



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 07:19 AM JST

PDB ID : 7EGP / pdb_00007egp
EMDB ID : EMD-31137
Title : The structure of SWI/SNF-nucleosome complex
Authors : Chen, Z.C.; Chen, K.J.; He, Z.Y.; Ye, Y.P.
Deposited on : 2021-03-24
Resolution : 6.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

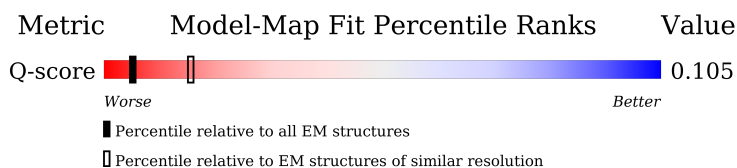
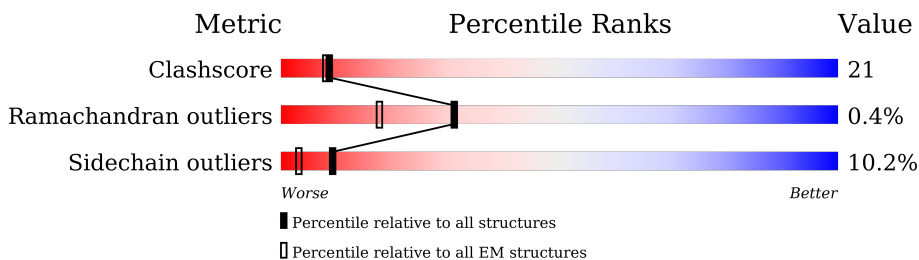
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	479 (6.40 - 7.40)

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	B	1093	
2	C	918	
3	D	836	
3	E	836	
4	H	566	

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Mol	Chain	Length	Quality of chain
5	I	332	
6	J	634	
7	A	982	
8	L	157	
9	M	477	
10	N	467	
11	O	135	
11	S	135	
12	P	102	
12	T	102	
13	Q	129	
13	U	129	
14	R	122	
14	V	122	
15	W	235	
16	X	235	

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

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

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 44871 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 13 discrepancies between the modelled and reference sequences:

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

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

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

There are 22 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

There are 11 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 11 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

- Molecule 12 is a protein called Histone H4.

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

- Molecule 13 is a protein called Histone H2A.

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

- Molecule 14 is a protein called Histone H2B 1.1.

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

There are 2 discrepancies between the modelled and reference sequences:

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

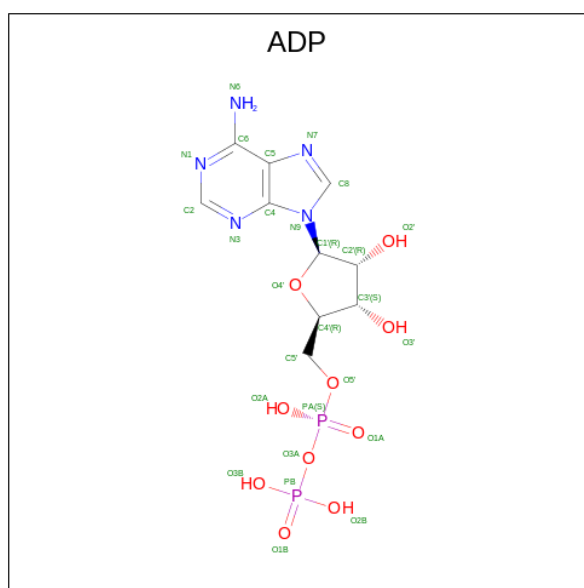
- Molecule 15 is a DNA chain called DNA (239-MER).

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

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

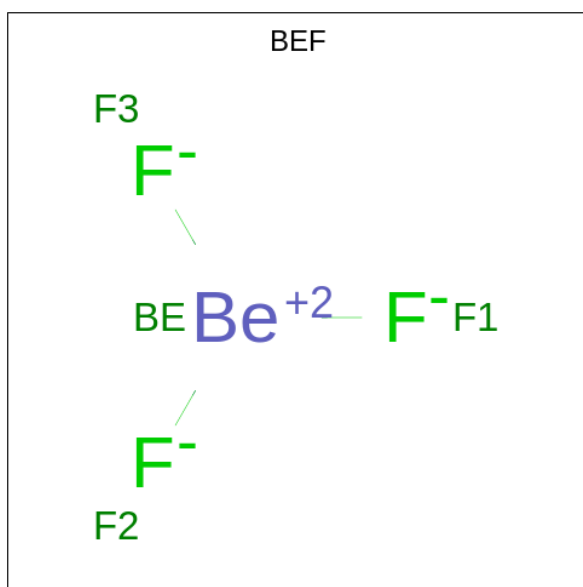
Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	166	Total	C	N	O	P	0	0
			3413	1618	632	997	166		

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



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

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



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

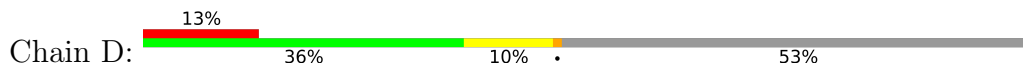
- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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



[illegible]

- Molecule 3: SWI/SNF complex subunit SWI3



MET	GLU	ASN	ASN	THR	LEU	GLY	GLU	GLY	SER	SER	THR	VAL	ASN	ASN	ALA	ALA	VAL	ASN	ASN	ASP	ASP	ASN	ASN	GLN	HIS	GLY	ASN	ASP	ASP	ASN	ASN	ALA	ALA	ALA	ALA	VAL	VAL	GLY	VAL	VAL	GLU	GLU	SER	SER	GLN	GLN	GLN	ASP	ASP	GLU	GLU	SER	LEU	LYS	ASP	GLU	ALA	GLU	THR	VAL
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PRO	ASN	THR	ARG	ASP	ALA	GLU	SER	GLU	ALA	ILE	THR	VAL	THR	ALA	LYS	GLN	GLN	PRO	THR	MET	GLN	ASN	LYS	LEU	ASP	SER	GLN	GLU	THR	PRO	SER	THR	GLU	GLU	SER	ALA	ALA	GLN	ASN	VAL	PHE	GLY	GLN	ASP	ASN	LEU	PHE	GLY	THR	GLU	SER
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VAL	LYS	GLU	GLU	SER	GLN	PRO	ASP	ASP	GLU	VAL	GLU	GLU	ASP	ASP	ASP	GLN	PRO	PRO	ASP	ASN	ASN	ILE	ILE	PHE	THR	THR	ASP	ASP	GLY	GLY	ASN	THR	SER	SER	SER	VAL	ALA	ASN	THR	PRO	PRO	GLU	GLU	ILE	PRO
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ASP	ALA	HIS	LYS	ALA	GLU	GLN	GLU	GLU	ASP	ASP	ILE	ILE	GLU	LYS	THR	GLU	SER	SER	VAL	ASP	LYS	LYS	VAL	ASP	SER	SER	GLY	GLU	GLU	ARG	ASN	ASN	GLN	GLU	ARG	GLU	ILE	ILE	MET	ASN	ASP	HIS	SER	SER	LYS	SER	SER	ALA	ASN	ASN	PRO	PRO	LYS	LYS	THR	THR	ILE	THR	ARG	VAL	GLU	PRO	GLU	THR	PHE	GLU	1299
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Q301	A302	T305	V306	S311	K312	S321	Q325	S326	L327	P328	N333	T339	S363	T366	R369	N370	V371	S372	G373	D374	K387	Q394	S397	N403	T404	A405	D417	G421	L422	F423	P424	F425	E426	S427	G428	K429	P430	S431	V432	Q433	L434	P435	D436	D437
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A438	A439	L440	K441	K442	N445	T446	S447	D448	S449	E450	L453	K458	E459	R462	K463	Y464	D465	E466	I467	T468	HIS	PRO	PRO	SER	THR	THR	ASP	ASP	GLU	ASN	ASN	GLY	GLY	LYS	MET	ASN	ASN	GLU	VAL	SER	THR	THR	THR	SER	MET	THR	GLY	ASP	ALA
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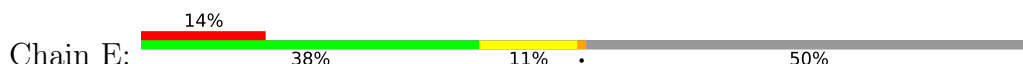
LEU LEU GLU GLU GLU GLU THR SER PARG L514 L515 K516 V517 K518 K519 D524 D525 L535 L36 K37 G538 I539 Q540 Q541 F542 G543 A544 D545 W546 N555 L556 R564 F565 L566 Q567 L568 P569 I570 E571 F574 L575 Y576 G579 ASN LYS GLY GLY ASP ASN ASP N587 G588

SLY	6766	6767	6768	6769	6770	6771	6772	6773	6774	6775	6776	6777	6778	6779	6780	6781	6782	6783	6784	6785	6786	6787	6788	6789	6790	6791	6792	6793	6794	6795	6796	6797	6798	6799	6800	6801	6802	6803	6804	6805	6806	6807	6808	6809	6810	6811	6812	6813	6814	6815	6816	6817	6818	6819	6820	6821	6822	6823	6824	6825	6826	6827	6828	6829	6830	6831	6832	6833	6834	6835	6836	6837	6838	6839	6840	6841	6842	6843	6844	6845	6846	6847	6848	6849	6850	6851	6852	6853	6854	6855	6856	6857	6858	6859	6860	6861	6862	6863	6864	6865	6866	6867	6868	6869	6870	6871	6872	6873	6874	6875	6876	6877	6878	6879	6880	6881	6882	6883	6884	6885	6886	6887	6888	6889	6890	6891	6892	6893	6894	6895	6896	6897	6898	6899	6900	6901	6902	6903	6904	6905	6906	6907	6908	6909	6910	6911	6912	6913	6914	6915	6916	6917	6918	6919	6920	6921	6922	6923	6924	6925	6926	6927	6928	6929	6930	6931	6932	6933	6934	6935	6936	6937	6938	6939	6940	6941	6942	6943	6944	6945	6946	6947	6948	6949	6950	6951	6952	6953	6954	6955	6956	6957	6958	6959	6960	6961	6962	6963	6964	6965	6966	6967	6968	6969	6970	6971	6972	6973	6974	6975	6976	6977	6978	6979	6980	6981	6982	6983	6984	6985	6986	6987	6988	6989	6990	6991	6992	6993	6994	6995	6996	6997	6998	6999	7000
6766	6767	6768	6769	6770	6771	6772	6773	6774	6775	6776	6777	6778	6779	6780	6781	6782	6783	6784	6785	6786	6787	6788	6789	6790	6791	6792	6793	6794	6795	6796	6797	6798	6799	6800	6801	6802	6803	6804	6805	6806	6807	6808	6809	6810	6811	6812	6813	6814	6815	6816	6817	6818	6819	6820	6821	6822	6823	6824	6825	6826	6827	6828	6829	6830	6831	6832	6833	6834	6835	6836	6837	6838	6839	6840	6841	6842	6843	6844	6845	6846	6847	6848	6849	6850	6851	6852	6853	6854	6855	6856	6857	6858	6859	6860	6861	6862	6863	6864	6865	6866	6867	6868	6869	6870	6871	6872	6873	6874	6875	6876	6877	6878	6879	6880	6881	6882	6883	6884	6885	6886	6887	6888	6889	6890	6891	6892	6893	6894	6895	6896	6897	6898	6899	6900	6901	6902	6903	6904	6905	6906	6907	6908	6909	6910	6911	6912	6913	6914	6915	6916	6917	6918	6919	6920	6921	6922	6923	6924	6925	6926	6927	6928	6929	6930	6931	6932	6933	6934	6935	6936																																																																	

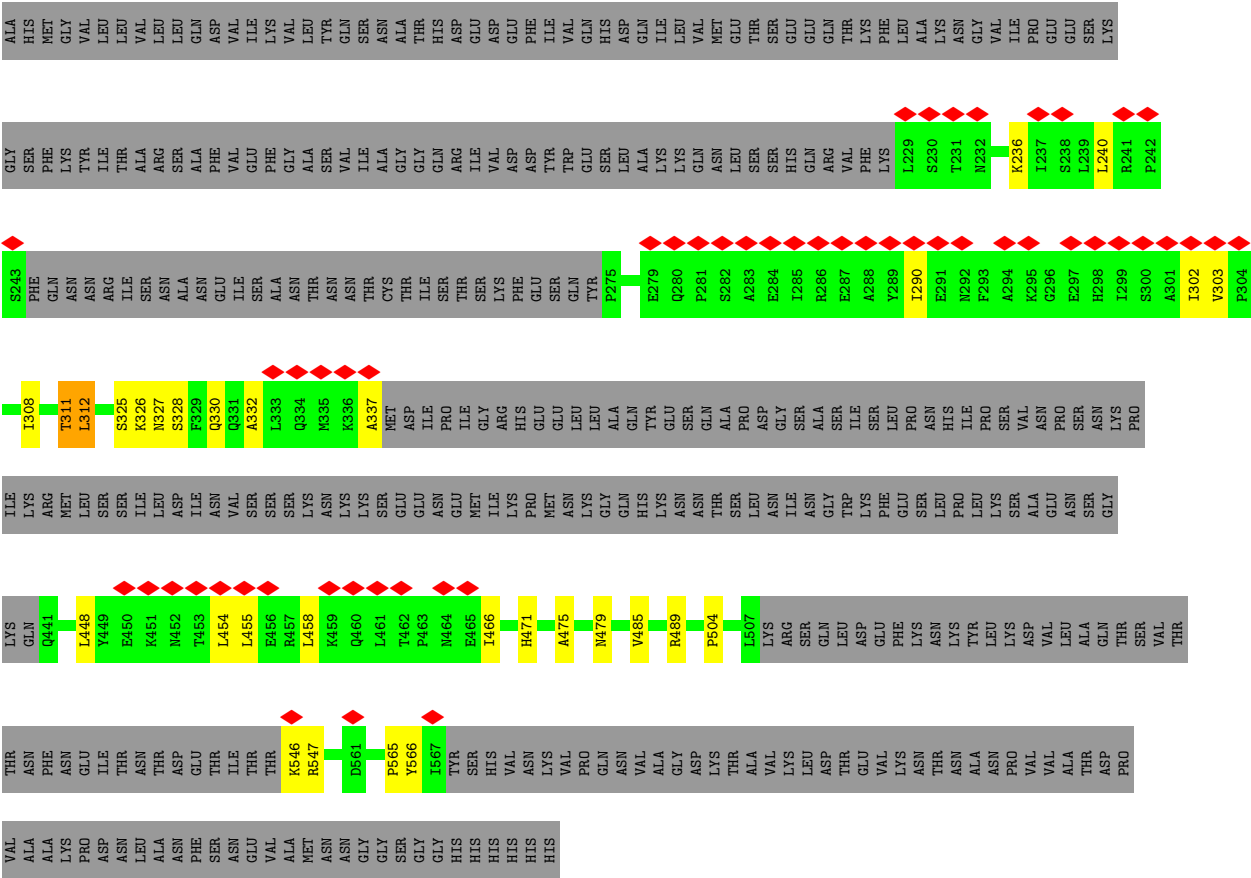
	PER	ASN	TILE	ASN	ASN	PER	VAL	ALA	GLU	-YS	PER	PRO	ASN	ASN	TILE	GLN	THR	GLY	ASN	ASN	GLN	PER	TILE	PER	ASN			
	7681	7672	7663	7664	7665	7666	7667	7668	7669	7670	7671	7672	7673	7674	7675	7676	7677	7678	7679	7680	7681	7682	7683	7684	7685	7686	7687	7688

LYS	PRO	ILE	SER	ILE	GLU	ALA	PRO	GLN	PHE	TYR	ARG	TYR	TRP	SER	ALA	GLY	GLY	SER	GLY	GLY	HIS	HIS	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

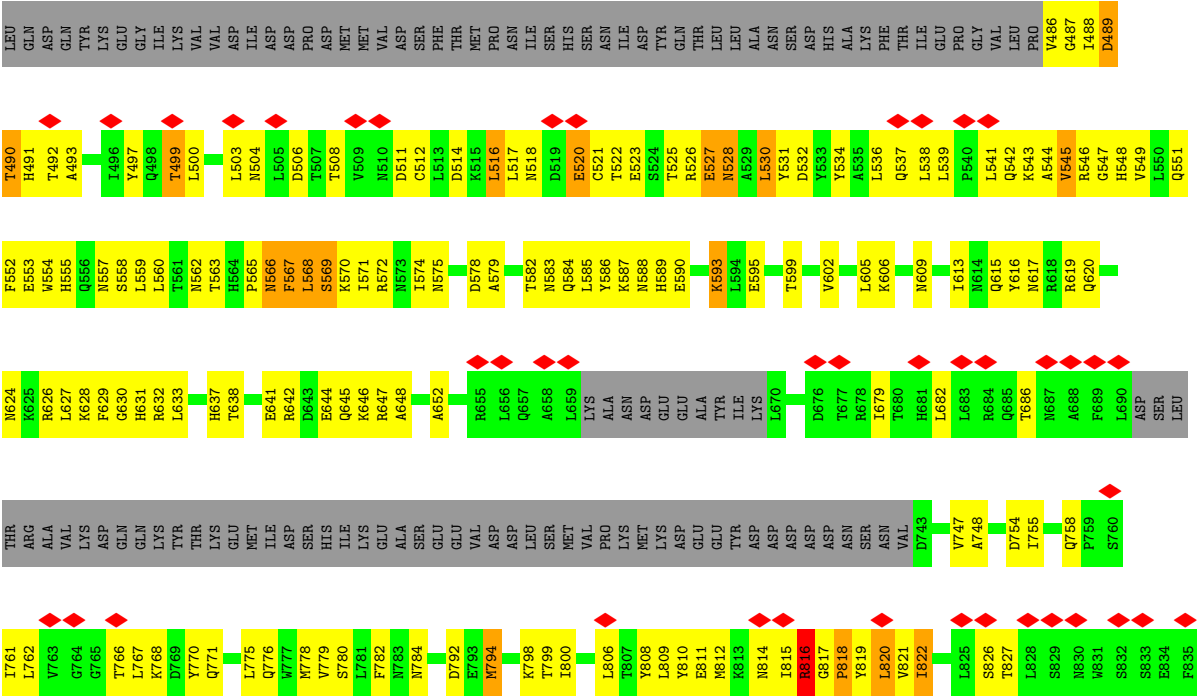
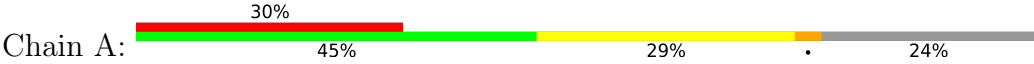
- Molecule 3: SWI/SNF complex subunit SWI3

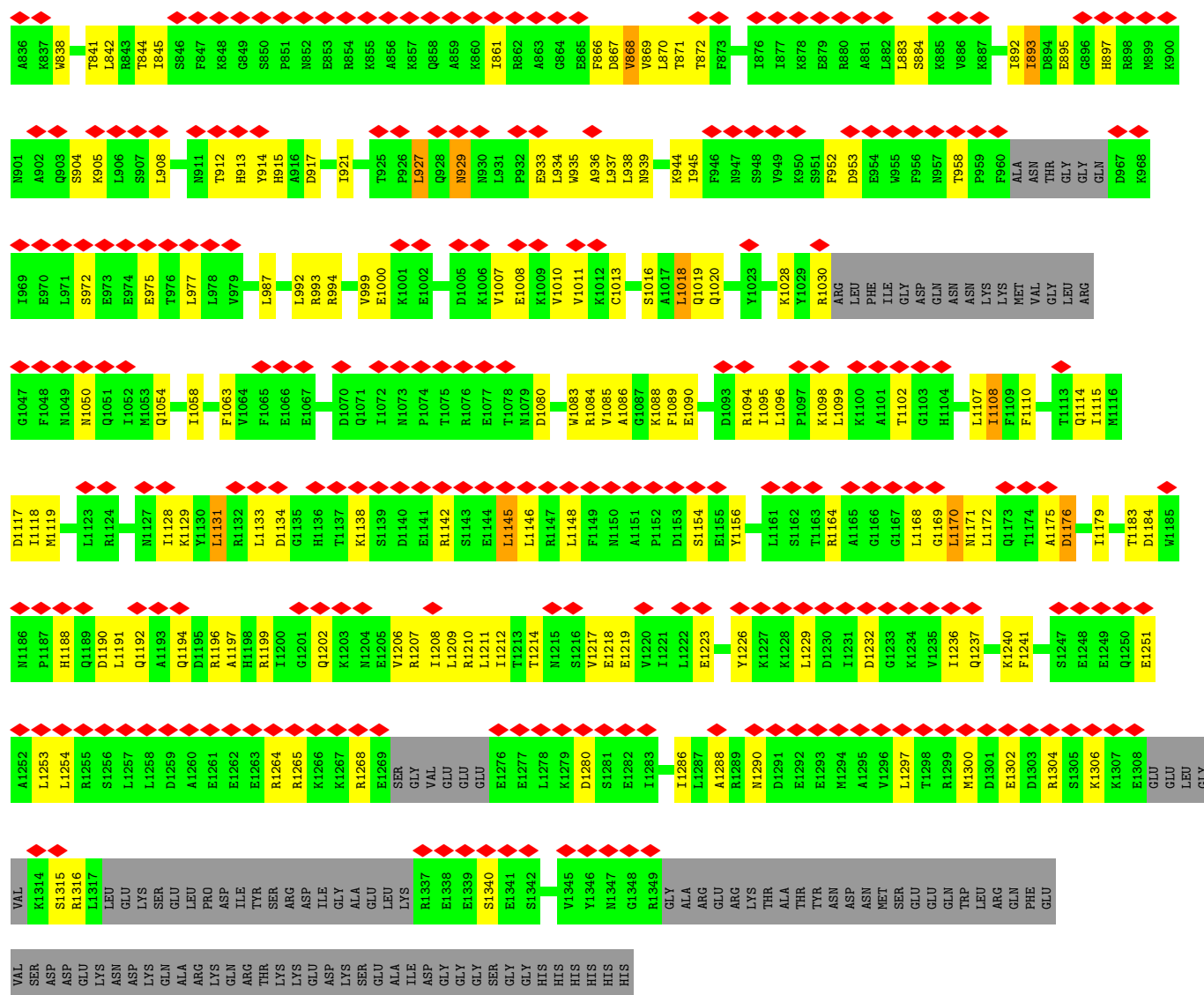




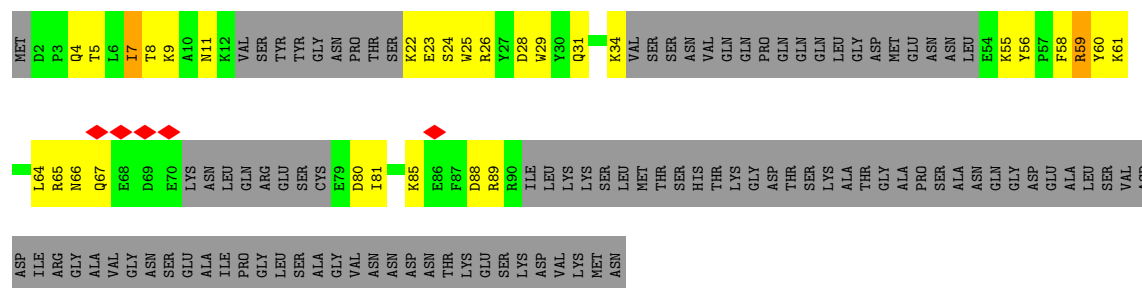


● Molecule 7: Transcription regulatory protein SNF2



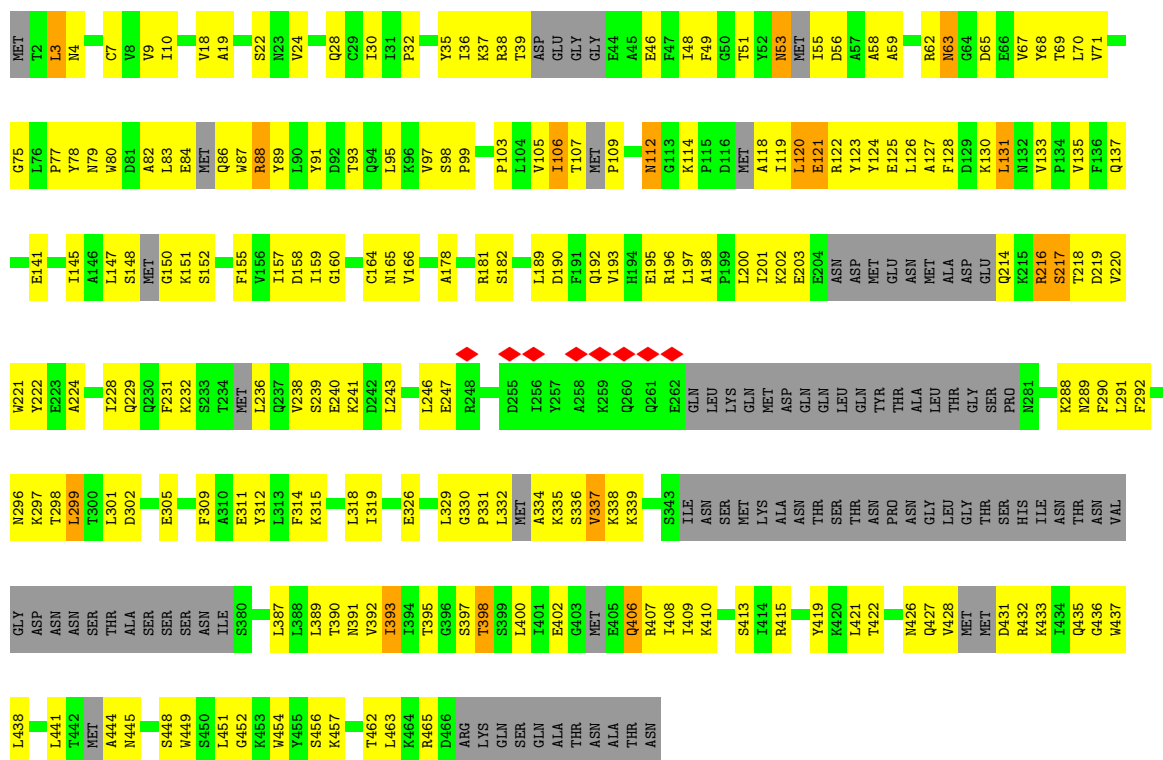


• Molecule 8: Regulator of Ty1 transposition protein 102

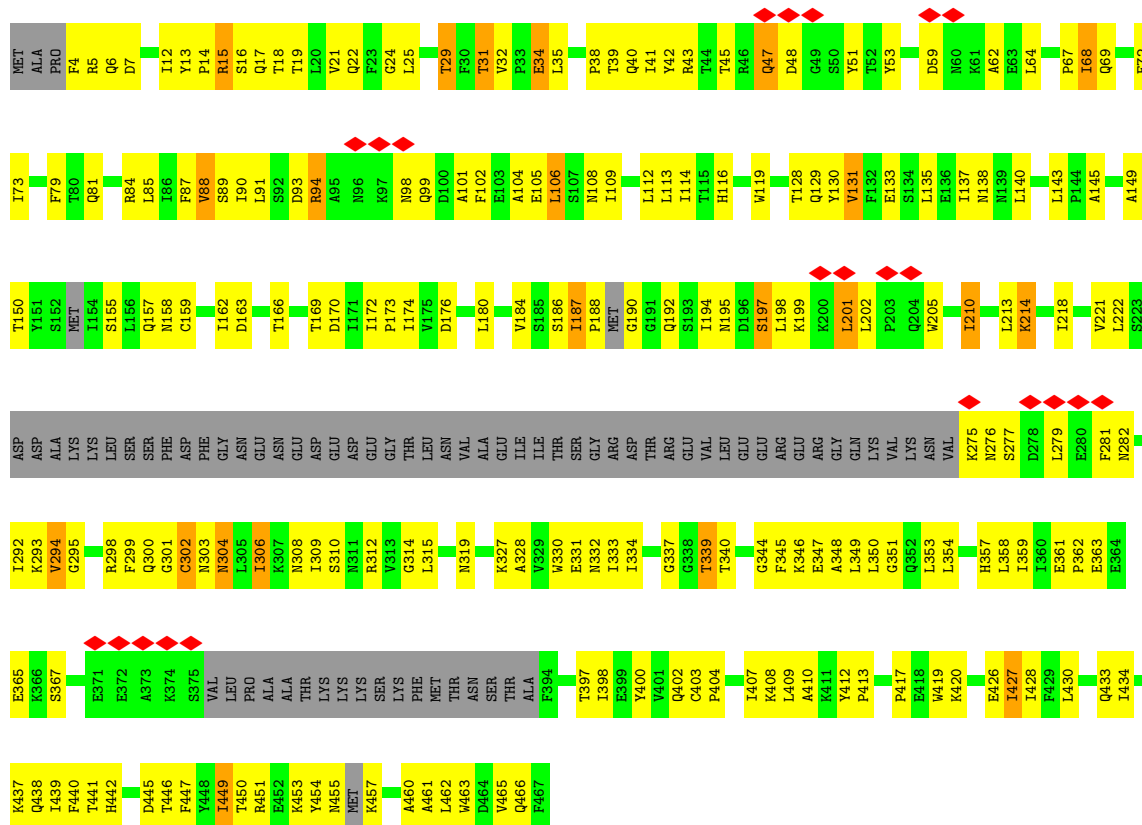


• Molecule 9: Actin-related protein 7

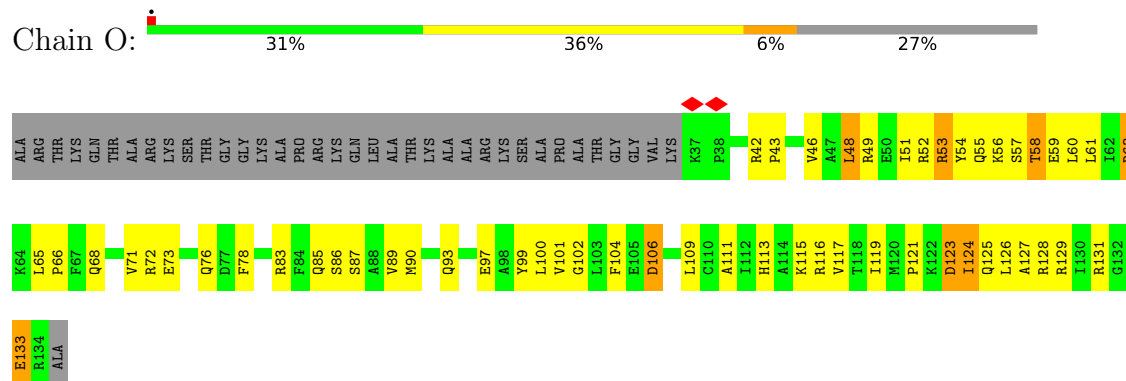




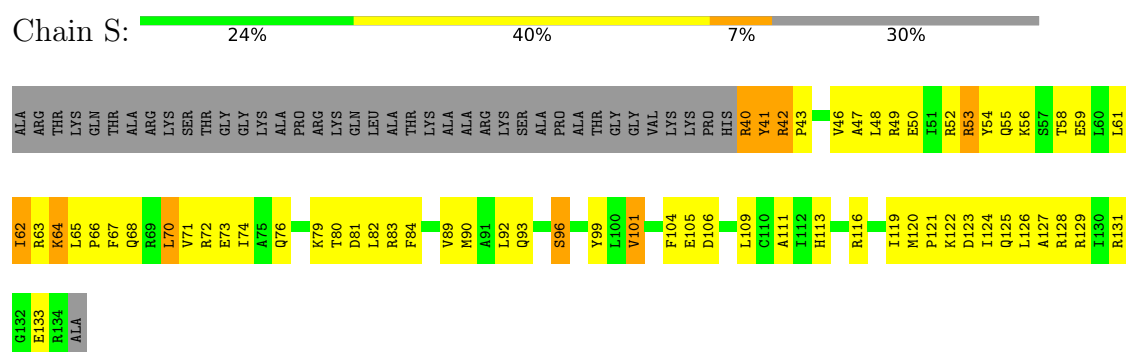
• Molecule 10: Actin-like protein ARP9



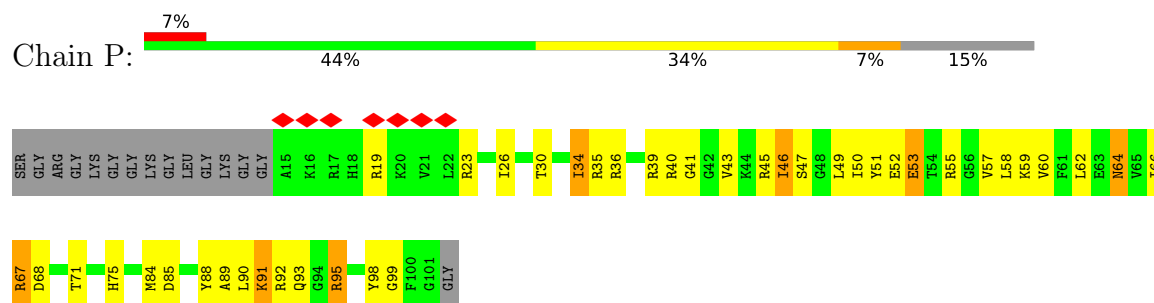
• Molecule 11: Histone H3.2



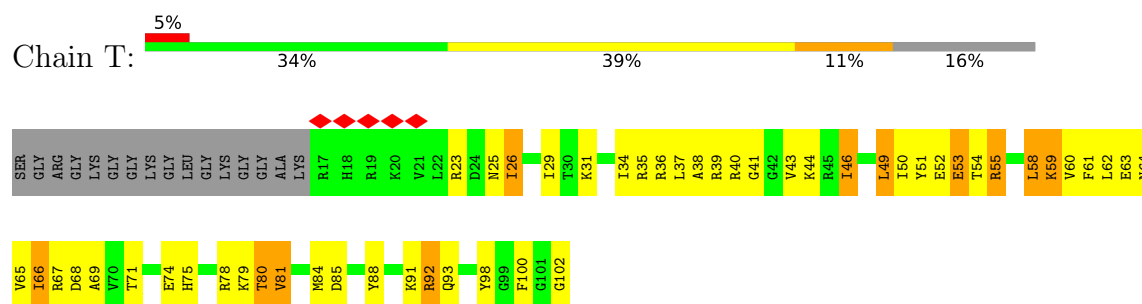
• Molecule 11: Histone H3.2



• Molecule 12: Histone H4

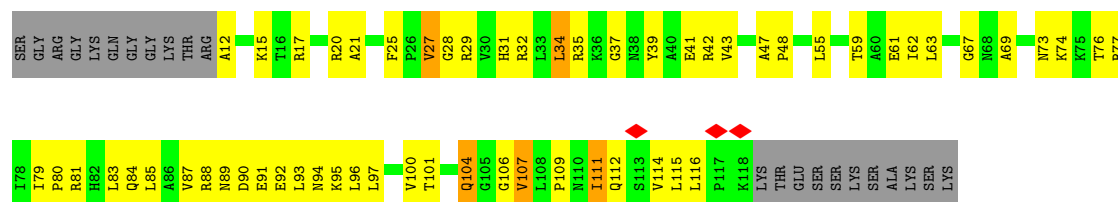


• Molecule 12: Histone H4

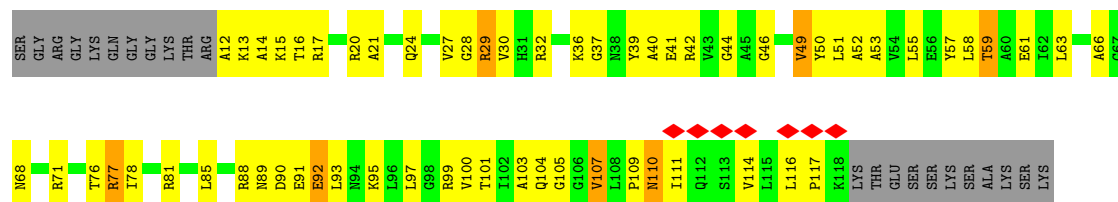


• Molecule 13: Histone H2A

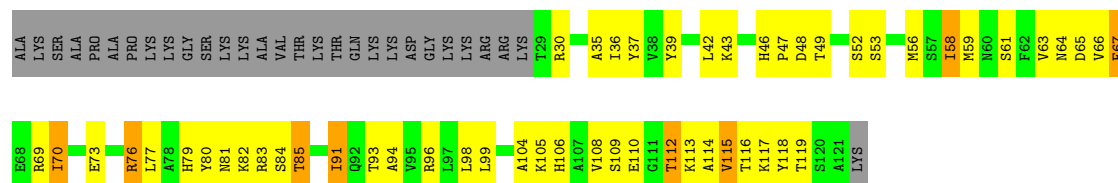




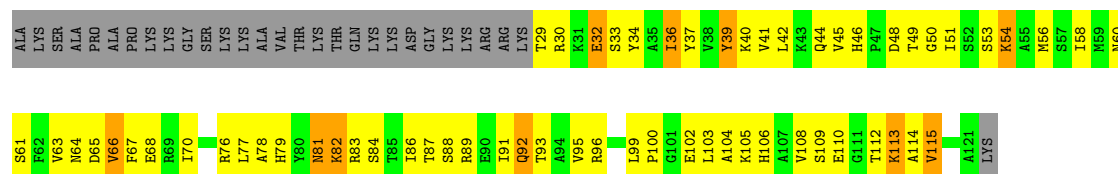
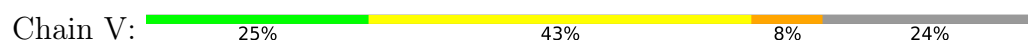
• Molecule 13: Histone H2A



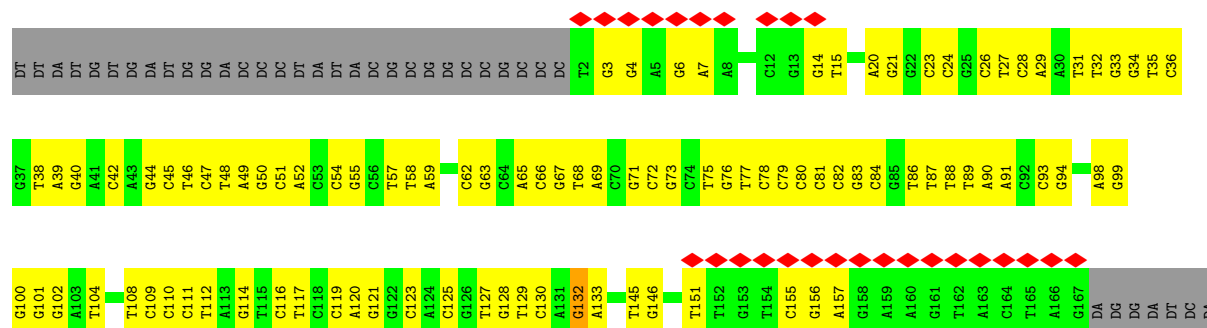
• Molecule 14: Histone H2B 1.1



• Molecule 14: Histone H2B 1.1



• Molecule 15: DNA (239-MER)



4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.26	0/4171	0.54	0/5648
2	C	0.29	0/2926	0.55	0/3953
3	D	0.26	0/3318	0.54	2/4465 (0.0%)
3	E	0.22	0/3526	0.50	0/4747
4	H	0.20	0/3201	0.48	0/4322
5	I	0.19	0/902	0.53	2/1211 (0.2%)
6	J	0.19	0/1390	0.46	0/1874
7	A	0.30	0/6256	0.59	0/8415
8	L	0.29	0/493	0.61	0/659
9	M	0.31	0/3197	0.57	0/4313
10	N	0.31	0/3234	0.59	0/4382
11	O	0.40	0/812	0.69	0/1091
11	S	0.39	0/788	0.76	2/1057 (0.2%)
12	P	0.37	0/711	0.70	0/950
12	T	0.36	0/680	0.68	0/912
13	Q	0.34	0/821	0.61	0/1112
13	U	0.36	0/825	0.65	0/1116
14	R	0.39	0/729	0.68	0/985
14	V	0.37	0/737	0.65	0/993
15	W	0.73	0/3804	0.82	1/5866 (0.0%)
16	X	0.75	0/3830	0.93	2/5912 (0.0%)
All	All	0.40	0/46351	0.64	9/63983 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	397	SER	CA-C-N	5.61	132.25	121.54
3	D	397	SER	C-N-CA	5.61	132.25	121.54
5	I	94	ILE	CA-C-N	5.38	131.81	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	94	ILE	C-N-CA	5.38	131.81	121.54
11	S	41	TYR	CA-C-N	5.34	132.38	121.48
11	S	41	TYR	C-N-CA	5.34	132.38	121.48
16	X	30	DG	C4'-C3'-O3'	-5.34	101.99	110.00
16	X	64	DG	C3'-C2'-C1'	-5.11	93.94	101.60
15	W	132	DG	O4'-C1'-N9	5.10	116.04	108.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4098	0	4239	194	0
2	C	2873	0	2807	111	0
3	D	3250	0	3301	178	0
3	E	3454	0	3511	79	0
4	H	3145	0	3143	49	0
5	I	888	0	867	10	0
6	J	1360	0	1400	47	0
7	A	6162	0	6271	511	0
8	L	482	0	455	31	0
9	M	3131	0	3129	182	0
10	N	3167	0	3149	159	0
11	O	800	0	829	57	0
11	S	778	0	813	74	0
12	P	703	0	757	42	0
12	T	672	0	698	58	0
13	Q	811	0	849	55	0
13	U	815	0	860	60	0
14	R	718	0	725	55	0
14	V	726	0	747	53	0
15	W	3393	0	1863	183	0
16	X	3413	0	1865	177	0
17	A	27	0	10	27	0
18	A	4	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	1	0	0	0	0
All	All	44871	0	42288	1750	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 (1750) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:ARG:HH12	1:B:985:LEU:CD1	1.02	1.64
3:D:565:PHE:CZ	7:A:542:GLN:HB2	1.36	1.57
9:M:214:GLN:NE2	9:M:216:ARG:CG	1.68	1.50
3:D:565:PHE:CE1	7:A:542:GLN:HB2	1.43	1.50
3:D:540:GLN:NE2	7:A:537:GLN:HB3	1.23	1.48
3:D:540:GLN:HE21	7:A:537:GLN:CB	1.27	1.44
1:B:941:ASN:ND2	1:B:944:LEU:H	1.07	1.44
1:B:940:ARG:NH1	1:B:985:LEU:HD13	1.15	1.42
3:D:609:SER:OG	7:A:488:ILE:CG1	1.67	1.40
1:B:941:ASN:HD21	1:B:944:LEU:N	1.24	1.33
7:A:584:GLN:HA	7:A:587:LYS:CE	1.59	1.31
2:C:554:GLN:O	2:C:655:ILE:N	1.62	1.30
9:M:216:ARG:HD3	9:M:220:VAL:CG2	1.46	1.30
1:B:723:ASN:OD1	7:A:559:LEU:HD21	1.32	1.30
9:M:214:GLN:NE2	9:M:216:ARG:HG3	0.98	1.29
7:A:915:HIS:CE1	7:A:917:ASP:OD1	1.85	1.29
3:D:609:SER:CB	7:A:488:ILE:HG12	1.63	1.27
3:D:605:ASN:O	7:A:488:ILE:CD1	1.81	1.27
3:D:570:ILE:CG2	7:A:539:LEU:HD22	1.64	1.26
7:A:808:TYR:HA	7:A:811:GLU:OE1	1.13	1.25
15:W:93:DC:O2	16:X:55:DG:N2	1.70	1.25
3:D:605:ASN:O	7:A:488:ILE:HD11	1.10	1.22
3:D:605:ASN:C	7:A:488:ILE:HD11	1.63	1.22
3:D:565:PHE:CE1	7:A:542:GLN:CB	2.22	1.22
1:B:907:ALA:HB2	7:A:557:ASN:ND2	1.54	1.22
1:B:1048:SER:O	7:A:589:HIS:NE2	1.73	1.21
2:C:663:LEU:HD12	2:C:666:ASP:OD2	1.38	1.21
3:E:444:MET:SD	7:A:503:LEU:HD13	1.79	1.21
7:A:584:GLN:CA	7:A:587:LYS:HE2	1.70	1.20
3:E:444:MET:CG	7:A:503:LEU:HD13	1.71	1.19
1:B:1049:LEU:HB3	1:B:1051:LYS:CD	1.71	1.19
3:D:540:GLN:HG2	7:A:538:LEU:CD2	1.71	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:584:GLN:NE2	7:A:587:LYS:NZ	1.91	1.19
7:A:808:TYR:O	7:A:811:GLU:HG2	1.42	1.18
7:A:915:HIS:NE2	7:A:917:ASP:OD1	1.75	1.18
9:M:216:ARG:CD	9:M:220:VAL:HG23	1.73	1.18
1:B:723:ASN:OD1	7:A:559:LEU:CD2	1.92	1.17
3:D:570:ILE:CD1	7:A:539:LEU:HD13	1.73	1.17
9:M:216:ARG:O	9:M:219:ASP:N	1.78	1.17
1:B:1051:LYS:HB2	1:B:1052:PRO:HD3	1.27	1.17
7:A:584:GLN:NE2	7:A:587:LYS:HZ1	1.41	1.17
2:C:654:GLN:O	2:C:655:ILE:HG23	1.45	1.15
1:B:1049:LEU:HB3	1:B:1051:LYS:HD2	1.22	1.15
3:D:540:GLN:HG2	7:A:538:LEU:HD21	1.18	1.14
1:B:940:ARG:NH1	1:B:985:LEU:CD1	1.78	1.14
7:A:810:TYR:O	7:A:814:ASN:N	1.80	1.14
3:D:565:PHE:CZ	7:A:542:GLN:CB	2.31	1.14
1:B:1145:THR:HG22	7:A:586:TYR:CZ	1.84	1.13
3:D:609:SER:OG	7:A:488:ILE:HG12	0.98	1.13
4:H:556:ASN:ND2	7:A:553:GLU:OE1	1.80	1.13
1:B:941:ASN:ND2	1:B:944:LEU:N	1.85	1.12
3:E:444:MET:SD	7:A:503:LEU:HD22	1.89	1.12
3:D:422:LEU:O	7:A:555:HIS:CD2	2.02	1.12
3:E:444:MET:HG3	7:A:503:LEU:HD13	1.29	1.12
15:W:88:DT:C4	16:X:60:DA:N1	2.17	1.12
7:A:808:TYR:O	7:A:811:GLU:CG	1.96	1.11
3:D:516:LYS:HE2	7:A:511:ASP:OD2	1.50	1.11
15:W:45:DC:O2	16:X:103:DG:N2	1.83	1.11
7:A:808:TYR:CA	7:A:811:GLU:OE1	1.98	1.10
1:B:1051:LYS:HG2	1:B:1052:PRO:HD2	1.13	1.10
15:W:121:DG:N2	16:X:27:DC:O2	1.83	1.10
3:D:540:GLN:NE2	7:A:537:GLN:CB	1.92	1.10
3:D:566:LEU:HD22	7:A:546:ARG:HG3	1.14	1.09
3:D:539:ILE:HG22	7:A:538:LEU:HG	1.24	1.09
3:D:566:LEU:HD22	7:A:546:ARG:CG	1.81	1.08
15:W:88:DT:N3	16:X:60:DA:N1	2.01	1.08
1:B:940:ARG:NH1	1:B:985:LEU:CB	2.15	1.07
1:B:940:ARG:NH1	1:B:985:LEU:HB3	1.68	1.07
3:D:570:ILE:HD12	7:A:539:LEU:HD13	1.13	1.06
9:M:217:SER:O	9:M:221:TRP:HB3	1.54	1.06
7:A:810:TYR:CZ	7:A:819:TYR:CE2	2.44	1.06
1:B:940:ARG:HH11	1:B:985:LEU:HB3	1.11	1.05
3:D:570:ILE:HD12	7:A:539:LEU:CD1	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:426:GLU:OE2	7:A:548:HIS:CD2	2.10	1.04
7:A:798:LYS:HG3	17:A:1501:ADP:O2B	1.57	1.04
3:D:570:ILE:HG21	7:A:539:LEU:CD2	1.88	1.03
7:A:585:LEU:O	7:A:588:ASN:OD1	1.75	1.03
15:W:114:DG:N2	16:X:34:DC:O2	1.91	1.03
15:W:35:DT:N3	16:X:113:DA:N1	2.07	1.02
15:W:129:DT:C4	16:X:19:DA:N1	2.27	1.02
2:C:652:LEU:HB2	6:J:312:LEU:O	1.56	1.02
1:B:940:ARG:CZ	1:B:985:LEU:HD13	1.90	1.02
7:A:798:LYS:HB2	17:A:1501:ADP:O3B	1.57	1.02
1:B:1049:LEU:CB	1:B:1051:LYS:HD2	1.90	1.01
1:B:940:ARG:HH12	1:B:985:LEU:CG	1.72	1.01
7:A:1199:ARG:NH2	18:A:1502:BEF:F2	1.83	1.01
3:D:565:PHE:O	7:A:542:GLN:NE2	1.94	1.01
1:B:1051:LYS:CG	1:B:1052:PRO:HD2	1.91	1.01
3:D:605:ASN:C	7:A:488:ILE:CD1	2.30	1.01
2:C:555:ASN:HA	2:C:654:GLN:HA	1.44	1.00
1:B:927:ASN:HD21	7:A:569:SER:HB3	1.26	1.00
10:N:169:THR:HG1	10:N:190:GLY:N	1.56	1.00
15:W:129:DT:N3	16:X:19:DA:N1	2.10	1.00
1:B:1051:LYS:HG2	1:B:1052:PRO:CD	1.92	0.99
7:A:810:TYR:CD2	7:A:816:ARG:HA	1.96	0.99
15:W:79:DC:O2	16:X:69:DG:N2	1.95	0.99
3:D:566:LEU:CD2	7:A:546:ARG:HG3	1.93	0.99
15:W:100:DG:N2	16:X:48:DC:O2	1.96	0.98
1:B:936:ARG:HB2	1:B:940:ARG:NH2	1.77	0.98
1:B:1145:THR:HG21	7:A:586:TYR:CE2	1.99	0.98
15:W:129:DT:O4	16:X:19:DA:N6	1.96	0.98
3:D:570:ILE:HG21	7:A:539:LEU:HD22	1.01	0.98
3:D:540:GLN:NE2	7:A:537:GLN:CG	2.27	0.97
7:A:584:GLN:HA	7:A:587:LYS:HE2	0.97	0.97
7:A:808:TYR:C	7:A:811:GLU:HG2	1.89	0.97
1:B:940:ARG:NH1	1:B:985:LEU:CG	2.28	0.96
3:E:444:MET:HG3	7:A:503:LEU:CD1	1.93	0.96
1:B:1051:LYS:CB	1:B:1052:PRO:HD3	1.94	0.96
7:A:583:ASN:O	7:A:587:LYS:HG3	1.65	0.95
3:D:606:PRO:HA	7:A:488:ILE:CD1	1.97	0.95
1:B:1051:LYS:CG	1:B:1052:PRO:CD	2.44	0.95
3:D:426:GLU:OE2	7:A:548:HIS:NE2	2.00	0.95
1:B:1049:LEU:CB	1:B:1051:LYS:CD	2.42	0.95
7:A:584:GLN:NE2	7:A:587:LYS:CE	2.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:99:DG:N2	16:X:49:DC:O2	1.99	0.95
15:W:110:DC:O2	16:X:38:DG:N2	1.98	0.95
1:B:1051:LYS:O	1:B:1055:ASN:ND2	2.00	0.94
7:A:810:TYR:OH	7:A:819:TYR:CE2	2.20	0.94
15:W:42:DC:O2	16:X:106:DG:N2	2.01	0.94
7:A:1199:ARG:NH1	18:A:1502:BEF:F3	1.90	0.94
2:C:652:LEU:HD12	6:J:312:LEU:HB2	1.46	0.94
2:C:652:LEU:HD12	6:J:312:LEU:CB	1.98	0.94
3:D:610:THR:OG1	7:A:487:GLY:HA3	1.67	0.93
3:D:540:GLN:CG	7:A:538:LEU:HD21	1.97	0.93
7:A:810:TYR:CD2	7:A:816:ARG:CA	2.51	0.93
1:B:1051:LYS:CB	1:B:1052:PRO:CD	2.46	0.93
7:A:810:TYR:O	7:A:814:ASN:CA	2.17	0.92
1:B:941:ASN:ND2	1:B:944:LEU:CB	2.31	0.92
7:A:810:TYR:O	7:A:814:ASN:HA	1.70	0.92
9:M:214:GLN:NE2	9:M:216:ARG:HG2	1.83	0.92
3:E:444:MET:SD	7:A:503:LEU:CD1	2.58	0.92
15:W:38:DT:N3	16:X:110:DA:N1	2.16	0.92
15:W:73:DG:N2	16:X:75:DC:O2	2.01	0.92
9:M:216:ARG:CD	9:M:220:VAL:CG2	2.23	0.91
7:A:808:TYR:HA	7:A:811:GLU:CD	1.95	0.91
1:B:940:ARG:CZ	1:B:985:LEU:CD1	2.48	0.91
10:N:169:THR:HB	10:N:187:ILE:O	1.71	0.91
9:M:214:GLN:OE1	9:M:216:ARG:NE	2.05	0.89
1:B:1049:LEU:CG	1:B:1051:LYS:HD3	2.01	0.89
1:B:1145:THR:CG2	7:A:586:TYR:CE2	2.55	0.89
2:C:652:LEU:HB2	6:J:312:LEU:HB3	1.53	0.89
7:A:766:THR:OG1	17:A:1501:ADP:N1	1.80	0.89
9:M:67:VAL:HB	9:M:217:SER:HB2	1.53	0.89
2:C:467:ASP:OD2	2:C:662:ARG:NH2	2.05	0.89
1:B:1145:THR:CG2	7:A:586:TYR:CZ	2.55	0.89
9:M:67:VAL:HB	9:M:217:SER:CB	2.03	0.89
9:M:214:GLN:HE21	9:M:216:ARG:HG3	1.17	0.89
3:D:602:LYS:HA	7:A:488:ILE:HB	1.52	0.89
1:B:1051:LYS:HB2	1:B:1052:PRO:CD	2.03	0.88
7:A:810:TYR:CE2	7:A:816:ARG:HA	2.07	0.88
1:B:1049:LEU:HD23	1:B:1051:LYS:HD3	1.54	0.88
3:D:601:SER:HB3	3:D:604:GLU:HB2	1.55	0.88
2:C:654:GLN:O	2:C:655:ILE:CG2	2.21	0.88
7:A:584:GLN:HE21	7:A:587:LYS:NZ	1.60	0.87
3:E:440:LEU:HD13	7:A:499:THR:HG21	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:67:VAL:N	9:M:217:SER:OG	2.06	0.87
3:D:537:LYS:CG	7:A:534:TYR:HE2	1.86	0.87
15:W:33:DG:N2	16:X:115:DC:O2	2.08	0.86
12:T:88:TYR:O	12:T:92:ARG:HB2	1.74	0.86
3:D:422:LEU:O	7:A:555:HIS:HD2	1.55	0.86
1:B:907:ALA:HB2	7:A:557:ASN:HD22	1.37	0.86
3:D:606:PRO:CA	7:A:488:ILE:HD11	2.06	0.86
2:C:558:ILE:HD12	2:C:653:LEU:HD11	1.55	0.86
2:C:652:LEU:CB	6:J:312:LEU:HB3	2.05	0.86
3:D:601:SER:C	7:A:488:ILE:HG21	2.00	0.86
7:A:584:GLN:NE2	7:A:587:LYS:HE3	1.88	0.86
7:A:584:GLN:CD	7:A:587:LYS:HE3	1.99	0.86
7:A:810:TYR:HD2	7:A:816:ARG:CB	1.88	0.86
9:M:214:GLN:CD	9:M:216:ARG:HG3	2.01	0.86
15:W:51:DC:O2	16:X:97:DG:N2	2.07	0.86
2:C:652:LEU:CD1	6:J:489:ARG:HH22	1.89	0.85
7:A:584:GLN:HA	7:A:587:LYS:HE3	1.58	0.85
1:B:940:ARG:N	1:B:940:ARG:HD2	1.92	0.85
1:B:941:ASN:ND2	1:B:941:ASN:O	2.08	0.85
9:M:216:ARG:HD3	9:M:220:VAL:HG23	0.85	0.85
3:E:444:MET:SD	7:A:503:LEU:CD2	2.65	0.85
1:B:723:ASN:CG	7:A:559:LEU:HD21	2.01	0.85
6:J:566:TYR:CZ	7:A:545:VAL:HG12	2.12	0.85
1:B:907:ALA:HB3	7:A:554:TRP:CZ3	2.10	0.85
9:M:35:TYR:O	9:M:67:VAL:HA	1.75	0.85
15:W:78:DC:O2	16:X:70:DG:N2	2.10	0.85
1:B:1048:SER:HB2	7:A:589:HIS:CE1	2.12	0.85
2:C:558:ILE:HD12	2:C:653:LEU:CD1	2.06	0.84
15:W:116:DC:O2	16:X:32:DG:N2	2.10	0.84
15:W:88:DT:N3	16:X:60:DA:C2	2.46	0.84
15:W:123:DC:O2	16:X:25:DG:N2	2.10	0.84
3:D:537:LYS:HG3	7:A:534:TYR:HE2	1.42	0.84
1:B:936:ARG:CB	1:B:940:ARG:NH2	2.41	0.83
3:D:606:PRO:O	7:A:486:VAL:O	1.96	0.83
2:C:652:LEU:HD11	6:J:489:ARG:HH22	1.41	0.83
15:W:34:DG:N2	16:X:114:DC:O2	2.10	0.83
1:B:1048:SER:O	7:A:589:HIS:CE1	2.30	0.83
15:W:130:DC:O2	16:X:18:DG:N2	2.11	0.83
3:D:537:LYS:HG3	7:A:534:TYR:CE2	2.13	0.83
7:A:810:TYR:HD2	7:A:816:ARG:HB3	1.40	0.83
9:M:67:VAL:CA	9:M:217:SER:OG	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1171:ASN:ND2	17:A:1501:ADP:O1A	2.12	0.83
3:D:602:LYS:HA	7:A:488:ILE:HD12	1.61	0.82
7:A:798:LYS:HD2	17:A:1501:ADP:O3B	1.79	0.82
1:B:1049:LEU:CD2	1:B:1051:LYS:HD3	2.08	0.82
3:D:570:ILE:CG2	7:A:539:LEU:CD2	2.50	0.82
7:A:489:ASP:O	7:A:491:HIS:N	2.12	0.82
3:D:536:LEU:HB3	7:A:534:TYR:HB3	1.60	0.82
15:W:63:DG:N2	16:X:85:DC:O2	2.12	0.82
2:C:652:LEU:CG	6:J:312:LEU:HB3	2.10	0.81
3:D:430:PRO:HG2	6:J:566:TYR:HB3	1.61	0.81
3:D:606:PRO:CA	7:A:488:ILE:CD1	2.58	0.81
7:A:810:TYR:OH	7:A:819:TYR:CD2	2.33	0.81
3:D:609:SER:OG	7:A:488:ILE:HG13	1.78	0.81
7:A:800:ILE:HD11	17:A:1501:ADP:C8	2.15	0.81
1:B:1048:SER:O	7:A:589:HIS:CD2	2.34	0.81
11:S:72:ARG:O	11:S:76:GLN:HB2	1.81	0.81
7:A:1196:ARG:NH2	18:A:1502:BEF:F2	2.04	0.81
9:M:216:ARG:HD2	9:M:220:VAL:H	1.44	0.81
3:D:565:PHE:CE1	7:A:542:GLN:CA	2.64	0.80
6:J:240:LEU:O	7:A:537:GLN:NE2	2.13	0.80
6:J:240:LEU:HD21	7:A:516:LEU:HD11	1.63	0.80
3:E:425:PHE:CD1	7:A:543:LYS:HG3	2.15	0.80
15:W:94:DG:N2	16:X:54:DC:O2	2.13	0.80
3:D:426:GLU:HG2	7:A:551:GLN:OE1	1.82	0.80
1:B:1051:LYS:CD	1:B:1051:LYS:H	1.95	0.79
15:W:109:DC:O2	16:X:39:DG:N2	2.15	0.79
1:B:936:ARG:HB2	1:B:940:ARG:HH22	1.44	0.79
15:W:81:DC:O2	16:X:67:DG:N2	2.14	0.79
1:B:927:ASN:OD1	7:A:569:SER:HB2	1.81	0.79
1:B:1051:LYS:HB3	1:B:1051:LYS:NZ	1.98	0.79
9:M:214:GLN:OE1	9:M:216:ARG:CZ	2.31	0.79
1:B:1149:VAL:CG2	7:A:586:TYR:HE1	1.96	0.78
7:A:798:LYS:CB	17:A:1501:ADP:O3B	2.31	0.78
2:C:663:LEU:CD1	2:C:666:ASP:OD2	2.26	0.78
7:A:584:GLN:HE21	7:A:587:LYS:HZ1	0.81	0.78
2:C:663:LEU:O	2:C:666:ASP:N	2.15	0.78
15:W:129:DT:C4	16:X:19:DA:C6	2.72	0.78
9:M:216:ARG:O	9:M:218:THR:N	2.17	0.78
9:M:216:ARG:C	9:M:218:THR:N	2.38	0.77
1:B:723:ASN:CG	7:A:559:LEU:CD2	2.57	0.77
7:A:810:TYR:CD2	7:A:816:ARG:HB3	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:ARG:CB	1:B:940:ARG:HH22	1.95	0.77
15:W:35:DT:C4	16:X:113:DA:N1	2.52	0.77
15:W:80:DC:O2	16:X:68:DG:N2	2.17	0.77
15:W:125:DC:O2	16:X:23:DG:N2	2.16	0.77
15:W:83:DG:N1	16:X:65:DC:N3	2.30	0.76
2:C:652:LEU:CD1	6:J:489:ARG:NH2	2.48	0.76
9:M:214:GLN:NE2	9:M:216:ARG:CD	2.49	0.76
1:B:907:ALA:HB3	7:A:554:TRP:HZ3	1.47	0.76
3:D:540:GLN:HE21	7:A:537:GLN:HB3	0.59	0.76
15:W:93:DC:N3	16:X:55:DG:N1	2.31	0.76
13:Q:15:LYS:H	15:W:31:DT:H4'	1.50	0.76
1:B:936:ARG:CA	1:B:940:ARG:NH2	2.49	0.76
2:C:654:GLN:O	2:C:655:ILE:HG13	1.85	0.76
2:C:663:LEU:HD12	2:C:666:ASP:CG	2.11	0.76
15:W:72:DC:O2	16:X:76:DG:N2	2.15	0.76
1:B:927:ASN:ND2	7:A:569:SER:HB3	2.02	0.75
1:B:1145:THR:HG21	7:A:586:TYR:CD2	2.21	0.75
3:E:444:MET:CE	7:A:503:LEU:HD13	2.15	0.75
3:D:426:GLU:CD	7:A:548:HIS:CD2	2.64	0.75
3:E:606:PRO:HA	7:A:486:VAL:HG13	1.68	0.75
3:D:609:SER:HB3	7:A:488:ILE:HG12	1.64	0.75
9:M:67:VAL:O	9:M:217:SER:CB	2.33	0.75
3:D:540:GLN:HG2	7:A:538:LEU:HD22	1.68	0.75
15:W:62:DC:O2	16:X:86:DG:N2	2.16	0.75
1:B:1233:LEU:HD11	7:A:579:ALA:CB	2.16	0.75
9:M:216:ARG:C	9:M:218:THR:H	1.92	0.74
15:W:48:DT:O2	16:X:101:DG:N2	2.20	0.74
15:W:129:DT:C2	16:X:19:DA:C2	2.75	0.74
1:B:941:ASN:ND2	1:B:944:LEU:HB2	2.02	0.74
15:W:88:DT:C2	16:X:60:DA:C2	2.75	0.74
3:D:606:PRO:N	7:A:488:ILE:HD11	2.02	0.74
4:H:566:MET:HE1	7:A:549:VAL:CG2	2.17	0.74
3:D:602:LYS:CA	7:A:488:ILE:HB	2.16	0.74
7:A:810:TYR:CD2	7:A:816:ARG:CB	2.70	0.74
7:A:810:TYR:CE2	7:A:819:TYR:CE2	2.76	0.74
3:D:423:PHE:CD1	7:A:552:PHE:CE1	2.76	0.73
6:J:566:TYR:CE1	7:A:545:VAL:HG12	2.23	0.73
15:W:44:DG:N2	16:X:104:DC:O2	2.19	0.73
1:B:1049:LEU:CB	1:B:1051:LYS:HD3	2.16	0.73
2:C:468:ARG:HH12	2:C:662:ARG:NE	1.86	0.73
3:D:422:LEU:C	7:A:555:HIS:HE2	1.96	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:518:LYS:O	3:E:522:GLN:HB2	1.89	0.73
11:S:43:PRO:HG3	16:X:68:DG:H21	1.54	0.73
1:B:1051:LYS:HE2	1:B:1051:LYS:N	2.03	0.73
7:A:1171:ASN:HD21	17:A:1501:ADP:C5'	2.00	0.73
7:A:572:ARG:HD2	7:A:575:ASN:HD21	1.54	0.73
7:A:808:TYR:O	7:A:811:GLU:HG3	1.87	0.73
2:C:654:GLN:NE2	6:J:311:THR:HG22	2.03	0.73
3:D:565:PHE:HZ	7:A:538:LEU:O	1.71	0.73
3:D:570:ILE:HG22	7:A:539:LEU:HD22	1.66	0.72
9:M:67:VAL:C	9:M:217:SER:OG	2.32	0.72
11:S:47:ALA:O	11:S:50:GLU:HB2	1.90	0.72
4:H:566:MET:HE1	7:A:549:VAL:HG21	1.72	0.72
7:A:566:ASN:O	7:A:568:LEU:N	2.22	0.72
1:B:941:ASN:ND2	1:B:944:LEU:CA	2.52	0.72
1:B:1233:LEU:HD11	7:A:579:ALA:HB3	1.71	0.72
15:W:104:DT:N3	16:X:44:DA:C2	2.58	0.72
15:W:109:DC:N3	16:X:39:DG:N1	2.38	0.72
7:A:798:LYS:HD2	17:A:1501:ADP:PB	2.30	0.72
3:D:424:PRO:HD3	7:A:552:PHE:HD1	1.55	0.71
9:M:243:LEU:O	9:M:247:GLU:HB2	1.89	0.71
1:B:734:ALA:CB	7:A:567:PHE:CZ	2.72	0.71
3:E:606:PRO:HA	7:A:486:VAL:CG1	2.19	0.71
7:A:818:PRO:HA	7:A:866:PHE:CE1	2.25	0.71
3:D:606:PRO:HA	7:A:488:ILE:HD12	1.70	0.71
1:B:1049:LEU:HD23	1:B:1051:LYS:CD	2.21	0.71
7:A:566:ASN:O	7:A:567:PHE:C	2.30	0.71
7:A:817:GLY:O	7:A:867:ASP:O	2.08	0.71
1:B:734:ALA:HB3	7:A:567:PHE:HZ	1.55	0.71
1:B:936:ARG:HA	1:B:940:ARG:NH2	2.06	0.70
1:B:1049:LEU:CA	1:B:1051:LYS:HD2	2.21	0.70
2:C:652:LEU:HB3	6:J:312:LEU:H	1.55	0.70
3:D:424:PRO:CD	7:A:552:PHE:HD1	2.05	0.70
1:B:727:ASN:HD21	7:A:558:SER:C	2.00	0.70
10:N:162:ILE:HA	10:N:170:ASP:O	1.92	0.70
2:C:654:GLN:CD	6:J:311:THR:HG22	2.16	0.70
2:C:676:ARG:HH12	13:U:61:GLU:HG2	1.57	0.69
1:B:907:ALA:CB	7:A:557:ASN:ND2	2.45	0.69
7:A:516:LEU:O	7:A:526:ARG:NH2	2.26	0.69
1:B:676:GLY:HA2	3:D:604:GLU:HG3	1.72	0.69
1:B:727:ASN:OD1	7:A:559:LEU:C	2.36	0.69
3:D:610:THR:OG1	7:A:486:VAL:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:236:LYS:HE3	7:A:526:ARG:HH12	1.57	0.69
2:C:654:GLN:C	2:C:655:ILE:HG13	2.18	0.69
3:D:602:LYS:HA	7:A:488:ILE:CB	2.21	0.69
1:B:734:ALA:CB	7:A:567:PHE:HZ	2.05	0.69
1:B:940:ARG:NH2	1:B:985:LEU:CD1	2.55	0.69
7:A:770:TYR:HB3	7:A:999:VAL:HG11	1.75	0.68
11:S:54:TYR:HB3	12:T:40:ARG:HE	1.57	0.68
3:D:565:PHE:O	7:A:542:GLN:CD	2.36	0.68
4:H:115:PRO:HG3	3:E:721:ASN:HB2	1.76	0.68
7:A:523:GLU:HA	7:A:526:ARG:HB3	1.76	0.68
9:M:232:LYS:HA	9:M:236:LEU:HG	1.75	0.68
10:N:453:LYS:O	10:N:457:LYS:N	2.27	0.68
11:S:125:GLN:NE2	12:T:53:GLU:OE1	2.27	0.68
3:D:605:ASN:O	7:A:488:ILE:HD13	1.88	0.68
13:U:42:ARG:NH2	15:W:111:DC:O2	2.27	0.68
9:M:99:PRO:HB2	9:M:133:VAL:HG22	1.75	0.67
9:M:214:GLN:CD	9:M:216:ARG:NE	2.52	0.67
7:A:1176:ASP:N	7:A:1176:ASP:OD1	2.28	0.67
7:A:810:TYR:CE2	7:A:819:TYR:CD2	2.83	0.67
12:P:23:ARG:HH12	12:P:30:THR:HG22	1.58	0.67
1:B:940:ARG:HH12	1:B:985:LEU:HD13	0.50	0.67
1:B:941:ASN:HD22	1:B:944:LEU:H	1.35	0.67
2:C:652:LEU:HD12	6:J:312:LEU:HB3	1.76	0.67
2:C:652:LEU:HB2	6:J:312:LEU:C	2.20	0.67
2:C:652:LEU:CB	6:J:312:LEU:O	2.38	0.67
7:A:810:TYR:CZ	7:A:819:TYR:HE2	2.12	0.67
7:A:915:HIS:NE2	7:A:917:ASP:CG	2.51	0.67
7:A:1129:LYS:HB3	7:A:1156:TYR:HB3	1.77	0.67
9:M:214:GLN:OE1	9:M:216:ARG:NH1	2.27	0.67
7:A:637:HIS:HE1	10:N:434:ILE:HD13	1.58	0.67
3:D:422:LEU:O	7:A:555:HIS:NE2	2.27	0.67
3:E:596:PRO:HG2	7:A:489:ASP:OD2	1.94	0.67
3:D:424:PRO:HB3	7:A:555:HIS:HB2	1.77	0.66
3:D:537:LYS:HA	7:A:534:TYR:CE2	2.30	0.66
15:W:50:DG:N2	16:X:99:DT:O2	2.28	0.66
1:B:927:ASN:HD21	7:A:569:SER:CB	2.07	0.66
1:B:1051:LYS:HD2	1:B:1051:LYS:H	1.60	0.66
1:B:1145:THR:HG22	7:A:586:TYR:CE1	2.31	0.66
3:D:602:LYS:HA	7:A:488:ILE:CD1	2.25	0.66
11:S:59:GLU:O	12:T:40:ARG:NH1	2.28	0.66
3:D:430:PRO:CG	6:J:566:TYR:HB3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:224:ALA:HA	9:M:228:ILE:HB	1.77	0.66
3:D:609:SER:CB	7:A:488:ILE:CG1	2.56	0.66
13:Q:115:LEU:HG	12:T:44:LYS:HB2	1.76	0.65
15:W:86:DT:N3	16:X:62:DA:C2	2.64	0.65
15:W:45:DC:N3	16:X:103:DG:N1	2.42	0.65
15:W:129:DT:N3	16:X:19:DA:C6	2.64	0.65
7:A:798:LYS:CG	17:A:1501:ADP:O2B	2.40	0.65
7:A:810:TYR:CZ	7:A:819:TYR:CD2	2.85	0.65
9:M:291:LEU:O	10:N:402:GLN:NE2	2.30	0.65
2:C:663:LEU:O	2:C:665:LYS:N	2.29	0.65
7:A:1171:ASN:ND2	17:A:1501:ADP:H5'1	2.12	0.65
9:M:67:VAL:O	9:M:217:SER:OG	2.15	0.65
3:D:429:LYS:HG3	6:J:565:PRO:O	1.97	0.64
7:A:798:LYS:CD	17:A:1501:ADP:O3B	2.45	0.64
10:N:449:ILE:HG12	10:N:465:VAL:HG21	1.80	0.64
1:B:1138:PRO:HB2	7:A:574:ILE:HG22	1.79	0.64
13:Q:17:ARG:HB2	13:Q:27:VAL:HB	1.79	0.64
13:U:24:GLN:HB3	14:V:40:LYS:HD3	1.78	0.64
15:W:114:DG:N1	16:X:34:DC:N3	2.42	0.64
1:B:940:ARG:HH22	1:B:985:LEU:CD1	2.10	0.64
9:M:315:LYS:HE2	9:M:318:LEU:HD11	1.79	0.64
12:P:99:GLY:HA3	14:V:54:LYS:HZ3	1.60	0.64
15:W:79:DC:O2	16:X:70:DG:N2	2.30	0.64
1:B:1051:LYS:CG	1:B:1052:PRO:HD3	2.21	0.64
3:D:426:GLU:CD	7:A:548:HIS:HD2	2.06	0.64
3:D:565:PHE:HE1	7:A:542:GLN:CA	2.11	0.64
7:A:1164:ARG:NH2	15:W:54:DC:O2	2.30	0.64
11:O:109:LEU:O	11:O:113:HIS:HB2	1.98	0.64
11:O:129:ARG:NH1	11:O:129:ARG:O	2.31	0.64
15:W:129:DT:C4	16:X:19:DA:N6	2.65	0.64
7:A:584:GLN:N	7:A:587:LYS:HE2	2.12	0.64
1:B:1049:LEU:C	1:B:1051:LYS:HD2	2.23	0.64
3:D:422:LEU:C	7:A:555:HIS:NE2	2.55	0.64
3:D:441:LYS:NZ	7:A:506:ASP:OD2	2.30	0.64
7:A:800:ILE:CD1	17:A:1501:ADP:C8	2.80	0.64
9:M:55:ILE:O	9:M:59:ALA:N	2.30	0.64
10:N:198:LEU:HB3	10:N:210:ILE:HG12	1.78	0.64
10:N:7:ASP:HA	10:N:24:GLY:HA2	1.80	0.64
9:M:448:SER:HB3	9:M:451:LEU:HG	1.80	0.64
15:W:35:DT:N3	16:X:113:DA:C2	2.66	0.64
3:D:537:LYS:CB	7:A:534:TYR:HE2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:290:PHE:HB3	9:M:299:LEU:HB2	1.80	0.64
1:B:1049:LEU:HD23	1:B:1051:LYS:HG3	1.79	0.64
1:B:1051:LYS:HB3	1:B:1051:LYS:HZ3	1.60	0.64
3:E:444:MET:HE2	7:A:503:LEU:CD1	2.27	0.63
1:B:1049:LEU:HD23	1:B:1051:LYS:CG	2.28	0.63
7:A:915:HIS:HE2	7:A:917:ASP:CG	2.06	0.63
3:E:425:PHE:CD1	7:A:543:LYS:CG	2.78	0.63
3:E:444:MET:SD	7:A:503:LEU:CG	2.87	0.63
12:P:91:LYS:HZ2	14:R:76:ARG:HH21	1.44	0.63
1:B:940:ARG:NH2	1:B:985:LEU:HD12	2.13	0.63
2:C:669:ARG:HH11	14:V:102:GLU:HB2	1.63	0.63
15:W:121:DG:N1	16:X:27:DC:N3	2.44	0.63
2:C:652:LEU:CD1	6:J:312:LEU:HB3	2.28	0.63
9:M:311:GLU:OE1	9:M:407:ARG:NH2	2.32	0.63
10:N:131:VAL:HG13	10:N:137:ILE:HB	1.81	0.63
11:O:54:TYR:HB3	12:P:40:ARG:HE	1.63	0.63
14:V:79:HIS:O	14:V:82:LYS:NZ	2.31	0.63
2:C:496:LEU:HD23	2:C:510:ILE:HG22	1.80	0.63
3:D:601:SER:O	7:A:488:ILE:HD13	1.97	0.63
7:A:816:ARG:HD3	7:A:842:LEU:CD2	2.28	0.63
8:L:23:GLU:O	10:N:451:ARG:NH2	2.32	0.63
15:W:44:DG:N1	16:X:104:DC:N3	2.44	0.63
3:E:440:LEU:CD1	7:A:499:THR:HG21	2.28	0.63
9:M:164:CYS:H	9:M:182:SER:HB3	1.64	0.63
11:O:51:ILE:O	11:O:55:GLN:NE2	2.32	0.63
15:W:86:DT:C2	16:X:62:DA:C2	2.86	0.63
15:W:99:DG:N1	16:X:49:DC:N3	2.42	0.63
7:A:815:ILE:O	7:A:816:ARG:C	2.41	0.62
10:N:84:ARG:O	10:N:88:VAL:HB	1.99	0.62
1:B:940:ARG:CZ	1:B:985:LEU:HD12	2.29	0.62
3:E:444:MET:CG	7:A:503:LEU:CD1	2.56	0.62
7:A:798:LYS:HG3	17:A:1501:ADP:PB	2.38	0.62
9:M:53:ASN:ND2	9:M:89:TYR:OH	2.32	0.62
15:W:47:DC:H4'	15:W:48:DT:H5'	1.81	0.62
15:W:35:DT:C2	16:X:113:DA:C2	2.87	0.62
15:W:57:DT:O2	16:X:92:DG:N2	2.32	0.62
15:W:130:DC:N3	16:X:18:DG:N1	2.44	0.62
2:C:663:LEU:O	2:C:664:ASP:C	2.42	0.62
3:D:565:PHE:CE1	7:A:542:GLN:HA	2.33	0.62
7:A:776:GLN:HA	7:A:779:VAL:HB	1.82	0.62
15:W:104:DT:C4	16:X:44:DA:N1	2.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:291:LEU:HD23	10:N:359:ILE:HG13	1.81	0.62
3:D:576:TYR:HB2	7:A:497:TYR:OH	1.99	0.62
9:M:216:ARG:HD3	9:M:220:VAL:HG21	1.67	0.62
2:C:554:GLN:C	2:C:655:ILE:H	1.94	0.62
7:A:584:GLN:CA	7:A:587:LYS:CE	2.48	0.62
13:Q:21:ALA:HB1	14:R:114:ALA:HB1	1.81	0.62
1:B:936:ARG:O	1:B:940:ARG:HD3	1.99	0.61
1:B:941:ASN:HD21	1:B:944:LEU:CA	2.09	0.61
9:M:231:PHE:O	9:M:236:LEU:N	2.33	0.61
10:N:39:THR:HG21	10:N:68:ILE:HB	1.82	0.61
11:S:59:GLU:OE2	12:T:40:ARG:NH2	2.33	0.61
3:D:565:PHE:HE1	7:A:542:GLN:HA	1.63	0.61
10:N:47:GLN:H	10:N:47:GLN:CD	2.06	0.61
2:C:475:ASP:OD2	3:E:368:ARG:NH1	2.34	0.61
3:D:540:GLN:HE22	7:A:537:GLN:CG	2.13	0.61
15:W:94:DG:N1	16:X:54:DC:N3	2.46	0.61
13:U:29:ARG:NH2	14:V:37:TYR:OH	2.33	0.61
15:W:68:DT:N3	16:X:80:DA:C2	2.69	0.61
1:B:1049:LEU:HB3	1:B:1051:LYS:CG	2.30	0.61
7:A:798:LYS:CG	17:A:1501:ADP:O3B	2.48	0.61
7:A:808:TYR:CB	7:A:811:GLU:OE1	2.49	0.61
12:P:35:ARG:NH2	16:X:82:DG:OP2	2.34	0.61
15:W:68:DT:C4	16:X:80:DA:N1	2.68	0.61
2:C:652:LEU:HB2	6:J:312:LEU:CB	2.27	0.61
1:B:724:THR:HG21	3:D:422:LEU:HA	1.83	0.61
1:B:1041:ASP:OD2	7:A:574:ILE:HD12	2.01	0.61
3:D:606:PRO:CB	7:A:486:VAL:N	2.64	0.61
7:A:613:ILE:HG13	9:M:150:GLY:HA3	1.82	0.61
10:N:42:TYR:HB3	10:N:62:ALA:HB1	1.83	0.61
15:W:51:DC:N3	16:X:97:DG:N1	2.48	0.61
3:E:440:LEU:HD13	7:A:499:THR:CG2	2.31	0.61
10:N:41:ILE:HD11	10:N:53:TYR:HB3	1.81	0.61
11:S:83:ARG:HD3	15:W:101:DG:H5'	1.83	0.61
12:P:75:HIS:CG	14:R:93:THR:HG1	2.19	0.60
3:E:444:MET:HE2	7:A:503:LEU:HD13	1.82	0.60
7:A:816:ARG:HG3	7:A:816:ARG:O	2.00	0.60
2:C:654:GLN:O	2:C:655:ILE:CB	2.50	0.60
2:C:676:ARG:NH1	13:U:57:TYR:O	2.34	0.60
7:A:585:LEU:O	7:A:589:HIS:ND1	2.32	0.60
9:M:67:VAL:HB	9:M:217:SER:OG	2.01	0.60
12:T:52:GLU:OE2	12:T:55:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:68:ASN:HA	13:U:71:ARG:HH21	1.64	0.60
1:B:913:LEU:HD12	7:A:559:LEU:HD11	1.84	0.60
3:E:596:PRO:HG3	7:A:492:THR:OG1	2.00	0.60
7:A:585:LEU:C	7:A:588:ASN:OD1	2.44	0.60
7:A:798:LYS:NZ	17:A:1501:ADP:O2B	2.20	0.60
8:L:28:ASP:HB3	8:L:64:LEU:HD12	1.84	0.60
11:S:53:ARG:NH2	11:S:59:GLU:OE2	2.34	0.60
3:D:605:ASN:HB3	3:D:608:LEU:HB3	1.84	0.60
3:D:539:ILE:HG22	7:A:538:LEU:CG	2.15	0.60
7:A:798:LYS:CG	17:A:1501:ADP:PB	2.90	0.60
7:A:821:VAL:HG12	7:A:892:ILE:HB	1.83	0.60
9:M:214:GLN:NE2	9:M:216:ARG:NE	2.48	0.60
10:N:166:THR:HG22	10:N:192:GLN:HE21	1.67	0.60
14:V:30:ARG:NH1	16:X:26:DC:O2	2.33	0.60
2:C:652:LEU:HD12	6:J:489:ARG:NH2	2.15	0.60
7:A:758:GLN:HB3	7:A:767:LEU:HD21	1.84	0.60
9:M:332:LEU:O	9:M:336:SER:HB2	2.02	0.60
2:C:433:GLY:O	2:C:435:ARG:NH2	2.34	0.60
9:M:35:TYR:OH	9:M:79:ASN:ND2	2.34	0.60
10:N:116[A]:HIS:NE2	10:N:170:ASP:OD2	2.35	0.60
12:P:71:THR:O	14:R:96:ARG:NH2	2.34	0.60
13:U:50:TYR:OH	14:V:92:GLN:NE2	2.34	0.60
1:B:1048:SER:HB2	7:A:589:HIS:HE1	1.62	0.59
1:B:1049:LEU:HG	1:B:1051:LYS:HD3	1.83	0.59
3:D:602:LYS:N	7:A:488:ILE:HG21	2.16	0.59
14:R:104:ALA:O	14:R:108:VAL:N	2.35	0.59
11:S:40:ARG:NH2	15:W:83:DG:N3	2.36	0.59
13:U:63:LEU:HD22	14:V:42:LEU:HD13	1.83	0.59
3:D:570:ILE:CB	7:A:539:LEU:HD13	2.32	0.59
11:S:52:ARG:O	11:S:56:LYS:N	2.35	0.59
9:M:122:ARG:O	9:M:125:GLU:HB2	2.02	0.59
3:E:305:ILE:HA	3:E:394:GLN:HE22	1.67	0.59
9:M:216:ARG:HD2	9:M:220:VAL:N	2.17	0.59
9:M:67:VAL:CB	9:M:217:SER:OG	2.50	0.59
14:R:64:ASN:HA	14:R:67:PHE:HB3	1.83	0.59
15:W:78:DC:N3	16:X:70:DG:N1	2.45	0.59
7:A:1300:MET:HB3	7:A:1304:ARG:HE	1.68	0.59
9:M:426:ASN:ND2	9:M:435:GLN:OE1	2.35	0.59
12:T:64:ASN:O	12:T:67:ARG:NH1	2.36	0.59
15:W:110:DC:N3	16:X:38:DG:N1	2.43	0.59
14:R:112:THR:O	14:R:116:THR:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:584:GLN:CD	7:A:587:LYS:CE	2.71	0.59
12:P:46:ILE:N	16:X:82:DG:OP1	2.36	0.59
15:W:68:DT:C2	16:X:80:DA:C2	2.90	0.59
1:B:940:ARG:HD2	1:B:940:ARG:H	1.68	0.58
3:E:443:MET:HE3	7:A:500:LEU:HD22	1.83	0.58
7:A:629:PHE:HA	7:A:632:ARG:HE	1.68	0.58
7:A:514:ASP:O	7:A:518:ASN:ND2	2.36	0.58
9:M:122:ARG:O	9:M:126:LEU:N	2.36	0.58
10:N:4:PHE:N	10:N:440:PHE:O	2.36	0.58
15:W:86:DT:C4	16:X:62:DA:N1	2.71	0.58
1:B:941:ASN:ND2	1:B:944:LEU:HB3	2.17	0.58
2:C:391:ARG:NH2	2:C:392:MET:SD	2.76	0.58
3:D:701:LEU:HD21	3:E:705:GLU:HG2	1.84	0.58
9:M:83:LEU:O	9:M:87:TRP:N	2.36	0.58
13:U:85:LEU:O	13:U:89:ASN:ND2	2.36	0.58
16:X:122:DG:H4'	16:X:123:DC:H5'	1.85	0.58
9:M:148:SER:OG	9:M:435:GLN:NE2	2.36	0.58
15:W:98:DA:C2	16:X:50:DT:N3	2.72	0.58
7:A:808:TYR:CA	7:A:811:GLU:HG2	2.32	0.58
10:N:39:THR:HG22	10:N:67:PRO:HD2	1.86	0.58
7:A:794:MET:SD	7:A:1196:ARG:NH2	2.75	0.58
1:B:1051:LYS:H	1:B:1051:LYS:CE	2.16	0.58
6:J:312:LEU:HD23	6:J:485:VAL:HG11	1.86	0.58
8:L:60:TYR:HB2	9:M:103:PRO:HD3	1.85	0.58
9:M:120:LEU:O	9:M:124:TYR:N	2.33	0.58
9:M:239:SER:HB2	9:M:246:LEU:HD12	1.86	0.58
3:D:537:LYS:HA	7:A:534:TYR:CD2	2.38	0.58
11:S:82:LEU:HB3	12:T:81:VAL:HG22	1.86	0.58
16:X:66:DG:H2''	16:X:67:DG:H2'	1.86	0.58
3:D:731:GLN:NE2	3:D:732:ASN:OD1	2.37	0.58
10:N:13:TYR:HB2	10:N:114:ILE:HD12	1.85	0.58
15:W:38:DT:N3	16:X:110:DA:C2	2.71	0.58
1:B:730:LEU:HD11	7:A:567:PHE:CE2	2.39	0.58
2:C:654:GLN:O	2:C:655:ILE:CG1	2.51	0.58
7:A:642:ARG:HA	7:A:645:GLN:HB2	1.86	0.58
7:A:816:ARG:NH1	7:A:841:THR:OG1	2.37	0.58
11:S:70:LEU:HB2	12:T:25:ASN:HB2	1.86	0.58
15:W:88:DT:O4	16:X:60:DA:N1	2.34	0.58
1:B:941:ASN:HD22	1:B:944:LEU:HB3	1.67	0.57
7:A:593:LYS:HD2	7:A:593:LYS:O	2.03	0.57
10:N:457:LYS:HB2	10:N:461:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:55:GLN:NE2	13:U:110:ASN:O	2.36	0.57
12:T:39:ARG:NH1	12:T:43:VAL:O	2.37	0.57
15:W:77:DT:C4	16:X:71:DA:N1	2.72	0.57
15:W:79:DC:N3	16:X:69:DG:N1	2.47	0.57
1:B:1051:LYS:H	1:B:1051:LYS:HE2	1.68	0.57
2:C:679:ARG:NH2	14:V:45:VAL:O	2.36	0.57
7:A:525:THR:HA	7:A:528:ASN:HD22	1.69	0.57
9:M:229:GLN:HA	9:M:232:LYS:HB2	1.86	0.57
11:O:71:VAL:HG11	11:O:89:VAL:HG22	1.86	0.57
13:Q:12:ALA:N	15:W:31:DT:O2	2.38	0.57
1:B:734:ALA:HB3	7:A:567:PHE:CZ	2.38	0.57
9:M:18:VAL:HG22	9:M:30:ILE:HG23	1.86	0.57
9:M:91:TYR:HA	9:M:95:LEU:HB2	1.87	0.57
10:N:214:LYS:NZ	10:N:339:THR:OG1	2.33	0.57
14:R:113:LYS:O	14:R:117:LYS:N	2.37	0.57
15:W:57:DT:C4	16:X:91:DA:N1	2.72	0.57
9:M:51:THR:O	9:M:55:ILE:N	2.37	0.57
10:N:188:PRO:O	10:N:190:GLY:N	2.37	0.57
10:N:295:GLY:O	10:N:298:ARG:NH1	2.36	0.57
7:A:1028:LYS:O	7:A:1030:ARG:NH1	2.37	0.57
10:N:12:ILE:HG22	10:N:14:PRO:HD3	1.87	0.57
10:N:22:GLN:NE2	10:N:31:THR:OG1	2.36	0.57
14:R:77:LEU:O	14:R:81:ASN:ND2	2.38	0.57
3:D:540:GLN:NE2	7:A:537:GLN:CD	2.62	0.57
7:A:806:LEU:O	7:A:810:TYR:HB2	2.05	0.57
9:M:121:GLU:O	9:M:124:TYR:HB2	2.05	0.57
10:N:169:THR:HG21	10:N:309:ILE:HG12	1.86	0.57
14:R:93:THR:OG1	14:R:96:ARG:NH1	2.36	0.57
15:W:90:DA:H4'	15:W:91:DA:H5'	1.85	0.57
10:N:438:GLN:O	10:N:442:HIS:ND1	2.37	0.57
13:Q:88:ARG:NH2	13:Q:100:VAL:O	2.37	0.57
15:W:129:DT:N3	16:X:19:DA:C2	2.71	0.57
7:A:686:THR:HG22	7:A:784:ASN:HB3	1.87	0.57
9:M:88:ARG:HH11	9:M:131:LEU:HD22	1.69	0.57
14:V:39:TYR:OH	16:X:21:DA:OP2	2.21	0.57
3:E:628:GLN:O	3:E:640:GLN:NE2	2.37	0.57
9:M:82:ALA:O	9:M:86:GLN:N	2.38	0.57
7:A:1171:ASN:ND2	17:A:1501:ADP:C5'	2.68	0.57
11:O:104:PHE:HD2	12:P:41:GLY:HA3	1.70	0.57
12:T:60:VAL:O	12:T:64:ASN:ND2	2.37	0.57
8:L:31:GLN:NE2	8:L:56:TYR:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:73:GLU:HG2	14:R:98:LEU:HD11	1.86	0.56
12:T:58:LEU:O	12:T:61:PHE:HB3	2.05	0.56
2:C:652:LEU:N	6:J:312:LEU:O	2.38	0.56
2:C:756:ASN:OD1	6:J:546:LYS:N	2.38	0.56
3:D:570:ILE:CG1	7:A:539:LEU:HD13	2.34	0.56
13:U:88:ARG:NH1	13:U:97:LEU:O	2.37	0.56
1:B:1138:PRO:HB2	7:A:574:ILE:CG2	2.35	0.56
1:B:1233:LEU:CD1	7:A:579:ALA:CB	2.82	0.56
3:D:609:SER:OG	7:A:488:ILE:CB	2.52	0.56
7:A:489:ASP:O	7:A:490:THR:C	2.49	0.56
7:A:794:MET:HE1	7:A:1192:GLN:HA	1.86	0.56
7:A:820:LEU:HG	7:A:913:HIS:HE1	1.69	0.56
7:A:1088:LYS:NZ	7:A:1211:LEU:O	2.37	0.56
8:L:11:ASN:HA	10:N:108:ASN:HA	1.87	0.56
9:M:71:VAL:HA	9:M:77:PRO:HA	1.86	0.56
12:T:68:ASP:O	12:T:71:THR:HB	2.05	0.56
13:U:42:ARG:HG2	15:W:112:DT:H4'	1.87	0.56
13:U:92:GLU:HA	13:U:95:LYS:HE2	1.86	0.56
15:W:100:DG:N2	16:X:49:DC:O2	2.38	0.56
1:B:941:ASN:HD22	1:B:944:LEU:CB	2.12	0.56
3:D:606:PRO:N	7:A:488:ILE:CD1	2.65	0.56
7:A:1226:TYR:HA	7:A:1229:LEU:HB2	1.86	0.56
10:N:101:ALA:HB1	10:N:105:GLU:HB2	1.87	0.56
10:N:359:ILE:HD13	10:N:404:PRO:HG2	1.86	0.56
10:N:413:PRO:HD2	10:N:427:ILE:HD11	1.86	0.56
13:Q:81:ARG:NH1	13:Q:107:VAL:O	2.38	0.56
11:S:61:LEU:HD13	12:T:36:ARG:HB3	1.88	0.56
15:W:116:DC:N3	16:X:32:DG:N1	2.40	0.56
2:C:438:TYR:O	3:E:387:LYS:NZ	2.39	0.56
9:M:112:ASN:OD1	9:M:112:ASN:N	2.33	0.56
12:P:34:ILE:HG21	12:P:51:TYR:HA	1.86	0.56
15:W:100:DG:N1	16:X:48:DC:N3	2.46	0.56
3:D:422:LEU:C	7:A:555:HIS:CD2	2.82	0.56
7:A:798:LYS:CD	17:A:1501:ADP:PB	2.93	0.56
9:M:9:VAL:O	9:M:437:TRP:NE1	2.38	0.56
11:S:49:ARG:O	11:S:52:ARG:HB2	2.06	0.56
7:A:629:PHE:HB2	7:A:632:ARG:HH21	1.71	0.56
8:L:65:ARG:O	8:L:67:GLN:NE2	2.39	0.56
10:N:15:ARG:NH1	10:N:426:GLU:OE2	2.39	0.56
9:M:53:ASN:N	9:M:53:ASN:OD1	2.37	0.56
9:M:165:ASN:HA	9:M:181:ARG:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:196:ARG:NH1	9:M:312:TYR:OH	2.39	0.56
11:O:58:THR:HB	13:U:81:ARG:HD3	1.88	0.56
14:R:93:THR:HA	14:R:96:ARG:HB2	1.87	0.56
7:A:780:SER:O	7:A:784:ASN:ND2	2.38	0.56
12:T:71:THR:O	14:V:96:ARG:NH2	2.39	0.56
2:C:504:ALA:O	2:C:508:GLN:NE2	2.36	0.56
2:C:658:ALA:O	2:C:659:GLU:HG3	2.06	0.56
11:O:59:GLU:O	12:P:40:ARG:NH1	2.39	0.56
12:P:52:GLU:OE1	12:P:55:ARG:NH1	2.39	0.56
3:E:531:ASP:OD1	3:E:531:ASP:N	2.39	0.55
8:L:58:PHE:HB3	9:M:456:SER:HA	1.88	0.55
10:N:149:ALA:HB2	10:N:428:ILE:HG12	1.87	0.55
10:N:194:ILE:HG12	10:N:302:CYS:HA	1.88	0.55
1:B:916:ASP:OD2	7:A:562:ASN:OD1	2.23	0.55
10:N:138:ASN:HB3	10:N:451:ARG:HB2	1.89	0.55
10:N:294:VAL:O	10:N:298:ARG:NH1	2.39	0.55
13:Q:32:ARG:HH11	15:W:29:DA:H3'	1.70	0.55
1:B:1142:GLN:HG2	7:A:582:THR:HG21	1.86	0.55
9:M:38:ARG:HB3	9:M:46:GLU:HB3	1.88	0.55
12:T:29:ILE:O	12:T:55:ARG:NH2	2.36	0.55
13:U:41:GLU:HB3	14:V:84:SER:HB2	1.88	0.55
1:B:1149:VAL:HG21	7:A:586:TYR:HE1	1.71	0.55
7:A:808:TYR:HA	7:A:811:GLU:CG	2.37	0.55
8:L:89:ARG:N	10:N:34:GLU:O	2.36	0.55
10:N:304:ASN:O	10:N:308:ASN:ND2	2.39	0.55
14:V:48:ASP:OD2	14:V:48:ASP:N	2.38	0.55
15:W:101:DG:H4'	15:W:102:DG:H5'	1.88	0.55
3:D:516:LYS:HA	7:A:508:THR:HG23	1.87	0.55
3:E:444:MET:CG	7:A:503:LEU:HB3	2.37	0.55
7:A:526:ARG:O	7:A:530:LEU:N	2.37	0.55
7:A:935:TRP:O	7:A:939:ASN:N	2.40	0.55
9:M:105:VAL:HG21	9:M:444:ALA:HB2	1.88	0.55
9:M:201:ILE:HG13	9:M:203:GLU:H	1.71	0.55
9:M:311:GLU:OE1	9:M:315:LYS:NZ	2.31	0.55
13:Q:88:ARG:NH1	13:Q:97:LEU:O	2.39	0.55
7:A:542:GLN:HG2	7:A:546:ARG:HD3	1.89	0.55
9:M:32:PRO:O	9:M:86:GLN:NE2	2.38	0.55
13:Q:29:ARG:NH2	14:R:37:TYR:OH	2.40	0.55
13:U:12:ALA:N	16:X:32:DG:N3	2.54	0.55
15:W:80:DC:H4'	15:W:81:DC:H5'	1.89	0.55
1:B:892:LYS:NZ	4:H:58:ASP:OD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:LYS:O	1:B:915:ASN:ND2	2.39	0.55
3:D:537:LYS:CG	7:A:534:TYR:CE2	2.75	0.55
7:A:609:ASN:ND2	9:M:152:SER:OG	2.39	0.55
9:M:87:TRP:HB3	9:M:131:LEU:HD11	1.87	0.55
12:T:26:ILE:HD11	12:T:58:LEU:HD21	1.88	0.55
12:T:65:VAL:HA	12:T:93:GLN:HE22	1.71	0.55
15:W:129:DT:C2	16:X:19:DA:N1	2.75	0.55
3:D:430:PRO:HG3	7:A:544:ALA:HB1	1.87	0.55
7:A:1084:ARG:NH2	7:A:1315:SER:O	2.40	0.55
9:M:35:TYR:HE2	9:M:37:LYS:HE3	1.72	0.55
2:C:659:GLU:OE2	2:C:728:ARG:NH1	2.40	0.55
5:I:50:TYR:OH	5:I:71:GLN:NE2	2.39	0.55
3:E:726:ARG:O	3:E:730:ASN:ND2	2.40	0.55
7:A:616:TYR:HA	7:A:619:ARG:HD2	1.87	0.55
9:M:119:ILE:O	9:M:123:TYR:N	2.36	0.55
10:N:6:GLN:HE22	10:N:437:LYS:HE3	1.72	0.55
13:Q:111:ILE:HD11	11:S:52:ARG:HG3	1.89	0.55
12:T:37:LEU:O	12:T:41:GLY:N	2.40	0.55
13:U:30:VAL:HG21	13:U:52:ALA:HB2	1.89	0.55
7:A:615:GLN:NE2	9:M:445:ASN:O	2.40	0.55
10:N:281:PHE:HA	10:N:294:VAL:O	2.07	0.55
10:N:310:SER:O	10:N:357:HIS:NE2	2.40	0.55
11:S:64:LYS:HZ1	11:S:93:GLN:HE22	1.53	0.55
11:S:83:ARG:HD2	15:W:100:DG:H4'	1.89	0.55
13:U:39:TYR:OH	14:V:68:GLU:OE1	2.25	0.55
7:A:1086:ALA:O	7:A:1316:ARG:NH1	2.40	0.54
7:A:1212:ILE:HG23	7:A:1218:GLU:HG3	1.89	0.54
8:L:23:GLU:OE1	8:L:25:TRP:NE1	2.40	0.54
8:L:85:LYS:NZ	10:N:93:ASP:OD1	2.30	0.54
14:R:114:ALA:O	14:R:118:TYR:N	2.38	0.54
15:W:28:DC:H4'	15:W:29:DA:H5'	1.89	0.54
3:D:540:GLN:CA	7:A:538:LEU:HD21	2.37	0.54
7:A:897:HIS:HE1	7:A:1168:LEU:HD11	1.71	0.54
9:M:216:ARG:HD2	9:M:216:ARG:C	2.32	0.54
1:B:966:ARG:NH1	7:A:565:PRO:HB2	2.22	0.54
3:D:602:LYS:CA	7:A:488:ILE:HD12	2.36	0.54
7:A:1094:ARG:NH1	7:A:1280:ASP:OD1	2.40	0.54
7:A:1102:THR:HG23	7:A:1297:LEU:HD21	1.88	0.54
7:A:1197:ALA:O	7:A:1202:GLN:NE2	2.40	0.54
8:L:4:GLN:OE1	10:N:84:ARG:NH2	2.39	0.54
2:C:659:GLU:CD	2:C:728:ARG:NH1	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:565:PHE:CD1	7:A:542:GLN:HG3	2.43	0.54
3:D:570:ILE:HD13	7:A:539:LEU:HB2	1.89	0.54
8:L:26:ARG:NH1	8:L:65:ARG:O	2.41	0.54
11:O:60:LEU:HD22	11:O:93:GLN:HG2	1.90	0.54
15:W:104:DT:C2	16:X:44:DA:C2	2.95	0.54
15:W:151:DT:O2	16:X:-2:DG:N2	2.41	0.54
1:B:936:ARG:CA	1:B:940:ARG:HH21	2.19	0.54
11:S:104:PHE:HD2	12:T:41:GLY:HA3	1.71	0.54
15:W:89:DT:H4'	15:W:90:DA:H5'	1.89	0.54
16:X:87:DT:H2''	16:X:88:DT:H5''	1.88	0.54
10:N:306:ILE:HD11	10:N:345:PHE:HA	1.89	0.54
2:C:633:ILE:HD11	2:C:638:VAL:HG23	1.88	0.54
7:A:627:LEU:O	7:A:631:HIS:ND1	2.41	0.54
7:A:1063:PHE:HB2	7:A:1118:ILE:HD13	1.90	0.54
9:M:387:LEU:O	9:M:391:ASN:HB2	2.08	0.54
11:S:111:ALA:O	11:S:116:ARG:N	2.38	0.54
13:U:59:THR:HB	14:V:41:VAL:HG11	1.89	0.54
9:M:18:VAL:HG13	9:M:30:ILE:HG12	1.89	0.54
14:R:39:TYR:HE2	15:W:21:DG:H3'	1.73	0.54
15:W:69:DA:H2	16:X:80:DA:H2	1.56	0.54
15:W:77:DT:C2	16:X:71:DA:C2	2.96	0.54
16:X:101:DG:H4'	16:X:102:DA:H5'	1.89	0.54
7:A:768:LYS:HZ2	17:A:1501:ADP:N6	2.06	0.54
9:M:145:ILE:HD13	9:M:395:THR:HG21	1.90	0.54
11:O:102:GLY:O	11:O:131:ARG:NH2	2.40	0.54
13:Q:77:ARG:N	16:X:132:DC:OP1	2.41	0.54
13:U:92:GLU:HG3	13:U:95:LYS:HZ1	1.72	0.54
7:A:1288:ALA:O	7:A:1290:ASN:ND2	2.41	0.54
9:M:159:ILE:HG22	9:M:398:THR:HB	1.90	0.54
9:M:126:LEU:HA	9:M:130:LYS:HB2	1.89	0.53
13:Q:43:VAL:N	16:X:113:DA:OP1	2.37	0.53
13:U:55:LEU:O	13:U:59:THR:OG1	2.22	0.53
1:B:1081:ASP:HA	1:B:1084:LEU:HB2	1.90	0.53
7:A:755:ILE:H	7:A:776:GLN:HG2	1.73	0.53
11:O:54:TYR:O	12:P:40:ARG:NH2	2.40	0.53
3:D:426:GLU:HG2	7:A:551:GLN:CD	2.33	0.53
6:J:240:LEU:CD2	7:A:516:LEU:HD11	2.36	0.53
7:A:1171:ASN:HD21	17:A:1501:ADP:PA	2.31	0.53
9:M:214:GLN:HB3	9:M:217:SER:HB3	1.90	0.53
13:U:21:ALA:HB1	14:V:114:ALA:HB1	1.89	0.53
15:W:49:DA:H2	16:X:100:DA:H2	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:87:DT:C4	16:X:61:DA:N1	2.76	0.53
1:B:865:PRO:O	1:B:946:ARG:NH2	2.41	0.53
3:D:424:PRO:HD3	7:A:555:HIS:CD2	2.44	0.53
7:A:518:ASN:OD1	7:A:521:CYS:N	2.42	0.53
7:A:884:SER:HB2	7:A:913:HIS:HA	1.90	0.53
17:A:1501:ADP:O1B	18:A:1502:BEF:F3	2.16	0.53
12:P:90:LEU:HD22	12:P:95:ARG:HB2	1.90	0.53
1:B:730:LEU:HD22	1:B:920:THR:HG23	1.90	0.53
10:N:18:THR:HA	10:N:38:PRO:HA	1.90	0.53
14:R:83:ARG:HD3	14:R:85:THR:HG22	1.89	0.53
2:C:558:ILE:CD1	2:C:653:LEU:HD11	2.32	0.53
13:Q:42:ARG:NH1	16:X:111:DC:O2	2.41	0.53
11:S:71:VAL:HG11	11:S:89:VAL:HA	1.91	0.53
2:C:600:GLN:HA	2:C:603:MET:HG2	1.91	0.53
3:D:459:GLU:OE2	3:D:462:ARG:NH2	2.42	0.53
7:A:527:GLU:HA	7:A:530:LEU:HB3	1.91	0.53
14:R:109:SER:O	14:R:113:LYS:N	2.40	0.53
11:S:41:TYR:HB2	15:W:83:DG:H4'	1.91	0.53
9:M:400:LEU:HG	9:M:432:ARG:HD2	1.88	0.53
10:N:173:PRO:HG2	10:N:180:LEU:HB2	1.91	0.53
11:S:72:ARG:NH2	16:X:51:DT:OP2	2.37	0.53
4:H:159:ARG:HA	4:H:281:LEU:O	2.09	0.53
7:A:768:LYS:O	7:A:771:GLN:NE2	2.41	0.53
15:W:117:DT:O2	16:X:32:DG:N2	2.42	0.53
3:D:426:GLU:OE2	7:A:548:HIS:HD2	1.82	0.53
3:D:537:LYS:CB	7:A:534:TYR:CE2	2.92	0.53
3:D:587:ASN:OD1	3:D:587:ASN:N	2.42	0.53
9:M:107:THR:HB	9:M:141:GLU:HB2	1.91	0.53
13:Q:34:LEU:HB3	13:Q:43:VAL:HG11	1.91	0.53
11:S:43:PRO:HG3	16:X:68:DG:N2	2.23	0.53
1:B:676:GLY:HA3	3:D:601:SER:HB2	1.91	0.52
1:B:1149:VAL:CG2	7:A:586:TYR:CE1	2.85	0.52
2:C:555:ASN:OD1	2:C:654:GLN:CB	2.58	0.52
4:H:307:PHE:O	4:H:419:GLN:NE2	2.41	0.52
3:E:447:SER:HB3	3:E:450:GLU:HB3	1.90	0.52
7:A:1171:ASN:HD21	17:A:1501:ADP:H5'1	1.68	0.52
10:N:81:GLN:NE2	10:N:130:TYR:OH	2.42	0.52
13:Q:62:ILE:HD13	14:R:59:MET:HE1	1.91	0.52
13:Q:97:LEU:HB3	13:Q:100:VAL:HB	1.91	0.52
14:R:69:ARG:NH2	12:T:98:TYR:OH	2.42	0.52
3:D:540:GLN:HE22	7:A:537:GLN:HG2	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:732:ASN:ND2	3:E:779:THR:O	2.42	0.52
7:A:1098:LYS:HD2	7:A:1297:LEU:HD13	1.91	0.52
12:P:51:TYR:O	12:P:55:ARG:NH1	2.41	0.52
13:U:88:ARG:NH2	13:U:100:VAL:O	2.42	0.52
9:M:189:LEU:HA	9:M:192:GLN:HB2	1.90	0.52
9:M:197:LEU:HD13	9:M:299:LEU:HD12	1.91	0.52
9:M:330:GLY:O	9:M:334:ALA:N	2.42	0.52
12:P:59:LYS:HA	12:P:62:LEU:HD12	1.91	0.52
13:U:81:ARG:NH1	13:U:107:VAL:O	2.42	0.52
7:A:682:LEU:HD13	7:A:748:ALA:HB2	1.92	0.52
7:A:754:ASP:N	7:A:754:ASP:OD1	2.41	0.52
11:O:78:PHE:HE1	12:P:66:ILE:HB	1.75	0.52
2:C:529:TYR:HB2	2:C:615:PHE:HB2	1.91	0.52
3:D:544:ALA:HB2	7:A:541:LEU:HD21	1.91	0.52
10:N:222:LEU:HG	10:N:299:PHE:HB3	1.91	0.52
11:O:106:ASP:OD1	11:O:106:ASP:N	2.43	0.52
13:U:32:ARG:NH2	14:V:32:GLU:OE2	2.42	0.52
1:B:940:ARG:NH1	1:B:985:LEU:HD12	2.04	0.52
9:M:200:LEU:HB3	9:M:299:LEU:HD22	1.92	0.52
13:Q:85:LEU:O	13:Q:89:ASN:ND2	2.43	0.52
13:Q:90:ASP:OD2	13:Q:93:LEU:N	2.38	0.52
13:Q:90:ASP:HB3	13:Q:93:LEU:HB2	1.92	0.52
15:W:108:DT:O2	16:X:41:DG:N2	2.42	0.52
1:B:1256:GLU:HG3	1:B:1265:ILE:HG12	1.92	0.52
11:S:127:ALA:O	11:S:131:ARG:N	2.36	0.52
11:S:128:ARG:HA	11:S:131:ARG:HB2	1.92	0.52
12:T:78:ARG:NH2	12:T:85:ASP:OD2	2.43	0.52
15:W:63:DG:N1	16:X:85:DC:N3	2.53	0.52
2:C:481:LYS:NZ	2:C:524:PHE:O	2.43	0.52
2:C:496:LEU:HD21	2:C:513:ILE:HD12	1.91	0.52
14:V:102:GLU:OE1	14:V:105:LYS:NZ	2.42	0.52
2:C:483:ASP:OD1	3:E:380:ARG:NH2	2.43	0.52
2:C:673:ARG:NH1	14:V:109:SER:OG	2.38	0.52
7:A:826:SER:HA	7:A:1142:ARG:HD3	1.92	0.52
11:S:109:LEU:O	11:S:113:HIS:HB2	2.10	0.52
12:T:67:ARG:O	12:T:71:THR:OG1	2.28	0.52
14:V:33:SER:OG	14:V:34:TYR:N	2.43	0.52
3:D:321:SER:O	3:D:325:GLN:NE2	2.42	0.52
5:I:103:PHE:CE2	7:A:565:PRO:HG3	2.45	0.52
3:E:440:LEU:CD2	7:A:499:THR:HB	2.40	0.52
3:E:442:LYS:NZ	3:E:579:GLY:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:1501:ADP:O1A	18:A:1502:BEF:F3	2.18	0.52
10:N:6:GLN:HB3	10:N:25:LEU:HB2	1.92	0.52
13:Q:116:LEU:HA	11:S:48:LEU:HD13	1.92	0.52
2:C:558:ILE:CD1	2:C:653:LEU:CD1	2.84	0.51
7:A:1184:ASP:OD2	7:A:1210:ARG:NH1	2.44	0.51
10:N:359:ILE:HG12	10:N:402:GLN:HB2	1.91	0.51
15:W:58:DT:H4'	15:W:59:DA:H5'	1.92	0.51
15:W:108:DT:H2''	15:W:109:DC:C5	2.45	0.51
1:B:723:ASN:HB3	7:A:558:SER:O	2.10	0.51
11:O:106:ASP:OD1	11:S:129:ARG:NH2	2.43	0.51
15:W:48:DT:N3	16:X:100:DA:C2	2.78	0.51
1:B:723:ASN:CG	7:A:559:LEU:HD23	2.34	0.51
2:C:659:GLU:CD	2:C:728:ARG:HH11	2.18	0.51
7:A:768:LYS:NZ	17:A:1501:ADP:N6	2.58	0.51
7:A:1083:TRP:HE3	7:A:1090:GLU:HA	1.75	0.51
9:M:84:GLU:HA	9:M:87:TRP:HB2	1.91	0.51
10:N:91:LEU:HD23	10:N:106:LEU:HD22	1.93	0.51
10:N:114:ILE:HD13	10:N:428:ILE:HG22	1.92	0.51
1:B:940:ARG:NH2	1:B:985:LEU:HD13	2.20	0.51
3:D:516:LYS:HA	7:A:508:THR:CG2	2.41	0.51
7:A:778:MET:O	7:A:782:PHE:N	2.41	0.51
9:M:214:GLN:CD	9:M:216:ARG:HE	2.15	0.51
16:X:38:DG:H1'	16:X:39:DG:C5	2.45	0.51
1:B:988:ILE:HD11	1:B:1046:LEU:HD13	1.92	0.51
7:A:609:ASN:O	7:A:613:ILE:N	2.36	0.51
1:B:927:ASN:CG	7:A:569:SER:HB2	2.36	0.51
3:D:785:ASN:ND2	3:D:787:PHE:O	2.42	0.51
6:J:325:SER:OG	6:J:326:LYS:N	2.43	0.51
7:A:1013:CYS:N	7:A:1212:ILE:O	2.43	0.51
7:A:1117:ASP:OD2	12:P:19:ARG:NH1	2.43	0.51
9:M:35:TYR:CZ	9:M:68:TYR:HB2	2.46	0.51
10:N:340:THR:O	10:N:346:LYS:NZ	2.41	0.51
4:H:130:SER:HA	4:H:434:THR:HB	1.93	0.51
7:A:806:LEU:HD22	7:A:810:TYR:CE2	2.46	0.51
7:A:1170:LEU:HD22	7:A:1172:LEU:HD11	1.92	0.51
10:N:43:ARG:O	10:N:62:ALA:HA	2.10	0.51
10:N:417:PRO:HA	10:N:420:LYS:HB3	1.93	0.51
12:P:35:ARG:NH2	12:P:51:TYR:OH	2.35	0.51
7:A:516:LEU:HD22	7:A:530:LEU:HA	1.91	0.51
12:P:43:VAL:HG11	12:P:46:ILE:HG23	1.93	0.51
15:W:48:DT:C4	16:X:100:DA:N1	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:946:ARG:O	1:B:950:ASP:HB2	2.11	0.51
2:C:640:ARG:NH2	3:D:369:ARG:O	2.42	0.51
3:D:606:PRO:HB3	7:A:486:VAL:N	2.26	0.51
10:N:218:ILE:O	10:N:276:ASN:ND2	2.44	0.51
11:O:42:ARG:HG2	15:W:68:DT:H5''	1.92	0.51
11:S:61:LEU:HB2	12:T:37:LEU:HG	1.92	0.51
1:B:747:GLU:HB2	2:C:439:LEU:HD13	1.92	0.51
1:B:1122:VAL:HG12	1:B:1132:LEU:HB3	1.93	0.51
3:D:598:LEU:HD22	7:A:490:THR:HG21	1.92	0.51
3:E:594:TYR:O	7:A:493:ALA:CB	2.59	0.51
12:T:35:ARG:NH1	12:T:51:TYR:OH	2.44	0.51
4:H:117:LEU:HD11	3:E:724:ILE:HD11	1.92	0.50
7:A:599:THR:HA	7:A:602:VAL:HB	1.92	0.50
7:A:1016:SER:O	7:A:1020:GLN:N	2.43	0.50
10:N:85:LEU:O	10:N:89:SER:OG	2.21	0.50
10:N:350:LEU:HB2	10:N:409:LEU:HD21	1.92	0.50
11:O:68:GLN:HG2	11:O:72:ARG:HE	1.76	0.50
14:R:61:SER:OG	12:T:100:PHE:N	2.41	0.50
4:H:295:ILE:HB	4:H:423:ILE:HG23	1.93	0.50
10:N:412:TYR:HD1	10:N:427:ILE:HD12	1.76	0.50
13:Q:17:ARG:HH22	13:Q:31:HIS:HD2	1.60	0.50
13:Q:63:LEU:HD22	14:R:42:LEU:HD13	1.94	0.50
14:R:70:ILE:HG12	14:R:94:ALA:HB1	1.92	0.50
13:U:93:LEU:O	13:U:97:LEU:N	2.44	0.50
15:W:120:DA:N7	16:X:27:DC:N4	2.59	0.50
1:B:927:ASN:ND2	7:A:569:SER:CB	2.69	0.50
2:C:502:GLU:O	2:C:505:THR:OG1	2.29	0.50
3:E:422:LEU:HD11	7:A:554:TRP:HD1	1.76	0.50
9:M:292:PHE:O	9:M:296:ASN:N	2.44	0.50
10:N:16:SER:HA	10:N:69:GLN:HA	1.93	0.50
13:Q:92:GLU:O	13:Q:96:LEU:HB2	2.11	0.50
14:R:109:SER:OG	14:R:110:GLU:N	2.44	0.50
16:X:66:DG:H1'	16:X:67:DG:H5'	1.93	0.50
1:B:936:ARG:O	1:B:940:ARG:CD	2.60	0.50
1:B:1149:VAL:HG21	7:A:586:TYR:CE1	2.45	0.50
2:C:652:LEU:HB2	6:J:312:LEU:CA	2.41	0.50
2:C:677:GLN:NE2	14:V:110:GLU:OE2	2.45	0.50
3:D:424:PRO:HG3	7:A:552:PHE:HA	1.92	0.50
7:A:1146:LEU:HD22	7:A:1170:LEU:HB3	1.93	0.50
7:A:1190:ASP:OD2	7:A:1210:ARG:NH2	2.45	0.50
8:L:25:TRP:HA	8:L:66:ASN:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:240:GLU:HG3	9:M:246:LEU:HD11	1.94	0.50
9:M:326:GLU:HA	9:M:331:PRO:HB2	1.91	0.50
11:O:59:GLU:H	12:P:40:ARG:HH22	1.59	0.50
12:T:66:ILE:HA	12:T:69:ALA:HB3	1.92	0.50
5:I:150:HIS:O	5:I:153:LYS:NZ	2.44	0.50
3:E:444:MET:HG2	7:A:503:LEU:HB3	1.93	0.50
9:M:157:ILE:HG12	9:M:166:VAL:HG22	1.93	0.50
10:N:362:PRO:HD2	10:N:365:GLU:HB2	1.94	0.50
13:Q:42:ARG:N	14:R:84:SER:O	2.45	0.50
11:S:42:ARG:NH1	16:X:69:DG:OP1	2.44	0.50
11:S:62:ILE:HG23	12:T:29:ILE:HD12	1.92	0.50
15:W:86:DT:C2	16:X:62:DA:H2	2.28	0.50
16:X:30:DG:H1'	16:X:31:DA:H5'	1.92	0.50
1:B:734:ALA:HB2	7:A:567:PHE:CZ	2.47	0.50
7:A:938:LEU:HD21	7:A:987:LEU:HD21	1.93	0.50
9:M:441:LEU:O	9:M:445:ASN:ND2	2.40	0.50
11:O:101:VAL:HG13	12:P:41:GLY:HA2	1.94	0.50
13:U:27:VAL:HG11	13:U:49:VAL:HG22	1.94	0.50
3:D:601:SER:O	7:A:488:ILE:CD1	2.60	0.50
3:E:567:GLN:O	3:E:629:ARG:NH2	2.45	0.50
7:A:522:THR:O	7:A:526:ARG:N	2.43	0.50
10:N:279:LEU:O	10:N:298:ARG:NH2	2.45	0.50
10:N:460:ALA:HA	10:N:463:TRP:HD1	1.77	0.50
14:V:42:LEU:O	14:V:46:HIS:N	2.44	0.50
1:B:940:ARG:HH22	1:B:985:LEU:HD12	1.74	0.50
2:C:669:ARG:NH1	13:U:92:GLU:OE1	2.40	0.50
3:D:682:LEU:HD11	5:I:149:GLN:HG3	1.93	0.50
7:A:595:GLU:HA	7:A:595:GLU:OE2	2.12	0.50
7:A:1080:ASP:OD1	7:A:1083:TRP:NE1	2.43	0.50
7:A:1095:ILE:O	7:A:1099:LEU:N	2.35	0.50
7:A:1209:LEU:HD11	7:A:1286:ILE:HG21	1.93	0.50
10:N:114:ILE:HA	10:N:143:LEU:O	2.12	0.50
12:P:64:ASN:O	12:P:67:ARG:NE	2.45	0.50
11:S:128:ARG:HB3	11:S:133:GLU:HB2	1.92	0.50
15:W:48:DT:C2	16:X:100:DA:C2	3.00	0.50
6:J:327:ASN:HB3	6:J:330:GLN:HE21	1.77	0.50
3:E:444:MET:CE	7:A:503:LEU:CD1	2.82	0.50
7:A:593:LYS:C	7:A:593:LYS:HE3	2.37	0.50
10:N:7:ASP:HB3	10:N:105:GLU:HG2	1.92	0.50
11:O:56:LYS:HA	13:U:109:PRO:HG3	1.94	0.50
15:W:73:DG:N1	16:X:75:DC:N3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:602:LYS:CB	7:A:488:ILE:HB	2.41	0.49
3:D:672:ALA:O	3:D:677:ARG:NH2	2.44	0.49
8:L:25:TRP:O	10:N:129:GLN:NE2	2.45	0.49
8:L:88:ASP:HA	10:N:35:LEU:HA	1.94	0.49
9:M:216:ARG:O	9:M:217:SER:C	2.55	0.49
9:M:241:LYS:HG3	9:M:410:LYS:HG2	1.93	0.49
12:P:89:ALA:O	12:P:93:GLN:N	2.37	0.49
14:R:37:TYR:OH	16:X:122:DG:O5'	2.29	0.49
12:T:38:ALA:HB1	12:T:43:VAL:HB	1.94	0.49
12:T:43:VAL:HG11	12:T:46:ILE:HG23	1.94	0.49
1:B:964:CYS:SG	1:B:965:ASN:N	2.85	0.49
3:D:565:PHE:CZ	7:A:538:LEU:O	2.58	0.49
4:H:313:GLN:HE21	4:H:387:THR:HG23	1.77	0.49
3:E:440:LEU:HD21	7:A:499:THR:HB	1.93	0.49
9:M:214:GLN:HE21	9:M:216:ARG:CG	1.85	0.49
10:N:4:PHE:HB2	10:N:440:PHE:HB3	1.95	0.49
11:S:55:GLN:NE2	12:T:40:ARG:O	2.45	0.49
16:X:54:DC:H2''	16:X:55:DG:C8	2.47	0.49
2:C:460:ILE:HD13	2:C:517:ILE:HG23	1.93	0.49
4:H:185:ILE:HG12	4:H:297:ILE:HG23	1.94	0.49
6:J:236:LYS:HE3	7:A:526:ARG:NH1	2.27	0.49
6:J:332:ALA:HB1	6:J:337:ALA:HB3	1.94	0.49
7:A:489:ASP:C	7:A:491:HIS:N	2.68	0.49
9:M:147:LEU:O	9:M:150:GLY:N	2.45	0.49
11:O:97:GLU:HA	11:O:100:LEU:HD12	1.94	0.49
11:S:121:PRO:HA	11:S:124:ILE:HG13	1.93	0.49
13:U:29:ARG:NH1	14:V:32:GLU:OE1	2.46	0.49
14:V:53:SER:HA	14:V:56:MET:HB3	1.93	0.49
15:W:77:DT:N3	16:X:71:DA:C2	2.80	0.49
15:W:87:DT:C2	16:X:61:DA:C2	3.00	0.49
1:B:905:ARG:NE	1:B:905:ARG:HA	2.27	0.49
3:D:602:LYS:N	7:A:488:ILE:CG2	2.75	0.49
10:N:315:LEU:O	10:N:319:ASN:ND2	2.45	0.49
11:O:48:LEU:HD23	13:U:111:ILE:HG21	1.94	0.49
11:S:62:ILE:HG12	12:T:29:ILE:HG23	1.95	0.49
13:U:32:ARG:HH11	13:U:36:LYS:HE2	1.77	0.49
7:A:845:ILE:HB	7:A:869:VAL:HG22	1.94	0.49
9:M:202:LYS:HZ2	9:M:297:LYS:HD2	1.77	0.49
9:M:332:LEU:O	9:M:336:SER:CB	2.61	0.49
10:N:133:GLU:OE1	10:N:454:TYR:OH	2.28	0.49
11:O:129:ARG:NH2	11:S:106:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:129:ARG:O	11:S:129:ARG:NH1	2.42	0.49
12:T:92:ARG:NH1	12:T:92:ARG:O	2.45	0.49
13:U:76:THR:N	15:W:132:DG:OP1	2.45	0.49
1:B:770:TYR:O	1:B:771:HIS:ND1	2.46	0.49
1:B:929:SER:OG	1:B:981:ASN:ND2	2.42	0.49
1:B:1233:LEU:CD1	7:A:579:ALA:HB1	2.43	0.49
4:H:130:SER:OG	4:H:161:GLU:OE1	2.30	0.49
3:E:365:THR:HG22	3:E:368:ARG:HH22	1.77	0.49
9:M:56:ASP:OD2	10:N:312:ARG:NH2	2.45	0.49
10:N:29:THR:HG21	10:N:417:PRO:HD2	1.94	0.49
10:N:101:ALA:O	10:N:106:LEU:N	2.31	0.49
7:A:817:GLY:O	7:A:819:TYR:N	2.44	0.49
9:M:216:ARG:CD	9:M:216:ARG:C	2.86	0.49
10:N:303:ASN:HA	10:N:306:ILE:HB	1.95	0.49
14:R:43:LYS:NZ	14:R:47:PRO:O	2.45	0.49
11:S:101:VAL:HG13	12:T:41:GLY:HA2	1.95	0.49
15:W:87:DT:H2''	15:W:88:DT:C5	2.48	0.49
16:X:3:DA:H2''	16:X:4:DG:C8	2.48	0.49
7:A:904:SER:OG	7:A:905:LYS:N	2.45	0.49
13:Q:87:VAL:HG13	13:Q:93:LEU:HB3	1.95	0.49
1:B:747:GLU:OE2	2:C:442:LYS:NZ	2.44	0.49
2:C:429:GLN:HE22	2:C:436:LYS:HA	1.77	0.49
3:D:537:LYS:CA	7:A:534:TYR:CE2	2.96	0.49
3:D:570:ILE:HG22	7:A:539:LEU:CD2	2.34	0.49
4:H:92:ARG:HG2	3:E:704:LEU:HD13	1.95	0.49
7:A:809:LEU:HA	7:A:812:MET:HE2	1.94	0.49
7:A:820:LEU:HG	7:A:913:HIS:CE1	2.47	0.49
9:M:118:ALA:O	9:M:122:ARG:N	2.41	0.49
10:N:21:VAL:HB	10:N:35:LEU:HB2	1.95	0.49
15:W:65:DA:H1'	15:W:66:DC:H5'	1.95	0.49
7:A:816:ARG:HD3	7:A:842:LEU:HD21	1.94	0.48
9:M:409:ILE:O	9:M:413:SER:OG	2.31	0.48
16:X:130:DG:H1'	16:X:131:DG:C5	2.48	0.48
1:B:1239:ILE:HG23	1:B:1298:GLN:HG3	1.93	0.48
15:W:42:DC:N3	16:X:106:DG:N1	2.51	0.48
3:D:570:ILE:HB	7:A:539:LEU:HD13	1.95	0.48
10:N:353:LEU:HB3	10:N:407:ILE:HG21	1.95	0.48
10:N:363:GLU:O	10:N:367:SER:OG	2.31	0.48
12:P:75:HIS:HB2	14:R:96:ARG:HH22	1.78	0.48
2:C:665:LYS:NZ	13:U:91:GLU:OE1	2.43	0.48
3:E:444:MET:SD	7:A:503:LEU:HB3	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:52:ARG:HG3	13:U:111:ILE:HD11	1.94	0.48
14:R:53:SER:HA	14:R:56:MET:HB3	1.95	0.48
2:C:655:ILE:C	2:C:655:ILE:HD12	2.39	0.48
3:D:566:LEU:HA	7:A:542:GLN:HE21	1.77	0.48
4:H:131:ASN:N	4:H:131:ASN:OD1	2.46	0.48
9:M:198:ALA:HA	9:M:201:ILE:HG12	1.96	0.48
10:N:445:ASP:O	10:N:453:LYS:NZ	2.41	0.48
11:O:113:HIS:CE1	11:S:122:LYS:HE2	2.49	0.48
13:U:29:ARG:CZ	14:V:32:GLU:HB2	2.44	0.48
2:C:465:ASP:OD2	2:C:468:ARG:NH2	2.46	0.48
3:D:779:THR:OG1	3:D:780:LEU:N	2.46	0.48
3:E:444:MET:HE2	7:A:503:LEU:HD11	1.94	0.48
3:E:593:LYS:H	3:E:593:LYS:HG3	1.48	0.48
7:A:758:GLN:HB2	7:A:762:LEU:HD23	1.96	0.48
11:S:70:LEU:HA	11:S:73:GLU:HB3	1.96	0.48
1:B:926:ARG:HH11	1:B:977:ILE:HD12	1.79	0.48
2:C:555:ASN:OD1	2:C:654:GLN:HB3	2.14	0.48
3:D:609:SER:OG	7:A:488:ILE:CA	2.62	0.48
3:E:688:ARG:NE	3:E:692:GLU:OE2	2.46	0.48
7:A:648:ALA:O	7:A:652:ALA:N	2.45	0.48
10:N:294:VAL:HG13	10:N:298:ARG:HD3	1.95	0.48
11:O:58:THR:O	11:O:58:THR:OG1	2.23	0.48
14:R:116:THR:HA	14:R:119:THR:HG22	1.95	0.48
15:W:45:DC:C2	16:X:103:DG:N2	2.59	0.48
1:B:1047:PHE:HB3	1:B:1149:VAL:HG11	1.95	0.48
9:M:89:TYR:O	9:M:93:THR:OG1	2.29	0.48
15:W:120:DA:C2	16:X:28:DT:N3	2.79	0.48
16:X:89:DT:H1'	16:X:90:DA:C4	2.49	0.48
7:A:630:GLY:O	10:N:155:SER:OG	2.29	0.48
7:A:800:ILE:CD1	17:A:1501:ADP:N7	2.77	0.48
9:M:216:ARG:O	9:M:216:ARG:HD2	2.13	0.48
9:M:390:THR:HG23	9:M:419:TYR:HB3	1.95	0.48
10:N:130:TYR:O	10:N:135:LEU:N	2.36	0.48
12:P:39:ARG:HH12	12:P:46:ILE:HG12	1.79	0.48
13:Q:84:GLN:NE2	13:Q:106:GLY:O	2.47	0.48
1:B:733:SER:O	7:A:570:LYS:HE3	2.14	0.48
2:C:661:GLU:O	2:C:662:ARG:HG3	2.13	0.48
12:P:39:ARG:NH1	12:P:43:VAL:O	2.47	0.48
13:Q:20:ARG:NH2	15:W:32:DT:OP1	2.47	0.48
11:S:63:ARG:HD3	11:S:63:ARG:HA	1.63	0.48
3:D:421:GLY:O	7:A:555:HIS:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:944:LYS:HG2	7:A:945:ILE:HG23	1.95	0.47
7:A:1251:GLU:HA	7:A:1254:LEU:HB2	1.96	0.47
11:O:123:ASP:N	11:O:123:ASP:OD1	2.45	0.47
13:Q:37:GLY:HA3	13:Q:39:TYR:CZ	2.49	0.47
13:Q:104:GLN:NE2	11:S:58:THR:O	2.47	0.47
12:T:75:HIS:CG	14:V:93:THR:HG1	2.28	0.47
15:W:119:DC:H2''	15:W:120:DA:C5	2.49	0.47
16:X:88:DT:H2''	16:X:89:DT:C5	2.48	0.47
4:H:89:ILE:O	4:H:92:ARG:HB3	2.14	0.47
4:H:318:ILE:HD11	4:H:332:ILE:HG23	1.95	0.47
3:E:433:GLN:O	3:E:437:MET:N	2.47	0.47
9:M:80:TRP:CD2	9:M:122:ARG:HD2	2.49	0.47
9:M:190:ASP:HA	9:M:228:ILE:HG21	1.94	0.47
11:O:61:LEU:HD22	12:P:36:ARG:HB3	1.96	0.47
11:O:106:ASP:HA	11:O:109:LEU:HD12	1.96	0.47
16:X:26:DC:H4'	16:X:27:DC:H5'	1.96	0.47
1:B:727:ASN:CG	7:A:560:LEU:HG	2.40	0.47
1:B:1002:ILE:HD11	1:B:1109:VAL:HA	1.96	0.47
4:H:169:GLN:HG3	4:H:172:ASP:HB2	1.96	0.47
4:H:388:LEU:O	4:H:414:HIS:NE2	2.38	0.47
10:N:101:ALA:O	10:N:105:GLU:N	2.47	0.47
13:U:16:THR:HG22	16:X:30:DG:H4'	1.96	0.47
16:X:113:DA:H1'	16:X:114:DC:H5'	1.97	0.47
16:X:116:DA:H1'	16:X:117:DA:H5'	1.96	0.47
2:C:628:ARG:HH22	2:C:724:ALA:HB2	1.80	0.47
4:H:92:ARG:NH1	3:E:708:MET:SD	2.87	0.47
3:E:624:GLN:HB3	3:E:632:GLN:HG2	1.96	0.47
7:A:935:TRP:HE1	7:A:952:PHE:HB2	1.79	0.47
1:B:1145:THR:CG2	7:A:586:TYR:CE1	2.96	0.47
2:C:413:SER:OG	2:C:414:GLY:N	2.47	0.47
7:A:770:TYR:O	7:A:994:ARG:NH2	2.48	0.47
10:N:199:LYS:HG3	10:N:210:ILE:HD13	1.96	0.47
15:W:48:DT:H2''	15:W:49:DA:C5	2.50	0.47
15:W:51:DC:H2'	15:W:52:DA:C8	2.49	0.47
16:X:31:DA:H4'	16:X:32:DG:H5'	1.96	0.47
7:A:958:THR:HA	7:A:975:GLU:HB3	1.95	0.47
10:N:314:GLY:HA3	10:N:357:HIS:CE1	2.50	0.47
11:O:90:MET:SD	11:O:90:MET:N	2.88	0.47
3:D:430:PRO:CG	7:A:544:ALA:HB1	2.45	0.47
4:H:182:ILE:HG21	4:H:185:ILE:HG13	1.95	0.47
3:E:444:MET:HG3	7:A:503:LEU:HD12	1.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1131:LEU:HD13	7:A:1145:LEU:HD12	1.96	0.47
10:N:73:ILE:H	10:N:119:TRP:CD1	2.32	0.47
10:N:354:LEU:HA	10:N:358:LEU:HB2	1.97	0.47
12:P:75:HIS:ND1	14:R:93:THR:OG1	2.39	0.47
3:D:574:PHE:HZ	7:A:508:THR:CB	2.27	0.47
4:H:299:ARG:NH1	4:H:305:GLU:OE1	2.41	0.47
4:H:313:GLN:HE22	4:H:388:LEU:HD12	1.79	0.47
4:H:332:ILE:HA	4:H:335:TYR:HB3	1.96	0.47
3:E:311:SER:OG	3:E:388:TRP:O	2.30	0.47
10:N:201:LEU:HD13	10:N:300:GLN:HB3	1.96	0.47
7:A:605:LEU:O	7:A:609:ASN:ND2	2.48	0.47
7:A:1241:PHE:HD2	7:A:1253:LEU:HD12	1.80	0.47
9:M:7:CYS:O	9:M:22:SER:N	2.39	0.47
10:N:354:LEU:HD23	10:N:358:LEU:HD13	1.96	0.47
11:O:117:VAL:N	15:W:71:DG:OP1	2.48	0.47
14:R:80:TYR:O	14:R:82:LYS:NZ	2.31	0.47
11:S:40:ARG:NH1	15:W:83:DG:H21	2.12	0.47
14:V:51:ILE:HG21	14:V:56:MET:HE2	1.96	0.47
15:W:82:DC:H2''	15:W:83:DG:N7	2.30	0.47
1:B:727:ASN:HB3	7:A:560:LEU:CD1	2.44	0.47
1:B:1049:LEU:CD2	1:B:1051:LYS:CD	2.88	0.47
2:C:529:TYR:HA	2:C:532:LEU:HB2	1.97	0.47
4:H:75:PHE:O	4:H:78:LEU:HB2	2.15	0.47
8:L:11:ASN:HD21	10:N:109:ILE:HB	1.80	0.47
11:O:121:PRO:HA	11:O:124:ILE:HG13	1.96	0.47
15:W:132:DG:H1'	15:W:133:DA:C8	2.50	0.47
15:W:145:DT:H2'	15:W:146:DG:C8	2.50	0.47
1:B:936:ARG:HB2	1:B:940:ARG:HH21	1.71	0.46
4:H:127:ILE:HA	4:H:161:GLU:O	2.16	0.46
4:H:129:ILE:HD13	4:H:295:ILE:HD13	1.97	0.46
3:E:423:PHE:CD2	7:A:547:GLY:HA3	2.50	0.46
9:M:165:ASN:HB3	9:M:181:ARG:HG2	1.97	0.46
10:N:202:LEU:HB2	10:N:210:ILE:HD11	1.97	0.46
12:P:84:MET:HE3	12:P:84:MET:HB3	1.88	0.46
12:T:39:ARG:HH12	12:T:46:ILE:HG12	1.80	0.46
16:X:24:DT:H2''	16:X:25:DG:C8	2.50	0.46
1:B:907:ALA:HB2	7:A:557:ASN:HD21	1.65	0.46
6:J:308:ILE:HD11	6:J:489:ARG:HD2	1.96	0.46
9:M:155:PHE:HD2	9:M:392:VAL:HG13	1.80	0.46
10:N:330:TRP:NE1	10:N:404:PRO:HB3	2.30	0.46
14:R:35:ALA:O	14:R:39:TYR:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:79:LYS:NZ	11:S:80:THR:O	2.42	0.46
13:U:14:ALA:N	16:X:30:DG:H21	2.12	0.46
16:X:88:DT:H2''	16:X:89:DT:C6	2.49	0.46
3:D:424:PRO:HD3	7:A:552:PHE:CD1	2.44	0.46
7:A:933:GLU:HB3	7:A:936:ALA:HB3	1.97	0.46
9:M:70:LEU:O	9:M:78:TYR:N	2.40	0.46
9:M:178:ALA:HA	9:M:339:LYS:HE2	1.97	0.46
13:U:28:GLY:HA3	16:X:31:DA:OP2	2.14	0.46
3:D:565:PHE:CE1	7:A:542:GLN:CG	2.97	0.46
4:H:118:ASN:OD1	4:H:118:ASN:N	2.40	0.46
7:A:1188:HIS:HE1	7:A:1236:ILE:HD13	1.80	0.46
9:M:390:THR:O	9:M:422:THR:OG1	2.32	0.46
10:N:22:GLN:OE1	10:N:433:GLN:NE2	2.40	0.46
10:N:169:THR:O	10:N:186:SER:HA	2.15	0.46
13:Q:77:ARG:HD3	15:W:20:DA:H5''	1.98	0.46
11:S:74:ILE:HD13	12:T:62:LEU:HB3	1.96	0.46
15:W:38:DT:C2	16:X:110:DA:C2	3.04	0.46
1:B:932:ASP:OD1	1:B:932:ASP:N	2.48	0.46
1:B:936:ARG:C	1:B:940:ARG:HH21	2.23	0.46
9:M:39:THR:O	9:M:62:ARG:NH2	2.34	0.46
14:R:66:VAL:HA	14:R:69:ARG:HD2	1.98	0.46
12:T:75:HIS:ND1	14:V:93:THR:OG1	2.37	0.46
15:W:23:DC:H1'	15:W:24:DC:H5'	1.97	0.46
3:D:424:PRO:HD2	7:A:552:PHE:HD1	1.78	0.46
3:E:771:LYS:O	3:E:775:SER:HB2	2.16	0.46
13:Q:109:PRO:HG3	11:S:56:LYS:HA	1.98	0.46
11:S:83:ARG:HB3	16:X:50:DT:H5''	1.97	0.46
1:B:697:LEU:HD22	1:B:702:LEU:HD23	1.98	0.46
1:B:730:LEU:CD1	7:A:567:PHE:CE2	2.99	0.46
3:D:387:LYS:HA	3:D:387:LYS:HD3	1.75	0.46
3:E:520:LEU:HD11	3:E:645:SER:HA	1.97	0.46
7:A:590:GLU:OE1	7:A:590:GLU:HA	2.15	0.46
7:A:641:GLU:O	7:A:645:GLN:N	2.47	0.46
9:M:314:PHE:HA	9:M:329:LEU:H	1.80	0.46
10:N:437:LYS:O	10:N:441:THR:OG1	2.28	0.46
12:T:85:ASP:OD1	12:T:85:ASP:N	2.48	0.46
15:W:108:DT:H2'	15:W:108:DT:OP2	2.16	0.46
3:D:370:ASN:OD1	6:J:471:HIS:ND1	2.45	0.46
6:J:475:ALA:O	6:J:479:ASN:ND2	2.49	0.46
9:M:58:ALA:HB1	9:M:222:TYR:HB2	1.97	0.46
9:M:335:LYS:HA	9:M:338:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:12:ALA:N	15:W:32:DT:O2	2.49	0.46
14:R:84:SER:N	15:W:40:DG:OP1	2.49	0.46
15:W:127:DT:H2'	15:W:128:DG:C8	2.51	0.46
7:A:644:GLU:OE1	7:A:647:ARG:NH1	2.49	0.46
7:A:1008:GLU:HA	7:A:1208:ILE:HB	1.97	0.46
7:A:1207:ARG:HD3	7:A:1207:ARG:HA	1.80	0.46
8:L:31:GLN:HG2	8:L:55:LYS:HD2	1.98	0.46
9:M:334:ALA:HB2	9:M:415:ARG:HD3	1.98	0.46
11:O:48:LEU:HG	11:O:51:ILE:HD12	1.98	0.46
11:O:52:ARG:O	11:O:56:LYS:N	2.47	0.46
11:S:49:ARG:O	11:S:53:ARG:N	2.40	0.46
11:S:106:ASP:OD2	11:S:131:ARG:NE	2.45	0.46
12:T:59:LYS:HA	12:T:62:LEU:HD12	1.97	0.46
2:C:663:LEU:HB3	2:C:666:ASP:HB2	1.97	0.46
3:D:458:LYS:O	3:D:462:ARG:HB2	2.16	0.46
5:I:125:THR:O	5:I:125:THR:OG1	2.31	0.46
13:U:58:LEU:HD23	13:U:61:GLU:HG3	1.96	0.46
15:W:77:DT:H2''	15:W:78:DC:C2	2.51	0.46
4:H:186:VAL:O	4:H:296:SER:OG	2.28	0.45
7:A:929:ASN:HA	7:A:1232:ASP:HB3	1.98	0.45
9:M:428:VAL:O	9:M:431:ASP:N	2.49	0.45
10:N:159:CYS:HA	10:N:332:ASN:HB2	1.98	0.45
11:O:57:SER:O	13:U:81:ARG:NH1	2.49	0.45
13:Q:67:GLY:HA2	14:R:49:THR:HG21	1.97	0.45
14:V:112:THR:O	14:V:115:VAL:HB	2.16	0.45
2:C:556:GLN:HB3	2:C:653:LEU:O	2.15	0.45
7:A:1264:ARG:HG3	7:A:1268:ARG:HH12	1.80	0.45
8:L:29:TRP:HE3	8:L:59:ARG:HB2	1.81	0.45
9:M:63:ASN:OD1	9:M:63:ASN:N	2.48	0.45
11:O:125:GLN:NE2	12:P:53:GLU:OE1	2.50	0.45
14:R:99:LEU:HD12	14:R:104:ALA:HA	1.99	0.45
11:S:42:ARG:HB3	16:X:68:DG:H4'	1.98	0.45
1:B:952:LEU:HG	1:B:996:LEU:HB3	1.97	0.45
3:D:736:ILE:O	3:D:740:LEU:HB2	2.15	0.45
3:D:786:PRO:O	4:H:167:ASN:ND2	2.48	0.45
3:E:614:LEU:HD12	3:E:660:ALA:HB1	1.99	0.45
7:A:822:ILE:HG23	7:A:893:ILE:HA	1.97	0.45
9:M:118:ALA:O	9:M:121:GLU:HB3	2.16	0.45
9:M:337:VAL:HG11	9:M:389:LEU:HD11	1.97	0.45
10:N:87:PHE:O	10:N:91:LEU:HG	2.16	0.45
10:N:166:THR:O	10:N:192:GLN:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:337:GLY:O	10:N:340:THR:OG1	2.30	0.45
13:Q:112:GLN:HE21	13:Q:112:GLN:HB3	1.59	0.45
11:S:73:GLU:HG3	12:T:23:ARG:HA	1.98	0.45
1:B:941:ASN:HD22	1:B:944:LEU:N	2.01	0.45
2:C:652:LEU:CD1	6:J:312:LEU:CB	2.79	0.45
10:N:5:ARG:NE	10:N:104:ALA:O	2.50	0.45
12:P:47:SER:HB3	12:P:50:ILE:HG12	1.99	0.45
11:S:67:PHE:HE2	11:S:90:MET:HA	1.82	0.45
14:V:102:GLU:HA	14:V:105:LYS:HD2	1.98	0.45
1:B:781:ASP:N	1:B:781:ASP:OD1	2.50	0.45
2:C:527:ASN:HB3	2:C:531:GLU:HG2	1.98	0.45
7:A:489:ASP:C	7:A:491:HIS:H	2.25	0.45
7:A:810:TYR:CE2	7:A:819:TYR:HE2	2.28	0.45
7:A:1164:ARG:HH12	16:X:95:DG:H21	1.63	0.45
3:D:423:PHE:CD1	7:A:552:PHE:CD1	3.04	0.45
4:H:115:PRO:O	4:H:116:HIS:ND1	2.50	0.45
4:H:160:ILE:HB	4:H:281:LEU:HB3	1.99	0.45
7:A:619:ARG:HH22	9:M:438:LEU:HB3	1.80	0.45
7:A:808:TYR:HA	7:A:811:GLU:HG2	1.97	0.45
9:M:126:LEU:HA	9:M:130:LYS:HD3	1.98	0.45
11:O:58:THR:O	13:U:104:GLN:NE2	2.49	0.45
12:T:75:HIS:O	14:V:89:ARG:NH2	2.50	0.45
9:M:75:GLY:HA3	9:M:109:PRO:HG3	1.99	0.45
9:M:127:ALA:O	9:M:133:VAL:N	2.50	0.45
13:Q:55:LEU:O	13:Q:59:THR:OG1	2.26	0.45
15:W:86:DT:H6	15:W:86:DT:H2'	1.67	0.45
1:B:1149:VAL:HG23	7:A:586:TYR:HE1	1.78	0.45
2:C:652:LEU:HG	6:J:312:LEU:HB3	1.94	0.45
7:A:844:THR:HA	7:A:868:VAL:HG12	1.99	0.45
9:M:151:LYS:HD2	9:M:393:ILE:HD11	1.98	0.45
9:M:335:LYS:HE3	9:M:339:LYS:HZ2	1.82	0.45
10:N:145:ALA:HB1	10:N:428:ILE:HD13	1.98	0.45
11:O:85:GLN:OE1	11:O:87:SER:OG	2.34	0.45
15:W:38:DT:C4	16:X:110:DA:N1	2.84	0.45
2:C:622:ASP:HB3	2:C:625:ILE:HG13	1.99	0.45
2:C:652:LEU:HB3	6:J:312:LEU:N	2.28	0.45
4:H:89:ILE:O	4:H:93:ASN:ND2	2.50	0.45
4:H:440:LEU:HD23	4:H:440:LEU:HA	1.86	0.45
7:A:642:ARG:HG2	7:A:646:LYS:HD3	1.99	0.45
10:N:112:LEU:HD21	10:N:143:LEU:HD23	1.99	0.45
10:N:333:ILE:HB	10:N:409:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:34:LEU:HA	13:Q:39:TYR:HE1	1.81	0.45
16:X:57:DT:H2''	16:X:58:DT:C6	2.52	0.45
1:B:760:LEU:HD23	1:B:950:ASP:HB3	1.98	0.45
1:B:905:ARG:HA	1:B:905:ARG:HE	1.80	0.45
1:B:916:ASP:OD2	7:A:562:ASN:CG	2.60	0.45
1:B:923:MET:HE2	7:A:567:PHE:O	2.16	0.45
3:E:685:GLU:OE2	3:E:688:ARG:NH2	2.43	0.45
8:L:7:ILE:HD13	10:N:135:LEU:HA	1.99	0.45
8:L:34:LYS:HG2	8:L:56:TYR:CZ	2.52	0.45
9:M:335:LYS:HB3	9:M:335:LYS:HE2	1.73	0.45
10:N:158:ASN:HA	10:N:174:ILE:O	2.17	0.45
10:N:197:SER:OG	10:N:301:GLY:O	2.28	0.45
11:S:40:ARG:HB3	15:W:84:DC:H4'	1.98	0.45
1:B:1030:LEU:HD21	1:B:1036:GLN:HE22	1.82	0.44
1:B:1040:VAL:HG21	1:B:1139:VAL:HG23	2.00	0.44
7:A:811:GLU:HG3	7:A:812:MET:HG3	1.98	0.44
7:A:1134:ASP:OD1	7:A:1134:ASP:N	2.51	0.44
10:N:31:THR:O	10:N:419:TRP:NE1	2.50	0.44
10:N:87:PHE:HE1	10:N:109:ILE:HD12	1.81	0.44
10:N:205:TRP:HZ3	10:N:213:LEU:HB2	1.82	0.44
10:N:365:GLU:OE1	10:N:400:TYR:OH	2.35	0.44
12:P:57:VAL:HA	12:P:60:VAL:HB	2.00	0.44
13:Q:47:ALA:HB1	14:R:91:ILE:HD11	1.99	0.44
13:Q:81:ARG:NH2	11:S:56:LYS:O	2.51	0.44
11:S:84:PHE:N	16:X:50:DT:O3'	2.50	0.44
14:V:113:LYS:HE3	14:V:113:LYS:HB3	1.76	0.44
2:C:545:ARG:NH1	2:C:560:GLN:OE1	2.45	0.44
4:H:158:MET:HG3	4:H:283:ILE:HB	1.99	0.44
15:W:49:DA:C2	16:X:100:DA:H2	2.33	0.44
15:W:98:DA:N1	16:X:50:DT:C4	2.85	0.44
1:B:941:ASN:ND2	1:B:941:ASN:C	2.73	0.44
7:A:953:ASP:OD1	7:A:953:ASP:N	2.49	0.44
9:M:314:PHE:HZ	9:M:408:ILE:HG12	1.83	0.44
10:N:169:THR:OG1	10:N:190:GLY:N	2.36	0.44
12:T:31:LYS:HA	12:T:34:ILE:HD12	2.00	0.44
15:W:34:DG:N2	16:X:115:DC:O2	2.51	0.44
15:W:75:DT:H6	15:W:75:DT:H2'	1.64	0.44
1:B:916:ASP:CB	7:A:562:ASN:ND2	2.81	0.44
2:C:739:MET:SD	3:E:370:ASN:ND2	2.91	0.44
4:H:136:GLN:HG2	4:H:154:ALA:HA	1.99	0.44
7:A:1196:ARG:HH21	7:A:1199:ARG:HH22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1219:GLU:O	7:A:1223:GLU:N	2.45	0.44
10:N:450:THR:H	10:N:453:LYS:HB2	1.83	0.44
15:W:46:DT:H2'	15:W:46:DT:OP2	2.17	0.44
15:W:78:DC:H4'	15:W:79:DC:H5'	2.00	0.44
1:B:707:LEU:HD12	2:C:428:PRO:HB3	1.99	0.44
2:C:467:ASP:OD2	2:C:662:ARG:CZ	2.65	0.44
3:D:600:PHE:HZ	4:H:519:ILE:HG23	1.82	0.44
3:D:610:THR:OG1	7:A:487:GLY:CA	2.53	0.44
10:N:102:PHE:HA	10:N:106:LEU:HB2	2.00	0.44
14:R:30:ARG:HH12	15:W:27:DT:H1'	1.82	0.44
1:B:927:ASN:OD1	7:A:569:SER:CB	2.58	0.44
1:B:930:PHE:CE2	7:A:570:LYS:HB3	2.53	0.44
1:B:1138:PRO:CB	7:A:574:ILE:HG22	2.47	0.44
2:C:655:ILE:HD12	2:C:655:ILE:O	2.18	0.44
3:D:576:TYR:CB	7:A:497:TYR:OH	2.66	0.44
9:M:137:GLN:HE21	9:M:452:GLY:HA3	1.82	0.44
10:N:131:VAL:HG11	10:N:140:LEU:HD22	1.99	0.44
10:N:214:LYS:HE2	10:N:214:LYS:HB3	1.61	0.44
12:P:68:ASP:HB3	12:P:92:ARG:HH22	1.82	0.44
12:T:84:MET:HE3	12:T:84:MET:HB3	1.86	0.44
14:V:104:ALA:O	14:V:108:VAL:N	2.43	0.44
15:W:109:DC:C2	16:X:39:DG:N2	2.80	0.44
1:B:1251:LYS:HD3	1:B:1251:LYS:HA	1.74	0.44
3:D:423:PHE:CE1	7:A:552:PHE:CZ	3.06	0.44
3:D:537:LYS:CA	7:A:534:TYR:CD2	3.00	0.44
3:D:570:ILE:HB	7:A:539:LEU:CD1	2.48	0.44
7:A:637:HIS:CE1	10:N:434:ILE:HG21	2.53	0.44
7:A:826:SER:HB3	7:A:1169:GLY:HA2	1.99	0.44
10:N:15:ARG:HE	10:N:15:ARG:HB2	1.43	0.44
10:N:45:THR:HG23	10:N:51:TYR:HE1	1.82	0.44
10:N:128:THR:HG22	10:N:454:TYR:HE1	1.82	0.44
14:R:112:THR:O	14:R:115:VAL:HB	2.18	0.44
15:W:117:DT:H6	15:W:117:DT:H2'	1.54	0.44
1:B:936:ARG:CB	1:B:940:ARG:HH21	2.29	0.44
4:H:377:SER:O	4:H:403:LEU:N	2.47	0.44
7:A:626:ARG:NE	10:N:176:ASP:O	2.51	0.44
7:A:1108:ILE:HG23	7:A:1179:ILE:HB	1.99	0.44
10:N:172:ILE:HA	10:N:184:VAL:HG22	2.00	0.44
13:Q:95:LYS:HD2	13:Q:95:LYS:HA	1.67	0.44
16:X:119:DT:H2''	16:X:120:DG:N7	2.33	0.44
2:C:673:ARG:HD3	14:V:106:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:331:PRO:O	9:M:335:LYS:HB3	2.18	0.44
10:N:275:LYS:HZ1	10:N:277:SER:HB3	1.83	0.44
10:N:306:ILE:HD13	10:N:348:ALA:HB3	2.00	0.44
14:V:54:LYS:HZ2	14:V:58:ILE:HD11	1.82	0.44
1:B:907:ALA:CB	7:A:554:TRP:CZ3	2.93	0.43
1:B:1023:LEU:HD11	1:B:1200:ILE:HD13	2.00	0.43
1:B:1049:LEU:HB2	1:B:1053:ASN:HD22	1.83	0.43
3:D:312:LYS:HE3	3:D:312:LYS:HB3	1.83	0.43
3:D:606:PRO:CA	7:A:488:ILE:HD12	2.38	0.43
4:H:452:PHE:O	4:H:455:THR:OG1	2.34	0.43
3:E:514:LEU:O	3:E:518:LYS:HB2	2.18	0.43
10:N:462:LEU:O	10:N:466:GLN:NE2	2.43	0.43
13:U:76:THR:O	14:V:50:GLY:N	2.51	0.43
5:I:40:SER:OG	5:I:41:LEU:N	2.52	0.43
3:E:335:ILE:HG22	3:E:337:SER:H	1.83	0.43
3:E:417:ASP:OD1	3:E:417:ASP:N	2.49	0.43
7:A:816:ARG:NH1	7:A:841:THR:CB	2.81	0.43
7:A:1145:LEU:HD13	7:A:1148:LEU:HD12	1.99	0.43
10:N:419:TRP:CD1	10:N:430:LEU:HD13	2.53	0.43
13:Q:83:LEU:HD13	14:R:58:ILE:HG21	1.98	0.43
13:Q:111:ILE:HG21	11:S:48:LEU:HB3	2.00	0.43
11:S:43:PRO:HD3	16:X:67:DG:H21	1.83	0.43
13:U:66:ALA:HB1	13:U:78:ILE:HG21	1.99	0.43
15:W:54:DC:O2	16:X:95:DG:N2	2.51	0.43
2:C:558:ILE:HD12	2:C:653:LEU:HD13	1.97	0.43
2:C:583:LEU:HB3	2:C:585:LEU:HD13	2.01	0.43
3:E:778:GLU:H	3:E:778:GLU:HG3	1.61	0.43
7:A:810:TYR:CD2	7:A:816:ARG:N	2.86	0.43
8:L:24:SER:C	8:L:66:ASN:HB2	2.44	0.43
8:L:64:LEU:HD23	9:M:4:ASN:HD22	1.83	0.43
11:S:83:ARG:O	12:T:80:THR:OG1	2.29	0.43
13:U:37:GLY:HA3	13:U:39:TYR:CZ	2.53	0.43
2:C:653:LEU:H	2:C:653:LEU:HG	1.50	0.43
3:E:314:PHE:HE1	3:E:347:ARG:HD2	1.84	0.43
7:A:799:THR:HB	7:A:838:TRP:HZ3	1.84	0.43
7:A:808:TYR:C	7:A:811:GLU:CG	2.71	0.43
10:N:327:LYS:HA	10:N:330:TRP:HB2	2.01	0.43
13:Q:91:GLU:O	13:Q:95:LYS:HB2	2.18	0.43
13:U:52:ALA:HA	13:U:55:LEU:HD12	2.01	0.43
13:U:77:ARG:CZ	16:X:20:DC:H4'	2.49	0.43
14:V:95:VAL:HG13	14:V:99:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1274:ASN:HD21	4:H:95:HIS:HD2	1.65	0.43
2:C:564:ASP:N	3:D:374:ASP:OD1	2.52	0.43
2:C:654:GLN:C	2:C:655:ILE:CG1	2.83	0.43
3:D:539:ILE:CG2	7:A:538:LEU:HG	2.18	0.43
6:J:546:LYS:NZ	6:J:547:ARG:O	2.49	0.43
7:A:613:ILE:O	7:A:617:ASN:N	2.50	0.43
7:A:792:ASP:HA	7:A:993:ARG:HG3	2.00	0.43
9:M:189:LEU:HD22	9:M:309:PHE:HB3	1.99	0.43
10:N:344:GLY:HA2	10:N:347:GLU:HB3	2.01	0.43
10:N:363:GLU:O	10:N:367:SER:CB	2.66	0.43
11:O:119:ILE:HD11	12:P:50:ILE:HG21	2.00	0.43
2:C:743:VAL:HG21	6:J:290:ILE:HD11	2.00	0.43
3:D:709:GLU:OE1	3:D:712:ARG:NH1	2.51	0.43
7:A:810:TYR:N	7:A:810:TYR:CD1	2.86	0.43
10:N:131:VAL:HA	10:N:135:LEU:HB2	2.00	0.43
13:Q:17:ARG:HA	13:Q:20:ARG:HD2	2.00	0.43
11:S:128:ARG:NE	11:S:133:GLU:OE1	2.52	0.43
16:X:144:DC:H2''	16:X:145:DC:C6	2.54	0.43
2:C:663:LEU:C	2:C:665:LYS:N	2.77	0.43
7:A:1302:GLU:HA	7:A:1306:LYS:HB3	2.00	0.43
8:L:26:ARG:HH21	8:L:64:LEU:HD13	1.84	0.43
12:P:85:ASP:HA	12:P:88:TYR:HB2	2.00	0.43
11:S:64:LYS:NZ	11:S:93:GLN:HE22	2.17	0.43
13:U:53:ALA:HB2	14:V:114:ALA:HB3	2.01	0.43
14:V:37:TYR:HA	14:V:40:LYS:HD2	2.00	0.43
16:X:58:DT:H4'	16:X:59:DA:H5'	2.00	0.43
3:D:423:PHE:HD1	7:A:552:PHE:CD1	2.37	0.43
3:D:537:LYS:HB2	7:A:531:TYR:HE1	1.83	0.43
7:A:531:TYR:HA	7:A:534:TYR:HB2	2.00	0.43
7:A:1094:ARG:O	7:A:1098:LYS:NZ	2.49	0.43
9:M:119:ILE:HA	9:M:122:ARG:HB2	2.00	0.43
9:M:397:SER:HA	9:M:433:LYS:HG2	1.99	0.43
12:T:38:ALA:O	12:T:43:VAL:N	2.51	0.43
16:X:110:DA:OP2	16:X:110:DA:H2''	2.19	0.43
2:C:655:ILE:C	2:C:655:ILE:CD1	2.92	0.43
5:I:126:VAL:O	3:E:667:ARG:NH1	2.51	0.43
7:A:816:ARG:HH12	7:A:841:THR:HB	1.83	0.43
7:A:1007:VAL:HG11	7:A:1206:VAL:HB	2.01	0.43
9:M:3:LEU:HD22	9:M:449:TRP:HD1	1.82	0.43
9:M:160:GLY:HA2	9:M:397:SER:H	1.83	0.43
15:W:27:DT:H2''	15:W:28:DC:C2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:144:TYR:OH	3:E:695:ASP:OD2	2.36	0.43
7:A:972:SER:O	7:A:977:LEU:N	2.46	0.43
11:S:116:ARG:NH1	11:S:120:MET:SD	2.92	0.43
12:T:26:ILE:HD12	12:T:26:ILE:HA	1.82	0.43
15:W:34:DG:H2'	15:W:35:DT:C6	2.54	0.43
16:X:78:DG:H4'	16:X:79:DT:H5'	2.01	0.43
3:D:540:GLN:CB	7:A:538:LEU:HD21	2.48	0.42
5:I:84:ARG:O	7:A:575:ASN:ND2	2.52	0.42
3:E:596:PRO:CG	7:A:489:ASP:OD2	2.66	0.42
7:A:568:LEU:H	7:A:568:LEU:HG	1.59	0.42
11:O:128:ARG:O	11:O:133:GLU:N	2.52	0.42
12:T:64:ASN:OD1	12:T:67:ARG:NH2	2.52	0.42
15:W:84:DC:H6	15:W:84:DC:H2'	1.71	0.42
1:B:1051:LYS:N	1:B:1051:LYS:CE	2.73	0.42
7:A:816:ARG:HD3	7:A:842:LEU:HD23	1.96	0.42
9:M:84:GLU:O	9:M:87:TRP:N	2.52	0.42
10:N:94:ARG:HB2	10:N:106:LEU:HD11	2.01	0.42
10:N:282:ASN:O	10:N:293:LYS:HA	2.20	0.42
16:X:37:DG:H1'	16:X:38:DG:C4	2.54	0.42
16:X:87:DT:H6	16:X:87:DT:H2'	1.73	0.42
6:J:325:SER:HB3	6:J:328:SER:HB2	2.01	0.42
7:A:927:LEU:HB2	7:A:937:LEU:HD11	2.01	0.42
7:A:1237:GLN:HA	7:A:1240:LYS:HE3	2.01	0.42
9:M:3:LEU:HD21	9:M:448:SER:HA	2.01	0.42
9:M:288:LYS:HE2	9:M:288:LYS:HB3	1.75	0.42
9:M:462:THR:HG22	9:M:465:ARG:HH22	1.84	0.42
10:N:17:GLN:O	10:N:39:THR:N	2.38	0.42
10:N:40:GLN:HB2	10:N:64:LEU:HD11	2.02	0.42
10:N:163:ASP:O	10:N:169:THR:HA	2.19	0.42
10:N:361:GLU:HB2	10:N:397:THR:HG23	2.01	0.42
11:O:83:ARG:HD2	16:X:101:DG:H5'	2.01	0.42
13:Q:88:ARG:HA	13:Q:88:ARG:HD3	1.77	0.42
11:S:49:ARG:HA	11:S:52:ARG:HD2	2.00	0.42
14:V:77:LEU:O	14:V:81:ASN:ND2	2.52	0.42
16:X:17:DT:H2''	16:X:18:DG:C5	2.54	0.42
16:X:130:DG:H1'	16:X:131:DG:C6	2.55	0.42
1:B:983:SER:HA	1:B:986:LEU:HB2	2.02	0.42
4:H:82:GLU:OE2	3:E:697:LYS:NZ	2.40	0.42
4:H:267:LYS:HE3	4:H:267:LYS:HB3	1.90	0.42
8:L:61:LYS:HE2	8:L:61:LYS:HB3	1.90	0.42
8:L:85:LYS:HE2	8:L:85:LYS:HB2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:157:GLN:HG3	10:N:176:ASP:HA	2.00	0.42
11:O:43:PRO:HG3	15:W:67:DG:H21	1.85	0.42
11:O:53:ARG:O	11:O:57:SER:N	2.49	0.42
13:U:81:ARG:HA	13:U:105:GLY:HA2	2.01	0.42
13:U:91:GLU:O	13:U:95:LYS:CB	2.67	0.42
1:B:792:HIS:HE1	3:D:328:PRO:HD2	1.83	0.42
3:D:606:PRO:HA	7:A:488:ILE:CG1	2.47	0.42
7:A:1013:CYS:O	7:A:1214:THR:N	2.44	0.42
9:M:302:ASP:OD1	9:M:305:GLU:N	2.50	0.42
9:M:406:GLN:HE21	9:M:406:GLN:HB2	1.69	0.42
11:O:46:VAL:HA	11:O:49:ARG:HH21	1.84	0.42
13:U:51:LEU:HD21	14:V:67:PHE:HD1	1.83	0.42
3:D:731:GLN:HE21	3:D:731:GLN:HB3	1.60	0.42
3:E:446:THR:OG1	3:E:447:SER:N	2.52	0.42
7:A:895:GLU:HB3	7:A:897:HIS:CE1	2.55	0.42
10:N:306:ILE:HG23	10:N:349:LEU:HA	2.00	0.42
11:O:43:PRO:HB2	12:P:45:ARG:HH21	1.84	0.42
14:R:37:TYR:OH	16:X:123:DC:OP1	2.38	0.42
14:R:85:THR:N	15:W:40:DG:OP1	2.51	0.42
13:U:40:ALA:HB2	14:V:86:ILE:HG13	2.01	0.42
14:V:41:VAL:HA	14:V:44:GLN:HB2	2.01	0.42
1:B:901:LYS:HB3	1:B:904:THR:CG2	2.50	0.42
2:C:652:LEU:CB	6:J:312:LEU:CB	2.87	0.42
3:D:363:SER:OG	3:D:366:THR:OG1	2.31	0.42
7:A:845:ILE:O	7:A:870:LEU:N	2.51	0.42
7:A:1265:ARG:HD3	7:A:1268:ARG:HD2	2.01	0.42
10:N:439:ILE:HG21	10:N:447:PHE:HB2	2.01	0.42
12:P:98:TYR:N	13:U:101:THR:O	2.43	0.42
13:Q:69:ALA:O	13:Q:73:ASN:ND2	2.37	0.42
15:W:47:DC:H1'	15:W:48:DT:C2	2.55	0.42
15:W:90:DA:H2	16:X:59:DA:C2	2.38	0.42
15:W:116:DC:H6	15:W:116:DC:H2'	1.72	0.42
3:D:574:PHE:HZ	7:A:508:THR:HB	1.85	0.42
5:I:138:SER:OG	5:I:139:GLU:N	2.52	0.42
3:E:618:VAL:HG11	3:E:663:SER:HB2	2.01	0.42
3:E:701:LEU:HD23	3:E:704:LEU:HD12	2.02	0.42
7:A:633:LEU:HD21	10:N:438:GLN:HB2	2.00	0.42
7:A:679:ILE:HG23	7:A:747:VAL:HG11	2.02	0.42
7:A:816:ARG:HH12	7:A:841:THR:CB	2.32	0.42
7:A:1164:ARG:HD2	15:W:54:DC:H4'	2.00	0.42
11:O:68:GLN:HG3	11:O:89:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:LYS:O	1:B:904:THR:HG23	2.20	0.42
2:C:555:ASN:OD1	2:C:654:GLN:HB2	2.19	0.42
2:C:573:GLU:OE2	2:C:598:ARG:NH2	2.53	0.42
7:A:520:GLU:H	7:A:520:GLU:HG3	1.43	0.42
7:A:806:LEU:O	7:A:810:TYR:CG	2.73	0.42
9:M:409:ILE:O	9:M:413:SER:CB	2.68	0.42
10:N:218:ILE:HD12	10:N:282:ASN:HB3	2.01	0.42
11:O:106:ASP:HA	11:O:109:LEU:HB2	2.02	0.42
11:S:124:ILE:HD11	12:T:50:ILE:HD12	2.02	0.42
12:T:34:ILE:HD11	12:T:55:ARG:HD2	2.01	0.42
14:V:100:PRO:HG2	14:V:103:LEU:HD12	2.00	0.42
15:W:14:DG:H1'	15:W:15:DT:H5'	2.01	0.42
16:X:28:DT:H1'	16:X:29:DG:C5	2.55	0.42
1:B:1145:THR:CG2	7:A:586:TYR:CD2	2.95	0.42
3:D:568:LEU:HD23	3:D:568:LEU:HA	1.94	0.42
9:M:135:VAL:HG22	9:M:454:TRP:HE3	1.84	0.42
10:N:166:THR:HG23	10:N:214:LYS:NZ	2.34	0.42
13:U:90:ASP:HB3	13:U:93:LEU:HB2	2.01	0.42
15:W:132:DG:H4'	15:W:133:DA:H5'	2.01	0.42
3:D:423:PHE:HA	7:A:552:PHE:CE1	2.55	0.41
6:J:302:ILE:HD12	6:J:302:ILE:HA	1.95	0.41
3:E:728:ASN:O	3:E:732:ASN:ND2	2.53	0.41
8:L:29:TRP:CE3	8:L:59:ARG:HB2	2.54	0.41
9:M:197:LEU:HD21	9:M:301:LEU:HG	2.02	0.41
1:B:1051:LYS:CD	1:B:1051:LYS:N	2.73	0.41
3:D:424:PRO:HD3	7:A:555:HIS:CG	2.54	0.41
6:J:566:TYR:CD2	7:A:541:LEU:HD11	2.55	0.41
3:E:422:LEU:HD11	7:A:554:TRP:CD1	2.54	0.41
7:A:543:LYS:HA	7:A:546:ARG:HB2	2.02	0.41
7:A:770:TYR:OH	17:A:1501:ADP:N7	2.53	0.41
7:A:1018:LEU:HD11	7:A:1085:VAL:HG23	2.00	0.41
8:L:22:LYS:HG3	10:N:451:ARG:CZ	2.50	0.41
10:N:328:ALA:O	10:N:332:ASN:ND2	2.40	0.41
13:Q:28:GLY:HA3	15:W:31:DT:P	2.60	0.41
11:S:83:ARG:HH22	15:W:99:DG:N2	2.18	0.41
13:U:46:GLY:HA2	13:U:49:VAL:HG23	2.01	0.41
15:W:156:DG:H2''	15:W:157:DA:C8	2.55	0.41
2:C:525:GLN:HE22	2:C:528:PRO:HG3	1.85	0.41
11:O:109:LEU:O	11:O:113:HIS:CB	2.68	0.41
11:O:111:ALA:O	11:O:116:ARG:N	2.53	0.41
12:T:49:LEU:H	12:T:49:LEU:HG	1.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:66:VAL:HG12	14:V:70:ILE:HG13	2.02	0.41
14:V:78:ALA:O	14:V:83:ARG:N	2.52	0.41
16:X:65:DC:H1'	16:X:66:DG:C5	2.56	0.41
1:B:868:ILE:HD11	1:B:954:LEU:HD13	2.01	0.41
3:D:306:VAL:N	3:D:394:GLN:OE1	2.53	0.41
4:H:382:ASP:H	4:H:385:LEU:HB2	1.85	0.41
3:E:445:ASN:OD1	7:A:504:ASN:ND2	2.53	0.41
3:E:465:ASP:O	3:E:469:HIS:ND1	2.54	0.41
9:M:7:CYS:N	9:M:22:SER:OG	2.52	0.41
9:M:36:ILE:O	9:M:48:ILE:HB	2.20	0.41
13:Q:25:PHE:HZ	13:Q:59:THR:HG21	1.84	0.41
14:R:106:HIS:O	14:R:109:SER:OG	2.27	0.41
11:S:92:LEU:O	11:S:96:SER:OG	2.38	0.41
12:T:46:ILE:N	15:W:82:DC:OP1	2.52	0.41
16:X:65:DC:H1'	16:X:66:DG:N7	2.36	0.41
4:H:566:MET:HE1	7:A:549:VAL:HG22	2.01	0.41
8:L:60:TYR:OH	9:M:4:ASN:O	2.30	0.41
10:N:73:ILE:HG13	10:N:119:TRP:CE2	2.55	0.41
10:N:351:GLY:HA2	10:N:354:LEU:HD12	2.03	0.41
13:Q:80:PRO:HA	13:Q:83:LEU:HD12	2.01	0.41
14:V:63:VAL:O	14:V:67:PHE:HB3	2.20	0.41
14:V:64:ASN:HA	14:V:67:PHE:HB3	2.03	0.41
7:A:999:VAL:HG23	7:A:1000:GLU:HG3	2.03	0.41
9:M:70:LEU:HD23	9:M:79:ASN:HB3	2.03	0.41
9:M:141:GLU:HG3	9:M:436:GLY:HA3	2.03	0.41
9:M:158:ASP:OD2	9:M:165:ASN:ND2	2.54	0.41
14:R:105:LYS:O	14:R:108:VAL:HB	2.21	0.41
15:W:3:DG:H2''	15:W:4:DG:C8	2.55	0.41
15:W:77:DT:H2''	15:W:78:DC:C6	2.55	0.41
2:C:564:ASP:OD1	2:C:566:SER:OG	2.38	0.41
7:A:516:LEU:HA	7:A:526:ARG:HA	2.03	0.41
7:A:532:ASP:O	7:A:536:LEU:N	2.49	0.41
7:A:754:ASP:HA	7:A:776:GLN:HG2	2.01	0.41
7:A:992:LEU:HD21	7:A:994:ARG:HH12	1.85	0.41
9:M:400:LEU:HD23	9:M:400:LEU:HA	1.78	0.41
11:O:133:GLU:H	11:O:133:GLU:HG3	1.56	0.41
14:R:64:ASN:N	12:T:102:GLY:O	2.54	0.41
13:U:44:GLY:HA3	14:V:87:THR:HG22	2.02	0.41
15:W:155:DC:H2''	15:W:156:DG:C8	2.56	0.41
16:X:-7:DG:H2''	16:X:-6:DA:C8	2.55	0.41
16:X:127:DC:H2'	16:X:128:DT:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:61:ILE:HG21	4:H:72:LEU:HG	2.03	0.41
3:E:536:LEU:HD21	3:E:631:ILE:HG22	2.02	0.41
7:A:619:ARG:HH12	9:M:438:LEU:HB3	1.86	0.41
7:A:775:LEU:O	7:A:779:VAL:N	2.39	0.41
9:M:67:VAL:O	9:M:217:SER:HB2	2.20	0.41
9:M:164:CYS:HB3	9:M:329:LEU:HD13	2.03	0.41
14:R:52:SER:O	14:R:56:MET:N	2.41	0.41
11:S:83:ARG:HG2	16:X:50:DT:H4'	2.03	0.41
15:W:75:DT:H2''	15:W:76:DG:C8	2.56	0.41
1:B:867:PRO:HD3	1:B:946:ARG:NH2	2.36	0.41
1:B:1138:PRO:HA	7:A:579:ALA:HB2	2.03	0.41
4:H:89:ILE:HG22	4:H:93:ASN:HD21	1.85	0.41
3:E:640:GLN:HA	3:E:643:GLU:HG2	2.03	0.41
7:A:816:ARG:NH1	7:A:841:THR:HB	2.35	0.41
7:A:871:THR:OG1	7:A:872:THR:N	2.50	0.41
7:A:1010:VAL:HG12	7:A:1210:ARG:HD2	2.02	0.41
7:A:1191:LEU:HA	7:A:1194:GLN:HB2	2.03	0.41
8:L:23:GLU:N	10:N:455:ASN:OD1	2.54	0.41
9:M:19:ALA:O	9:M:28:GLN:N	2.54	0.41
9:M:128:PHE:O	9:M:457:LYS:NZ	2.54	0.41
10:N:94:ARG:HA	10:N:94:ARG:HD3	1.91	0.41
10:N:116[A]:HIS:HB3	10:N:119:TRP:CD1	2.56	0.41
10:N:330:TRP:CZ3	10:N:353:LEU:HD22	2.56	0.41
11:O:63:ARG:HB2	11:O:66:PRO:HD2	2.02	0.41
11:O:83:ARG:HB3	15:W:50:DG:H4'	2.02	0.41
12:P:91:LYS:HE3	12:P:91:LYS:HB3	1.65	0.41
13:Q:34:LEU:HD22	13:Q:39:TYR:HE1	1.86	0.41
13:Q:41:GLU:HB3	14:R:84:SER:HB2	2.03	0.41
14:R:58:ILE:HA	12:T:98:TYR:HB3	2.02	0.41
11:S:48:LEU:O	11:S:52:ARG:N	2.50	0.41
11:S:84:PHE:H	16:X:51:DT:P	2.44	0.41
12:T:35:ARG:NH1	15:W:82:DC:OP2	2.54	0.41
13:U:88:ARG:HA	13:U:88:ARG:HD3	1.88	0.41
15:W:55:DG:H5'	15:W:55:DG:C8	2.56	0.41
1:B:901:LYS:HB3	1:B:904:THR:HG21	2.02	0.41
2:C:652:LEU:HD23	2:C:652:LEU:HA	1.74	0.41
2:C:675:ARG:H	2:C:675:ARG:HG2	1.68	0.41
3:D:602:LYS:HA	7:A:488:ILE:CG1	2.51	0.41
7:A:1050:ASN:ND2	7:A:1054:GLN:OE1	2.54	0.41
8:L:5:THR:O	8:L:9:LYS:HB2	2.20	0.41
8:L:81:ILE:HG23	10:N:88:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:70:LEU:HD13	9:M:83:LEU:HD12	2.02	0.41
9:M:121:GLU:HA	9:M:124:TYR:HB2	2.03	0.41
9:M:160:GLY:O	9:M:398:THR:OG1	2.31	0.41
9:M:292:PHE:HB2	9:M:299:LEU:HD11	2.02	0.41
10:N:13:TYR:O	10:N:19:THR:HA	2.21	0.41
10:N:98:ASN:HD22	10:N:101:ALA:HB2	1.85	0.41
10:N:192:GLN:NE2	10:N:195:ASN:OD1	2.53	0.41
10:N:331:GLU:HA	10:N:408:LYS:H	1.85	0.41
13:Q:34:LEU:HG	13:Q:48:PRO:HG3	2.03	0.41
14:R:30:ARG:CZ	16:X:122:DG:H21	2.34	0.41
14:R:35:ALA:HB1	14:R:56:MET:HE3	2.03	0.41
11:S:66:PRO:HB3	12:T:25:ASN:HB3	2.02	0.41
14:V:36:ILE:HA	14:V:39:TYR:HB2	2.03	0.41
14:V:58:ILE:O	14:V:61:SER:OG	2.33	0.41
16:X:14:DA:H2''	16:X:15:DT:H5'	2.04	0.41
7:A:1175:ALA:HB3	7:A:1197:ALA:HA	2.03	0.40
12:P:66:ILE:H	12:P:66:ILE:HG13	1.70	0.40
13:Q:31:HIS:CD2	13:Q:35:ARG:HE	2.39	0.40
14:R:48:ASP:N	14:R:48:ASP:OD1	2.54	0.40
11:S:63:ARG:HB3	11:S:66:PRO:HD2	2.03	0.40
11:S:104:PHE:CD2	12:T:41:GLY:HA3	2.54	0.40
11:S:128:ARG:O	11:S:133:GLU:N	2.54	0.40
15:W:6:DG:H2''	15:W:7:DA:C8	2.56	0.40
15:W:109:DC:O2	16:X:39:DG:C2	2.74	0.40
16:X:112:DG:H1'	16:X:113:DA:C8	2.56	0.40
2:C:544:ILE:HD12	2:C:544:ILE:HA	1.78	0.40
3:D:540:GLN:NE2	7:A:537:GLN:HG2	2.21	0.40
7:A:935:TRP:HE1	7:A:952:PHE:HD2	1.68	0.40
9:M:55:ILE:HG21	10:N:315:LEU:HD22	2.03	0.40
10:N:79:PHE:HZ	10:N:113:LEU:HD11	1.86	0.40
11:O:127:ALA:O	11:O:131:ARG:HB2	2.20	0.40
14:R:59:MET:O	14:R:63:VAL:HG23	2.22	0.40
11:S:48:LEU:H	11:S:48:LEU:HG	1.61	0.40
13:U:17:ARG:HA	13:U:20:ARG:HD2	2.02	0.40
13:U:116:LEU:HA	13:U:117:PRO:HD3	1.97	0.40
15:W:26:DC:H1'	15:W:27:DT:C2	2.56	0.40
15:W:36:DC:H6	15:W:36:DC:H2'	1.63	0.40
15:W:39:DA:H2	16:X:110:DA:H2	1.68	0.40
15:W:87:DT:H3	16:X:62:DA:H2	1.69	0.40
16:X:27:DC:H2''	16:X:28:DT:C5	2.57	0.40
1:B:759:LEU:HD23	1:B:759:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:663:LEU:HD13	2:C:663:LEU:HA	1.91	0.40
3:D:669:HIS:CD2	3:D:670:ILE:HG13	2.56	0.40
3:D:777:PRO:HG2	4:H:321:LYS:HB3	2.04	0.40
7:A:893:ILE:HG23	7:A:921:ILE:HG12	2.04	0.40
7:A:1019:GLN:NE2	7:A:1058:ILE:O	2.42	0.40
7:A:1110:PHE:HE1	7:A:1119:MET:HE3	1.86	0.40
9:M:178:ALA:O	9:M:336:SER:OG	2.33	0.40
10:N:334:ILE:HG12	10:N:410:ALA:HB3	2.03	0.40
11:O:71:VAL:HG21	11:O:89:VAL:HG13	2.03	0.40
11:O:72:ARG:HH12	15:W:51:DC:P	2.44	0.40
11:O:116:ARG:NH2	11:O:123:ASP:OD1	2.53	0.40
14:R:46:HIS:ND1	14:R:48:ASP:OD1	2.54	0.40
14:R:105:LYS:HA	14:R:108:VAL:HB	2.03	0.40
15:W:121:DG:N2	16:X:27:DC:C2	2.69	0.40
16:X:-16:DG:H1'	16:X:-15:DT:H5'	2.03	0.40
2:C:541:ASP:OD1	2:C:541:ASP:N	2.54	0.40
3:D:570:ILE:HG21	7:A:539:LEU:CG	2.49	0.40
4:H:311:SER:HB3	4:H:414:HIS:HB3	2.02	0.40
9:M:10:ILE:HB	9:M:106:ILE:HG22	2.03	0.40
9:M:193:VAL:HB	9:M:228:ILE:HG23	2.04	0.40
9:M:427[B]:GLN:HE21	9:M:427[B]:GLN:HB3	1.60	0.40
11:O:124:ILE:HD11	12:P:50:ILE:HD12	2.04	0.40
12:P:75:HIS:CE1	14:R:93:THR:HG1	2.34	0.40
13:Q:59:THR:HA	13:Q:62:ILE:HG22	2.03	0.40
13:Q:111:ILE:HD13	13:Q:116:LEU:HD21	2.02	0.40
13:U:103:ALA:O	14:V:54:LYS:NZ	2.35	0.40
15:W:109:DC:C2	16:X:39:DG:N1	2.89	0.40
16:X:118:DT:H2''	16:X:119:DT:C6	2.56	0.40
1:B:679:ILE:HA	1:B:682:ILE:HB	2.04	0.40
1:B:757:MET:HE3	1:B:757:MET:HB3	1.91	0.40
1:B:966:ARG:HH12	7:A:565:PRO:HB2	1.85	0.40
3:D:709:GLU:OE2	3:D:713:LYS:NZ	2.37	0.40
4:H:172:ASP:HB3	4:H:175:ARG:HD3	2.03	0.40
9:M:289:ASN:HB3	9:M:298:THR:HG23	2.03	0.40
9:M:409:ILE:HA	9:M:421:LEU:HD12	2.03	0.40
14:V:83:ARG:HD3	14:V:83:ARG:HA	1.97	0.40
15:W:100:DG:C2	16:X:48:DC:O2	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

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	B	489/1093 (45%)	460 (94%)	25 (5%)	4 (1%)	16	54
2	C	347/918 (38%)	309 (89%)	36 (10%)	2 (1%)	21	59
3	D	385/836 (46%)	372 (97%)	13 (3%)	0	100	100
3	E	414/836 (50%)	389 (94%)	24 (6%)	1 (0%)	43	78
4	H	376/566 (66%)	345 (92%)	30 (8%)	1 (0%)	36	72
5	I	102/332 (31%)	93 (91%)	8 (8%)	1 (1%)	12	48
6	J	159/634 (25%)	147 (92%)	11 (7%)	1 (1%)	21	59
7	A	734/982 (75%)	682 (93%)	46 (6%)	6 (1%)	16	54
8	L	45/157 (29%)	42 (93%)	3 (7%)	0	100	100
9	M	360/477 (76%)	344 (96%)	15 (4%)	1 (0%)	36	72
10	N	381/467 (82%)	358 (94%)	22 (6%)	1 (0%)	36	72
11	O	96/135 (71%)	90 (94%)	6 (6%)	0	100	100
11	S	93/135 (69%)	84 (90%)	9 (10%)	0	100	100
12	P	85/102 (83%)	81 (95%)	4 (5%)	0	100	100
12	T	84/102 (82%)	79 (94%)	5 (6%)	0	100	100
13	Q	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
13	U	105/129 (81%)	101 (96%)	4 (4%)	0	100	100
14	R	91/122 (75%)	86 (94%)	5 (6%)	0	100	100
14	V	91/122 (75%)	90 (99%)	1 (1%)	0	100	100
All	All	4542/8274 (55%)	4254 (94%)	270 (6%)	18 (0%)	31	67

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	868	ILE
1	B	1051	LYS

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Mol	Chain	Res	Type
2	C	655	ILE
2	C	664	ASP
7	A	490	THR
7	A	563	THR
10	N	48	ASP
7	A	489	ASP
7	A	567	PHE
9	M	217	SER
4	H	62	PRO
7	A	816	ARG
7	A	818	PRO
1	B	1052	PRO
6	J	504	PRO
5	I	39	PRO
3	E	401	PRO
1	B	867	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	484/1017 (48%)	440 (91%)	44 (9%)	9	27
2	C	321/832 (39%)	286 (89%)	35 (11%)	6	20
3	D	368/758 (48%)	334 (91%)	34 (9%)	8	26
3	E	393/758 (52%)	357 (91%)	36 (9%)	8	26
4	H	360/517 (70%)	322 (89%)	38 (11%)	6	21
5	I	102/288 (35%)	94 (92%)	8 (8%)	11	32
6	J	150/565 (26%)	142 (95%)	8 (5%)	20	41
7	A	678/889 (76%)	623 (92%)	55 (8%)	11	31
8	L	52/140 (37%)	48 (92%)	4 (8%)	12	32
9	M	345/420 (82%)	318 (92%)	27 (8%)	11	32
10	N	359/423 (85%)	326 (91%)	33 (9%)	8	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	O	84/110 (76%)	69 (82%)	15 (18%)	2	9
11	S	82/110 (74%)	65 (79%)	17 (21%)	1	6
12	P	72/78 (92%)	62 (86%)	10 (14%)	3	14
12	T	67/78 (86%)	51 (76%)	16 (24%)	1	4
13	Q	81/101 (80%)	69 (85%)	12 (15%)	3	13
13	U	82/101 (81%)	71 (87%)	11 (13%)	4	14
14	R	77/102 (76%)	66 (86%)	11 (14%)	3	13
14	V	79/102 (78%)	62 (78%)	17 (22%)	1	6
All	All	4236/7389 (57%)	3805 (90%)	431 (10%)	9	23

All (431) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	718	ASN
1	B	738	LEU
1	B	747	GLU
1	B	760	LEU
1	B	768	VAL
1	B	792	HIS
1	B	800	PHE
1	B	803	VAL
1	B	882	THR
1	B	900	THR
1	B	926	ARG
1	B	940	ARG
1	B	941	ASN
1	B	950	ASP
1	B	955	VAL
1	B	960	GLU
1	B	970	ASN
1	B	975	LEU
1	B	979	LEU
1	B	981	ASN
1	B	986	LEU
1	B	1029	GLN
1	B	1034	LYS
1	B	1050	GLU
1	B	1051	LYS
1	B	1084	LEU

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Mol	Chain	Res	Type
1	B	1091	LEU
1	B	1105	LEU
1	B	1106	LEU
1	B	1107	ASN
1	B	1113	LEU
1	B	1125	GLN
1	B	1131	LEU
1	B	1133	ILE
1	B	1134	ASP
1	B	1139	VAL
1	B	1154	ILE
1	B	1197	GLU
1	B	1214	ILE
1	B	1258	CYS
1	B	1259	LEU
1	B	1260	ASN
1	B	1265	ILE
1	B	1292	ASP
2	C	368	PHE
2	C	385	GLN
2	C	387	LEU
2	C	408	TRP
2	C	422	THR
2	C	430	VAL
2	C	432	VAL
2	C	451	ASN
2	C	468	ARG
2	C	473	LEU
2	C	478	LEU
2	C	489	GLU
2	C	496	LEU
2	C	505	THR
2	C	531	GLU
2	C	544	ILE
2	C	548	LEU
2	C	581	GLN
2	C	585	LEU
2	C	608	LEU
2	C	620	ILE
2	C	623	ASP
2	C	633	ILE
2	C	635	LEU

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Mol	Chain	Res	Type
2	C	640	ARG
2	C	647	ILE
2	C	649	THR
2	C	652	LEU
2	C	653	LEU
2	C	655	ILE
2	C	663	LEU
2	C	664	ASP
2	C	745	VAL
2	C	750	GLU
2	C	754	LEU
3	D	305	ILE
3	D	311	SER
3	D	325	GLN
3	D	327	LEU
3	D	339	THR
3	D	363	SER
3	D	366	THR
3	D	371	VAL
3	D	372	SER
3	D	417	ASP
3	D	432	VAL
3	D	450	GLU
3	D	453	LEU
3	D	466	GLU
3	D	514	LEU
3	D	517	VAL
3	D	519	ILE
3	D	523	ILE
3	D	525	GLU
3	D	535	LEU
3	D	542	PHE
3	D	563	LEU
3	D	587	ASN
3	D	617	LEU
3	D	635	GLU
3	D	640	GLN
3	D	694	LEU
3	D	695	ASP
3	D	719	GLN
3	D	731	GLN
3	D	735	LYS

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Mol	Chain	Res	Type
3	D	740	LEU
3	D	773	MET
3	D	780	LEU
4	H	64	HIS
4	H	72	LEU
4	H	78	LEU
4	H	118	ASN
4	H	122	VAL
4	H	127	ILE
4	H	130	SER
4	H	134	GLU
4	H	182	ILE
4	H	187	VAL
4	H	266	VAL
4	H	282	ASP
4	H	283	ILE
4	H	317	ILE
4	H	321	LYS
4	H	329	ILE
4	H	332	ILE
4	H	343	THR
4	H	383	THR
4	H	384	GLN
4	H	388	LEU
4	H	389	LEU
4	H	397	SER
4	H	403	LEU
4	H	410	ILE
4	H	413	THR
4	H	415	LEU
4	H	418	LEU
4	H	423	ILE
4	H	426	THR
4	H	427	VAL
4	H	429	VAL
4	H	431	LYS
4	H	434	THR
4	H	439	VAL
4	H	485	LYS
4	H	538	ASP
4	H	561	LEU
5	I	89	GLN

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Mol	Chain	Res	Type
5	I	90	LEU
5	I	97	GLU
5	I	98	SER
5	I	109	LYS
5	I	125	THR
5	I	136	LEU
5	I	140	LYS
6	J	303	VAL
6	J	311	THR
6	J	312	LEU
6	J	448	LEU
6	J	454	LEU
6	J	455	LEU
6	J	458	LEU
6	J	466	ILE
3	E	329	GLU
3	E	339	THR
3	E	360	GLU
3	E	363	SER
3	E	366	THR
3	E	391	ILE
3	E	415	ARG
3	E	417	ASP
3	E	420	ARG
3	E	432	VAL
3	E	445	ASN
3	E	453	LEU
3	E	466	GLU
3	E	516	LYS
3	E	518	LYS
3	E	522	GLN
3	E	530	GLU
3	E	531	ASP
3	E	532	LEU
3	E	556	LYS
3	E	557	SER
3	E	589	LEU
3	E	593	LYS
3	E	602	LYS
3	E	622	THR
3	E	638	LYS
3	E	644	ILE

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Mol	Chain	Res	Type
3	E	689	LEU
3	E	691	MET
3	E	703	LYS
3	E	715	LEU
3	E	716	GLU
3	E	723	LEU
3	E	744	LEU
3	E	746	LEU
3	E	778	GLU
7	A	499	THR
7	A	512	CYS
7	A	516	LEU
7	A	517	LEU
7	A	520	GLU
7	A	527	GLU
7	A	528	ASN
7	A	530	LEU
7	A	545	VAL
7	A	566	ASN
7	A	568	LEU
7	A	569	SER
7	A	571	ILE
7	A	578	ASP
7	A	593	LYS
7	A	606	LYS
7	A	620	GLN
7	A	624	ASN
7	A	628	LYS
7	A	638	THR
7	A	761	ILE
7	A	794	MET
7	A	816	ARG
7	A	820	LEU
7	A	822	ILE
7	A	827	THR
7	A	861	ILE
7	A	868	VAL
7	A	883	LEU
7	A	893	ILE
7	A	908	LEU
7	A	912	THR
7	A	914	TYR

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Mol	Chain	Res	Type
7	A	927	LEU
7	A	929	ASN
7	A	934	LEU
7	A	1011	VAL
7	A	1018	LEU
7	A	1089	PHE
7	A	1096	LEU
7	A	1107	LEU
7	A	1108	ILE
7	A	1114	GLN
7	A	1115	ILE
7	A	1128	ILE
7	A	1131	LEU
7	A	1133	LEU
7	A	1138	LYS
7	A	1145	LEU
7	A	1154	SER
7	A	1170	LEU
7	A	1176	ASP
7	A	1183	THR
7	A	1217	VAL
7	A	1340	SER
8	L	7	ILE
8	L	8	THR
8	L	59	ARG
8	L	80	ASP
9	M	3	LEU
9	M	24	VAL
9	M	49	PHE
9	M	53	ASN
9	M	63	ASN
9	M	65	ASP
9	M	69	THR
9	M	88	ARG
9	M	97	VAL
9	M	98	SER
9	M	106	ILE
9	M	112	ASN
9	M	114	LYS
9	M	120	LEU
9	M	121	GLU
9	M	131	LEU

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Mol	Chain	Res	Type
9	M	195	GLU
9	M	216	ARG
9	M	238	VAL
9	M	299	LEU
9	M	319	ILE
9	M	337	VAL
9	M	393	ILE
9	M	398	THR
9	M	402	GLU
9	M	406	GLN
9	M	463	LEU
10	N	15	ARG
10	N	29	THR
10	N	31	THR
10	N	32	VAL
10	N	34	GLU
10	N	47	GLN
10	N	59	ASP
10	N	68	ILE
10	N	72	GLU
10	N	88	VAL
10	N	90	ILE
10	N	94	ARG
10	N	99	GLN
10	N	106	LEU
10	N	131	VAL
10	N	150	THR
10	N	187	ILE
10	N	197	SER
10	N	201	LEU
10	N	210	ILE
10	N	214	LYS
10	N	221	VAL
10	N	292	ILE
10	N	294	VAL
10	N	302	CYS
10	N	304	ASN
10	N	306	ILE
10	N	339	THR
10	N	398	ILE
10	N	403	CYS
10	N	427	ILE

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Mol	Chain	Res	Type
10	N	446	THR
10	N	449	ILE
11	O	48	LEU
11	O	53	ARG
11	O	58	THR
11	O	63	ARG
11	O	65	LEU
11	O	73	GLU
11	O	76	GLN
11	O	86	SER
11	O	99	TYR
11	O	106	ASP
11	O	115	LYS
11	O	123	ASP
11	O	124	ILE
11	O	126	LEU
11	O	133	GLU
12	P	26	ILE
12	P	34	ILE
12	P	46	ILE
12	P	49	LEU
12	P	53	GLU
12	P	58	LEU
12	P	64	ASN
12	P	67	ARG
12	P	91	LYS
12	P	95	ARG
13	Q	27	VAL
13	Q	34	LEU
13	Q	61	GLU
13	Q	74	LYS
13	Q	76	THR
13	Q	79	ILE
13	Q	94	ASN
13	Q	101	THR
13	Q	104	GLN
13	Q	107	VAL
13	Q	111	ILE
13	Q	114	VAL
14	R	36	ILE
14	R	58	ILE
14	R	65	ASP

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Mol	Chain	Res	Type
14	R	67	PHE
14	R	70	ILE
14	R	76	ARG
14	R	79	HIS
14	R	85	THR
14	R	91	ILE
14	R	112	THR
14	R	115	VAL
11	S	40	ARG
11	S	42	ARG
11	S	46	VAL
11	S	53	ARG
11	S	62	ILE
11	S	64	LYS
11	S	65	LEU
11	S	68	GLN
11	S	70	LEU
11	S	81	ASP
11	S	96	SER
11	S	99	TYR
11	S	101	VAL
11	S	105	GLU
11	S	119	ILE
11	S	123	ASP
11	S	126	LEU
12	T	26	ILE
12	T	46	ILE
12	T	49	LEU
12	T	53	GLU
12	T	54	THR
12	T	55	ARG
12	T	58	LEU
12	T	59	LYS
12	T	63	GLU
12	T	66	ILE
12	T	74	GLU
12	T	79	LYS
12	T	80	THR
12	T	81	VAL
12	T	91	LYS
12	T	92	ARG
13	U	13	LYS

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Mol	Chain	Res	Type
13	U	15	LYS
13	U	29	ARG
13	U	49	VAL
13	U	59	THR
13	U	77	ARG
13	U	92	GLU
13	U	99	ARG
13	U	107	VAL
13	U	110	ASN
13	U	114	VAL
14	V	29	THR
14	V	32	GLU
14	V	36	ILE
14	V	39	TYR
14	V	49	THR
14	V	54	LYS
14	V	60	ASN
14	V	65	ASP
14	V	66	VAL
14	V	76	ARG
14	V	81	ASN
14	V	82	LYS
14	V	88	SER
14	V	91	ILE
14	V	92	GLN
14	V	113	LYS
14	V	115	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	706	ASN
1	B	708	HIS
1	B	737	ASN
1	B	758	ASN
1	B	792	HIS
1	B	873	ASN
1	B	941	ASN
1	B	970	ASN
1	B	984	HIS
1	B	1055	ASN
1	B	1093	ASN

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Mol	Chain	Res	Type
1	B	1107	ASN
1	B	1120	GLN
1	B	1142	GLN
1	B	1188	ASN
1	B	1213	ASN
1	B	1238	ASN
1	B	1274	ASN
1	B	1294	GLN
1	B	1307	ASN
2	C	370	ASN
2	C	385	GLN
2	C	421	ASN
2	C	434	ASN
2	C	567	ASN
2	C	654	GLN
3	D	325	GLN
3	D	416	HIS
3	D	540	GLN
3	D	552	ASN
3	D	560	GLN
3	D	640	GLN
3	D	680	ASN
3	D	690	GLN
3	D	719	GLN
3	D	725	GLN
3	D	731	GLN
3	D	766	GLN
4	H	93	ASN
4	H	167	ASN
4	H	498	ASN
4	H	549	ASN
4	H	563	ASN
5	I	48	ASN
5	I	49	ASN
5	I	71	GLN
5	I	89	GLN
5	I	115	ASN
5	I	119	ASN
6	J	280	GLN
6	J	292	ASN
6	J	327	ASN
3	E	359	ASN

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Mol	Chain	Res	Type
3	E	394	GLN
3	E	445	ASN
3	E	522	GLN
3	E	533	GLN
3	E	555	ASN
3	E	560	GLN
3	E	567	GLN
3	E	628	GLN
3	E	678	GLN
3	E	680	ASN
3	E	690	GLN
3	E	700	HIS
3	E	730	ASN
3	E	732	ASN
3	E	766	GLN
7	A	498	GLN
7	A	504	ASN
7	A	528	ASN
7	A	542	GLN
7	A	555	HIS
7	A	556	GLN
7	A	557	ASN
7	A	562	ASN
7	A	573	ASN
7	A	575	ASN
7	A	584	GLN
7	A	609	ASN
7	A	624	ASN
7	A	637	HIS
7	A	639	ASN
7	A	657	GLN
7	A	681	HIS
7	A	749	HIS
7	A	939	ASN
7	A	1050	ASN
7	A	1071	GLN
7	A	1150	ASN
7	A	1171	ASN
7	A	1284	ASN
8	L	11	ASN
8	L	31	GLN
8	L	67	GLN

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Mol	Chain	Res	Type
9	M	4	ASN
9	M	12	ASN
9	M	28	GLN
9	M	53	ASN
9	M	74	GLN
9	M	79	ASN
9	M	229	GLN
9	M	237	GLN
9	M	253	GLN
9	M	406	GLN
10	N	6	GLN
10	N	17	GLN
10	N	26	ASN
10	N	139	ASN
10	N	167	HIS
10	N	179	GLN
10	N	192	GLN
10	N	304	ASN
11	O	55	GLN
11	O	113	HIS
13	Q	94	ASN
13	Q	110	ASN
13	Q	112	GLN
11	S	85	GLN
11	S	93	GLN
11	S	108	ASN
14	V	79	HIS
14	V	81	ASN
14	V	92	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	ADP	A	1501	19,7	27,29,29	1.38	4 (14%)	42,45,45	1.97	10 (23%)
18	BEF	A	1502	-	0,3,3	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	A	1501	19,7	-	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)
17	A	1501	ADP	C5-C4	4.60	1.47	1.39
17	A	1501	ADP	C5-C6	2.68	1.48	1.41
17	A	1501	ADP	C8-N7	2.39	1.36	1.31
17	A	1501	ADP	C5-N7	-2.27	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1501	ADP	C5-C4-N3	-6.23	118.62	126.75
17	A	1501	ADP	N3-C4-N9	4.94	135.22	127.08
17	A	1501	ADP	C2-N3-C4	3.85	120.86	111.75
17	A	1501	ADP	PA-O3A-PB	-3.33	121.41	132.83
17	A	1501	ADP	C4-C5-N7	-3.23	106.68	110.62
17	A	1501	ADP	N3-C2-N1	-3.09	123.78	128.60
17	A	1501	ADP	C5-N7-C8	2.77	107.44	103.51
17	A	1501	ADP	C4-N9-C8	2.57	108.51	105.73
17	A	1501	ADP	C3'-C2'-C1'	2.42	106.03	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1501	ADP	C6-C5-N7	2.11	135.96	132.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

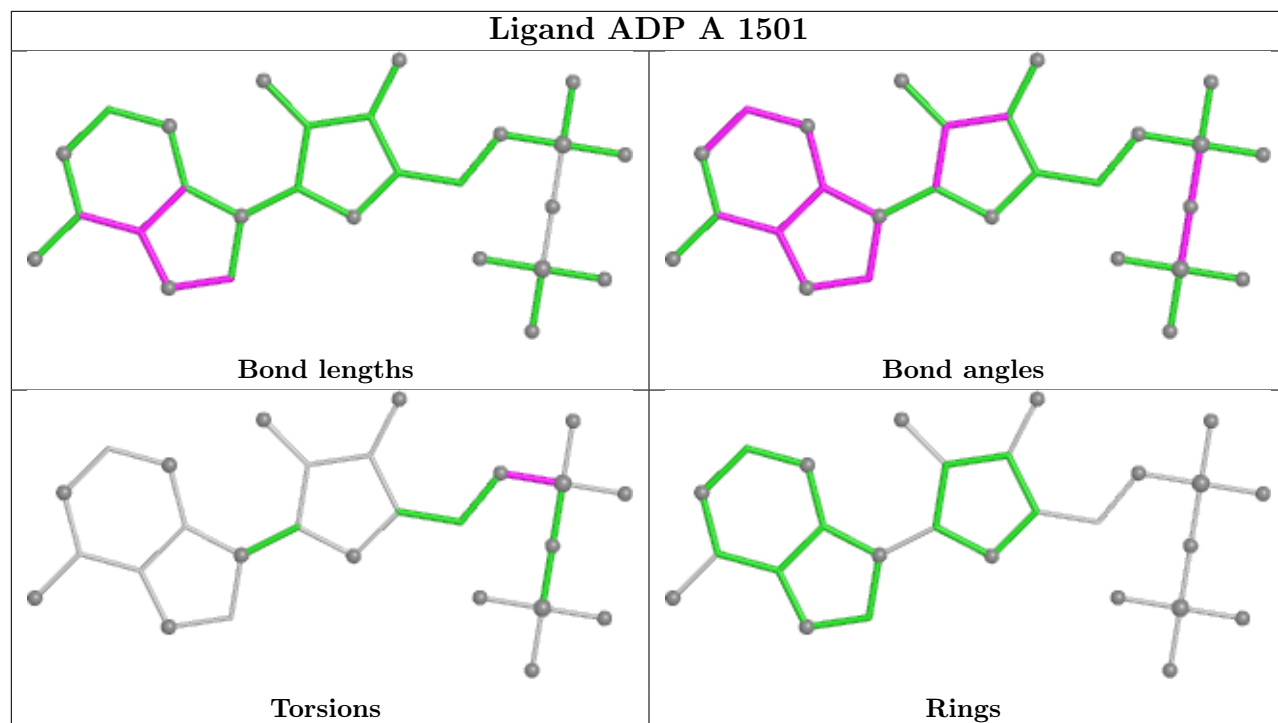
Mol	Chain	Res	Type	Atoms
17	A	1501	ADP	C5'-O5'-PA-O1A

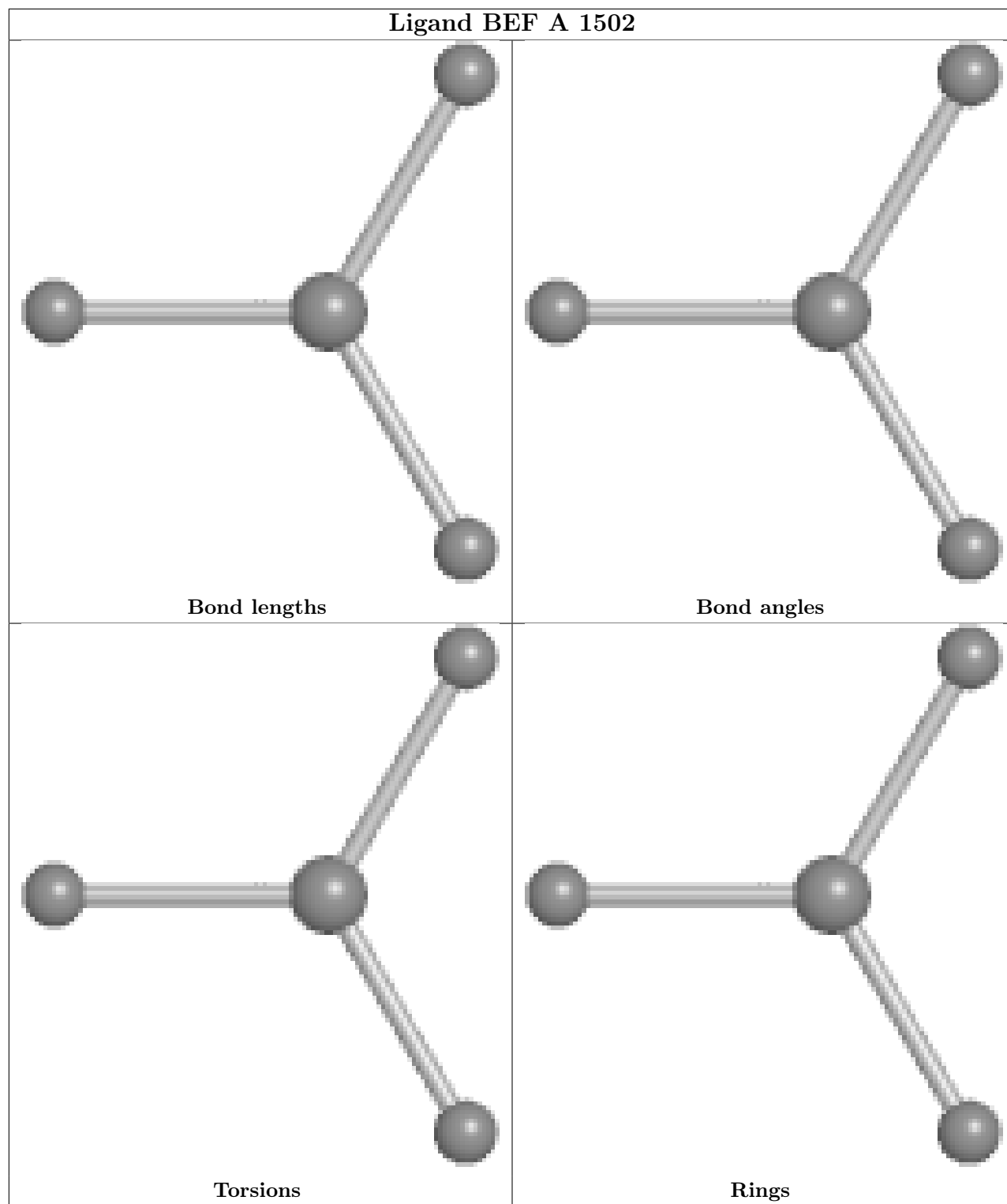
There are no ring outliers.

2 monomers are involved in 30 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

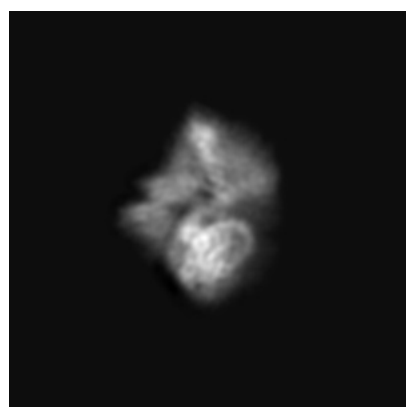
6 Map visualisation [i](#)

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

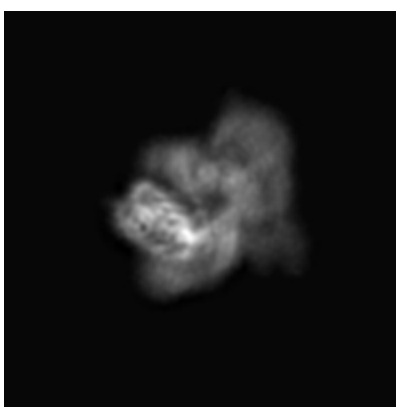
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

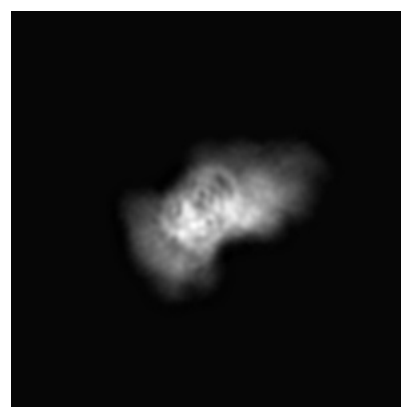
6.1.1 Primary map



X



Y

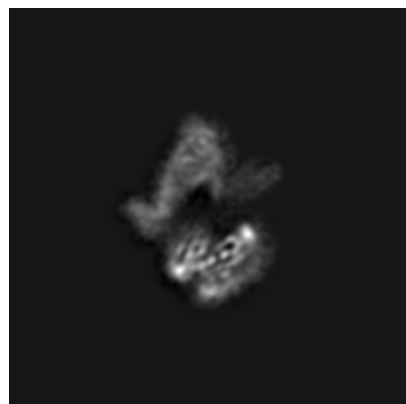


Z

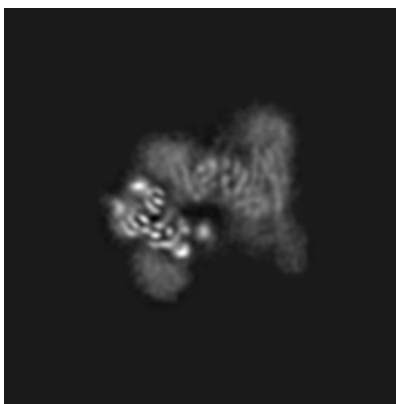
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

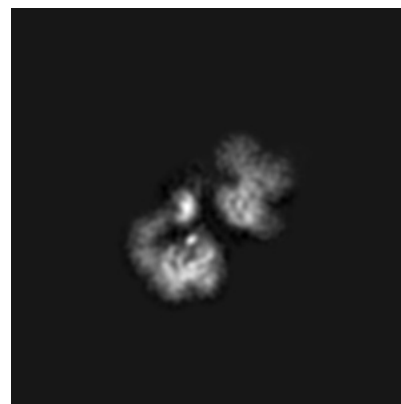
6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

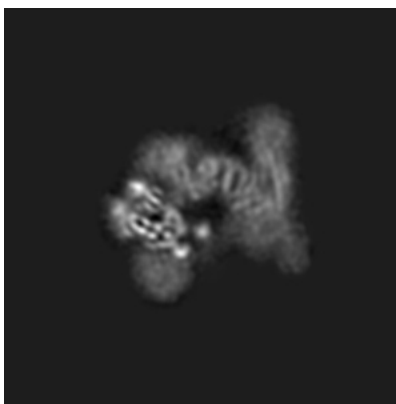
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 87



Y Index: 98

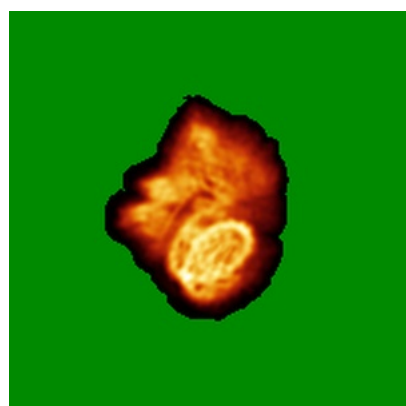


Z Index: 90

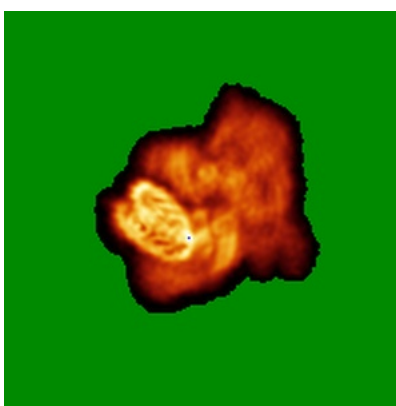
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

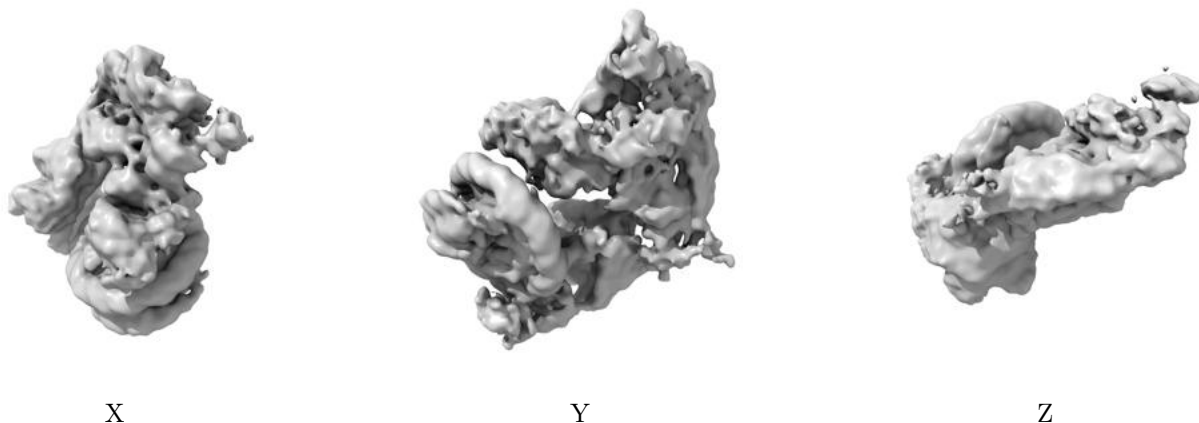


Z

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 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

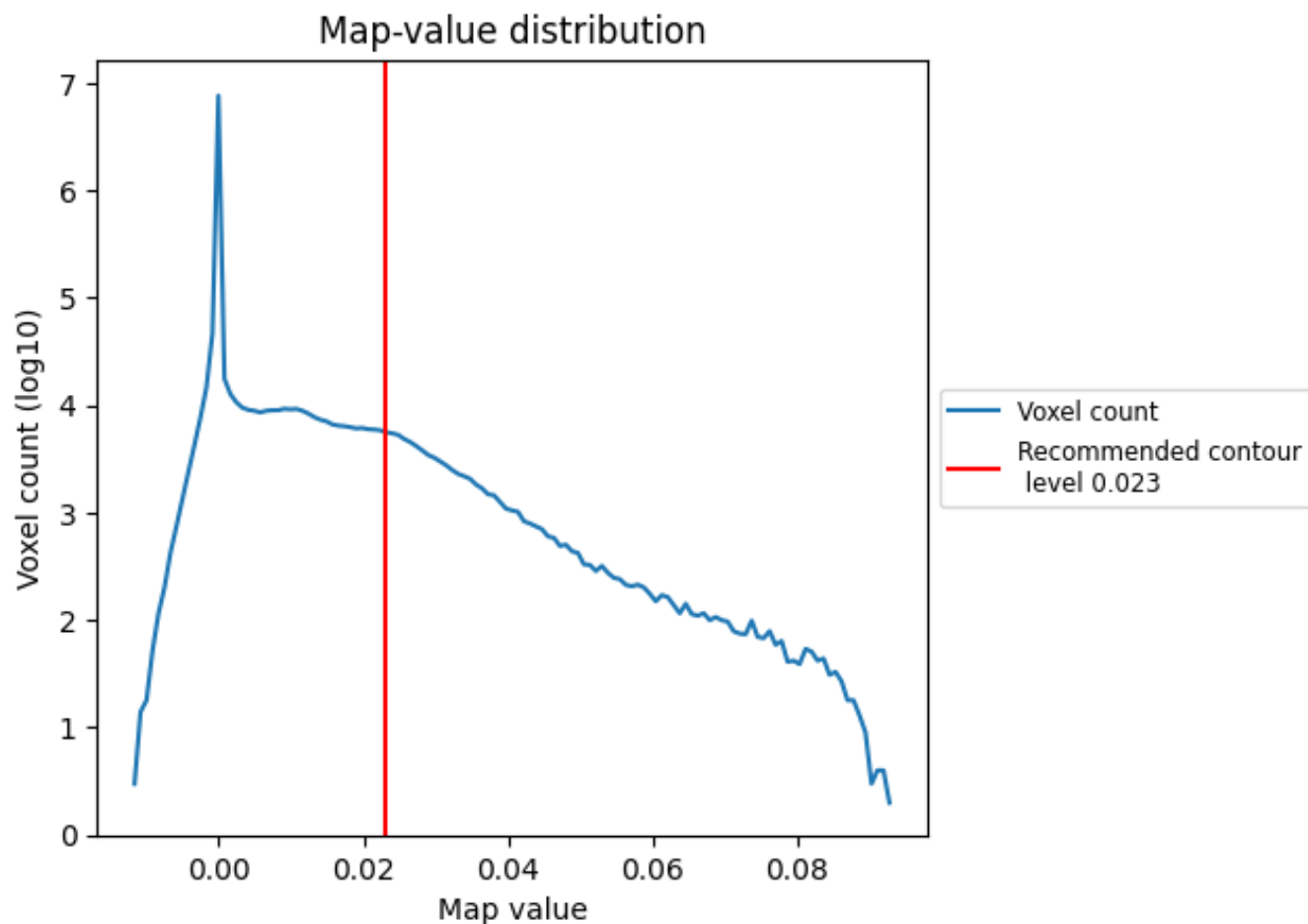
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

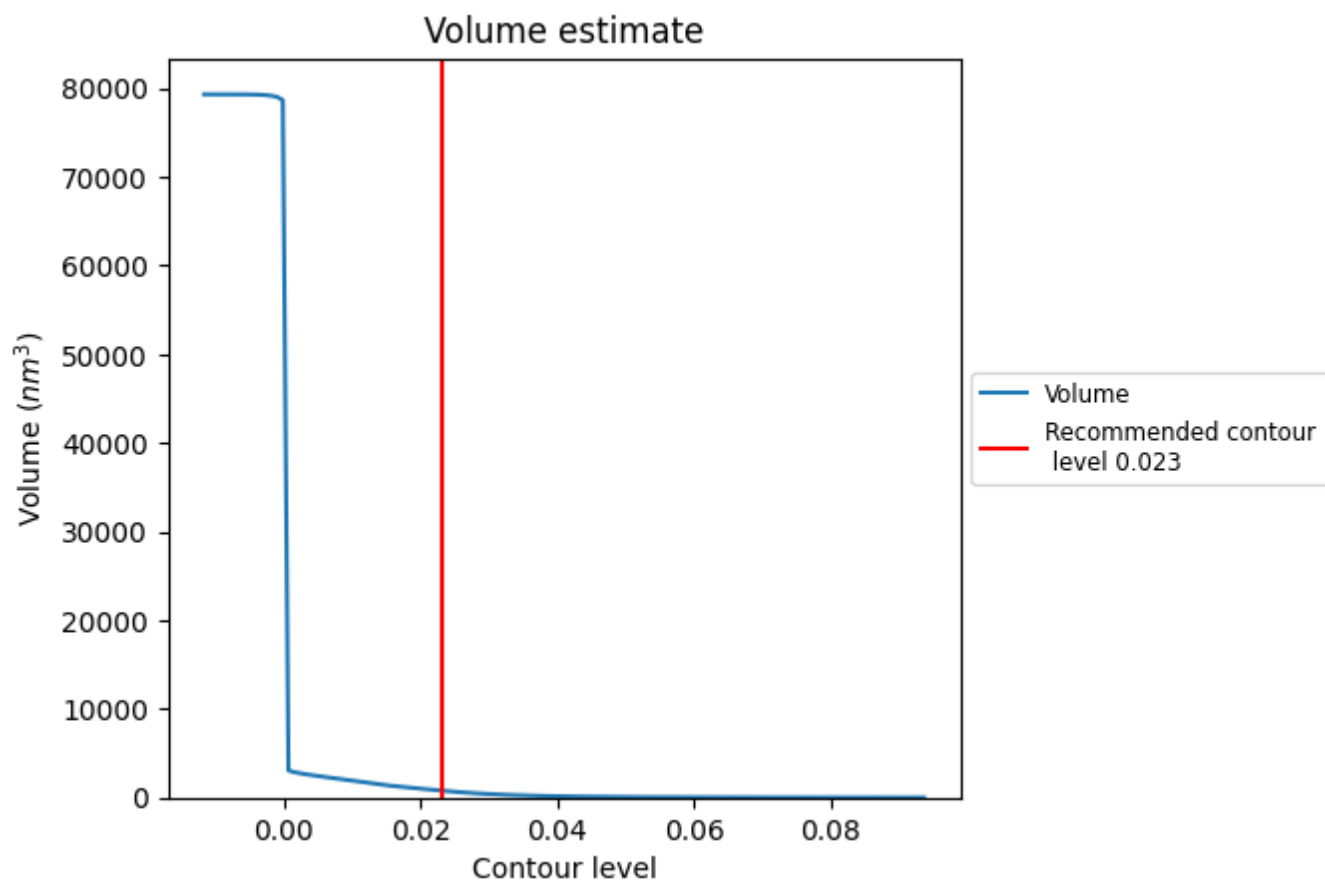
This section contains the results of statistical analysis of the map.

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.

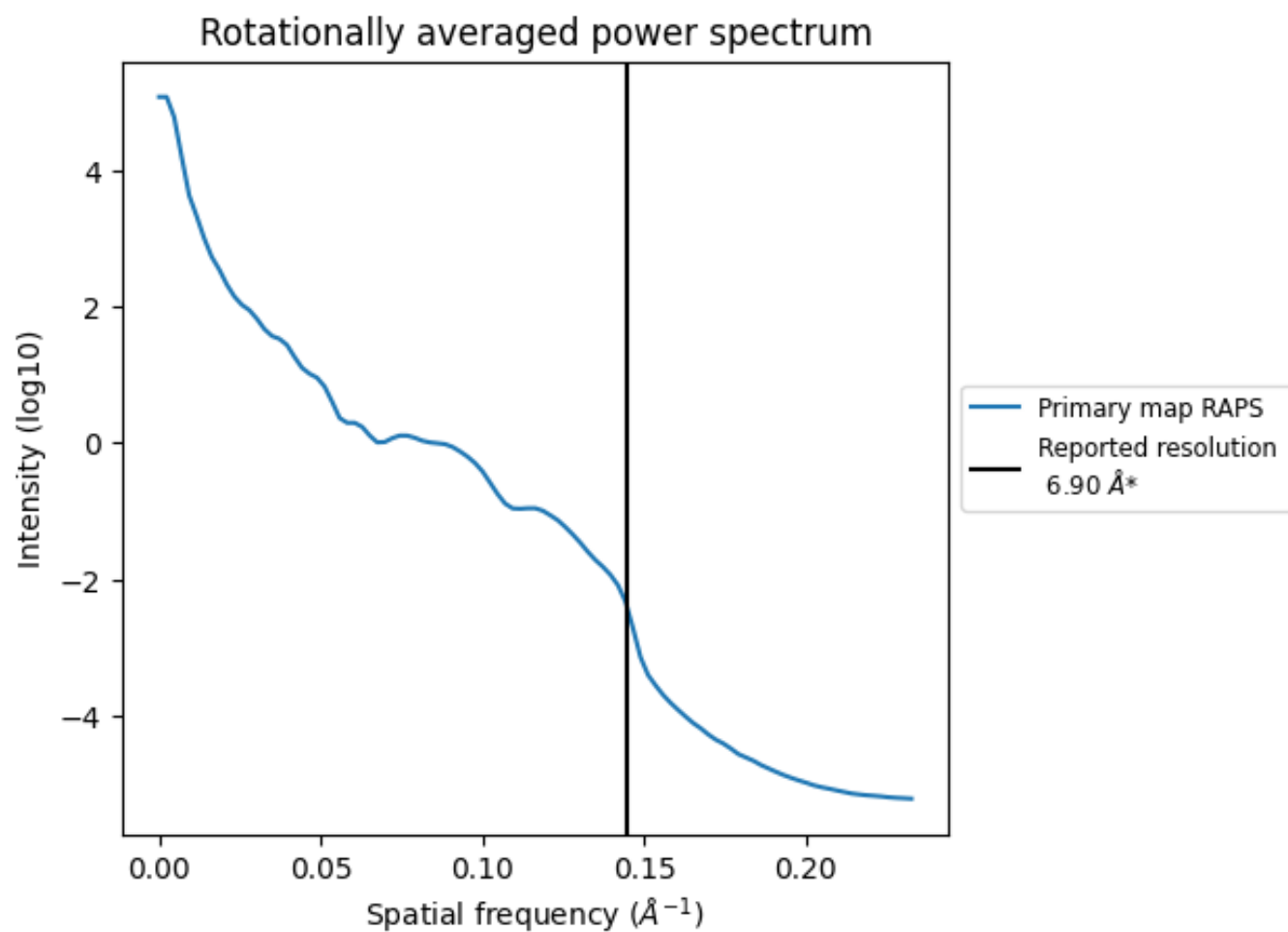
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 786 nm³; this corresponds to an approximate mass of 710 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.145 Å⁻¹

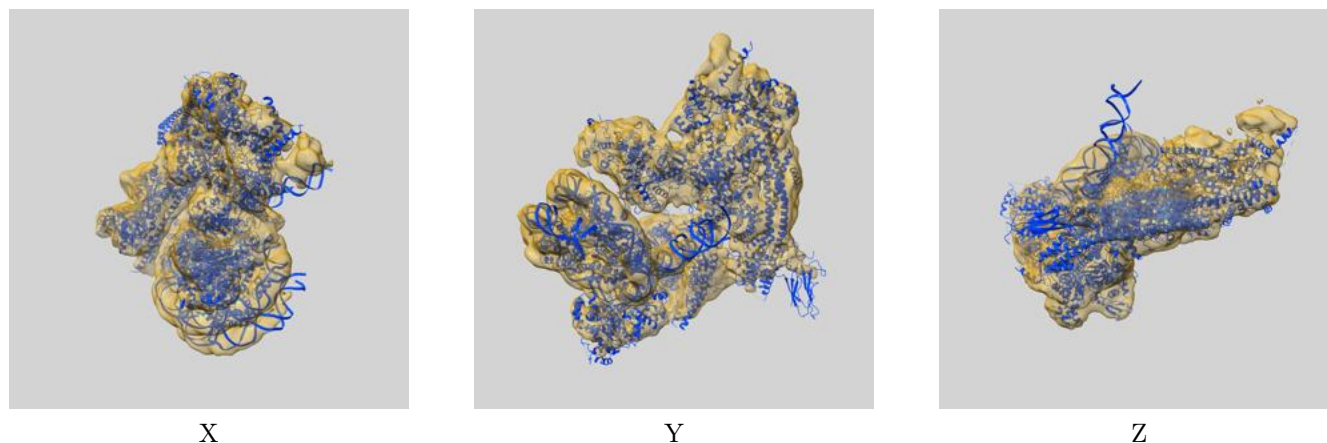
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

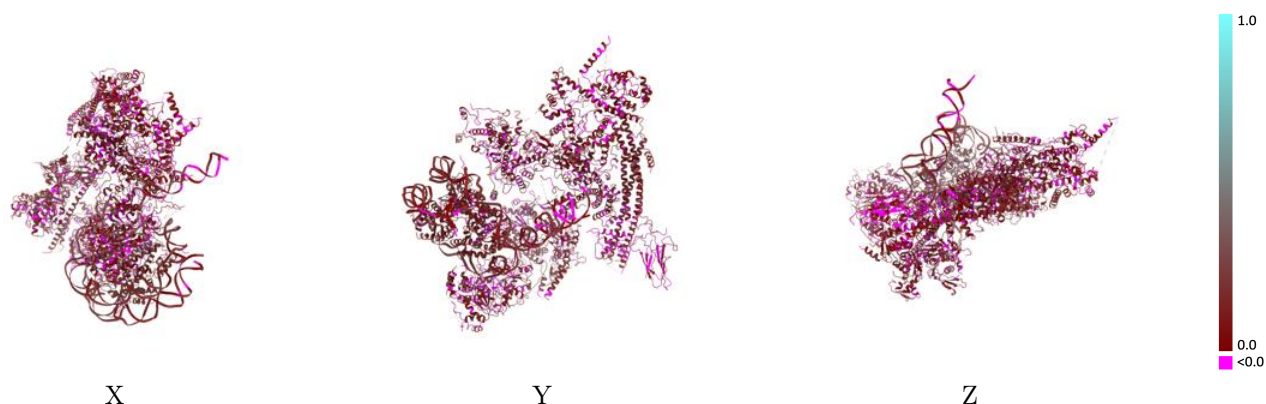
This section contains information regarding the fit between EMDB map EMD-31137 and PDB model 7EGP. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



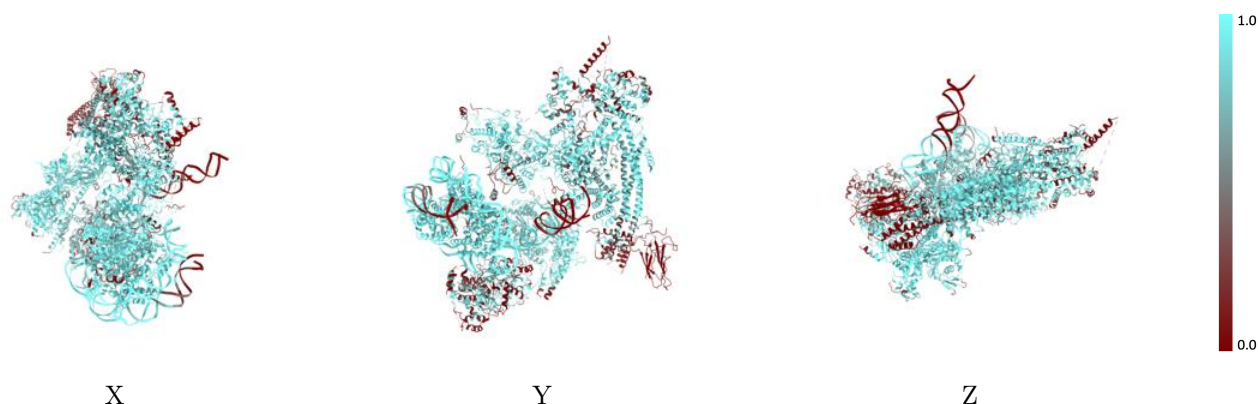
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



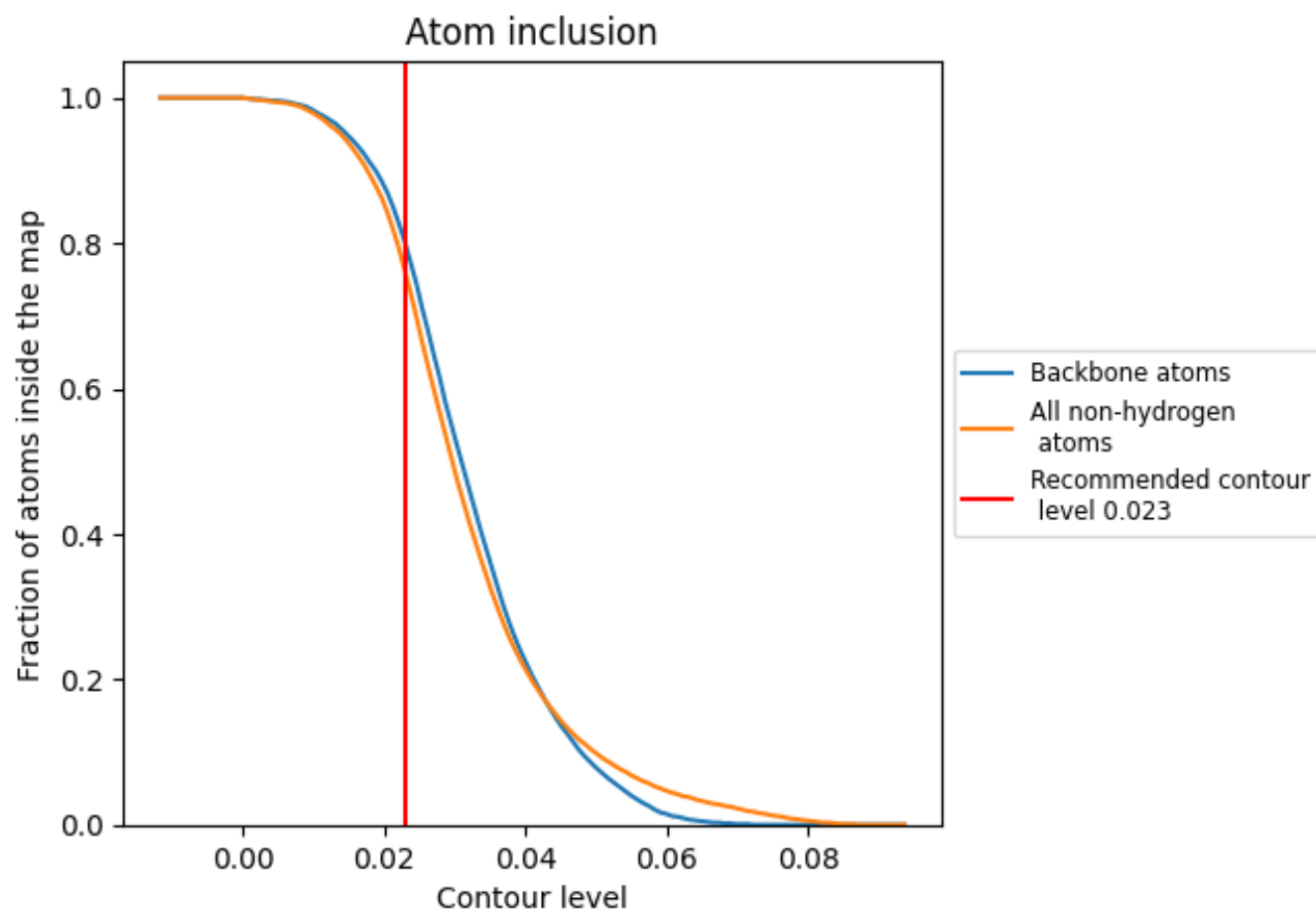
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.7590	 0.1050
A	 0.5670	 0.0840
B	 0.8200	 0.1060
C	 0.8180	 0.1010
D	 0.6600	 0.0800
E	 0.6790	 0.0780
H	 0.4470	 0.0690
I	 0.6480	 0.0950
J	 0.6680	 0.0770
L	 0.8690	 0.0480
M	 0.9660	 0.1100
N	 0.9120	 0.0950
O	 0.9440	 0.1280
P	 0.8870	 0.1410
Q	 0.9500	 0.1460
R	 0.9930	 0.1800
S	 0.9770	 0.1450
T	 0.9170	 0.1440
U	 0.8950	 0.1320
V	 0.9620	 0.1690
W	 0.8090	 0.1400
X	 0.7980	 0.1480

