Full wwPDB EM Validation Report

Nov 22, 2022 – 02:05 PM JST

PDB ID	:	7EGP
EMDB ID	:	EMD-31137
Title	:	The structure of SWI/SNF-nucleosome complex
Authors	:	Chen, Z.C.; Chen, K.J.; He, Z.Y.; Ye, Y.P.
Deposited on	:	2021-03-24
Resolution	:	6.90 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:

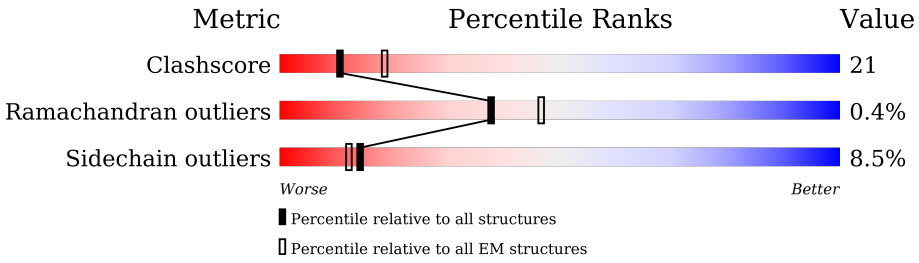
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	1093	36% 9% 54%
2	C	918	5% 27% 9% 62%
3	D	836	13% 37% 9% 53%
3	E	836	14% 39% 11% 50%
4	H	566	34% 54% 12% 31%
5	I	332	9% 25% 7% 68%
6	J	634	9% 22% 74%
7	A	982	30% 46% 28% 24%

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Mol	Chain	Length	Quality of chain
8	L	157	16% 17% 66%
9	M	477	40% 38% 19%
10	N	467	5% 40% 40% 16%
11	O	135	33% 34% 5% 27%
11	S	135	27% 39% 30%
12	P	102	7% 45% 34% 6% 15%
12	T	102	5% 35% 40% 9% 16%
13	Q	129	39% 42% 17%
13	U	129	5% 36% 43% 17%
14	R	122	33% 39% 5% 24%
14	V	122	27% 42% 7% 24%
15	W	235	11% 21% 30% 20% 29%
16	X	235	14% 22% 27% 22% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	ADP	A	1501	-	-	X	-
18	BEF	A	1502	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 44871 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 SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	507	4098	2663	672	752	11	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1315	GLY	-	expression tag	UNP P09547
B	1316	GLY	-	expression tag	UNP P09547
B	1317	SER	-	expression tag	UNP P09547
B	1318	GLY	-	expression tag	UNP P09547
B	1319	GLY	-	expression tag	UNP P09547
B	1320	TRP	-	expression tag	UNP P09547
B	1321	SER	-	expression tag	UNP P09547
B	1322	HIS	-	expression tag	UNP P09547
B	1323	PRO	-	expression tag	UNP P09547
B	1324	GLN	-	expression tag	UNP P09547
B	1325	PHE	-	expression tag	UNP P09547
B	1326	GLU	-	expression tag	UNP P09547
B	1327	LYS	-	expression tag	UNP P09547
B	1328	TRP	-	expression tag	UNP P09547
B	1329	SER	-	expression tag	UNP P09547
B	1330	HIS	-	expression tag	UNP P09547
B	1331	PRO	-	expression tag	UNP P09547
B	1332	GLN	-	expression tag	UNP P09547
B	1333	PHE	-	expression tag	UNP P09547
B	1334	GLU	-	expression tag	UNP P09547
B	1335	LYS	-	expression tag	UNP P09547
B	1336	TRP	-	expression tag	UNP P09547
B	1337	SER	-	expression tag	UNP P09547
B	1338	HIS	-	expression tag	UNP P09547
B	1339	PRO	-	expression tag	UNP P09547
B	1340	GLN	-	expression tag	UNP P09547
B	1341	PHE	-	expression tag	UNP P09547

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1342	GLU	-	expression tag	UNP P09547
B	1343	LYS	-	expression tag	UNP P09547

- Molecule 2 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	351	Total	C	N	O	S	0	0
			2873	1794	506	563	10		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	906	GLY	-	expression tag	UNP P18480
C	907	GLY	-	expression tag	UNP P18480
C	908	SER	-	expression tag	UNP P18480
C	909	GLY	-	expression tag	UNP P18480
C	910	GLY	-	expression tag	UNP P18480
C	911	ASP	-	expression tag	UNP P18480
C	912	TYR	-	expression tag	UNP P18480
C	913	LYS	-	expression tag	UNP P18480
C	914	ASP	-	expression tag	UNP P18480
C	915	ASP	-	expression tag	UNP P18480
C	916	ASP	-	expression tag	UNP P18480
C	917	ASP	-	expression tag	UNP P18480
C	918	LYS	-	expression tag	UNP P18480

- Molecule 3 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	395	Total	C	N	O	S	0	0
			3250	2082	560	597	11		
3	E	422	Total	C	N	O	S	0	0
			3454	2208	593	641	12		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	826	GLY	-	expression tag	UNP P32591
D	827	GLY	-	expression tag	UNP P32591
D	828	SER	-	expression tag	UNP P32591
D	829	GLY	-	expression tag	UNP P32591
D	830	GLY	-	expression tag	UNP P32591

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Chain	Residue	Modelled	Actual	Comment	Reference
D	831	HIS	-	expression tag	UNP P32591
D	832	HIS	-	expression tag	UNP P32591
D	833	HIS	-	expression tag	UNP P32591
D	834	HIS	-	expression tag	UNP P32591
D	835	HIS	-	expression tag	UNP P32591
D	836	HIS	-	expression tag	UNP P32591
E	826	GLY	-	expression tag	UNP P32591
E	827	GLY	-	expression tag	UNP P32591
E	828	SER	-	expression tag	UNP P32591
E	829	GLY	-	expression tag	UNP P32591
E	830	GLY	-	expression tag	UNP P32591
E	831	HIS	-	expression tag	UNP P32591
E	832	HIS	-	expression tag	UNP P32591
E	833	HIS	-	expression tag	UNP P32591
E	834	HIS	-	expression tag	UNP P32591
E	835	HIS	-	expression tag	UNP P32591
E	836	HIS	-	expression tag	UNP P32591

- Molecule 4 is a protein called Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	388	Total	C	N	O	S	0	0
			3145	1995	536	603	11		

- Molecule 5 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	106	Total	C	N	O	S	0	0
			888	553	158	173	4		

- Molecule 6 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	167	Total	C	N	O	S	0	0
			1360	877	241	240	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	624	GLY	-	expression tag	UNP P43554
J	625	GLY	-	expression tag	UNP P43554

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Chain	Residue	Modelled	Actual	Comment	Reference
J	626	SER	-	expression tag	UNP P43554
J	627	GLY	-	expression tag	UNP P43554
J	628	GLY	-	expression tag	UNP P43554
J	629	HIS	-	expression tag	UNP P43554
J	630	HIS	-	expression tag	UNP P43554
J	631	HIS	-	expression tag	UNP P43554
J	632	HIS	-	expression tag	UNP P43554
J	633	HIS	-	expression tag	UNP P43554
J	634	HIS	-	expression tag	UNP P43554

- Molecule 7 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	750	Total	C	N	O	S	0	0
			6162	3900	1101	1141	20		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1401	GLY	-	expression tag	UNP P22082
A	1402	GLY	-	expression tag	UNP P22082
A	1403	SER	-	expression tag	UNP P22082
A	1404	GLY	-	expression tag	UNP P22082
A	1405	GLY	-	expression tag	UNP P22082
A	1406	HIS	-	expression tag	UNP P22082
A	1407	HIS	-	expression tag	UNP P22082
A	1408	HIS	-	expression tag	UNP P22082
A	1409	HIS	-	expression tag	UNP P22082
A	1410	HIS	-	expression tag	UNP P22082
A	1411	HIS	-	expression tag	UNP P22082

- Molecule 8 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	53	Total	C	N	O	0	0
			482	308	83	91		

- Molecule 9 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	387	Total	C	N	O	S	3	0
			3131	2020	516	591	4		

- Molecule 10 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	392	Total	C	N	O	S	1	0
			3167	2033	519	611	4		

- Molecule 11 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	98	Total	C	N	O	S	0	0
			800	505	153	139	3		
11	S	95	Total	C	N	O	S	0	0
			778	491	148	136	3		

- Molecule 12 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
12	T	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 13 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Q	107	Total	C	N	O	0	0
			811	510	158	143		
13	U	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 14 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
14	V	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	29	THR	SER	engineered mutation	UNP P02281
V	29	THR	SER	engineered mutation	UNP P02281

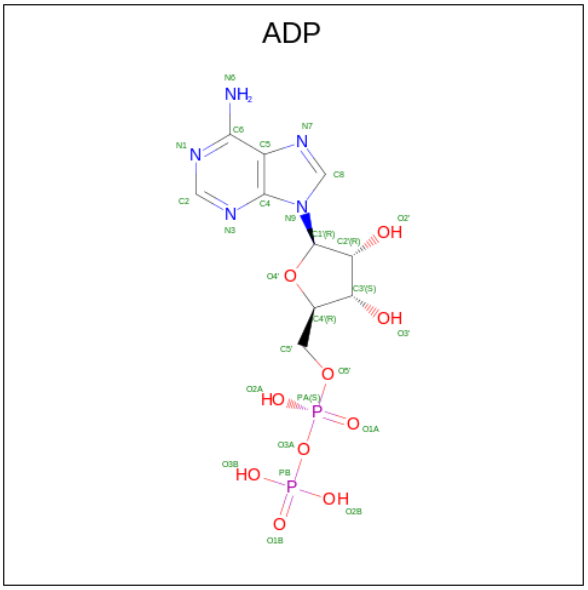
- Molecule 15 is a DNA chain called DNA (239-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	W	166	3393	1611	621	995	166	0	0

- Molecule 16 is a DNA chain called DNA (239-MER).

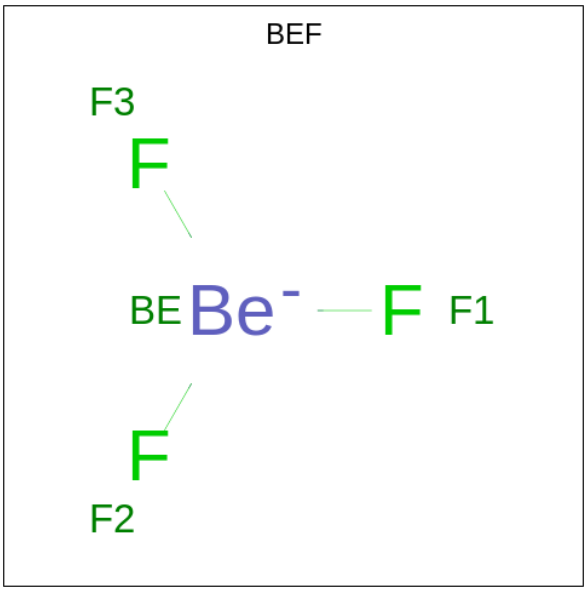
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	X	166	3413	1618	632	997	166	0	0

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	A	1	27	10	5	10	2	0

- Molecule 18 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	Be	F	0
			4	1	3	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

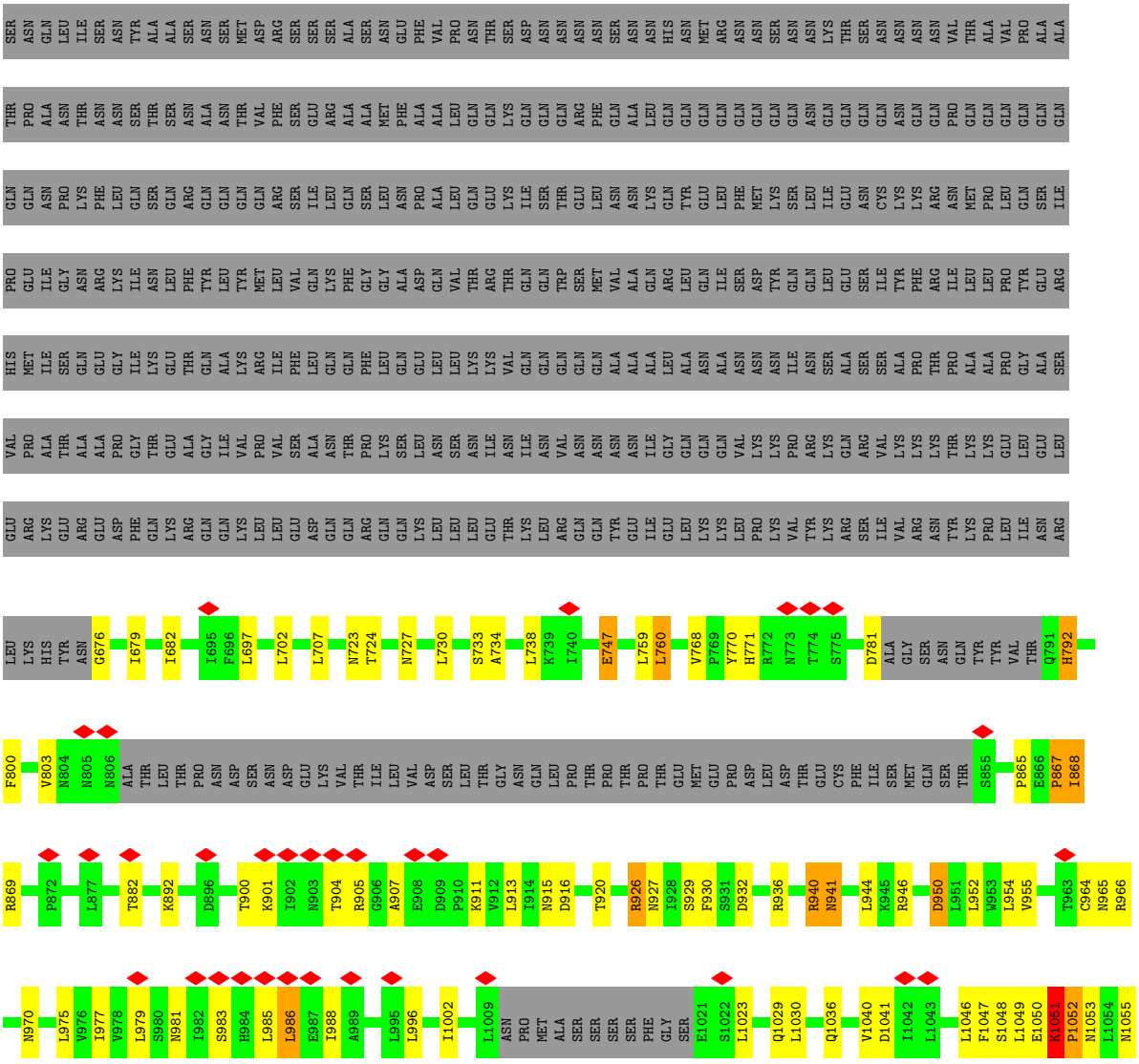
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	

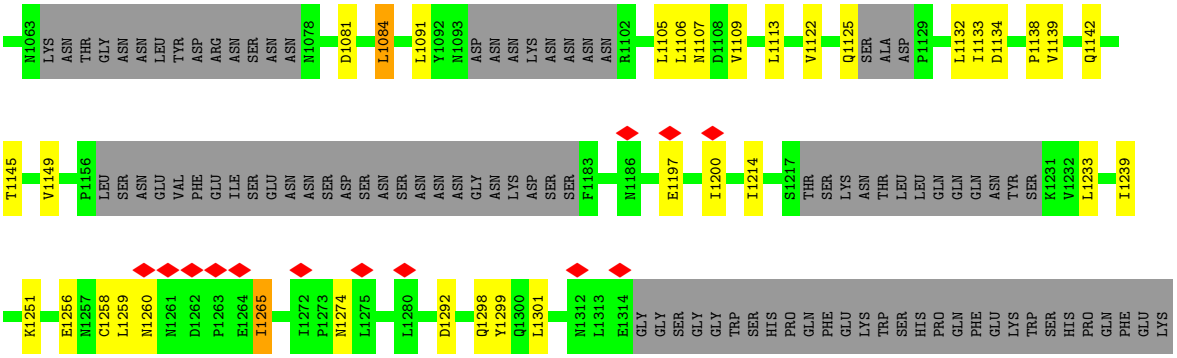
3 Residue-property plots (i)

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.

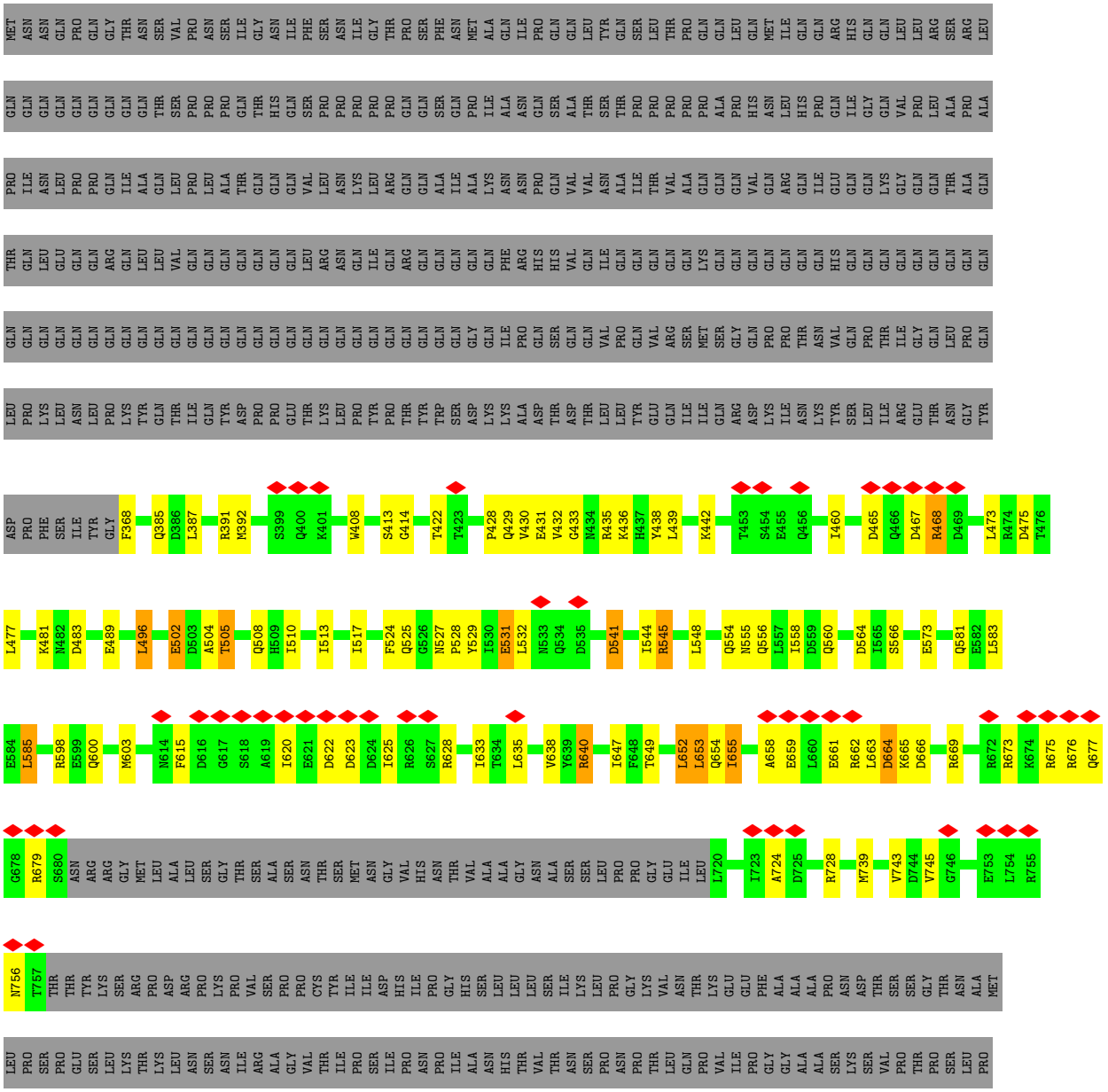
- Molecule 1: SWI/SNF chromatin-remodeling complex subunit SWI1

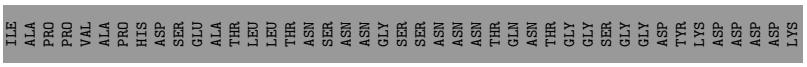
Chain B:





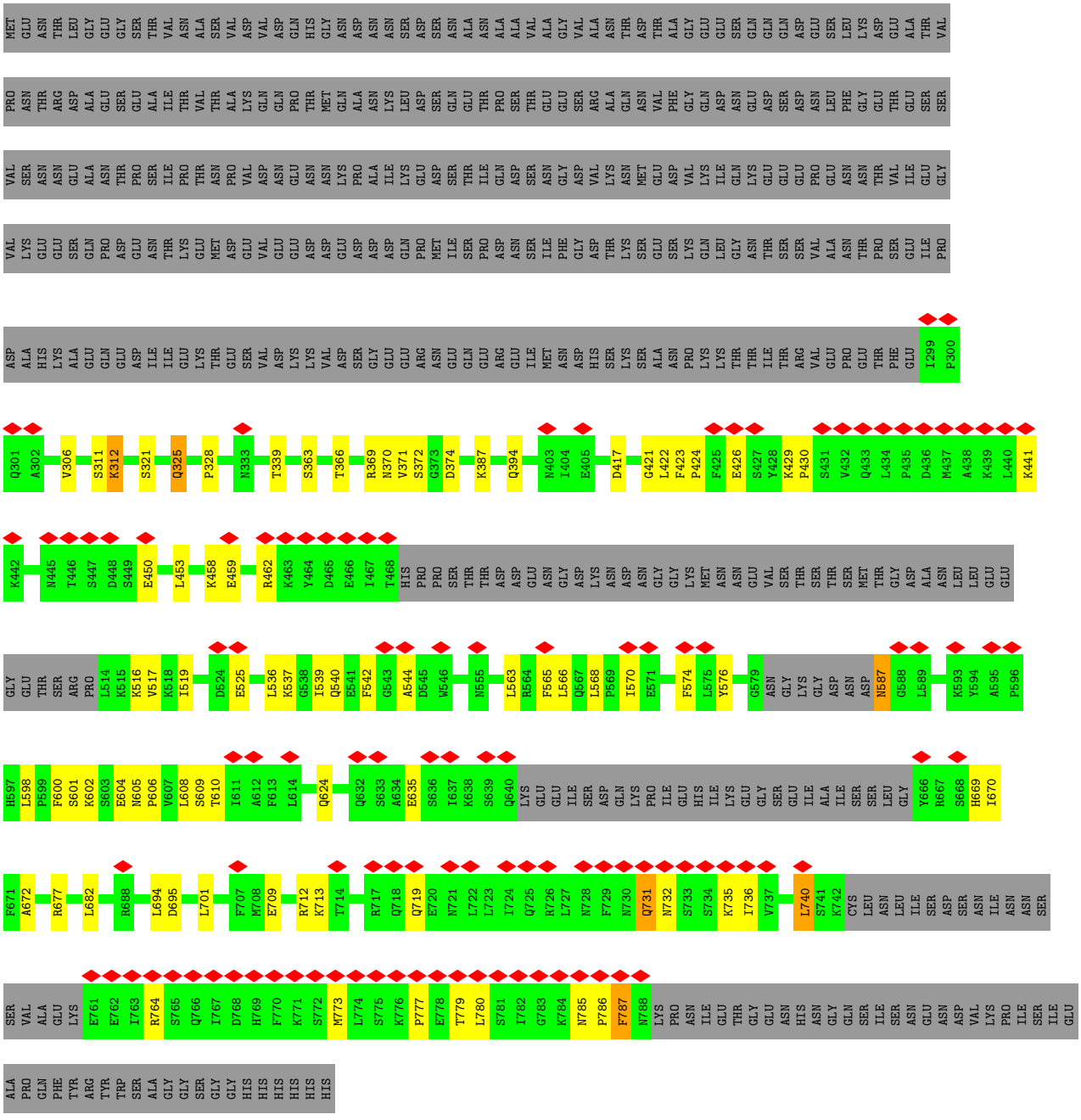
• Molecule 2: SWI/SNF chromatin-remodeling complex subunit SNF5





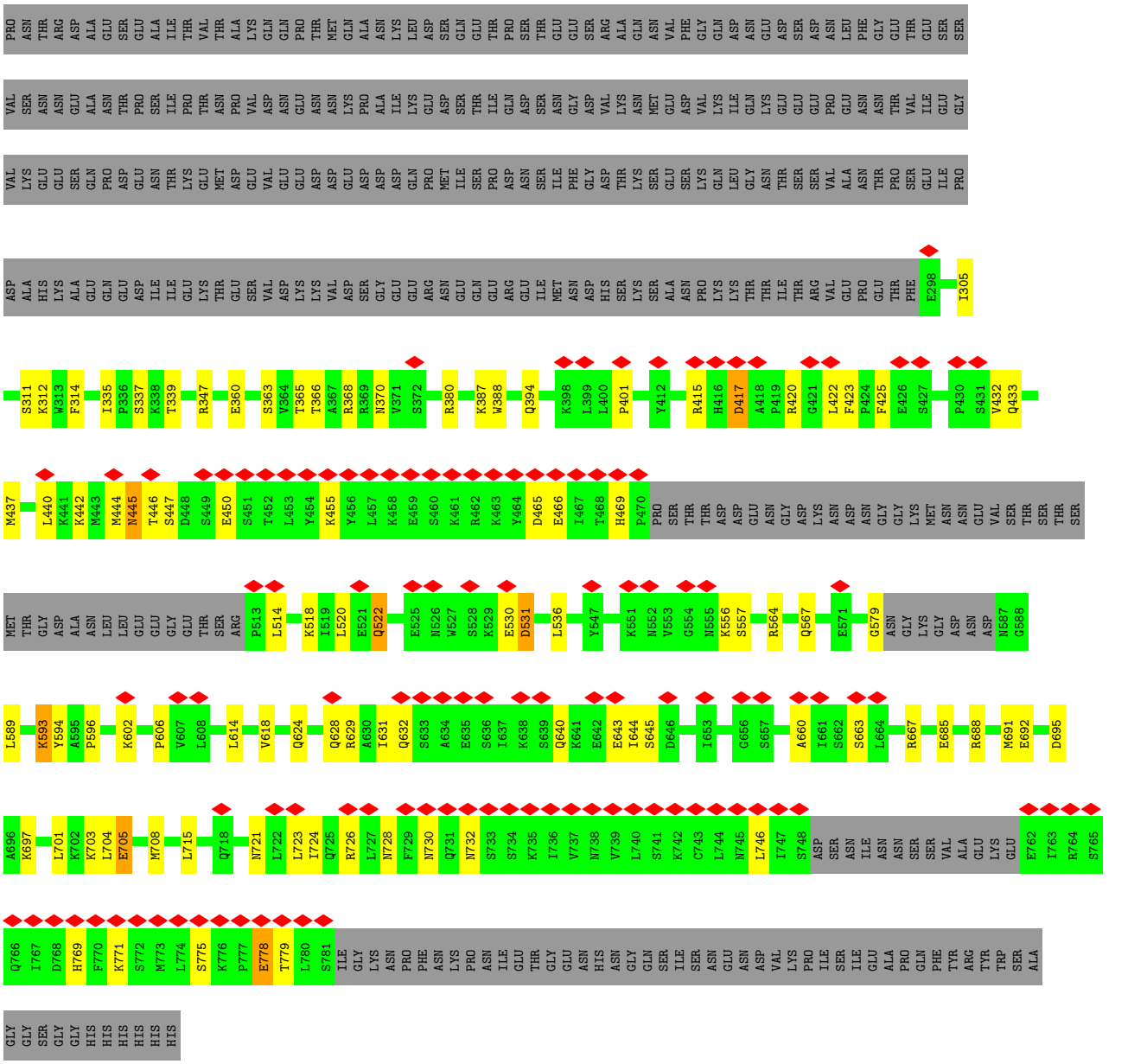
• Molecule 3: SWI/SNF complex subunit SWI3

Chain D:

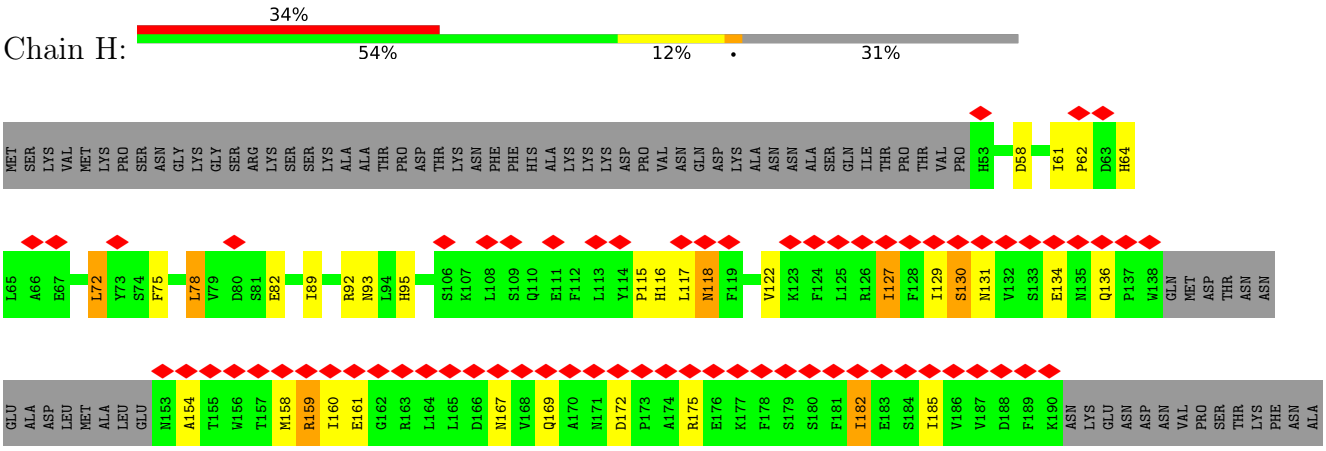


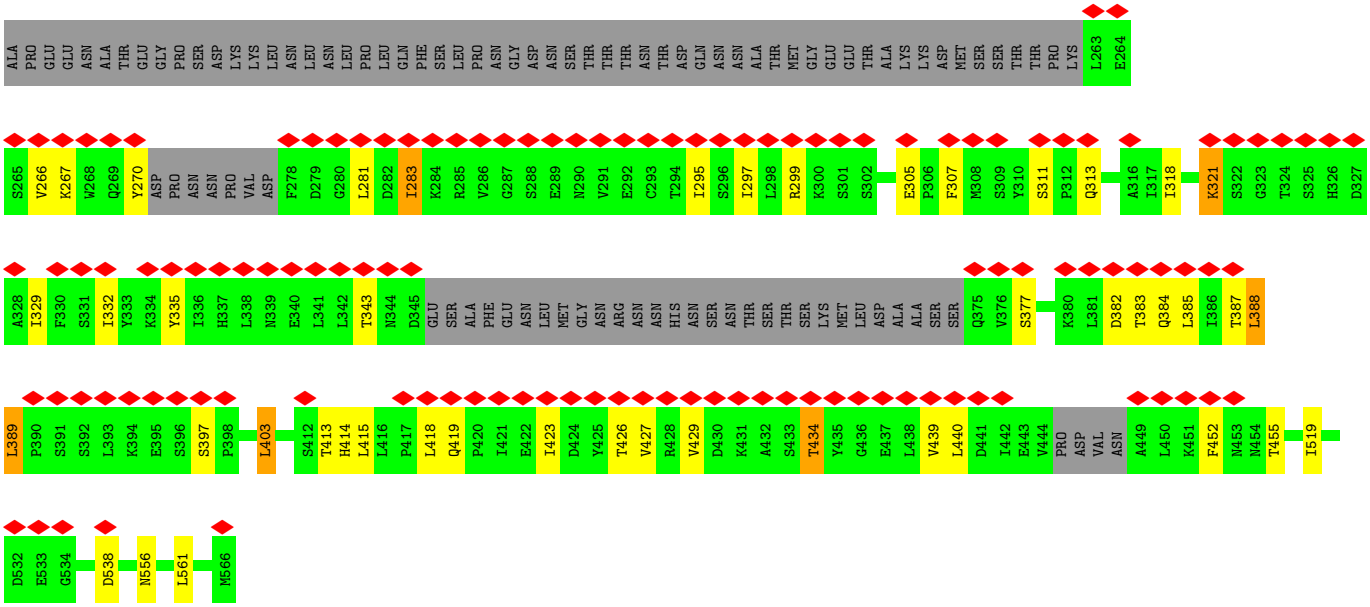
• Molecule 3: SWI/SNF complex subunit SWI3

Chain E:



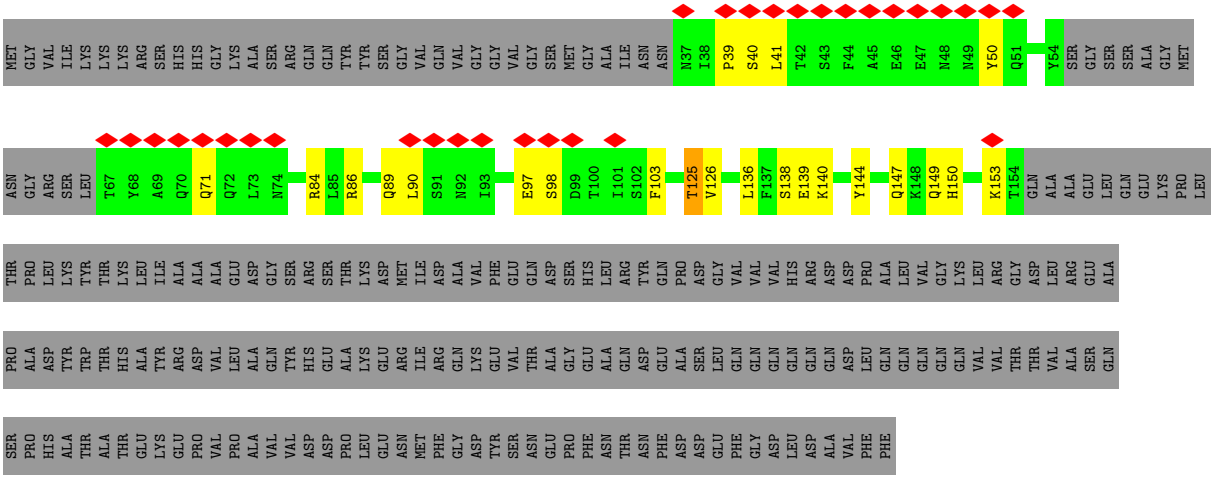
• Molecule 4: Transcription regulatory protein SNF12





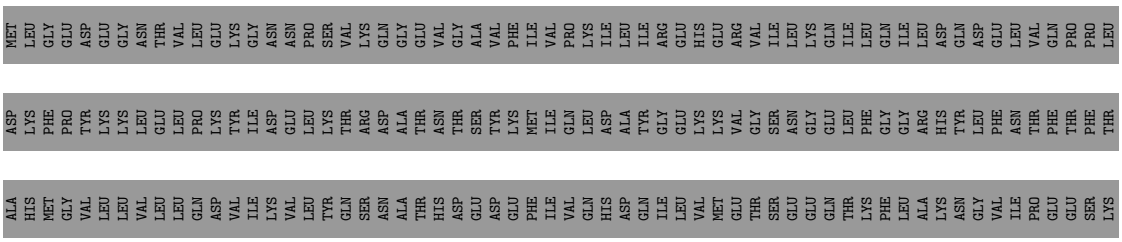
• Molecule 5: Transcription regulatory protein SNF6

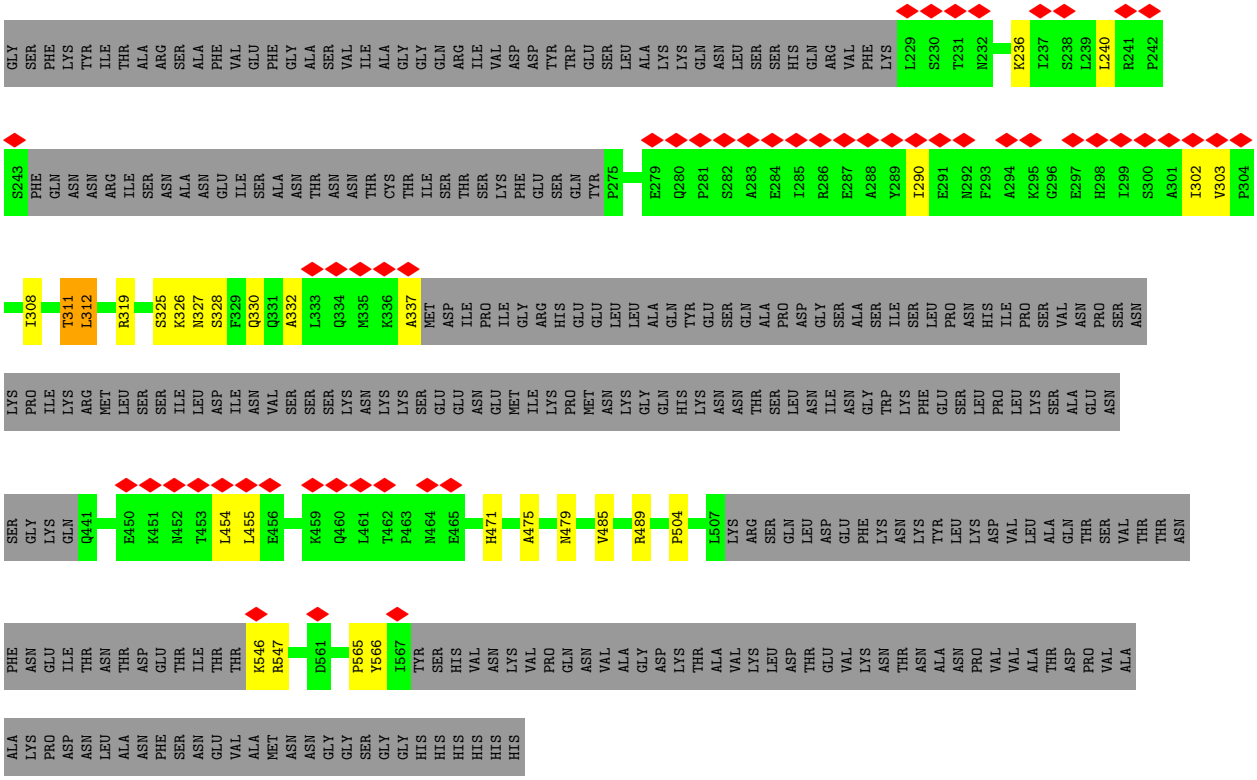
Chain I:



• Molecule 6: SWI/SNF global transcription activator complex subunit SWP82

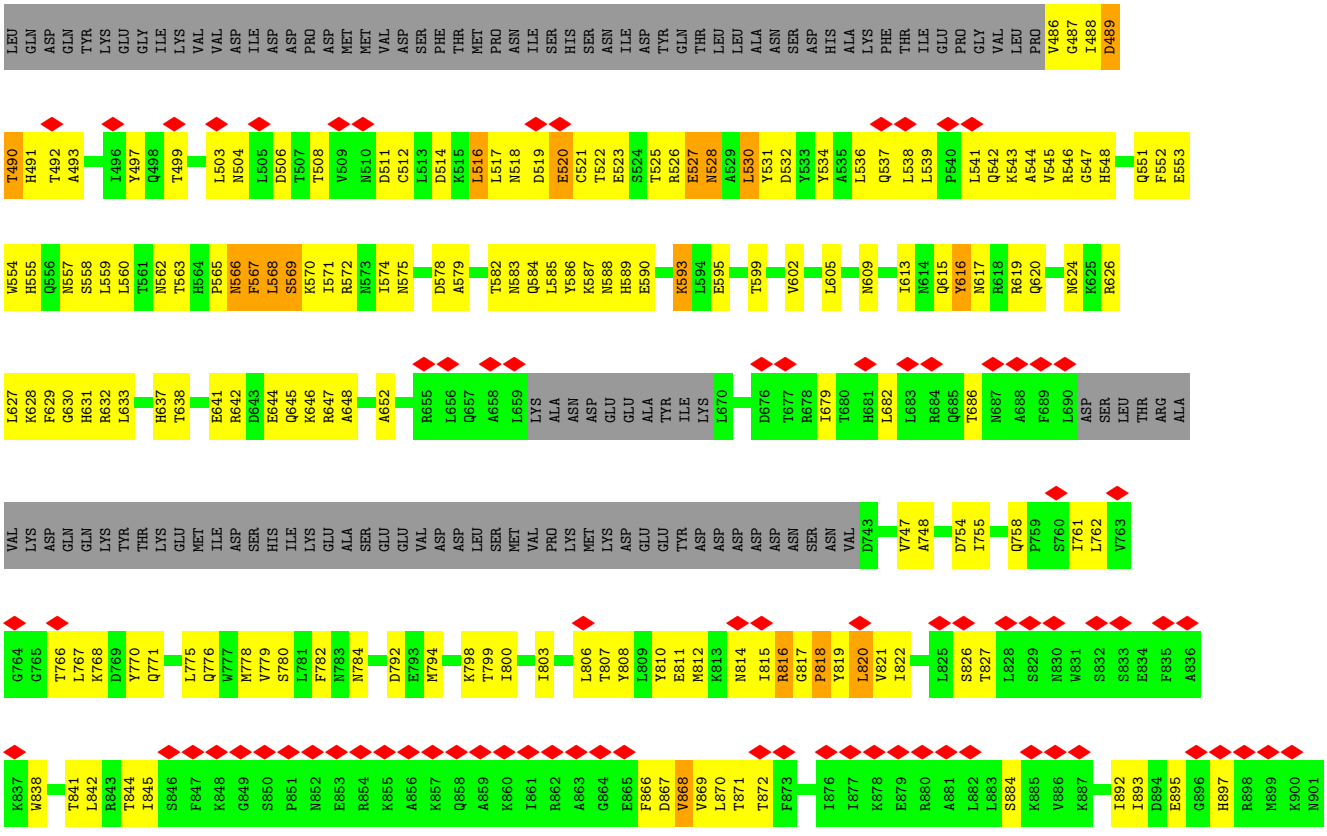
Chain J:

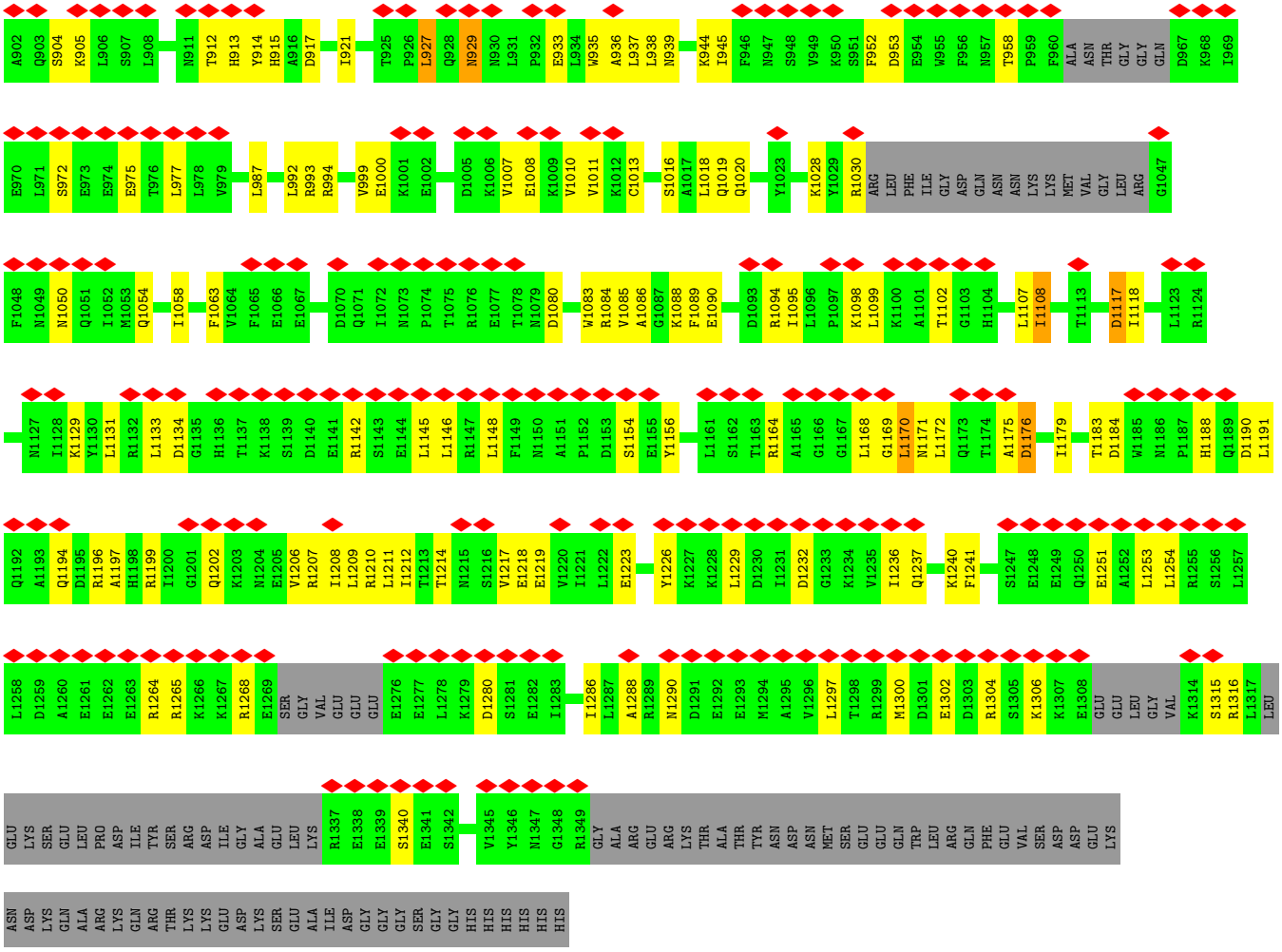




• Molecule 7: Transcription regulatory protein SNF2

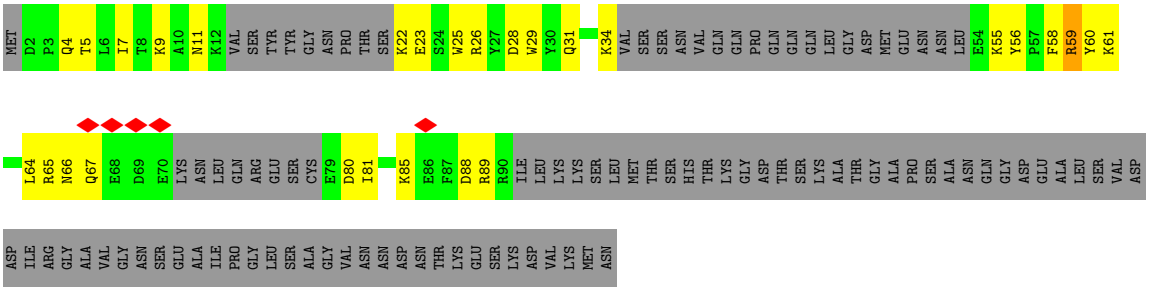
Chain A:





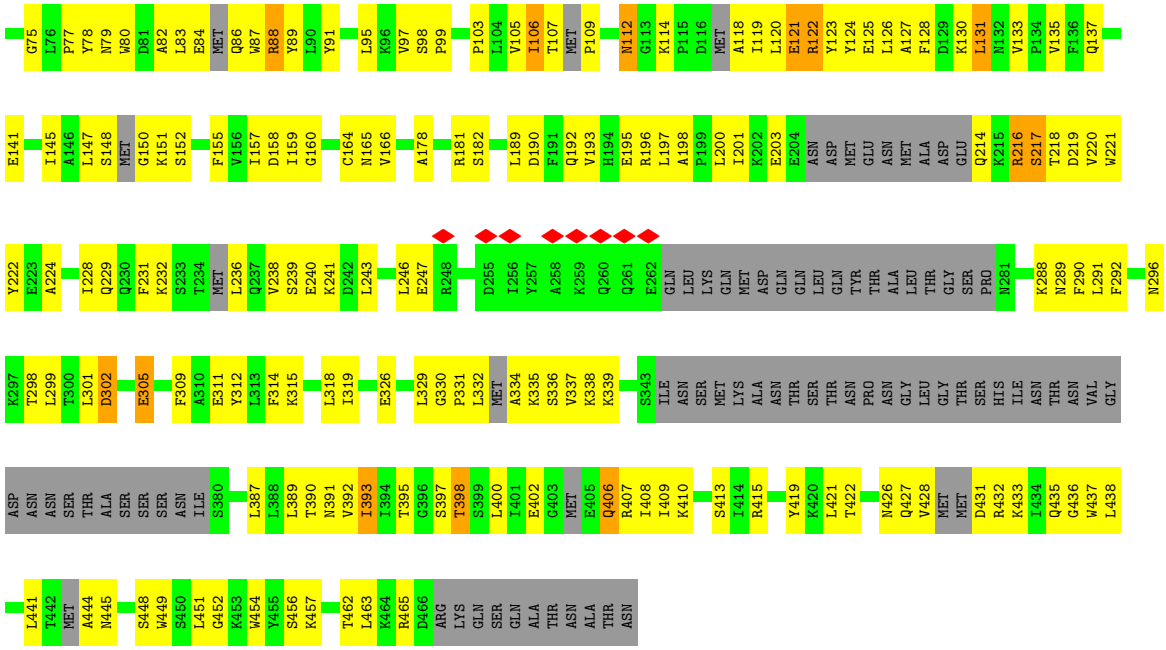
• Molecule 8: Regulator of Ty1 transposition protein 102

Chain L:

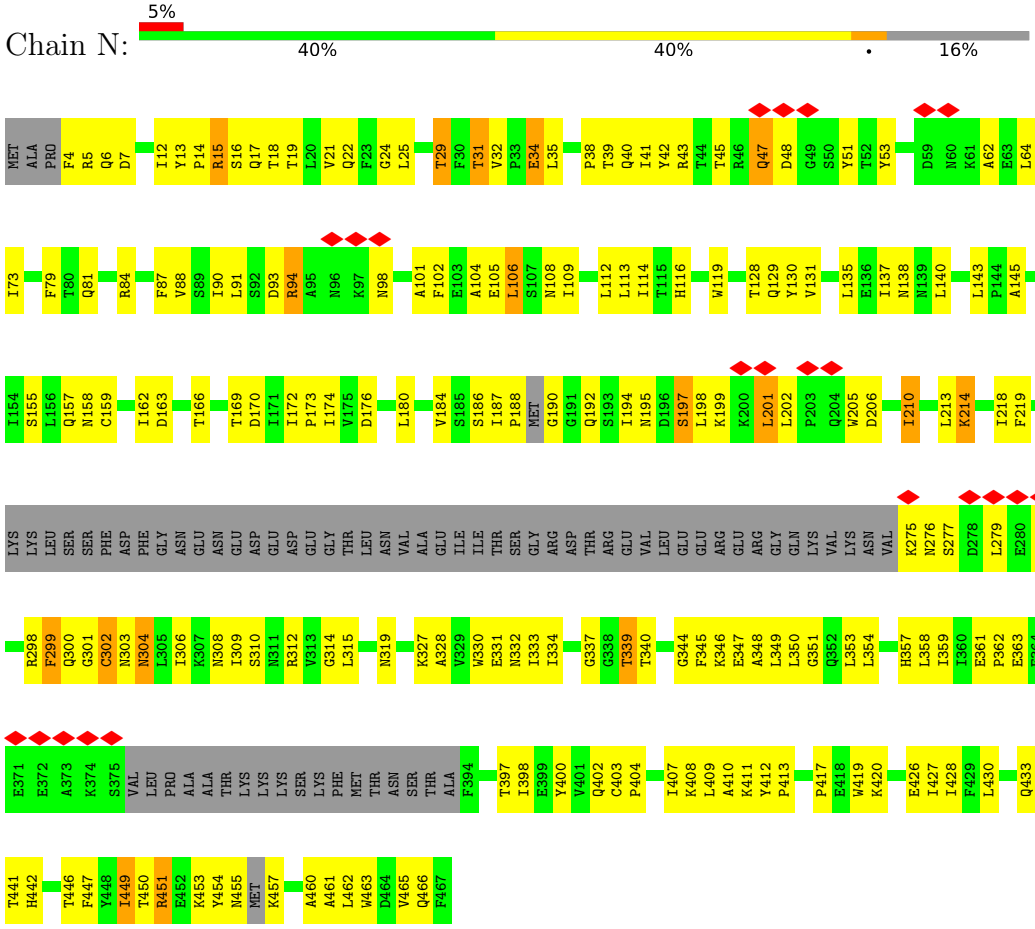


• Molecule 9: Actin-related protein 7

Chain M:

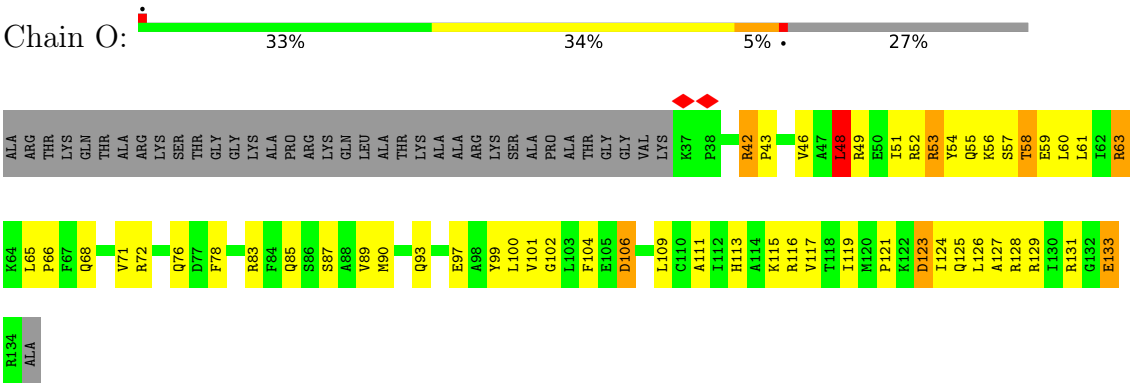


• Molecule 10: Actin-like protein ARP9



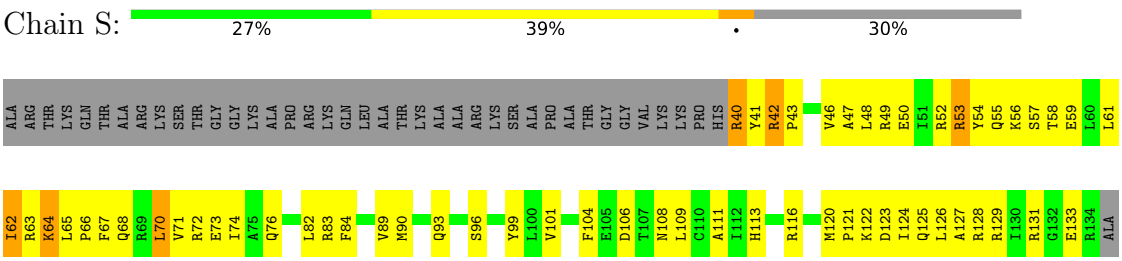
• Molecule 11: Histone H3.2

Chain O:



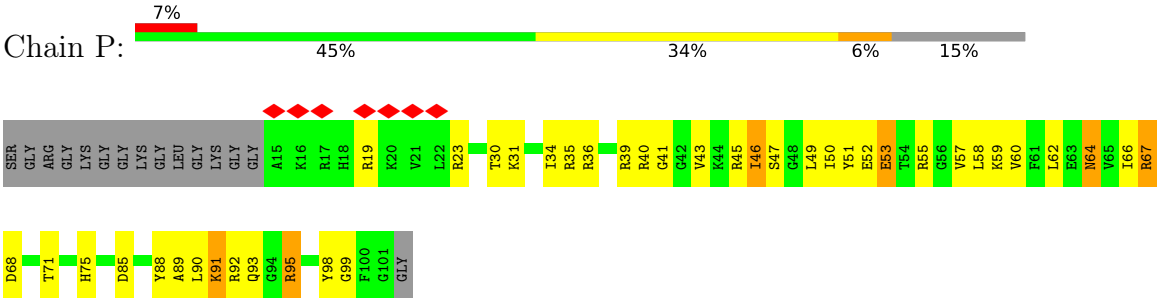
• Molecule 11: Histone H3.2

Chain S:



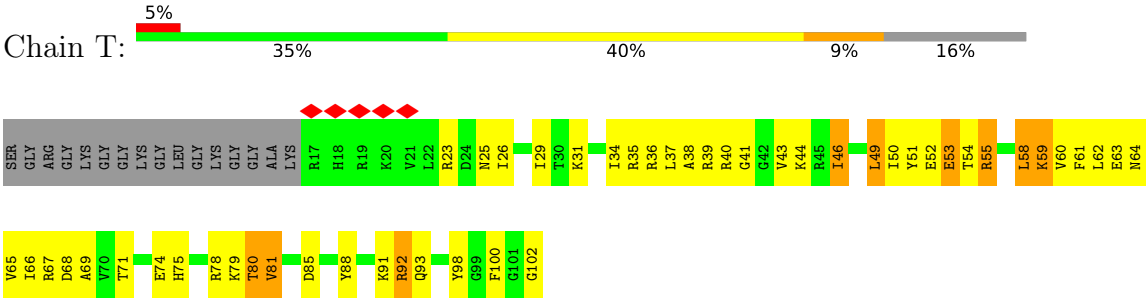
• Molecule 12: Histone H4

Chain P:



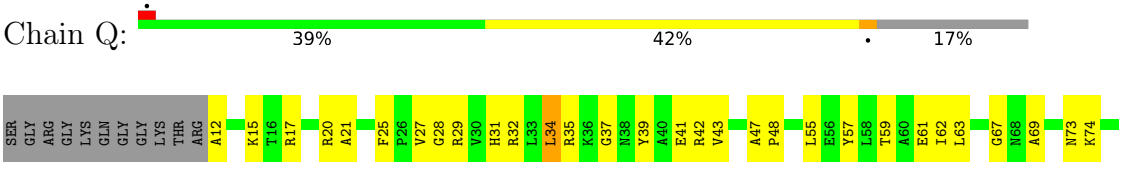
• Molecule 12: Histone H4

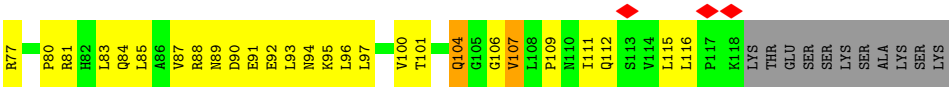
Chain T:



• Molecule 13: Histone H2A

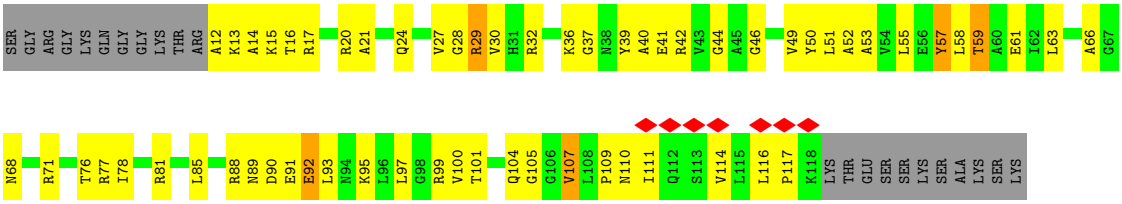
Chain Q:





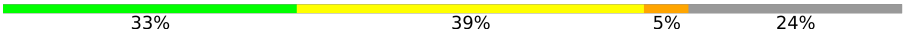
• Molecule 13: Histone H2A

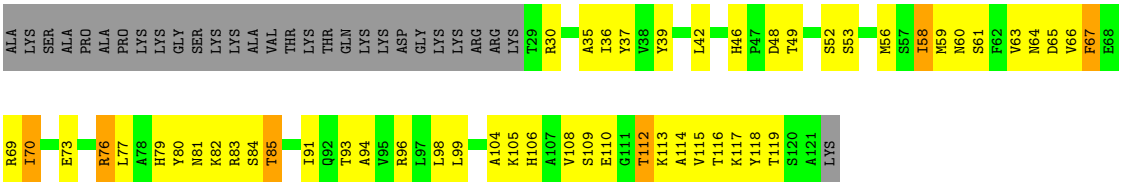
Chain U:



• Molecule 14: Histone H2B 1.1

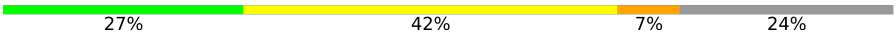
Chain R:

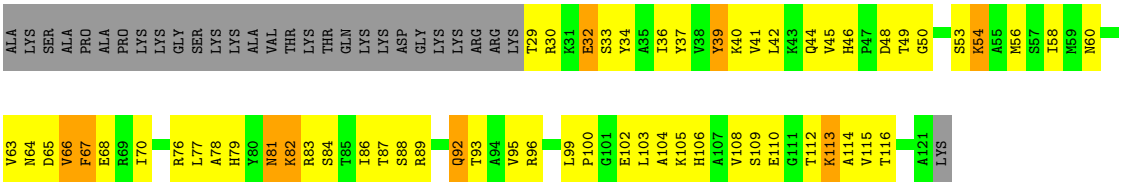




• Molecule 14: Histone H2B 1.1

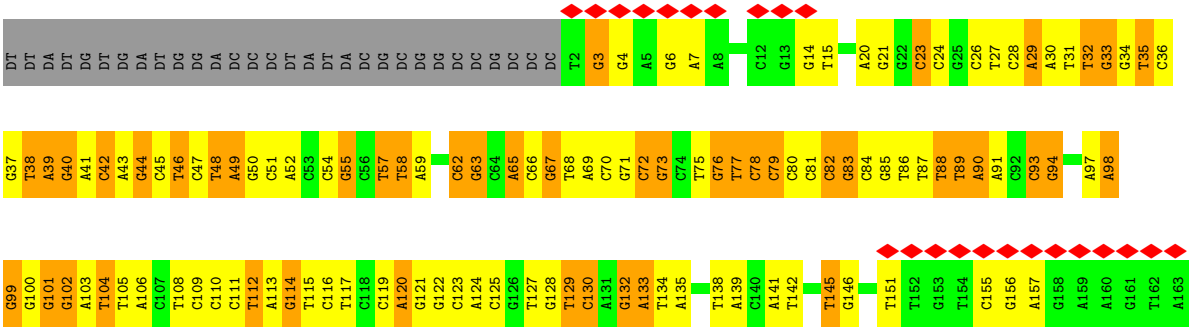
Chain V:

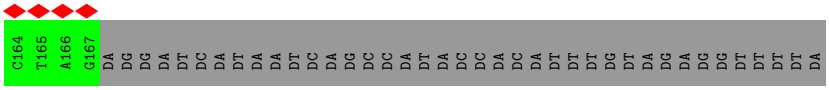




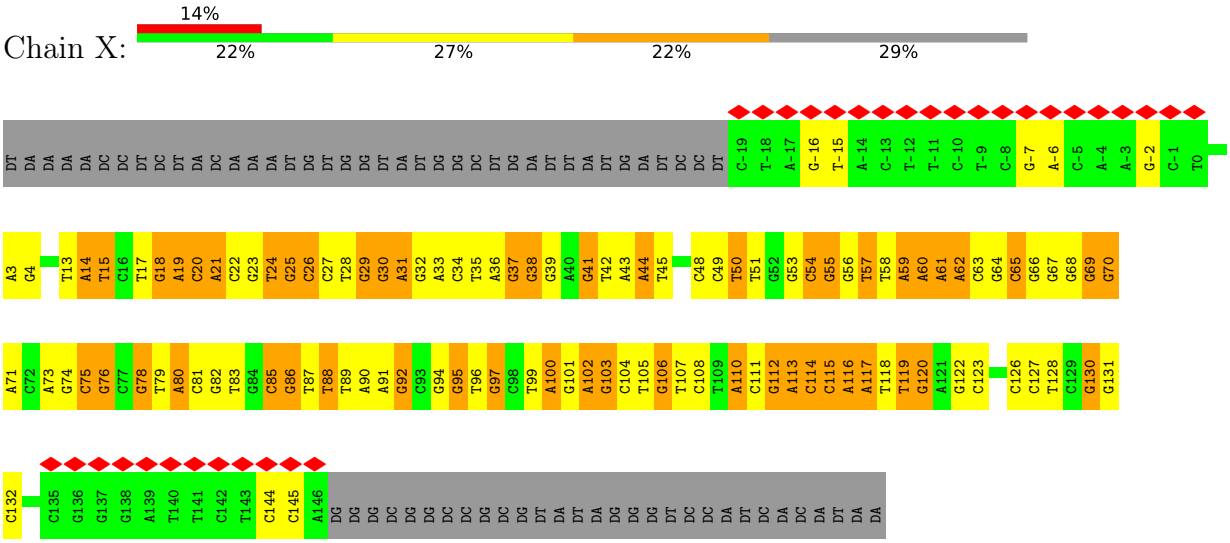
• Molecule 15: DNA (239-MER)

Chain W:





• Molecule 16: DNA (239-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229461	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	429.68002, 429.68002, 429.68002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.1484, 2.1484, 2.1484	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.29	0/4171	0.49	1/5648 (0.0%)
2	C	0.31	0/2926	0.49	0/3953
3	D	0.30	0/3318	0.45	0/4465
3	E	0.29	0/3526	0.47	0/4747
4	H	0.26	0/3201	0.47	1/4322 (0.0%)
5	I	0.25	0/902	0.48	0/1211
6	J	0.27	0/1390	0.47	0/1874
7	A	0.32	0/6256	0.52	0/8415
8	L	0.36	0/493	0.59	0/659
9	M	0.38	0/3197	0.57	0/4313
10	N	0.35	0/3234	0.56	1/4382 (0.0%)
11	O	0.42	0/812	0.63	1/1091 (0.1%)
11	S	0.40	0/788	0.68	0/1057
12	P	0.39	0/711	0.59	0/950
12	T	0.39	0/680	0.61	0/912
13	Q	0.37	0/821	0.57	0/1112
13	U	0.41	0/825	0.60	0/1116
14	R	0.47	0/729	0.60	0/985
14	V	0.45	0/737	0.63	0/993
15	W	1.63	70/3804 (1.8%)	1.37	37/5866 (0.6%)
16	X	1.67	77/3830 (2.0%)	1.48	56/5912 (0.9%)
All	All	0.74	147/46351 (0.3%)	0.77	97/63983 (0.2%)

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	55	DG	N9-C4	-10.06	1.29	1.38
16	X	33	DA	N9-C4	-9.92	1.31	1.37
16	X	61	DA	C3'-O3'	-9.43	1.31	1.44
16	X	14	DA	N9-C4	-9.01	1.32	1.37
15	W	106	DA	N9-C4	-8.95	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	W	124	DA	N9-C4	-8.47	1.32	1.37
15	W	49	DA	N9-C4	-8.45	1.32	1.37
15	W	130	DC	C3'-O3'	-8.37	1.33	1.44
15	W	98	DA	N9-C4	-8.26	1.32	1.37
16	X	55	DG	C2-N3	-8.12	1.26	1.32
16	X	30	DG	C3'-O3'	-8.10	1.33	1.44
15	W	88	DT	C3'-O3'	-8.09	1.33	1.44
15	W	44	DG	N9-C4	-7.86	1.31	1.38
15	W	122	DG	C3'-O3'	-7.78	1.33	1.44
15	W	65	DA	N9-C4	-7.70	1.33	1.37
16	X	69	DG	N9-C4	-7.61	1.31	1.38
15	W	139	DA	N9-C4	-7.56	1.33	1.37
16	X	57	DT	C3'-O3'	-7.55	1.34	1.44
15	W	57	DT	C3'-O3'	-7.54	1.34	1.44
16	X	43	DA	N9-C4	-7.53	1.33	1.37
16	X	116	DA	N9-C4	-7.49	1.33	1.37
15	W	135	DA	N9-C4	-7.43	1.33	1.37
16	X	97	DG	N9-C4	-7.30	1.32	1.38
15	W	33	DG	N9-C4	-7.23	1.32	1.38
15	W	49	DA	N3-C4	-7.23	1.30	1.34
16	X	44	DA	N9-C4	-7.20	1.33	1.37
16	X	100	DA	N9-C4	-7.09	1.33	1.37
16	X	18	DG	N9-C4	-7.05	1.32	1.38
15	W	103	DA	N9-C4	-7.00	1.33	1.37
16	X	110	DA	N9-C4	-6.96	1.33	1.37
15	W	99	DG	N9-C4	-6.93	1.32	1.38
15	W	99	DG	C2-N3	-6.87	1.27	1.32
16	X	110	DA	C2-N3	-6.86	1.27	1.33
15	W	134	DT	N1-C2	-6.74	1.32	1.38
15	W	115	DT	N1-C2	-6.71	1.32	1.38
16	X	76	DG	N9-C4	-6.71	1.32	1.38
16	X	106	DG	N9-C4	-6.71	1.32	1.38
16	X	97	DG	C2-N3	-6.66	1.27	1.32
16	X	120	DG	N9-C4	-6.65	1.32	1.38
16	X	105	DT	N1-C2	-6.63	1.32	1.38
16	X	103	DG	N9-C4	-6.63	1.32	1.38
16	X	24	DT	N1-C2	-6.61	1.32	1.38
16	X	103	DG	C3'-O3'	-6.59	1.35	1.44
16	X	38	DG	N9-C4	-6.56	1.32	1.38
16	X	107	DT	N1-C2	-6.55	1.32	1.38
15	W	29	DA	N9-C4	-6.51	1.33	1.37
16	X	113	DA	N9-C4	-6.42	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	102	DA	N9-C4	-6.42	1.33	1.37
15	W	113	DA	N9-C4	-6.40	1.34	1.37
15	W	102	DG	C3'-O3'	-6.34	1.35	1.44
15	W	105	DT	N1-C2	-6.34	1.32	1.38
16	X	62	DA	C3'-O3'	-6.31	1.35	1.44
16	X	45	DT	N1-C2	-6.31	1.33	1.38
16	X	35	DT	N1-C2	-6.29	1.33	1.38
15	W	85	DG	C5-C6	-6.28	1.36	1.42
15	W	133	DA	N9-C4	-6.26	1.34	1.37
15	W	85	DG	C8-N7	-6.21	1.27	1.30
16	X	103	DG	C2-N3	-6.21	1.27	1.32
16	X	69	DG	C2-N3	-6.17	1.27	1.32
16	X	38	DG	C2-N3	-6.14	1.27	1.32
15	W	67	DG	C2-N3	-6.11	1.27	1.32
16	X	25	DG	N9-C4	-6.09	1.33	1.38
16	X	18	DG	C2-N3	-6.08	1.27	1.32
15	W	70	DC	C3'-O3'	-6.07	1.36	1.44
15	W	46	DT	N1-C2	-6.07	1.33	1.38
15	W	55	DG	C5-C6	-6.06	1.36	1.42
15	W	39	DA	N9-C4	-6.05	1.34	1.37
15	W	138	DT	N1-C2	-6.03	1.33	1.38
15	W	77	DT	C3'-O3'	-6.03	1.36	1.44
16	X	13	DT	N1-C2	-6.01	1.33	1.38
15	W	35	DT	N1-C2	-5.99	1.33	1.38
15	W	38	DT	N1-C2	-5.97	1.33	1.38
15	W	3	DG	C1'-N9	-5.96	1.39	1.47
16	X	21	DA	N9-C4	-5.94	1.34	1.37
15	W	104	DT	N1-C2	-5.89	1.33	1.38
15	W	85	DG	C1'-N9	-5.88	1.39	1.47
16	X	117	DA	N9-C4	-5.86	1.34	1.37
16	X	83	DT	N1-C2	-5.85	1.33	1.38
16	X	64	DG	N9-C4	-5.81	1.33	1.38
16	X	120	DG	C2-N3	-5.81	1.28	1.32
16	X	100	DA	N3-C4	-5.80	1.31	1.34
15	W	94	DG	N9-C4	-5.78	1.33	1.38
15	W	44	DG	C2-N3	-5.77	1.28	1.32
16	X	108	DC	C3'-O3'	-5.75	1.36	1.44
16	X	65	DC	C2-N3	-5.73	1.31	1.35
16	X	56	DG	N9-C4	-5.72	1.33	1.38
16	X	94	DG	C3'-O3'	5.72	1.51	1.44
16	X	74	DG	N9-C4	-5.68	1.33	1.38
16	X	112	DG	N9-C4	-5.68	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	41	DG	C3'-O3'	-5.67	1.36	1.44
16	X	19	DA	N9-C4	-5.67	1.34	1.37
16	X	73	DA	N9-C4	-5.67	1.34	1.37
16	X	81	DC	C3'-O3'	-5.65	1.36	1.44
16	X	62	DA	N3-C4	-5.63	1.31	1.34
15	W	113	DA	N7-C5	-5.63	1.35	1.39
15	W	43	DA	N9-C4	-5.61	1.34	1.37
15	W	41	DA	N9-C4	-5.61	1.34	1.37
15	W	114	DG	N9-C4	-5.60	1.33	1.38
16	X	80	DA	C3'-O3'	-5.57	1.36	1.44
15	W	63	DG	N9-C4	-5.55	1.33	1.38
16	X	86	DG	N9-C4	-5.55	1.33	1.38
16	X	33	DA	N3-C4	-5.53	1.31	1.34
15	W	79	DC	C3'-O3'	-5.50	1.36	1.44
16	X	31	DA	N9-C4	-5.47	1.34	1.37
15	W	32	DT	N1-C2	-5.47	1.33	1.38
16	X	20	DC	C3'-O3'	-5.46	1.36	1.44
16	X	36	DA	N9-C4	-5.46	1.34	1.37
15	W	76	DG	N9-C4	-5.45	1.33	1.38
15	W	49	DA	C2-N3	-5.45	1.28	1.33
16	X	107	DT	C1'-N1	-5.44	1.39	1.47
16	X	78	DG	N9-C4	-5.43	1.33	1.38
15	W	83	DG	N3-C4	-5.40	1.31	1.35
16	X	94	DG	N9-C4	-5.39	1.33	1.38
16	X	110	DA	N3-C4	-5.39	1.31	1.34
15	W	141	DA	C3'-O3'	-5.38	1.36	1.44
15	W	83	DG	C6-N1	-5.37	1.35	1.39
15	W	97	DA	C3'-O3'	-5.36	1.36	1.44
15	W	78	DC	C2-N3	-5.32	1.31	1.35
15	W	55	DG	N7-C5	-5.32	1.36	1.39
16	X	25	DG	C3'-O3'	-5.31	1.37	1.44
15	W	85	DG	N9-C4	-5.31	1.33	1.38
16	X	33	DA	C2-N3	-5.31	1.28	1.33
15	W	33	DG	C2-N3	-5.31	1.28	1.32
15	W	90	DA	C3'-O3'	-5.29	1.37	1.44
15	W	73	DG	N9-C4	-5.29	1.33	1.38
15	W	97	DA	N9-C4	-5.28	1.34	1.37
15	W	141	DA	N9-C4	-5.28	1.34	1.37
15	W	120	DA	N9-C4	-5.23	1.34	1.37
15	W	120	DA	C2-N3	-5.23	1.28	1.33
15	W	48	DT	C3'-O3'	-5.23	1.37	1.44
16	X	92	DG	N9-C4	-5.22	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	55	DG	N3-C4	-5.20	1.31	1.35
16	X	95	DG	N9-C4	-5.18	1.33	1.38
15	W	67	DG	N9-C4	-5.18	1.33	1.38
16	X	37	DG	N9-C4	-5.17	1.33	1.38
16	X	105	DT	C2-N3	-5.17	1.33	1.37
16	X	59	DA	N9-C4	-5.14	1.34	1.37
16	X	14	DA	N3-C4	-5.11	1.31	1.34
15	W	58	DT	C3'-O3'	-5.10	1.37	1.44
15	W	93	DC	N1-C2	-5.09	1.35	1.40
16	X	96	DT	N1-C2	-5.09	1.33	1.38
16	X	14	DA	C2-N3	-5.09	1.28	1.33
16	X	114	DC	C3'-O3'	-5.06	1.37	1.44
15	W	55	DG	C8-N7	-5.04	1.27	1.30
15	W	89	DT	C3'-O3'	-5.03	1.37	1.44
15	W	77	DT	N1-C2	-5.02	1.34	1.38
16	X	29	DG	C3'-O3'	-5.01	1.37	1.44

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	132	DG	O4'-C1'-N9	11.49	116.04	108.00
15	W	90	DA	O4'-C1'-N9	10.17	115.12	108.00
16	X	74	DG	O4'-C1'-N9	8.79	114.16	108.00
16	X	42	DT	O4'-C1'-N1	8.61	114.03	108.00
16	X	65	DC	O4'-C4'-C3'	-8.13	101.12	106.00
16	X	35	DT	O4'-C4'-C3'	-8.01	101.20	106.00
15	W	40	DG	O4'-C1'-N9	7.91	113.54	108.00
16	X	22	DC	O4'-C1'-N1	7.89	113.53	108.00
15	W	112	DT	O4'-C1'-N1	7.77	113.44	108.00
16	X	88	DT	O4'-C4'-C3'	-7.75	101.35	106.00
4	H	389	LEU	CA-CB-CG	7.19	131.84	115.30
16	X	64	DG	C3'-C2'-C1'	-7.13	93.94	102.50
16	X	13	DT	O4'-C1'-N1	7.07	112.95	108.00
16	X	55	DG	N3-C4-N9	-7.07	121.76	126.00
15	W	37	DG	O4'-C4'-C3'	-6.96	101.72	104.50
16	X	105	DT	C3'-C2'-C1'	-6.91	94.20	102.50
16	X	130	DG	O4'-C4'-C3'	-6.88	101.75	104.50
16	X	70	DG	OP2-P-O3'	6.83	120.22	105.20
16	X	26	DC	O4'-C1'-N1	6.76	112.73	108.00
15	W	67	DG	O4'-C4'-C3'	-6.70	101.82	104.50
16	X	74	DG	C1'-O4'-C4'	-6.69	103.41	110.10
10	N	411	LYS	C-N-CA	6.64	138.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	X	105	DT	O4'-C1'-N1	6.62	112.63	108.00
16	X	42	DT	C1'-O4'-C4'	-6.57	103.53	110.10
16	X	31	DA	O4'-C1'-N9	6.45	112.51	108.00
16	X	22	DC	C1'-O4'-C4'	-6.44	103.66	110.10
16	X	94	DG	OP1-P-O3'	6.44	119.36	105.20
15	W	101	DG	C1'-O4'-C4'	-6.42	103.69	110.10
15	W	23	DC	O4'-C4'-C3'	-6.40	101.94	104.50
15	W	35	DT	O4'-C4'-C3'	-6.39	101.95	104.50
15	W	42	DC	C3'-C2'-C1'	-6.32	94.92	102.50
16	X	60	DA	OP2-P-O3'	6.23	118.90	105.20
16	X	15	DT	OP1-P-O3'	6.16	118.76	105.20
16	X	62	DA	O4'-C1'-N9	6.16	112.31	108.00
16	X	13	DT	C1'-O4'-C4'	-6.15	103.95	110.10
16	X	70	DG	O4'-C4'-C3'	-6.11	102.05	104.50
15	W	101	DG	O4'-C1'-N9	6.11	112.28	108.00
16	X	97	DG	N3-C4-N9	-6.08	122.35	126.00
16	X	85	DC	C1'-O4'-C4'	-6.03	104.08	110.10
16	X	88	DT	C4'-C3'-C2'	-6.00	97.70	103.10
15	W	82	DC	C3'-C2'-C1'	-6.00	95.30	102.50
16	X	85	DC	C3'-C2'-C1'	-6.00	95.30	102.50
16	X	94	DG	P-O3'-C3'	5.99	126.89	119.70
16	X	85	DC	O4'-C1'-N1	5.97	112.18	108.00
15	W	129	DT	OP1-P-O3'	5.97	118.33	105.20
16	X	112	DG	C3'-C2'-C1'	-5.94	95.37	102.50
15	W	55	DG	O4'-C4'-C3'	-5.91	102.14	104.50
16	X	112	DG	O4'-C1'-N9	5.88	112.12	108.00
16	X	70	DG	P-O3'-C3'	5.83	126.69	119.70
16	X	69	DG	N3-C4-N9	-5.82	122.51	126.00
15	W	99	DG	N3-C4-N9	-5.79	122.52	126.00
15	W	30	DA	OP2-P-O3'	5.75	117.85	105.20
16	X	115	DC	C1'-O4'-C4'	-5.69	104.41	110.10
15	W	40	DG	C1'-O4'-C4'	-5.68	104.42	110.10
15	W	62	DC	C3'-C2'-C1'	-5.68	95.69	102.50
15	W	132	DG	C3'-C2'-C1'	-5.62	95.76	102.50
16	X	115	DC	O4'-C1'-N1	5.52	111.86	108.00
16	X	75	DC	C3'-C2'-C1'	-5.51	95.89	102.50
16	X	31	DA	C1'-O4'-C4'	-5.49	104.61	110.10
16	X	107	DT	C3'-C2'-C1'	-5.45	95.96	102.50
15	W	94	DG	P-O3'-C3'	5.44	126.23	119.70
15	W	112	DT	C1'-O4'-C4'	-5.43	104.67	110.10
16	X	55	DG	N9-C4-C5	5.43	107.57	105.40
16	X	54	DC	C3'-C2'-C1'	-5.42	96.00	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	40	DG	C3'-C2'-C1'	-5.42	96.00	102.50
15	W	104	DT	N3-C4-O4	5.39	123.14	119.90
16	X	92	DG	C3'-C2'-C1'	-5.36	96.06	102.50
16	X	105	DT	C1'-O4'-C4'	-5.35	104.75	110.10
11	O	48	LEU	CA-CB-CG	-5.35	103.00	115.30
16	X	50	DT	N3-C4-O4	5.32	123.09	119.90
15	W	105	DT	C3'-C2'-C1'	-5.31	96.13	102.50
16	X	97	DG	C3'-C2'-C1'	-5.24	96.22	102.50
15	W	88	DT	N3-C4-O4	5.23	123.04	119.90
16	X	61	DA	OP1-P-OP2	-5.23	111.76	119.60
15	W	37	DG	C3'-C2'-C1'	-5.21	96.25	102.50
16	X	15	DT	P-O3'-C3'	5.21	125.95	119.70
15	W	72	DC	O4'-C1'-N1	5.20	111.64	108.00
16	X	38	DG	N3-C4-N9	-5.18	122.89	126.00
15	W	129	DT	C5-C4-O4	-5.17	121.28	124.90
15	W	132	DG	C1'-O4'-C4'	-5.16	104.94	110.10
16	X	115	DC	C3'-C2'-C1'	-5.14	96.33	102.50
16	X	53	DG	C3'-C2'-C1'	-5.14	96.33	102.50
1	B	1301	LEU	CA-CB-CG	5.14	127.12	115.30
16	X	126	DC	P-O3'-C3'	5.13	125.85	119.70
15	W	89	DT	N3-C4-O4	5.12	122.97	119.90
16	X	42	DT	C3'-C2'-C1'	-5.10	96.38	102.50
16	X	55	DG	C3'-C2'-C1'	-5.09	96.39	102.50
16	X	63	DC	C1'-O4'-C4'	-5.09	105.01	110.10
15	W	94	DG	OP2-P-O3'	5.07	116.35	105.20
15	W	112	DT	C3'-C2'-C1'	-5.07	96.42	102.50
16	X	119	DT	N3-C4-O4	5.07	122.94	119.90
16	X	74	DG	C3'-C2'-C1'	-5.04	96.45	102.50
15	W	37	DG	C4'-C3'-C2'	-5.02	98.58	103.10
15	W	142	DT	O4'-C1'-N1	5.02	111.51	108.00
15	W	88	DT	C5-C4-O4	-5.02	121.39	124.90
15	W	35	DT	C5-C4-O4	-5.01	121.39	124.90
15	W	145	DT	O4'-C4'-C3'	-5.01	102.50	104.50

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	B	4098	0	4239	190	0
2	C	2873	0	2807	107	0
3	D	3250	0	3301	177	0
3	E	3454	0	3511	76	0
4	H	3145	0	3143	45	0
5	I	888	0	867	10	0
6	J	1360	0	1400	47	0
7	A	6162	0	6271	497	0
8	L	482	0	455	31	0
9	M	3131	0	3129	180	0
10	N	3167	0	3149	155	0
11	O	800	0	829	57	0
11	S	778	0	813	73	0
12	P	703	0	757	40	0
12	T	672	0	698	57	0
13	Q	811	0	849	54	0
13	U	815	0	860	59	0
14	R	718	0	725	51	0
14	V	726	0	747	51	0
15	W	3393	0	1863	183	0
16	X	3413	0	1865	177	0
17	A	27	0	10	27	0
18	A	4	0	0	5	0
19	A	1	0	0	0	0
All	All	44871	0	42288	1714	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 21.

All (1714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:ARG:HH12	1:B:985:LEU:CD1	1.02	1.64
3:D:565:PHE:CZ	7:A:542:GLN:HB2	1.36	1.57
9:M:214:GLN:NE2	9:M:216:ARG:CG	1.68	1.50
3:D:565:PHE:CE1	7:A:542:GLN:HB2	1.43	1.50
3:D:540:GLN:NE2	7:A:537:GLN:HB3	1.23	1.48
3:D:540:GLN:HE21	7:A:537:GLN:CB	1.27	1.44
1:B:941:ASN:ND2	1:B:944:LEU:H	1.07	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:ARG:NH1	1:B:985:LEU:HD13	1.15	1.42
3:D:609:SER:OG	7:A:488:ILE:CG1	1.67	1.40
1:B:941:ASN:HD21	1:B:944:LEU:N	1.24	1.33
7:A:584:GLN:HA	7:A:587:LYS:CE	1.59	1.31
2:C:554:GLN:O	2:C:655:ILE:N	1.62	1.30
9:M:216:ARG:HD3	9:M:220:VAL:CG2	1.46	1.30
1:B:723:ASN:OD1	7:A:559:LEU:HD21	1.32	1.30
9:M:214:GLN:NE2	9:M:216:ARG:HG3	0.98	1.29
7:A:915:HIS:CE1	7:A:917:ASP:OD1	1.85	1.29
3:D:609:SER:CB	7:A:488:ILE:HG12	1.63	1.27
3:D:605:ASN:O	7:A:488:ILE:CD1	1.81	1.27
3:D:570:ILE:CG2	7:A:539:LEU:HD22	1.64	1.26
7:A:808:TYR:HA	7:A:811:GLU:OE1	1.13	1.25
15:W:93:DC:O2	16:X:55:DG:N2	1.70	1.25
3:D:605:ASN:O	7:A:488:ILE:HD11	1.10	1.22
3:D:565:PHE:CE1	7:A:542:GLN:CB	2.22	1.22
1:B:907:ALA:HB2	7:A:557:ASN:ND2	1.54	1.22
1:B:1048:SER:O	7:A:589:HIS:NE2	1.73	1.21
2:C:663:LEU:HD12	2:C:666:ASP:OD2	1.38	1.21
3:E:444:MET:SD	7:A:503:LEU:HD13	1.79	1.21
7:A:584:GLN:CA	7:A:587:LYS:HE2	1.70	1.20
3:E:444:MET:CG	7:A:503:LEU:HD13	1.71	1.19
1:B:1049:LEU:HB3	1:B:1051:LYS:CD	1.71	1.19
3:D:540:GLN:HG2	7:A:538:LEU:CD2	1.71	1.19
7:A:584:GLN:NE2	7:A:587:LYS:NZ	1.91	1.19
7:A:808:TYR:O	7:A:811:GLU:HG2	1.42	1.18
7:A:915:HIS:NE2	7:A:917:ASP:OD1	1.75	1.18
9:M:216:ARG:CD	9:M:220:VAL:HG23	1.73	1.18
3:D:605:ASN:C	7:A:488:ILE:HD11	1.63	1.18
1:B:723:ASN:OD1	7:A:559:LEU:CD2	1.92	1.17
3:D:570:ILE:CD1	7:A:539:LEU:HD13	1.73	1.17
9:M:216:ARG:O	9:M:219:ASP:N	1.78	1.17
1:B:1051:LYS:HB2	1:B:1052:PRO:HD3	1.27	1.17
7:A:584:GLN:NE2	7:A:587:LYS:HZ1	1.42	1.16
2:C:654:GLN:O	2:C:655:ILE:HG23	1.45	1.15
1:B:1049:LEU:HB3	1:B:1051:LYS:HD2	1.22	1.15
3:D:540:GLN:HG2	7:A:538:LEU:HD21	1.18	1.14
1:B:940:ARG:NH1	1:B:985:LEU:CD1	1.78	1.14
7:A:810:TYR:O	7:A:814:ASN:N	1.80	1.14
3:D:565:PHE:CZ	7:A:542:GLN:CB	2.31	1.14
1:B:1145:THR:HG22	7:A:586:TYR:CZ	1.84	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:609:SER:OG	7:A:488:ILE:HG12	0.98	1.13
4:H:556:ASN:ND2	7:A:553:GLU:OE1	1.80	1.13
1:B:941:ASN:ND2	1:B:944:LEU:N	1.85	1.12
3:E:444:MET:SD	7:A:503:LEU:HD22	1.89	1.12
3:D:422:LEU:O	7:A:555:HIS:CD2	2.02	1.12
3:E:444:MET:HG3	7:A:503:LEU:HD13	1.29	1.12
15:W:88:DT:C4	16:X:60:DA:N1	2.17	1.12
7:A:808:TYR:O	7:A:811:GLU:CG	1.96	1.11
3:D:516:LYS:HE2	7:A:511:ASP:OD2	1.50	1.11
15:W:45:DC:O2	16:X:103:DG:N2	1.83	1.11
7:A:808:TYR:CA	7:A:811:GLU:OE1	1.98	1.10
1:B:1051:LYS:HG2	1:B:1052:PRO:HD2	1.13	1.10
15:W:121:DG:N2	16:X:27:DC:O2	1.83	1.10
3:D:540:GLN:NE2	7:A:537:GLN:CB	1.92	1.10
3:D:566:LEU:HD22	7:A:546:ARG:HG3	1.14	1.09
3:D:539:ILE:HG22	7:A:538:LEU:HG	1.24	1.09
3:D:566:LEU:HD22	7:A:546:ARG:CG	1.81	1.08
15:W:88:DT:N3	16:X:60:DA:N1	2.01	1.08
1:B:940:ARG:NH1	1:B:985:LEU:CB	2.15	1.07
1:B:940:ARG:NH1	1:B:985:LEU:HB3	1.68	1.07
3:D:570:ILE:HD12	7:A:539:LEU:HD13	1.13	1.06
9:M:217:SER:O	9:M:221:TRP:HB3	1.54	1.06
7:A:810:TYR:CZ	7:A:819:TYR:CE2	2.44	1.06
1:B:940:ARG:HH11	1:B:985:LEU:HB3	1.11	1.05
3:D:570:ILE:HD12	7:A:539:LEU:CD1	1.86	1.05
3:D:426:GLU:OE2	7:A:548:HIS:CD2	2.10	1.04
7:A:798:LYS:HG3	17:A:1501:ADP:O2B	1.57	1.04
3:D:570:ILE:HG21	7:A:539:LEU:CD2	1.88	1.03
7:A:585:LEU:O	7:A:588:ASN:OD1	1.75	1.03
15:W:114:DG:N2	16:X:34:DC:O2	1.91	1.03
15:W:35:DT:N3	16:X:113:DA:N1	2.07	1.02
15:W:129:DT:C4	16:X:19:DA:N1	2.27	1.02
2:C:652:LEU:HB2	6:J:312:LEU:O	1.56	1.02
1:B:940:ARG:CZ	1:B:985:LEU:HD13	1.90	1.02
7:A:798:LYS:HB2	17:A:1501:ADP:O3B	1.57	1.02
1:B:1049:LEU:CB	1:B:1051:LYS:HD2	1.90	1.01
1:B:940:ARG:HH12	1:B:985:LEU:CG	1.72	1.01
7:A:1199:ARG:NH2	18:A:1502:BEF:F2	1.83	1.01
3:D:565:PHE:O	7:A:542:GLN:NE2	1.94	1.01
1:B:1051:LYS:CG	1:B:1052:PRO:HD2	1.91	1.01
2:C:555:ASN:HA	2:C:654:GLN:HA	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:ASN:HD21	7:A:569:SER:HB3	1.26	1.00
10:N:169:THR:HG1	10:N:190:GLY:N	1.56	1.00
15:W:129:DT:N3	16:X:19:DA:N1	2.10	1.00
1:B:1051:LYS:HG2	1:B:1052:PRO:CD	1.92	0.99
7:A:810:TYR:CD2	7:A:816:ARG:HA	1.96	0.99
15:W:79:DC:O2	16:X:69:DG:N2	1.95	0.99
3:D:566:LEU:CD2	7:A:546:ARG:HG3	1.93	0.99
15:W:100:DG:N2	16:X:48:DC:O2	1.96	0.98
1:B:936:ARG:HB2	1:B:940:ARG:NH2	1.77	0.98
1:B:1145:THR:HG21	7:A:586:TYR:CE2	1.99	0.98
15:W:129:DT:O4	16:X:19:DA:N6	1.96	0.98
3:D:570:ILE:HG21	7:A:539:LEU:HD22	1.01	0.98
3:D:540:GLN:NE2	7:A:537:GLN:CG	2.27	0.97
7:A:584:GLN:HA	7:A:587:LYS:HE2	0.97	0.97
1:B:940:ARG:NH1	1:B:985:LEU:CG	2.28	0.96
3:E:444:MET:HG3	7:A:503:LEU:CD1	1.93	0.96
1:B:1051:LYS:CB	1:B:1052:PRO:HD3	1.94	0.96
7:A:583:ASN:O	7:A:587:LYS:HG3	1.65	0.95
3:D:606:PRO:HA	7:A:488:ILE:CD1	1.97	0.95
1:B:1051:LYS:CG	1:B:1052:PRO:CD	2.44	0.95
3:D:426:GLU:OE2	7:A:548:HIS:NE2	2.00	0.95
1:B:1049:LEU:CB	1:B:1051:LYS:CD	2.42	0.95
7:A:584:GLN:NE2	7:A:587:LYS:CE	2.29	0.95
15:W:99:DG:N2	16:X:49:DC:O2	1.99	0.95
15:W:110:DC:O2	16:X:38:DG:N2	1.98	0.95
1:B:1051:LYS:O	1:B:1055:ASN:ND2	2.00	0.94
7:A:810:TYR:OH	7:A:819:TYR:CE2	2.20	0.94
15:W:42:DC:O2	16:X:106:DG:N2	2.01	0.94
7:A:1199:ARG:NH1	18:A:1502:BEF:F3	1.90	0.94
2:C:652:LEU:HD12	6:J:312:LEU:HB2	1.46	0.94
2:C:652:LEU:HD12	6:J:312:LEU:CB	1.98	0.94
3:D:610:THR:OG1	7:A:487:GLY:HA3	1.67	0.93
3:D:540:GLN:CG	7:A:538:LEU:HD21	1.97	0.93
7:A:810:TYR:CD2	7:A:816:ARG:CA	2.51	0.93
1:B:1051:LYS:CB	1:B:1052:PRO:CD	2.46	0.93
7:A:810:TYR:O	7:A:814:ASN:CA	2.17	0.92
1:B:941:ASN:ND2	1:B:944:LEU:CB	2.31	0.92
7:A:808:TYR:C	7:A:811:GLU:HG2	1.89	0.92
7:A:810:TYR:O	7:A:814:ASN:HA	1.70	0.92
9:M:214:GLN:NE2	9:M:216:ARG:HG2	1.83	0.92
3:E:444:MET:SD	7:A:503:LEU:CD1	2.58	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:38:DT:N3	16:X:110:DA:N1	2.16	0.92
15:W:73:DG:N2	16:X:75:DC:O2	2.01	0.92
9:M:216:ARG:CD	9:M:220:VAL:CG2	2.23	0.91
1:B:940:ARG:CZ	1:B:985:LEU:CD1	2.48	0.91
3:D:605:ASN:C	7:A:488:ILE:CD1	2.30	0.91
10:N:169:THR:HB	10:N:187:ILE:O	1.71	0.91
9:M:214:GLN:OE1	9:M:216:ARG:NE	2.05	0.89
1:B:1049:LEU:CG	1:B:1051:LYS:HD3	2.01	0.89
1:B:1145:THR:CG2	7:A:586:TYR:CE2	2.55	0.89
2:C:652:LEU:HB2	6:J:312:LEU:HB3	1.53	0.89
7:A:766:THR:OG1	17:A:1501:ADP:N1	1.80	0.89
9:M:67:VAL:HB	9:M:217:SER:HB2	1.53	0.89
2:C:467:ASP:OD2	2:C:662:ARG:NH2	2.05	0.89
1:B:1145:THR:CG2	7:A:586:TYR:CZ	2.55	0.89
9:M:67:VAL:HB	9:M:217:SER:CB	2.03	0.89
9:M:214:GLN:HE21	9:M:216:ARG:HG3	1.17	0.89
3:D:602:LYS:HA	7:A:488:ILE:HB	1.52	0.89
1:B:1051:LYS:HB2	1:B:1052:PRO:CD	2.03	0.88
7:A:810:TYR:CE2	7:A:816:ARG:HA	2.07	0.88
1:B:1049:LEU:HD23	1:B:1051:LYS:HD3	1.54	0.88
3:D:601:SER:HB3	3:D:604:GLU:HB2	1.55	0.88
2:C:654:GLN:O	2:C:655:ILE:CG2	2.21	0.88
7:A:584:GLN:HE21	7:A:587:LYS:NZ	1.60	0.87
3:E:440:LEU:HD13	7:A:499:THR:HG21	1.57	0.87
9:M:67:VAL:N	9:M:217:SER:OG	2.06	0.87
3:D:537:LYS:CG	7:A:534:TYR:HE2	1.86	0.87
15:W:33:DG:N2	16:X:115:DC:O2	2.08	0.86
12:T:88:TYR:O	12:T:92:ARG:HB2	1.74	0.86
3:D:422:LEU:O	7:A:555:HIS:HD2	1.55	0.86
7:A:808:TYR:HA	7:A:811:GLU:CD	1.95	0.86
1:B:907:ALA:HB2	7:A:557:ASN:HD22	1.37	0.86
3:D:606:PRO:CA	7:A:488:ILE:HD11	2.06	0.86
2:C:558:ILE:HD12	2:C:653:LEU:HD11	1.55	0.86
2:C:652:LEU:CB	6:J:312:LEU:HB3	2.05	0.86
7:A:584:GLN:NE2	7:A:587:LYS:HE3	1.88	0.86
7:A:810:TYR:HD2	7:A:816:ARG:CB	1.88	0.86
15:W:51:DC:O2	16:X:97:DG:N2	2.07	0.86
2:C:652:LEU:CD1	6:J:489:ARG:HH22	1.89	0.85
7:A:584:GLN:HA	7:A:587:LYS:HE3	1.58	0.85
1:B:940:ARG:N	1:B:940:ARG:HD2	1.92	0.85
1:B:941:ASN:ND2	1:B:941:ASN:O	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:216:ARG:HD3	9:M:220:VAL:HG23	0.85	0.85
3:E:444:MET:SD	7:A:503:LEU:CD2	2.65	0.85
6:J:566:TYR:CZ	7:A:545:VAL:HG12	2.12	0.85
1:B:907:ALA:HB3	7:A:554:TRP:CZ3	2.10	0.85
9:M:35:TYR:O	9:M:67:VAL:HA	1.75	0.85
15:W:78:DC:O2	16:X:70:DG:N2	2.10	0.85
1:B:1048:SER:HB2	7:A:589:HIS:CE1	2.12	0.85
2:C:558:ILE:HD12	2:C:653:LEU:CD1	2.06	0.84
15:W:116:DC:O2	16:X:32:DG:N2	2.10	0.84
15:W:88:DT:N3	16:X:60:DA:C2	2.46	0.84
15:W:123:DC:O2	16:X:25:DG:N2	2.10	0.84
3:D:537:LYS:HG3	7:A:534:TYR:HE2	1.42	0.84
1:B:936:ARG:CB	1:B:940:ARG:NH2	2.41	0.83
3:D:606:PRO:O	7:A:486:VAL:O	1.96	0.83
2:C:652:LEU:HD11	6:J:489:ARG:HH22	1.41	0.83
15:W:34:DG:N2	16:X:114:DC:O2	2.10	0.83
1:B:1048:SER:O	7:A:589:HIS:CE1	2.30	0.83
15:W:130:DC:O2	16:X:18:DG:N2	2.11	0.83
3:D:537:LYS:HG3	7:A:534:TYR:CE2	2.13	0.83
7:A:810:TYR:HD2	7:A:816:ARG:HB3	1.40	0.83
9:M:67:VAL:CA	9:M:217:SER:OG	2.27	0.83
7:A:1171:ASN:ND2	17:A:1501:ADP:O1A	2.12	0.83
3:D:602:LYS:HA	7:A:488:ILE:HD12	1.61	0.82
7:A:798:LYS:HD2	17:A:1501:ADP:O3B	1.79	0.82
1:B:1049:LEU:CD2	1:B:1051:LYS:HD3	2.08	0.82
3:D:570:ILE:CG2	7:A:539:LEU:CD2	2.50	0.82
7:A:489:ASP:O	7:A:491:HIS:N	2.12	0.82
3:D:536:LEU:HB3	7:A:534:TYR:HB3	1.60	0.82
15:W:63:DG:N2	16:X:85:DC:O2	2.12	0.82
2:C:652:LEU:CG	6:J:312:LEU:HB3	2.10	0.81
3:D:430:PRO:HG2	6:J:566:TYR:HB3	1.61	0.81
3:D:606:PRO:CA	7:A:488:ILE:CD1	2.58	0.81
7:A:810:TYR:OH	7:A:819:TYR:CD2	2.33	0.81
3:D:601:SER:C	7:A:488:ILE:HG21	2.00	0.81
3:D:609:SER:OG	7:A:488:ILE:HG13	1.78	0.81
7:A:584:GLN:CD	7:A:587:LYS:HE3	1.99	0.81
7:A:800:ILE:HD11	17:A:1501:ADP:C8	2.15	0.81
1:B:1048:SER:O	7:A:589:HIS:CD2	2.34	0.81
11:S:72:ARG:O	11:S:76:GLN:HB2	1.81	0.81
7:A:1196:ARG:NH2	18:A:1502:BEF:F2	2.04	0.81
9:M:216:ARG:HD2	9:M:220:VAL:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:565:PHE:CE1	7:A:542:GLN:CA	2.64	0.80
6:J:240:LEU:O	7:A:537:GLN:NE2	2.13	0.80
1:B:723:ASN:CG	7:A:559:LEU:HD21	2.01	0.80
6:J:240:LEU:HD21	7:A:516:LEU:HD11	1.63	0.80
3:E:425:PHE:CD1	7:A:543:LYS:HG3	2.15	0.80
15:W:94:DG:N2	16:X:54:DC:O2	2.13	0.80
3:D:426:GLU:HG2	7:A:551:GLN:OE1	1.82	0.80
1:B:1051:LYS:CD	1:B:1051:LYS:H	1.95	0.79
15:W:109:DC:O2	16:X:39:DG:N2	2.15	0.79
1:B:936:ARG:HB2	1:B:940:ARG:HH22	1.44	0.79
15:W:81:DC:O2	16:X:67:DG:N2	2.14	0.79
1:B:927:ASN:OD1	7:A:569:SER:HB2	1.81	0.79
1:B:1051:LYS:HB3	1:B:1051:LYS:NZ	1.98	0.79
7:A:584:GLN:HE21	7:A:587:LYS:HZ1	0.82	0.79
9:M:214:GLN:OE1	9:M:216:ARG:CZ	2.31	0.79
1:B:1149:VAL:CG2	7:A:586:TYR:HE1	1.96	0.78
7:A:798:LYS:CB	17:A:1501:ADP:O3B	2.31	0.78
2:C:663:LEU:CD1	2:C:666:ASP:OD2	2.26	0.78
2:C:663:LEU:O	2:C:666:ASP:N	2.15	0.78
15:W:129:DT:C4	16:X:19:DA:C6	2.72	0.78
9:M:216:ARG:O	9:M:218:THR:N	2.17	0.78
7:A:810:TYR:CD2	7:A:816:ARG:HB3	2.20	0.77
1:B:936:ARG:CB	1:B:940:ARG:HH22	1.95	0.77
15:W:35:DT:C4	16:X:113:DA:N1	2.52	0.77
15:W:80:DC:O2	16:X:68:DG:N2	2.17	0.77
15:W:125:DC:O2	16:X:23:DG:N2	2.16	0.77
15:W:83:DG:N1	16:X:65:DC:N3	2.30	0.76
2:C:652:LEU:CD1	6:J:489:ARG:NH2	2.48	0.76
9:M:214:GLN:NE2	9:M:216:ARG:CD	2.49	0.76
1:B:907:ALA:HB3	7:A:554:TRP:HZ3	1.47	0.76
3:D:540:GLN:HE21	7:A:537:GLN:HB3	0.59	0.76
15:W:93:DC:N3	16:X:55:DG:N1	2.31	0.76
13:Q:15:LYS:H	15:W:31:DT:H4'	1.50	0.76
1:B:936:ARG:CA	1:B:940:ARG:NH2	2.49	0.76
2:C:654:GLN:O	2:C:655:ILE:HG13	1.85	0.76
15:W:72:DC:O2	16:X:76:DG:N2	2.15	0.76
1:B:927:ASN:ND2	7:A:569:SER:HB3	2.02	0.75
1:B:1145:THR:HG21	7:A:586:TYR:CD2	2.21	0.75
3:E:444:MET:CE	7:A:503:LEU:HD13	2.15	0.75
3:E:606:PRO:HA	7:A:486:VAL:HG13	1.68	0.75
3:D:609:SER:HB3	7:A:488:ILE:HG12	1.64	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:67:VAL:O	9:M:217:SER:CB	2.33	0.75
3:D:540:GLN:HG2	7:A:538:LEU:HD22	1.68	0.75
15:W:62:DC:O2	16:X:86:DG:N2	2.16	0.75
1:B:1233:LEU:HD11	7:A:579:ALA:CB	2.16	0.75
15:W:48:DT:O2	16:X:101:DG:N2	2.20	0.74
15:W:129:DT:C2	16:X:19:DA:C2	2.75	0.74
1:B:941:ASN:ND2	1:B:944:LEU:HB2	2.02	0.74
15:W:88:DT:C2	16:X:60:DA:C2	2.75	0.74
3:D:606:PRO:N	7:A:488:ILE:HD11	2.02	0.74
3:D:602:LYS:CA	7:A:488:ILE:HB	2.16	0.74
7:A:810:TYR:CD2	7:A:816:ARG:CB	2.70	0.74
7:A:810:TYR:CE2	7:A:819:TYR:CE2	2.76	0.74
3:D:423:PHE:CD1	7:A:552:PHE:CE1	2.76	0.73
6:J:566:TYR:CE1	7:A:545:VAL:HG12	2.23	0.73
15:W:44:DG:N2	16:X:104:DC:O2	2.19	0.73
1:B:1049:LEU:CB	1:B:1051:LYS:HD3	2.16	0.73
2:C:468:ARG:HH12	2:C:662:ARG:NE	1.86	0.73
3:E:518:LYS:O	3:E:522:GLN:HB2	1.89	0.73
9:M:216:ARG:C	9:M:218:THR:N	2.38	0.73
11:S:43:PRO:HG3	16:X:68:DG:H21	1.54	0.73
1:B:1051:LYS:HE2	1:B:1051:LYS:N	2.03	0.73
9:M:214:GLN:CD	9:M:216:ARG:HG3	2.01	0.73
7:A:1171:ASN:HD21	17:A:1501:ADP:C5'	2.00	0.73
7:A:572:ARG:HD2	7:A:575:ASN:HD21	1.54	0.73
7:A:808:TYR:O	7:A:811:GLU:HG3	1.87	0.73
2:C:654:GLN:NE2	6:J:311:THR:HG22	2.03	0.73
3:D:565:PHE:HZ	7:A:538:LEU:O	1.71	0.73
1:B:723:ASN:CG	7:A:559:LEU:CD2	2.57	0.72
3:D:570:ILE:HG22	7:A:539:LEU:HD22	1.66	0.72
11:S:47:ALA:O	11:S:50:GLU:HB2	1.90	0.72
7:A:566:ASN:O	7:A:568:LEU:N	2.22	0.72
1:B:941:ASN:ND2	1:B:944:LEU:CA	2.52	0.72
1:B:1233:LEU:HD11	7:A:579:ALA:HB3	1.71	0.72
15:W:104:DT:N3	16:X:44:DA:C2	2.58	0.72
15:W:109:DC:N3	16:X:39:DG:N1	2.38	0.72
7:A:798:LYS:HD2	17:A:1501:ADP:PB	2.30	0.72
3:D:424:PRO:HD3	7:A:552:PHE:HD1	1.55	0.71
9:M:243:LEU:O	9:M:247:GLU:HB2	1.89	0.71
1:B:734:ALA:CB	7:A:567:PHE:CZ	2.72	0.71
3:E:606:PRO:HA	7:A:486:VAL:CG1	2.19	0.71
7:A:818:PRO:HA	7:A:866:PHE:CE1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:606:PRO:HA	7:A:488:ILE:HD12	1.70	0.71
1:B:1049:LEU:HD23	1:B:1051:LYS:CD	2.21	0.71
2:C:663:LEU:HD12	2:C:666:ASP:CG	2.11	0.71
7:A:817:GLY:O	7:A:867:ASP:O	2.08	0.71
1:B:734:ALA:HB3	7:A:567:PHE:HZ	1.55	0.71
1:B:936:ARG:HA	1:B:940:ARG:NH2	2.06	0.70
3:D:426:GLU:CD	7:A:548:HIS:CD2	2.64	0.70
1:B:1049:LEU:CA	1:B:1051:LYS:HD2	2.21	0.70
2:C:652:LEU:HB3	6:J:312:LEU:H	1.55	0.70
3:D:424:PRO:CD	7:A:552:PHE:HD1	2.05	0.70
9:M:216:ARG:C	9:M:218:THR:H	1.92	0.70
10:N:162:ILE:HA	10:N:170:ASP:O	1.92	0.70
2:C:676:ARG:HH12	13:U:61:GLU:HG2	1.57	0.69
1:B:907:ALA:CB	7:A:557:ASN:ND2	2.45	0.69
7:A:516:LEU:O	7:A:526:ARG:NH2	2.26	0.69
1:B:676:GLY:HA2	3:D:604:GLU:HG3	1.72	0.69
3:D:610:THR:OG1	7:A:486:VAL:O	2.10	0.69
6:J:236:LYS:HE3	7:A:526:ARG:HH12	1.57	0.69
3:D:602:LYS:HA	7:A:488:ILE:CB	2.21	0.69
1:B:734:ALA:CB	7:A:567:PHE:HZ	2.05	0.69
1:B:940:ARG:NH2	1:B:985:LEU:CD1	2.55	0.69
7:A:770:TYR:HB3	7:A:999:VAL:HG11	1.75	0.68
11:S:54:TYR:HB3	12:T:40:ARG:HE	1.57	0.68
9:M:67:VAL:C	9:M:217:SER:OG	2.32	0.68
4:H:115:PRO:HG3	3:E:721:ASN:HB2	1.76	0.68
7:A:523:GLU:HA	7:A:526:ARG:HB3	1.76	0.68
9:M:232:LYS:HA	9:M:236:LEU:HG	1.75	0.68
10:N:453:LYS:O	10:N:457:LYS:N	2.27	0.68
11:S:125:GLN:NE2	12:T:53:GLU:OE1	2.27	0.68
3:D:605:ASN:O	7:A:488:ILE:HD13	1.88	0.68
13:U:42:ARG:NH2	15:W:111:DC:O2	2.27	0.68
9:M:99:PRO:HB2	9:M:133:VAL:HG22	1.75	0.67
7:A:1176:ASP:N	7:A:1176:ASP:OD1	2.28	0.67
7:A:810:TYR:CE2	7:A:819:TYR:CD2	2.83	0.67
12:P:23:ARG:HH12	12:P:30:THR:HG22	1.58	0.67
1:B:940:ARG:HH12	1:B:985:LEU:HD13	0.50	0.67
1:B:941:ASN:HD22	1:B:944:LEU:H	1.35	0.67
2:C:652:LEU:HD12	6:J:312:LEU:HB3	1.76	0.67
2:C:652:LEU:CB	6:J:312:LEU:O	2.38	0.67
7:A:810:TYR:CZ	7:A:819:TYR:HE2	2.12	0.67
7:A:1129:LYS:HB3	7:A:1156:TYR:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:214:GLN:OE1	9:M:216:ARG:NH1	2.27	0.67
7:A:637:HIS:HE1	10:N:434:ILE:HD13	1.58	0.67
3:D:422:LEU:O	7:A:555:HIS:NE2	2.27	0.67
3:E:596:PRO:HG2	7:A:489:ASP:OD2	1.94	0.67
3:D:424:PRO:HB3	7:A:555:HIS:HB2	1.77	0.66
3:D:537:LYS:HA	7:A:534:TYR:CE2	2.30	0.66
15:W:50:DG:N2	16:X:99:DT:O2	2.28	0.66
1:B:927:ASN:HD21	7:A:569:SER:CB	2.07	0.66
1:B:1051:LYS:HD2	1:B:1051:LYS:H	1.60	0.66
1:B:1145:THR:HG22	7:A:586:TYR:CE1	2.31	0.66
3:D:602:LYS:HA	7:A:488:ILE:CD1	2.25	0.66
7:A:566:ASN:O	7:A:567:PHE:C	2.30	0.66
11:S:59:GLU:O	12:T:40:ARG:NH1	2.28	0.66
3:D:430:PRO:CG	6:J:566:TYR:HB3	2.26	0.66
9:M:224:ALA:HA	9:M:228:ILE:HB	1.77	0.66
3:D:609:SER:CB	7:A:488:ILE:CG1	2.56	0.66
13:Q:115:LEU:HG	12:T:44:LYS:HB2	1.76	0.65
15:W:86:DT:N3	16:X:62:DA:C2	2.64	0.65
15:W:45:DC:N3	16:X:103:DG:N1	2.42	0.65
15:W:129:DT:N3	16:X:19:DA:C6	2.64	0.65
2:C:654:GLN:CD	6:J:311:THR:HG22	2.16	0.65
7:A:798:LYS:CG	17:A:1501:ADP:O2B	2.40	0.65
7:A:810:TYR:CZ	7:A:819:TYR:CD2	2.85	0.65
9:M:291:LEU:O	10:N:402:GLN:NE2	2.30	0.65
2:C:663:LEU:O	2:C:665:LYS:N	2.29	0.65
7:A:1171:ASN:ND2	17:A:1501:ADP:H5'1	2.12	0.65
9:M:67:VAL:O	9:M:217:SER:OG	2.15	0.65
1:B:727:ASN:OD1	7:A:559:LEU:C	2.36	0.64
3:D:429:LYS:HG3	6:J:565:PRO:O	1.97	0.64
7:A:798:LYS:CD	17:A:1501:ADP:O3B	2.45	0.64
10:N:449:ILE:HG12	10:N:465:VAL:HG21	1.80	0.64
1:B:1138:PRO:HB2	7:A:574:ILE:HG22	1.79	0.64
13:Q:17:ARG:HB2	13:Q:27:VAL:HB	1.79	0.64
13:U:24:GLN:HB3	14:V:40:LYS:HD3	1.78	0.64
15:W:114:DG:N1	16:X:34:DC:N3	2.42	0.64
1:B:940:ARG:HH22	1:B:985:LEU:CD1	2.10	0.64
9:M:315:LYS:HE2	9:M:318:LEU:HD11	1.79	0.64
15:W:79:DC:O2	16:X:70:DG:N2	2.30	0.64
1:B:727:ASN:HD21	7:A:558:SER:C	2.00	0.64
1:B:1051:LYS:CG	1:B:1052:PRO:HD3	2.21	0.64
3:D:565:PHE:HE1	7:A:542:GLN:CA	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1164:ARG:NH2	15:W:54:DC:O2	2.30	0.64
11:O:109:LEU:O	11:O:113:HIS:HB2	1.98	0.64
11:O:129:ARG:NH1	11:O:129:ARG:O	2.31	0.64
15:W:129:DT:C4	16:X:19:DA:N6	2.65	0.64
7:A:584:GLN:N	7:A:587:LYS:HE2	2.12	0.64
3:D:441:LYS:NZ	7:A:506:ASP:OD2	2.30	0.64
7:A:800:ILE:CD1	17:A:1501:ADP:C8	2.80	0.64
9:M:55:ILE:O	9:M:59:ALA:N	2.30	0.64
10:N:198:LEU:HB3	10:N:210:ILE:HG12	1.78	0.64
10:N:7:ASP:HA	10:N:24:GLY:HA2	1.80	0.64
9:M:448:SER:HB3	9:M:451:LEU:HG	1.80	0.64
15:W:35:DT:N3	16:X:113:DA:C2	2.66	0.64
3:D:537:LYS:CB	7:A:534:TYR:HE2	2.11	0.64
9:M:290:PHE:HB3	9:M:299:LEU:HB2	1.80	0.64
1:B:1049:LEU:HD23	1:B:1051:LYS:HG3	1.79	0.64
1:B:1051:LYS:HB3	1:B:1051:LYS:HZ3	1.60	0.64
1:B:1049:LEU:HD23	1:B:1051:LYS:CG	2.28	0.63
3:E:425:PHE:CD1	7:A:543:LYS:CG	2.78	0.63
3:E:444:MET:SD	7:A:503:LEU:CG	2.87	0.63
12:P:91:LYS:HZ2	14:R:76:ARG:HH21	1.44	0.63
1:B:940:ARG:NH2	1:B:985:LEU:HD12	2.13	0.63
2:C:669:ARG:HH11	14:V:102:GLU:HB2	1.63	0.63
15:W:121:DG:N1	16:X:27:DC:N3	2.44	0.63
2:C:652:LEU:CD1	6:J:312:LEU:HB3	2.28	0.63
9:M:311:GLU:OE1	9:M:407:ARG:NH2	2.32	0.63
10:N:131:VAL:HG13	10:N:137:ILE:HB	1.81	0.63
11:O:54:TYR:HB3	12:P:40:ARG:HE	1.63	0.63
2:C:496:LEU:HD23	2:C:510:ILE:HG22	1.80	0.63
3:D:565:PHE:O	7:A:542:GLN:CD	2.36	0.63
3:D:601:SER:O	7:A:488:ILE:HD13	1.97	0.63
7:A:816:ARG:HD3	7:A:842:LEU:CD2	2.28	0.63
8:L:23:GLU:O	10:N:451:ARG:NH2	2.32	0.63
15:W:44:DG:N1	16:X:104:DC:N3	2.44	0.63
3:E:440:LEU:CD1	7:A:499:THR:HG21	2.28	0.63
9:M:164:CYS:H	9:M:182:SER:HB3	1.64	0.63
11:O:51:ILE:O	11:O:55:GLN:NE2	2.32	0.63
15:W:86:DT:C2	16:X:62:DA:C2	2.86	0.63
15:W:99:DG:N1	16:X:49:DC:N3	2.42	0.63
9:M:214:GLN:CD	9:M:216:ARG:NE	2.52	0.62
10:N:84:ARG:O	10:N:88:VAL:HB	1.99	0.62
1:B:940:ARG:CZ	1:B:985:LEU:HD12	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:654:GLN:C	2:C:655:ILE:HG13	2.18	0.62
3:E:444:MET:CG	7:A:503:LEU:CD1	2.56	0.62
7:A:798:LYS:HG3	17:A:1501:ADP:PB	2.38	0.62
9:M:53:ASN:ND2	9:M:89:TYR:OH	2.32	0.62
15:W:47:DC:H4'	15:W:48:DT:H5'	1.81	0.62
15:W:35:DT:C2	16:X:113:DA:C2	2.87	0.62
15:W:57:DT:O2	16:X:92:DG:N2	2.32	0.62
15:W:130:DC:N3	16:X:18:DG:N1	2.44	0.62
7:A:915:HIS:NE2	7:A:917:ASP:CG	2.51	0.62
2:C:652:LEU:HB2	6:J:312:LEU:C	2.20	0.62
3:D:565:PHE:CE1	7:A:542:GLN:HA	2.33	0.62
7:A:776:GLN:HA	7:A:779:VAL:HB	1.82	0.62
15:W:104:DT:C4	16:X:44:DA:N1	2.68	0.62
9:M:291:LEU:HD23	10:N:359:ILE:HG13	1.81	0.62
3:D:576:TYR:HB2	7:A:497:TYR:OH	1.99	0.62
9:M:216:ARG:HD3	9:M:220:VAL:HG21	1.67	0.62
7:A:584:GLN:CA	7:A:587:LYS:CE	2.48	0.62
13:Q:21:ALA:HB1	14:R:114:ALA:HB1	1.81	0.62
1:B:936:ARG:O	1:B:940:ARG:HD3	1.99	0.61
1:B:941:ASN:HD21	1:B:944:LEU:CA	2.09	0.61
9:M:231:PHE:O	9:M:236:LEU:N	2.33	0.61
10:N:39:THR:HG21	10:N:68:ILE:HB	1.82	0.61
11:S:59:GLU:OE2	12:T:40:ARG:NH2	2.33	0.61
3:D:565:PHE:HE1	7:A:542:GLN:HA	1.63	0.61
2:C:475:ASP:OD2	3:E:368:ARG:NH1	2.34	0.61
3:D:540:GLN:HE22	7:A:537:GLN:CG	2.13	0.61
15:W:94:DG:N1	16:X:54:DC:N3	2.46	0.61
13:U:29:ARG:NH2	14:V:37:TYR:OH	2.33	0.61
15:W:68:DT:N3	16:X:80:DA:C2	2.69	0.61
1:B:1049:LEU:HB3	1:B:1051:LYS:CG	2.30	0.61
7:A:798:LYS:CG	17:A:1501:ADP:O3B	2.48	0.61
7:A:808:TYR:CB	7:A:811:GLU:OE1	2.49	0.61
12:P:35:ARG:NH2	16:X:82:DG:OP2	2.34	0.61
15:W:68:DT:C4	16:X:80:DA:N1	2.68	0.61
2:C:652:LEU:HB2	6:J:312:LEU:CB	2.27	0.61
1:B:724:THR:HG21	3:D:422:LEU:HA	1.83	0.61
1:B:1041:ASP:OD2	7:A:574:ILE:HD12	2.01	0.61
3:D:606:PRO:CB	7:A:486:VAL:N	2.64	0.61
7:A:613:ILE:HG13	9:M:150:GLY:HA3	1.82	0.61
10:N:42:TYR:HB3	10:N:62:ALA:HB1	1.83	0.61
15:W:51:DC:N3	16:X:97:DG:N1	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:440:LEU:HD13	7:A:499:THR:CG2	2.31	0.61
10:N:41:ILE:HD11	10:N:53:TYR:HB3	1.81	0.61
11:S:83:ARG:HD3	15:W:101:DG:H5'	1.83	0.61
7:A:816:ARG:HG3	7:A:816:ARG:O	2.00	0.60
14:V:79:HIS:O	14:V:82:LYS:NZ	2.31	0.60
2:C:654:GLN:O	2:C:655:ILE:CB	2.50	0.60
2:C:676:ARG:NH1	13:U:57:TYR:O	2.34	0.60
7:A:585:LEU:O	7:A:589:HIS:ND1	2.32	0.60
9:M:67:VAL:HB	9:M:217:SER:OG	2.01	0.60
12:T:52:GLU:OE2	12:T:55:ARG:NH1	2.34	0.60
13:U:68:ASN:HA	13:U:71:ARG:HH21	1.64	0.60
1:B:913:LEU:HD12	7:A:559:LEU:HD11	1.84	0.60
3:E:596:PRO:HG3	7:A:492:THR:OG1	2.00	0.60
7:A:798:LYS:NZ	17:A:1501:ADP:O2B	2.20	0.60
8:L:28:ASP:HB3	8:L:64:LEU:HD12	1.84	0.60
11:S:53:ARG:NH2	11:S:59:GLU:OE2	2.34	0.60
3:D:605:ASN:HB3	3:D:608:LEU:HB3	1.84	0.60
3:D:539:ILE:HG22	7:A:538:LEU:CG	2.15	0.60
7:A:798:LYS:CG	17:A:1501:ADP:PB	2.90	0.60
7:A:821:VAL:HG12	7:A:892:ILE:HB	1.83	0.60
9:M:214:GLN:NE2	9:M:216:ARG:NE	2.48	0.60
10:N:166:THR:HG22	10:N:192:GLN:HE21	1.67	0.60
14:V:30:ARG:NH1	16:X:26:DC:O2	2.33	0.60
2:C:652:LEU:HD12	6:J:489:ARG:NH2	2.15	0.60
7:A:758:GLN:HB3	7:A:767:LEU:HD21	1.84	0.60
9:M:332:LEU:O	9:M:336:SER:HB2	2.02	0.60
2:C:433:GLY:O	2:C:435:ARG:NH2	2.34	0.60
9:M:35:TYR:OH	9:M:79:ASN:ND2	2.34	0.60
10:N:116[A]:HIS:NE2	10:N:170:ASP:OD2	2.35	0.60
12:P:71:THR:O	14:R:96:ARG:NH2	2.34	0.60
13:U:50:TYR:OH	14:V:92:GLN:NE2	2.34	0.60
1:B:1048:SER:HB2	7:A:589:HIS:HE1	1.62	0.59
1:B:1049:LEU:HG	1:B:1051:LYS:HD3	1.83	0.59
3:D:602:LYS:N	7:A:488:ILE:HG21	2.16	0.59
14:R:104:ALA:O	14:R:108:VAL:N	2.35	0.59
11:S:40:ARG:NH2	15:W:83:DG:N3	2.36	0.59
13:U:63:LEU:HD22	14:V:42:LEU:HD13	1.83	0.59
3:D:570:ILE:CB	7:A:539:LEU:HD13	2.32	0.59
11:S:52:ARG:O	11:S:56:LYS:N	2.35	0.59
3:D:426:GLU:CD	7:A:548:HIS:HD2	2.06	0.59
9:M:122:ARG:O	9:M:125:GLU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1049:LEU:C	1:B:1051:LYS:HD2	2.23	0.59
3:D:422:LEU:C	7:A:555:HIS:NE2	2.55	0.59
3:E:305:ILE:HA	3:E:394:GLN:HE22	1.67	0.59
9:M:216:ARG:HD2	9:M:220:VAL:N	2.17	0.59
9:M:67:VAL:CB	9:M:217:SER:OG	2.50	0.59
14:R:64:ASN:HA	14:R:67:PHE:HB3	1.83	0.59
15:W:78:DC:N3	16:X:70:DG:N1	2.45	0.59
7:A:1300:MET:HB3	7:A:1304:ARG:HE	1.68	0.59
9:M:426:ASN:ND2	9:M:435:GLN:OE1	2.35	0.59
12:T:64:ASN:O	12:T:67:ARG:NH1	2.36	0.59
15:W:110:DC:N3	16:X:38:DG:N1	2.43	0.59
14:R:112:THR:O	14:R:116:THR:N	2.33	0.59
12:P:46:ILE:N	16:X:82:DG:OP1	2.36	0.59
15:W:68:DT:C2	16:X:80:DA:C2	2.90	0.59
1:B:940:ARG:HD2	1:B:940:ARG:H	1.68	0.58
7:A:629:PHE:HA	7:A:632:ARG:HE	1.68	0.58
7:A:514:ASP:O	7:A:518:ASN:ND2	2.36	0.58
9:M:122:ARG:O	9:M:126:LEU:N	2.36	0.58
10:N:4:PHE:N	10:N:440:PHE:O	2.36	0.58
15:W:86:DT:C4	16:X:62:DA:N1	2.71	0.58
1:B:941:ASN:ND2	1:B:944:LEU:HB3	2.17	0.58
2:C:391:ARG:NH2	2:C:392:MET:SD	2.76	0.58
3:D:701:LEU:HD21	3:E:705:GLU:HG2	1.84	0.58
9:M:83:LEU:O	9:M:87:TRP:N	2.36	0.58
13:U:85:LEU:O	13:U:89:ASN:ND2	2.36	0.58
16:X:122:DG:H4'	16:X:123:DC:H5'	1.85	0.58
9:M:148:SER:OG	9:M:435:GLN:NE2	2.36	0.58
15:W:98:DA:C2	16:X:50:DT:N3	2.72	0.58
7:A:808:TYR:CA	7:A:811:GLU:HG2	2.32	0.58
10:N:39:THR:HG22	10:N:67:PRO:HD2	1.86	0.58
7:A:794:MET:SD	7:A:1196:ARG:NH2	2.75	0.58
10:N:47:GLN:H	10:N:47:GLN:CD	2.06	0.58
1:B:1051:LYS:H	1:B:1051:LYS:CE	2.16	0.58
6:J:312:LEU:HD23	6:J:485:VAL:HG11	1.86	0.58
8:L:60:TYR:HB2	9:M:103:PRO:HD3	1.85	0.58
9:M:120:LEU:O	9:M:124:TYR:N	2.33	0.58
9:M:239:SER:HB2	9:M:246:LEU:HD12	1.86	0.58
3:D:537:LYS:HA	7:A:534:TYR:CD2	2.38	0.58
7:A:815:ILE:O	7:A:816:ARG:C	2.41	0.58
11:S:82:LEU:HB3	12:T:81:VAL:HG22	1.86	0.58
16:X:66:DG:H2"	16:X:67:DG:H2'	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:731:GLN:NE2	3:D:732:ASN:OD1	2.37	0.58
10:N:13:TYR:HB2	10:N:114:ILE:HD12	1.85	0.58
15:W:38:DT:N3	16:X:110:DA:C2	2.71	0.58
1:B:730:LEU:HD11	7:A:567:PHE:CE2	2.39	0.58
2:C:654:GLN:O	2:C:655:ILE:CG1	2.51	0.58
7:A:642:ARG:HA	7:A:645:GLN:HB2	1.86	0.58
7:A:816:ARG:NH1	7:A:841:THR:OG1	2.37	0.58
11:S:70:LEU:HB2	12:T:25:ASN:HB2	1.86	0.58
15:W:88:DT:O4	16:X:60:DA:N1	2.34	0.58
1:B:941:ASN:HD22	1:B:944:LEU:HB3	1.67	0.57
7:A:593:LYS:HD2	7:A:593:LYS:O	2.03	0.57
10:N:457:LYS:HB2	10:N:461:ALA:HB2	1.85	0.57
11:O:55:GLN:NE2	13:U:110:ASN:O	2.36	0.57
12:T:39:ARG:NH1	12:T:43:VAL:O	2.37	0.57
15:W:77:DT:C4	16:X:71:DA:N1	2.72	0.57
15:W:79:DC:N3	16:X:69:DG:N1	2.47	0.57
1:B:1051:LYS:H	1:B:1051:LYS:HE2	1.68	0.57
2:C:679:ARG:NH2	14:V:45:VAL:O	2.36	0.57
7:A:525:THR:HA	7:A:528:ASN:HD22	1.69	0.57
9:M:229:GLN:HA	9:M:232:LYS:HB2	1.86	0.57
11:O:71:VAL:HG11	11:O:89:VAL:HG22	1.86	0.57
13:Q:12:ALA:N	15:W:31:DT:O2	2.38	0.57
1:B:734:ALA:HB3	7:A:567:PHE:CZ	2.38	0.57
2:C:663:LEU:O	2:C:664:ASP:C	2.42	0.57
9:M:18:VAL:HG22	9:M:30:ILE:HG23	1.86	0.57
9:M:91:TYR:HA	9:M:95:LEU:HB2	1.87	0.57
10:N:214:LYS:NZ	10:N:339:THR:OG1	2.33	0.57
14:R:113:LYS:O	14:R:117:LYS:N	2.37	0.57
15:W:57:DT:C4	16:X:91:DA:N1	2.72	0.57
9:M:51:THR:O	9:M:55:ILE:N	2.37	0.57
10:N:188:PRO:O	10:N:190:GLY:N	2.37	0.57
10:N:295:GLY:O	10:N:298:ARG:NH1	2.36	0.57
7:A:1028:LYS:O	7:A:1030:ARG:NH1	2.37	0.57
10:N:12:ILE:HG22	10:N:14:PRO:HD3	1.87	0.57
10:N:22:GLN:NE2	10:N:31:THR:OG1	2.36	0.57
14:R:77:LEU:O	14:R:81:ASN:ND2	2.38	0.57
7:A:806:LEU:O	7:A:810:TYR:HB2	2.05	0.57
7:A:915:HIS:HE2	7:A:917:ASP:CG	2.06	0.57
9:M:121:GLU:O	9:M:124:TYR:HB2	2.05	0.57
10:N:169:THR:HG21	10:N:309:ILE:HG12	1.86	0.57
14:R:93:THR:OG1	14:R:96:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:90:DA:H4'	15:W:91:DA:H5'	1.85	0.57
10:N:438:GLN:O	10:N:442:HIS:ND1	2.37	0.57
13:Q:88:ARG:NH2	13:Q:100:VAL:O	2.37	0.57
15:W:129:DT:N3	16:X:19:DA:C2	2.71	0.57
7:A:686:THR:HG22	7:A:784:ASN:HB3	1.87	0.57
9:M:88:ARG:HH11	9:M:131:LEU:HD22	1.69	0.57
14:V:39:TYR:OH	16:X:21:DA:OP2	2.21	0.57
3:E:628:GLN:O	3:E:640:GLN:NE2	2.37	0.57
9:M:82:ALA:O	9:M:86:GLN:N	2.38	0.57
7:A:1171:ASN:ND2	17:A:1501:ADP:C5'	2.68	0.57
11:O:104:PHE:HD2	12:P:41:GLY:HA3	1.70	0.57
12:T:60:VAL:O	12:T:64:ASN:ND2	2.37	0.57
8:L:31:GLN:NE2	8:L:56:TYR:O	2.38	0.56
14:R:73:GLU:HG2	14:R:98:LEU:HD11	1.86	0.56
12:T:58:LEU:O	12:T:61:PHE:HB3	2.05	0.56
2:C:652:LEU:N	6:J:312:LEU:O	2.38	0.56
2:C:756:ASN:OD1	6:J:546:LYS:N	2.38	0.56
3:D:570:ILE:CG1	7:A:539:LEU:HD13	2.34	0.56
3:E:444:MET:CE	7:A:503:LEU:CD1	2.82	0.56
13:U:88:ARG:NH1	13:U:97:LEU:O	2.37	0.56
1:B:1138:PRO:HB2	7:A:574:ILE:CG2	2.35	0.56
1:B:1233:LEU:CD1	7:A:579:ALA:CB	2.82	0.56
3:D:609:SER:OG	7:A:488:ILE:CB	2.52	0.56
7:A:820:LEU:HG	7:A:913:HIS:HE1	1.69	0.56
7:A:1088:LYS:NZ	7:A:1211:LEU:O	2.37	0.56
8:L:11:ASN:HA	10:N:108:ASN:HA	1.87	0.56
9:M:71:VAL:HA	9:M:77:PRO:HA	1.86	0.56
12:T:68:ASP:O	12:T:71:THR:HB	2.05	0.56
13:U:42:ARG:HG2	15:W:112:DT:H4'	1.87	0.56
13:U:92:GLU:HA	13:U:95:LYS:HE2	1.86	0.56
15:W:100:DG:N2	16:X:49:DC:O2	2.38	0.56
1:B:941:ASN:HD22	1:B:944:LEU:CB	2.12	0.56
3:D:606:PRO:N	7:A:488:ILE:CD1	2.65	0.56
7:A:1226:TYR:HA	7:A:1229:LEU:HB2	1.86	0.56
10:N:101:ALA:HB1	10:N:105:GLU:HB2	1.87	0.56
10:N:359:ILE:HD13	10:N:404:PRO:HG2	1.86	0.56
10:N:413:PRO:HD2	10:N:427:ILE:HD11	1.86	0.56
13:Q:81:ARG:NH1	13:Q:107:VAL:O	2.38	0.56
11:S:61:LEU:HD13	12:T:36:ARG:HB3	1.88	0.56
15:W:116:DC:N3	16:X:32:DG:N1	2.40	0.56
2:C:438:TYR:O	3:E:387:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:112:ASN:OD1	9:M:112:ASN:N	2.33	0.56
12:P:34:ILE:HG21	12:P:51:TYR:HA	1.86	0.56
15:W:100:DG:N1	16:X:48:DC:N3	2.46	0.56
7:A:798:LYS:CD	17:A:1501:ADP:PB	2.93	0.56
9:M:9:VAL:O	9:M:437:TRP:NE1	2.38	0.56
11:S:49:ARG:O	11:S:52:ARG:HB2	2.06	0.56
7:A:629:PHE:HB2	7:A:632:ARG:HH21	1.71	0.56
8:L:65:ARG:O	8:L:67:GLN:NE2	2.39	0.56
10:N:15:ARG:NH1	10:N:426:GLU:OE2	2.39	0.56
9:M:53:ASN:N	9:M:53:ASN:OD1	2.37	0.56
9:M:165:ASN:HA	9:M:181:ARG:HA	1.87	0.56
9:M:196:ARG:NH1	9:M:312:TYR:OH	2.39	0.56
11:O:58:THR:HB	13:U:81:ARG:HD3	1.88	0.56
14:R:93:THR:HA	14:R:96:ARG:HB2	1.87	0.56
7:A:780:SER:O	7:A:784:ASN:ND2	2.38	0.56
12:T:71:THR:O	14:V:96:ARG:NH2	2.39	0.56
2:C:504:ALA:O	2:C:508:GLN:NE2	2.36	0.56
2:C:658:ALA:O	2:C:659:GLU:HG3	2.06	0.56
11:O:59:GLU:O	12:P:40:ARG:NH1	2.39	0.56
12:P:52:GLU:OE1	12:P:55:ARG:NH1	2.39	0.56
3:E:531:ASP:OD1	3:E:531:ASP:N	2.39	0.55
7:A:585:LEU:C	7:A:588:ASN:OD1	2.44	0.55
8:L:58:PHE:HB3	9:M:456:SER:HA	1.88	0.55
10:N:149:ALA:HB2	10:N:428:ILE:HG12	1.87	0.55
10:N:194:ILE:HG12	10:N:302:CYS:HA	1.88	0.55
12:P:75:HIS:CG	14:R:93:THR:HG1	2.25	0.55
1:B:916:ASP:OD2	7:A:562:ASN:OD1	2.23	0.55
10:N:138:ASN:HB3	10:N:451:ARG:HB2	1.89	0.55
10:N:294:VAL:O	10:N:298:ARG:NH1	2.39	0.55
13:Q:32:ARG:HH11	15:W:29:DA:H3'	1.70	0.55
1:B:1142:GLN:HG2	7:A:582:THR:HG21	1.86	0.55
9:M:38:ARG:HB3	9:M:46:GLU:HB3	1.88	0.55
12:T:29:ILE:O	12:T:55:ARG:NH2	2.36	0.55
13:U:41:GLU:HB3	14:V:84:SER:HB2	1.88	0.55
1:B:1149:VAL:HG21	7:A:586:TYR:HE1	1.71	0.55
7:A:808:TYR:HA	7:A:811:GLU:CG	2.37	0.55
8:L:89:ARG:N	10:N:34:GLU:O	2.36	0.55
10:N:304:ASN:O	10:N:308:ASN:ND2	2.39	0.55
14:V:48:ASP:OD2	14:V:48:ASP:N	2.38	0.55
15:W:101:DG:H4'	15:W:102:DG:H5'	1.88	0.55
3:D:516:LYS:HA	7:A:508:THR:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:444:MET:CG	7:A:503:LEU:HB3	2.37	0.55
7:A:526:ARG:O	7:A:530:LEU:N	2.37	0.55
7:A:935:TRP:O	7:A:939:ASN:N	2.40	0.55
9:M:105:VAL:HG21	9:M:444:ALA:HB2	1.88	0.55
9:M:201:ILE:HG13	9:M:203:GLU:H	1.71	0.55
9:M:311:GLU:OE1	9:M:315:LYS:NZ	2.31	0.55
13:Q:88:ARG:NH1	13:Q:97:LEU:O	2.39	0.55
7:A:542:GLN:HG2	7:A:546:ARG:HD3	1.89	0.55
9:M:32:PRO:O	9:M:86:GLN:NE2	2.38	0.55
13:Q:29:ARG:NH2	14:R:37:TYR:OH	2.40	0.55
13:U:12:ALA:N	16:X:32:DG:N3	2.54	0.55
15:W:80:DC:H4'	15:W:81:DC:H5'	1.89	0.55
1:B:892:LYS:NZ	4:H:58:ASP:OD2	2.40	0.55
1:B:911:LYS:O	1:B:915:ASN:ND2	2.39	0.55
3:D:537:LYS:CG	7:A:534:TYR:CE2	2.75	0.55
7:A:609:ASN:ND2	9:M:152:SER:OG	2.39	0.55
9:M:87:TRP:HB3	9:M:131:LEU:HD11	1.87	0.55
12:T:26:ILE:HD11	12:T:58:LEU:HD21	1.88	0.55
12:T:65:VAL:HA	12:T:93:GLN:HE22	1.71	0.55
15:W:129:DT:C2	16:X:19:DA:N1	2.75	0.55
3:D:430:PRO:HG3	7:A:544:ALA:HB1	1.87	0.55
7:A:1084:ARG:NH2	7:A:1315:SER:O	2.40	0.55
9:M:35:TYR:HE2	9:M:37:LYS:HE3	1.72	0.55
2:C:659:GLU:OE2	2:C:728:ARG:NH1	2.40	0.55
5:I:50:TYR:OH	5:I:71:GLN:NE2	2.39	0.55
3:E:726:ARG:O	3:E:730:ASN:ND2	2.40	0.55
7:A:616:TYR:HA	7:A:619:ARG:HD2	1.87	0.55
9:M:119:ILE:O	9:M:123:TYR:N	2.36	0.55
10:N:6:GLN:HE22	10:N:437:LYS:HE3	1.72	0.55
13:Q:111:ILE:HD11	11:S:52:ARG:HG3	1.89	0.55
12:T:37:LEU:O	12:T:41:GLY:N	2.40	0.55
13:U:30:VAL:HG21	13:U:52:ALA:HB2	1.89	0.55
7:A:615:GLN:NE2	9:M:445:ASN:O	2.40	0.55
10:N:281:PHE:HA	10:N:294:VAL:O	2.07	0.55
10:N:310:SER:O	10:N:357:HIS:NE2	2.40	0.55
11:S:64:LYS:HZ1	11:S:93:GLN:HE22	1.53	0.55
11:S:83:ARG:HD2	15:W:100:DG:H4'	1.89	0.55
13:U:39:TYR:OH	14:V:68:GLU:OE1	2.25	0.55
7:A:1086:ALA:O	7:A:1316:ARG:NH1	2.40	0.54
7:A:1212:ILE:HG23	7:A:1218:GLU:HG3	1.89	0.54
8:L:23:GLU:OE1	8:L:25:TRP:NE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:85:LYS:NZ	10:N:93:ASP:OD1	2.30	0.54
12:P:75:HIS:CE1	14:R:93:THR:HG1	2.25	0.54
14:R:114:ALA:O	14:R:118:TYR:N	2.38	0.54
15:W:28:DC:H4'	15:W:29:DA:H5'	1.89	0.54
3:D:540:GLN:CA	7:A:538:LEU:HD21	2.37	0.54
7:A:897:HIS:HE1	7:A:1168:LEU:HD11	1.71	0.54
1:B:966:ARG:NH1	7:A:565:PRO:HB2	2.22	0.54
3:D:602:LYS:CA	7:A:488:ILE:HD12	2.36	0.54
7:A:1094:ARG:NH1	7:A:1280:ASP:OD1	2.40	0.54
7:A:1102:THR:HG23	7:A:1297:LEU:HD21	1.88	0.54
7:A:1197:ALA:O	7:A:1202:GLN:NE2	2.40	0.54
8:L:4:GLN:OE1	10:N:84:ARG:NH2	2.39	0.54
3:D:565:PHE:CD1	7:A:542:GLN:HG3	2.43	0.54
3:D:570:ILE:HD13	7:A:539:LEU:HB2	1.89	0.54
8:L:26:ARG:NH1	8:L:65:ARG:O	2.41	0.54
11:O:60:LEU:HD22	11:O:93:GLN:HG2	1.90	0.54
15:W:104:DT:C2	16:X:44:DA:C2	2.95	0.54
15:W:151:DT:O2	16:X:-2:DG:N2	2.41	0.54
1:B:936:ARG:CA	1:B:940:ARG:HH21	2.19	0.54
11:S:104:PHE:HD2	12:T:41:GLY:HA3	1.71	0.54
15:W:89:DT:H4'	15:W:90:DA:H5'	1.89	0.54
16:X:87:DT:H2"	16:X:88:DT:H5"	1.88	0.54
10:N:306:ILE:HD11	10:N:345:PHE:HA	1.89	0.54
2:C:633:ILE:HD11	2:C:638:VAL:HG23	1.88	0.54
7:A:627:LEU:O	7:A:631:HIS:ND1	2.41	0.54
7:A:1063:PHE:HB2	7:A:1118:ILE:HD13	1.90	0.54
9:M:387:LEU:O	9:M:391:ASN:HB2	2.08	0.54
11:S:111:ALA:O	11:S:116:ARG:N	2.38	0.54
13:U:59:THR:HB	14:V:41:VAL:HG11	1.89	0.54
9:M:18:VAL:HG13	9:M:30:ILE:HG12	1.89	0.54
14:R:39:TYR:HE2	15:W:21:DG:H3'	1.73	0.54
15:W:69:DA:H2	16:X:80:DA:H2	1.56	0.54
15:W:77:DT:C2	16:X:71:DA:C2	2.96	0.54
16:X:101:DG:H4'	16:X:102:DA:H5'	1.89	0.54
9:M:145:ILE:HD13	9:M:395:THR:HG21	1.90	0.54
11:O:102:GLY:O	11:O:131:ARG:NH2	2.40	0.54
13:Q:77:ARG:N	16:X:132:DC:OP1	2.41	0.54
7:A:1288:ALA:O	7:A:1290:ASN:ND2	2.41	0.54
9:M:159:ILE:HG22	9:M:398:THR:HB	1.90	0.54
9:M:126:LEU:HA	9:M:130:LYS:HB2	1.89	0.53
13:Q:43:VAL:N	16:X:113:DA:OP1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:55:LEU:O	13:U:59:THR:OG1	2.22	0.53
1:B:1081:ASP:HA	1:B:1084:LEU:HB2	1.90	0.53
7:A:755:ILE:H	7:A:776:GLN:HG2	1.73	0.53
11:O:54:TYR:O	12:P:40:ARG:NH2	2.40	0.53
6:J:240:LEU:CD2	7:A:516:LEU:HD11	2.36	0.53
7:A:1171:ASN:HD21	17:A:1501:ADP:PA	2.31	0.53
9:M:214:GLN:HB3	9:M:217:SER:HB3	1.90	0.53
13:U:21:ALA:HB1	14:V:114:ALA:HB1	1.89	0.53
15:W:49:DA:H2	16:X:100:DA:H2	1.55	0.53
15:W:87:DT:C4	16:X:61:DA:N1	2.76	0.53
1:B:865:PRO:O	1:B:946:ARG:NH2	2.41	0.53
3:D:424:PRO:HD3	7:A:555:HIS:CD2	2.44	0.53
7:A:518:ASN:OD1	7:A:521:CYS:N	2.42	0.53
7:A:884:SER:HB2	7:A:913:HIS:HA	1.90	0.53
17:A:1501:ADP:O1B	18:A:1502:BEF:F3	2.16	0.53
12:P:90:LEU:HD22	12:P:95:ARG:HB2	1.90	0.53
1:B:730:LEU:HD22	1:B:920:THR:HG23	1.90	0.53
10:N:18:THR:HA	10:N:38:PRO:HA	1.90	0.53
14:R:83:ARG:HD3	14:R:85:THR:HG22	1.89	0.53
2:C:558:ILE:CD1	2:C:653:LEU:HD11	2.32	0.53
13:Q:42:ARG:NH1	16:X:111:DC:O2	2.41	0.53
11:S:71:VAL:HG11	11:S:89:VAL:HA	1.91	0.53
2:C:600:GLN:HA	2:C:603:MET:HG2	1.91	0.53
3:D:459:GLU:OE2	3:D:462:ARG:NH2	2.42	0.53
7:A:527:GLU:HA	7:A:530:LEU:HB3	1.91	0.53
14:R:109:SER:O	14:R:113:LYS:N	2.40	0.53
11:S:41:TYR:HB2	15:W:83:DG:H4'	1.91	0.53
9:M:400:LEU:HG	9:M:432:ARG:HD2	1.88	0.53
10:N:173:PRO:HG2	10:N:180:LEU:HB2	1.91	0.53
12:P:99:GLY:HA3	14:V:54:LYS:HZ3	1.74	0.53
11:S:72:ARG:NH2	16:X:51:DT:OP2	2.37	0.53
4:H:159:ARG:HA	4:H:281:LEU:O	2.09	0.53
7:A:768:LYS:O	7:A:771:GLN:NE2	2.41	0.53
15:W:117:DT:O2	16:X:32:DG:N2	2.42	0.53
3:D:426:GLU:OE2	7:A:548:HIS:HD2	1.82	0.53
3:D:537:LYS:CB	7:A:534:TYR:CE2	2.92	0.53
3:D:587:ASN:OD1	3:D:587:ASN:N	2.42	0.53
9:M:107:THR:HB	9:M:141:GLU:HB2	1.91	0.53
13:Q:34:LEU:HB3	13:Q:43:VAL:HG11	1.91	0.53
11:S:43:PRO:HG3	16:X:68:DG:N2	2.23	0.53
1:B:676:GLY:HA3	3:D:601:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1149:VAL:CG2	7:A:586:TYR:CE1	2.85	0.52
2:C:555:ASN:OD1	2:C:654:GLN:CB	2.58	0.52
4:H:307:PHE:O	4:H:419:GLN:NE2	2.41	0.52
3:E:447:SER:HB3	3:E:450:GLU:HB3	1.90	0.52
7:A:1171:ASN:HD21	17:A:1501:ADP:H5'1	1.68	0.52
10:N:81:GLN:NE2	10:N:130:TYR:OH	2.42	0.52
13:Q:97:LEU:HB3	13:Q:100:VAL:HB	1.91	0.52
14:R:69:ARG:NH2	12:T:98:TYR:OH	2.42	0.52
3:D:540:GLN:NE2	7:A:537:GLN:CD	2.62	0.52
3:D:540:GLN:HE22	7:A:537:GLN:HG2	1.72	0.52
3:D:732:ASN:ND2	3:E:779:THR:O	2.42	0.52
7:A:1098:LYS:HD2	7:A:1297:LEU:HD13	1.91	0.52
12:P:51:TYR:O	12:P:55:ARG:NH1	2.41	0.52
13:U:88:ARG:NH2	13:U:100:VAL:O	2.42	0.52
9:M:189:LEU:HA	9:M:192:GLN:HB2	1.90	0.52
9:M:197:LEU:HD13	9:M:299:LEU:HD12	1.91	0.52
9:M:330:GLY:O	9:M:334:ALA:N	2.42	0.52
11:O:106:ASP:OD1	11:O:106:ASP:N	2.43	0.52
12:P:59:LYS:HA	12:P:62:LEU:HD12	1.91	0.52
13:U:81:ARG:NH1	13:U:107:VAL:O	2.42	0.52
7:A:682:LEU:HD13	7:A:748:ALA:HB2	1.92	0.52
7:A:754:ASP:N	7:A:754:ASP:OD1	2.41	0.52
11:O:78:PHE:HE1	12:P:66:ILE:HB	1.75	0.52
2:C:529:TYR:HB2	2:C:615:PHE:HB2	1.91	0.52
3:D:544:ALA:HB2	7:A:541:LEU:HD21	1.91	0.52
10:N:222:LEU:HG	10:N:299:PHE:HB3	1.91	0.52
13:U:32:ARG:NH2	14:V:32:GLU:OE2	2.42	0.52
1:B:940:ARG:NH1	1:B:985:LEU:HD12	2.04	0.52
9:M:200:LEU:HB3	9:M:299:LEU:HD22	1.92	0.52
13:Q:85:LEU:O	13:Q:89:ASN:ND2	2.43	0.52
13:Q:90:ASP:OD2	13:Q:93:LEU:N	2.38	0.52
13:Q:90:ASP:HB3	13:Q:93:LEU:HB2	1.92	0.52
15:W:108:DT:O2	16:X:41:DG:N2	2.42	0.52
1:B:1256:GLU:HG3	1:B:1265:ILE:HG12	1.92	0.52
11:S:127:ALA:O	11:S:131:ARG:N	2.36	0.52
11:S:128:ARG:HA	11:S:131:ARG:HB2	1.92	0.52
12:T:78:ARG:NH2	12:T:85:ASP:OD2	2.43	0.52
15:W:63:DG:N1	16:X:85:DC:N3	2.53	0.52
2:C:481:LYS:NZ	2:C:524:PHE:O	2.43	0.52
2:C:496:LEU:HD21	2:C:513:ILE:HD12	1.91	0.52
2:C:483:ASP:OD1	3:E:380:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:673:ARG:NH1	14:V:109:SER:OG	2.38	0.52
7:A:826:SER:HA	7:A:1142:ARG:HD3	1.92	0.52
9:M:67:VAL:C	9:M:217:SER:HG	2.12	0.52
11:S:109:LEU:O	11:S:113:HIS:HB2	2.10	0.52
12:T:67:ARG:O	12:T:71:THR:OG1	2.28	0.52
14:V:33:SER:OG	14:V:34:TYR:N	2.43	0.52
3:D:321:SER:O	3:D:325:GLN:NE2	2.42	0.52
5:I:103:PHE:CE2	7:A:565:PRO:HG3	2.45	0.52
3:E:440:LEU:CD2	7:A:499:THR:HB	2.40	0.52
7:A:489:ASP:O	7:A:490:THR:C	2.49	0.52
17:A:1501:ADP:O1A	18:A:1502:BEF:F3	2.18	0.52
10:N:6:GLN:HB3	10:N:25:LEU:HB2	1.92	0.52
13:Q:116:LEU:HA	11:S:48:LEU:HD13	1.92	0.52
2:C:558:ILE:CD1	2:C:653:LEU:CD1	2.84	0.51
7:A:1184:ASP:OD2	7:A:1210:ARG:NH1	2.44	0.51
10:N:359:ILE:HG12	10:N:402:GLN:HB2	1.91	0.51
15:W:58:DT:H4'	15:W:59:DA:H5'	1.92	0.51
15:W:108:DT:H2"	15:W:109:DC:C5	2.45	0.51
1:B:723:ASN:HB3	7:A:558:SER:O	2.10	0.51
11:O:106:ASP:OD1	11:S:129:ARG:NH2	2.43	0.51
15:W:48:DT:N3	16:X:100:DA:C2	2.78	0.51
7:A:768:LYS:NZ	17:A:1501:ADP:N6	2.58	0.51
7:A:1083:TRP:HE3	7:A:1090:GLU:HA	1.75	0.51
9:M:84:GLU:HA	9:M:87:TRP:HB2	1.91	0.51
10:N:91:LEU:HD23	10:N:106:LEU:HD22	1.93	0.51
10:N:114:ILE:HD13	10:N:428:ILE:HG22	1.92	0.51
1:B:940:ARG:NH2	1:B:985:LEU:HD13	2.20	0.51
3:D:422:LEU:C	7:A:555:HIS:CD2	2.82	0.51
3:D:516:LYS:HA	7:A:508:THR:CG2	2.41	0.51
7:A:778:MET:O	7:A:782:PHE:N	2.41	0.51
16:X:38:DG:H1'	16:X:39:DG:C5	2.45	0.51
1:B:988:ILE:HD11	1:B:1046:LEU:HD13	1.92	0.51
7:A:609:ASN:O	7:A:613:ILE:N	2.36	0.51
3:D:785:ASN:ND2	3:D:787:PHE:O	2.42	0.51
6:J:325:SER:OG	6:J:326:LYS:N	2.43	0.51
7:A:768:LYS:HZ2	17:A:1501:ADP:N6	2.09	0.51
7:A:1013:CYS:N	7:A:1212:ILE:O	2.43	0.51
7:A:1117:ASP:OD2	12:P:19:ARG:NH1	2.43	0.51
9:M:35:TYR:CZ	9:M:68:TYR:HB2	2.46	0.51
10:N:340:THR:O	10:N:346:LYS:NZ	2.41	0.51
4:H:130:SER:HA	4:H:434:THR:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:806:LEU:HD22	7:A:810:TYR:CE2	2.46	0.51
7:A:1170:LEU:HD22	7:A:1172:LEU:HD11	1.92	0.51
10:N:43:ARG:O	10:N:62:ALA:HA	2.10	0.51
10:N:417:PRO:HA	10:N:420:LYS:HB3	1.93	0.51
12:P:35:ARG:NH2	12:P:51:TYR:OH	2.35	0.51
7:A:516:LEU:HD22	7:A:530:LEU:HA	1.91	0.51
12:P:43:VAL:HG11	12:P:46:ILE:HG23	1.93	0.51
15:W:48:DT:C4	16:X:100:DA:N1	2.79	0.51
1:B:946:ARG:O	1:B:950:ASP:HB2	2.11	0.51
2:C:640:ARG:NH2	3:D:369:ARG:O	2.42	0.51
3:D:606:PRO:HB3	7:A:486:VAL:N	2.26	0.51
10:N:218:ILE:O	10:N:276:ASN:ND2	2.44	0.51
11:O:42:ARG:HG2	15:W:68:DT:H5"	1.92	0.51
11:S:61:LEU:HB2	12:T:37:LEU:HG	1.92	0.51
1:B:747:GLU:HB2	2:C:439:LEU:HD13	1.92	0.51
1:B:1122:VAL:HG12	1:B:1132:LEU:HB3	1.93	0.51
3:D:598:LEU:HD22	7:A:490:THR:HG21	1.92	0.51
3:E:594:TYR:O	7:A:493:ALA:CB	2.59	0.51
14:R:80:TYR:O	14:R:82:LYS:NZ	2.31	0.51
12:T:35:ARG:NH1	12:T:51:TYR:OH	2.44	0.51
4:H:117:LEU:HD11	3:E:724:ILE:HD11	1.92	0.50
7:A:599:THR:HA	7:A:602:VAL:HB	1.92	0.50
7:A:1016:SER:O	7:A:1020:GLN:N	2.43	0.50
10:N:350:LEU:HB2	10:N:409:LEU:HD21	1.92	0.50
11:O:68:GLN:HG2	11:O:72:ARG:HE	1.76	0.50
14:R:61:SER:OG	12:T:100:PHE:N	2.41	0.50
4:H:295:ILE:HB	4:H:423:ILE:HG23	1.93	0.50
10:N:412:TYR:HD1	10:N:427:ILE:HD12	1.76	0.50
13:Q:17:ARG:HH22	13:Q:31:HIS:HD2	1.60	0.50
13:Q:63:LEU:HD22	14:R:42:LEU:HD13	1.94	0.50
14:R:70:ILE:HG12	14:R:94:ALA:HB1	1.92	0.50
13:U:93:LEU:O	13:U:97:LEU:N	2.44	0.50
15:W:120:DA:N7	16:X:27:DC:N4	2.59	0.50
1:B:927:ASN:ND2	7:A:569:SER:CB	2.69	0.50
2:C:502:GLU:O	2:C:505:THR:OG1	2.29	0.50
3:E:422:LEU:HD11	7:A:554:TRP:HD1	1.76	0.50
9:M:292:PHE:O	9:M:296:ASN:N	2.44	0.50
10:N:16:SER:HA	10:N:69:GLN:HA	1.93	0.50
13:Q:92:GLU:O	13:Q:96:LEU:HB2	2.11	0.50
14:R:109:SER:OG	14:R:110:GLU:N	2.44	0.50
16:X:66:DG:H1'	16:X:67:DG:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:ARG:O	1:B:940:ARG:CD	2.60	0.50
1:B:1149:VAL:HG21	7:A:586:TYR:CE1	2.45	0.50
2:C:652:LEU:HB2	6:J:312:LEU:CA	2.41	0.50
2:C:677:GLN:NE2	14:V:110:GLU:OE2	2.45	0.50
3:D:424:PRO:HG3	7:A:552:PHE:HA	1.92	0.50
7:A:1146:LEU:HD22	7:A:1170:LEU:HB3	1.93	0.50
7:A:1190:ASP:OD2	7:A:1210:ARG:NH2	2.45	0.50
8:L:25:TRP:HA	8:L:66:ASN:H	1.76	0.50
9:M:240:GLU:HG3	9:M:246:LEU:HD11	1.94	0.50
9:M:326:GLU:HA	9:M:331:PRO:HB2	1.91	0.50
11:O:59:GLU:H	12:P:40:ARG:HH22	1.59	0.50
12:T:66:ILE:HA	12:T:69:ALA:HB3	1.92	0.50
5:I:150:HIS:O	5:I:153:LYS:NZ	2.44	0.50
3:E:444:MET:HG2	7:A:503:LEU:HB3	1.93	0.50
9:M:157:ILE:HG12	9:M:166:VAL:HG22	1.93	0.50
10:N:362:PRO:HD2	10:N:365:GLU:HB2	1.94	0.50
13:Q:42:ARG:N	14:R:84:SER:O	2.45	0.50
11:S:42:ARG:NH1	16:X:69:DG:OP1	2.44	0.50
11:S:62:ILE:HG23	12:T:29:ILE:HD12	1.92	0.50
15:W:86:DT:C2	16:X:62:DA:H2	2.28	0.50
16:X:30:DG:H1'	16:X:31:DA:H5'	1.92	0.50
1:B:734:ALA:HB2	7:A:567:PHE:CZ	2.47	0.50
7:A:938:LEU:HD21	7:A:987:LEU:HD21	1.93	0.50
9:M:441:LEU:O	9:M:445:ASN:ND2	2.40	0.50
11:O:101:VAL:HG13	12:P:41:GLY:HA2	1.94	0.50
13:U:27:VAL:HG11	13:U:49:VAL:HG22	1.94	0.50
3:D:601:SER:O	7:A:488:ILE:CD1	2.60	0.50
3:E:567:GLN:O	3:E:629:ARG:NH2	2.45	0.50
7:A:522:THR:O	7:A:526:ARG:N	2.43	0.50
10:N:279:LEU:O	10:N:298:ARG:NH2	2.45	0.50
10:N:460:ALA:HA	10:N:463:TRP:HD1	1.77	0.50
14:V:42:LEU:O	14:V:46:HIS:N	2.44	0.50
1:B:940:ARG:HH22	1:B:985:LEU:HD12	1.74	0.50
2:C:669:ARG:NH1	13:U:92:GLU:OE1	2.40	0.50
3:D:682:LEU:HD11	5:I:149:GLN:HG3	1.93	0.50
7:A:595:GLU:HA	7:A:595:GLU:OE2	2.12	0.50
7:A:1080:ASP:OD1	7:A:1083:TRP:NE1	2.43	0.50
7:A:1095:ILE:O	7:A:1099:LEU:N	2.35	0.50
7:A:1209:LEU:HD11	7:A:1286:ILE:HG21	1.93	0.50
10:N:114:ILE:HA	10:N:143:LEU:O	2.12	0.50
12:P:64:ASN:O	12:P:67:ARG:NE	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:128:ARG:HB3	11:S:133:GLU:HB2	1.92	0.50
15:W:48:DT:C2	16:X:100:DA:C2	3.00	0.50
6:J:327:ASN:HB3	6:J:330:GLN:HE21	1.77	0.50
9:M:216:ARG:HD2	9:M:216:ARG:C	2.32	0.50
10:N:7:ASP:HB3	10:N:105:GLU:HG2	1.92	0.50
11:O:56:LYS:HA	13:U:109:PRO:HG3	1.94	0.50
15:W:73:DG:N1	16:X:75:DC:N3	2.40	0.50
3:D:602:LYS:CB	7:A:488:ILE:HB	2.41	0.49
3:D:672:ALA:O	3:D:677:ARG:NH2	2.44	0.49
8:L:25:TRP:O	10:N:129:GLN:NE2	2.45	0.49
8:L:88:ASP:HA	10:N:35:LEU:HA	1.94	0.49
9:M:241:LYS:HG3	9:M:410:LYS:HG2	1.93	0.49
12:P:89:ALA:O	12:P:93:GLN:N	2.37	0.49
12:T:38:ALA:HB1	12:T:43:VAL:HB	1.94	0.49
12:T:43:VAL:HG11	12:T:46:ILE:HG23	1.94	0.49
1:B:964:CYS:SG	1:B:965:ASN:N	2.85	0.49
2:C:659:GLU:CD	2:C:728:ARG:NH1	2.65	0.49
3:D:565:PHE:CZ	7:A:538:LEU:O	2.58	0.49
4:H:313:GLN:HE21	4:H:387:THR:HG23	1.77	0.49
3:E:440:LEU:HD21	7:A:499:THR:HB	1.93	0.49
9:M:214:GLN:HE21	9:M:216:ARG:CG	1.85	0.49
10:N:4:PHE:HB2	10:N:440:PHE:HB3	1.95	0.49
11:S:55:GLN:NE2	12:T:40:ARG:O	2.45	0.49
16:X:54:DC:H2"	16:X:55:DG:C8	2.47	0.49
2:C:460:ILE:HD13	2:C:517:ILE:HG23	1.93	0.49
4:H:185:ILE:HG12	4:H:297:ILE:HG23	1.94	0.49
6:J:236:LYS:HE3	7:A:526:ARG:NH1	2.27	0.49
6:J:332:ALA:HB1	6:J:337:ALA:HB3	1.94	0.49
9:M:147:LEU:O	9:M:150:GLY:N	2.45	0.49
11:O:97:GLU:HA	11:O:100:LEU:HD12	1.94	0.49
14:R:37:TYR:OH	16:X:122:DG:O5'	2.29	0.49
11:S:121:PRO:HA	11:S:124:ILE:HG13	1.93	0.49
13:U:29:ARG:NH1	14:V:32:GLU:OE1	2.46	0.49
14:V:53:SER:HA	14:V:56:MET:HB3	1.93	0.49
15:W:77:DT:N3	16:X:71:DA:C2	2.80	0.49
15:W:87:DT:C2	16:X:61:DA:C2	3.00	0.49
1:B:905:ARG:NE	1:B:905:ARG:HA	2.27	0.49
3:D:602:LYS:N	7:A:488:ILE:CG2	2.75	0.49
10:N:315:LEU:O	10:N:319:ASN:ND2	2.45	0.49
11:O:48:LEU:HD23	13:U:111:ILE:HG21	1.94	0.49
11:S:62:ILE:HG12	12:T:29:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:32:ARG:HH11	13:U:36:LYS:HE2	1.77	0.49
3:E:442:LYS:NZ	3:E:579:GLY:O	2.43	0.49
7:A:845:ILE:HB	7:A:869:VAL:HG22	1.94	0.49
9:M:332:LEU:O	9:M:336:SER:CB	2.61	0.49
11:O:129:ARG:NH2	11:S:106:ASP:OD1	2.45	0.49
11:S:129:ARG:O	11:S:129:ARG:NH1	2.42	0.49
12:T:92:ARG:NH1	12:T:92:ARG:O	2.45	0.49
13:U:76:THR:N	15:W:132:DG:OP1	2.45	0.49
1:B:770:TYR:O	1:B:771:HIS:ND1	2.46	0.49
1:B:929:SER:OG	1:B:981:ASN:ND2	2.42	0.49
1:B:1233:LEU:CD1	7:A:579:ALA:HB1	2.43	0.49
4:H:130:SER:OG	4:H:161:GLU:OE1	2.30	0.49
3:E:365:THR:HG22	3:E:368:ARG:HH22	1.77	0.49
9:M:56:ASP:OD2	10:N:312:ARG:NH2	2.45	0.49
10:N:29:THR:HG21	10:N:417:PRO:HD2	1.94	0.49
10:N:101:ALA:O	10:N:106:LEU:N	2.31	0.49
14:V:54:LYS:HZ2	14:V:58:ILE:HD11	1.78	0.49
7:A:817:GLY:O	7:A:819:TYR:N	2.44	0.49
10:N:303:ASN:HA	10:N:306:ILE:HB	1.95	0.49
11:S:101:VAL:HG13	12:T:41:GLY:HA2	1.95	0.49
15:W:87:DT:H2"	15:W:88:DT:C5	2.48	0.49
16:X:3:DA:H2"	16:X:4:DG:C8	2.48	0.49
7:A:904:SER:OG	7:A:905:LYS:N	2.45	0.49
13:Q:87:VAL:HG13	13:Q:93:LEU:HB3	1.95	0.49
1:B:747:GLU:OE2	2:C:442:LYS:NZ	2.44	0.49
2:C:429:GLN:HE22	2:C:436:LYS:HA	1.77	0.49
3:D:537:LYS:CA	7:A:534:TYR:CE2	2.96	0.49
3:D:570:ILE:HG22	7:A:539:LEU:CD2	2.34	0.49
4:H:92:ARG:HG2	3:E:704:LEU:HD13	1.95	0.49
7:A:820:LEU:HG	7:A:913:HIS:CE1	2.47	0.49
9:M:118:ALA:O	9:M:122:ARG:N	2.41	0.49
10:N:21:VAL:HB	10:N:35:LEU:HB2	1.95	0.49
15:W:65:DA:H1'	15:W:66:DC:H5'	1.95	0.49
3:D:426:GLU:HG2	7:A:551:GLN:CD	2.33	0.48
7:A:816:ARG:HD3	7:A:842:LEU:HD21	1.94	0.48
16:X:130:DG:H1'	16:X:131:DG:C5	2.48	0.48
1:B:1239:ILE:HG23	1:B:1298:GLN:HG3	1.93	0.48
15:W:42:DC:N3	16:X:106:DG:N1	2.51	0.48
3:D:570:ILE:HB	7:A:539:LEU:HD13	1.95	0.48
10:N:353:LEU:HB3	10:N:407:ILE:HG21	1.95	0.48
10:N:363:GLU:O	10:N:367:SER:OG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:75:HIS:HB2	14:R:96:ARG:HH22	1.78	0.48
2:C:665:LYS:NZ	13:U:91:GLU:OE1	2.43	0.48
3:E:444:MET:SD	7:A:503:LEU:HB3	2.53	0.48
11:O:52:ARG:HG3	13:U:111:ILE:HD11	1.94	0.48
14:R:53:SER:HA	14:R:56:MET:HB3	1.95	0.48
3:D:566:LEU:HA	7:A:542:GLN:HE21	1.77	0.48
4:H:131:ASN:N	4:H:131:ASN:OD1	2.46	0.48
3:E:444:MET:HE2	7:A:503:LEU:HD13	1.95	0.48
9:M:198:ALA:HA	9:M:201:ILE:HG12	1.96	0.48
11:O:113:HIS:CE1	11:S:122:LYS:HE2	2.49	0.48
13:U:29:ARG:CZ	14:V:32:GLU:HB2	2.44	0.48
2:C:465:ASP:OD2	2:C:468:ARG:NH2	2.46	0.48
3:D:779:THR:OG1	3:D:780:LEU:N	2.46	0.48
3:E:593:LYS:H	3:E:593:LYS:HG3	1.48	0.48
7:A:758:GLN:HB2	7:A:762:LEU:HD23	1.96	0.48
11:S:70:LEU:HA	11:S:73:GLU:HB3	1.96	0.48
1:B:723:ASN:CG	7:A:559:LEU:HD23	2.34	0.48
1:B:926:ARG:HH11	1:B:977:ILE:HD12	1.79	0.48
2:C:555:ASN:OD1	2:C:654:GLN:HB3	2.14	0.48
3:D:609:SER:OG	7:A:488:ILE:CA	2.62	0.48
3:E:688:ARG:NE	3:E:692:GLU:OE2	2.46	0.48
7:A:648:ALA:O	7:A:652:ALA:N	2.45	0.48
10:N:294:VAL:HG13	10:N:298:ARG:HD3	1.95	0.48
11:O:58:THR:O	11:O:58:THR:OG1	2.23	0.48
14:R:116:THR:HA	14:R:119:THR:HG22	1.95	0.48
15:W:45:DC:C2	16:X:103:DG:N2	2.59	0.48
1:B:1047:PHE:HB3	1:B:1149:VAL:HG11	1.95	0.48
15:W:120:DA:C2	16:X:28:DT:N3	2.79	0.48
16:X:89:DT:H1'	16:X:90:DA:C4	2.49	0.48
7:A:630:GLY:O	10:N:155:SER:OG	2.29	0.48
7:A:800:ILE:CD1	17:A:1501:ADP:N7	2.77	0.48
9:M:216:ARG:O	9:M:216:ARG:HD2	2.13	0.48
9:M:390:THR:HG23	9:M:419:TYR:HB3	1.95	0.48
10:N:130:TYR:O	10:N:135:LEU:N	2.36	0.48
12:P:39:ARG:HH12	12:P:46:ILE:HG12	1.79	0.48
13:Q:84:GLN:NE2	13:Q:106:GLY:O	2.47	0.48
1:B:733:SER:O	7:A:570:LYS:HE3	2.14	0.48
2:C:661:GLU:O	2:C:662:ARG:HG3	2.13	0.48
12:P:39:ARG:NH1	12:P:43:VAL:O	2.47	0.48
13:Q:20:ARG:NH2	15:W:32:DT:OP1	2.47	0.48
11:S:63:ARG:HD3	11:S:63:ARG:HA	1.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:421:GLY:O	7:A:555:HIS:NE2	2.47	0.47
7:A:944:LYS:HG2	7:A:945:ILE:HG23	1.95	0.47
7:A:1251:GLU:HA	7:A:1254:LEU:HB2	1.96	0.47
11:O:123:ASP:N	11:O:123:ASP:OD1	2.45	0.47
13:Q:37:GLY:HA3	13:Q:39:TYR:CZ	2.49	0.47
13:Q:104:GLN:NE2	11:S:58:THR:O	2.47	0.47
15:W:119:DC:H2"	15:W:120:DA:C5	2.49	0.47
16:X:88:DT:H2"	16:X:89:DT:C5	2.48	0.47
4:H:89:ILE:O	4:H:92:ARG:HB3	2.14	0.47
4:H:318:ILE:HD11	4:H:332:ILE:HG23	1.95	0.47
3:E:433:GLN:O	3:E:437:MET:N	2.47	0.47
9:M:80:TRP:CD2	9:M:122:ARG:HD2	2.49	0.47
9:M:190:ASP:HA	9:M:228:ILE:HG21	1.94	0.47
11:O:61:LEU:HD22	12:P:36:ARG:HB3	1.96	0.47
11:O:106:ASP:HA	11:O:109:LEU:HD12	1.96	0.47
16:X:26:DC:H4'	16:X:27:DC:H5'	1.96	0.47
1:B:1002:ILE:HD11	1:B:1109:VAL:HA	1.96	0.47
4:H:169:GLN:HG3	4:H:172:ASP:HB2	1.96	0.47
4:H:388:LEU:O	4:H:414:HIS:NE2	2.38	0.47
10:N:101:ALA:O	10:N:105:GLU:N	2.47	0.47
13:U:16:THR:HG22	16:X:30:DG:H4'	1.96	0.47
16:X:113:DA:H1'	16:X:114:DC:H5'	1.97	0.47
16:X:116:DA:H1'	16:X:117:DA:H5'	1.96	0.47
2:C:628:ARG:HH22	2:C:724:ALA:HB2	1.80	0.47
4:H:92:ARG:NH1	3:E:708:MET:SD	2.87	0.47
3:E:624:GLN:HB3	3:E:632:GLN:HG2	1.96	0.47
7:A:935:TRP:HE1	7:A:952:PHE:HB2	1.79	0.47
1:B:1145:THR:CG2	7:A:586:TYR:CE1	2.96	0.47
2:C:413:SER:OG	2:C:414:GLY:N	2.47	0.47
7:A:770:TYR:O	7:A:994:ARG:NH2	2.48	0.47
10:N:199:LYS:HG3	10:N:210:ILE:HD13	1.96	0.47
12:T:75:HIS:CG	14:V:93:THR:HG1	2.29	0.47
15:W:48:DT:H2"	15:W:49:DA:C5	2.50	0.47
15:W:51:DC:H2'	15:W:52:DA:C8	2.49	0.47
16:X:31:DA:H4'	16:X:32:DG:H5'	1.96	0.47
7:A:958:THR:HA	7:A:975:GLU:HB3	1.95	0.47
10:N:314:GLY:HA3	10:N:357:HIS:CE1	2.50	0.47
11:O:90:MET:SD	11:O:90:MET:N	2.88	0.47
3:D:430:PRO:CG	7:A:544:ALA:HB1	2.45	0.47
3:D:709:GLU:OE2	3:D:713:LYS:NZ	2.37	0.47
4:H:182:ILE:HG21	4:H:185:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:444:MET:HG3	7:A:503:LEU:HD12	1.92	0.47
7:A:1131:LEU:HD13	7:A:1145:LEU:HD12	1.96	0.47
8:L:31:GLN:O	8:L:55:LYS:NZ	2.39	0.47
10:N:354:LEU:HA	10:N:358:LEU:HB2	1.97	0.47
2:C:659:GLU:CD	2:C:728:ARG:HH11	2.18	0.47
3:D:574:PHE:HZ	7:A:508:THR:CB	2.27	0.47
4:H:299:ARG:NH1	4:H:305:GLU:OE1	2.41	0.47
4:H:313:GLN:HE22	4:H:388:LEU:HD12	1.79	0.47
4:H:332:ILE:HA	4:H:335:TYR:HB3	1.96	0.47
10:N:201:LEU:HD13	10:N:300:GLN:HB3	1.96	0.47
7:A:605:LEU:O	7:A:609:ASN:ND2	2.48	0.47
7:A:1241:PHE:HD2	7:A:1253:LEU:HD12	1.80	0.47
9:M:7:CYS:O	9:M:22:SER:N	2.39	0.47
10:N:354:LEU:HD23	10:N:358:LEU:HD13	1.96	0.47
11:O:117:VAL:N	15:W:71:DG:OP1	2.48	0.47
11:S:40:ARG:NH1	15:W:83:DG:H21	2.12	0.47
15:W:82:DC:H2"	15:W:83:DG:N7	2.30	0.47
1:B:727:ASN:HB3	7:A:560:LEU:CD1	2.44	0.47
1:B:1049:LEU:CD2	1:B:1051:LYS:CD	2.88	0.47
2:C:529:TYR:HA	2:C:532:LEU:HB2	1.97	0.47
4:H:75:PHE:O	4:H:78:LEU:HB2	2.15	0.47
8:L:11:ASN:HD21	10:N:109:ILE:HB	1.80	0.47
11:O:121:PRO:HA	11:O:124:ILE:HG13	1.96	0.47
15:W:132:DG:H1'	15:W:133:DA:C8	2.50	0.47
15:W:145:DT:H2'	15:W:146:DG:C8	2.50	0.47
1:B:936:ARG:HB2	1:B:940:ARG:HH21	1.71	0.46
4:H:127:ILE:HA	4:H:161:GLU:O	2.16	0.46
4:H:129:ILE:HD13	4:H:295:ILE:HD13	1.97	0.46
3:E:423:PHE:CD2	7:A:547:GLY:HA3	2.50	0.46
9:M:165:ASN:HB3	9:M:181:ARG:HG2	1.97	0.46
9:M:214:GLN:CD	9:M:216:ARG:HE	2.15	0.46
10:N:202:LEU:HB2	10:N:210:ILE:HD11	1.97	0.46
12:T:39:ARG:HH12	12:T:46:ILE:HG12	1.80	0.46
16:X:24:DT:H2"	16:X:25:DG:C8	2.50	0.46
1:B:907:ALA:HB2	7:A:557:ASN:HD21	1.65	0.46
6:J:308:ILE:HD11	6:J:489:ARG:HD2	1.96	0.46
9:M:155:PHE:HD2	9:M:392:VAL:HG13	1.80	0.46
10:N:330:TRP:NE1	10:N:404:PRO:HB3	2.30	0.46
14:R:35:ALA:O	14:R:39:TYR:HB2	2.14	0.46
13:U:14:ALA:N	16:X:30:DG:H21	2.12	0.46
16:X:88:DT:H2"	16:X:89:DT:C6	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:ASN:CG	7:A:569:SER:HB2	2.36	0.46
3:D:424:PRO:HD3	7:A:552:PHE:CD1	2.44	0.46
7:A:933:GLU:HB3	7:A:936:ALA:HB3	1.97	0.46
9:M:70:LEU:O	9:M:78:TYR:N	2.40	0.46
9:M:178:ALA:HA	9:M:339:LYS:HE2	1.97	0.46
13:U:28:GLY:HA3	16:X:31:DA:OP2	2.14	0.46
13:U:92:GLU:HG3	13:U:95:LYS:HZ1	1.80	0.46
3:D:565:PHE:CE1	7:A:542:GLN:CG	2.97	0.46
4:H:118:ASN:OD1	4:H:118:ASN:N	2.40	0.46
7:A:1188:HIS:HE1	7:A:1236:ILE:HD13	1.80	0.46
9:M:390:THR:O	9:M:422:THR:OG1	2.32	0.46
10:N:22:GLN:OE1	10:N:433:GLN:NE2	2.40	0.46
10:N:169:THR:O	10:N:186:SER:HA	2.15	0.46
13:Q:77:ARG:HD3	15:W:20:DA:H5”	1.98	0.46
11:S:74:ILE:HD13	12:T:62:LEU:HB3	1.96	0.46
15:W:38:DT:C2	16:X:110:DA:C2	3.04	0.46
1:B:932:ASP:OD1	1:B:932:ASP:N	2.48	0.46
9:M:39:THR:O	9:M:62:ARG:NH2	2.34	0.46
14:R:66:VAL:HA	14:R:69:ARG:HD2	1.98	0.46
12:T:75:HIS:ND1	14:V:93:THR:OG1	2.37	0.46
15:W:23:DC:H1’	15:W:24:DC:H5’	1.97	0.46
3:D:424:PRO:HD2	7:A:552:PHE:HD1	1.78	0.46
3:E:771:LYS:O	3:E:775:SER:HB2	2.16	0.46
13:Q:109:PRO:HG3	11:S:56:LYS:HA	1.98	0.46
11:S:83:ARG:HB3	16:X:50:DT:H5”	1.97	0.46
1:B:697:LEU:HD22	1:B:702:LEU:HD23	1.98	0.46
1:B:730:LEU:CD1	7:A:567:PHE:CE2	2.99	0.46
3:D:387:LYS:HA	3:D:387:LYS:HD3	1.75	0.46
3:E:520:LEU:HD11	3:E:645:SER:HA	1.97	0.46
7:A:590:GLU:OE1	7:A:590:GLU:HA	2.15	0.46
7:A:641:GLU:O	7:A:645:GLN:N	2.47	0.46
9:M:314:PHE:HA	9:M:329:LEU:H	1.80	0.46
12:T:85:ASP:OD1	12:T:85:ASP:N	2.48	0.46
15:W:108:DT:H2’	15:W:108:DT:OP2	2.16	0.46
3:D:370:ASN:OD1	6:J:471:HIS:ND1	2.45	0.46
6:J:475:ALA:O	6:J:479:ASN:ND2	2.49	0.46
9:M:58:ALA:HB1	9:M:222:TYR:HB2	1.97	0.46
9:M:335:LYS:HA	9:M:338:LYS:HD2	1.98	0.46
13:Q:12:ALA:N	15:W:32:DT:O2	2.49	0.46
14:R:84:SER:N	15:W:40:DG:OP1	2.49	0.46
15:W:127:DT:H2’	15:W:128:DG:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:644:GLU:OE1	7:A:647:ARG:NH1	2.49	0.46
7:A:1008:GLU:HA	7:A:1208:ILE:HB	1.97	0.46
7:A:1207:ARG:HD3	7:A:1207:ARG:HA	1.80	0.46
8:L:31:GLN:HG2	8:L:55:LYS:HD2	1.98	0.46
9:M:334:ALA:HB2	9:M:415:ARG:HD3	1.98	0.46
11:O:48:LEU:HG	11:O:51:ILE:HD12	1.98	0.46
11:O:52:ARG:O	11:O:56:LYS:N	2.47	0.46
11:S:49:ARG:O	11:S:53:ARG:N	2.40	0.46
11:S:106:ASP:OD2	11:S:131:ARG:NE	2.45	0.46
12:T:59:LYS:HA	12:T:62:LEU:HD12	1.97	0.46
2:C:663:LEU:HB3	2:C:666:ASP:HB2	1.97	0.46
3:D:458:LYS:O	3:D:462:ARG:HB2	2.16	0.46
5:I:125:THR:O	5:I:125:THR:OG1	2.31	0.46
13:U:58:LEU:HD23	13:U:61:GLU:HG3	1.96	0.46
14:V:113:LYS:O	14:V:116:THR:OG1	2.27	0.46
15:W:77:DT:H2"	15:W:78:DC:C2	2.51	0.46
7:A:929:ASN:HA	7:A:1232:ASP:HB3	1.98	0.45
9:M:428:VAL:O	9:M:431:ASP:N	2.49	0.45
10:N:159:CYS:HA	10:N:332:ASN:HB2	1.98	0.45
11:O:57:SER:O	13:U:81:ARG:NH1	2.49	0.45
13:Q:67:GLY:HA2	14:R:49:THR:HG21	1.97	0.45
14:V:112:THR:O	14:V:115:VAL:HB	2.16	0.45
2:C:556:GLN:HB3	2:C:653:LEU:O	2.15	0.45
7:A:953:ASP:N	7:A:953:ASP:OD1	2.49	0.45
7:A:1264:ARG:HG3	7:A:1268:ARG:HH12	1.80	0.45
8:L:29:TRP:HE3	8:L:59:ARG:HB2	1.81	0.45
9:M:63:ASN:OD1	9:M:63:ASN:N	2.48	0.45
11:O:125:GLN:NE2	12:P:53:GLU:OE1	2.50	0.45
14:R:99:LEU:HD12	14:R:104:ALA:HA	1.99	0.45
11:S:42:ARG:HB3	16:X:68:DG:H4'	1.98	0.45
1:B:952:LEU:HG	1:B:996:LEU:HB3	1.97	0.45
3:D:736:ILE:O	3:D:740:LEU:HB2	2.15	0.45
3:D:786:PRO:O	4:H:167:ASN:ND2	2.48	0.45
3:E:614:LEU:HD12	3:E:660:ALA:HB1	1.99	0.45
7:A:822:ILE:HG23	7:A:893:ILE:HA	1.97	0.45
9:M:118:ALA:O	9:M:121:GLU:HB3	2.16	0.45
9:M:337:VAL:HG11	9:M:389:LEU:HD11	1.97	0.45
10:N:87:PHE:O	10:N:91:LEU:HG	2.16	0.45
10:N:166:THR:O	10:N:192:GLN:N	2.47	0.45
13:Q:112:GLN:HE21	13:Q:112:GLN:HB3	1.59	0.45
11:S:73:GLU:HG3	12:T:23:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:941:ASN:HD22	1:B:944:LEU:N	2.01	0.45
2:C:652:LEU:CD1	6:J:312:LEU:CB	2.79	0.45
10:N:5:ARG:NE	10:N:104:ALA:O	2.50	0.45
12:P:47:SER:HB3	12:P:50:ILE:HG12	1.99	0.45
11:S:67:PHE:HE2	11:S:90:MET:HA	1.82	0.45
14:V:102:GLU:HA	14:V:105:LYS:HD2	1.98	0.45
1:B:781:ASP:N	1:B:781:ASP:OD1	2.50	0.45
2:C:527:ASN:HB3	2:C:531:GLU:HG2	1.98	0.45
7:A:810:TYR:CE2	7:A:819:TYR:HE2	2.28	0.45
7:A:1164:ARG:HH12	16:X:95:DG:H21	1.63	0.45
3:D:423:PHE:CD1	7:A:552:PHE:CD1	3.04	0.45
4:H:115:PRO:O	4:H:116:HIS:ND1	2.50	0.45
4:H:160:ILE:HB	4:H:281:LEU:HB3	1.99	0.45
7:A:593:LYS:C	7:A:593:LYS:HE3	2.37	0.45
7:A:619:ARG:HH22	9:M:438:LEU:HB3	1.80	0.45
7:A:808:TYR:HA	7:A:811:GLU:HG2	1.97	0.45
9:M:126:LEU:HA	9:M:130:LYS:HD3	1.98	0.45
11:O:58:THR:O	13:U:104:GLN:NE2	2.49	0.45
12:T:75:HIS:O	14:V:89:ARG:NH2	2.50	0.45
9:M:75:GLY:HA3	9:M:109:PRO:HG3	1.99	0.45
9:M:127:ALA:O	9:M:133:VAL:N	2.50	0.45
13:Q:55:LEU:O	13:Q:59:THR:OG1	2.26	0.45
15:W:86:DT:H6	15:W:86:DT:H2'	1.67	0.45
1:B:1149:VAL:HG23	7:A:586:TYR:HE1	1.78	0.45
2:C:652:LEU:HG	6:J:312:LEU:HB3	1.94	0.45
7:A:844:THR:HA	7:A:868:VAL:HG12	1.99	0.45
9:M:151:LYS:HD2	9:M:393:ILE:HD11	1.98	0.45
9:M:216:ARG:O	9:M:217:SER:C	2.55	0.45
10:N:145:ALA:HB1	10:N:428:ILE:HD13	1.98	0.45
11:O:85:GLN:OE1	11:O:87:SER:OG	2.34	0.45
15:W:38:DT:C4	16:X:110:DA:N1	2.84	0.45
2:C:622:ASP:HB3	2:C:625:ILE:HG13	1.99	0.45
2:C:652:LEU:HB3	6:J:312:LEU:N	2.28	0.45
4:H:89:ILE:O	4:H:93:ASN:ND2	2.50	0.45
4:H:440:LEU:HD23	4:H:440:LEU:HA	1.86	0.45
7:A:642:ARG:HG2	7:A:646:LYS:HD3	1.99	0.45
9:M:216:ARG:CD	9:M:216:ARG:C	2.86	0.45
10:N:112:LEU:HD21	10:N:143:LEU:HD23	1.99	0.45
10:N:333:ILE:HB	10:N:409:LEU:HD23	1.99	0.45
13:Q:34:LEU:HA	13:Q:39:TYR:HE1	1.81	0.45
16:X:57:DT:H2"	16:X:58:DT:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:LEU:HD23	1:B:950:ASP:HB3	1.98	0.45
1:B:905:ARG:HA	1:B:905:ARG:HE	1.80	0.45
3:E:685:GLU:OE2	3:E:688:ARG:NH2	2.43	0.45
7:A:489:ASP:C	7:A:491:HIS:N	2.68	0.45
8:L:7:ILE:HD13	10:N:135:LEU:HA	1.99	0.45
8:L:34:LYS:HG2	8:L:56:TYR:CZ	2.52	0.45
9:M:335:LYS:HB3	9:M:335:LYS:HE2	1.73	0.45
10:N:158:ASN:HA	10:N:174:ILE:O	2.17	0.45
10:N:197:SER:OG	10:N:301:GLY:O	2.28	0.45
11:S:40:ARG:HB3	15:W:84:DC:H4'	1.98	0.45
1:B:1030:LEU:HD21	1:B:1036:GLN:HE22	1.82	0.44
1:B:1040:VAL:HG21	1:B:1139:VAL:HG23	2.00	0.44
7:A:811:GLU:HG3	7:A:812:MET:HG3	1.98	0.44
7:A:1134:ASP:N	7:A:1134:ASP:OD1	2.51	0.44
10:N:31:THR:O	10:N:419:TRP:NE1	2.50	0.44
10:N:87:PHE:HE1	10:N:109:ILE:HD12	1.81	0.44
10:N:205:TRP:HZ3	10:N:213:LEU:HB2	1.82	0.44
10:N:365:GLU:OE1	10:N:400:TYR:OH	2.35	0.44
12:P:57:VAL:HA	12:P:60:VAL:HB	2.00	0.44
13:Q:47:ALA:HB1	14:R:91:ILE:HD11	1.99	0.44
13:Q:81:ARG:NH2	11:S:56:LYS:O	2.51	0.44
11:S:84:PHE:N	16:X:50:DT:O3'	2.50	0.44
14:V:113:LYS:HE3	14:V:113:LYS:HB3	1.76	0.44
2:C:545:ARG:NH1	2:C:560:GLN:OE1	2.45	0.44
4:H:158:MET:HG3	4:H:283:ILE:HB	1.99	0.44
15:W:49:DA:C2	16:X:100:DA:H2	2.33	0.44
15:W:98:DA:N1	16:X:50:DT:C4	2.85	0.44
9:M:314:PHE:HZ	9:M:408:ILE:HG12	1.83	0.44
10:N:169:THR:OG1	10:N:190:GLY:N	2.36	0.44
12:T:31:LYS:HA	12:T:34:ILE:HD12	2.00	0.44
15:W:34:DG:N2	16:X:115:DC:O2	2.51	0.44
15:W:75:DT:H6	15:W:75:DT:H2'	1.64	0.44
1:B:916:ASP:CB	7:A:562:ASN:ND2	2.81	0.44
2:C:739:MET:SD	3:E:370:ASN:ND2	2.91	0.44
4:H:136:GLN:HG2	4:H:154:ALA:HA	1.99	0.44
7:A:1196:ARG:HH21	7:A:1199:ARG:HH22	1.64	0.44
7:A:1219:GLU:O	7:A:1223:GLU:N	2.45	0.44
10:N:450:THR:H	10:N:453:LYS:HB2	1.83	0.44
15:W:46:DT:H2'	15:W:46:DT:OP2	2.17	0.44
15:W:78:DC:H4'	15:W:79:DC:H5'	2.00	0.44
1:B:707:LEU:HD12	2:C:428:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:467:ASP:OD2	2:C:662:ARG:CZ	2.65	0.44
3:D:600:PHE:HZ	4:H:519:ILE:HG23	1.82	0.44
3:D:610:THR:OG1	7:A:487:GLY:CA	2.53	0.44
10:N:102:PHE:HA	10:N:106:LEU:HB2	2.00	0.44
14:R:30:ARG:HH12	15:W:27:DT:H1'	1.82	0.44
1:B:927:ASN:OD1	7:A:569:SER:CB	2.58	0.44
1:B:930:PHE:CE2	7:A:570:LYS:HB3	2.53	0.44
1:B:1138:PRO:CB	7:A:574:ILE:HG22	2.47	0.44
2:C:655:ILE:HD12	2:C:655:ILE:O	2.18	0.44
3:D:576:TYR:CB	7:A:497:TYR:OH	2.66	0.44
9:M:137:GLN:HE21	9:M:452:GLY:HA3	1.82	0.44
10:N:131:VAL:HG11	10:N:140:LEU:HD22	1.99	0.44
10:N:214:LYS:HE2	10:N:214:LYS:HB3	1.61	0.44
12:P:68:ASP:HB3	12:P:92:ARG:HH22	1.82	0.44
14:V:104:ALA:O	14:V:108:VAL:N	2.43	0.44
15:W:109:DC:C2	16:X:39:DG:N2	2.80	0.44
1:B:1251:LYS:HD3	1:B:1251:LYS:HA	1.74	0.44
3:D:423:PHE:CE1	7:A:552:PHE:CZ	3.06	0.44
3:D:537:LYS:CA	7:A:534:TYR:CD2	3.00	0.44
3:D:570:ILE:HB	7:A:539:LEU:CD1	2.48	0.44
7:A:637:HIS:CE1	10:N:434:ILE:HG21	2.53	0.44
7:A:803:ILE:O	7:A:807:THR:OG1	2.29	0.44
7:A:826:SER:HB3	7:A:1169:GLY:HA2	1.99	0.44
10:N:15:ARG:HE	10:N:15:ARG:HB2	1.43	0.44
10:N:45:THR:HG23	10:N:51:TYR:HE1	1.82	0.44
10:N:128:THR:HG22	10:N:454:TYR:HE1	1.82	0.44
10:N:275:LYS:HZ1	10:N:277:SER:HB3	1.83	0.44
14:R:112:THR:O	14:R:115:VAL:HB	2.18	0.44
15:W:117:DT:H6	15:W:117:DT:H2'	1.54	0.44
1:B:936:ARG:CB	1:B:940:ARG:HH21	2.29	0.44
4:H:377:SER:O	4:H:403:LEU:N	2.47	0.44
7:A:626:ARG:NE	10:N:176:ASP:O	2.51	0.44
7:A:1108:ILE:HG23	7:A:1179:ILE:HB	1.99	0.44
10:N:172:ILE:HA	10:N:184:VAL:HG22	2.00	0.44
13:Q:95:LYS:HD2	13:Q:95:LYS:HA	1.67	0.44
16:X:119:DT:H2"	16:X:120:DG:N7	2.33	0.44
2:C:673:ARG:HD3	14:V:106:HIS:HB3	1.99	0.44
9:M:331:PRO:O	9:M:335:LYS:HB3	2.18	0.44
10:N:306:ILE:HD13	10:N:348:ALA:HB3	2.00	0.44
1:B:907:ALA:CB	7:A:554:TRP:CZ3	2.93	0.43
1:B:1023:LEU:HD11	1:B:1200:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1049:LEU:HB2	1:B:1053:ASN:HD22	1.83	0.43
3:D:312:LYS:HE3	3:D:312:LYS:HB3	1.83	0.43
3:D:606:PRO:CA	7:A:488:ILE:HD12	2.38	0.43
4:H:452:PHE:O	4:H:455:THR:OG1	2.34	0.43
3:E:514:LEU:O	3:E:518:LYS:HB2	2.18	0.43
10:N:462:LEU:O	10:N:466:GLN:NE2	2.43	0.43
13:U:76:THR:O	14:V:50:GLY:N	2.51	0.43
14:V:102:GLU:OE1	14:V:105:LYS:NZ	2.42	0.43
5:I:40:SER:OG	5:I:41:LEU:N	2.52	0.43
3:E:335:ILE:HG22	3:E:337:SER:H	1.83	0.43
3:E:417:ASP:N	3:E:417:ASP:OD1	2.49	0.43
7:A:816:ARG:NH1	7:A:841:THR:CB	2.81	0.43
7:A:1145:LEU:HD13	7:A:1148:LEU:HD12	1.99	0.43
10:N:419:TRP:CD1	10:N:430:LEU:HD13	2.53	0.43
13:Q:83:LEU:HD13	14:R:58:ILE:HG21	1.98	0.43
13:Q:111:ILE:HG21	11:S:48:LEU:HB3	2.00	0.43
11:S:43:PRO:HD3	16:X:67:DG:H21	1.83	0.43
13:U:66:ALA:HB1	13:U:78:ILE:HG21	1.99	0.43
15:W:54:DC:O2	16:X:95:DG:N2	2.51	0.43
2:C:558:ILE:HD12	2:C:653:LEU:HD13	1.97	0.43
2:C:583:LEU:HB3	2:C:585:LEU:HD13	2.01	0.43
2:C:655:ILE:HD12	2:C:655:ILE:C	2.39	0.43
3:E:778:GLU:H	3:E:778:GLU:HG3	1.61	0.43
7:A:810:TYR:CD2	7:A:816:ARG:N	2.86	0.43
8:L:64:LEU:HD23	9:M:4:ASN:HD22	1.83	0.43
11:S:83:ARG:O	12:T:80:THR:OG1	2.29	0.43
13:U:37:GLY:HA3	13:U:39:TYR:CZ	2.53	0.43
2:C:653:LEU:H	2:C:653:LEU:HG	1.50	0.43
3:E:314:PHE:HE1	3:E:347:ARG:HD2	1.84	0.43
7:A:799:THR:HB	7:A:838:TRP:HZ3	1.84	0.43
10:N:327:LYS:HA	10:N:330:TRP:HB2	2.01	0.43
13:Q:91:GLU:O	13:Q:95:LYS:HB2	2.18	0.43
13:U:52:ALA:HA	13:U:55:LEU:HD12	2.01	0.43
13:U:77:ARG:CZ	16:X:20:DC:H4'	2.49	0.43
14:V:95:VAL:HG13	14:V:99:LEU:HD12	2.00	0.43
1:B:1274:ASN:HD21	4:H:95:HIS:HD2	1.65	0.43
2:C:564:ASP:N	3:D:374:ASP:OD1	2.52	0.43
3:D:539:ILE:CG2	7:A:538:LEU:HG	2.18	0.43
6:J:546:LYS:NZ	6:J:547:ARG:O	2.49	0.43
7:A:613:ILE:O	7:A:617:ASN:N	2.50	0.43
7:A:792:ASP:HA	7:A:993:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:189:LEU:HD22	9:M:309:PHE:HB3	1.99	0.43
10:N:344:GLY:HA2	10:N:347:GLU:HB3	2.01	0.43
10:N:363:GLU:O	10:N:367:SER:CB	2.66	0.43
11:O:119:ILE:HD11	12:P:50:ILE:HG21	2.00	0.43
2:C:743:VAL:HG21	6:J:290:ILE:HD11	2.00	0.43
3:D:709:GLU:OE1	3:D:712:ARG:NH1	2.51	0.43
7:A:810:TYR:N	7:A:810:TYR:CD1	2.86	0.43
7:A:871:THR:OG1	7:A:872:THR:N	2.50	0.43
10:N:131:VAL:HA	10:N:135:LEU:HB2	2.00	0.43
13:Q:17:ARG:HA	13:Q:20:ARG:HD2	2.00	0.43
11:S:128:ARG:NE	11:S:133:GLU:OE1	2.52	0.43
16:X:144:DC:H2"	16:X:145:DC:C6	2.54	0.43
7:A:1302:GLU:HA	7:A:1306:LYS:HB3	2.00	0.43
8:L:26:ARG:HH21	8:L:64:LEU:HD13	1.84	0.43
12:P:85:ASP:HA	12:P:88:TYR:HB2	2.00	0.43
11:S:64:LYS:NZ	11:S:93:GLN:HE22	2.17	0.43
13:U:53:ALA:HB2	14:V:114:ALA:HB3	2.01	0.43
14:V:37:TYR:HA	14:V:40:LYS:HD2	2.00	0.43
16:X:58:DT:H4'	16:X:59:DA:H5'	2.00	0.43
3:D:423:PHE:HD1	7:A:552:PHE:CD1	2.37	0.43
3:D:537:LYS:HB2	7:A:531:TYR:HE1	1.83	0.43
7:A:531:TYR:HA	7:A:534:TYR:HB2	2.00	0.43
7:A:1094:ARG:O	7:A:1098:LYS:NZ	2.49	0.43
9:M:119:ILE:HA	9:M:122:ARG:HB2	2.00	0.43
9:M:397:SER:HA	9:M:433:LYS:HG2	1.99	0.43
12:T:38:ALA:O	12:T:43:VAL:N	2.51	0.43
16:X:110:DA:OP2	16:X:110:DA:H2'	2.19	0.43
5:I:126:VAL:O	3:E:667:ARG:NH1	2.51	0.43
7:A:816:ARG:HH12	7:A:841:THR:HB	1.83	0.43
7:A:1007:VAL:HG11	7:A:1206:VAL:HB	2.01	0.43
9:M:3:LEU:HD22	9:M:449:TRP:HD1	1.82	0.43
9:M:160:GLY:HA2	9:M:397:SER:H	1.83	0.43
15:W:27:DT:H2"	15:W:28:DC:C2	2.54	0.43
5:I:144:TYR:OH	3:E:695:ASP:OD2	2.36	0.43
7:A:972:SER:O	7:A:977:LEU:N	2.46	0.43
11:S:116:ARG:NH1	11:S:120:MET:SD	2.92	0.43
12:T:26:ILE:HD12	12:T:26:ILE:HA	1.82	0.43
15:W:34:DG:H2'	15:W:35:DT:C6	2.54	0.43
16:X:78:DG:H4'	16:X:79:DT:H5'	2.01	0.43
1:B:727:ASN:CG	7:A:560:LEU:HG	2.40	0.42
3:D:540:GLN:CB	7:A:538:LEU:HD21	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:84:ARG:O	7:A:575:ASN:ND2	2.52	0.42
3:E:596:PRO:CG	7:A:489:ASP:OD2	2.66	0.42
7:A:568:LEU:H	7:A:568:LEU:HG	1.59	0.42
11:O:128:ARG:O	11:O:133:GLU:N	2.52	0.42
12:T:64:ASN:OD1	12:T:67:ARG:NH2	2.52	0.42
15:W:84:DC:H6	15:W:84:DC:H2'	1.71	0.42
1:B:1051:LYS:N	1:B:1051:LYS:CE	2.73	0.42
7:A:816:ARG:HD3	7:A:842:LEU:HD23	1.96	0.42
9:M:84:GLU:O	9:M:87:TRP:N	2.52	0.42
10:N:94:ARG:HB2	10:N:106:LEU:HD11	2.01	0.42
10:N:282:ASN:O	10:N:293:LYS:HA	2.20	0.42
10:N:337:GLY:O	10:N:340:THR:OG1	2.30	0.42
16:X:37:DG:H1'	16:X:38:DG:C4	2.54	0.42
16:X:87:DT:H6	16:X:87:DT:H2'	1.73	0.42
6:J:325:SER:HB3	6:J:328:SER:HB2	2.01	0.42
7:A:927:LEU:HB2	7:A:937:LEU:HD11	2.01	0.42
7:A:1237:GLN:HA	7:A:1240:LYS:HE3	2.01	0.42
9:M:3:LEU:HD21	9:M:448:SER:HA	2.01	0.42
9:M:288:LYS:HE2	9:M:288:LYS:HB3	1.75	0.42
9:M:462:THR:HG22	9:M:465:ARG:HH22	1.84	0.42
10:N:17:GLN:O	10:N:39:THR:N	2.38	0.42
10:N:40:GLN:HB2	10:N:64:LEU:HD11	2.02	0.42
10:N:163:ASP:O	10:N:169:THR:HA	2.19	0.42
10:N:361:GLU:HB2	10:N:397:THR:HG23	2.01	0.42
11:O:83:ARG:HD2	16:X:101:DG:H5'	2.01	0.42
13:Q:88:ARG:HA	13:Q:88:ARG:HD3	1.77	0.42
11:S:49:ARG:HA	11:S:52:ARG:HD2	2.00	0.42
14:V:77:LEU:O	14:V:81:ASN:ND2	2.52	0.42
16:X:17:DT:H2"	16:X:18:DG:C5	2.54	0.42
16:X:130:DG:H1'	16:X:131:DG:C6	2.55	0.42
1:B:983:SER:HA	1:B:986:LEU:HB2	2.02	0.42
4:H:82:GLU:OE2	3:E:697:LYS:NZ	2.40	0.42
4:H:267:LYS:HE3	4:H:267:LYS:HB3	1.90	0.42
8:L:61:LYS:HE2	8:L:61:LYS:HB3	1.90	0.42
8:L:85:LYS:HE2	8:L:85:LYS:HB2	1.77	0.42
10:N:157:GLN:HG3	10:N:176:ASP:HA	2.00	0.42
10:N:437:LYS:O	10:N:441:THR:OG1	2.28	0.42
11:O:43:PRO:HG3	15:W:67:DG:H21	1.85	0.42
11:O:53:ARG:O	11:O:57:SER:N	2.49	0.42
13:U:81:ARG:HA	13:U:105:GLY:HA2	2.01	0.42
13:U:91:GLU:O	13:U:95:LYS:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:HIS:HE1	3:D:328:PRO:HD2	1.83	0.42
3:D:606:PRO:HA	7:A:488:ILE:CG1	2.47	0.42
7:A:1013:CYS:O	7:A:1214:THR:N	2.44	0.42
9:M:302:ASP:OD1	9:M:305:GLU:N	2.50	0.42
9:M:406:GLN:HE21	9:M:406:GLN:HB2	1.69	0.42
11:O:46:VAL:HA	11:O:49:ARG:HH21	1.84	0.42
13:U:51:LEU:HD21	14:V:67:PHE:HD1	1.83	0.42
3:D:731:GLN:HE21	3:D:731:GLN:HB3	1.60	0.42
3:E:446:THR:OG1	3:E:447:SER:N	2.52	0.42
7:A:895:GLU:HB3	7:A:897:HIS:CE1	2.55	0.42
10:N:306:ILE:HG23	10:N:349:LEU:HA	2.00	0.42
11:O:43:PRO:HB2	12:P:45:ARG:HH21	1.84	0.42
14:R:37:TYR:OH	16:X:123:DC:OP1	2.38	0.42
14:R:85:THR:N	15:W:40:DG:OP1	2.51	0.42
13:U:40:ALA:HB2	14:V:86:ILE:HG13	2.01	0.42
14:V:41:VAL:HA	14:V:44:GLN:HB2	2.01	0.42
1:B:901:LYS:HB3	1:B:904:THR:CG2	2.50	0.42
2:C:652:LEU:CB	6:J:312:LEU:CB	2.87	0.42
3:D:363:SER:OG	3:D:366:THR:OG1	2.31	0.42
7:A:845:ILE:O	7:A:870:LEU:N	2.51	0.42
7:A:1265:ARG:HD3	7:A:1268:ARG:HD2	2.01	0.42
9:M:409:ILE:O	9:M:413:SER:OG	2.31	0.42
10:N:439:ILE:HG21	10:N:447:PHE:HB2	2.01	0.42
12:P:98:TYR:N	13:U:101:THR:O	2.43	0.42
13:Q:69:ALA:O	13:Q:73:ASN:ND2	2.37	0.42
15:W:47:DC:H1'	15:W:48:DT:C2	2.55	0.42
15:W:90:DA:H2	16:X:59:DA:C2	2.38	0.42
15:W:116:DC:H6	15:W:116:DC:H2'	1.72	0.42
3:D:574:PHE:HZ	7:A:508:THR:HB	1.85	0.42
5:I:138:SER:OG	5:I:139:GLU:N	2.52	0.42
3:E:618:VAL:HG11	3:E:663:SER:HB2	2.01	0.42
3:E:701:LEU:HD23	3:E:704:LEU:HD12	2.02	0.42
7:A:633:LEU:HD21	10:N:438:GLN:HB2	2.00	0.42
7:A:679:ILE:HG23	7:A:747:VAL:HG11	2.02	0.42
7:A:816:ARG:HH12	7:A:841:THR:CB	2.32	0.42
7:A:1164:ARG:HD2	15:W:54:DC:H4'	2.00	0.42
11:O:68:GLN:HG3	11:O:89:VAL:HG21	2.01	0.42
11:S:53:ARG:HH21	11:S:57:SER:HG	1.60	0.42
1:B:901:LYS:O	1:B:904:THR:HG23	2.20	0.42
2:C:555:ASN:OD1	2:C:654:GLN:HB2	2.19	0.42
2:C:573:GLU:OE2	2:C:598:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:520:GLU:H	7:A:520:GLU:HG3	1.43	0.42
7:A:806:LEU:O	7:A:810:TYR:CG	2.73	0.42
9:M:409:ILE:O	9:M:413:SER:CB	2.68	0.42
10:N:218:ILE:HD12	10:N:282:ASN:HB3	2.01	0.42
11:O:106:ASP:HA	11:O:109:LEU:HB2	2.02	0.42
11:S:124:ILE:HD11	12:T:50:ILE:HD12	2.02	0.42
12:T:34:ILE:HD11	12:T:55:ARG:HD2	2.01	0.42
14:V:100:PRO:HG2	14:V:103:LEU:HD12	2.00	0.42
15:W:14:DG:H1'	15:W:15:DT:H5'	2.01	0.42
16:X:28:DT:H1'	16:X:29:DG:C5	2.55	0.42
1:B:1145:THR:CG2	7:A:586:TYR:CD2	2.95	0.42
3:D:568:LEU:HD23	3:D:568:LEU:HA	1.94	0.42
3:E:311:SER:OG	3:E:388:TRP:O	2.30	0.42
9:M:135:VAL:HG22	9:M:454:TRP:HE3	1.84	0.42
10:N:166:THR:HG23	10:N:214:LYS:NZ	2.34	0.42
13:U:90:ASP:HB3	13:U:93:LEU:HB2	2.01	0.42
15:W:132:DG:H4'	15:W:133:DA:H5'	2.01	0.42
3:D:423:PHE:HA	7:A:552:PHE:CE1	2.55	0.41
6:J:302:ILE:HD12	6:J:302:ILE:HA	1.95	0.41
3:E:728:ASN:O	3:E:732:ASN:ND2	2.53	0.41
8:L:29:TRP:CE3	8:L:59:ARG:HB2	2.54	0.41
9:M:197:LEU:HD21	9:M:301:LEU:HG	2.02	0.41
1:B:1051:LYS:CD	1:B:1051:LYS:N	2.73	0.41
3:D:424:PRO:HD3	7:A:555:HIS:CG	2.54	0.41
6:J:566:TYR:CD2	7:A:541:LEU:HD11	2.55	0.41
3:E:422:LEU:HD11	7:A:554:TRP:CD1	2.54	0.41
7:A:543:LYS:HA	7:A:546:ARG:HB2	2.02	0.41
7:A:770:TYR:OH	17:A:1501:ADP:N7	2.53	0.41
7:A:1018:LEU:HD11	7:A:1085:VAL:HG23	2.00	0.41
8:L:22:LYS:HG3	10:N:451:ARG:CZ	2.50	0.41
10:N:328:ALA:O	10:N:332:ASN:ND2	2.40	0.41
13:Q:28:GLY:HA3	15:W:31:DT:P	2.60	0.41
11:S:83:ARG:HH22	15:W:99:DG:N2	2.18	0.41
13:U:46:GLY:HA2	13:U:49:VAL:HG23	2.01	0.41
15:W:156:DG:H2"	15:W:157:DA:C8	2.55	0.41
2:C:525:GLN:HE22	2:C:528:PRO:HG3	1.85	0.41
11:O:109:LEU:O	11:O:113:HIS:CB	2.68	0.41
11:O:111:ALA:O	11:O:116:ARG:N	2.53	0.41
12:T:49:LEU:H	12:T:49:LEU:HG	1.45	0.41
14:V:66:VAL:HG12	14:V:70:ILE:HG13	2.02	0.41
14:V:78:ALA:O	14:V:83:ARG:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X:65:DC:H1'	16:X:66:DG:C5	2.56	0.41
1:B:868:ILE:HD11	1:B:954:LEU:HD13	2.01	0.41
3:D:306:VAL:N	3:D:394:GLN:OE1	2.53	0.41
4:H:382:ASP:H	4:H:385:LEU:HB2	1.85	0.41
3:E:445:ASN:OD1	7:A:504:ASN:ND2	2.53	0.41
3:E:465:ASP:O	3:E:469:HIS:ND1	2.54	0.41
9:M:7:CYS:N	9:M:22:SER:OG	2.52	0.41
9:M:36:ILE:O	9:M:48:ILE:HB	2.20	0.41
13:Q:25:PHE:HZ	13:Q:59:THR:HG21	1.84	0.41
14:R:106:HIS:O	14:R:109:SER:OG	2.27	0.41
12:T:46:ILE:N	15:W:82:DC:OP1	2.52	0.41
16:X:65:DC:H1'	16:X:66:DG:N7	2.36	0.41
8:L:60:TYR:OH	9:M:4:ASN:O	2.30	0.41
10:N:73:ILE:HG13	10:N:119:TRP:CE2	2.55	0.41
10:N:351:GLY:HA2	10:N:354:LEU:HD12	2.03	0.41
13:Q:80:PRO:HA	13:Q:83:LEU:HD12	2.01	0.41
14:V:63:VAL:O	14:V:67:PHE:HB3	2.20	0.41
14:V:64:ASN:HA	14:V:67:PHE:HB3	2.03	0.41
7:A:999:VAL:HG23	7:A:1000:GLU:HG3	2.03	0.41
9:M:70:LEU:HD23	9:M:79:ASN:HB3	2.03	0.41
9:M:141:GLU:HG3	9:M:436:GLY:HA3	2.03	0.41
9:M:158:ASP:OD2	9:M:165:ASN:ND2	2.54	0.41
14:R:105:LYS:O	14:R:108:VAL:HB	2.21	0.41
15:W:3:DG:H2"	15:W:4:DG:C8	2.55	0.41
15:W:77:DT:H2"	15:W:78:DC:C6	2.55	0.41
2:C:564:ASP:OD1	2:C:566:SER:OG	2.38	0.41
7:A:516:LEU:HA	7:A:526:ARG:HA	2.03	0.41
7:A:532:ASP:O	7:A:536:LEU:N	2.49	0.41
7:A:754:ASP:HA	7:A:776:GLN:HG2	2.01	0.41
7:A:992:LEU:HD21	7:A:994:ARG:HH12	1.85	0.41
9:M:400:LEU:HD23	9:M:400:LEU:HA	1.78	0.41
11:O:133:GLU:H	11:O:133:GLU:HG3	1.56	0.41
14:R:64:ASN:N	12:T:102:GLY:O	2.54	0.41
13:U:44:GLY:HA3	14:V:87:THR:HG22	2.02	0.41
15:W:155:DC:H2"	15:W:156:DG:C8	2.56	0.41
16:X:-7:DG:H2"	16:X:-6:DA:C8	2.55	0.41
16:X:127:DC:H2'	16:X:128:DT:C6	2.56	0.41
4:H:61:ILE:HG21	4:H:72:LEU:HG	2.03	0.41
3:E:536:LEU:HD21	3:E:631:ILE:HG22	2.02	0.41
7:A:619:ARG:HH12	9:M:438:LEU:HB3	1.86	0.41
7:A:775:LEU:O	7:A:779:VAL:N	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:67:VAL:O	9:M:217:SER:HB2	2.20	0.41
9:M:164:CYS:HB3	9:M:329:LEU:HD13	2.03	0.41
14:R:52:SER:O	14:R:56:MET:N	2.41	0.41
11:S:83:ARG:HG2	16:X:50:DT:H4'	2.03	0.41
15:W:75:DT:H2"	15:W:76:DG:C8	2.56	0.41
1:B:867:PRO:HD3	1:B:946:ARG:NH2	2.36	0.41
1:B:1138:PRO:HA	7:A:579:ALA:HB2	2.03	0.41
4:H:89:ILE:HG22	4:H:93:ASN:HD21	1.85	0.41
3:E:640:GLN:HA	3:E:643:GLU:HG2	2.03	0.41
7:A:816:ARG:NH1	7:A:841:THR:HB	2.35	0.41
7:A:1010:VAL:HG12	7:A:1210:ARG:HD2	2.02	0.41
7:A:1191:LEU:HA	7:A:1194:GLN:HB2	2.03	0.41
8:L:23:GLU:N	10:N:455:ASN:OD1	2.54	0.41
9:M:19:ALA:O	9:M:28:GLN:N	2.54	0.41
9:M:128:PHE:O	9:M:457:LYS:NZ	2.54	0.41
10:N:94:ARG:HA	10:N:94:ARG:HD3	1.91	0.41
10:N:116[A]:HIS:HB3	10:N:119:TRP:CD1	2.56	0.41
10:N:330:TRP:CZ3	10:N:353:LEU:HD22	2.56	0.41
11:O:63:ARG:HB2	11:O:66:PRO:HD2	2.02	0.41
11:O:83:ARG:HB3	15:W:50:DG:H4'	2.02	0.41
12:P:91:LYS:HE3	12:P:91:LYS:HB3	1.65	0.41
13:Q:34:LEU:HD22	13:Q:39:TYR:HE1	1.86	0.41
13:Q:41:GLU:HB3	14:R:84:SER:HB2	2.03	0.41
14:R:58:ILE:HA	12:T:98:TYR:HB3	2.02	0.41
11:S:48:LEU:O	11:S:52:ARG:N	2.50	0.41
11:S:84:PHE:H	16:X:51:DT:P	2.44	0.41
12:T:35:ARG:NH1	15:W:82:DC:OP2	2.54	0.41
13:U:88:ARG:HA	13:U:88:ARG:HD3	1.88	0.41
15:W:55:DG:H5'	15:W:55:DG:C8	2.56	0.41
1:B:901:LYS:HB3	1:B:904:THR:HG21	2.02	0.41
2:C:652:LEU:HD23	2:C:652:LEU:HA	1.74	0.41
2:C:675:ARG:H	2:C:675:ARG:HG2	1.68	0.41
3:D:602:LYS:HA	7:A:488:ILE:CG1	2.51	0.41
7:A:1050:ASN:ND2	7:A:1054:GLN:OE1	2.54	0.41
8:L:5:THR:O	8:L:9:LYS:HB2	2.20	0.41
8:L:81:ILE:HG23	10:N:88:VAL:HG12	2.03	0.41
9:M:70:LEU:HD13	9:M:83:LEU:HD12	2.02	0.41
9:M:121:GLU:HA	9:M:124:TYR:HB2	2.03	0.41
9:M:160:GLY:O	9:M:398:THR:OG1	2.31	0.41
9:M:292:PHE:HB2	9:M:299:LEU:HD11	2.02	0.41
10:N:13:TYR:O	10:N:19:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:98:ASN:HD22	10:N:101:ALA:HB2	1.85	0.41
10:N:192:GLN:NE2	10:N:195:ASN:OD1	2.53	0.41
10:N:331:GLU:HA	10:N:408:LYS:H	1.85	0.41
13:Q:34:LEU:HG	13:Q:48:PRO:HG3	2.03	0.41
14:R:30:ARG:CZ	16:X:122:DG:H21	2.34	0.41
11:S:66:PRO:HB3	12:T:25:ASN:HB3	2.02	0.41
14:V:36:ILE:HA	14:V:39:TYR:HB2	2.03	0.41
16:X:14:DA:H2"	16:X:15:DT:H5'	2.04	0.41
7:A:1175:ALA:HB3	7:A:1197:ALA:HA	2.03	0.40
9:M:335:LYS:HE3	9:M:339:LYS:HZ2	1.86	0.40
12:P:66:ILE:H	12:P:66:ILE:HG13	1.70	0.40
13:Q:31:HIS:CD2	13:Q:35:ARG:HE	2.39	0.40
14:R:48:ASP:N	14:R:48:ASP:OD1	2.54	0.40
11:S:63:ARG:HB3	11:S:66:PRO:HD2	2.03	0.40
11:S:104:PHE:CD2	12:T:41:GLY:HA3	2.54	0.40
11:S:128:ARG:O	11:S:133:GLU:N	2.54	0.40
15:W:6:DG:H2"	15:W:7:DA:C8	2.56	0.40
15:W:109:DC:O2	16:X:39:DG:C2	2.74	0.40
16:X:112:DG:H1'	16:X:113:DA:C8	2.56	0.40
2:C:544:ILE:HD12	2:C:544:ILE:HA	1.78	0.40
3:D:540:GLN:NE2	7:A:537:GLN:HG2	2.21	0.40
7:A:935:TRP:HE1	7:A:952:PHE:HD2	1.68	0.40
9:M:55:ILE:HG21	10:N:315:LEU:HD22	2.03	0.40
10:N:79:PHE:HZ	10:N:113:LEU:HD11	1.86	0.40
11:O:127:ALA:O	11:O:131:ARG:HB2	2.20	0.40
14:R:59:MET:O	14:R:63:VAL:HG23	2.22	0.40
11:S:48:LEU:H	11:S:48:LEU:HG	1.61	0.40
13:U:17:ARG:HA	13:U:20:ARG:HD2	2.02	0.40
13:U:116:LEU:HA	13:U:117:PRO:HD3	1.97	0.40
15:W:26:DC:H1'	15:W:27:DT:C2	2.56	0.40
15:W:36:DC:H6	15:W:36:DC:H2'	1.63	0.40
15:W:39:DA:H2	16:X:110:DA:H2	1.68	0.40
15:W:87:DT:H3	16:X:62:DA:H2	1.69	0.40
16:X:27:DC:H2"	16:X:28:DT:C5	2.57	0.40
1:B:759:LEU:HD23	1:B:759:LEU:HA	1.91	0.40
1:B:936:ARG:C	1:B:940:ARG:HH21	2.23	0.40
2:C:663:LEU:HD13	2:C:663:LEU:HA	1.91	0.40
3:D:669:HIS:CD2	3:D:670:ILE:HG13	2.56	0.40
3:D:777:PRO:HG2	4:H:321:LYS:HB3	2.04	0.40
7:A:893:ILE:HG23	7:A:921:ILE:HG12	2.04	0.40
7:A:1019:GLN:NE2	7:A:1058:ILE:O	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:334:ILE:HG12	10:N:410:ALA:HB3	2.03	0.40
11:O:71:VAL:HG21	11:O:89:VAL:HG13	2.03	0.40
11:O:72:ARG:HH12	15:W:51:DC:P	2.44	0.40
11:O:116:ARG:NH2	11:O:123:ASP:OD1	2.53	0.40
14:R:46:HIS:ND1	14:R:48:ASP:OD1	2.54	0.40
14:R:105:LYS:HA	14:R:108:VAL:HB	2.03	0.40
15:W:121:DG:N2	16:X:27:DC:C2	2.69	0.40
16:X:-16:DG:H1'	16:X:-15:DT:H5'	2.03	0.40
2:C:541:ASP:OD1	2:C:541:ASP:N	2.54	0.40
3:D:570:ILE:HG21	7:A:539:LEU:CG	2.49	0.40
4:H:311:SER:HB3	4:H:414:HIS:HB3	2.02	0.40
9:M:10:ILE:HB	9:M:106:ILE:HG22	2.03	0.40
9:M:193:VAL:HB	9:M:228:ILE:HG23	2.04	0.40
9:M:427[B]:GLN:HE21	9:M:427[B]:GLN:HB3	1.60	0.40
11:O:124:ILE:HD11	12:P:50:ILE:HD12	2.04	0.40
13:Q:59:THR:HA	13:Q:62:ILE:HG22	2.03	0.40
13:Q:111:ILE:HD13	13:Q:116:LEU:HD21	2.02	0.40
15:W:109:DC:C2	16:X:39:DG:N1	2.89	0.40
16:X:118:DT:H2"	16:X:119:DT:C6	2.56	0.40
1:B:679:ILE:HA	1:B:682:ILE:HB	2.04	0.40
1:B:966:ARG:HH12	7:A:565:PRO:HB2	1.85	0.40
4:H:172:ASP:HB3	4:H:175:ARG:HD3	2.03	0.40
9:M:289:ASN:HB3	9:M:298:THR:HG23	2.03	0.40
9:M:409:ILE:HA	9:M:421:LEU:HD12	2.03	0.40
14:V:83:ARG:HD3	14:V:83:ARG:HA	1.97	0.40
15:W:100:DG:C2	16:X:48:DC:O2	2.70	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	B	489/1093 (45%)	460 (94%)	25 (5%)	4 (1%)	19 60
2	C	347/918 (38%)	309 (89%)	36 (10%)	2 (1%)	25 66
3	D	385/836 (46%)	372 (97%)	13 (3%)	0	100 100
3	E	414/836 (50%)	389 (94%)	24 (6%)	1 (0%)	47 81
4	H	376/566 (66%)	345 (92%)	30 (8%)	1 (0%)	41 77
5	I	102/332 (31%)	93 (91%)	8 (8%)	1 (1%)	15 54
6	J	159/634 (25%)	147 (92%)	11 (7%)	1 (1%)	25 66
7	A	734/982 (75%)	682 (93%)	46 (6%)	6 (1%)	19 60
8	L	45/157 (29%)	42 (93%)	3 (7%)	0	100 100
9	M	360/477 (76%)	344 (96%)	15 (4%)	1 (0%)	41 77
10	N	381/467 (82%)	358 (94%)	22 (6%)	1 (0%)	41 77
11	O	96/135 (71%)	90 (94%)	6 (6%)	0	100 100
11	S	93/135 (69%)	84 (90%)	9 (10%)	0	100 100
12	P	85/102 (83%)	81 (95%)	4 (5%)	0	100 100
12	T	84/102 (82%)	79 (94%)	5 (6%)	0	100 100
13	Q	105/129 (81%)	102 (97%)	3 (3%)	0	100 100
13	U	105/129 (81%)	101 (96%)	4 (4%)	0	100 100
14	R	91/122 (75%)	86 (94%)	5 (6%)	0	100 100
14	V	91/122 (75%)	90 (99%)	1 (1%)	0	100 100
All	All	4542/8274 (55%)	4254 (94%)	270 (6%)	18 (0%)	38 72

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	868	ILE
1	B	1051	LYS
2	C	655	ILE
2	C	664	ASP
7	A	490	THR
7	A	563	THR
10	N	48	ASP
7	A	489	ASP
7	A	567	PHE
9	M	217	SER
4	H	62	PRO
7	A	816	ARG

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Mol	Chain	Res	Type
7	A	818	PRO
1	B	1052	PRO
6	J	504	PRO
5	I	39	PRO
3	E	401	PRO
1	B	867	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	484/1017 (48%)	445 (92%)	39 (8%)	11 35
2	C	321/832 (39%)	291 (91%)	30 (9%)	9 28
3	D	368/758 (48%)	342 (93%)	26 (7%)	14 39
3	E	393/758 (52%)	363 (92%)	30 (8%)	13 37
4	H	360/517 (70%)	328 (91%)	32 (9%)	9 30
5	I	102/288 (35%)	93 (91%)	9 (9%)	10 31
6	J	150/565 (26%)	144 (96%)	6 (4%)	31 55
7	A	678/889 (76%)	639 (94%)	39 (6%)	20 45
8	L	52/140 (37%)	50 (96%)	2 (4%)	33 57
9	M	345/420 (82%)	317 (92%)	28 (8%)	11 35
10	N	359/423 (85%)	333 (93%)	26 (7%)	14 39
11	O	84/110 (76%)	71 (84%)	13 (16%)	2 14
11	S	82/110 (74%)	68 (83%)	14 (17%)	2 11
12	P	72/78 (92%)	63 (88%)	9 (12%)	4 19
12	T	67/78 (86%)	53 (79%)	14 (21%)	1 6
13	Q	81/101 (80%)	73 (90%)	8 (10%)	8 26
13	U	82/101 (81%)	73 (89%)	9 (11%)	6 22
14	R	77/102 (76%)	67 (87%)	10 (13%)	4 18
14	V	79/102 (78%)	64 (81%)	15 (19%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4236/7389 (57%)	3877 (92%)	359 (8%)	14 33

All (359) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	738	LEU
1	B	747	GLU
1	B	760	LEU
1	B	768	VAL
1	B	792	HIS
1	B	800	PHE
1	B	803	VAL
1	B	869	ARG
1	B	882	THR
1	B	900	THR
1	B	926	ARG
1	B	940	ARG
1	B	941	ASN
1	B	950	ASP
1	B	955	VAL
1	B	970	ASN
1	B	975	LEU
1	B	979	LEU
1	B	986	LEU
1	B	1029	GLN
1	B	1050	GLU
1	B	1051	LYS
1	B	1084	LEU
1	B	1091	LEU
1	B	1105	LEU
1	B	1106	LEU
1	B	1107	ASN
1	B	1113	LEU
1	B	1125	GLN
1	B	1133	ILE
1	B	1134	ASP
1	B	1197	GLU
1	B	1214	ILE
1	B	1258	CYS
1	B	1259	LEU
1	B	1260	ASN
1	B	1265	ILE

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Mol	Chain	Res	Type
1	B	1292	ASP
1	B	1299	TYR
2	C	368	PHE
2	C	385	GLN
2	C	387	LEU
2	C	408	TRP
2	C	422	THR
2	C	430	VAL
2	C	431	GLU
2	C	432	VAL
2	C	468	ARG
2	C	473	LEU
2	C	477	LEU
2	C	489	GLU
2	C	496	LEU
2	C	502	GLU
2	C	505	THR
2	C	531	GLU
2	C	541	ASP
2	C	545	ARG
2	C	548	LEU
2	C	581	GLN
2	C	585	LEU
2	C	620	ILE
2	C	623	ASP
2	C	635	LEU
2	C	640	ARG
2	C	647	ILE
2	C	649	THR
2	C	652	LEU
2	C	653	LEU
2	C	745	VAL
3	D	311	SER
3	D	312	LYS
3	D	325	GLN
3	D	339	THR
3	D	371	VAL
3	D	372	SER
3	D	417	ASP
3	D	450	GLU
3	D	453	LEU
3	D	517	VAL

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Mol	Chain	Res	Type
3	D	519	ILE
3	D	525	GLU
3	D	542	PHE
3	D	563	LEU
3	D	587	ASN
3	D	624	GLN
3	D	635	GLU
3	D	694	LEU
3	D	695	ASP
3	D	719	GLN
3	D	731	GLN
3	D	735	LYS
3	D	740	LEU
3	D	764	ARG
3	D	773	MET
3	D	787	PHE
4	H	64	HIS
4	H	72	LEU
4	H	78	LEU
4	H	118	ASN
4	H	122	VAL
4	H	127	ILE
4	H	130	SER
4	H	134	GLU
4	H	159	ARG
4	H	182	ILE
4	H	266	VAL
4	H	270	TYR
4	H	283	ILE
4	H	321	LYS
4	H	329	ILE
4	H	343	THR
4	H	383	THR
4	H	384	GLN
4	H	388	LEU
4	H	389	LEU
4	H	397	SER
4	H	403	LEU
4	H	413	THR
4	H	415	LEU
4	H	418	LEU
4	H	426	THR

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Mol	Chain	Res	Type
4	H	427	VAL
4	H	429	VAL
4	H	434	THR
4	H	439	VAL
4	H	538	ASP
4	H	561	LEU
5	I	86	ARG
5	I	89	GLN
5	I	90	LEU
5	I	97	GLU
5	I	98	SER
5	I	125	THR
5	I	136	LEU
5	I	140	LYS
5	I	147	GLN
6	J	303	VAL
6	J	311	THR
6	J	312	LEU
6	J	319	ARG
6	J	454	LEU
6	J	455	LEU
3	E	312	LYS
3	E	339	THR
3	E	360	GLU
3	E	363	SER
3	E	366	THR
3	E	415	ARG
3	E	417	ASP
3	E	420	ARG
3	E	432	VAL
3	E	445	ASN
3	E	455	LYS
3	E	466	GLU
3	E	522	GLN
3	E	530	GLU
3	E	531	ASP
3	E	556	LYS
3	E	557	SER
3	E	564	ARG
3	E	589	LEU
3	E	593	LYS
3	E	602	LYS

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Mol	Chain	Res	Type
3	E	644	ILE
3	E	691	MET
3	E	703	LYS
3	E	705	GLU
3	E	715	LEU
3	E	723	LEU
3	E	746	LEU
3	E	769	HIS
3	E	778	GLU
7	A	512	CYS
7	A	516	LEU
7	A	517	LEU
7	A	519	ASP
7	A	520	GLU
7	A	527	GLU
7	A	528	ASN
7	A	530	LEU
7	A	566	ASN
7	A	568	LEU
7	A	569	SER
7	A	571	ILE
7	A	578	ASP
7	A	593	LYS
7	A	616	TYR
7	A	620	GLN
7	A	624	ASN
7	A	628	LYS
7	A	638	THR
7	A	761	ILE
7	A	820	LEU
7	A	827	THR
7	A	868	VAL
7	A	912	THR
7	A	914	TYR
7	A	927	LEU
7	A	929	ASN
7	A	1011	VAL
7	A	1089	PHE
7	A	1107	LEU
7	A	1108	ILE
7	A	1117	ASP
7	A	1133	LEU

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Mol	Chain	Res	Type
7	A	1154	SER
7	A	1170	LEU
7	A	1176	ASP
7	A	1183	THR
7	A	1217	VAL
7	A	1340	SER
8	L	59	ARG
8	L	80	ASP
9	M	3	LEU
9	M	24	VAL
9	M	49	PHE
9	M	53	ASN
9	M	63	ASN
9	M	65	ASP
9	M	69	THR
9	M	72	ASP
9	M	88	ARG
9	M	97	VAL
9	M	98	SER
9	M	106	ILE
9	M	112	ASN
9	M	114	LYS
9	M	121	GLU
9	M	122	ARG
9	M	131	LEU
9	M	195	GLU
9	M	216	ARG
9	M	238	VAL
9	M	302	ASP
9	M	305	GLU
9	M	319	ILE
9	M	393	ILE
9	M	398	THR
9	M	402	GLU
9	M	406	GLN
9	M	463	LEU
10	N	15	ARG
10	N	29	THR
10	N	31	THR
10	N	32	VAL
10	N	34	GLU
10	N	47	GLN

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Mol	Chain	Res	Type
10	N	72	GLU
10	N	90	ILE
10	N	94	ARG
10	N	106	LEU
10	N	150	THR
10	N	197	SER
10	N	201	LEU
10	N	206	ASP
10	N	210	ILE
10	N	214	LYS
10	N	219	PHE
10	N	299	PHE
10	N	302	CYS
10	N	304	ASN
10	N	339	THR
10	N	398	ILE
10	N	403	CYS
10	N	446	THR
10	N	449	ILE
10	N	451	ARG
11	O	42	ARG
11	O	48	LEU
11	O	53	ARG
11	O	58	THR
11	O	63	ARG
11	O	65	LEU
11	O	76	GLN
11	O	99	TYR
11	O	106	ASP
11	O	115	LYS
11	O	123	ASP
11	O	126	LEU
11	O	133	GLU
12	P	31	LYS
12	P	46	ILE
12	P	49	LEU
12	P	53	GLU
12	P	58	LEU
12	P	64	ASN
12	P	67	ARG
12	P	91	LYS
12	P	95	ARG

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Mol	Chain	Res	Type
13	Q	34	LEU
13	Q	57	TYR
13	Q	61	GLU
13	Q	74	LYS
13	Q	94	ASN
13	Q	101	THR
13	Q	104	GLN
13	Q	107	VAL
14	R	36	ILE
14	R	58	ILE
14	R	60	ASN
14	R	65	ASP
14	R	67	PHE
14	R	70	ILE
14	R	76	ARG
14	R	79	HIS
14	R	85	THR
14	R	112	THR
11	S	40	ARG
11	S	42	ARG
11	S	46	VAL
11	S	53	ARG
11	S	62	ILE
11	S	64	LYS
11	S	65	LEU
11	S	68	GLN
11	S	70	LEU
11	S	96	SER
11	S	99	TYR
11	S	108	ASN
11	S	123	ASP
11	S	126	LEU
12	T	46	ILE
12	T	49	LEU
12	T	53	GLU
12	T	54	THR
12	T	55	ARG
12	T	58	LEU
12	T	59	LYS
12	T	63	GLU
12	T	74	GLU
12	T	79	LYS

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Mol	Chain	Res	Type
12	T	80	THR
12	T	81	VAL
12	T	91	LYS
12	T	92	ARG
13	U	13	LYS
13	U	15	LYS
13	U	29	ARG
13	U	57	TYR
13	U	59	THR
13	U	92	GLU
13	U	99	ARG
13	U	107	VAL
13	U	114	VAL
14	V	29	THR
14	V	32	GLU
14	V	39	TYR
14	V	49	THR
14	V	54	LYS
14	V	60	ASN
14	V	65	ASP
14	V	66	VAL
14	V	67	PHE
14	V	76	ARG
14	V	81	ASN
14	V	82	LYS
14	V	88	SER
14	V	92	GLN
14	V	113	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	708	HIS
1	B	718	ASN
1	B	765	GLN
1	B	792	HIS
1	B	933	ASN
1	B	941	ASN
1	B	970	ASN
1	B	1055	ASN
1	B	1107	ASN
1	B	1120	GLN

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Mol	Chain	Res	Type
1	B	1142	GLN
1	B	1213	ASN
1	B	1294	GLN
1	B	1307	ASN
2	C	570	ASN
3	D	325	GLN
3	D	416	HIS
3	D	540	GLN
3	D	560	GLN
3	D	605	ASN
3	D	640	GLN
3	D	719	GLN
3	D	731	GLN
3	D	766	GLN
3	D	785	ASN
4	H	93	ASN
4	H	95	HIS
4	H	167	ASN
4	H	419	GLN
4	H	453	ASN
4	H	460	GLN
4	H	563	ASN
5	I	48	ASN
5	I	71	GLN
5	I	89	GLN
5	I	119	ASN
6	J	280	GLN
6	J	327	ASN
3	E	359	ASN
3	E	394	GLN
3	E	445	ASN
3	E	522	GLN
3	E	567	GLN
3	E	587	ASN
3	E	597	HIS
3	E	680	ASN
3	E	690	GLN
3	E	730	ASN
7	A	504	ASN
7	A	528	ASN
7	A	542	GLN
7	A	555	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	557	ASN
7	A	562	ASN
7	A	575	ASN
7	A	584	GLN
7	A	609	ASN
7	A	614	ASN
7	A	617	ASN
7	A	637	HIS
7	A	681	HIS
7	A	939	ASN
7	A	1050	ASN
7	A	1171	ASN
8	L	11	ASN
8	L	67	GLN
9	M	28	GLN
9	M	53	ASN
9	M	74	GLN
9	M	79	ASN
9	M	237	GLN
9	M	253	GLN
9	M	406	GLN
10	N	6	GLN
10	N	129	GLN
10	N	139	ASN
10	N	179	GLN
10	N	192	GLN
10	N	195	ASN
10	N	304	ASN
10	N	319	ASN
10	N	438	GLN
11	O	55	GLN
11	O	113	HIS
13	Q	31	HIS
13	Q	94	ASN
13	Q	112	GLN
11	S	93	GLN
11	S	108	ASN
14	V	81	ASN
14	V	92	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
18	BEF	A	1502	-	0,3,3	-	-	-		
17	ADP	A	1501	7,19	24,29,29	0.97	1 (4%)	29,45,45	1.44	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	A	1501	7,19	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1501	ADP	C5-C4	2.52	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	1501	ADP	C3'-C2'-C1'	3.36	106.03	100.98
17	A	1501	ADP	PA-O3A-PB	-3.33	121.41	132.83
17	A	1501	ADP	N3-C2-N1	-3.14	123.78	128.68
17	A	1501	ADP	C4-C5-N7	-2.61	106.68	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	1501	ADP	C5'-O5'-PA-O1A

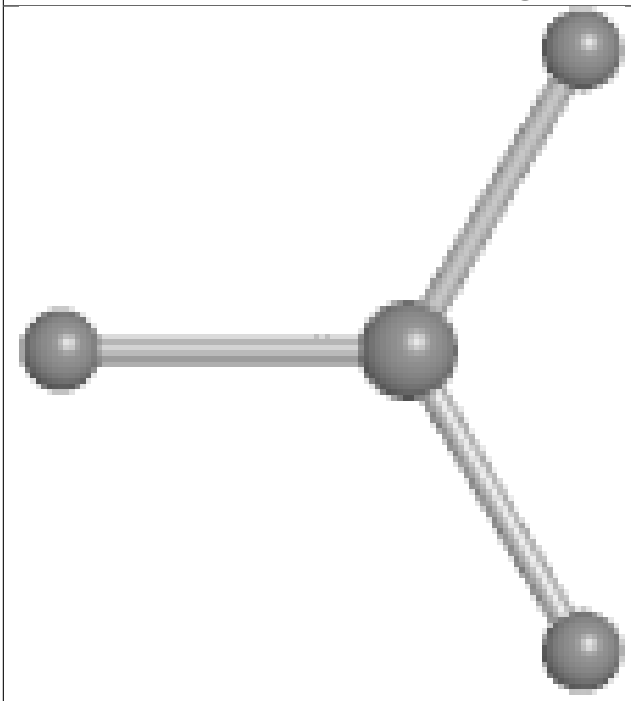
There are no ring outliers.

2 monomers are involved in 30 short contacts:

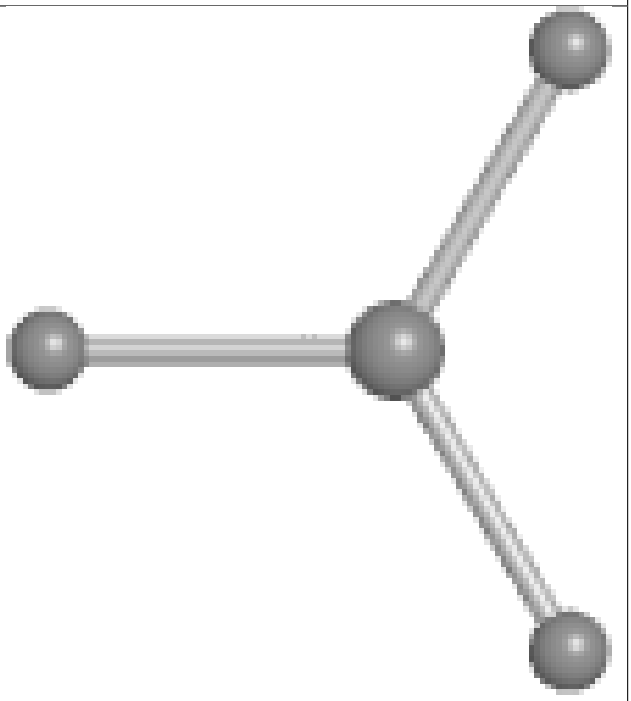
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1502	BEF	5	0
17	A	1501	ADP	27	0

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.

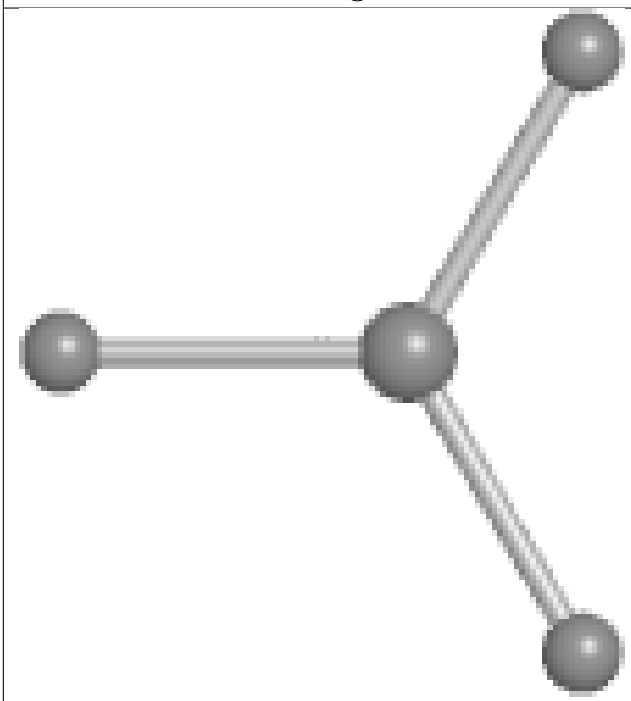
Ligand BEF A 1502



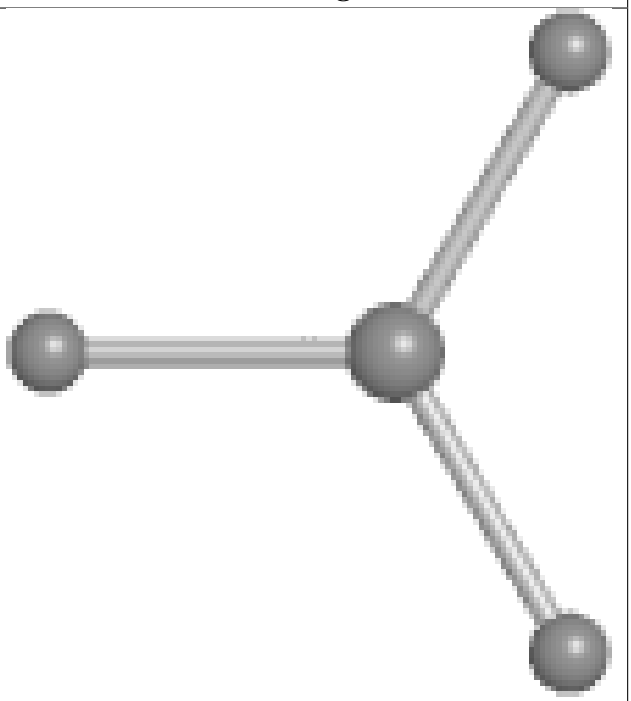
Bond lengths



Bond angles

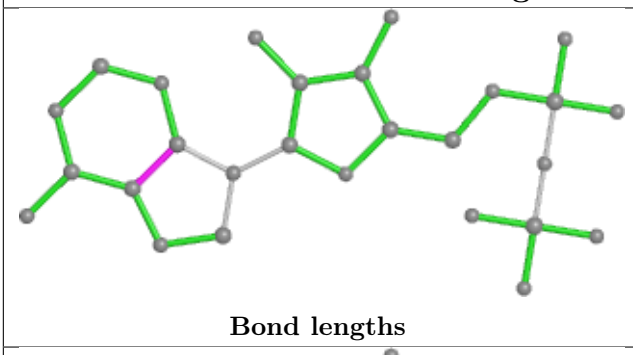


Torsions

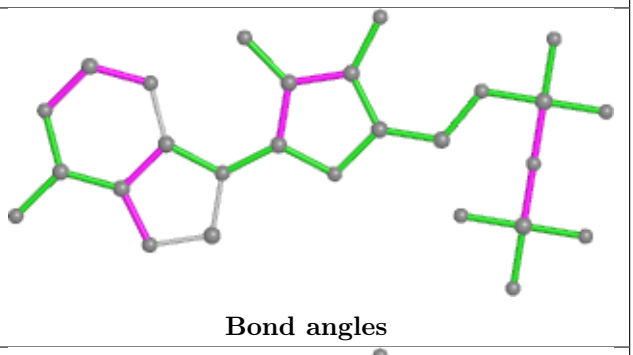


Rings

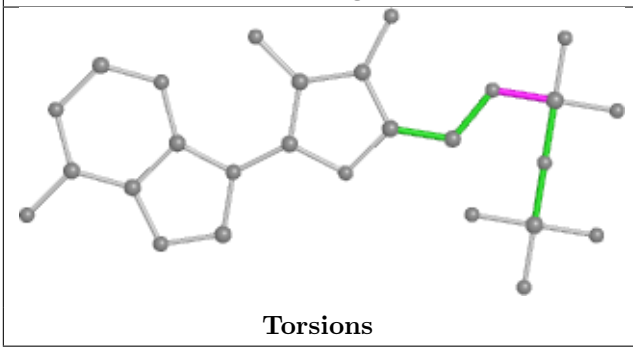
Ligand ADP A 1501



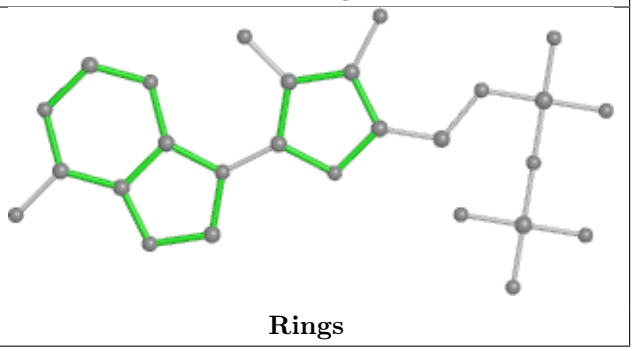
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

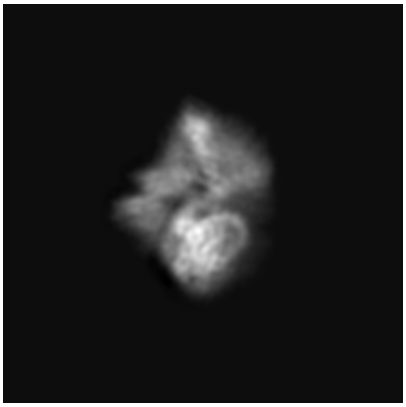
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31137. These allow visual inspection of the internal detail of the map and identification of artifacts.

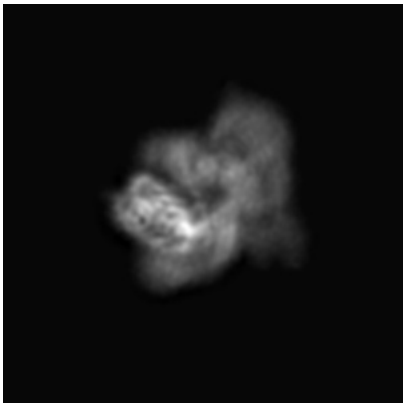
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

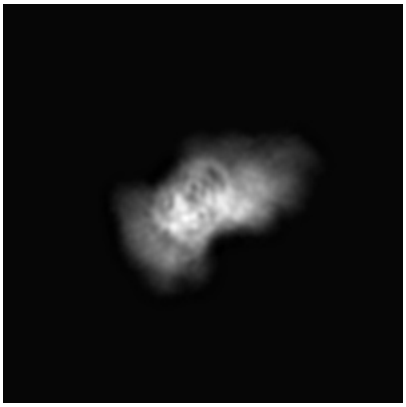
6.1.1 Primary map



X



Y

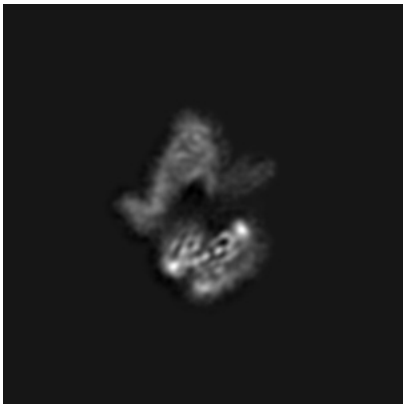


Z

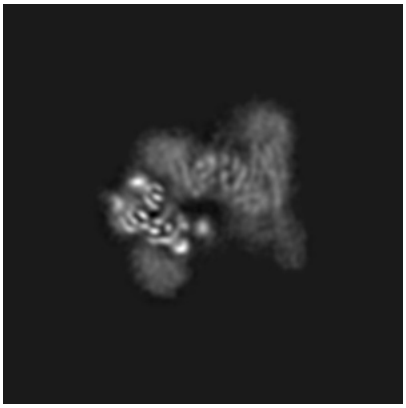
The images above show the map projected in three orthogonal directions.

6.2 Central slices

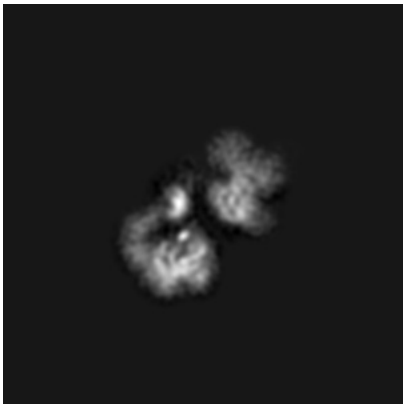
6.2.1 Primary map



X Index: 100



Y Index: 100



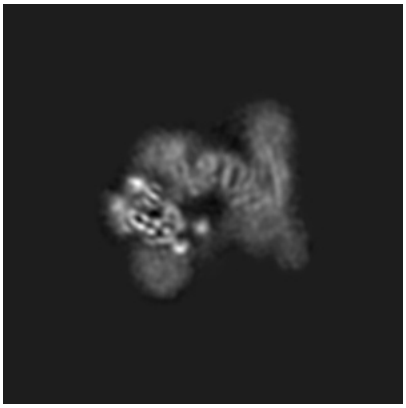
Z Index: 100

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

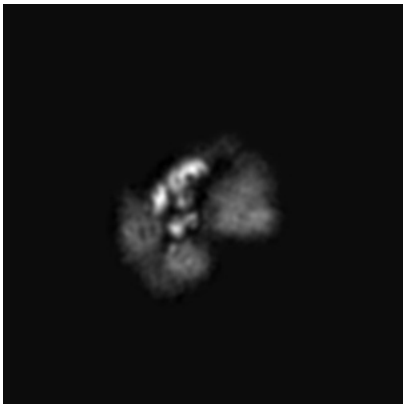
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 87



Y Index: 98

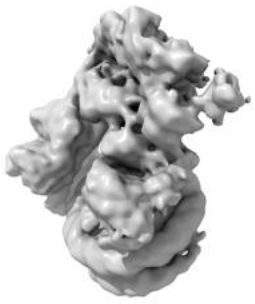


Z Index: 90

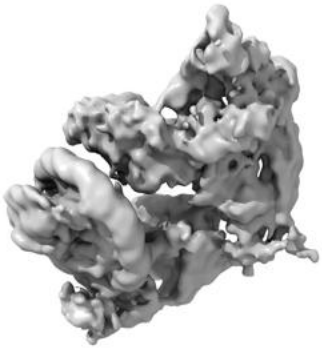
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

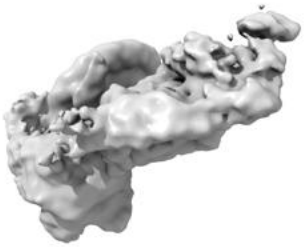
6.4.1 Primary map



X



Y



Z

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

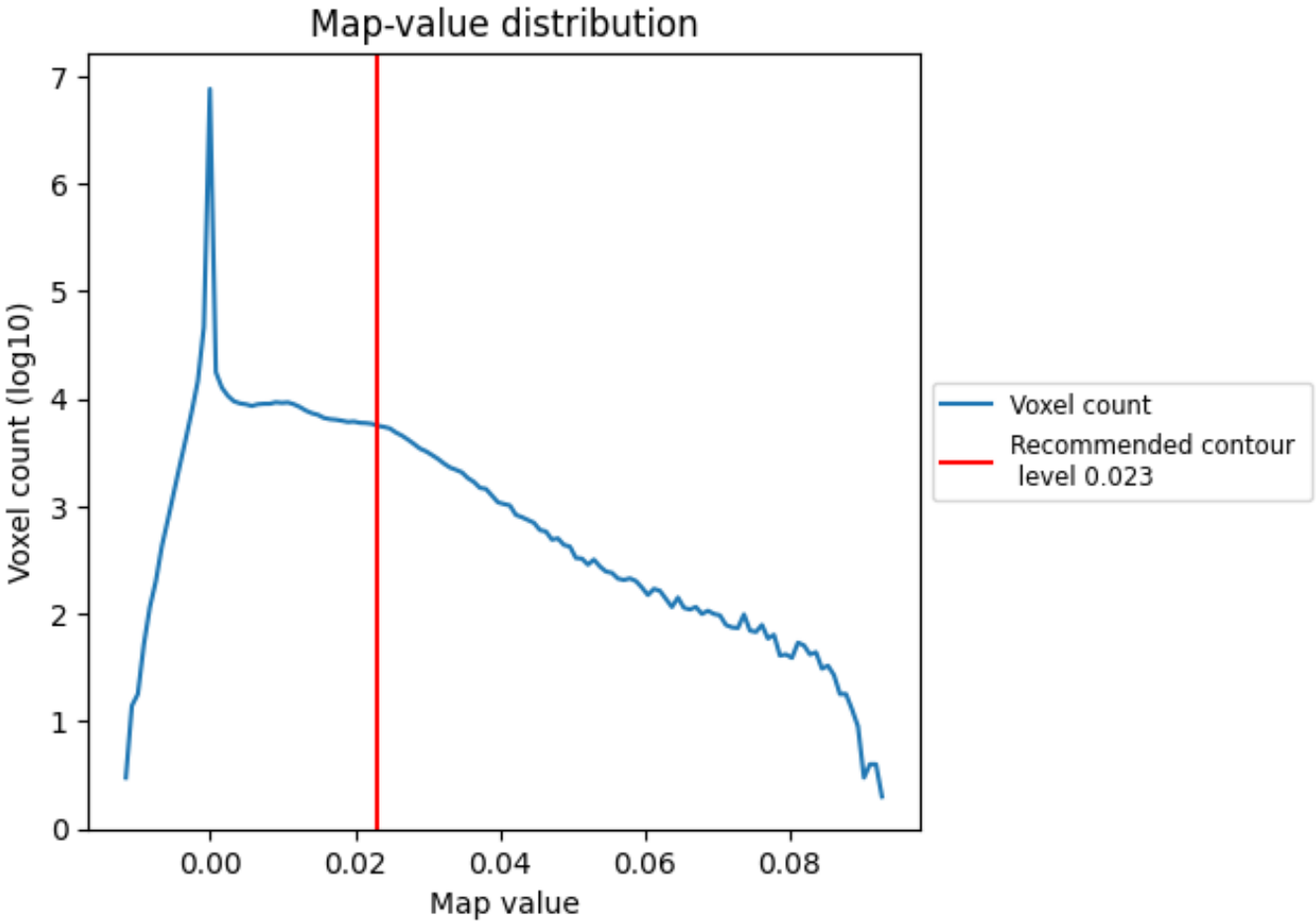
6.5 Mask visualisation (i)

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

7 Map analysis

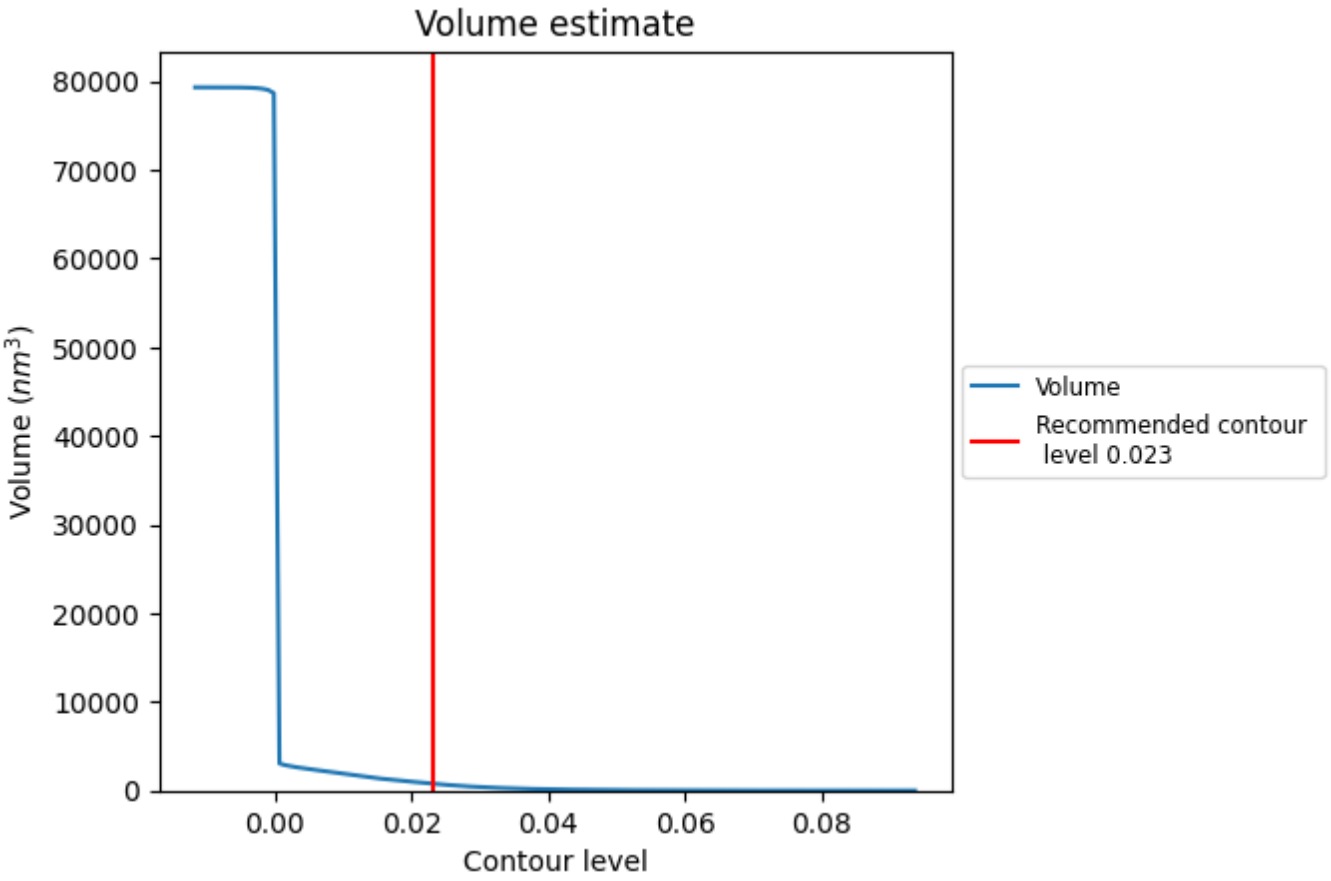
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

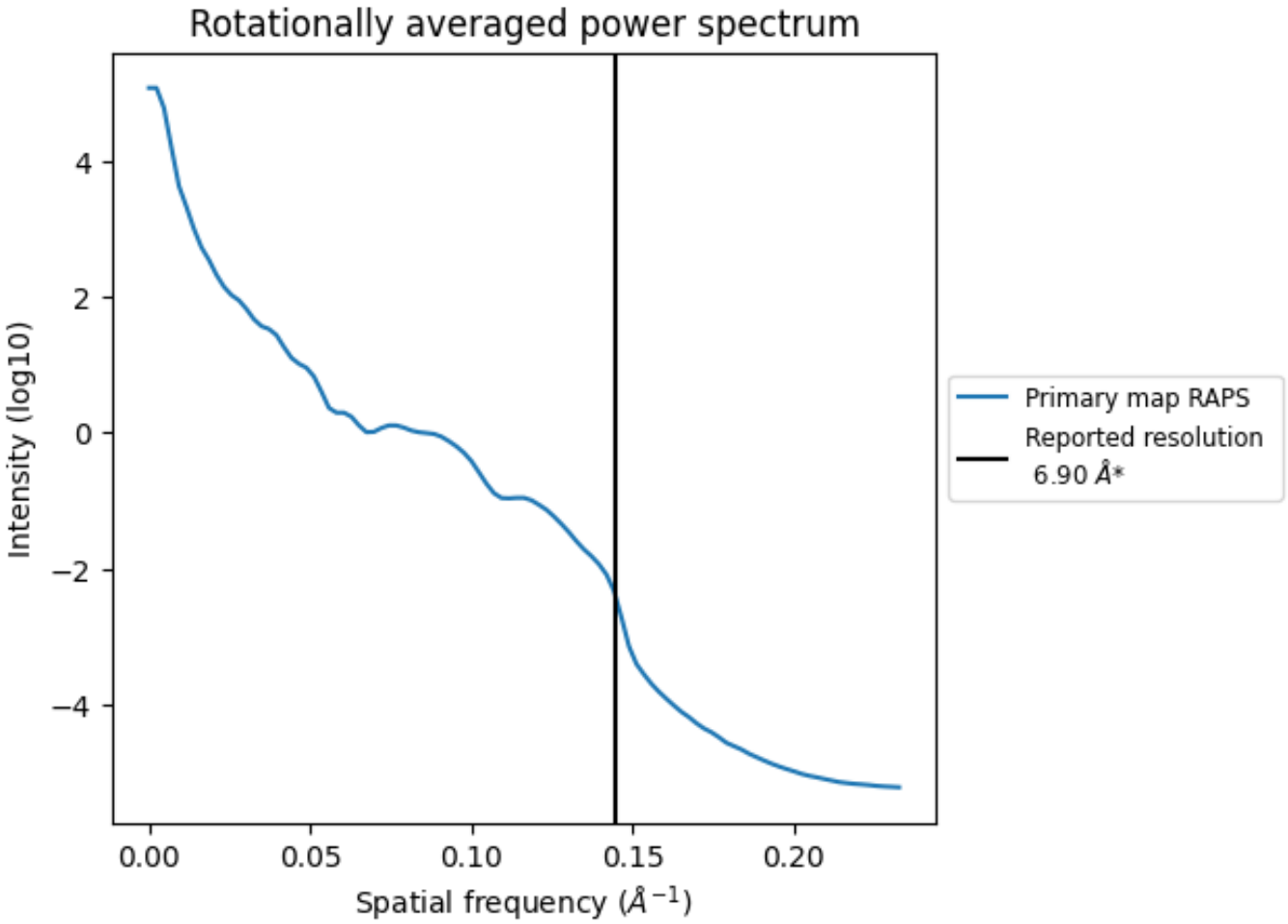
7.2 Volume estimate



The volume at the recommended contour level is 786 nm^3; this corresponds to an approximate mass of 710 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 0.145 Å^{-1}

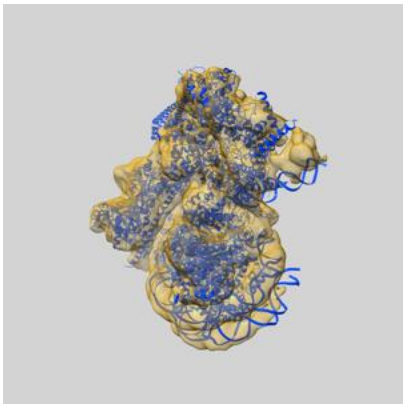
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

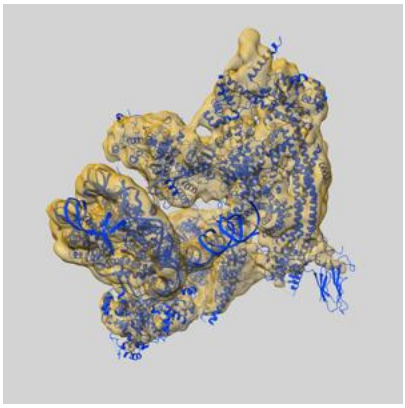
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31137 and PDB model 7EGP. Per-residue inclusion information can be found in section 3 on page 11.

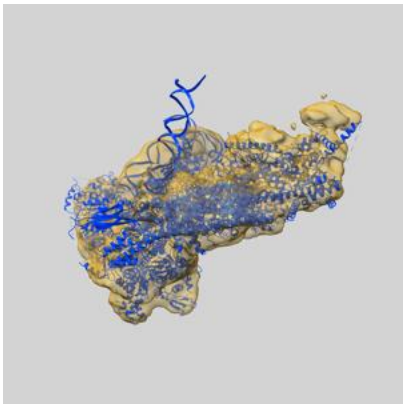
9.1 Map-model overlay



X



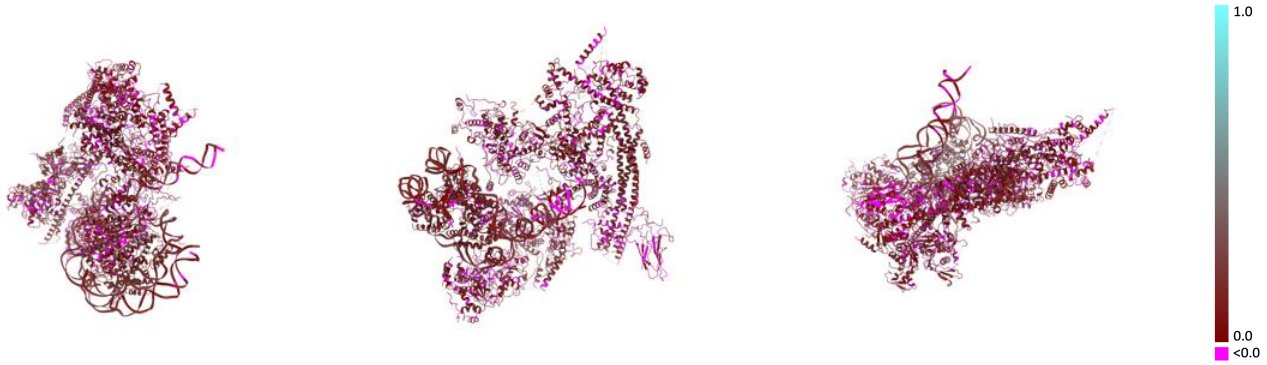
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

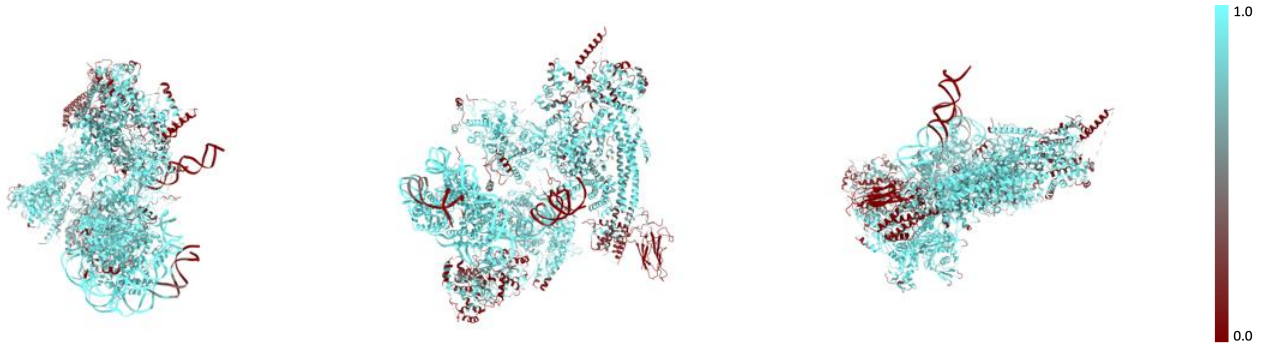
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

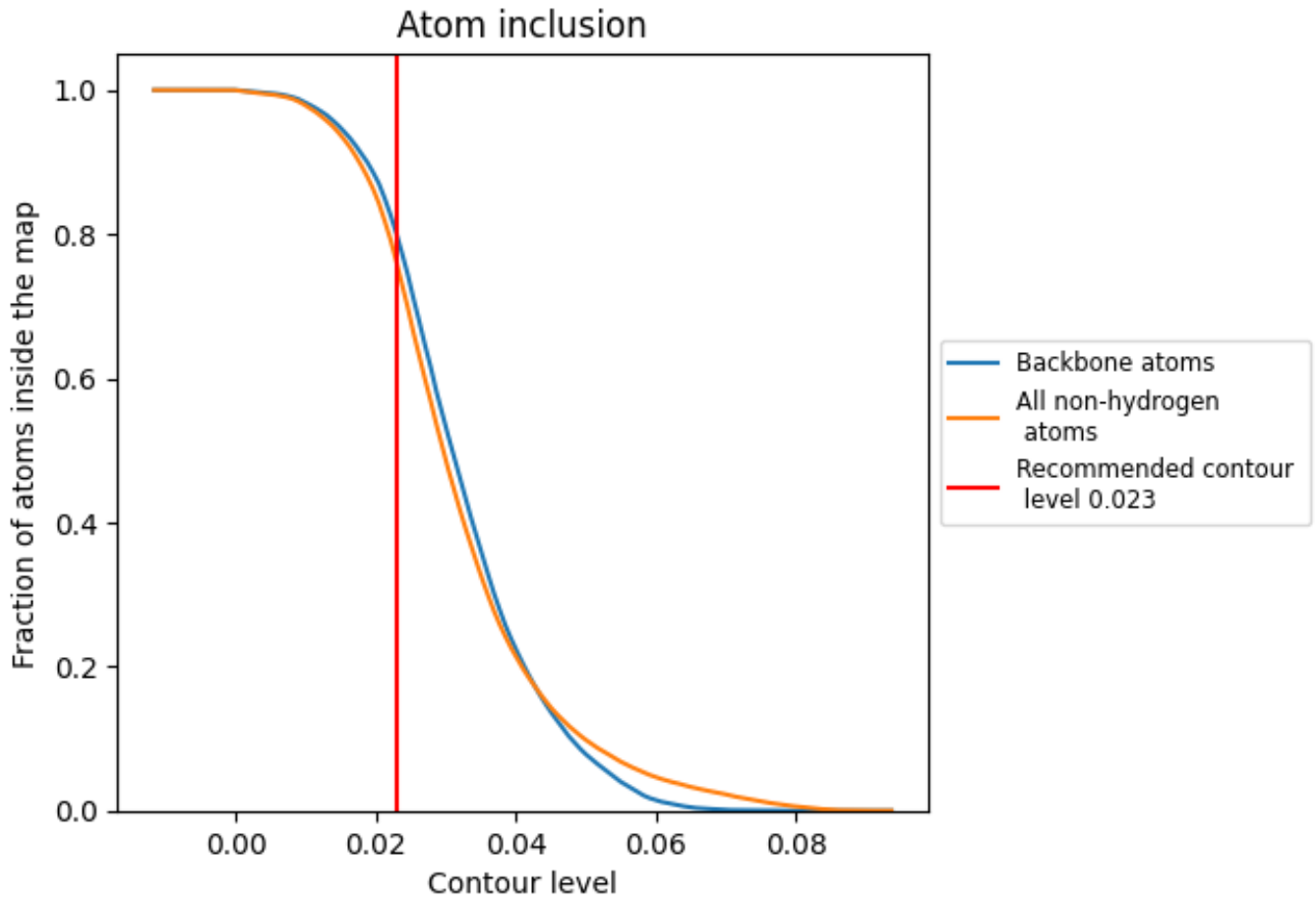
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.023).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7591	0.1050
A	0.5666	0.0840
B	0.8195	0.1060
C	0.8179	0.1010
D	0.6605	0.0800
E	0.6794	0.0780
H	0.4470	0.0690
I	0.6482	0.0950
J	0.6682	0.0770
L	0.8688	0.0480
M	0.9657	0.1100
N	0.9125	0.0950
O	0.9442	0.1280
P	0.8871	0.1410
Q	0.9504	0.1460
R	0.9929	0.1800
S	0.9773	0.1450
T	0.9167	0.1440
U	0.8949	0.1320
V	0.9619	0.1690
W	0.8087	0.1400
X	0.7981	0.1480