



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 04:22 PM EDT

PDB ID : 6UXW / pdb_00006uxw
EMDB ID : EMD-20934
Title : SWI/SNF nucleosome complex with ADP-BeFx
Authors : He, Y.; Han, Y.
Deposited on : 2019-11-08
Resolution : 8.96 Å (reported)
Based on initial models : 4I6M, 5Z3V

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:

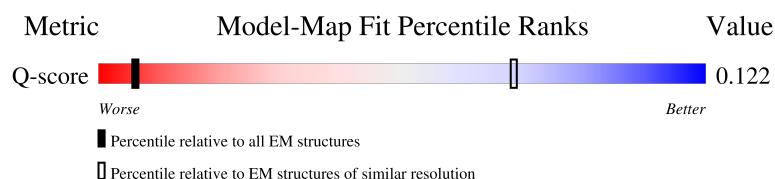
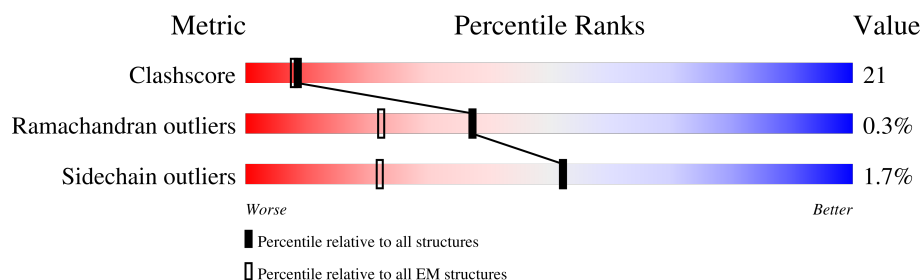
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 8.96 Å.

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



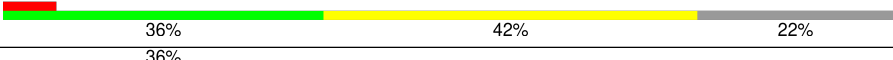
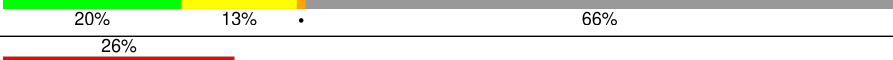
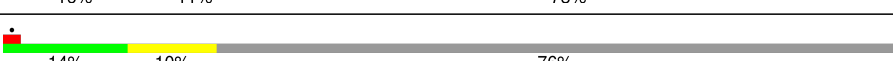
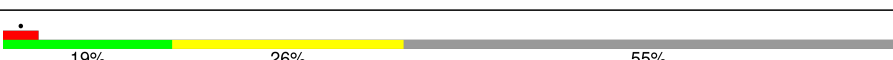
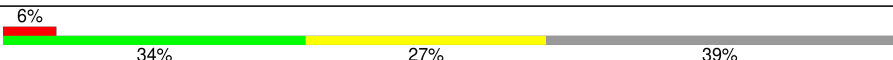
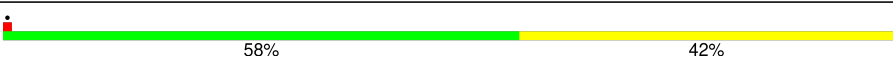
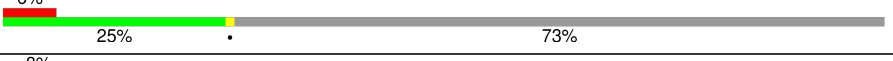
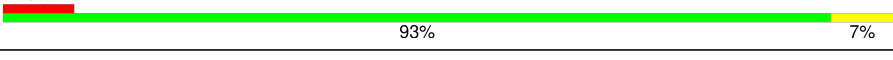
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	236 (8.47 - 9.40)

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

Mol	Chain	Length	Quality of chain
1	R	135	21% 59% 14% 27%
1	V	135	8% 56% 15% 30%
2	S	102	19% 60% 21% 20%
2	W	102	11% 60% 18% 23%

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Mol	Chain	Length	Quality of chain
3	T	129	
3	X	129	
4	U	122	
4	Y	122	
5	a	185	
6	b	200	
7	P	477	
8	Q	467	
9	Z	157	
10	A	1703	
11	B	1314	
12	C	905	
13	D	825	
13	E	825	
13	F	825	
13	G	825	
14	H	566	
15	I	179	
16	J	67	
16	K	67	
16	L	67	
16	N	67	
16	O	67	
17	M	83	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	BEF	A	1803	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 41275 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
1	V	95	Total	C	N	O	S	0	0
			779	492	148	136	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	102	ALA	GLY	conflict	UNP P84233
V	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	82	Total	C	N	O	S	0	0
			653	413	127	112	1		
2	W	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	T	107	Total	C	N	O	0	0
			811	510	158	143		
3	X	107	Total	C	N	O	0	0
			815	513	159	143		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	99	ARG	GLY	conflict	UNP P06897
T	123	SER	ALA	conflict	UNP P06897
X	99	ARG	GLY	conflict	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
X	123	SER	ALA	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	Y	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
U	29	THR	SER	conflict	UNP P02281
Y	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called 601 sequence bottom strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	155	Total	C	N	O	P	0	0
			3160	1502	574	929	155		

- Molecule 6 is a DNA chain called 601 sequence top strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	155	Total	C	N	O	P	0	0
			3195	1514	595	931	155		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	399	Total	C	N	O	S	3	0
			3227	2081	528	603	15		

- Molecule 8 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	396	Total	C	N	O	S	1	0
			3198	2053	523	615	7		

- Molecule 9 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	54	Total	C	N	O	S	0	0
			490	313	84	92	1		

- Molecule 10 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	778	Total	C	N	O	S	1	0
			6385	4041	1139	1185	20		

- Molecule 11 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	482	Total	C	N	O	S	0	0
			3890	2519	637	723	11		

- Molecule 12 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	245	Total	C	N	O	S	0	0
			2005	1256	346	395	8		

- Molecule 13 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	159	Total	C	N	O	S	0	0
			1322	853	225	239	5		
13	E	139	Total	C	N	O	S	0	0
			1152	746	198	205	3		
13	F	221	Total	C	N	O	S	0	0
			1583	987	287	304	5		
13	G	197	Total	C	N	O	S	0	0
			1435	904	258	268	5		

- Molecule 14 is a protein called Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	257	Total	C	N	O	S	0	0
			2085	1323	355	400	7		

- Molecule 15 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	109	Total	C	N	O	S	0	0
			818	504	155	156	3		

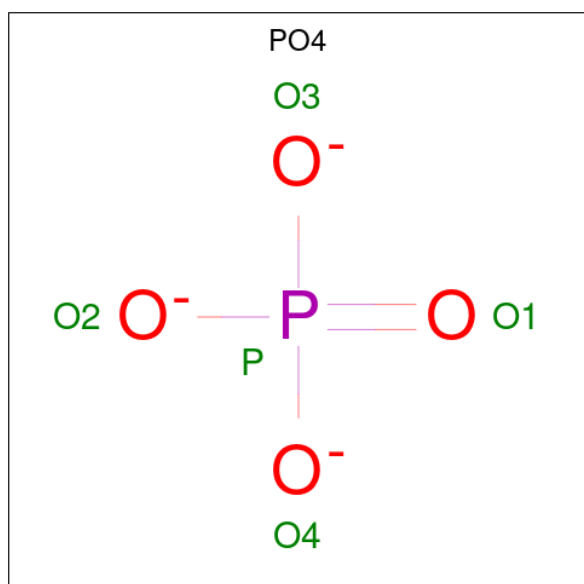
- Molecule 16 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	J	67	Total	C	N	O	0	0
			336	201	67	68		
16	K	28	Total	C	N	O	0	0
			140	84	28	28		
16	L	18	Total	C	N	O	0	0
			90	54	18	18		
16	N	30	Total	C	N	O	0	0
			150	90	30	30		
16	O	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 17 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

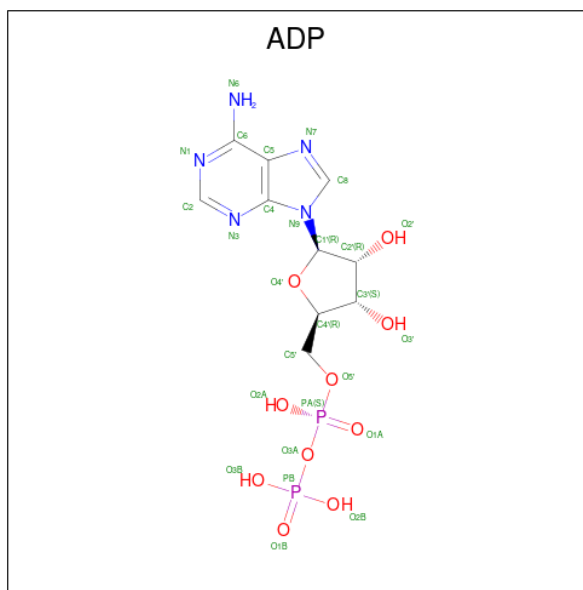
Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	83	Total	C	N	O	0	0
			416	249	83	84		

- Molecule 18 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



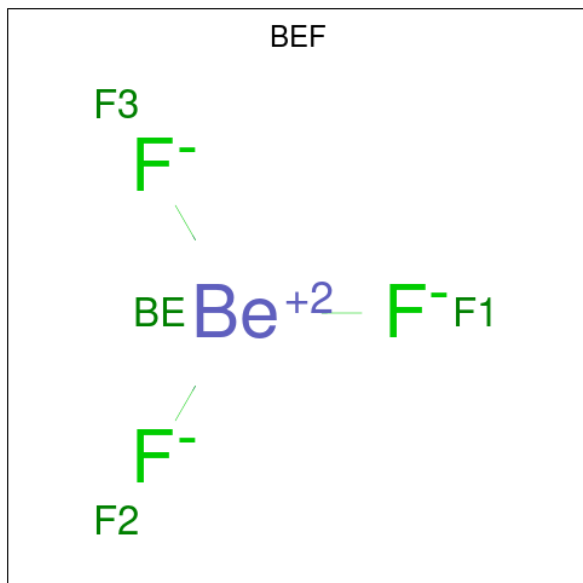
Mol	Chain	Residues	Atoms			AltConf
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	A	1	Total	O	P	0
			5	4	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 20 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



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

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

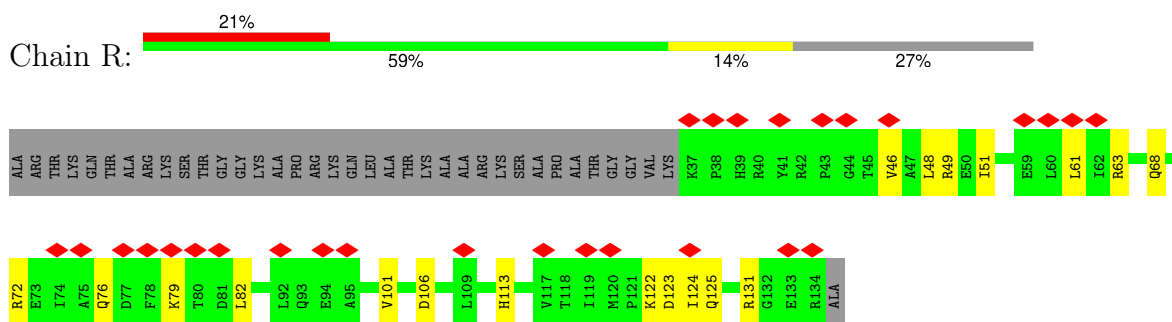
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	P	33	Total	O	0
			33	33	
22	Q	51	Total	O	0
			51	51	
22	Z	2	Total	O	0
			2	2	

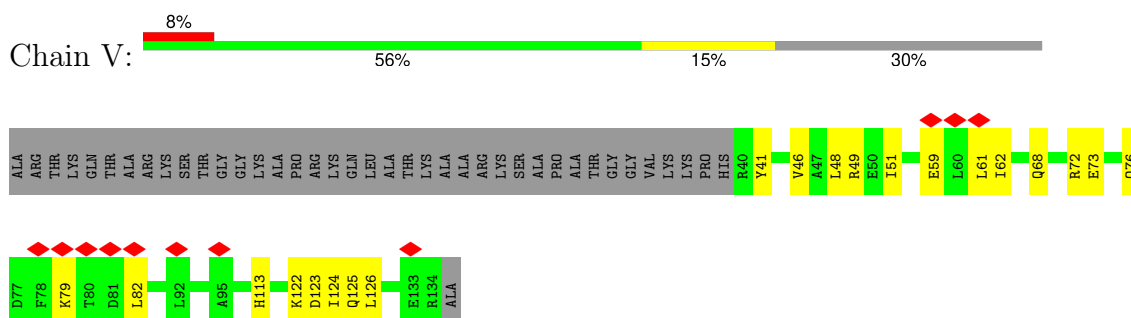
3 Residue-property plots

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

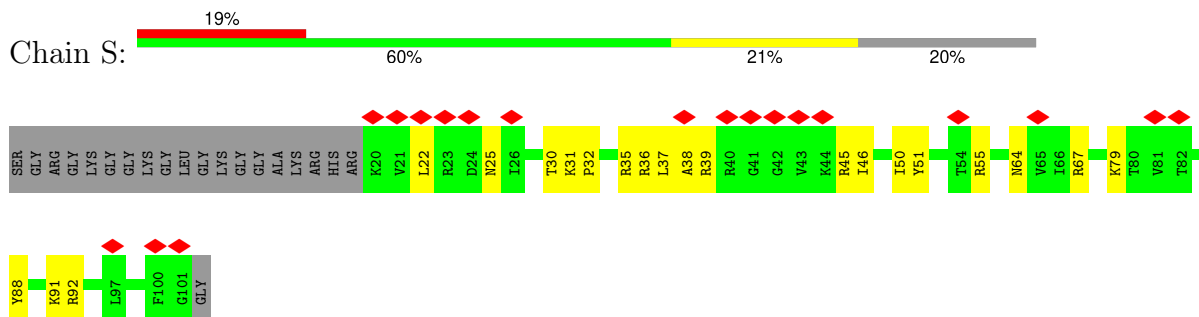
• Molecule 1: Histone H3.2



• Molecule 1: Histone H3.2

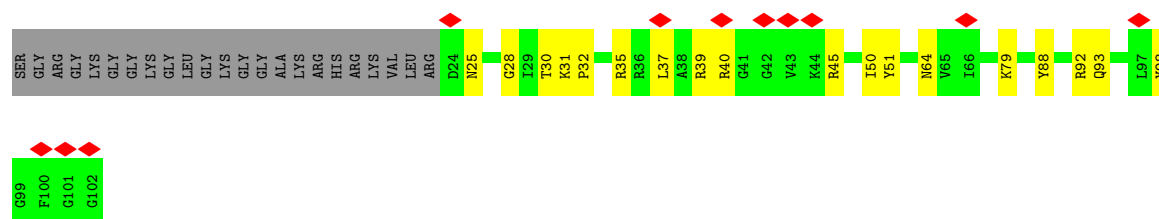


• Molecule 2: Histone H4

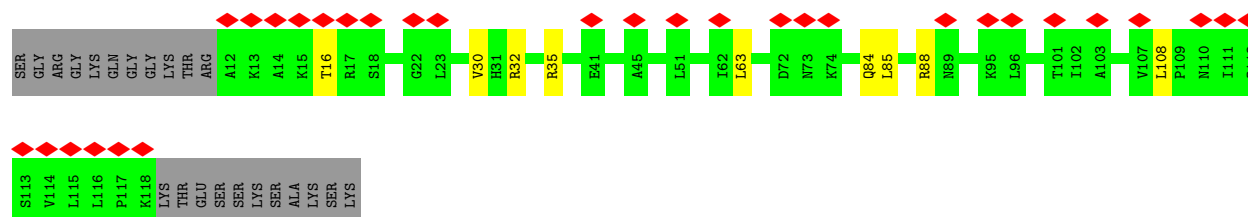
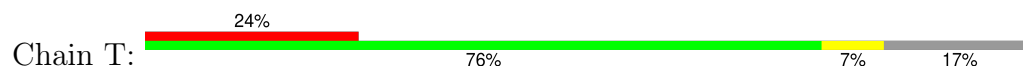


• Molecule 2: Histone H4

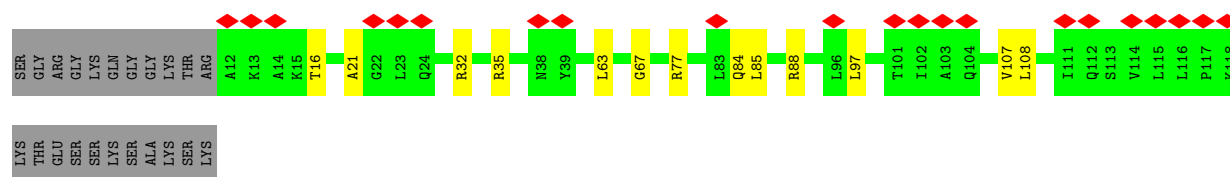
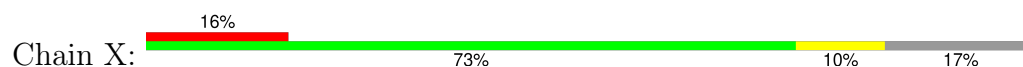




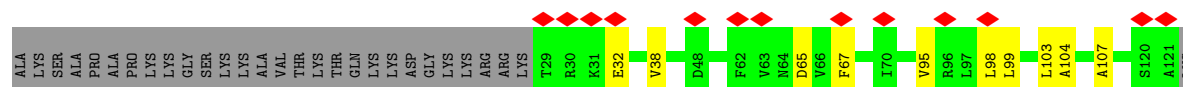
- Molecule 3: Histone H2A type 1



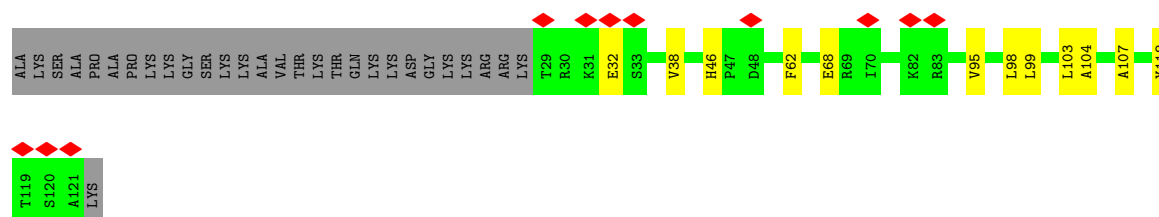
- Molecule 3: Histone H2A type 1



- Molecule 4: Histone H2B 1.1

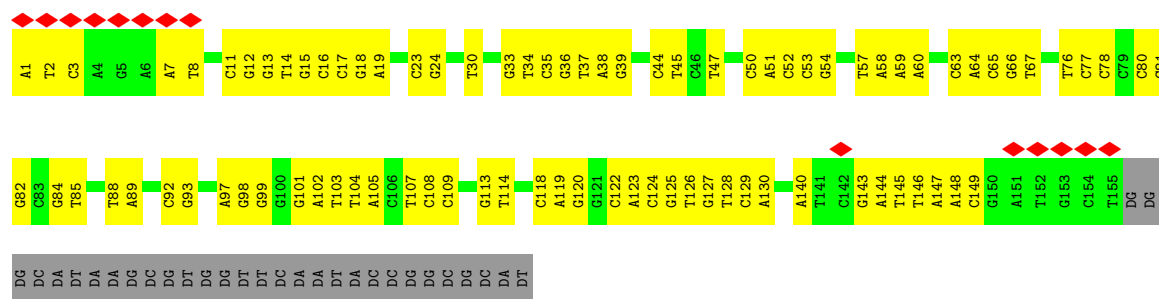


- Molecule 4: Histone H2B 1.1

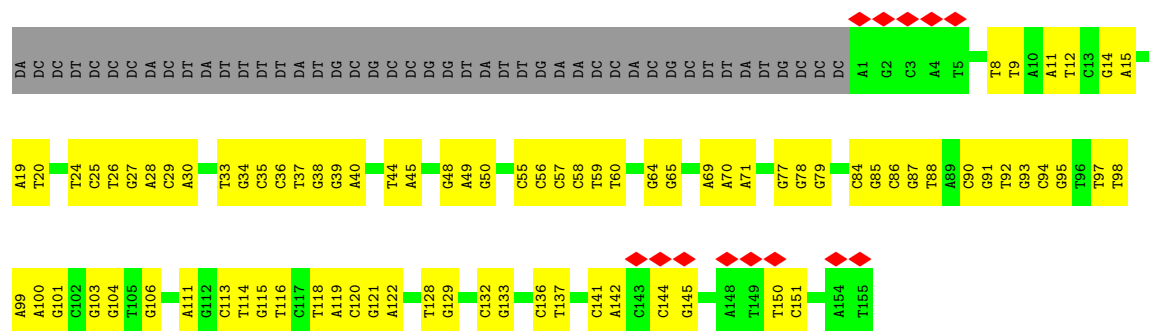


- Molecule 5: 601 sequence bottom strand

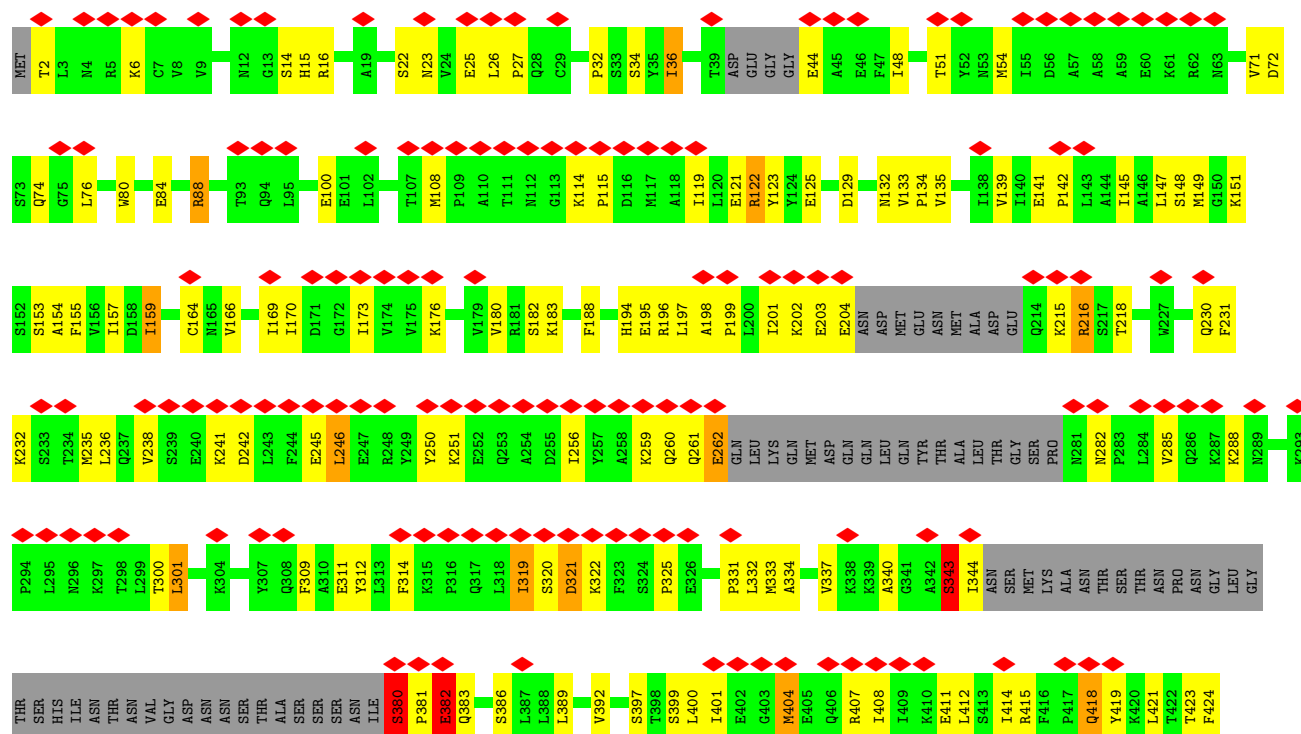


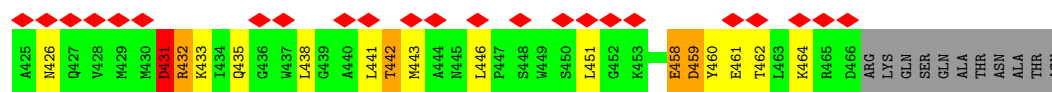


• Molecule 6: 601 sequence top strand

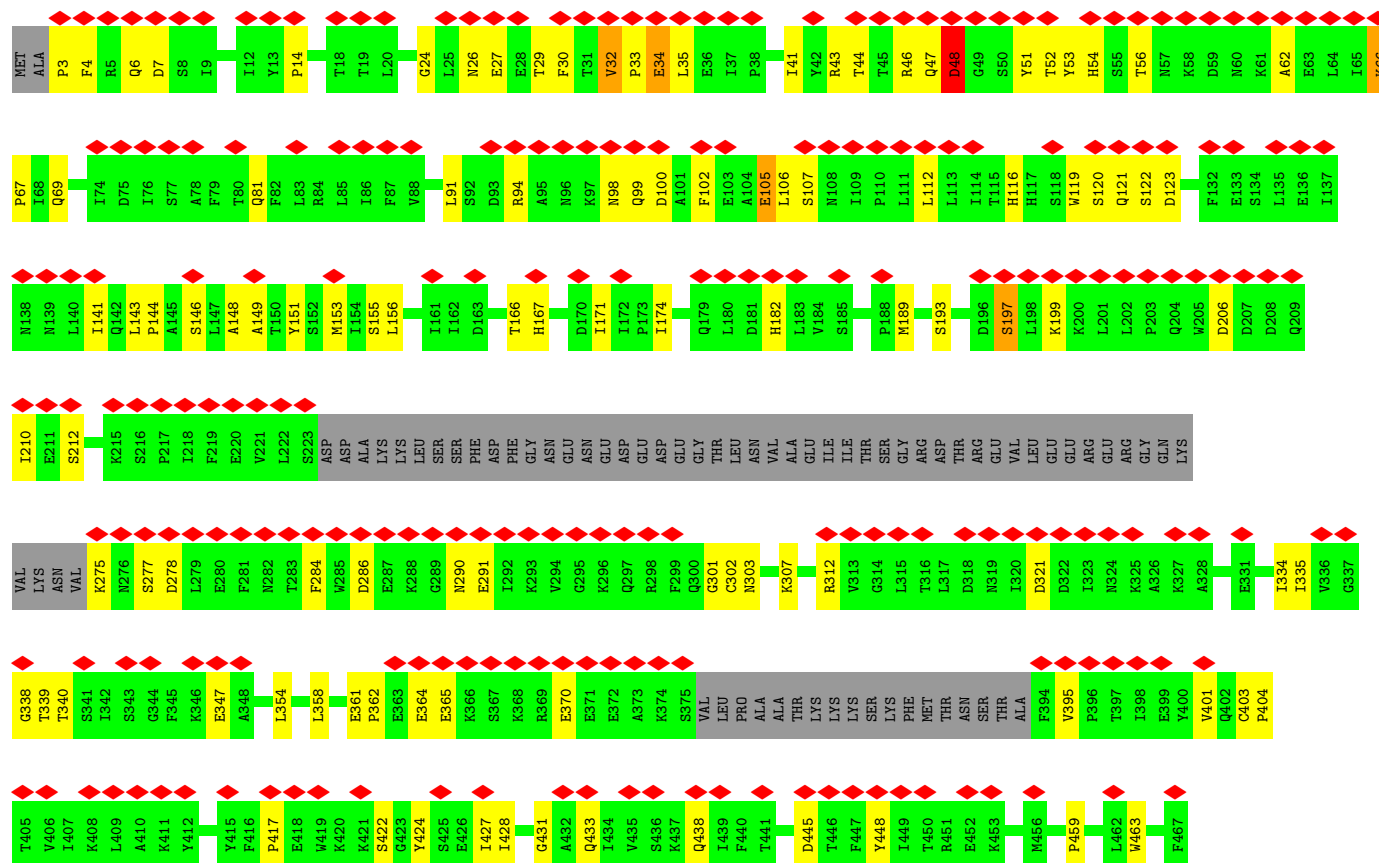


• Molecule 7: Actin-related protein 7

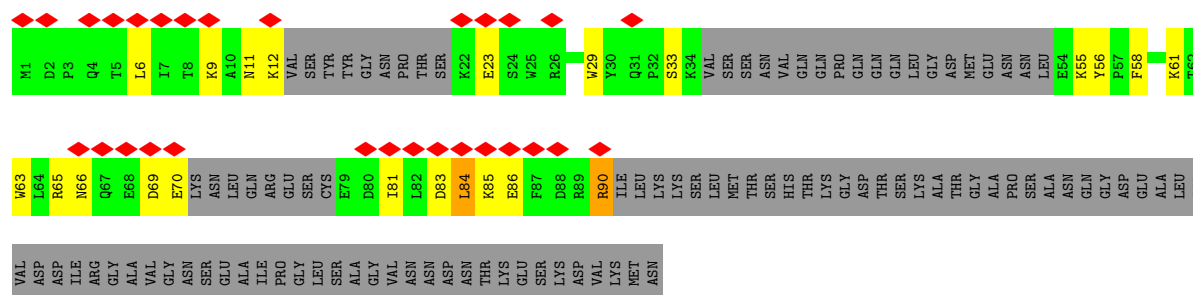




• Molecule 8: Actin-like protein ARP9



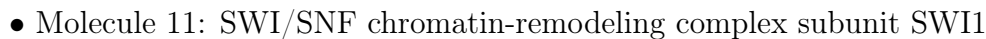
• Molecule 9: Regulator of Ty1 transposition protein 102



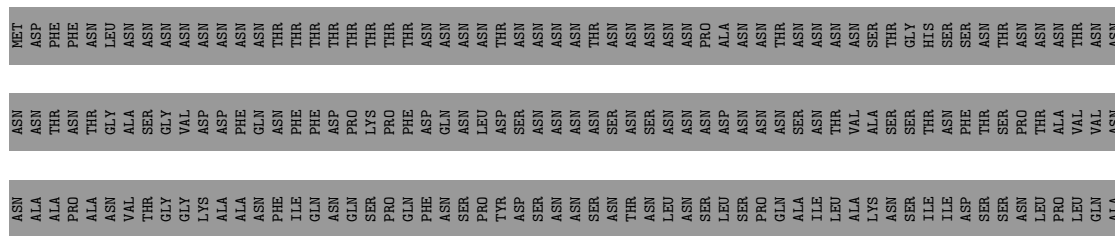
• Molecule 10: Transcription regulatory protein SNF2



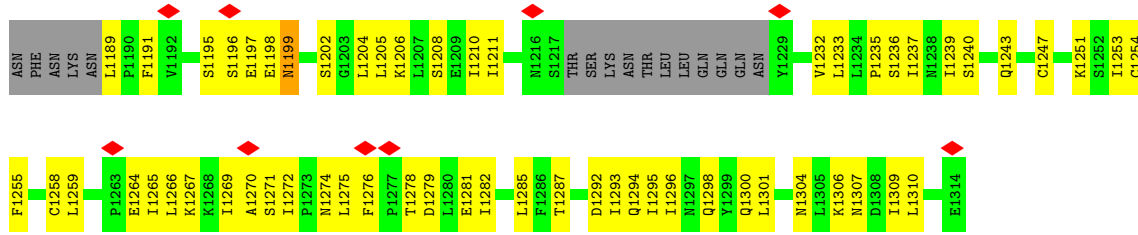
[illegible]



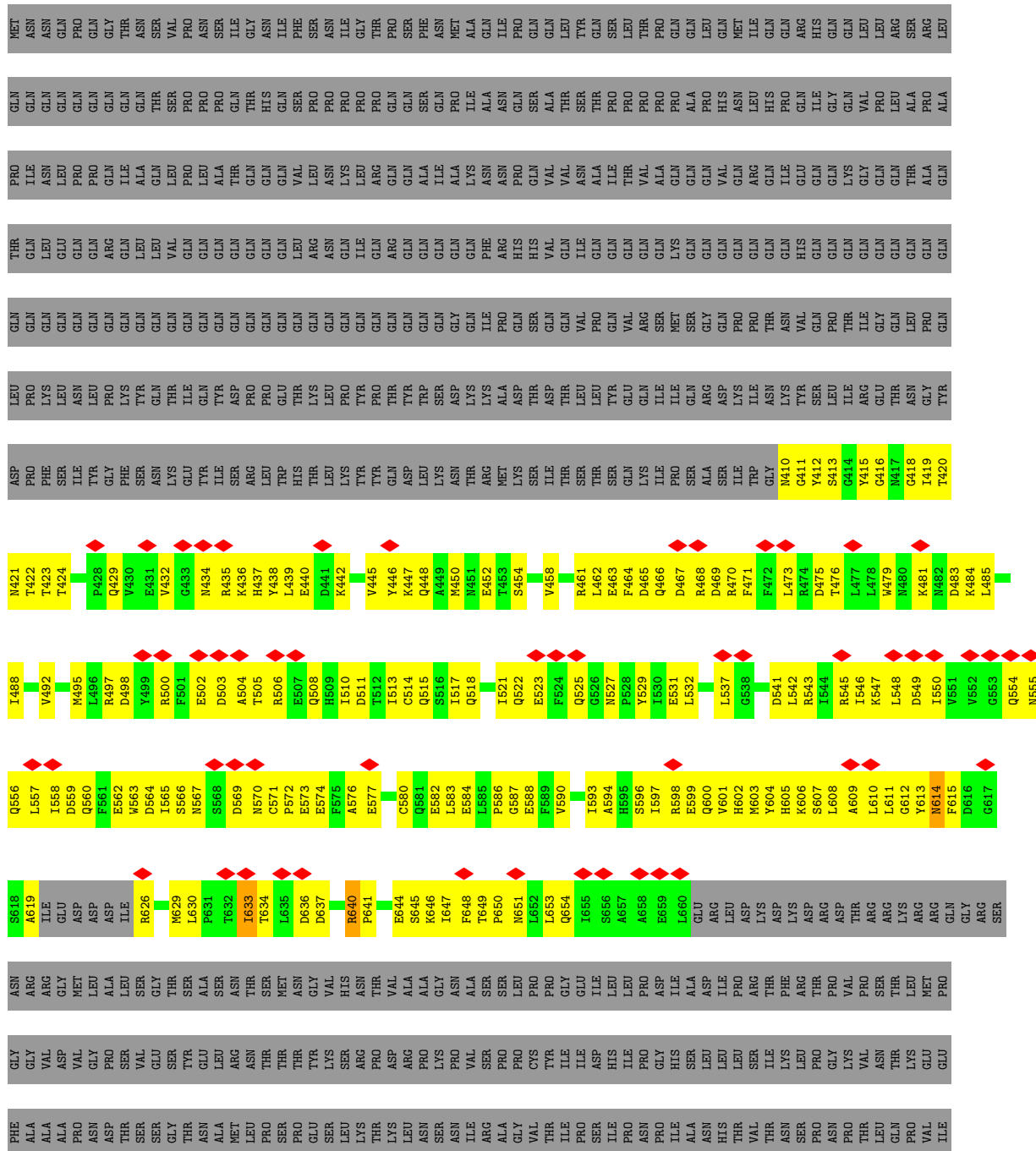
Frequency	Percentage
Often	15%
Sometimes	21%
Rarely/Not at all	63%



P1118	N1053	E987	I921	THR	Q791	N723	VAL	LYS	ALA	TYR	LYS	GLN	ASN
L1119	L1054	I988	S922	SER	H792	T724	ARG	LYS	PRO	PHE	LYS	GLN	GLN
Q1120	N1055	A989	M923	PRO	D793	A725	ASN	LYS	THR	ILE	THR	GLN	GLN
V1121	Y1056	I990	I924	ALA	D793	L726	TYR	LYS	ALA	ILE	ASN	GLN	GLN
V1122	F1057	S991	L925	V858	D794	N727	LYS	LYS	ALA	LEU	ASN	GLN	GLN
S1123	K1058	S991	R926	V861	D796	T728	PRO	LYS	ALA	LEU	PRO	GLN	GLN
S1124	S1059	I992	N927	D862	V796	L729	LEU	GLU	PRO	TYR	VAL	GLN	GLN
Q1125	I1060	D993	N927	L863	D797	L730	ILE	LEU	GLY	TYR	PRO	GLN	GLN
S1126	L1061	I996	S929	L864	D797	V731	ASN	GLU	ALA	GLU	ALA	GLN	GLN
A1127	L1062	I997	S929	P865	K798	T732	ARG	GLU	VAL	HIS	THR	GLN	GLN
S1130	N1063	I997	D932	E866	E801	D735	LEU	LYS	PRO	MET	PRO	ASN	ASN
D1134	K1064	I998	N933	E869	N805	S736	HIS	ARG	ALA	ILE	ALA	GLN	GLN
Q1135	THR	I999	N934	R869	N806	S737	TYR	GLU	THR	SER	ASN	LEU	SER
F1136	GLY	L1000	S935	Q874	ALA	N737	ASN	ARG	ALA	GLN	LYS	THR	GLY
S1137	ASN	I1001	R936	F875	THR	K738	GLY	GLU	ALA	GLU	ASN	SER	ILE
P1138	ASN	I1002	M938	P876	LEU	K739	TYR	ASP	PRO	GLY	LYS	ASN	ALA
V1139	LEU	Q1006	S939	L877	THR	I740	ILE	PHE	THR	ILE	ILE	SER	ASN
I1140	TYR	F1007	R940	K878	PRO	S741	ASN	LYS	GLU	LYS	LEU	ALA	ASP
S1141	ASP	K1008	N941	I879	ASN	L742	TYR	ARG	ALA	THR	ASN	VAL	ASN
Q1142	ARG	LEU	F942	I879	ASP	V743	ILE	GLN	GLY	GLN	ALA	ASN	VAL
S1143	ASN	ASN	Y943	H880	SER	K744	ILE	GLN	GLN	GLN	TYR	ASN	ILE
L1144	SER	PRO	L944	R881	ASN	V745	SER	GLN	ILE	ALA	ILE	ASN	THR
T1145	ASN	MET	K945	T882	ASP	V746	LYS	LYS	VAL	LYS	TYR	THR	PRO
S1146	ASN	ALA	R946	P883	GLU	E747	ILE	LEU	PRO	ARG	VAL	ASP	HIS
I1147	N1078	SER	F947	T886	LYS	L748	GLY	LEU	VAL	ILE	VAL	PHE	PHE
Q1152	H1079	SER	I948	S887	VAL	L749	GLU	GLU	SER	PHE	SER	VAL	ILE
LYS	K1080	SER	L951	S887	THR	D750	LYS	ASP	ALA	GLN	ILE	GLU	THR
ILE	D1081	PHE	L952	K889	ILE	S751	ILE	GLN	THR	GLN	PHE	GLN	ASN
LEU	K1082	GLY	N953	K890	VAL	I754	ASP	ARG	PRO	PHE	GLY	SER	GLN
PRO	K1083	SER	L954	I891	ASP	N758	ASN	GLN	LYS	LEU	ALA	ASN	GLU
ASN	L1084	ILE	V955	K892	SER	L760	LYS	GLN	SER	GLN	ALA	LEU	ASN
ASN	L1087	E1021	L956	D893	THR	S761	PRO	LYS	LEU	LEU	ASP	PRO	ALA
ASN	R1088	S1022	L957	D893	THR	N762	ILE	LEU	ASN	LEU	GLN	ALA	VAL
GLU	L1091	L1023	H958	E894	GLY	L763	PHE	LEU	ASN	SER	VAL	LEU	ASN
PHE	Y1092	F1025	I895	T895	THR	S764	LEU	LEU	ASN	LYS	THR	GLN	ASN
VAL	N1093	N1026	P959	D896	ASN	V767	ASN	GLU	ASN	GLN	ARG	GLN	ASN
GLU	ASP	E1027	N961	D897	LEU	H771	PRO	THR	ASN	GLN	THR	GLN	ASN
ILE	ASN	F1028	P898	F899	PRO	H772	THR	PRO	ASN	GLN	MET	ASN	ASN
SER	LYS	Q1029	F899	T900	THR	D776	PRO	THR	ASN	GLN	THR	ASN	ASN
GLU	ASN	L1030	C964	K901	PRO	Y777	PRO	THR	ASN	GLN	THR	ASN	ASN
ASN	ASN	Q1031	N965	I902	THR	Y778	THR	THR	ASN	GLN	THR	ASN	ASN
ASN	ASN	Q1032	N903	N903	THR	Y779	THR	THR	ASN	GLN	THR	ASN	ASN
ASN	ASN	K1034	T904	T904	GLU	E780	GLU	GLU	ASN	GLN	THR	ASN	ASN
ASP	ARG	Y1035	R905	G906	MET	D781	PRO	PRO	ASN	GLN	THR	ASN	ASN
SER	H1103	Q1036	K973	A907	GLU	A782	THR	ASP	ALA	ALA	ALA	ASN	ASN
ASN	N1104	T1037	D974	P910	GLU	G783	GLU	ASP	GLY	LEU	GLN	GLN	GLN
SER	L1105	F1038	L975	V912	LEU	S711	LEU	LEU	GLY	LEU	TYR	GLN	GLN
ASN	L1106	Y978	V976	T914	THR	M712	LYS	LYS	ALA	ALA	ASN	GLN	GLN
ASN	V1109	G1039	N981	N915	CYS	Q715	VAL	VAL	ALA	ASN	ASN	GLN	GLN
GLY	W1110	D1041	L913	N915	GLU	S716	THR	THR	ILE	ASN	ASN	GLN	GLN
ASN	S1111	L1046	N915	D916	ILE	K717	GLU	GLU	ALA	ASN	ASN	GLN	GLN
LYS	S1115	F1047	N915	Q917	PHE	N718	LYS	PRO	ALA	ASN	ASN	GLN	GLN
ASP	ASP	S1048	S983	L918	SER	L719	ARG	LYS	ARG	ASN	ASN	GLN	GLN
SER	A1116	L1049	H984	L985	MET	Q786	LYS	LYS	LYS	LEU	LEU	GLN	GLN
SER	I1117	E1050	L986	L986	GLN	Y787	ILE	ILE	VAL	GLU	GLU	GLN	GLN
PHE		K1051			SER	Y788			ARG	SER	SER	GLN	GLN
		P1052				T790			VAL	SER	SER	GLN	GLN



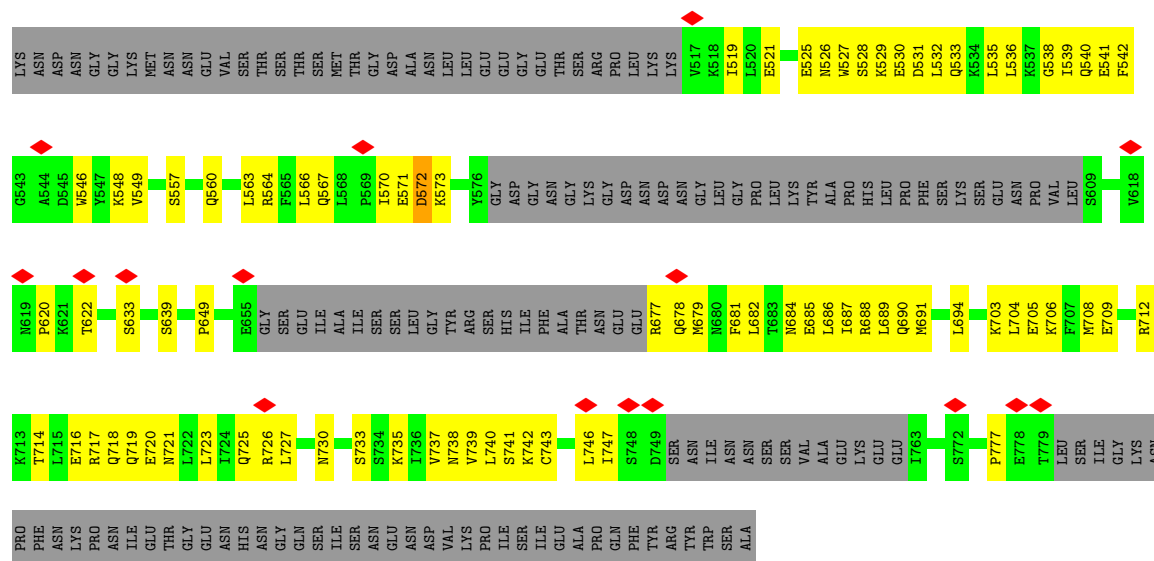
• Molecule 12: SWI/SNF chromatin-remodeling complex subunit SNF5



Chain D: 8% 11% 81%

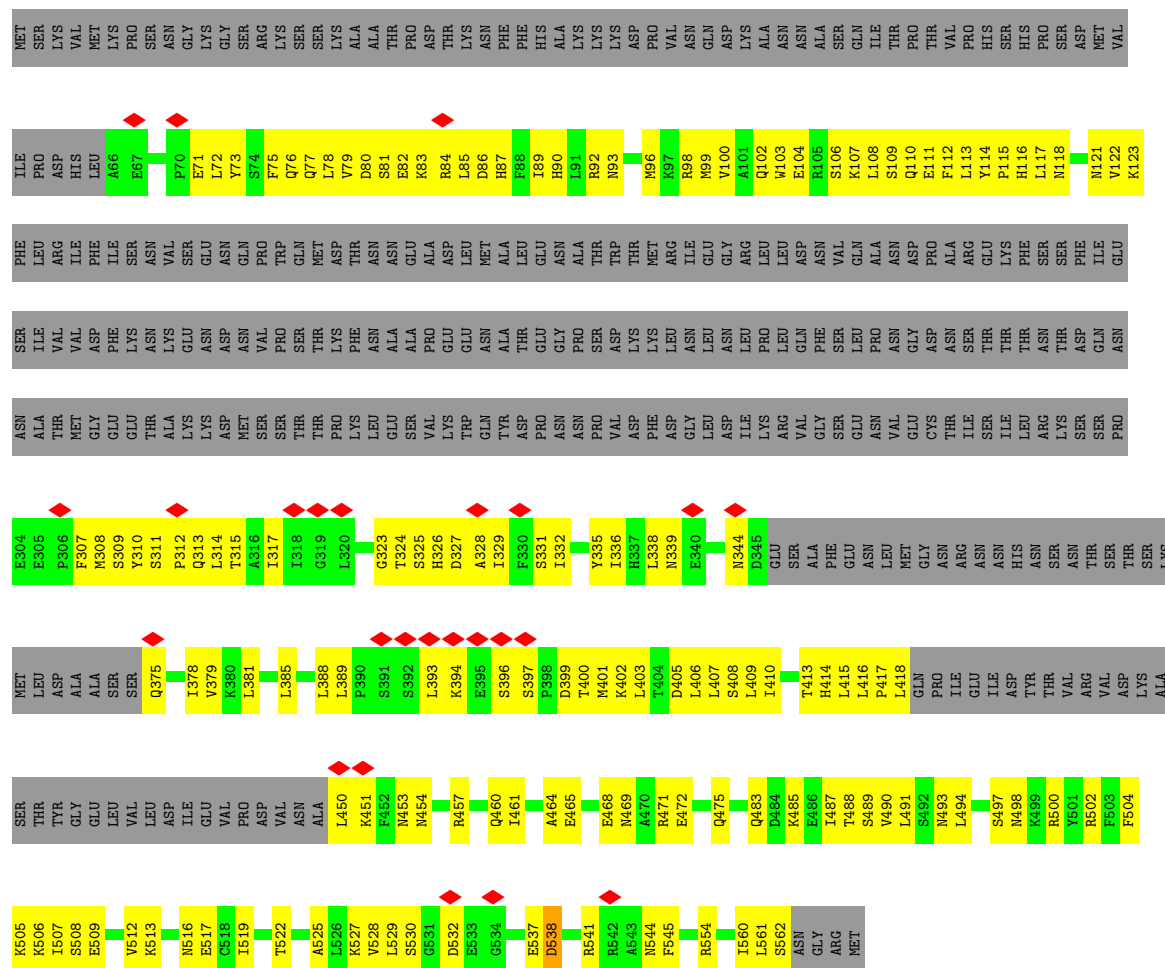




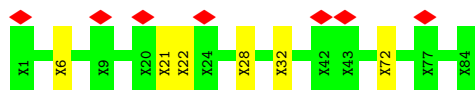


• Molecule 14: Transcription regulatory protein SNF12

Chain H: 19% 26% 55%



• Molecule 15: Transcription regulatory protein SNF6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion.	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	76.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	430.08002, 430.08002, 430.08002	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.24, 2.24, 2.24	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ADP, MG, BEF

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	R	0.11	0/813	0.31	0/1093
1	V	0.11	0/789	0.31	0/1059
2	S	0.12	0/660	0.34	0/885
2	W	0.12	0/634	0.34	0/848
3	T	0.12	0/821	0.29	0/1112
3	X	0.12	0/825	0.29	0/1116
4	U	0.10	0/729	0.27	0/985
4	Y	0.10	0/737	0.27	0/993
5	a	0.23	0/3541	0.44	0/5458
6	b	0.21	0/3587	0.43	0/5539
7	P	0.56	1/3303 (0.0%)	0.90	6/4465 (0.1%)
8	Q	0.58	0/3269	0.88	2/4432 (0.0%)
9	Z	0.45	0/501	0.83	0/669
10	A	0.24	0/6488	0.49	1/8732 (0.0%)
11	B	0.35	0/3958	0.53	0/5364
12	C	0.31	0/2040	0.64	2/2756 (0.1%)
13	D	0.26	0/1359	0.45	0/1838
13	E	0.34	0/1189	0.53	0/1616
13	F	0.30	0/1596	0.58	5/2154 (0.2%)
13	G	0.32	0/1446	0.58	3/1949 (0.2%)
14	H	0.33	1/2119 (0.0%)	0.47	0/2856
15	I	0.29	0/682	0.45	0/913
All	All	0.33	2/41086 (0.0%)	0.57	19/56832 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	380	SER	C-N	5.23	1.40	1.34
14	H	544	ASN	CA-C	-5.03	1.44	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	640	ARG	CA-C-N	10.77	133.30	119.84
12	C	640	ARG	C-N-CA	10.77	133.30	119.84
13	F	649	PRO	N-CA-CB	8.29	110.56	103.35
13	F	606	PRO	N-CA-CB	8.00	111.65	103.25
13	F	599	PRO	N-CA-CB	7.19	110.38	103.19
7	P	431	ASP	N-CA-C	6.96	121.38	112.34
10	A	959	PRO	N-CA-CB	6.42	109.99	103.25
13	F	777	PRO	N-CA-CB	6.25	110.15	103.52
13	F	620	PRO	N-CA-CB	6.16	109.72	103.25
13	G	777	PRO	N-CA-CB	6.12	110.07	103.33
13	G	649	PRO	N-CA-CB	6.07	110.00	103.33
13	G	620	PRO	N-CA-CB	5.94	110.64	103.45
7	P	380	SER	CA-C-N	-5.67	113.07	118.97
7	P	380	SER	C-N-CA	-5.67	113.07	118.97
7	P	176	LYS	N-CA-C	5.40	117.16	111.28
7	P	215	LYS	N-CA-C	-5.34	106.70	113.43
7	P	404	MET	N-CA-C	5.13	116.56	111.07
8	Q	66	LYS	CA-C-N	5.10	124.41	118.85
8	Q	66	LYS	C-N-CA	5.10	124.41	118.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	B	776	ASP	Peptide
11	B	932	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	801	0	831	18	0
1	V	779	0	815	17	0
2	S	653	0	695	16	0
2	W	627	0	663	16	0
3	T	811	0	849	7	0
3	X	815	0	860	12	0
4	U	718	0	725	8	0
4	Y	726	0	747	10	0
5	a	3160	0	1741	83	0
6	b	3195	0	1742	77	0
7	P	3227	0	3251	175	0
8	Q	3198	0	3187	71	0
9	Z	490	0	467	19	0
10	A	6385	0	6494	341	0
11	B	3890	0	4008	265	0
12	C	2005	0	1939	171	0
13	D	1322	0	1325	99	0
13	E	1152	0	1137	87	0
13	F	1583	0	1397	78	0
13	G	1435	0	1294	62	0
14	H	2085	0	2104	147	0
15	I	818	0	708	69	0
16	J	336	0	70	19	0
16	K	140	0	33	3	0
16	L	90	0	21	0	0
16	N	150	0	41	3	0
16	O	90	0	21	2	0
17	M	416	0	92	4	0
18	A	5	0	0	0	0
18	P	25	0	0	0	0
18	Q	30	0	0	1	0
19	A	27	0	12	6	0
20	A	4	0	0	4	0
21	A	1	0	0	0	0
22	P	33	0	0	4	0
22	Q	51	0	0	4	0
22	Z	2	0	0	0	0
All	All	41275	0	37269	1666	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 (1666) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:238:VAL:HG21	7:P:404:MET:SD	1.34	1.68
7:P:36:ILE:HD12	7:P:54:MET:CE	1.34	1.52
7:P:36:ILE:CD1	7:P:54:MET:HE3	1.52	1.39
7:P:155:PHE:CE2	7:P:333:MET:HE3	1.60	1.35
13:D:412:TYR:CD1	14:H:560:ILE:HG23	1.62	1.35
13:D:412:TYR:CD1	14:H:560:ILE:CG2	2.12	1.33
7:P:238:VAL:CG2	7:P:404:MET:SD	2.19	1.28
7:P:76:LEU:CD2	7:P:108:MET:HE1	1.63	1.28
10:A:594:LEU:O	10:A:598:LYS:HD3	1.35	1.27
7:P:76:LEU:CD2	7:P:108:MET:CE	2.15	1.25
7:P:36:ILE:CD1	7:P:54:MET:CE	2.11	1.18
7:P:157:ILE:CD1	7:P:333:MET:HE2	1.74	1.16
7:P:36:ILE:CG1	7:P:54:MET:HE1	1.76	1.14
7:P:36:ILE:CB	7:P:54:MET:HE1	1.76	1.14
7:P:451:LEU:HD13	10:A:608:MET:SD	1.88	1.14
7:P:155:PHE:CE2	7:P:333:MET:CE	2.31	1.12
7:P:157:ILE:HG12	7:P:333:MET:HE1	1.23	1.10
7:P:343:SER:CB	7:P:344:ILE:HA	1.81	1.09
7:P:76:LEU:HD22	7:P:108:MET:HE1	1.11	1.09
10:A:594:LEU:HG	10:A:598:LYS:HE3	1.32	1.08
7:P:343:SER:HB3	7:P:344:ILE:HA	1.09	1.05
10:A:594:LEU:CG	10:A:598:LYS:HE3	1.87	1.05
10:A:876:ILE:O	10:A:880:ARG:HB3	1.56	1.05
5:a:1:DA:H2"	5:a:2:DT:C7	1.87	1.04
7:P:216:ARG:HG2	7:P:216:ARG:HH11	1.17	1.04
7:P:157:ILE:HG12	7:P:333:MET:CE	1.87	1.03
7:P:114:LYS:HG3	7:P:115:PRO:HD3	1.37	1.03
13:D:412:TYR:CG	14:H:560:ILE:HG21	1.93	1.03
13:D:412:TYR:CD1	14:H:560:ILE:HG21	1.95	1.01
7:P:122:ARG:HH11	7:P:122:ARG:HG2	1.25	1.00
5:a:2:DT:H2"	5:a:3:DC:C5	1.97	0.99
7:P:25:GLU:O	10:A:619:ARG:NH2	1.96	0.98
7:P:76:LEU:HD21	7:P:108:MET:HE3	1.46	0.97
10:A:570:LYS:HE2	15:I:90:LEU:H	1.25	0.97
10:A:1190:ASP:O	10:A:1194:GLN:HB2	1.63	0.97
7:P:343:SER:HB3	7:P:344:ILE:CA	1.95	0.97
7:P:76:LEU:HD22	7:P:108:MET:CE	1.86	0.97
7:P:76:LEU:CD2	7:P:108:MET:HE3	1.93	0.96
13:D:412:TYR:HD1	14:H:560:ILE:HG23	1.16	0.96
7:P:155:PHE:HE2	7:P:333:MET:HE3	1.16	0.95
10:A:801:GLN:O	10:A:805:LEU:HB2	1.67	0.95
10:A:673:GLN:O	10:A:677:THR:HB	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:157:ILE:HD11	7:P:333:MET:HE2	1.49	0.94
10:A:1253:LEU:O	10:A:1257:LEU:HB3	1.66	0.94
10:A:807:THR:O	10:A:811:GLU:HB2	1.68	0.93
7:P:36:ILE:CG1	7:P:54:MET:CE	2.41	0.93
10:A:875:TYR:O	10:A:879:GLU:HB2	1.68	0.93
7:P:157:ILE:CG1	7:P:333:MET:HE1	1.99	0.92
7:P:108:MET:SD	22:P:606:HOH:O	2.27	0.91
11:B:933:ASN:HB2	11:B:936:ARG:HE	1.34	0.91
7:P:157:ILE:CD1	7:P:333:MET:CE	2.48	0.91
13:D:412:TYR:CG	14:H:560:ILE:CG2	2.54	0.90
7:P:155:PHE:CZ	7:P:333:MET:HE3	2.07	0.90
10:A:972:SER:O	10:A:976:THR:HB	1.71	0.90
7:P:166:VAL:HG21	7:P:333:MET:SD	2.13	0.89
12:C:641:PRO:HG2	13:D:372:SER:OG	1.72	0.89
7:P:84:GLU:OE2	7:P:88:ARG:NH1	2.05	0.89
10:A:594:LEU:CD1	10:A:598:LYS:HE3	2.03	0.88
13:G:519:ILE:HD12	13:G:572:ASP:HB3	1.55	0.88
5:a:1:DA:H2"	5:a:2:DT:H72	1.56	0.88
10:A:794:MET:HE1	10:A:1192:GLN:HA	1.57	0.87
5:a:1:DA:C2'	5:a:2:DT:H72	2.03	0.87
8:Q:303:ASN:HD21	8:Q:307:LYS:HZ1	1.19	0.87
12:C:432:VAL:HG12	12:C:436:LYS:H	1.40	0.86
12:C:644:GLU:HA	12:C:647:ILE:CG1	2.04	0.86
10:A:771:GLN:O	10:A:775:LEU:HB2	1.76	0.86
5:a:143:DG:C2	6:b:14:DG:C2	2.64	0.85
11:B:887:SER:O	11:B:890:LYS:HB3	1.76	0.85
10:A:974:GLU:O	10:A:978:LEU:HB2	1.77	0.85
12:C:439:LEU:HD22	13:E:387:LYS:HG2	1.59	0.85
7:P:157:ILE:CG1	7:P:333:MET:CE	2.52	0.84
5:a:1:DA:H2"	5:a:2:DT:H73	1.61	0.83
7:P:36:ILE:N	7:P:54:MET:HE1	1.92	0.83
10:A:1188:HIS:O	10:A:1192:GLN:HB2	1.78	0.83
13:G:677:ARG:HH11	13:G:678:GLN:H	1.25	0.83
7:P:157:ILE:HD13	7:P:333:MET:HE2	1.60	0.83
10:A:557:ASN:HB3	11:B:907:ALA:H	1.44	0.83
10:A:570:LYS:NZ	15:I:88:GLU:O	2.13	0.82
12:C:644:GLU:HA	12:C:647:ILE:HG13	1.61	0.81
7:P:36:ILE:CA	7:P:54:MET:HE1	2.10	0.81
10:A:684:ARG:O	10:A:688:ALA:HB3	1.81	0.81
12:C:505:THR:HA	12:C:508:GLN:HB2	1.63	0.81
7:P:166:VAL:CG2	7:P:333:MET:SD	2.68	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:712:MET:HE3	13:E:310:TYR:HB3	1.63	0.81
7:P:147:LEU:CD2	7:P:443:MET:SD	2.68	0.81
7:P:36:ILE:HD12	7:P:54:MET:SD	2.22	0.80
10:A:597:LYS:HB2	10:A:597:LYS:NZ	1.95	0.80
10:A:505:LEU:HB2	13:G:573:LYS:HE2	1.64	0.79
13:D:412:TYR:HB2	14:H:560:ILE:HG22	1.65	0.79
5:a:1:DA:C2'	5:a:2:DT:C7	2.59	0.79
12:C:504:ALA:O	12:C:508:GLN:NE2	2.15	0.78
7:P:36:ILE:HD12	7:P:54:MET:HE3	0.78	0.78
7:P:159:ILE:HD11	7:P:408:ILE:HD11	1.65	0.78
8:Q:459:PRO:HG2	9:Z:63:TRP:CD2	2.18	0.78
13:D:414:THR:OG1	13:E:309:SER:N	2.15	0.78
13:D:434:LEU:HD12	13:D:435:PRO:HD2	1.65	0.78
10:A:597:LYS:HA	10:A:600:GLU:HB2	1.66	0.78
7:P:36:ILE:N	7:P:54:MET:CE	2.47	0.77
7:P:114:LYS:HG3	7:P:115:PRO:CD	2.14	0.77
13:E:402:LYS:NZ	13:E:403:ASN:O	2.16	0.77
10:A:793:GLU:O	10:A:794:MET:HG3	1.85	0.76
10:A:768:LYS:H	10:A:771:GLN:HE22	1.32	0.76
10:A:935:TRP:HE1	10:A:952:PHE:HB2	1.49	0.76
14:H:394:LYS:NZ	14:H:401:MET:SD	2.58	0.76
7:P:122:ARG:HH11	7:P:122:ARG:CG	1.99	0.76
12:C:557:LEU:HD11	12:C:651:ASN:HB3	1.68	0.76
10:A:1253:LEU:O	10:A:1257:LEU:CB	2.34	0.75
13:E:341:GLU:OE1	13:E:341:GLU:N	2.20	0.75
7:P:100:GLU:HG2	7:P:132:ASN:HB3	1.68	0.75
8:Q:303:ASN:HD21	8:Q:307:LYS:NZ	1.85	0.75
15:I:110:ASN:OD1	15:I:113:SER:OG	2.04	0.75
11:B:747:GLU:OE2	12:C:429:GLN:NE2	2.20	0.74
11:B:1103:HIS:O	11:B:1104:ASN:ND2	2.20	0.74
7:P:36:ILE:HB	7:P:54:MET:HE1	1.69	0.74
10:A:674:THR:O	10:A:678:ARG:HB2	1.88	0.74
10:A:855:LYS:O	10:A:859:ALA:CB	2.35	0.74
12:C:434:ASN:H	12:C:436:LYS:HG3	1.53	0.74
7:P:216:ARG:HG2	7:P:216:ARG:NH1	1.94	0.74
13:F:700:HIS:HA	13:F:703:LYS:HD2	1.69	0.74
6:b:11:DA:H5''	6:b:11:DA:H8	1.52	0.74
11:B:1084:LEU:O	11:B:1087:ARG:HB3	1.87	0.74
11:B:1051:LYS:HZ2	11:B:1053:ASN:HB2	1.52	0.74
13:F:525:GLU:OE2	13:F:564:ARG:NH1	2.21	0.74
7:P:147:LEU:HD22	7:P:443:MET:SD	2.28	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:540:GLN:HG3	13:G:541:GLU:HG3	1.70	0.73
15:I:143:ARG:HA	15:I:146:MET:HE2	1.68	0.73
12:C:562:GLU:HG2	12:C:634:THR:HG21	1.70	0.73
10:A:1254:LEU:O	10:A:1258:LEU:CB	2.35	0.73
12:C:633:ILE:HD12	12:C:633:ILE:H	1.54	0.73
14:H:504:PHE:HA	14:H:507:ILE:HD12	1.69	0.73
10:A:798:LYS:HD3	10:A:922:LEU:HB3	1.71	0.73
10:A:572:ARG:NH2	15:I:93:ILE:O	2.21	0.73
10:A:1022:MET:O	10:A:1026:MET:HB3	1.87	0.73
13:D:414:THR:HG22	13:D:416:HIS:CE1	2.23	0.73
10:A:1004:PRO:HB2	10:A:1205:GLU:HG3	1.71	0.73
11:B:1294:GLN:OE1	11:B:1294:GLN:N	2.18	0.73
10:A:1023:TYR:O	10:A:1027:LEU:HB3	1.89	0.73
18:Q:504:PO4:O2	22:Q:601:HOH:O	2.06	0.72
11:B:715:GLN:HE22	11:B:717:LYS:HB3	1.52	0.72
11:B:938:MET:HE1	11:B:940:ARG:HH21	1.55	0.72
11:B:732:THR:HG21	11:B:924:ILE:HG13	1.71	0.72
12:C:574:GLU:OE1	12:C:574:GLU:N	2.21	0.72
13:D:412:TYR:HB2	14:H:560:ILE:CG2	2.18	0.72
7:P:108:MET:HE2	7:P:119:ILE:HG21	1.72	0.72
12:C:605:HIS:O	12:C:609:ALA:N	2.22	0.72
10:A:921:ILE:HD12	10:A:941:VAL:HG22	1.71	0.72
12:C:502:GLU:O	12:C:508:GLN:NE2	2.23	0.71
12:C:630:LEU:O	12:C:633:ILE:HD11	1.89	0.71
14:H:79:VAL:O	14:H:83:LYS:NZ	2.23	0.71
7:P:157:ILE:HD11	7:P:333:MET:CE	2.18	0.71
13:E:318:LYS:O	13:E:347:ARG:NH2	2.22	0.71
9:Z:84:LEU:O	9:Z:85:LYS:HB2	1.89	0.71
10:A:673:GLN:O	10:A:677:THR:CB	2.37	0.71
13:F:739:VAL:HA	13:F:742:LYS:HD2	1.72	0.71
3:T:32:ARG:NH2	4:U:32:GLU:OE2	2.24	0.71
7:P:76:LEU:HD21	7:P:108:MET:CE	2.04	0.71
10:A:1254:LEU:O	10:A:1258:LEU:HB2	1.90	0.71
12:C:475:ASP:OD1	13:E:369:ARG:NH1	2.23	0.71
8:Q:14:PRO:O	8:Q:116[B]:HIS:HE1	1.72	0.71
12:C:421:ASN:OD1	13:D:415:ARG:NH2	2.24	0.71
12:C:573:GLU:N	12:C:573:GLU:OE2	2.24	0.71
14:H:78:LEU:O	14:H:81:SER:OG	2.08	0.70
14:H:379:VAL:O	14:H:400:THR:HA	1.90	0.70
10:A:533:TYR:CZ	10:A:537:GLN:OE1	2.45	0.70
13:E:312:LYS:HG2	14:H:560:ILE:CD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:393:LEU:HG	14:H:396:SER:HB3	1.74	0.70
5:a:50:DC:H2'	5:a:51:DA:C8	2.27	0.70
7:P:344:ILE:O	7:P:344:ILE:HG23	1.92	0.70
11:B:789:VAL:HG12	11:B:790:THR:H	1.56	0.70
12:C:549:ASP:HA	12:C:557:LEU:O	1.92	0.70
12:C:481:LYS:NZ	12:C:521:ILE:O	2.18	0.70
13:F:597:HIS:N	13:F:600:PHE:O	2.25	0.70
7:P:51:THR:HB	22:P:623:HOH:O	1.91	0.70
12:C:576:ALA:HB1	12:C:590:VAL:HB	1.73	0.70
15:I:157:UNK:O	15:I:161:UNK:N	2.25	0.70
7:P:401:ILE:O	7:P:404:MET:HG2	1.91	0.70
12:C:556:GLN:NE2	12:C:654:GLN:OE1	2.25	0.70
11:B:964:CYS:HB3	11:B:967:LYS:HG2	1.74	0.69
13:G:712:ARG:NH2	14:H:106:SER:OG	2.24	0.69
7:P:183:LYS:O	7:P:183:LYS:HG2	1.91	0.69
10:A:976:THR:O	10:A:980:ILE:HB	1.92	0.69
7:P:14:SER:HA	7:P:71:VAL:HB	1.74	0.69
10:A:1112:MET:HE1	10:A:1134:ASP:HB2	1.74	0.69
13:D:341:GLU:HA	13:D:344:MET:HE2	1.74	0.69
10:A:597:LYS:O	10:A:597:LYS:HE3	1.92	0.69
10:A:594:LEU:O	10:A:598:LYS:CD	2.29	0.69
10:A:789:ILE:HD11	10:A:941:VAL:HG21	1.74	0.69
10:A:855:LYS:O	10:A:859:ALA:HB3	1.92	0.69
12:C:582:GLU:N	12:C:582:GLU:OE1	2.26	0.69
12:C:633:ILE:HD12	12:C:633:ILE:N	2.07	0.69
13:E:308:PRO:O	13:E:311:SER:OG	2.11	0.69
13:G:720:GLU:HA	13:G:723:LEU:HD12	1.75	0.69
5:a:2:DT:H2''	5:a:3:DC:H5	1.56	0.69
10:A:993:ARG:HD3	10:A:1240:LYS:HA	1.75	0.69
7:P:392:VAL:HB	7:P:423:THR:HG22	1.75	0.68
10:A:552:PHE:O	14:H:554:ARG:NH1	2.25	0.68
10:A:807:THR:O	10:A:811:GLU:CB	2.40	0.68
5:a:147:DA:H2'	5:a:147:DA:OP2	1.94	0.68
8:Q:98:ASN:O	8:Q:99:GLN:HG2	1.93	0.68
10:A:792:ASP:HB2	10:A:796:LEU:HD22	1.76	0.68
12:C:546:ILE:O	12:C:560:GLN:HA	1.94	0.68
10:A:547:GLY:HA3	13:E:420:ARG:HD2	1.74	0.68
10:A:570:LYS:HE2	15:I:90:LEU:N	2.07	0.68
11:B:797:ASP:O	11:B:801:GLU:N	2.18	0.68
10:A:952:PHE:HA	10:A:955:TRP:HE3	1.58	0.68
13:F:667:ARG:NH2	13:G:639:SER:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:74:ASN:HA	15:I:77:ARG:HE	1.59	0.68
10:A:1184:ASP:HB3	10:A:1190:ASP:HB2	1.75	0.68
14:H:453:ASN:HB2	14:H:457:ARG:HH12	1.59	0.68
10:A:1264:ARG:HA	10:A:1267:LYS:HB2	1.76	0.68
12:C:422:THR:HG22	12:C:423:THR:H	1.59	0.68
10:A:1190:ASP:OD2	10:A:1210:ARG:NH2	2.26	0.67
7:P:311:GLU:OE2	7:P:407:ARG:NH2	2.28	0.67
11:B:1036:GLN:OE1	11:B:1036:GLN:N	2.27	0.67
11:B:1137:SER:HA	11:B:1140:ILE:HD12	1.77	0.67
8:Q:275:LYS:HB3	8:Q:278:ASP:OD2	1.95	0.67
10:A:976:THR:HG23	10:A:980:ILE:HD12	1.74	0.67
10:A:594:LEU:HD11	10:A:598:LYS:HE3	1.77	0.67
13:G:538:GLY:O	13:G:542:PHE:HB2	1.95	0.67
16:J:19:UNK:O	16:J:23:UNK:N	2.27	0.67
10:A:498:GLN:HA	10:A:501:ILE:HD12	1.76	0.67
10:A:1023:TYR:O	10:A:1027:LEU:CB	2.43	0.67
2:S:45:ARG:HE	5:a:80:DC:H4'	1.60	0.67
8:Q:303:ASN:ND2	8:Q:307:LYS:HZ1	1.91	0.67
12:C:559:ASP:OD1	12:C:560:GLN:N	2.28	0.67
10:A:557:ASN:ND2	11:B:907:ALA:O	2.28	0.66
11:B:958:HIS:CE1	11:B:960:GLU:HA	2.30	0.66
8:Q:107:SER:O	9:Z:11:ASN:HA	1.95	0.66
8:Q:303:ASN:ND2	8:Q:307:LYS:NZ	2.43	0.66
10:A:999:VAL:HG23	10:A:1000:GLU:HG3	1.78	0.66
10:A:973:GLU:O	10:A:977:LEU:HB2	1.94	0.66
11:B:891:ILE:O	11:B:895:ILE:N	2.28	0.66
7:P:382:GLU:CD	7:P:382:GLU:H	2.03	0.66
17:M:28:UNK:O	17:M:32:UNK:N	2.28	0.66
14:H:82:GLU:HA	14:H:85:LEU:HD13	1.78	0.66
7:P:458:GLU:HG2	7:P:459:ASP:N	2.10	0.66
10:A:602:VAL:O	10:A:605:LEU:HD23	1.96	0.66
10:A:570:LYS:HG3	15:I:90:LEU:C	2.20	0.66
11:B:929:SER:O	11:B:981:ASN:ND2	2.29	0.66
13:E:402:LYS:NZ	16:J:59:UNK:O	2.26	0.66
11:B:1307:ASN:HA	11:B:1310:LEU:HD12	1.76	0.65
15:I:136:LEU:O	15:I:139:GLU:HG2	1.96	0.65
2:W:45:ARG:HE	6:b:90:DC:H4'	1.62	0.65
7:P:180:VAL:HG11	7:P:332:LEU:HG	1.78	0.65
10:A:546:ARG:NH2	13:G:566:LEU:O	2.25	0.65
11:B:923:MET:O	11:B:927:ASN:ND2	2.30	0.65
12:C:646:LYS:O	12:C:649:THR:N	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:365:THR:HB	13:E:368:ARG:HH21	1.62	0.65
15:I:78:GLN:O	15:I:82:ARG:HG2	1.96	0.65
6:b:106:DG:OP2	10:A:900:LYS:NZ	2.21	0.64
12:C:465:ASP:OD1	12:C:473:LEU:N	2.30	0.64
3:X:32:ARG:NH2	4:Y:32:GLU:OE2	2.30	0.64
10:A:592:LEU:O	10:A:596:ARG:HG3	1.98	0.64
12:C:584:GLU:HG3	12:C:586:PRO:HD3	1.79	0.64
7:P:36:ILE:CD1	7:P:54:MET:HE1	2.05	0.64
13:F:688:ARG:HH11	14:H:86:ASP:HB2	1.62	0.64
13:G:570:ILE:HG13	13:G:570:ILE:O	1.97	0.64
10:A:1168:LEU:HA	10:A:1196:ARG:HH11	1.61	0.64
11:B:974:ASP:HA	11:B:977:ILE:HD12	1.80	0.64
10:A:594:LEU:CD1	10:A:598:LYS:CE	2.75	0.64
10:A:597:LYS:HB2	10:A:597:LYS:HZ1	1.61	0.64
10:A:1050:ASN:O	10:A:1054:GLN:N	2.25	0.64
11:B:896:ASP:C	15:I:110:ASN:HD22	2.06	0.64
1:V:59:GLU:O	2:W:40:ARG:NH2	2.28	0.64
10:A:559:LEU:HA	11:B:726:LEU:HD12	1.78	0.64
10:A:594:LEU:O	10:A:597:LYS:HG3	1.98	0.64
13:E:306:VAL:O	13:E:394:GLN:NE2	2.31	0.64
10:A:826:SER:HB3	10:A:1169:GLY:HA2	1.80	0.64
10:A:1061:HIS:HB2	10:A:1064:VAL:HG13	1.79	0.64
11:B:1196:SER:N	11:B:1197:GLU:OE2	2.27	0.64
12:C:545:ARG:HH12	12:C:649:THR:HG22	1.62	0.64
13:E:404:ILE:HD11	13:E:408:LEU:HD22	1.79	0.64
11:B:933:ASN:O	11:B:936:ARG:HG2	1.99	0.63
11:B:986:LEU:HD11	11:B:1046:LEU:HD13	1.80	0.63
13:F:686:LEU:HD22	15:I:133:LYS:HG2	1.80	0.63
10:A:594:LEU:HG	10:A:598:LYS:CE	2.18	0.63
10:A:1300:MET:HB3	10:A:1304:ARG:HE	1.63	0.63
11:B:1081:ASP:OD1	11:B:1082:LYS:N	2.31	0.63
11:B:990:SER:O	11:B:993:ASP:N	2.31	0.63
11:B:1300:GLN:OE1	11:B:1304:ASN:ND2	2.31	0.63
13:G:525:GLU:O	13:G:564:ARG:NH2	2.25	0.63
16:J:5:UNK:O	16:J:9:UNK:N	2.31	0.63
10:A:790:LEU:HD23	10:A:798:LYS:HG2	1.80	0.63
12:C:511:ASP:N	12:C:511:ASP:OD1	2.31	0.63
12:C:602:HIS:HA	12:C:605:HIS:NE2	2.13	0.63
11:B:719:LEU:HD13	14:H:554:ARG:HH21	1.64	0.63
13:D:426:GLU:HB3	13:E:413:SER:H	1.64	0.63
13:E:354:TYR:OH	13:E:394:GLN:N	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:555:HIS:HB2	13:D:422:LEU:HD13	1.79	0.63
11:B:1145:THR:HG21	11:B:1239:ILE:HD11	1.80	0.63
13:D:417:ASP:OD2	16:J:64:UNK:N	2.29	0.63
13:E:309:SER:O	13:E:312:LYS:N	2.23	0.63
7:P:148:SER:HB2	7:P:442:THR:HG21	1.79	0.63
10:A:771:GLN:O	10:A:775:LEU:CB	2.47	0.63
13:D:412:TYR:CB	14:H:560:ILE:CG2	2.77	0.63
7:P:121:GLU:O	7:P:125:GLU:HG3	1.98	0.63
12:C:515:GLN:OE1	12:C:518:GLN:NE2	2.31	0.63
13:E:308:PRO:HB2	13:E:310:TYR:CE2	2.34	0.63
11:B:915:ASN:HD21	11:B:962:PHE:HA	1.62	0.62
13:D:354:TYR:OH	13:D:394:GLN:NE2	2.32	0.62
5:a:146:DT:H2''	5:a:147:DA:H5'	1.81	0.62
11:B:982:ILE:HB	11:B:1046:LEU:HD11	1.80	0.62
12:C:583:LEU:HD23	12:C:584:GLU:HG2	1.80	0.62
13:F:676:GLU:OE2	13:F:677:ARG:NH2	2.30	0.62
13:D:427:SER:OG	13:D:428:TYR:N	2.32	0.62
14:H:309:SER:OG	14:H:416:LEU:O	2.12	0.62
6:b:59:DT:H2'	6:b:60:DT:H71	1.82	0.62
11:B:706:ASN:OD1	11:B:707:LEU:N	2.33	0.62
7:P:76:LEU:HD23	7:P:108:MET:HE1	1.73	0.62
10:A:1094:ARG:NH1	10:A:1280:ASP:OD1	2.33	0.62
11:B:1092:TYR:O	11:B:1093:ASN:ND2	2.32	0.62
12:C:454:SER:HB3	13:E:335:ILE:HB	1.80	0.62
13:E:301:GLN:HE21	13:E:303:HIS:H	1.47	0.62
7:P:76:LEU:HD23	7:P:108:MET:CE	2.23	0.62
10:A:584:GLN:O	10:A:588:ASN:ND2	2.33	0.62
10:A:829:SER:HG	10:A:1143:SER:HG	1.45	0.62
13:F:670:ILE:HG21	14:H:508:SER:HB3	1.82	0.62
5:a:108:DC:H2''	5:a:109:DC:C5	2.35	0.62
13:G:528:SER:N	13:G:531:ASP:OD2	2.32	0.62
7:P:153:SER:HA	7:P:169:ILE:O	1.99	0.61
7:P:203:GLU:O	7:P:204:GLU:HB2	2.00	0.61
13:E:374:ASP:OD1	13:E:375:ALA:N	2.33	0.61
13:F:673:THR:O	13:F:677:ARG:HG2	2.00	0.61
5:a:143:DG:C2	6:b:14:DG:N2	2.69	0.61
7:P:343:SER:CB	7:P:344:ILE:CA	2.66	0.61
8:Q:14:PRO:O	8:Q:116[B]:HIS:CE1	2.53	0.61
10:A:1141:GLU:HA	10:A:1144:GLU:HB3	1.81	0.61
11:B:886:THR:O	11:B:889:LYS:HB2	1.99	0.61
13:D:339:THR:HG23	13:D:342:VAL:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:16:THR:HA	5:a:30:DT:H5"	1.80	0.61
7:P:256:ILE:O	7:P:260:GLN:HB2	2.01	0.61
11:B:896:ASP:CG	15:I:110:ASN:HB3	2.24	0.61
12:C:471:PHE:HB3	12:C:473:LEU:HG	1.81	0.61
11:B:1034:LYS:O	11:B:1037:THR:OG1	2.16	0.61
11:B:1195:SER:H	11:B:1251:LYS:HE2	1.65	0.61
16:J:4:UNK:O	16:J:8:UNK:N	2.33	0.61
3:T:16:THR:HA	6:b:40:DA:H5"	1.82	0.61
11:B:979:LEU:HA	11:B:982:ILE:HD12	1.82	0.61
13:D:308:PRO:O	13:D:311:SER:OG	2.17	0.61
11:B:919:SER:O	11:B:922:SER:OG	2.16	0.61
11:B:1029:GLN:OE1	11:B:1029:GLN:N	2.22	0.61
13:G:557:SER:N	13:G:560:GLN:OE1	2.30	0.61
14:H:457:ARG:HA	14:H:461:ILE:HD11	1.82	0.61
8:Q:47:GLN:O	8:Q:48:ASP:HB3	2.00	0.61
11:B:889:LYS:O	11:B:893:ASP:N	2.29	0.61
11:B:1051:LYS:NZ	11:B:1053:ASN:HD22	1.99	0.61
11:B:1140:ILE:O	11:B:1143:SER:OG	2.17	0.61
10:A:1230:ASP:OD2	10:A:1268:ARG:NH2	2.30	0.61
12:C:465:ASP:O	12:C:470:ARG:NH2	2.34	0.61
13:E:415:ARG:HE	13:E:416:HIS:CE1	2.18	0.61
1:V:41:TYR:HA	5:a:143:DG:H5"	1.82	0.60
6:b:115:DG:H2"	6:b:116:DT:H5"	1.83	0.60
7:P:36:ILE:HG13	7:P:54:MET:HE1	1.75	0.60
10:A:552:PHE:C	14:H:554:ARG:HH11	2.08	0.60
10:A:792:ASP:HA	10:A:993:ARG:HA	1.81	0.60
11:B:744:LYS:HG3	12:C:437:HIS:CE1	2.36	0.60
11:B:1028:PHE:HZ	11:B:1033:GLY:H	1.48	0.60
10:A:594:LEU:HD11	10:A:598:LYS:CE	2.31	0.60
13:D:332:THR:HG23	13:D:334:ARG:H	1.65	0.60
15:I:104:ARG:HH12	16:K:9:UNK:HA	1.64	0.60
7:P:238:VAL:HG21	7:P:404:MET:CG	2.28	0.60
10:A:533:TYR:OH	10:A:537:GLN:OE1	2.16	0.60
13:F:710:LEU:HD23	13:F:713:LYS:HZ3	1.65	0.60
5:a:148:DA:OP2	5:a:148:DA:H8	1.84	0.60
10:A:1199:ARG:NH2	20:A:1803:BEF:F2	2.22	0.60
13:D:318:LYS:O	13:D:347:ARG:NH2	2.34	0.60
5:a:143:DG:N1	6:b:14:DG:N1	2.50	0.60
7:P:108:MET:CE	7:P:119:ILE:HG21	2.31	0.60
13:F:673:THR:O	13:F:677:ARG:NH1	2.34	0.60
11:B:743:VAL:O	11:B:744:LYS:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:410:ASN:HB2	13:D:415:ARG:HD3	1.82	0.60
12:C:564:ASP:OD1	12:C:565:ILE:N	2.33	0.60
13:D:318:LYS:HG2	13:D:319:ILE:H	1.66	0.60
11:B:1206:LYS:O	11:B:1210:ILE:HG12	2.01	0.60
13:G:536:LEU:HA	13:G:539:ILE:HG12	1.82	0.60
13:D:422:LEU:HD23	13:D:422:LEU:H	1.67	0.60
16:J:49:UNK:O	16:J:53:UNK:N	2.34	0.60
7:P:400:LEU:HD12	7:P:433:LYS:HE2	1.84	0.60
12:C:411:GLY:O	12:C:420:THR:OG1	2.19	0.60
12:C:644:GLU:OE1	12:C:644:GLU:N	2.28	0.60
10:A:768:LYS:N	10:A:771:GLN:HE22	2.00	0.59
12:C:564:ASP:OD1	12:C:566:SER:N	2.31	0.59
13:D:371:VAL:HG13	13:D:373:GLY:H	1.67	0.59
13:F:706:LYS:O	13:F:710:LEU:HG	2.01	0.59
6:b:11:DA:H5"	6:b:11:DA:C8	2.36	0.59
10:A:567:PHE:HB2	11:B:926:ARG:CZ	2.32	0.59
10:A:1027:LEU:HA	10:A:1054:GLN:HE22	1.67	0.59
6:b:103:DG:H5"	10:A:905:LYS:HD3	1.82	0.59
11:B:1233:LEU:O	11:B:1236:SER:OG	2.14	0.59
13:E:302:ALA:O	13:E:303:HIS:ND1	2.35	0.59
14:H:76:GLN:HG3	14:H:78:LEU:HD23	1.84	0.59
14:H:99:MET:HA	14:H:102:GLN:HE21	1.68	0.59
14:H:109:SER:HA	14:H:112:PHE:CD2	2.37	0.59
10:A:1301:ASP:O	10:A:1305:SER:OG	2.19	0.59
11:B:896:ASP:O	15:I:110:ASN:ND2	2.32	0.59
10:A:1079:ASN:OD1	10:A:1080:ASP:N	2.35	0.59
12:C:543:ARG:HA	12:C:564:ASP:HA	1.84	0.59
12:C:646:LYS:NZ	13:D:370:ASN:O	2.35	0.59
15:I:138:SER:O	15:I:141:THR:OG1	2.18	0.59
7:P:155:PHE:CE2	7:P:333:MET:HE1	2.34	0.59
9:Z:29:TRP:CD2	9:Z:61:LYS:HD3	2.38	0.59
10:A:1170:LEU:HD13	10:A:1172:LEU:HG	1.85	0.59
11:B:750:ASP:O	11:B:754:ILE:HG12	2.03	0.59
13:D:426:GLU:OE2	13:E:413:SER:N	2.36	0.59
14:H:71:GLU:OE1	14:H:73:TYR:N	2.35	0.59
7:P:166:VAL:HG22	7:P:333:MET:SD	2.43	0.59
8:Q:35:LEU:HD11	9:Z:84:LEU:HD13	1.84	0.59
8:Q:53:TYR:CD1	8:Q:81:GLN:HG3	2.37	0.59
11:B:1294:GLN:O	11:B:1298:GLN:HG2	2.02	0.59
12:C:466:GLN:HE21	12:C:468:ARG:HH21	1.50	0.59
13:F:661:ILE:HA	13:F:664:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:11:UNK:O	16:J:15:UNK:N	2.36	0.59
11:B:976:VAL:HA	11:B:979:LEU:HD12	1.84	0.59
8:Q:44:THR:OG1	8:Q:62:ALA:HB2	2.02	0.58
13:G:519:ILE:CD1	13:G:572:ASP:HB3	2.32	0.58
13:G:677:ARG:HH11	13:G:678:GLN:N	1.98	0.58
6:b:86:DC:H2"	6:b:87:DG:C8	2.38	0.58
11:B:1197:GLU:H	11:B:1199:ASN:CG	2.12	0.58
8:Q:182:HIS:HE1	22:Q:628:HOH:O	1.85	0.58
11:B:1293:ILE:HA	11:B:1296:ILE:HD12	1.86	0.58
12:C:550:ILE:O	12:C:556:GLN:HA	2.03	0.58
7:P:155:PHE:CZ	7:P:333:MET:CE	2.77	0.58
7:P:381:PRO:C	7:P:383:GLN:H	2.11	0.58
7:P:389:LEU:HB3	7:P:421:LEU:HD23	1.84	0.58
10:A:538:LEU:HD13	10:A:541:LEU:HD13	1.85	0.58
11:B:1196:SER:OG	11:B:1251:LYS:NZ	2.37	0.58
13:F:663:SER:HA	13:F:666:TYR:CD2	2.38	0.58
15:I:91:SER:OG	15:I:92:ASN:N	2.36	0.58
2:S:79:LYS:N	5:a:101:DG:OP1	2.36	0.58
5:a:118:DC:H2"	5:a:119:DA:N7	2.17	0.58
10:A:1339:GLU:O	10:A:1343:ALA:HB2	2.03	0.58
13:E:311:SER:O	13:E:313:TRP:N	2.32	0.58
7:P:36:ILE:HG13	7:P:54:MET:CE	2.32	0.58
13:F:667:ARG:HA	13:F:670:ILE:HD12	1.85	0.58
4:U:65:ASP:OD2	2:W:98:TYR:OH	2.18	0.58
7:P:380:SER:O	7:P:383:GLN:HB2	2.03	0.58
11:B:869:ARG:HA	11:B:953:TRP:CZ3	2.38	0.58
11:B:1064:LYS:HG3	11:B:1104:ASN:ND2	2.19	0.58
13:G:723:LEU:O	13:G:727:LEU:HG	2.03	0.58
13:G:743:CYS:O	13:G:747:ILE:HG13	2.02	0.58
10:A:542:GLN:OE1	10:A:546:ARG:NH2	2.36	0.58
10:A:1254:LEU:O	10:A:1258:LEU:HB3	2.02	0.58
11:B:926:ARG:O	11:B:929:SER:OG	2.19	0.58
7:P:334:ALA:HB2	7:P:415:ARG:HD3	1.86	0.58
10:A:1171:ASN:ND2	19:A:1802:ADP:O1A	2.37	0.58
11:B:944:LEU:O	11:B:948:ILE:HG12	2.04	0.58
12:C:537:LEU:N	13:D:334:ARG:HH22	2.02	0.58
13:E:374:ASP:OD1	13:E:376:ALA:N	2.37	0.58
13:F:692:GLU:HB3	14:H:89:ILE:HG21	1.85	0.58
10:A:595:GLU:HA	10:A:598:LYS:HB2	1.86	0.58
13:F:732:ASN:O	13:F:736:ILE:HG13	2.04	0.58
13:G:678:GLN:HB2	13:G:679:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1261:GLU:O	10:A:1265:ARG:HG2	2.04	0.57
12:C:461:ARG:NH1	16:N:31:UNK:O	2.36	0.57
5:a:125:DG:H2'	5:a:126:DT:C6	2.38	0.57
7:P:44:GLU:O	7:P:44:GLU:HG2	2.04	0.57
8:Q:199:LYS:HD2	8:Q:210:ILE:HD13	1.85	0.57
10:A:556:GLN:OE1	14:H:554:ARG:NH1	2.37	0.57
11:B:1051:LYS:HZ3	11:B:1053:ASN:HD22	1.51	0.57
14:H:324:THR:HG23	14:H:327:ASP:H	1.69	0.57
5:a:143:DG:N2	6:b:14:DG:C2	2.72	0.57
7:P:159:ILE:HG23	7:P:164:CYS:SG	2.44	0.57
11:B:866:GLU:OE1	11:B:866:GLU:N	2.30	0.57
12:C:517:ILE:O	12:C:521:ILE:HG23	2.03	0.57
13:G:519:ILE:HD12	13:G:572:ASP:CB	2.32	0.57
10:A:1084:ARG:NH2	10:A:1315:SER:O	2.37	0.57
14:H:111:GLU:HA	14:H:114:TYR:CD2	2.39	0.57
7:P:155:PHE:HE2	7:P:333:MET:CE	1.94	0.57
8:Q:141:ILE:HG12	8:Q:448:TYR:HB3	1.85	0.57
10:A:483:VAL:HG13	10:A:485:PRO:HD3	1.85	0.57
10:A:773:LYS:O	10:A:777:TRP:HB2	2.04	0.57
10:A:798:LYS:HB3	10:A:922:LEU:HD13	1.86	0.57
11:B:874:GLN:HE22	11:B:959:PRO:HD2	1.70	0.57
11:B:880:HIS:CE1	11:B:958:HIS:HB3	2.39	0.57
11:B:1199:ASN:OD1	11:B:1199:ASN:N	2.31	0.57
11:B:1264:GLU:HA	11:B:1267:LYS:HD3	1.85	0.57
12:C:469:ASP:HB2	12:C:471:PHE:HE2	1.68	0.57
14:H:308:MET:HE2	14:H:417:PRO:HD3	1.87	0.57
10:A:595:GLU:HA	10:A:598:LYS:HG2	1.87	0.57
10:A:796:LEU:HD21	10:A:994:ARG:HB2	1.85	0.57
13:E:354:TYR:CD2	13:E:391:ILE:HA	2.40	0.57
13:E:364:VAL:HB	13:E:382:HIS:CG	2.39	0.57
15:I:139:GLU:O	15:I:143:ARG:HD3	2.04	0.57
6:b:118:DT:H2''	6:b:119:DA:N7	2.18	0.57
7:P:216:ARG:HA	7:P:216:ARG:NE	2.20	0.57
7:P:381:PRO:HG2	7:P:382:GLU:OE2	2.04	0.57
7:P:418:GLN:O	7:P:418:GLN:HG3	2.03	0.57
10:A:559:LEU:HD21	11:B:722:ILE:HG23	1.86	0.57
10:A:1339:GLU:O	10:A:1343:ALA:CB	2.53	0.57
11:B:1058:LYS:HA	11:B:1061:LEU:HD12	1.87	0.57
11:B:1237:ILE:O	11:B:1240:SER:OG	2.18	0.57
13:E:420:ARG:O	13:E:420:ARG:NH1	2.37	0.57
1:R:68:GLN:HE21	1:R:72:ARG:HH21	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:968:LYS:O	10:A:972:SER:OG	2.20	0.57
11:B:864:LEU:HB2	11:B:865:PRO:HD3	1.86	0.57
11:B:1292:ASP:OD1	11:B:1292:ASP:N	2.37	0.57
12:C:464:PHE:HB2	12:C:473:LEU:HB2	1.85	0.57
12:C:488:ILE:O	12:C:492:VAL:HG23	2.05	0.57
12:C:514:CYS:HA	12:C:517:ILE:HD12	1.87	0.57
8:Q:34:GLU:CD	8:Q:34:GLU:H	2.13	0.56
10:A:1212:ILE:HG23	10:A:1218:GLU:HG3	1.85	0.56
11:B:761:SER:O	11:B:764:SER:OG	2.18	0.56
10:A:855:LYS:O	10:A:859:ALA:HB2	2.05	0.56
11:B:1301:LEU:HA	11:B:1304:ASN:HD22	1.69	0.56
13:E:420:ARG:HD3	13:E:420:ARG:N	2.19	0.56
14:H:519:ILE:O	14:H:522:THR:OG1	2.20	0.56
7:P:241:LYS:NZ	7:P:245:GLU:HB3	2.19	0.56
10:A:555:HIS:O	10:A:558:SER:OG	2.20	0.56
11:B:935:SER:HA	11:B:938:MET:HB2	1.86	0.56
12:C:593:ILE:O	12:C:596:SER:OG	2.22	0.56
13:D:406:PRO:HA	13:E:352:ASN:HD21	1.70	0.56
13:D:412:TYR:CB	14:H:560:ILE:HG21	2.33	0.56
13:F:657:SER:O	13:F:661:ILE:HG12	2.05	0.56
14:H:490:VAL:HA	14:H:493:ASN:HD22	1.69	0.56
7:P:194:HIS:NE2	7:P:203:GLU:OE1	2.39	0.56
10:A:1199:ARG:NH1	20:A:1803:BEF:F3	2.28	0.56
13:D:324:VAL:HG23	13:D:331:PHE:CD1	2.40	0.56
13:E:308:PRO:HD3	13:E:393:TYR:CE2	2.39	0.56
10:A:589:HIS:ND1	11:B:1050:GLU:HG2	2.20	0.56
12:C:570:ASN:HD21	13:D:380:ARG:NE	2.04	0.56
7:P:72:ASP:OD1	7:P:74:GLN:HB2	2.05	0.56
11:B:785:ASN:HB3	13:E:345:ARG:NH2	2.21	0.56
13:F:690:GLN:HB3	13:F:691:MET:HE2	1.88	0.56
14:H:498:ASN:O	14:H:502:ARG:HG2	2.05	0.56
3:T:63:LEU:HD11	4:U:38:VAL:HG13	1.87	0.56
10:A:525:THR:HA	10:A:528:ASN:ND2	2.20	0.56
13:F:702:LYS:HD3	13:F:706:LYS:HZ1	1.70	0.56
14:H:117:LEU:O	14:H:118:ASN:ND2	2.39	0.56
15:I:138:SER:O	15:I:142:ILE:HG12	2.06	0.56
10:A:821:VAL:HG12	10:A:892:ILE:HB	1.88	0.56
1:V:68:GLN:HE21	1:V:72:ARG:HH21	1.52	0.56
5:a:23:DC:H2"	5:a:24:DG:C8	2.41	0.56
10:A:546:ARG:CZ	14:H:541:ARG:HE	2.18	0.56
13:D:363:SER:OG	13:D:364:VAL:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:437:MET:O	13:D:441:LYS:N	2.37	0.56
7:P:26:LEU:HB3	7:P:27:PRO:HD2	1.88	0.56
10:A:1134:ASP:OD2	10:A:1136:HIS:NE2	2.39	0.56
15:I:170:UNK:O	15:I:174:UNK:N	2.39	0.56
10:A:880:ARG:O	10:A:884:SER:OG	2.17	0.55
11:B:880:HIS:HE1	11:B:958:HIS:O	1.89	0.55
13:G:530:GLU:HA	13:G:533:GLN:HB2	1.88	0.55
14:H:532:ASP:OD1	14:H:532:ASP:N	2.37	0.55
6:b:48:DG:H2''	6:b:49:DA:C8	2.42	0.55
6:b:128:DT:H2''	6:b:129:DG:N7	2.20	0.55
7:P:36:ILE:H	7:P:54:MET:CE	2.19	0.55
11:B:999:ILE:O	11:B:1002:ILE:HG22	2.06	0.55
12:C:584:GLU:HB2	13:D:401:PRO:HG3	1.88	0.55
14:H:512:VAL:O	14:H:516:ASN:ND2	2.39	0.55
1:R:124:ILE:HD11	2:S:50:ILE:HG23	1.88	0.55
7:P:426:ASN:HB3	7:P:432:ARG:HG2	1.88	0.55
10:A:944:LYS:HG2	10:A:945:ILE:HG23	1.88	0.55
10:A:1096:LEU:HD23	10:A:1128:ILE:HD13	1.87	0.55
11:B:745:TYR:N	11:B:745:TYR:CD1	2.74	0.55
12:C:567:ASN:ND2	12:C:570:ASN:OD1	2.40	0.55
13:D:438:ALA:O	13:D:442:LYS:N	2.40	0.55
14:H:307:PHE:HD2	14:H:323:GLY:HA2	1.71	0.55
11:B:941:ASN:O	11:B:944:LEU:N	2.39	0.55
14:H:335:TYR:O	14:H:339:ASN:ND2	2.39	0.55
9:Z:69:ASP:O	9:Z:70:GLU:HG3	2.06	0.55
10:A:1019:GLN:HE22	10:A:1062:PRO:HB3	1.70	0.55
10:A:822:ILE:HD11	10:A:873:PHE:HA	1.89	0.55
13:G:735:LYS:O	13:G:739:VAL:HG23	2.06	0.55
10:A:1003:LEU:HD12	10:A:1004:PRO:HD2	1.88	0.55
11:B:1243:GLN:NE2	11:B:1247:CYS:SG	2.79	0.55
12:C:649:THR:OG1	13:D:369:ARG:HA	2.06	0.55
10:A:471:ASN:CG	15:I:129:ASP:HB3	2.32	0.55
14:H:399:ASP:HB2	14:H:401:MET:HG2	1.89	0.55
7:P:48:ILE:HB	7:P:54:MET:SD	2.47	0.55
11:B:1278:THR:OG1	11:B:1281:GLU:HG2	2.07	0.55
5:a:37:DT:H2''	5:a:38:DA:N7	2.22	0.54
8:Q:43:ARG:HG3	8:Q:53:TYR:CE2	2.42	0.54
10:A:505:LEU:O	10:A:508:THR:OG1	2.17	0.54
13:G:519:ILE:CD1	13:G:572:ASP:CB	2.85	0.54
6:b:136:DC:H2'	6:b:137:DT:C6	2.42	0.54
13:E:306:VAL:H	13:E:394:GLN:NE2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:424:PRO:HG2	13:E:425:PHE:CE2	2.42	0.54
14:H:311:SER:OG	14:H:314:LEU:HG	2.08	0.54
10:A:1088:LYS:O	10:A:1092:LEU:HB2	2.07	0.54
11:B:947:PHE:HD2	11:B:948:ILE:HD13	1.72	0.54
12:C:475:ASP:OD1	12:C:476:THR:N	2.40	0.54
7:P:147:LEU:HD23	7:P:443:MET:SD	2.47	0.54
11:B:742:LEU:HB2	11:B:745:TYR:CZ	2.42	0.54
11:B:912:VAL:HG12	11:B:963:THR:HG21	1.88	0.54
13:D:426:GLU:HB3	13:E:412:TYR:HA	1.90	0.54
13:G:546:TRP:HA	13:G:549:VAL:HG22	1.90	0.54
8:Q:275:LYS:HE3	8:Q:277:SER:H	1.73	0.54
10:A:685:GLN:HA	10:A:689:PHE:HD2	1.71	0.54
10:A:1109:PHE:HB3	10:A:1163:THR:HG22	1.89	0.54
10:A:1170:LEU:HD12	10:A:1196:ARG:HD2	1.88	0.54
15:I:71:GLN:O	15:I:74:ASN:HB2	2.08	0.54
7:P:196:ARG:NH2	7:P:312:TYR:OH	2.39	0.54
10:A:1262:GLU:OE2	10:A:1266:LYS:NZ	2.37	0.54
11:B:1232:VAL:C	11:B:1235:PRO:HD2	2.33	0.54
12:C:415:TYR:CE2	12:C:418:GLY:HA2	2.42	0.54
10:A:1094:ARG:O	10:A:1098:LYS:NZ	2.38	0.54
11:B:745:TYR:CD2	11:B:936:ARG:HD3	2.42	0.54
13:F:719:GLN:HA	13:F:722:LEU:HD12	1.90	0.54
10:A:1173:GLN:NE2	19:A:1802:ADP:O2'	2.41	0.54
12:C:527:ASN:HB3	12:C:531:GLU:CD	2.33	0.54
12:C:609:ALA:HA	12:C:614:ASN:HD21	1.72	0.54
13:F:666:TYR:O	13:F:670:ILE:HG13	2.07	0.54
7:P:16[A]:ARG:NH2	22:P:602:HOH:O	2.40	0.54
10:A:1264:ARG:HG3	10:A:1268:ARG:HH12	1.73	0.54
13:F:710:LEU:HB3	14:H:107:LYS:HD3	1.88	0.54
13:D:412:TYR:HD1	14:H:560:ILE:CG2	1.83	0.54
13:D:448:ASP:OD1	13:D:448:ASP:N	2.40	0.54
10:A:499:THR:HG21	13:E:427:SER:HB3	1.89	0.53
13:F:708:MET:HG3	13:F:712:ARG:HH21	1.71	0.53
14:H:465:GLU:O	14:H:469:ASN:ND2	2.42	0.53
17:M:21:UNK:HA	17:M:22:UNK:C	2.37	0.53
6:b:56:DC:H2''	6:b:57:DC:C5	2.44	0.53
10:A:504:ASN:O	10:A:507:THR:OG1	2.22	0.53
12:C:464:PHE:HB2	12:C:473:LEU:HD12	1.90	0.53
13:D:449:SER:HA	13:D:452:THR:HB	1.90	0.53
13:F:703:LYS:HA	13:F:707:PHE:CE2	2.43	0.53
5:a:81:DC:H2''	5:a:82:DG:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:261:GLN:HB2	7:P:262:GLU:OE1	2.09	0.53
10:A:1057:LYS:HB3	10:A:1064:VAL:HG21	1.90	0.53
11:B:952:LEU:HD12	11:B:996:LEU:HD12	1.90	0.53
5:a:84:DG:H2'	5:a:85:DT:H71	1.90	0.53
5:a:102:DA:H2'	5:a:103:DT:H71	1.90	0.53
11:B:710:LEU:HD22	11:B:747:GLU:HG3	1.90	0.53
15:I:115:ASN:OD1	15:I:119:ASN:ND2	2.29	0.53
1:R:63:ARG:NH2	6:b:69:DA:H5''	2.23	0.53
15:I:133:LYS:HD2	15:I:133:LYS:N	2.24	0.53
8:Q:43:ARG:HD3	8:Q:51:TYR:CD1	2.43	0.53
19:A:1802:ADP:O3B	20:A:1803:BEF:F3	2.16	0.53
11:B:741:SER:O	11:B:936:ARG:NH2	2.36	0.53
11:B:915:ASN:ND2	11:B:963:THR:HG23	2.23	0.53
11:B:1136:PHE:CE2	11:B:1140:ILE:HD11	2.44	0.53
16:J:27:UNK:O	16:J:31:UNK:N	2.41	0.53
6:b:78:DG:H2''	6:b:79:DG:C8	2.44	0.53
5:a:1:DA:C2'	5:a:2:DT:H73	2.35	0.53
5:a:54:DG:OP1	10:A:1162:SER:OG	2.24	0.53
6:b:132:DC:H2''	6:b:133:DG:C8	2.43	0.53
7:P:241:LYS:O	7:P:242:ASP:C	2.52	0.53
10:A:958:THR:HA	10:A:975:GLU:HB3	1.90	0.53
12:C:641:PRO:HG2	12:C:646:LYS:HD3	1.91	0.53
13:D:447:SER:OG	13:D:451:SER:N	2.36	0.53
10:A:761:ILE:HG22	10:A:839:ALA:HB1	1.91	0.53
11:B:1055:ASN:OD1	11:B:1055:ASN:N	2.38	0.53
11:B:1279:ASP:HA	11:B:1282:ILE:HD12	1.91	0.53
5:a:140:DA:H5'	5:a:140:DA:C8	2.44	0.53
7:P:438:LEU:O	7:P:442:THR:HG23	2.08	0.53
10:A:941:VAL:HG12	10:A:942:LEU:HG	1.91	0.53
11:B:939:SER:OG	11:B:985:LEU:O	2.17	0.53
11:B:953:TRP:CD1	11:B:957:ILE:HD12	2.44	0.53
12:C:577:GLU:O	12:C:580:CYS:HB3	2.09	0.52
7:P:399:SER:OG	7:P:432:ARG:NH1	2.42	0.52
10:A:505:LEU:O	10:A:509:VAL:HG23	2.08	0.52
10:A:1062:PRO:HG3	10:A:1085:VAL:HG21	1.91	0.52
11:B:1127:ALA:O	11:B:1130:SER:OG	2.20	0.52
11:B:1143:SER:O	11:B:1146:SER:OG	2.19	0.52
3:X:77:ARG:HE	5:a:19:DA:H4'	1.74	0.52
10:A:1022:MET:HE1	10:A:1343:ALA:HB1	1.91	0.52
12:C:439:LEU:O	12:C:442:LYS:HG2	2.10	0.52
12:C:518:GLN:HA	12:C:521:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:549:VAL:HA	13:F:552:ASN:HD22	1.75	0.52
13:F:733:SER:O	13:F:737:VAL:HG23	2.09	0.52
13:G:738:ASN:O	13:G:741:SER:OG	2.23	0.52
6:b:37:DT:H2"	6:b:38:DG:C8	2.44	0.52
10:A:473:ASP:CG	10:A:475:ALA:H	2.16	0.52
11:B:866:GLU:H	11:B:866:GLU:CD	2.16	0.52
11:B:1037:THR:OG1	11:B:1038:PHE:N	2.41	0.52
12:C:469:ASP:HB2	12:C:471:PHE:CE2	2.44	0.52
13:E:417:ASP:HB3	13:E:419:PRO:HD2	1.90	0.52
6:b:87:DG:H2"	6:b:88:DT:H72	1.92	0.52
6:b:120:DC:H2"	6:b:121:DG:C8	2.44	0.52
10:A:575:ASN:N	10:A:578:ASP:OD2	2.43	0.52
10:A:1161:LEU:HD21	10:A:1166:GLY:C	2.35	0.52
7:P:241:LYS:HZ2	7:P:245:GLU:HB3	1.74	0.52
14:H:98:ARG:O	14:H:102:GLN:HG3	2.10	0.52
14:H:485:LYS:O	14:H:488:THR:OG1	2.26	0.52
7:P:6:LYS:HE3	8:Q:121:GLN:OE1	2.10	0.52
10:A:497:TYR:CE2	10:A:501:ILE:HD11	2.45	0.52
19:A:1802:ADP:O1A	20:A:1803:BEF:F3	2.18	0.52
13:D:344:MET:HG2	13:D:347:ARG:HH12	1.73	0.52
13:D:365:THR:HA	13:D:368:ARG:HG3	1.91	0.52
13:D:449:SER:O	13:D:453:LEU:N	2.28	0.52
13:F:681:PHE:HE1	14:H:497:SER:HB2	1.73	0.52
13:G:564:ARG:HA	13:G:567:GLN:HE21	1.75	0.52
7:P:197:LEU:HD11	7:P:231:PHE:CZ	2.45	0.52
13:G:689:LEU:HB3	15:I:143:ARG:HE	1.73	0.52
14:H:375:GLN:HG2	14:H:402:LYS:HE3	1.91	0.52
14:H:464:ALA:O	14:H:468:GLU:HG3	2.10	0.52
15:I:73:LEU:O	15:I:77:ARG:HG3	2.10	0.52
7:P:80:TRP:NE1	7:P:122:ARG:HD3	2.25	0.52
7:P:426:ASN:O	7:P:432:ARG:NE	2.35	0.52
10:A:1207:ARG:NH1	10:A:1286:ILE:O	2.43	0.52
11:B:1029:GLN:HE21	11:B:1032:TRP:HE1	1.57	0.52
7:P:36:ILE:CB	7:P:54:MET:CE	2.68	0.52
10:A:572:ARG:NH1	15:I:95:HIS:HB2	2.24	0.52
11:B:745:TYR:CD1	11:B:746:PRO:HD3	2.45	0.52
12:C:644:GLU:CA	12:C:647:ILE:HG12	2.38	0.52
13:F:702:LYS:HD3	13:F:706:LYS:HE3	1.91	0.52
16:J:42:UNK:O	16:J:46:UNK:N	2.43	0.52
1:R:61:LEU:HD12	2:S:37:LEU:HD23	1.92	0.51
1:V:61:LEU:HD12	2:W:37:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:641:GLU:O	10:A:645:GLN:HG3	2.10	0.51
11:B:715:GLN:OE1	11:B:717:LYS:N	2.43	0.51
11:B:963:THR:OG1	11:B:964:CYS:N	2.41	0.51
12:C:461:ARG:C	12:C:462:LEU:HD22	2.34	0.51
2:W:30:THR:HB	2:W:32:PRO:HD2	1.91	0.51
5:a:16:DC:H2"	5:a:17:DC:C5	2.46	0.51
11:B:932:ASP:HA	11:B:934:ASN:OD1	2.11	0.51
12:C:483:ASP:OD1	12:C:484:LYS:N	2.43	0.51
12:C:497:ARG:HH12	12:C:503:ASP:HA	1.75	0.51
13:D:361:TYR:HB2	13:D:395:VAL:HG11	1.91	0.51
14:H:310:TYR:HB3	14:H:314:LEU:HB2	1.91	0.51
7:P:201:ILE:O	7:P:202:LYS:HB2	2.11	0.51
7:P:446:LEU:HD22	10:A:608:MET:SD	2.50	0.51
11:B:745:TYR:HD2	11:B:936:ARG:HD3	1.76	0.51
13:D:365:THR:OG1	13:D:368:ARG:NH2	2.43	0.51
13:D:426:GLU:CB	13:E:413:SER:H	2.23	0.51
6:b:33:DT:H2"	6:b:34:DG:C8	2.45	0.51
7:P:133:VAL:HG13	7:P:134:PRO:HD2	1.91	0.51
8:Q:32:VAL:HG23	8:Q:33:PRO:HD2	1.92	0.51
10:A:598:LYS:CD	10:A:598:LYS:N	2.73	0.51
11:B:727:ASN:O	11:B:731:VAL:HG23	2.10	0.51
12:C:646:LYS:O	12:C:650:PRO:HD3	2.11	0.51
13:F:735:LYS:O	13:F:739:VAL:HG23	2.11	0.51
14:H:497:SER:HA	14:H:500:ARG:HD3	1.92	0.51
2:S:30:THR:HB	2:S:32:PRO:HD2	1.91	0.51
8:Q:47:GLN:O	8:Q:48:ASP:CB	2.59	0.51
9:Z:85:LYS:O	9:Z:90:ARG:NH1	2.44	0.51
10:A:984:HIS:O	10:A:988:ARG:HG3	2.10	0.51
11:B:1064:LYS:HG3	11:B:1104:ASN:HD22	1.76	0.51
6:b:44:DT:H2"	6:b:45:DA:C8	2.44	0.51
11:B:879:ILE:O	11:B:881:ARG:NE	2.35	0.51
13:E:339:THR:HG22	13:E:342:VAL:HG12	1.93	0.51
6:b:77:DG:H2"	6:b:78:DG:C8	2.46	0.51
7:P:320:SER:OG	7:P:322:LYS:N	2.38	0.51
10:A:1016:SER:O	10:A:1020:GLN:N	2.40	0.51
10:A:1057:LYS:O	10:A:1061:HIS:N	2.43	0.51
10:A:1223:GLU:O	10:A:1227:LYS:HG2	2.09	0.51
11:B:1134:ASP:O	11:B:1138:PRO:HD3	2.11	0.51
12:C:547:LYS:O	12:C:548:LEU:HD23	2.10	0.51
7:P:418:GLN:HG2	7:P:419:TYR:CE1	2.46	0.51
10:A:892:ILE:HD12	10:A:920:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1293:GLU:HA	10:A:1296:VAL:HG22	1.92	0.51
12:C:438:TYR:HB2	13:E:383:LYS:HD2	1.92	0.51
13:F:525:GLU:HB2	13:F:564:ARG:CZ	2.41	0.51
10:A:778:MET:HE2	10:A:920:LEU:HD22	1.92	0.51
10:A:1024:GLN:O	10:A:1028:LYS:HB2	2.11	0.51
10:A:1098:LYS:HG2	10:A:1297:LEU:HD22	1.93	0.51
12:C:510:ILE:HA	12:C:513:ILE:HD12	1.91	0.51
14:H:505:LYS:O	14:H:508:SER:OG	2.16	0.51
14:H:506:LYS:HA	14:H:509:GLU:HG2	1.93	0.51
15:I:74:ASN:O	15:I:78:GLN:HG2	2.11	0.51
10:A:866:PHE:CE1	10:A:869:VAL:HG23	2.46	0.51
11:B:1047:PHE:CE1	11:B:1058:LYS:HD2	2.46	0.51
11:B:1054:LEU:HA	11:B:1057:PHE:CD2	2.45	0.51
12:C:450:MET:HG2	12:C:485:LEU:HD11	1.92	0.51
12:C:597:ILE:O	12:C:601:VAL:HG12	2.11	0.51
13:D:364:VAL:O	13:D:367:ALA:N	2.43	0.51
13:E:350:MET:O	13:E:353:SER:OG	2.25	0.51
15:I:78:GLN:HG3	16:O:3:UNK:C	2.40	0.51
11:B:1202:SER:OG	11:B:1204:LEU:HB2	2.11	0.50
12:C:603:MET:O	12:C:607:SER:N	2.26	0.50
13:F:565:PHE:HE1	13:F:634:ALA:H	1.59	0.50
13:G:691:MET:HA	13:G:694:LEU:HD12	1.92	0.50
13:G:705:GLU:O	13:G:709:GLU:HG2	2.11	0.50
14:H:311:SER:HB3	14:H:414:HIS:HB3	1.93	0.50
5:a:128:DT:H2'	5:a:129:DC:C5	2.46	0.50
6:b:24:DT:H4'	6:b:25:DC:OP1	2.11	0.50
8:Q:335:ILE:HG22	8:Q:340:THR:HG21	1.93	0.50
10:A:570:LYS:NZ	10:A:571:ILE:HG12	2.26	0.50
12:C:588:GLU:HA	13:E:369:ARG:O	2.11	0.50
12:C:636:ASP:OD1	12:C:637:ASP:N	2.44	0.50
13:D:317:GLU:OE1	13:D:317:GLU:N	2.44	0.50
10:A:563:THR:HG22	10:A:564:HIS:H	1.74	0.50
10:A:795:GLY:HA2	10:A:1199:ARG:HH11	1.76	0.50
11:B:1080:LYS:HA	11:B:1083:LYS:HG2	1.93	0.50
7:P:22:SER:HA	7:P:441:LEU:CD1	2.42	0.50
7:P:141:GLU:HB3	7:P:142:PRO:HD3	1.94	0.50
10:A:551:GLN:HG3	13:E:419:PRO:HG3	1.91	0.50
12:C:458:VAL:N	12:C:479:TRP:O	2.44	0.50
12:C:603:MET:HA	12:C:606:LYS:HB3	1.94	0.50
13:D:344:MET:HG2	13:D:347:ARG:NH1	2.26	0.50
10:A:470:ALA:O	15:I:128:CYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:715:GLN:NE2	11:B:717:LYS:HB3	2.22	0.50
14:H:75:PHE:HA	14:H:78:LEU:HD21	1.93	0.50
14:H:381:LEU:HD11	14:H:401:MET:SD	2.52	0.50
15:I:74:ASN:HA	15:I:77:ARG:NE	2.26	0.50
5:a:122:DC:H2''	5:a:123:DA:C8	2.46	0.50
8:Q:102:PHE:HZ	9:Z:6:LEU:CD2	2.25	0.50
10:A:467:THR:OG1	10:A:468:LEU:N	2.44	0.50
10:A:1026:MET:HA	10:A:1029:TYR:CD2	2.47	0.50
11:B:1205:LEU:O	11:B:1208:SER:OG	2.25	0.50
12:C:529:TYR:HA	12:C:532:LEU:HB2	1.92	0.50
13:F:674:ASN:OD1	14:H:504:PHE:HB3	2.11	0.50
13:G:525:GLU:C	13:G:527:TRP:H	2.18	0.50
2:S:92:ARG:NH2	4:U:98:LEU:HD23	2.27	0.50
7:P:407:ARG:O	7:P:411:GLU:HB2	2.12	0.50
11:B:1105:LEU:HD23	11:B:1106:LEU:HD23	1.94	0.50
11:B:1258:CYS:SG	11:B:1259:LEU:N	2.84	0.50
5:a:76:DT:H2''	5:a:77:DC:C6	2.46	0.50
10:A:564:HIS:CD2	11:B:966:ARG:HH12	2.30	0.50
10:A:1288:ALA:C	10:A:1290:ASN:H	2.20	0.50
13:D:350:MET:O	13:D:353:SER:OG	2.27	0.50
13:G:527:TRP:CD1	13:G:564:ARG:HH21	2.30	0.50
13:G:712:ARG:O	13:G:716:GLU:HG2	2.12	0.50
16:J:44:UNK:O	16:J:48:UNK:N	2.45	0.50
6:b:64:DG:H2''	6:b:65:DG:C8	2.46	0.50
7:P:238:VAL:HG22	7:P:404:MET:SD	2.39	0.50
10:A:565:PRO:HG2	10:A:567:PHE:HE1	1.77	0.50
10:A:968:LYS:O	10:A:972:SER:CB	2.59	0.50
12:C:613:TYR:CE1	12:C:619:ALA:HA	2.46	0.50
13:D:415:ARG:NH1	13:D:416:HIS:O	2.45	0.50
13:E:389:GLY:O	13:E:393:TYR:HB2	2.12	0.50
6:b:144:DC:H2''	6:b:145:DG:C8	2.47	0.49
7:P:418:GLN:HB3	22:P:610:HOH:O	2.10	0.49
11:B:1028:PHE:CE2	11:B:1030:LEU:HA	2.47	0.49
10:A:766:THR:HB	19:A:1802:ADP:HN62	1.77	0.49
10:A:1026:MET:HG2	10:A:1054:GLN:OE1	2.12	0.49
12:C:410:ASN:HB2	13:D:415:ARG:CD	2.42	0.49
13:F:707:PHE:O	13:F:711:GLU:HG2	2.13	0.49
14:H:85:LEU:O	14:H:89:ILE:HG12	2.12	0.49
14:H:336:ILE:HD11	14:H:385:LEU:HD21	1.93	0.49
5:a:33:DG:H2'	5:a:34:DT:C6	2.47	0.49
7:P:183:LYS:O	7:P:183:LYS:CG	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:460:TYR:CZ	7:P:464:LYS:HE3	2.47	0.49
8:Q:171:ILE:HD13	8:Q:312:ARG:CG	2.42	0.49
10:A:488:ILE:HD11	13:G:622:THR:HA	1.94	0.49
10:A:566:ASN:HD22	15:I:94:ILE:HG12	1.77	0.49
11:B:956:LEU:HD12	11:B:996:LEU:HD13	1.95	0.49
11:B:1059:SER:O	11:B:1062:LEU:HB2	2.13	0.49
13:D:327:LEU:HB3	13:D:329:GLU:OE2	2.12	0.49
13:E:332:THR:HG23	13:E:334:ARG:H	1.75	0.49
13:E:362:PHE:N	13:E:392:ASN:OD1	2.41	0.49
13:F:709:GLU:C	13:F:713:LYS:HZ2	2.19	0.49
1:R:113:HIS:NE2	1:V:123:ASP:OD1	2.46	0.49
11:B:869:ARG:HG2	11:B:953:TRP:CD2	2.48	0.49
11:B:1035:TYR:O	11:B:1038:PHE:N	2.45	0.49
11:B:1189:LEU:HB2	11:B:1191:PHE:CE2	2.48	0.49
11:B:1292:ASP:O	11:B:1296:ILE:HG13	2.13	0.49
12:C:518:GLN:O	12:C:522:GLN:HG2	2.13	0.49
12:C:613:TYR:C	12:C:615:PHE:H	2.19	0.49
13:F:675:GLU:O	13:F:679:MET:HG2	2.13	0.49
15:I:139:GLU:HG3	15:I:143:ARG:NH1	2.27	0.49
2:S:91:LYS:NZ	4:Y:68:GLU:OE1	2.46	0.49
5:a:144:DA:H2''	5:a:145:DT:H5'	1.95	0.49
11:B:742:LEU:HB2	11:B:745:TYR:CE1	2.47	0.49
13:D:361:TYR:CG	13:D:362:PHE:N	2.80	0.49
13:F:530:GLU:H	13:F:530:GLU:CD	2.18	0.49
13:F:643:GLU:O	13:F:647:GLN:N	2.33	0.49
2:W:92:ARG:NH2	4:Y:98:LEU:HD23	2.28	0.49
10:A:570:LYS:O	15:I:92:ASN:ND2	2.46	0.49
10:A:1261:GLU:HA	10:A:1264:ARG:HG2	1.94	0.49
14:H:100:VAL:O	14:H:104:GLU:HG3	2.11	0.49
16:J:18:UNK:O	16:J:22:UNK:N	2.46	0.49
7:P:170:ILE:O	7:P:173:ILE:HG22	2.13	0.49
5:a:98:DG:H2''	5:a:99:DG:N7	2.28	0.49
7:P:389:LEU:O	7:P:421:LEU:HA	2.13	0.49
8:Q:286:ASP:HB2	8:Q:290:ASN:HB2	1.95	0.49
9:Z:83:ASP:C	9:Z:84:LEU:O	2.52	0.49
10:A:597:LYS:CD	10:A:597:LYS:C	2.86	0.49
11:B:915:ASN:ND2	11:B:963:THR:H	2.11	0.49
12:C:445:VAL:O	12:C:448:GLN:NE2	2.45	0.49
2:W:31:LYS:HB3	2:W:32:PRO:HD3	1.94	0.49
8:Q:153:MET:HG3	8:Q:334:ILE:HD13	1.95	0.49
10:A:541:LEU:O	10:A:545:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1090:GLU:O	10:A:1094:ARG:HG2	2.13	0.49
11:B:952:LEU:HB3	11:B:996:LEU:HD12	1.94	0.49
10:A:755:ILE:HG22	10:A:757:LYS:H	1.78	0.49
10:A:977:LEU:HB3	10:A:981:ARG:NH1	2.28	0.49
10:A:1111:GLN:HG3	10:A:1112:MET:H	1.78	0.49
12:C:411:GLY:O	13:D:415:ARG:NH2	2.45	0.49
12:C:412:TYR:HB2	12:C:419:ILE:HA	1.94	0.49
14:H:512:VAL:HG13	14:H:513:LYS:H	1.78	0.49
6:b:26:DT:H2''	6:b:27:DG:N7	2.27	0.48
6:b:103:DG:H2''	6:b:104:DG:O5'	2.12	0.48
10:A:830:ASN:O	10:A:833:SER:N	2.46	0.48
10:A:890:HIS:NE2	10:A:892:ILE:HD11	2.28	0.48
11:B:1056:TYR:O	11:B:1060:ILE:HG13	2.13	0.48
13:E:402:LYS:HA	16:J:59:UNK:CB	2.43	0.48
13:F:659:ILE:HD13	13:G:633:SER:H	1.77	0.48
13:F:724:ILE:O	13:F:727:LEU:HG	2.12	0.48
13:F:738:ASN:O	13:F:741:SER:OG	2.26	0.48
3:X:21:ALA:HB2	4:Y:118:TYR:HB2	1.95	0.48
10:A:937:LEU:O	10:A:941:VAL:HG23	2.13	0.48
11:B:745:TYR:HE2	11:B:936:ARG:HB2	1.78	0.48
12:C:518:GLN:O	12:C:521:ILE:HG12	2.13	0.48
13:G:721:ASN:O	13:G:725:GLN:HG2	2.13	0.48
13:G:730:ASN:O	13:G:733:SER:OG	2.27	0.48
14:H:328:ALA:O	14:H:331:SER:OG	2.20	0.48
10:A:921:ILE:HD11	10:A:940:PHE:HD2	1.77	0.48
10:A:1232:ASP:O	10:A:1236:ILE:N	2.46	0.48
12:C:645:SER:O	12:C:648:PHE:HD2	1.96	0.48
13:G:682:LEU:HA	13:G:685:GLU:CD	2.38	0.48
14:H:92:ARG:O	14:H:96:MET:HG2	2.13	0.48
14:H:326:HIS:O	14:H:329:ILE:HG12	2.13	0.48
14:H:329:ILE:HA	14:H:332:ILE:HG12	1.96	0.48
6:b:98:DT:H2''	6:b:99:DA:C8	2.48	0.48
7:P:458:GLU:O	7:P:459:ASP:C	2.56	0.48
10:A:542:GLN:HG3	10:A:543:LYS:N	2.28	0.48
10:A:837:LYS:HG3	10:A:838:TRP:CD1	2.48	0.48
10:A:891:MET:HE2	10:A:916:ALA:HB3	1.94	0.48
10:A:939:ASN:ND2	10:A:945:ILE:HG13	2.28	0.48
13:F:563:LEU:O	13:F:567:GLN:N	2.47	0.48
13:F:655:GLU:HA	13:F:658:GLU:CD	2.38	0.48
15:I:81:GLU:HB2	15:I:82:ARG:NH1	2.28	0.48
11:B:1278:THR:HG21	14:H:113:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:381:PRO:HG2	7:P:382:GLU:CD	2.39	0.48
10:A:776:GLN:HA	10:A:779:VAL:HB	1.96	0.48
10:A:846:SER:HA	10:A:870:LEU:O	2.13	0.48
11:B:1006:GLN:NE2	11:B:1029:GLN:HE22	2.12	0.48
13:F:691:MET:HE1	15:I:135:ARG:NH1	2.29	0.48
13:G:703:LYS:O	13:G:706:LYS:HG3	2.13	0.48
14:H:90:HIS:HA	14:H:93:ASN:OD1	2.14	0.48
15:I:88:GLU:OE2	15:I:89:GLN:NE2	2.37	0.48
8:Q:148:ALA:O	8:Q:431:GLY:HA3	2.14	0.48
10:A:1096:LEU:HD12	10:A:1099:LEU:HD12	1.96	0.48
11:B:902:ILE:O	11:B:904:THR:N	2.46	0.48
13:F:725:GLN:HE22	13:F:728:ASN:HD22	1.62	0.48
8:Q:286:ASP:HB3	8:Q:290:ASN:H	1.79	0.48
10:A:650:LYS:HE2	10:A:650:LYS:HA	1.95	0.48
11:B:1124:SER:OG	11:B:1126:SER:O	2.31	0.48
13:D:340:PRO:O	13:D:344:MET:HG3	2.14	0.48
13:E:335:ILE:HD12	13:E:336:PRO:HD2	1.96	0.48
13:F:662:SER:OG	13:F:663:SER:N	2.46	0.48
15:I:125:THR:OG1	15:I:126:VAL:N	2.47	0.48
1:V:46:VAL:HG22	1:V:49:ARG:HH22	1.78	0.48
2:W:88:TYR:O	2:W:92:ARG:HB2	2.14	0.48
5:a:1:DA:C1'	5:a:2:DT:H72	2.44	0.48
6:b:36:DC:H2''	6:b:37:DT:C5	2.48	0.48
10:A:1106:VAL:HB	10:A:1158:CYS:SG	2.53	0.48
11:B:786:GLN:HG2	11:B:787:TYR:H	1.77	0.48
11:B:942:PHE:HA	11:B:945:LYS:HE3	1.95	0.48
11:B:993:ASP:O	11:B:997:ILE:HG12	2.14	0.48
11:B:1275:LEU:HG	11:B:1276:PHE:CG	2.48	0.48
13:G:532:LEU:O	13:G:536:LEU:HG	2.14	0.48
14:H:76:GLN:HG3	14:H:78:LEU:H	1.79	0.48
14:H:76:GLN:HE21	14:H:78:LEU:HA	1.79	0.48
14:H:410:ILE:HD13	14:H:414:HIS:HB2	1.95	0.48
15:I:139:GLU:HG3	15:I:143:ARG:HH12	1.79	0.48
6:b:29:DC:H2''	6:b:30:DA:C8	2.49	0.48
10:A:492:THR:OG1	10:A:493:ALA:N	2.47	0.48
10:A:801:GLN:O	10:A:805:LEU:CB	2.52	0.48
10:A:895:GLU:HG3	10:A:1168:LEU:HD13	1.96	0.48
7:P:381:PRO:C	7:P:383:GLN:N	2.72	0.47
8:Q:30:PHE:HB3	8:Q:433:GLN:OE1	2.14	0.47
11:B:761:SER:OG	11:B:762:ASN:N	2.47	0.47
11:B:1106:LEU:HA	11:B:1109:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:364:VAL:HB	13:E:382:HIS:ND1	2.29	0.47
13:F:727:LEU:HD21	14:H:122:VAL:HG21	1.96	0.47
14:H:529:LEU:HD21	15:I:107:LEU:HB3	1.96	0.47
3:X:32:ARG:HA	3:X:35:ARG:HE	1.79	0.47
5:a:88:DT:H2"	5:a:89:DA:C8	2.48	0.47
7:P:458:GLU:O	7:P:461:GLU:N	2.47	0.47
10:A:570:LYS:O	10:A:572:ARG:N	2.47	0.47
10:A:602:VAL:HA	10:A:605:LEU:HD22	1.96	0.47
10:A:938:LEU:HD23	10:A:944:LYS:NZ	2.29	0.47
12:C:416:GLY:N	13:E:393:TYR:CZ	2.82	0.47
13:F:651:GLU:O	13:F:655:GLU:HG2	2.14	0.47
13:G:685:GLU:HA	13:G:688:ARG:HH12	1.79	0.47
7:P:216:ARG:NH1	7:P:216:ARG:CG	2.69	0.47
8:Q:151:TYR:CD1	10:A:633:LEU:HD12	2.50	0.47
10:A:586:TYR:CZ	11:B:1048:SER:HA	2.49	0.47
10:A:1110:PHE:CE2	10:A:1160:ILE:HG12	2.50	0.47
10:A:1257:LEU:HD12	10:A:1260:ALA:HB3	1.96	0.47
11:B:939:SER:O	11:B:945:LYS:NZ	2.46	0.47
11:B:973:LYS:O	11:B:977:ILE:HG13	2.13	0.47
11:B:1088:LEU:HA	11:B:1091:LEU:HB2	1.95	0.47
11:B:1144:LEU:O	11:B:1147:ILE:HG22	2.14	0.47
12:C:440:GLU:OE1	12:C:440:GLU:N	2.29	0.47
14:H:123:LYS:HD2	14:H:454:ASN:ND2	2.29	0.47
1:R:46:VAL:HG22	1:R:49:ARG:HH22	1.78	0.47
7:P:188:PHE:HZ	7:P:319:ILE:HD13	1.80	0.47
8:Q:120:SER:HB2	8:Q:123:ASP:H	1.78	0.47
10:A:921:ILE:HD11	10:A:940:PHE:CD2	2.49	0.47
11:B:898:PRO:HB2	11:B:899:PHE:CE2	2.48	0.47
13:D:358:PRO:HB2	13:D:394:GLN:NE2	2.28	0.47
14:H:75:PHE:CZ	14:H:77:GLN:HA	2.50	0.47
4:Y:95:VAL:HG13	4:Y:99:LEU:HD12	1.96	0.47
5:a:66:DG:H2"	5:a:67:DT:C6	2.49	0.47
7:P:15:HIS:ND1	7:P:16[B]:ARG:HG2	2.29	0.47
11:B:718:ASN:HB2	11:B:770:TYR:CD2	2.49	0.47
13:F:563:LEU:O	13:F:568:LEU:N	2.44	0.47
14:H:313:GLN:H	14:H:313:GLN:CD	2.22	0.47
8:Q:26:ASN:O	8:Q:27:GLU:HB2	2.15	0.47
8:Q:417:PRO:HD2	22:Q:622:HOH:O	2.15	0.47
11:B:703:GLY:O	12:C:424:THR:HG23	2.14	0.47
11:B:762:ASN:HB2	11:B:767:VAL:HG13	1.97	0.47
11:B:1062:LEU:HD23	11:B:1106:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1306:LYS:O	11:B:1310:LEU:HG	2.14	0.47
12:C:498:ASP:O	12:C:500:ARG:NH1	2.48	0.47
13:D:318:LYS:NZ	13:D:319:ILE:O	2.48	0.47
13:E:348:ASN:HA	13:E:351:VAL:HG12	1.97	0.47
3:T:32:ARG:HA	3:T:35:ARG:HE	1.80	0.47
7:P:337:VAL:O	7:P:340:ALA:HB3	2.15	0.47
8:Q:364:GLU:HG2	8:Q:365:GLU:N	2.29	0.47
9:Z:9:LYS:HD2	9:Z:12:LYS:HE2	1.97	0.47
10:A:562:ASN:OD1	10:A:563:THR:N	2.48	0.47
10:A:681:HIS:HD2	10:A:684:ARG:HB2	1.80	0.47
10:A:755:ILE:O	10:A:776:GLN:NE2	2.47	0.47
10:A:1219:GLU:O	10:A:1223:GLU:HG2	2.14	0.47
11:B:901:LYS:HA	11:B:901:LYS:HD3	1.63	0.47
13:D:433:GLN:N	13:D:433:GLN:OE1	2.48	0.47
14:H:99:MET:O	14:H:102:GLN:NE2	2.48	0.47
14:H:453:ASN:O	14:H:457:ARG:NH1	2.47	0.47
2:W:25:ASN:O	2:W:28:GLY:N	2.37	0.47
3:X:63:LEU:HD11	4:Y:38:VAL:HG13	1.96	0.47
8:Q:403:CYS:HB2	8:Q:404:PRO:HA	1.97	0.47
10:A:674:THR:O	10:A:678:ARG:CB	2.62	0.47
10:A:1056:LYS:HD3	10:A:1185:TRP:HZ2	1.79	0.47
11:B:789:VAL:HG12	11:B:790:THR:N	2.28	0.47
12:C:446:TYR:CE1	12:C:485:LEU:HB3	2.50	0.47
12:C:446:TYR:HE1	12:C:485:LEU:HB3	1.79	0.47
12:C:562:GLU:CG	12:C:634:THR:HG21	2.43	0.47
12:C:594:ALA:O	12:C:597:ILE:HB	2.13	0.47
12:C:602:HIS:HA	12:C:605:HIS:CE1	2.49	0.47
12:C:630:LEU:O	12:C:633:ILE:CD1	2.59	0.47
12:C:640:ARG:HA	12:C:641:PRO:HD3	1.45	0.47
13:D:429:LYS:HE3	13:E:420:ARG:HH22	1.79	0.47
13:D:458:LYS:HA	13:D:461:LYS:HE2	1.97	0.47
13:F:683:THR:HA	15:I:133:LYS:HE3	1.97	0.47
1:V:73:GLU:OE1	2:W:25:ASN:HB2	2.14	0.47
2:W:64:ASN:HB3	2:W:93:GLN:HE22	1.80	0.47
5:a:50:DC:H2'	5:a:51:DA:H8	1.74	0.47
10:A:490:THR:OG1	10:A:491:HIS:N	2.48	0.47
10:A:894:ASP:OD1	10:A:895:GLU:N	2.48	0.47
11:B:863:LEU:H	11:B:863:LEU:HD23	1.80	0.47
11:B:1028:PHE:HE1	11:B:1032:TRP:HD1	1.63	0.47
13:F:689:LEU:O	13:F:693:LYS:HG2	2.15	0.47
4:U:95:VAL:HG13	4:U:99:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:97:DA:C8	5:a:97:DA:H5'	2.50	0.47
14:H:308:MET:SD	14:H:415:LEU:HG	2.55	0.47
1:V:124:ILE:HD11	2:W:50:ILE:HG23	1.97	0.46
7:P:259:LYS:HD2	7:P:259:LYS:O	2.14	0.46
10:A:825:LEU:HD23	10:A:872:THR:HG21	1.96	0.46
11:B:1051:LYS:O	11:B:1053:ASN:N	2.45	0.46
11:B:1195:SER:H	11:B:1251:LYS:CE	2.28	0.46
12:C:447:LYS:HD2	13:E:328:PRO:HG3	1.97	0.46
13:D:374:ASP:O	13:D:378:LEU:HG	2.15	0.46
13:E:306:VAL:H	13:E:394:GLN:HE22	1.60	0.46
13:G:527:TRP:CG	13:G:564:ARG:HH21	2.33	0.46
14:H:489:SER:O	14:H:493:ASN:ND2	2.49	0.46
6:b:49:DA:H2''	6:b:50:DG:H8	1.80	0.46
8:Q:370:GLU:HG3	8:Q:395:VAL:HG21	1.97	0.46
12:C:605:HIS:HA	12:C:608:LEU:HB3	1.96	0.46
12:C:653:LEU:HB2	16:N:13:UNK:HA	1.97	0.46
13:D:307:ILE:HD11	13:D:312:LYS:HA	1.96	0.46
13:G:714:THR:O	13:G:718:GLN:HG3	2.15	0.46
13:G:742:LYS:O	13:G:746:LEU:HG	2.14	0.46
15:I:104:ARG:NH1	16:K:9:UNK:HA	2.30	0.46
3:X:67:GLY:HA3	4:Y:46:HIS:CD2	2.51	0.46
13:F:557:SER:H	13:F:560:GLN:CD	2.24	0.46
14:H:78:LEU:HD13	14:H:84:ARG:NH1	2.31	0.46
1:V:62:ILE:HD11	2:W:37:LEU:HD11	1.97	0.46
7:P:6:LYS:HD2	7:P:23:ASN:ND2	2.30	0.46
8:Q:302:CYS:HB2	22:Q:635:HOH:O	2.16	0.46
10:A:678:ARG:HA	10:A:681:HIS:HB3	1.97	0.46
11:B:920:THR:O	11:B:924:ILE:HG22	2.15	0.46
12:C:646:LYS:HG2	13:D:372:SER:HB3	1.97	0.46
13:D:426:GLU:HB3	13:E:413:SER:N	2.28	0.46
5:a:126:DT:H2'	5:a:127:DG:C8	2.51	0.46
5:a:143:DG:N3	6:b:14:DG:N2	2.64	0.46
6:b:103:DG:H2'	6:b:104:DG:C8	2.51	0.46
7:P:325:PRO:O	7:P:331:PRO:HG2	2.15	0.46
10:A:556:GLN:HB3	11:B:718:ASN:HD21	1.81	0.46
10:A:1061:HIS:CE1	10:A:1089:PHE:HZ	2.34	0.46
12:C:466:GLN:O	12:C:470:ARG:NH2	2.45	0.46
10:A:471:ASN:HB3	15:I:129:ASP:HB3	1.97	0.46
10:A:756:LYS:HG2	10:A:772:ILE:HG21	1.97	0.46
10:A:1237:GLN:HA	10:A:1240:LYS:HE3	1.97	0.46
13:E:361:TYR:CG	13:E:362:PHE:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:23:GLU:OE2	9:Z:65:ARG:HD3	2.16	0.46
10:A:1170:LEU:HD22	10:A:1172:LEU:HD11	1.98	0.46
12:C:523:GLU:O	12:C:606:LYS:HE3	2.15	0.46
13:F:655:GLU:HA	13:F:658:GLU:OE1	2.15	0.46
13:F:708:MET:HG3	13:F:712:ARG:NH2	2.30	0.46
13:G:563:LEU:HG	13:G:567:GLN:NE2	2.30	0.46
5:a:14:DT:H2''	5:a:15:DG:C8	2.51	0.46
6:b:26:DT:H2''	6:b:27:DG:C8	2.50	0.46
7:P:164:CYS:HB2	7:P:182:SER:HB3	1.98	0.46
11:B:724:THR:O	11:B:728:THR:HG22	2.15	0.46
12:C:563:TRP:HZ3	13:D:376:ALA:HB2	1.81	0.46
1:R:113:HIS:CG	1:V:126:LEU:HD22	2.51	0.46
2:S:30:THR:HG21	6:b:70:DA:H5''	1.98	0.46
5:a:11:DC:H2''	5:a:12:DG:C8	2.51	0.46
10:A:540:PRO:HB2	13:D:430:PRO:O	2.16	0.46
11:B:735:ASP:OD1	11:B:735:ASP:N	2.49	0.46
11:B:899:PHE:HE1	14:H:517:GLU:HB2	1.81	0.46
13:F:549:VAL:HA	13:F:552:ASN:ND2	2.29	0.46
14:H:314:LEU:HA	14:H:317:ILE:HD12	1.97	0.46
15:I:133:LYS:HD2	15:I:133:LYS:H	1.81	0.46
8:Q:143:LEU:HD12	8:Q:144:PRO:HD2	1.98	0.46
8:Q:424:TYR:CD1	8:Q:427:ILE:HD12	2.51	0.46
9:Z:33:SER:HB3	9:Z:55:LYS:HD3	1.98	0.46
11:B:1197:GLU:N	11:B:1199:ASN:OD1	2.39	0.46
11:B:1198:GLU:O	14:H:98:ARG:NH1	2.42	0.46
13:F:528:SER:H	13:F:531:ASP:HB2	1.80	0.46
13:G:677:ARG:HD2	13:G:677:ARG:HA	1.68	0.46
5:a:47:DT:H5'	5:a:47:DT:C6	2.51	0.45
6:b:150:DT:H2''	6:b:151:DC:C6	2.51	0.45
7:P:236:LEU:HD22	7:P:309:PHE:CD2	2.51	0.45
10:A:1083:TRP:HB2	10:A:1089:PHE:HB3	1.98	0.45
11:B:1255:PHE:HA	11:B:1258:CYS:SG	2.56	0.45
12:C:466:GLN:H	12:C:466:GLN:CD	2.24	0.45
12:C:644:GLU:CA	12:C:647:ILE:CG1	2.85	0.45
7:P:334:ALA:CB	7:P:415:ARG:HD3	2.46	0.45
8:Q:121:GLN:HG2	8:Q:463:TRP:CH2	2.52	0.45
8:Q:286:ASP:CB	8:Q:290:ASN:H	2.29	0.45
9:Z:56:TYR:HB3	9:Z:58:PHE:CE2	2.50	0.45
10:A:570:LYS:HG3	15:I:90:LEU:O	2.16	0.45
10:A:974:GLU:HG2	10:A:978:LEU:HD12	1.98	0.45
10:A:1141:GLU:O	10:A:1145:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1188:HIS:O	10:A:1192:GLN:CB	2.57	0.45
11:B:718:ASN:O	11:B:722:ILE:HG12	2.16	0.45
12:C:640:ARG:NH2	17:M:72:UNK:O	2.49	0.45
13:D:321:SER:HA	13:D:324:VAL:HG12	1.97	0.45
13:F:685:GLU:O	13:F:689:LEU:HG	2.15	0.45
1:R:63:ARG:HH21	6:b:69:DA:H5"	1.82	0.45
1:R:72:ARG:O	1:R:76:GLN:HG3	2.17	0.45
5:a:119:DA:H1'	5:a:120:DG:C5	2.51	0.45
7:P:320:SER:OG	7:P:321:ASP:N	2.49	0.45
8:Q:30:PHE:N	8:Q:30:PHE:CD1	2.85	0.45
8:Q:212:SER:HB3	8:Q:284:PHE:HE2	1.81	0.45
11:B:708:HIS:CE1	11:B:710:LEU:HD11	2.51	0.45
12:C:463:GLU:HA	12:C:473:LEU:O	2.16	0.45
13:D:315:ASN:C	13:D:317:GLU:H	2.25	0.45
13:F:528:SER:N	13:F:531:ASP:OD2	2.50	0.45
14:H:99:MET:HE3	14:H:103:TRP:HE1	1.81	0.45
5:a:1:DA:C2	5:a:1:DA:OP1	2.68	0.45
5:a:147:DA:OP2	5:a:147:DA:H8	2.00	0.45
7:P:419:TYR:N	7:P:419:TYR:CD1	2.84	0.45
10:A:766:THR:O	19:A:1802:ADP:N6	2.49	0.45
10:A:973:GLU:HA	10:A:977:LEU:HD12	1.98	0.45
10:A:1264:ARG:O	10:A:1268:ARG:HG3	2.16	0.45
13:F:683:THR:O	13:F:687:ILE:HG12	2.15	0.45
14:H:121:ASN:OD1	14:H:122:VAL:HG23	2.17	0.45
1:R:113:HIS:HE1	1:V:122:LYS:HG3	1.81	0.45
6:b:100:DA:H2"	6:b:101:DG:H8	1.82	0.45
8:Q:354:LEU:HD22	8:Q:358:LEU:HD22	1.99	0.45
10:A:1061:HIS:CD2	10:A:1115:ILE:HA	2.52	0.45
11:B:907:ALA:CB	11:B:913:LEU:HB2	2.46	0.45
12:C:529:TYR:CD1	12:C:532:LEU:HB2	2.51	0.45
12:C:613:TYR:OH	12:C:626:ARG:HG2	2.16	0.45
13:E:429:LYS:NZ	13:E:433:GLN:HE21	2.14	0.45
13:F:527:TRP:HE3	13:F:531:ASP:HB3	1.81	0.45
13:G:687:ILE:HA	13:G:690:GLN:OE1	2.16	0.45
14:H:378:ILE:HB	14:H:400:THR:HG22	1.98	0.45
14:H:525:ALA:HA	14:H:528:VAL:HG12	1.97	0.45
14:H:537:GLU:HG3	14:H:538:ASP:H	1.82	0.45
3:X:84:GLN:HE21	3:X:88:ARG:HG3	1.81	0.45
5:a:77:DC:H2"	5:a:78:DC:C5	2.52	0.45
6:b:104:DG:OP2	10:A:904:SER:OG	2.35	0.45
11:B:758:ASN:O	11:B:761:SER:OG	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:917:GLN:O	11:B:921:ILE:HG12	2.16	0.45
14:H:71:GLU:O	14:H:72:LEU:HD23	2.15	0.45
15:I:88:GLU:HB3	15:I:89:GLN:HE22	1.82	0.45
2:S:51:TYR:HB3	2:S:55:ARG:HH12	1.82	0.45
3:T:84:GLN:HE21	3:T:88:ARG:HG3	1.81	0.45
1:V:72:ARG:O	1:V:76:GLN:HG3	2.16	0.45
5:a:59:DA:H2''	5:a:60:DA:C8	2.52	0.45
5:a:148:DA:H2''	5:a:149:DC:C6	2.52	0.45
6:b:94:DC:H2''	6:b:95:DG:C8	2.51	0.45
5:a:7:DA:H2'	5:a:8:DT:H71	1.98	0.45
5:a:35:DC:H2''	5:a:36:DG:C8	2.52	0.45
6:b:39:DG:H2''	6:b:40:DA:H8	1.82	0.45
6:b:92:DT:H2''	6:b:93:DG:C8	2.52	0.45
7:P:282:ASN:O	7:P:285:VAL:HG22	2.16	0.45
10:A:595:GLU:HA	10:A:598:LYS:CG	2.45	0.45
10:A:1079:ASN:H	10:A:1082:ILE:HD12	1.81	0.45
10:A:1176:ASP:OD1	10:A:1176:ASP:N	2.50	0.45
12:C:527:ASN:OD1	12:C:531:GLU:N	2.50	0.45
13:F:676:GLU:CD	13:F:677:ARG:HH22	2.24	0.45
14:H:77:GLN:OE1	14:H:79:VAL:HB	2.17	0.45
14:H:99:MET:CE	14:H:103:TRP:HE1	2.30	0.45
4:Y:99:LEU:O	4:Y:104:ALA:HB2	2.17	0.45
5:a:65:DC:H2''	5:a:66:DG:C8	2.52	0.45
8:Q:146:SER:HB2	8:Q:174:ILE:HD11	1.99	0.45
10:A:522:THR:C	10:A:524:SER:H	2.25	0.45
11:B:1266:LEU:O	11:B:1270:ALA:N	2.45	0.45
14:H:528:VAL:C	14:H:530:SER:H	2.25	0.45
15:I:71:GLN:HA	15:I:74:ASN:CG	2.42	0.45
15:I:75:LYS:HA	16:O:3:UNK:N	2.32	0.45
7:P:145:ILE:O	7:P:149:MET:HG2	2.17	0.45
9:Z:33:SER:HB3	9:Z:55:LYS:CD	2.46	0.45
11:B:710:LEU:HD12	11:B:711:SER:N	2.32	0.45
11:B:934:ASN:O	11:B:938:MET:N	2.49	0.45
13:G:737:VAL:O	13:G:740:LEU:HG	2.17	0.45
6:b:35:DC:H2''	6:b:36:DC:C5	2.52	0.44
10:A:473:ASP:OD1	10:A:474:HIS:N	2.50	0.44
10:A:1013:CYS:HB2	10:A:1213:THR:HG22	1.99	0.44
10:A:1209:LEU:HD21	10:A:1286:ILE:HG21	1.99	0.44
11:B:785:ASN:HD22	13:E:341:GLU:HB3	1.82	0.44
11:B:1265:ILE:HG13	11:B:1266:LEU:H	1.82	0.44
12:C:466:GLN:O	12:C:468:ARG:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:324:VAL:HG12	13:E:331:PHE:CZ	2.52	0.44
13:G:677:ARG:HH12	13:G:679:MET:HE2	1.81	0.44
14:H:86:ASP:OD1	14:H:87:HIS:N	2.50	0.44
5:a:104:DT:H2''	5:a:105:DA:C8	2.51	0.44
10:A:546:ARG:NH1	14:H:541:ARG:HE	2.15	0.44
10:A:575:ASN:O	11:B:1135:GLN:NE2	2.51	0.44
10:A:589:HIS:CE1	11:B:1050:GLU:HG2	2.53	0.44
10:A:1061:HIS:HD2	10:A:1115:ILE:HG13	1.82	0.44
11:B:748:LEU:O	11:B:751:SER:OG	2.33	0.44
12:C:587:GLY:O	12:C:590:VAL:HG22	2.16	0.44
13:E:312:LYS:HG2	14:H:560:ILE:HD11	1.97	0.44
13:F:654:LYS:O	13:F:657:SER:OG	2.28	0.44
14:H:325:SER:HB3	14:H:415:LEU:HD22	2.00	0.44
6:b:70:DA:H2''	6:b:71:DA:H8	1.81	0.44
7:P:232:LYS:HA	7:P:236:LEU:HG	1.99	0.44
10:A:770:TYR:HB3	10:A:999:VAL:HG12	2.00	0.44
10:A:1173:GLN:HA	10:A:1199:ARG:HB3	1.99	0.44
11:B:795:MET:O	11:B:798:LYS:HB2	2.17	0.44
12:C:651:ASN:HD21	13:D:368:ARG:HH22	1.66	0.44
13:D:381:LEU:O	13:D:385:LEU:HG	2.17	0.44
13:G:726:ARG:HG2	13:G:730:ASN:HD21	1.82	0.44
14:H:111:GLU:O	14:H:114:TYR:N	2.46	0.44
4:U:99:LEU:O	4:U:104:ALA:HB2	2.17	0.44
3:X:97:LEU:HD21	4:Y:62:PHE:HE1	1.82	0.44
5:a:107:DT:H2''	5:a:108:DC:C6	2.52	0.44
6:b:14:DG:H2''	6:b:15:DA:C8	2.53	0.44
6:b:38:DG:H2''	6:b:39:DG:C8	2.52	0.44
8:Q:102:PHE:HZ	9:Z:6:LEU:HD23	1.82	0.44
8:Q:338:GLY:O	8:Q:339:THR:C	2.59	0.44
10:A:558:SER:O	10:A:559:LEU:HD23	2.18	0.44
10:A:680:THR:O	10:A:684:ARG:HG2	2.18	0.44
11:B:718:ASN:HD22	11:B:719:LEU:HD23	1.83	0.44
11:B:1119:LEU:H	11:B:1122:VAL:HG22	1.82	0.44
12:C:571:CYS:HB2	12:C:574:GLU:OE2	2.18	0.44
12:C:613:TYR:C	12:C:615:PHE:N	2.74	0.44
13:E:323:GLU:O	13:E:327:LEU:N	2.51	0.44
14:H:81:SER:HA	14:H:83:LYS:HE2	1.98	0.44
14:H:111:GLU:O	14:H:112:PHE:C	2.61	0.44
14:H:389:LEU:HB2	14:H:409:LEU:HD21	1.98	0.44
5:a:147:DA:OP2	5:a:147:DA:C8	2.70	0.44
9:Z:66:ASN:HB3	9:Z:70:GLU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1055:LEU:HA	10:A:1058:ILE:HG12	1.98	0.44
11:B:1034:LYS:HA	11:B:1034:LYS:HD3	1.74	0.44
12:C:475:ASP:OD2	13:E:368:ARG:NH1	2.48	0.44
13:D:343:TYR:HA	13:D:346:TYR:CD2	2.53	0.44
13:D:407:PRO:C	13:D:408:LEU:HD22	2.41	0.44
13:F:685:GLU:OE2	14:H:83:LYS:HD3	2.17	0.44
14:H:418:LEU:HD23	14:H:418:LEU:HA	1.82	0.44
10:A:876:ILE:O	10:A:880:ARG:CB	2.46	0.44
10:A:902:ALA:O	10:A:907:SER:OG	2.32	0.44
11:B:903:ASN:ND2	11:B:906:GLY:O	2.51	0.44
11:B:1027:GLU:HG3	11:B:1118:PRO:HD2	1.99	0.44
12:C:570:ASN:CG	13:D:376:ALA:HB1	2.43	0.44
14:H:338:LEU:HD12	14:H:339:ASN:N	2.32	0.44
15:I:115:ASN:O	15:I:119:ASN:ND2	2.51	0.44
1:R:106:ASP:OD2	1:R:131:ARG:NH2	2.39	0.44
6:b:103:DG:H2'	6:b:104:DG:H8	1.82	0.44
10:A:566:ASN:OD1	10:A:566:ASN:N	2.51	0.44
10:A:1087:GLY:HA2	10:A:1316:ARG:HH12	1.83	0.44
11:B:878:LYS:HG2	11:B:881:ARG:HD3	1.99	0.44
11:B:897:ASP:C	11:B:899:PHE:H	2.26	0.44
11:B:919:SER:O	11:B:923:MET:HG3	2.18	0.44
13:F:694:LEU:HD23	13:F:697:LYS:HZ1	1.83	0.44
13:G:743:CYS:HA	13:G:746:LEU:HD12	1.98	0.44
1:R:46:VAL:HG21	5:a:82:DG:H3'	1.98	0.44
6:b:90:DC:H2''	6:b:91:DG:C8	2.53	0.44
7:P:147:LEU:C	7:P:149:MET:H	2.26	0.44
10:A:1216:SER:OG	10:A:1219:GLU:OE1	2.28	0.44
11:B:862:ASP:OD1	11:B:862:ASP:N	2.49	0.44
11:B:1030:LEU:N	11:B:1120:GLN:OE1	2.51	0.44
13:D:308:PRO:HD3	13:D:393:TYR:CD2	2.53	0.44
13:F:545:ASP:OD1	13:F:545:ASP:N	2.51	0.44
5:a:53:DC:H5''	10:A:1112:MET:HB2	2.00	0.44
10:A:597:LYS:HD3	10:A:598:LYS:HD2	1.99	0.44
10:A:1055:LEU:HD23	10:A:1058:ILE:HD11	2.00	0.44
11:B:1023:LEU:HD22	11:B:1111:SER:HB3	1.99	0.44
12:C:466:GLN:C	12:C:468:ARG:H	2.25	0.44
13:D:369:ARG:NH2	13:D:370:ASN:HD21	2.16	0.44
13:F:530:GLU:OE2	13:F:530:GLU:N	2.28	0.44
13:G:535:LEU:O	13:G:539:ILE:HG23	2.17	0.44
1:V:79:LYS:HD3	1:V:82:LEU:HD21	2.00	0.43
6:b:113:DC:C6	6:b:114:DT:H72	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:129:ASP:OD2	7:P:460:TYR:HE2	2.01	0.43
8:Q:286:ASP:HB2	8:Q:290:ASN:O	2.18	0.43
9:Z:83:ASP:O	9:Z:86:GLU:HG3	2.18	0.43
11:B:711:SER:OG	11:B:712:MET:N	2.51	0.43
11:B:745:TYR:HD1	11:B:745:TYR:H	1.64	0.43
11:B:1091:LEU:HD23	11:B:1091:LEU:HA	1.85	0.43
12:C:452:GLU:HA	13:E:334:ARG:NH1	2.32	0.43
12:C:572:PRO:HD2	12:C:598:ARG:HH22	1.83	0.43
13:D:402:LYS:O	13:D:404:ILE:HG23	2.17	0.43
13:G:521:GLU:N	13:G:521:GLU:OE1	2.51	0.43
14:H:483:GLN:O	14:H:487:ILE:HG12	2.18	0.43
15:I:138:SER:OG	15:I:139:GLU:N	2.51	0.43
1:R:122:LYS:HA	1:R:125:GLN:HG2	2.00	0.43
5:a:18:DG:H2''	5:a:19:DA:C8	2.53	0.43
10:A:496:ILE:HG13	10:A:497:TYR:N	2.32	0.43
10:A:1184:ASP:HB3	10:A:1190:ASP:CB	2.46	0.43
11:B:1117:ILE:HB	11:B:1118:PRO:HD3	2.00	0.43
12:C:599:GLU:O	12:C:603:MET:HE3	2.18	0.43
13:D:347:ARG:HG3	13:D:348:ASN:N	2.32	0.43
14:H:491:LEU:HD23	14:H:491:LEU:HA	1.70	0.43
14:H:513:LYS:HA	14:H:516:ASN:HD22	1.83	0.43
1:V:122:LYS:HA	1:V:125:GLN:HG2	2.00	0.43
6:b:69:DA:H2''	6:b:70:DA:C8	2.54	0.43
10:A:1261:GLU:HG3	10:A:1264:ARG:HH21	1.82	0.43
11:B:777:TYR:CD1	11:B:777:TYR:N	2.86	0.43
11:B:984:HIS:O	11:B:986:LEU:HD12	2.18	0.43
13:D:352:ASN:O	13:D:356:LEU:HG	2.18	0.43
13:E:379:PHE:CZ	13:E:383:LYS:HD3	2.53	0.43
15:I:142:ILE:HA	15:I:145:LEU:HG	1.99	0.43
2:S:31:LYS:HB3	2:S:32:PRO:HD3	2.01	0.43
2:S:88:TYR:O	2:S:92:ARG:HB2	2.17	0.43
7:P:151:LYS:HE3	7:P:424:PHE:CE1	2.53	0.43
11:B:1049:LEU:HD23	11:B:1049:LEU:HA	1.77	0.43
12:C:547:LYS:HB2	12:C:560:GLN:NE2	2.33	0.43
12:C:548:LEU:HD21	12:C:600:GLN:HG3	1.99	0.43
13:E:416:HIS:CE1	16:J:36:UNK:HA	2.53	0.43
14:H:344:ASN:N	14:H:344:ASN:OD1	2.52	0.43
14:H:403:LEU:O	14:H:407:LEU:HG	2.17	0.43
2:S:38:ALA:HB3	2:S:46:ILE:HD11	2.00	0.43
3:X:77:ARG:NE	5:a:19:DA:H4'	2.33	0.43
6:b:141:DC:H2''	6:b:142:DA:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:261:GLN:HB2	7:P:262:GLU:CD	2.43	0.43
10:A:1233:GLY:O	10:A:1237:GLN:HB2	2.18	0.43
11:B:770:TYR:C	11:B:771:HIS:CG	2.96	0.43
11:B:910:PRO:O	11:B:913:LEU:HB3	2.17	0.43
12:C:435:ARG:NH1	12:C:438:TYR:OH	2.51	0.43
12:C:511:ASP:O	12:C:515:GLN:HG2	2.19	0.43
12:C:525:GLN:N	12:C:525:GLN:OE1	2.51	0.43
12:C:549:ASP:HB2	12:C:558:ILE:HD13	2.01	0.43
12:C:554:GLN:NE2	12:C:555:ASN:HB2	2.33	0.43
16:J:30:UNK:O	16:J:34:UNK:N	2.51	0.43
8:Q:197:SER:HB3	8:Q:301:GLY:HA2	1.99	0.43
10:A:503:LEU:O	10:A:507:THR:HG23	2.19	0.43
10:A:522:THR:O	10:A:526:ARG:HG3	2.18	0.43
10:A:770:TYR:HB2	10:A:994:ARG:NE	2.33	0.43
11:B:890:LYS:HB3	11:B:890:LYS:HE3	1.88	0.43
12:C:446:TYR:CD1	12:C:485:LEU:HD22	2.53	0.43
13:D:339:THR:HG22	13:D:342:VAL:HG22	2.00	0.43
1:R:79:LYS:HD3	1:R:82:LEU:HD21	2.00	0.43
5:a:51:DA:H2'	5:a:52:DC:C6	2.54	0.43
5:a:59:DA:H2''	5:a:60:DA:H8	1.84	0.43
8:Q:66:LYS:HA	8:Q:67:PRO:HD3	1.78	0.43
10:A:514:ASP:OD1	10:A:515:LYS:N	2.52	0.43
10:A:745:TYR:HA	10:A:749:HIS:HD2	1.82	0.43
10:A:913:HIS:O	10:A:913:HIS:ND1	2.51	0.43
11:B:879:ILE:HG22	11:B:880:HIS:N	2.34	0.43
12:C:582:GLU:O	12:C:583:LEU:C	2.62	0.43
12:C:641:PRO:HB2	12:C:646:LYS:CE	2.49	0.43
13:G:529:LYS:O	13:G:533:GLN:HG3	2.19	0.43
14:H:413:THR:HB	14:H:414:HIS:CE1	2.53	0.43
1:R:48:LEU:HD23	1:R:51:ILE:HD12	2.00	0.43
7:P:122:ARG:HG2	7:P:122:ARG:NH1	2.06	0.43
7:P:180:VAL:CG1	7:P:332:LEU:HG	2.48	0.43
7:P:314:PHE:CZ	7:P:407:ARG:HG3	2.54	0.43
10:A:570:LYS:HZ2	10:A:571:ILE:HG12	1.84	0.43
10:A:603:ALA:O	10:A:604:ARG:C	2.62	0.43
10:A:1054:GLN:HG3	10:A:1055:LEU:HG	2.01	0.43
11:B:1202:SER:H	11:B:1274:ASN:CB	2.31	0.43
12:C:607:SER:HA	12:C:610:LEU:HG	2.00	0.43
13:D:308:PRO:HG3	13:D:393:TYR:CE1	2.54	0.43
13:D:311:SER:O	13:D:313:TRP:N	2.49	0.43
14:H:80:ASP:O	14:H:82:GLU:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:48:LEU:HD23	1:V:51:ILE:HD12	2.00	0.43
5:a:63:DC:H2''	5:a:64:DA:C8	2.54	0.43
10:A:929:ASN:ND2	10:A:1228:LYS:HB3	2.33	0.43
11:B:779:TYR:O	13:E:319:ILE:HG12	2.18	0.43
11:B:982:ILE:C	11:B:1046:LEU:HD21	2.43	0.43
12:C:467:ASP:HA	12:C:470:ARG:NH2	2.34	0.43
11:B:763:LEU:HD11	11:B:961:ASN:HB2	2.00	0.43
11:B:1064:LYS:NZ	11:B:1103:HIS:O	2.44	0.43
11:B:1211:ILE:HG21	11:B:1237:ILE:HB	2.00	0.43
13:E:327:LEU:HD23	13:E:327:LEU:HA	1.81	0.43
14:H:312:PRO:HA	14:H:315:THR:HG22	2.01	0.43
14:H:512:VAL:HG13	14:H:513:LYS:N	2.34	0.43
15:I:136:LEU:O	15:I:140:LYS:HG2	2.19	0.43
6:b:97:DT:H2''	6:b:98:DT:H5'	2.01	0.42
6:b:150:DT:H2''	6:b:151:DC:C5	2.53	0.42
8:Q:46:ARG:O	8:Q:47:GLN:C	2.62	0.42
10:A:1247:SER:O	10:A:1250:GLN:HG2	2.18	0.42
11:B:992:ILE:O	11:B:996:LEU:HD23	2.18	0.42
11:B:1285:LEU:C	11:B:1287:THR:H	2.27	0.42
13:E:386:THR:OG1	13:E:391:ILE:HD11	2.18	0.42
14:H:388:LEU:HG	14:H:414:HIS:CE1	2.54	0.42
14:H:460:GLN:CD	14:H:460:GLN:H	2.26	0.42
15:I:79:ASP:O	15:I:83:VAL:HG12	2.18	0.42
2:S:22:LEU:HB3	2:S:25:ASN:ND2	2.34	0.42
6:b:29:DC:H2''	6:b:30:DA:H8	1.83	0.42
10:A:1097:PRO:O	10:A:1101:ALA:HB2	2.19	0.42
11:B:760:LEU:HD11	11:B:951:LEU:HA	2.01	0.42
11:B:990:SER:O	11:B:991:SER:C	2.62	0.42
11:B:990:SER:OG	11:B:991:SER:N	2.52	0.42
13:E:339:THR:HG23	13:E:342:VAL:H	1.84	0.42
14:H:335:TYR:O	14:H:338:LEU:HG	2.19	0.42
14:H:468:GLU:HA	14:H:471:ARG:NH1	2.33	0.42
5:a:38:DA:H2''	5:a:39:DG:C8	2.54	0.42
5:a:113:DG:H2'	5:a:114:DT:H71	2.01	0.42
7:P:32:PRO:C	7:P:34:SER:H	2.26	0.42
7:P:198:ALA:N	7:P:199:PRO:HD2	2.34	0.42
8:Q:6:GLN:O	8:Q:24:GLY:HA2	2.19	0.42
10:A:539:LEU:HD13	13:G:570:ILE:HG21	1.99	0.42
10:A:559:LEU:HD21	11:B:722:ILE:HD12	2.02	0.42
10:A:851:PRO:O	10:A:855:LYS:HG3	2.19	0.42
10:A:1179:ILE:HG23	10:A:1211:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:706:ASN:CG	11:B:707:LEU:N	2.77	0.42
11:B:787:TYR:CE1	13:E:345:ARG:HB3	2.55	0.42
11:B:1253:ILE:HG13	11:B:1254:CYS:N	2.33	0.42
13:D:420:ARG:O	13:D:420:ARG:HG3	2.19	0.42
14:H:397:SER:HB2	14:H:399:ASP:OD1	2.19	0.42
6:b:39:DG:H2''	6:b:40:DA:C8	2.54	0.42
7:P:80:TRP:CE2	7:P:122:ARG:HD3	2.53	0.42
7:P:300:THR:C	7:P:301:LEU:HD23	2.44	0.42
10:A:559:LEU:HD12	11:B:916:ASP:OD1	2.18	0.42
10:A:563:THR:C	10:A:564:HIS:CG	2.97	0.42
10:A:678:ARG:O	10:A:682:LEU:HG	2.20	0.42
10:A:1095:ILE:O	10:A:1099:LEU:HG	2.19	0.42
10:A:1110:PHE:CZ	10:A:1119:MET:HG2	2.55	0.42
11:B:899:PHE:CE2	14:H:506:LYS:HD2	2.54	0.42
11:B:1267:LYS:HB3	13:G:717:ARG:CZ	2.50	0.42
12:C:541:ASP:OD1	12:C:541:ASP:N	2.52	0.42
13:E:415:ARG:NH2	16:J:39:UNK:C	2.82	0.42
15:I:102:SER:O	15:I:105:SER:N	2.51	0.42
3:T:30:VAL:HG13	4:U:67:PHE:HE1	1.85	0.42
6:b:84:DC:H2''	6:b:85:DG:C8	2.54	0.42
6:b:99:DA:H2''	6:b:100:DA:N7	2.33	0.42
9:Z:9:LYS:HD2	9:Z:12:LYS:NZ	2.34	0.42
10:A:513:LEU:O	10:A:516:LEU:HG	2.18	0.42
10:A:536:LEU:HD13	10:A:536:LEU:HA	1.78	0.42
11:B:882:THR:HA	11:B:883:PRO:HD3	1.87	0.42
11:B:1121:GLN:CD	11:B:1130:SER:HA	2.44	0.42
12:C:412:TYR:HB2	12:C:420:THR:H	1.83	0.42
13:E:362:PHE:CE1	13:E:366:THR:HB	2.55	0.42
13:G:681:PHE:HA	13:G:684:ASN:ND2	2.34	0.42
14:H:84:ARG:O	14:H:87:HIS:HB2	2.19	0.42
14:H:115:PRO:HG2	14:H:116:HIS:CD2	2.54	0.42
5:a:92:DC:H2''	5:a:93:DG:H8	1.84	0.42
6:b:55:DC:H2''	6:b:56:DC:C6	2.55	0.42
7:P:431:ASP:O	7:P:435:GLN:HB2	2.19	0.42
11:B:1035:TYR:N	11:B:1036:GLN:OE1	2.52	0.42
11:B:1053:ASN:HB3	11:B:1057:PHE:CZ	2.54	0.42
12:C:469:ASP:N	12:C:469:ASP:OD1	2.50	0.42
13:D:347:ARG:O	13:D:351:VAL:HG12	2.19	0.42
13:D:402:LYS:HE2	13:D:402:LYS:HB2	1.71	0.42
5:a:145:DT:H2''	5:a:146:DT:C6	2.55	0.42
8:Q:91:LEU:CD2	8:Q:106:LEU:HD22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:445:ASP:HA	8:Q:448:TYR:CE1	2.55	0.42
11:B:985:LEU:C	11:B:986:LEU:HD12	2.44	0.42
11:B:1295:ILE:H	11:B:1295:ILE:HD12	1.84	0.42
12:C:415:TYR:OH	12:C:419:ILE:N	2.52	0.42
12:C:613:TYR:CZ	12:C:619:ALA:HA	2.55	0.42
13:F:670:ILE:CG2	14:H:508:SER:HB3	2.47	0.42
14:H:541:ARG:HG2	14:H:545:PHE:HE2	1.84	0.42
15:I:144:TYR:HA	15:I:147:GLN:NE2	2.34	0.42
2:W:79:LYS:N	6:b:111:DA:OP1	2.52	0.42
5:a:57:DT:H2"	5:a:58:DA:N7	2.34	0.42
10:A:1337:ARG:O	10:A:1340:SER:N	2.52	0.42
11:B:1051:LYS:C	11:B:1053:ASN:H	2.27	0.42
11:B:1265:ILE:O	11:B:1269:ILE:N	2.30	0.42
12:C:555:ASN:OD1	12:C:654:GLN:N	2.48	0.42
13:F:726:ARG:CZ	15:I:161:UNK:HA	2.49	0.42
5:a:101:DG:H2"	5:a:102:DA:H8	1.85	0.42
6:b:114:DT:H2"	6:b:115:DG:C8	2.54	0.42
10:A:531:TYR:HA	10:A:534:TYR:CD2	2.55	0.42
13:F:532:LEU:HA	13:F:535:LEU:HB3	2.02	0.42
13:G:682:LEU:O	13:G:686:LEU:HG	2.20	0.42
14:H:378:ILE:HA	14:H:401:MET:C	2.45	0.42
15:I:110:ASN:HA	15:I:113:SER:OG	2.20	0.42
1:R:101:VAL:HG11	3:X:107:VAL:HG21	2.02	0.42
10:A:469:LEU:HA	15:I:128:CYS:SG	2.60	0.42
10:A:595:GLU:HA	10:A:598:LYS:CB	2.49	0.42
10:A:978:LEU:O	10:A:982:ARG:HG2	2.20	0.42
11:B:952:LEU:HA	11:B:955:VAL:HG12	2.01	0.42
12:C:567:ASN:OD1	12:C:569:ASP:N	2.46	0.42
13:F:718:GLN:HE22	13:G:719:GLN:HB2	1.85	0.42
15:I:102:SER:O	15:I:105:SER:OG	2.20	0.42
3:X:85:LEU:HD23	3:X:108:LEU:HD23	2.02	0.41
5:a:129:DC:H2"	5:a:130:DA:N7	2.35	0.41
6:b:19:DA:C8	6:b:20:DT:H72	2.55	0.41
7:P:197:LEU:HD11	7:P:231:PHE:CE1	2.55	0.41
8:Q:361:GLU:HA	8:Q:362:PRO:HD3	1.94	0.41
10:A:546:ARG:NH1	10:A:546:ARG:HB2	2.35	0.41
10:A:586:TYR:OH	11:B:1048:SER:HA	2.20	0.41
10:A:884:SER:HB2	10:A:913:HIS:HA	2.02	0.41
10:A:988:ARG:HB2	10:A:989:PRO:HD3	2.00	0.41
10:A:1019:GLN:OE1	10:A:1058:ILE:HB	2.20	0.41
12:C:505:THR:OG1	12:C:506:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:551:LYS:HA	13:F:551:LYS:HD3	1.62	0.41
13:G:526:ASN:O	13:G:527:TRP:HD1	2.02	0.41
14:H:86:ASP:HA	14:H:89:ILE:HG12	2.02	0.41
15:I:71:GLN:O	15:I:75:LYS:HG3	2.20	0.41
15:I:74:ASN:HA	15:I:77:ARG:HH21	1.85	0.41
1:R:123:ASP:OD1	1:V:113:HIS:NE2	2.52	0.41
6:b:27:DG:H2''	6:b:28:DA:C8	2.55	0.41
10:A:564:HIS:HB3	11:B:966:ARG:HH22	1.85	0.41
10:A:818:PRO:HB3	10:A:866:PHE:CZ	2.55	0.41
10:A:1137:THR:OG1	10:A:1141:GLU:OE2	2.36	0.41
10:A:1149:PHE:CZ	10:A:1172:LEU:HD13	2.55	0.41
10:A:1228:LYS:HA	10:A:1231:ILE:HD12	2.02	0.41
11:B:724:THR:O	11:B:725:ALA:C	2.63	0.41
11:B:745:TYR:O	11:B:746:PRO:C	2.63	0.41
11:B:1202:SER:H	11:B:1274:ASN:ND2	2.17	0.41
12:C:413:SER:H	12:C:420:THR:HG23	1.84	0.41
12:C:495:MET:HE2	13:E:365:THR:HG22	2.01	0.41
12:C:588:GLU:HG3	13:E:370:ASN:HD22	1.85	0.41
12:C:636:ASP:HA	13:D:337:SER:OG	2.20	0.41
13:D:329:GLU:OE1	13:D:329:GLU:N	2.42	0.41
13:E:323:GLU:H	13:E:323:GLU:HG2	1.72	0.41
2:S:35:ARG:O	2:S:39:ARG:HG2	2.19	0.41
6:b:121:DG:H2''	6:b:122:DA:C8	2.55	0.41
7:P:418:GLN:HG2	7:P:419:TYR:CD1	2.56	0.41
10:A:530:LEU:HG	10:A:534:TYR:CE2	2.55	0.41
10:A:758:GLN:HB3	10:A:767:LEU:HD21	2.02	0.41
10:A:895:GLU:N	10:A:922:LEU:O	2.53	0.41
13:D:453:LEU:HD12	13:D:456:TYR:HB2	2.01	0.41
13:F:699:ASN:HB2	13:F:703:LYS:HZ1	1.85	0.41
13:F:726:ARG:HD3	13:F:726:ARG:HA	1.94	0.41
14:H:106:SER:O	14:H:110:GLN:HG2	2.19	0.41
4:Y:103:LEU:O	4:Y:107:ALA:CB	2.69	0.41
5:a:148:DA:OP2	5:a:148:DA:C8	2.70	0.41
6:b:11:DA:H2'	6:b:12:DT:C6	2.55	0.41
7:P:235:MET:SD	8:Q:401:VAL:HG21	2.60	0.41
10:A:1120:GLU:HG2	10:A:1130:TYR:CE2	2.55	0.41
10:A:1303:ASP:OD1	10:A:1304:ARG:N	2.49	0.41
12:C:541:ASP:CG	12:C:542:LEU:HG	2.46	0.41
12:C:541:ASP:HA	12:C:543:ARG:HH11	1.85	0.41
13:D:420:ARG:NH2	17:M:6:UNK:H	2.18	0.41
13:E:424:PRO:HG2	13:E:425:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:702:LYS:HD3	13:F:706:LYS:NZ	2.35	0.41
14:H:405:ASP:O	14:H:408:SER:OG	2.36	0.41
14:H:527:LYS:HD2	14:H:527:LYS:HA	1.74	0.41
15:I:81:GLU:HB2	15:I:82:ARG:HH12	1.83	0.41
16:J:34:UNK:O	16:J:35:UNK:C	2.67	0.41
16:J:35:UNK:O	16:J:36:UNK:C	2.69	0.41
6:b:8:DT:H2"	6:b:9:DT:C5	2.56	0.41
7:P:147:LEU:C	7:P:149:MET:N	2.77	0.41
10:A:681:HIS:HE1	10:A:944:LYS:HA	1.86	0.41
10:A:1237:GLN:O	10:A:1240:LYS:HG2	2.21	0.41
11:B:876:PRO:O	11:B:877:LEU:HD22	2.20	0.41
11:B:897:ASP:N	11:B:897:ASP:OD1	2.53	0.41
11:B:1027:GLU:HG2	11:B:1115:SER:HA	2.03	0.41
11:B:1292:ASP:HB2	11:B:1295:ILE:HB	2.02	0.41
12:C:608:LEU:HD12	12:C:629:MET:HE2	2.03	0.41
13:D:355:ARG:O	13:D:358:PRO:HD3	2.20	0.41
13:G:542:PHE:CD2	13:G:548:LYS:HD3	2.56	0.41
14:H:379:VAL:C	14:H:400:THR:HA	2.45	0.41
14:H:528:VAL:C	14:H:530:SER:N	2.79	0.41
16:J:27:UNK:O	16:J:28:UNK:C	2.68	0.41
1:R:122:LYS:HG3	1:V:113:HIS:HE1	1.84	0.41
7:P:108:MET:SD	7:P:123:TYR:HE2	2.43	0.41
10:A:834:GLU:O	10:A:838:TRP:HB2	2.20	0.41
11:B:1271:SER:O	11:B:1272:ILE:HD13	2.20	0.41
12:C:498:ASP:OD2	13:E:363:SER:HB2	2.21	0.41
14:H:99:MET:HG3	14:H:103:TRP:CD1	2.55	0.41
15:I:121:LEU:HD23	15:I:121:LEU:HA	1.74	0.41
2:S:64:ASN:O	2:S:67:ARG:HG2	2.21	0.41
6:b:70:DA:H2"	6:b:71:DA:C8	2.54	0.41
7:P:412:LEU:HD12	7:P:412:LEU:HA	1.76	0.41
8:Q:3:PRO:HA	8:Q:4:PHE:HA	1.67	0.41
10:A:1061:HIS:NE2	10:A:1115:ILE:HG23	2.36	0.41
10:A:1071:GLN:HE22	10:A:1343:ALA:HA	1.86	0.41
13:E:312:LYS:HD2	13:E:312:LYS:HA	1.83	0.41
13:G:704:LEU:O	13:G:708:MET:HG2	2.21	0.41
16:J:3:UNK:O	16:J:7:UNK:N	2.54	0.41
5:a:1:DA:OP1	5:a:1:DA:H2	2.04	0.41
8:Q:112:LEU:HD12	8:Q:141:ILE:HD12	2.02	0.41
8:Q:166:THR:HG22	8:Q:167:HIS:CE1	2.56	0.41
8:Q:189:MET:HE3	8:Q:193:SER:OG	2.21	0.41
10:A:479:ILE:HG12	16:K:23:UNK:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:447:LYS:CD	13:E:328:PRO:HG3	2.51	0.41
13:D:320:HIS:HD2	13:D:321:SER:N	2.19	0.41
13:E:329:GLU:OE2	13:E:380:ARG:NE	2.48	0.41
5:a:53:DC:H3'	10:A:1112:MET:HG3	2.02	0.41
5:a:122:DC:H2''	5:a:123:DA:N7	2.35	0.41
5:a:124:DC:H2''	5:a:125:DG:H8	1.86	0.41
6:b:49:DA:H2''	6:b:50:DG:C8	2.56	0.41
6:b:57:DC:H2''	6:b:58:DC:C5	2.56	0.41
6:b:91:DG:H2'	6:b:92:DT:H71	2.03	0.41
6:b:144:DC:H2''	6:b:145:DG:H8	1.84	0.41
7:P:203:GLU:O	7:P:204:GLU:CB	2.66	0.41
7:P:235:MET:HE1	7:P:288:LYS:HB3	2.01	0.41
7:P:458:GLU:O	7:P:460:TYR:N	2.53	0.41
8:Q:26:ASN:HB3	8:Q:29:THR:O	2.21	0.41
9:Z:84:LEU:O	9:Z:85:LYS:CB	2.61	0.41
10:A:611:SER:O	10:A:615:GLN:HG3	2.21	0.41
10:A:840:PRO:O	10:A:841:THR:OG1	2.34	0.41
10:A:895:GLU:OE1	10:A:897:HIS:NE2	2.51	0.41
10:A:928:GLN:NE2	10:A:929:ASN:HD22	2.19	0.41
10:A:1149:PHE:CE2	10:A:1172:LEU:HD13	2.56	0.41
11:B:861:TRP:HD1	12:C:447:LYS:HE2	1.86	0.41
11:B:879:ILE:HG22	11:B:880:HIS:CD2	2.55	0.41
11:B:883:PRO:O	11:B:886:THR:HG23	2.21	0.41
11:B:905:ARG:HA	11:B:905:ARG:NE	2.36	0.41
11:B:933:ASN:O	11:B:937:ILE:HG13	2.21	0.41
11:B:1309:ILE:HD13	11:B:1309:ILE:HA	1.82	0.41
12:C:584:GLU:HG3	12:C:586:PRO:CD	2.50	0.41
12:C:606:LYS:O	12:C:609:ALA:HB3	2.21	0.41
12:C:653:LEU:HD12	16:N:13:UNK:HA	2.03	0.41
13:D:376:ALA:C	13:D:380:ARG:HE	2.28	0.41
13:E:315:ASN:HB2	13:E:318:LYS:HG2	2.03	0.41
13:F:702:LYS:HD3	13:F:706:LYS:CE	2.50	0.41
14:H:109:SER:HA	14:H:112:PHE:CE2	2.56	0.41
14:H:309:SER:O	14:H:415:LEU:HD12	2.21	0.41
14:H:406:LEU:O	14:H:410:ILE:N	2.45	0.41
14:H:450:LEU:HG	14:H:451:LYS:H	1.85	0.41
15:I:123:LEU:HD23	15:I:123:LEU:HA	1.82	0.41
15:I:142:ILE:HG22	15:I:146:MET:SD	2.60	0.41
2:W:31:LYS:HG3	2:W:51:TYR:CE2	2.56	0.41
2:W:35:ARG:O	2:W:39:ARG:HG2	2.21	0.41
6:b:64:DG:H2''	6:b:65:DG:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:381:PRO:O	7:P:383:GLN:N	2.53	0.41
7:P:446:LEU:CD2	10:A:608:MET:SD	3.09	0.41
7:P:451:LEU:CD1	10:A:608:MET:SD	2.82	0.41
10:A:493:ALA:HA	10:A:496:ILE:HG12	2.02	0.41
10:A:598:LYS:N	10:A:598:LYS:HD2	2.34	0.41
11:B:958:HIS:HE1	11:B:960:GLU:OE1	2.04	0.41
11:B:1233:LEU:H	11:B:1233:LEU:HG	1.65	0.41
14:H:108:LEU:HD23	14:H:108:LEU:HA	1.90	0.41
3:T:85:LEU:HD23	3:T:108:LEU:HD23	2.02	0.40
6:b:99:DA:H2"	6:b:100:DA:C8	2.56	0.40
7:P:154:ALA:N	7:P:169:ILE:O	2.53	0.40
8:Q:105:GLU:H	8:Q:105:GLU:HG3	1.62	0.40
8:Q:146:SER:O	8:Q:149:ALA:HB3	2.21	0.40
8:Q:156:LEU:HA	8:Q:156:LEU:HD23	1.76	0.40
10:A:546:ARG:NH1	14:H:541:ARG:HH11	2.19	0.40
10:A:556:GLN:HG3	11:B:719:LEU:HD22	2.03	0.40
10:A:930:ASN:C	10:A:932:PRO:HD3	2.46	0.40
10:A:1019:GLN:NE2	10:A:1062:PRO:HB3	2.35	0.40
11:B:741:SER:OG	11:B:742:LEU:N	2.53	0.40
11:B:878:LYS:HG2	11:B:881:ARG:CZ	2.51	0.40
12:C:411:GLY:O	13:D:415:ARG:NE	2.50	0.40
13:E:376:ALA:HB1	13:E:380:ARG:HH12	1.86	0.40
4:U:103:LEU:O	4:U:107:ALA:CB	2.69	0.40
7:P:36:ILE:HB	7:P:54:MET:CE	2.42	0.40
7:P:389:LEU:HD22	7:P:421:LEU:CD2	2.52	0.40
8:Q:119:TRP:N	8:Q:119:TRP:CD1	2.89	0.40
10:A:938:LEU:HD23	10:A:944:LYS:HZ3	1.86	0.40
11:B:1046:LEU:HA	11:B:1046:LEU:HD23	1.75	0.40
12:C:438:TYR:HB3	13:E:383:LYS:HZ1	1.86	0.40
12:C:602:HIS:O	12:C:603:MET:C	2.64	0.40
12:C:604:TYR:O	12:C:607:SER:OG	2.26	0.40
13:G:716:GLU:O	13:G:717:ARG:C	2.64	0.40
14:H:311:SER:CB	14:H:414:HIS:HB3	2.51	0.40
14:H:472:GLU:O	14:H:475:GLN:HB3	2.21	0.40
5:a:13:DG:C8	5:a:14:DT:H72	2.57	0.40
5:a:92:DC:H2"	5:a:93:DG:C8	2.57	0.40
7:P:139:VAL:HG11	7:P:443:MET:HG3	2.03	0.40
7:P:246:LEU:HD13	7:P:250:TYR:HE2	1.87	0.40
8:Q:148:ALA:HB1	8:Q:428:ILE:O	2.22	0.40
10:A:572:ARG:HH22	15:I:95:HIS:N	2.19	0.40
10:A:1250:GLN:O	10:A:1254:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:785:ASN:HB3	13:E:345:ARG:HH21	1.86	0.40
11:B:1057:PHE:O	11:B:1061:LEU:HG	2.20	0.40
11:B:1275:LEU:HD12	11:B:1276:PHE:H	1.85	0.40
13:F:681:PHE:CZ	14:H:498:ASN:HA	2.56	0.40
2:S:32:PRO:O	2:S:36:ARG:HG3	2.22	0.40
5:a:52:DC:H2'	5:a:53:DC:C6	2.57	0.40
8:Q:206:ASP:OD1	8:Q:206:ASP:C	2.64	0.40
8:Q:354:LEU:HD23	8:Q:354:LEU:HA	1.89	0.40
10:A:572:ARG:HH22	15:I:95:HIS:H	1.67	0.40
11:B:701:GLU:O	11:B:702:LEU:HD23	2.20	0.40
11:B:1025:PHE:HD1	11:B:1025:PHE:HA	1.67	0.40
12:C:550:ILE:HD12	12:C:550:ILE:HA	1.96	0.40
13:E:304:GLU:OE1	13:E:304:GLU:N	2.54	0.40
13:F:567:GLN:O	13:F:568:LEU:HD23	2.21	0.40
14:H:78:LEU:HB3	14:H:84:ARG:HH12	1.87	0.40
5:a:44:DC:C6	5:a:45:DT:H72	2.56	0.40
7:P:188:PHE:CZ	7:P:319:ILE:HD13	2.57	0.40
7:P:381:PRO:HG2	7:P:382:GLU:H	1.86	0.40
10:A:567:PHE:O	11:B:926:ARG:NE	2.54	0.40
11:B:896:ASP:OD2	15:I:110:ASN:HB3	2.21	0.40
11:B:964:CYS:SG	11:B:966:ARG:HB3	2.61	0.40
11:B:1141:SER:O	11:B:1145:THR:HG22	2.20	0.40
12:C:630:LEU:O	12:C:633:ILE:CG1	2.69	0.40
13:D:414:THR:HG1	13:E:309:SER:N	2.15	0.40
14:H:121:ASN:OD1	14:H:122:VAL:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	R	96/135 (71%)	92 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	93/135 (69%)	89 (96%)	4 (4%)	0	100	100
2	S	80/102 (78%)	76 (95%)	4 (5%)	0	100	100
2	W	77/102 (76%)	73 (95%)	4 (5%)	0	100	100
3	T	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
3	X	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
4	U	91/122 (75%)	88 (97%)	3 (3%)	0	100	100
4	Y	91/122 (75%)	89 (98%)	2 (2%)	0	100	100
7	P	392/477 (82%)	369 (94%)	18 (5%)	5 (1%)	9	42
8	Q	391/467 (84%)	367 (94%)	22 (6%)	2 (0%)	24	63
9	Z	46/157 (29%)	43 (94%)	2 (4%)	1 (2%)	5	29
10	A	763/1703 (45%)	667 (87%)	96 (13%)	0	100	100
11	B	468/1314 (36%)	364 (78%)	104 (22%)	0	100	100
12	C	241/905 (27%)	176 (73%)	63 (26%)	2 (1%)	16	54
13	D	157/825 (19%)	130 (83%)	27 (17%)	0	100	100
13	E	137/825 (17%)	113 (82%)	24 (18%)	0	100	100
13	F	215/825 (26%)	186 (86%)	27 (13%)	2 (1%)	14	51
13	G	189/825 (23%)	164 (87%)	24 (13%)	1 (0%)	24	63
14	H	249/566 (44%)	217 (87%)	32 (13%)	0	100	100
15	I	78/179 (44%)	66 (85%)	12 (15%)	0	100	100
All	All	4064/10044 (40%)	3573 (88%)	478 (12%)	13 (0%)	37	72

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Q	48	ASP
13	F	606	PRO
7	P	343	SER
12	C	614	ASN
7	P	382	GLU
7	P	459	ASP
9	Z	84	LEU
13	G	572	ASP
7	P	431	ASP
7	P	458	GLU
8	Q	155	SER

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Mol	Chain	Res	Type
13	F	648	LYS
12	C	612	GLY

5.3.2 Protein sidechains ⓘ

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	R	84/110 (76%)	84 (100%)	0	100	100
1	V	82/110 (74%)	82 (100%)	0	100	100
2	S	67/78 (86%)	67 (100%)	0	100	100
2	W	64/78 (82%)	64 (100%)	0	100	100
3	T	81/101 (80%)	81 (100%)	0	100	100
3	X	82/101 (81%)	82 (100%)	0	100	100
4	U	77/102 (76%)	77 (100%)	0	100	100
4	Y	79/102 (78%)	79 (100%)	0	100	100
7	P	357/420 (85%)	331 (93%)	26 (7%)	13	34
8	Q	363/423 (86%)	344 (95%)	19 (5%)	21	42
9	Z	53/140 (38%)	51 (96%)	2 (4%)	29	50
10	A	705/1520 (46%)	698 (99%)	7 (1%)	68	78
11	B	460/1218 (38%)	459 (100%)	1 (0%)	87	87
12	C	222/823 (27%)	220 (99%)	2 (1%)	70	79
13	D	150/751 (20%)	150 (100%)	0	100	100
13	E	129/751 (17%)	129 (100%)	0	100	100
13	F	138/751 (18%)	138 (100%)	0	100	100
13	G	127/751 (17%)	126 (99%)	1 (1%)	73	80
14	H	239/517 (46%)	235 (98%)	4 (2%)	53	69
15	I	79/133 (59%)	79 (100%)	0	100	100
All	All	3638/8980 (40%)	3576 (98%)	62 (2%)	52	69

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	P	2	THR
7	P	36	ILE
7	P	88	ARG
7	P	122	ARG
7	P	135	VAL
7	P	159	ILE
7	P	195	GLU
7	P	216	ARG
7	P	218	THR
7	P	230	GLN
7	P	246	LEU
7	P	251	LYS
7	P	262	GLU
7	P	301	LEU
7	P	319	ILE
7	P	321	ASP
7	P	343	SER
7	P	380	SER
7	P	382	GLU
7	P	386	SER
7	P	397	SER
7	P	414	ILE
7	P	418	GLN
7	P	432	ARG
7	P	442	THR
7	P	462	THR
8	Q	7	ASP
8	Q	32	VAL
8	Q	34	GLU
8	Q	41	ILE
8	Q	48	ASP
8	Q	52	THR
8	Q	54	HIS
8	Q	56	THR
8	Q	69	GLN
8	Q	94	ARG
8	Q	100	ASP
8	Q	105	GLU
8	Q	122	SER
8	Q	197	SER
8	Q	291	GLU
8	Q	321	ASP

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Mol	Chain	Res	Type
8	Q	347	GLU
8	Q	422	SER
8	Q	438	GLN
9	Z	81	ILE
9	Z	90	ARG
10	A	597	LYS
10	A	598	LYS
10	A	605	LEU
10	A	607	SER
10	A	649	GLU
10	A	650	LYS
10	A	659	LEU
11	B	1199	ASN
12	C	611	LEU
12	C	633	ILE
13	G	571	GLU
14	H	494	LEU
14	H	538	ASP
14	H	561	LEU
14	H	562	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	68	GLN
2	S	25	ASN
3	T	82	HIS
4	U	46	HIS
1	V	68	GLN
2	W	27	GLN
2	W	93	GLN
4	Y	46	HIS
7	P	15	HIS
7	P	137	GLN
8	Q	17	GLN
8	Q	167	HIS
8	Q	300	GLN
8	Q	303	ASN
8	Q	304	ASN
8	Q	433	GLN
10	A	460	HIS
10	A	504	ASN

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Mol	Chain	Res	Type
10	A	510	ASN
10	A	528	ASN
10	A	548	HIS
10	A	564	HIS
10	A	588	ASN
10	A	657	GLN
10	A	681	HIS
10	A	749	HIS
10	A	784	ASN
10	A	929	ASN
10	A	939	ASN
10	A	1019	GLN
10	A	1054	GLN
10	A	1071	GLN
10	A	1104	HIS
10	A	1171	ASN
10	A	1173	GLN
10	A	1194	GLN
10	A	1202	GLN
11	B	718	ASN
11	B	727	ASN
11	B	804	ASN
11	B	874	GLN
11	B	880	HIS
11	B	915	ASN
11	B	984	HIS
11	B	1006	GLN
11	B	1026	ASN
11	B	1053	ASN
11	B	1063	ASN
11	B	1078	ASN
11	B	1093	ASN
11	B	1104	ASN
11	B	1142	GLN
11	B	1215	ASN
11	B	1243	GLN
11	B	1274	ASN
11	B	1300	GLN
11	B	1304	ASN
12	C	417	ASN
12	C	437	HIS
12	C	448	GLN

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Mol	Chain	Res	Type
12	C	466	GLN
12	C	508	GLN
12	C	520	GLN
12	C	595	HIS
12	C	614	ASN
13	D	333	ASN
13	D	348	ASN
13	D	392	ASN
13	D	394	GLN
13	D	416	HIS
13	E	348	ASN
13	E	352	ASN
13	E	357	ASN
13	E	411	GLN
13	E	433	GLN
13	F	540	GLN
13	F	552	ASN
13	F	718	GLN
13	F	725	GLN
13	F	738	ASN
13	G	555	ASN
13	G	567	GLN
13	G	725	GLN
13	G	730	ASN
13	G	745	ASN
14	H	76	GLN
14	H	102	GLN
14	H	110	GLN
14	H	116	HIS
14	H	118	ASN
14	H	313	GLN
14	H	469	ASN
14	H	475	GLN
14	H	493	ASN
14	H	516	ASN
15	I	76	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	PO4	Q	505	-	4,4,4	0.91	0	6,6,6	0.45	0
18	PO4	P	503	-	4,4,4	1.01	0	6,6,6	0.51	0
18	PO4	P	504	-	4,4,4	0.89	0	6,6,6	0.64	0
18	PO4	Q	501	-	4,4,4	1.03	0	6,6,6	0.64	0
18	PO4	Q	503	-	4,4,4	0.89	0	6,6,6	0.60	0
18	PO4	P	502	-	4,4,4	0.84	0	6,6,6	0.58	0
18	PO4	Q	504	-	4,4,4	0.93	0	6,6,6	0.44	0
18	PO4	A	1801	-	4,4,4	0.83	0	6,6,6	0.84	0
18	PO4	Q	502	-	4,4,4	0.88	0	6,6,6	0.49	0
18	PO4	P	501	-	4,4,4	0.94	0	6,6,6	0.68	0
19	ADP	A	1802	21	28,29,29	1.41	4 (14%)	43,45,45	1.83	8 (18%)
20	BEF	A	1803	-	0,3,3	-	-	-	-	-
18	PO4	Q	506	-	4,4,4	0.86	0	6,6,6	0.62	0
18	PO4	P	505	-	4,4,4	0.93	0	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	A	1802	21	-	1/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1802	ADP	C5-C4	4.69	1.47	1.39
19	A	1802	ADP	C5-C6	2.71	1.48	1.41
19	A	1802	ADP	C5-N7	-2.31	1.34	1.39
19	A	1802	ADP	C8-N7	2.25	1.36	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	1802	ADP	C5-C4-N3	-5.85	118.66	126.72
19	A	1802	ADP	N3-C4-N9	4.69	135.14	127.17
19	A	1802	ADP	C2-N3-C4	3.66	120.78	111.83
19	A	1802	ADP	C4-C5-N7	-3.40	106.69	110.58
19	A	1802	ADP	N3-C2-N1	-3.18	123.77	128.58
19	A	1802	ADP	C4-N9-C8	2.64	108.51	105.74
19	A	1802	ADP	C5-N7-C8	2.52	107.41	103.45
19	A	1802	ADP	C3'-C2'-C1'	2.39	105.99	101.46

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1802	ADP	C5'-O5'-PA-O1A

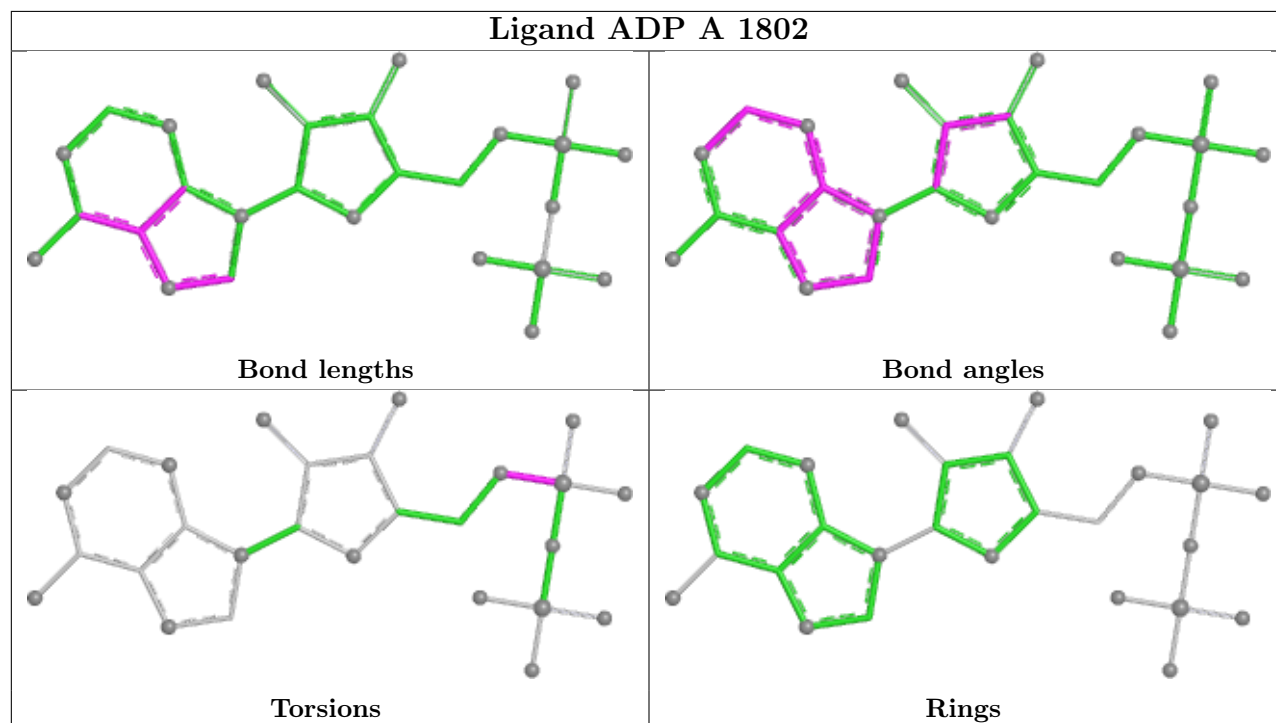
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Q	504	PO4	1	0
19	A	1802	ADP	6	0
20	A	1803	BEF	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	I	1
17	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	150:HIS	C	152:UNK	N	20.17
1	M	22:UNK	C	24:UNK	N	7.86

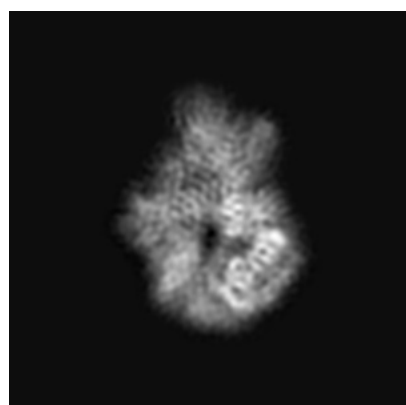
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20934. These allow visual inspection of the internal detail of the map and identification of artifacts.

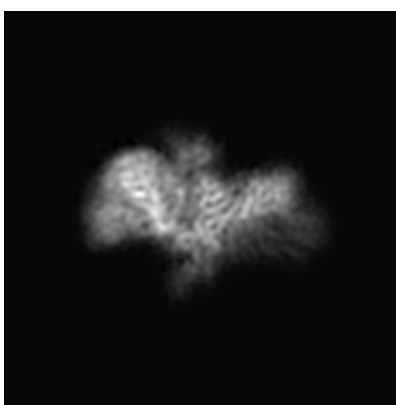
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

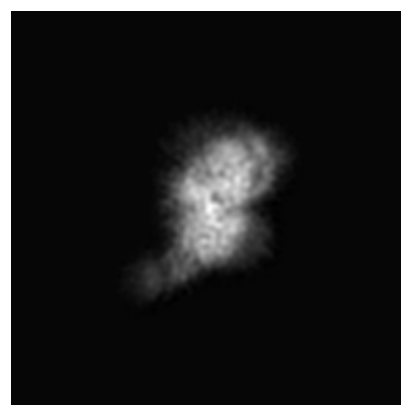
6.1.1 Primary map



X



Y

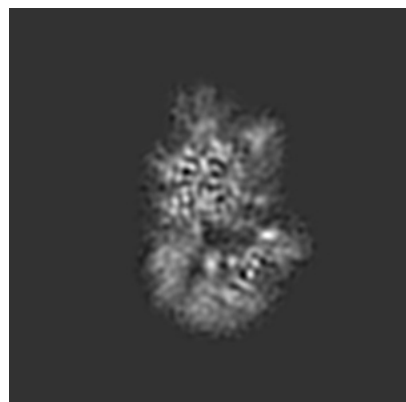


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 96



Y Index: 96

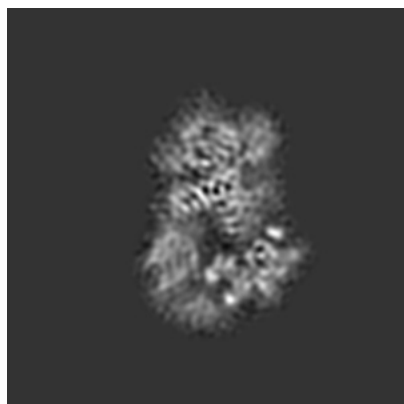


Z Index: 96

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: 102



Y Index: 107



Z Index: 97

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

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

6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

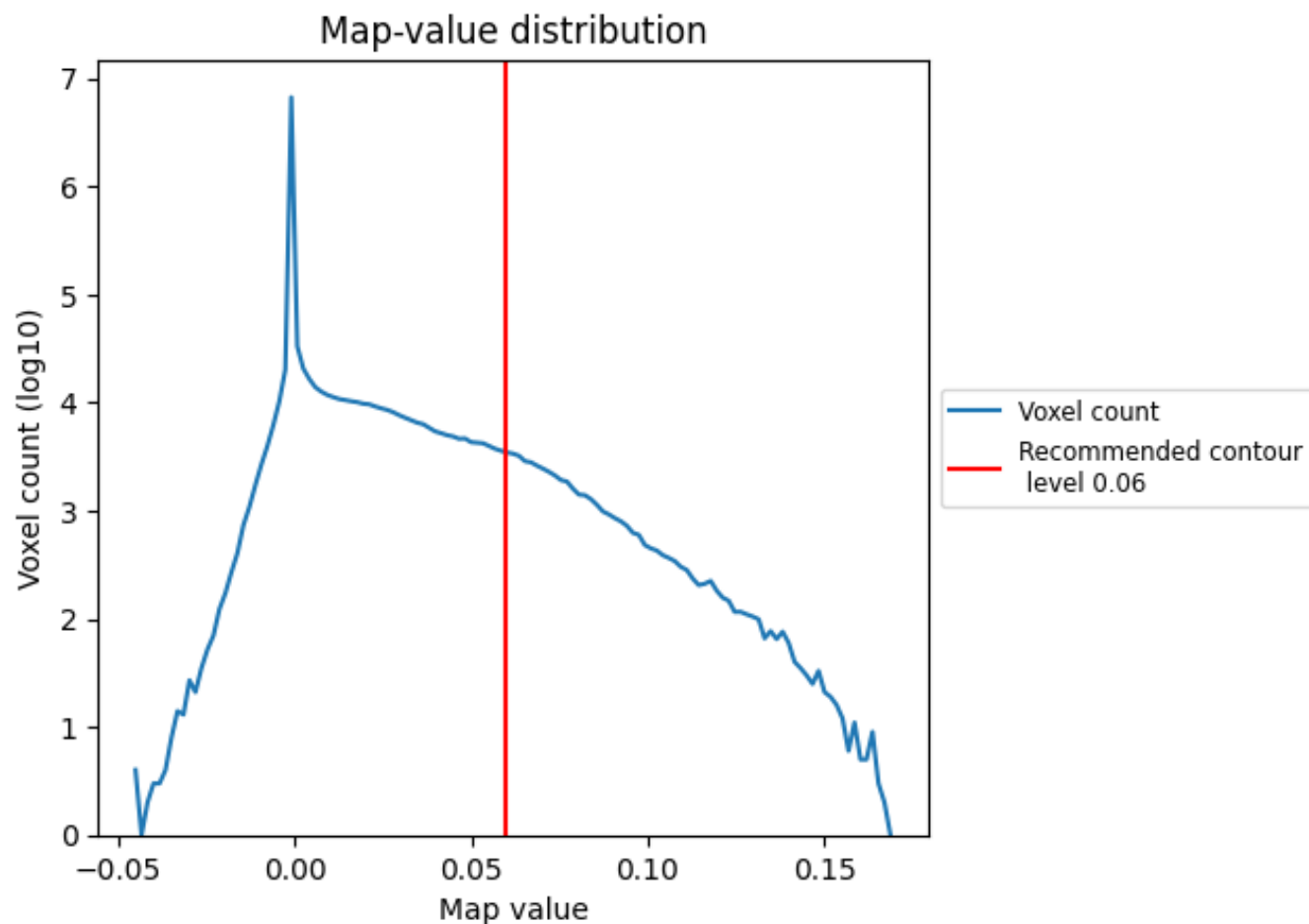
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

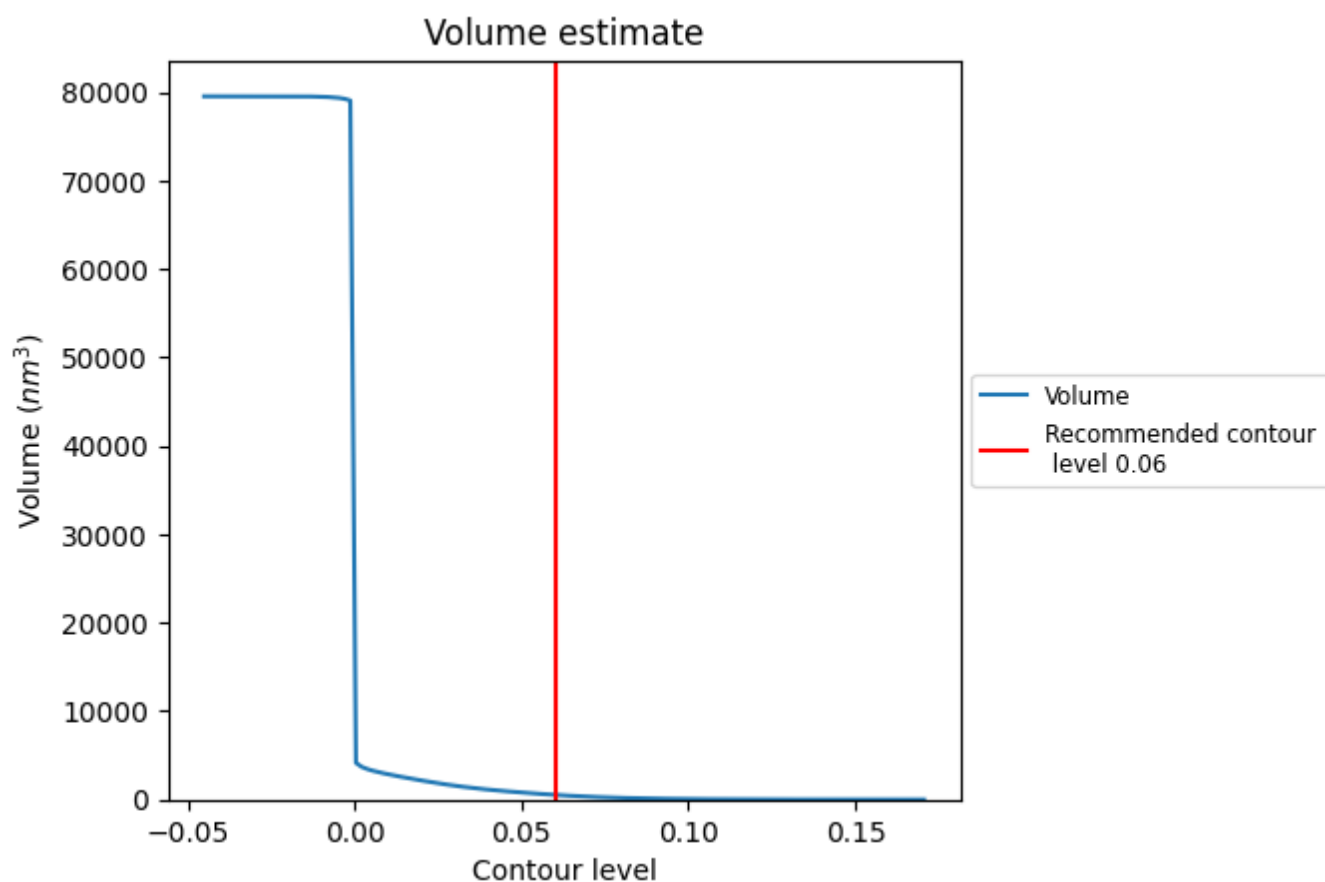
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

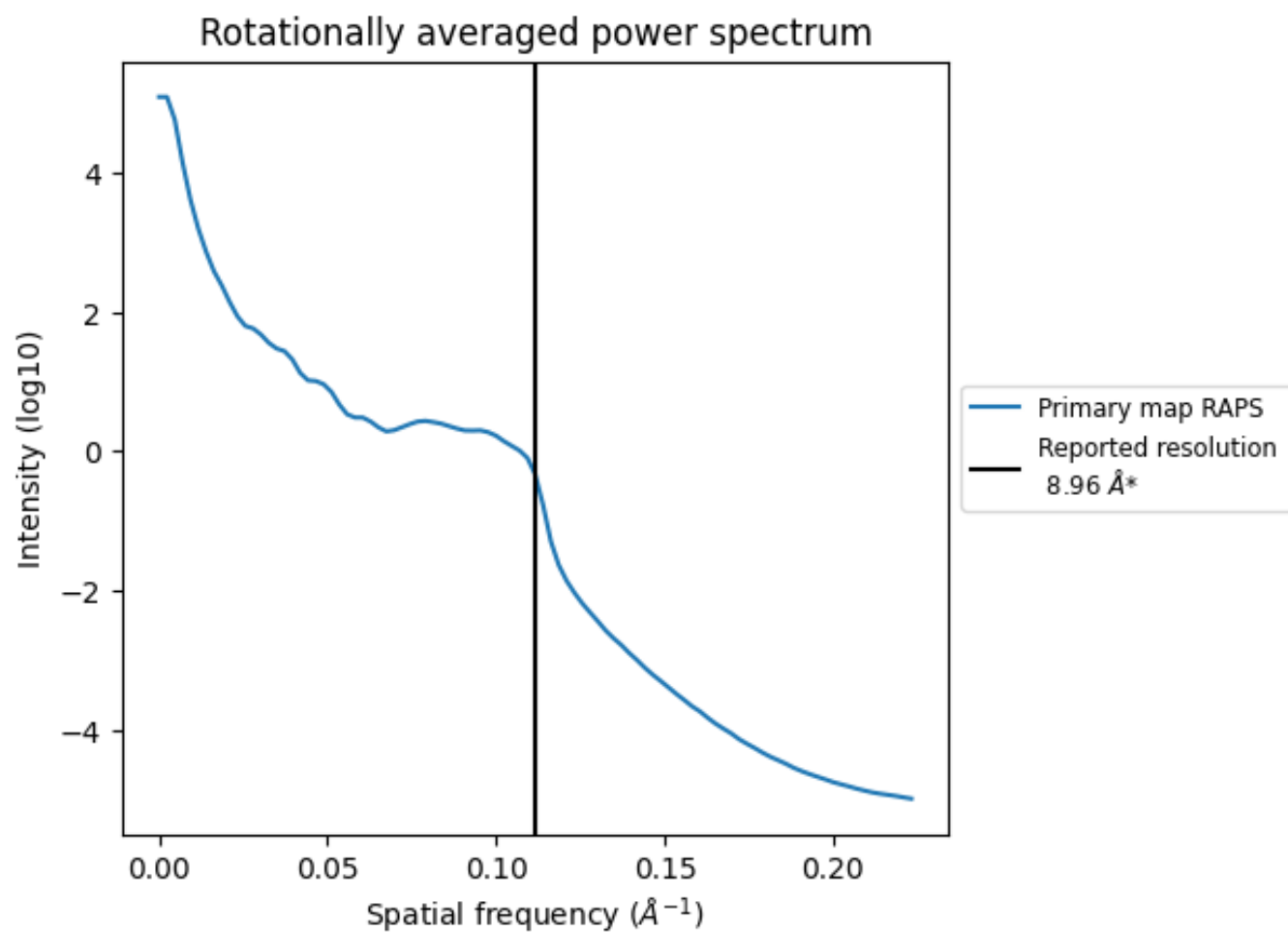
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 531 nm³; this corresponds to an approximate mass of 480 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

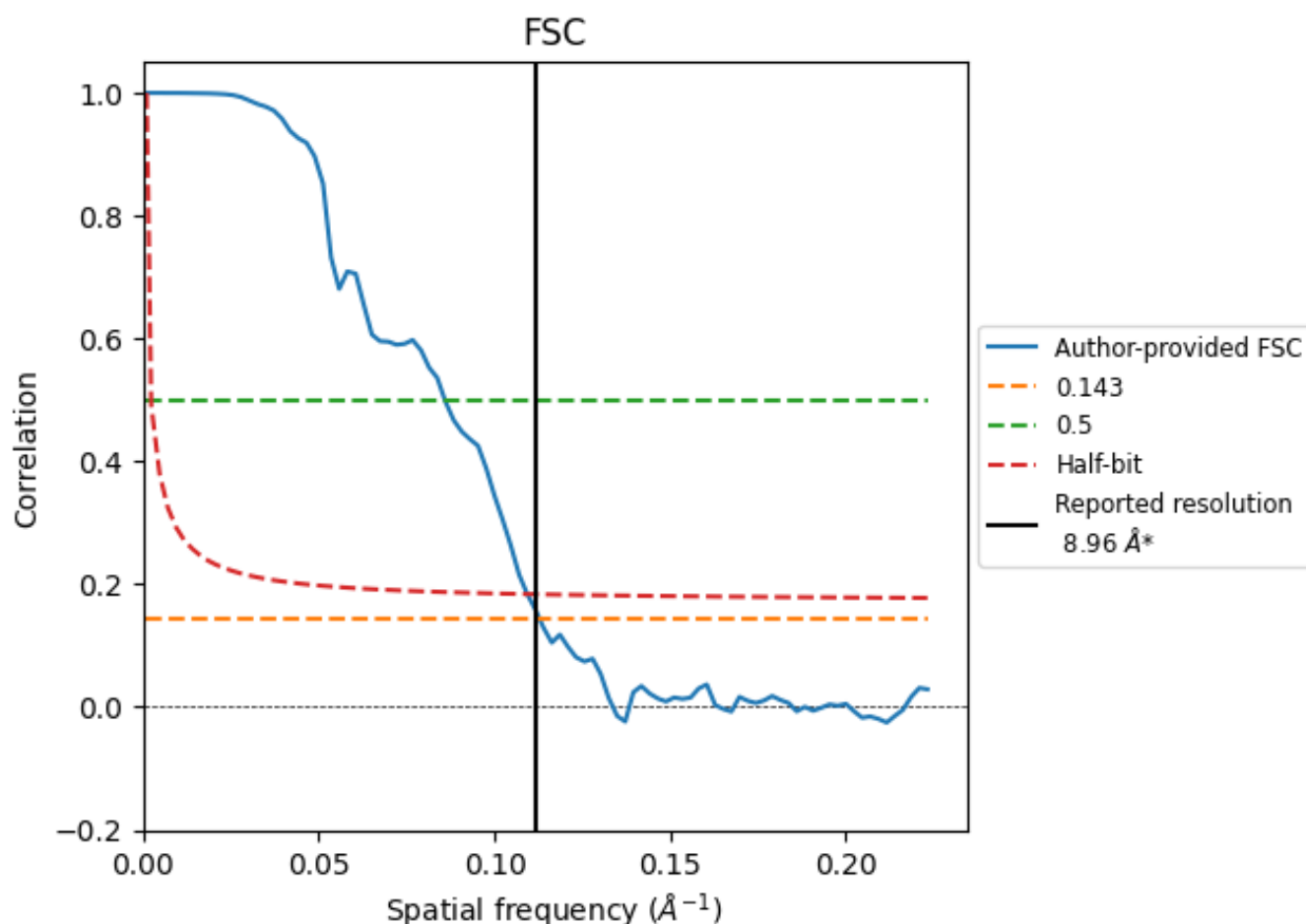


*Reported resolution corresponds to spatial frequency of 0.112 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.112 Å⁻¹

8.2 Resolution estimates [i](#)

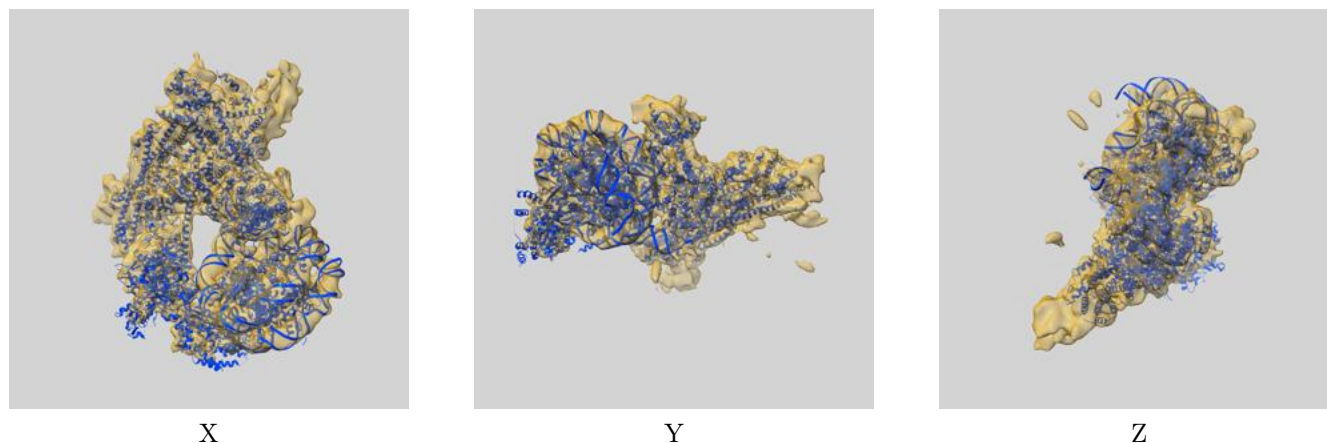
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.96	-	-
Author-provided FSC curve	8.86	11.64	9.15
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

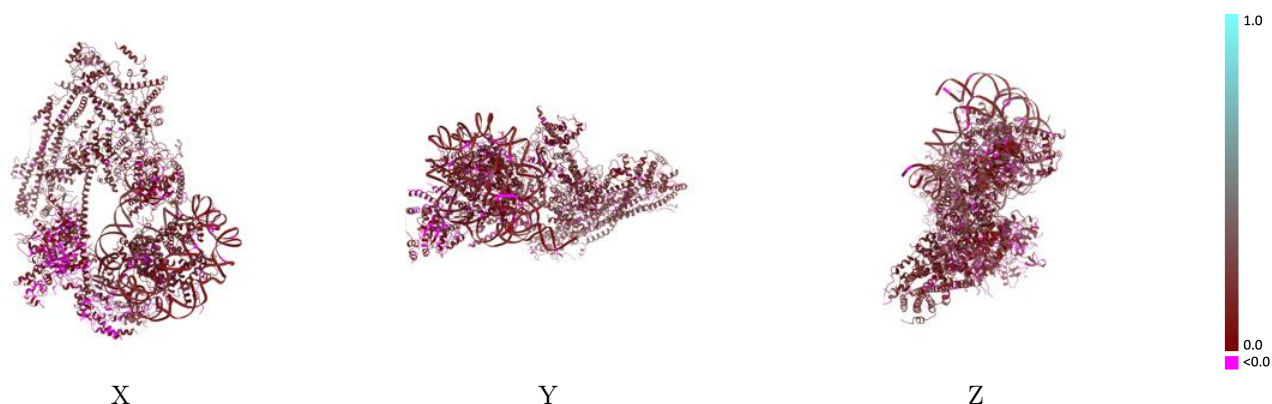
This section contains information regarding the fit between EMDB map EMD-20934 and PDB model 6UXW. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



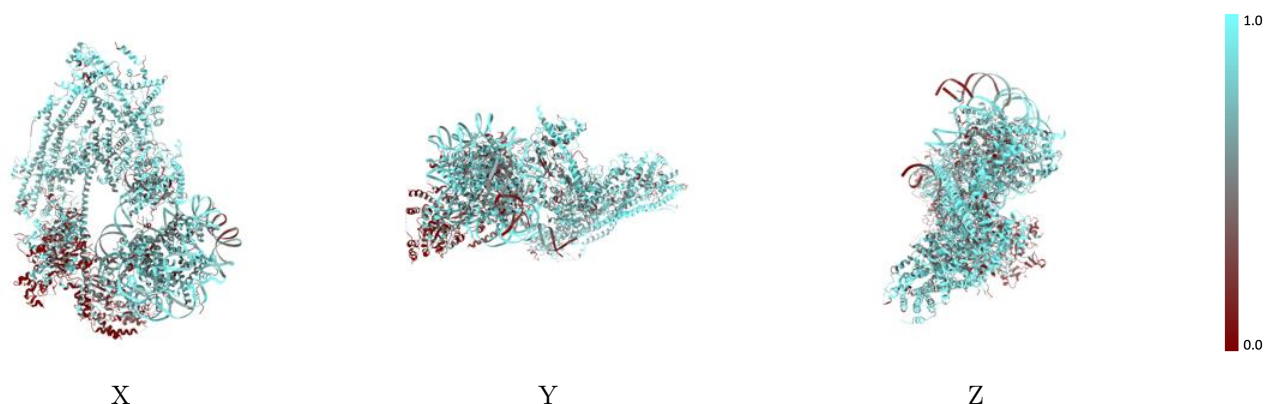
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



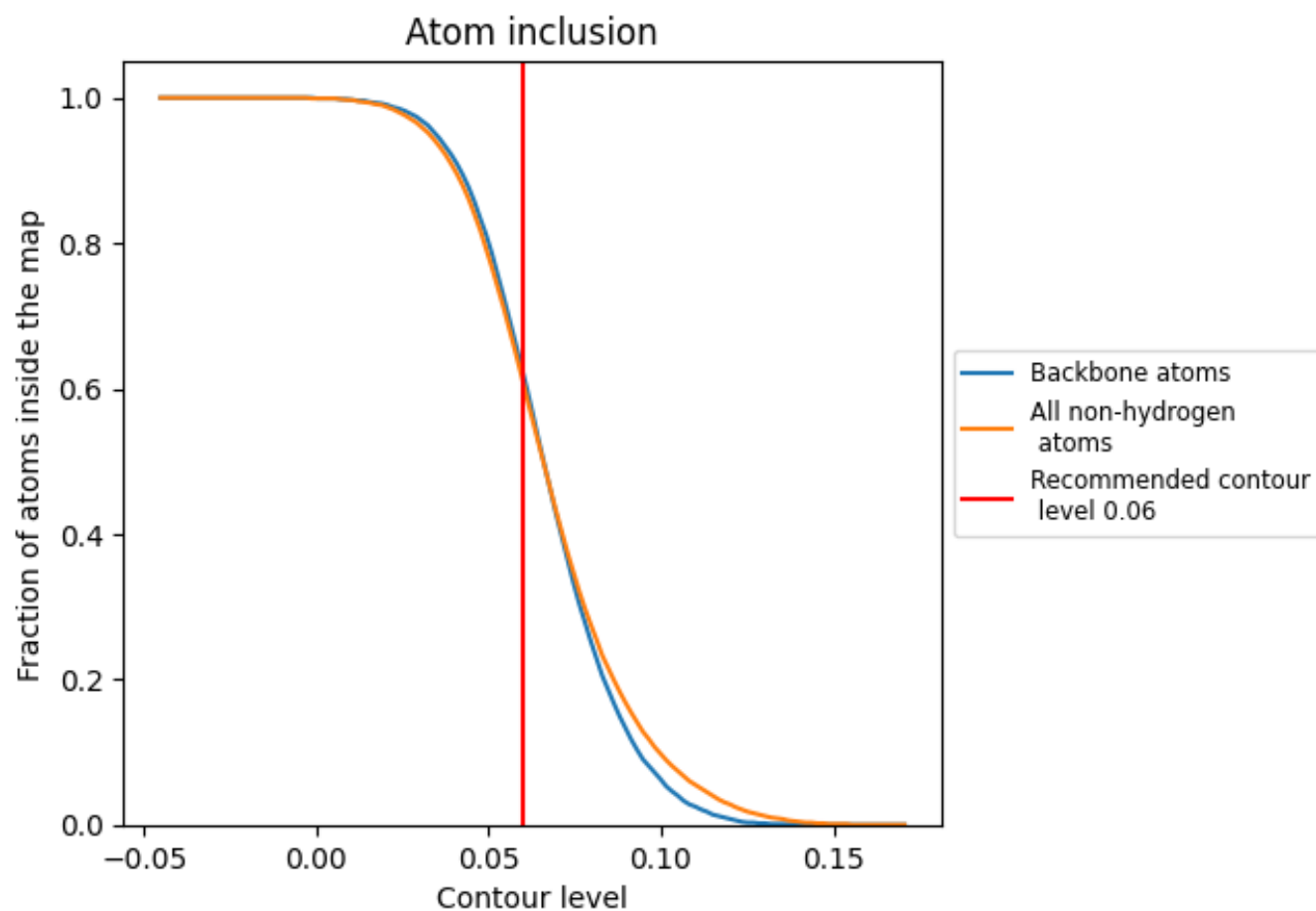
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 61% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6090	 0.1220
A	 0.3700	 0.0820
B	 0.6980	 0.1540
C	 0.6370	 0.1420
D	 0.7220	 0.1270
E	 0.7080	 0.1410
F	 0.7600	 0.1580
G	 0.7540	 0.1690
H	 0.7300	 0.1660
I	 0.7700	 0.1710
J	 0.9670	 0.2740
K	 0.8860	 0.2370
L	 0.3000	 0.1970
M	 0.8890	 0.2170
N	 0.4270	 0.0640
O	 0.7440	 0.1650
P	 0.5240	 0.0750
Q	 0.3550	 0.0520
R	 0.5820	 0.1120
S	 0.6010	 0.1060
T	 0.5800	 0.1100
U	 0.6930	 0.1590
V	 0.6590	 0.1260
W	 0.6770	 0.1050
X	 0.6730	 0.1180
Y	 0.7000	 0.1370
Z	 0.4380	 0.0930
a	 0.7290	 0.1300
b	 0.7540	 0.1380

