Full wwPDB EM Validation Report (i)

Dec 5, 2022 – 03:34 pm GMT

PDB ID	:	8AV6
EMDB ID	:	EMD-4278
Title	:	CryoEM structure of INO80 core nucleosome complex in closed grappler conformation
Authors	:	Kunert, F.; Metzner, F.J.; Eustermann, S.; Jung, J.; Woike, S.; Schall, K.; Kostrewa, D.; Hopfner, K.P.
Deposited on	:	2022-08-26
Resolution	:	4.68 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 (i) 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 (1)) were used in the production of this report:

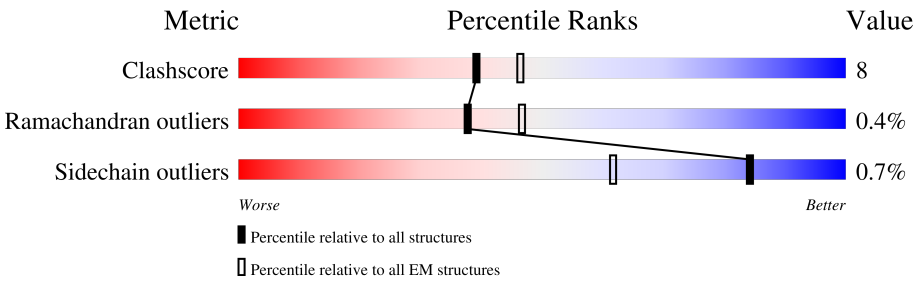
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.68 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	462	87% 10% •
1	B	462	83% 11% 5%
1	C	462	87% 13% •
2	D	488	81% 9% 10%
2	E	488	78% 12% 10%
2	F	488	80% 9% 10%
3	G	1856	29% 9% • 61%
4	H	492	5% 13% 5% • 80%

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Mol	Chain	Length	Quality of chain
5	I	219	41% 9% 50%
6	J	769	6% 70% 13% 16%
7	K	227	33% 24% 10% 33%
8	L	227	29% 31% 7% 33%
9	M	135	59% 11% 30%
9	Q	135	48% 23% 28%
10	N	102	69% 7% 25%
10	R	102	74% 24%
11	O	129	76% 6% 18%
11	S	129	53% 29% 16%
12	P	125	68% 6% 26%
12	T	125	54% 18% 27%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 45567 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 RuvB-like helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	449	3432	2154	610	653	15	0	0
1	B	438	3352	2103	597	637	15	0	0
1	C	459	3511	2199	627	670	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	439	3383	2117	595	656	15	0	0
2	E	441	3396	2124	598	659	15	0	0
2	F	437	3376	2113	594	654	15	0	0

- Molecule 3 is a protein called Ino80.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	724	5917	3770	1050	1063	34	0	0

- Molecule 4 is a protein called PAPA-1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	98	762	466	153	137	6	0	0

- Molecule 5 is a protein called YL1_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	109	875	550	167	154	4	0	0

- Molecule 6 is a protein called DASH complex subunit DAD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	647	5253	3307	960	965	21	0	0

- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	K	152	3101	1473	561	915	152	0	0

- Molecule 8 is a DNA chain called DNA (208-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	L	152	3131	1482	588	909	152	0	0

- Molecule 9 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	94	773	488	147	135	3	0	0
9	Q	97	801	505	155	138	3	0	0

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	77	618	391	119	107	1	0	0
10	R	78	622	393	120	108	1	0	0

- Molecule 11 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	O	106	812	514	157	141	0	0

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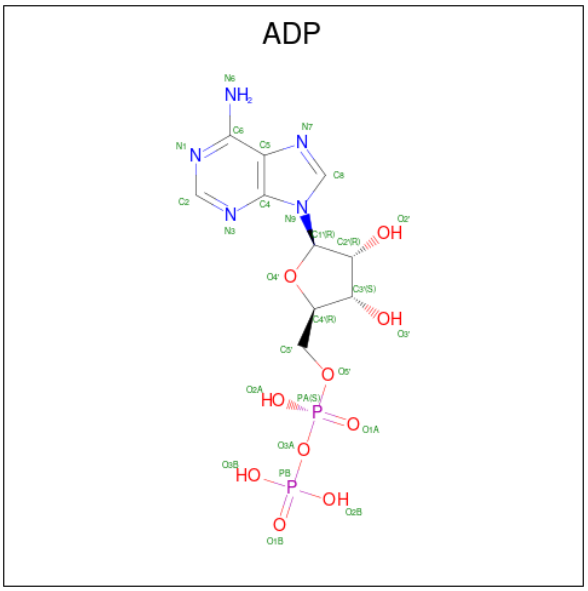
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	S	108	826	523	160	143	0	0

- Molecule 12 is a protein called Histone H2B type 1-C/E/F/G/I.

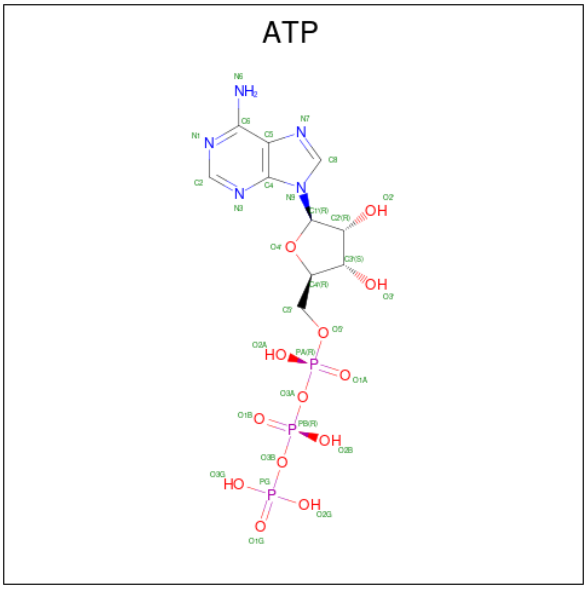
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	93	725	455	130	138	2	0	0
			Total	C	N	O	S		
12	T	91	708	446	125	135	2	0	0

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	A	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	B	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	C	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	D	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	E	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	F	1	27	10	5	10	2	0

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



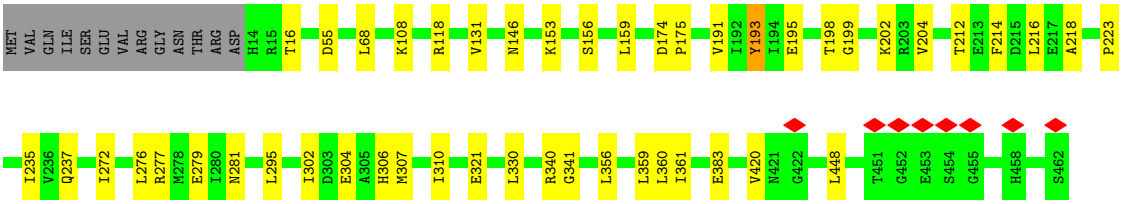
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
14	J	1	31	10	5	13	3	0

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.

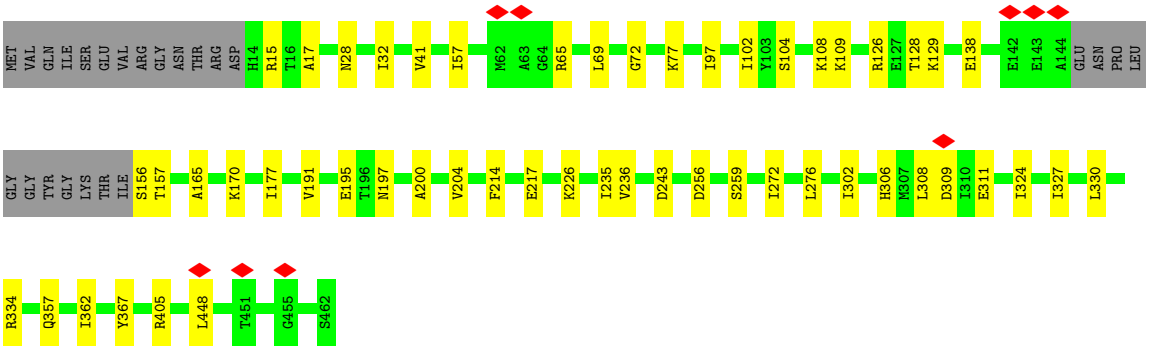
- Molecule 1: RuvB-like helicase

Chain A:



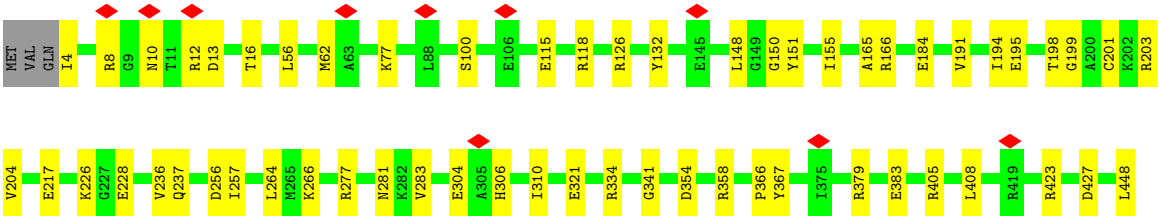
- Molecule 1: RuvB-like helicase

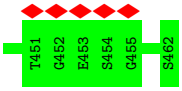
Chain B:



- Molecule 1: RuvB-like helicase

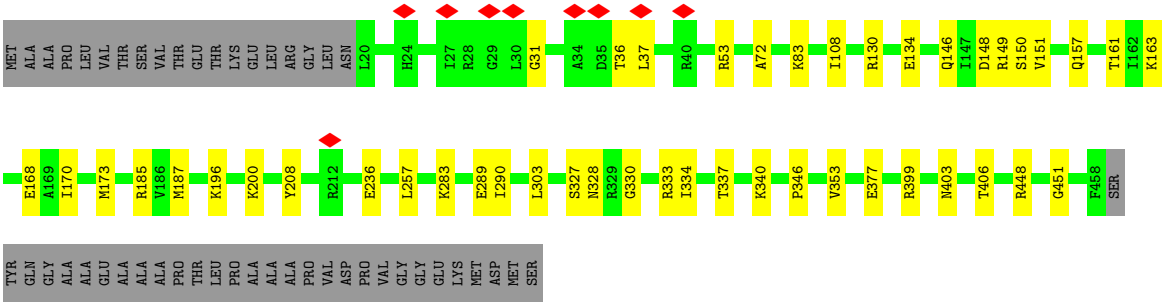
Chain C:





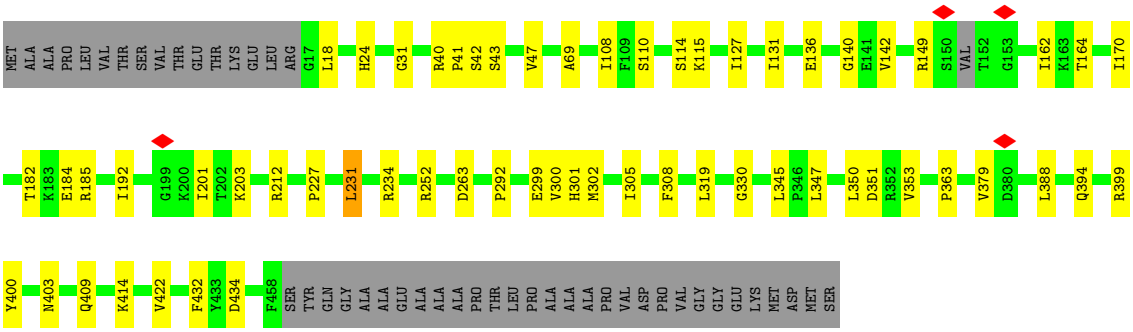
• Molecule 2: RuvB-like helicase

Chain D:



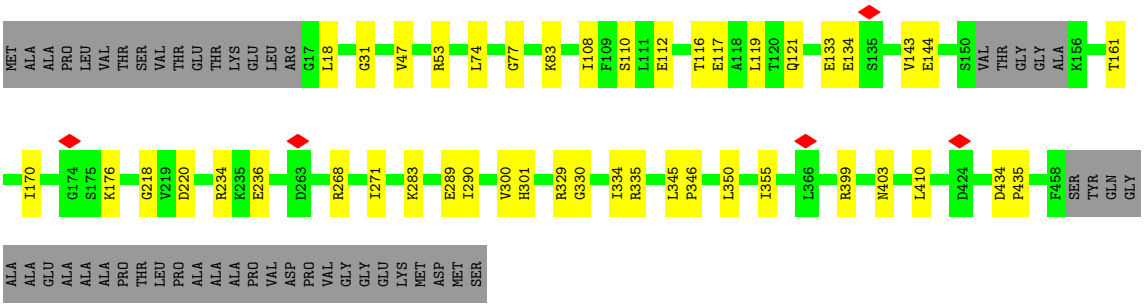
• Molecule 2: RuvB-like helicase

Chain E:



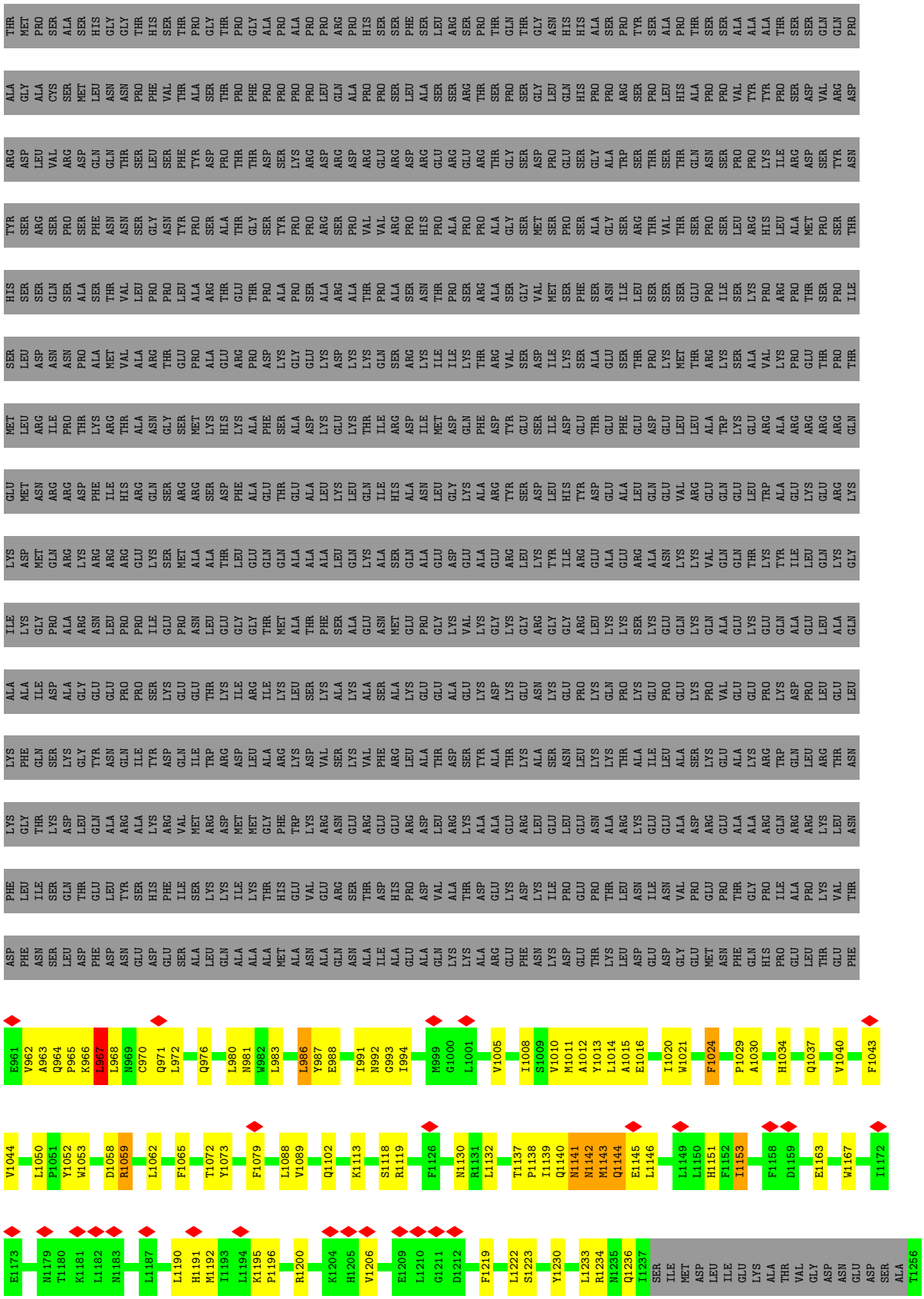
• Molecule 2: RuvB-like helicase

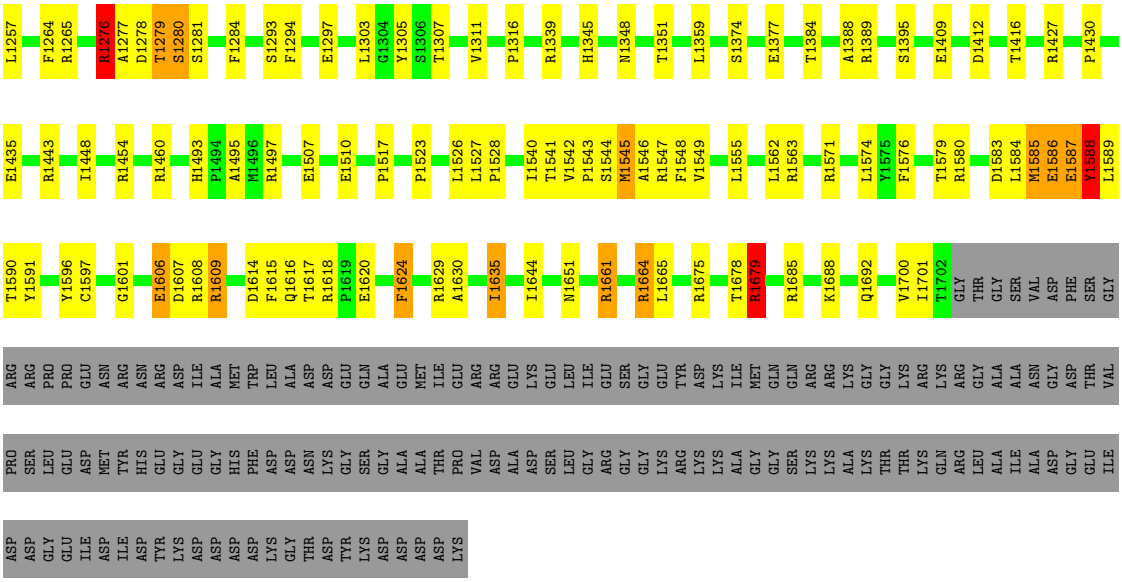
Chain F:



• Molecule 3: Ino80

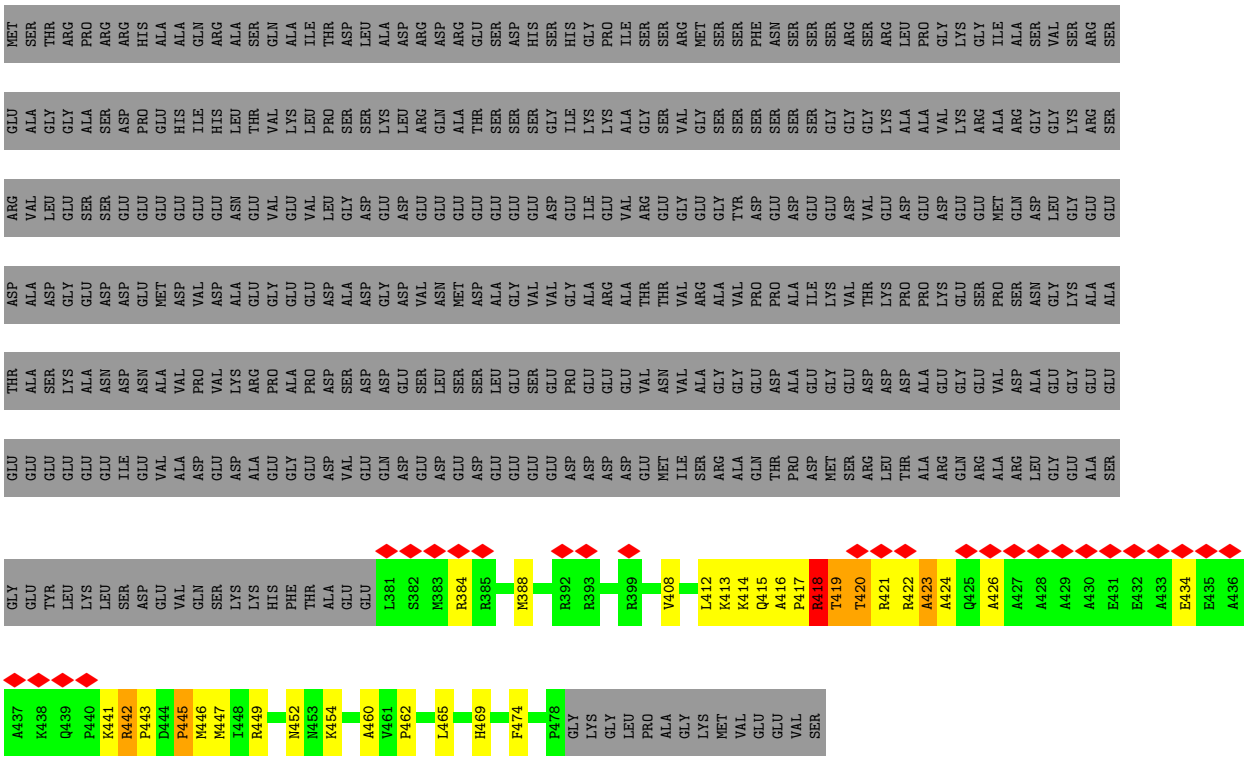
Chain G:


THR MET PRO SER ALA SER HIS GLY GLY THR HIS SER THR PRO GLY THR PRO GLY ALA PRO ALA PRO PRO ARG PRO HIS SER SER PHE SER LEU ARG SER PRO THR GLN THR GLY ASN HIS HIS ALA SER PRO TYR SER ALA PRO THR SER SER ALA ALA THR SER SER GLN GLN PRO
ALA GLY ALA CYS SER MET LEU ASN ASN PRO PHE VAL THR ALA SER THR PRO PHE PRO PRO PRO PRO LEU GLN ALA PRO PRO SER PRO LEU ALA SER SER ARG THR SER PRO SER GLY LEU GLN HIS PRO PRO ARG SER PRO LEU HIS ALA PRO PRO PRO VAL TYR TYR PRO SER ASP VAL ARG ASP
ARG ASP LEU VAL ARG ASP GLN GLN THR SER LEU SER PHE TYR ASP PRO THR THR ASP SER LYS ARG ASP ARG ASP ARG GLU ARG ASP ARG GLU ARG GLU ARG THR GLY SER ASP PRO GLU SER GLY ALA TRP SER THR SER THR GLN ASN SER PRO LYS ILE ARG ASP SER THR ASN
TYR SER ARG SER PRO SER PHE ASN ASN SER SER GLY ASN TYR PRO SER ALA THR GLY SER TYR PRO PRO ARG SER PRO VAL VAL ARG PRO HIS PRO ALA PRO PRO ALA GLY SER MET SER PRO SER ALA GLY ARG THR SER VAL THR SER PRO SER LEU ARG HIS LEU ALA MET PRO SER THR
HIS SER SER GLN SER ALA SER THR VAL LEU PRO PRO LEU ALA ARG THR GLU THR PRO ALA PRO SER ALA ARG ALA THR PRO ASN THR PRO SER GLY VAL MET SER PHE SER ASN ILE LEU SER SER GLU GLY SER PRO ILE SER LYS PRO THR SER PRO ILE
SER LEU ASP ASN ASN PRO ALA MET VAL ALA ARG THR GLU PRO ALA LYS GLY GLU LYS ASP LYS LYS LYS GLN SER ARG LYS ILE ILE LYS THR ARG ARG VAL SER ASP ILE LYS SER ALA GLU SER THR PRO SER LYS SER ALA VAL LYS PRO GLU THR PRO THR
MET LEU ARG ILE PRO THR LYS ARG THR ALA ASN GLY SER MET LYS HIS LYS ALA PHE SER ALA ASP LYS GLU LYS THR ILE ARG ASP ILE MET ASP GLN PHE ASP TYR GLU SER ILE ASP GLU THR GLU PHE ALA LEU LEU TRP LYS GLU GLU ARG ARG ARG ARG ARG GLN
GLU MET ASN ARG ARG ASP PHE ILE HIS ARG GLN SER ARG SER ASP PHE ALA GLU THR GLU ALA LEU LYS LEU GLN ILE HIS ALA ALA ASN LEU GLY LYS ARG TYR SER ASP LEU HIS TYR ASP GLU ALA LEU GLN GLU VAL ARG GLU GLN GLU LEU TRP ALA ALA GLU LYS GLU ARG LYS
LYS ASP MET GLN ARG LYS ARG ARG GLU LYS SER MET ALA ALA THR LEU GLU GLN GLN LYS ALA SER GLN ALA ALA GLU ASP GLU ARG LEU LYS TYR ILE ARG GLU ALA GLU ARG ALA ASN ASN LYS LYS VAL GLN GLN THR LYS TYR ILE LEU GLN LYS GLY
ILE LYS GLY PRO ALA ARG ASN LEU PRO PRO ILE GLU PRO ASN LEU GLU GLY GLY THR MET ALA THR PHE SER ALA GLU ASN MET GLU PRO GLY LYS VAL LYS GLY LYS GLY ARG GLY GLY ARG LEU LYS LYS SER LYS GLU GLN LYS GLN ALA GLU LEU ALA GLN
ALA ALA ILE ASP ALA GLY GLU GLU PRO PRO SER LYS LYS ILE ARG ILE LYS LEU SER LYS ALA LYS ALA SER ALA ALA LYS GLU PRO GLU ALA ASP LYS GLU PRO LYS GLN PRO LYS GLU PRO GLU VAL LEU LEU ALA ALA GLU ARG GLU GLN GLU LEU GLU LEU
LYS PHE GLN SER LYS GLY TYR ASN GLN ILE TYR ASP GLN ILE TRP ARG ASP LEU ALA ARG LYS ASP VAL SER LYS VAL PHE ARG LEU ALA THR ASP SER TYR ALA THR LYS ASN SER ALA ALA LYS LYS THR ALA ILE ILE LEU ALA SER LYS GLU LEU ALA ALA ARG ALA ARG ARG ARG
LYS GLY THR LYS ASP LEU GLN ALA ARG ALA ARG ARG ASN GLU ARG GLU GLU ARG ASP LEU ARG LYS ALA ASP ALA ALA GLU LYS ARG LEU GLU LYS LYS THR LYS ALA GLU GLU ASN LYS GLU GLU ALA ASP ARG GLU ALA ALA ARG ARG ARG ARG ASN
PHE LEU ILE SER GLN THR GLU LEU TYR SER HIS PHE ILE SER LYS LYS ILE LYS THR HIS GLU VAL GLU ARG SER THR ASP HIS PRO ASP VAL ALA THR ASP GLU LYS ASP LYS ILE PRO GLU PRO THR LEU ASN ILE ASN VAL PRO GLU ILE ALA ILE ILE ASN ILE LYS LEU ASN VAL THR
ASP PHE ASN SER LEU ASP PHE ASN SER GLU GLN ASN ALA ILE ALA GLU GLN ALA THR LYS ALA ALA MET ALA ASN ASP GLU THR LYS LEU ASP GLU GLU GLU ALA GLN LYS LYS ASN ALA ALA ILE ASP GLY GLU MET ASN PHE GLN HIS PRO GLU ARG LEU ARG ARG ARG PHE



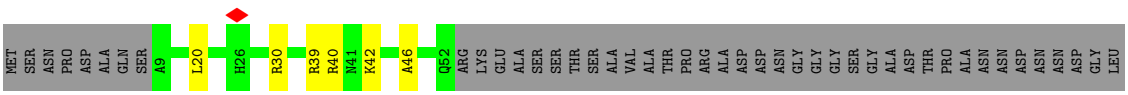
• Molecule 4: PAPA-1 domain-containing protein

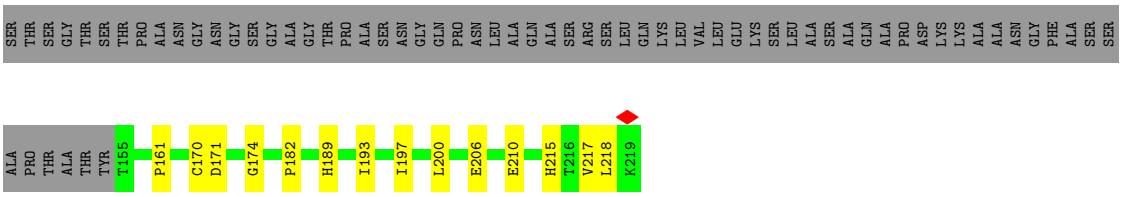
Chain H:



• Molecule 5: YL1_C domain-containing protein

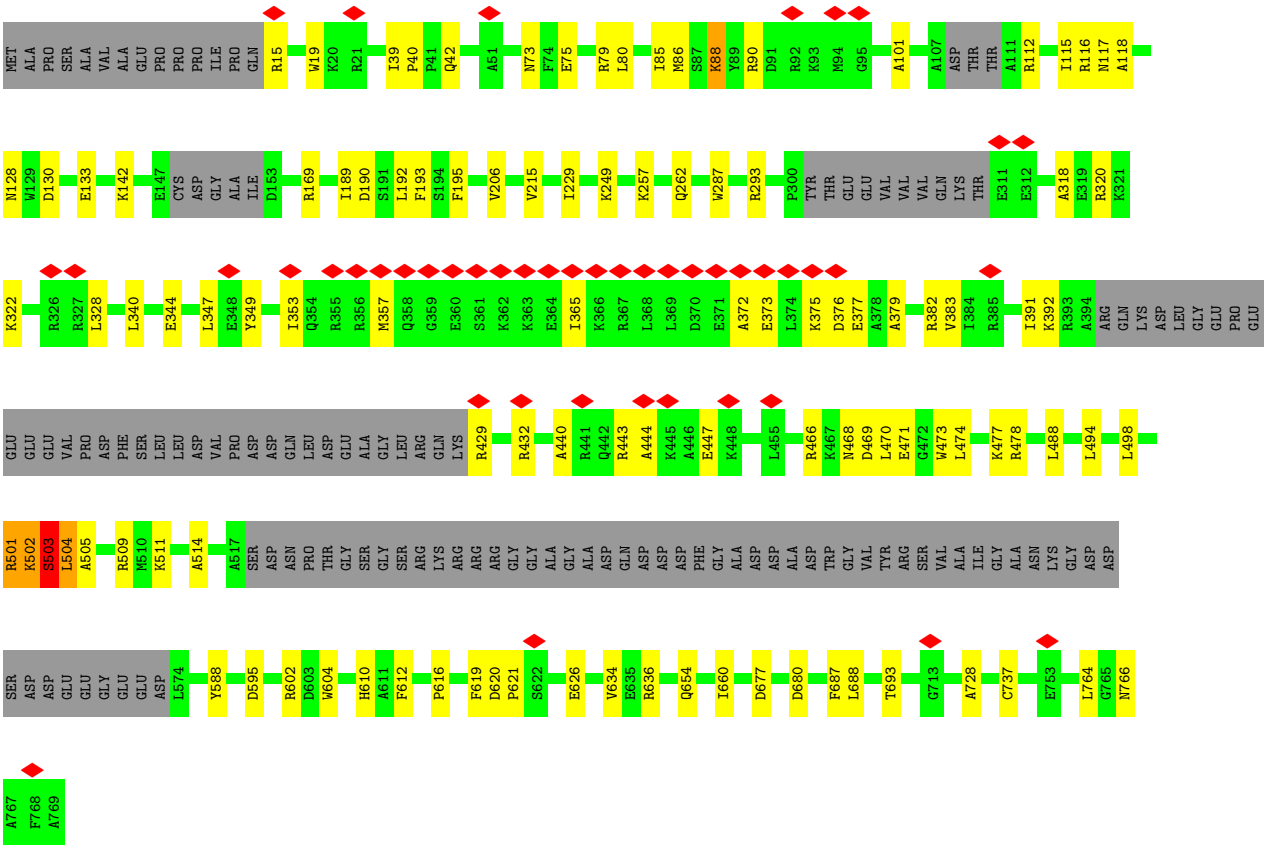
Chain I:





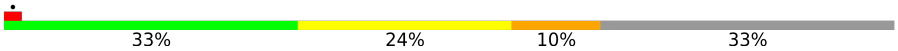
• Molecule 6: DASH complex subunit DAD4

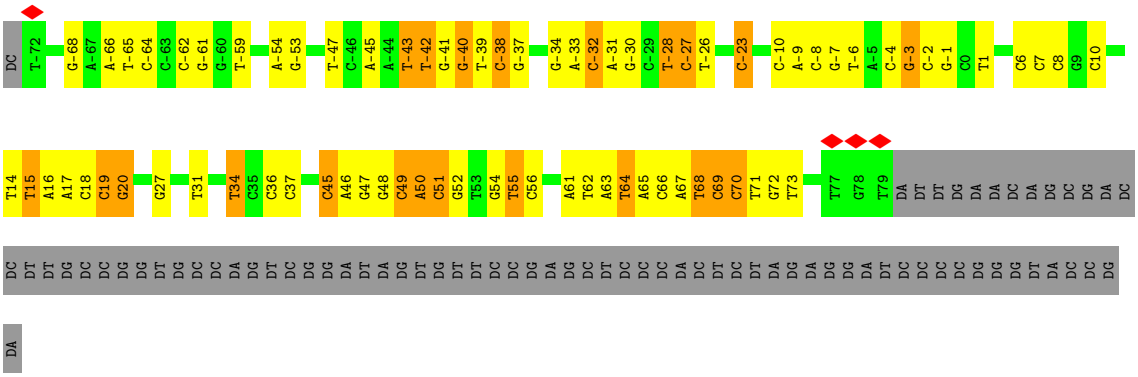
Chain J:



• Molecule 7: DNA

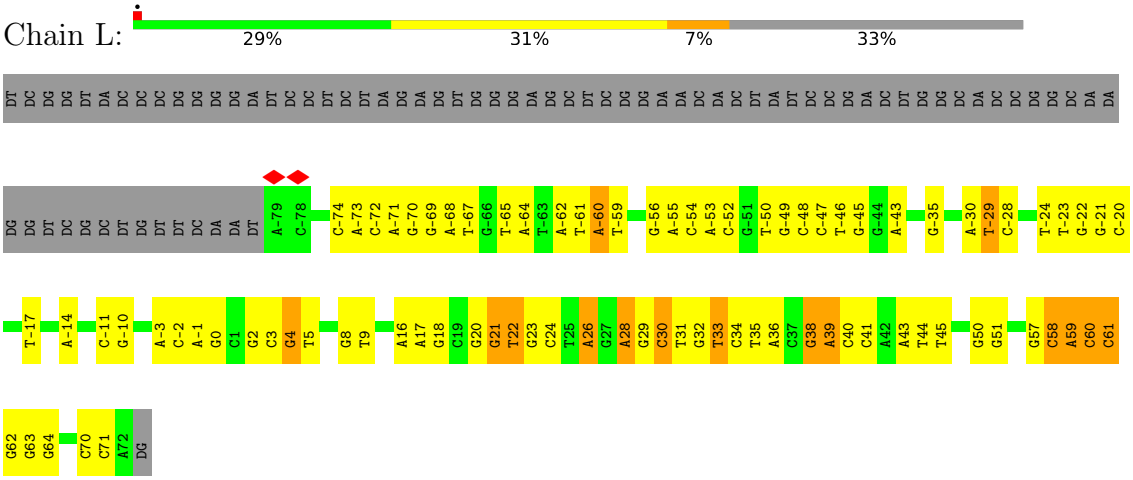
Chain K:





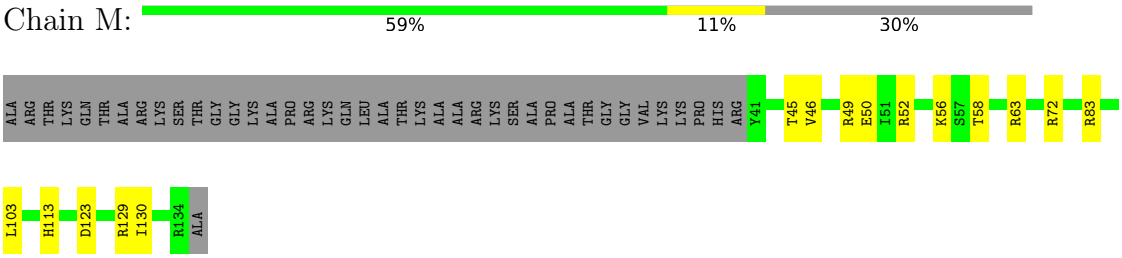
- Molecule 8: DNA (208-MER)

Chain L:



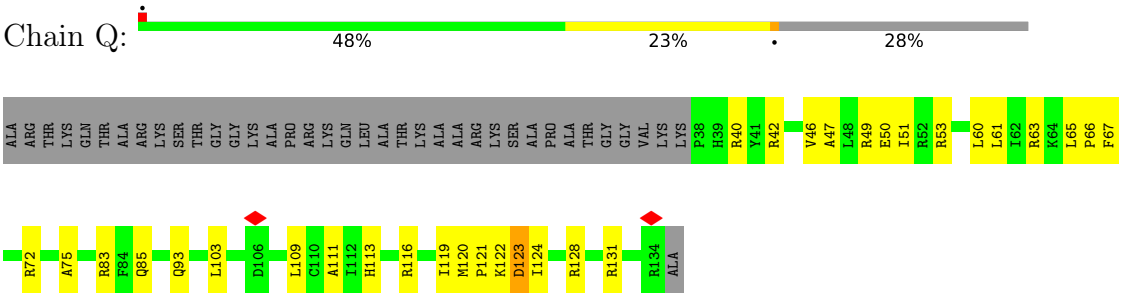
- Molecule 9: Histone H3.2

Chain M:



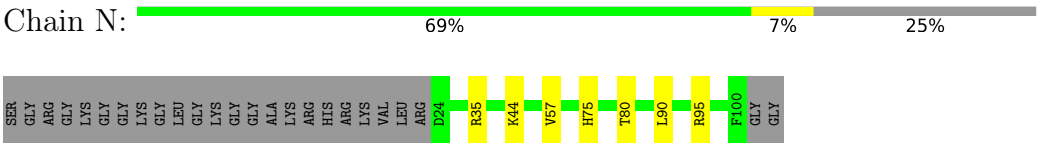
- Molecule 9: Histone H3.2

Chain Q:



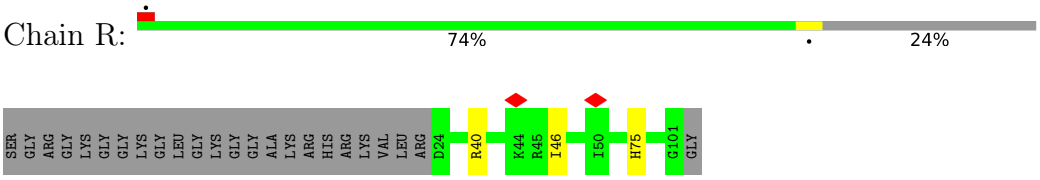
- Molecule 10: Histone H4

Chain N:



- Molecule 10: Histone H4

Chain R:

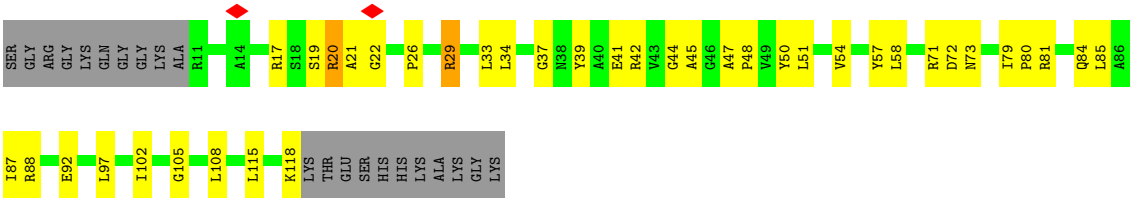


- Molecule 11: Histone H2A

Chain O:

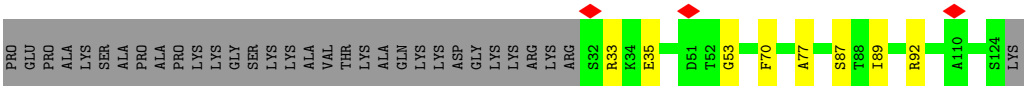
- Molecule 11: Histone H2A

Chain S:



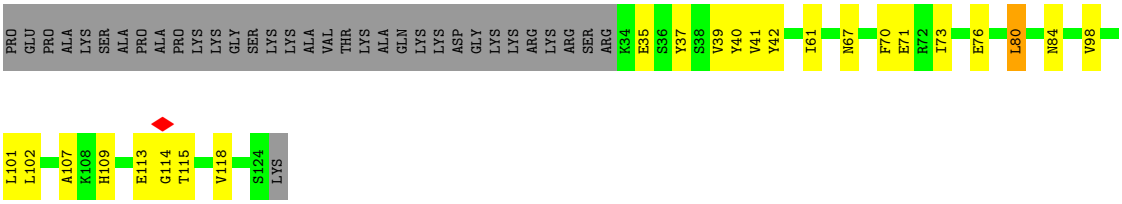
- Molecule 12: Histone H2B type 1-C/E/F/G/I

Chain P:



- Molecule 12: Histone H2B type 1-C/E/F/G/I

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16287	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 ($e^-/Å^2$)	59.6	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.067	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	360.4, 360.4, 360.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.50	0/3481	0.61	1/4703 (0.0%)
1	B	0.50	0/3398	0.59	0/4589
1	C	0.47	0/3560	0.58	0/4809
2	D	0.46	0/3426	0.60	2/4614 (0.0%)
2	E	0.49	0/3438	0.61	1/4628 (0.0%)
2	F	0.47	0/3418	0.58	1/4601 (0.0%)
3	G	0.71	2/6054 (0.0%)	1.10	25/8183 (0.3%)
4	H	0.59	0/771	0.72	0/1032
5	I	0.47	0/895	0.61	0/1209
6	J	0.52	3/5354 (0.1%)	0.60	4/7203 (0.1%)
7	K	0.90	0/3474	1.56	67/5356 (1.3%)
8	L	0.89	0/3516	1.58	75/5428 (1.4%)
9	M	0.28	0/783	0.55	0/1050
9	Q	0.25	0/813	0.53	0/1090
10	N	0.30	0/625	0.61	0/838
10	R	0.29	0/629	0.57	0/843
11	O	0.28	0/822	0.51	0/1110
11	S	0.36	0/836	0.74	1/1128 (0.1%)
12	P	0.29	0/736	0.50	0/990
12	T	0.43	0/719	0.64	0/968
All	All	0.58	5/46748 (0.0%)	0.91	177/64372 (0.3%)

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
3	G	0	12
4	H	0	1
6	J	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	K	0	4
8	L	0	1
11	S	0	1
All	All	0	23

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	112	ARG	CG-CD	-6.63	1.35	1.51
6	J	112	ARG	CZ-NH1	6.55	1.41	1.33
3	G	1223	SER	CA-CB	-6.48	1.43	1.52
6	J	503	SER	CA-CB	-5.58	1.44	1.52
3	G	1151	HIS	CG-CD2	-5.02	1.27	1.35

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1059	ARG	NE-CZ-NH2	-13.40	113.60	120.30
3	G	1265	ARG	NE-CZ-NH2	-12.47	114.07	120.30
8	L	26	DA	P-O3'-C3'	-11.59	105.80	119.70
8	L	-14	DA	P-O3'-C3'	-11.01	106.49	119.70
3	G	1059	ARG	NE-CZ-NH1	10.57	125.58	120.30
6	J	503	SER	CA-C-N	-10.47	94.16	117.20
6	J	504	LEU	N-CA-CB	-10.27	89.86	110.40
8	L	-64	DA	N1-C6-N6	-9.00	113.20	118.60
11	S	29	ARG	NE-CZ-NH1	8.89	124.75	120.30
7	K	48	DG	P-O3'-C3'	-8.52	109.48	119.70
7	K	-23	DC	P-O3'-C3'	-8.28	109.77	119.70
8	L	-68	DA	N1-C6-N6	-8.27	113.64	118.60
3	G	1073	TYR	CB-CG-CD1	8.23	125.94	121.00
8	L	21	DG	P-O3'-C3'	-8.04	110.05	119.70
7	K	65	DA	N1-C6-N6	-8.03	113.78	118.60
8	L	-52	DC	P-O3'-C3'	-7.95	110.16	119.70
8	L	-71	DA	N1-C6-N6	-7.91	113.85	118.60
8	L	26	DA	O4'-C1'-N9	-7.87	102.49	108.00
3	G	1119	ARG	NE-CZ-NH1	-7.86	116.37	120.30
8	L	-70	DG	O4'-C1'-N9	7.84	113.49	108.00
3	G	1119	ARG	NE-CZ-NH2	-7.82	116.39	120.30
3	G	1276	ARG	NE-CZ-NH2	-7.76	116.42	120.30
7	K	67	DA	C5-C6-N1	7.72	121.56	117.70
3	G	1679	ARG	NE-CZ-NH2	7.65	124.12	120.30
7	K	67	DA	N1-C6-N6	-7.60	114.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	65	DA	C5-C6-N1	7.56	121.48	117.70
7	K	54	DG	C8-N9-C1'	7.54	136.80	127.00
7	K	15	DT	P-O3'-C3'	-7.54	110.66	119.70
7	K	31	DT	P-O3'-C3'	-7.52	110.67	119.70
7	K	54	DG	C4-N9-C1'	-7.50	116.75	126.50
7	K	54	DG	P-O3'-C3'	-7.47	110.73	119.70
7	K	49	DC	P-O3'-C3'	-7.41	110.81	119.70
7	K	19	DC	P-O3'-C3'	-7.39	110.83	119.70
8	L	71	DC	O4'-C1'-N1	7.39	113.18	108.00
7	K	69	DC	N3-C2-O2	-7.38	116.73	121.90
8	L	51	DG	O4'-C1'-N9	7.38	113.16	108.00
8	L	-49	DG	P-O3'-C3'	-7.36	110.87	119.70
3	G	1024	PHE	N-CA-CB	-7.33	97.40	110.60
8	L	-73	DA	C5-C6-N1	7.33	121.36	117.70
7	K	-10	DC	P-O3'-C3'	-7.33	110.91	119.70
7	K	-45	DA	P-O3'-C3'	-7.32	110.91	119.70
7	K	-28	DT	P-O3'-C3'	-7.21	111.04	119.70
7	K	55	DT	P-O3'-C3'	-7.21	111.04	119.70
8	L	38	DG	P-O3'-C3'	-7.19	111.07	119.70
8	L	-73	DA	N1-C6-N6	-7.15	114.31	118.60
8	L	-68	DA	C5-C6-N1	7.11	121.25	117.70
8	L	-50	DT	P-O3'-C3'	-7.10	111.19	119.70
7	K	-3	DG	P-O3'-C3'	-7.08	111.21	119.70
8	L	-72	DC	N3-C2-O2	-7.04	116.97	121.90
7	K	-68	DG	O4'-C1'-N9	7.03	112.92	108.00
7	K	-30	DG	P-O3'-C3'	-7.03	111.26	119.70
7	K	73	DT	O4'-C1'-N1	7.03	112.92	108.00
7	K	66	DC	N3-C2-O2	-6.99	117.01	121.90
3	G	1119	ARG	NH1-CZ-NH2	6.97	127.07	119.40
8	L	60	DC	P-O3'-C3'	-6.97	111.33	119.70
3	G	1679	ARG	NE-CZ-NH1	-6.94	116.83	120.30
3	G	1608	ARG	NE-CZ-NH1	-6.93	116.84	120.30
8	L	24	DC	P-O3'-C3'	-6.92	111.39	119.70
7	K	-42	DT	P-O3'-C3'	-6.92	111.40	119.70
7	K	-8	DC	P-O3'-C3'	-6.92	111.40	119.70
8	L	2	DG	P-O3'-C3'	-6.87	111.46	119.70
8	L	-53	DA	P-O3'-C3'	-6.85	111.48	119.70
8	L	-71	DA	C5-C6-N1	6.82	121.11	117.70
8	L	0	DG	P-O3'-C3'	-6.82	111.52	119.70
8	L	62	DG	P-O3'-C3'	-6.82	111.52	119.70
8	L	58	DC	O5'-P-OP1	-6.81	99.57	105.70
2	D	37	LEU	CA-CB-CG	6.79	130.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	-17	DT	P-O3'-C3'	-6.73	111.63	119.70
8	L	-64	DA	C5-C6-N1	6.72	121.06	117.70
8	L	-48	DC	P-O3'-C3'	-6.64	111.73	119.70
2	D	257	LEU	CA-CB-CG	6.63	130.55	115.30
8	L	58	DC	P-O3'-C3'	-6.63	111.75	119.70
6	J	503	SER	C-N-CA	-6.62	105.15	121.70
8	L	63	DG	P-O3'-C3'	-6.61	111.77	119.70
8	L	-64	DA	C4-C5-C6	-6.60	113.70	117.00
8	L	-20	DC	P-O3'-C3'	-6.59	111.79	119.70
7	K	-40	DG	P-O3'-C3'	-6.54	111.86	119.70
7	K	-1	DG	P-O3'-C3'	-6.53	111.86	119.70
7	K	27	DG	O4'-C1'-N9	6.51	112.55	108.00
7	K	-2	DC	P-O3'-C3'	-6.50	111.91	119.70
7	K	65	DA	C4-C5-C6	-6.47	113.76	117.00
7	K	-62	DC	P-O3'-C3'	-6.38	112.05	119.70
7	K	70	DC	N3-C2-O2	-6.32	117.47	121.90
8	L	22	DT	P-O3'-C3'	-6.32	112.11	119.70
8	L	45	DT	P-O3'-C3'	-6.28	112.16	119.70
7	K	50	DA	P-O3'-C3'	-6.26	112.19	119.70
8	L	59	DA	P-O3'-C3'	-6.25	112.20	119.70
3	G	1119	ARG	N-CA-CB	-6.24	99.37	110.60
8	L	4	DG	P-O3'-C3'	-6.22	112.23	119.70
7	K	73	DT	N3-C2-O2	-6.19	118.59	122.30
3	G	1597	CYS	CB-CA-C	-6.18	98.05	110.40
7	K	20	DG	P-O3'-C3'	-6.18	112.29	119.70
8	L	43	DA	P-O3'-C3'	-6.18	112.29	119.70
3	G	1591	TYR	CB-CG-CD2	-6.16	117.30	121.00
7	K	64	DT	C6-C5-C7	-6.15	119.21	122.90
7	K	-59	DT	P-O3'-C3'	-6.13	112.34	119.70
8	L	-22	DG	C1'-O4'-C4'	-6.11	103.99	110.10
7	K	-32	DC	P-O3'-C3'	-6.10	112.38	119.70
8	L	39	DA	P-O3'-C3'	-6.07	112.41	119.70
7	K	-64	DC	P-O3'-C3'	-6.07	112.42	119.70
8	L	-68	DA	C4-C5-C6	-6.07	113.97	117.00
8	L	-21	DG	P-O3'-C3'	-6.07	112.42	119.70
8	L	-67	DT	C6-C5-C7	-6.06	119.27	122.90
7	K	51	DC	P-O3'-C3'	-6.04	112.45	119.70
7	K	73	DT	C6-C5-C7	-6.04	119.28	122.90
8	L	-73	DA	C4-C5-C6	-6.01	114.00	117.00
7	K	69	DC	N1-C2-O2	5.99	122.50	118.90
7	K	1	DT	P-O3'-C3'	-5.98	112.53	119.70
8	L	44	DT	P-O3'-C3'	-5.95	112.56	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	64	DG	P-O3'-C3'	-5.94	112.57	119.70
7	K	68	DT	C6-C5-C7	-5.93	119.34	122.90
8	L	9	DT	P-O3'-C3'	-5.92	112.59	119.70
8	L	-2	DC	P-O3'-C3'	-5.89	112.63	119.70
7	K	71	DT	C6-C5-C7	-5.87	119.38	122.90
7	K	-41	DG	P-O3'-C3'	-5.87	112.66	119.70
7	K	71	DT	N3-C2-O2	-5.85	118.79	122.30
8	L	-71	DA	C4-C5-C6	-5.85	114.08	117.00
3	G	1119	ARG	CG-CD-NE	-5.83	99.55	111.80
6	J	503	SER	O-C-N	5.80	131.99	122.70
3	G	1624	PHE	CB-CG-CD2	-5.78	116.75	120.80
8	L	-54	DC	P-O3'-C3'	-5.75	112.80	119.70
8	L	-29	DT	C1'-O4'-C4'	-5.75	104.36	110.10
7	K	-61	DG	P-O3'-C3'	-5.74	112.81	119.70
7	K	-27	DC	P-O3'-C3'	-5.73	112.82	119.70
7	K	-38	DC	P-O3'-C3'	-5.65	112.92	119.70
7	K	67	DA	C4-C5-C6	-5.63	114.19	117.00
8	L	30	DC	P-O3'-C3'	-5.62	112.95	119.70
3	G	1359	LEU	CA-CB-CG	5.61	128.21	115.30
3	G	1571	ARG	NE-CZ-NH1	5.60	123.10	120.30
7	K	-43	DT	P-O3'-C3'	-5.60	112.98	119.70
7	K	-7	DG	P-O3'-C3'	-5.57	113.02	119.70
8	L	-56	DG	P-O3'-C3'	-5.56	113.03	119.70
8	L	-65	DT	C6-C5-C7	-5.53	119.58	122.90
8	L	-3	DA	P-O3'-C3'	-5.52	113.07	119.70
8	L	-1	DA	P-O3'-C3'	-5.51	113.09	119.70
3	G	1052	TYR	CB-CG-CD2	5.48	124.29	121.00
7	K	-65	DT	O4'-C1'-N1	5.48	111.83	108.00
8	L	-55	DA	P-O3'-C3'	-5.46	113.15	119.70
8	L	23	DG	P-O3'-C3'	-5.46	113.15	119.70
8	L	16	DA	O4'-C1'-N9	5.43	111.80	108.00
2	F	410	LEU	CB-CG-CD2	-5.42	101.78	111.00
7	K	45	DC	P-O3'-C3'	-5.40	113.22	119.70
7	K	64	DT	N3-C2-O2	-5.40	119.06	122.30
7	K	14	DT	P-O3'-C3'	-5.37	113.25	119.70
8	L	-22	DG	O4'-C1'-N9	5.37	111.76	108.00
7	K	64	DT	O4'-C1'-N1	5.35	111.74	108.00
1	A	159	LEU	CA-CB-CG	5.34	127.58	115.30
8	L	-72	DC	O4'-C1'-N1	5.34	111.73	108.00
8	L	57	DG	OP1-P-O3'	5.32	116.90	105.20
7	K	-6	DT	P-O3'-C3'	-5.31	113.33	119.70
7	K	34	DT	P-O3'-C3'	-5.31	113.33	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	-72	DC	N1-C2-O2	5.27	122.06	118.90
8	L	-67	DT	N3-C2-O2	-5.27	119.14	122.30
8	L	29	DG	P-O3'-C3'	-5.26	113.39	119.70
8	L	33	DT	P-O3'-C3'	-5.25	113.39	119.70
7	K	-65	DT	C1'-O4'-C4'	-5.23	104.87	110.10
3	G	1029	PRO	N-CD-CG	-5.22	95.37	103.20
3	G	1588	TYR	CB-CG-CD2	-5.22	117.87	121.00
8	L	-74	DC	C2'-C3'-O3'	-5.20	95.44	112.60
7	K	47	DG	P-O3'-C3'	-5.17	113.50	119.70
8	L	61	DC	P-O3'-C3'	-5.13	113.54	119.70
8	L	40	DC	P-O3'-C3'	-5.13	113.54	119.70
8	L	-60	DA	O4'-C1'-N9	5.12	111.59	108.00
8	L	28	DA	P-O3'-C3'	-5.12	113.55	119.70
3	G	1265	ARG	NH1-CZ-NH2	5.12	125.03	119.40
3	G	1664	ARG	CG-CD-NE	-5.12	101.05	111.80
7	K	-9	DA	P-O3'-C3'	-5.09	113.59	119.70
8	L	-35	DG	P-O3'-C3'	-5.08	113.60	119.70
8	L	32	DG	P-O3'-C3'	-5.08	113.61	119.70
7	K	64	DT	C4'-C3'-C2'	-5.06	98.55	103.10
7	K	-33	DA	P-O3'-C3'	-5.06	113.63	119.70
7	K	-26	DT	P-O3'-C3'	-5.05	113.64	119.70
8	L	-70	DG	N1-C6-O6	-5.04	116.88	119.90
7	K	-47	DT	P-O3'-C3'	-5.02	113.67	119.70
8	L	41	DC	P-O3'-C3'	-5.02	113.67	119.70
2	E	231	LEU	CA-CB-CG	5.01	126.82	115.30
3	G	1073	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	1024	PHE	Sidechain
3	G	1059	ARG	Sidechain
3	G	1234	ARG	Sidechain
3	G	1276	ARG	Sidechain
3	G	1563	ARG	Sidechain
3	G	1580	ARG	Sidechain
3	G	1661	ARG	Sidechain
3	G	1675	ARG	Sidechain
3	G	1679	ARG	Sidechain
3	G	1685	ARG	Sidechain
3	G	1692	GLN	Mainchain

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Mol	Chain	Res	Type	Group
3	G	986	LEU	Mainchain
4	H	418	ARG	Sidechain
6	J	382	ARG	Sidechain
6	J	478	ARG	Sidechain
6	J	501	ARG	Sidechain
6	J	503	SER	Mainchain
7	K	68	DT	Sidechain
7	K	69	DC	Sidechain
7	K	70	DC	Sidechain
7	K	72	DG	Sidechain
8	L	-69	DG	Sidechain
11	S	20	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	3432	0	3518	39	0
1	B	3352	0	3438	35	0
1	C	3511	0	3595	46	0
2	D	3383	0	3458	33	0
2	E	3396	0	3466	47	0
2	F	3376	0	3450	35	0
3	G	5917	0	5925	186	0
4	H	762	0	793	55	0
5	I	875	0	879	15	0
6	J	5253	0	5245	100	0
7	K	3101	0	1708	58	0
8	L	3131	0	1705	78	0
9	M	773	0	811	34	0
9	Q	801	0	839	44	0
10	N	618	0	657	6	0
10	R	622	0	660	5	0
11	O	812	0	871	8	0
11	S	826	0	884	58	0
12	P	725	0	743	13	0
12	T	708	0	725	21	0
13	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	27	0	12	2	0
13	C	27	0	12	3	0
13	D	27	0	12	2	0
13	E	27	0	12	1	0
13	F	27	0	12	4	0
14	J	31	0	12	0	0
All	All	45567	0	43454	695	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 8.

All (695) 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)
3:G:1065:PHE:HZ	4:H:408:VAL:CG1	1.07	1.59
3:G:1065:PHE:CZ	4:H:408:VAL:HG11	1.44	1.53
3:G:1065:PHE:CZ	4:H:408:VAL:CG1	1.90	1.50
7:K:18:DC:OP2	9:Q:65:LEU:CD1	1.67	1.41
7:K:-53:DG:OP1	12:P:53:GLY:HA3	1.38	1.17
3:G:1651:ASN:HB2	7:K:64:DT:H5"	1.23	1.17
8:L:17:DA:O3'	9:M:63:ARG:NH1	1.83	1.11
3:G:1065:PHE:CZ	4:H:408:VAL:HG13	1.70	1.09
3:G:1629:ARG:HH12	7:K:64:DT:H5'	1.05	1.08
2:E:212:ARG:NE	11:S:71:ARG:NH2	2.02	1.08
1:A:223:PRO:HD3	3:G:1590:THR:HG21	1.34	1.06
8:L:17:DA:O3'	9:M:63:ARG:CZ	2.04	1.05
7:K:-53:DG:OP1	12:P:53:GLY:CA	2.05	1.02
3:G:1601:GLY:H	8:L:-61:DT:P	1.83	1.02
3:G:1601:GLY:HA3	8:L:-61:DT:OP2	1.59	1.01
6:J:340:LEU:HD21	6:J:444:ALA:HB2	1.42	1.01
3:G:1065:PHE:CE1	4:H:408:VAL:HG13	1.96	1.00
3:G:1113:LYS:NZ	7:K:63:DA:H3'	1.76	0.99
2:E:212:ARG:NE	11:S:71:ARG:HH22	1.61	0.98
3:G:1601:GLY:N	8:L:-61:DT:OP1	1.96	0.98
8:L:18:DG:OP1	9:M:63:ARG:NE	1.96	0.98
3:G:1601:GLY:CA	8:L:-61:DT:OP2	2.13	0.97
8:L:-43:DA:OP1	11:S:17:ARG:N	2.00	0.95
8:L:18:DG:H5'	9:M:63:ARG:HH11	1.27	0.95
3:G:1629:ARG:NH1	7:K:64:DT:H5'	1.82	0.95
6:J:357:MET:SD	6:J:365:ILE:HG23	2.08	0.93
8:L:18:DG:H5'	9:M:63:ARG:NH1	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:212:ARG:CZ	11:S:71:ARG:NH2	2.30	0.92
8:L:18:DG:C5'	9:M:63:ARG:HH11	1.83	0.92
6:J:392:LYS:HA	6:J:447:GLU:HB3	1.52	0.92
3:G:1113:LYS:HZ1	7:K:63:DA:H3'	1.33	0.91
3:G:987:TYR:HE1	3:G:1130:ASN:OD1	1.54	0.90
7:K:18:DC:OP2	9:Q:65:LEU:HD13	0.73	0.90
4:H:413:LYS:HA	4:H:417:PRO:HG2	1.53	0.89
3:G:1279:THR:HB	3:G:1542:VAL:HG13	1.55	0.89
3:G:1601:GLY:N	8:L:-61:DT:P	2.46	0.88
2:E:212:ARG:CZ	11:S:71:ARG:HH22	1.84	0.88
7:K:8:DC:OP1	10:R:46:ILE:O	1.90	0.87
11:S:102:ILE:HG23	12:T:61:ILE:HD13	1.57	0.86
3:G:1065:PHE:CE1	4:H:408:VAL:CG1	2.55	0.86
3:G:1629:ARG:HH12	7:K:64:DT:C5'	1.87	0.85
3:G:987:TYR:CE1	3:G:1130:ASN:OD1	2.29	0.84
7:K:17:DA:H3'	9:Q:65:LEU:HD22	1.59	0.84
3:G:1579:THR:OG1	8:L:-62:DA:H5'	1.79	0.82
3:G:1065:PHE:HZ	4:H:408:VAL:HG11	0.66	0.82
3:G:1037:GLN:HE22	4:H:416:ALA:HB1	1.45	0.80
1:A:131:VAL:HG12	1:A:193:TYR:HE2	1.46	0.80
3:G:1279:THR:HA	3:G:1542:VAL:HA	1.66	0.78
6:J:373:GLU:OE2	11:S:118:LYS:O	2.01	0.78
3:G:1058:ASP:OD1	4:H:414:LYS:NZ	2.16	0.78
3:G:1651:ASN:CB	7:K:64:DT:H5"	2.11	0.77
1:C:150:GLY:HA2	4:H:442:ARG:HD3	1.64	0.77
3:G:1601:GLY:HA3	8:L:-61:DT:P	2.23	0.77
8:L:-23:DT:H5"	9:Q:83:ARG:HG2	1.66	0.77
7:K:-66:DA:H4'	9:Q:49:ARG:NH1	2.01	0.76
3:G:964:GLN:OE1	3:G:971:GLN:HA	1.84	0.76
3:G:1037:GLN:NE2	4:H:416:ALA:HB1	2.00	0.75
4:H:413:LYS:HA	4:H:417:PRO:CG	2.16	0.75
3:G:1651:ASN:HB2	7:K:64:DT:C5'	2.11	0.75
11:S:87:ILE:HD12	11:S:102:ILE:HD11	1.68	0.75
4:H:422:ARG:C	4:H:424:ALA:H	1.91	0.75
7:K:17:DA:H3'	9:Q:65:LEU:HB2	1.69	0.74
3:G:1601:GLY:N	8:L:-61:DT:OP2	2.20	0.74
4:H:413:LYS:O	4:H:417:PRO:HB2	1.88	0.74
8:L:18:DG:P	9:M:63:ARG:HE	2.11	0.73
8:L:26:DA:H4'	9:M:83:ARG:NH1	2.03	0.73
3:G:1618:ARG:NH1	3:G:1620:GLU:OE1	2.21	0.73
6:J:429:ARG:HA	6:J:432:ARG:HD2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:416:ALA:HB3	4:H:417:PRO:HD3	1.69	0.73
9:Q:119:ILE:HA	9:Q:123:ASP:OD2	1.89	0.73
3:G:1609:ARG:HH12	4:H:419:THR:CG2	2.02	0.73
9:M:123:ASP:OD1	9:Q:113:HIS:NE2	2.20	0.71
3:G:1279:THR:HB	3:G:1542:VAL:CG1	2.20	0.71
8:L:18:DG:P	9:M:63:ARG:NE	2.64	0.71
6:J:340:LEU:HD21	6:J:444:ALA:CB	2.21	0.70
3:G:1141:ASN:ND2	7:K:64:DT:OP2	2.25	0.70
1:A:131:VAL:HG12	1:A:193:TYR:CE2	2.25	0.69
7:K:17:DA:C3'	9:Q:65:LEU:HD22	2.22	0.69
3:G:1601:GLY:CA	8:L:-61:DT:P	2.77	0.69
3:G:1609:ARG:HH12	4:H:419:THR:HG21	1.58	0.69
7:K:-54:DA:H4'	11:O:77:ARG:NE	2.08	0.69
7:K:-23:DC:OP1	9:M:72:ARG:NH2	2.24	0.69
8:L:18:DG:P	9:M:63:ARG:NH1	2.66	0.68
11:S:81:ARG:HD2	11:S:105:GLY:O	1.94	0.68
4:H:441:LYS:HA	4:H:442:ARG:NH1	2.08	0.68
9:M:52:ARG:NH2	9:M:56:LYS:NZ	2.40	0.68
4:H:412:LEU:O	4:H:417:PRO:HD2	1.94	0.68
9:Q:116:ARG:HH22	9:Q:123:ASP:CG	1.98	0.67
3:G:1020:ILE:CG2	3:G:1102:GLN:HG2	2.25	0.67
11:S:47:ALA:HB3	11:S:48:PRO:HD3	1.77	0.67
3:G:1008:ILE:HA	3:G:1011:MET:HE2	1.74	0.67
1:C:118:ARG:HH22	1:C:281:ASN:HD21	1.42	0.67
12:T:102:LEU:O	12:T:107:ALA:HB2	1.95	0.67
1:A:218:ALA:HB2	2:D:196:LYS:HG2	1.77	0.66
3:G:1034:HIS:CE1	4:H:418:ARG:NE	2.63	0.66
2:D:149:ARG:O	4:H:447:MET:HA	1.95	0.66
2:F:399:ARG:HH21	13:F:501:ADP:H5'2	1.60	0.66
1:B:17:ALA:HA	2:E:69:ALA:HB2	1.77	0.66
3:G:1190:LEU:O	3:G:1191:HIS:C	2.29	0.66
2:E:184:GLU:HG3	2:E:201:ILE:HB	1.78	0.66
8:L:18:DG:P	9:M:63:ARG:HH11	2.17	0.65
9:M:52:ARG:HH21	9:M:56:LYS:HZ1	1.42	0.65
6:J:503:SER:C	6:J:505:ALA:N	2.49	0.65
7:K:-53:DG:P	12:P:53:GLY:HA3	2.35	0.65
3:G:1279:THR:HB	3:G:1542:VAL:HG22	1.78	0.65
3:G:1587:GLU:O	3:G:1590:THR:N	2.30	0.65
6:J:320:ARG:HH12	8:L:-11:DC:H5"	1.61	0.65
3:G:1630:ALA:HB2	8:L:-61:DT:OP1	1.95	0.65
3:G:1541:THR:HG22	3:G:1542:VAL:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:212:ARG:NE	11:S:71:ARG:CZ	2.53	0.64
3:G:1614:ASP:O	3:G:1616:GLN:N	2.30	0.64
6:J:116:ARG:NH1	8:L:-30:DA:H5"	2.13	0.63
3:G:986:LEU:HD21	3:G:993:GLY:HA3	1.78	0.63
6:J:116:ARG:HH12	8:L:-30:DA:H5"	1.63	0.63
7:K:10:DC:H5'	9:Q:40:ARG:NH2	2.14	0.63
1:A:131:VAL:CG1	1:A:193:TYR:CE2	2.81	0.63
6:J:488:LEU:HD21	6:J:602:ARG:NH2	2.14	0.63
1:B:126:ARG:HG2	1:B:236:VAL:HG12	1.79	0.63
11:S:19:SER:C	11:S:21:ALA:N	2.51	0.63
2:D:148:ASP:HB2	2:D:157:GLN:HB2	1.82	0.62
2:D:187:MET:SD	4:H:452:ASN:ND2	2.73	0.62
2:F:399:ARG:NH2	13:F:501:ADP:O2A	2.33	0.62
3:G:1113:LYS:HZ2	7:K:63:DA:H3'	1.60	0.62
2:E:192:ILE:HG22	2:E:203:LYS:HG2	1.82	0.62
6:J:116:ARG:HH11	8:L:-30:DA:P	2.23	0.62
4:H:423:ALA:O	4:H:426:ALA:N	2.33	0.62
3:G:1279:THR:CB	3:G:1542:VAL:HG13	2.27	0.62
3:G:963:ALA:O	3:G:964:GLN:C	2.35	0.62
7:K:17:DA:H2"	7:K:18:DC:H6	1.65	0.62
7:K:17:DA:C2'	9:Q:65:LEU:HD22	2.30	0.61
3:G:1037:GLN:NE2	4:H:416:ALA:CB	2.62	0.61
8:L:58:DC:OP1	11:O:75:LYS:HB3	1.99	0.61
6:J:73:ASN:ND2	6:J:737:CYS:SG	2.72	0.61
2:D:134:GLU:HG2	2:D:236:GLU:HG2	1.83	0.61
3:G:1279:THR:CB	3:G:1542:VAL:HG22	2.30	0.61
1:B:109:LYS:NZ	1:B:309:ASP:OD2	2.32	0.61
5:I:210:GLU:HB2	5:I:215:HIS:HD2	1.66	0.61
3:G:1555:LEU:HD13	3:G:1585:MET:HE1	1.82	0.61
3:G:1050:LEU:CD1	3:G:1062:LEU:HD22	2.31	0.60
6:J:190:ASP:HB2	6:J:728:ALA:HB1	1.82	0.60
3:G:962:VAL:HG23	3:G:981:ASN:OD1	2.01	0.60
6:J:473:TRP:CZ2	6:J:477:LYS:HE3	2.35	0.60
9:M:52:ARG:CG	9:M:56:LYS:HE3	2.31	0.60
3:G:1614:ASP:O	3:G:1615:PHE:C	2.39	0.60
11:S:34:LEU:HA	11:S:39:TYR:CD2	2.36	0.60
1:B:311:GLU:OE2	2:F:335:ARG:NH2	2.34	0.60
11:S:85:LEU:HD22	11:S:108:LEU:HD23	1.83	0.60
4:H:422:ARG:O	4:H:424:ALA:N	2.35	0.60
6:J:392:LYS:HA	6:J:447:GLU:CB	2.29	0.60
1:C:150:GLY:HA3	4:H:442:ARG:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:58:DC:H2"	8:L:59:DA:C8	2.37	0.60
9:Q:60:LEU:HD23	9:Q:93:GLN:HG2	1.82	0.60
9:Q:103:LEU:HD11	9:Q:128:ARG:HG2	1.83	0.60
3:G:1609:ARG:NH1	4:H:419:THR:CG2	2.64	0.59
2:D:333:ARG:NH2	2:D:337:THR:O	2.34	0.59
3:G:1140:GLN:O	3:G:1141:ASN:HB2	2.01	0.59
10:R:75:HIS:HD2	12:T:84:ASN:ND2	2.00	0.59
11:S:54:VAL:HG21	12:T:98:VAL:HG21	1.83	0.59
12:T:37:TYR:O	12:T:41:VAL:HG23	2.01	0.59
1:A:279:GLU:HG2	3:G:1311:VAL:HG13	1.85	0.59
6:J:443:ARG:O	6:J:447:GLU:HG2	2.02	0.59
3:G:1278:ASP:O	3:G:1279:THR:C	2.41	0.59
2:E:212:ARG:HE	11:S:71:ARG:NH2	1.99	0.59
3:G:1139:ILE:HG12	3:G:1146:LEU:HB2	1.85	0.59
2:E:185:ARG:HH21	3:G:1303:LEU:HD23	1.67	0.59
7:K:15:DT:H2"	7:K:16:DA:C8	2.38	0.59
6:J:494:LEU:O	6:J:498:LEU:HG	2.02	0.58
2:F:161:THR:HG22	2:F:170:ILE:HG12	1.84	0.58
6:J:349:TYR:CZ	6:J:353:ILE:HD11	2.38	0.58
8:L:18:DG:P	9:M:63:ARG:CZ	2.92	0.58
4:H:422:ARG:C	4:H:424:ALA:N	2.56	0.58
9:Q:50:GLU:HG2	9:Q:53:ARG:NH1	2.18	0.58
6:J:514:ALA:HB3	11:S:72:ASP:HB3	1.84	0.58
3:G:1548:PHE:HZ	3:G:1584:LEU:HB3	1.67	0.58
6:J:90:ARG:NH2	8:L:-28:DC:OP1	2.36	0.58
3:G:1549:VAL:HG12	3:G:1549:VAL:O	2.03	0.58
8:L:34:DC:H2"	8:L:35:DT:H71	1.84	0.58
3:G:1142:ASN:OD1	3:G:1142:ASN:N	2.29	0.58
11:S:44:GLY:O	11:S:48:PRO:HD2	2.04	0.58
1:B:243:ASP:OD2	3:G:1339:ARG:NH1	2.37	0.58
4:H:413:LYS:HA	4:H:417:PRO:CD	2.34	0.58
6:J:116:ARG:NH1	8:L:-30:DA:C5'	2.67	0.58
12:P:77:ALA:HB1	12:P:89:ILE:HG23	1.84	0.58
1:B:195:GLU:HB2	1:B:200:ALA:H	1.69	0.58
8:L:50:DG:OP1	12:P:33:ARG:HA	2.04	0.58
10:R:75:HIS:CD2	12:T:84:ASN:ND2	2.72	0.58
1:C:100:SER:O	2:F:116:THR:OG1	2.17	0.57
3:G:1053:TRP:O	4:H:415:GLN:NE2	2.37	0.57
3:G:1544:SER:O	3:G:1546:ALA:N	2.37	0.57
4:H:415:GLN:O	4:H:418:ARG:HG2	2.03	0.57
6:J:469:ASP:OD1	6:J:470:LEU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:511:LYS:HA	11:S:72:ASP:HB3	1.86	0.57
2:E:299:GLU:OE1	2:E:301:HIS:NE2	2.34	0.57
3:G:965:PRO:HD3	3:G:980:LEU:CD2	2.34	0.57
3:G:1701:ILE:HG22	3:G:1701:ILE:O	2.04	0.57
1:A:321:GLU:OE1	2:E:24:HIS:ND1	2.36	0.57
11:S:87:ILE:HD12	11:S:102:ILE:CD1	2.34	0.57
2:E:136:GLU:HG2	2:E:234:ARG:HG2	1.86	0.57
3:G:1527:LEU:HD12	3:G:1528:PRO:HD2	1.85	0.57
6:J:340:LEU:CD2	6:J:444:ALA:HB2	2.28	0.57
6:J:344:GLU:OE2	6:J:440:ALA:HB1	2.05	0.57
2:D:83:LYS:NZ	2:D:328:ASN:OD1	2.32	0.56
9:Q:47:ALA:O	9:Q:51:ILE:HG13	2.05	0.56
1:A:223:PRO:CD	3:G:1590:THR:HG21	2.22	0.56
6:J:466:ARG:C	6:J:468:ASN:H	2.08	0.56
7:K:-4:DC:H2"	7:K:-3:DG:C8	2.40	0.56
1:B:72:GLY:O	1:B:77:LYS:NZ	2.39	0.56
9:M:113:HIS:NE2	9:Q:116:ARG:NH1	2.53	0.56
2:F:283:LYS:HD2	2:F:290:ILE:HD12	1.87	0.56
3:G:1279:THR:HB	3:G:1542:VAL:CG2	2.36	0.56
5:I:174:GLY:HA3	6:J:634:VAL:HG11	1.86	0.56
6:J:88:LYS:NZ	8:L:-29:DT:P	2.79	0.56
7:K:55:DT:H2"	7:K:56:DC:C5	2.40	0.56
11:S:26:PRO:HG3	12:T:40:TYR:CE2	2.41	0.56
1:C:115:GLU:OE2	1:C:277:ARG:NH2	2.33	0.56
4:H:413:LYS:HA	4:H:417:PRO:HD2	1.87	0.56
6:J:375:LYS:O	6:J:376:ASP:OD1	2.24	0.56
1:A:193:TYR:CE2	1:A:195:GLU:OE1	2.59	0.56
11:S:102:ILE:CG2	12:T:61:ILE:HD13	2.34	0.55
1:A:235:ILE:HD12	1:A:237:GLN:HE21	1.71	0.55
1:B:367:TYR:OH	13:B:501:ADP:N7	2.36	0.55
3:G:968:LEU:HD12	3:G:1043:PHE:O	2.06	0.55
1:C:304:GLU:OE1	1:C:306:HIS:NE2	2.40	0.55
3:G:994:ILE:HG12	3:G:1153:ILE:CD1	2.37	0.55
6:J:501:ARG:CZ	11:S:92:GLU:OE1	2.54	0.55
2:E:149:ARG:HH22	2:E:182:THR:HG21	1.71	0.55
7:K:17:DA:H2'	9:Q:65:LEU:HD22	1.88	0.55
1:A:108:LYS:HB3	2:E:110:SER:HA	1.88	0.55
6:J:488:LEU:HD21	6:J:602:ARG:HH22	1.70	0.55
1:C:132:TYR:HB2	1:C:194:ILE:HB	1.89	0.55
2:E:363:PRO:HB3	2:E:394:GLN:HE21	1.72	0.55
3:G:1409:GLU:HB2	3:G:1412:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1618:ARG:O	3:G:1618:ARG:HG3	2.07	0.55
1:A:16:THR:HG21	1:A:383:GLU:HG2	1.88	0.55
4:H:384:ARG:O	4:H:388:MET:HG2	2.06	0.55
1:A:310:ILE:HG22	1:A:341:GLY:HA3	1.89	0.55
1:C:448:LEU:HD11	2:F:330:GLY:HA2	1.88	0.55
11:O:51:LEU:HD21	12:P:70:PHE:CD1	2.42	0.54
12:T:76:GLU:O	12:T:80:LEU:HD12	2.07	0.54
2:F:301:HIS:CE1	2:F:329:ARG:HE	2.25	0.54
7:K:17:DA:H3'	9:Q:65:LEU:CD2	2.34	0.54
8:L:70:DC:H3'	9:Q:42:ARG:HD2	1.88	0.54
1:A:304:GLU:OE1	1:A:306:HIS:NE2	2.36	0.54
3:G:1020:ILE:HG21	3:G:1102:GLN:HG2	1.88	0.54
6:J:514:ALA:O	11:S:73:ASN:ND2	2.39	0.54
12:T:109:HIS:O	12:T:113:GLU:HG2	2.07	0.54
3:G:1050:LEU:HD12	3:G:1062:LEU:HD22	1.90	0.54
9:Q:120:MET:HB3	9:Q:121:PRO:HD2	1.90	0.54
1:C:8:ARG:NH1	2:F:289:GLU:OE1	2.41	0.54
2:E:142:VAL:HA	2:E:162:ILE:HG22	1.90	0.54
11:S:50:TYR:CE1	12:T:114:GLY:HA3	2.43	0.54
1:C:126:ARG:HG2	1:C:236:VAL:HG12	1.90	0.54
2:D:399:ARG:HH21	13:D:501:ADP:H5'2	1.72	0.54
2:E:399:ARG:NH2	13:E:501:ADP:O1A	2.40	0.54
9:Q:111:ALA:HB2	9:Q:123:ASP:OD2	2.08	0.54
1:B:165:ALA:HB3	1:B:226:LYS:HA	1.89	0.53
2:D:146:GLN:NE2	4:H:449:ARG:HH21	2.05	0.53
5:I:42:LYS:HE3	5:I:46:ALA:HB1	1.91	0.53
7:K:-32:DC:H2"	7:K:-31:DA:C8	2.43	0.53
1:C:321:GLU:OE2	1:C:358:ARG:NH1	2.34	0.53
1:B:138:GLU:OE2	1:B:170:LYS:NZ	2.40	0.53
8:L:60:DC:H2"	8:L:61:DC:C6	2.44	0.53
2:E:379:VAL:HG22	2:E:409:GLN:HE21	1.74	0.53
7:K:-53:DG:OP1	12:P:53:GLY:HA2	2.02	0.53
1:A:202:LYS:HD2	3:G:1540:ILE:O	2.08	0.53
1:C:198:THR:O	2:D:185:ARG:NH1	2.41	0.53
4:H:446:MET:HA	4:H:465:LEU:HD11	1.91	0.53
6:J:466:ARG:C	6:J:468:ASN:N	2.61	0.53
1:C:367:TYR:OH	13:C:501:ADP:N7	2.38	0.53
2:D:31:GLY:O	2:D:53:ARG:NH2	2.42	0.53
3:G:1013:TYR:O	3:G:1014:LEU:C	2.46	0.53
3:G:1701:ILE:O	3:G:1701:ILE:CG2	2.56	0.53
11:S:19:SER:C	11:S:21:ALA:H	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:50:GLU:HG2	9:Q:53:ARG:HH12	1.74	0.53
3:G:1542:VAL:CG1	3:G:1543:PRO:HD2	2.38	0.53
1:B:357:GLN:HA	2:F:435:PRO:HG2	1.91	0.52
3:G:967:LEU:N	3:G:1016:GLU:OE2	2.38	0.52
3:G:1517:PRO:HG3	4:H:469:HIS:CD2	2.44	0.52
1:C:13:ASP:O	2:F:283:LYS:NZ	2.37	0.52
3:G:1544:SER:C	3:G:1546:ALA:N	2.61	0.52
6:J:15:ARG:NH2	6:J:595:ASP:OD2	2.42	0.52
3:G:1030:ALA:HB3	8:L:-59:DT:P	2.49	0.52
3:G:1541:THR:HG22	3:G:1542:VAL:N	2.24	0.52
5:I:161:PRO:HA	6:J:654:GLN:HA	1.90	0.52
6:J:318:ALA:O	6:J:322:LYS:HG3	2.09	0.52
11:S:44:GLY:O	11:S:48:PRO:CD	2.57	0.52
1:B:15:ARG:HH12	2:E:292:PRO:HB3	1.74	0.52
2:E:140:GLY:H	2:E:227:PRO:HG2	1.74	0.52
6:J:621:PRO:HD2	6:J:626:GLU:HG2	1.92	0.52
7:K:-66:DA:H4'	9:Q:49:ARG:CZ	2.39	0.52
1:A:156:SER:HA	1:A:175:PRO:HG3	1.92	0.52
8:L:33:DT:C6	8:L:33:DT:H5'	2.44	0.52
1:A:118:ARG:HH22	1:A:281:ASN:HD21	1.58	0.51
1:A:307:MET:SD	1:A:340:ARG:NH1	2.83	0.51
2:F:268:ARG:HH21	2:F:271:ILE:HD11	1.74	0.51
6:J:15:ARG:CZ	6:J:595:ASP:OD1	2.59	0.51
1:A:356:LEU:HD12	1:A:359:LEU:HD12	1.92	0.51
1:C:77:LYS:NZ	13:C:501:ADP:O1B	2.36	0.51
1:C:148:LEU:HD12	4:H:460:ALA:HB2	1.93	0.51
2:E:164:THR:HG23	2:E:231:LEU:HD12	1.93	0.51
3:G:1583:ASP:O	3:G:1584:LEU:C	2.46	0.51
8:L:-60:DA:H2"	8:L:-59:DT:H5"	1.90	0.51
9:M:52:ARG:NH2	9:M:56:LYS:HZ1	2.02	0.51
1:A:55:ASP:OD2	2:E:414:LYS:NZ	2.41	0.51
6:J:466:ARG:NH1	6:J:588:TYR:CE1	2.79	0.51
2:E:212:ARG:CD	11:S:71:ARG:HH22	2.24	0.51
2:F:31:GLY:O	2:F:53:ARG:NH2	2.44	0.51
6:J:505:ALA:O	6:J:509:ARG:HG3	2.11	0.51
12:T:73:ILE:HA	12:T:101:LEU:CD2	2.41	0.51
1:A:360:LEU:HD11	2:E:403:ASN:HB3	1.93	0.51
1:C:256:ASP:OD1	1:C:256:ASP:N	2.44	0.51
3:G:1549:VAL:O	3:G:1549:VAL:CG1	2.59	0.51
3:G:1614:ASP:O	3:G:1617:THR:N	2.42	0.51
11:S:34:LEU:HA	11:S:39:TYR:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:ASP:OD1	4:H:449:ARG:HG2	2.11	0.51
1:B:214:PHE:HB2	1:B:217:GLU:HG3	1.93	0.51
8:L:17:DA:O3'	9:M:63:ARG:NE	2.44	0.51
9:Q:120:MET:SD	9:Q:122:LYS:HE2	2.50	0.51
2:E:108:ILE:HG22	2:E:115:LYS:HG2	1.91	0.50
2:F:77:GLY:O	2:F:83:LYS:NZ	2.42	0.50
3:G:1030:ALA:HB3	8:L:-59:DT:OP1	2.11	0.50
3:G:1113:LYS:HE2	7:K:64:DT:OP2	2.10	0.50
7:K:-34:DG:OP1	12:P:87:SER:N	2.31	0.50
1:B:65:ARG:NH1	2:F:403:ASN:OD1	2.44	0.50
3:G:1614:ASP:C	3:G:1616:GLN:N	2.64	0.50
7:K:17:DA:H2"	7:K:18:DC:C6	2.45	0.50
1:B:306:HIS:CD2	1:B:334:ARG:HE	2.29	0.50
2:F:47:VAL:O	13:F:501:ADP:N6	2.44	0.50
6:J:353:ILE:O	6:J:357:MET:HG3	2.12	0.50
1:B:128:THR:O	1:B:197:ASN:ND2	2.44	0.50
3:G:964:GLN:O	3:G:965:PRO:C	2.49	0.50
3:G:1195:LYS:N	3:G:1196:PRO:CD	2.75	0.50
7:K:61:DA:H2"	7:K:62:DT:H5'	1.92	0.50
1:B:156:SER:OG	1:B:157:THR:N	2.41	0.50
7:K:17:DA:H5"	9:Q:66:PRO:HD3	1.94	0.50
3:G:987:TYR:O	3:G:988:GLU:C	2.47	0.50
8:L:-43:DA:OP1	11:S:17:ARG:HB2	2.11	0.50
1:B:302:ILE:HB	1:B:330:LEU:HD23	1.94	0.49
3:G:986:LEU:CD2	3:G:993:GLY:HA3	2.42	0.49
3:G:1139:ILE:HD11	3:G:1146:LEU:HD22	1.94	0.49
11:O:47:ALA:HB2	12:P:89:ILE:O	2.12	0.49
11:S:19:SER:O	11:S:21:ALA:N	2.44	0.49
1:A:193:TYR:HE2	1:A:195:GLU:OE1	1.95	0.49
1:C:56:LEU:HG	1:C:62:MET:HB2	1.95	0.49
2:D:83:LYS:NZ	2:D:327:SER:O	2.40	0.49
3:G:991:ILE:HG22	3:G:992:ASN:O	2.11	0.49
3:G:1585:MET:O	3:G:1586:GLU:C	2.49	0.49
6:J:503:SER:C	6:J:505:ALA:H	2.15	0.49
1:A:131:VAL:CG1	1:A:193:TYR:HE2	2.16	0.49
3:G:966:LYS:C	3:G:968:LEU:H	2.15	0.49
3:G:1348:ASN:HB3	3:G:1351:THR:HG23	1.94	0.49
7:K:51:DC:H2"	7:K:52:DG:H5"	1.94	0.49
3:G:1163:GLU:HG2	3:G:1167:TRP:CE2	2.48	0.49
8:L:-43:DA:OP2	11:S:17:ARG:NE	2.39	0.49
8:L:4:DG:H2"	8:L:5:DT:H71	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:THR:HG21	1:C:383:GLU:HG2	1.94	0.49
3:G:1233:LEU:HB3	3:G:1264:PHE:CE1	2.48	0.49
6:J:192:LEU:HB3	6:J:764:LEU:HD22	1.95	0.49
7:K:8:DC:P	10:R:46:ILE:O	2.71	0.49
11:S:41:GLU:HG2	11:S:42:ARG:HG3	1.94	0.49
1:C:150:GLY:CA	4:H:442:ARG:HD3	2.39	0.49
1:C:423:ARG:NH1	1:C:427:ASP:OD2	2.45	0.49
9:Q:103:LEU:CD1	9:Q:128:ARG:HG2	2.42	0.49
11:S:87:ILE:HD13	11:S:97:LEU:HD13	1.95	0.49
1:C:10:ASN:O	1:C:12:ARG:NH1	2.46	0.49
3:G:1606:GLU:OE1	3:G:1607:ASP:N	2.44	0.49
5:I:206:GLU:HB3	5:I:215:HIS:NE2	2.27	0.49
6:J:15:ARG:NH2	6:J:595:ASP:CG	2.66	0.49
6:J:320:ARG:NH1	8:L:-11:DC:H5"	2.28	0.49
6:J:511:LYS:HA	11:S:72:ASP:CG	2.33	0.49
9:M:52:ARG:HG3	9:M:56:LYS:HE3	1.95	0.48
10:N:75:HIS:O	12:P:92:ARG:NH2	2.46	0.48
11:S:19:SER:O	11:S:22:GLY:N	2.41	0.48
11:S:29:ARG:O	11:S:33:LEU:HG	2.12	0.48
2:F:108:ILE:HD13	2:F:119:LEU:HD12	1.95	0.48
3:G:1012:ALA:HB2	3:G:1044:VAL:HG11	1.95	0.48
2:F:220:ASP:OD1	3:G:1345:HIS:NE2	2.46	0.48
3:G:1542:VAL:HG12	3:G:1543:PRO:HD2	1.95	0.48
6:J:206:VAL:HG22	6:J:215:VAL:HG22	1.95	0.48
9:M:52:ARG:HH21	9:M:56:LYS:NZ	2.04	0.48
1:B:57:ILE:HG12	1:B:327:ILE:HG21	1.94	0.48
1:B:97:ILE:HD11	1:B:302:ILE:HG12	1.96	0.48
1:C:310:ILE:HG22	1:C:341:GLY:HA3	1.95	0.48
6:J:118:ALA:HA	6:J:128:ASN:HB3	1.95	0.48
6:J:466:ARG:NH1	6:J:588:TYR:CZ	2.81	0.48
1:A:198:THR:OG1	1:A:199:GLY:N	2.46	0.48
3:G:994:ILE:CG1	3:G:1153:ILE:CD1	2.92	0.48
6:J:392:LYS:CA	6:J:447:GLU:HB3	2.33	0.48
6:J:677:ASP:HB3	6:J:680:ASP:HB2	1.94	0.48
7:K:-28:DT:H2"	7:K:-27:DC:C6	2.49	0.48
7:K:49:DC:H2"	7:K:50:DA:C8	2.49	0.48
8:L:4:DG:H2"	8:L:5:DT:C7	2.44	0.48
10:N:44:LYS:HB2	11:S:115:LEU:HD13	1.96	0.48
1:C:195:GLU:HG2	1:C:199:GLY:H	1.79	0.48
11:S:79:ILE:HB	11:S:80:PRO:HD2	1.95	0.48
1:C:165:ALA:HB3	1:C:226:LYS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1143:MET:SD	3:G:1700:VAL:HG21	2.54	0.47
1:C:264:LEU:HD21	3:G:1389:ARG:HE	1.77	0.47
6:J:471:GLU:O	6:J:474:LEU:N	2.47	0.47
12:T:35:GLU:HG3	12:T:35:GLU:O	2.12	0.47
3:G:1008:ILE:HD13	3:G:1040:VAL:HA	1.97	0.47
3:G:1435:GLU:HA	3:G:1443:ARG:HD3	1.96	0.47
3:G:1544:SER:C	3:G:1546:ALA:H	2.16	0.47
6:J:349:TYR:CE1	6:J:353:ILE:HD11	2.50	0.47
11:S:79:ILE:HB	11:S:80:PRO:CD	2.45	0.47
11:S:87:ILE:HD13	11:S:97:LEU:CD1	2.44	0.47
3:G:1384:THR:HB	3:G:1388:ALA:HB3	1.95	0.47
4:H:423:ALA:O	4:H:424:ALA:C	2.51	0.47
6:J:15:ARG:NH1	6:J:595:ASP:OD1	2.48	0.47
2:F:399:ARG:O	2:F:403:ASN:ND2	2.47	0.47
3:G:1219:PHE:CD1	3:G:1679:ARG:HG2	2.50	0.47
7:K:-34:DG:OP1	12:P:87:SER:OG	2.30	0.47
11:S:17:ARG:HA	11:S:20:ARG:HH21	1.79	0.47
1:A:68:LEU:HD23	1:A:361:ILE:HG12	1.97	0.47
1:B:69:LEU:HD23	1:B:362:ILE:HB	1.97	0.47
2:D:399:ARG:NH2	13:D:501:ADP:O1A	2.47	0.47
3:G:1140:GLN:O	3:G:1141:ASN:CB	2.62	0.47
3:G:1233:LEU:HD23	3:G:1236:GLN:HE22	1.78	0.47
6:J:86:MET:HA	6:J:101:ALA:HA	1.97	0.47
9:Q:61:LEU:HD13	10:R:40:ARG:HH11	1.80	0.47
2:E:185:ARG:NH1	3:G:1297:GLU:OE1	2.48	0.47
2:F:47:VAL:H	13:F:501:ADP:HN62	1.62	0.47
5:I:40:ARG:NH2	6:J:130:ASP:OD1	2.48	0.47
9:M:46:VAL:O	9:M:50:GLU:HG3	2.15	0.47
6:J:169:ARG:HH22	6:J:766:ASN:HD22	1.62	0.47
8:L:33:DT:H5'	8:L:33:DT:H6	1.80	0.47
1:B:448:LEU:HD11	2:E:330:GLY:HA2	1.96	0.47
8:L:30:DC:C6	8:L:31:DT:H72	2.50	0.47
9:M:103:LEU:CD2	10:N:57:VAL:HG11	2.45	0.47
1:C:191:VAL:HG23	1:C:204:VAL:HB	1.96	0.46
3:G:964:GLN:OE1	3:G:972:LEU:N	2.45	0.46
5:I:30:ARG:NH1	6:J:133:GLU:OE2	2.47	0.46
6:J:501:ARG:O	6:J:503:SER:N	2.48	0.46
5:I:20:LEU:HD23	6:J:39:ILE:HD12	1.96	0.46
6:J:15:ARG:NH1	6:J:595:ASP:OD2	2.49	0.46
6:J:88:LYS:HZ3	8:L:-29:DT:P	2.38	0.46
6:J:466:ARG:O	6:J:468:ASN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:HG23	1:A:204:VAL:HB	1.97	0.46
1:B:129:LYS:HD3	1:B:235:ILE:HD12	1.97	0.46
2:E:300:VAL:HG13	2:E:345:LEU:HD21	1.97	0.46
3:G:983:LEU:CD2	3:G:1132:LEU:HD13	2.45	0.46
6:J:470:LEU:O	6:J:473:TRP:HB3	2.15	0.46
8:L:34:DC:H2"	8:L:35:DT:C7	2.43	0.46
3:G:1688:LYS:HB3	3:G:1688:LYS:HE2	1.73	0.46
1:A:448:LEU:HD11	2:D:330:GLY:HA2	1.97	0.46
3:G:1586:GLU:HG2	3:G:1596:TYR:OH	2.14	0.46
1:B:108:LYS:HB3	2:F:110:SER:HA	1.97	0.46
1:B:177:ILE:HB	2:F:218:GLY:HA2	1.98	0.46
3:G:1635:ILE:HD13	3:G:1635:ILE:HG21	1.42	0.46
8:L:38:DG:H2"	8:L:39:DA:C8	2.50	0.46
9:M:45:THR:O	9:M:49:ARG:HG3	2.16	0.46
3:G:1279:THR:H	3:G:1542:VAL:HG13	1.80	0.46
5:I:197:ILE:HA	5:I:200:LEU:HD23	1.98	0.46
7:K:16:DA:H1'	7:K:17:DA:C8	2.51	0.46
7:K:17:DA:H3'	9:Q:65:LEU:CB	2.41	0.46
11:S:85:LEU:HD22	11:S:108:LEU:CD2	2.45	0.46
3:G:1276:ARG:HG2	3:G:1277:ALA:N	2.31	0.46
3:G:1279:THR:N	3:G:1543:PRO:HD2	2.31	0.46
6:J:117:ASN:O	6:J:128:ASN:ND2	2.41	0.46
8:L:-23:DT:OP1	9:Q:83:ARG:HA	2.15	0.46
9:M:52:ARG:NH2	9:M:56:LYS:HZ2	2.12	0.46
8:L:35:DT:H2"	8:L:36:DA:N7	2.31	0.46
1:C:334:ARG:NH1	2:D:451:GLY:O	2.49	0.46
3:G:1142:ASN:OD1	3:G:1145:GLU:HG3	2.16	0.46
4:H:420:THR:O	4:H:421:ARG:CG	2.64	0.46
3:G:983:LEU:HD13	3:G:1010:VAL:CG2	2.46	0.45
2:F:74:LEU:HD23	2:F:355:ILE:HG12	1.98	0.45
3:G:1280:SER:O	3:G:1281:SER:HB3	2.16	0.45
6:J:365:ILE:HG21	6:J:377:GLU:OE1	2.16	0.45
7:K:18:DC:H2"	7:K:19:DC:C6	2.52	0.45
8:L:58:DC:H2"	8:L:59:DA:H8	1.78	0.45
1:C:354:ASP:OD2	2:D:328:ASN:ND2	2.50	0.45
7:K:45:DC:H2"	7:K:46:DA:N7	2.31	0.45
9:Q:116:ARG:NH2	9:Q:123:ASP:OD2	2.44	0.45
1:A:302:ILE:HB	1:A:330:LEU:HD23	1.99	0.45
3:G:1280:SER:OG	3:G:1281:SER:N	2.49	0.45
7:K:-43:DT:C2'	7:K:-42:DT:H71	2.46	0.45
3:G:965:PRO:HD3	3:G:980:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1278:ASP:OD1	3:G:1279:THR:HG22	2.17	0.45
3:G:1493:HIS:CE1	3:G:1495:ALA:HB3	2.52	0.45
6:J:287:TRP:HZ3	6:J:616:PRO:HA	1.82	0.45
1:C:4:ILE:HG22	2:F:133:GLU:HB2	1.98	0.45
2:D:334:ILE:HD13	2:D:346:PRO:HG3	1.99	0.45
8:L:58:DC:OP1	11:O:75:LYS:CB	2.64	0.45
9:Q:116:ARG:CZ	9:Q:122:LYS:HE3	2.47	0.45
3:G:1034:HIS:CE1	4:H:418:ARG:HE	2.33	0.45
2:D:283:LYS:HD2	2:D:290:ILE:HD12	1.98	0.45
6:J:511:LYS:HA	11:S:72:ASP:CB	2.46	0.45
7:K:-38:DC:H2"	7:K:-37:DG:C8	2.52	0.45
11:S:34:LEU:HA	11:S:39:TYR:CE2	2.52	0.45
6:J:19:TRP:CZ3	6:J:604:TRP:CZ2	3.04	0.45
6:J:379:ALA:O	6:J:383:VAL:HG23	2.17	0.45
9:Q:123:ASP:OD1	9:Q:123:ASP:N	2.49	0.45
3:G:1630:ALA:HB2	8:L:-61:DT:H5"	1.98	0.44
1:A:174:ASP:OD2	3:G:1305:TYR:N	2.48	0.44
1:B:272:ILE:HG23	1:B:276:LEU:HD23	2.00	0.44
3:G:1279:THR:OG1	3:G:1542:VAL:HG22	2.17	0.44
4:H:418:ARG:O	4:H:419:THR:HB	2.16	0.44
6:J:189:ILE:HB	6:J:192:LEU:HD12	1.98	0.44
6:J:353:ILE:HD13	6:J:372:ALA:HB2	1.99	0.44
10:N:90:LEU:HB3	10:N:95:ARG:O	2.17	0.44
3:G:1058:ASP:CG	4:H:414:LYS:HZ3	2.21	0.44
3:G:1139:ILE:HD11	3:G:1700:VAL:HG11	2.00	0.44
3:G:1143:MET:O	3:G:1144:GLN:C	2.55	0.44
3:G:1507:GLU:HA	3:G:1510:GLU:HG2	2.00	0.44
12:T:115:THR:O	12:T:118:VAL:HG12	2.18	0.44
1:B:191:VAL:HG23	1:B:204:VAL:HB	1.98	0.44
1:C:283:VAL:HG21	3:G:1448:ILE:HD11	1.99	0.44
6:J:88:LYS:NZ	8:L:-29:DT:OP1	2.48	0.44
9:Q:72:ARG:O	9:Q:75:ALA:N	2.50	0.44
3:G:966:LYS:O	3:G:968:LEU:N	2.51	0.44
11:S:57:TYR:CD2	11:S:58:LEU:HD23	2.52	0.44
8:L:-47:DC:H2"	8:L:-46:DT:C5	2.52	0.44
3:G:994:ILE:CG1	3:G:1153:ILE:HD12	2.48	0.44
3:G:1058:ASP:CG	4:H:414:LYS:NZ	2.69	0.44
6:J:88:LYS:HZ1	8:L:-29:DT:P	2.41	0.44
11:S:33:LEU:HB2	12:T:70:PHE:CZ	2.52	0.44
8:L:-24:DT:O5'	9:Q:85:GLN:HA	2.18	0.44
11:S:51:LEU:HD21	12:T:70:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASN:HD22	1:B:32:ILE:HB	1.83	0.44
2:D:130:ARG:NH2	2:D:289:GLU:OE1	2.49	0.44
3:G:1395:SER:HB3	3:G:1523:PRO:HG2	2.00	0.44
6:J:116:ARG:HD2	8:L:-30:DA:OP1	2.18	0.44
6:J:257:LYS:O	6:J:262:GLN:NE2	2.51	0.44
8:L:26:DA:C4'	9:M:83:ARG:NH1	2.79	0.44
2:D:108:ILE:HD12	2:D:303:LEU:HD21	1.99	0.43
3:G:967:LEU:H	3:G:1016:GLU:CD	2.21	0.43
3:G:1587:GLU:O	3:G:1588:TYR:C	2.57	0.43
6:J:40:PRO:HB2	6:J:42:GLN:HG3	1.99	0.43
8:L:3:DC:H2"	8:L:4:DG:C8	2.53	0.43
8:L:28:DA:OP1	10:N:80:THR:N	2.51	0.43
9:M:129:ARG:HG2	9:Q:109:LEU:HD13	2.00	0.43
9:Q:124:ILE:O	9:Q:128:ARG:HG3	2.18	0.43
2:E:40:ARG:HA	2:E:41:PRO:HD3	1.85	0.43
2:E:347:LEU:HD23	2:E:350:LEU:HD12	2.00	0.43
8:L:-11:DC:H2"	8:L:-10:DG:C8	2.54	0.43
1:A:193:TYR:CG	1:A:193:TYR:O	2.71	0.43
3:G:1585:MET:HE3	3:G:1585:MET:HB2	1.57	0.43
5:I:170:CYS:SG	5:I:171:ASP:N	2.91	0.43
9:Q:122:LYS:HG3	9:Q:123:ASP:OD1	2.18	0.43
1:A:420:VAL:HG13	2:D:36:THR:HA	2.00	0.43
6:J:373:GLU:CD	11:S:118:LYS:O	2.55	0.43
6:J:392:LYS:HG3	6:J:447:GLU:OE1	2.18	0.43
3:G:976:GLN:NE2	3:G:1005:VAL:HG11	2.34	0.43
3:G:1222:LEU:CD2	3:G:1678:THR:HG21	2.48	0.43
9:M:113:HIS:CE1	9:Q:116:ARG:HH12	2.36	0.43
1:C:151:TYR:HE2	4:H:449:ARG:HH11	1.65	0.43
3:G:966:LYS:N	3:G:1016:GLU:OE1	2.51	0.43
1:C:151:TYR:HD1	4:H:462:PRO:HA	1.83	0.43
2:D:333:ARG:HA	2:D:340:LYS:HA	2.01	0.43
6:J:75:GLU:OE2	6:J:79:ARG:NH2	2.44	0.43
7:K:6:DC:H1'	7:K:7:DC:C6	2.54	0.43
2:E:42:SER:HA	2:E:47:VAL:HG22	2.01	0.43
6:J:190:ASP:HA	6:J:193:PHE:HD2	1.82	0.43
7:K:18:DC:H2"	7:K:19:DC:H6	1.84	0.43
8:L:17:DA:H4'	9:M:63:ARG:NH2	2.33	0.43
1:A:146:ASN:HB2	1:A:153:LYS:HD3	2.00	0.43
3:G:1293:SER:OG	3:G:1294:PHE:N	2.52	0.43
9:Q:46:VAL:O	9:Q:50:GLU:HG3	2.19	0.43
2:E:252:ARG:HH22	2:E:263:ASP:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:983:LEU:HD21	3:G:1132:LEU:HD13	2.01	0.43
3:G:1088:LEU:HD23	3:G:1088:LEU:HA	1.90	0.43
3:G:1562:LEU:HD23	3:G:1562:LEU:HA	1.83	0.43
6:J:80:LEU:HD11	6:J:142:LYS:HB2	2.00	0.43
6:J:501:ARG:C	6:J:503:SER:N	2.71	0.43
6:J:620:ASP:OD1	6:J:620:ASP:N	2.44	0.43
1:B:41:VAL:H	13:B:501:ADP:HN62	1.67	0.42
1:C:195:GLU:OE2	1:C:198:THR:OG1	2.37	0.42
1:C:257:ILE:HG13	3:G:1526:LEU:HB3	2.01	0.42
2:D:377:GLU:OE1	2:D:406:THR:OG1	2.35	0.42
2:F:300:VAL:HG13	2:F:345:LEU:HD21	2.01	0.42
4:H:413:LYS:CA	4:H:417:PRO:HD2	2.49	0.42
4:H:416:ALA:HB3	4:H:417:PRO:CD	2.43	0.42
6:J:169:ARG:NH2	6:J:766:ASN:HD22	2.17	0.42
7:K:-43:DT:H4'	11:O:14:ALA:HB1	1.99	0.42
7:K:19:DC:H2"	7:K:20:DG:C8	2.54	0.42
1:B:405:ARG:HD2	2:E:351:ASP:HB3	2.01	0.42
3:G:1020:ILE:HG23	3:G:1072:THR:HG23	2.01	0.42
3:G:1416:THR:HG22	3:G:1427:ARG:HE	1.84	0.42
3:G:1544:SER:O	3:G:1547:ARG:N	2.53	0.42
5:I:39:ARG:NH1	7:K:34:DT:OP1	2.52	0.42
5:I:215:HIS:ND1	5:I:217:VAL:HG22	2.34	0.42
2:F:345:LEU:HD12	2:F:350:LEU:HD21	2.01	0.42
1:B:302:ILE:HG21	1:B:308:LEU:HD11	2.01	0.42
2:F:134:GLU:HG2	2:F:236:GLU:HG2	2.01	0.42
3:G:1137:THR:O	3:G:1138:PRO:C	2.58	0.42
3:G:1257:LEU:HD23	3:G:1257:LEU:HA	1.86	0.42
1:A:193:TYR:O	1:A:193:TYR:CD2	2.72	0.42
1:C:184:GLU:HG2	1:C:203:ARG:H	1.83	0.42
7:K:36:DC:H1'	7:K:37:DC:C6	2.54	0.42
12:T:67:ASN:O	12:T:71:GLU:HG3	2.20	0.42
3:G:1276:ARG:HH21	3:G:1276:ARG:HD3	1.66	0.42
5:I:218:LEU:HD21	12:T:118:VAL:CG1	2.50	0.42
6:J:229:ILE:HG21	6:J:660:ILE:HD12	2.02	0.42
11:O:32:ARG:HH12	12:P:35:GLU:CD	2.23	0.42
11:O:79:ILE:HB	11:O:80:PRO:HD2	2.01	0.42
11:S:33:LEU:O	11:S:37:GLY:HA3	2.19	0.42
1:A:175:PRO:HB2	3:G:1497:ARG:HH22	1.85	0.42
1:C:150:GLY:HA3	4:H:442:ARG:CG	2.48	0.42
2:D:150:SER:OG	2:D:151:VAL:N	2.53	0.42
2:E:388:LEU:HD22	2:E:422:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:434:ASP:OD1	2:F:434:ASP:N	2.52	0.42
3:G:994:ILE:HG12	3:G:1153:ILE:HD12	2.02	0.42
9:M:130:ILE:CG2	9:Q:131:ARG:HG3	2.49	0.42
1:A:216:LEU:HD23	2:D:173:MET:HG2	2.02	0.42
1:B:102:ILE:HD13	1:B:308:LEU:HD23	2.01	0.42
2:E:127:ILE:HD13	2:E:319:LEU:HB3	2.02	0.42
2:E:162:ILE:HD11	2:E:231:LEU:HD21	2.01	0.42
9:Q:46:VAL:HG22	9:Q:49:ARG:NH2	2.35	0.42
1:C:237:GLN:HE21	3:G:1430:PRO:HB3	1.84	0.41
5:I:189:HIS:HB3	5:I:193:ILE:HD12	2.01	0.41
9:M:113:HIS:CE1	9:Q:116:ARG:NH1	2.88	0.41
2:D:399:ARG:O	2:D:403:ASN:ND2	2.54	0.41
2:F:117:GLU:OE2	2:F:121:GLN:NE2	2.53	0.41
4:H:417:PRO:O	4:H:418:ARG:HB3	2.20	0.41
7:K:-40:DG:H2"	7:K:-39:DT:H5'	2.02	0.41
8:L:-60:DA:H2"	8:L:-59:DT:C5'	2.49	0.41
8:L:-46:DT:H2"	8:L:-45:DG:C8	2.54	0.41
8:L:30:DC:H2"	8:L:31:DT:H5'	2.02	0.41
2:D:163:LYS:HG2	2:D:168:GLU:HA	2.01	0.41
2:E:31:GLY:O	2:E:43:SER:OG	2.36	0.41
2:F:143:VAL:HG12	2:F:144:GLU:HG3	2.02	0.41
3:G:1584:LEU:N	3:G:1584:LEU:HD23	2.35	0.41
8:L:35:DT:H2"	8:L:36:DA:C8	2.55	0.41
1:A:272:ILE:HG23	1:A:276:LEU:HD23	2.01	0.41
1:A:277:ARG:O	1:A:281:ASN:ND2	2.53	0.41
1:A:295:LEU:HD22	2:E:18:LEU:HD12	2.03	0.41
1:B:256:ASP:OD2	1:B:259:SER:OG	2.26	0.41
1:C:166:ARG:HH22	1:C:228:GLU:HG2	1.85	0.41
2:E:305:ILE:HA	2:E:308:PHE:HD2	1.86	0.41
3:G:966:LYS:N	3:G:1016:GLU:OE2	2.54	0.41
3:G:1542:VAL:HG12	3:G:1543:PRO:CD	2.49	0.41
3:G:1587:GLU:O	3:G:1589:LEU:N	2.52	0.41
9:M:58:THR:HG21	11:S:81:ARG:HB2	2.02	0.41
12:T:73:ILE:HG12	12:T:101:LEU:CD2	2.50	0.41
1:C:266:LYS:NZ	2:F:112:GLU:OE2	2.52	0.41
2:D:161:THR:HG22	2:D:170:ILE:HG12	2.03	0.41
6:J:392:LYS:HA	6:J:447:GLU:CG	2.50	0.41
11:S:19:SER:O	11:S:20:ARG:C	2.57	0.41
6:J:116:ARG:NH1	8:L:-30:DA:H3'	2.35	0.41
6:J:347:LEU:HD22	6:J:391:ILE:HD12	2.03	0.41
11:S:47:ALA:HB3	11:S:48:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:400:TYR:OH	2:E:432:PHE:O	2.28	0.41
6:J:116:ARG:NH1	8:L:-30:DA:OP1	2.48	0.41
8:L:21:DG:C8	8:L:22:DT:H72	2.55	0.41
11:S:45:ALA:O	11:S:48:PRO:HD2	2.20	0.41
1:B:104:SER:HA	2:E:114:SER:HB3	2.02	0.41
2:E:170:ILE:HD11	5:I:182:PRO:HB3	2.03	0.41
2:E:302:MET:HB3	2:E:302:MET:HE2	1.87	0.41
2:E:434:ASP:OD1	2:E:434:ASP:N	2.53	0.41
3:G:1574:LEU:HG	3:G:1576:PHE:CE1	2.55	0.41
6:J:249:LYS:HE2	6:J:612:PHE:CZ	2.56	0.41
8:L:8:DG:P	10:N:35:ARG:HH12	2.43	0.41
8:L:20:DG:H4'	8:L:21:DG:OP1	2.21	0.41
9:Q:67:PHE:CZ	9:Q:93:GLN:HA	2.55	0.41
1:C:194:ILE:HG12	1:C:201:CYS:HB3	2.02	0.41
1:C:366:PRO:HG3	2:D:448:ARG:HD3	2.02	0.41
2:E:131:ILE:HD11	3:G:1316:PRO:HG2	2.02	0.41
2:F:134:GLU:OE1	2:F:234:ARG:NH2	2.53	0.41
2:F:334:ILE:HD13	2:F:346:PRO:HG3	2.03	0.41
3:G:1374:SER:H	3:G:1377:GLU:HB2	1.86	0.41
3:G:1665:LEU:HD23	3:G:1665:LEU:HA	1.92	0.41
6:J:15:ARG:CZ	6:J:595:ASP:CG	2.89	0.41
6:J:85:ILE:HG23	6:J:115:ILE:HG23	2.03	0.41
6:J:195:PHE:HD1	6:J:687:PHE:HE1	1.69	0.41
7:K:-34:DG:P	12:P:87:SER:OG	2.79	0.41
11:S:33:LEU:CB	12:T:70:PHE:CZ	3.04	0.41
1:B:324:ILE:HD11	2:F:18:LEU:HD22	2.03	0.41
2:D:200:LYS:HD3	3:G:1454:ARG:HH12	1.86	0.41
3:G:1011:MET:HE2	3:G:1011:MET:HB2	1.92	0.41
3:G:1644:ILE:HD13	3:G:1644:ILE:HG21	1.73	0.41
6:J:501:ARG:O	6:J:502:LYS:C	2.59	0.41
11:S:26:PRO:HD3	12:T:40:TYR:CG	2.56	0.41
11:S:108:LEU:HD23	11:S:108:LEU:HA	1.93	0.41
3:G:1651:ASN:CB	7:K:64:DT:C5'	2.87	0.40
6:J:293:ARG:O	6:J:636:ARG:NH1	2.51	0.40
11:S:84:GLN:O	11:S:88:ARG:HG2	2.21	0.40
1:C:405:ARG:NH2	13:C:501:ADP:O2A	2.43	0.40
3:G:964:GLN:NE2	3:G:970:CYS:O	2.54	0.40
4:H:418:ARG:O	4:H:419:THR:CB	2.70	0.40
1:C:217:GLU:OE1	2:F:176:LYS:N	2.52	0.40
1:C:379:ARG:HG2	1:C:408:LEU:HD22	2.04	0.40
2:D:72:ALA:HB3	2:D:353:VAL:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:350:LEU:HA	2:E:353:VAL:HG22	2.02	0.40
3:G:1050:LEU:HD11	3:G:1062:LEU:HD22	2.02	0.40
3:G:1635:ILE:HG12	3:G:1661:ARG:CD	2.51	0.40
6:J:688:LEU:HB3	6:J:693:THR:HG21	2.04	0.40
3:G:1233:LEU:CB	3:G:1264:PHE:CE1	3.04	0.40
3:G:1284:PHE:HZ	3:G:1307:THR:HG23	1.85	0.40
1:A:212:THR:HG22	1:A:214:PHE:H	1.86	0.40
1:C:155:ILE:HD12	4:H:474:PHE:HD1	1.85	0.40
2:D:208:TYR:OH	4:H:454:LYS:HD3	2.21	0.40
6:J:116:ARG:NH1	8:L:-30:DA:O5'	2.55	0.40
6:J:610:HIS:HE1	6:J:619:PHE:HA	1.86	0.40
8:L:26:DA:H4'	9:M:83:ARG:HH12	1.79	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	447/462 (97%)	418 (94%)	29 (6%)	0	100	100
1	B	434/462 (94%)	404 (93%)	30 (7%)	0	100	100
1	C	457/462 (99%)	428 (94%)	29 (6%)	0	100	100
2	D	437/488 (90%)	409 (94%)	28 (6%)	0	100	100
2	E	437/488 (90%)	410 (94%)	27 (6%)	0	100	100
2	F	433/488 (89%)	402 (93%)	31 (7%)	0	100	100
3	G	720/1856 (39%)	647 (90%)	63 (9%)	10 (1%)	11	47
4	H	96/492 (20%)	84 (88%)	7 (7%)	5 (5%)	2	22
5	I	105/219 (48%)	99 (94%)	6 (6%)	0	100	100
6	J	635/769 (83%)	600 (94%)	33 (5%)	2 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	M	92/135 (68%)	92 (100%)	0	0	100	100
9	Q	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
10	N	75/102 (74%)	73 (97%)	2 (3%)	0	100	100
10	R	76/102 (74%)	73 (96%)	3 (4%)	0	100	100
11	O	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
11	S	106/129 (82%)	103 (97%)	3 (3%)	0	100	100
12	P	91/125 (73%)	90 (99%)	1 (1%)	0	100	100
12	T	89/125 (71%)	84 (94%)	4 (4%)	1 (1%)	14	52
All	All	4929/7168 (69%)	4612 (94%)	299 (6%)	18 (0%)	38	72

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	967	LEU
3	G	1141	ASN
3	G	1545	MET
4	H	423	ALA
6	J	504	LEU
4	H	419	THR
4	H	445	PRO
12	T	39	VAL
3	G	1015	ALA
3	G	1279	THR
3	G	1586	GLU
3	G	1587	GLU
3	G	1588	TYR
3	G	1280	SER
3	G	1144	GLN
6	J	502	LYS
4	H	420	THR
4	H	443	PRO

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	365/377 (97%)	364 (100%)	1 (0%)	92	95
1	B	357/377 (95%)	357 (100%)	0	100	100
1	C	374/377 (99%)	374 (100%)	0	100	100
2	D	367/402 (91%)	367 (100%)	0	100	100
2	E	368/402 (92%)	368 (100%)	0	100	100
2	F	367/402 (91%)	367 (100%)	0	100	100
3	G	645/1604 (40%)	625 (97%)	20 (3%)	40	62
4	H	77/398 (19%)	73 (95%)	4 (5%)	23	50
5	I	93/171 (54%)	93 (100%)	0	100	100
6	J	546/644 (85%)	544 (100%)	2 (0%)	91	94
9	M	82/110 (74%)	82 (100%)	0	100	100
9	Q	85/110 (77%)	83 (98%)	2 (2%)	49	69
10	N	64/78 (82%)	64 (100%)	0	100	100
10	R	64/78 (82%)	64 (100%)	0	100	100
11	O	82/98 (84%)	82 (100%)	0	100	100
11	S	83/98 (85%)	83 (100%)	0	100	100
12	P	80/105 (76%)	80 (100%)	0	100	100
12	T	78/105 (74%)	76 (97%)	2 (3%)	46	67
All	All	4177/5936 (70%)	4146 (99%)	31 (1%)	84	90

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	TYR
3	G	967	LEU
3	G	1021	TRP
3	G	1079	PHE
3	G	1089	VAL
3	G	1118	SER
3	G	1142	ASN
3	G	1143	MET
3	G	1153	ILE
3	G	1192	MET
3	G	1200	ARG
3	G	1206	VAL

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Mol	Chain	Res	Type
3	G	1230	TYR
3	G	1460	ARG
3	G	1545	MET
3	G	1585	MET
3	G	1606	GLU
3	G	1609	ARG
3	G	1624	PHE
3	G	1635	ILE
3	G	1664	ARG
4	H	418	ARG
4	H	434	GLU
4	H	442	ARG
4	H	445	PRO
6	J	88	LYS
6	J	328	LEU
9	Q	63	ARG
9	Q	123	ASP
12	T	42	TYR
12	T	80	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	248	ASN
1	A	281	ASN
1	B	28	ASN
1	C	28	ASN
1	C	242	HIS
2	D	146	GLN
2	D	274	GLN
2	E	394	GLN
2	E	409	GLN
3	G	1037	GLN
3	G	1402	HIS
3	G	1697	GLN
6	J	73	ASN
6	J	762	HIS
12	P	84	ASN
9	Q	68	GLN
10	R	75	HIS
12	T	84	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	A	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.43	4 (13%)
13	ADP	C	501	-	24,29,29	1.00	1 (4%)	29,45,45	1.49	4 (13%)
13	ADP	B	501	-	24,29,29	1.07	2 (8%)	29,45,45	1.57	3 (10%)
13	ADP	E	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.61	4 (13%)
14	ATP	J	801	-	26,33,33	1.02	2 (7%)	31,52,52	1.60	5 (16%)
13	ADP	D	501	-	24,29,29	0.99	2 (8%)	29,45,45	1.56	5 (17%)
13	ADP	F	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.50	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	A	501	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	C	501	-	-	3/12/32/32	0/3/3/3
13	ADP	B	501	-	-	1/12/32/32	0/3/3/3
13	ADP	E	501	-	-	0/12/32/32	0/3/3/3
14	ATP	J	801	-	-	3/18/38/38	0/3/3/3
13	ADP	D	501	-	-	0/12/32/32	0/3/3/3
13	ADP	F	501	-	-	0/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	801	ATP	C2'-C1'	-2.36	1.50	1.53
13	B	501	ADP	C2'-C1'	-2.27	1.50	1.53
14	J	801	ATP	C5-C4	2.24	1.46	1.40
13	D	501	ADP	C5-C4	2.24	1.46	1.40
13	C	501	ADP	C2'-C1'	-2.18	1.50	1.53
13	B	501	ADP	C5-C4	2.18	1.46	1.40
13	E	501	ADP	C2'-C1'	-2.15	1.50	1.53
13	D	501	ADP	C2'-C1'	-2.10	1.50	1.53
13	F	501	ADP	C5-C4	2.08	1.46	1.40
13	A	501	ADP	C2'-C1'	-2.01	1.50	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	501	ADP	PA-O3A-PB	-4.57	117.15	132.83
13	E	501	ADP	PA-O3A-PB	-4.45	117.56	132.83
13	C	501	ADP	PA-O3A-PB	-4.21	118.38	132.83
13	F	501	ADP	PA-O3A-PB	-3.95	119.26	132.83
14	J	801	ATP	PA-O3A-PB	-3.94	119.31	132.83
13	A	501	ADP	PA-O3A-PB	-3.85	119.60	132.83
14	J	801	ATP	PB-O3B-PG	-3.82	119.72	132.83
13	D	501	ADP	PA-O3A-PB	-3.74	119.98	132.83
13	D	501	ADP	N3-C2-N1	-3.26	123.58	128.68
13	E	501	ADP	N3-C2-N1	-3.25	123.59	128.68
13	F	501	ADP	C3'-C2'-C1'	3.22	105.82	100.98
14	J	801	ATP	N3-C2-N1	-3.18	123.70	128.68
13	E	501	ADP	C3'-C2'-C1'	2.99	105.48	100.98
13	B	501	ADP	N3-C2-N1	-2.91	124.13	128.68
13	D	501	ADP	C3'-C2'-C1'	2.85	105.28	100.98
13	C	501	ADP	C3'-C2'-C1'	2.80	105.19	100.98
13	A	501	ADP	N3-C2-N1	-2.73	124.42	128.68
13	F	501	ADP	N3-C2-N1	-2.72	124.43	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	501	ADP	N3-C2-N1	-2.68	124.48	128.68
13	A	501	ADP	C3'-C2'-C1'	2.45	104.67	100.98
14	J	801	ATP	C2'-C3'-C4'	2.40	107.30	102.64
14	J	801	ATP	C4-C5-N7	-2.39	106.91	109.40
13	A	501	ADP	C4-C5-N7	-2.35	106.95	109.40
13	F	501	ADP	C4-C5-N7	-2.26	107.04	109.40
13	D	501	ADP	C4-C5-N7	-2.20	107.10	109.40
13	E	501	ADP	C4-C5-N7	-2.13	107.18	109.40
13	B	501	ADP	C2'-C3'-C4'	2.12	106.77	102.64
13	C	501	ADP	C4-C5-N7	-2.08	107.23	109.40
13	D	501	ADP	O3B-PB-O2B	2.06	115.51	107.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	501	ADP	C5'-O5'-PA-O1A
13	C	501	ADP	C5'-O5'-PA-O1A
13	C	501	ADP	C5'-O5'-PA-O2A
14	J	801	ATP	C5'-O5'-PA-O1A
14	J	801	ATP	C5'-O5'-PA-O2A
13	C	501	ADP	C5'-O5'-PA-O3A
14	J	801	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

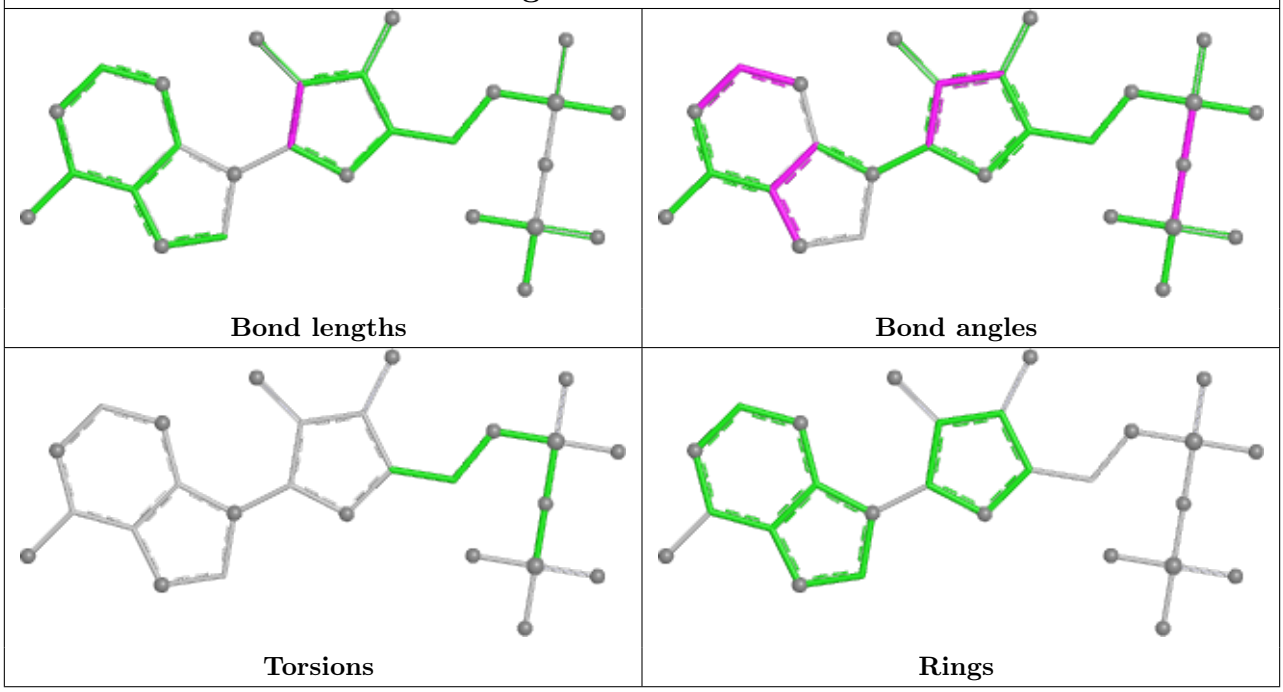
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	501	ADP	3	0
13	B	501	ADP	2	0
13	E	501	ADP	1	0
13	D	501	ADP	2	0
13	F	501	ADP	4	0

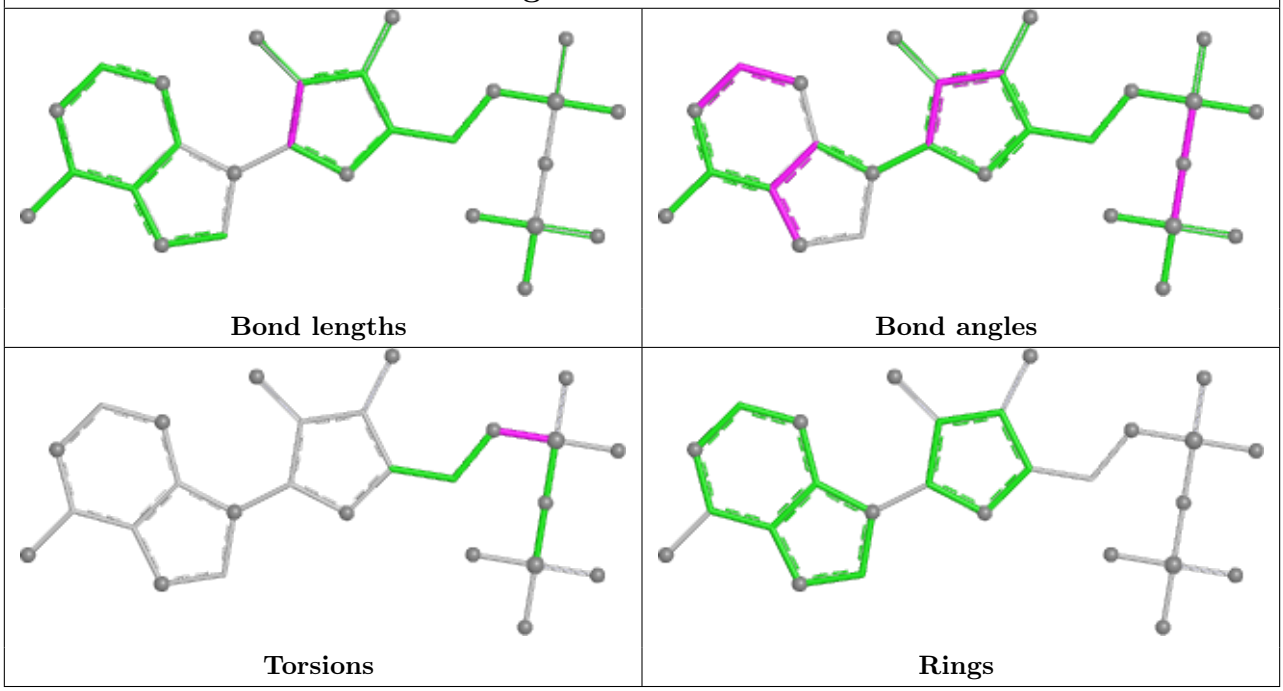
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A 501



Ligand ADP C 501



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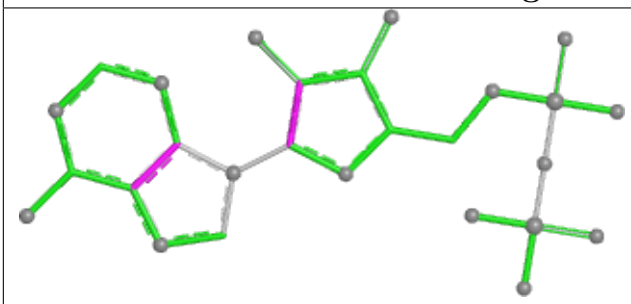
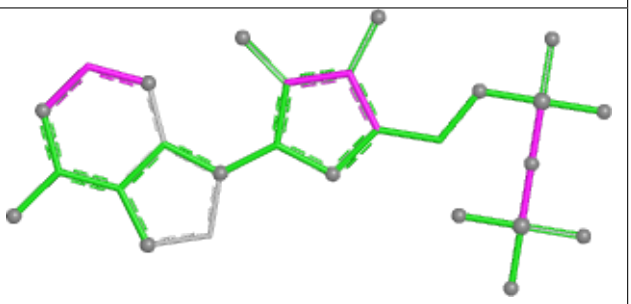
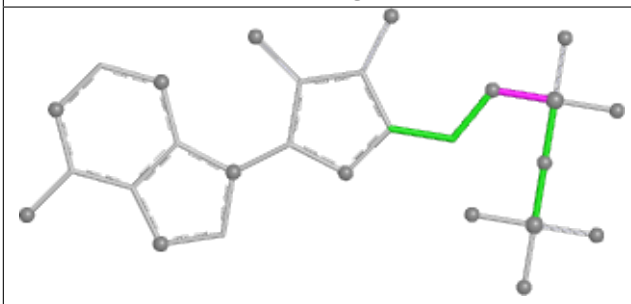
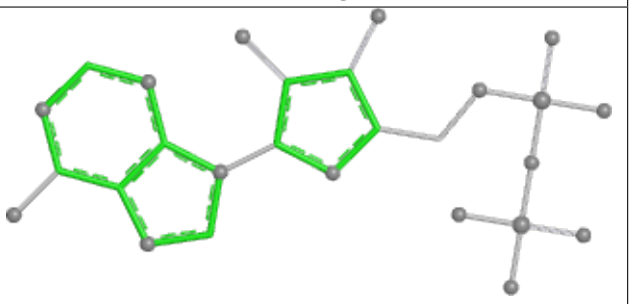
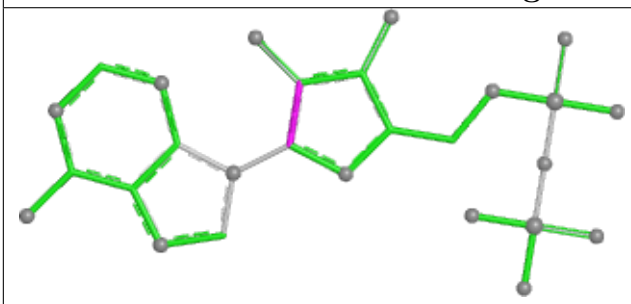
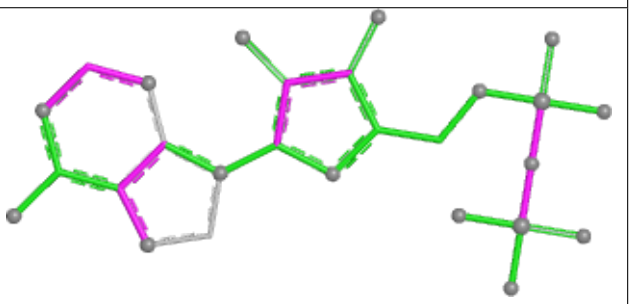
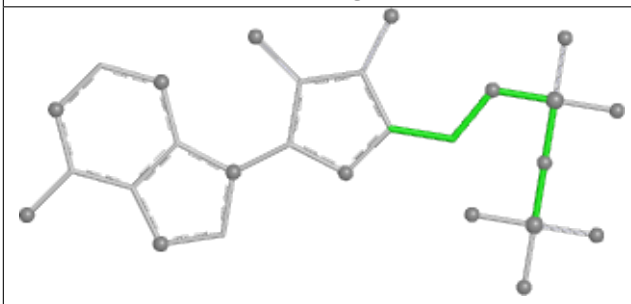
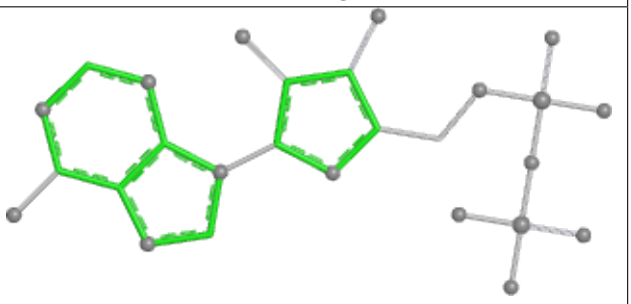
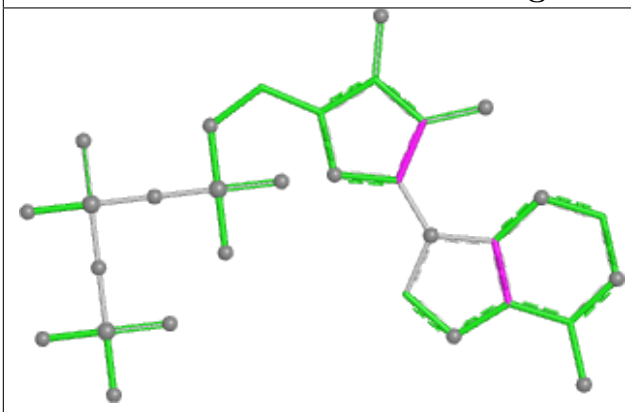
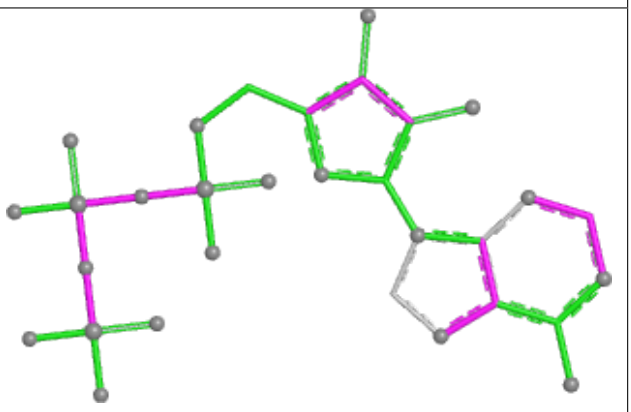
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

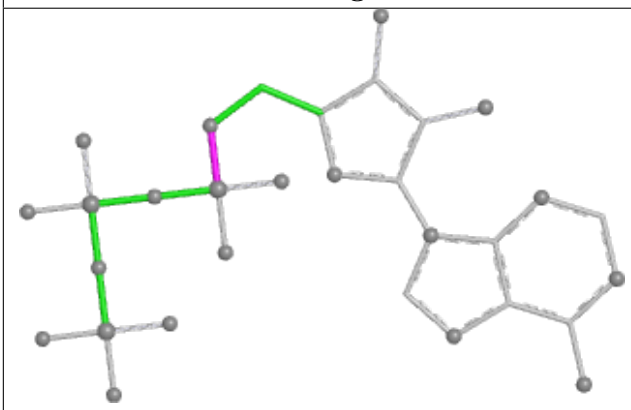
Ligand ATP J 801



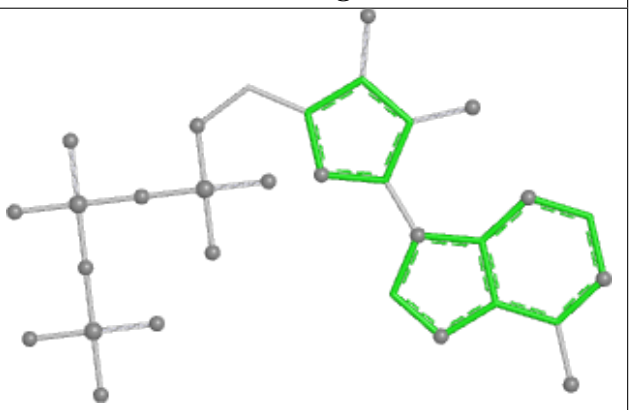
Bond lengths



Bond angles

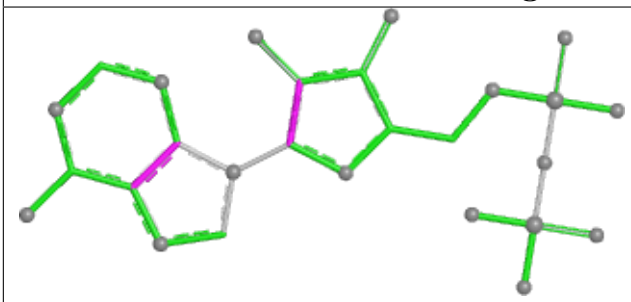


Torsions

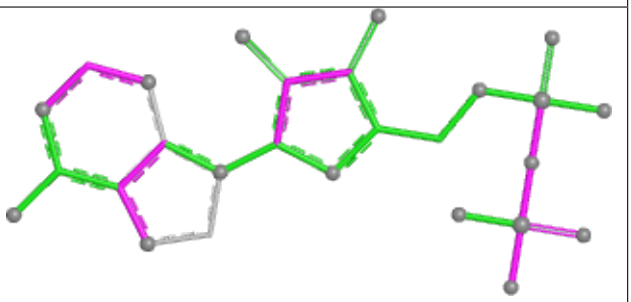


Rings

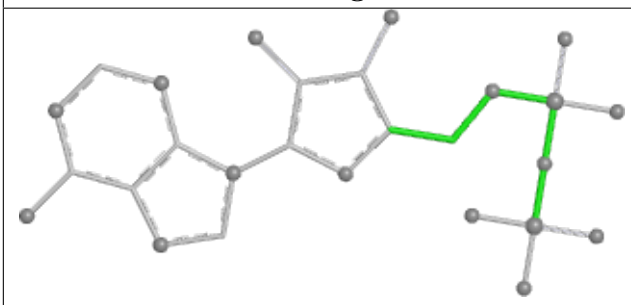
Ligand ADP D 501



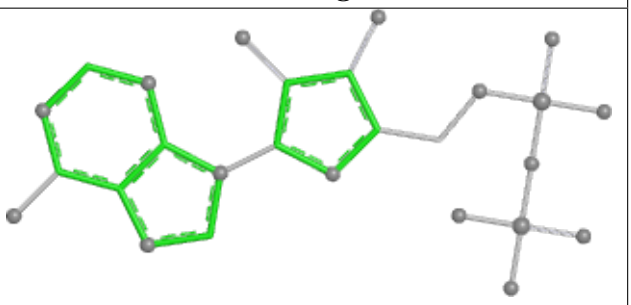
Bond lengths



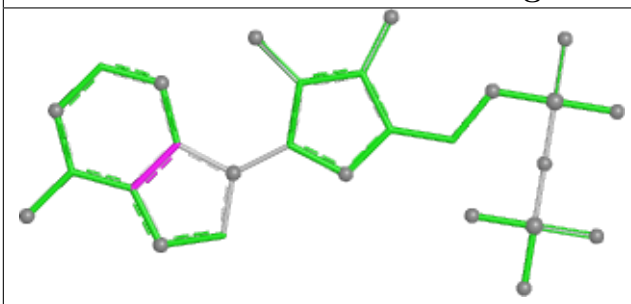
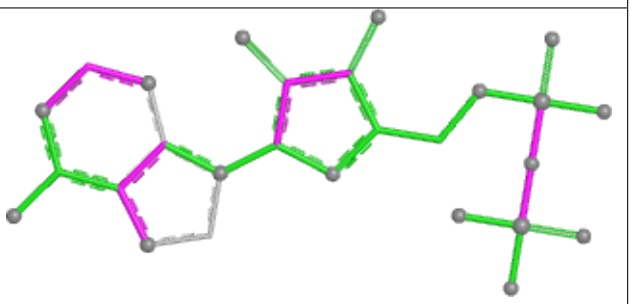
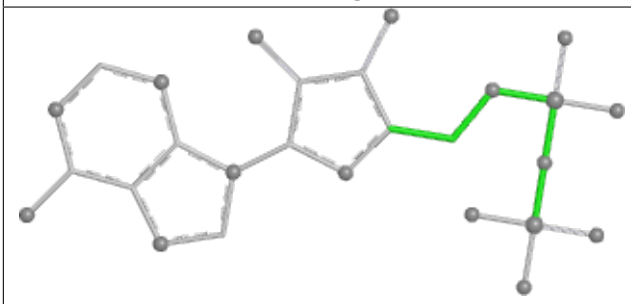
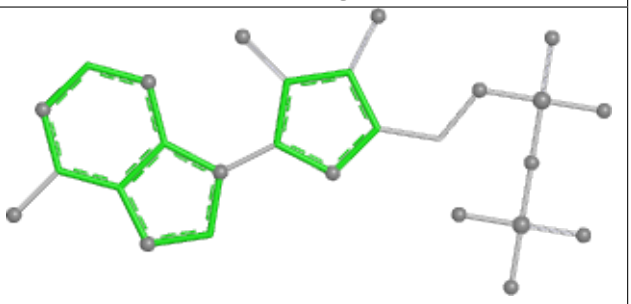
Bond angles



Torsions



Rings

Ligand ADP F 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

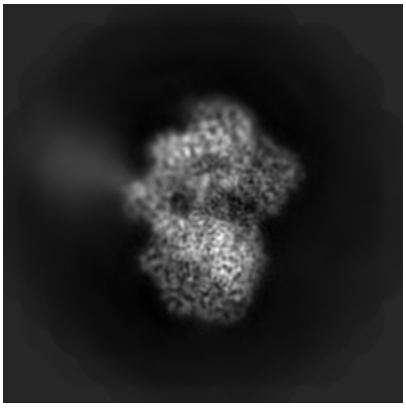
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4278. These allow visual inspection of the internal detail of the map and identification of artifacts.

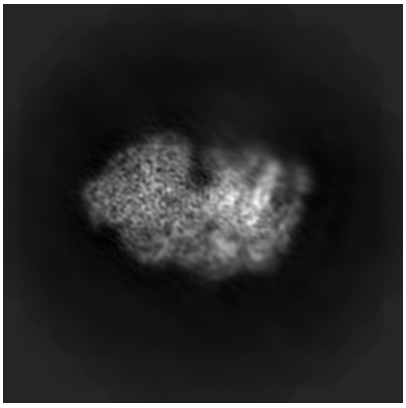
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

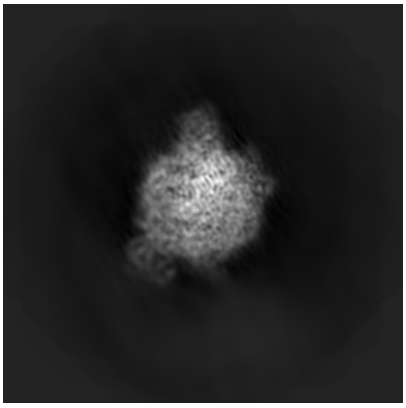
6.1.1 Primary map



X



Y

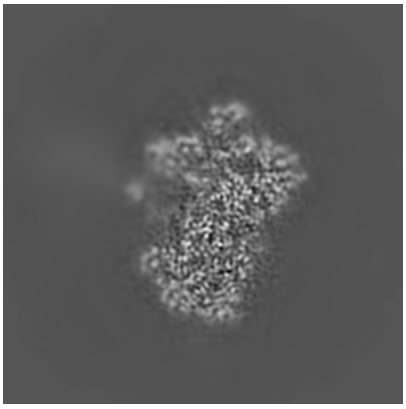


Z

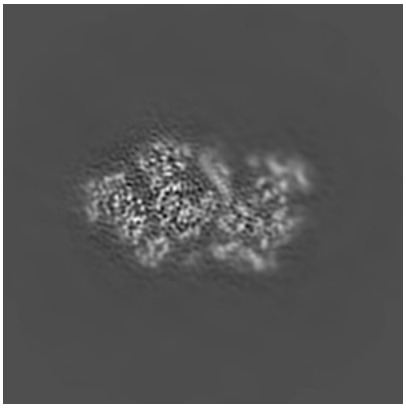
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

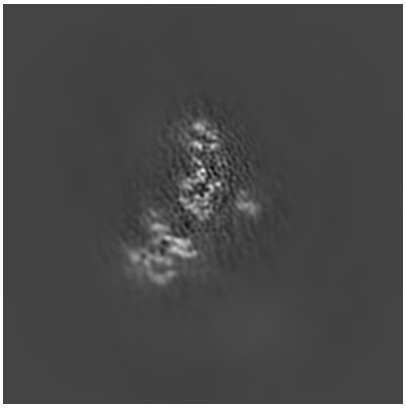
6.2.1 Primary map



X Index: 170



Y Index: 170

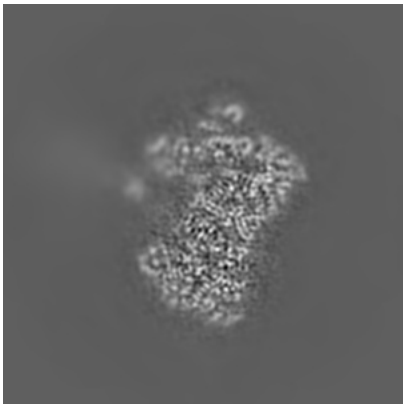


Z Index: 170

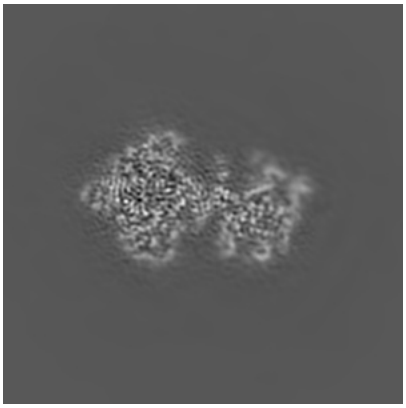
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

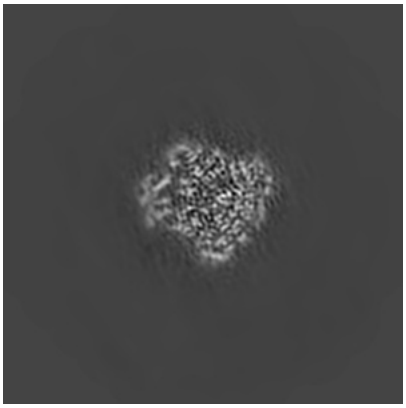
6.3.1 Primary map



X Index: 173



Y Index: 189

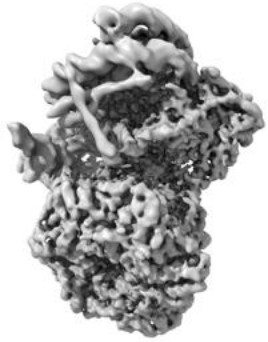


Z Index: 128

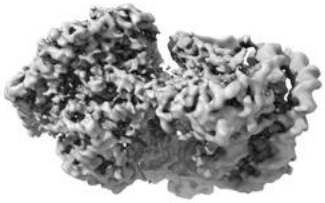
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

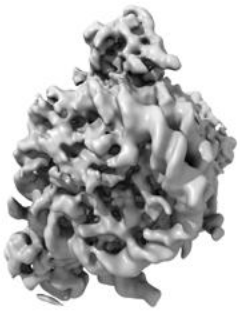
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

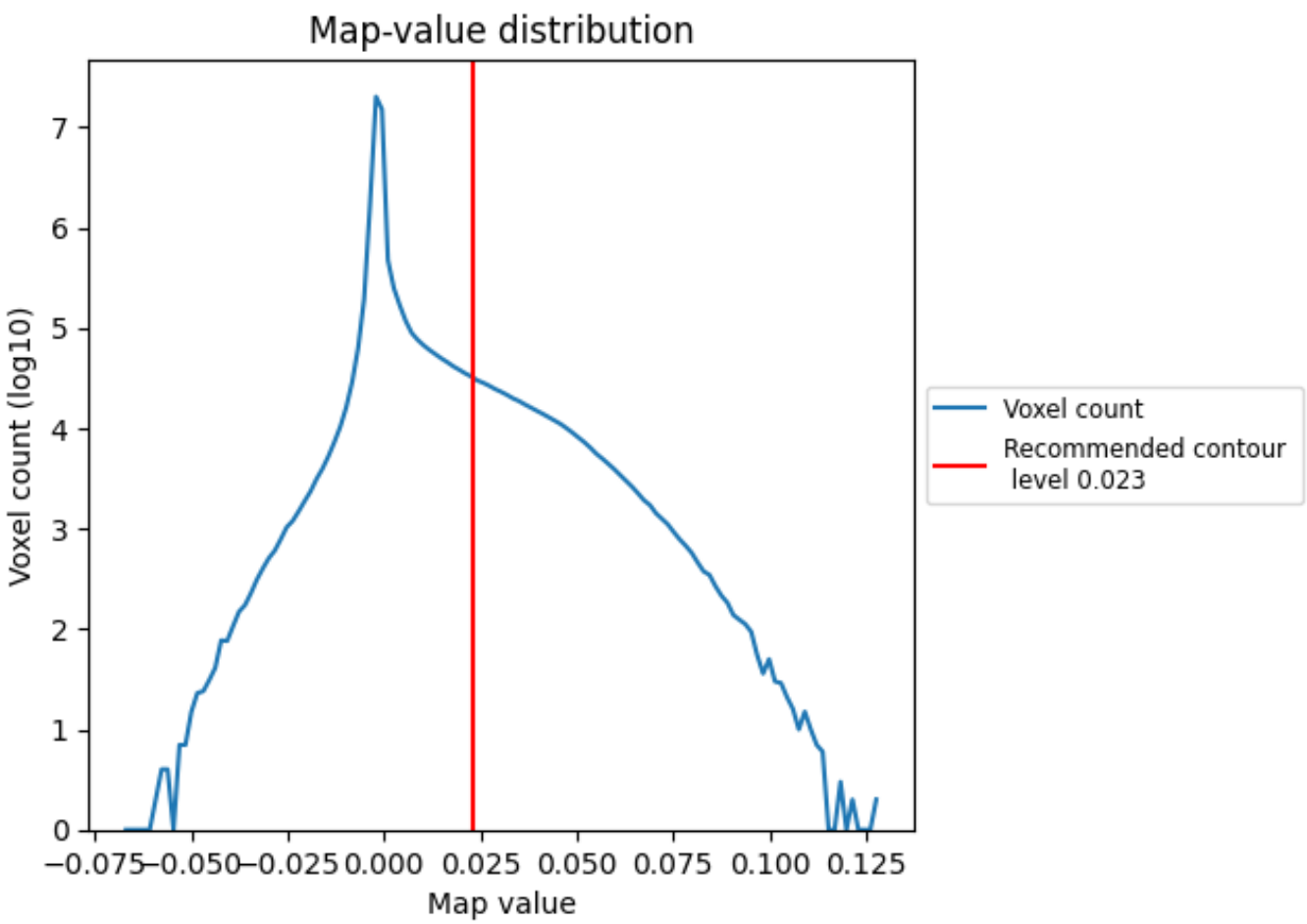
6.5 Mask visualisation (i)

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

7 Map analysis (i)

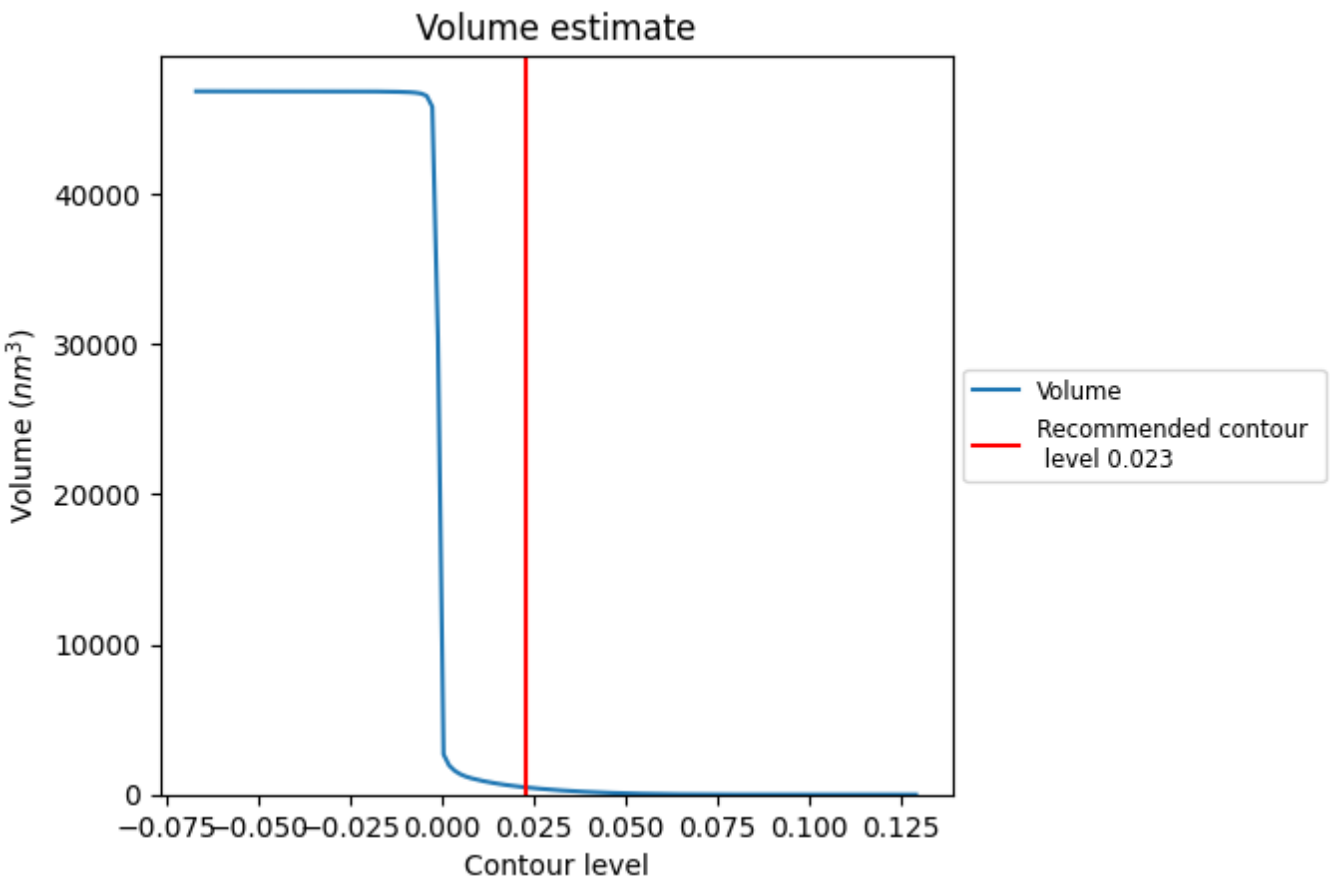
This section contains the results of statistical analysis of the map.

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.

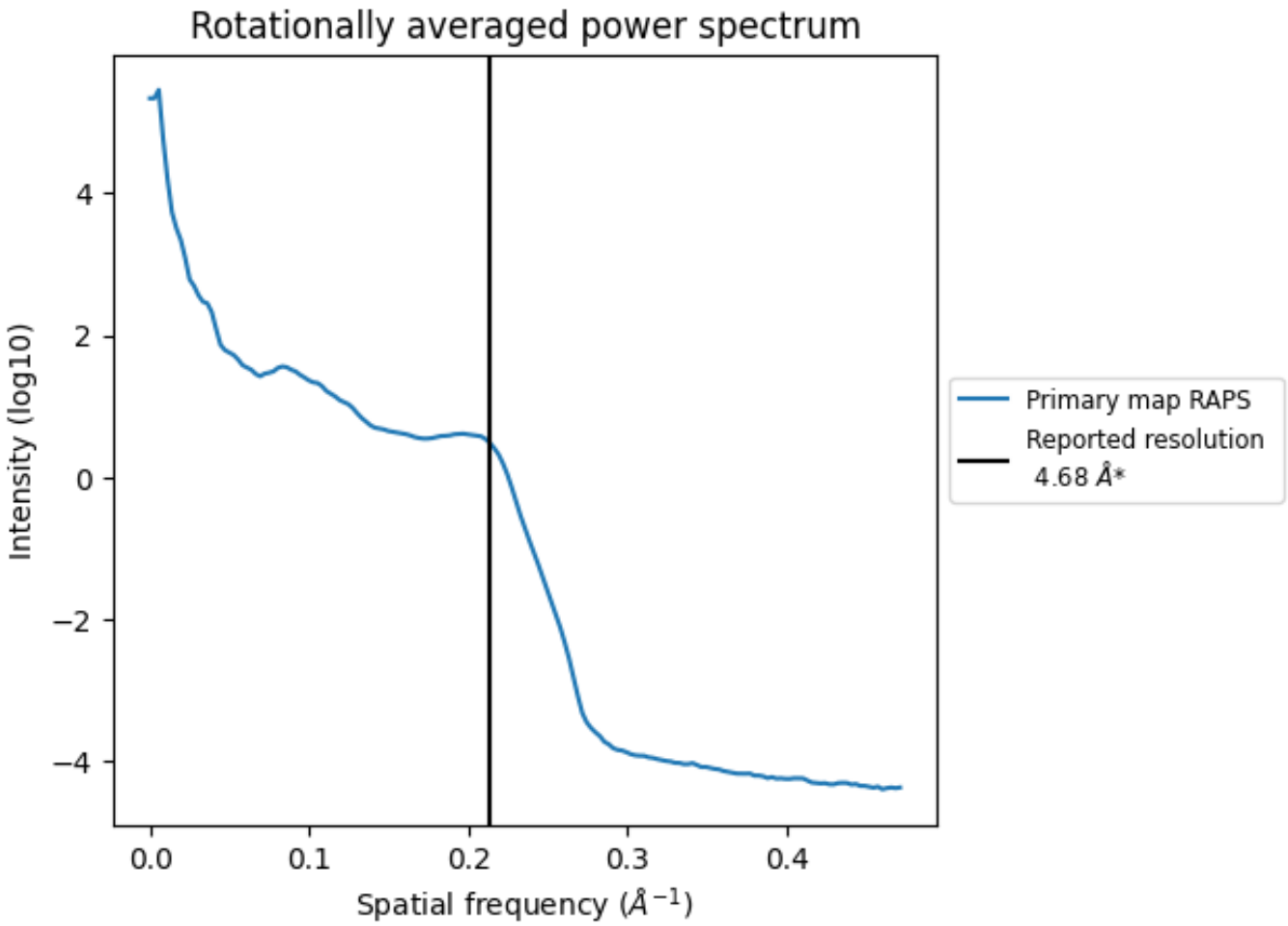
7.2 Volume estimate (i)



The volume at the recommended contour level is 477 nm^3; this corresponds to an approximate mass of 431 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)

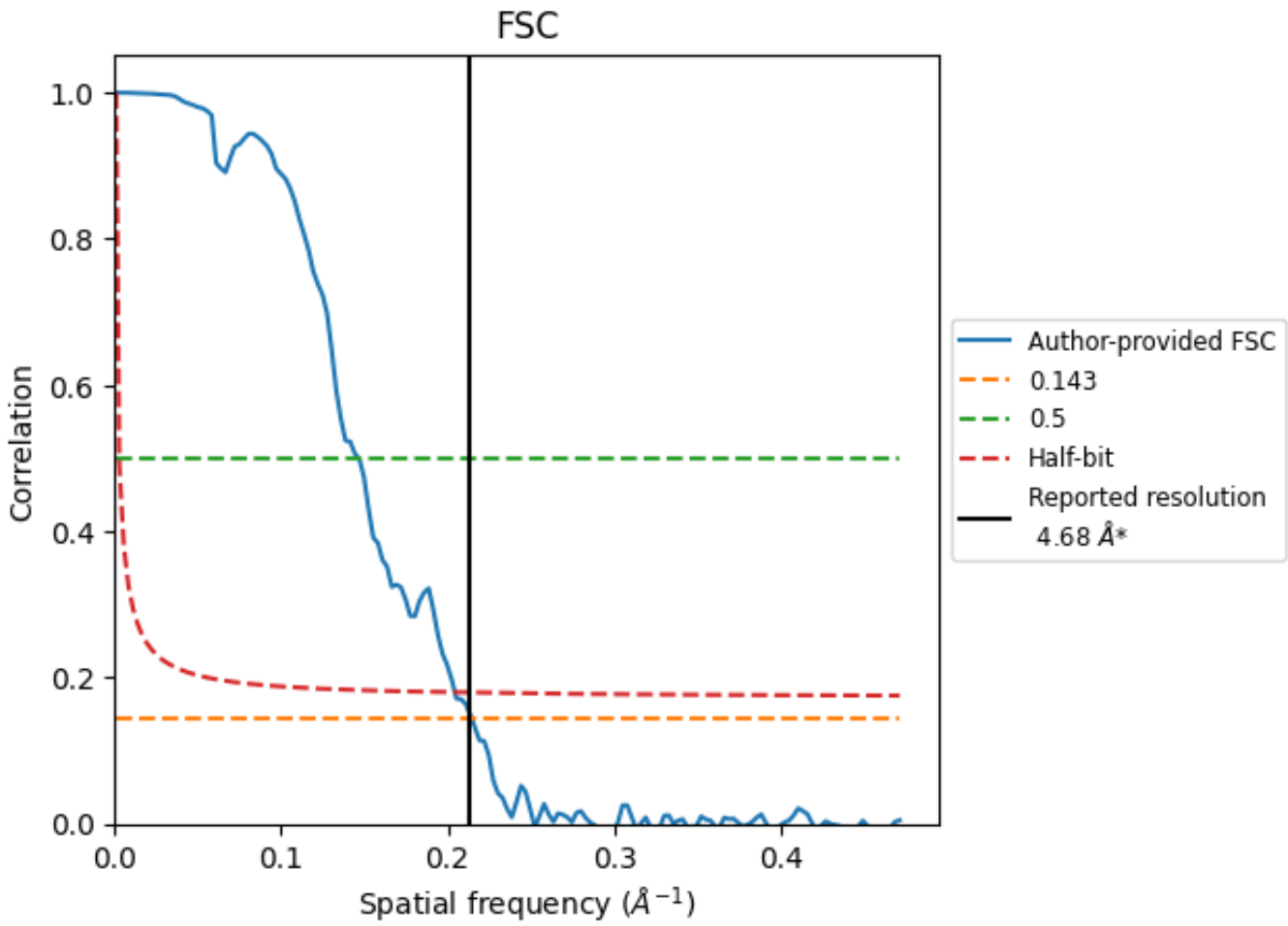


*Reported resolution corresponds to spatial frequency of 0.214 Å^{-1}

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 0.214 Å^{-1}

8.2 Resolution estimates (i)

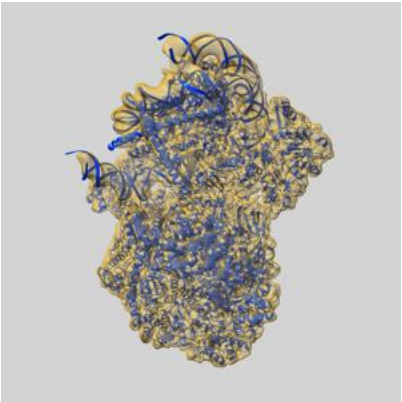
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.68	-	-
Author-provided FSC curve	4.66	6.83	4.89
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

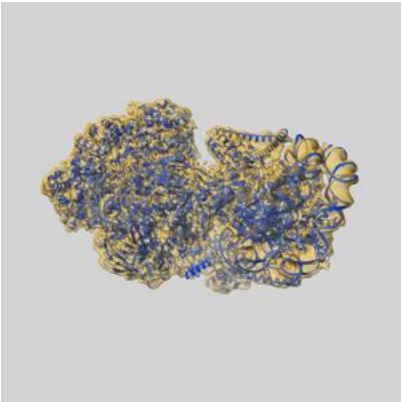
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4278 and PDB model 8AV6. Per-residue inclusion information can be found in section 3 on page 8.

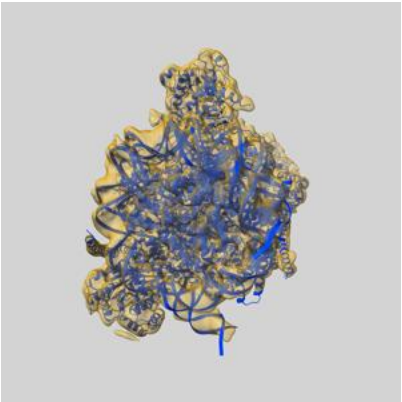
9.1 Map-model overlay (i)



X



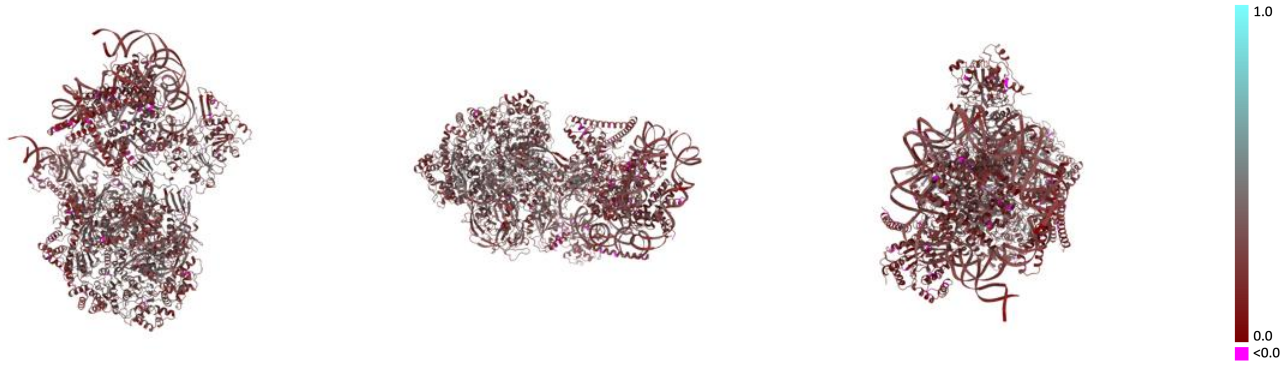
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 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.

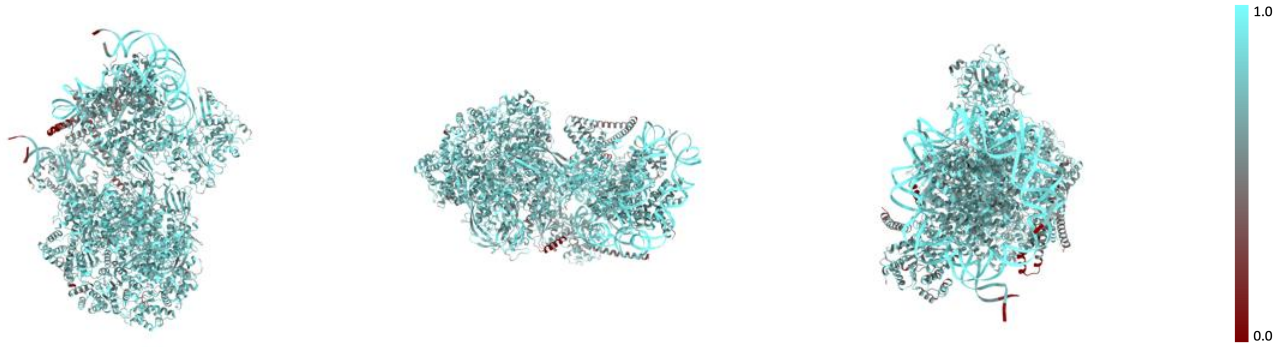
9.2 Q-score mapped to coordinate model (i)



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.

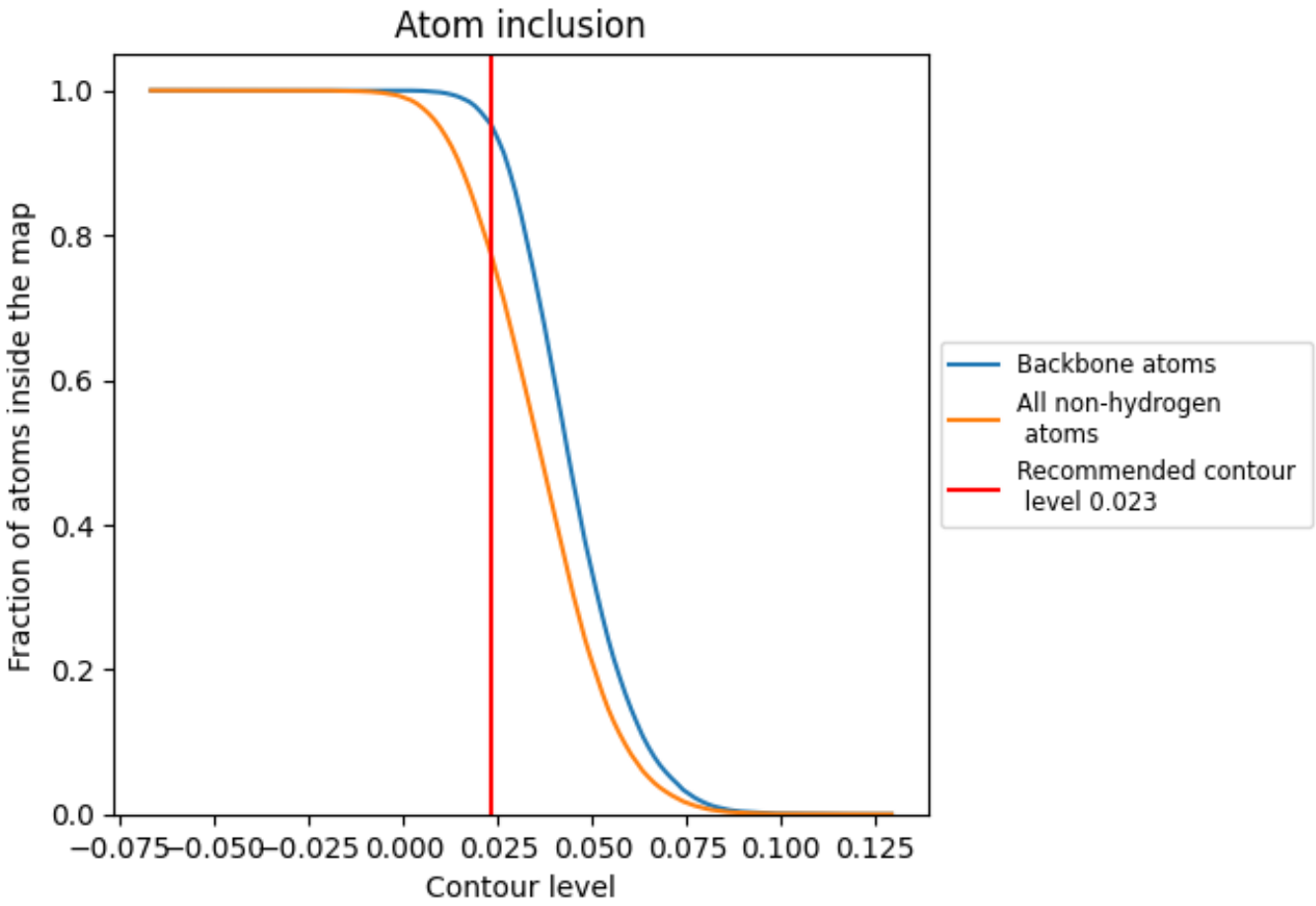
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.023).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7763	0.2830
A	0.7818	0.3220
B	0.7908	0.3210
C	0.7664	0.3060
D	0.7502	0.2960
E	0.7867	0.3150
F	0.7758	0.3290
G	0.7420	0.2600
H	0.5455	0.2250
I	0.7789	0.2840
J	0.7140	0.2540
K	0.9049	0.2630
L	0.9249	0.2700
M	0.7151	0.2170
N	0.7273	0.2310
O	0.7376	0.2450
P	0.7571	0.2490
Q	0.7195	0.2070
R	0.7742	0.2480
S	0.7746	0.2720
T	0.7893	0.2790