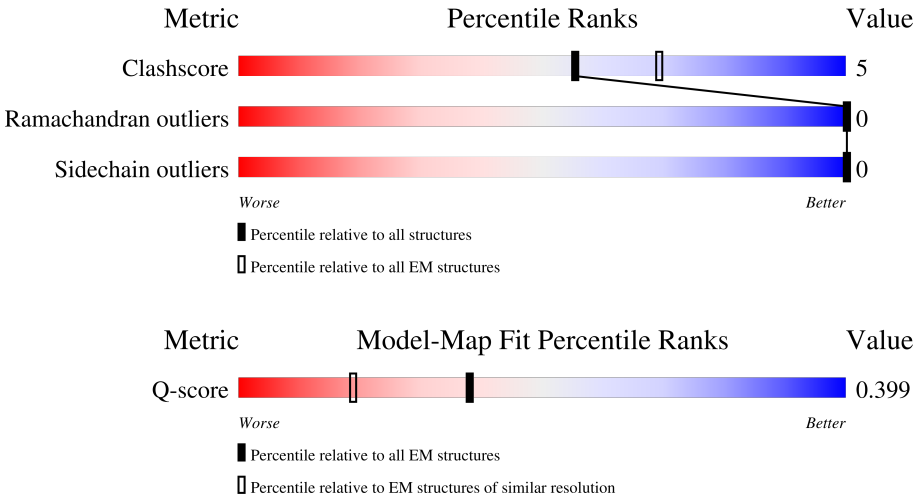
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.16 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	14474 (2.66 - 3.66)

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 <=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	A	136	56% 15% 29%
1	E	136	56% 15% 29%
2	B	103	62% 15% 23%
2	F	103	57% 19% 23%

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Mol	Chain	Length	Quality of chain
3	C	132	70% 10% 20%
3	G	132	65% 15% 18%
4	D	131	63% 8% 29%
4	H	131	54% 16% 29%
5	I	227	54% 11% 35%
6	J	227	53% 11% 35%
7	Q	1489	37% 8% 56%
8	R	755	65% 5% 30%
9	S	166	69% 7% 25%
10	T	463	84% 10% 6%
10	V	463	83% 12% 5%
10	X	463	85% 10%
11	U	460	89% 8%
11	W	460	87% 9%
11	Y	460	89% 6% 5%
12	Z	320	16% 82%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 43084 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 Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	97	Total 801	C 508	N 155	O 138	0	0
1	E	97	Total 801	C 508	N 155	O 138	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total 624	C 392	N 121	O 110	S 1	0	0
2	F	79	Total 620	C 389	N 120	O 110	S 1	0	0

- Molecule 3 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	106	Total 819	C 514	N 161	O 144	0	0
3	G	108	Total 827	C 517	N 164	O 146	0	0

- Molecule 4 is a protein called Histone H2B.1.

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

- Molecule 5 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	147	Total	C	N	O	P	0	0
			3030	1434	567	882	147		

- Molecule 6 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	147	Total	C	N	O	P	0	0
			2997	1423	545	882	147		

- Molecule 7 is a protein called Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	659	Total	C	N	O	S	0	0
			5278	3374	902	978	24		

- Molecule 8 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	525	Total	C	N	O	S	0	0
			3963	2510	681	761	11		

- Molecule 9 is a protein called Chromatin-remodeling complex subunit IES6.

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

- Molecule 10 is a protein called RuvB-like protein 1.

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

- Molecule 11 is a protein called RuvB-like protein 2.

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

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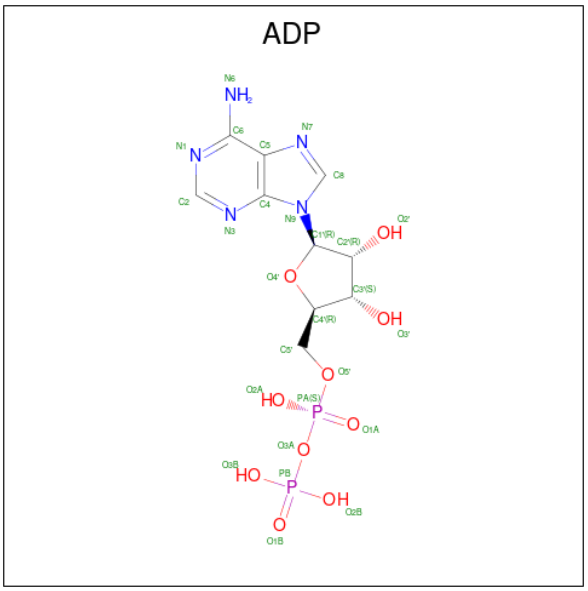
Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	442	Total	C	N	O	S	0	0
			3398	2123	590	673	12		
11	Y	436	Total	C	N	O	S	0	0
			3350	2098	583	658	11		

- Molecule 12 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	56	Total	C	N	O	S	0	0
			387	241	73	71	2		

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



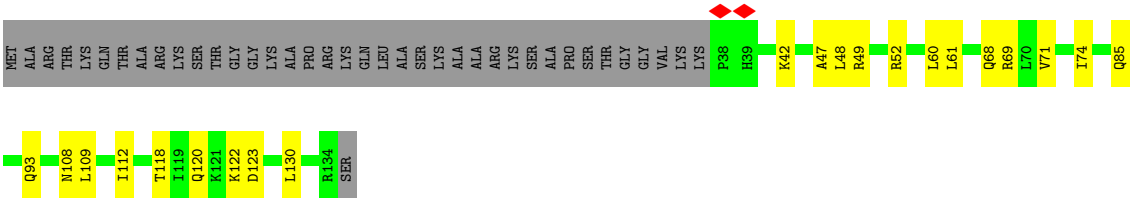
Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

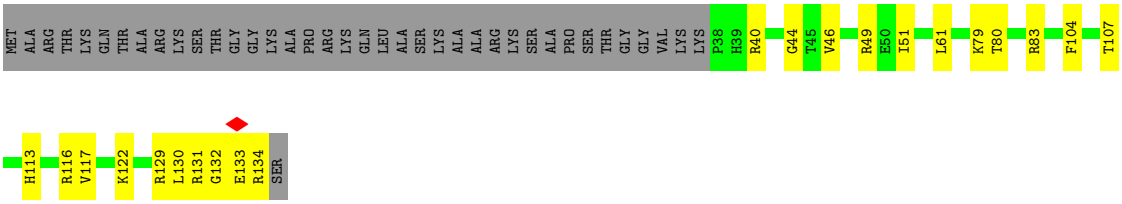
• Molecule 1: Histone H3

Chain A:



• Molecule 1: Histone H3

Chain E:

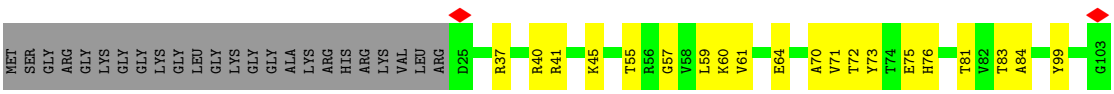


• Molecule 2: Histone H4

Chain B:

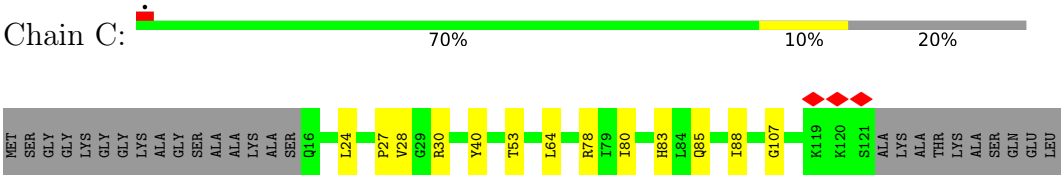
• Molecule 2: Histone H4

Chain F:



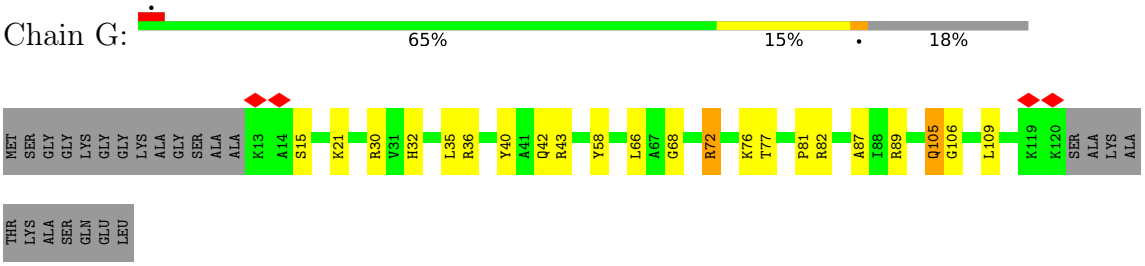
• Molecule 3: Histone H2A.1

Chain C:



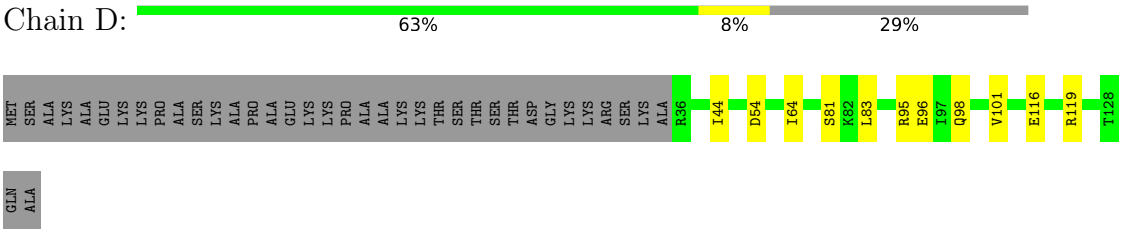
• Molecule 3: Histone H2A.1

Chain G:



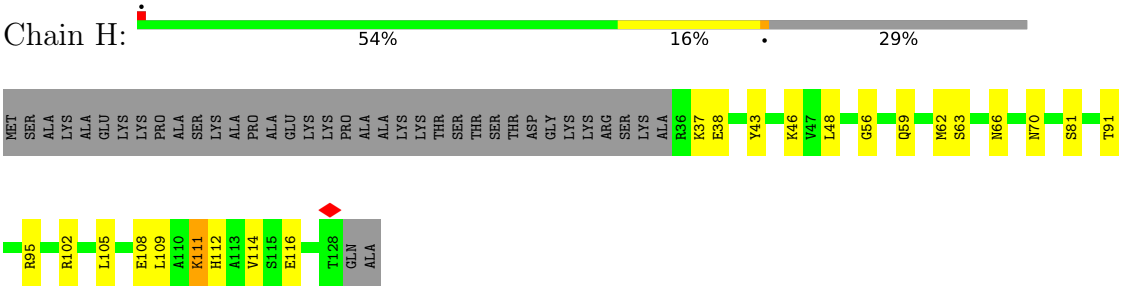
• Molecule 4: Histone H2B.1

Chain D:



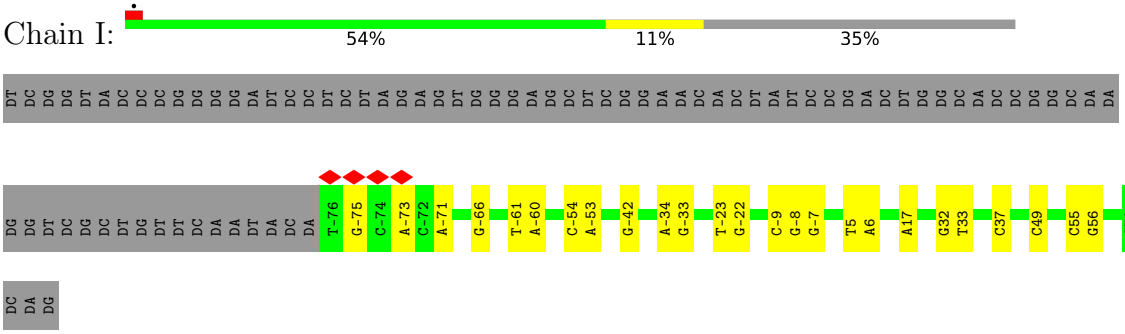
• Molecule 4: Histone H2B.1

Chain H:



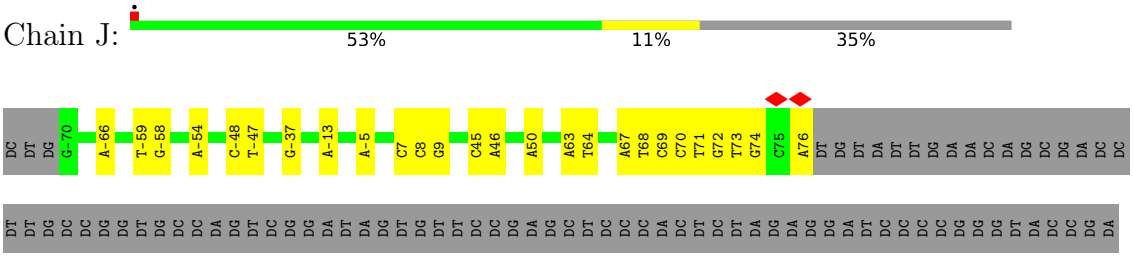
• Molecule 5: DNA (227-MER)

Chain I:



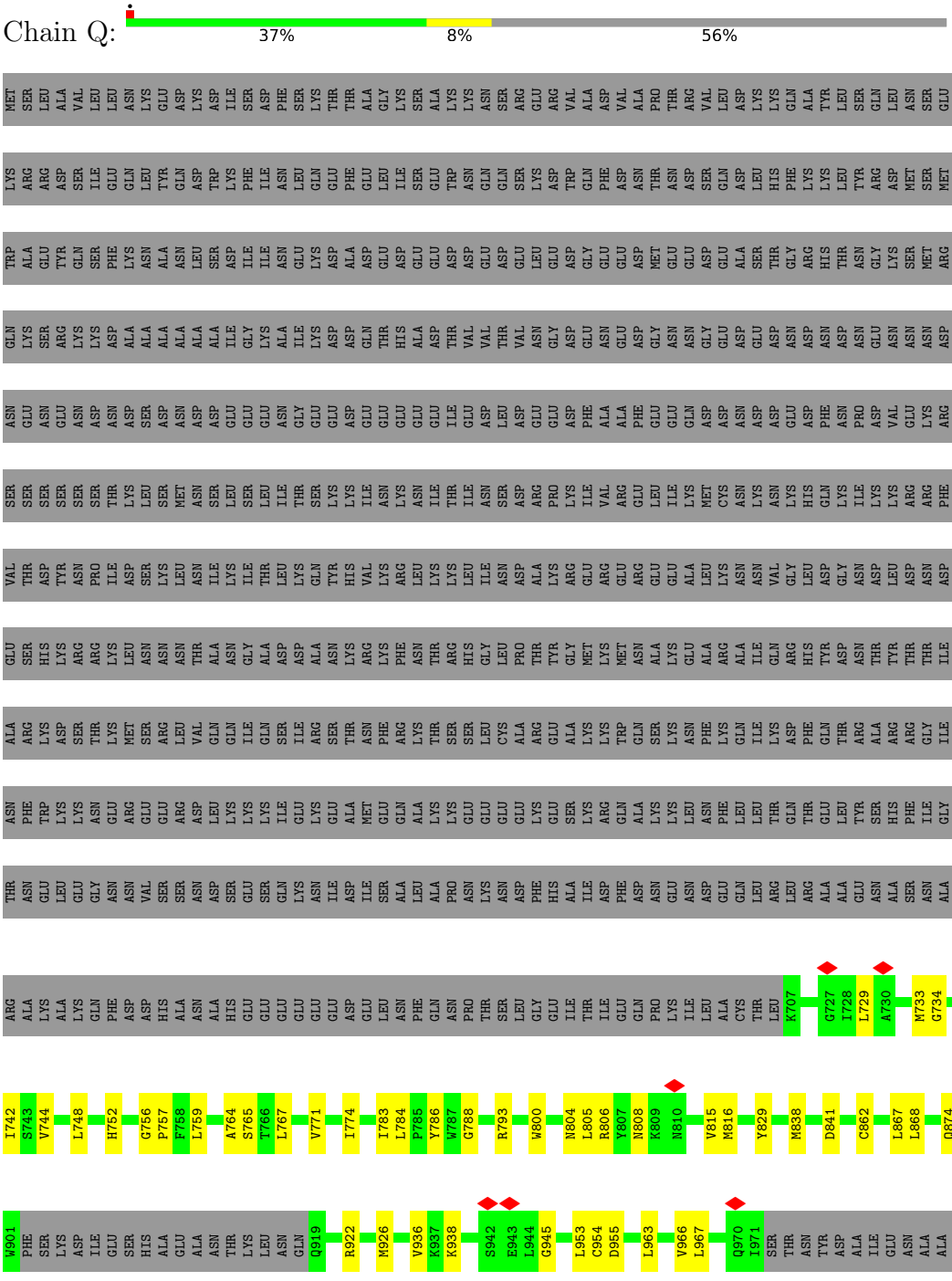
• Molecule 6: DNA (227-MER)

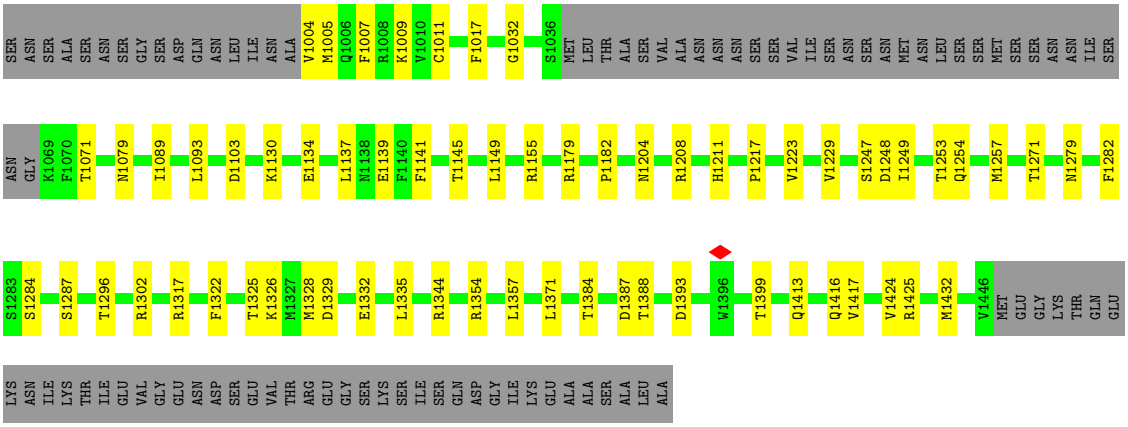
Chain J:



• Molecule 7: Chromatin-remodeling ATPase INO80

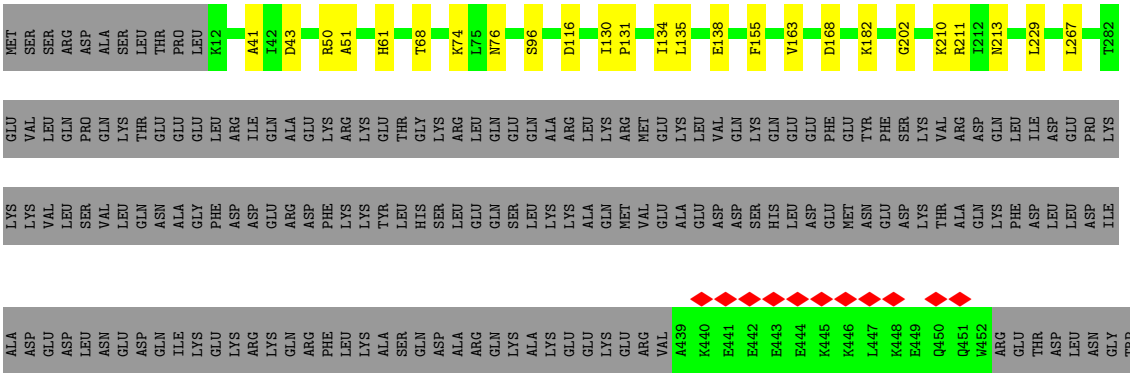
Chain Q:





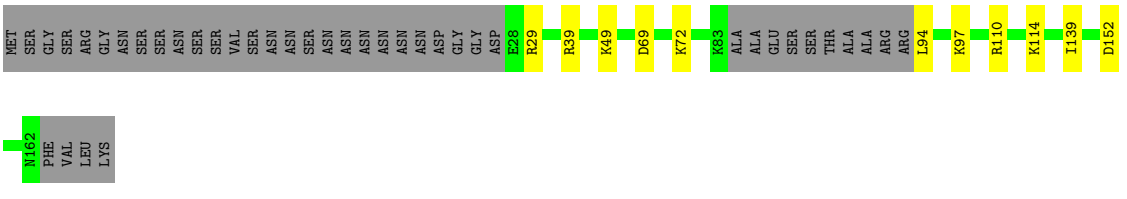
• Molecule 8: Actin-related protein 5

Chain R:



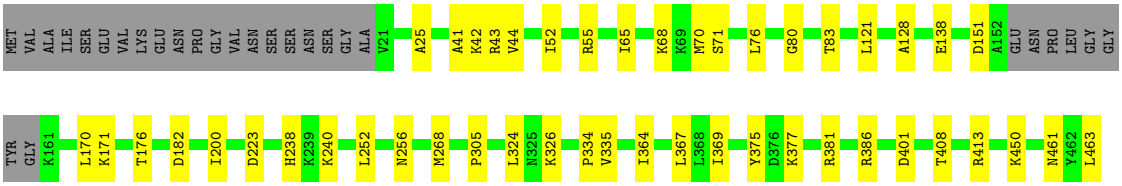
• Molecule 9: Chromatin-remodeling complex subunit IES6

Chain S:



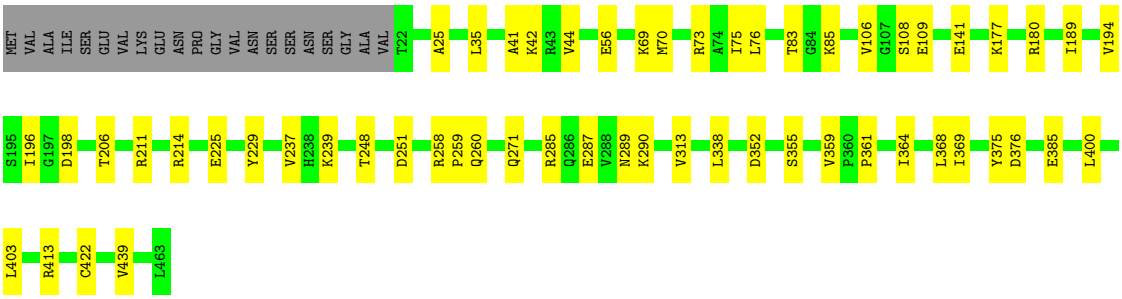
• Molecule 10: RuvB-like protein 1

Chain T:



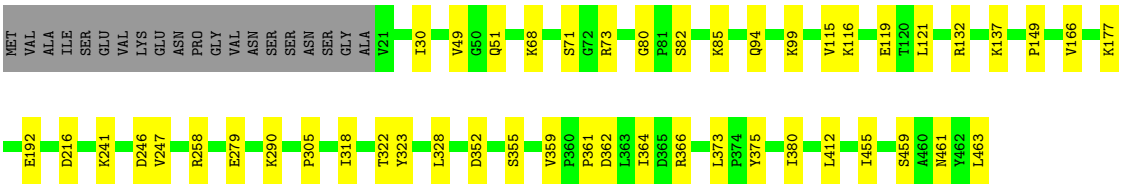
• Molecule 10: RuvB-like protein 1

Chain V:



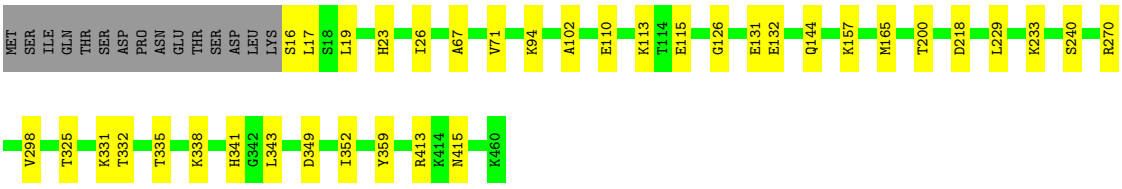
• Molecule 10: RuvB-like protein 1

Chain X:



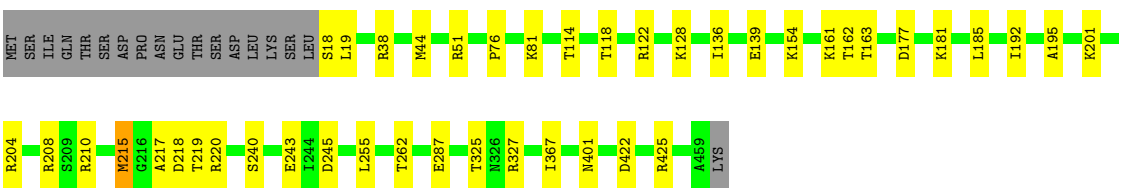
• Molecule 11: RuvB-like protein 2

Chain U:



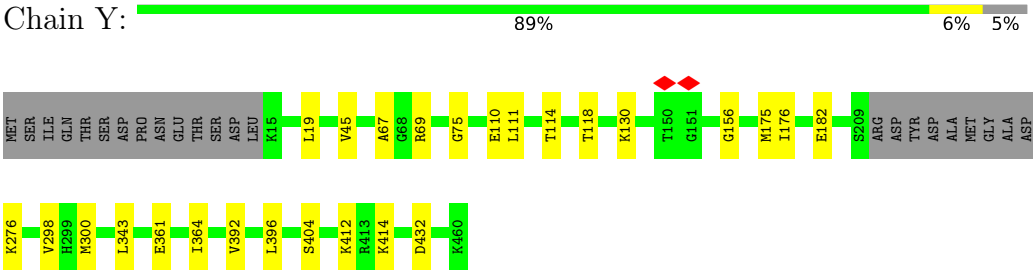
• Molecule 11: RuvB-like protein 2

Chain W:



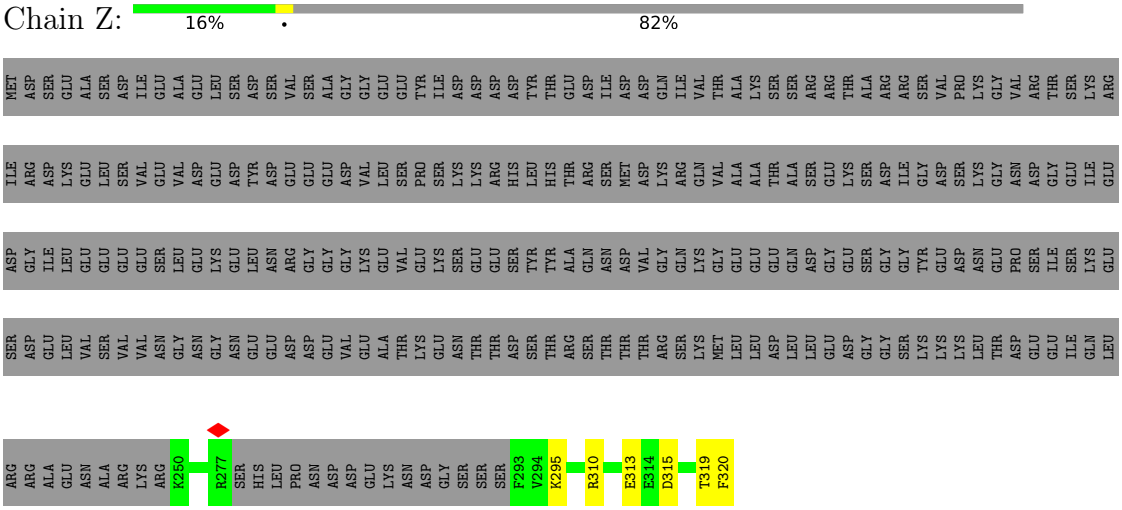
• Molecule 11: RuvB-like protein 2

Chain Y:



• Molecule 12: Ino eighty subunit 2

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73064	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 ($e^-/Å^2$)	45.8	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	1.122	Depositor
Minimum map value	-0.359	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	374.08, 374.08, 374.08	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/812	0.67	0/1086
1	E	0.21	0/812	0.56	1/1086 (0.1%)
2	B	0.31	0/631	0.77	0/844
2	F	0.30	0/627	0.83	0/840
3	C	0.24	0/830	0.54	0/1121
3	G	0.30	0/838	0.75	4/1131 (0.4%)
4	D	0.32	0/736	0.71	0/991
4	H	0.29	0/736	0.78	2/991 (0.2%)
5	I	0.26	0/3402	0.48	0/5253
6	J	0.23	0/3358	0.43	0/5176
7	Q	0.26	0/5396	0.57	0/7324
8	R	0.22	0/4051	0.47	0/5521
9	S	0.21	0/1036	0.55	0/1392
10	T	0.16	0/3378	0.43	0/4569
10	V	0.18	0/3439	0.48	0/4652
10	X	0.19	0/3446	0.51	0/4662
11	U	0.17	0/3459	0.43	0/4662
11	W	0.22	0/3436	0.49	3/4632 (0.1%)
11	Y	0.19	0/3386	0.46	1/4561 (0.0%)
12	Z	0.19	0/392	0.46	0/529
All	All	0.22	0/44201	0.52	11/61023 (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
11	W	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	W	218	ASP	N-CA-C	-9.57	95.86	110.70
11	W	215	MET	CB-CA-C	-6.66	108.88	116.54
4	H	48	LEU	CA-CB-CG	6.03	137.40	116.30
1	E	117	VAL	N-CA-C	-5.87	107.03	113.43
11	W	218	ASP	CB-CA-C	-5.83	103.04	111.91
3	G	105	GLN	CA-CB-CG	5.54	125.19	114.10
11	Y	175	MET	CB-CG-SD	5.47	129.10	112.70
3	G	72	ARG	CA-CB-CG	5.22	124.55	114.10
3	G	42	GLN	CA-CB-CG	5.14	124.38	114.10
4	H	111	LYS	CA-CB-CG	5.12	124.35	114.10
3	G	72	ARG	CG-CD-NE	5.02	123.05	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	W	220	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	A	801	0	851	19	0
1	E	801	0	851	17	0
2	B	624	0	654	15	0
2	F	620	0	643	14	0
3	C	819	0	865	10	0
3	G	827	0	865	15	0
4	D	726	0	748	9	0
4	H	726	0	748	18	0
5	I	3030	0	1650	25	0
6	J	2997	0	1650	36	0
7	Q	5278	0	5183	74	0
8	R	3963	0	3623	25	0
9	S	1014	0	1050	10	0
10	T	3339	0	3468	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	V	3397	0	3533	42	0
10	X	3404	0	3542	35	0
11	U	3421	0	3499	26	0
11	W	3398	0	3470	47	0
11	Y	3350	0	3444	18	0
12	Z	387	0	301	5	0
13	T	27	0	12	2	0
13	U	27	0	12	1	0
13	V	27	0	12	2	0
13	W	27	0	12	0	0
13	X	27	0	12	2	0
13	Y	27	0	12	1	0
All	All	43084	0	40710	411	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 5.

All (411) 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)
11:W:185:LEU:HD11	11:W:215:MET:CE	1.20	1.58
11:W:185:LEU:CD1	11:W:215:MET:CE	1.81	1.54
11:W:185:LEU:CD1	11:W:215:MET:HE2	1.44	1.38
11:W:185:LEU:CD1	11:W:215:MET:HE1	1.75	1.16
11:W:185:LEU:HD11	11:W:215:MET:HE3	1.23	1.14
11:W:185:LEU:HD13	11:W:215:MET:CE	1.83	1.07
11:W:185:LEU:CD2	11:W:215:MET:HE1	1.93	0.97
11:W:185:LEU:HD13	11:W:215:MET:HE2	1.45	0.94
1:A:123:ASP:OD1	1:E:113:HIS:HE1	1.51	0.93
5:I:-73:DA:C2	6:J:74:DG:N2	2.40	0.90
7:Q:1182:PRO:HD3	10:V:206:THR:HG22	1.55	0.86
5:I:-71:DA:C2	6:J:72:DG:N2	2.44	0.86
6:J:67:DA:H2"	6:J:68:DT:H71	1.59	0.84
5:I:-71:DA:C2	6:J:72:DG:C2	2.65	0.84
7:Q:1130:LYS:HE2	11:U:131:GLU:OE1	1.75	0.83
7:Q:1004:VAL:HG12	7:Q:1005:MET:H	1.43	0.83
1:A:123:ASP:OD1	1:E:113:HIS:CE1	2.31	0.82
11:W:185:LEU:HD11	11:W:215:MET:HE2	0.96	0.81
2:F:61:VAL:O	2:F:64:GLU:HB3	1.82	0.79
5:I:-73:DA:C2	6:J:74:DG:C2	2.72	0.77
7:Q:1004:VAL:HG12	7:Q:1005:MET:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-66:DG:C2	6:J:67:DA:C2	2.73	0.76
11:W:185:LEU:CD2	11:W:215:MET:CE	2.64	0.74
7:Q:1182:PRO:HD3	10:V:206:THR:CG2	2.19	0.72
11:W:185:LEU:CG	11:W:215:MET:CE	2.68	0.71
10:X:115:VAL:HG11	10:X:119:GLU:HG2	1.72	0.70
11:W:185:LEU:CG	11:W:215:MET:HE1	2.21	0.70
11:W:217:ALA:C	11:W:219:THR:H	1.99	0.69
11:W:185:LEU:HD21	11:W:215:MET:CE	2.26	0.66
11:W:185:LEU:HD22	11:W:215:MET:HE1	1.76	0.65
7:Q:874:GLN:HG3	7:Q:1399:THR:HG21	1.80	0.64
5:I:-66:DG:N2	6:J:67:DA:C2	2.67	0.63
4:D:116:GLU:HG3	4:D:119:ARG:HH21	1.62	0.63
1:A:108:ASN:HB2	2:B:44:VAL:HG12	1.82	0.62
11:U:165:MET:HE3	11:U:229:LEU:HB3	1.82	0.61
11:W:185:LEU:HD13	11:W:215:MET:HE1	1.55	0.61
6:J:63:DA:H2"	6:J:64:DT:C7	2.31	0.61
3:C:40:TYR:HB3	4:D:81:SER:HB2	1.82	0.61
8:R:211:ARG:HH21	8:R:213:ASN:HD21	1.48	0.61
7:Q:838:MET:HE2	7:Q:862:CYS:HB3	1.84	0.60
1:A:47:ALA:HB1	2:B:40:ARG:HH22	1.65	0.60
6:J:70:DC:H2"	6:J:71:DT:H71	1.84	0.60
3:G:66:LEU:HB3	3:G:87:ALA:HB1	1.84	0.59
7:Q:1223:VAL:HB	7:Q:1229:VAL:HG11	1.85	0.59
6:J:67:DA:H2"	6:J:68:DT:C7	2.31	0.59
3:C:64:LEU:HD11	4:D:44:ILE:HG13	1.85	0.58
3:C:78:ARG:HH12	6:J:-54:DA:H4'	1.68	0.58
11:W:76:PRO:O	11:W:81:LYS:NZ	2.36	0.58
3:G:30:ARG:NH1	4:H:38:GLU:OE1	2.36	0.58
6:J:64:DT:H5"	7:Q:1432:MET:HE1	1.86	0.58
7:Q:954:CYS:SG	7:Q:955:ASP:N	2.78	0.57
6:J:67:DA:C2'	6:J:68:DT:H71	2.32	0.57
10:T:268:MET:SD	10:T:268:MET:N	2.76	0.57
2:F:70:ALA:O	2:F:73:TYR:HB2	2.05	0.57
11:W:208:ARG:HE	11:W:210:ARG:HB3	1.69	0.57
11:Y:130:LYS:HG2	11:Y:236:VAL:HG22	1.87	0.57
1:E:44:GLY:HA3	2:F:45:LYS:HE3	1.86	0.57
4:H:108:GLU:HG3	4:H:111:LYS:HZ1	1.70	0.57
7:Q:1103:ASP:N	7:Q:1103:ASP:OD1	2.38	0.57
6:J:63:DA:H2"	6:J:64:DT:H71	1.86	0.56
7:Q:922:ARG:HH21	7:Q:926:MET:HG3	1.70	0.56
4:H:102:ARG:HH21	4:H:114:VAL:HG21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:68:THR:HB	8:R:96:SER:HA	1.87	0.56
10:V:385:GLU:HG3	10:V:400:LEU:HD21	1.87	0.56
10:V:35:LEU:HD23	10:V:41:ALA:CA	2.35	0.56
10:X:51:GLN:NE2	10:X:373:LEU:O	2.39	0.56
7:Q:1089:ILE:O	7:Q:1093:LEU:HB2	2.06	0.56
3:G:68:GLY:O	3:G:72:ARG:NH1	2.39	0.56
7:Q:1130:LYS:CE	11:U:131:GLU:OE1	2.49	0.56
10:X:322:THR:HG21	11:Y:300:MET:HG3	1.88	0.56
3:C:30:ARG:NH2	5:I:49:DC:OP1	2.38	0.55
10:V:42:LYS:NZ	10:V:44:VAL:O	2.39	0.55
4:H:37:LYS:NZ	6:J:50:DA:OP1	2.39	0.55
7:Q:748:LEU:HD22	7:Q:752:HIS:HE2	1.71	0.55
7:Q:771:VAL:HG23	7:Q:783:ILE:HG21	1.88	0.55
1:E:46:VAL:HG23	1:E:49:ARG:HH21	1.70	0.55
5:I:37:DC:H41	6:J:-37:DG:H1	1.54	0.55
10:X:71:SER:HB2	11:Y:19:LEU:HD12	1.88	0.55
2:B:92:LYS:HA	2:B:97:THR:HG22	1.88	0.55
9:S:69:ASP:HA	9:S:72:LYS:HG2	1.89	0.55
9:S:152:ASP:OD2	9:S:152:ASP:N	2.38	0.55
8:R:602:ASP:OD1	8:R:602:ASP:N	2.40	0.55
10:T:170:LEU:HD11	10:T:200:ILE:HD11	1.88	0.55
2:F:76:HIS:HE1	4:H:95:ARG:HG3	1.72	0.55
10:V:35:LEU:HD23	10:V:41:ALA:HA	1.88	0.55
10:V:285:ARG:O	10:V:289:ASN:ND2	2.40	0.55
7:Q:1137:LEU:HB2	11:U:200:THR:HB	1.89	0.54
10:X:380:ILE:HD12	10:X:412:LEU:HD13	1.89	0.54
6:J:63:DA:H2"	6:J:64:DT:C5	2.43	0.54
10:V:35:LEU:CD2	10:V:41:ALA:HB2	2.38	0.54
10:X:461:ASN:OD1	10:X:461:ASN:N	2.41	0.54
8:R:754:GLU:HG2	9:S:97:LYS:HB2	1.89	0.54
1:A:109:LEU:HD23	1:A:112:ILE:HD11	1.90	0.54
7:Q:733:MET:HE3	7:Q:734:GLY:H	1.72	0.54
9:S:114:LYS:NZ	10:T:223:ASP:OD1	2.41	0.54
11:U:110:GLU:N	11:U:110:GLU:OE2	2.41	0.54
1:A:69:ARG:NH2	5:I:17:DA:OP2	2.40	0.53
7:Q:1179:ARG:HH12	10:V:260:GLN:HB3	1.72	0.53
10:T:182:ASP:OD1	10:T:182:ASP:N	2.42	0.53
10:V:196:ILE:O	10:V:214:ARG:NH1	2.40	0.53
10:X:361:PRO:HA	10:X:364:ILE:HB	1.89	0.53
7:Q:1204:ASN:ND2	11:W:195:ALA:O	2.40	0.53
11:U:126:GLY:HA2	11:U:240:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:ARG:HH12	6:J:-66:DA:H4'	1.74	0.53
2:B:37:ARG:NH2	6:J:-13:DA:OP1	2.42	0.53
4:H:108:GLU:HA	4:H:111:LYS:HE3	1.90	0.53
7:Q:788:GLY:O	7:Q:793:ARG:NH2	2.41	0.53
3:G:72:ARG:NH2	3:G:76:LYS:O	2.38	0.53
12:Z:310:ARG:NH1	12:Z:315:ASP:OD2	2.41	0.53
1:A:42:LYS:NZ	6:J:-5:DA:OP1	2.43	0.52
10:T:381:ARG:NH1	10:T:401:ASP:OD1	2.43	0.52
4:H:66:ASN:O	4:H:70:ASN:ND2	2.42	0.52
11:U:218:ASP:OD1	11:U:218:ASP:N	2.36	0.52
1:A:49:ARG:HA	1:A:52:ARG:HE	1.73	0.52
2:B:36:ARG:NH2	2:B:52:TYR:OH	2.43	0.52
7:Q:1384:THR:O	7:Q:1413:GLN:NE2	2.43	0.52
8:R:640:GLU:HG3	9:S:110:ARG:HH21	1.75	0.52
11:Y:432:ASP:OD1	11:Y:432:ASP:N	2.42	0.52
5:I:-23:DT:H2"	5:I:-22:DG:H5"	1.92	0.52
7:Q:1005:MET:O	7:Q:1009:LYS:HG2	2.10	0.52
10:T:463:LEU:HD22	11:Y:75:GLY:HA2	1.92	0.52
4:H:111:LYS:HA	4:H:114:VAL:HG22	1.92	0.51
7:Q:1211:HIS:HE2	7:Q:1287:SER:HG	1.55	0.51
10:T:43:ARG:HG2	10:T:44:VAL:HG23	1.91	0.51
10:T:71:SER:HB3	11:U:19:LEU:HB2	1.93	0.51
10:V:361:PRO:HA	10:V:364:ILE:HB	1.91	0.51
4:H:59:GLN:OE1	4:H:59:GLN:N	2.43	0.51
7:Q:1387:ASP:HB2	7:Q:1417:VAL:HA	1.91	0.51
10:V:180:ARG:HE	11:W:210:ARG:HH11	1.56	0.51
8:R:210:LYS:HG3	8:R:641:LEU:HD22	1.92	0.51
11:U:67:ALA:HB3	10:V:25:ALA:HB2	1.92	0.51
10:V:106:VAL:HB	10:V:109:GLU:HG3	1.91	0.51
8:R:168:ASP:OD1	8:R:168:ASP:N	2.41	0.51
10:V:376:ASP:OD1	10:V:376:ASP:N	2.44	0.51
11:W:18:SER:OG	11:W:19:LEU:N	2.42	0.51
1:E:79:LYS:NZ	1:E:80:THR:O	2.44	0.51
2:F:57:GLY:HA2	2:F:60:LYS:HE2	1.93	0.51
7:Q:1011:CYS:SG	7:Q:1424:VAL:HG21	2.51	0.51
7:Q:1071:THR:OG1	10:X:177:LYS:NZ	2.44	0.51
11:U:115:GLU:OE2	11:U:270:ARG:NH2	2.44	0.51
10:X:375:TYR:OH	13:X:1001:ADP:N7	2.42	0.51
10:V:85:LYS:NZ	13:V:1001:ADP:O2B	2.39	0.51
7:Q:1393:ASP:OD1	7:Q:1393:ASP:N	2.43	0.50
10:V:35:LEU:HD23	10:V:41:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:156:GLY:HA3	11:Y:176:ILE:HD11	1.92	0.50
5:I:-71:DA:N3	6:J:72:DG:N2	2.59	0.50
10:V:106:VAL:HG12	10:V:108:SER:H	1.76	0.50
2:B:100:GLY:O	4:H:63:SER:OG	2.27	0.50
7:Q:1317:ARG:O	7:Q:1388:THR:OG1	2.29	0.50
10:V:180:ARG:HE	11:W:210:ARG:NH1	2.09	0.50
8:R:155:PHE:O	8:R:731:LYS:NZ	2.45	0.50
7:Q:1032:GLY:HA3	11:Y:182:GLU:HA	1.93	0.50
10:T:252:LEU:O	10:T:256:ASN:ND2	2.45	0.50
8:R:138:GLU:OE2	8:R:749:ASN:ND2	2.44	0.49
3:G:40:TYR:HB3	4:H:81:SER:HB2	1.93	0.49
10:V:198:ASP:OD2	10:V:211:ARG:NH2	2.45	0.49
2:F:83:THR:OG1	2:F:84:ALA:N	2.45	0.49
11:W:185:LEU:HD21	11:W:215:MET:HE3	1.95	0.49
10:V:422:CYS:SG	10:V:439:VAL:HG22	2.52	0.49
10:T:377:LYS:HG3	10:T:408:THR:HG21	1.94	0.49
11:Y:364:ILE:HG12	11:Y:396:LEU:HD13	1.95	0.49
1:E:83:ARG:HB2	2:F:81:THR:HB	1.95	0.49
1:E:132:GLY:HA2	1:E:134:ARG:HH12	1.78	0.49
1:A:120:GLN:OE1	1:A:122:LYS:NZ	2.45	0.49
7:Q:936:VAL:HG13	7:Q:938:LYS:H	1.77	0.49
10:V:225:GLU:OE1	10:V:229:TYR:OH	2.31	0.49
5:I:-66:DG:N2	6:J:67:DA:N3	2.61	0.48
1:A:60:LEU:HD22	1:A:93:GLN:HE22	1.78	0.48
2:F:41:ARG:O	2:F:41:ARG:NE	2.45	0.48
11:W:262:THR:O	11:W:262:THR:OG1	2.29	0.48
7:Q:1155:ARG:HH22	10:V:271:GLN:HE21	1.59	0.48
11:W:136:ILE:HB	11:W:192:ILE:HB	1.95	0.48
11:W:422:ASP:N	11:W:422:ASP:OD1	2.46	0.48
3:C:24:LEU:HD21	4:D:119:ARG:HH22	1.77	0.48
1:A:130:LEU:HD12	1:E:130:LEU:HD12	1.96	0.48
11:W:139:GLU:OE1	11:W:161:LYS:NZ	2.46	0.48
7:Q:1326:LYS:HA	7:Q:1329:ASP:HB2	1.95	0.48
10:X:362:ASP:OD1	10:X:362:ASP:N	2.42	0.48
12:Z:319:THR:OG1	12:Z:320:PHE:N	2.46	0.48
3:G:32:HIS:CD2	3:G:36:ARG:HE	2.31	0.48
10:T:171:LYS:HG3	10:T:176:THR:HG22	1.95	0.48
11:W:128:LYS:HB3	11:W:287:GLU:HG2	1.95	0.47
11:Y:110:GLU:HG3	11:Y:111:LEU:HG	1.95	0.47
8:R:51:ALA:HB3	8:R:61:HIS:HB2	1.95	0.47
11:U:349:ASP:OD2	10:V:413:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:49:VAL:H	13:X:1001:ADP:HN62	1.61	0.47
3:G:77:THR:O	4:H:56:GLY:N	2.42	0.47
5:I:-75:DG:N2	6:J:76:DA:C2	2.83	0.47
10:V:83:THR:O	10:V:375:TYR:OH	2.33	0.47
1:E:104:PHE:HA	1:E:107:THR:HG22	1.97	0.47
2:B:83:THR:OG1	2:B:84:ALA:N	2.45	0.47
2:F:71:VAL:O	2:F:75:GLU:N	2.47	0.47
7:Q:765:SER:OG	7:Q:1354:ARG:NH1	2.46	0.47
7:Q:805:LEU:HG	7:Q:806:ARG:H	1.80	0.47
8:R:116:ASP:OD2	9:S:49:LYS:NZ	2.44	0.47
10:V:56:GLU:OE1	11:W:425:ARG:NH2	2.41	0.47
10:X:355:SER:OG	10:X:359:VAL:O	2.25	0.47
5:I:-73:DA:N3	6:J:74:DG:N2	2.62	0.47
8:R:267:LEU:HD11	8:R:587:ARG:HG2	1.96	0.47
4:H:105:LEU:HD12	4:H:109:LEU:HB3	1.95	0.46
10:X:318:ILE:O	10:X:322:THR:OG1	2.31	0.46
3:G:82:ARG:NH1	3:G:106:GLY:O	2.48	0.46
8:R:134:ILE:HB	8:R:163:VAL:HG12	1.96	0.46
11:W:208:ARG:NH2	12:Z:313:GLU:O	2.48	0.46
1:E:116:ARG:HH12	1:E:122:LYS:HZ1	1.63	0.46
4:H:43:TYR:HA	4:H:46:LYS:HE2	1.95	0.46
7:Q:1004:VAL:CG1	7:Q:1005:MET:H	2.15	0.46
11:U:131:GLU:HG2	11:U:132:GLU:N	2.30	0.46
10:X:362:ASP:O	10:X:366:ARG:NH1	2.43	0.46
10:X:80:GLY:O	10:X:85:LYS:NZ	2.48	0.46
5:I:-7:DG:H1	6:J:7:DC:H42	1.63	0.46
7:Q:867:LEU:HG	7:Q:887:ILE:HD11	1.98	0.46
10:T:413:ARG:NH2	13:T:1001:ADP:O3A	2.48	0.46
11:U:332:THR:OG1	11:U:335:THR:OG1	2.33	0.46
10:X:290:LYS:HB2	10:X:290:LYS:HE3	1.73	0.46
7:Q:759:LEU:HB3	7:Q:838:MET:HA	1.98	0.46
7:Q:1208:ARG:NH1	7:Q:1284:SER:O	2.49	0.46
10:V:35:LEU:HD23	10:V:41:ALA:CB	2.46	0.46
10:V:73:ARG:NH2	11:W:401:ASN:OD1	2.48	0.46
11:W:38:ARG:O	11:W:51:ARG:NH2	2.39	0.46
7:Q:786:TYR:HB2	7:Q:816:MET:HE2	1.97	0.46
10:T:68:LYS:HG2	10:T:305:PRO:HD2	1.98	0.46
11:U:16:SER:OG	11:U:17:LEU:N	2.49	0.46
5:I:-75:DG:C2	6:J:76:DA:C2	3.04	0.46
10:T:41:ALA:HB3	10:T:52:ILE:HG23	1.98	0.46
10:X:116:LYS:HE2	10:X:279:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ARG:NH1	2:B:81:THR:O	2.49	0.45
11:W:240:SER:HB3	11:W:243:GLU:HG3	1.98	0.45
10:X:68:LYS:HG2	10:X:305:PRO:HD2	1.97	0.45
1:E:46:VAL:HA	1:E:49:ARG:HE	1.81	0.45
3:G:15:SER:OG	5:I:-42:DG:OP1	2.31	0.45
3:G:81:PRO:HD2	3:G:105:GLN:HE22	1.81	0.45
1:A:61:LEU:HD13	2:B:37:ARG:HB3	1.98	0.45
5:I:32:DG:C5	5:I:33:DT:C4	3.04	0.45
7:Q:783:ILE:HA	7:Q:815:VAL:HG23	1.97	0.45
10:X:115:VAL:HG12	10:X:116:LYS:N	2.31	0.45
10:T:364:ILE:HA	10:T:367:LEU:HD12	1.97	0.45
4:D:54:ASP:OD1	4:D:54:ASP:N	2.47	0.45
10:X:99:LYS:HE3	10:X:132:ARG:HE	1.82	0.45
10:V:313:VAL:HG11	10:V:338:LEU:HB3	1.98	0.45
10:V:355:SER:OG	10:V:359:VAL:O	2.30	0.45
11:W:181:LYS:HA	11:W:181:LYS:HD2	1.81	0.45
11:U:71:VAL:HG12	11:U:352:ILE:HG13	1.99	0.45
3:C:85:GLN:NE2	3:C:107:GLY:O	2.49	0.45
8:R:714:MET:H	8:R:714:MET:HG2	1.61	0.45
10:T:375:TYR:OH	13:T:1001:ADP:N7	2.43	0.45
11:U:144:GLN:HB3	11:U:157:LYS:HB2	1.99	0.45
3:C:27:PRO:HB2	3:C:30:ARG:HB2	1.99	0.45
4:D:98:GLN:HA	4:D:101:VAL:HG22	1.99	0.45
11:Y:361:GLU:HG3	11:Y:392:VAL:HG11	1.98	0.45
11:Y:412:LYS:O	11:Y:414:LYS:NZ	2.50	0.45
7:Q:729:LEU:HD12	7:Q:868:LEU:HD22	1.99	0.44
7:Q:764:ALA:HA	7:Q:767:LEU:HD12	1.99	0.44
7:Q:963:LEU:HA	7:Q:966:VAL:HB	1.99	0.44
9:S:39:ARG:O	9:S:39:ARG:NE	2.48	0.44
10:T:76:LEU:O	10:T:369:ILE:HA	2.17	0.44
10:V:141:GLU:OE2	10:V:239:LYS:NZ	2.50	0.44
10:V:189:ILE:HG23	10:V:194:VAL:HB	2.00	0.44
11:Y:114:THR:O	11:Y:118:THR:OG1	2.34	0.44
3:G:35:LEU:HD23	3:G:35:LEU:HA	1.88	0.44
7:Q:733:MET:HE1	7:Q:737:LYS:H	1.83	0.44
7:Q:1141:PHE:O	7:Q:1145:THR:OG1	2.30	0.44
10:X:82:SER:O	10:X:82:SER:OG	2.29	0.44
3:C:28:VAL:HG22	3:C:53:THR:HG21	1.99	0.44
9:S:29:ARG:H	9:S:29:ARG:HG3	1.66	0.44
1:A:48:LEU:HB3	1:A:52:ARG:HH21	1.82	0.44
3:G:43:ARG:HG2	4:H:91:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:21:LYS:HE2	3:G:21:LYS:HB3	1.82	0.44
7:Q:1325:THR:HA	7:Q:1328:MET:HE2	1.99	0.44
8:R:135:LEU:HB3	8:R:714:MET:HE3	2.00	0.44
10:V:177:LYS:HB3	10:V:237:VAL:HG11	2.00	0.44
11:W:162:THR:OG1	11:W:163:THR:N	2.50	0.44
10:X:30:ILE:O	10:X:94:GLN:NE2	2.47	0.44
7:Q:1249:ILE:HG13	7:Q:1271:THR:HG21	2.00	0.44
7:Q:1322:PHE:HE2	7:Q:1371:LEU:HD22	1.82	0.44
10:V:76:LEU:O	10:V:369:ILE:HA	2.18	0.44
4:H:108:GLU:O	4:H:112:HIS:ND1	2.51	0.44
11:U:413:ARG:HH21	11:U:415:ASN:HD22	1.66	0.44
10:T:65:ILE:HG12	10:T:335:VAL:HG21	2.00	0.44
10:T:151:ASP:OD1	10:T:151:ASP:N	2.42	0.43
11:U:331:LYS:HA	11:U:338:LYS:HA	1.99	0.43
10:X:73:ARG:HH12	11:Y:404:SER:HB3	1.82	0.43
7:Q:841:ASP:HA	7:Q:868:LEU:HB2	2.00	0.43
10:X:192:GLU:OE2	10:X:192:GLU:N	2.50	0.43
1:E:61:LEU:HD22	2:F:37:ARG:HG2	2.00	0.43
7:Q:1279:ASN:HB2	7:Q:1282:PHE:HD1	1.83	0.43
8:R:643:GLU:O	8:R:647:LEU:HB2	2.19	0.43
10:T:42:LYS:O	10:T:55:ARG:NH2	2.45	0.43
10:V:287:GLU:HA	10:V:290:LYS:HG2	2.01	0.43
10:X:149:PRO:HB3	10:X:166:VAL:HG22	2.01	0.43
4:D:83:LEU:HD22	4:D:96:GLU:HB3	1.99	0.43
10:T:138:GLU:HG3	10:T:240:LYS:HG3	2.01	0.43
1:A:68:GLN:HA	1:A:71:VAL:HG22	2.01	0.43
1:A:85:GLN:HB3	2:B:83:THR:HA	2.01	0.43
2:B:36:ARG:O	2:B:40:ARG:HG2	2.18	0.43
3:C:88:ILE:HD12	3:C:88:ILE:HA	1.86	0.43
5:I:-34:DA:H1'	5:I:-33:DG:H5'	2.01	0.43
7:Q:804:ASN:CB	7:Q:808:ASN:HD21	2.32	0.43
6:J:8:DC:H2"	6:J:9:DG:C8	2.54	0.43
11:U:94:LYS:HD2	11:U:94:LYS:HA	1.86	0.43
11:W:255:LEU:HD12	11:W:255:LEU:HA	1.89	0.43
6:J:68:DT:H2"	6:J:69:DC:C6	2.54	0.43
7:Q:1079:ASN:ND2	7:Q:1217:PRO:O	2.52	0.43
8:R:43:ASP:HB3	8:R:50:ARG:HB2	2.00	0.43
10:X:216:ASP:O	12:Z:295:LYS:NZ	2.40	0.43
1:A:71:VAL:HA	1:A:74:ILE:HG22	2.00	0.43
6:J:70:DC:H2"	6:J:71:DT:C6	2.54	0.43
7:Q:1247:SER:OG	7:Q:1248:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:359:TYR:OH	13:U:1001:ADP:N7	2.46	0.43
10:X:115:VAL:HG11	10:X:119:GLU:CG	2.46	0.42
1:E:129:ARG:O	1:E:129:ARG:NH1	2.49	0.42
7:Q:806:ARG:HD3	7:Q:806:ARG:HA	1.93	0.42
8:R:135:LEU:HD13	8:R:714:MET:HB2	2.01	0.42
10:T:70:MET:HE3	10:T:70:MET:HB3	1.82	0.42
10:T:326:LYS:HD2	11:U:102:ALA:HB2	2.00	0.42
11:U:325:THR:HG21	11:U:341:HIS:HB3	2.00	0.42
10:V:403:LEU:HD23	10:V:403:LEU:HA	1.92	0.42
7:Q:744:VAL:O	7:Q:748:LEU:HB2	2.19	0.42
7:Q:1009:LYS:HG3	7:Q:1017:PHE:CE2	2.54	0.42
9:S:139:ILE:HD13	9:S:139:ILE:HA	1.91	0.42
10:V:248:THR:OG1	10:V:251:ASP:OD2	2.33	0.42
10:X:137:LYS:HB2	10:X:241:LYS:HG3	2.01	0.42
11:Y:276:LYS:HD3	11:Y:276:LYS:HA	1.76	0.42
5:I:32:DG:C8	5:I:33:DT:C7	3.02	0.42
7:Q:1253:THR:O	7:Q:1257:MET:HG3	2.19	0.42
10:X:455:ILE:O	10:X:459:SER:OG	2.33	0.42
7:Q:945:GLY:O	7:Q:1416:GLN:NE2	2.52	0.42
11:U:23:HIS:HB2	11:U:26:ILE:HD12	2.02	0.42
11:W:201:LYS:HD3	11:W:219:THR:HG21	2.00	0.42
5:I:55:DC:H2"	5:I:56:DG:N7	2.34	0.42
11:W:217:ALA:C	11:W:219:THR:N	2.63	0.42
10:X:258:ARG:HD2	10:X:258:ARG:HA	1.89	0.42
5:I:-54:DC:H2'	5:I:-53:DA:C8	2.55	0.42
7:Q:1387:ASP:OD1	7:Q:1387:ASP:N	2.52	0.42
8:R:182:LYS:O	8:R:202:GLY:N	2.50	0.42
8:R:753:PHE:HB3	9:S:94:LEU:HD22	2.01	0.42
1:A:61:LEU:HB3	2:B:37:ARG:HD2	2.02	0.42
2:B:76:HIS:O	4:D:95:ARG:NH2	2.52	0.42
7:Q:967:LEU:HD22	7:Q:1007:PHE:HB3	2.02	0.42
1:A:118:THR:HA	2:B:46:ARG:HB3	2.02	0.42
8:R:599:ARG:HA	8:R:599:ARG:HD3	1.78	0.42
3:C:80:ILE:HG13	3:C:83:HIS:H	1.83	0.41
4:D:64:ILE:HA	2:F:99:TYR:HB3	2.02	0.41
6:J:69:DC:H2"	6:J:70:DC:C6	2.55	0.41
7:Q:1296:THR:HB	7:Q:1302:ARG:HH21	1.85	0.41
11:U:113:LYS:H	11:U:113:LYS:HG3	1.69	0.41
11:W:204:ARG:HB3	11:W:219:THR:OG1	2.19	0.41
10:X:352:ASP:OD1	10:X:352:ASP:N	2.52	0.41
1:A:74:ILE:HD13	2:B:63:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:742:ILE:HD12	7:Q:774:ILE:HG12	2.00	0.41
7:Q:953:LEU:O	7:Q:1425:ARG:NH2	2.53	0.41
8:R:229:LEU:HD12	8:R:229:LEU:HA	1.84	0.41
4:H:62:MET:HE2	4:H:62:MET:HB2	1.77	0.41
7:Q:739:VAL:HA	7:Q:742:ILE:HG22	2.03	0.41
7:Q:1134:GLU:HG2	7:Q:1139:GLU:HG2	2.01	0.41
7:Q:1357:LEU:HD23	7:Q:1357:LEU:HA	1.94	0.41
10:T:450:LYS:HE2	10:T:450:LYS:HB3	1.84	0.41
11:W:122:ARG:NH1	11:W:245:ASP:OD2	2.53	0.41
2:F:55:THR:O	2:F:59:LEU:HG	2.21	0.41
8:R:41:ALA:HB1	8:R:714:MET:HE2	2.03	0.41
11:U:298:VAL:HG13	11:U:343:LEU:HD21	2.02	0.41
3:G:89:ARG:HB2	3:G:109:LEU:HD21	2.02	0.41
5:I:-9:DC:H2"	5:I:-8:DG:C8	2.56	0.41
10:T:386:ARG:HE	10:T:386:ARG:HB2	1.57	0.41
11:W:44:MET:HE2	11:W:44:MET:HB3	1.95	0.41
10:X:121:LEU:HD23	10:X:323:TYR:HD2	1.84	0.41
6:J:67:DA:H2"	6:J:68:DT:C5	2.55	0.41
7:Q:1249:ILE:O	7:Q:1254:GLN:NE2	2.53	0.41
8:R:74:LYS:HE3	8:R:76:ASN:ND2	2.35	0.41
11:W:114:THR:O	11:W:118:THR:OG1	2.34	0.41
11:Y:45:VAL:O	13:Y:1001:ADP:N6	2.54	0.41
1:E:40:ARG:NH2	6:J:9:DG:N3	2.58	0.41
6:J:-59:DT:H2"	6:J:-58:DG:C8	2.56	0.41
7:Q:784:LEU:HD12	7:Q:784:LEU:HA	1.96	0.41
10:T:80:GLY:O	10:T:83:THR:OG1	2.33	0.41
10:T:121:LEU:HD21	10:T:324:LEU:HD13	2.02	0.41
11:W:185:LEU:HD21	11:W:215:MET:HE1	1.81	0.41
10:X:246:ASP:C	10:X:247:VAL:HG13	2.46	0.41
1:E:51:ILE:HG13	2:F:40:ARG:HD2	2.03	0.41
6:J:72:DG:H2"	6:J:73:DT:C6	2.56	0.41
7:Q:756:GLY:HA3	7:Q:757:PRO:HD3	1.85	0.41
7:Q:1328:MET:HB2	7:Q:1344:ARG:HE	1.86	0.41
10:T:461:ASN:OD1	10:T:461:ASN:N	2.54	0.41
5:I:5:DT:H2"	5:I:6:DA:N7	2.36	0.41
10:T:138:GLU:OE2	10:T:238:HIS:NE2	2.54	0.41
2:F:72:THR:HA	2:F:75:GLU:HB2	2.03	0.40
10:T:25:ALA:HB2	11:Y:67:ALA:HB3	2.03	0.40
10:V:258:ARG:NE	10:V:259:PRO:O	2.54	0.40
10:V:352:ASP:OD1	10:V:352:ASP:N	2.54	0.40
10:V:413:ARG:NH2	13:V:1001:ADP:O3B	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:367:ILE:HD13	11:W:367:ILE:HA	1.92	0.40
10:X:328:LEU:HD23	10:X:328:LEU:HA	1.90	0.40
11:U:233:LYS:HB2	11:U:233:LYS:HE2	1.90	0.40
10:V:69:LYS:HB3	10:V:70:MET:HE2	2.02	0.40
11:Y:298:VAL:HG13	11:Y:343:LEU:HD21	2.04	0.40
6:J:45:DC:H2"	6:J:46:DA:N7	2.36	0.40
7:Q:1332:GLU:HA	7:Q:1335:LEU:HD12	2.03	0.40
10:T:128:ALA:HB3	10:T:334:PRO:HG3	2.03	0.40
1:E:131:ARG:NE	1:E:133:GLU:OE2	2.54	0.40
3:G:58:TYR:HB2	4:H:116:GLU:HG2	2.03	0.40
5:I:-61:DT:H2'	5:I:-60:DA:C8	2.55	0.40
8:R:130:ILE:HA	8:R:131:PRO:HD3	1.92	0.40
11:W:76:PRO:HD3	10:X:463:LEU:HG	2.03	0.40
11:Y:69:ARG:HD3	11:Y:69:ARG:HA	1.89	0.40
12:Z:313:GLU:OE1	12:Z:313:GLU:N	2.54	0.40
6:J:-48:DC:H2"	6:J:-47:DT:C4	2.57	0.40
7:Q:800:TRP:HZ2	7:Q:829:TYR:CD1	2.40	0.40
7:Q:1149:LEU:HD12	7:Q:1149:LEU:HA	1.92	0.40
10:V:75:ILE:HD13	10:V:368:LEU:HB2	2.03	0.40
11:W:154:LYS:NZ	11:W:177:ASP:OD1	2.49	0.40
11:W:325:THR:HG22	11:W:327:ARG:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
1	E	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
2	B	77/103 (75%)	73 (95%)	4 (5%)	0	100	100
2	F	77/103 (75%)	73 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	104/132 (79%)	97 (93%)	7 (7%)	0	100	100
3	G	106/132 (80%)	101 (95%)	5 (5%)	0	100	100
4	D	91/131 (70%)	89 (98%)	2 (2%)	0	100	100
4	H	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
7	Q	651/1489 (44%)	612 (94%)	39 (6%)	0	100	100
8	R	515/755 (68%)	508 (99%)	7 (1%)	0	100	100
9	S	121/166 (73%)	116 (96%)	5 (4%)	0	100	100
10	T	431/463 (93%)	421 (98%)	10 (2%)	0	100	100
10	V	440/463 (95%)	423 (96%)	17 (4%)	0	100	100
10	X	441/463 (95%)	420 (95%)	21 (5%)	0	100	100
11	U	443/460 (96%)	422 (95%)	21 (5%)	0	100	100
11	W	440/460 (96%)	423 (96%)	17 (4%)	0	100	100
11	Y	432/460 (94%)	413 (96%)	19 (4%)	0	100	100
12	Z	52/320 (16%)	52 (100%)	0	0	100	100
All	All	4702/6503 (72%)	4521 (96%)	181 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/113 (75%)	85 (100%)	0	100	100
1	E	85/113 (75%)	85 (100%)	0	100	100
2	B	63/79 (80%)	63 (100%)	0	100	100
2	F	62/79 (78%)	62 (100%)	0	100	100
3	C	85/99 (86%)	85 (100%)	0	100	100
3	G	84/99 (85%)	84 (100%)	0	100	100
4	D	81/109 (74%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	81/109 (74%)	81 (100%)	0	100	100
7	Q	582/1350 (43%)	582 (100%)	0	100	100
8	R	394/682 (58%)	394 (100%)	0	100	100
9	S	109/142 (77%)	109 (100%)	0	100	100
10	T	367/391 (94%)	367 (100%)	0	100	100
10	V	374/391 (96%)	374 (100%)	0	100	100
10	X	375/391 (96%)	375 (100%)	0	100	100
11	U	378/394 (96%)	378 (100%)	0	100	100
11	W	375/394 (95%)	375 (100%)	0	100	100
11	Y	371/394 (94%)	371 (100%)	0	100	100
12	Z	27/285 (10%)	27 (100%)	0	100	100
All	All	3978/5614 (71%)	3978 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
3	C	85	GLN
1	E	39	HIS
1	E	113	HIS
3	G	114	GLN
7	Q	753	ASN
7	Q	808	ASN
7	Q	856	ASN
7	Q	875	ASN
7	Q	895	HIS
7	Q	899	ASN
7	Q	1254	GLN
7	Q	1416	GLN
7	Q	1438	GLN
8	R	31	GLN
8	R	76	ASN
8	R	109	ASN
8	R	653	GLN
8	R	666	ASN
8	R	745	HIS

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Mol	Chain	Res	Type
9	S	153	GLN
10	T	205	ASN
11	U	144	GLN
11	U	173	ASN
11	U	252	GLN
11	U	326	ASN
11	U	408	GLN
11	U	453	ASN
10	V	298	GLN
11	W	23	HIS
11	W	49	GLN
11	W	173	ASN
11	W	242	HIS
11	W	360	ASN
11	W	362	GLN

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	ADP	X	1001	-	28,29,29	1.40	4 (14%)	43,45,45	1.82	7 (16%)
13	ADP	T	1001	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	8 (18%)
13	ADP	W	1001	-	28,29,29	1.42	4 (14%)	43,45,45	1.86	8 (18%)
13	ADP	V	1001	-	28,29,29	1.38	4 (14%)	43,45,45	1.82	9 (20%)
13	ADP	Y	1001	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)
13	ADP	U	1001	-	28,29,29	1.38	4 (14%)	43,45,45	1.83	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	X	1001	-	-	1/16/32/32	0/3/3/3
13	ADP	T	1001	-	-	1/16/32/32	0/3/3/3
13	ADP	W	1001	-	-	3/16/32/32	0/3/3/3
13	ADP	V	1001	-	-	3/16/32/32	0/3/3/3
13	ADP	Y	1001	-	-	3/16/32/32	0/3/3/3
13	ADP	U	1001	-	-	4/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	1001	ADP	C5-C4	4.67	1.47	1.39
13	Y	1001	ADP	C5-C4	4.62	1.47	1.39
13	T	1001	ADP	C5-C4	4.57	1.47	1.39
13	X	1001	ADP	C5-C4	4.55	1.47	1.39
13	V	1001	ADP	C5-C4	4.53	1.47	1.39
13	U	1001	ADP	C5-C4	4.49	1.47	1.39
13	U	1001	ADP	C5-C6	2.64	1.48	1.41
13	V	1001	ADP	C5-C6	2.62	1.48	1.41
13	X	1001	ADP	C5-C6	2.60	1.48	1.41
13	W	1001	ADP	C5-C6	2.58	1.48	1.41
13	T	1001	ADP	C5-C6	2.57	1.48	1.41
13	W	1001	ADP	C5-N7	-2.56	1.34	1.39
13	Y	1001	ADP	C5-C6	2.54	1.48	1.41
13	Y	1001	ADP	C5-N7	-2.48	1.34	1.39
13	X	1001	ADP	C5-N7	-2.42	1.34	1.39
13	V	1001	ADP	C5-N7	-2.42	1.34	1.39
13	T	1001	ADP	C5-N7	-2.41	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	U	1001	ADP	C5-N7	-2.41	1.34	1.39
13	U	1001	ADP	C8-N7	2.32	1.36	1.31
13	V	1001	ADP	C8-N7	2.31	1.36	1.31
13	T	1001	ADP	C8-N7	2.20	1.35	1.31
13	X	1001	ADP	C8-N7	2.20	1.35	1.31
13	Y	1001	ADP	C8-N7	2.17	1.35	1.31
13	W	1001	ADP	C8-N7	2.15	1.35	1.31

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	W	1001	ADP	C5-C4-N3	-6.13	118.28	126.72
13	Y	1001	ADP	C5-C4-N3	-5.83	118.70	126.72
13	X	1001	ADP	C5-C4-N3	-5.82	118.70	126.72
13	T	1001	ADP	C5-C4-N3	-5.75	118.80	126.72
13	V	1001	ADP	C5-C4-N3	-5.71	118.85	126.72
13	U	1001	ADP	C5-C4-N3	-5.70	118.87	126.72
13	W	1001	ADP	N3-C4-N9	4.99	135.65	127.17
13	Y	1001	ADP	N3-C4-N9	4.76	135.27	127.17
13	T	1001	ADP	N3-C4-N9	4.70	135.15	127.17
13	X	1001	ADP	N3-C4-N9	4.69	135.15	127.17
13	V	1001	ADP	N3-C4-N9	4.56	134.92	127.17
13	U	1001	ADP	N3-C4-N9	4.51	134.84	127.17
13	U	1001	ADP	C2-N3-C4	3.70	120.88	111.83
13	W	1001	ADP	C2-N3-C4	3.70	120.86	111.83
13	X	1001	ADP	C2-N3-C4	3.69	120.84	111.83
13	V	1001	ADP	C2-N3-C4	3.68	120.81	111.83
13	Y	1001	ADP	C2-N3-C4	3.67	120.80	111.83
13	T	1001	ADP	C2-N3-C4	3.62	120.67	111.83
13	U	1001	ADP	C4-C5-N7	-3.40	106.69	110.58
13	V	1001	ADP	C4-C5-N7	-3.38	106.72	110.58
13	X	1001	ADP	C4-C5-N7	-3.31	106.80	110.58
13	T	1001	ADP	C4-C5-N7	-3.30	106.81	110.58
13	U	1001	ADP	N3-C2-N1	-3.30	123.59	128.58
13	V	1001	ADP	N3-C2-N1	-3.29	123.61	128.58
13	Y	1001	ADP	C4-C5-N7	-3.29	106.83	110.58
13	Y	1001	ADP	N3-C2-N1	-3.26	123.65	128.58
13	W	1001	ADP	C4-C5-N7	-3.22	106.91	110.58
13	X	1001	ADP	N3-C2-N1	-3.21	123.72	128.58
13	T	1001	ADP	N3-C2-N1	-3.20	123.74	128.58
13	W	1001	ADP	N3-C2-N1	-3.06	123.96	128.58
13	T	1001	ADP	C4-N9-C8	2.85	108.73	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	1001	ADP	C4-N9-C8	2.76	108.63	105.74
13	U	1001	ADP	C4-N9-C8	2.76	108.63	105.74
13	Y	1001	ADP	C4-N9-C8	2.75	108.62	105.74
13	X	1001	ADP	C4-N9-C8	2.61	108.48	105.74
13	U	1001	ADP	C5-N7-C8	2.52	107.41	103.45
13	T	1001	ADP	C5-N7-C8	2.49	107.36	103.45
13	V	1001	ADP	C5-N7-C8	2.49	107.36	103.45
13	Y	1001	ADP	C5-N7-C8	2.48	107.35	103.45
13	X	1001	ADP	C5-N7-C8	2.45	107.30	103.45
13	W	1001	ADP	C4-N9-C8	2.44	108.30	105.74
13	W	1001	ADP	C5-N7-C8	2.42	107.26	103.45
13	W	1001	ADP	C3'-C2'-C1'	2.38	105.96	101.46
13	Y	1001	ADP	C3'-C2'-C1'	2.17	105.58	101.46
13	U	1001	ADP	C6-C5-N7	2.14	136.22	132.09
13	U	1001	ADP	N9-C8-N7	-2.08	110.98	113.94
13	V	1001	ADP	C6-C5-N7	2.07	136.08	132.09
13	T	1001	ADP	N9-C8-N7	-2.03	111.05	113.94
13	V	1001	ADP	N9-C8-N7	-2.03	111.06	113.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

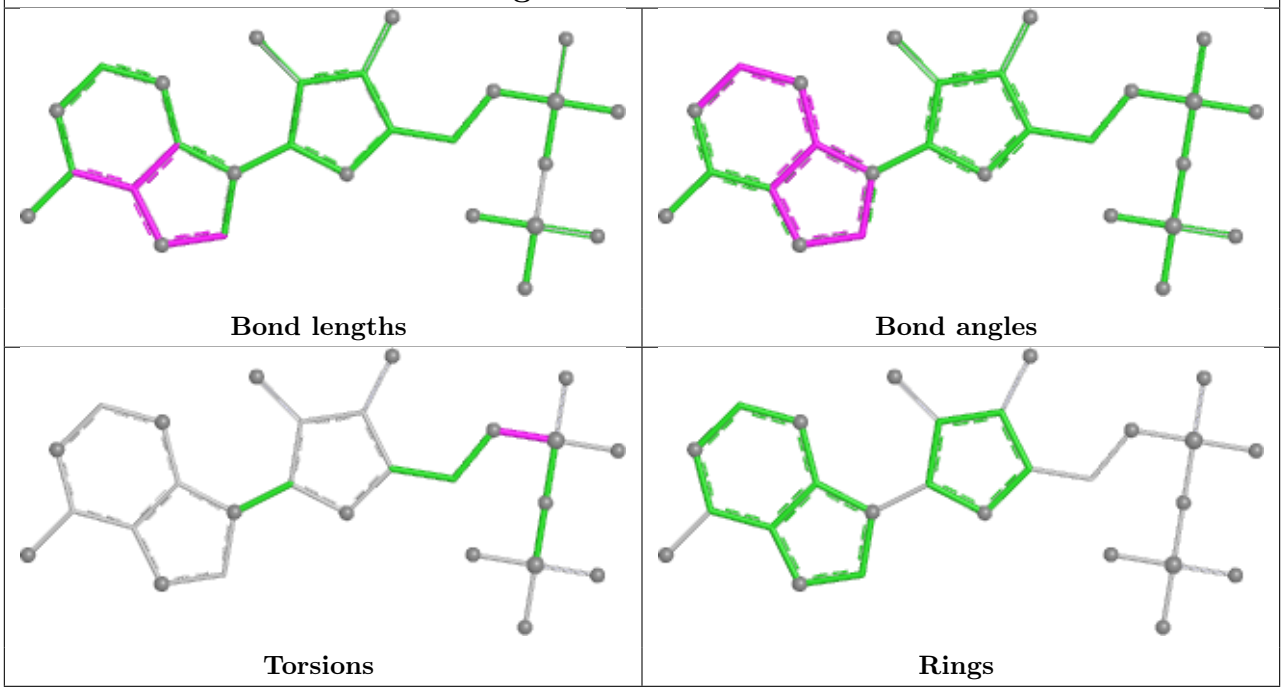
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	X	1001	ADP	2	0
13	T	1001	ADP	2	0
13	V	1001	ADP	2	0
13	Y	1001	ADP	1	0
13	U	1001	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 then 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.

Ligand ADP X 1001



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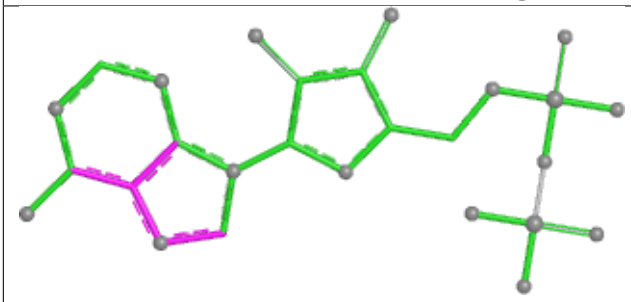
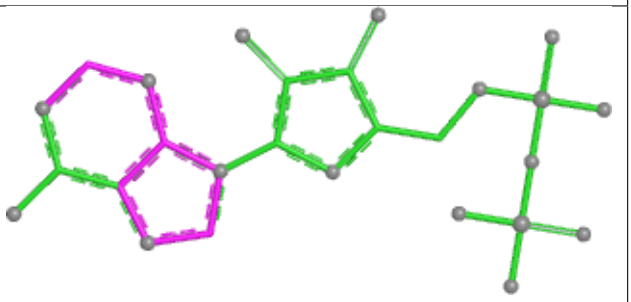
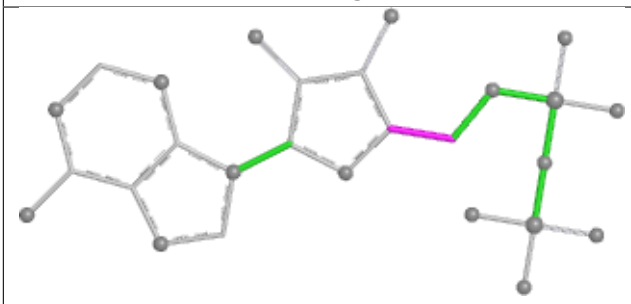
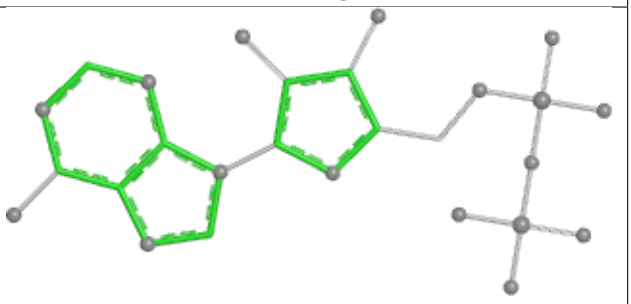
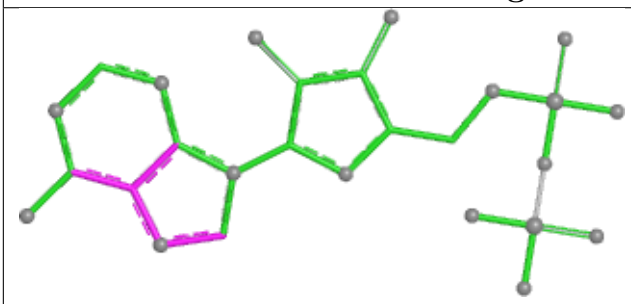
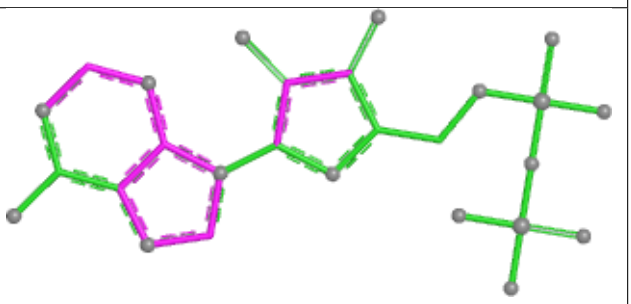
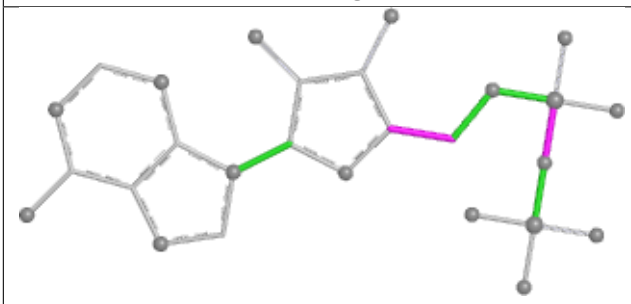
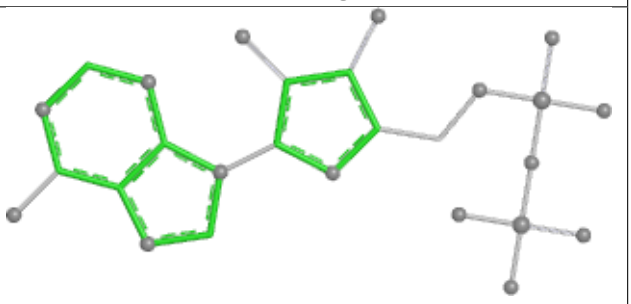
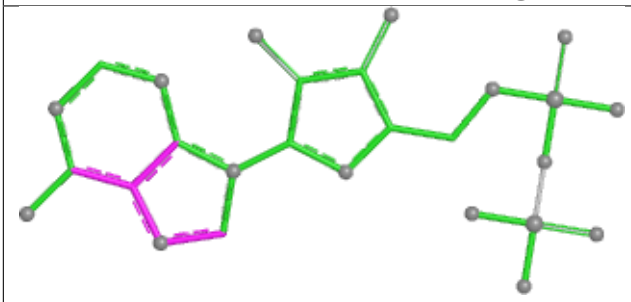
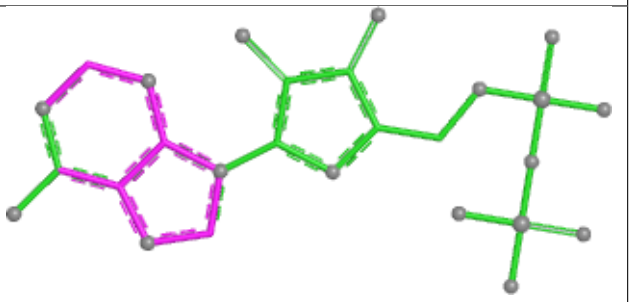
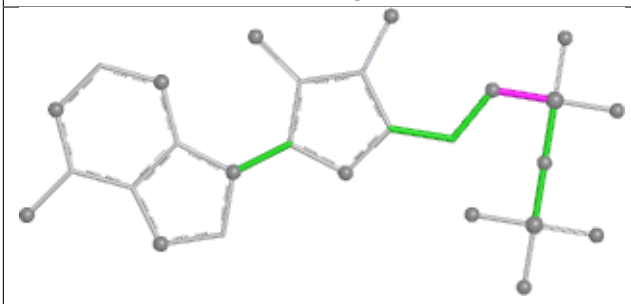
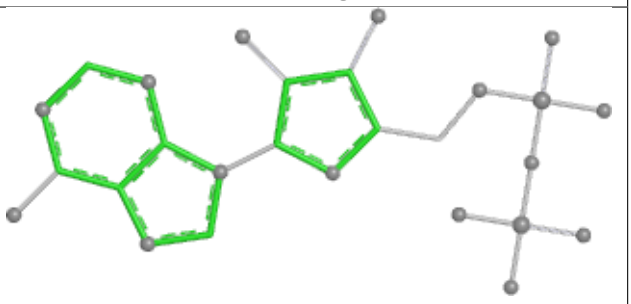
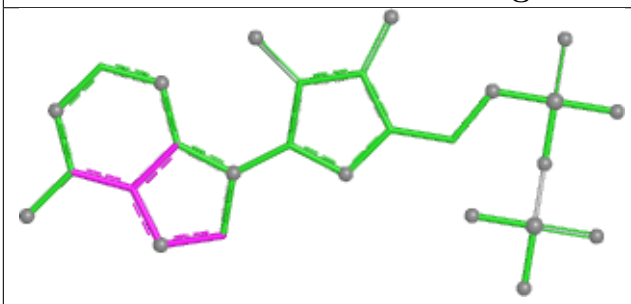
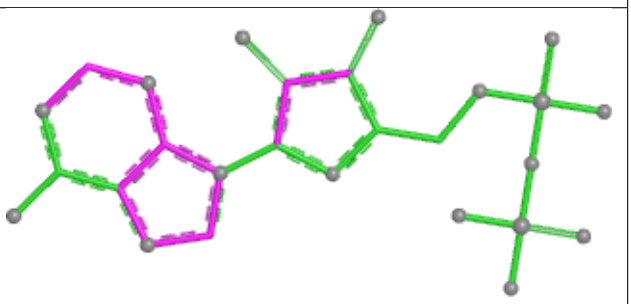
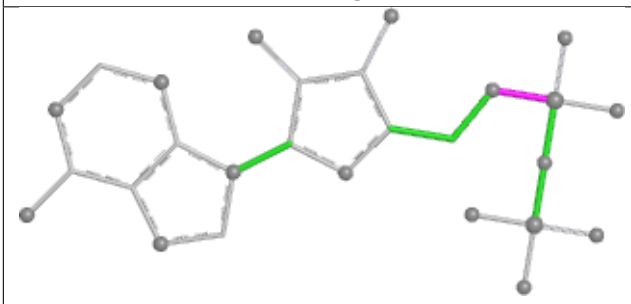
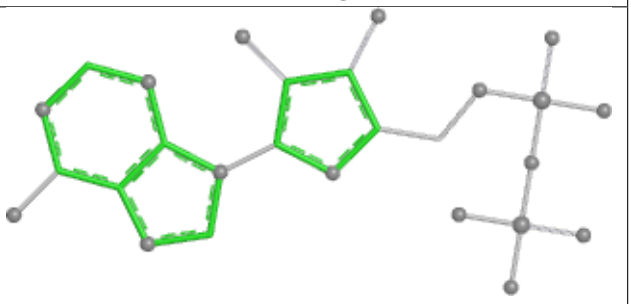
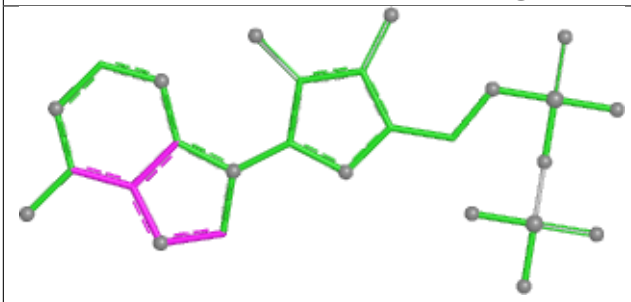
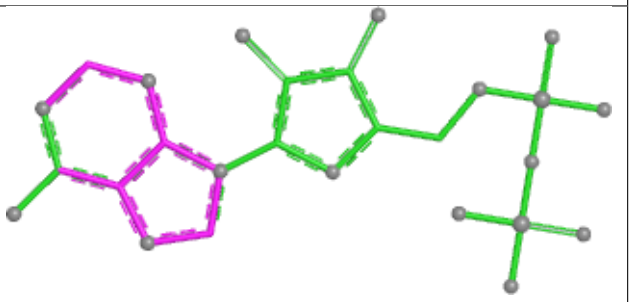
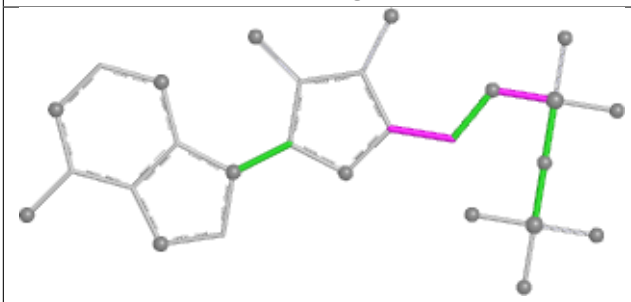
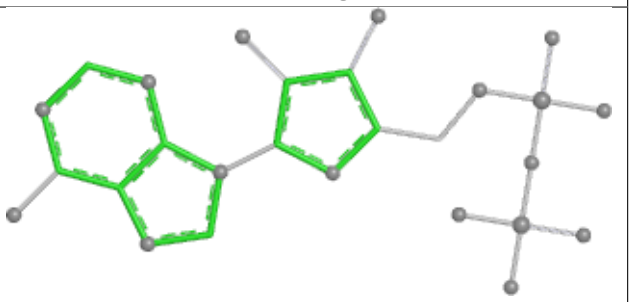
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP W 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP V 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Y 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP U 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

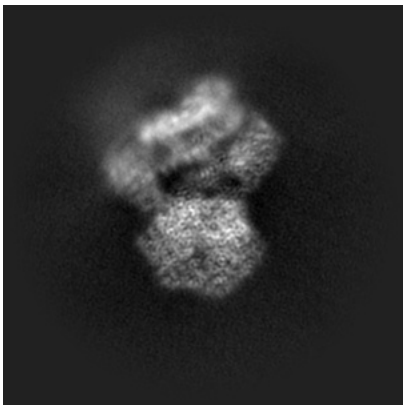
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45370. 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

6.1.1 Primary map



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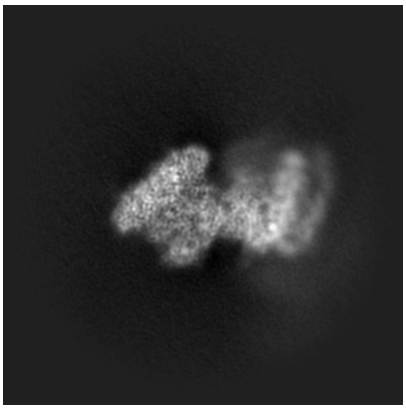

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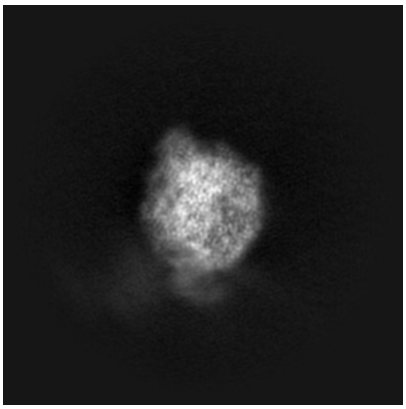
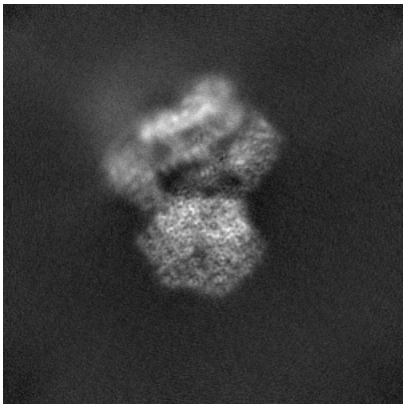


Z

6.1.2 Raw map



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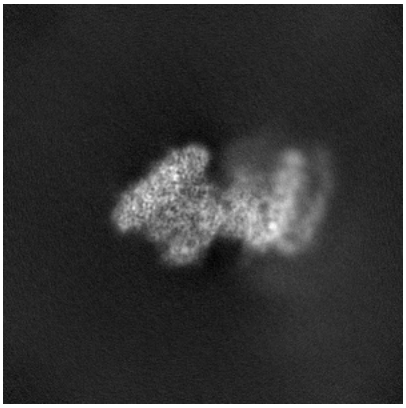

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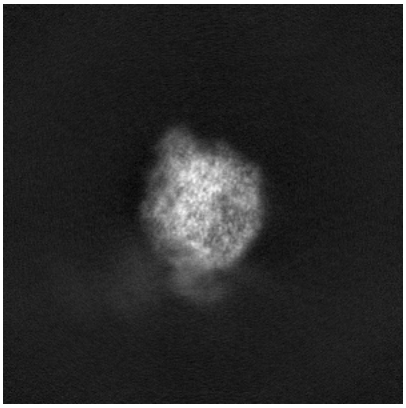
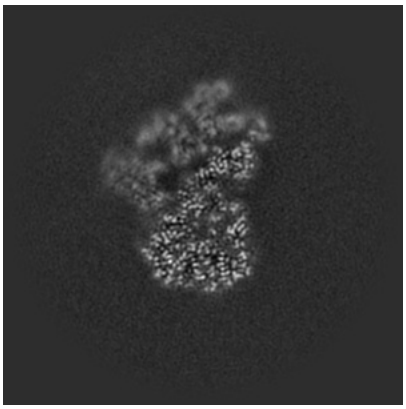


Z

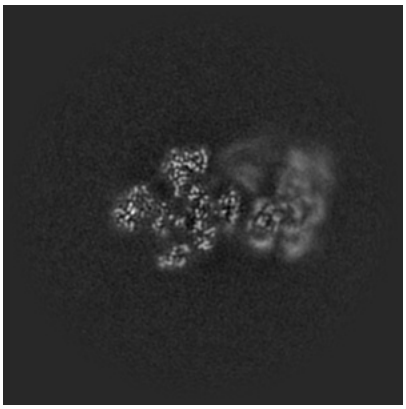
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

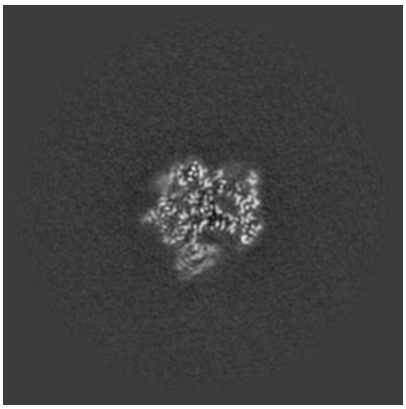
6.2.1 Primary map



X Index: 224

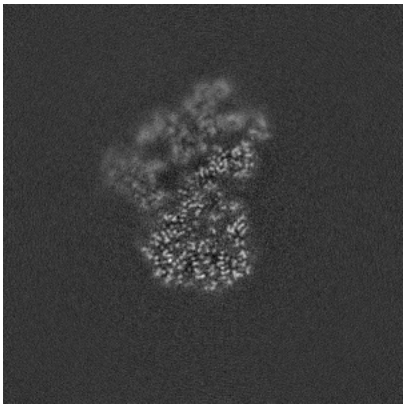


Y Index: 224



Z Index: 224

6.2.2 Raw map



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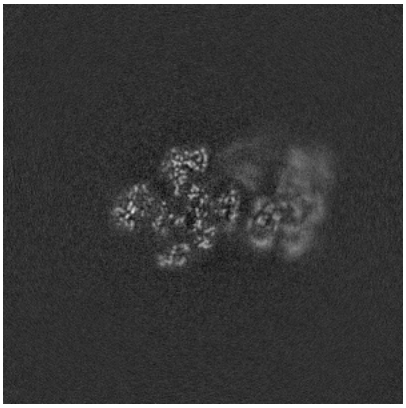

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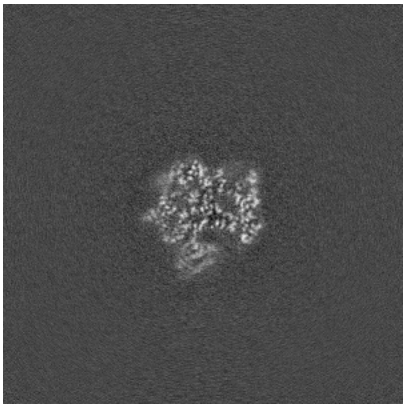
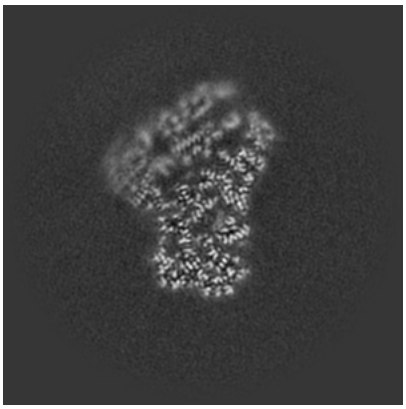


Z Index: 224

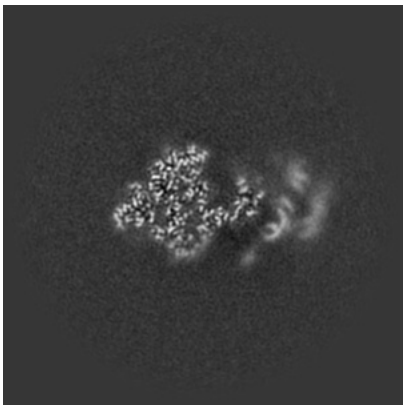
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

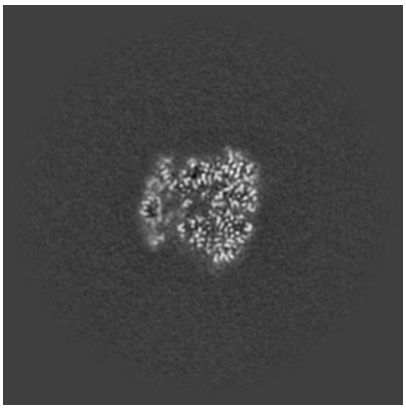
6.3.1 Primary map



X Index: 213

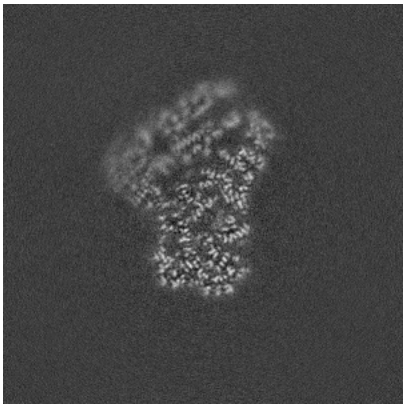


Y Index: 251

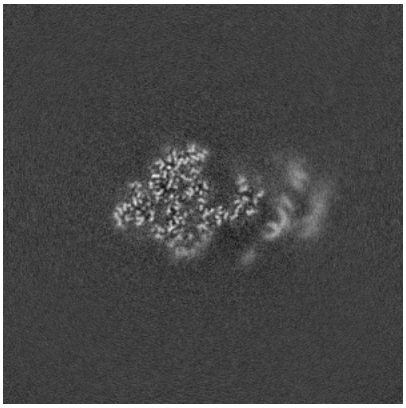


Z Index: 194

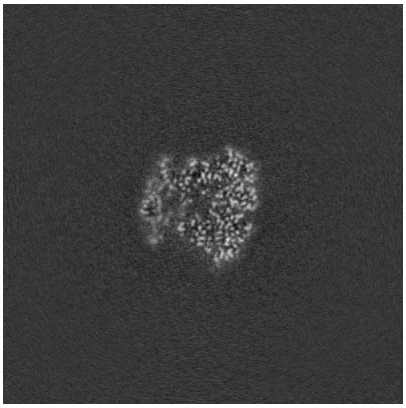
6.3.2 Raw map



X Index: 213



Y Index: 251

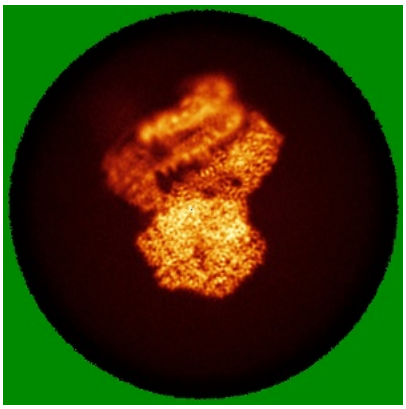


Z Index: 193

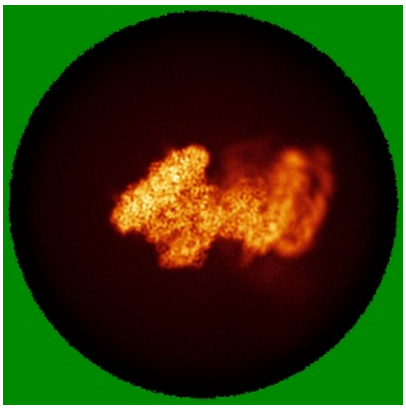
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

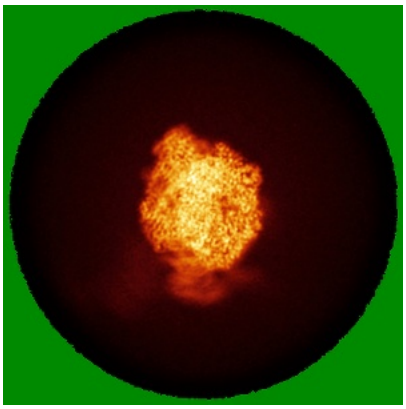
6.4.1 Primary map



X

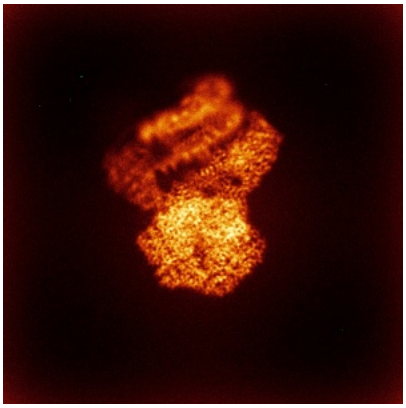


Y

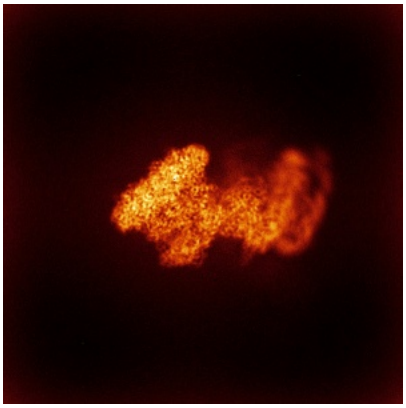


Z

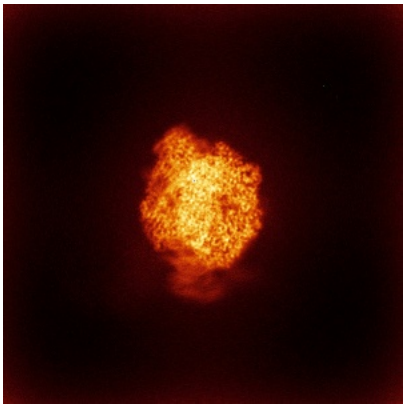
6.4.2 Raw map



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.

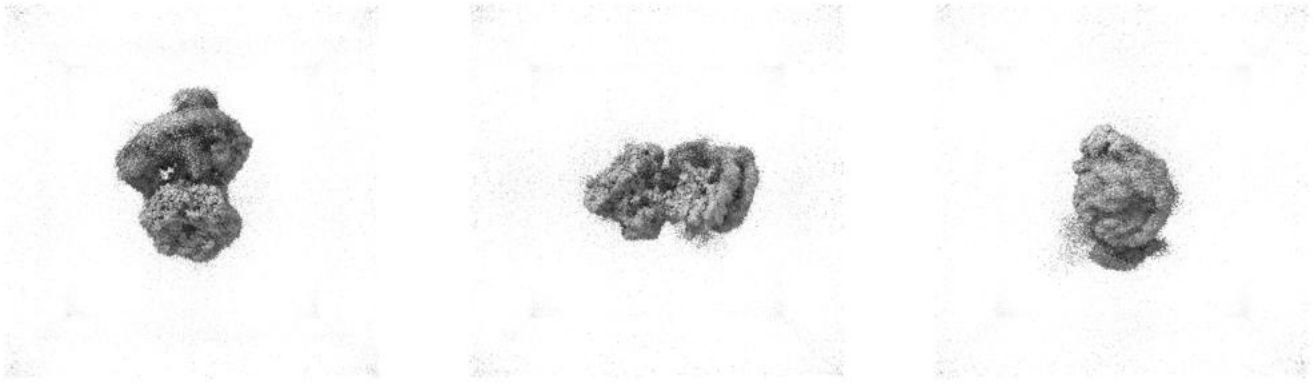
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

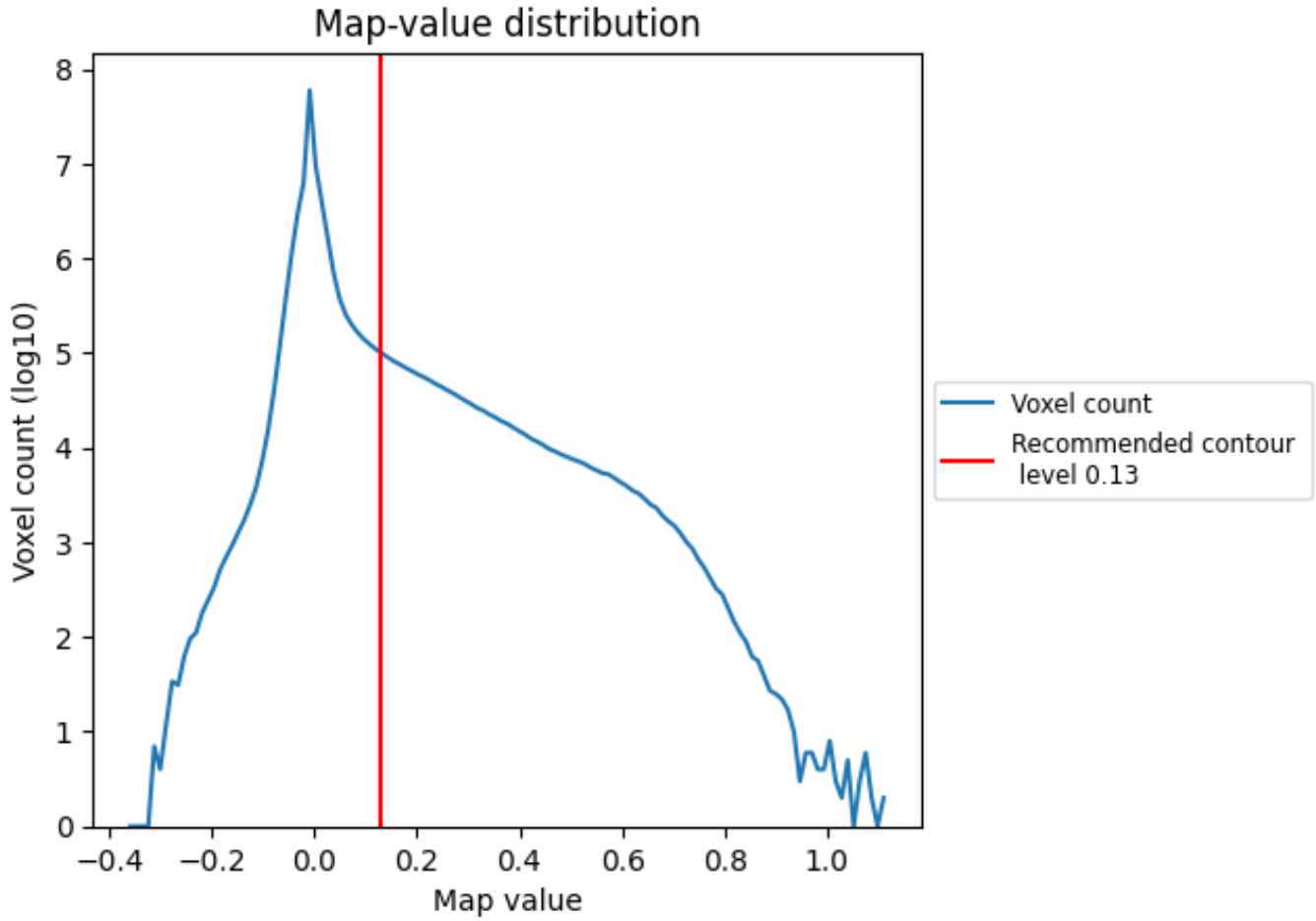
6.6 Mask visualisation (i)

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

7 Map analysis

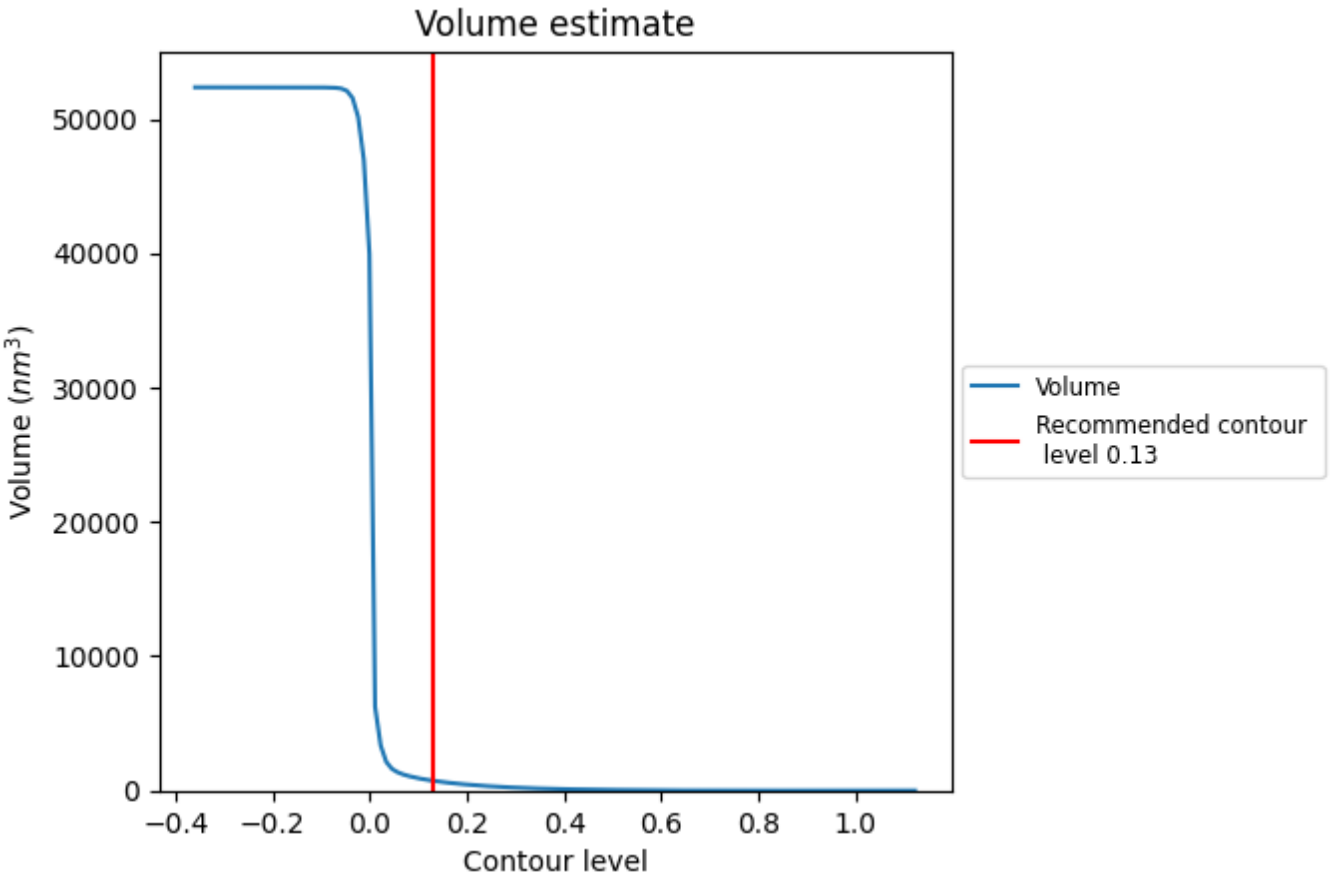
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

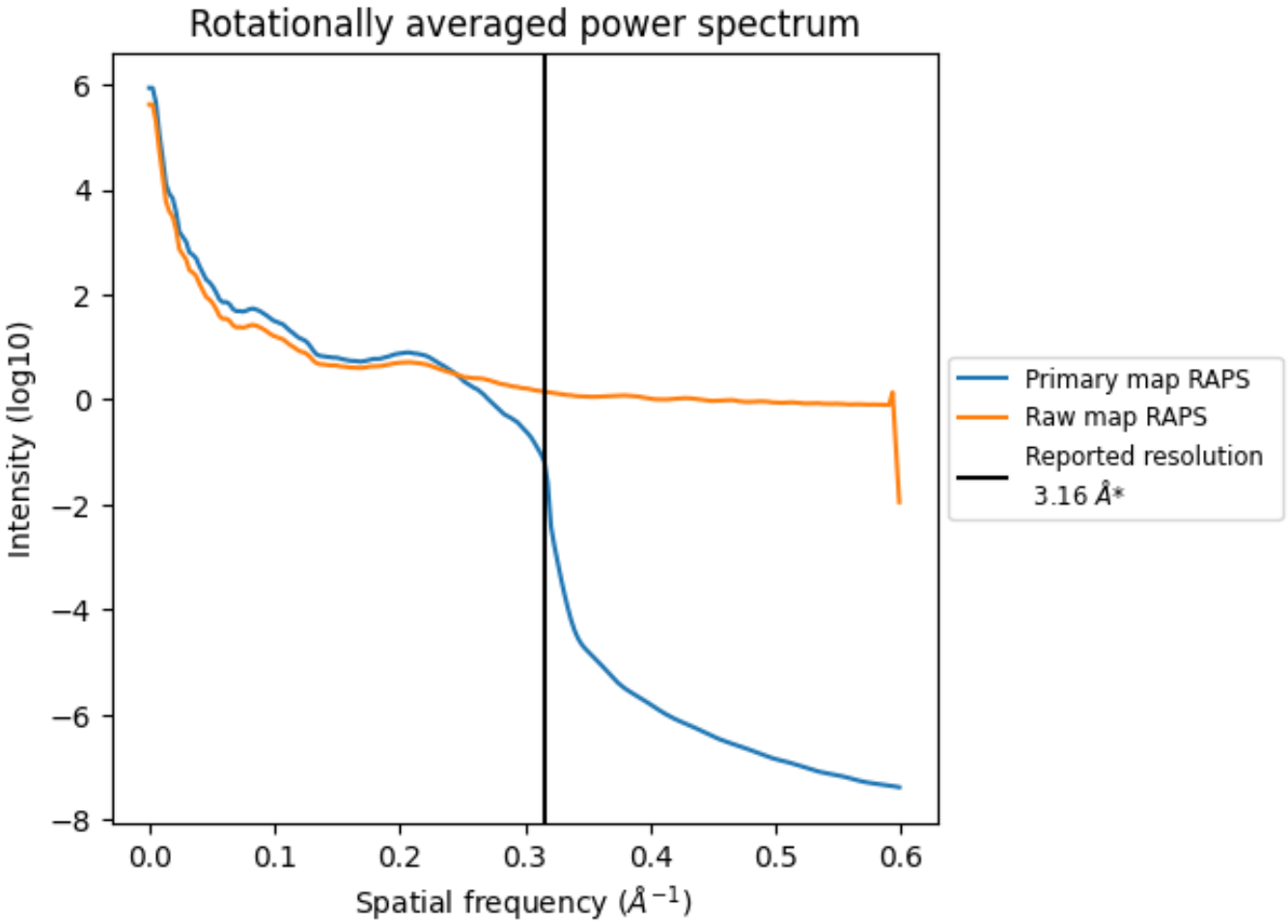
7.2 Volume estimate



The volume at the recommended contour level is 732 nm^3; this corresponds to an approximate mass of 662 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

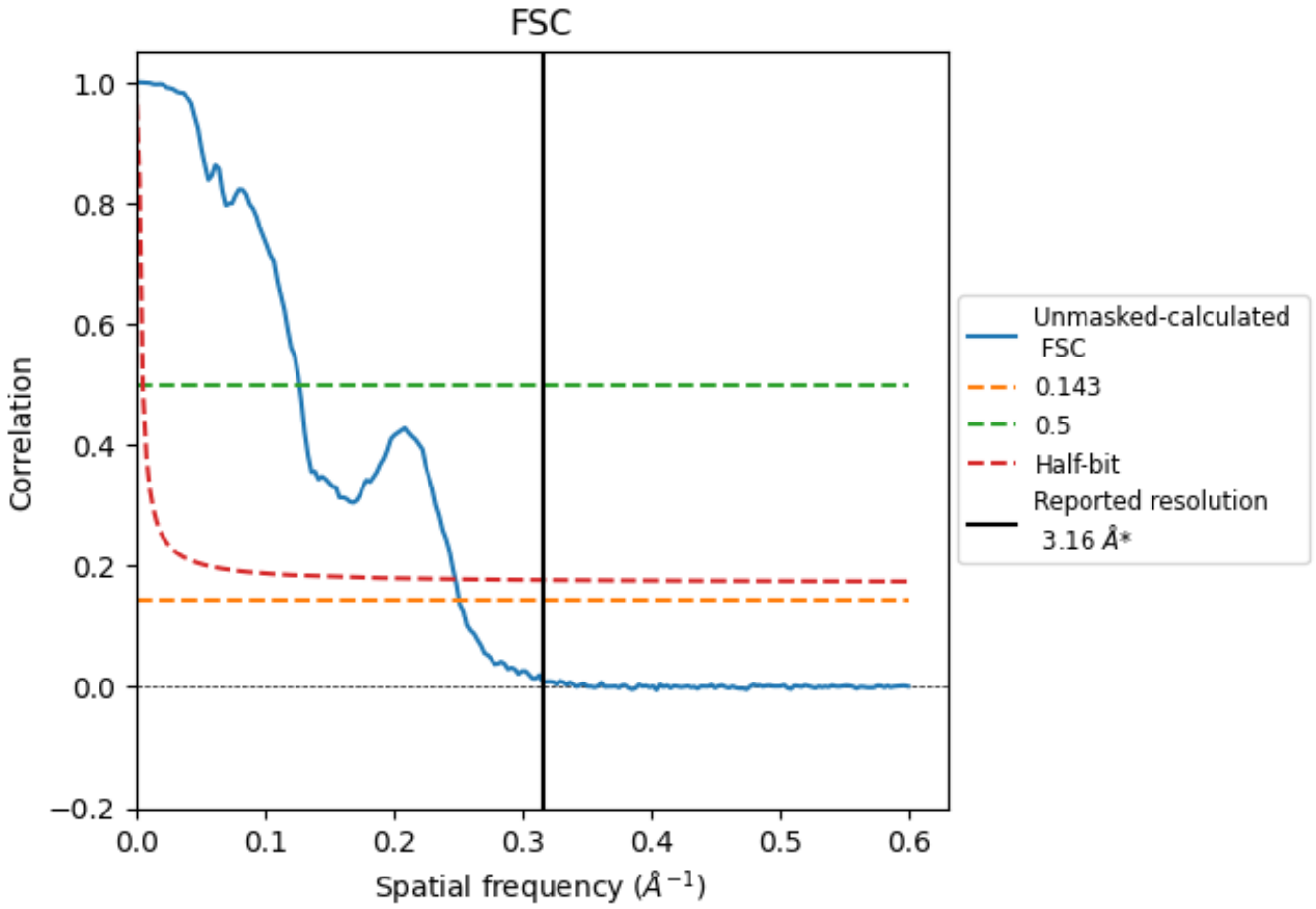


*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8.2 Resolution estimates (i)

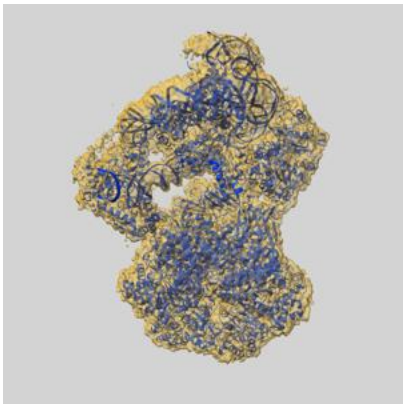
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	7.89	4.04

*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 3.99 differs from the reported value 3.16 by more than 10 %

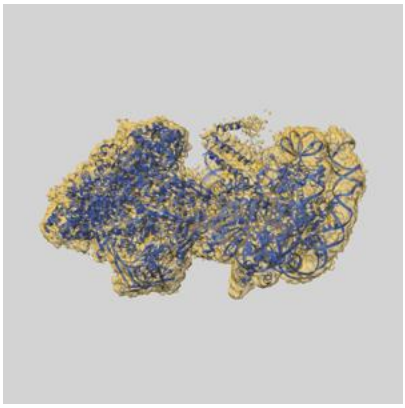
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45370 and PDB model 9C9T. Per-residue inclusion information can be found in section 3 on page 7.

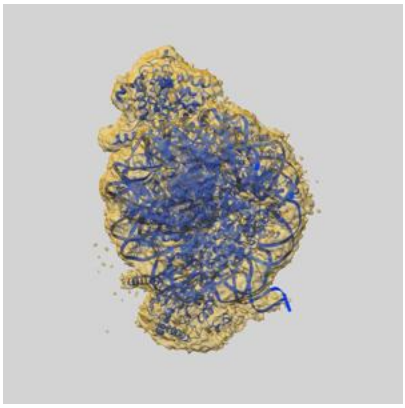
9.1 Map-model overlay



X



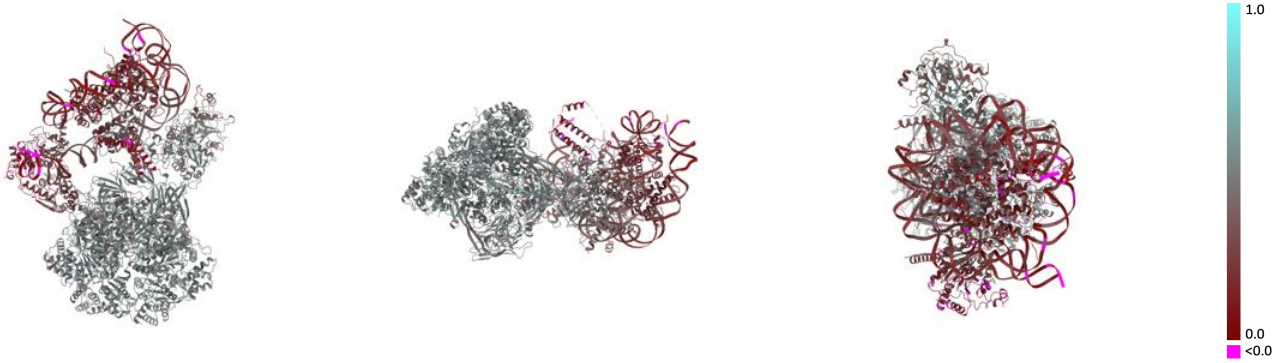
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

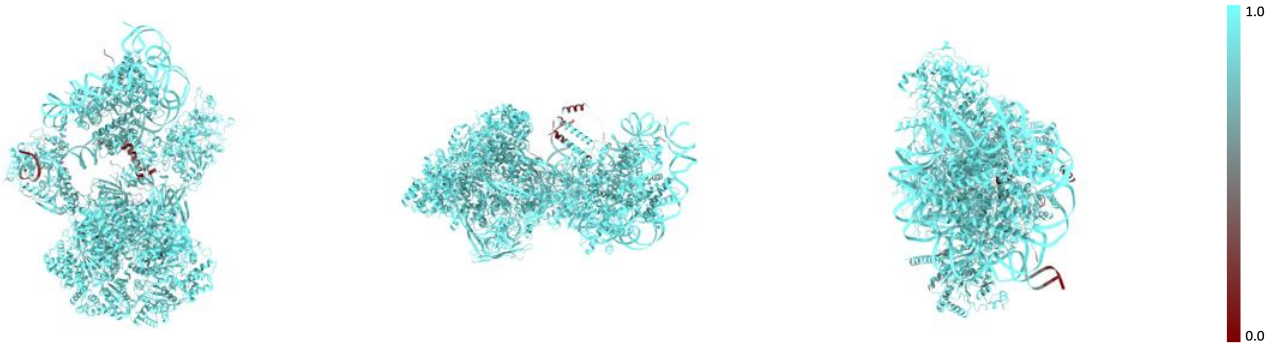
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

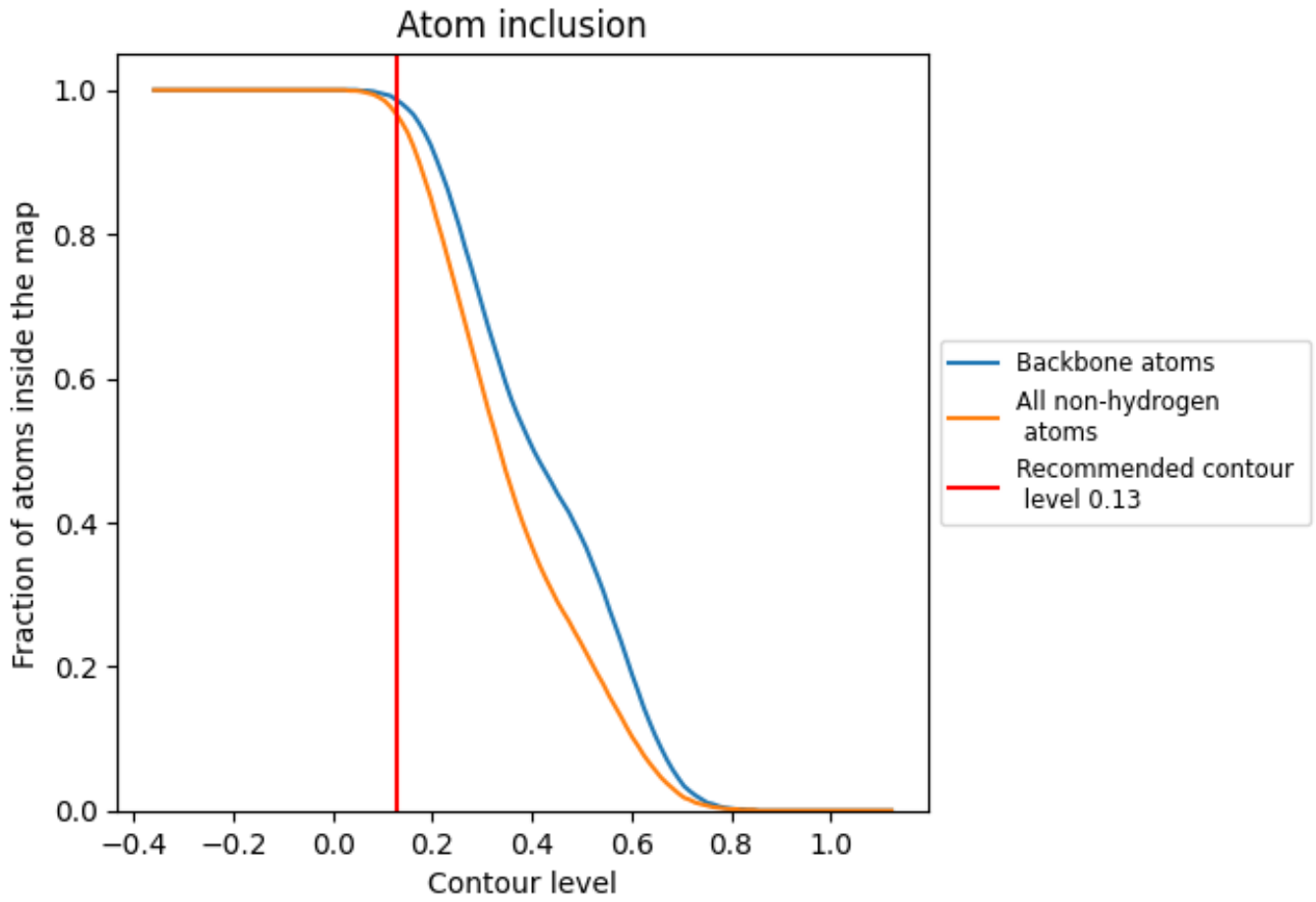
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.9640	0.3990
A	0.9650	0.1920
B	0.9800	0.2070
C	0.9540	0.2210
D	0.9650	0.2280
E	0.9560	0.2000
F	0.9480	0.2710
G	0.9140	0.3220
H	0.9300	0.3580
I	0.9540	0.2140
J	0.9640	0.2160
Q	0.9230	0.3330
R	0.9540	0.4210
S	0.9850	0.4380
T	0.9790	0.5110
U	0.9890	0.5060
V	0.9800	0.4940
W	0.9860	0.5080
X	0.9780	0.5170
Y	0.9720	0.5090
Z	0.9470	0.4230