Full wwPDB EM Validation Report (i)

Aug 3, 2026 – 01:47 PM EDT

PDB ID	:	9E2R / pdb_00009e2r
EMDB ID	:	EMD-47462
Title	:	Cryo-EM structure of human DNMT3A2-DNMT3B3 complex bound to a di-nucleosome and an histone-3 peptide
Authors	:	Xie, X.; Liu, M.; Zhou, X.E.; Worden, E.; Jones, P.
Deposited on	:	2024-10-22
Resolution	:	7.71 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 (i)) were used in the production of this report:

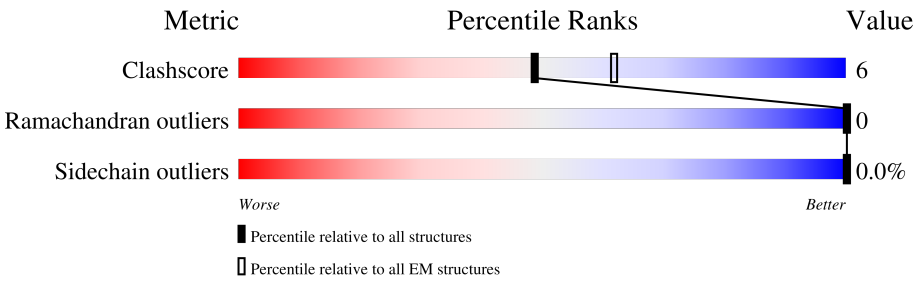
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

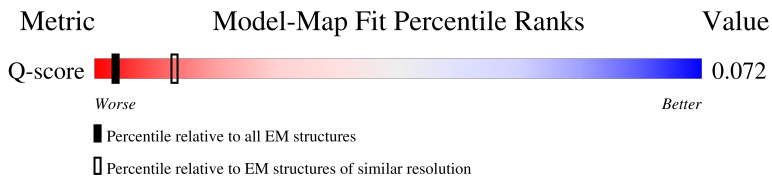
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.71 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	355 (7.23 - 8.21)

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	135	60% 11% 29%
1	E	135	62% 10% 28%
1	M	135	• 66% 7% 27%
1	Q	135	60% 10% 30%

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Mol	Chain	Length	Quality of chain
2	B	103	66% 11% 23%
2	F	103	66% 10% 24%
2	N	103	63% 13% 24%
2	R	103	69% 7% 24%
3	C	129	62% 15% 23%
3	G	129	67% 9% 24%
3	O	129	67% 9% 24%
3	S	129	64% 12% 24%
4	D	123	67% 8% 25%
4	H	123	69% 6% 25%
4	P	123	67% 7% 26%
4	T	123	67% 7% 25%
5	I	321	78% 22%
6	J	319	82% 18%
7	L	773	7% 35% 10% 55%
7	V	773	40% 5% 55%
7	X	773	21% 76%
7	Z	773	21% 76%
8	K	689	16% 72% 9% 20%
8	U	689	52% 9% 38%
8	W	689	51% 10% 39%
8	Y	689	71% 9% 19%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 49041 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 H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	96	795	501	154	137	3	0	0
1	E	97	802	506	155	138	3	0	0
1	M	99	820	518	159	140	3	0	0
1	Q	95	785	495	151	136	3	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP Q71DI3
E	102	ALA	GLY	conflict	UNP Q71DI3
M	102	ALA	GLY	conflict	UNP Q71DI3
Q	102	ALA	GLY	conflict	UNP Q71DI3

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	79	633	399	124	109	1	0	0
2	F	78	622	393	120	108	1	0	0
2	N	78	622	393	120	108	1	0	0
2	R	78	622	393	120	108	1	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	99	764	479	151	134	0	0
3	G	98	755	474	149	132	0	0
3	O	98	755	474	149	132	0	0
3	S	98	752	473	148	131	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	92	719	453	129	135	2	0	0
4	H	92	719	453	129	135	2	0	0
4	P	91	708	447	125	134	2	0	0
4	T	92	719	453	129	135	2	0	0

- Molecule 5 is a DNA chain called DNA (321-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	321	6614	3127	1244	1922	321	0	0

- Molecule 6 is a DNA chain called DNA (319-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	319	6506	3086	1183	1918	319	0	0

- Molecule 7 is a protein called Isoform 3 of DNA (cytosine-5)-methyltransferase 3B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	V	347	2776	1764	488	498	26	0	0
7	Z	182	1478	964	255	253	6	0	0
7	L	348	2777	1759	489	503	26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	X	184	1495	974	262	254	5	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	391	LYS	-	insertion	UNP Q9UBC3
V	392	ASP	-	insertion	UNP Q9UBC3
V	393	TYR	-	insertion	UNP Q9UBC3
Z	391	LYS	-	insertion	UNP Q9UBC3
Z	392	ASP	-	insertion	UNP Q9UBC3
Z	393	TYR	-	insertion	UNP Q9UBC3
L	391	LYS	-	insertion	UNP Q9UBC3
L	392	ASP	-	insertion	UNP Q9UBC3
L	393	TYR	-	insertion	UNP Q9UBC3
X	391	LYS	-	insertion	UNP Q9UBC3
X	392	ASP	-	insertion	UNP Q9UBC3
X	393	TYR	-	insertion	UNP Q9UBC3

- Molecule 8 is a protein called DNA (cytosine-5)-methyltransferase 3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	U	424	3404	2156	604	609	35	0	0
8	Y	555	4451	2839	784	786	42	0	0
8	W	423	3400	2154	603	608	35	0	0
8	K	552	4426	2824	778	782	42	0	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	V	3	3	3	0
9	U	3	3	3	0
9	Y	3	3	3	0
9	L	3	3	3	0

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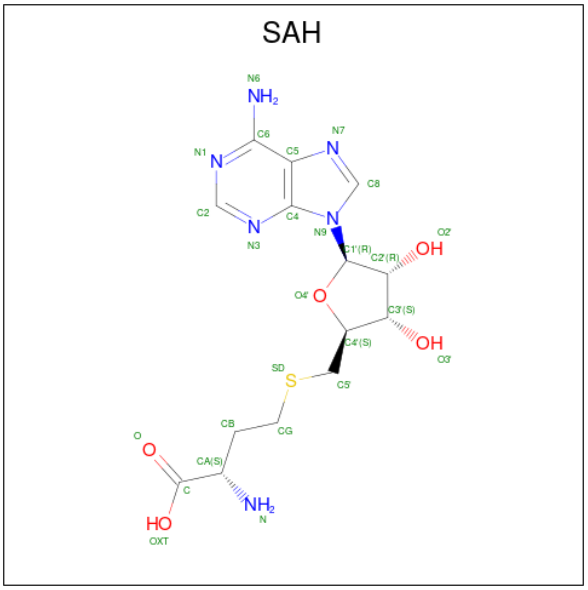
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	W	3	3	3	0
			Total	Zn	
9	K	3	3	3	0

- Molecule 10 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



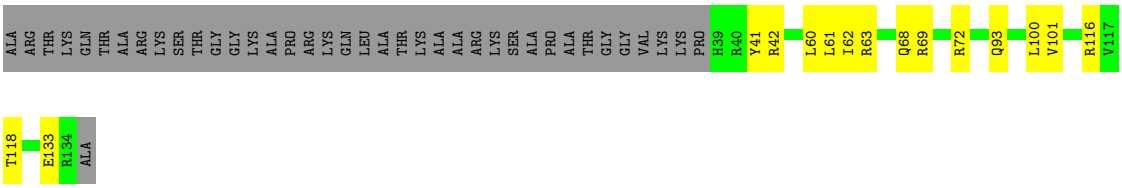
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
10	U	1	26	14	6	5	1	0
			Total	C	N	O	S	
10	Y	1	26	14	6	5	1	0
			Total	C	N	O	S	
10	W	1	26	14	6	5	1	0
			Total	C	N	O	S	
10	K	1	26	14	6	5	1	0

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.

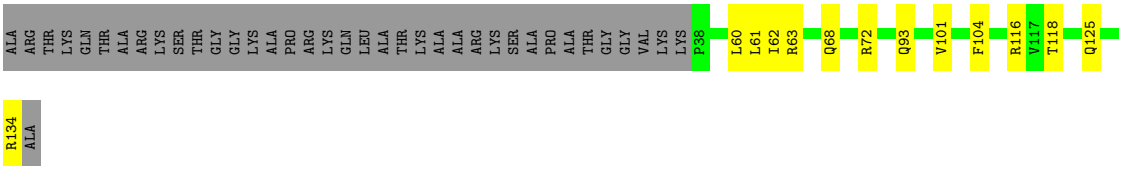
- Molecule 1: Histone H3.2

Chain A:



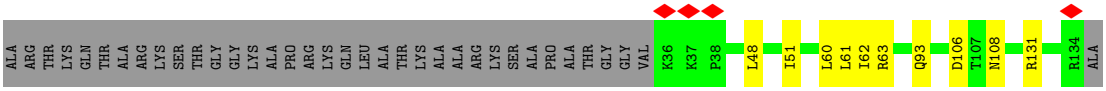
- Molecule 1: Histone H3.2

Chain E:



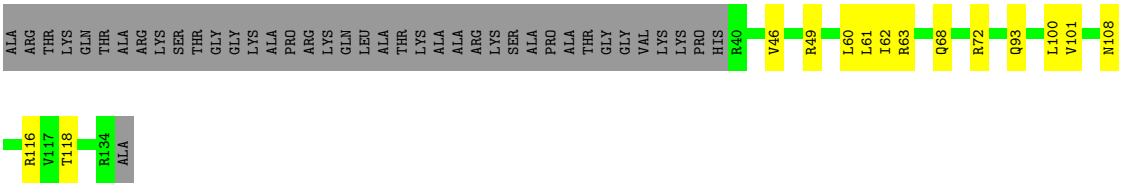
- Molecule 1: Histone H3.2

Chain M:



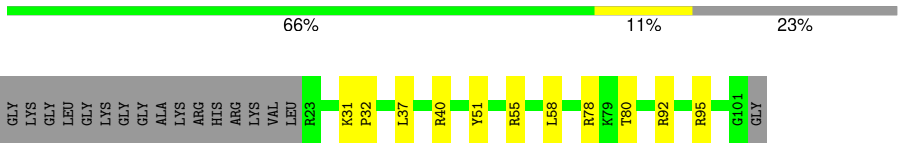
- Molecule 1: Histone H3.2

Chain Q:



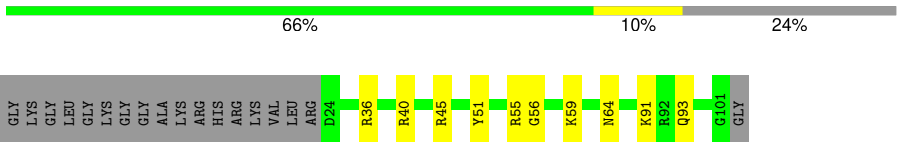
- Molecule 2: Histone H4

Chain B:



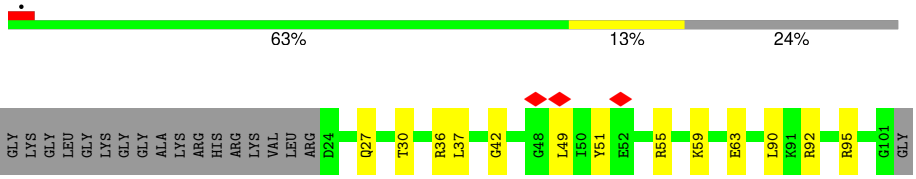
- Molecule 2: Histone H4

Chain F:



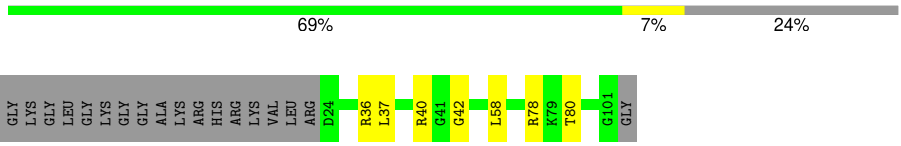
- Molecule 2: Histone H4

Chain N:



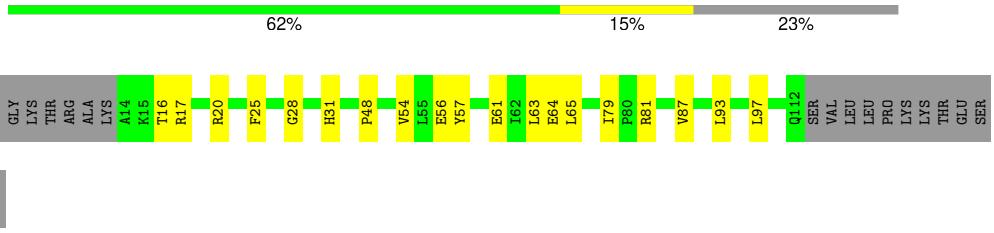
- Molecule 2: Histone H4

Chain R:



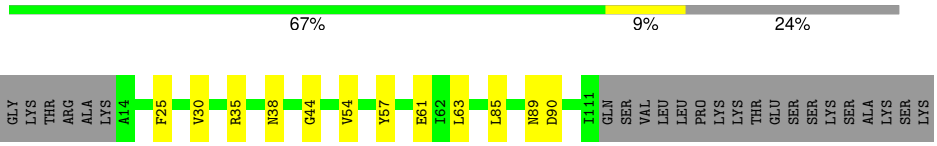
- Molecule 3: Histone H2A

Chain C:



- Molecule 3: Histone H2A

Chain G:

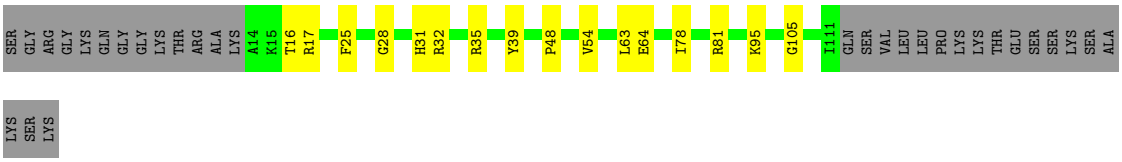


- Molecule 3: Histone H2A

Chain O:

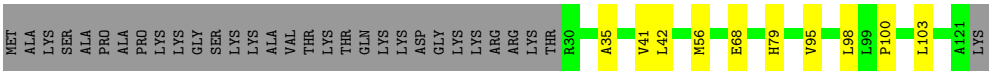
• Molecule 3: Histone H2A

Chain S:



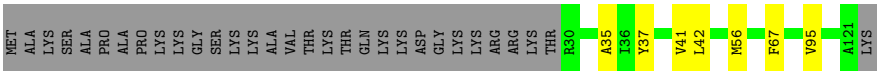
• Molecule 4: Histone H2B

Chain D:



• Molecule 4: Histone H2B

Chain H:



• Molecule 4: Histone H2B

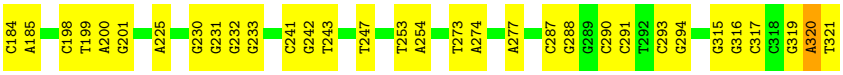
Chain P:

• Molecule 4: Histone H2B

Chain T:

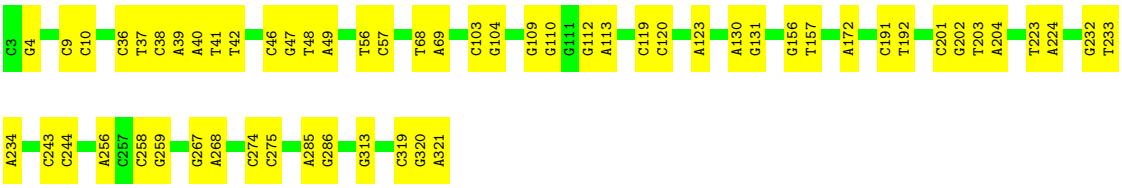
• Molecule 5: DNA (321-MER)

Chain I:



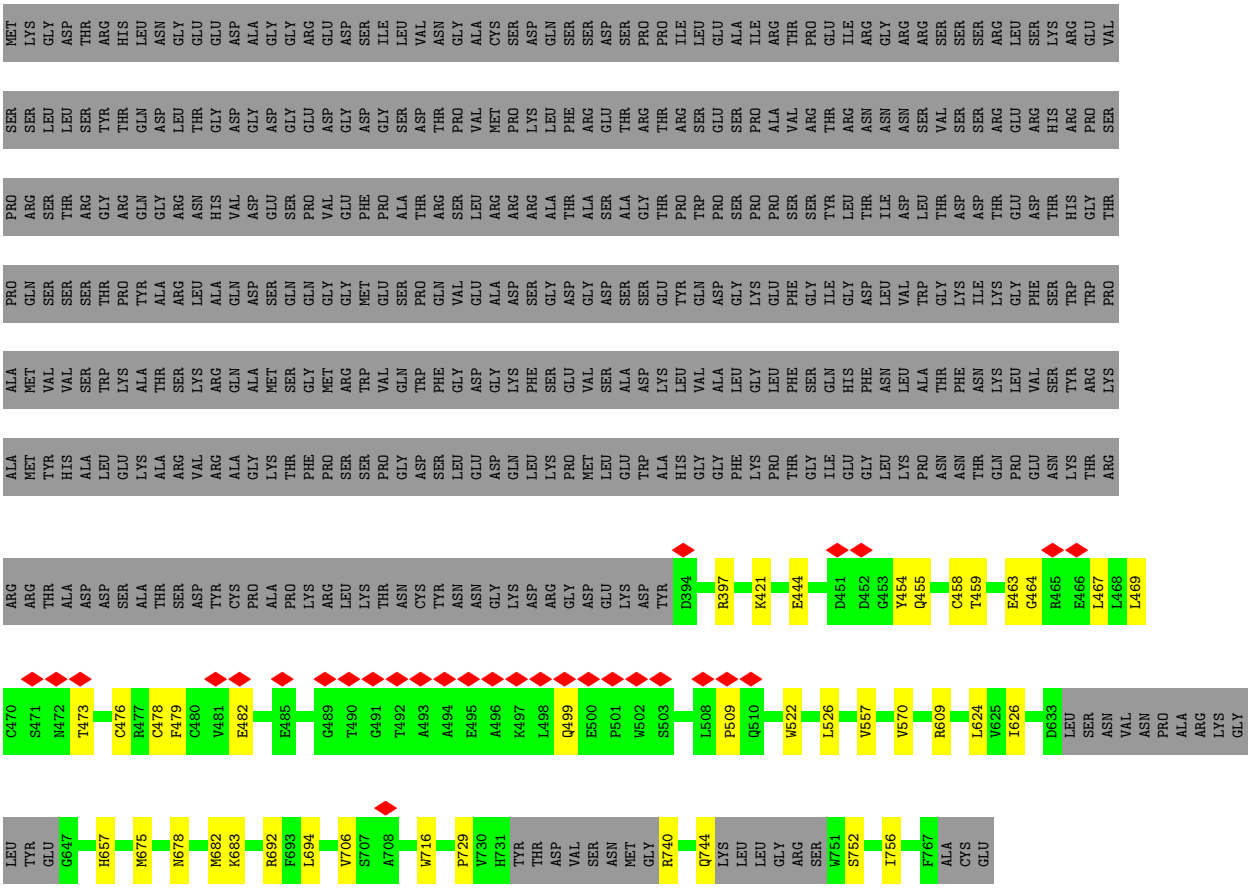
• Molecule 6: DNA (319-MER)

Chain J:



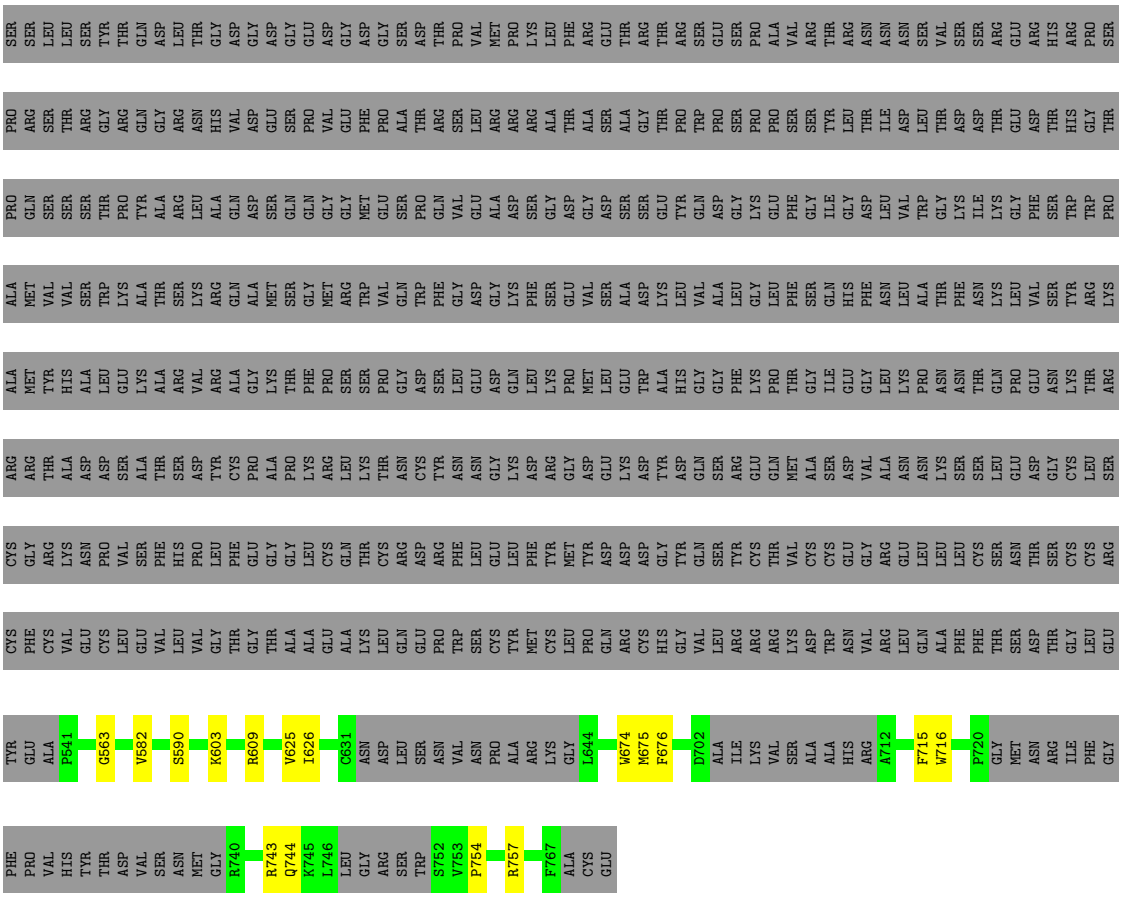
• Molecule 7: Isoform 3 of DNA (cytosine-5)-methyltransferase 3B

Chain V:



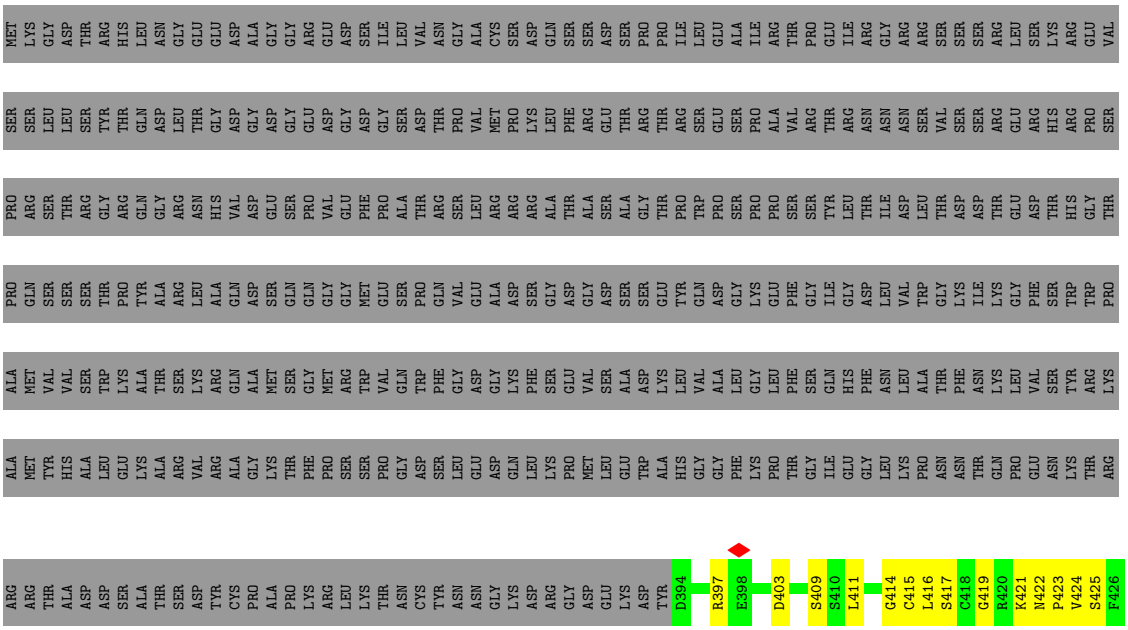
• Molecule 7: Isoform 3 of DNA (cytosine-5)-methyltransferase 3B

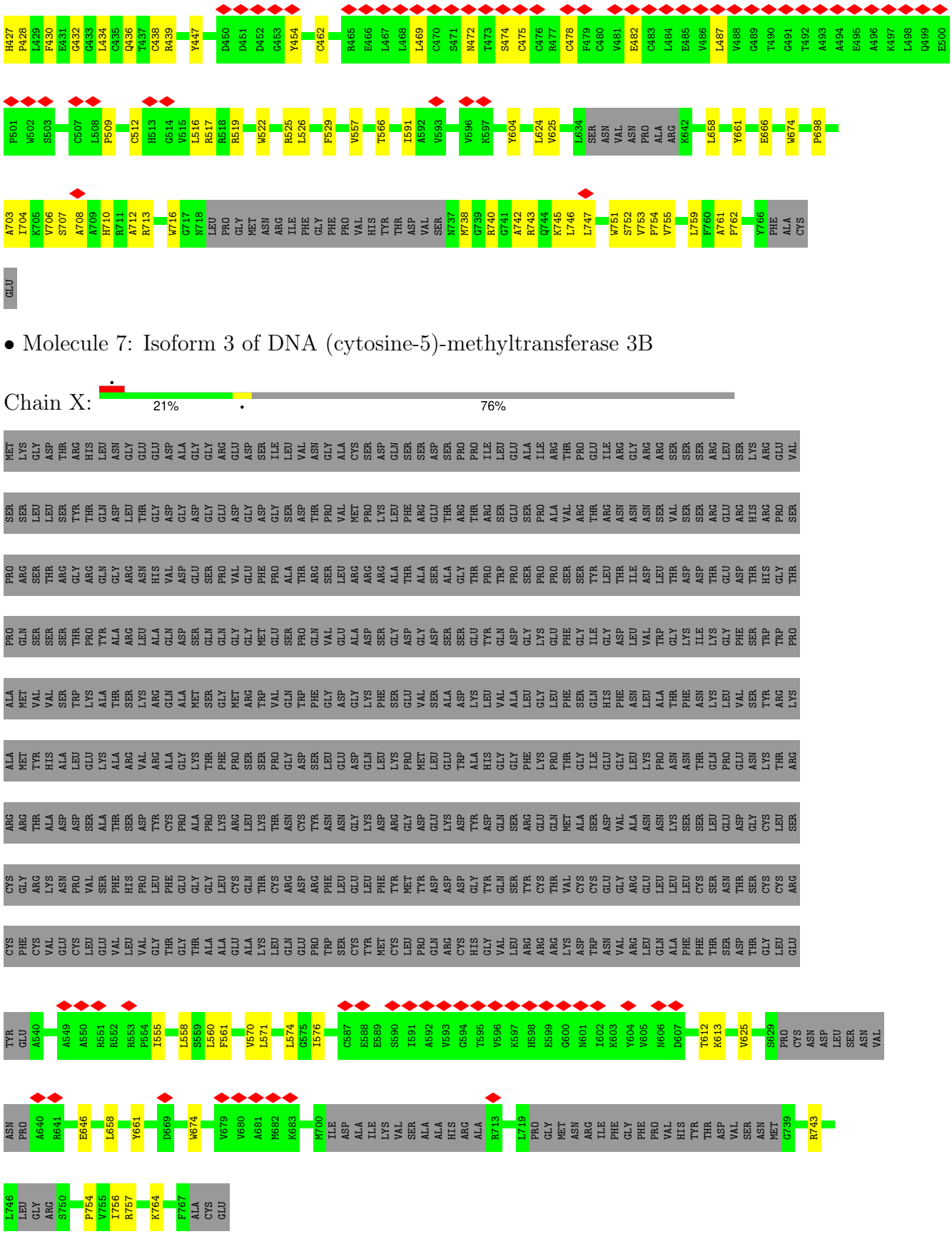
Chain Z:



• Molecule 7: Isoform 3 of DNA (cytosine-5)-methyltransferase 3B

Chain L:





• Molecule 7: Isoform 3 of DNA (cytosine-5)-methyltransferase 3B

Chain X: 21% 76%

• Molecule 8: DNA (cytosine-5)-methyltransferase 3A

Chain U: 52% 9% 38%

MET ASN ALA VAL GLU GLU ASN GLN GLY PRO GLY GLU SER GLN LYS VAL GLU GLU ALA SER PRO PRO ALA VAL GLN GLN PRO THR ASP PRO ALA SER PRO THR VAL ALA THR THR PRO GLU PRO VAL GLY SER ASP ALA GLY ASP LYS ASN ALA THR LYS ALA GLY ASP GLU PRO GLU

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

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

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

LYS PRO LYS VAL LYS GLU ILE ILE ASP GLU ARG THR R476 R484 I493 E505 L522 Q527 C537 V546 C557 F558 C559 L566 Q573 I576 Y584 L594 L595 W601 P602 S603 R604 M607 F608 V636 L637 S638 L639 F640 V649 Y660

S663 I681 V684 G685 D686 V687 R688 S689 V690 L703 V704 N711 I715 V716 N717 R720 L730 E733 L737 L754 V758 V759 A760 M761 G762 V763 D768 I769 F772 D781 A782 K783 H789 R790 A791 R792 T832 ILE THR THR ARG SER ASN

SER ILE LYS GLN GLY LYS ASP Q846 H847 F848 E856 W860 R891 S892 I898 L901 V912

• Molecule 8: DNA (cytosine-5)-methyltransferase 3A

Chain Y: 71% 9% 19%

MET ASN ALA VAL GLU GLU ASN GLN GLY PRO GLY GLU SER GLN LYS VAL GLU GLU ALA SER PRO PRO ALA VAL GLN GLN PRO THR ASP PRO ALA SER PRO THR VAL ALA THR THR PRO GLU PRO VAL GLY SER ASP ALA GLY ASP LYS ASN ALA THR LYS ALA GLY ASP ASP GLU PRO E9

F16 R35 R52 M55 L73 Y96 P111 VAL CYS HIS ASP SER ASP GLU SER ASP THR ALA LYS A124 N129 S143 G144 P145 L148 P151 GLU GLU GLU LYS ASN PRO TYR LYS GLU VAL TYR THR ASP MET TRP VAL GLU PRO GLU GLU ALA ALA ALA TYR

ALA PRO PRO PRO PRO ALA LYS LYS PRO ARG LYS SER THR ALA GLU LYS PRO LYS VAL LYS GLU ILE ILE ASP GLU ARG THR R476 R484 H506 M513 K518 N519 Y533 Q534 C537 V546 G550 C555 C559 L566 W581 K589 G590 T591 L594

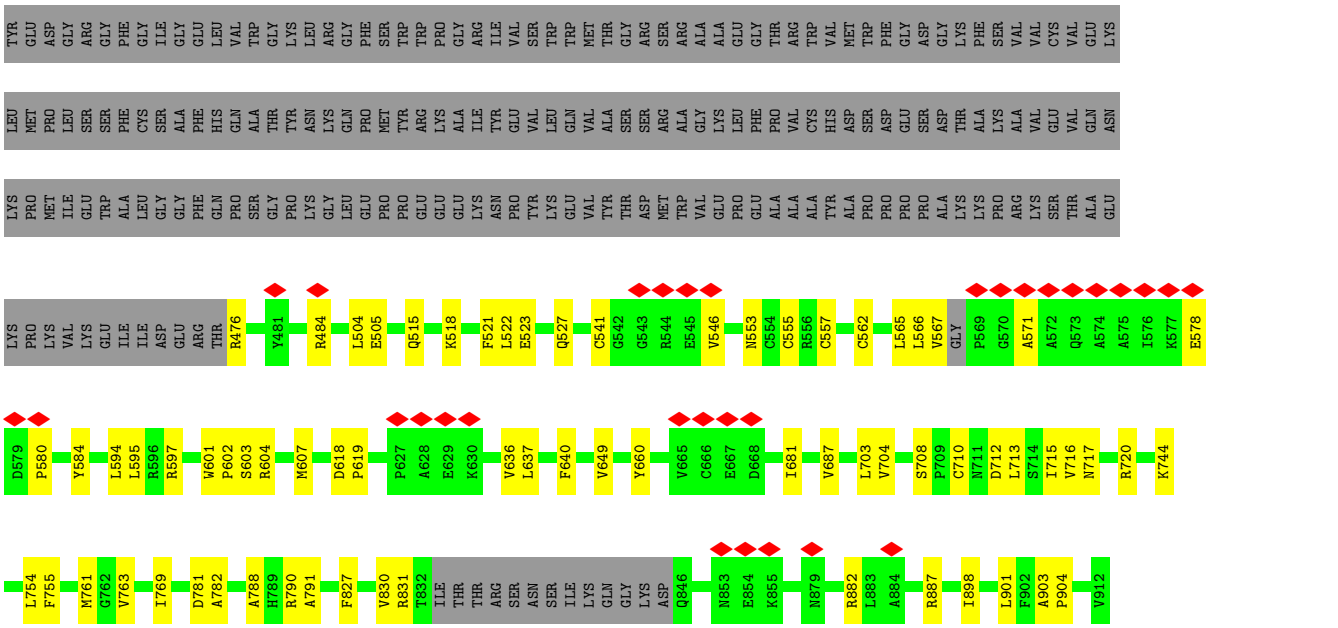
L595 R598 V636 L637 S638 L639 F640 D641 G642 I643 A644 S669 R676 L703 V704 F731 F734 M761 G762 V763 I769 S770 R771 P777 D781 A782 S786 A787 A788 H789 R790 A791 W795 K829 V830 R831 T832 ILE THR THR ARG SER ASN SER ILE LYS

GLN GLY LYS ASP Q846 R866 V867 F870 P871 V872 H873 S878 S892 V912

• Molecule 8: DNA (cytosine-5)-methyltransferase 3A

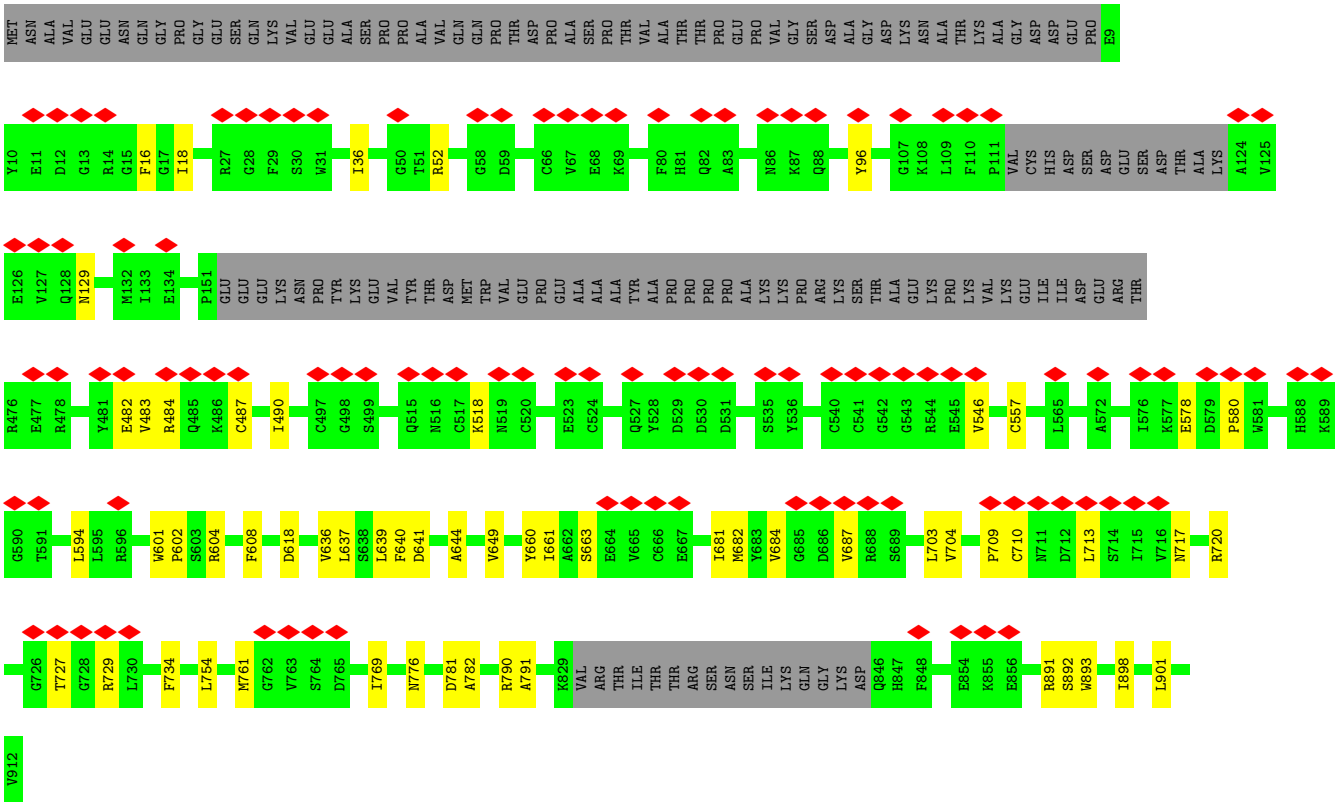
Chain W: 51% 10% 39%

MET ASN ALA VAL GLU GLU ASN GLN GLY PRO GLY GLU SER GLN LYS VAL GLU GLU ALA SER PRO PRO ALA VAL GLN GLN PRO THR ASP PRO ALA SER PRO THR VAL ALA THR THR PRO GLU PRO VAL GLY SER ASP ALA GLY ASP LYS ASN ALA THR LYS ALA GLY ASP ASP GLU PRO GLU



• Molecule 8: DNA (cytosine-5)-methyltransferase 3A

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44359	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	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: ZN, SAH

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	0.89	0/806	1.28	0/1081
1	E	0.90	0/814	1.26	0/1092
1	M	0.88	0/832	1.27	0/1115
1	Q	0.89	0/795	1.29	0/1066
2	B	0.89	0/640	1.25	0/857
2	F	0.90	0/629	1.28	0/843
2	N	0.90	0/629	1.25	0/843
2	R	0.90	0/629	1.24	0/843
3	C	0.90	0/773	1.24	0/1043
3	G	0.90	0/764	1.26	0/1031
3	O	0.90	0/764	1.26	0/1031
3	S	0.90	0/761	1.28	0/1027
4	D	0.92	0/730	1.34	0/983
4	H	0.92	0/730	1.35	0/983
4	P	0.92	0/719	1.35	0/969
4	T	0.93	0/730	1.36	0/983
5	I	0.27	0/7428	0.57	1/11471 (0.0%)
6	J	0.27	0/7290	0.53	1/11241 (0.0%)
7	L	0.98	0/2840	1.34	0/3830
7	V	0.97	0/2843	1.32	2/3837 (0.1%)
7	X	0.96	0/1532	1.27	0/2061
7	Z	0.95	0/1515	1.26	0/2041
8	K	0.96	0/4545	1.26	0/6142
8	U	0.96	0/3487	1.27	0/4712
8	W	0.96	0/3482	1.30	0/4703
8	Y	0.97	0/4570	1.25	0/6176
All	All	0.81	0/51277	1.11	4/72004 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	752	SER	CA-C-N	6.03	125.16	120.33
7	V	752	SER	C-N-CA	6.03	125.16	120.33
5	I	320	DA	C2'-C3'-O3'	-5.43	103.35	111.50
6	J	313	DG	C2'-C3'-O3'	-5.35	103.47	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	795	0	833	11	0
1	E	802	0	841	9	0
1	M	820	0	866	7	0
1	Q	785	0	826	13	0
2	B	633	0	673	9	0
2	F	622	0	660	9	0
2	N	622	0	660	14	0
2	R	622	0	660	7	0
3	C	764	0	808	17	0
3	G	755	0	800	12	0
3	O	755	0	800	9	0
3	S	752	0	796	13	0
4	D	719	0	740	10	0
4	H	719	0	740	6	0
4	P	708	0	727	7	0
4	T	719	0	740	12	0
5	I	6614	0	3597	52	0
6	J	6506	0	3578	36	0
7	L	2777	0	2711	93	0
7	V	2776	0	2696	35	0
7	X	1495	0	1504	18	0
7	Z	1478	0	1487	13	0
8	K	4426	0	4307	44	0
8	U	3404	0	3317	58	0
8	W	3400	0	3314	63	0
8	Y	4451	0	4336	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	3	0	0	0	0
9	L	3	0	0	0	0
9	U	3	0	0	0	0
9	V	3	0	0	0	0
9	W	3	0	0	0	0
9	Y	3	0	0	0	0
10	K	26	0	19	4	0
10	U	26	0	19	2	0
10	W	26	0	19	0	0
10	Y	26	0	19	1	0
All	All	49041	0	43093	529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (529) 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)
7:L:707:SER:HB2	7:L:746:LEU:HD23	1.25	1.16
7:L:713:ARG:NH2	7:L:752:SER:HB3	1.64	1.12
7:L:474:SER:HB3	7:L:708:ALA:HB1	1.45	0.97
8:K:639:LEU:HD12	8:K:734:PHE:CD1	1.98	0.97
7:L:415:CYS:O	7:L:419:GLY:HA2	1.64	0.96
7:L:425:SER:CB	7:L:439:ARG:HD2	1.98	0.94
7:L:474:SER:CB	7:L:708:ALA:HB1	1.98	0.93
8:U:687:VAL:HG13	8:U:737:LEU:HD12	1.52	0.91
8:U:759:VAL:HB	8:U:791:ALA:O	1.70	0.91
7:L:713:ARG:HH22	7:L:752:SER:HB3	1.33	0.90
7:L:428:PRO:HB3	7:L:525:ARG:HB3	1.52	0.90
7:L:707:SER:HB2	7:L:746:LEU:CD2	2.01	0.90
8:K:640:PHE:CE1	8:K:687:VAL:HG21	2.08	0.89
3:O:56:GLU:OE2	7:V:740:ARG:NH2	2.11	0.83
7:L:707:SER:CB	7:L:746:LEU:HD23	2.07	0.83
8:K:639:LEU:HD12	8:K:734:PHE:HD1	1.44	0.82
8:W:522:LEU:HB2	8:W:763:VAL:HG21	1.62	0.81
8:K:640:PHE:CZ	8:K:687:VAL:HG21	2.14	0.81
4:P:101:GLY:O	4:P:105:LYS:HG3	1.81	0.81
7:L:745:LYS:HD3	7:L:754:PRO:HD3	1.62	0.81
7:L:706:VAL:HG12	7:L:746:LEU:CD2	2.12	0.80
3:C:61:GLU:HB3	7:Z:743:ARG:HH21	1.47	0.79
7:L:706:VAL:HG12	7:L:746:LEU:HD21	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:44:GLN:OE1	7:V:740:ARG:NH1	2.14	0.79
6:J:4:DG:H8	8:W:887:ARG:NH1	1.80	0.79
8:W:522:LEU:HB3	8:W:763:VAL:CG2	2.13	0.79
8:W:522:LEU:HB3	8:W:763:VAL:HG22	1.65	0.78
7:L:425:SER:HB2	7:L:439:ARG:HD2	1.66	0.78
8:W:522:LEU:CB	8:W:763:VAL:CG2	2.62	0.77
8:U:758:VAL:HA	8:U:792:ARG:CD	2.15	0.77
8:U:687:VAL:CG1	8:U:733:GLU:HB3	2.14	0.77
7:L:472:ASN:HB3	7:L:475:CYS:HB3	1.67	0.77
7:L:713:ARG:HH21	7:L:752:SER:HB3	1.50	0.76
7:L:427:HIS:HB3	7:L:434:LEU:HD22	1.68	0.76
7:V:421:LYS:HD3	8:Y:143:SER:O	1.86	0.75
7:L:417:SER:HB3	7:L:438:CYS:SG	2.26	0.74
8:W:555:CYS:SG	8:W:831:ARG:NH1	2.60	0.74
5:I:315:DG:OP2	8:W:882:ARG:NH1	2.15	0.74
7:L:703:ALA:HB3	7:L:751:TRP:CZ3	2.23	0.74
8:W:640:PHE:CZ	8:W:687:VAL:HG21	2.23	0.74
3:O:61:GLU:OE2	7:V:744:GLN:NE2	2.20	0.73
7:L:474:SER:O	7:L:710:HIS:CE1	2.41	0.73
7:L:707:SER:CB	7:L:746:LEU:HB3	2.18	0.73
7:V:454:TYR:CD2	7:V:469:LEU:HD22	2.22	0.73
8:W:522:LEU:CB	8:W:763:VAL:HG21	2.18	0.73
2:N:49:LEU:HD11	7:V:499:GLN:NE2	2.04	0.73
7:X:560:LEU:HD11	7:X:658:LEU:HD22	1.71	0.72
3:G:90:ASP:OD1	7:L:743:ARG:NH1	2.23	0.72
8:Y:787:ALA:O	8:Y:829:LYS:HA	1.90	0.72
8:K:636:VAL:HA	8:K:703:LEU:O	1.91	0.71
8:W:603:SER:O	8:W:607:MET:HG3	1.91	0.71
8:Y:639:LEU:HD22	8:Y:734:PHE:CD1	2.25	0.71
8:Y:788:ALA:HA	8:Y:830:VAL:H	1.56	0.71
8:U:522:LEU:HD23	8:U:763:VAL:HB	1.74	0.70
8:W:640:PHE:CE1	8:W:687:VAL:HG21	2.27	0.70
5:I:2:DC:H4'	8:U:711:ASN:HD21	1.55	0.70
8:U:687:VAL:HG13	8:U:737:LEU:CD1	2.20	0.70
5:I:2:DC:H2"	5:I:3:DG:C8	2.27	0.69
7:L:411:LEU:HD11	7:L:432:GLY:H	1.56	0.69
8:U:758:VAL:HA	8:U:792:ARG:HD2	1.74	0.69
7:L:447:TYR:CE2	7:L:712:ALA:HB2	2.28	0.68
5:I:320:DA:H2"	5:I:321:DT:C5	2.29	0.68
7:L:447:TYR:CD2	7:L:712:ALA:HB2	2.29	0.68
8:W:527:GLN:HE21	8:W:715:ILE:HG13	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:484:ARG:HB3	8:W:594:LEU:HD11	1.76	0.67
7:L:428:PRO:CB	7:L:525:ARG:HB3	2.25	0.66
3:S:39:TYR:HB3	4:T:75:SER:HB2	1.78	0.66
8:Y:643:ILE:HD11	8:Y:892:SER:HB2	1.77	0.66
7:L:415:CYS:O	7:L:419:GLY:CA	2.42	0.66
8:W:527:GLN:NE2	8:W:715:ILE:HG13	2.11	0.65
8:U:603:SER:O	8:U:607:MET:HG2	1.96	0.65
8:K:640:PHE:CE1	8:K:687:VAL:CG2	2.79	0.65
7:L:474:SER:HB2	7:L:708:ALA:HB1	1.76	0.65
7:L:425:SER:HB3	7:L:439:ARG:HD2	1.78	0.64
8:W:527:GLN:HG2	8:W:715:ILE:HG23	1.79	0.64
7:L:713:ARG:HH22	7:L:752:SER:CB	2.10	0.64
7:L:522:TRP:HZ3	7:L:704:ILE:HD13	1.63	0.64
7:L:454:TYR:CD2	7:L:469:LEU:HD23	2.32	0.63
8:Y:643:ILE:HD11	8:Y:892:SER:CB	2.28	0.63
6:J:4:DG:H8	8:W:887:ARG:HH12	1.45	0.63
8:U:484:ARG:HB3	8:U:594:LEU:HD11	1.79	0.63
8:W:527:GLN:HA	8:W:716:VAL:HG12	1.80	0.63
8:K:636:VAL:HG22	8:K:703:LEU:HB3	1.80	0.63
8:U:759:VAL:CB	8:U:791:ALA:O	2.46	0.62
2:F:45:ARG:HE	5:I:90:DC:H4'	1.63	0.62
8:Y:788:ALA:HB2	8:Y:867:VAL:CG1	2.29	0.62
8:W:515:GLN:HA	8:W:518:LYS:HE2	1.81	0.62
8:Y:642:GLY:O	8:Y:669:SER:HB2	1.98	0.62
1:E:125:GLN:HG2	1:E:134:ARG:HH12	1.64	0.62
8:U:892:SER:HA	10:U:1004:SAH:C	2.30	0.62
3:S:32:ARG:NH1	6:J:40:DA:OP2	2.33	0.62
7:L:454:TYR:CG	7:L:469:LEU:HD23	2.34	0.62
7:L:430:PHE:O	7:L:519:ARG:NE	2.33	0.61
1:Q:68:GLN:HE21	1:Q:72:ARG:HH21	1.48	0.61
8:U:687:VAL:HG11	8:U:733:GLU:HB3	1.81	0.61
8:K:16:PHE:HB2	8:K:52:ARG:HE	1.64	0.61
5:I:2:DC:H4'	8:U:711:ASN:ND2	2.15	0.61
7:X:558:LEU:HD21	7:X:658:LEU:HD23	1.82	0.61
1:E:62:ILE:O	1:E:93:GLN:NE2	2.34	0.60
8:U:781:ASP:HA	8:U:791:ALA:HA	1.83	0.60
7:L:411:LEU:HD11	7:L:432:GLY:N	2.17	0.60
7:V:397:ARG:HH22	7:V:482:GLU:HG2	1.67	0.59
8:U:522:LEU:HD23	8:U:763:VAL:CB	2.32	0.59
8:K:663:SER:HA	8:K:684:VAL:HB	1.84	0.59
4:D:68:GLU:OE1	2:F:91:LYS:NZ	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:707:SER:OG	7:L:746:LEU:HB3	2.02	0.59
3:C:57:TYR:OH	7:Z:743:ARG:HB2	2.03	0.59
3:S:35:ARG:NH2	5:I:277:DA:OP2	2.36	0.58
7:X:754:PRO:HA	7:X:757:ARG:HG2	1.85	0.58
8:W:476:ARG:HH11	8:W:565:LEU:HD23	1.68	0.58
8:K:637:LEU:HB3	8:K:704:VAL:HG22	1.84	0.58
1:A:68:GLN:HE21	1:A:72:ARG:HH21	1.51	0.58
1:Q:46:VAL:HG21	5:I:247:DT:H3'	1.86	0.58
3:G:57:TYR:HE1	7:L:740:ARG:O	1.86	0.58
8:W:515:GLN:HA	8:W:518:LYS:CE	2.34	0.57
8:Y:534:GLN:HG3	8:Y:555:CYS:O	2.04	0.57
7:X:625:VAL:O	7:X:674:TRP:HA	2.04	0.57
8:K:641:ASP:OD1	8:K:644:ALA:HA	2.05	0.57
7:L:428:PRO:HA	7:L:519:ARG:HD2	1.87	0.57
7:L:474:SER:O	7:L:710:HIS:HE1	1.88	0.57
7:X:646:GLU:HB3	8:K:729:ARG:HH22	1.69	0.57
8:U:783:LYS:HD3	8:U:789:HIS:CD2	2.40	0.57
7:L:487:LEU:HD13	7:L:516:LEU:HB2	1.86	0.57
7:V:464:GLY:HA2	7:V:467:LEU:HD11	1.87	0.56
7:L:707:SER:HB3	7:L:751:TRP:HZ2	1.69	0.56
8:U:687:VAL:HG12	8:U:733:GLU:HB3	1.85	0.56
8:W:636:VAL:HG22	8:W:703:LEU:HB3	1.88	0.56
1:Q:60:LEU:O	1:Q:63:ARG:NH2	2.38	0.56
8:Y:782:ALA:O	8:Y:786:SER:OG	2.18	0.56
8:Y:782:ALA:HB3	8:Y:790:ARG:HB3	1.87	0.56
7:L:755:VAL:HG12	7:L:759:LEU:HD12	1.88	0.56
8:W:562:CYS:O	8:W:566:LEU:HG	2.06	0.56
1:A:42:ARG:NH1	5:I:154:DC:OP1	2.39	0.56
8:Y:589:LYS:NZ	8:Y:591:THR:OG1	2.38	0.56
7:L:707:SER:HB2	7:L:746:LEU:HB3	1.88	0.56
7:V:459:THR:HB	7:V:479:PHE:CE1	2.41	0.55
8:Y:639:LEU:HD12	8:Y:639:LEU:N	2.21	0.55
7:L:422:ASN:N	7:L:423:PRO:HD3	2.21	0.55
2:B:92:ARG:HH21	4:D:98:LEU:HD23	1.72	0.55
3:C:65:LEU:HD21	7:Z:744:GLN:OE1	2.07	0.55
1:Q:62:ILE:O	1:Q:93:GLN:NE2	2.40	0.55
4:D:100:PRO:HD2	4:D:103:LEU:HD23	1.88	0.55
7:L:424:VAL:HB	7:L:436:GLN:HB2	1.89	0.55
8:U:684:VAL:HG12	8:U:685:GLY:N	2.22	0.55
8:W:566:LEU:HD13	8:W:595:LEU:HD22	1.88	0.55
8:W:636:VAL:HA	8:W:703:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:116:ARG:NH1	1:Q:118:THR:O	2.40	0.54
7:V:626:ILE:HA	7:V:675:MET:O	2.07	0.54
7:L:746:LEU:HD12	7:L:746:LEU:N	2.23	0.54
8:K:637:LEU:O	8:K:704:VAL:HA	2.07	0.54
2:N:49:LEU:CD1	7:V:499:GLN:NE2	2.70	0.54
8:Y:550:GLY:N	8:Y:581:TRP:O	2.39	0.54
8:K:754:LEU:HD11	8:K:901:LEU:HD13	1.88	0.54
7:V:692:ARG:HG3	8:U:688:ARG:HD2	1.90	0.54
7:L:428:PRO:CB	7:L:525:ARG:CB	2.85	0.54
8:W:578:GLU:HG2	8:W:580:PRO:HD2	1.90	0.54
1:A:133:GLU:OE2	2:B:95:ARG:NH1	2.34	0.54
6:J:4:DG:C8	8:W:887:ARG:NH1	2.69	0.54
7:L:403:ASP:HB3	7:L:409:SER:HB3	1.89	0.54
7:L:591:ILE:HD13	7:L:604:TYR:HB2	1.90	0.54
8:K:892:SER:HA	10:K:1004:SAH:OXT	2.08	0.54
5:I:231:DG:H2"	5:I:232:DG:C8	2.43	0.54
3:C:54:VAL:HG21	4:D:95:VAL:HG21	1.89	0.53
1:E:60:LEU:O	1:E:63:ARG:NH2	2.41	0.53
7:L:417:SER:CB	7:L:438:CYS:SG	2.94	0.53
8:K:482:GLU:HB3	8:K:487:CYS:HB2	1.89	0.53
1:A:60:LEU:O	1:A:63:ARG:NH2	2.41	0.53
8:K:483:VAL:HG11	8:K:490:ILE:HD13	1.90	0.53
2:F:51:TYR:HB3	2:F:55:ARG:HH12	1.72	0.53
8:Y:761:MET:HE1	8:Y:769:ILE:HD12	1.90	0.53
7:L:625:VAL:O	7:L:674:TRP:HA	2.07	0.53
8:Y:676:ARG:NH2	8:Y:873:HIS:O	2.42	0.53
3:G:35:ARG:NH2	5:I:122:DA:OP2	2.40	0.53
3:G:54:VAL:HG21	4:H:95:VAL:HG21	1.89	0.53
7:V:421:LYS:CE	8:Y:145:PRO:HD2	2.39	0.53
1:E:116:ARG:NH1	1:E:118:THR:O	2.42	0.53
8:Y:781:ASP:HA	8:Y:791:ALA:HA	1.91	0.53
7:L:706:VAL:CG1	7:L:746:LEU:HD21	2.35	0.53
8:K:892:SER:HA	10:K:1004:SAH:C	2.38	0.53
8:W:522:LEU:HB2	8:W:763:VAL:CG2	2.29	0.53
7:L:707:SER:HB3	7:L:751:TRP:CZ2	2.44	0.52
1:A:62:ILE:O	1:A:93:GLN:NE2	2.42	0.52
7:L:397:ARG:HG3	7:L:416:LEU:HD23	1.91	0.52
8:W:618:ASP:OD1	8:W:619:PRO:HD2	2.09	0.52
8:U:684:VAL:HG11	8:U:690:VAL:HG22	1.89	0.52
6:J:36:DC:H2"	6:J:37:DT:C5	2.45	0.52
8:U:754:LEU:HD11	8:U:901:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:513:MET:HE2	8:Y:518:LYS:HA	1.91	0.52
8:W:754:LEU:HD11	8:W:901:LEU:HD13	1.91	0.52
8:W:637:LEU:HB3	8:W:704:VAL:HG22	1.92	0.52
5:I:290:DC:H4'	5:I:291:DC:OP1	2.09	0.52
1:A:69:ARG:NH2	6:J:256:DA:OP1	2.40	0.52
8:W:522:LEU:HD13	8:W:763:VAL:CG1	2.39	0.52
8:W:567:VAL:HG21	8:W:571:ALA:HB3	1.92	0.52
8:W:604:ARG:HA	8:W:607:MET:CE	2.40	0.52
6:J:320:DG:H2"	6:J:321:DA:N7	2.24	0.51
7:V:694:LEU:HD22	7:V:716:TRP:HB3	1.92	0.51
7:L:522:TRP:CZ3	7:L:704:ILE:HD13	2.44	0.51
7:L:738:MET:O	7:L:738:MET:HG3	2.10	0.51
8:W:527:GLN:CG	8:W:715:ILE:HG23	2.39	0.51
8:K:604:ARG:O	8:K:608:PHE:HB2	2.10	0.51
2:N:59:LYS:NZ	2:N:63:GLU:OE2	2.44	0.51
3:G:30:VAL:HG13	4:H:67:PHE:HE1	1.76	0.51
7:L:666:GLU:HB2	8:W:744:LYS:HD3	1.91	0.51
7:L:522:TRP:O	7:L:526:LEU:HB2	2.10	0.51
8:U:687:VAL:CG1	8:U:737:LEU:HD12	2.34	0.51
7:L:755:VAL:HG12	7:L:759:LEU:CD1	2.39	0.51
7:L:469:LEU:HG	7:L:478:CYS:SG	2.51	0.51
8:Y:643:ILE:HD11	8:Y:870:PHE:CZ	2.47	0.50
8:U:636:VAL:HG22	8:U:703:LEU:HB3	1.92	0.50
8:Y:787:ALA:HA	8:Y:829:LYS:NZ	2.26	0.50
3:C:65:LEU:HD11	7:Z:744:GLN:HE22	1.77	0.50
3:G:63:LEU:HD22	4:H:42:LEU:HD13	1.92	0.50
8:U:522:LEU:CD2	8:U:763:VAL:HG23	2.41	0.50
8:Y:637:LEU:O	8:Y:704:VAL:HA	2.12	0.50
3:C:20:ARG:NH2	5:I:41:DG:OP1	2.44	0.50
8:Y:643:ILE:CD1	8:Y:892:SER:CB	2.88	0.50
7:L:747:LEU:C	7:L:747:LEU:HD23	2.36	0.50
2:N:51:TYR:HB3	2:N:55:ARG:HH12	1.75	0.50
8:U:636:VAL:HA	8:U:703:LEU:O	2.11	0.50
7:L:713:ARG:NH2	7:L:752:SER:CB	2.56	0.50
1:A:116:ARG:NH1	1:A:118:THR:O	2.45	0.50
1:M:106:ASP:OD2	1:M:131:ARG:NH2	2.45	0.50
3:O:42:ARG:HG2	6:J:123:DA:H5'	1.94	0.50
5:I:4:DG:N2	6:J:319:DC:O2	2.44	0.50
7:L:397:ARG:HH22	7:L:482:GLU:HB3	1.76	0.50
5:I:23:DA:H2"	5:I:24:DT:H5"	1.94	0.49
6:J:103:DC:H2"	6:J:104:DG:H5"	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:676:PHE:HB3	7:Z:716:TRP:HB2	1.94	0.49
8:U:759:VAL:CG1	8:U:791:ALA:O	2.60	0.49
6:J:130:DA:H2"	6:J:131:DG:C8	2.47	0.49
8:U:758:VAL:HA	8:U:792:ARG:HD3	1.92	0.49
7:L:462:CYS:O	7:L:462:CYS:SG	2.70	0.49
6:J:9:DC:H2'	6:J:10:DC:C6	2.47	0.49
1:M:61:LEU:HD13	2:N:36:ARG:HB3	1.94	0.49
8:U:637:LEU:HB3	8:U:704:VAL:HG22	1.94	0.49
8:U:663:SER:OG	8:U:685:GLY:O	2.27	0.49
8:U:608:PHE:C	8:U:608:PHE:CD2	2.91	0.49
7:L:512:CYS:SG	7:L:517:ARG:HG2	2.53	0.49
8:W:504:LEU:HG	8:W:505:GLU:O	2.13	0.49
7:Z:563:GLY:HA3	7:Z:590:SER:HB3	1.95	0.49
8:Y:636:VAL:HG22	8:Y:703:LEU:HB3	1.95	0.49
8:K:761:MET:HE1	8:K:769:ILE:HD12	1.95	0.49
3:O:54:VAL:HG21	4:P:95:VAL:HG21	1.95	0.49
3:G:57:TYR:CE1	7:L:740:ARG:O	2.66	0.48
1:Q:46:VAL:HG22	1:Q:49:ARG:HH21	1.78	0.48
2:B:51:TYR:HB3	2:B:55:ARG:HH12	1.79	0.48
3:C:57:TYR:HE2	4:D:103:LEU:HD12	1.78	0.48
8:W:717:ASN:HB3	8:W:720:ARG:HB3	1.96	0.48
6:J:232:DG:H2"	6:J:233:DT:C5	2.49	0.48
8:U:761:MET:HE1	8:U:769:ILE:HD12	1.96	0.48
8:W:761:MET:HE1	8:W:769:ILE:HD12	1.95	0.48
7:V:522:TRP:O	7:V:526:LEU:HB2	2.13	0.48
7:X:571:LEU:HD22	7:X:576:ILE:HD11	1.96	0.48
7:V:444:GLU:HG2	7:V:683:LYS:HA	1.96	0.48
7:L:411:LEU:HD23	7:L:411:LEU:C	2.38	0.48
7:L:746:LEU:HG	7:L:751:TRP:CZ2	2.48	0.48
7:X:574:LEU:HD21	7:X:757:ARG:HB2	1.95	0.48
1:Q:61:LEU:HD13	2:R:36:ARG:HB3	1.94	0.48
3:S:16:THR:HA	6:J:41:DT:H5"	1.95	0.48
1:A:101:VAL:HG21	2:B:40:ARG:HD2	1.95	0.47
8:W:566:LEU:HD22	8:W:595:LEU:HD13	1.95	0.47
8:U:717:ASN:HB3	8:U:720:ARG:HB3	1.96	0.47
2:N:92:ARG:HH11	4:P:98:LEU:HD23	1.78	0.47
5:I:29:DC:H2"	5:I:30:DA:C8	2.49	0.47
8:W:553:ASN:OD1	8:W:827:PHE:CD1	2.67	0.47
8:W:710:CYS:HA	8:W:713:LEU:HB2	1.96	0.47
7:L:428:PRO:HB2	7:L:525:ARG:HB2	1.97	0.47
8:K:717:ASN:HB3	8:K:720:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:59:LYS:HD3	7:L:509:PRO:HB3	1.97	0.47
6:J:46:DC:H2"	6:J:47:DG:C8	2.49	0.47
7:Z:582:VAL:HG22	7:Z:603:LYS:HB2	1.96	0.47
8:Y:533:TYR:HA	8:Y:555:CYS:HB3	1.95	0.47
8:W:523:GLU:O	8:W:715:ILE:HG21	2.12	0.47
8:K:484:ARG:HB3	8:K:594:LEU:HD11	1.95	0.47
3:S:64:GLU:HA	4:T:46:HIS:HE1	1.79	0.47
5:I:184:DC:H2"	5:I:185:DA:C8	2.50	0.47
8:U:860:TRP:CE2	8:Y:878:SER:HA	2.49	0.47
1:E:61:LEU:HD13	2:F:36:ARG:HB3	1.97	0.46
5:I:319:DG:H2"	5:I:320:DA:H8	1.79	0.46
7:V:706:VAL:HA	7:V:729:PRO:HG2	1.98	0.46
7:L:427:HIS:HB3	7:L:434:LEU:CD2	2.42	0.46
8:W:708:SER:H	8:W:755:PHE:HE1	1.63	0.46
7:Z:626:ILE:HB	7:Z:675:MET:HE3	1.96	0.46
8:U:566:LEU:HB3	8:U:595:LEU:HB2	1.96	0.46
8:Y:506:HIS:O	8:Y:598:ARG:NE	2.49	0.46
8:W:522:LEU:CD1	8:W:763:VAL:HG21	2.46	0.46
3:G:25:PHE:CE2	4:H:41:VAL:HG21	2.51	0.46
4:T:103:LEU:HD23	7:X:743:ARG:HD2	1.96	0.46
6:J:285:DA:H2"	6:J:286:DG:C8	2.50	0.46
3:C:25:PHE:CE2	4:D:41:VAL:HG21	2.50	0.46
5:I:273:DT:H2"	5:I:274:DA:C8	2.51	0.46
6:J:201:DC:H2"	6:J:202:DG:C8	2.50	0.46
7:V:609:ARG:NH2	8:U:768:ASP:OD1	2.48	0.46
8:K:781:ASP:HA	8:K:791:ALA:HA	1.96	0.46
8:U:505:GLU:OE1	8:U:604:ARG:NH1	2.49	0.46
3:C:31:HIS:HD2	3:C:48:PRO:HG3	1.80	0.46
3:O:17:ARG:HH21	3:O:28:GLY:HA2	1.81	0.46
6:J:112:DG:H2"	6:J:113:DA:H5"	1.98	0.46
6:J:191:DC:H2"	6:J:192:DT:C5	2.51	0.46
7:V:458:CYS:HB3	7:V:463:GLU:H	1.80	0.46
3:C:17:ARG:HH21	3:C:28:GLY:HA2	1.81	0.46
8:Y:484:ARG:HB3	8:Y:594:LEU:HD11	1.97	0.46
7:L:427:HIS:CB	7:L:434:LEU:HD22	2.44	0.46
8:W:504:LEU:HG	8:W:505:GLU:N	2.30	0.46
3:S:25:PHE:CE2	4:T:41:VAL:HG21	2.51	0.46
6:J:41:DT:H2'	6:J:42:DT:H71	1.98	0.46
7:V:467:LEU:HA	7:V:479:PHE:O	2.16	0.46
7:V:570:VAL:HG11	7:V:756:ILE:HG22	1.98	0.46
7:V:692:ARG:HG3	8:U:688:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:609:ARG:HD2	8:Y:771:ARG:HG3	1.97	0.46
8:W:546:VAL:HB	8:W:557:CYS:HB3	1.98	0.46
4:P:99:LEU:HB2	4:P:104:ALA:HB2	1.98	0.46
3:S:54:VAL:HG21	4:T:95:VAL:HG21	1.98	0.46
8:Y:777:PRO:HB3	8:Y:795:TRP:CE2	2.51	0.46
7:L:707:SER:HB2	7:L:746:LEU:CB	2.45	0.46
6:J:267:DG:H2"	6:J:268:DA:H5"	1.98	0.45
7:L:753:VAL:N	7:L:754:PRO:HD2	2.32	0.45
8:W:782:ALA:HB3	8:W:790:ARG:HB3	1.99	0.45
6:J:258:DC:H2"	6:J:259:DG:H5"	1.99	0.45
7:Z:754:PRO:HA	7:Z:757:ARG:HG2	1.98	0.45
8:Y:35:ARG:HD3	8:Y:55:MET:HE2	1.97	0.45
7:L:746:LEU:N	7:L:746:LEU:CD1	2.80	0.45
4:D:79:HIS:CE1	3:G:38:ASN:HD22	2.34	0.45
8:Y:639:LEU:HD22	8:Y:734:PHE:HD1	1.80	0.45
4:T:103:LEU:CD2	7:X:743:ARG:NE	2.79	0.45
7:Z:625:VAL:O	7:Z:674:TRP:HA	2.17	0.45
8:W:527:GLN:HE21	8:W:715:ILE:CG1	2.25	0.45
2:N:30:THR:HG21	5:I:225:DA:H5"	1.99	0.45
5:I:138:DC:H2"	5:I:139:DG:C8	2.51	0.45
8:Y:788:ALA:CB	8:Y:830:VAL:HB	2.46	0.45
7:L:397:ARG:HG3	7:L:416:LEU:CD2	2.47	0.45
8:U:546:VAL:HB	8:U:557:CYS:HB3	1.97	0.45
7:L:704:ILE:HG13	7:L:710:HIS:CD2	2.51	0.45
1:E:101:VAL:HG21	2:F:40:ARG:HD2	1.99	0.45
2:N:90:LEU:HB3	2:N:95:ARG:HB2	1.98	0.45
5:I:26:DT:H2"	5:I:27:DG:C8	2.52	0.45
8:U:566:LEU:HD13	8:U:595:LEU:HD13	1.99	0.45
8:U:640:PHE:CZ	8:U:730:LEU:HB3	2.52	0.45
7:L:447:TYR:CD2	7:L:712:ALA:CB	2.99	0.45
8:W:523:GLU:O	8:W:715:ILE:HG12	2.17	0.45
4:H:37:TYR:OH	5:I:131:DG:OP1	2.31	0.44
1:Q:101:VAL:HG21	2:R:40:ARG:HD2	1.99	0.44
5:I:253:DT:H2"	5:I:254:DA:N7	2.32	0.44
8:K:782:ALA:HB3	8:K:790:ARG:HB3	2.00	0.44
3:G:61:GLU:OE2	7:L:743:ARG:NH2	2.50	0.44
5:I:200:DA:H2"	5:I:201:DG:C8	2.52	0.44
1:M:62:ILE:O	1:M:93:GLN:NE2	2.49	0.44
3:S:78:ILE:HD12	4:T:42:LEU:HD11	1.99	0.44
1:A:100:LEU:HD11	2:B:58:LEU:HD22	1.99	0.44
5:I:230:DG:H2"	5:I:231:DG:H5"	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:421:LYS:HE2	8:Y:145:PRO:HD2	1.99	0.44
8:K:639:LEU:CD1	8:K:734:PHE:HD1	2.23	0.44
1:A:41:TYR:OH	6:J:172:DA:H5"	2.18	0.44
3:C:79:ILE:HG22	3:C:81:ARG:H	1.81	0.44
3:C:87:VAL:HG13	3:C:93:LEU:HB3	1.97	0.44
5:I:36:DC:H2"	5:I:37:DT:C5	2.53	0.44
7:L:566:THR:HG21	7:L:753:VAL:HA	1.99	0.44
1:M:108:ASN:ND2	2:N:42:GLY:O	2.51	0.44
2:N:59:LYS:HD3	7:V:509:PRO:HB3	1.99	0.44
7:X:658:LEU:HA	7:X:661:TYR:HD2	1.82	0.44
2:F:56:GLY:HA2	7:L:509:PRO:HB2	2.00	0.44
5:I:2:DC:H5'	8:U:711:ASN:OD1	2.18	0.44
5:I:69:DA:H2"	5:I:70:DA:C8	2.53	0.44
7:V:557:VAL:HA	7:V:624:LEU:O	2.17	0.44
8:U:537:CYS:HB2	8:U:559:CYS:HB3	1.99	0.44
7:X:574:LEU:HD22	7:X:764:LYS:HD2	2.00	0.44
8:K:546:VAL:HB	8:K:557:CYS:HB3	1.99	0.44
8:K:710:CYS:HA	8:K:713:LEU:HB2	1.98	0.44
3:S:95:LYS:HD2	4:T:100:PRO:HB3	2.00	0.44
6:J:233:DT:H2"	6:J:234:DA:C8	2.53	0.44
7:L:526:LEU:O	7:L:529:PHE:HB3	2.17	0.44
3:C:87:VAL:HG11	3:C:97:LEU:HD12	2.00	0.43
4:H:35:ALA:HA	4:H:56:MET:SD	2.58	0.43
1:Q:100:LEU:HD11	2:R:58:LEU:HD22	1.99	0.43
5:I:132:DC:H2"	5:I:133:DG:C8	2.52	0.43
7:L:557:VAL:HG22	7:L:624:LEU:HB3	1.99	0.43
7:X:570:VAL:HG21	7:X:756:ILE:HB	2.00	0.43
8:W:604:ARG:HA	8:W:607:MET:HE3	1.99	0.43
4:D:35:ALA:HA	4:D:56:MET:SD	2.58	0.43
1:M:48:LEU:HA	1:M:51:ILE:HD12	2.01	0.43
8:U:522:LEU:HD23	8:U:763:VAL:CG2	2.48	0.43
8:U:558:PHE:HE2	8:U:584:TYR:H	1.66	0.43
8:U:601:TRP:CG	8:U:602:PRO:HD3	2.53	0.43
8:Y:641:ASP:CG	8:Y:644:ALA:HA	2.42	0.43
7:L:428:PRO:HA	7:L:519:ARG:CD	2.48	0.43
7:X:555:ILE:HG13	7:X:576:ILE:HD12	2.00	0.43
8:K:518:LYS:HG3	8:K:608:PHE:HZ	1.81	0.43
8:K:660:TYR:HB3	8:K:681:ILE:HD12	1.99	0.43
2:B:31:LYS:HB3	2:B:32:PRO:HD3	2.00	0.43
3:O:85:LEU:O	3:O:89:ASN:ND2	2.52	0.43
5:I:232:DG:H2"	5:I:233:DG:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:48:DT:H2"	6:J:49:DA:C8	2.53	0.43
6:J:119:DC:H2"	6:J:120:DC:C5	2.53	0.43
7:V:421:LYS:CE	8:Y:144:GLY:HA3	2.49	0.43
7:V:626:ILE:HG22	7:V:675:MET:HB3	2.00	0.43
8:W:781:ASP:HA	8:W:791:ALA:HA	2.00	0.43
2:B:92:ARG:NH2	4:D:98:LEU:HA	2.32	0.43
5:I:178:DA:H2"	5:I:179:DT:H5"	1.99	0.43
6:J:38:DC:H2"	6:J:39:DA:C8	2.54	0.43
6:J:274:DC:H2"	6:J:275:DC:C5	2.53	0.43
8:Y:639:LEU:N	8:Y:639:LEU:CD1	2.82	0.43
8:Y:782:ALA:HB1	8:Y:786:SER:OG	2.18	0.43
7:X:612:THR:HG22	7:X:613:LYS:N	2.34	0.43
3:S:63:LEU:HD22	4:T:42:LEU:HD12	1.99	0.43
7:V:454:TYR:CG	7:V:469:LEU:HD22	2.53	0.43
8:U:660:TYR:HB3	8:U:681:ILE:HD12	1.99	0.43
3:G:44:GLY:HA2	5:I:121:DG:H5"	2.01	0.43
5:I:293:DC:H2"	5:I:294:DG:C8	2.53	0.43
6:J:243:DC:H2"	6:J:244:DC:C5	2.54	0.43
8:Y:641:ASP:OD2	8:Y:644:ALA:HA	2.18	0.43
8:Y:731:PHE:O	8:Y:734:PHE:HB3	2.19	0.43
7:L:703:ALA:HB1	7:L:706:VAL:CG2	2.48	0.43
5:I:316:DG:H4'	5:I:317:DC:OP1	2.18	0.43
5:I:321:DT:H2"	8:W:712:ASP:OD2	2.19	0.43
7:L:414:GLY:HA2	7:L:421:LYS:HA	2.01	0.43
7:L:428:PRO:HB2	7:L:525:ARG:CB	2.49	0.43
7:L:742:ALA:O	7:L:746:LEU:HD13	2.19	0.43
8:W:584:TYR:O	8:W:597:ARG:NH1	2.52	0.43
8:K:661:ILE:HG13	8:K:682:MET:HB2	2.00	0.43
2:R:78:ARG:NH1	2:R:80:THR:O	2.52	0.43
3:S:81:ARG:NH1	3:S:105:GLY:O	2.47	0.43
8:Y:546:VAL:HA	8:Y:559:CYS:HA	2.00	0.43
8:W:788:ALA:HA	8:W:830:VAL:H	1.84	0.43
8:K:709:PRO:HG2	8:K:727:THR:HB	2.00	0.43
2:F:64:ASN:HB3	2:F:93:GLN:HE22	1.83	0.42
3:O:31:HIS:HD2	3:O:48:PRO:HG3	1.84	0.42
7:V:455:GLN:O	7:V:478:CYS:SG	2.66	0.42
7:V:678:ASN:HD21	7:V:682:MET:HE3	1.84	0.42
8:K:649:VAL:HG11	8:K:898:ILE:HG22	1.99	0.42
2:N:59:LYS:CD	7:V:509:PRO:HB3	2.49	0.42
7:V:473:THR:HA	7:V:476:CYS:SG	2.59	0.42
8:W:604:ARG:N	8:W:607:MET:HE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:660:TYR:HB3	8:W:681:ILE:HD12	2.01	0.42
8:K:482:GLU:O	8:K:487:CYS:N	2.51	0.42
3:C:63:LEU:HD22	4:D:42:LEU:HD13	2.02	0.42
6:J:68:DT:H2"	6:J:69:DA:N7	2.34	0.42
1:M:60:LEU:O	1:M:63:ARG:NH2	2.52	0.42
8:Y:787:ALA:HA	8:Y:829:LYS:HZ3	1.85	0.42
7:L:747:LEU:HD23	7:L:747:LEU:O	2.19	0.42
7:X:646:GLU:HB3	8:K:729:ARG:NH2	2.34	0.42
8:K:601:TRP:CG	8:K:602:PRO:HD3	2.54	0.42
2:B:78:ARG:NH1	2:B:80:THR:O	2.53	0.42
8:U:783:LYS:HB3	8:U:789:HIS:HA	2.01	0.42
3:C:64:GLU:CD	7:Z:744:GLN:HG3	2.44	0.42
7:V:657:HIS:CE1	8:U:772:PHE:HD1	2.36	0.42
7:L:428:PRO:HG3	7:L:525:ARG:O	2.20	0.42
1:E:68:GLN:HE21	1:E:72:ARG:HH21	1.67	0.42
5:I:98:DT:H2"	5:I:99:DA:C8	2.55	0.42
6:J:109:DG:H2"	6:J:110:DG:N7	2.35	0.42
6:J:203:DT:H2"	6:J:204:DA:C8	2.54	0.42
7:X:561:PHE:O	7:X:561:PHE:CG	2.72	0.42
3:O:39:TYR:HB3	4:P:75:SER:HB2	2.02	0.42
4:T:69:ARG:HB3	4:T:98:LEU:HD13	2.02	0.42
7:Z:675:MET:HG2	7:Z:715:PHE:HE1	1.85	0.42
1:E:61:LEU:HD22	2:F:36:ARG:HD2	2.02	0.42
6:J:223:DT:H2"	6:J:224:DA:N7	2.35	0.42
8:U:522:LEU:HD23	8:U:763:VAL:HG23	2.01	0.42
8:U:527:GLN:HE21	8:U:715:ILE:HG13	1.85	0.42
8:K:893:TRP:NE1	10:K:1004:SAH:N	2.68	0.42
1:A:61:LEU:HD12	2:B:37:LEU:HD23	2.02	0.41
3:C:16:THR:HA	5:I:40:DA:H5"	2.02	0.41
3:O:32:ARG:NH2	4:P:32:GLU:OE1	2.53	0.41
1:Q:61:LEU:HD12	2:R:37:LEU:HD23	2.02	0.41
8:K:518:LYS:HG3	8:K:608:PHE:CZ	2.55	0.41
1:M:61:LEU:HD12	2:N:37:LEU:HD23	2.01	0.41
1:Q:108:ASN:ND2	2:R:42:GLY:O	2.52	0.41
5:I:86:DC:H2"	5:I:87:DG:C8	2.55	0.41
8:U:639:LEU:HD22	8:U:687:VAL:HG22	2.00	0.41
8:U:649:VAL:HG11	8:U:898:ILE:HG22	2.02	0.41
8:K:96:TYR:HB2	8:K:129:ASN:HD21	1.86	0.41
2:N:90:LEU:HB3	2:N:95:ARG:O	2.20	0.41
4:T:103:LEU:HD21	7:X:743:ARG:NE	2.34	0.41
5:I:287:DC:H2"	5:I:288:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:578:GLU:HG2	8:K:580:PRO:HD2	2.01	0.41
4:T:103:LEU:HD23	7:X:743:ARG:CD	2.50	0.41
8:U:891:ARG:HD3	10:U:1004:SAH:H3'	2.01	0.41
8:Y:73:LEU:HD23	8:Y:148:LEU:HD22	2.01	0.41
8:Y:96:TYR:HB2	8:Y:129:ASN:HD21	1.86	0.41
8:Y:537:CYS:HB2	8:Y:559:CYS:HB3	2.01	0.41
8:W:601:TRP:CG	8:W:602:PRO:HD3	2.55	0.41
3:S:31:HIS:HD2	3:S:48:PRO:HG3	1.85	0.41
7:V:421:LYS:HE2	8:Y:144:GLY:HA3	2.02	0.41
8:Y:566:LEU:HD13	8:Y:595:LEU:HD13	2.01	0.41
8:W:527:GLN:CA	8:W:716:VAL:HG12	2.48	0.41
8:Y:866:ARG:HE	8:Y:872:VAL:HG12	1.85	0.41
8:W:521:PHE:HA	8:W:541:CYS:SG	2.60	0.41
2:N:27:GLN:O	2:N:27:GLN:HG3	2.20	0.41
8:W:505:GLU:OE1	8:W:604:ARG:NH1	2.53	0.41
8:W:649:VAL:HG11	8:W:898:ILE:HG22	2.03	0.41
8:K:891:ARG:HD3	10:K:1004:SAH:H3'	2.03	0.41
7:L:698:PRO:HA	7:L:716:TRP:HE1	1.86	0.41
3:S:17:ARG:HH21	3:S:28:GLY:HA2	1.86	0.41
5:I:45:DA:H2"	5:I:46:DG:C8	2.56	0.41
5:I:241:DC:H2"	5:I:242:DG:C8	2.55	0.41
5:I:242:DG:H2"	5:I:243:DT:C6	2.55	0.41
5:I:320:DA:H2"	5:I:321:DT:C6	2.56	0.41
6:J:56:DT:H2"	6:J:57:DC:C6	2.56	0.41
10:Y:1004:SAH:HN1	10:Y:1004:SAH:HG1	1.67	0.41
1:Q:46:VAL:HB	5:I:247:DT:P	2.61	0.41
5:I:43:DC:H2'	5:I:44:DT:C6	2.55	0.41
8:K:18:ILE:HA	8:K:36:ILE:HG22	2.03	0.41
1:E:101:VAL:HA	1:E:104:PHE:HD2	1.86	0.40
5:I:198:DC:H2'	5:I:199:DT:C6	2.55	0.40
5:I:320:DA:H2"	5:I:321:DT:C7	2.51	0.40
7:V:454:TYR:CE1	7:V:469:LEU:HD13	2.56	0.40
8:Y:641:ASP:OD1	8:Y:644:ALA:HB2	2.22	0.40
5:I:75:DG:H2"	5:I:76:DG:H5"	2.04	0.40
8:U:527:GLN:NE2	8:U:715:ILE:HG13	2.36	0.40
8:U:848:PHE:HB2	8:U:856:GLU:HB3	2.03	0.40
8:Y:16:PHE:HB2	8:Y:52:ARG:HE	1.86	0.40
7:L:658:LEU:HA	7:L:661:TYR:HD2	1.85	0.40
8:W:903:ALA:HB3	8:W:904:PRO:HD3	2.03	0.40
8:K:618:ASP:O	8:K:776:ASN:ND2	2.54	0.40
3:C:25:PHE:CE2	3:C:56:GLU:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:85:LEU:O	3:G:89:ASN:ND2	2.54	0.40
5:I:253:DT:H2"	5:I:254:DA:C8	2.56	0.40
6:J:39:DA:H2"	6:J:40:DA:C8	2.56	0.40
1:Q:61:LEU:HD22	2:R:36:ARG:HD2	2.02	0.40
5:I:157:DC:H2"	5:I:158:DA:C8	2.56	0.40
6:J:156:DG:H2"	6:J:157:DT:H2'	2.03	0.40
8:W:522:LEU:HD13	8:W:763:VAL:HG13	2.03	0.40
8:K:483:VAL:HG12	8:K:594:LEU:HD22	2.04	0.40
5:I:11:DC:H2"	5:I:12:DA:C8	2.57	0.40
8:U:493:ILE:HD12	8:U:493:ILE:HA	1.95	0.40
8:U:573:GLN:HA	8:U:576:ILE:HD12	2.03	0.40
8:Y:519:ASN:HB3	8:Y:763:VAL:HG21	2.04	0.40
7:L:761:ALA:N	7:L:762:PRO:HD2	2.35	0.40
8:K:18:ILE:HA	8:K:36:ILE:CG2	2.52	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	94/135 (70%)	91 (97%)	3 (3%)	0	100	100
1	E	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
1	M	97/135 (72%)	96 (99%)	1 (1%)	0	100	100
1	Q	93/135 (69%)	91 (98%)	2 (2%)	0	100	100
2	B	77/103 (75%)	76 (99%)	1 (1%)	0	100	100
2	F	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
2	N	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
2	R	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
3	C	97/129 (75%)	95 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	96/129 (74%)	93 (97%)	3 (3%)	0	100	100
3	O	96/129 (74%)	92 (96%)	4 (4%)	0	100	100
3	S	96/129 (74%)	93 (97%)	3 (3%)	0	100	100
4	D	90/123 (73%)	85 (94%)	5 (6%)	0	100	100
4	H	90/123 (73%)	88 (98%)	2 (2%)	0	100	100
4	P	89/123 (72%)	88 (99%)	1 (1%)	0	100	100
4	T	90/123 (73%)	89 (99%)	1 (1%)	0	100	100
7	L	342/773 (44%)	325 (95%)	17 (5%)	0	100	100
7	V	339/773 (44%)	327 (96%)	12 (4%)	0	100	100
7	X	174/773 (22%)	164 (94%)	10 (6%)	0	100	100
7	Z	172/773 (22%)	166 (96%)	6 (4%)	0	100	100
8	K	544/689 (79%)	520 (96%)	24 (4%)	0	100	100
8	U	420/689 (61%)	405 (96%)	15 (4%)	0	100	100
8	W	417/689 (60%)	400 (96%)	17 (4%)	0	100	100
8	Y	547/689 (79%)	527 (96%)	20 (4%)	0	100	100
All	All	4383/7808 (56%)	4227 (96%)	156 (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	84/110 (76%)	84 (100%)	0	100	100
1	E	85/110 (77%)	85 (100%)	0	100	100
1	M	87/110 (79%)	87 (100%)	0	100	100
1	Q	83/110 (76%)	83 (100%)	0	100	100
2	B	65/79 (82%)	65 (100%)	0	100	100
2	F	64/79 (81%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	64/79 (81%)	64 (100%)	0	100	100
2	R	64/79 (81%)	64 (100%)	0	100	100
3	C	77/101 (76%)	77 (100%)	0	100	100
3	G	76/101 (75%)	76 (100%)	0	100	100
3	O	76/101 (75%)	76 (100%)	0	100	100
3	S	75/101 (74%)	75 (100%)	0	100	100
4	D	78/103 (76%)	78 (100%)	0	100	100
4	H	78/103 (76%)	78 (100%)	0	100	100
4	P	77/103 (75%)	77 (100%)	0	100	100
4	T	78/103 (76%)	78 (100%)	0	100	100
7	L	300/660 (46%)	300 (100%)	0	100	100
7	V	300/660 (46%)	300 (100%)	0	100	100
7	X	156/660 (24%)	156 (100%)	0	100	100
7	Z	157/660 (24%)	157 (100%)	0	100	100
8	K	475/591 (80%)	475 (100%)	0	100	100
8	U	372/591 (63%)	371 (100%)	1 (0%)	86	86
8	W	372/591 (63%)	372 (100%)	0	100	100
8	Y	478/591 (81%)	478 (100%)	0	100	100
All	All	3821/6576 (58%)	3820 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
8	U	608	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	GLN
1	A	108	ASN
3	C	24	GLN
3	C	31	HIS
3	C	110	ASN
4	D	64	ASN

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Mol	Chain	Res	Type
1	E	39	HIS
1	E	68	GLN
2	F	93	GLN
3	G	31	HIS
3	G	38	ASN
3	G	73	ASN
3	G	82	HIS
4	H	64	ASN
4	H	106	HIS
1	M	108	ASN
2	N	27	GLN
2	N	93	GLN
3	O	31	HIS
3	O	73	ASN
3	O	82	HIS
3	O	89	ASN
3	O	110	ASN
4	P	64	ASN
4	P	106	HIS
1	Q	68	GLN
1	Q	108	ASN
3	S	31	HIS
4	T	64	ASN
4	T	106	HIS
7	V	499	GLN
7	V	510	GLN
7	Z	598	HIS
7	Z	601	ASN
8	U	527	GLN
8	U	739	HIS
8	U	789	HIS
8	U	802	ASN
8	U	900	HIS
8	Y	82	GLN
8	Y	129	ASN
8	Y	816	GLN
8	Y	847	HIS
8	Y	900	HIS
7	L	513	HIS
7	L	678	ASN
7	L	710	HIS
7	X	601	ASN

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Mol	Chain	Res	Type
8	W	527	GLN
8	W	739	HIS
8	W	816	GLN
8	W	821	HIS
8	W	886	GLN
8	W	900	HIS
8	K	82	GLN
8	K	129	ASN
8	K	612	ASN
8	K	694	HIS
8	K	900	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 18 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
10	SAH	U	1004	-	27,28,28	0.44	0	36,40,40	0.29	0
10	SAH	K	1004	-	27,28,28	0.44	0	36,40,40	0.29	0
10	SAH	Y	1004	-	27,28,28	0.43	0	36,40,40	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	SAH	W	1004	-	27,28,28	0.44	0	36,40,40	0.29	0

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
10	SAH	U	1004	-	-	7/15/31/31	0/3/3/3
10	SAH	K	1004	-	-	6/15/31/31	0/3/3/3
10	SAH	Y	1004	-	-	7/15/31/31	0/3/3/3
10	SAH	W	1004	-	-	7/15/31/31	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	U	1004	SAH	N-CA-CB-CG
10	Y	1004	SAH	N-CA-CB-CG
10	W	1004	SAH	N-CA-CB-CG
10	K	1004	SAH	N-CA-CB-CG
10	U	1004	SAH	C2'-C1'-N9-C8
10	Y	1004	SAH	C2'-C1'-N9-C8
10	W	1004	SAH	C2'-C1'-N9-C8
10	K	1004	SAH	C2'-C1'-N9-C8
10	U	1004	SAH	C-CA-CB-CG
10	Y	1004	SAH	C-CA-CB-CG
10	W	1004	SAH	C-CA-CB-CG
10	K	1004	SAH	C-CA-CB-CG
10	U	1004	SAH	C2'-C1'-N9-C4
10	Y	1004	SAH	C2'-C1'-N9-C4
10	W	1004	SAH	C2'-C1'-N9-C4
10	K	1004	SAH	C2'-C1'-N9-C4
10	U	1004	SAH	OXT-C-CA-CB
10	Y	1004	SAH	OXT-C-CA-CB
10	W	1004	SAH	OXT-C-CA-CB
10	K	1004	SAH	OXT-C-CA-CB
10	U	1004	SAH	O4'-C1'-N9-C8

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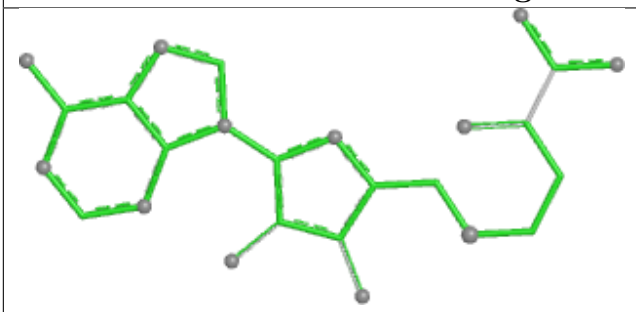
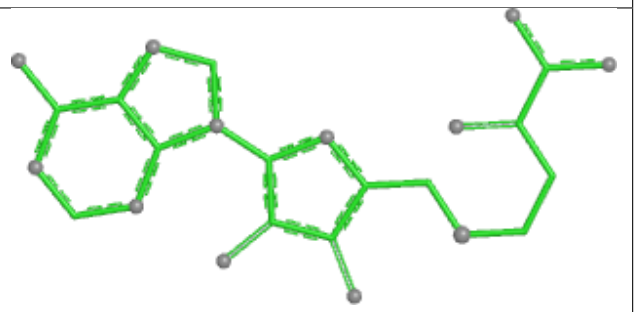
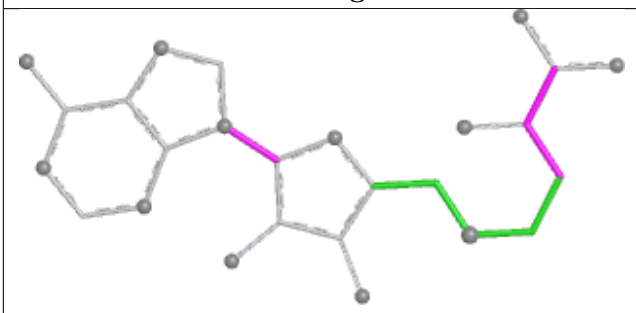
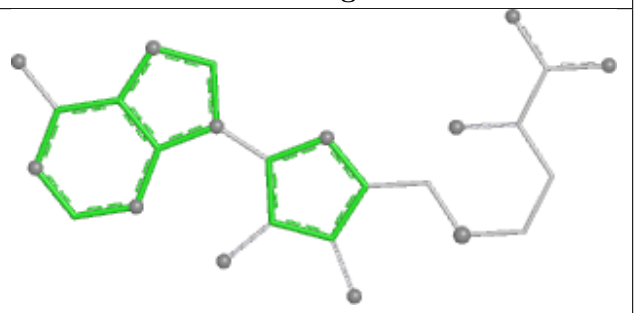
Mol	Chain	Res	Type	Atoms
10	Y	1004	SAH	O4'-C1'-N9-C8
10	W	1004	SAH	O4'-C1'-N9-C8
10	K	1004	SAH	O4'-C1'-N9-C8
10	U	1004	SAH	O-C-CA-CB
10	Y	1004	SAH	O-C-CA-CB
10	W	1004	SAH	O-C-CA-CB

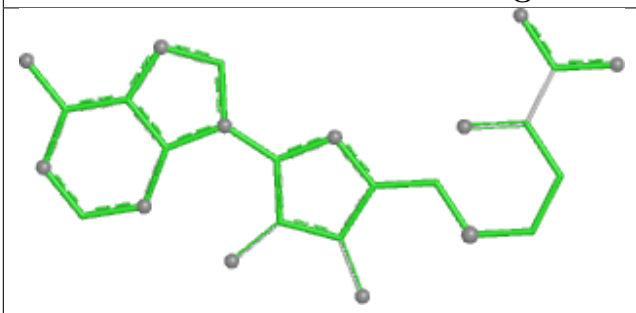
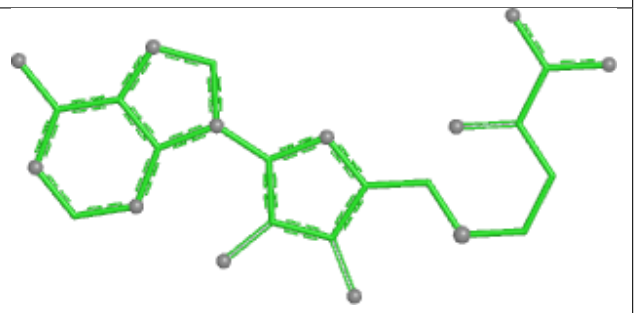
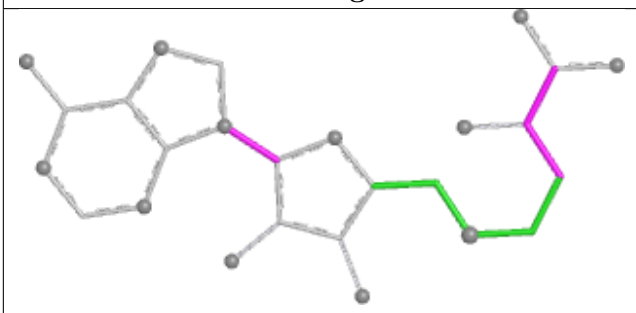
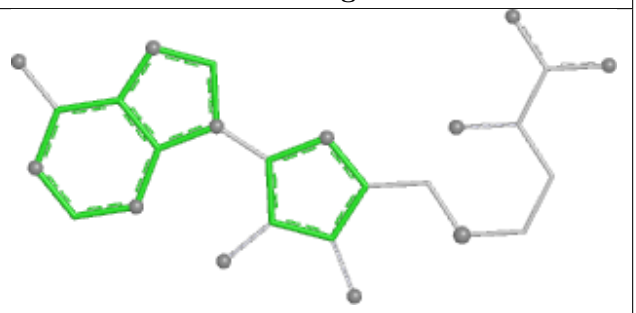
There are no ring outliers.

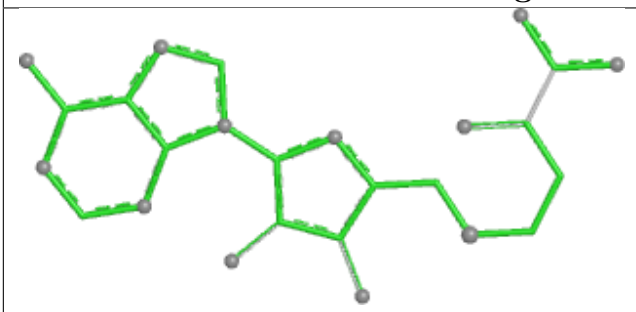
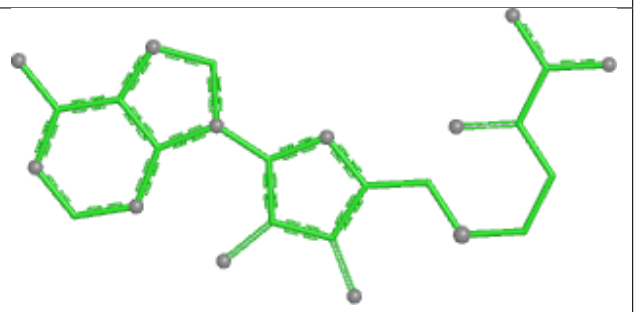
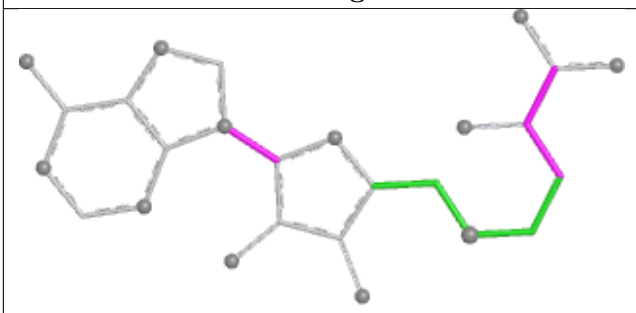
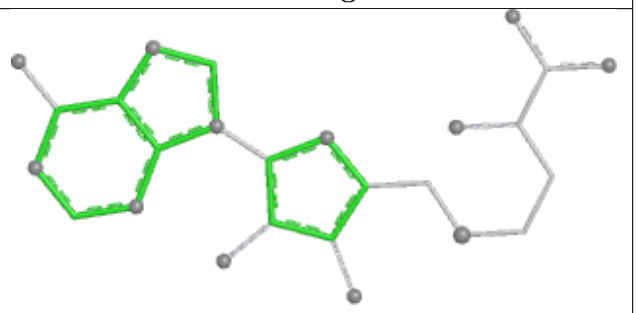
3 monomers are involved in 7 short contacts:

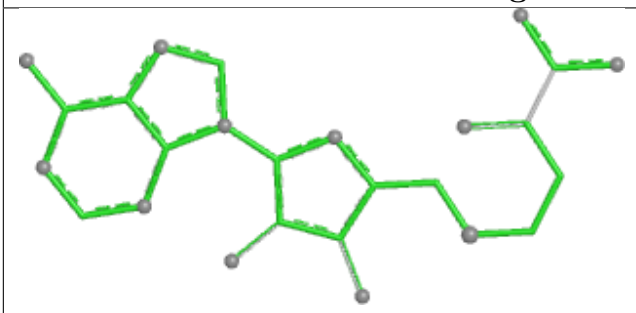
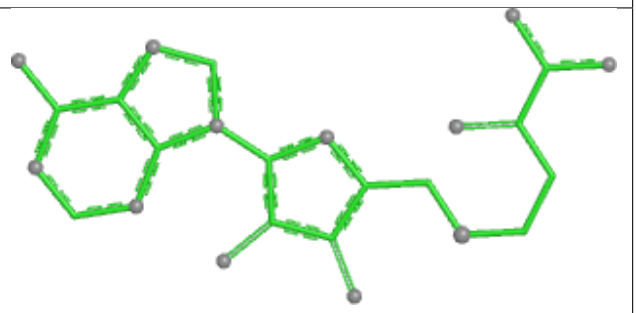
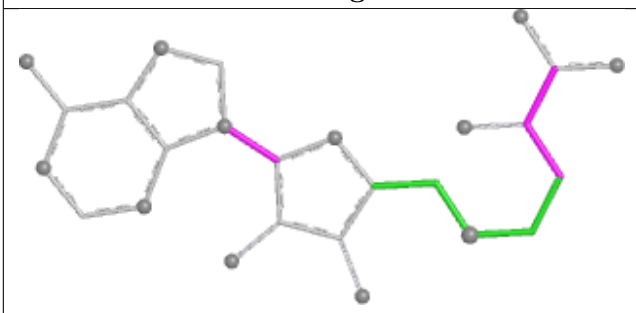
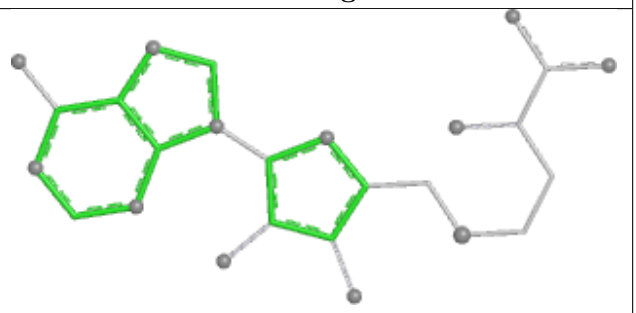
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	U	1004	SAH	2	0
10	K	1004	SAH	4	0
10	Y	1004	SAH	1	0

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 SAH U 1004	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH K 1004	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH Y 1004	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH W 1004	
 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.

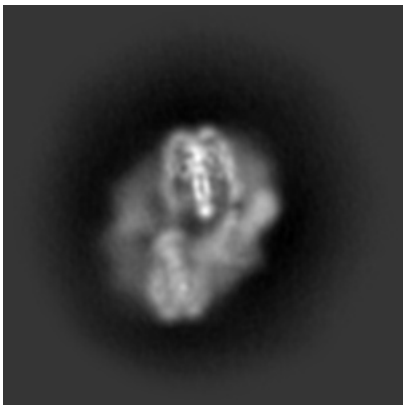
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-47462. These allow visual inspection of the internal detail of the map and identification of artifacts.

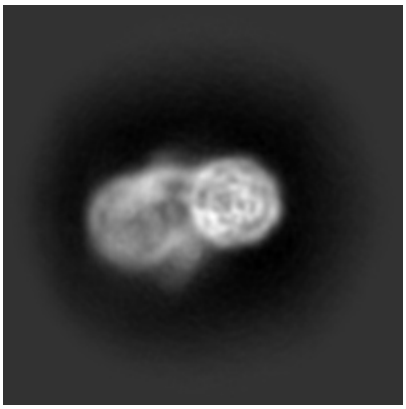
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

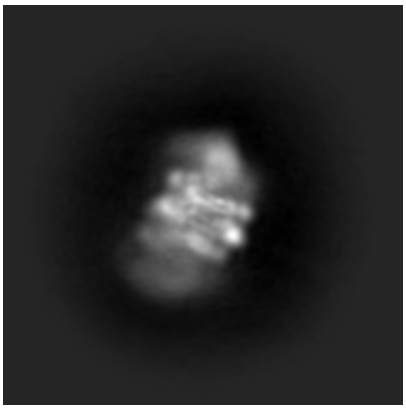
6.1.1 Primary map



X

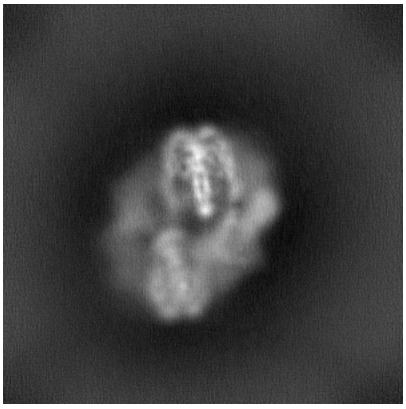


Y

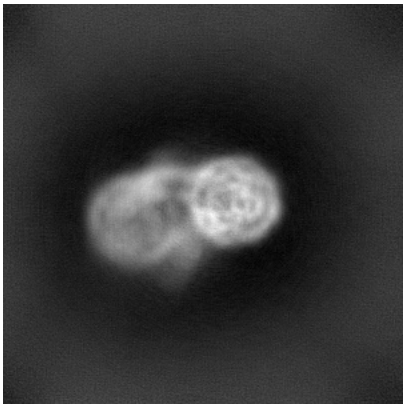


Z

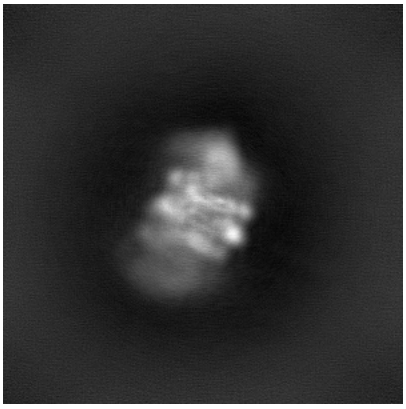
6.1.2 Raw map



X



Y

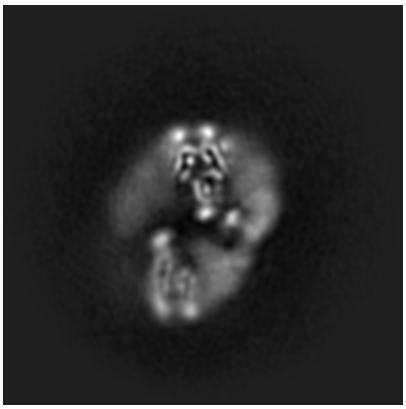


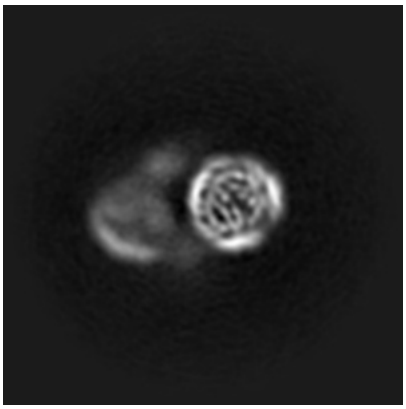
Z

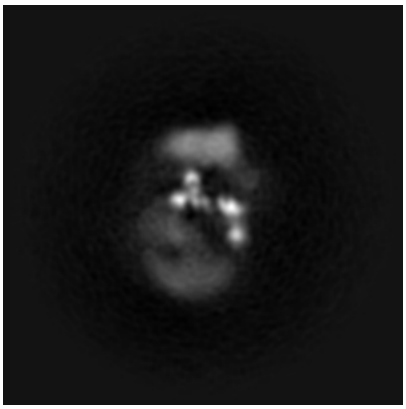
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

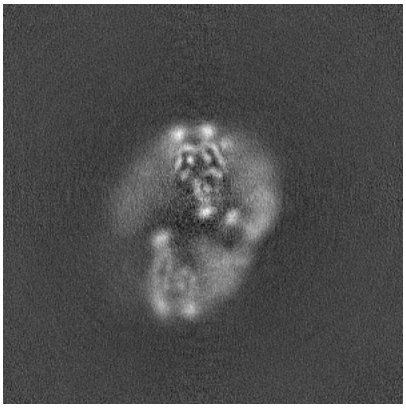
6.2.1 Primary map

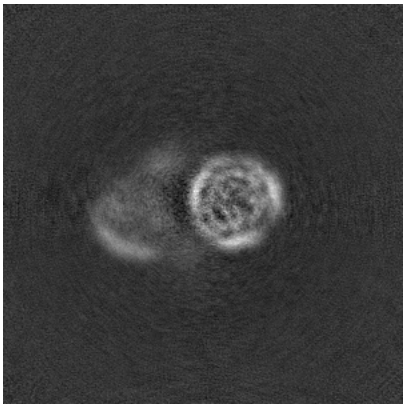

X Index: 240

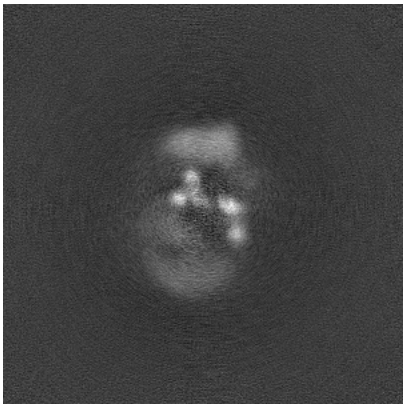

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

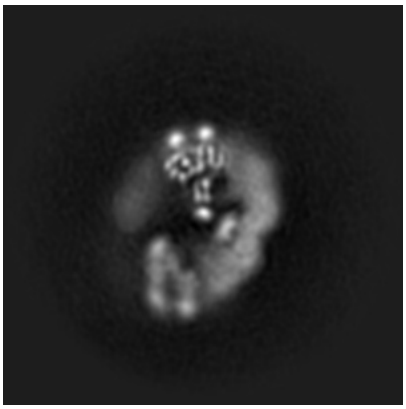

Y Index: 240

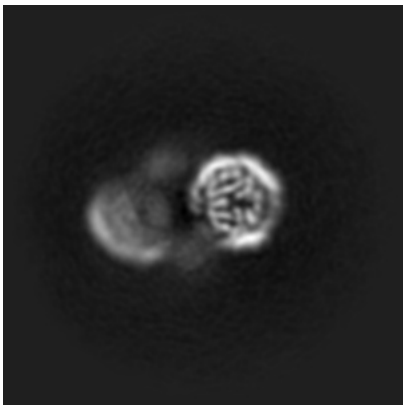

Z Index: 240

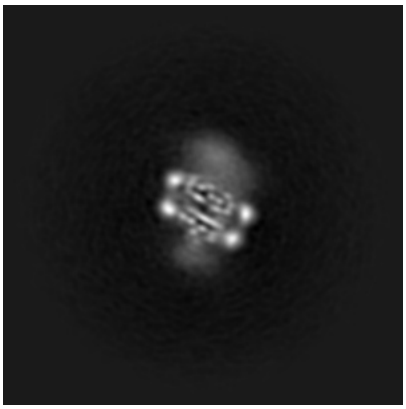
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

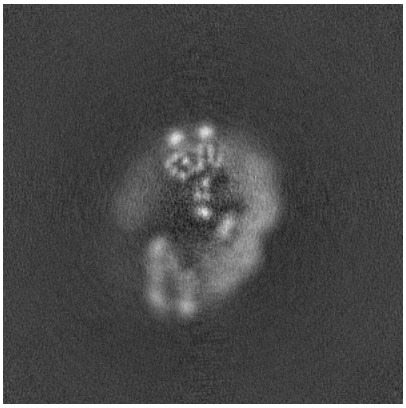
6.3.1 Primary map

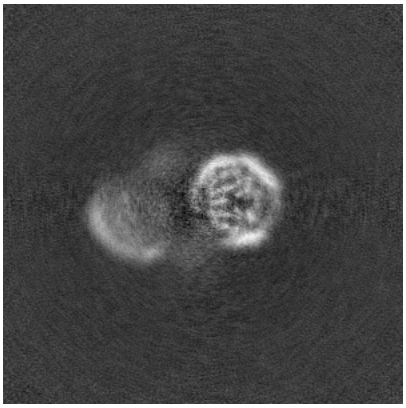

X Index: 251

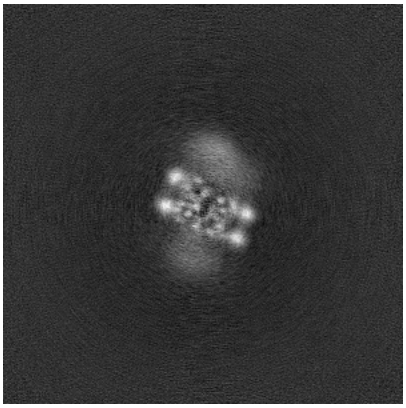

Y Index: 233


Z Index: 292

6.3.2 Raw map


X Index: 251

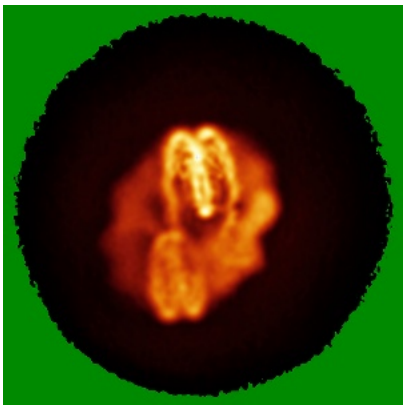

Y Index: 233

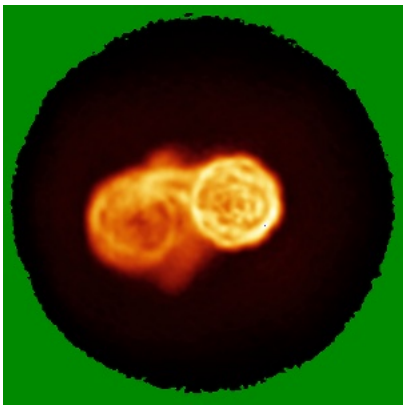

Z Index: 280

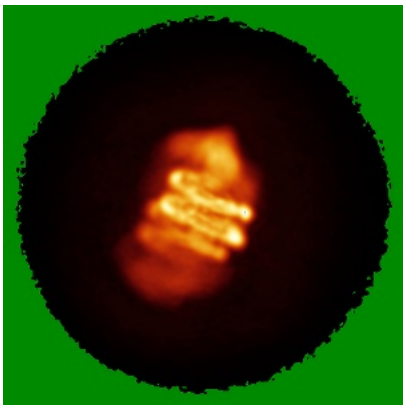
The images above show the largest variance slices of the map in three orthogonal directions.

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

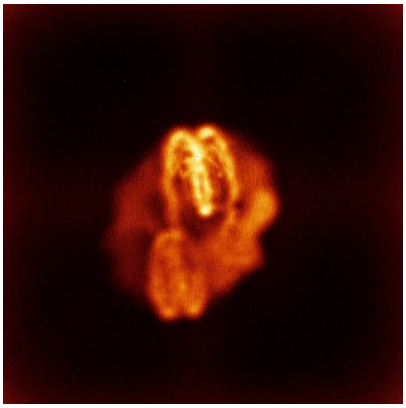
6.4.1 Primary map

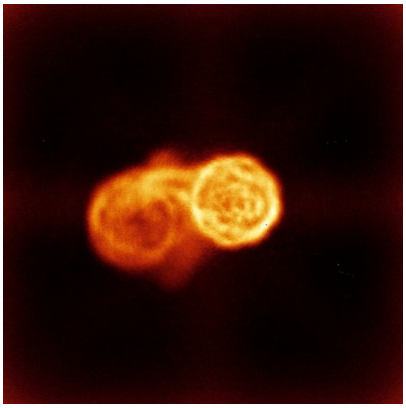

X

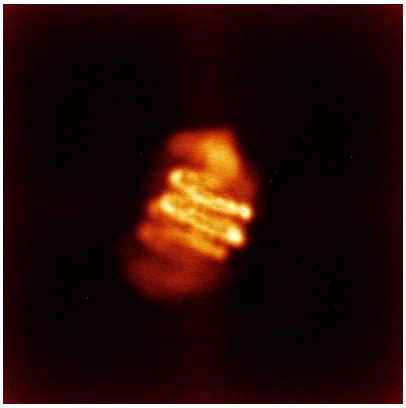

Y


Z

6.4.2 Raw map


X

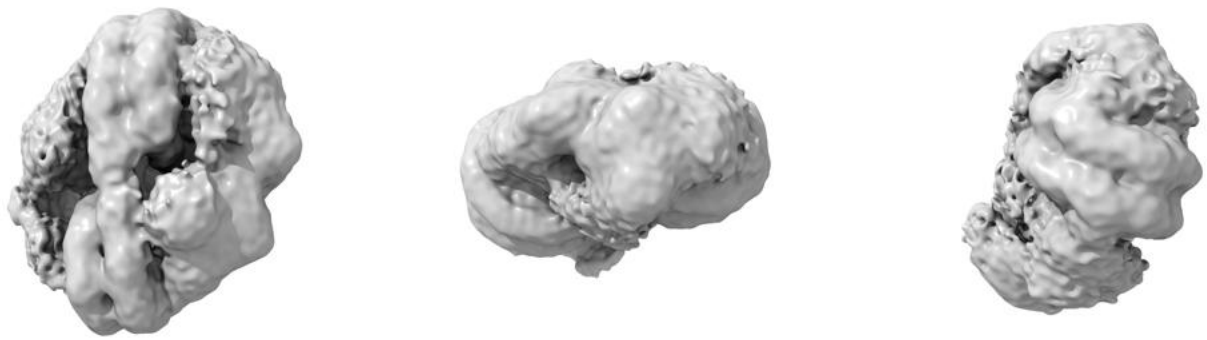

Y


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)

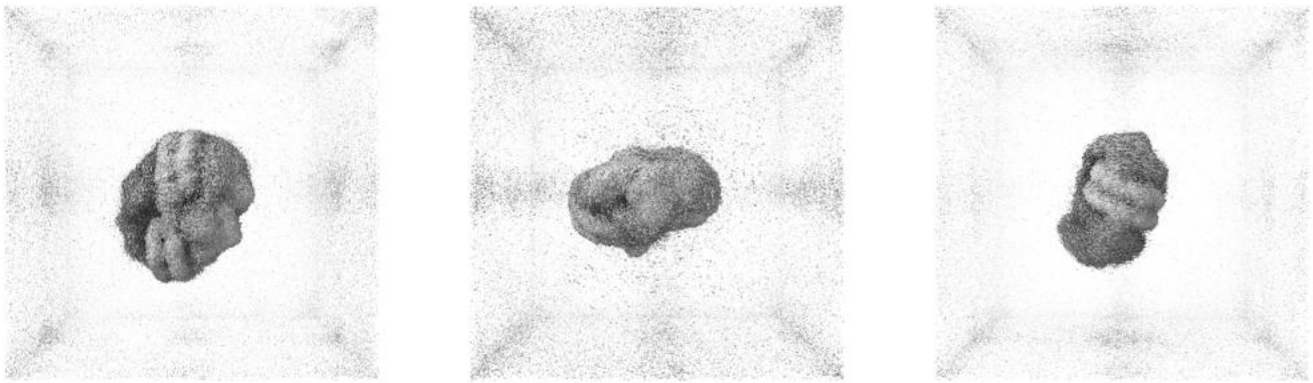
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

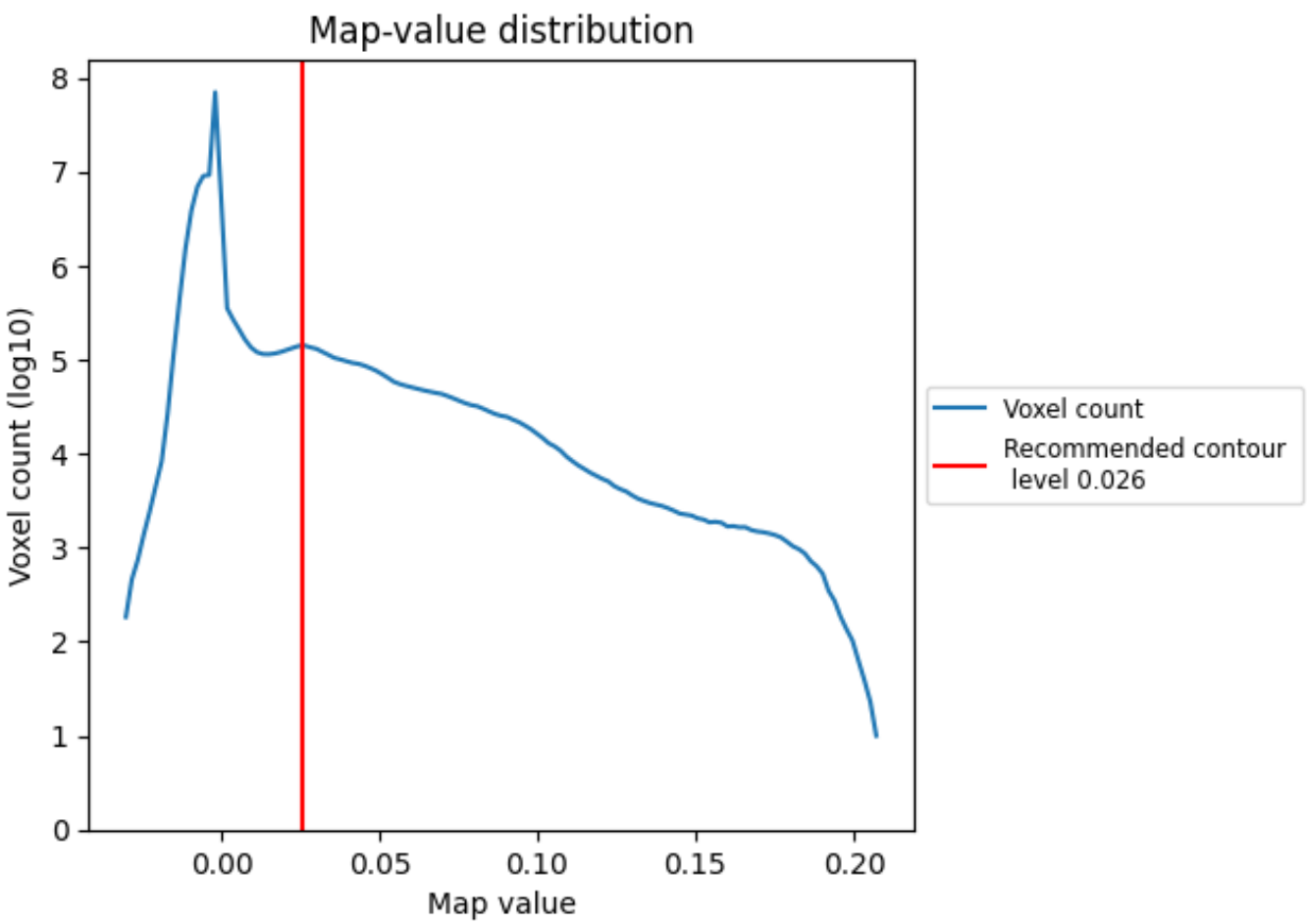
6.6 Mask visualisation (i)

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

7 Map analysis (i)

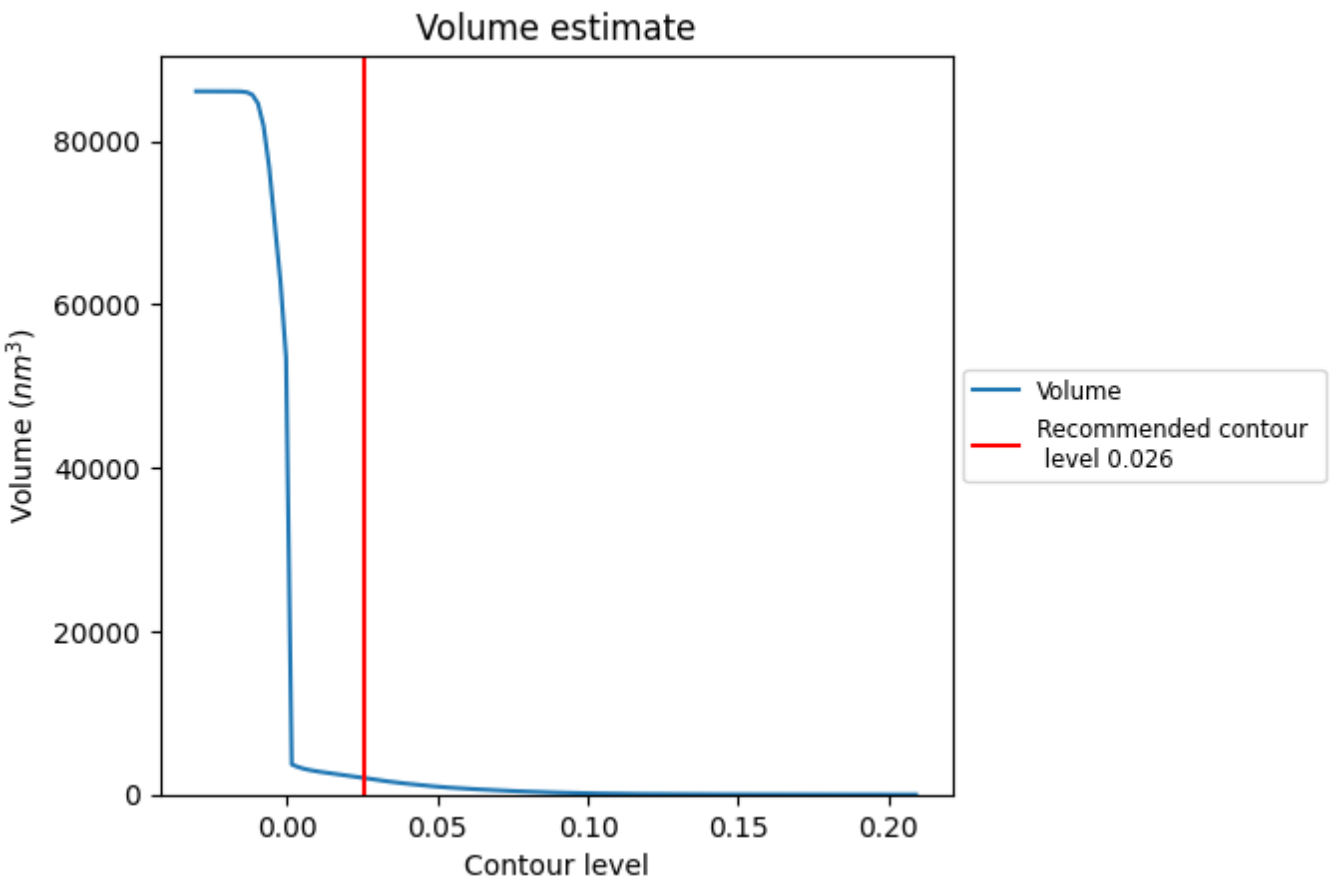
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

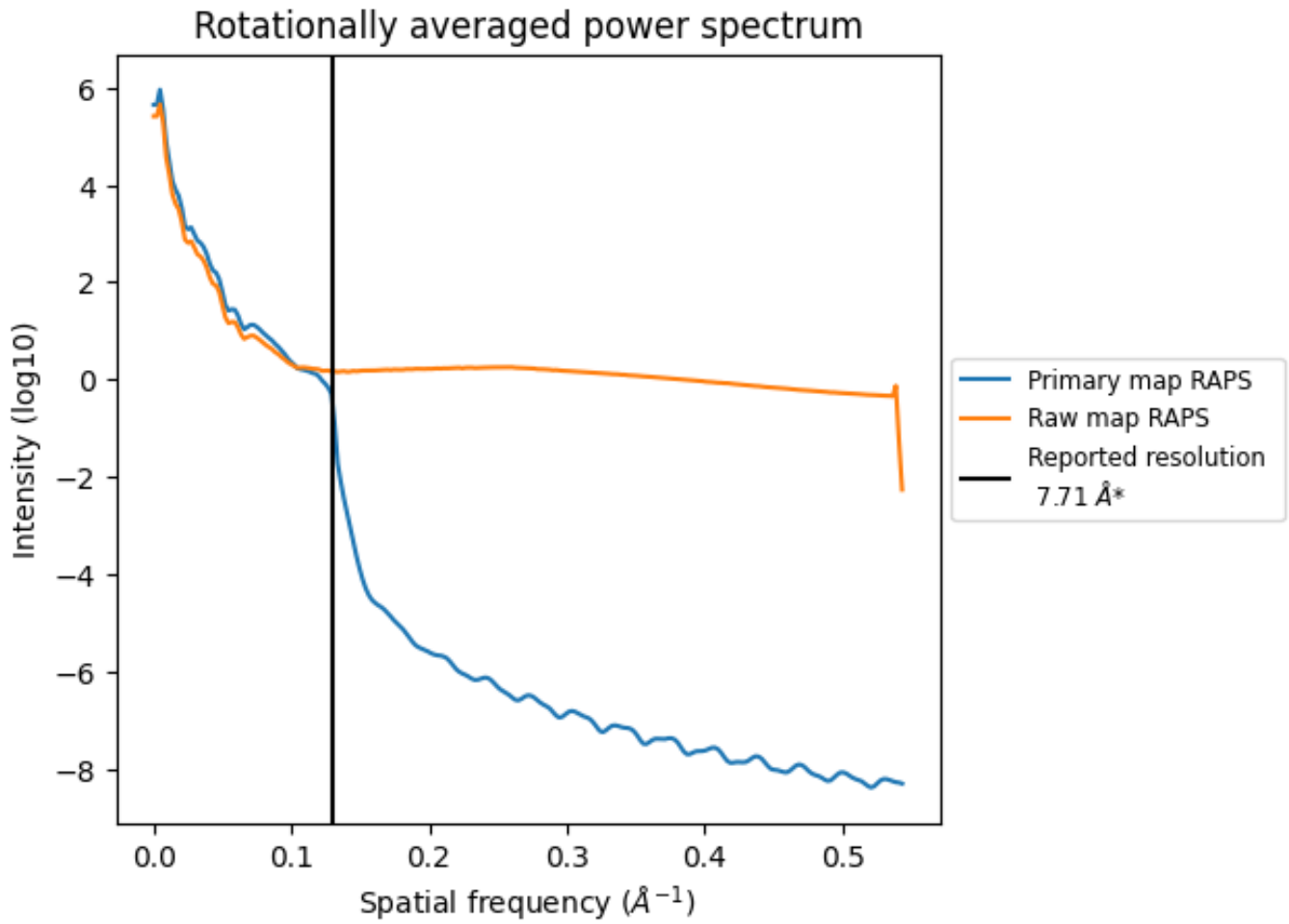
7.2 Volume estimate (i)



The volume at the recommended contour level is 2027 nm^3; this corresponds to an approximate mass of 1831 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)

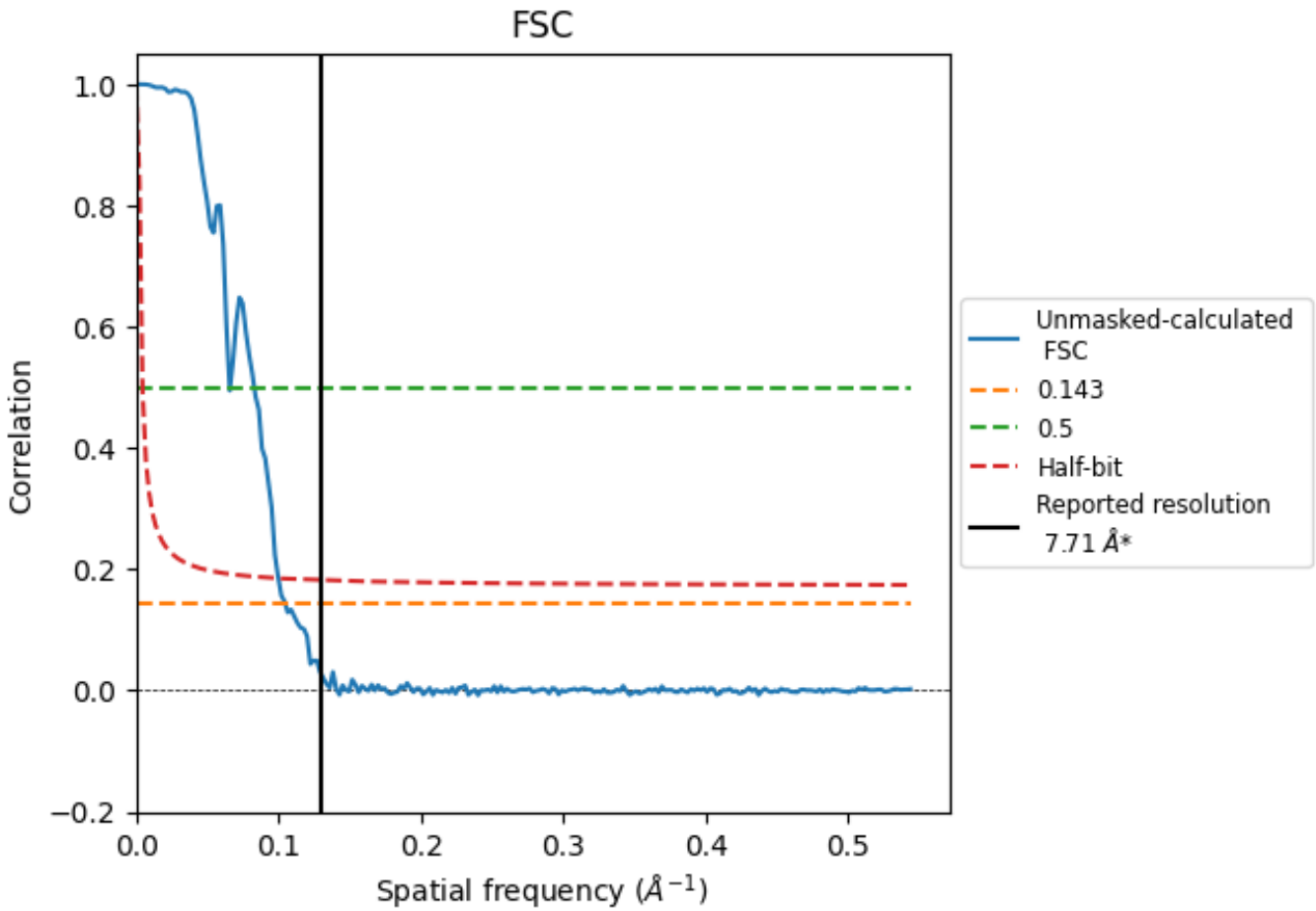


*Reported resolution corresponds to spatial frequency of 0.130 Å^{-1}

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 0.130 Å^{-1}

8.2 Resolution estimates (i)

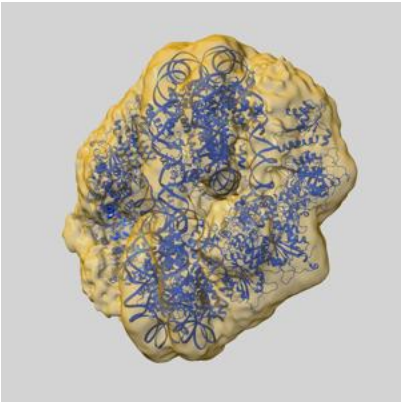
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.56	15.24	10.01

*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 9.56 differs from the reported value 7.71 by more than 10 %

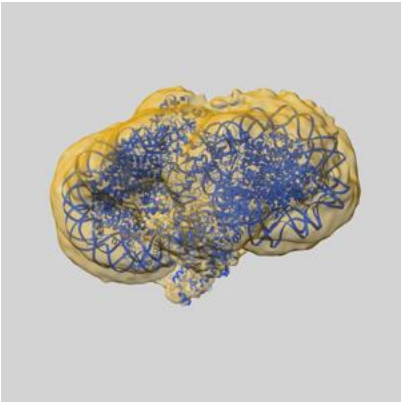
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-47462 and PDB model 9E2R. Per-residue inclusion information can be found in section 3 on page 8.

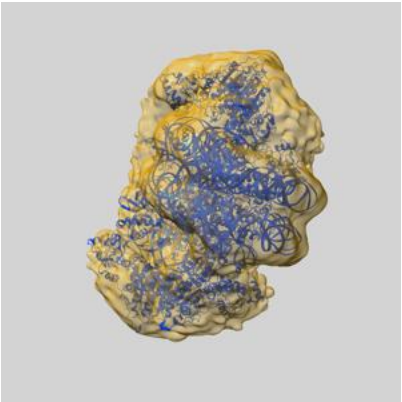
9.1 Map-model overlay (i)



X



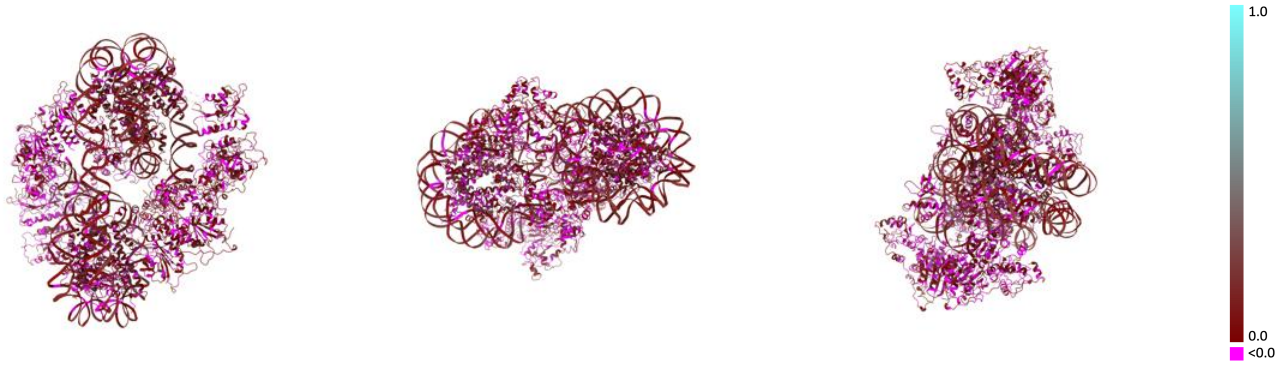
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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.

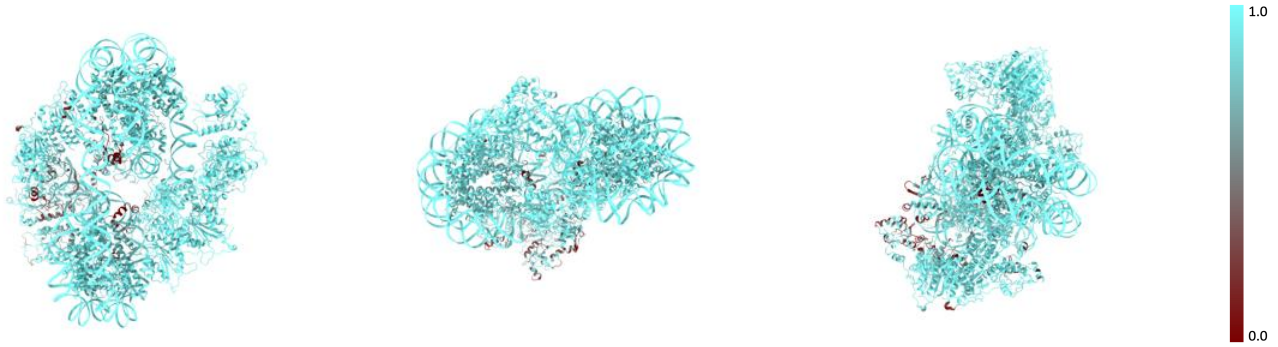
9.2 Q-score mapped to coordinate model (i)



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.

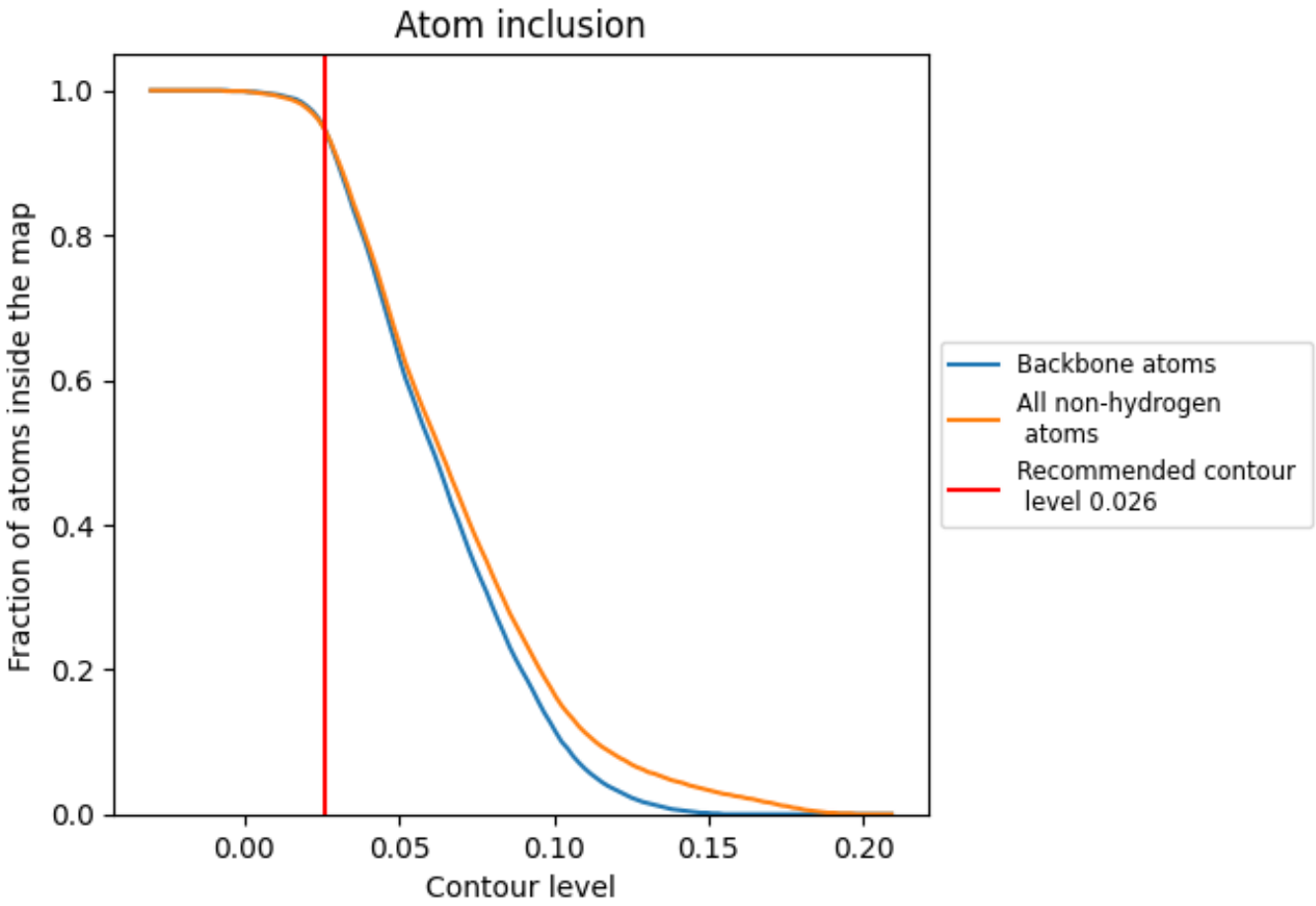
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.0720
A	0.9880	0.1270
B	0.9900	0.1130
C	0.9640	0.1000
D	0.9860	0.1180
E	0.9820	0.1350
F	0.9880	0.1230
G	0.9630	0.0910
H	0.9840	0.1090
I	0.9920	0.1200
J	0.9840	0.1070
K	0.7800	0.0260
L	0.8520	0.0320
M	0.9510	0.0740
N	0.9480	0.0710
O	0.9360	0.0640
P	0.9930	0.0490
Q	0.9890	0.0920
R	0.9930	0.0750
S	0.9900	0.0320
T	1.0000	0.0740
U	0.9920	0.0570
V	0.9170	0.0600
W	0.9150	0.0200
X	0.8230	0.0200
Y	0.9930	0.0600
Z	1.0000	0.0430