



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 07:29 PM UTC

PDB ID : 8TAS / pdb_00008tas
EMDB ID : EMD-41141
Title : PRC2 monomer bound to nucleosome
Authors : Sauer, P.V.; Pavlenko, E.; Nogales, E.; Poepsel, S.
Deposited on : 2023-06-27
Resolution : 4.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

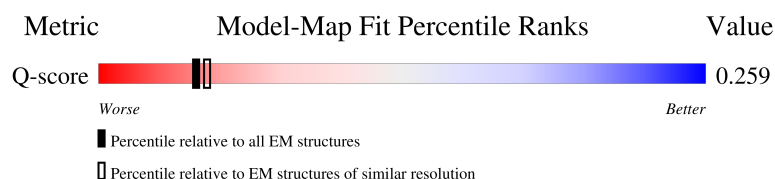
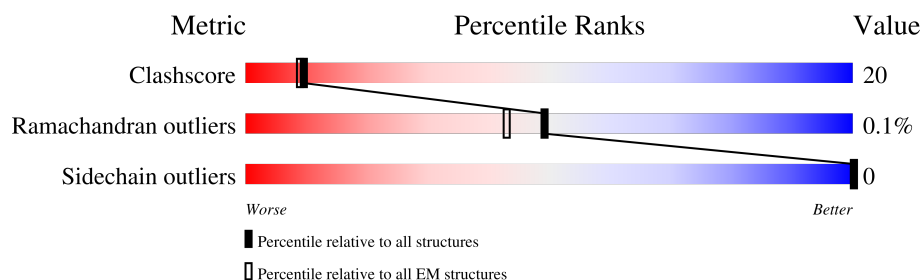
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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.



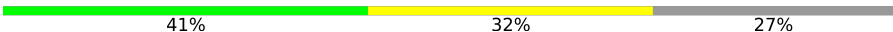
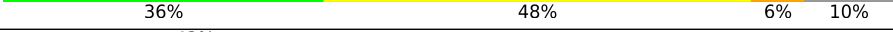
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	D	619	35% 51% 20% 29%
2	E	753	47% 29% 24%
3	G	441	37% 45% 18%
4	I	136	51% 33% 16%

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Mol	Chain	Length	Quality of chain
4	W	136	
5	H	215	
6	J	106	
6	X	106	
7	R	133	
7	U	133	
8	S	123	
8	V	123	
9	T	215	
10	O	425	
11	Y	303	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29440 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 Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	439	Total	C	N	O	S	0	0
			3633	2309	652	645	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	67	MET	-	initiating methionine	UNP Q15022

- Molecule 2 is a protein called Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	570	Total	C	N	O	S	0	0
			4580	2871	821	846	42		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP Q15910
E	0	ASN	-	expression tag	UNP Q15910
E	1	ALA	-	expression tag	UNP Q15910
E	14	ALA	CYS	conflict	UNP Q15910
E	15	CYS	TRP	conflict	UNP Q15910

- Molecule 3 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	362	Total	C	N	O	S	0	0
			2930	1855	513	541	21		

- Molecule 4 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	114	Total	C	N	O	S	0	0
			917	576	179	159	3		
4	W	99	Total	C	N	O	S	0	0
			817	515	158	141	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	102	ALA	GLY	conflict	UNP P84233
W	102	ALA	GLY	conflict	UNP P84233

- Molecule 5 is a DNA chain called DNA (226-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	193	Total	C	N	O	P	0	0
			3972	1873	761	1145	193		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	83	Total	C	N	O	S	0	0
			661	418	129	113	1		
6	X	87	Total	C	N	O	S	0	0
			666	419	129	117	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	103	SER	-	expression tag	UNP P62799
J	104	SER	-	expression tag	UNP P62799
J	105	GLY	-	expression tag	UNP P62799
X	103	SER	-	expression tag	UNP P62799
X	104	SER	-	expression tag	UNP P62799
X	105	GLY	-	expression tag	UNP P62799

- Molecule 7 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	108	Total	C	N	O	S	0	0
			829	522	162	144	1		
7	U	108	Total	C	N	O	S	0	0
			825	519	161	144	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	SER	-	expression tag	UNP Q6AZJ8
R	-2	ASN	-	expression tag	UNP Q6AZJ8
R	-1	ALA	-	expression tag	UNP Q6AZJ8
R	119	CYS	LYS	conflict	UNP Q6AZJ8
U	-3	SER	-	expression tag	UNP Q6AZJ8
U	-2	ASN	-	expression tag	UNP Q6AZJ8
U	-1	ALA	-	expression tag	UNP Q6AZJ8
U	119	CYS	LYS	conflict	UNP Q6AZJ8

- Molecule 8 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	96	Total	C	N	O	S	0	0
			742	466	133	141	2		
8	V	95	Total	C	N	O	S	0	0
			737	463	132	140	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	MET	-	initiating methionine	UNP P02281
S	29	THR	SER	conflict	UNP P02281
V	0	MET	-	initiating methionine	UNP P02281
V	29	THR	SER	conflict	UNP P02281

- Molecule 9 is a DNA chain called DNA (226-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	193	Total	C	N	O	P	0	0
			3919	1853	724	1149	193		

- Molecule 10 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	395	Total	C	N	O	S	0	0
			3139	1981	535	613	10		

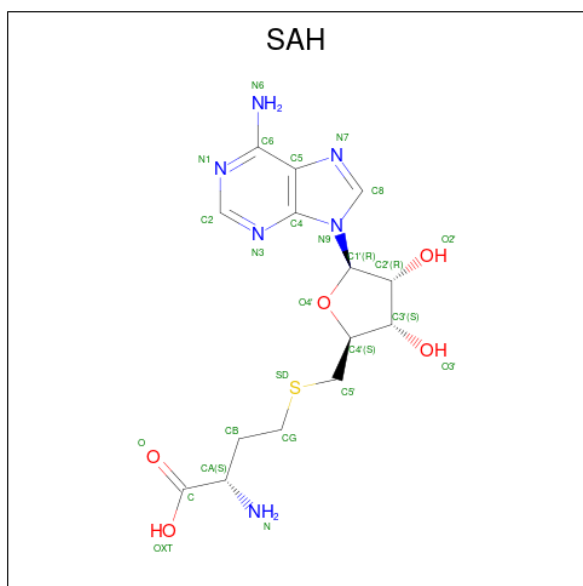
- Molecule 11 is a protein called Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	126	Total	C	N	O	S	0	0
			1047	664	206	174	3		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	7	SER	-	expression tag	UNP Q6ZN18
Y	8	ASN	-	expression tag	UNP Q6ZN18
Y	9	ALA	-	expression tag	UNP Q6ZN18
Y	10	TYR	-	expression tag	UNP Q6ZN18
Y	11	THR	-	expression tag	UNP Q6ZN18
Y	12	ARG	-	expression tag	UNP Q6ZN18
Y	13	ARG	-	expression tag	UNP Q6ZN18
Y	14	TYR	-	expression tag	UNP Q6ZN18
Y	15	SER	-	expression tag	UNP Q6ZN18

- Molecule 12 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).

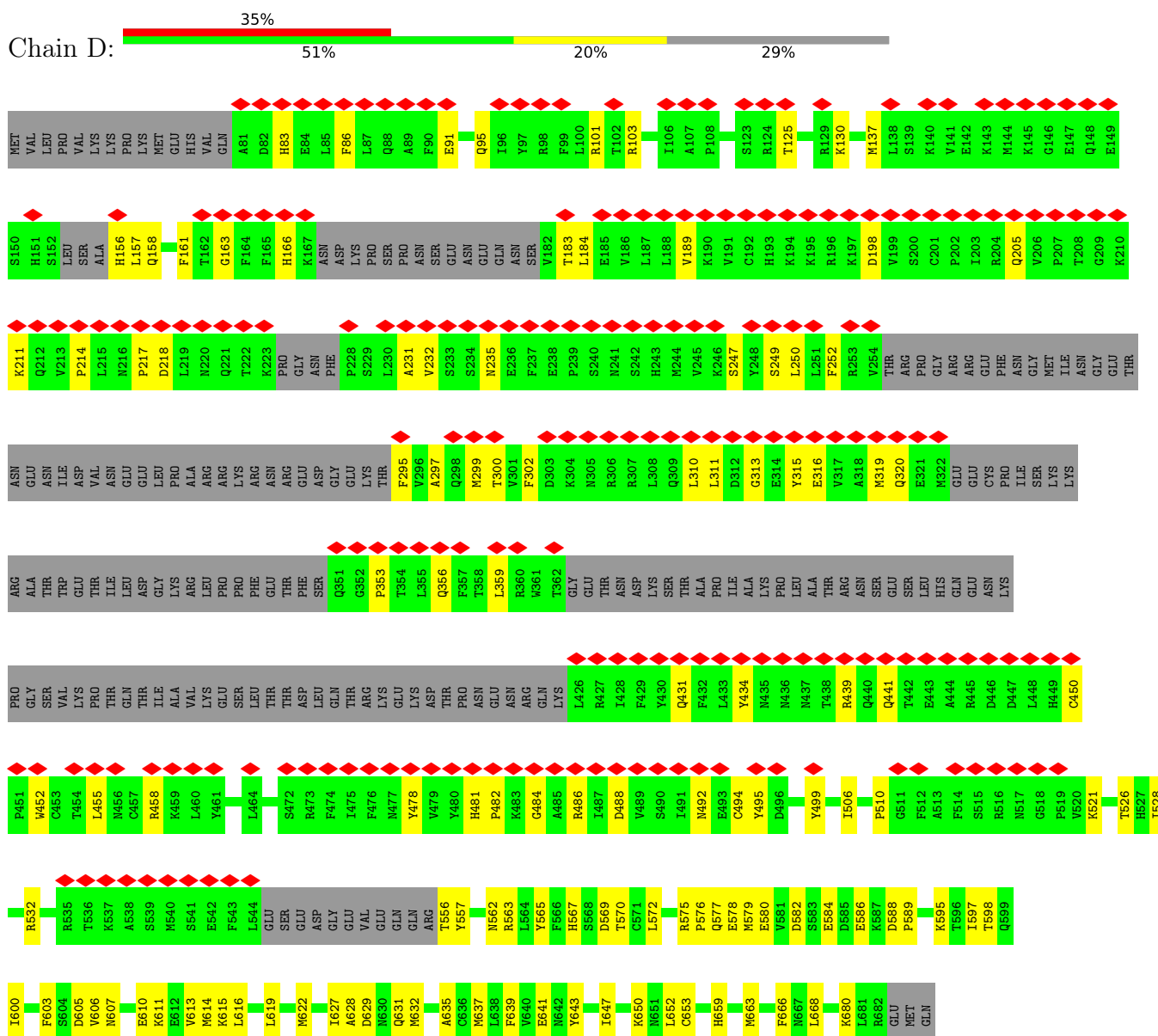


Mol	Chain	Residues	Atoms					AltConf
12	E	1	Total	C	N	O	S	0
			26	14	6	5	1	

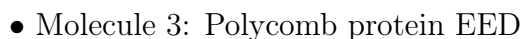
3 Residue-property plots

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.

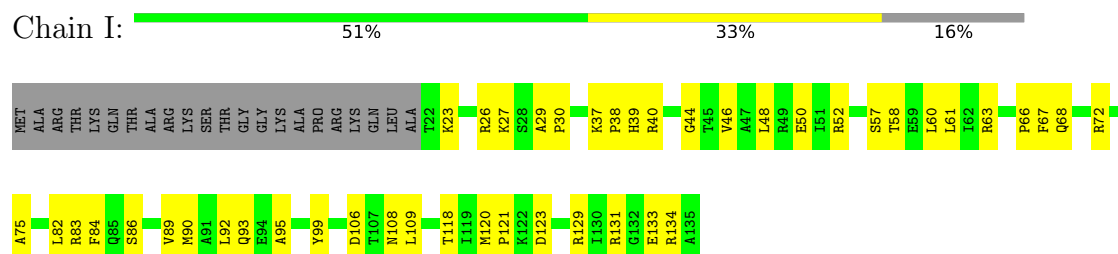
• Molecule 1: Polycomb protein SUZ12



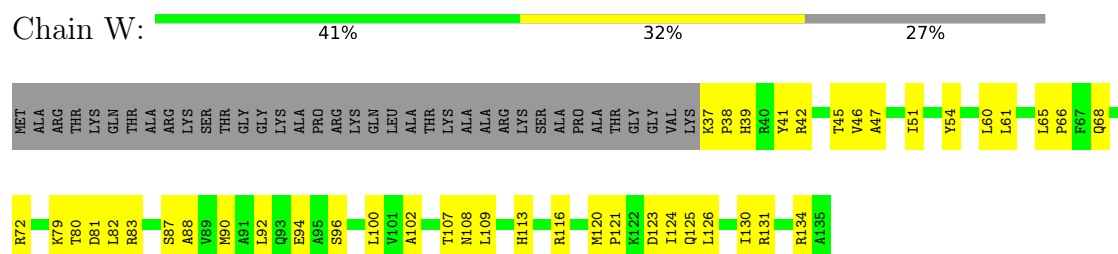
• Molecule 2: Histone-lysine N-methyltransferase EZH2



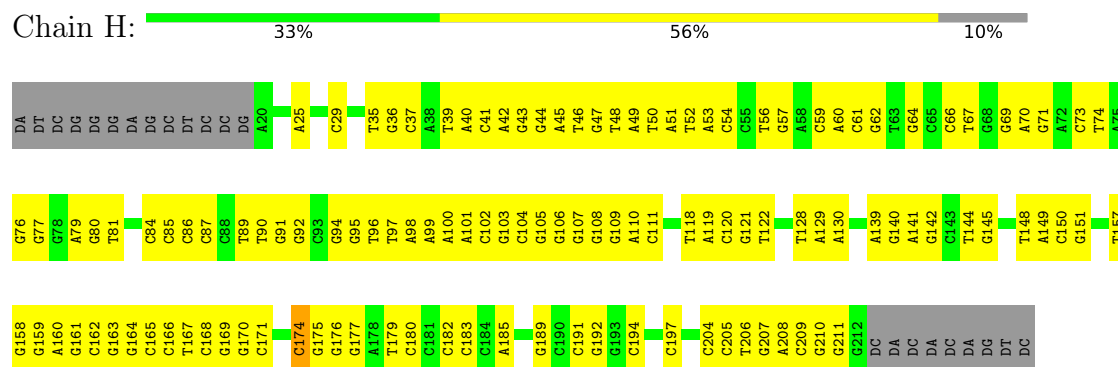
- Molecule 4: Histone H3.2



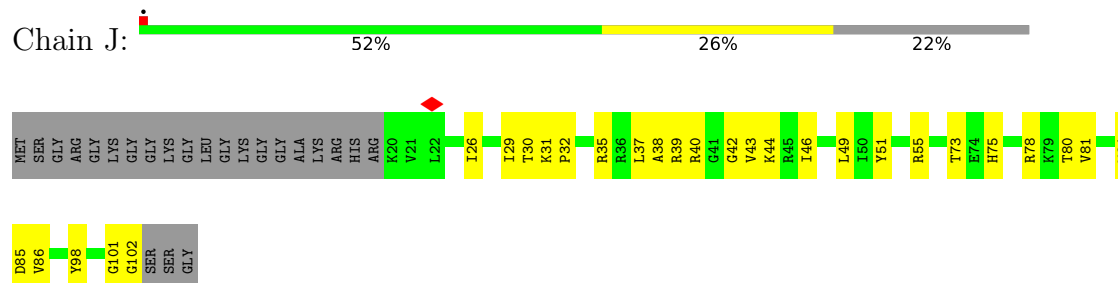
- Molecule 4: Histone H3.2



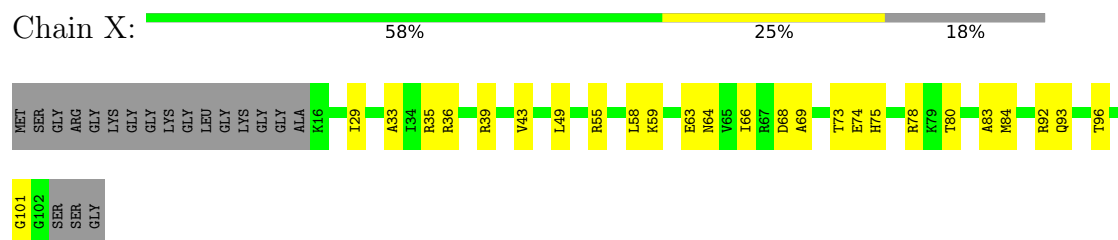
- Molecule 5: DNA (226-MER)



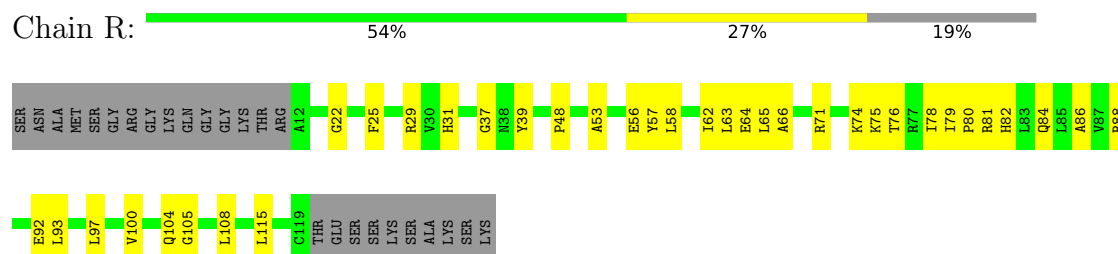
- Molecule 6: Histone H4



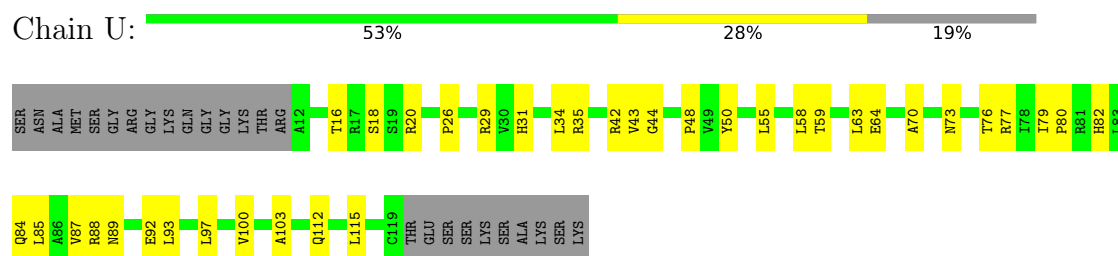
- Molecule 6: Histone H4



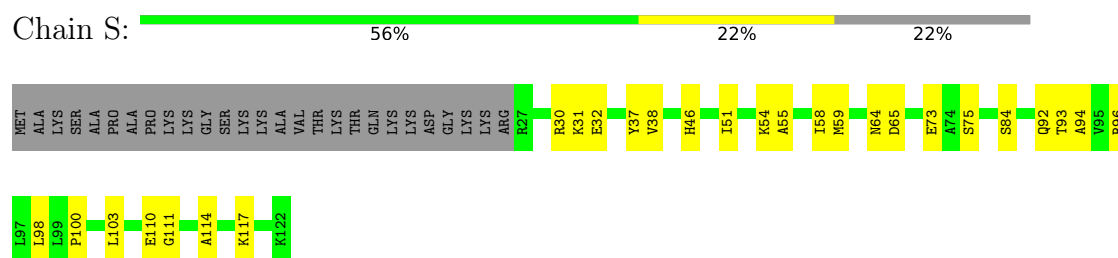
- Molecule 7: Histone H2A



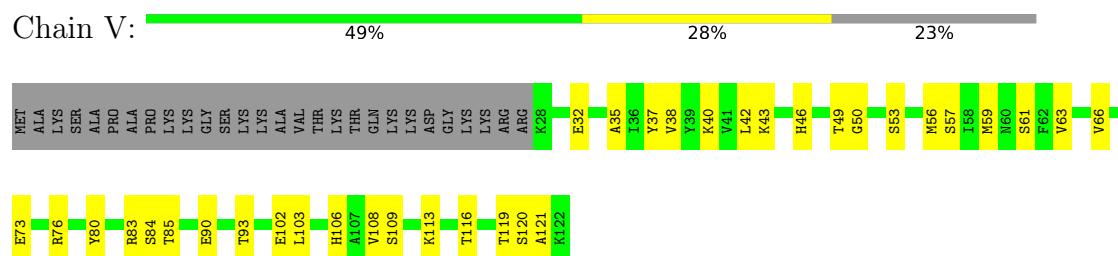
- Molecule 7: Histone H2A



- Molecule 8: Histone H2B 1.1



- Molecule 8: Histone H2B 1.1



- Molecule 9: DNA (226-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	505.88998, 505.88998, 505.88998	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.533, 1.533, 1.533	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	D	0.13	0/3713	0.34	0/4992
2	E	0.18	0/4682	0.39	0/6308
3	G	0.15	0/3005	0.38	0/4070
4	I	0.31	0/930	0.47	0/1246
4	W	0.38	0/829	0.50	0/1111
5	H	0.27	0/4463	0.80	2/6888 (0.0%)
6	J	0.40	0/668	0.48	0/894
6	X	0.43	0/673	0.52	0/904
7	R	0.39	0/839	0.49	0/1132
7	U	0.39	0/835	0.52	0/1128
8	S	0.43	0/753	0.54	0/1014
8	V	0.41	0/748	0.54	0/1007
9	T	0.28	0/4391	0.84	15/6763 (0.2%)
10	O	0.13	0/3225	0.36	0/4394
11	Y	0.12	0/1070	0.41	0/1437
All	All	0.26	0/30824	0.58	17/43288 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	T	67	DC	OP1-P-O3'	6.62	127.86	108.00
9	T	46	DG	OP1-P-O3'	6.34	127.03	108.00
9	T	150	DC	OP1-P-O3'	6.32	126.96	108.00
5	H	104	DC	OP1-P-O3'	6.23	126.69	108.00
9	T	120	DC	OP1-P-O3'	6.17	126.50	108.00
9	T	109	DA	OP1-P-O3'	6.14	126.43	108.00
5	H	174	DC	OP1-P-O3'	5.96	125.86	108.00
9	T	80	DG	OP1-P-O3'	5.84	125.51	108.00
9	T	61	DG	OP1-P-O3'	5.83	125.49	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	58	DC	OP1-P-O3'	5.82	125.47	108.00
9	T	104	DC	OP1-P-O3'	5.81	125.44	108.00
9	T	57	DC	OP1-P-O3'	5.43	124.28	108.00
9	T	93	DC	OP1-P-O3'	5.40	124.20	108.00
9	T	82	DC	OP1-P-O3'	5.30	123.91	108.00
9	T	117	DT	OP1-P-O3'	5.23	123.69	108.00
9	T	133	DC	OP1-P-O3'	5.14	123.43	108.00
9	T	98	DT	OP1-P-O3'	5.14	123.41	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3633	0	3628	100	0
2	E	4580	0	4483	173	0
3	G	2930	0	2839	154	0
4	I	917	0	971	46	0
4	W	817	0	858	38	0
5	H	3972	0	2154	135	0
6	J	661	0	709	31	0
6	X	666	0	679	21	0
7	R	829	0	887	41	0
7	U	825	0	876	40	0
8	S	742	0	753	24	0
8	V	737	0	751	33	0
9	T	3919	0	2153	133	0
10	O	3139	0	2986	103	0
11	Y	1047	0	1102	23	0
12	E	26	0	19	5	0
All	All	29440	0	25848	907	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 20.

All (907) 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:191:ASN:HB3	3:G:211:LYS:HB3	1.50	0.92
3:G:175:ILE:HG13	3:G:182:CYS:HB2	1.54	0.90
7:U:84:GLN:HE21	7:U:88:ARG:HE	1.19	0.87
11:Y:243:TRP:HB2	11:Y:248:ILE:HG21	1.60	0.84
1:D:629:ASP:HA	1:D:632:MET:HE2	1.60	0.82
5:H:169:DG:N2	9:T:58:DC:O2	2.15	0.79
4:W:61:LEU:HD12	6:X:36:ARG:HB3	1.64	0.79
7:R:78:ILE:HG22	8:S:51:ILE:HA	1.65	0.79
1:D:576:PRO:HA	1:D:579:MET:HE3	1.63	0.79
2:E:326:GLY:O	2:E:328:GLN:N	2.17	0.78
1:D:619:LEU:HA	1:D:622:MET:HE3	1.66	0.78
3:G:145:GLU:HB2	3:G:168:SER:HB2	1.66	0.77
10:O:180:GLY:HA3	10:O:197:SER:HA	1.65	0.77
5:H:205:DC:O2	9:T:22:DG:N2	2.14	0.77
3:G:330:CYS:H	3:G:354:GLY:HA3	1.48	0.76
6:X:84:MET:HE1	6:X:101:GLY:HA3	1.68	0.76
2:E:682:ALA:O	2:E:690:ARG:NH1	2.19	0.75
5:H:182:DC:H42	9:T:45:DA:H61	1.32	0.75
7:R:25:PHE:HE2	7:R:56:GLU:HA	1.52	0.74
7:U:87:VAL:HG11	7:U:97:LEU:HD12	1.67	0.74
1:D:319:MET:HB2	1:D:353:PRO:HB2	1.69	0.74
2:E:512:GLN:HA	2:E:516:ASP:HB2	1.68	0.74
5:H:97:DT:H4'	5:H:98:DA:H5'	1.69	0.74
5:H:64:DG:O6	9:T:163:DC:N4	2.20	0.73
10:O:160:LYS:HD3	10:O:161:PRO:HD2	1.70	0.73
4:W:121:PRO:O	4:W:125:GLN:NE2	2.21	0.73
5:H:54:DC:H42	9:T:173:DA:H61	1.33	0.73
9:T:153:DA:OP2	7:U:35:ARG:NH2	2.22	0.73
2:E:448:LEU:HD13	2:E:459:ILE:HD12	1.69	0.72
7:U:42:ARG:HB2	8:V:85:THR:HG22	1.70	0.72
1:D:650:LYS:HB2	1:D:652:LEU:HD22	1.71	0.72
3:G:172:ILE:HB	3:G:186:TYR:HB2	1.72	0.71
5:H:80:DG:N2	9:T:148:DC:O2	2.24	0.71
2:E:60:TRP:HE1	3:G:105:SER:H	1.39	0.71
6:J:98:TYR:OH	8:S:65:ASP:OD2	2.07	0.71
4:I:106:ASP:HA	4:I:109:LEU:HD12	1.73	0.70
5:H:194:DC:O2	9:T:33:DG:N2	2.17	0.70
1:D:613:VAL:HG12	1:D:652:LEU:HD12	1.74	0.69
2:E:575:GLN:NE2	9:T:44:DG:O3'	2.21	0.69
5:H:109:DG:N2	9:T:119:DC:O2	2.26	0.69
2:E:585:CYS:HB2	2:E:590:CYS:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:176:ASN:HB3	3:G:179:THR:HG22	1.75	0.69
9:T:152:DC:H5''	7:U:44:GLY:HA2	1.74	0.69
5:H:179:DT:H2''	5:H:180:DC:H5'	1.75	0.68
6:X:64:ASN:O	6:X:93:GLN:NE2	2.25	0.68
1:D:158:GLN:HE22	1:D:232:VAL:HG13	1.58	0.68
3:G:210:SER:OG	3:G:212:ASP:OD1	2.11	0.68
4:I:37:LYS:NZ	4:I:38:PRO:O	2.24	0.68
5:H:84:DC:H42	9:T:143:DA:H61	1.41	0.68
5:H:37:DC:O2	9:T:190:DG:N2	2.20	0.68
3:G:264:ARG:NH2	3:G:340:ILE:O	2.27	0.68
8:V:116:THR:HA	8:V:119:THR:HG22	1.74	0.68
8:V:35:ALA:HA	8:V:56:MET:HE3	1.76	0.67
10:O:386:GLU:HB3	10:O:389:VAL:HG12	1.76	0.67
7:R:62:ILE:HG13	7:R:93:LEU:HD21	1.76	0.67
10:O:318:ASP:OD2	10:O:338:THR:OG1	2.10	0.67
10:O:133:MET:HE2	10:O:135:GLN:HB2	1.76	0.67
10:O:77:ASN:ND2	10:O:125:GLY:O	2.26	0.67
5:H:189:DG:N2	9:T:38:DC:O2	2.19	0.67
3:G:99:VAL:HG11	3:G:428:VAL:HG21	1.77	0.66
3:G:281:ASN:HB3	3:G:284:LYS:HG2	1.77	0.66
5:H:189:DG:N1	9:T:38:DC:N3	2.36	0.66
4:I:67:PHE:CD2	4:I:93:GLN:HG3	2.31	0.66
6:J:51:TYR:O	6:J:55:ARG:NH2	2.29	0.66
5:H:57:DG:O6	9:T:169:DC:N4	2.28	0.66
10:O:198:ASP:HA	10:O:229:VAL:HG13	1.76	0.66
2:E:586:ASP:HB3	2:E:589:LEU:HB2	1.78	0.66
6:J:39:ARG:NH1	6:J:44:LYS:O	2.28	0.66
3:G:86:ASN:ND2	3:G:130:GLY:O	2.28	0.66
4:I:123:ASP:OD1	4:W:113:HIS:NE2	2.28	0.66
5:H:51:DA:N6	9:T:176:DT:O4	2.20	0.66
10:O:204:LEU:O	10:O:220:LYS:N	2.26	0.66
3:G:211:LYS:HA	3:G:238:GLU:HG3	1.77	0.66
4:I:60:LEU:HD13	4:I:93:GLN:OE1	1.96	0.66
1:D:521:LYS:HD3	1:D:577:GLN:HG3	1.77	0.65
2:E:541:CYS:SG	2:E:560:ASN:ND2	2.68	0.65
5:H:192:DG:O6	9:T:34:DC:N4	2.29	0.65
2:E:236:THR:O	2:E:240:LEU:N	2.29	0.65
7:U:79:ILE:HG22	7:U:82:HIS:HD2	1.61	0.65
2:E:521:HIS:O	2:E:545:GLN:NE2	2.30	0.65
2:E:501:HIS:HA	2:E:504:TRP:CD1	2.32	0.65
7:R:25:PHE:HD2	7:R:56:GLU:HG2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:106:HIS:O	8:V:109:SER:OG	2.12	0.65
2:E:181:TYR:OH	2:E:220:SER:OG	2.15	0.64
10:O:93:PHE:HB2	11:Y:171:LYS:HD3	1.79	0.64
1:D:526:THR:HG23	10:O:36:MET:HE1	1.79	0.64
2:E:71:LEU:HB2	3:G:136:GLN:HG2	1.78	0.64
2:E:330:TYR:HE1	2:E:457:CYS:HB2	1.63	0.64
3:G:242:ALA:O	3:G:313:ARG:NH2	2.31	0.64
6:J:78:ARG:NH2	6:J:85:ASP:OD2	2.28	0.64
3:G:245:ASP:OD2	3:G:250:LYS:N	2.24	0.64
5:H:80:DG:OP2	8:V:83:ARG:NH2	2.29	0.64
7:U:20:ARG:NH1	8:V:121:ALA:O	2.30	0.64
4:W:102:ALA:O	4:W:131:ARG:NH2	2.29	0.64
2:E:620:LEU:HD11	2:E:634:LYS:HB3	1.80	0.64
2:E:624:SER:N	2:E:628:GLY:O	2.31	0.64
7:R:29:ARG:NH1	8:S:32:GLU:OE2	2.31	0.64
10:O:188:ASN:HB2	10:O:240:GLU:HB3	1.79	0.64
10:O:85:GLN:HB2	10:O:114:LYS:HB3	1.79	0.63
2:E:288:ARG:NH2	2:E:709:GLY:O	2.25	0.63
3:G:207:LEU:HB2	3:G:217:LEU:HD12	1.80	0.63
10:O:106:GLY:N	10:O:109:GLY:O	2.30	0.63
2:E:567:CYS:O	2:E:592:THR:OG1	2.10	0.63
7:R:64:GLU:HA	8:S:46:HIS:HE1	1.61	0.63
5:H:41:DC:H2"	5:H:42:DA:C8	2.34	0.63
11:Y:224:SER:OG	11:Y:259:ARG:NH1	2.31	0.63
6:J:44:LYS:HB2	7:R:115:LEU:HD13	1.81	0.62
1:D:586:GLU:HG2	1:D:588:ASP:H	1.64	0.62
6:J:84:MET:HA	6:J:84:MET:HE3	1.81	0.62
1:D:125:THR:HB	10:O:410:ASN:HD21	1.65	0.62
10:O:292:GLY:HA2	10:O:298:VAL:HA	1.79	0.62
1:D:641:GLU:HA	1:D:680:LYS:HE2	1.82	0.62
6:X:29:ILE:O	6:X:55:ARG:NH1	2.33	0.62
3:G:89:LYS:HA	3:G:433:SER:HA	1.82	0.61
5:H:37:DC:N3	9:T:190:DG:N1	2.36	0.61
2:E:671:LEU:HD13	2:E:681:ASP:HB3	1.82	0.61
8:V:38:VAL:HB	8:V:56:MET:HE1	1.81	0.61
5:H:142:DG:N2	9:T:86:DC:O2	2.33	0.61
2:E:160:ASP:HA	3:G:306:ARG:HE	1.66	0.61
10:O:81:ILE:HB	10:O:119:ILE:HB	1.83	0.61
2:E:653:GLN:OE1	4:I:26:ARG:NE	2.33	0.61
2:E:664:ASP:OD1	2:E:741:TYR:OH	2.16	0.61
2:E:528:CYS:HB2	2:E:540:PRO:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:38:ALA:HB1	6:J:43:VAL:HB	1.83	0.61
1:D:556:THR:OG1	11:Y:173:ARG:NH2	2.34	0.61
2:E:529:ASP:HA	2:E:553:GLN:HB2	1.82	0.61
2:E:701:TYR:CZ	2:E:716:PHE:HB2	2.36	0.61
3:G:86:ASN:HB3	3:G:436:ARG:HB3	1.82	0.61
10:O:251:LYS:HE2	10:O:268:SER:HB3	1.83	0.61
2:E:502:ARG:NH1	4:I:39:HIS:O	2.33	0.61
9:T:32:DC:H2'	9:T:33:DG:C8	2.36	0.60
9:T:193:DC:H2'	9:T:194:DG:C8	2.36	0.60
10:O:281:PHE:CD1	10:O:289:LEU:HD13	2.36	0.60
2:E:86:THR:HA	2:E:93:THR:HG23	1.83	0.60
2:E:100:THR:HG23	3:G:141:ALA:HB3	1.83	0.60
2:E:554:CYS:HB3	2:E:558:CYS:HB2	1.84	0.60
3:G:201:ARG:NH1	3:G:247:LEU:O	2.34	0.60
5:H:182:DC:O2	9:T:46:DG:N2	2.35	0.60
6:J:84:MET:HE1	6:J:101:GLY:HA3	1.83	0.60
9:T:98:DT:H2''	9:T:99:DA:C8	2.37	0.60
9:T:122:DC:H2'	9:T:123:DG:C8	2.38	0.59
10:O:79:LEU:HD21	10:O:140:ILE:HD11	1.83	0.59
2:E:556:SER:O	2:E:561:ARG:NH2	2.34	0.59
8:S:73:GLU:HG3	8:S:98:LEU:HD21	1.84	0.59
2:E:660:GLY:O	2:E:664:ASP:N	2.29	0.59
4:I:108:ASN:ND2	6:J:42:GLY:O	2.36	0.59
4:I:61:LEU:HD12	6:J:37:LEU:HD23	1.83	0.59
10:O:169:PRO:HG2	10:O:215:LYS:HZ3	1.66	0.59
5:H:40:DA:N6	9:T:186:DG:O6	2.36	0.59
2:E:587:PRO:HA	2:E:595:ALA:HB1	1.83	0.59
2:E:610:SER:O	2:E:614:GLY:N	2.35	0.59
2:E:693:ASN:OD1	12:E:801:SAH:N6	2.35	0.59
5:H:50:DT:H2'	5:H:51:DA:C8	2.37	0.59
7:R:97:LEU:HD22	7:R:100:VAL:HG11	1.84	0.59
6:J:29:ILE:O	6:J:55:ARG:NH1	2.36	0.59
10:O:178:LYS:NZ	10:O:199:ASP:OD1	2.29	0.59
2:E:336:ALA:HB1	2:E:472:TYR:HE2	1.68	0.58
10:O:393:VAL:HG13	10:O:399:MET:HE1	1.83	0.58
1:D:247:SER:HB2	1:D:302:PHE:HB3	1.84	0.58
7:U:79:ILE:HG22	7:U:82:HIS:CD2	2.37	0.58
10:O:127:VAL:HG13	10:O:142:THR:HG23	1.84	0.58
1:D:189:VAL:HG23	1:D:205:GLN:HG3	1.84	0.58
10:O:61:PHE:HB2	10:O:85:GLN:HB3	1.83	0.58
10:O:65:ARG:HA	10:O:83:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:92:GLN:NE2	8:S:96:ARG:HH12	2.02	0.58
8:V:90:GLU:N	8:V:90:GLU:OE2	2.36	0.58
2:E:52:ARG:HD3	3:G:246:LEU:HB2	1.86	0.58
2:E:289:CYS:HB2	2:E:297:HIS:NE2	2.19	0.58
2:E:470:GLN:HA	2:E:473:GLU:HB2	1.86	0.58
2:E:647:CYS:SG	2:E:687:ASN:ND2	2.75	0.58
3:G:338:ASP:HA	3:G:342:LYS:HE2	1.84	0.58
1:D:157:LEU:HD11	1:D:359:LEU:HD11	1.85	0.58
3:G:240:LEU:O	3:G:367:ARG:NH2	2.37	0.58
7:U:84:GLN:NE2	7:U:88:ARG:HE	1.97	0.58
10:O:236:HIS:HA	10:O:281:PHE:CD2	2.38	0.58
5:H:47:DG:H2'	5:H:48:DT:H71	1.86	0.58
7:U:34:LEU:HB3	7:U:43:VAL:HG21	1.84	0.58
1:D:103:ARG:NH1	11:Y:283:ASN:O	2.37	0.57
3:G:383:VAL:HG23	3:G:385:LYS:HG3	1.85	0.57
6:X:73:THR:HG23	6:X:78:ARG:HB2	1.86	0.57
1:D:572:LEU:HD11	3:G:225:LEU:HD22	1.86	0.57
2:E:624:SER:HB3	2:E:630:GLY:HA3	1.86	0.57
9:T:89:DA:H1'	9:T:90:DG:C8	2.39	0.57
5:H:29:DC:H42	9:T:197:DC:H42	1.50	0.57
9:T:163:DC:H2''	9:T:164:DA:H8	1.69	0.57
2:E:163:CYS:SG	2:E:167:ASN:ND2	2.77	0.57
7:R:25:PHE:CE2	7:R:56:GLU:HA	2.38	0.57
9:T:162:DG:OP1	8:V:37:TYR:OH	2.19	0.57
1:D:605:ASP:HA	2:E:257:PRO:HD3	1.85	0.57
10:O:36:MET:HB3	10:O:401:VAL:HB	1.87	0.57
1:D:570:THR:O	3:G:216:ARG:NH1	2.38	0.57
7:R:31:HIS:HD2	7:R:48:PRO:HG3	1.70	0.57
10:O:341:ARG:HE	10:O:371:GLY:HA3	1.69	0.57
1:D:569:ASP:N	1:D:584:GLU:OE1	2.37	0.57
5:H:168:DC:H2''	5:H:169:DG:C8	2.40	0.56
6:J:78:ARG:HH22	6:J:85:ASP:CG	2.13	0.56
7:U:16:THR:HG22	7:U:18:SER:H	1.70	0.56
3:G:119:ASN:HB2	3:G:140:ASP:HB3	1.87	0.56
5:H:46:DT:O3'	4:W:41:TYR:OH	2.23	0.56
10:O:148:ASP:OD2	10:O:172:ARG:NH1	2.32	0.56
1:D:647:ILE:HA	1:D:652:LEU:HD21	1.87	0.56
3:G:160:HIS:HB3	3:G:178:ILE:HD13	1.87	0.56
5:H:207:DG:H2''	5:H:208:DA:C8	2.39	0.56
3:G:145:GLU:OE1	3:G:168:SER:N	2.38	0.56
2:E:228:SER:HB3	2:E:234:LYS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:501:HIS:HA	2:E:504:TRP:HD1	1.69	0.56
2:E:675:ASN:OD1	2:E:678:PHE:N	2.31	0.56
3:G:406:HIS:HB2	3:G:437:TRP:CZ2	2.41	0.56
4:I:92:LEU:HD22	6:J:86:VAL:HG11	1.87	0.56
7:R:79:ILE:HB	7:R:82:HIS:HD1	1.71	0.56
10:O:293:SER:OG	10:O:297:THR:OG1	2.19	0.56
3:G:193:ILE:HG12	3:G:210:SER:HB3	1.87	0.56
10:O:49:TRP:NE1	10:O:391:CYS:SG	2.79	0.56
2:E:433:GLU:H	2:E:470:GLN:HG2	1.70	0.56
9:T:88:DC:H2''	9:T:89:DA:C8	2.40	0.56
1:D:214:PRO:HD2	1:D:217:PRO:HG3	1.87	0.56
10:O:196:ALA:HB1	10:O:230:VAL:HG13	1.86	0.56
6:X:59:LYS:NZ	6:X:63:GLU:OE2	2.38	0.56
10:O:24:TRP:CE2	10:O:372:GLY:HA3	2.40	0.56
3:G:116:VAL:HG12	3:G:121:VAL:HG12	1.87	0.55
11:Y:243:TRP:HD1	11:Y:248:ILE:HD12	1.72	0.55
4:W:79:LYS:HD3	6:X:74:GLU:OE2	2.06	0.55
2:E:663:TYR:O	2:E:667:MET:N	2.40	0.55
3:G:311:CYS:HB2	3:G:322:LYS:HB2	1.88	0.55
1:D:184:LEU:HD22	1:D:211:LYS:HE2	1.88	0.55
1:D:431:GLN:HG2	1:D:441:GLN:HG3	1.89	0.55
3:G:423:SER:HA	3:G:439:ARG:HB3	1.89	0.55
9:T:50:DC:H2''	9:T:51:DC:H5''	1.87	0.55
10:O:382:TRP:HE3	10:O:390:ILE:HG12	1.71	0.55
9:T:153:DA:OP1	7:U:35:ARG:NH1	2.40	0.55
2:E:121:MET:HA	2:E:650:ILE:HB	1.88	0.55
5:H:56:DT:H2''	5:H:57:DG:N7	2.22	0.55
9:T:133:DC:H2'	9:T:134:DG:C8	2.42	0.55
10:O:132:TYR:HB3	10:O:140:ILE:HG22	1.88	0.55
5:H:148:DT:H3	9:T:79:DA:H61	1.53	0.55
3:G:226:VAL:HG12	3:G:227:ALA:H	1.71	0.55
7:R:31:HIS:CD2	7:R:48:PRO:HG3	2.42	0.55
1:D:450:CYS:HB3	1:D:455:LEU:H	1.72	0.54
2:E:631:ILE:HG13	2:E:689:ILE:HA	1.90	0.54
3:G:118:SER:OG	3:G:146:ASN:ND2	2.41	0.54
2:E:673:ASN:N	4:I:27:LYS:O	2.32	0.54
9:T:126:DT:H2''	9:T:127:DT:H5'	1.89	0.54
10:O:281:PHE:CE1	10:O:289:LEU:HD13	2.42	0.54
1:D:481:HIS:ND1	1:D:486:ARG:HD3	2.23	0.54
2:E:46:ARG:NH1	3:G:391:LEU:O	2.40	0.54
2:E:562:PHE:CD1	2:E:583:ARG:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:22:GLY:HA3	8:S:117:LYS:NZ	2.23	0.54
3:G:389:TRP:NE1	3:G:401:CYS:SG	2.76	0.54
10:O:327:PRO:HD3	10:O:382:TRP:CD1	2.43	0.54
1:D:632:MET:HE3	1:D:668:LEU:HB2	1.90	0.54
2:E:643:ILE:HG22	2:E:644:SER:H	1.72	0.54
3:G:412:ALA:O	3:G:430:ASP:N	2.34	0.54
4:W:100:LEU:HD11	6:X:58:LEU:HD13	1.89	0.54
1:D:631:GLN:HG2	2:E:599:TRP:CE2	2.43	0.54
2:E:39:LYS:NZ	3:G:393:VAL:O	2.40	0.54
2:E:105:ALA:O	3:G:169:ARG:NH2	2.41	0.54
2:E:331:GLN:O	2:E:469:ARG:NH2	2.41	0.54
3:G:379:LEU:O	3:G:387:TYR:N	2.33	0.54
2:E:296:LEU:HD23	2:E:296:LEU:H	1.73	0.53
1:D:562:ASN:OD1	1:D:563:ARG:N	2.41	0.53
3:G:90:GLU:HG3	3:G:92:HIS:H	1.73	0.53
3:G:127:HIS:HB2	3:G:131:GLU:HB3	1.90	0.53
3:G:384:GLY:HA2	3:G:413:ILE:HG12	1.91	0.53
5:H:54:DC:N4	9:T:173:DA:H61	2.05	0.53
6:J:75:HIS:HB2	8:V:93:THR:HG21	1.91	0.53
2:E:599:TRP:HA	2:E:613:ARG:NH2	2.23	0.53
5:H:77:DG:H1	9:T:150:DC:H42	1.57	0.53
4:I:39:HIS:NE2	5:H:183:DC:H4'	2.23	0.53
4:I:57:SER:O	6:J:40:ARG:NH2	2.38	0.53
9:T:17:DC:H1'	9:T:18:DG:H5'	1.89	0.53
3:G:406:HIS:HB2	3:G:437:TRP:HZ2	1.74	0.53
5:H:150:DC:H1'	5:H:151:DG:C8	2.44	0.53
2:E:659:ARG:NH1	2:E:681:ASP:OD2	2.42	0.53
2:E:700:CYS:HA	2:E:717:ALA:HA	1.90	0.53
10:O:318:ASP:CG	10:O:319:GLU:H	2.17	0.53
1:D:607:ASN:HB2	1:D:610:GLU:HG2	1.91	0.53
2:E:570:GLN:HB2	2:E:606:CYS:HA	1.89	0.53
2:E:657:ASP:OD1	4:I:26:ARG:NH1	2.31	0.53
3:G:153:THR:HG21	3:G:174:ILE:HD11	1.91	0.53
3:G:169:ARG:NH1	3:G:171:ILE:HD12	2.24	0.53
10:O:271:ALA:HB3	10:O:276:VAL:HG21	1.90	0.53
3:G:80:TYR:HA	3:G:402:THR:HG21	1.91	0.53
3:G:164:ALA:HA	3:G:174:ILE:HA	1.91	0.53
9:T:76:DC:H2''	9:T:77:DG:C8	2.44	0.53
1:D:532:ARG:HH21	10:O:93:PHE:HZ	1.57	0.52
5:H:66:DC:H2''	5:H:67:DT:C5	2.44	0.52
5:H:139:DA:H2''	5:H:140:DG:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:274:ALA:HB3	10:O:295:ASP:HB2	1.91	0.52
3:G:96:LEU:HG	3:G:432:ALA:HA	1.90	0.52
9:T:68:DC:H4'	9:T:69:DT:OP1	2.08	0.52
10:O:177:GLN:N	10:O:199:ASP:OD2	2.42	0.52
1:D:499:TYR:HB3	1:D:506:ILE:HD11	1.90	0.52
4:W:125:GLN:HA	4:W:134:ARG:NH1	2.24	0.52
10:O:316:HIS:NE2	10:O:335:SER:OG	2.43	0.52
1:D:478:TYR:OH	1:D:484:GLY:O	2.27	0.52
1:D:643:TYR:O	1:D:647:ILE:HG12	2.09	0.52
7:R:57:TYR:HB2	8:S:110:GLU:HG3	1.90	0.52
10:O:170:ASP:HA	10:O:215:LYS:HE2	1.91	0.52
10:O:313:PHE:HB3	10:O:345:TRP:CZ2	2.44	0.52
1:D:575:ARG:NH1	1:D:578:GLU:OE1	2.41	0.52
2:E:221:ASP:HA	2:E:224:PHE:CD2	2.43	0.52
2:E:224:PHE:HB3	2:E:237:ALA:H	1.75	0.52
11:Y:225:THR:N	11:Y:242:HIS:O	2.42	0.52
5:H:101:DA:OP2	6:J:30:THR:OG1	2.28	0.52
2:E:507:HIS:ND1	2:E:559:GLN:O	2.41	0.52
5:H:166:DC:N3	9:T:60:DA:N6	2.58	0.52
1:D:607:ASN:ND2	2:E:261:THR:O	2.36	0.52
3:G:252:MET:SD	3:G:262:LEU:HB3	2.50	0.52
4:I:48:LEU:HB3	4:I:52:ARG:NH2	2.24	0.52
2:E:683:THR:O	2:E:690:ARG:NH1	2.43	0.51
2:E:704:VAL:HG22	2:E:713:ILE:HG22	1.92	0.51
5:H:35:DT:H2''	5:H:36:DG:C8	2.45	0.51
7:R:104:GLN:HE22	8:S:54:LYS:NZ	2.07	0.51
5:H:194:DC:H42	9:T:32:DC:H42	1.56	0.51
1:D:250:LEU:N	1:D:299:MET:O	2.36	0.51
4:I:46:VAL:HB	9:T:123:DG:OP2	2.10	0.51
10:O:43:PRO:O	10:O:71:HIS:N	2.43	0.51
6:J:35:ARG:HG3	6:J:46:ILE:HD12	1.90	0.51
9:T:69:DT:H2''	9:T:70:DA:C8	2.46	0.51
4:W:107:THR:HG21	4:W:124:ILE:HG12	1.92	0.51
10:O:68:LEU:HB2	10:O:80:VAL:HG13	1.93	0.51
1:D:311:LEU:HD12	1:D:313:GLY:H	1.75	0.51
2:E:273:GLN:HA	2:E:446:ARG:HD2	1.91	0.51
2:E:475:ARG:HA	2:E:478:GLU:HB2	1.93	0.51
7:U:100:VAL:HG12	6:X:96:THR:OG1	2.10	0.51
6:X:39:ARG:NH1	6:X:43:VAL:O	2.44	0.51
10:O:36:MET:HE3	10:O:37:THR:N	2.26	0.51
2:E:29:LEU:HA	2:E:32:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:500:LYS:HG3	2:E:502:ARG:H	1.75	0.51
2:E:503:LEU:O	2:E:507:HIS:N	2.33	0.51
3:G:177:PRO:O	3:G:180:MET:HE2	2.10	0.51
9:T:66:DC:H2''	9:T:67:DC:C5	2.45	0.51
2:E:236:THR:HG23	2:E:239:GLU:H	1.75	0.51
2:E:628:GLY:HA3	12:E:801:SAH:C	2.40	0.51
3:G:406:HIS:NE2	3:G:408:LYS:HB2	2.25	0.51
5:H:191:DC:H2''	5:H:192:DG:C8	2.45	0.51
4:W:83:ARG:O	6:X:80:THR:HA	2.10	0.51
2:E:437:TRP:HE1	2:E:466:LYS:HG2	1.76	0.51
2:E:643:ILE:HG12	2:E:716:PHE:HA	1.92	0.51
4:I:37:LYS:HD2	4:I:38:PRO:HD2	1.92	0.51
7:R:25:PHE:CD2	7:R:56:GLU:HG2	2.45	0.51
9:T:172:DG:H4'	7:U:77:ARG:HH21	1.76	0.51
4:W:116:ARG:NH2	4:W:123:ASP:OD1	2.43	0.51
7:R:80:PRO:HD3	8:S:55:ALA:HB2	1.94	0.50
2:E:54:GLU:O	2:E:58:GLN:NE2	2.26	0.50
3:G:237:ASP:HB2	3:G:257:ASP:HB2	1.92	0.50
5:H:79:DA:OP1	8:V:84:SER:OG	2.23	0.50
7:U:79:ILE:HG13	7:U:80:PRO:HD2	1.92	0.50
10:O:118:GLU:O	10:O:159:SER:OG	2.29	0.50
3:G:82:PHE:HB2	3:G:404:LEU:HD21	1.92	0.50
3:G:90:GLU:HB3	3:G:432:ALA:HB1	1.94	0.50
3:G:222:THR:HG21	3:G:278:TYR:HA	1.93	0.50
3:G:386:LEU:HB2	3:G:404:LEU:HB2	1.93	0.50
3:G:387:TYR:HB3	3:G:389:TRP:CZ3	2.46	0.50
5:H:25:DA:N6	9:T:201:DA:N1	2.59	0.50
9:T:124:DC:H2''	9:T:125:DG:H8	1.77	0.50
7:U:31:HIS:HD1	7:U:48:PRO:HG3	1.75	0.50
1:D:652:LEU:H	1:D:652:LEU:HD23	1.75	0.50
9:T:77:DG:H4'	9:T:78:DT:H5'	1.94	0.50
3:G:230:GLY:O	3:G:295:HIS:ND1	2.27	0.50
5:H:166:DC:H1'	5:H:167:DT:C6	2.47	0.50
8:V:40:LYS:O	8:V:43:LYS:N	2.44	0.50
8:V:76:ARG:O	8:V:80:TYR:N	2.39	0.50
10:O:350:ILE:HA	10:O:365:GLU:HB3	1.94	0.50
3:G:239:VAL:HA	3:G:255:GLY:HA3	1.93	0.50
1:D:569:ASP:OD1	1:D:570:THR:N	2.45	0.50
3:G:206:LEU:HB3	3:G:220:ILE:HD11	1.94	0.50
3:G:311:CYS:O	3:G:322:LYS:N	2.43	0.50
3:G:332:LYS:HD3	3:G:336:MET:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:79:ILE:HG22	7:R:81:ARG:H	1.76	0.50
7:U:58:LEU:HD23	8:V:66:VAL:HG11	1.94	0.50
4:W:109:LEU:O	4:W:113:HIS:N	2.40	0.50
2:E:108:PRO:HG2	2:E:629:TRP:CE2	2.46	0.50
3:G:169:ARG:HH12	3:G:171:ILE:HD12	1.76	0.50
4:I:40:ARG:HD2	9:T:124:DC:H5"	1.94	0.50
9:T:77:DG:H1'	9:T:78:DT:C6	2.47	0.50
9:T:108:DT:H2"	9:T:109:DA:C8	2.47	0.50
1:D:156:HIS:CE1	1:D:235:ASN:HB2	2.47	0.49
9:T:171:DA:H2"	9:T:172:DG:C8	2.47	0.49
10:O:404:MET:SD	10:O:404:MET:N	2.84	0.49
5:H:52:DT:H2'	5:H:53:DA:C8	2.48	0.49
5:H:106:DG:H2"	5:H:107:DG:N7	2.27	0.49
7:R:63:LEU:HA	7:R:66:ALA:HB3	1.94	0.49
1:D:295:PHE:HA	1:D:320:GLN:O	2.13	0.49
2:E:470:GLN:O	2:E:474:PHE:HB2	2.12	0.49
2:E:649:GLU:O	2:E:680:VAL:HA	2.13	0.49
5:H:161:DG:OP1	8:S:37:TYR:OH	2.24	0.49
5:H:185:DA:N6	9:T:42:DC:H42	2.10	0.49
11:Y:229:LYS:HG2	11:Y:239:LEU:HD22	1.94	0.49
1:D:249:SER:HA	1:D:300:THR:HA	1.94	0.49
2:E:99:LYS:HB3	3:G:138:TYR:CD1	2.47	0.49
2:E:437:TRP:NE1	2:E:466:LYS:HG2	2.27	0.49
2:E:619:LEU:HD13	2:E:631:ILE:HG21	1.93	0.49
3:G:99:VAL:O	3:G:417:SER:OG	2.20	0.49
3:G:207:LEU:HA	3:G:217:LEU:HA	1.94	0.49
10:O:173:LEU:HB3	10:O:205:TRP:CE2	2.47	0.49
11:Y:205:PHE:HE1	11:Y:280:LEU:HD12	1.78	0.49
3:G:114:ALA:HA	3:G:123:LEU:HA	1.95	0.49
3:G:171:ILE:HG12	3:G:187:VAL:HG23	1.94	0.49
1:D:481:HIS:CG	1:D:482:PRO:HD2	2.47	0.49
7:U:73:ASN:HB3	7:U:82:HIS:HE1	1.78	0.49
10:O:70:THR:OG1	10:O:78:HIS:O	2.21	0.49
1:D:631:GLN:O	1:D:635:ALA:N	2.40	0.49
2:E:636:PRO:HB3	2:E:722:GLN:HA	1.94	0.49
5:H:56:DT:H1'	5:H:57:DG:C5	2.47	0.49
7:R:88:ARG:HB2	7:R:108:LEU:HD21	1.94	0.49
1:D:627:ILE:HD13	2:E:612:GLN:NE2	2.28	0.49
1:D:637:MET:HE2	1:D:637:MET:HA	1.95	0.49
3:G:304:ILE:HD11	3:G:350:VAL:HG11	1.94	0.49
5:H:141:DA:H2"	5:H:142:DG:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:63:LEU:HD21	8:V:59:MET:HE3	1.94	0.49
4:W:120:MET:N	4:W:123:ASP:OD2	2.35	0.49
10:O:215:LYS:HD3	10:O:215:LYS:O	2.11	0.49
2:E:84:SER:HA	2:E:95:VAL:HA	1.95	0.49
3:G:113:PHE:CZ	3:G:124:TYR:HB2	2.48	0.49
7:R:88:ARG:NH2	7:R:100:VAL:O	2.46	0.49
1:D:565:TYR:HA	2:E:622:ALA:HB2	1.94	0.48
2:E:706:MET:HE1	2:E:709:GLY:HA2	1.95	0.48
3:G:82:PHE:CE1	3:G:439:ARG:HB2	2.47	0.48
4:I:118:THR:N	5:H:110:DA:OP1	2.42	0.48
1:D:458:ARG:NE	10:O:357:GLU:OE2	2.43	0.48
5:H:73:DC:H2'	5:H:74:DT:C6	2.48	0.48
5:H:121:DG:H2'	5:H:122:DT:H71	1.95	0.48
9:T:127:DT:H1'	9:T:128:DT:C5	2.47	0.48
7:U:79:ILE:O	7:U:82:HIS:N	2.46	0.48
1:D:606:VAL:HG13	1:D:610:GLU:HG3	1.94	0.48
2:E:622:ALA:HB3	2:E:632:PHE:CE1	2.48	0.48
10:O:278:CYS:HB2	10:O:323:VAL:HG22	1.95	0.48
2:E:695:SER:HB3	2:E:698:PRO:HB3	1.95	0.48
3:G:86:ASN:HB3	3:G:436:ARG:HD3	1.94	0.48
4:I:67:PHE:HD2	4:I:93:GLN:HG3	1.75	0.48
5:H:185:DA:H61	9:T:42:DC:H42	1.61	0.48
9:T:191:DC:H2''	9:T:192:DA:C8	2.49	0.48
1:D:627:ILE:HD13	2:E:612:GLN:HE21	1.78	0.48
1:D:666:PHE:HB2	1:D:668:LEU:HD23	1.95	0.48
2:E:180:GLN:HE22	2:E:223:ILE:HG21	1.79	0.48
3:G:97:PHE:C	3:G:415:GLN:HG3	2.38	0.48
3:G:199:HIS:CE1	3:G:201:ARG:HB2	2.49	0.48
4:I:68:GLN:HG2	4:I:72:ARG:HE	1.79	0.48
4:I:72:ARG:HH12	5:H:90:DT:P	2.36	0.48
10:O:120:LYS:HB2	10:O:161:PRO:HD3	1.93	0.48
10:O:253:MET:SD	10:O:268:SER:OG	2.70	0.48
10:O:302:ASP:OD1	10:O:303:LEU:N	2.47	0.48
10:O:380:PHE:HA	10:O:392:SER:HA	1.96	0.48
1:D:567:HIS:HB3	1:D:569:ASP:OD1	2.12	0.48
2:E:52:ARG:HD2	3:G:246:LEU:HD12	1.95	0.48
2:E:287:ARG:HA	2:E:290:PHE:HA	1.95	0.48
2:E:670:PHE:HD2	2:E:683:THR:HA	1.79	0.48
3:G:371:ASP:CG	3:G:375:LYS:H	2.19	0.48
5:H:175:DG:O6	9:T:51:DC:N4	2.46	0.48
4:W:37:LYS:HB3	4:W:38:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:298:VAL:O	10:O:313:PHE:N	2.44	0.48
3:G:219:ASN:O	3:G:223:ASP:N	2.46	0.48
3:G:260:LEU:O	3:G:300:SER:HA	2.13	0.48
9:T:150:DC:H4'	9:T:151:DC:OP1	2.10	0.48
6:X:68:ASP:OD2	6:X:92:ARG:NH2	2.42	0.48
3:G:245:ASP:HB3	3:G:314:TRP:CD2	2.48	0.48
4:I:23:LYS:NZ	4:I:26:ARG:HD2	2.29	0.48
1:D:91:GLU:HB3	1:D:95:GLN:NE2	2.29	0.48
7:U:93:LEU:HD22	8:V:103:LEU:HD11	1.96	0.48
1:D:510:PRO:HG2	3:G:183:ILE:HG23	1.94	0.48
2:E:60:TRP:NE1	3:G:105:SER:H	2.07	0.48
2:E:160:ASP:HA	3:G:306:ARG:HH21	1.79	0.48
5:H:45:DA:H2'	5:H:46:DT:H71	1.95	0.48
5:H:86:DC:H2''	5:H:87:DC:C5	2.49	0.48
7:R:64:GLU:HA	8:S:46:HIS:CE1	2.47	0.48
9:T:48:DA:H2'	9:T:49:DT:C6	2.49	0.48
9:T:168:DG:H2''	9:T:169:DC:C6	2.49	0.48
10:O:49:TRP:CG	10:O:383:ASN:HB3	2.48	0.47
2:E:224:PHE:HB3	2:E:236:THR:HA	1.96	0.47
2:E:598:HIS:ND1	2:E:601:SER:HB2	2.28	0.47
4:W:92:LEU:O	4:W:96:SER:N	2.46	0.47
11:Y:293:LEU:HG	11:Y:294:LYS:HG2	1.96	0.47
7:R:71:ARG:O	7:R:74:LYS:HD2	2.14	0.47
2:E:38:VAL:HA	2:E:41:MET:HE2	1.97	0.47
3:G:320:LEU:HA	3:G:330:CYS:HA	1.95	0.47
3:G:358:TYR:HE2	3:G:361:CYS:HB3	1.78	0.47
5:H:79:DA:H2''	5:H:80:DG:C8	2.49	0.47
8:V:61:SER:OG	6:X:101:GLY:O	2.21	0.47
4:I:86:SER:OG	5:H:89:DT:OP2	2.23	0.47
5:H:40:DA:H61	9:T:187:DT:H3	1.63	0.47
10:O:175:GLY:HA3	10:O:219:ALA:HB2	1.97	0.47
5:H:165:DC:H2''	5:H:166:DC:H5'	1.96	0.47
5:H:194:DC:N3	9:T:33:DG:N1	2.55	0.47
9:T:163:DC:H2''	9:T:164:DA:C8	2.48	0.47
4:W:126:LEU:O	4:W:130:ILE:HD12	2.14	0.47
2:E:121:MET:HE2	2:E:295:PHE:C	2.40	0.47
3:G:193:ILE:HA	3:G:210:SER:HA	1.97	0.47
3:G:195:GLU:HB3	3:G:209:VAL:HB	1.97	0.47
5:H:176:DG:H2''	5:H:177:DG:C8	2.50	0.47
7:R:62:ILE:O	7:R:66:ALA:N	2.45	0.47
7:R:82:HIS:O	7:R:86:ALA:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:93:THR:HG21	6:X:75:HIS:HB2	1.97	0.47
9:T:16:DC:C2	9:T:17:DC:C4	3.03	0.47
9:T:90:DG:C4	9:T:91:DC:C5	3.03	0.47
9:T:122:DC:H4'	9:T:123:DG:OP1	2.14	0.47
7:U:77:ARG:HA	8:V:50:GLY:O	2.15	0.47
2:E:681:ASP:OD1	2:E:681:ASP:N	2.46	0.47
6:J:73:THR:HG21	6:J:81:VAL:HA	1.96	0.47
9:T:149:DC:H2''	9:T:150:DC:C6	2.49	0.47
4:W:121:PRO:HG2	6:X:49:LEU:HD23	1.95	0.47
10:O:194:LEU:HD13	10:O:233:VAL:HG22	1.96	0.47
3:G:197:LYS:HE2	3:G:243:ASP:HA	1.97	0.47
10:O:343:ASN:HD22	10:O:369:ILE:HG12	1.79	0.47
3:G:90:GLU:N	3:G:432:ALA:O	2.41	0.47
4:I:129:ARG:HD2	4:W:109:LEU:HD11	1.96	0.47
9:T:152:DC:H2''	9:T:153:DA:H8	1.80	0.47
10:O:327:PRO:HD3	10:O:382:TRP:NE1	2.30	0.47
2:E:696:VAL:HG22	2:E:745:GLU:HG3	1.98	0.46
2:E:704:VAL:HG23	4:I:29:ALA:HB3	1.95	0.46
9:T:17:DC:C4	9:T:18:DG:C6	3.03	0.46
8:V:73:GLU:OE2	8:V:76:ARG:NH2	2.48	0.46
1:D:431:GLN:NE2	1:D:439:ARG:HH12	2.13	0.46
2:E:333:LEU:HD12	2:E:469:ARG:NH1	2.30	0.46
3:G:250:LYS:HZ2	3:G:264:ARG:HG2	1.80	0.46
5:H:79:DA:H61	9:T:148:DC:H42	1.63	0.46
5:H:98:DA:C6	5:H:99:DA:C6	3.03	0.46
5:H:108:DG:N2	9:T:120:DC:O2	2.48	0.46
9:T:104:DC:H4'	9:T:105:DA:OP1	2.14	0.46
1:D:582:ASP:OD1	1:D:582:ASP:N	2.44	0.46
1:D:589:PRO:HG2	2:E:116:LEU:HA	1.96	0.46
2:E:673:ASN:HB2	4:I:26:ARG:HB3	1.97	0.46
2:E:734:SER:O	2:E:738:ALA:N	2.47	0.46
5:H:206:DT:O2	9:T:22:DG:N2	2.48	0.46
9:T:133:DC:H2''	9:T:134:DG:O5'	2.15	0.46
9:T:170:DC:H2''	9:T:171:DA:N9	2.30	0.46
11:Y:191:ASP:OD1	11:Y:192:ALA:N	2.48	0.46
2:E:524:ASN:HA	2:E:711:HIS:CD2	2.51	0.46
2:E:635:ASP:N	2:E:635:ASP:OD1	2.47	0.46
2:E:700:CYS:SG	2:E:715:ILE:HG22	2.56	0.46
3:G:371:ASP:OD1	3:G:375:LYS:N	2.39	0.46
2:E:98:LEU:HD23	3:G:139:VAL:HB	1.97	0.46
1:D:492:ASN:HB3	1:D:495:TYR:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:249:GLU:O	2:E:251:GLN:N	2.48	0.46
3:G:387:TYR:HB3	3:G:389:TRP:CH2	2.51	0.46
5:H:164:DG:N2	9:T:64:DC:O2	2.49	0.46
5:H:171:DC:H3'	7:R:75:LYS:HZ1	1.80	0.46
5:H:206:DT:O2	9:T:21:DA:H2	1.98	0.46
7:U:55:LEU:HD22	8:V:63:VAL:HG13	1.98	0.46
10:O:237:LEU:HG	10:O:281:PHE:HB2	1.98	0.46
1:D:218:ASP:OD1	1:D:218:ASP:N	2.49	0.46
2:E:701:TYR:CE1	2:E:703:LYS:HG3	2.51	0.46
5:H:162:DC:H2''	5:H:163:DG:C8	2.51	0.46
2:E:713:ILE:O	2:E:713:ILE:HG13	2.15	0.46
3:G:213:HIS:CD2	3:G:238:GLU:HA	2.51	0.46
3:G:261:LYS:HA	3:G:299:PHE:O	2.16	0.46
8:V:42:LEU:O	8:V:46:HIS:N	2.45	0.46
10:O:138:CYS:HA	10:O:154:TYR:CZ	2.51	0.46
5:H:54:DC:H42	9:T:173:DA:N6	2.09	0.46
9:T:168:DG:H2''	9:T:169:DC:N1	2.31	0.46
10:O:346:ASP:N	10:O:365:GLU:O	2.34	0.46
11:Y:214:LEU:HD12	11:Y:221:VAL:HG21	1.97	0.46
7:U:70:ALA:HA	7:U:82:HIS:CE1	2.51	0.46
1:D:528:ILE:HB	1:D:557:TYR:HB3	1.97	0.45
2:E:329:CYS:HA	2:E:468:CYS:HB3	1.98	0.45
2:E:625:ASP:HB2	2:E:746:ARG:NH1	2.31	0.45
5:H:52:DT:H2'	5:H:53:DA:H8	1.80	0.45
5:H:103:DG:H5'	5:H:103:DG:H8	1.81	0.45
7:R:97:LEU:HB3	7:R:100:VAL:CG1	2.46	0.45
3:G:83:LYS:HD3	3:G:440:LEU:HD21	1.98	0.45
5:H:118:DT:H2''	5:H:119:DA:N7	2.32	0.45
10:O:43:PRO:HG2	10:O:71:HIS:HB3	1.97	0.45
1:D:488:ASP:OD1	1:D:488:ASP:N	2.48	0.45
3:G:153:THR:HB	3:G:162:LEU:HB2	1.98	0.45
7:U:26:PRO:HD3	8:V:37:TYR:CG	2.51	0.45
5:H:122:DT:H3'	4:W:46:VAL:HG21	1.98	0.45
10:O:375:ALA:HB1	10:O:395:GLU:HB2	1.98	0.45
1:D:161:PHE:HZ	1:D:231:ALA:HB2	1.82	0.45
3:G:311:CYS:SG	3:G:367:ARG:HA	2.56	0.45
8:S:94:ALA:O	8:S:98:LEU:HG	2.16	0.45
9:T:20:DC:C4	9:T:21:DA:C6	3.04	0.45
10:O:300:LEU:HG	10:O:310:LEU:HB2	1.99	0.45
5:H:76:DG:H1'	5:H:77:DG:C4	2.52	0.45
9:T:134:DG:C5	9:T:135:DC:C4	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:318:ASP:HB3	10:O:339:ASP:HB3	1.99	0.45
1:D:565:TYR:CG	2:E:620:LEU:HD23	2.52	0.45
2:E:646:TYR:HB3	2:E:713:ILE:HD11	1.99	0.45
3:G:267:SER:O	3:G:270:MET:HG3	2.17	0.45
5:H:211:DG:N2	9:T:17:DC:N3	2.65	0.45
6:J:30:THR:OG1	6:J:32:PRO:HD2	2.17	0.45
1:D:161:PHE:CZ	1:D:231:ALA:HB2	2.52	0.45
1:D:311:LEU:HD12	1:D:313:GLY:N	2.31	0.45
1:D:632:MET:CE	1:D:668:LEU:HB2	2.47	0.45
2:E:737:ASP:HA	2:E:740:LYS:HB3	1.99	0.45
3:G:379:LEU:N	3:G:387:TYR:O	2.50	0.45
4:W:51:ILE:HD11	6:X:39:ARG:HD2	1.98	0.45
7:U:92:GLU:OE2	8:V:102:GLU:N	2.48	0.45
4:W:47:ALA:O	4:W:51:ILE:HG12	2.17	0.45
1:D:494:CYS:SG	11:Y:180:ARG:NH2	2.90	0.45
5:H:48:DT:H2''	5:H:49:DA:C8	2.51	0.45
5:H:71:DG:C8	5:H:71:DG:H5'	2.52	0.45
5:H:98:DA:H61	9:T:129:DT:H3	1.65	0.45
5:H:99:DA:H2''	5:H:100:DA:H8	1.82	0.45
5:H:208:DA:H2	9:T:19:DT:H3	1.65	0.45
8:V:53:SER:O	8:V:57:SER:N	2.46	0.45
1:D:163:GLY:HA2	1:D:217:PRO:HG2	1.99	0.44
2:E:565:CYS:HB3	2:E:590:CYS:CB	2.47	0.44
2:E:670:PHE:HB2	2:E:683:THR:OG1	2.17	0.44
5:H:39:DT:H2''	5:H:40:DA:C8	2.51	0.44
5:H:174:DC:H2'	5:H:175:DG:C8	2.52	0.44
9:T:176:DT:O4	9:T:177:DA:N6	2.50	0.44
1:D:101:ARG:HD3	1:D:452:TRP:O	2.17	0.44
6:J:98:TYR:CZ	7:R:100:VAL:HG21	2.52	0.44
8:S:38:VAL:HG11	8:S:59:MET:HG3	2.00	0.44
1:D:86:PHE:CE1	1:D:434:TYR:HB2	2.51	0.44
2:E:21:SER:O	2:E:25:ARG:HG2	2.16	0.44
5:H:105:DG:C2	5:H:106:DG:C2	3.05	0.44
6:J:31:LYS:HG3	6:J:51:TYR:CE1	2.52	0.44
6:J:73:THR:HG21	6:J:81:VAL:HG22	1.98	0.44
7:U:103:ALA:HB1	4:W:94:GLU:OE1	2.17	0.44
4:W:88:ALA:HB2	6:X:83:ALA:N	2.33	0.44
1:D:597:ILE:HA	1:D:600:ILE:HD12	2.00	0.44
2:E:748:MET:HE1	11:Y:180:ARG:N	2.32	0.44
3:G:375:LYS:O	3:G:376:MET:HE2	2.18	0.44
3:G:429:CYS:HB3	3:G:433:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:67:DC:H4'	9:T:68:DC:OP1	2.16	0.44
9:T:143:DA:H2'	9:T:144:DT:H71	1.99	0.44
7:U:29:ARG:CZ	8:V:32:GLU:HG2	2.48	0.44
2:E:289:CYS:O	2:E:291:LYS:HG3	2.17	0.44
2:E:616:LYS:HG3	2:E:617:LYS:O	2.17	0.44
3:G:360:GLN:HG2	3:G:381:ASN:HD21	1.83	0.44
4:I:121:PRO:HG2	6:J:49:LEU:HB3	2.00	0.44
5:H:71:DG:H5'	5:H:71:DG:H8	1.82	0.44
5:H:171:DC:OP1	7:R:76:THR:N	2.50	0.44
9:T:97:DC:H2'	9:T:98:DT:C6	2.53	0.44
9:T:206:DA:H2''	9:T:207:DT:C6	2.52	0.44
4:W:42:ARG:O	4:W:45:THR:HG22	2.17	0.44
2:E:120:PHE:O	2:E:650:ILE:N	2.24	0.44
9:T:92:DA:C5	9:T:93:DC:C4	3.06	0.44
9:T:133:DC:H2'	9:T:134:DG:H8	1.82	0.44
9:T:197:DC:H2'	9:T:198:DA:C8	2.53	0.44
7:U:29:ARG:NH2	8:V:32:GLU:HG2	2.32	0.44
11:Y:259:ARG:HG3	11:Y:260:HIS:ND1	2.32	0.44
1:D:663:MET:O	1:D:668:LEU:HG	2.17	0.44
2:E:626:VAL:HG22	2:E:746:ARG:HD3	2.00	0.44
3:G:147:PHE:HA	3:G:167:GLY:HA3	1.99	0.44
4:W:54:TYR:HE2	6:X:36:ARG:HD2	1.82	0.44
10:O:126:GLU:O	10:O:145:PRO:HD3	2.18	0.44
10:O:147:SER:HB3	10:O:176:HIS:O	2.17	0.44
11:Y:225:THR:O	11:Y:242:HIS:N	2.44	0.44
1:D:83:HIS:HA	1:D:86:PHE:HB3	1.99	0.44
1:D:607:ASN:O	1:D:611:LYS:N	2.51	0.44
1:D:647:ILE:HG22	1:D:653:CYS:SG	2.58	0.44
2:E:701:TYR:CD1	2:E:703:LYS:HG3	2.53	0.44
3:G:384:GLY:HA3	3:G:410:GLY:HA2	1.99	0.44
9:T:142:DG:C2	9:T:143:DA:C4	3.06	0.44
1:D:659:HIS:O	1:D:663:MET:HG2	2.17	0.44
2:E:565:CYS:HB3	2:E:590:CYS:HA	1.99	0.44
2:E:573:THR:HG23	2:E:575:GLN:HG2	1.99	0.44
3:G:245:ASP:CG	3:G:249:GLU:H	2.26	0.44
4:I:44:GLY:N	9:T:123:DG:OP1	2.43	0.44
5:H:59:DC:H2'	5:H:60:DA:C8	2.52	0.44
9:T:119:DC:H2''	9:T:120:DC:C6	2.53	0.44
10:O:287:PHE:HB3	10:O:302:ASP:OD1	2.18	0.44
1:D:249:SER:HG	1:D:299:MET:C	2.25	0.43
1:D:632:MET:HA	1:D:635:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:83:ARG:O	6:J:80:THR:HA	2.18	0.43
5:H:79:DA:H61	9:T:148:DC:N4	2.16	0.43
3:G:189:HIS:CE1	3:G:216:ARG:HB2	2.53	0.43
4:W:82:LEU:HD23	4:W:82:LEU:HA	1.72	0.43
6:X:35:ARG:O	6:X:39:ARG:HG2	2.18	0.43
10:O:52:ASP:CG	10:O:65:ARG:HH22	2.26	0.43
2:E:584:GLU:HG2	2:E:608:ASN:O	2.18	0.43
5:H:94:DG:H2''	5:H:95:DG:H8	1.83	0.43
5:H:171:DC:H3'	7:R:75:LYS:NZ	2.32	0.43
9:T:161:DG:C6	9:T:162:DG:C6	3.07	0.43
1:D:316:GLU:HB2	1:D:356:GLN:NE2	2.33	0.43
2:E:336:ALA:O	2:E:472:TYR:OH	2.18	0.43
2:E:660:GLY:HA2	2:E:663:TYR:CD1	2.54	0.43
3:G:264:ARG:HH22	3:G:343:ILE:HG22	1.84	0.43
4:I:63:ARG:HB2	4:I:66:PRO:HG2	2.00	0.43
5:H:61:DC:C2	5:H:62:DG:C8	3.06	0.43
5:H:76:DG:N2	9:T:152:DC:N3	2.63	0.43
7:R:65:LEU:HD23	7:R:65:LEU:HA	1.82	0.43
9:T:75:DT:H2''	9:T:76:DC:C6	2.53	0.43
7:U:76:THR:O	8:V:49:THR:HG23	2.19	0.43
10:O:232:ASP:OD1	10:O:233:VAL:N	2.51	0.43
2:E:102:ASN:O	3:G:173:ARG:NH1	2.48	0.43
2:E:575:GLN:NE2	9:T:44:DG:H4'	2.33	0.43
3:G:268:LYS:HA	3:G:271:MET:HE2	2.00	0.43
3:G:380:GLY:HA3	3:G:413:ILE:HG21	2.00	0.43
4:I:108:ASN:ND2	6:J:43:VAL:HA	2.33	0.43
6:J:102:GLY:O	8:S:64:ASN:ND2	2.23	0.43
9:T:80:DG:H2''	9:T:81:DA:H8	1.83	0.43
2:E:85:VAL:N	2:E:94:GLN:O	2.51	0.43
3:G:271:MET:HA	3:G:274:ILE:HB	2.00	0.43
3:G:326:ASN:HA	3:G:358:TYR:CZ	2.53	0.43
6:J:31:LYS:HE3	6:J:51:TYR:CE2	2.54	0.43
9:T:118:DC:H2''	9:T:119:DC:C5	2.54	0.43
11:Y:288:MET:HG2	11:Y:289:PRO:HD3	1.99	0.43
1:D:310:LEU:HD23	1:D:315:TYR:CE2	2.53	0.43
1:D:616:LEU:HG	1:D:639:PHE:HZ	1.84	0.43
2:E:502:ARG:HH21	9:T:47:DA:H5''	1.84	0.43
2:E:699:ASN:HB3	2:E:721:ILE:HD11	2.01	0.43
4:I:61:LEU:HD11	6:J:40:ARG:HD2	2.00	0.43
5:H:70:DA:H61	9:T:157:DC:H42	1.67	0.43
5:H:130:DA:OP1	4:W:66:PRO:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:84:SER:O	8:S:84:SER:OG	2.30	0.43
9:T:83:DA:C6	9:T:84:DG:C6	3.06	0.43
4:W:87:SER:HA	4:W:90:MET:HE2	2.00	0.43
11:Y:230:ARG:NE	11:Y:232:GLU:OE2	2.51	0.43
2:E:731:TYR:OH	12:E:801:SAH:H8	2.18	0.43
2:E:732:ARG:HD2	4:I:30:PRO:HD3	1.99	0.43
3:G:85:VAL:HG21	3:G:438:ASP:HB2	1.99	0.43
3:G:404:LEU:HD23	3:G:437:TRP:CZ3	2.54	0.43
5:H:85:DC:H2'	5:H:86:DC:C2	2.53	0.43
5:H:101:DA:H1'	5:H:102:DC:H5'	2.01	0.43
7:U:64:GLU:HG2	8:V:46:HIS:HE1	1.82	0.43
4:W:39:HIS:HE1	4:W:41:TYR:CD1	2.36	0.43
2:E:458:ALA:O	2:E:461:ARG:HG3	2.19	0.43
2:E:470:GLN:N	2:E:473:GLU:OE1	2.46	0.43
4:I:58:THR:OG1	7:R:104:GLN:O	2.33	0.43
5:H:119:DA:H2''	5:H:120:DC:C5	2.53	0.43
10:O:24:TRP:O	10:O:28:THR:OG1	2.24	0.43
1:D:628:ALA:HB2	2:E:587:PRO:HB2	2.00	0.43
5:H:97:DT:H1'	5:H:98:DA:C8	2.54	0.43
5:H:128:DT:H2''	5:H:129:DA:C8	2.53	0.43
5:H:149:DA:H2''	5:H:150:DC:C5	2.54	0.43
8:S:30:ARG:NH2	9:T:69:DT:OP1	2.34	0.43
9:T:61:DG:H4'	9:T:62:DG:OP1	2.19	0.43
10:O:236:HIS:HA	10:O:281:PHE:HD2	1.83	0.43
1:D:183:THR:OG1	1:D:211:LYS:O	2.35	0.42
3:G:216:ARG:HE	3:G:228:ILE:HD12	1.84	0.42
3:G:264:ARG:HG3	3:G:298:ASP:CG	2.44	0.42
3:G:333:PRO:HG2	3:G:340:ILE:HG22	2.01	0.42
4:I:131:ARG:HG3	4:W:130:ILE:HG22	2.01	0.42
5:H:157:DT:H2''	5:H:158:DG:C8	2.53	0.42
5:H:168:DC:H42	9:T:59:DG:H1	1.67	0.42
7:U:115:LEU:HD11	4:W:108:ASN:HD21	1.84	0.42
1:D:600:ILE:HD13	1:D:615:LYS:HG2	2.00	0.42
5:H:144:DT:H2''	5:H:145:DG:H5'	2.01	0.42
9:T:119:DC:H2''	9:T:120:DC:C5	2.54	0.42
10:O:279:LEU:HD12	10:O:291:THR:HG22	2.01	0.42
2:E:60:TRP:HA	2:E:63:ARG:HD3	2.00	0.42
2:E:171:PHE:HE2	2:E:243:LYS:HZ3	1.67	0.42
2:E:612:GLN:OE1	2:E:613:ARG:NH1	2.46	0.42
2:E:704:VAL:HA	2:E:713:ILE:HA	2.01	0.42
3:G:103:TRP:CH2	3:G:372:PHE:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:235:HIS:CD2	3:G:259:SER:HB2	2.53	0.42
4:W:39:HIS:HE1	4:W:41:TYR:CE1	2.37	0.42
4:W:68:GLN:NE2	4:W:72:ARG:HH21	2.17	0.42
1:D:252:PHE:HB2	1:D:297:ALA:HB3	2.00	0.42
2:E:456:PHE:HA	2:E:459:ILE:HG12	2.02	0.42
2:E:699:ASN:O	2:E:718:LYS:N	2.47	0.42
3:G:150:CYS:HB2	3:G:163:LEU:HD21	2.01	0.42
7:R:37:GLY:HA3	7:R:39:TYR:CE2	2.55	0.42
7:R:92:GLU:HG3	8:S:103:LEU:CD1	2.49	0.42
6:X:66:ILE:HA	6:X:69:ALA:HB3	2.01	0.42
10:O:49:TRP:HZ2	10:O:391:CYS:HB3	1.85	0.42
10:O:232:ASP:OD2	10:O:279:LEU:N	2.52	0.42
1:D:557:TYR:CZ	10:O:106:GLY:HA3	2.55	0.42
2:E:108:PRO:HG2	2:E:629:TRP:CD2	2.55	0.42
2:E:502:ARG:NH2	4:I:39:HIS:HB3	2.34	0.42
3:G:191:ASN:OD1	3:G:192:ALA:N	2.51	0.42
4:I:129:ARG:HB2	4:I:134:ARG:HD2	2.02	0.42
5:H:207:DG:N2	9:T:21:DA:O4'	2.53	0.42
6:J:35:ARG:HH11	6:J:39:ARG:NH2	2.17	0.42
8:V:116:THR:O	8:V:120:SER:N	2.51	0.42
3:G:151:ALA:O	3:G:163:LEU:HG	2.20	0.42
3:G:201:ARG:NH2	3:G:247:LEU:HD22	2.35	0.42
5:H:120:DC:N4	9:T:107:DG:H1	2.17	0.42
7:R:84:GLN:HG2	7:R:105:GLY:O	2.19	0.42
7:R:84:GLN:HE21	7:R:88:ARG:HG3	1.84	0.42
9:T:82:DC:H2''	9:T:83:DA:C8	2.55	0.42
7:U:63:LEU:HD11	8:V:38:VAL:HG13	2.01	0.42
10:O:49:TRP:CZ2	10:O:391:CYS:HB3	2.54	0.42
10:O:178:LYS:HE2	10:O:198:ASP:HB2	2.01	0.42
4:I:120:MET:HE1	5:H:111:DC:OP1	2.20	0.42
5:H:210:DG:C2	5:H:211:DG:C4	3.07	0.42
10:O:174:ARG:HG2	10:O:175:GLY:N	2.35	0.42
10:O:294:ALA:HA	10:O:319:GLU:HG2	2.01	0.42
2:E:110:MET:HB3	2:E:629:TRP:HE1	1.84	0.42
3:G:340:ILE:HG13	3:G:341:ASP:N	2.35	0.42
1:D:603:PHE:HE2	1:D:605:ASP:HB2	1.85	0.42
2:E:318:THR:HG23	2:E:320:LEU:HG	2.02	0.42
5:H:191:DC:O2	9:T:37:DG:N2	2.53	0.42
9:T:180:DC:H2''	9:T:181:DA:H8	1.85	0.42
7:U:55:LEU:O	7:U:59:THR:HG22	2.20	0.42
2:E:25:ARG:O	2:E:28:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:620:LEU:N	2:E:632:PHE:O	2.44	0.42
4:I:50:GLU:OE1	6:J:39:ARG:NE	2.50	0.42
4:I:75:ALA:HB1	4:I:82:LEU:HD12	2.02	0.42
5:H:43:DG:C6	5:H:44:DG:C6	3.08	0.42
5:H:80:DG:H2''	5:H:81:DT:C6	2.55	0.42
5:H:163:DG:OP1	8:S:31:LYS:N	2.51	0.42
5:H:208:DA:C5	5:H:209:DC:C4	3.08	0.42
6:J:26:ILE:HD11	6:J:55:ARG:O	2.19	0.42
9:T:93:DC:H2''	9:T:94:DC:H6	1.85	0.42
8:V:113:LYS:HA	8:V:116:THR:HG22	2.01	0.42
1:D:130:LYS:HB3	10:O:348:SER:HB2	2.02	0.41
2:E:273:GLN:HE21	2:E:276:GLN:HG3	1.85	0.41
5:H:159:DG:H1'	5:H:160:DA:C8	2.54	0.41
9:T:45:DA:H2'	9:T:46:DG:C8	2.55	0.41
6:X:33:ALA:HA	6:X:36:ARG:NH2	2.35	0.41
11:Y:287:THR:HG22	11:Y:289:PRO:HD2	2.02	0.41
1:D:198:ASP:N	1:D:198:ASP:OD1	2.53	0.41
1:D:595:LYS:O	1:D:598:THR:OG1	2.35	0.41
1:D:663:MET:SD	1:D:668:LEU:HD21	2.60	0.41
3:G:102:ASN:HB2	3:G:152:TRP:CH2	2.55	0.41
3:G:226:VAL:HG12	3:G:227:ALA:N	2.33	0.41
3:G:311:CYS:HB3	3:G:368:PHE:CE1	2.55	0.41
7:R:62:ILE:HD12	7:R:62:ILE:H	1.85	0.41
9:T:17:DC:H2''	9:T:18:DG:H8	1.85	0.41
7:U:26:PRO:HB3	8:V:37:TYR:CZ	2.55	0.41
2:E:584:GLU:OE2	2:E:609:CYS:HA	2.19	0.41
5:H:91:DG:C4	5:H:92:DG:C8	3.08	0.41
9:T:118:DC:H4'	9:T:119:DC:H5'	2.01	0.41
7:U:112:GLN:H	7:U:115:LEU:HD12	1.85	0.41
10:O:150:LEU:HB3	10:O:169:PRO:HB3	2.03	0.41
10:O:373:HIS:HD2	10:O:375:ALA:O	2.03	0.41
11:Y:243:TRP:H	11:Y:248:ILE:HD13	1.84	0.41
1:D:166:HIS:CD2	1:D:353:PRO:HG3	2.56	0.41
3:G:228:ILE:HG23	3:G:293:LYS:HA	2.02	0.41
3:G:269:ARG:HD3	3:G:292:GLN:OE1	2.20	0.41
4:I:95:ALA:O	4:I:99:TYR:N	2.43	0.41
5:H:122:DT:P	4:W:46:VAL:HB	2.60	0.41
5:H:185:DA:H61	9:T:42:DC:N4	2.17	0.41
9:T:170:DC:H2''	9:T:171:DA:O4'	2.21	0.41
4:W:60:LEU:C	4:W:61:LEU:HD22	2.46	0.41
4:W:80:THR:OG1	4:W:81:ASP:OD1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:575:ARG:NH1	3:G:286:ASN:O	2.53	0.41
2:E:558:CYS:HB3	2:E:561:ARG:NE	2.36	0.41
3:G:115:THR:HB	3:G:122:THR:HG23	2.02	0.41
7:R:39:TYR:O	8:S:75:SER:OG	2.29	0.41
7:U:85:LEU:O	7:U:89:ASN:HB2	2.20	0.41
10:O:56:PRO:HD2	10:O:62:SER:HA	2.02	0.41
5:H:61:DC:H2''	5:H:62:DG:H8	1.85	0.41
10:O:246:VAL:HG11	10:O:276:VAL:HG12	2.01	0.41
1:D:613:VAL:HG23	1:D:614:MET:SD	2.60	0.41
2:E:104:VAL:HG21	3:G:171:ILE:HG21	2.01	0.41
3:G:179:THR:HG23	3:G:181:GLN:H	1.86	0.41
3:G:229:PHE:HE2	3:G:251:ILE:HD12	1.86	0.41
5:H:160:DA:C6	5:H:161:DG:C6	3.08	0.41
8:S:58:ILE:HG22	8:S:59:MET:HE2	2.02	0.41
10:O:257:THR:O	10:O:258:ARG:HG2	2.20	0.41
2:E:629:TRP:N	12:E:801:SAH:OXT	2.43	0.41
3:G:95:PRO:HA	3:G:430:ASP:O	2.20	0.41
3:G:219:ASN:HB3	3:G:224:THR:HG22	2.01	0.41
3:G:240:LEU:HD23	3:G:255:GLY:HA2	2.01	0.41
5:H:89:DT:H6	5:H:89:DT:H2'	1.72	0.41
5:H:189:DG:C2	9:T:39:DG:C2	3.09	0.41
5:H:205:DC:N4	9:T:21:DA:H61	2.19	0.41
5:H:205:DC:H42	9:T:21:DA:H61	1.67	0.41
7:R:92:GLU:OE2	8:S:100:PRO:HG2	2.20	0.41
11:Y:244:MET:O	11:Y:246:GLU:HG3	2.21	0.41
1:D:137:MET:HE3	10:O:304:ARG:NH2	2.36	0.41
1:D:650:LYS:HB2	1:D:652:LEU:CD2	2.44	0.41
2:E:624:SER:OG	2:E:627:ALA:O	2.38	0.41
2:E:636:PRO:HD3	2:E:723:THR:OG1	2.20	0.41
3:G:206:LEU:C	3:G:217:LEU:HG	2.46	0.41
3:G:324:CYS:SG	3:G:364:TRP:HB3	2.61	0.41
3:G:326:ASN:HA	3:G:358:TYR:CE2	2.56	0.41
3:G:374:GLN:O	3:G:391:LEU:HD12	2.21	0.41
5:H:139:DA:H2''	5:H:140:DG:H8	1.84	0.41
5:H:197:DC:H42	9:T:29:DC:N4	2.19	0.41
7:R:53:ALA:O	7:R:56:GLU:HB2	2.20	0.41
9:T:93:DC:H4'	9:T:94:DC:OP1	2.19	0.41
9:T:122:DC:H2''	9:T:123:DG:O5'	2.21	0.41
7:U:50:TYR:OH	8:V:108:VAL:HA	2.21	0.41
10:O:183:LEU:HG	10:O:193:LEU:HD11	2.02	0.41
10:O:281:PHE:HD1	10:O:289:LEU:HD13	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:379:ASP:HB3	10:O:393:VAL:HB	2.03	0.41
11:Y:190:PHE:CE2	11:Y:195:LEU:HB2	2.56	0.41
1:D:580:GLU:N	1:D:580:GLU:OE1	2.54	0.41
1:D:663:MET:SD	1:D:668:LEU:HD11	2.61	0.41
2:E:539:CYS:HB3	2:E:542:VAL:HG23	2.02	0.41
3:G:373:TRP:CZ3	3:G:421:ASP:HA	2.56	0.41
3:G:411:ALA:HB3	3:G:429:CYS:SG	2.60	0.41
4:I:63:ARG:O	4:I:66:PRO:HD2	2.21	0.41
5:H:69:DG:H2''	5:H:70:DA:H8	1.85	0.41
8:S:111:GLY:O	8:S:114:ALA:N	2.54	0.41
9:T:78:DT:H2''	9:T:79:DA:C8	2.56	0.41
4:W:65:LEU:HB3	4:W:66:PRO:HD3	2.03	0.41
2:E:659:ARG:HB3	2:E:663:TYR:CZ	2.56	0.40
3:G:220:ILE:HD12	3:G:220:ILE:H	1.85	0.40
5:H:96:DT:H4'	5:H:97:DT:OP1	2.21	0.40
5:H:128:DT:H6	5:H:128:DT:H2'	1.72	0.40
5:H:204:DC:H2''	5:H:205:DC:C6	2.56	0.40
9:T:172:DG:H4'	7:U:77:ARG:HE	1.86	0.40
10:O:10:ASP:O	10:O:14:GLU:HG2	2.21	0.40
2:E:600:ASP:OD1	2:E:600:ASP:N	2.53	0.40
5:H:105:DG:C5	5:H:106:DG:C6	3.09	0.40
5:H:169:DG:H1'	5:H:170:DG:C8	2.56	0.40
4:W:61:LEU:HD13	4:W:61:LEU:HA	1.95	0.40
10:O:79:LEU:N	10:O:121:ILE:O	2.34	0.40
2:E:634:LYS:O	2:E:723:THR:HG23	2.21	0.40
3:G:250:LYS:HG2	3:G:264:ARG:HG2	2.03	0.40
3:G:275:LYS:HD3	3:G:275:LYS:HA	1.73	0.40
4:I:84:PHE:HD1	4:I:89:VAL:HG22	1.86	0.40
5:H:206:DT:H1'	5:H:207:DG:C8	2.55	0.40
9:T:100:DA:C2	9:T:101:DA:C4	3.09	0.40
9:T:158:DC:H6	9:T:158:DC:H2'	1.74	0.40
7:U:63:LEU:HA	7:U:63:LEU:HD23	1.84	0.40
2:E:83:CYS:HB3	2:E:98:LEU:HD11	2.04	0.40
3:G:230:GLY:N	3:G:294:ILE:O	2.54	0.40
3:G:409:CYS:HB2	3:G:435:TRP:CD2	2.57	0.40
4:I:99:TYR:OH	4:I:133:GLU:OE1	2.30	0.40
7:R:58:LEU:HD23	7:R:58:LEU:HA	1.92	0.40
9:T:65:DG:C5	9:T:66:DC:C4	3.09	0.40
10:O:133:MET:HE3	10:O:191:GLY:H	1.86	0.40
11:Y:240:LEU:HD13	11:Y:253:TRP:CE2	2.56	0.40
2:E:472:TYR:O	2:E:476:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:629:TRP:H	12:E:801:SAH:C	2.33	0.40
3:G:308:TYR:HB2	3:G:324:CYS:SG	2.62	0.40
4:I:90:MET:HE2	4:I:90:MET:HB2	1.94	0.40
10:O:129:ARG:N	10:O:143:LYS:HB2	2.36	0.40
10:O:224:THR:O	10:O:224:THR:HG22	2.22	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	D	423/619 (68%)	403 (95%)	20 (5%)	0	100	100
2	E	560/753 (74%)	511 (91%)	47 (8%)	2 (0%)	30	65
3	G	360/441 (82%)	329 (91%)	31 (9%)	0	100	100
4	I	112/136 (82%)	107 (96%)	5 (4%)	0	100	100
4	W	97/136 (71%)	92 (95%)	5 (5%)	0	100	100
6	J	81/106 (76%)	76 (94%)	5 (6%)	0	100	100
6	X	85/106 (80%)	78 (92%)	7 (8%)	0	100	100
7	R	106/133 (80%)	101 (95%)	5 (5%)	0	100	100
7	U	106/133 (80%)	103 (97%)	3 (3%)	0	100	100
8	S	94/123 (76%)	84 (89%)	10 (11%)	0	100	100
8	V	93/123 (76%)	85 (91%)	8 (9%)	0	100	100
10	O	391/425 (92%)	376 (96%)	15 (4%)	0	100	100
11	Y	124/303 (41%)	114 (92%)	9 (7%)	1 (1%)	16	52
All	All	2632/3537 (74%)	2459 (93%)	170 (6%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	327	PRO
11	Y	187	HIS
2	E	492	THR

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	D	411/575 (72%)	411 (100%)	0	100	100
2	E	507/672 (75%)	507 (100%)	0	100	100
3	G	324/392 (83%)	324 (100%)	0	100	100
4	I	95/111 (86%)	95 (100%)	0	100	100
4	W	86/111 (78%)	86 (100%)	0	100	100
6	J	68/81 (84%)	68 (100%)	0	100	100
6	X	64/81 (79%)	64 (100%)	0	100	100
7	R	85/104 (82%)	85 (100%)	0	100	100
7	U	84/104 (81%)	84 (100%)	0	100	100
8	S	79/103 (77%)	79 (100%)	0	100	100
8	V	79/103 (77%)	79 (100%)	0	100	100
10	O	351/375 (94%)	351 (100%)	0	100	100
11	Y	117/271 (43%)	117 (100%)	0	100	100
All	All	2350/3083 (76%)	2350 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	156	HIS
1	D	166	HIS
1	D	243	HIS
1	D	356	GLN

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Mol	Chain	Res	Type
1	D	431	GLN
1	D	449	HIS
1	D	456	ASN
1	D	477	ASN
1	D	517	ASN
1	D	664	HIS
1	D	667	ASN
2	E	45	ASN
2	E	102	ASN
2	E	117	GLN
2	E	118	GLN
2	E	119	ASN
2	E	180	GLN
2	E	273	GLN
2	E	512	GLN
2	E	520	ASN
2	E	553	GLN
2	E	560	ASN
3	G	146	ASN
3	G	157	ASN
3	G	160	HIS
3	G	185	HIS
3	G	189	HIS
3	G	272	ASN
3	G	283	ASN
3	G	406	HIS
4	I	108	ASN
7	R	31	HIS
7	R	104	GLN
8	S	92	GLN
8	S	106	HIS
7	U	82	HIS
7	U	84	GLN
8	V	79	HIS
8	V	92	GLN
4	W	39	HIS
4	W	125	GLN
10	O	48	GLN
10	O	78	HIS
10	O	188	ASN
10	O	329	ASN
10	O	403	GLN

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Mol	Chain	Res	Type
10	O	410	ASN
11	Y	283	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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$
12	SAH	E	801	-	27,28,28	1.11	4 (14%)	36,40,40	2.07	10 (27%)

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
12	SAH	E	801	-	-	4/15/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	801	SAH	C2-N3	2.55	1.38	1.33
12	E	801	SAH	C2-N1	2.51	1.38	1.33
12	E	801	SAH	OXT-C	-2.32	1.23	1.30
12	E	801	SAH	C8-N7	2.13	1.35	1.31

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	801	SAH	N3-C2-N1	-5.49	120.28	128.58
12	E	801	SAH	C5-C4-N3	-4.70	120.25	126.72
12	E	801	SAH	C5'-SD-CG	-4.16	89.91	102.26
12	E	801	SAH	N9-C8-N7	-3.66	108.74	113.94
12	E	801	SAH	C2-N3-C4	3.49	120.35	111.83
12	E	801	SAH	C5-N7-C8	3.28	108.61	103.45
12	E	801	SAH	N3-C4-N9	3.05	132.36	127.17
12	E	801	SAH	OXT-C-O	-2.61	118.17	124.08
12	E	801	SAH	C4-C5-N7	-2.36	107.88	110.58
12	E	801	SAH	C3'-C2'-C1'	2.15	105.52	101.46

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	E	801	SAH	C3'-C4'-C5'-SD
12	E	801	SAH	O4'-C4'-C5'-SD
12	E	801	SAH	C-CA-CB-CG
12	E	801	SAH	CA-CB-CG-SD

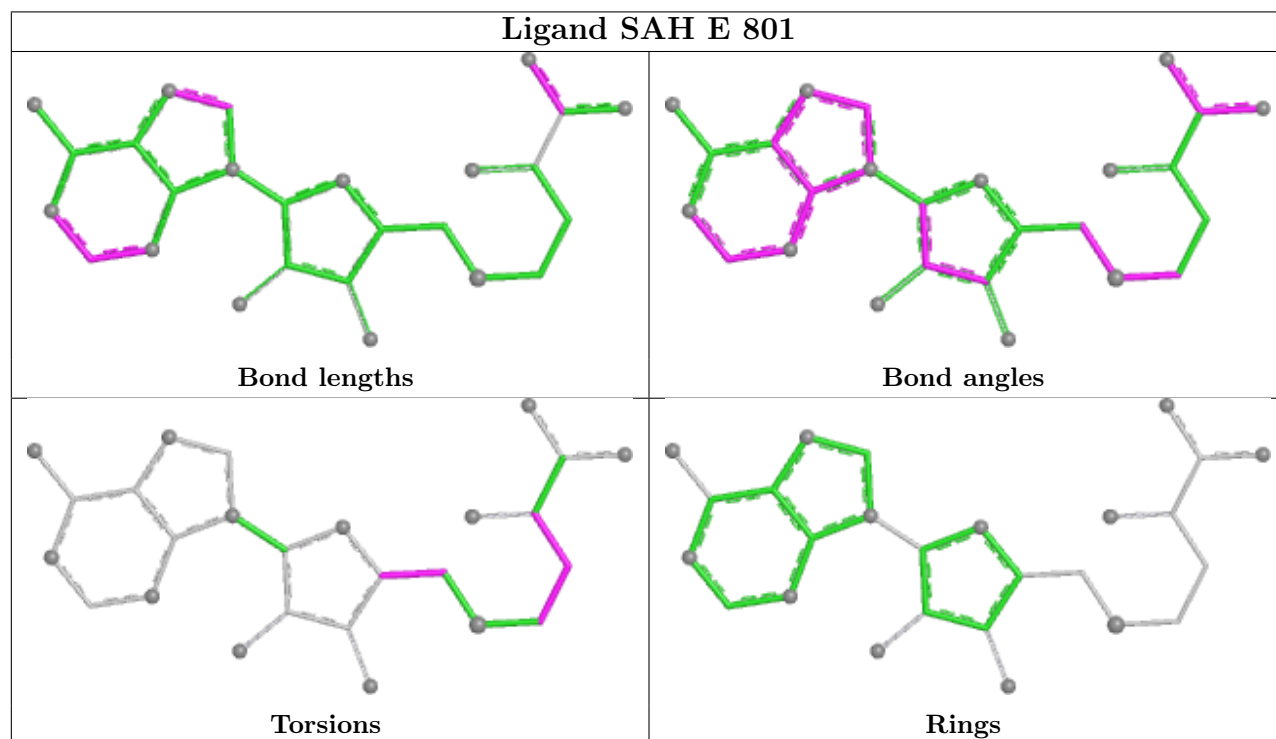
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	801	SAH	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

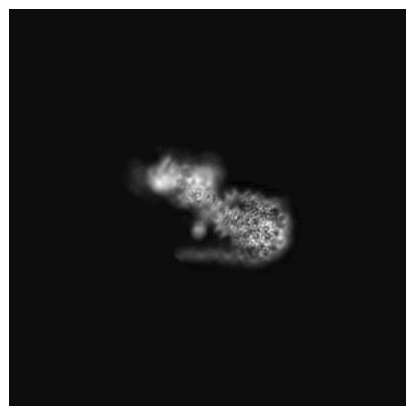
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41141. These allow visual inspection of the internal detail of the map and identification of artifacts.

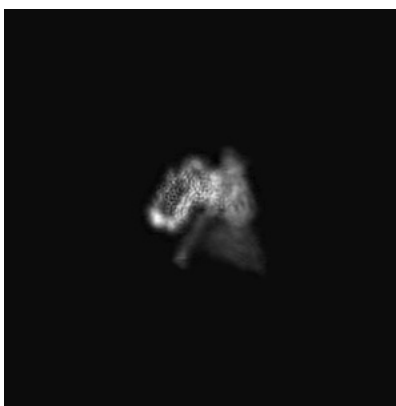
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

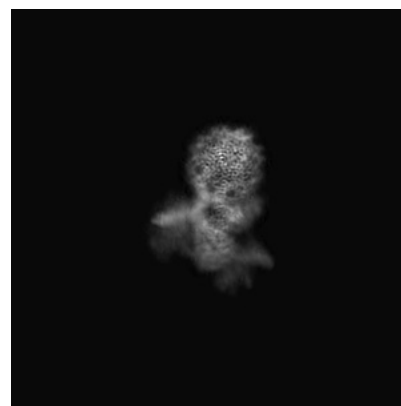
6.1.1 Primary map



X

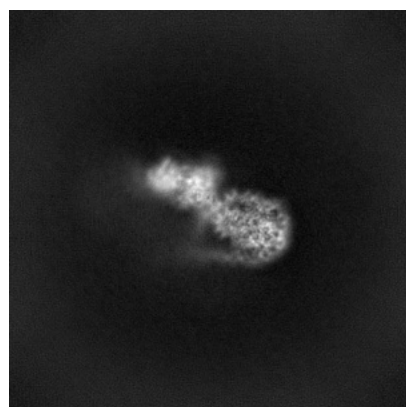


Y

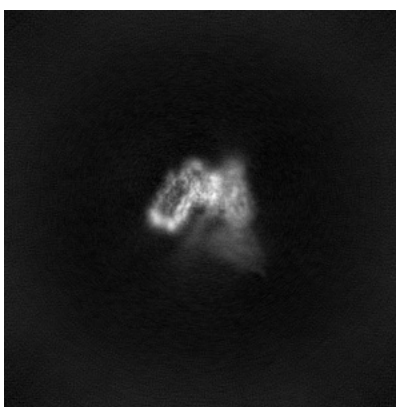


Z

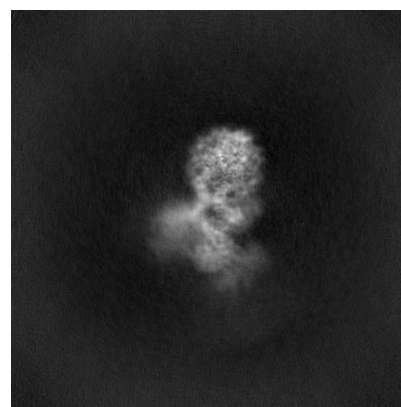
6.1.2 Raw map



X



Y

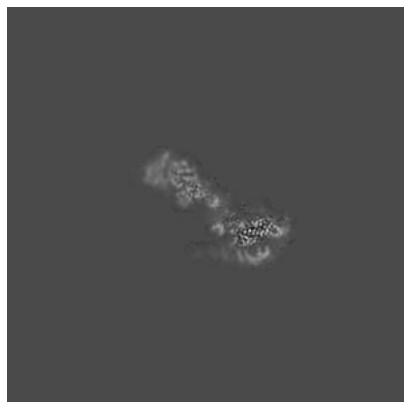


Z

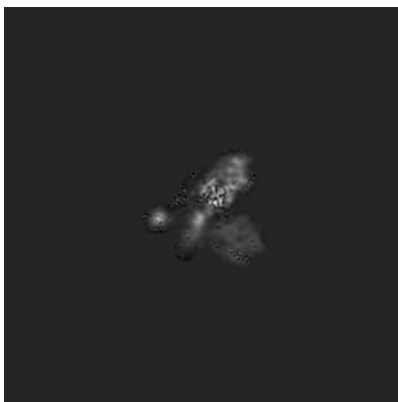
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

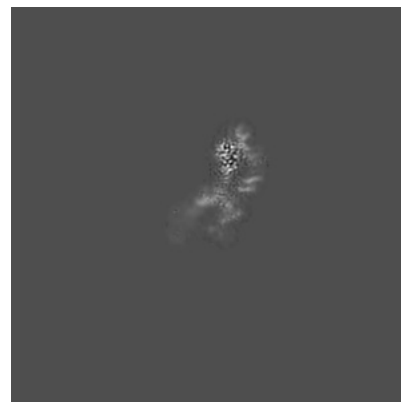
6.2.1 Primary map



X Index: 165



Y Index: 165

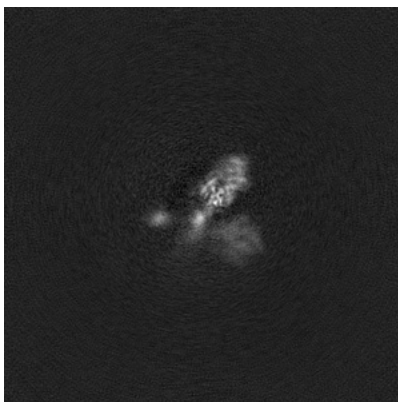


Z Index: 165

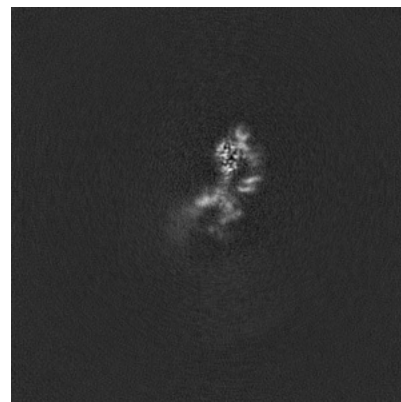
6.2.2 Raw map



X Index: 165



Y Index: 165

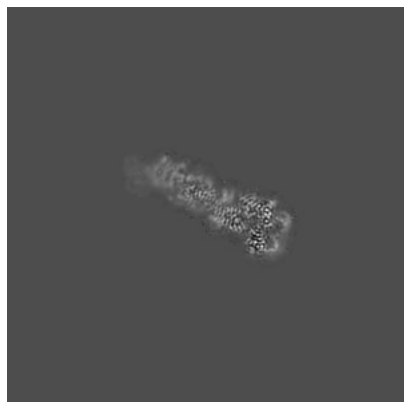


Z Index: 165

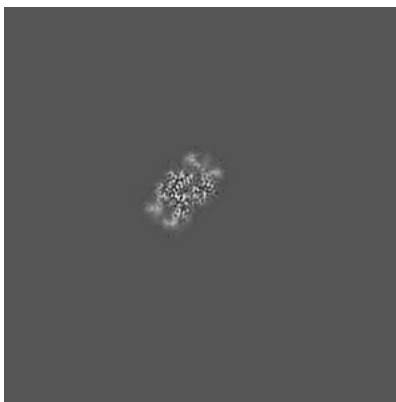
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

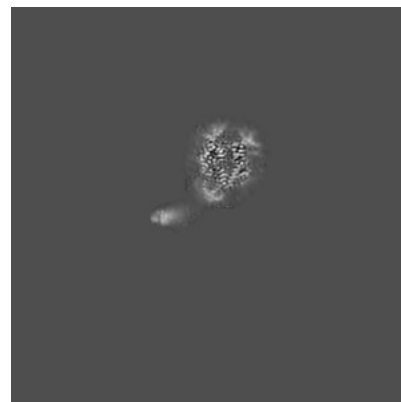
6.3.1 Primary map



X Index: 175

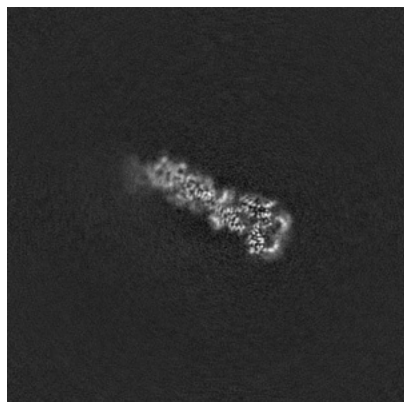


Y Index: 207

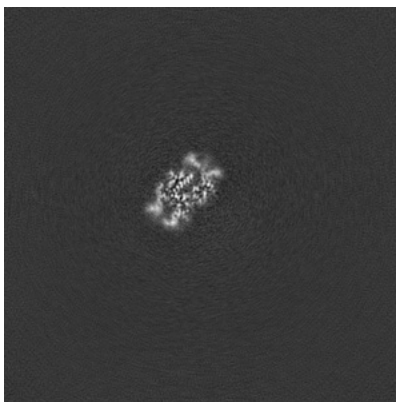


Z Index: 148

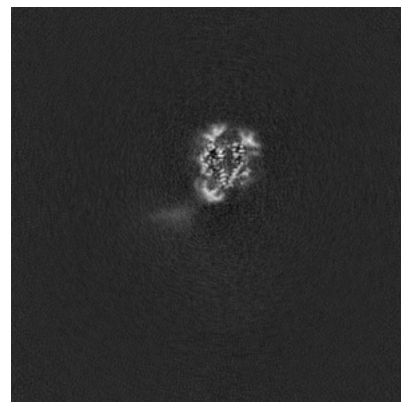
6.3.2 Raw map



X Index: 174



Y Index: 207

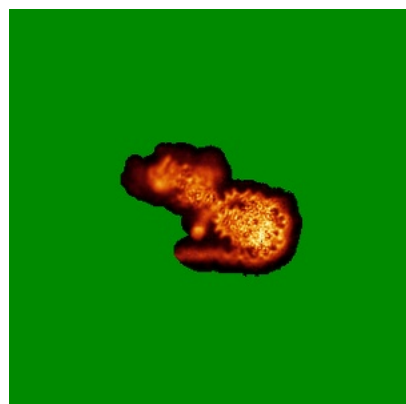


Z Index: 148

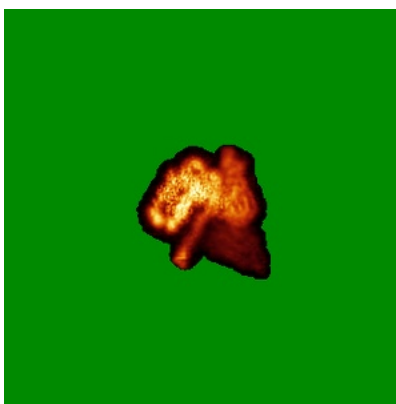
The images above show the largest variance slices of the map in three orthogonal directions.

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

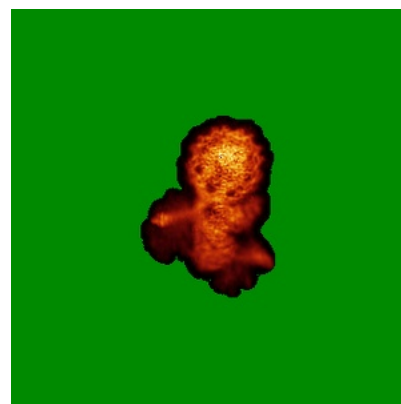
6.4.1 Primary map



X

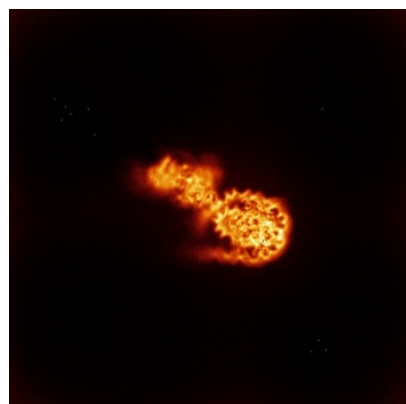


Y

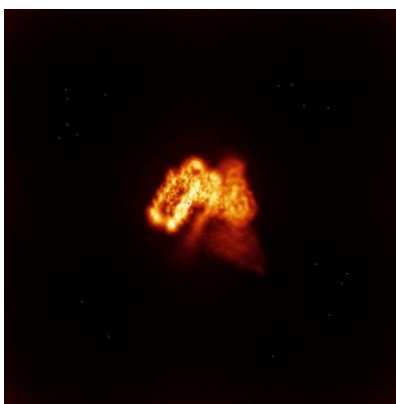


Z

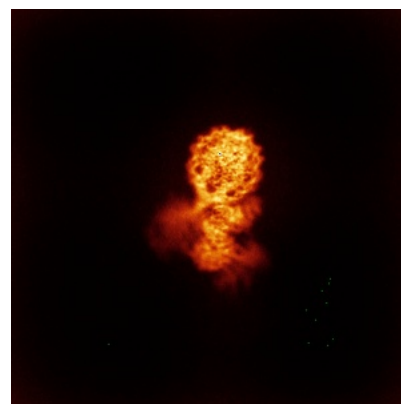
6.4.2 Raw map



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](#)

This section was not generated.

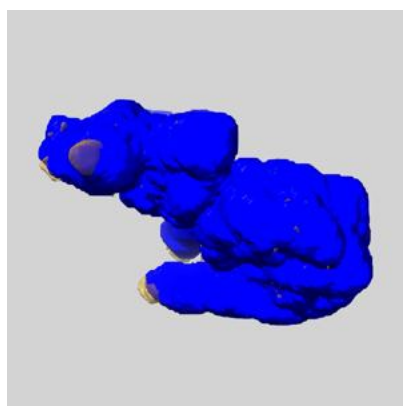
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

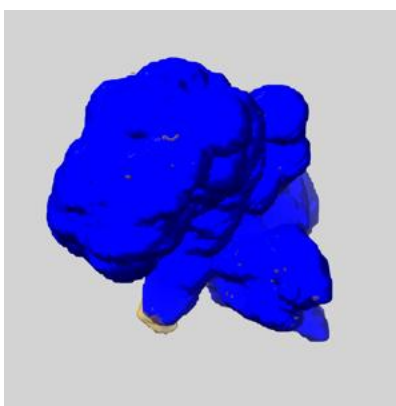
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

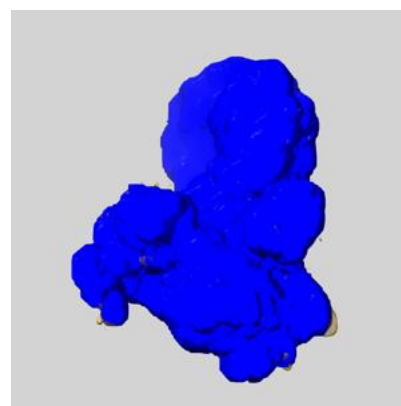
6.6.1 emd_41141_msk_1.map [i](#)



X



Y

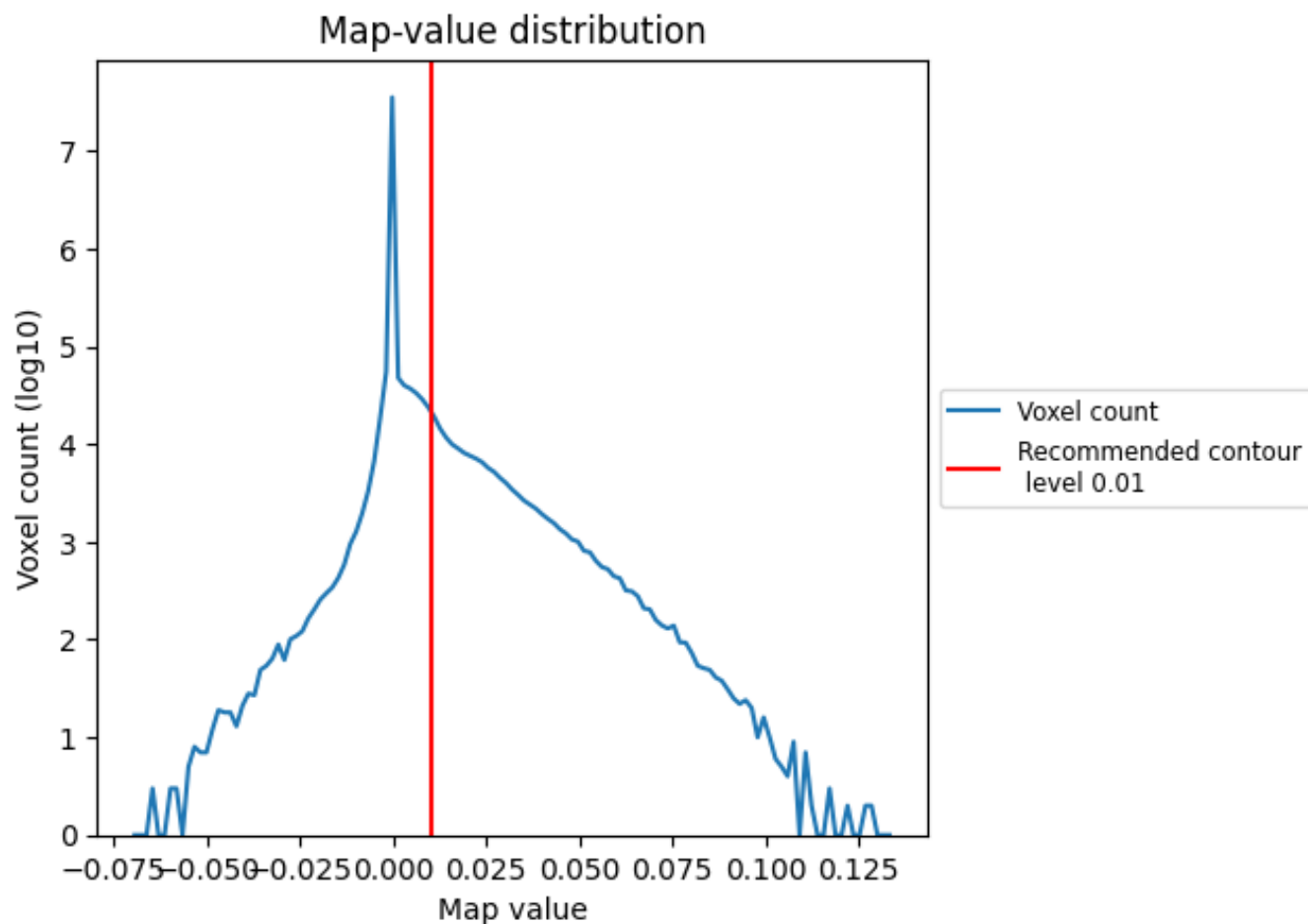


Z

7 Map analysis [i](#)

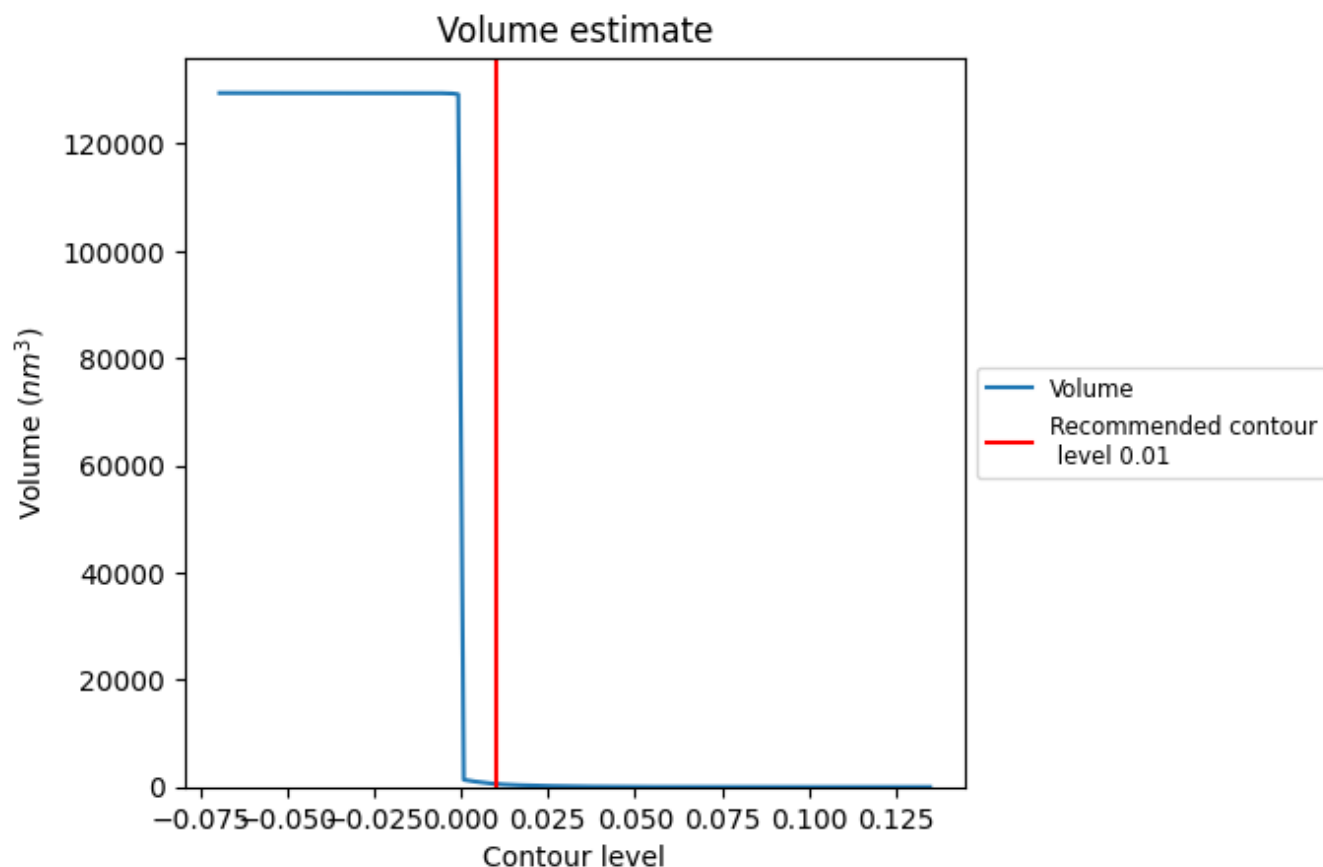
This section contains the results of statistical analysis of the map.

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.

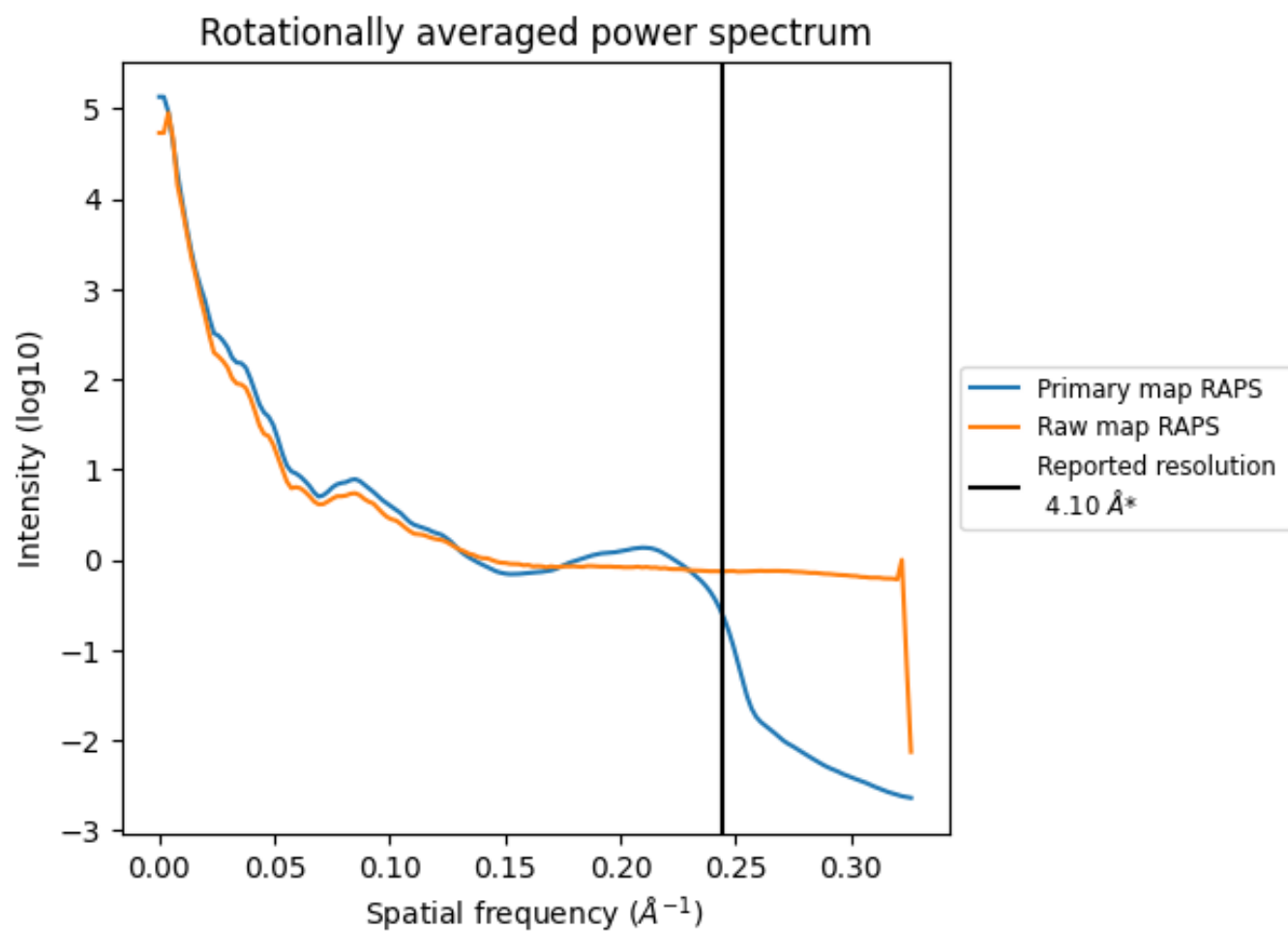
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 570 nm^3 ; this corresponds to an approximate mass of 515 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

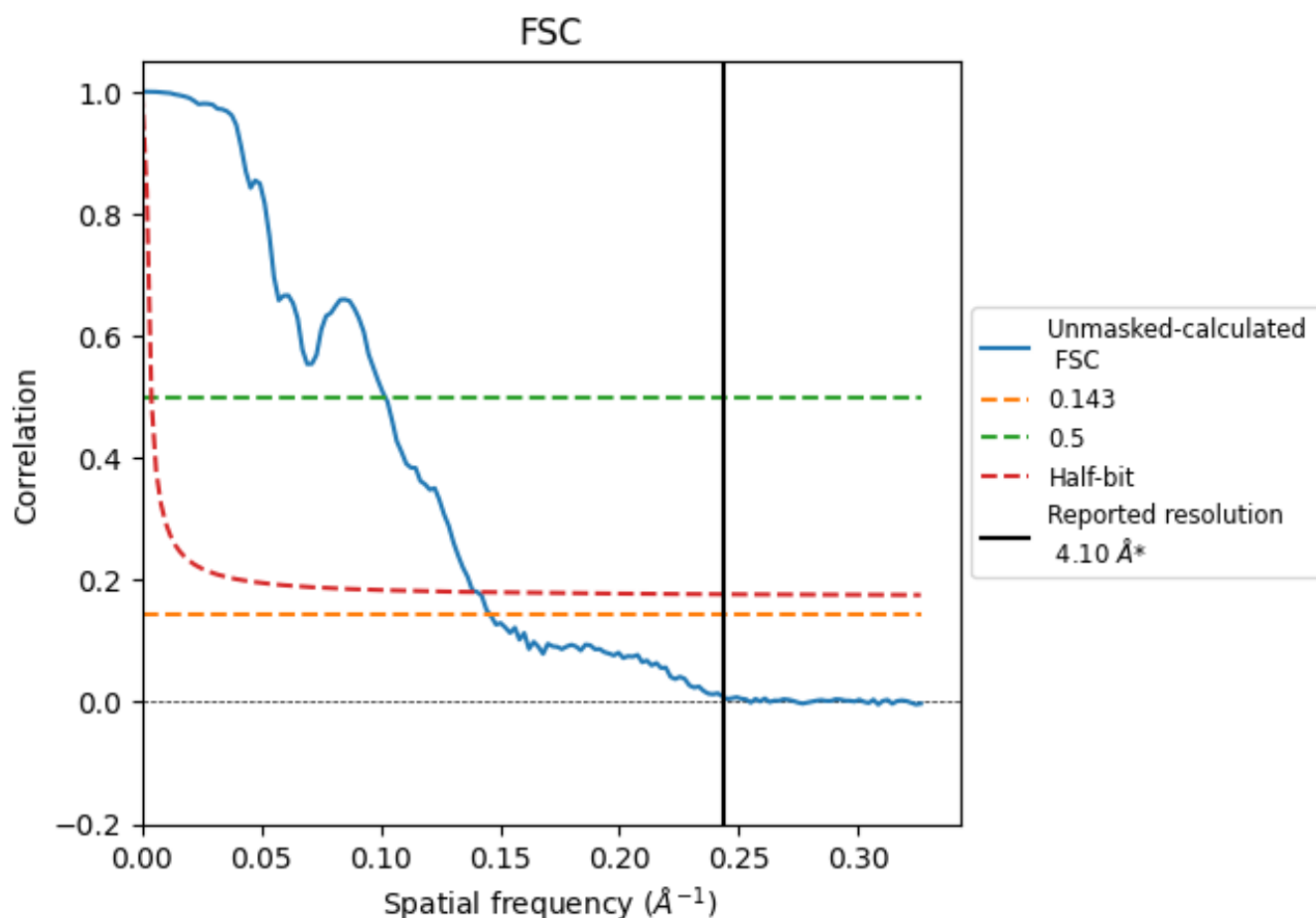


*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

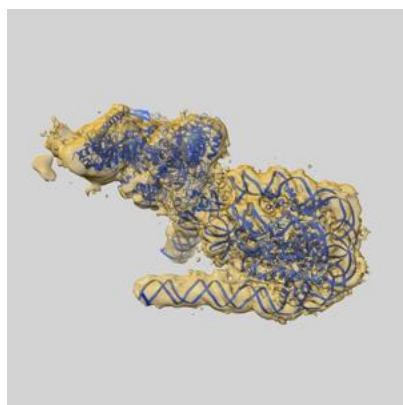
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.86	9.82	7.12

*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 6.86 differs from the reported value 4.1 by more than 10 %

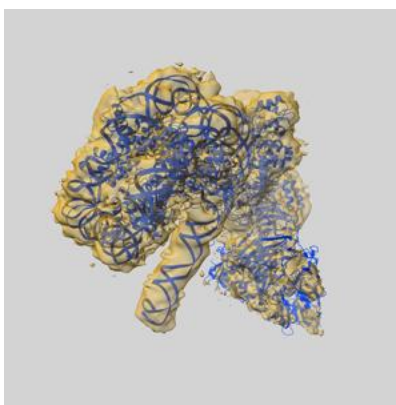
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41141 and PDB model 8TAS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

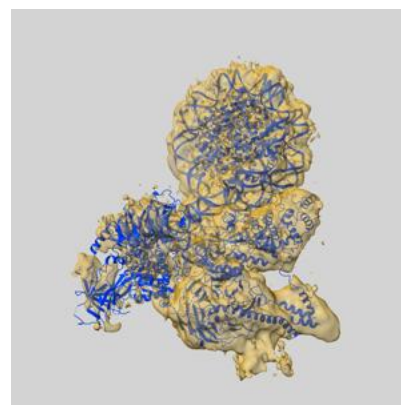
9.1 Map-model overlay [i](#)



X



Y



Z

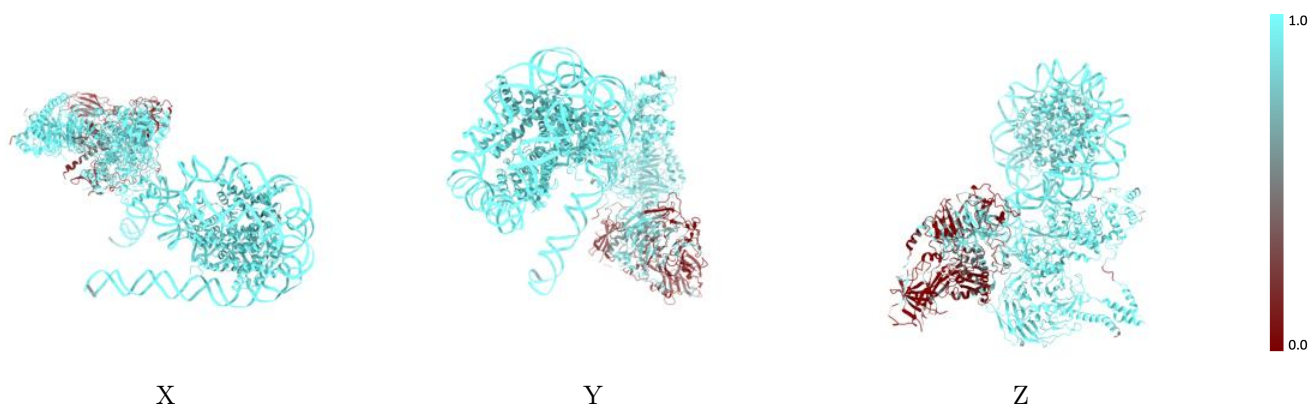
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



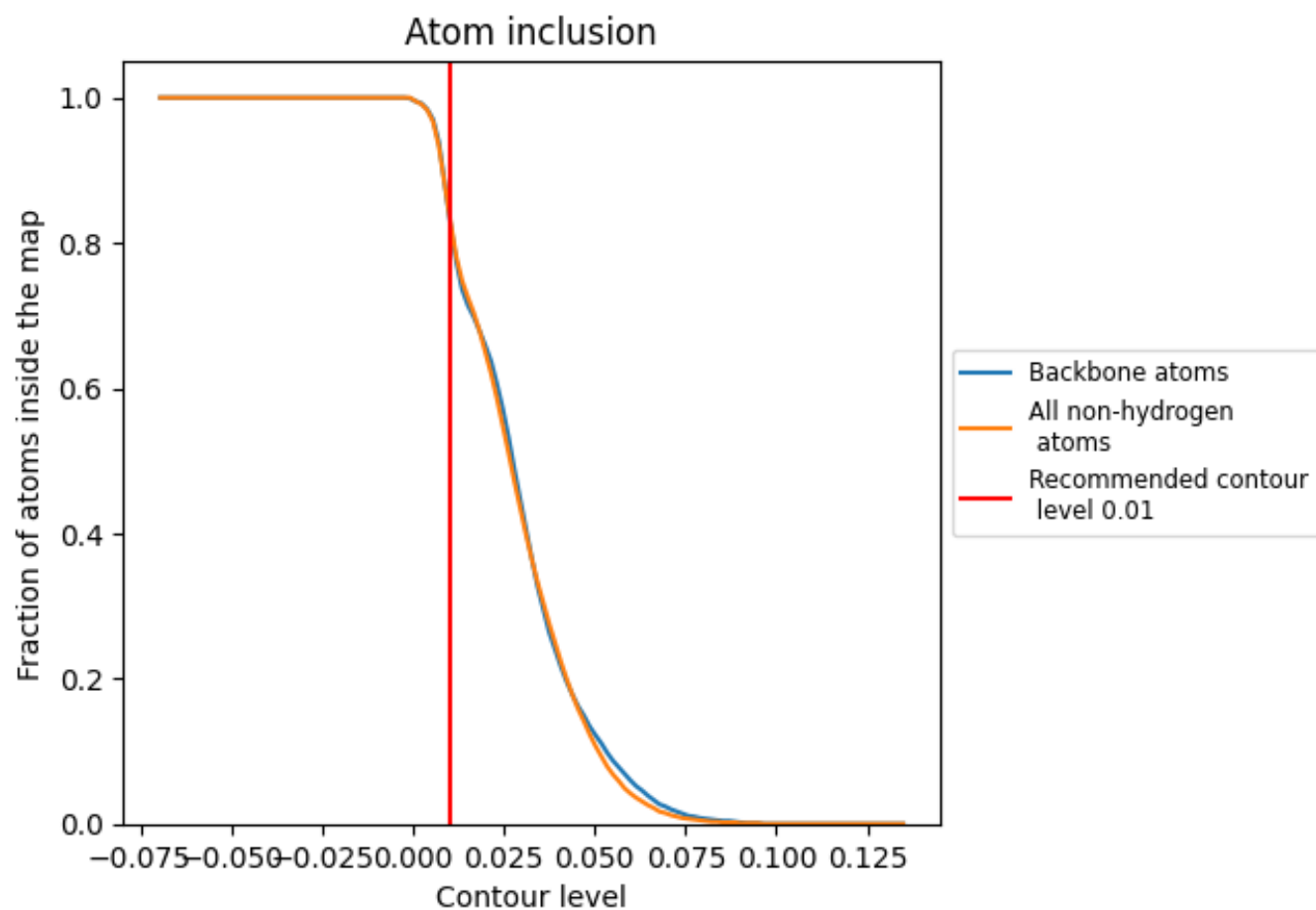
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8410	0.2590
D	0.4870	0.1280
E	0.9630	0.2310
G	0.9910	0.2000
H	0.9900	0.2930
I	0.9920	0.4530
J	0.9780	0.4400
O	0.4800	0.0920
R	0.9910	0.4540
S	0.9960	0.4590
T	0.9940	0.2910
U	0.9880	0.4640
V	0.9890	0.4610
W	0.9920	0.4520
X	0.9920	0.4630
Y	0.1680	0.1000

1.0

0.0

<0.0