



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 12:30 PM UTC

PDB ID : 7VDV / pdb_00007vdv
EMDB ID : EMD-31926
Title : The overall structure of human chromatin remodeling PBAF-nucleosome complex
Authors : Chen, Z.C.; Chen, K.J.; Yuan, J.J.
Deposited on : 2021-09-07
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

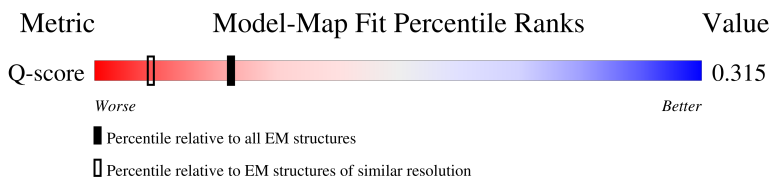
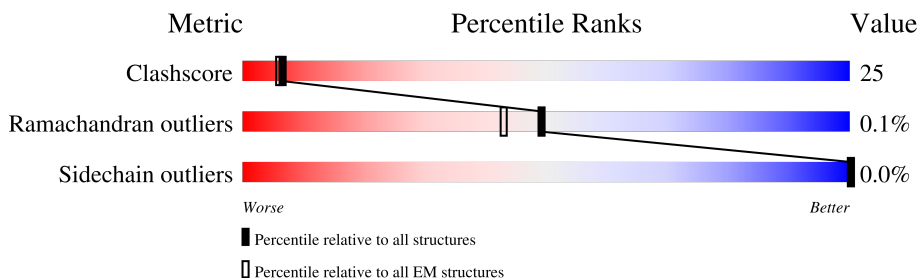
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	103	
1	F	103	
2	C	130	
2	G	130	

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Mol	Chain	Length	Quality of chain
3	D	126	
3	H	126	
4	E	136	
4	K	136	
5	I	207	
6	J	207	
7	A	1485	
8	N	429	
9	P	375	
10	Q	870	
11	R	514	
12	T	652	
13	U	7	
14	V	385	
15	W	1214	
15	X	1214	
16	Y	529	
17	Z	411	
18	a	1020	
19	M	16	

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
20	BEF	A	1701	-	-	X	-
22	ADP	A	1703	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 40028 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H4.

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

- Molecule 2 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	107	Total	C	N	O	0	0
			811	510	158	143		
2	G	108	Total	C	N	O	0	0
			828	522	162	144		

- Molecule 3 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	93	Total	C	N	O	S	0	0
			717	450	128	137	2		
3	H	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 4 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	95	Total	C	N	O	S	0	0
			779	492	148	136	3		
4	K	98	Total	C	N	O	S	0	0
			801	506	153	139	3		

- Molecule 5 is a DNA chain called DNA (207-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	135	Total	C	N	O	P	0	0
			2752	1307	499	811	135		

- Molecule 6 is a DNA chain called DNA (207-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	137	Total	C	N	O	P	0	0
			2827	1337	532	821	137		

- Molecule 7 is a protein called Isoform 2 of Transcription activator BRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	809	Total	C	N	O	S	0	0
			6652	4216	1208	1196	32		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	MET	-	initiating methionine	UNP P51532
A	1615	ALA	-	expression tag	UNP P51532
A	1616	SER	-	expression tag	UNP P51532
A	1617	GLY	-	expression tag	UNP P51532
A	1618	GLY	-	expression tag	UNP P51532
A	1619	SER	-	expression tag	UNP P51532
A	1620	TRP	-	expression tag	UNP P51532
A	1621	SER	-	expression tag	UNP P51532
A	1622	HIS	-	expression tag	UNP P51532
A	1623	PRO	-	expression tag	UNP P51532
A	1624	GLN	-	expression tag	UNP P51532
A	1625	PHE	-	expression tag	UNP P51532
A	1626	GLU	-	expression tag	UNP P51532
A	1627	LYS	-	expression tag	UNP P51532
A	1628	TRP	-	expression tag	UNP P51532
A	1629	SER	-	expression tag	UNP P51532
A	1630	HIS	-	expression tag	UNP P51532
A	1631	PRO	-	expression tag	UNP P51532
A	1632	GLN	-	expression tag	UNP P51532
A	1633	PHE	-	expression tag	UNP P51532
A	1634	GLU	-	expression tag	UNP P51532
A	1635	LYS	-	expression tag	UNP P51532
A	1636	TRP	-	expression tag	UNP P51532
A	1637	SER	-	expression tag	UNP P51532
A	1638	HIS	-	expression tag	UNP P51532

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1639	PRO	-	expression tag	UNP P51532
A	1640	GLN	-	expression tag	UNP P51532
A	1641	PHE	-	expression tag	UNP P51532
A	1642	GLU	-	expression tag	UNP P51532
A	1643	LYS	-	expression tag	UNP P51532

- Molecule 8 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	334	Total	C	N	O	S	0	0
			2612	1656	441	495	20		

- Molecule 9 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	317	Total	C	N	O	S	0	0
			2482	1575	409	480	18		

- Molecule 10 is a protein called AT-rich interactive domain-containing protein 2,AT-rich interactive domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	500	Total	C	N	O	S	0	0
			3981	2540	670	748	23		

- Molecule 11 is a protein called PHD finger protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	92	Total	C	N	O	S	0	0
			771	498	132	140	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-15	MET	-	expression tag	UNP Q8WUB8
R	-14	HIS	-	expression tag	UNP Q8WUB8
R	-13	HIS	-	expression tag	UNP Q8WUB8
R	-12	HIS	-	expression tag	UNP Q8WUB8
R	-11	HIS	-	expression tag	UNP Q8WUB8
R	-10	HIS	-	expression tag	UNP Q8WUB8
R	-9	HIS	-	expression tag	UNP Q8WUB8

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-8	HIS	-	expression tag	UNP Q8WUB8
R	-7	HIS	-	expression tag	UNP Q8WUB8
R	-6	HIS	-	expression tag	UNP Q8WUB8
R	-5	HIS	-	expression tag	UNP Q8WUB8
R	-4	HIS	-	expression tag	UNP Q8WUB8
R	-3	HIS	-	expression tag	UNP Q8WUB8
R	-2	GLY	-	expression tag	UNP Q8WUB8
R	-1	GLU	-	expression tag	UNP Q8WUB8
R	0	PHE	-	expression tag	UNP Q8WUB8

- Molecule 12 is a protein called Isoform 2 of Bromodomain-containing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	267	Total	C	N	O	S	3	0
			2166	1368	367	416	15		

- Molecule 13 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	U	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 14 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	238	Total	C	N	O	S	0	0
			1910	1191	336	370	13		

- Molecule 15 is a protein called SWI/SNF complex subunit SMARCC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	248	Total	C	N	O	S	0	0
			2056	1305	362	379	10		
15	X	252	Total	C	N	O	S	0	0
			2072	1320	363	378	11		

- Molecule 16 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	245	Total	C	N	O	S	0	0
			2057	1308	368	370	11		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	516	ALA	-	expression tag	UNP Q96GM5
Y	517	SER	-	expression tag	UNP Q96GM5
Y	518	HIS	-	expression tag	UNP Q96GM5
Y	519	HIS	-	expression tag	UNP Q96GM5
Y	520	HIS	-	expression tag	UNP Q96GM5
Y	521	HIS	-	expression tag	UNP Q96GM5
Y	522	HIS	-	expression tag	UNP Q96GM5
Y	523	HIS	-	expression tag	UNP Q96GM5
Y	524	HIS	-	expression tag	UNP Q96GM5
Y	525	HIS	-	expression tag	UNP Q96GM5
Y	526	HIS	-	expression tag	UNP Q96GM5
Y	527	HIS	-	expression tag	UNP Q96GM5
Y	528	HIS	-	expression tag	UNP Q96GM5
Y	529	HIS	-	expression tag	UNP Q96GM5

- Molecule 17 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	92	Total	C	N	O	S	0	0
			757	469	147	137	4		

- Molecule 18 is a protein called Protein polybromo-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	92	Total	C	N	O	S	0	0
			750	471	141	135	3		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	670	MET	-	initiating methionine	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86

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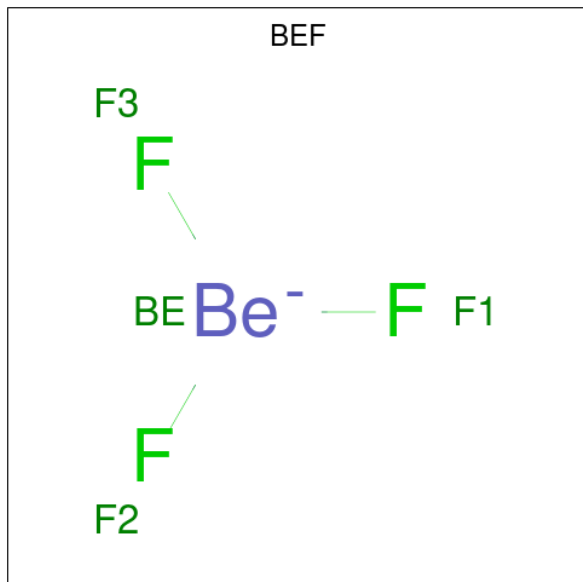
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Chain	Residue	Modelled	Actual	Comment	Reference
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	SER	deletion	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	SER	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	ARG	deletion	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	GLY	deletion	UNP Q86U86
a	?	-	THR	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	VAL	deletion	UNP Q86U86
a	?	-	GLY	deletion	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	LEU	deletion	UNP Q86U86
a	?	-	MET	deletion	UNP Q86U86
a	?	-	GLY	deletion	UNP Q86U86
a	?	-	VAL	deletion	UNP Q86U86
a	?	-	VAL	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	THR	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	MET	deletion	UNP Q86U86
a	?	-	GLY	deletion	UNP Q86U86
a	?	-	MET	deletion	UNP Q86U86
a	?	-	LEU	deletion	UNP Q86U86
a	?	-	ASN	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	LEU	deletion	UNP Q86U86
a	?	-	THR	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	VAL	deletion	UNP Q86U86

- Molecule 19 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	M	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 20 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).

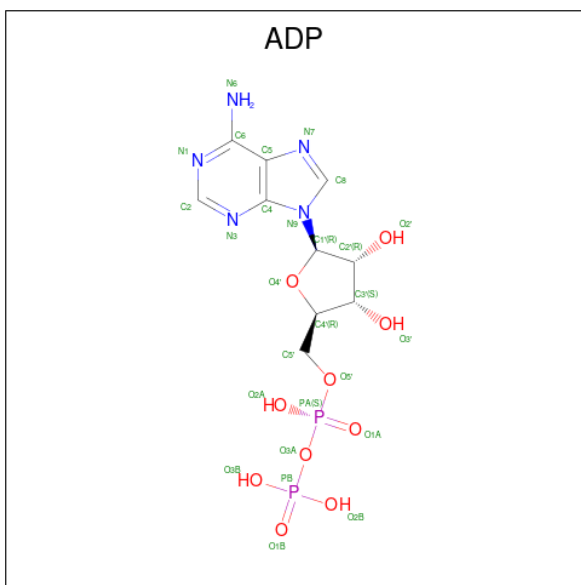


Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	Be	F	0
			4	1	3	

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

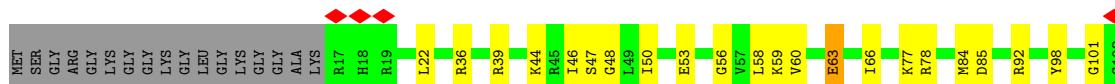
3 Residue-property plots

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

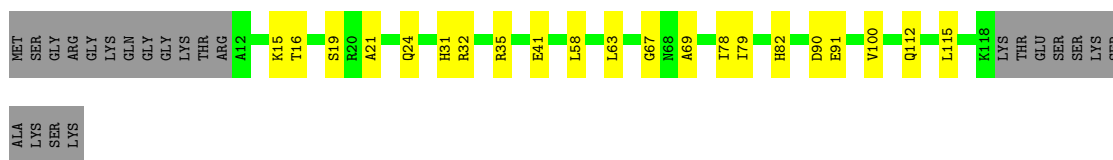
- Molecule 1: Histone H4



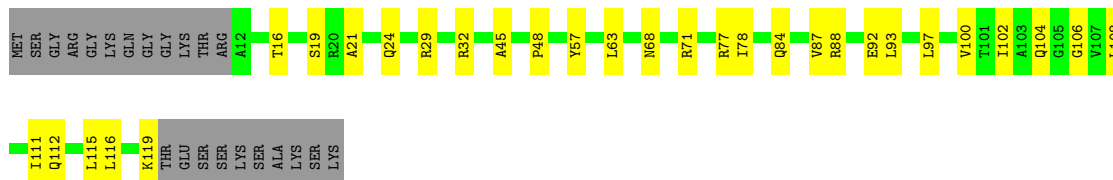
- Molecule 1: Histone H4



- Molecule 2: Histone H2A

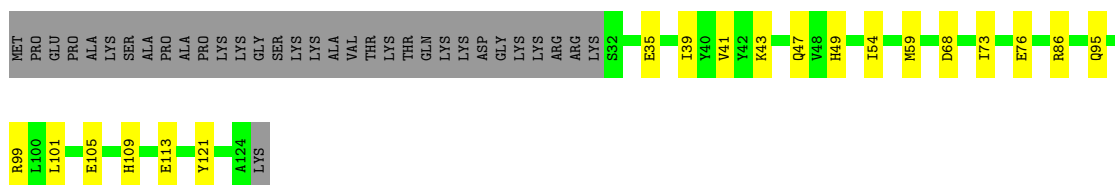


- Molecule 2: Histone H2A



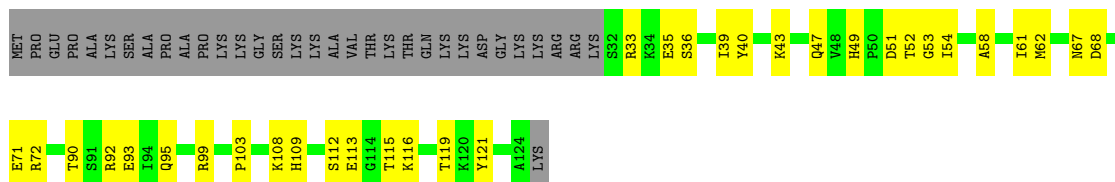
- Molecule 3: Histone H2B 1.1





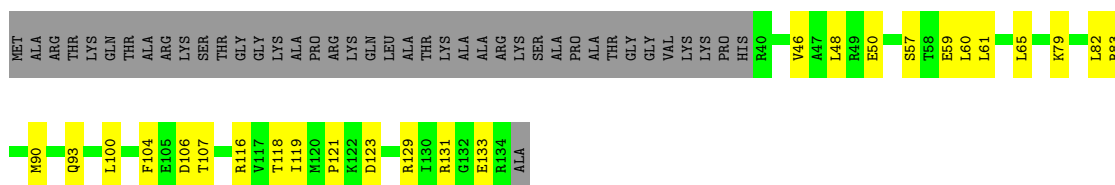
• Molecule 3: Histone H2B 1.1

Chain H: 48% 26% 26%



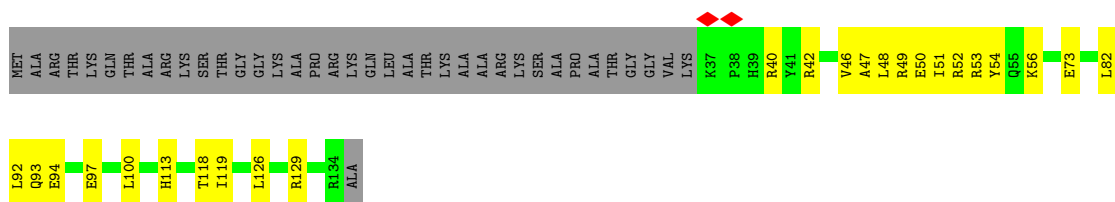
• Molecule 4: Histone H3

Chain E: 51% 18% 30%



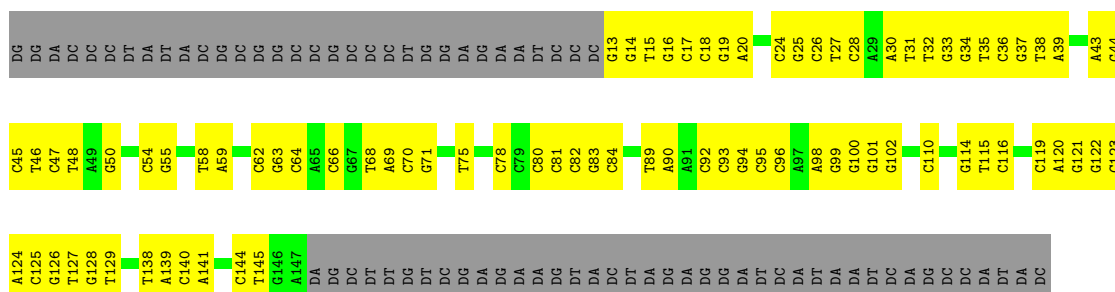
• Molecule 4: Histone H3

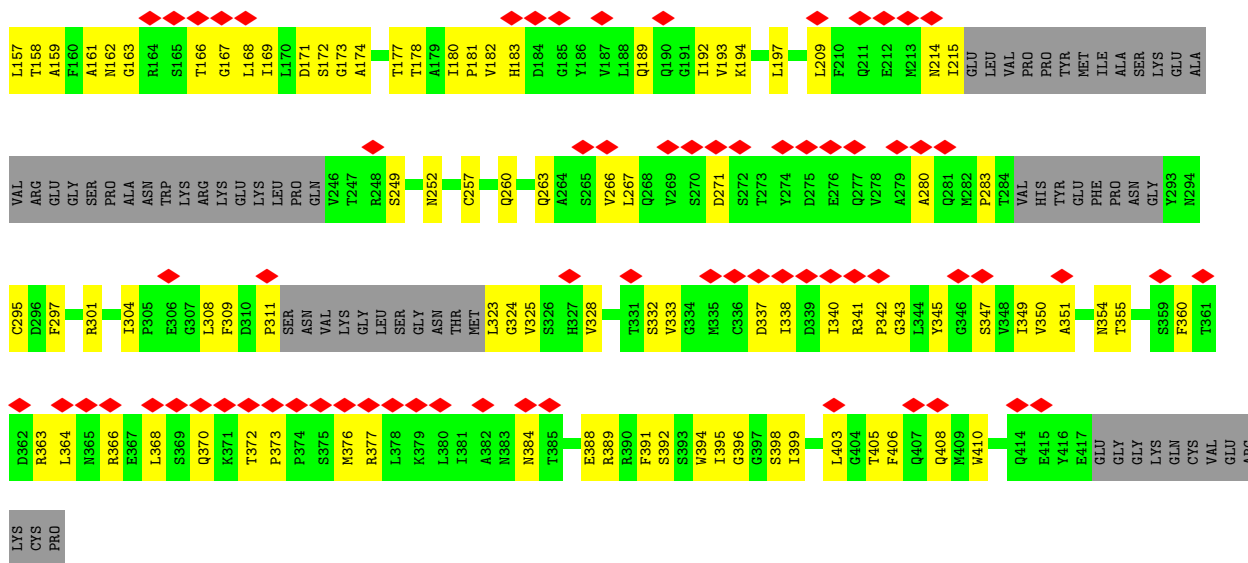
Chain K: 54% 18% 28%



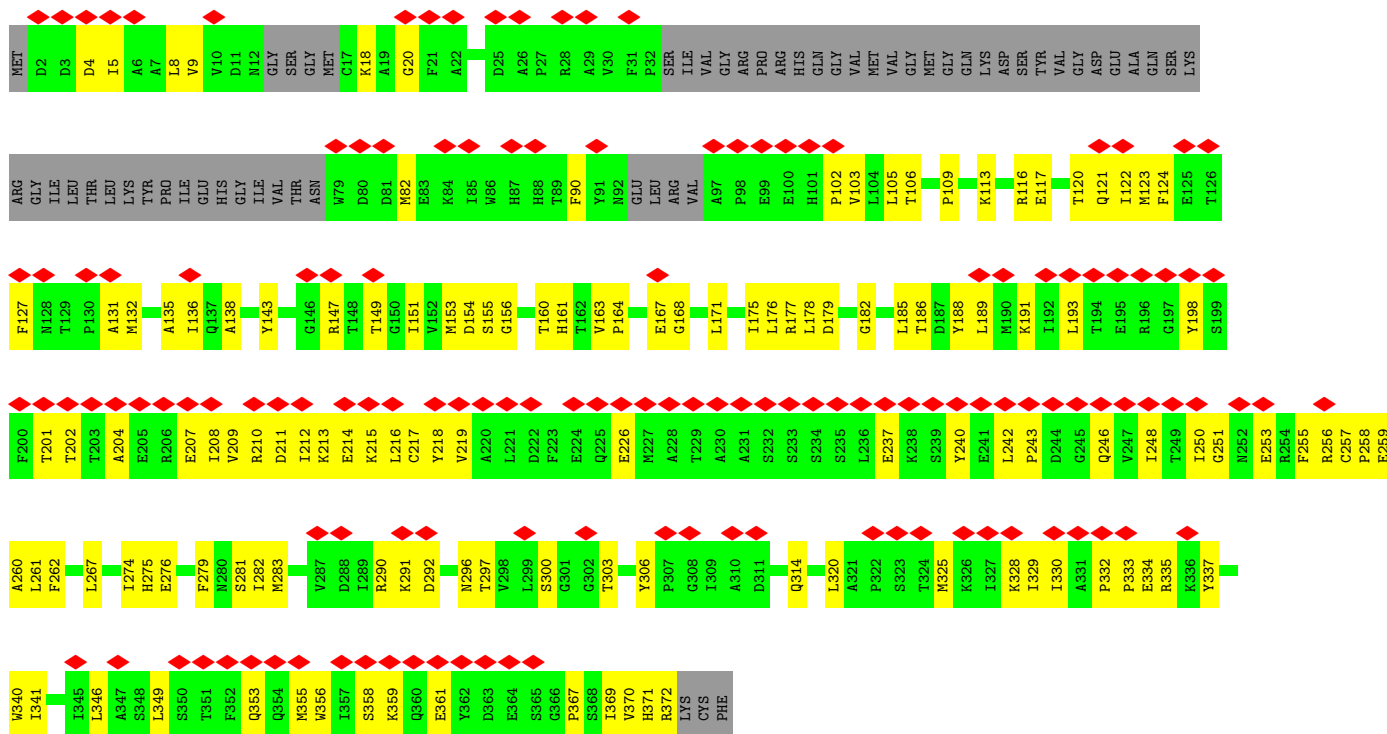
• Molecule 5: DNA (207-MER)

Chain I: 26% 40% 35%

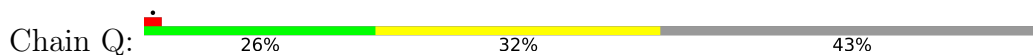




• Molecule 9: Actin, cytoplasmic 1

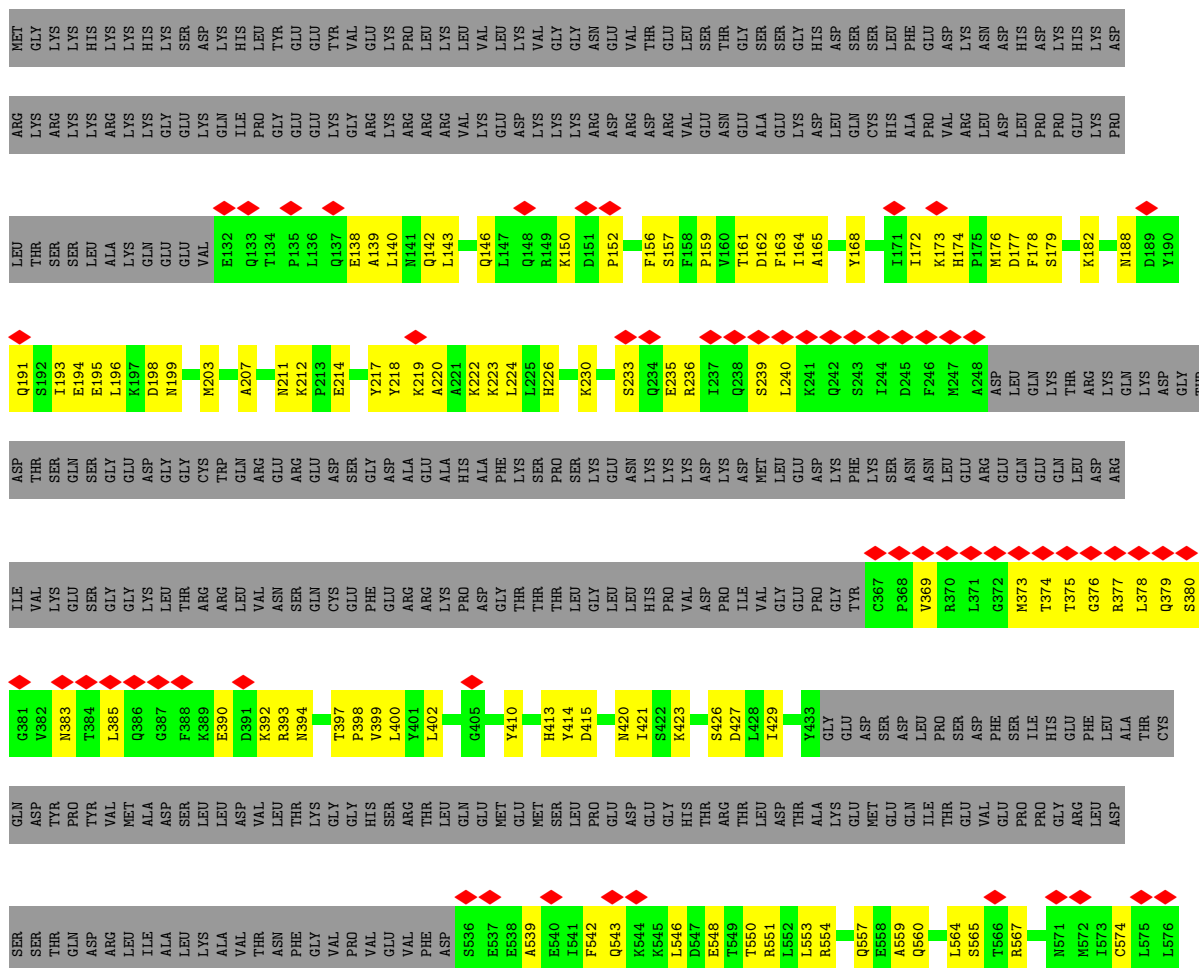


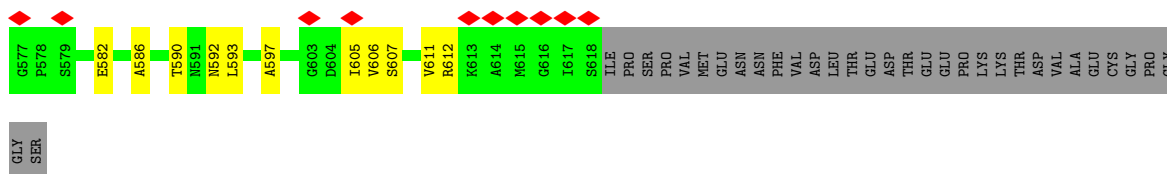
• Molecule 10: AT-rich interactive domain-containing protein 2, AT-rich interactive domain-containing protein 2



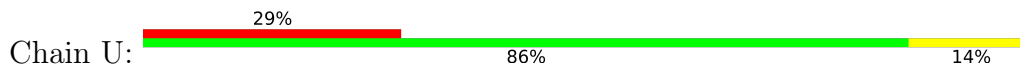


- Molecule 12: Isoform 2 of Bromodomain-containing protein 7

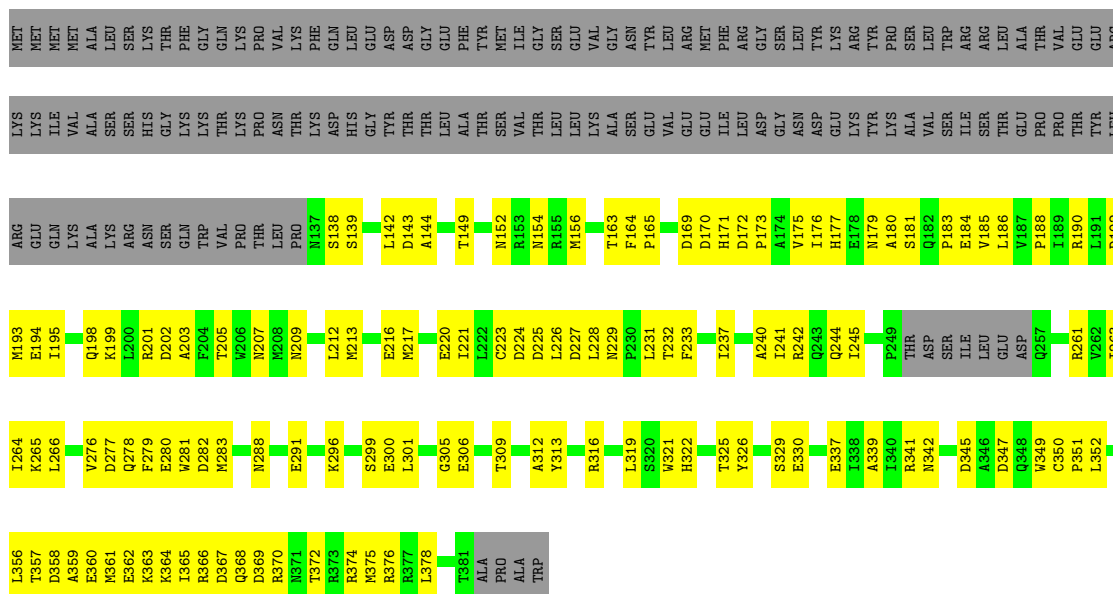
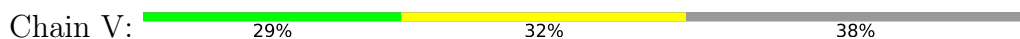




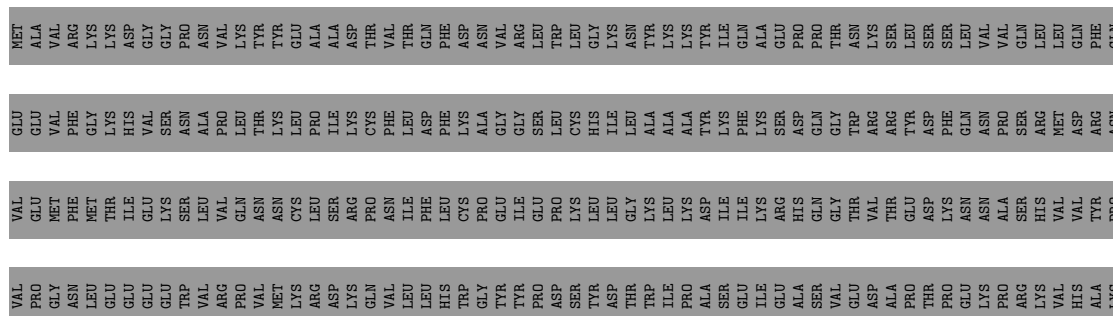
- Molecule 13: unknown



- Molecule 14: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



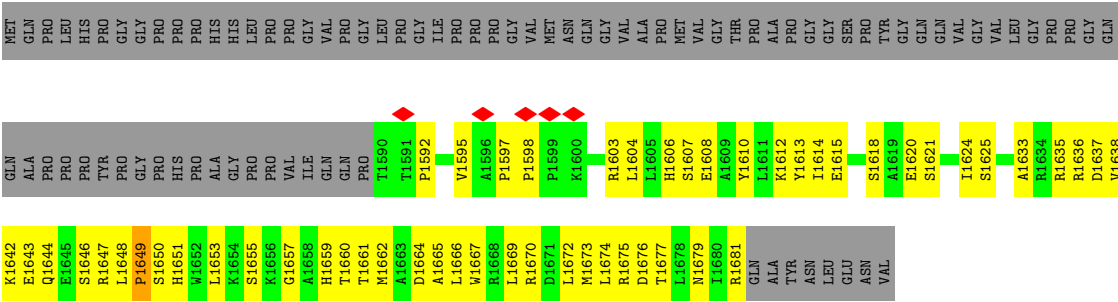
- Molecule 15: SWI/SNF complex subunit SMARCC2



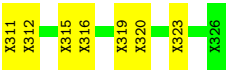








● Molecule 19: unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137659	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	0.056	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0062	Depositor
Map size ($\text{\AA}$)	389.69998, 389.69998, 389.69998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, 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	0.81	0/711	0.71	0/950
1	F	0.77	0/680	0.79	2/912 (0.2%)
2	C	0.66	0/821	0.56	0/1112
2	G	0.65	0/838	0.59	0/1131
3	D	0.73	0/728	0.63	0/983
3	H	0.73	0/736	0.68	0/991
4	E	0.72	0/789	0.67	0/1059
4	K	0.75	0/813	0.60	0/1093
5	I	0.59	0/3083	0.47	0/4752
6	J	0.59	0/3175	0.46	0/4903
7	A	0.30	0/6771	0.54	0/9102
8	N	0.19	0/2667	0.43	0/3615
9	P	0.16	0/2535	0.42	0/3436
10	Q	0.33	0/4051	0.53	0/5466
11	R	0.36	0/792	0.56	0/1072
12	T	0.20	0/2210	0.48	0/2977
14	V	0.43	0/1947	0.54	0/2638
15	W	0.38	0/2097	0.50	0/2831
15	X	0.26	0/2120	0.50	0/2869
16	Y	0.22	0/2097	0.44	0/2822
17	Z	0.24	0/765	0.50	0/1021
18	a	0.29	0/767	0.65	0/1037
All	All	0.44	0/41193	0.52	2/56772 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	GLU	N-CA-CB	6.07	119.04	110.12
1	F	63	GLU	CB-CA-C	-5.43	101.78	110.79

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	703	0	757	22	0
1	F	672	0	698	21	0
2	C	811	0	849	19	0
2	G	828	0	884	30	0
3	D	717	0	723	20	0
3	H	725	0	745	30	0
4	E	779	0	815	22	0
4	K	801	0	831	28	0
5	I	2752	0	1516	116	0
6	J	2827	0	1537	123	0
7	A	6652	0	6786	390	0
8	N	2612	0	2557	111	0
9	P	2482	0	2432	101	0
10	Q	3981	0	4002	259	0
11	R	771	0	774	77	0
12	T	2166	0	2163	99	0
13	U	35	0	10	2	0
14	V	1910	0	1860	129	0
15	W	2056	0	2028	119	0
15	X	2072	0	2052	160	0
16	Y	2057	0	2088	109	0
17	Z	757	0	786	50	0
18	a	750	0	761	57	0
19	M	80	0	18	4	0
20	A	4	0	0	3	0
21	A	1	0	0	0	0
22	A	27	0	12	11	0
All	All	40028	0	37684	1807	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 25.

All (1807) 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)
12:T:377:ARG:C	12:T:378:LEU:HD23	1.31	1.49
12:T:377:ARG:O	12:T:378:LEU:HD23	1.10	1.25
12:T:377:ARG:O	12:T:378:LEU:CD2	1.96	1.13
12:T:377:ARG:C	12:T:378:LEU:CD2	2.23	1.11
7:A:426:ARG:HA	11:R:262:PHE:HE1	1.27	0.98
7:A:1083:GLU:HB3	7:A:1301:LYS:HE3	1.42	0.98
5:I:99:DG:H1	6:J:49:DC:H42	1.11	0.97
14:V:357:THR:OG1	14:V:360:GLU:OE1	1.86	0.92
7:A:1076:TYR:HE1	7:A:1301:LYS:NZ	1.67	0.92
7:A:756:GLN:HE22	7:A:760:LYS:HE3	1.35	0.91
11:R:229:GLN:NE2	14:V:306:GLU:OE2	2.03	0.91
10:Q:1805:MET:HG3	10:Q:1806:GLU:H	1.37	0.89
7:A:1076:TYR:HE1	7:A:1301:LYS:HZ1	0.91	0.88
7:A:483:ALA:HB1	8:N:399:ILE:HG13	1.53	0.87
5:I:92:DC:H42	6:J:56:DG:H1	1.22	0.86
12:T:157:SER:HA	12:T:178:PHE:HB2	1.57	0.86
4:E:79:LYS:HB3	4:E:82:LEU:HD21	1.56	0.85
10:Q:407:LEU:HD12	10:Q:449:LEU:HD21	1.59	0.85
8:N:124:GLU:OE2	8:N:128:ASN:ND2	2.09	0.85
9:P:105:LEU:HD21	9:P:123:MET:HE1	1.57	0.84
9:P:120:THR:HG21	9:P:370:VAL:HG11	1.59	0.84
18:a:1653:LEU:HB2	18:a:1662:MET:HE3	1.58	0.83
10:Q:43:LYS:HG2	10:Q:77:ASN:HD22	1.43	0.83
5:I:78:DC:N3	6:J:70:DG:N1	2.27	0.82
15:W:901:ILE:HA	15:W:904:ARG:HE	1.41	0.82
5:I:32:DT:O4	6:J:116:DA:N6	2.11	0.82
7:A:969:HIS:HD2	7:A:1232:GLY:HA2	1.43	0.82
7:A:1076:TYR:CE1	7:A:1301:LYS:NZ	2.46	0.81
7:A:437:LYS:HE3	18:a:1603:ARG:HH22	1.43	0.81
15:X:616:TYR:HE2	15:X:619:ASP:H	1.28	0.81
7:A:1087:ARG:HE	7:A:1301:LYS:HE2	1.46	0.81
14:V:179:ASN:HD22	14:V:212:LEU:HD23	1.45	0.81
17:Z:201:ARG:HG3	17:Z:202:LEU:HD12	1.63	0.80
10:Q:242:ASP:OD1	10:Q:323:HIS:NE2	2.12	0.80
7:A:549:ARG:NH1	7:A:971:VAL:O	2.14	0.80
11:R:276:TYR:OH	12:T:159:PRO:O	1.99	0.80
7:A:1127:ASP:OD1	7:A:1128:GLY:N	2.14	0.80
5:I:125:DC:N3	6:J:23:DG:N1	2.29	0.79
5:I:58:DT:O4	6:J:90:DA:N6	2.13	0.79
1:B:98:TYR:OH	3:H:68:ASP:OD1	1.99	0.79
5:I:115:DT:O4	6:J:33:DA:N6	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:260:ALA:HB1	9:P:267:LEU:HB2	1.64	0.79
12:T:392:LYS:HB3	12:T:393:ARG:HH11	1.48	0.79
16:Y:476:GLU:OE1	16:Y:482:TYR:OH	2.00	0.79
18:a:1662:MET:HE2	18:a:1666:LEU:HD21	1.65	0.79
18:a:1661:THR:HG23	18:a:1664:ASP:H	1.48	0.78
10:Q:1792:ARG:HG3	15:X:918:GLU:HG2	1.64	0.78
11:R:275:ARG:HG2	11:R:283:LEU:HD12	1.65	0.78
10:Q:1769:ARG:NH1	10:Q:1805:MET:SD	2.56	0.78
7:A:197:PRO:HG3	15:W:651:ASP:HA	1.66	0.78
4:K:50:GLU:O	4:K:54:TYR:N	2.17	0.78
11:R:220:GLU:HG3	11:R:221:GLU:OE1	1.84	0.78
11:R:270:SER:OG	11:R:272:ASP:OD1	2.02	0.77
5:I:127:DT:N3	6:J:21:DA:N1	2.32	0.77
7:A:1003:LEU:HB3	7:A:1303:ARG:HH11	1.49	0.77
12:T:548:GLU:OE1	12:T:592:ASN:ND2	2.18	0.77
5:I:116:DC:N3	6:J:32:DG:N1	2.33	0.77
8:N:166:THR:HA	8:N:183:HIS:HA	1.67	0.77
10:Q:321:HIS:HE2	10:Q:358:THR:HG1	1.26	0.77
7:A:1083:GLU:CB	7:A:1301:LYS:HE3	2.15	0.77
7:A:757:TYR:O	7:A:979:ARG:NH1	2.19	0.76
10:Q:80:ARG:HB2	11:R:223:ARG:HH22	1.50	0.76
10:Q:82:CYS:HB3	10:Q:85:ALA:HB2	1.67	0.76
5:I:34:DG:H1	6:J:114:DC:H42	1.34	0.76
5:I:99:DG:N2	6:J:49:DC:N3	2.34	0.76
12:T:564:LEU:HA	12:T:567:ARG:HH21	1.50	0.76
16:Y:137:ILE:HD13	16:Y:438:ARG:HH22	1.50	0.76
5:I:116:DC:N4	6:J:32:DG:O6	2.18	0.76
5:I:69:DA:N6	6:J:79:DT:O4	2.19	0.75
15:X:925:GLN:NE2	16:Y:321:GLN:OE1	2.18	0.75
7:A:544:GLN:O	7:A:548:LYS:NZ	2.19	0.75
3:D:109:HIS:HD2	7:A:1335:GLY:HA2	1.51	0.75
5:I:127:DT:O4	6:J:21:DA:N6	2.20	0.75
7:A:412:PHE:HA	18:a:1597:PRO:HB3	1.69	0.74
11:R:216:ARG:NH2	11:R:220:GLU:OE2	2.20	0.74
15:X:474:ARG:HA	15:X:477:PRO:HG3	1.69	0.74
7:A:1192:ARG:NH2	20:A:1701:BEF:F1	2.10	0.74
15:X:469:MET:HE1	15:X:501:HIS:HA	1.70	0.74
7:A:451:ARG:NH1	10:Q:1806:GLU:O	2.19	0.74
10:Q:404:ILE:HA	10:Q:407:LEU:HD23	1.68	0.74
17:Z:264:ASP:O	17:Z:268:ASN:ND2	2.21	0.74
11:R:211:ASN:HD21	15:X:481:LEU:HA	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:244:PRO:HG2	11:R:247:ARG:HG3	1.71	0.73
7:A:934:LYS:NZ	7:A:940:GLU:O	2.21	0.73
15:W:451:ASN:HB3	15:W:453:LYS:HG2	1.71	0.73
9:P:213:LYS:NZ	9:P:257:CYS:SG	2.61	0.73
10:Q:1784:GLU:HA	10:Q:1787:ARG:HE	1.54	0.73
10:Q:1761:GLU:OE1	10:Q:1769:ARG:NH2	2.22	0.73
8:N:18:ILE:HG22	8:N:88:LEU:HD11	1.70	0.73
16:Y:133:LEU:HD12	16:Y:134:PRO:HD2	1.71	0.73
7:A:785:LYS:N	22:A:1703:ADP:O3A	2.21	0.73
9:P:160:THR:OG1	9:P:178:LEU:O	2.07	0.72
10:Q:1790:LEU:HD23	10:Q:1818:LEU:HD13	1.71	0.72
11:R:222:ARG:NE	14:V:301:LEU:O	2.17	0.72
8:N:12:GLY:O	8:N:118:HIS:ND1	2.23	0.72
8:N:17:ASP:OD2	8:N:24:ARG:NH1	2.22	0.72
7:A:1053:GLN:HA	7:A:1056:GLU:HB3	1.71	0.72
7:A:450:ALA:O	7:A:453:THR:OG1	2.06	0.72
8:N:333:VAL:HG11	8:N:345:TYR:HE1	1.55	0.72
7:A:426:ARG:HA	11:R:262:PHE:CE1	2.19	0.72
7:A:1003:LEU:HB3	7:A:1303:ARG:NH1	2.04	0.72
7:A:1180:PRO:HG3	7:A:1218:ALA:HB1	1.71	0.71
10:Q:214:LEU:HB3	14:V:173:PRO:HB2	1.70	0.71
5:I:75:DT:O4	6:J:73:DA:N6	2.17	0.71
18:a:1647:ARG:NH1	18:a:1649:PRO:HA	2.06	0.71
12:T:390:GLU:OE1	12:T:393:ARG:N	2.24	0.71
7:A:1192:ARG:NH1	22:A:1703:ADP:O1B	2.24	0.71
9:P:182:GLY:O	9:P:186:THR:N	2.23	0.71
7:A:1265:ASP:HB3	7:A:1268:THR:HB	1.71	0.71
8:N:283:PRO:HA	8:N:295:CYS:HB2	1.73	0.71
15:X:892:VAL:HA	15:X:895:GLN:HB3	1.73	0.71
9:P:131:ALA:HA	9:P:358:SER:HA	1.73	0.71
10:Q:466:LYS:HB2	10:Q:521:GLU:HB2	1.73	0.70
7:A:906:ARG:NH2	7:A:927:PHE:O	2.24	0.70
7:A:1077:ARG:HG2	7:A:1301:LYS:O	1.91	0.70
8:N:263:GLN:HA	8:N:267:LEU:HD13	1.72	0.70
14:V:198:GLN:NE2	14:V:199:LYS:O	2.24	0.70
14:V:229:ASN:ND2	14:V:232:THR:OG1	2.23	0.70
9:P:333:PRO:O	9:P:335:ARG:NH1	2.24	0.70
2:C:90:ASP:OD2	2:C:91:GLU:N	2.24	0.70
10:Q:38:PRO:HB3	10:Q:92:TYR:HE1	1.56	0.70
12:T:410:TYR:HA	16:Y:155:ARG:HE	1.56	0.70
7:A:952:GLU:OE2	7:A:1227:LYS:NZ	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:1665:ALA:O	18:a:1669:LEU:N	2.24	0.70
10:Q:243:ASP:HB3	10:Q:246:VAL:HG22	1.74	0.69
5:I:115:DT:N3	6:J:33:DA:N1	2.41	0.69
9:P:82:MET:HE1	9:P:122:ILE:HG21	1.74	0.69
15:W:448:GLU:OE2	15:W:499:ARG:NE	2.25	0.69
10:Q:81:SER:HB2	11:R:224:ALA:H	1.58	0.69
7:A:1200:ARG:HD2	7:A:1275:ARG:HE	1.57	0.69
10:Q:63:VAL:HG13	10:Q:68:GLN:HB2	1.74	0.69
16:Y:136:ARG:HB3	16:Y:435:LYS:HD2	1.74	0.69
10:Q:325:ILE:HG22	10:Q:329:GLN:HE22	1.58	0.69
11:R:257:LEU:HD12	15:X:538:PRO:HD2	1.73	0.69
15:X:504:LEU:HD22	15:X:509:LEU:HD22	1.74	0.69
10:Q:240:ILE:HD11	10:Q:324:PHE:HB3	1.74	0.69
7:A:744:LYS:NZ	7:A:763:GLU:OE1	2.25	0.69
9:P:8:LEU:HB3	9:P:103:VAL:HG12	1.73	0.68
4:E:121:PRO:HB3	1:F:53:GLU:HG3	1.74	0.68
8:N:20:SER:HB2	8:N:174:ALA:H	1.58	0.68
11:R:227:ASP:OD2	11:R:230:THR:OG1	2.12	0.68
5:I:17:DC:OP1	7:A:900:HIS:NE2	2.21	0.68
7:A:175:ASN:O	7:A:178:HIS:ND1	2.25	0.68
2:G:21:ALA:HB2	3:H:121:TYR:HB2	1.76	0.68
7:A:939:PHE:O	7:A:941:GLN:NE2	2.26	0.68
11:R:282:ALA:O	18:a:1655:SER:OG	2.11	0.68
16:Y:472:ASN:ND2	16:Y:476:GLU:OE2	2.26	0.68
7:A:374:LEU:HD11	15:W:648:TYR:HB3	1.76	0.68
7:A:486:PHE:HB3	8:N:399:ILE:HD11	1.75	0.68
9:P:155:SER:HA	9:P:160:THR:HG22	1.76	0.68
9:P:213:LYS:HB3	9:P:306:TYR:HE1	1.57	0.68
10:Q:1805:MET:HG3	10:Q:1806:GLU:N	2.09	0.68
12:T:188:ASN:O	12:T:191:GLN:NE2	2.27	0.68
7:A:419:GLU:HA	7:A:422:VAL:HG22	1.75	0.67
9:P:349:LEU:O	9:P:353:GLN:NE2	2.27	0.67
5:I:99:DG:H21	5:I:100:DG:N2	1.92	0.67
7:A:914:LEU:HD23	7:A:921:LEU:HD22	1.77	0.67
5:I:125:DC:N4	6:J:23:DG:O6	2.18	0.67
5:I:31:DT:H2'	5:I:32:DT:H71	1.76	0.67
5:I:78:DC:O2	6:J:70:DG:N2	2.22	0.67
7:A:943:PHE:HA	7:A:956:LEU:HD21	1.77	0.67
7:A:1287:ASP:OD1	7:A:1288:LEU:N	2.27	0.67
16:Y:300:ARG:HE	16:Y:346:ILE:HG12	1.59	0.67
15:X:502:ALA:O	15:X:506:GLN:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:913:MET:O	15:X:917:ARG:NH2	2.28	0.67
6:J:34:DC:H2'	6:J:35:DT:H71	1.76	0.67
7:A:834:TYR:OH	7:A:866:ASP:OD2	2.12	0.67
10:Q:201:THR:O	10:Q:205:ALA:N	2.23	0.67
15:X:609:LEU:HA	15:X:627:VAL:HG11	1.75	0.67
1:B:66:ILE:HD11	4:K:92:LEU:HD11	1.77	0.67
5:I:78:DC:N4	6:J:70:DG:O6	2.19	0.66
7:A:476:LEU:HG	8:N:405:THR:HG21	1.76	0.66
12:T:164:ILE:HD12	18:a:1672:LEU:HD21	1.77	0.66
7:A:1043:ARG:NH1	7:A:1176:SER:O	2.27	0.66
7:A:1239:SER:O	7:A:1243:ARG:NH2	2.27	0.66
14:V:375:MET:HA	14:V:375:MET:HE3	1.77	0.66
15:X:446:LEU:HD13	15:X:500:VAL:HG12	1.77	0.66
15:X:624:SER:OG	15:X:630:ARG:O	2.11	0.66
9:P:123:MET:HA	9:P:127:PHE:HB3	1.76	0.66
14:V:220:GLU:OE2	14:V:221:ILE:HG13	1.95	0.66
14:V:356:LEU:HD12	14:V:360:GLU:HB3	1.77	0.66
17:Z:228:LYS:HA	17:Z:231:VAL:HB	1.77	0.66
7:A:1047:ASN:OD1	7:A:1081:LYS:NZ	2.29	0.66
10:Q:335:LEU:HA	10:Q:338:ILE:HG22	1.76	0.66
7:A:969:HIS:CD2	7:A:1232:GLY:HA2	2.29	0.66
8:N:155:ALA:HB2	8:N:180:ILE:HD12	1.77	0.66
8:N:351:ALA:HB2	8:N:389:ARG:HH21	1.59	0.66
15:X:434:ASP:OD2	15:X:437:SER:N	2.28	0.66
10:Q:240:ILE:HG23	10:Q:241:VAL:HG23	1.76	0.66
8:N:351:ALA:HA	8:N:389:ARG:HE	1.60	0.66
10:Q:459:PRO:HD2	10:Q:460:ASP:H	1.60	0.66
15:X:904:ARG:O	15:X:907:GLU:HG2	1.96	0.66
18:a:1635:ARG:HH11	18:a:1637:ASP:HB3	1.59	0.66
4:E:90:MET:HE2	4:E:90:MET:HA	1.78	0.66
4:E:61:LEU:HD12	1:F:36:ARG:HB3	1.78	0.66
11:R:211:ASN:HD22	15:X:481:LEU:HD12	1.60	0.66
11:R:274:LEU:HD23	11:R:277:LEU:HD21	1.78	0.66
3:D:68:ASP:OD1	1:F:98:TYR:OH	2.14	0.65
16:Y:305:LEU:HD12	16:Y:318:ALA:HB1	1.77	0.65
16:Y:480:GLU:HA	16:Y:483:PHE:HD1	1.61	0.65
2:G:29:ARG:NH1	3:H:36:SER:O	2.27	0.65
7:A:479:ILE:HG23	8:N:403:LEU:HD13	1.78	0.65
11:R:213:ASN:OD1	11:R:216:ARG:NH1	2.26	0.65
5:I:81:DC:N4	6:J:66:DG:O6	2.29	0.65
5:I:92:DC:N4	6:J:56:DG:H1	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:309:ASN:OD1	10:Q:310:ARG:N	2.28	0.65
7:A:797:MET:SD	7:A:798:GLU:HG2	2.35	0.65
15:W:608:LEU:HB3	15:W:627:VAL:HG22	1.77	0.65
16:Y:438:ARG:O	16:Y:442:LEU:N	2.27	0.65
7:A:748:LEU:HD21	7:A:798:GLU:HG3	1.79	0.65
7:A:915:GLN:HA	7:A:1181:HIS:CE1	2.32	0.65
15:W:601:TRP:CH2	15:W:630:ARG:HG3	2.32	0.65
15:W:442:GLU:OE1	15:W:462:TYR:OH	2.15	0.65
15:X:892:VAL:O	15:X:896:MET:N	2.25	0.65
5:I:83:DG:H1	6:J:65:DC:H42	1.45	0.65
6:J:91:DA:H2''	6:J:92:DG:C8	2.32	0.65
7:A:787:ILE:HD13	22:A:1703:ADP:C8	2.32	0.65
7:A:1163:LEU:H	7:A:1189:ARG:HH21	1.45	0.64
7:A:1310:LEU:HB3	7:A:1311:PRO:HD2	1.78	0.64
14:V:277:ASP:OD1	14:V:278:GLN:N	2.30	0.64
7:A:1177:ASP:OD2	7:A:1178:TRP:N	2.29	0.64
15:X:921:GLU:O	15:X:925:GLN:N	2.24	0.64
16:Y:435:LYS:HA	16:Y:438:ARG:NH1	2.12	0.64
8:N:41:ILE:HD11	8:N:98:SER:HB2	1.79	0.64
9:P:237:GLU:HA	9:P:251:GLY:HA2	1.77	0.64
14:V:171:HIS:HB2	14:V:176:ILE:HD11	1.78	0.64
15:X:534:LEU:HB3	15:X:541:LEU:HD22	1.79	0.64
16:Y:501:GLN:O	16:Y:504:GLN:NE2	2.25	0.64
7:A:445:GLN:O	10:Q:518:ILE:N	2.28	0.64
14:V:261:ARG:NE	14:V:280:GLU:OE1	2.25	0.64
2:G:84:GLN:NE2	2:G:106:GLY:O	2.27	0.64
5:I:128:DG:H1	6:J:20:DC:H42	1.44	0.64
7:A:1286:MET:HA	7:A:1289:ASP:HB2	1.78	0.64
7:A:441:ARG:NH1	10:Q:299:GLU:OE2	2.21	0.64
9:P:163:VAL:HG12	9:P:175:ILE:HG23	1.80	0.64
14:V:341:ARG:HH21	15:X:490:LEU:C	2.05	0.64
1:F:60:VAL:HA	1:F:63:GLU:OE1	1.97	0.64
9:P:202:THR:HG22	9:P:204:ALA:H	1.63	0.64
2:C:78:ILE:HB	3:D:54:ILE:HD12	1.80	0.64
7:A:466:ARG:O	7:A:470:GLN:NE2	2.30	0.64
10:Q:1776:LEU:HA	10:Q:1779:ILE:HB	1.79	0.64
5:I:100:DG:H2''	5:I:101:DG:H5''	1.79	0.63
11:R:259:PRO:HG2	18:a:1606:HIS:HE1	1.63	0.63
5:I:145:DT:O4	6:J:3:DA:N6	2.19	0.63
6:J:77:DC:H2''	6:J:78:DG:C8	2.32	0.63
7:A:425:ARG:NH2	7:A:427:ASP:OD1	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1211:GLU:HA	7:A:1214:ILE:HG22	1.79	0.63
10:Q:1816:TYR:O	10:Q:1820:PHE:N	2.32	0.63
14:V:172:ASP:HB3	14:V:175:VAL:HG22	1.81	0.63
2:C:115:LEU:HB3	1:F:44:LYS:HD2	1.81	0.63
7:A:1215:LEU:HG	7:A:1219:LYS:HE3	1.79	0.63
11:R:211:ASN:ND2	15:X:481:LEU:HD12	2.14	0.63
12:T:373:MET:HG3	12:T:374:THR:H	1.64	0.63
15:X:924:ARG:NH1	15:X:925:GLN:OE1	2.32	0.63
7:A:417:ARG:NH2	15:W:640:LEU:O	2.21	0.63
10:Q:296:LEU:O	10:Q:302:ASN:ND2	2.17	0.63
7:A:1239:SER:HB3	7:A:1243:ARG:HH21	1.63	0.63
14:V:282:ASP:N	15:X:493:ASP:OD1	2.24	0.63
14:V:291:GLU:OE2	14:V:316:ARG:NH1	2.31	0.62
8:N:368:LEU:O	8:N:372:THR:OG1	2.14	0.62
6:J:27:DC:H2"	6:J:28:DT:H71	1.81	0.62
6:J:123:DC:H2"	6:J:124:DG:C8	2.35	0.62
10:Q:407:LEU:HA	10:Q:415:VAL:HG23	1.80	0.62
10:Q:1813:LYS:HG2	16:Y:334:ARG:HB2	1.82	0.62
7:A:981:LYS:NZ	7:A:1191:HIS:O	2.33	0.62
15:W:930:ASP:O	15:X:931:ARG:NH2	2.32	0.62
2:C:24:GLN:NE2	3:D:47:GLN:HE22	1.98	0.62
7:A:1100:LEU:HD21	7:A:1171:VAL:HG22	1.82	0.62
9:P:147:ARG:NH1	9:P:296:ASN:OD1	2.32	0.62
10:Q:51:TYR:O	10:Q:55:THR:OG1	2.12	0.62
15:W:898:LYS:HD2	16:Y:417:ILE:HG23	1.81	0.62
17:Z:255:LYS:O	17:Z:258:LYS:HG2	1.99	0.62
7:A:1083:GLU:HB3	7:A:1301:LYS:CE	2.24	0.62
10:Q:1797:LEU:HD22	10:Q:1815:LEU:HD21	1.80	0.62
14:V:300:GLU:HA	15:X:520:PRO:HB3	1.82	0.62
14:V:364:LYS:O	14:V:368:GLN:HG2	2.00	0.62
15:W:633:ASP:OD1	15:W:634:GLU:N	2.32	0.62
17:Z:231:VAL:HG12	17:Z:235:MET:HE1	1.82	0.62
7:A:1000:MET:HE1	7:A:1005:ARG:HA	1.82	0.62
8:N:158:THR:HG21	8:N:169:ILE:HG21	1.80	0.62
15:W:458:THR:OG1	15:W:461:ILE:HG12	2.00	0.62
15:X:536:ASP:OD1	18:a:1625:SER:OG	2.18	0.62
7:A:1019:THR:OG1	7:A:1031:GLY:O	2.16	0.61
7:A:1047:ASN:ND2	7:A:1175:ASP:OD2	2.33	0.61
8:N:324:GLY:O	8:N:328:VAL:N	2.29	0.61
18:a:1610:TYR:O	18:a:1613:TYR:N	2.33	0.61
5:I:125:DC:H2"	5:I:126:DG:H5"	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:414:ARG:HH22	12:T:385:LEU:HG	1.65	0.61
7:A:1205:CYS:SG	7:A:1206:THR:N	2.73	0.61
10:Q:324:PHE:CE1	10:Q:327:LEU:HB2	2.35	0.61
16:Y:489:GLU:OE1	16:Y:493:ARG:NH1	2.33	0.61
12:T:376:GLY:O	12:T:378:LEU:CD2	2.48	0.61
9:P:151:ILE:HG21	9:P:282:ILE:HD11	1.82	0.61
10:Q:132:ASN:HB3	10:Q:135:GLN:HB2	1.80	0.61
7:A:784:GLY:HA2	22:A:1703:ADP:H5'1	1.82	0.61
10:Q:153:ASN:OD1	14:V:163:THR:OG1	2.16	0.61
7:A:967:ARG:O	7:A:971:VAL:HG23	2.00	0.61
7:A:1181:HIS:NE2	7:A:1225:ASP:OD2	2.24	0.61
18:a:1618:SER:HB3	18:a:1621:SER:HB3	1.82	0.61
7:A:483:ALA:HB2	8:N:403:LEU:HD21	1.83	0.61
7:A:1226:GLN:HA	7:A:1230:GLN:HB3	1.82	0.61
10:Q:136:HIS:NE2	14:V:227:ASP:OD1	2.32	0.61
11:R:227:ASP:HB3	11:R:234:GLN:HE22	1.66	0.61
6:J:56:DG:OP2	7:A:1135:ARG:NH2	2.34	0.61
5:I:145:DT:O2	6:J:4:DG:N2	2.33	0.61
8:N:350:VAL:O	8:N:389:ARG:NE	2.32	0.61
10:Q:367:ASP:HB3	10:Q:370:LEU:HD13	1.82	0.61
2:G:16:THR:O	2:G:19:SER:OG	2.14	0.60
10:Q:368:ARG:HG2	10:Q:372:MET:HE1	1.82	0.60
15:W:469:MET:HE1	15:W:500:VAL:HG12	1.83	0.60
11:R:263:GLN:HE22	11:R:265:TYR:HB3	1.66	0.60
7:A:1085:LEU:HD23	7:A:1088:ILE:HD11	1.82	0.60
3:D:109:HIS:CD2	7:A:1335:GLY:HA2	2.36	0.60
11:R:282:ALA:HB3	18:a:1653:LEU:HD23	1.83	0.60
14:V:143:ASP:OD1	14:V:144:ALA:N	2.33	0.60
14:V:365:ILE:HA	14:V:368:GLN:HE21	1.64	0.60
9:P:211:ASP:HA	9:P:214:GLU:HB2	1.84	0.60
14:V:369:ASP:OD1	14:V:370:ARG:N	2.35	0.60
9:P:153:MET:O	9:P:300:SER:OG	2.13	0.60
12:T:139:ALA:HB1	12:T:240:LEU:HD21	1.83	0.60
14:V:367:ASP:OD1	14:V:368:GLN:N	2.33	0.60
3:D:73:ILE:HD13	3:D:101:LEU:HD22	1.83	0.60
6:J:118:DT:H2''	6:J:119:DT:H71	1.84	0.60
7:A:441:ARG:O	10:Q:294:ARG:NH2	2.32	0.60
7:A:774:ASN:HB3	7:A:928:LEU:HD22	1.84	0.60
8:N:271:ASP:O	8:N:363:ARG:NH2	2.32	0.60
8:N:351:ALA:HB2	8:N:389:ARG:NH2	2.16	0.60
11:R:259:PRO:HG2	18:a:1606:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:423:HIS:O	15:W:513:GLN:NE2	2.35	0.60
5:I:62:DC:H2"	5:I:63:DG:H8	1.67	0.60
7:A:765:LEU:HB3	7:A:792:LEU:HD12	1.84	0.60
7:A:889:HIS:ND1	7:A:923:ALA:HB2	2.16	0.60
10:Q:24:ARG:O	10:Q:28:HIS:N	2.27	0.60
14:V:358:ASP:HA	14:V:361:MET:HE2	1.83	0.60
8:N:309:PHE:HA	8:N:324:GLY:HA2	1.82	0.60
10:Q:138:VAL:HG21	14:V:231:LEU:HD11	1.83	0.60
14:V:220:GLU:O	14:V:224:ASP:N	2.35	0.60
16:Y:300:ARG:HH21	16:Y:346:ILE:HA	1.67	0.60
17:Z:237:HIS:O	17:Z:241:LEU:N	2.27	0.60
7:A:485:ASP:HA	7:A:488:GLU:HB2	1.84	0.59
7:A:510:ASN:OD1	7:A:511:THR:N	2.35	0.59
7:A:891:CYS:HB3	7:A:894:THR:HG23	1.84	0.59
7:A:996:ILE:HD12	7:A:1084:LEU:HD11	1.82	0.59
10:Q:309:ASN:ND2	10:Q:311:THR:OG1	2.32	0.59
18:a:1675:ARG:HH21	18:a:1679:ASN:N	2.00	0.59
7:A:917:LYS:HB3	7:A:919:PRO:HD2	1.83	0.59
14:V:139:SER:HA	14:V:142:LEU:HD23	1.84	0.59
16:Y:507:GLU:OE2	18:a:1670:ARG:HD2	2.02	0.59
17:Z:244:GLU:HA	17:Z:247:GLN:HG3	1.84	0.59
18:a:1603:ARG:NH1	18:a:1607:SER:HB3	2.17	0.59
10:Q:43:LYS:HZ1	10:Q:45:LEU:HD12	1.67	0.59
10:Q:1815:LEU:O	10:Q:1819:ASN:N	2.32	0.59
5:I:126:DG:H2'	5:I:127:DT:H71	1.84	0.59
7:A:783:LEU:HD21	7:A:981:LYS:HG3	1.82	0.59
10:Q:47:LEU:HA	10:Q:50:LEU:HD23	1.85	0.59
11:R:265:TYR:HA	15:X:545:GLN:HE21	1.68	0.59
15:X:505:GLU:OE1	15:X:511:ASN:ND2	2.34	0.59
15:X:616:TYR:HD2	15:X:618:ASP:H	1.50	0.59
19:M:316:UNK:O	19:M:320:UNK:N	2.35	0.59
4:K:48:LEU:O	4:K:51:ILE:HG12	2.02	0.59
2:C:16:THR:O	2:C:19:SER:OG	2.20	0.59
5:I:99:DG:H1	6:J:49:DC:N4	1.91	0.59
7:A:1078:ALA:HA	7:A:1303:ARG:HE	1.67	0.59
9:P:282:ILE:HG22	9:P:290:ARG:HD2	1.84	0.59
1:B:24:ASP:HB3	1:B:27:GLN:HG2	1.85	0.59
1:F:78:ARG:NH2	1:F:85:ASP:OD2	2.35	0.59
7:A:1287:ASP:O	7:A:1291:ARG:HG3	2.02	0.59
7:A:881:ASP:OD1	7:A:882:GLU:N	2.36	0.59
7:A:1062:HIS:CD2	7:A:1310:LEU:HD11	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:343:GLY:O	8:N:347:SER:OG	2.16	0.59
10:Q:191:MET:HE1	10:Q:199:ILE:HD13	1.84	0.59
15:W:621:ASN:HA	15:W:632:GLN:HE21	1.68	0.59
7:A:1268:THR:O	7:A:1272:MET:N	2.35	0.59
5:I:50:DG:H1	6:J:98:DC:H42	1.49	0.59
8:N:96:TRP:HH2	8:N:136:LEU:HA	1.66	0.59
8:N:333:VAL:HG11	8:N:345:TYR:CE1	2.38	0.58
10:Q:344:LEU:HD11	10:Q:381:LEU:HD22	1.85	0.58
14:V:296:LYS:O	14:V:299:SER:OG	2.13	0.58
15:W:599:ARG:HD3	15:W:600:GLU:HB2	1.85	0.58
1:B:25:ASN:HD21	4:K:73:GLU:HG3	1.67	0.58
3:H:90:THR:OG1	3:H:93:GLU:OE1	2.17	0.58
10:Q:131:TYR:HB3	10:Q:133:TYR:CE1	2.38	0.58
10:Q:322:SER:O	10:Q:328:ARG:HD2	2.03	0.58
10:Q:131:TYR:OH	14:V:224:ASP:O	2.16	0.58
10:Q:186:GLU:HG3	10:Q:187:SER:H	1.69	0.58
10:Q:372:MET:O	10:Q:375:MET:N	2.36	0.58
14:V:177:HIS:O	14:V:181:SER:N	2.30	0.58
15:W:439:HIS:CE1	15:W:441:ILE:HG12	2.38	0.58
15:W:898:LYS:HA	15:W:901:ILE:HD12	1.85	0.58
15:X:449:PHE:HA	15:X:457:LYS:HB3	1.84	0.58
15:X:930:ASP:HA	15:X:933:ALA:HB3	1.85	0.58
7:A:460:GLN:HA	7:A:463:GLU:HB2	1.85	0.58
8:N:134:GLU:O	8:N:137:THR:OG1	2.18	0.58
10:Q:174:ASP:OD2	10:Q:285:ARG:NH2	2.36	0.58
5:I:82:DC:H42	6:J:66:DG:H1	1.52	0.58
7:A:489:TYR:O	7:A:492:SER:OG	2.17	0.58
8:N:15:VAL:HG21	8:N:398:SER:HA	1.86	0.58
10:Q:434:THR:O	10:Q:438:LYS:HG3	2.04	0.58
2:G:77:ARG:HE	5:I:20:DA:H4'	1.69	0.58
10:Q:249:LEU:HD21	10:Q:314:ARG:HD2	1.85	0.58
14:V:179:ASN:ND2	14:V:212:LEU:HD23	2.16	0.58
16:Y:428:ILE:HA	16:Y:431:ILE:HD12	1.84	0.58
8:N:342:PRO:HA	8:N:345:TYR:HB2	1.86	0.58
11:R:266:TYR:CD1	16:Y:493:ARG:HG2	2.38	0.58
14:V:149:THR:HG23	14:V:201:ARG:H	1.69	0.58
15:W:913:MET:HA	15:W:916:GLU:HG2	1.84	0.58
8:N:30:GLU:HB3	8:N:394:TRP:HH2	1.69	0.58
8:N:173:GLY:O	8:N:354:ASN:ND2	2.36	0.58
10:Q:422:LEU:HD23	10:Q:425:LEU:HD12	1.85	0.58
10:Q:454:ILE:HG22	10:Q:455:GLN:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:263:GLN:CD	11:R:265:TYR:H	2.09	0.58
14:V:183:PRO:O	14:V:209:ASN:ND2	2.37	0.58
15:X:458:THR:HG22	15:X:460:GLU:H	1.69	0.58
9:P:4:ASP:OD1	9:P:5:ILE:N	2.36	0.58
10:Q:406:HIS:HA	10:Q:409:LEU:HD23	1.86	0.58
15:W:931:ARG:HH21	15:X:923:GLN:NE2	2.02	0.58
5:I:114:DG:H2'	5:I:115:DT:H71	1.85	0.57
7:A:764:TRP:O	7:A:767:SER:OG	2.21	0.57
7:A:1210:VAL:HA	7:A:1213:LYS:HE2	1.86	0.57
14:V:202:ASP:OD1	14:V:203:ALA:N	2.36	0.57
14:V:202:ASP:OD2	15:W:487:ARG:NH1	2.26	0.57
15:X:447:PRO:O	15:X:451:ASN:N	2.37	0.57
15:X:449:PHE:HE2	15:X:461:ILE:HG22	1.68	0.57
7:A:1232:GLY:HA3	7:A:1234:PHE:CE2	2.40	0.57
12:T:194:GLU:O	12:T:198:ASP:N	2.34	0.57
12:T:539:ALA:O	12:T:543:GLN:N	2.35	0.57
15:W:438:VAL:HG22	15:W:443:ARG:HH21	1.70	0.57
15:X:513:GLN:N	15:X:513:GLN:OE1	2.37	0.57
15:W:620:TRP:CH2	15:W:636:ILE:HG13	2.39	0.57
16:Y:133:LEU:HD11	16:Y:137:ILE:HG21	1.84	0.57
7:A:549:ARG:HH12	7:A:971:VAL:C	2.12	0.57
15:W:903:LEU:HD11	15:X:899:LEU:HD11	1.86	0.57
18:a:1636:ARG:NH2	18:a:1664:ASP:OD1	2.37	0.57
7:A:953:LYS:HG2	7:A:1251:LEU:HB3	1.85	0.57
7:A:1198:GLU:HG3	7:A:1275:ARG:HD3	1.85	0.57
11:R:197:PRO:O	11:R:201:LYS:N	2.35	0.57
11:R:271:PRO:HB2	11:R:275:ARG:HH12	1.68	0.57
9:P:314:GLN:NE2	9:P:329:ILE:HG12	2.19	0.57
14:V:144:ALA:O	14:V:190:ARG:NH2	2.37	0.57
5:I:34:DG:H1	6:J:114:DC:N4	2.00	0.57
7:A:757:TYR:O	7:A:761:GLY:N	2.31	0.57
7:A:1077:ARG:NH1	7:A:1307:GLU:OE1	2.37	0.57
10:Q:81:SER:CB	11:R:224:ALA:H	2.18	0.57
15:X:454:ASN:OD1	15:X:456:SER:N	2.38	0.57
7:A:1225:ASP:OD1	7:A:1226:GLN:N	2.37	0.57
16:Y:500:GLN:CD	16:Y:503:ARG:HH22	2.13	0.57
7:A:838:PRO:HB2	7:A:842:ARG:HH12	1.69	0.56
7:A:1124:LEU:HD22	7:A:1138:LEU:HD22	1.87	0.56
9:P:102:PRO:HB2	9:P:356:TRP:CZ3	2.40	0.56
10:Q:321:HIS:NE2	10:Q:358:THR:OG1	2.22	0.56
11:R:202:LYS:HG3	11:R:206:LYS:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:173:LYS:HG2	12:T:174:HIS:CE1	2.40	0.56
15:X:897:LYS:O	15:X:901:ILE:HG12	2.04	0.56
6:J:102:DA:H2''	6:J:103:DG:H8	1.71	0.56
8:N:159:ALA:O	8:N:163:GLY:N	2.38	0.56
10:Q:81:SER:HB3	11:R:222:ARG:HA	1.86	0.56
15:W:895:GLN:HA	15:W:898:LYS:HZ2	1.71	0.56
7:A:474:GLU:HA	7:A:477:ASN:HB2	1.87	0.56
7:A:917:LYS:O	7:A:920:GLU:HB2	2.05	0.56
10:Q:211:ASP:HB3	10:Q:311:THR:CG2	2.36	0.56
10:Q:454:ILE:C	10:Q:456:MET:H	2.13	0.56
14:V:326:TYR:O	14:V:329:SER:OG	2.19	0.56
15:X:883:LYS:O	15:X:887:LEU:HB2	2.05	0.56
16:Y:133:LEU:O	16:Y:138:ARG:NH2	2.34	0.56
18:a:1646:SER:O	18:a:1647:ARG:HG3	2.06	0.56
10:Q:1784:GLU:HA	10:Q:1787:ARG:NE	2.20	0.56
18:a:1642:LYS:HE3	18:a:1644:GLN:HG2	1.87	0.56
8:N:193:VAL:HG22	8:N:332:SER:HB3	1.88	0.56
10:Q:221:PHE:HB3	10:Q:225:TRP:CE3	2.40	0.56
16:Y:494:TYR:O	16:Y:498:LYS:HG2	2.05	0.56
9:P:9:VAL:HG23	9:P:340:TRP:NE1	2.21	0.56
10:Q:246:VAL:HG12	10:Q:354:LEU:HD11	1.86	0.56
10:Q:368:ARG:HB3	12:T:415:ASP:OD1	2.05	0.56
10:Q:1787:ARG:O	10:Q:1791:LYS:HG2	2.05	0.56
16:Y:505:GLU:O	16:Y:509:ALA:N	2.32	0.56
10:Q:52:THR:O	10:Q:56:THR:N	2.38	0.56
10:Q:301:GLY:HA2	10:Q:304:LYS:NZ	2.20	0.56
14:V:152:ASN:OD1	14:V:154:ASN:ND2	2.39	0.56
15:W:611:GLU:OE1	15:W:626:HIS:NE2	2.35	0.56
15:W:895:GLN:HA	15:W:898:LYS:NZ	2.21	0.56
4:K:47:ALA:O	4:K:50:GLU:HG3	2.05	0.56
8:N:349:ILE:HG22	8:N:389:ARG:NH2	2.21	0.56
10:Q:293:LEU:O	10:Q:297:SER:N	2.39	0.56
15:X:443:ARG:HA	15:X:450:PHE:CD2	2.41	0.56
16:Y:147:TYR:O	16:Y:151:LEU:N	2.32	0.56
9:P:185:LEU:HD11	9:P:258:PRO:HA	1.88	0.56
10:Q:444:ASP:OD1	10:Q:445:MET:N	2.39	0.56
11:R:229:GLN:HG2	15:W:488:ARG:HD2	1.88	0.56
14:V:341:ARG:NH2	15:X:490:LEU:O	2.37	0.56
15:X:616:TYR:CE1	15:X:622:LYS:HG3	2.41	0.56
16:Y:323:ILE:HG23	16:Y:328:LEU:HB2	1.87	0.56
16:Y:443:SER:HA	16:Y:446:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:90:DA:H1'	6:J:91:DA:C8	2.40	0.55
14:V:264:ILE:HD11	14:V:319:LEU:HD11	1.87	0.55
2:G:87:VAL:HG21	2:G:97:LEU:HD12	1.87	0.55
10:Q:401:ARG:HD2	10:Q:402:GLU:N	2.21	0.55
10:Q:445:MET:SD	16:Y:166:LEU:HD23	2.47	0.55
17:Z:247:GLN:HA	17:Z:250:GLU:HG3	1.87	0.55
7:A:476:LEU:O	7:A:479:ILE:HG22	2.06	0.55
9:P:207:GLU:HB2	9:P:210:ARG:HH21	1.72	0.55
10:Q:95:ARG:HG3	10:Q:96:TYR:CE1	2.41	0.55
10:Q:454:ILE:O	10:Q:456:MET:N	2.38	0.55
17:Z:198:ARG:HD3	17:Z:202:LEU:HD13	1.89	0.55
7:A:805:PRO:HD2	7:A:876:LYS:HB2	1.88	0.55
7:A:807:LEU:HB2	7:A:875:TRP:CE3	2.41	0.55
5:I:39:DA:H61	6:J:109:DT:H3	1.54	0.55
6:J:70:DG:H2''	6:J:71:DA:C8	2.41	0.55
7:A:748:LEU:HD23	7:A:748:LEU:H	1.71	0.55
7:A:1011:MET:HA	7:A:1011:MET:HE3	1.87	0.55
8:N:197:LEU:HB3	8:N:308:LEU:HD23	1.88	0.55
11:R:217:GLU:HA	11:R:220:GLU:HG2	1.88	0.55
12:T:374:THR:O	12:T:377:ARG:NH1	2.32	0.55
16:Y:300:ARG:NE	16:Y:346:ILE:HG12	2.21	0.55
6:J:40:DA:H1'	6:J:41:DG:C8	2.42	0.55
8:N:16:PHE:O	8:N:122:MET:HA	2.07	0.55
15:X:515:ASP:O	15:X:519:ARG:NH2	2.36	0.55
16:Y:439:GLU:HA	16:Y:442:LEU:HB3	1.89	0.55
18:a:1647:ARG:HH11	18:a:1649:PRO:HA	1.71	0.55
3:D:39:ILE:H	3:D:39:ILE:HD12	1.72	0.55
6:J:67:DG:H2''	6:J:68:DG:C8	2.42	0.55
8:N:189:GLN:O	8:N:192:ILE:HG12	2.07	0.55
10:Q:467:LEU:HD11	10:Q:1764:ILE:HD11	1.89	0.55
7:A:364:VAL:HG23	7:A:365:GLU:HG2	1.89	0.55
9:P:155:SER:HB2	9:P:303:THR:HB	1.88	0.55
14:V:376:ARG:HG2	14:V:376:ARG:HH11	1.71	0.55
15:W:641:ARG:HD3	16:Y:483:PHE:CE2	2.41	0.55
5:I:83:DG:H5'	5:I:83:DG:H8	1.69	0.55
7:A:1260:GLU:O	7:A:1261:ASP:OD1	2.24	0.55
20:A:1701:BEF:F3	22:A:1703:ADP:O2B	2.14	0.55
8:N:20:SER:CB	8:N:174:ALA:H	2.19	0.55
12:T:397:THR:H	12:T:420:ASN:HB2	1.71	0.55
15:X:484:THR:HA	15:X:487:ARG:HG2	1.89	0.55
12:T:211:ASN:HD21	12:T:217:TYR:C	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:173:PRO:O	14:V:177:HIS:ND1	2.28	0.54
5:I:84:DC:H5'	4:K:40:ARG:HG3	1.89	0.54
7:A:741:ARG:HH11	7:A:763:GLU:HG2	1.73	0.54
7:A:949:MET:O	7:A:1220:TYR:OH	2.15	0.54
10:Q:243:ASP:O	10:Q:247:ARG:HG3	2.07	0.54
10:Q:356:PHE:HA	10:Q:359:VAL:HG12	1.89	0.54
12:T:161:THR:H	12:T:164:ILE:HG22	1.72	0.54
16:Y:459:GLN:OE1	17:Z:199:ASN:ND2	2.40	0.54
2:C:41:GLU:OE1	2:C:41:GLU:N	2.38	0.54
7:A:1052:PHE:O	7:A:1053:GLN:HG3	2.08	0.54
9:P:213:LYS:HB3	9:P:306:TYR:CE1	2.39	0.54
14:V:281:TRP:CZ2	14:V:288:ASN:HB3	2.41	0.54
14:V:360:GLU:O	14:V:364:LYS:HG2	2.08	0.54
6:J:57:DT:H5''	7:A:862:TYR:CE1	2.43	0.54
10:Q:444:ASP:O	10:Q:448:CYS:N	2.35	0.54
17:Z:244:GLU:HB2	17:Z:247:GLN:HE21	1.72	0.54
15:X:473:TYR:CG	15:X:510:ILE:HG13	2.42	0.54
7:A:196:LEU:HD12	7:A:200:LEU:HD22	1.90	0.54
10:Q:325:ILE:O	10:Q:328:ARG:N	2.39	0.54
14:V:169:ASP:OD1	14:V:170:ASP:N	2.41	0.54
17:Z:224:MET:HA	17:Z:227:LEU:HD12	1.88	0.54
3:H:116:LYS:HE3	14:V:378:LEU:HD11	1.89	0.54
7:A:868:HIS:CD2	7:A:869:ILE:HG23	2.42	0.54
16:Y:301:LEU:HD13	16:Y:346:ILE:HG21	1.89	0.54
3:H:115:THR:O	3:H:119:THR:HG23	2.08	0.54
7:A:180:LEU:HD21	12:T:542:PHE:HE1	1.71	0.54
14:V:342:ASN:ND2	14:V:345:ASP:OD2	2.39	0.54
4:K:53:ARG:HD3	4:K:54:TYR:CE1	2.43	0.54
3:H:49:HIS:HB3	3:H:52:THR:HG23	1.90	0.54
7:A:406:ALA:HB1	15:W:644:ILE:HG12	1.90	0.54
7:A:941:GLN:HB2	7:A:944:ASN:H	1.72	0.54
7:A:1083:GLU:CA	7:A:1301:LYS:HE3	2.38	0.54
9:P:178:LEU:HD23	9:P:274:ILE:HD13	1.90	0.54
15:X:612:ALA:HA	15:X:626:HIS:ND1	2.23	0.54
17:Z:188:MET:O	17:Z:191:THR:N	2.40	0.54
10:Q:94:LEU:HG	10:Q:98:GLU:HG3	1.90	0.54
10:Q:166:LEU:HD22	15:W:507:TRP:HZ2	1.73	0.54
5:I:14:DG:C2	5:I:15:DT:C2	2.97	0.53
7:A:781:MET:HE1	7:A:1184:LEU:HB3	1.90	0.53
14:V:351:PRO:HD3	15:X:487:ARG:NH2	2.23	0.53
15:W:622:LYS:HA	15:W:625:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:991:LYS:HD2	7:A:1191:HIS:ND1	2.23	0.53
7:A:1153:LEU:C	7:A:1154:LEU:HD12	2.33	0.53
9:P:164:PRO:HG3	9:P:281:SER:HB3	1.91	0.53
15:W:430:ALA:HB1	15:W:509:LEU:HD21	1.91	0.53
4:E:100:LEU:HD11	1:F:58:LEU:HD12	1.90	0.53
5:I:63:DG:N3	6:J:86:DG:N2	2.56	0.53
7:A:1074:ASP:O	7:A:1078:ALA:N	2.42	0.53
15:W:505:GLU:OE1	15:W:511:ASN:ND2	2.41	0.53
17:Z:225:GLN:O	17:Z:229:ARG:N	2.32	0.53
4:E:106:ASP:OD2	4:E:131:ARG:NH2	2.35	0.53
7:A:1065:PHE:CZ	7:A:1070:VAL:HG13	2.42	0.53
10:Q:1783:SER:O	10:Q:1786:GLY:N	2.40	0.53
15:W:636:ILE:HD13	16:Y:495:PHE:HZ	1.74	0.53
15:X:940:LYS:O	15:X:944:MET:HG2	2.09	0.53
16:Y:134:PRO:HG2	16:Y:137:ILE:HG12	1.90	0.53
19:M:312:UNK:O	19:M:316:UNK:N	2.42	0.53
5:I:110:DC:N4	6:J:38:DG:H1	2.06	0.53
7:A:487:LYS:HG2	8:N:399:ILE:HD13	1.90	0.53
12:T:399:VAL:HG21	12:T:414:TYR:HD2	1.74	0.53
12:T:410:TYR:HA	16:Y:155:ARG:NE	2.21	0.53
15:X:481:LEU:N	15:X:511:ASN:OD1	2.35	0.53
15:X:881:GLU:OE2	15:X:885:LYS:HE3	2.08	0.53
5:I:125:DC:O2	6:J:23:DG:N2	2.41	0.53
7:A:1073:LEU:HD22	7:A:1076:TYR:CD2	2.44	0.53
7:A:1088:ILE:HG13	7:A:1089:LEU:HD22	1.90	0.53
7:A:1270:ASN:OD1	7:A:1271:GLN:N	2.42	0.53
8:N:171:ASP:HA	8:N:351:ALA:HB3	1.90	0.53
10:Q:37:ILE:HG21	10:Q:44:GLU:CD	2.34	0.53
14:V:277:ASP:OD2	15:X:487:ARG:NH2	2.42	0.53
15:X:446:LEU:HD12	15:X:462:TYR:HE1	1.73	0.53
7:A:791:ALA:O	7:A:794:THR:OG1	2.24	0.53
11:R:235:VAL:N	15:X:524:GLY:O	2.22	0.53
5:I:34:DG:N2	6:J:114:DC:N3	2.47	0.53
8:N:138:GLU:HG2	8:N:142:GLU:HG3	1.90	0.53
10:Q:246:VAL:HG11	10:Q:321:HIS:CD2	2.44	0.53
16:Y:429:GLU:O	16:Y:433:GLN:HG3	2.09	0.53
7:A:1135:ARG:O	7:A:1139:LEU:HD13	2.08	0.53
10:Q:452:MET:HB2	10:Q:454:ILE:HG12	1.91	0.53
15:X:423:HIS:CG	15:X:424:ILE:H	2.27	0.53
15:X:482:THR:HB	15:X:484:THR:HG22	1.90	0.53
15:X:483:SER:HB3	15:X:501:HIS:CG	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:602:THR:HG22	15:X:604:GLN:H	1.74	0.53
15:X:897:LYS:HA	15:X:900:GLU:HB3	1.91	0.53
16:Y:300:ARG:NH1	16:Y:300:ARG:HB3	2.24	0.53
7:A:764:TRP:CZ2	7:A:768:LEU:HD11	2.44	0.52
9:P:116:ARG:HB3	9:P:371:HIS:HE1	1.74	0.52
10:Q:300:GLU:HG2	10:Q:301:GLY:N	2.24	0.52
2:C:35:ARG:HG3	2:C:35:ARG:HH11	1.73	0.52
3:H:58:ALA:O	3:H:62:MET:HG2	2.08	0.52
5:I:36:DC:H42	6:J:112:DG:H1	1.57	0.52
8:N:209:LEU:HD12	8:N:304:ILE:HD11	1.90	0.52
10:Q:1774:LEU:HD21	10:Q:1810:THR:HG21	1.91	0.52
15:W:876:LEU:O	15:W:879:VAL:HG22	2.09	0.52
6:J:91:DA:H2''	6:J:92:DG:H8	1.71	0.52
7:A:757:TYR:C	7:A:979:ARG:HH11	2.16	0.52
7:A:781:MET:O	20:A:1701:BEF:F3	2.18	0.52
7:A:805:PRO:HB2	7:A:875:TRP:CZ3	2.45	0.52
7:A:989:PRO:HB2	7:A:1198:GLU:HA	1.90	0.52
10:Q:74:GLU:CD	10:Q:80:ARG:HA	2.34	0.52
10:Q:128:PRO:HB2	14:V:152:ASN:OD1	2.09	0.52
14:V:276:VAL:N	14:V:352:LEU:O	2.42	0.52
15:X:605:GLU:O	15:X:609:LEU:N	2.42	0.52
15:X:620:TRP:CZ3	15:X:636:ILE:HD12	2.45	0.52
15:X:870:ALA:O	15:X:874:LYS:N	2.37	0.52
16:Y:443:SER:HA	16:Y:446:ARG:HE	1.75	0.52
7:A:547:ASP:OD1	7:A:548:LYS:N	2.42	0.52
7:A:1269:VAL:O	7:A:1273:ILE:HG13	2.08	0.52
12:T:553:LEU:O	12:T:557:GLN:HG3	2.10	0.52
15:W:898:LYS:HB3	15:W:902:LYS:NZ	2.24	0.52
5:I:45:DC:H1'	5:I:46:DT:H5'	1.91	0.52
7:A:1280:PHE:O	7:A:1284:MET:N	2.36	0.52
8:N:171:ASP:O	8:N:178:THR:N	2.31	0.52
10:Q:34:PHE:HZ	10:Q:37:ILE:HD12	1.75	0.52
12:T:390:GLU:HG2	12:T:394:ASN:HB3	1.90	0.52
7:A:780:GLU:HG2	7:A:781:MET:H	1.73	0.52
7:A:1126:LEU:HD11	7:A:1135:ARG:HG2	1.92	0.52
10:Q:244:ASN:OD1	10:Q:245:GLU:N	2.41	0.52
15:W:434:ASP:OD2	15:W:437:SER:HB3	2.09	0.52
15:X:877:ALA:CA	17:Z:224:MET:HE1	2.40	0.52
15:X:936:MET:O	15:X:940:LYS:N	2.33	0.52
3:H:95:GLN:OE1	3:H:99:ARG:NH2	2.43	0.52
7:A:824:LYS:HE2	7:A:825:TRP:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1267:GLU:O	7:A:1269:VAL:N	2.43	0.52
8:N:21:TYR:CD2	8:N:22:THR:HG23	2.44	0.52
14:V:264:ILE:O	14:V:278:GLN:HA	2.10	0.52
1:F:47:SER:OG	1:F:48:GLY:N	2.42	0.52
7:A:368:GLN:HB3	7:A:372:TYR:CZ	2.45	0.52
7:A:1280:PHE:HD1	7:A:1284:MET:HE3	1.74	0.52
9:P:18:LYS:HD3	9:P:337:TYR:CD1	2.44	0.52
10:Q:377:ILE:O	10:Q:381:LEU:N	2.36	0.52
14:V:325:THR:O	14:V:329:SER:N	2.43	0.52
15:X:906:PHE:O	15:X:910:GLU:HG2	2.08	0.52
1:F:46:ILE:HG22	1:F:47:SER:O	2.10	0.52
7:A:1109:MET:HE1	7:A:1155:SER:HB3	1.92	0.52
9:P:113:LYS:HB2	9:P:371:HIS:NE2	2.25	0.52
9:P:261:LEU:HB3	9:P:274:ILE:HG12	1.92	0.52
11:R:241:LYS:HE2	15:W:417:VAL:HG21	1.92	0.52
11:R:271:PRO:HA	11:R:274:LEU:HB2	1.91	0.52
12:T:163:PHE:CZ	18:a:1672:LEU:HB3	2.45	0.52
12:T:373:MET:CG	12:T:374:THR:H	2.23	0.52
16:Y:170:GLU:O	16:Y:173:LYS:HG3	2.10	0.52
4:K:53:ARG:O	4:K:56:LYS:HG2	2.10	0.52
7:A:1048:HIS:CE1	7:A:1050:TYR:HB2	2.45	0.52
8:N:130:ARG:HD2	8:N:133:ARG:HD2	1.91	0.52
9:P:120:THR:HB	9:P:124:PHE:CE2	2.45	0.52
15:X:469:MET:HA	15:X:472:THR:HG22	1.92	0.52
7:A:554:LEU:HD21	7:A:734:VAL:HB	1.92	0.51
7:A:830:VAL:O	7:A:854:ASN:HB2	2.11	0.51
9:P:256:ARG:HA	9:P:259:GLU:HG2	1.92	0.51
10:Q:34:PHE:CE1	10:Q:38:PRO:HD3	2.44	0.51
15:X:901:ILE:HA	15:X:904:ARG:HG2	1.92	0.51
18:a:1667:TRP:HA	18:a:1670:ARG:NH2	2.24	0.51
2:C:115:LEU:HD22	1:F:44:LYS:HB2	1.91	0.51
4:K:51:ILE:HG13	4:K:52:ARG:N	2.26	0.51
1:B:78:ARG:NH2	1:B:85:ASP:OD2	2.42	0.51
7:A:411:ASN:ND2	18:a:1595:VAL:O	2.43	0.51
10:Q:373:ARG:O	10:Q:377:ILE:HG12	2.10	0.51
10:Q:381:LEU:O	10:Q:387:ASN:ND2	2.33	0.51
4:E:104:PHE:HA	4:E:107:THR:HG22	1.91	0.51
6:J:100:DA:H2''	6:J:101:DG:C8	2.45	0.51
7:A:444:ARG:HH11	10:Q:517:GLU:HB2	1.76	0.51
7:A:1063:LEU:HD22	7:A:1065:PHE:HE1	1.74	0.51
12:T:559:ALA:HB1	12:T:582:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:83:ARG:HD3	5:I:50:DG:H4'	1.91	0.51
1:F:92:ARG:CZ	1:F:92:ARG:HB3	2.40	0.51
5:I:82:DC:N4	6:J:66:DG:H1	2.08	0.51
9:P:218:TYR:O	9:P:255:PHE:HA	2.10	0.51
12:T:378:LEU:HD11	18:a:1592:PRO:O	2.10	0.51
15:X:494:VAL:HA	15:X:497:ILE:HD12	1.93	0.51
6:J:35:DT:H2''	6:J:36:DA:C8	2.46	0.51
7:A:198:ASP:HA	7:A:201:GLN:OE1	2.11	0.51
7:A:444:ARG:HA	10:Q:519:ASP:HB3	1.93	0.51
7:A:963:LEU:HD22	7:A:966:ARG:HH12	1.75	0.51
9:P:198:TYR:HB2	9:P:248:ILE:HD12	1.92	0.51
11:R:265:TYR:HD2	16:Y:496:TYR:CE1	2.29	0.51
12:T:195:GLU:HA	12:T:198:ASP:HB2	1.92	0.51
12:T:400:LEU:HD11	12:T:415:ASP:HB2	1.93	0.51
14:V:364:LYS:HE2	14:V:364:LYS:HA	1.92	0.51
15:X:459:PRO:O	15:X:462:TYR:HB3	2.11	0.51
5:I:83:DG:H5'	5:I:83:DG:C8	2.45	0.51
7:A:1049:PRO:CG	7:A:1303:ARG:HH22	2.24	0.51
8:N:389:ARG:HD2	8:N:392:SER:HB3	1.93	0.51
14:V:263:ILE:HG23	14:V:265:LYS:NZ	2.25	0.51
15:W:479:GLU:OE2	15:W:480:TYR:N	2.44	0.51
3:D:59:MET:HA	3:D:59:MET:HE2	1.92	0.51
6:J:82:DG:H2''	6:J:83:DT:H5'	1.91	0.51
7:A:990:GLU:OE2	7:A:1200:ARG:NH2	2.43	0.51
7:A:1063:LEU:HD22	7:A:1065:PHE:CE1	2.46	0.51
8:N:127:TRP:CH2	8:N:192:ILE:HD12	2.46	0.51
10:Q:396:ASP:OD2	10:Q:397:GLN:N	2.41	0.51
11:R:271:PRO:HA	11:R:274:LEU:HD12	1.92	0.51
15:X:616:TYR:CZ	15:X:622:LYS:HG3	2.45	0.51
1:B:98:TYR:CE2	2:G:100:VAL:HG11	2.45	0.51
8:N:139:LEU:O	8:N:143:HIS:HB3	2.11	0.51
8:N:388:GLU:HG3	8:N:391:PHE:HD2	1.75	0.51
10:Q:415:VAL:O	10:Q:419:LEU:HG	2.10	0.51
16:Y:480:GLU:HA	16:Y:483:PHE:CD1	2.45	0.51
18:a:1643:GLU:O	18:a:1646:SER:OG	2.21	0.51
7:A:860:TYR:O	7:A:863:ILE:HG22	2.11	0.51
7:A:1275:ARG:N	7:A:1279:GLU:OE2	2.20	0.51
8:N:75:LEU:HD23	8:N:76:ARG:HG3	1.93	0.51
10:Q:147:GLY:O	10:Q:148:LEU:HD23	2.11	0.51
10:Q:301:GLY:O	10:Q:305:LEU:HD23	2.11	0.51
11:R:283:LEU:HD21	15:W:622:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:602:THR:O	15:W:606:THR:N	2.34	0.51
15:X:922:TYR:O	15:X:926:GLN:N	2.35	0.51
17:Z:247:GLN:O	17:Z:251:ARG:N	2.33	0.51
18:a:1636:ARG:HD3	18:a:1667:TRP:CE3	2.45	0.51
7:A:422:VAL:HA	7:A:425:ARG:HG2	1.93	0.50
7:A:427:ASP:OD1	7:A:428:THR:N	2.45	0.50
7:A:925:LEU:H	7:A:925:LEU:HD12	1.77	0.50
10:Q:365:SER:O	10:Q:371:LYS:NZ	2.24	0.50
11:R:210:PHE:HE2	15:X:485:ALA:HA	1.76	0.50
11:R:280:ASN:HB3	15:W:619:ASP:CB	2.40	0.50
14:V:138:SER:C	14:V:321:TRP:HD1	2.19	0.50
15:W:931:ARG:HH21	15:X:923:GLN:HE21	1.57	0.50
7:A:464:GLN:O	7:A:468:ARG:N	2.33	0.50
7:A:983:GLU:OE2	7:A:984:VAL:HG23	2.10	0.50
8:N:391:PHE:O	8:N:395:ILE:HG12	2.11	0.50
10:Q:211:ASP:HB3	10:Q:311:THR:HG21	1.94	0.50
10:Q:452:MET:SD	10:Q:453:ASP:N	2.85	0.50
11:R:266:TYR:OH	11:R:268:ARG:NE	2.43	0.50
16:Y:341:LYS:HG2	16:Y:342:TYR:N	2.27	0.50
7:A:411:ASN:OD1	7:A:412:PHE:N	2.45	0.50
8:N:377:ARG:NE	8:N:377:ARG:HA	2.25	0.50
14:V:347:ASP:HA	15:X:488:ARG:HH21	1.76	0.50
18:a:1612:LYS:O	18:a:1615:GLU:HG3	2.11	0.50
1:B:47:SER:OG	1:B:48:GLY:N	2.45	0.50
2:C:79:ILE:HG12	2:C:82:HIS:CE1	2.46	0.50
4:E:48:LEU:HD21	1:F:44:LYS:HE3	1.93	0.50
3:H:51:ASP:OD1	3:H:51:ASP:N	2.36	0.50
7:A:888:ASN:HB3	7:A:891:CYS:HB2	1.93	0.50
8:N:71:ASP:OD2	8:N:73:ASN:ND2	2.43	0.50
8:N:172:SER:HA	8:N:177:THR:HA	1.92	0.50
12:T:375:THR:HB	12:T:377:ARG:CZ	2.41	0.50
12:T:551:ARG:HA	12:T:551:ARG:NE	2.27	0.50
15:W:442:GLU:CD	15:W:462:TYR:HH	2.20	0.50
6:J:15:DT:H4'	6:J:16:DC:OP1	2.10	0.50
6:J:25:DG:N7	6:J:26:DC:N4	2.60	0.50
7:A:780:GLU:O	7:A:785:LYS:NZ	2.43	0.50
8:N:355:THR:HB	8:N:384:ASN:OD1	2.11	0.50
9:P:18:LYS:HD3	9:P:337:TYR:HD1	1.76	0.50
10:Q:429:GLY:O	10:Q:433:CYS:HB2	2.12	0.50
11:R:280:ASN:HB3	15:W:619:ASP:HB2	1.94	0.50
14:V:266:LEU:N	14:V:277:ASP:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:356:LEU:HD12	14:V:360:GLU:CB	2.42	0.50
15:X:437:SER:O	15:X:466:ARG:NH1	2.44	0.50
16:Y:142:PRO:O	16:Y:143:GLU:HG3	2.12	0.50
16:Y:329:GLN:HE21	16:Y:334:ARG:HB3	1.76	0.50
2:G:78:ILE:HB	3:H:54:ILE:HG13	1.94	0.50
7:A:1065:PHE:HZ	7:A:1070:VAL:HG13	1.77	0.50
7:A:1099:VAL:HG23	7:A:1170:THR:HG23	1.93	0.50
7:A:1268:THR:O	7:A:1271:GLN:HB3	2.12	0.50
9:P:143:TYR:HE2	9:P:346:LEU:HD13	1.77	0.50
9:P:151:ILE:HG22	9:P:164:PRO:HA	1.93	0.50
10:Q:63:VAL:O	10:Q:67:ASN:N	2.45	0.50
10:Q:132:ASN:N	14:V:227:ASP:OD2	2.34	0.50
15:W:603:GLU:HA	15:W:606:THR:HB	1.93	0.50
19:M:311:UNK:O	19:M:315:UNK:N	2.45	0.50
7:A:378:ILE:HG22	15:W:648:TYR:HE2	1.77	0.50
7:A:768:LEU:HD22	7:A:773:LEU:HB2	1.93	0.50
7:A:1088:ILE:HG22	7:A:1273:ILE:HD11	1.93	0.50
9:P:149:THR:HG22	9:P:167:GLU:H	1.77	0.50
10:Q:60:PHE:HB2	10:Q:93:TYR:CE1	2.47	0.50
10:Q:309:ASN:HD21	10:Q:311:THR:HG1	1.59	0.50
10:Q:400:TYR:HA	10:Q:403:ILE:HD12	1.93	0.50
14:V:360:GLU:HA	14:V:363:LYS:NZ	2.26	0.50
15:X:601:TRP:O	15:X:602:THR:OG1	2.22	0.50
15:X:896:MET:O	15:X:900:GLU:N	2.38	0.50
6:J:118:DT:H2''	6:J:119:DT:C7	2.42	0.50
7:A:185:MET:HB3	7:A:189:MET:HE1	1.93	0.50
8:N:249:SER:HA	8:N:252:ASN:HB2	1.94	0.50
14:V:276:VAL:HB	14:V:352:LEU:HB2	1.94	0.50
6:J:73:DA:H5'	6:J:73:DA:C8	2.46	0.50
7:A:417:ARG:HG2	15:W:640:LEU:HG	1.93	0.50
7:A:1009:ARG:O	7:A:1013:ALA:N	2.44	0.50
8:N:260:GLN:HA	8:N:263:GLN:HG2	1.93	0.50
10:Q:87:PHE:O	10:Q:91:GLN:HG2	2.12	0.50
11:R:212:SER:HA	15:X:479:GLU:OE2	2.11	0.50
5:I:123:DC:H2''	5:I:124:DA:C8	2.46	0.49
7:A:1162:GLY:HA2	7:A:1189:ARG:NH2	2.27	0.49
15:W:605:GLU:O	15:W:608:LEU:HB2	2.12	0.49
18:a:1610:TYR:O	18:a:1614:ILE:HD12	2.12	0.49
4:E:133:GLU:N	4:E:133:GLU:OE2	2.45	0.49
7:A:1223:ASN:HB3	7:A:1227:LYS:NZ	2.27	0.49
9:P:164:PRO:HB2	9:P:171:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:262:PHE:O	9:P:275:HIS:HE1	1.95	0.49
14:V:190:ARG:HB2	14:V:313:TYR:OH	2.12	0.49
14:V:279:PHE:HB2	15:X:494:VAL:HG21	1.94	0.49
7:A:197:PRO:HB2	7:A:199:HIS:CE1	2.47	0.49
16:Y:348:GLU:H	16:Y:360:ARG:HH22	1.58	0.49
3:D:95:GLN:OE1	3:D:99:ARG:NH2	2.45	0.49
7:A:1300:ARG:HB3	7:A:1300:ARG:NH1	2.27	0.49
11:R:258:ILE:H	11:R:261:GLN:NE2	2.11	0.49
14:V:241:ILE:O	14:V:245:ILE:HG13	2.12	0.49
14:V:362:GLU:HG3	14:V:366:ARG:HH11	1.76	0.49
14:V:363:LYS:HA	14:V:366:ARG:HG2	1.93	0.49
15:W:610:LEU:O	15:W:614:GLU:HG2	2.12	0.49
15:X:454:ASN:CG	15:X:457:LYS:HG3	2.37	0.49
18:a:1650:SER:O	18:a:1662:MET:HE1	2.12	0.49
3:H:39:ILE:HG13	3:H:40:TYR:N	2.27	0.49
5:I:82:DC:N3	6:J:66:DG:N2	2.53	0.49
7:A:783:LEU:N	22:A:1703:ADP:O3B	2.44	0.49
7:A:1049:PRO:HG2	7:A:1303:ARG:HH22	1.76	0.49
8:N:405:THR:HA	8:N:408:GLN:HG2	1.93	0.49
9:P:193:LEU:HD11	9:P:253:GLU:HG3	1.94	0.49
10:Q:94:LEU:HA	10:Q:98:GLU:HG2	1.94	0.49
10:Q:432:ALA:HA	10:Q:435:LYS:HG2	1.93	0.49
11:R:218:ARG:HD3	14:V:300:GLU:O	2.13	0.49
11:R:266:TYR:CZ	16:Y:489:GLU:HG3	2.47	0.49
11:R:276:TYR:HD1	11:R:284:TYR:HB2	1.76	0.49
14:V:312:ALA:O	14:V:316:ARG:HG3	2.11	0.49
5:I:101:DG:H2''	5:I:102:DG:C8	2.47	0.49
7:A:382:ILE:O	7:A:386:GLU:N	2.40	0.49
7:A:898:ASN:OD1	7:A:899:THR:N	2.45	0.49
8:N:72:THR:HG21	9:P:176:LEU:HD21	1.94	0.49
8:N:101:ALA:HA	8:N:104:ASP:HB3	1.94	0.49
15:W:424:ILE:HA	15:W:513:GLN:OE1	2.11	0.49
15:W:611:GLU:HA	15:W:614:GLU:HG2	1.94	0.49
15:X:631:THR:HG22	15:X:634:GLU:HG2	1.93	0.49
1:B:46:ILE:HG22	1:B:47:SER:O	2.13	0.49
5:I:34:DG:H5'	5:I:34:DG:C8	2.47	0.49
5:I:92:DC:N3	6:J:56:DG:N2	2.49	0.49
6:J:134:DC:H2''	6:J:135:DC:C5	2.48	0.49
7:A:383:GLN:O	7:A:387:ASN:ND2	2.46	0.49
8:N:19:GLY:HA3	8:N:24:ARG:CZ	2.43	0.49
10:Q:52:THR:HA	10:Q:55:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:166:LEU:HD22	15:W:507:TRP:CZ2	2.47	0.49
10:Q:231:ARG:NH1	10:Q:281:ILE:HD12	2.27	0.49
14:V:225:ASP:OD1	14:V:226:LEU:N	2.45	0.49
1:F:77:LYS:HE2	3:H:92:ARG:CZ	2.43	0.49
7:A:375:GLN:HG2	12:T:385:LEU:HB3	1.95	0.49
7:A:955:ASP:OD1	7:A:1227:LYS:HE3	2.13	0.49
10:Q:167:SER:OG	10:Q:172:GLU:OE2	2.19	0.49
10:Q:1778:ASN:HA	10:Q:1781:LYS:HB2	1.94	0.49
10:Q:1808:SER:HB2	16:Y:355:SER:HB3	1.94	0.49
12:T:611:VAL:O	12:T:612:ARG:HD2	2.12	0.49
15:X:913:MET:HA	15:X:916:GLU:OE1	2.13	0.49
4:E:46:VAL:O	4:E:50:GLU:HG3	2.13	0.49
5:I:54:DC:H2'	5:I:55:DG:C8	2.48	0.49
6:J:62:DA:H5'	6:J:62:DA:C8	2.48	0.49
7:A:790:ILE:HG12	7:A:822:PHE:HE1	1.77	0.49
7:A:1017:LEU:HD12	7:A:1018:LEU:H	1.78	0.49
10:Q:238:LYS:O	10:Q:247:ARG:NH2	2.46	0.49
15:W:435:TYR:CD2	15:X:529:SER:HB3	2.48	0.49
16:Y:137:ILE:HD13	16:Y:438:ARG:NH2	2.24	0.49
5:I:36:DC:H2''	5:I:37:DG:C8	2.47	0.49
7:A:454:GLU:OE2	10:Q:1770:LEU:HD13	2.12	0.49
7:A:501:THR:HG21	9:P:168:GLY:HA3	1.94	0.49
7:A:546:LYS:O	7:A:550:LEU:HD23	2.13	0.49
7:A:967:ARG:O	7:A:971:VAL:N	2.45	0.49
10:Q:192:GLN:HB3	10:Q:194:GLU:OE2	2.11	0.49
11:R:263:GLN:NE2	11:R:265:TYR:HB3	2.28	0.49
14:V:305:GLY:HA2	15:W:489:ASN:OD1	2.12	0.49
15:W:612:ALA:HA	15:W:626:HIS:CD2	2.48	0.49
15:X:478:GLN:O	15:X:514:VAL:HG12	2.12	0.49
15:X:616:TYR:OH	15:X:623:VAL:HG23	2.12	0.49
15:X:941:TYR:HA	15:X:944:MET:HE2	1.95	0.49
5:I:89:DT:H2''	5:I:90:DA:C8	2.48	0.48
5:I:98:DA:H2''	5:I:99:DG:C8	2.47	0.48
7:A:370:ARG:O	7:A:374:LEU:HD23	2.13	0.48
7:A:743:ASP:HB3	7:A:762:LEU:HD23	1.93	0.48
8:N:360:PHE:CE2	8:N:364:LEU:HD22	2.48	0.48
10:Q:50:LEU:C	10:Q:52:THR:H	2.19	0.48
15:X:535:ALA:HB2	15:X:544:LEU:HD23	1.94	0.48
2:G:57:TYR:HB2	3:H:113:GLU:OE1	2.13	0.48
6:J:124:DG:C6	6:J:125:DG:C6	3.00	0.48
7:A:790:ILE:HG12	7:A:822:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1048:HIS:CD2	7:A:1082:PHE:CE2	3.01	0.48
1:F:22:LEU:H	1:F:22:LEU:HD12	1.78	0.48
6:J:22:DC:H2''	6:J:23:DG:H8	1.78	0.48
7:A:774:ASN:OD1	7:A:905:ARG:NH1	2.45	0.48
8:N:23:VAL:HG12	8:N:37:PHE:O	2.13	0.48
12:T:369:VAL:O	12:T:369:VAL:HG12	2.13	0.48
12:T:392:LYS:CB	12:T:393:ARG:HH11	2.22	0.48
15:W:632:GLN:O	15:W:636:ILE:HD12	2.13	0.48
16:Y:153:PHE:HA	16:Y:156:LYS:HG3	1.96	0.48
1:B:84:MET:HA	1:B:84:MET:HE3	1.93	0.48
7:A:179:GLN:OE1	12:T:546:LEU:HD22	2.13	0.48
7:A:550:LEU:HD13	7:A:553:LEU:HD22	1.96	0.48
7:A:886:MET:HG3	7:A:894:THR:HG22	1.94	0.48
7:A:929:LEU:HB3	7:A:932:ILE:HB	1.93	0.48
7:A:988:LEU:HD13	7:A:989:PRO:HD2	1.95	0.48
14:V:142:LEU:HD21	14:V:321:TRP:CG	2.49	0.48
14:V:144:ALA:O	14:V:190:ARG:NH1	2.46	0.48
15:X:615:MET:SD	15:X:626:HIS:ND1	2.86	0.48
18:a:1674:LEU:O	18:a:1677:THR:OG1	2.28	0.48
4:K:52:ARG:O	4:K:56:LYS:HE3	2.13	0.48
4:E:129:ARG:NH1	4:E:129:ARG:O	2.46	0.48
5:I:58:DT:H4'	5:I:59:DA:H5'	1.95	0.48
7:A:943:PHE:O	7:A:956:LEU:HD11	2.13	0.48
7:A:1062:HIS:CE1	7:A:1310:LEU:HD21	2.47	0.48
9:P:337:TYR:O	9:P:341:ILE:HG12	2.13	0.48
9:P:358:SER:H	9:P:361:GLU:CD	2.22	0.48
9:P:369:ILE:O	9:P:372:ARG:HD2	2.12	0.48
10:Q:161:LEU:O	10:Q:164:SER:OG	2.26	0.48
11:R:267:LYS:NZ	18:a:1676:ASP:O	2.46	0.48
14:V:306:GLU:H	14:V:306:GLU:CD	2.20	0.48
14:V:358:ASP:OD2	14:V:359:ALA:N	2.46	0.48
15:X:877:ALA:HB2	17:Z:224:MET:HE1	1.94	0.48
18:a:1657:GLY:O	18:a:1659:HIS:ND1	2.30	0.48
2:G:87:VAL:HG23	2:G:93:LEU:HB3	1.96	0.48
7:A:552:TYR:HA	7:A:555:GLN:OE1	2.13	0.48
7:A:805:PRO:HB2	7:A:875:TRP:CE3	2.48	0.48
8:N:100:GLN:O	8:N:104:ASP:N	2.42	0.48
10:Q:43:LYS:NZ	10:Q:45:LEU:HD12	2.28	0.48
10:Q:431:VAL:O	10:Q:435:LYS:HG2	2.13	0.48
11:R:256:ALA:N	11:R:263:GLN:HB3	2.28	0.48
11:R:272:ASP:OD1	11:R:273:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:362:GLU:HG3	14:V:366:ARG:NH1	2.28	0.48
3:H:108:LYS:HG3	3:H:109:HIS:N	2.28	0.48
7:A:1039:ILE:H	7:A:1039:ILE:HD12	1.77	0.48
9:P:189:LEU:HD23	9:P:209:VAL:HB	1.95	0.48
10:Q:1769:ARG:HD2	10:Q:1805:MET:HE1	1.94	0.48
14:V:165:PRO:HB2	14:V:171:HIS:NE2	2.29	0.48
14:V:242:ARG:HA	14:V:245:ILE:HD12	1.95	0.48
15:W:894:THR:O	15:W:898:LYS:HG3	2.14	0.48
15:X:427:PRO:HG3	15:X:512:TYR:CZ	2.48	0.48
16:Y:500:GLN:NE2	16:Y:503:ARG:HH12	2.12	0.48
4:E:119:ILE:HG13	4:E:119:ILE:O	2.13	0.48
7:A:363:PRO:HB3	17:Z:193:THR:HG21	1.96	0.48
7:A:415:GLN:OE1	18:a:1597:PRO:HB2	2.14	0.48
7:A:785:LYS:HB3	7:A:909:LEU:HD23	1.95	0.48
7:A:1128:GLY:O	7:A:1129:THR:OG1	2.23	0.48
9:P:154:ASP:HB3	9:P:161:HIS:HB2	1.95	0.48
9:P:275:HIS:CD2	9:P:276:GLU:HG3	2.48	0.48
10:Q:316:LEU:O	10:Q:319:SER:OG	2.16	0.48
15:W:427:PRO:O	15:W:428:SER:OG	2.32	0.48
15:X:913:MET:C	15:X:917:ARG:HH21	2.19	0.48
15:X:914:ASP:OD2	15:X:915:ARG:N	2.46	0.48
16:Y:161:ILE:HG13	16:Y:162:MET:N	2.29	0.48
7:A:180:LEU:O	7:A:184:ILE:HG12	2.13	0.48
7:A:549:ARG:O	7:A:552:TYR:N	2.46	0.48
8:N:167:GLY:HA2	8:N:347:SER:OG	2.13	0.48
12:T:611:VAL:HG13	13:U:51:UNK:O	2.13	0.48
14:V:369:ASP:O	14:V:372:THR:OG1	2.21	0.48
2:G:111:ILE:HG12	4:K:51:ILE:HG21	1.96	0.48
5:I:15:DT:C2	5:I:16:DG:C8	3.01	0.48
8:N:172:SER:N	8:N:351:ALA:O	2.47	0.48
8:N:181:PRO:HD2	8:N:192:ILE:HG22	1.96	0.48
12:T:390:GLU:CD	12:T:394:ASN:H	2.21	0.48
12:T:611:VAL:HG22	13:U:51:UNK:O	2.13	0.48
15:W:878:ALA:O	15:W:882:ARG:HG2	2.14	0.48
17:Z:266:PHE:CZ	17:Z:270:LEU:HD21	2.49	0.48
7:A:196:LEU:HD23	7:A:196:LEU:H	1.79	0.47
9:P:219:VAL:HG11	9:P:262:PHE:CE2	2.48	0.47
10:Q:287:LEU:HD12	10:Q:324:PHE:CZ	2.49	0.47
15:W:601:TRP:CZ3	15:W:630:ARG:HG3	2.49	0.47
15:W:887:LEU:HD23	15:W:890:LEU:HD13	1.95	0.47
15:X:924:ARG:HH12	16:Y:317:GLN:NE2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:741:ARG:NH1	7:A:763:GLU:HG2	2.29	0.47
7:A:953:LYS:NZ	7:A:1255:GLU:OE2	2.41	0.47
10:Q:237:TRP:HB3	10:Q:250:ILE:HD13	1.96	0.47
10:Q:271:HIS:ND1	10:Q:272:PRO:HD2	2.30	0.47
10:Q:1794:GLU:O	10:Q:1798:SER:N	2.33	0.47
2:C:69:ALA:HA	7:A:1346:TYR:CD1	2.49	0.47
3:D:105:GLU:OE2	3:D:109:HIS:HE1	1.97	0.47
5:I:36:DC:N4	6:J:112:DG:H1	2.13	0.47
5:I:82:DC:H2''	5:I:83:DG:H8	1.79	0.47
5:I:83:DG:H1	6:J:65:DC:N4	2.11	0.47
7:A:869:ILE:HG13	7:A:870:LEU:HD22	1.95	0.47
7:A:1085:LEU:HD11	7:A:1174:PHE:HE2	1.79	0.47
8:N:100:GLN:HB3	8:N:139:LEU:HD11	1.95	0.47
9:P:20:GLY:HA3	9:P:340:TRP:HZ2	1.77	0.47
9:P:136:ILE:HG22	9:P:138:ALA:H	1.78	0.47
11:R:236:PRO:HB3	15:X:521:THR:OG1	2.12	0.47
15:W:600:GLU:O	15:W:630:ARG:NH1	2.47	0.47
16:Y:136:ARG:HG3	16:Y:438:ARG:NH2	2.29	0.47
6:J:27:DC:H2''	6:J:28:DT:C7	2.43	0.47
7:A:943:PHE:C	7:A:945:ALA:H	2.23	0.47
9:P:212:ILE:HG12	9:P:240:TYR:CD2	2.49	0.47
10:Q:24:ARG:NH1	10:Q:25:GLN:OE1	2.46	0.47
10:Q:1780:GLY:O	10:Q:1787:ARG:HD2	2.14	0.47
12:T:593:LEU:O	12:T:597:ALA:N	2.46	0.47
4:E:116:ARG:NH1	4:E:118:THR:O	2.48	0.47
3:H:67:ASN:O	3:H:71:GLU:OE1	2.33	0.47
5:I:119:DC:H2''	5:I:120:DA:N7	2.29	0.47
7:A:898:ASN:OD1	7:A:899:THR:HG23	2.14	0.47
7:A:978:ARG:HG3	7:A:979:ARG:H	1.79	0.47
7:A:899:THR:OG1	7:A:900:HIS:ND1	2.41	0.47
9:P:261:LEU:HB3	9:P:274:ILE:CG1	2.44	0.47
10:Q:281:ILE:HG13	10:Q:282:GLU:N	2.28	0.47
10:Q:450:VAL:HG21	10:Q:1776:LEU:HD11	1.96	0.47
14:V:185:VAL:O	14:V:207:ASN:HA	2.14	0.47
14:V:188:PRO:HG3	14:V:316:ARG:C	2.39	0.47
15:W:885:LYS:HA	15:W:888:VAL:HG12	1.96	0.47
15:X:619:ASP:HB3	15:X:622:LYS:HG2	1.97	0.47
16:Y:294:GLN:HE21	16:Y:310:GLN:C	2.23	0.47
16:Y:341:LYS:HG2	16:Y:342:TYR:H	1.80	0.47
16:Y:463:LEU:HB3	17:Z:196:PHE:CE1	2.50	0.47
1:B:35:ARG:O	1:B:39:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:HG2	4:K:118:THR:HG23	1.97	0.47
2:C:63:LEU:HD11	3:D:41:VAL:HG13	1.95	0.47
4:E:60:LEU:HD13	4:E:93:GLN:CD	2.40	0.47
3:H:62:MET:HE3	3:H:62:MET:HA	1.97	0.47
5:I:35:DT:H1'	5:I:36:DC:H5'	1.96	0.47
5:I:43:DA:C6	5:I:44:DG:C6	3.03	0.47
7:A:185:MET:HA	7:A:185:MET:HE2	1.96	0.47
7:A:1192:ARG:NH1	22:A:1703:ADP:O1A	2.48	0.47
9:P:20:GLY:HA3	9:P:340:TRP:CZ2	2.50	0.47
9:P:219:VAL:HG11	9:P:262:PHE:HE2	1.79	0.47
10:Q:286:VAL:HA	10:Q:289:ILE:HG22	1.96	0.47
10:Q:456:MET:HE3	10:Q:456:MET:HB3	1.79	0.47
14:V:169:ASP:OD1	14:V:169:ASP:C	2.58	0.47
14:V:288:ASN:HA	15:X:495:CYS:SG	2.55	0.47
15:W:610:LEU:HD12	15:W:611:GLU:N	2.30	0.47
15:W:924:ARG:NH2	17:Z:263:THR:HA	2.30	0.47
15:W:927:LEU:HD21	15:X:923:GLN:OE1	2.15	0.47
16:Y:158:ASP:HA	16:Y:161:ILE:HG12	1.95	0.47
16:Y:319:LEU:O	16:Y:323:ILE:HG12	2.15	0.47
17:Z:195:ARG:O	17:Z:198:ARG:HG2	2.14	0.47
6:J:17:DT:H2''	6:J:18:DG:N7	2.30	0.47
7:A:484:LYS:HE2	8:N:163:GLY:HA2	1.97	0.47
7:A:546:LYS:HG2	7:A:550:LEU:HD23	1.96	0.47
8:N:168:LEU:HA	8:N:181:PRO:HA	1.95	0.47
10:Q:51:TYR:HB2	10:Q:97:LEU:HD13	1.97	0.47
11:R:263:GLN:OE1	11:R:265:TYR:N	2.27	0.47
12:T:377:ARG:HB3	12:T:379:GLN:OE1	2.15	0.47
15:X:918:GLU:O	15:X:922:TYR:N	2.34	0.47
6:J:91:DA:C6	6:J:92:DG:C6	3.03	0.47
7:A:1047:ASN:HD22	7:A:1105:MET:CE	2.28	0.47
7:A:1098:LYS:NZ	7:A:1142:PHE:O	2.29	0.47
7:A:1100:LEU:HD23	7:A:1100:LEU:H	1.80	0.47
10:Q:138:VAL:HG23	10:Q:139:SER:N	2.30	0.47
10:Q:301:GLY:HA2	10:Q:304:LYS:HZ3	1.80	0.47
14:V:306:GLU:O	14:V:309:THR:N	2.47	0.47
16:Y:494:TYR:O	16:Y:497:SER:OG	2.27	0.47
9:P:90:PHE:HE1	9:P:103:VAL:HG11	1.80	0.47
9:P:279:PHE:CD2	9:P:320:LEU:HD22	2.50	0.47
10:Q:433:CYS:SG	10:Q:1779:ILE:HD13	2.55	0.47
14:V:183:PRO:HA	15:W:454:ASN:OD1	2.14	0.47
15:X:454:ASN:ND2	15:X:457:LYS:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:112:SER:OG	14:V:374:ARG:NH2	2.48	0.46
7:A:1090:PRO:O	7:A:1093:ARG:HB2	2.13	0.46
10:Q:54:VAL:HG11	10:Q:93:TYR:CE2	2.51	0.46
10:Q:304:LYS:HA	10:Q:341:GLU:HG2	1.97	0.46
15:W:931:ARG:HE	17:Z:270:LEU:HD12	1.81	0.46
3:D:39:ILE:O	3:D:43:LYS:HG3	2.15	0.46
6:J:53:DG:H2''	6:J:54:DC:H6	1.81	0.46
22:A:1703:ADP:O1B	22:A:1703:ADP:H5'2	2.14	0.46
9:P:367:PRO:O	9:P:370:VAL:HG22	2.15	0.46
15:W:608:LEU:O	15:W:612:ALA:N	2.46	0.46
15:X:465:TYR:CE2	15:X:490:LEU:HB3	2.50	0.46
2:G:77:ARG:HA	3:H:53:GLY:O	2.15	0.46
5:I:83:DG:OP1	4:K:46:VAL:HB	2.15	0.46
5:I:129:DT:H3	6:J:19:DA:N6	2.13	0.46
6:J:12:DA:H1'	6:J:13:DT:H5'	1.97	0.46
7:A:877:TYR:CD1	7:A:905:ARG:HB2	2.51	0.46
9:P:106:THR:HA	9:P:135:ALA:O	2.15	0.46
9:P:291:LYS:HA	9:P:325:MET:SD	2.56	0.46
10:Q:32:SER:HB3	10:Q:129:SER:HB2	1.98	0.46
10:Q:274:ARG:HH21	10:Q:280:ASP:HB2	1.80	0.46
12:T:233:SER:HB2	12:T:235:GLU:OE1	2.16	0.46
15:W:456:SER:O	15:W:461:ILE:HG13	2.15	0.46
15:W:476:ASN:OD1	15:W:478:GLN:NE2	2.48	0.46
15:X:485:ALA:O	15:X:488:ARG:HG2	2.14	0.46
16:Y:135:GLN:HA	16:Y:138:ARG:NE	2.31	0.46
5:I:82:DC:H2''	5:I:83:DG:C8	2.51	0.46
7:A:991:LYS:HB2	7:A:1191:HIS:CD2	2.51	0.46
8:N:107:TYR:OH	8:N:146:ILE:HD13	2.16	0.46
10:Q:62:LYS:O	10:Q:66:LYS:HG2	2.16	0.46
11:R:197:PRO:HB2	11:R:200:ILE:HG12	1.98	0.46
15:W:484:THR:HA	15:W:487:ARG:HG2	1.97	0.46
15:W:917:ARG:HD2	15:W:918:GLU:N	2.31	0.46
16:Y:440:PHE:HD1	16:Y:441:MET:HE2	1.80	0.46
7:A:446:SER:HA	10:Q:517:GLU:HA	1.97	0.46
7:A:785:LYS:H	22:A:1703:ADP:PB	2.39	0.46
10:Q:441:LYS:HD2	16:Y:163:ARG:NE	2.30	0.46
10:Q:1816:TYR:HB3	16:Y:334:ARG:NH1	2.30	0.46
15:X:908:GLU:O	15:X:912:ILE:HG12	2.16	0.46
16:Y:142:PRO:C	16:Y:144:SER:H	2.24	0.46
16:Y:463:LEU:HB3	17:Z:196:PHE:CZ	2.50	0.46
17:Z:198:ARG:HH11	17:Z:201:ARG:NH2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Z:230:GLN:O	17:Z:234:LEU:HD13	2.16	0.46
18:a:1620:GLU:N	18:a:1620:GLU:OE2	2.48	0.46
18:a:1670:ARG:HA	18:a:1673:MET:SD	2.55	0.46
4:K:42:ARG:HD3	4:K:42:ARG:N	2.31	0.46
1:F:56:GLY:O	1:F:59:LYS:HB3	2.15	0.46
5:I:26:DC:H2''	5:I:27:DT:C6	2.50	0.46
5:I:100:DG:C6	5:I:101:DG:N1	2.84	0.46
5:I:121:DG:H2''	5:I:122:DG:C8	2.50	0.46
6:J:94:DG:H2''	6:J:95:DG:O5'	2.14	0.46
7:A:787:ILE:H	7:A:787:ILE:HD12	1.81	0.46
7:A:991:LYS:HD2	7:A:1191:HIS:CG	2.51	0.46
7:A:1142:PHE:CE2	7:A:1152:PHE:HB2	2.51	0.46
8:N:280:ALA:HB2	8:N:301:ARG:HE	1.79	0.46
10:Q:131:TYR:CE1	14:V:227:ASP:HB2	2.50	0.46
10:Q:292:ILE:H	10:Q:292:ILE:HD12	1.81	0.46
16:Y:299:PRO:HA	16:Y:302:ALA:HB3	1.98	0.46
16:Y:427:THR:HG22	16:Y:431:ILE:HD11	1.97	0.46
6:J:37:DG:H2''	6:J:38:DG:N7	2.31	0.46
6:J:49:DC:C2	6:J:50:DT:C4	3.04	0.46
10:Q:422:LEU:HA	10:Q:425:LEU:HB2	1.98	0.46
12:T:398:PRO:HB3	12:T:421:ILE:HD11	1.97	0.46
18:a:1676:ASP:OD1	18:a:1677:THR:N	2.49	0.46
4:E:65:LEU:HD23	6:J:92:DG:OP2	2.16	0.46
10:Q:304:LYS:HG3	10:Q:305:LEU:HD22	1.96	0.46
10:Q:390:LEU:HD13	10:Q:394:TYR:HE2	1.80	0.46
12:T:399:VAL:HG12	12:T:426:SER:OG	2.15	0.46
5:I:18:DC:H2''	5:I:19:DG:C8	2.51	0.46
5:I:37:DG:H2''	5:I:38:DT:H72	1.98	0.46
7:A:170:THR:HG21	7:A:177:LEU:HB2	1.97	0.46
7:A:541:LEU:HB3	7:A:545:LYS:NZ	2.31	0.46
7:A:883:GLY:HA3	7:A:908:LEU:HD12	1.98	0.46
7:A:1280:PHE:CD1	7:A:1284:MET:HE3	2.51	0.46
8:N:157:LEU:O	8:N:161:ALA:N	2.39	0.46
8:N:373:PRO:HB2	8:N:376:MET:HE3	1.98	0.46
10:Q:65:GLU:H	10:Q:65:GLU:CD	2.24	0.46
16:Y:148:MET:SD	16:Y:149:ASP:N	2.89	0.46
6:J:92:DG:C4	6:J:93:DC:C5	3.04	0.46
7:A:785:LYS:HB2	22:A:1703:ADP:O2B	2.15	0.46
8:N:167:GLY:O	8:N:182:VAL:N	2.32	0.46
10:Q:416:ILE:HA	10:Q:419:LEU:HD12	1.97	0.46
11:R:266:TYR:HA	16:Y:496:TYR:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:924:ARG:HH22	17:Z:263:THR:HA	1.80	0.46
16:Y:163:ARG:HG2	16:Y:163:ARG:HH21	1.81	0.46
17:Z:185:GLY:HA2	17:Z:190:HIS:CD2	2.51	0.46
5:I:124:DA:H1'	5:I:125:DC:H5'	1.97	0.45
8:N:257:CYS:HA	8:N:260:GLN:OE1	2.16	0.45
9:P:177:ARG:NH2	9:P:179:ASP:OD1	2.49	0.45
9:P:328:LYS:HG2	9:P:330:ILE:HG23	1.97	0.45
10:Q:1764:ILE:O	10:Q:1768:ILE:HG13	2.16	0.45
11:R:274:LEU:HA	11:R:277:LEU:HG	1.97	0.45
12:T:193:ILE:HD13	12:T:240:LEU:HD23	1.98	0.45
15:W:622:LYS:O	15:W:626:HIS:N	2.37	0.45
17:Z:193:THR:O	17:Z:197:GLN:HG2	2.16	0.45
1:B:31:LYS:O	1:B:35:ARG:HG3	2.16	0.45
6:J:80:DA:H2''	6:J:81:DC:C5	2.51	0.45
7:A:1078:ALA:HB1	7:A:1303:ARG:HH21	1.81	0.45
7:A:1231:ALA:HA	7:A:1246:PHE:CD2	2.51	0.45
10:Q:336:GLY:O	10:Q:380:ASN:ND2	2.47	0.45
10:Q:1785:CYS:HA	10:Q:1788:ARG:HE	1.81	0.45
11:R:270:SER:OG	11:R:273:GLU:OE1	2.32	0.45
14:V:361:MET:O	14:V:365:ILE:HG23	2.17	0.45
15:X:536:ASP:OD2	18:a:1624:ILE:HB	2.15	0.45
16:Y:422:ASN:O	16:Y:426:GLU:HG2	2.16	0.45
2:G:112:GLN:HB2	2:G:115:LEU:HD23	1.97	0.45
5:I:24:DC:C2	6:J:125:DG:N2	2.84	0.45
5:I:32:DT:H2''	5:I:33:DG:H8	1.81	0.45
8:N:214:ASN:CG	8:N:215:ILE:H	2.25	0.45
14:V:229:ASN:HB3	14:V:232:THR:HB	1.98	0.45
2:G:88:ARG:HB2	2:G:108:LEU:HD21	1.97	0.45
6:J:98:DC:H5'	6:J:98:DC:H6	1.82	0.45
7:A:434:LEU:HD23	7:A:434:LEU:O	2.17	0.45
7:A:939:PHE:CE1	7:A:941:GLN:HG3	2.52	0.45
7:A:1010:HIS:O	7:A:1014:LYS:N	2.47	0.45
7:A:1300:ARG:HB3	7:A:1300:ARG:CZ	2.47	0.45
9:P:291:LYS:HG3	9:P:292:ASP:N	2.31	0.45
10:Q:54:VAL:HG11	10:Q:93:TYR:HE2	1.81	0.45
10:Q:68:GLN:HG2	10:Q:71:GLU:OE2	2.16	0.45
10:Q:75:GLU:OE2	10:Q:76:PHE:HB2	2.17	0.45
10:Q:184:SER:HB3	10:Q:292:ILE:HG23	1.98	0.45
10:Q:271:HIS:CG	10:Q:272:PRO:HD2	2.51	0.45
10:Q:351:THR:O	10:Q:355:MET:HG2	2.17	0.45
10:Q:465:VAL:HG23	10:Q:466:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:640:LEU:HD23	16:Y:482:TYR:CE1	2.51	0.45
15:W:893:GLU:O	15:W:897:LYS:HG3	2.17	0.45
16:Y:331:PRO:HA	16:Y:334:ARG:HD3	1.99	0.45
17:Z:232:GLN:OE1	17:Z:233:SER:OG	2.29	0.45
1:B:44:LYS:HD3	2:G:115:LEU:HD12	1.99	0.45
6:J:121:DA:C6	6:J:122:DG:C6	3.03	0.45
7:A:845:VAL:O	7:A:849:ARG:HG2	2.16	0.45
7:A:1087:ARG:O	7:A:1090:PRO:HD2	2.17	0.45
7:A:1200:ARG:NH2	7:A:1275:ARG:HG2	2.30	0.45
7:A:1293:GLU:O	7:A:1296:ARG:HD3	2.17	0.45
8:N:271:ASP:HA	8:N:363:ARG:HE	1.81	0.45
10:Q:26:PHE:O	10:Q:30:ARG:HD3	2.17	0.45
10:Q:445:MET:HE1	16:Y:167:ASP:OD1	2.16	0.45
14:V:330:GLU:CD	14:V:330:GLU:H	2.24	0.45
15:W:508:GLY:O	15:W:512:TYR:HB2	2.15	0.45
15:W:882:ARG:HH21	15:W:885:LYS:NZ	2.14	0.45
16:Y:303:ARG:NH1	16:Y:304:LEU:HB2	2.31	0.45
18:a:1659:HIS:O	18:a:1660:THR:OG1	2.30	0.45
4:K:46:VAL:O	4:K:49:ARG:HG2	2.16	0.45
3:D:109:HIS:O	3:D:113:GLU:HG2	2.17	0.45
5:I:26:DC:H2"	5:I:27:DT:H6	1.80	0.45
7:A:1082:PHE:O	7:A:1086:ASP:N	2.45	0.45
8:N:366:ARG:O	8:N:370:GLN:HG2	2.16	0.45
10:Q:40:VAL:O	10:Q:43:LYS:HG3	2.17	0.45
10:Q:292:ILE:O	10:Q:296:LEU:N	2.42	0.45
11:R:217:GLU:HA	11:R:220:GLU:CG	2.47	0.45
12:T:222:LYS:HG2	12:T:226[B]:HIS:CD2	2.52	0.45
16:Y:466:MET:HE1	17:Z:196:PHE:HB2	1.97	0.45
2:C:112:GLN:HB2	2:C:115:LEU:HD12	1.97	0.45
3:D:86:ARG:HG3	3:D:86:ARG:NH1	2.32	0.45
2:G:32:ARG:NH1	5:I:30:DA:OP1	2.49	0.45
7:A:908:LEU:C	7:A:909:LEU:HD12	2.42	0.45
8:N:33:PRO:HD3	8:N:394:TRP:CE3	2.52	0.45
8:N:158:THR:HG23	8:N:169:ILE:HG12	1.99	0.45
10:Q:235:LYS:HE2	10:Q:235:LYS:HA	1.98	0.45
11:R:276:TYR:CD1	11:R:284:TYR:HB2	2.51	0.45
12:T:379:GLN:O	12:T:380:SER:OG	2.32	0.45
12:T:383:ASN:OD1	18:a:1592:PRO:HA	2.17	0.45
14:V:193:MET:HE2	14:V:193:MET:N	2.31	0.45
15:W:928:LEU:O	15:W:932:GLN:HG3	2.17	0.45
16:Y:404:MET:O	16:Y:408:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:491:VAL:HA	16:Y:494:TYR:HB3	1.98	0.45
17:Z:247:GLN:NE2	17:Z:248:ILE:HG23	2.32	0.45
2:G:68:ASN:HD22	2:G:71:ARG:NH2	2.14	0.45
2:G:77:ARG:NE	5:I:20:DA:H4'	2.30	0.45
5:I:68:DT:H2''	5:I:69:DA:C8	2.52	0.45
7:A:409:LEU:HD23	18:a:1595:VAL:HG21	1.99	0.45
7:A:500:LEU:HD11	9:P:355:MET:HG3	1.99	0.45
7:A:838:PRO:HB2	7:A:842:ARG:NH1	2.31	0.45
7:A:978:ARG:O	7:A:979:ARG:HG3	2.17	0.45
7:A:991:LYS:HB2	7:A:1191:HIS:NE2	2.32	0.45
12:T:195:GLU:O	12:T:199:ASN:N	2.46	0.45
12:T:605:ILE:HG23	15:X:646:ASP:OD1	2.17	0.45
15:W:599:ARG:HD3	15:W:599:ARG:C	2.42	0.45
15:W:901:ILE:HA	15:W:904:ARG:NE	2.21	0.45
15:X:449:PHE:CE2	15:X:461:ILE:HG22	2.50	0.45
15:X:466:ARG:HB2	15:X:504:LEU:HD11	1.97	0.45
5:I:13:DG:C5	5:I:14:DG:C5	3.05	0.45
6:J:52:DG:C2	6:J:53:DG:C4	3.04	0.45
7:A:1073:LEU:O	7:A:1076:TYR:HB3	2.17	0.45
7:A:1131:LYS:HB3	7:A:1134:ASP:OD2	2.17	0.45
8:N:32:CYS:SG	8:N:33:PRO:HD2	2.56	0.45
10:Q:193:LEU:HD21	10:Q:296:LEU:HD11	1.98	0.45
10:Q:193:LEU:HD21	10:Q:296:LEU:HD21	1.99	0.45
12:T:567:ARG:NH1	12:T:574:CYS:SG	2.90	0.45
14:V:164:PHE:CE2	14:V:220:GLU:OE2	2.70	0.45
14:V:195:ILE:O	14:V:198:GLN:N	2.37	0.45
15:X:451:ASN:C	15:X:453:LYS:H	2.25	0.45
1:F:84:MET:HE1	1:F:101:GLY:O	2.17	0.45
8:N:89:LYS:HB2	8:N:94:GLU:HG3	1.98	0.45
10:Q:233:PHE:CE1	10:Q:282:GLU:HB2	2.52	0.45
10:Q:359:VAL:HG21	10:Q:378:LEU:HD21	1.98	0.45
14:V:288:ASN:HD21	15:X:493:ASP:CG	2.25	0.45
14:V:350:CYS:HB3	15:X:488:ARG:HE	1.82	0.45
15:W:931:ARG:NH2	15:X:927:LEU:HD13	2.32	0.45
16:Y:508:GLN:O	16:Y:508:GLN:NE2	2.41	0.45
7:A:460:GLN:HG3	7:A:463:GLU:OE1	2.17	0.44
7:A:764:TRP:CE3	7:A:977:LEU:HB2	2.52	0.44
7:A:998:CYS:SG	7:A:1084:LEU:HD13	2.57	0.44
7:A:1052:PHE:C	7:A:1054:HIS:H	2.25	0.44
10:Q:141:TYR:O	10:Q:145:SER:N	2.44	0.44
10:Q:433:CYS:O	10:Q:436:ILE:HB	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:441:LYS:HD2	16:Y:163:ARG:HE	1.82	0.44
12:T:586:ALA:O	12:T:590:THR:N	2.41	0.44
18:a:1648:LEU:O	18:a:1650:SER:N	2.50	0.44
2:G:104:GLN:N	4:K:94:GLU:OE2	2.43	0.44
5:I:47:DC:H2''	5:I:48:DT:C5	2.52	0.44
6:J:87:DT:H6	6:J:87:DT:H2'	1.61	0.44
7:A:781:MET:HE3	7:A:1188:ASP:OD1	2.17	0.44
10:Q:18:ALA:O	10:Q:19:PHE:HB3	2.16	0.44
10:Q:182:LEU:HD11	18:a:1610:TYR:HD2	1.83	0.44
14:V:194:GLU:HG2	14:V:199:LYS:HB3	1.98	0.44
15:W:910:GLU:HA	15:W:913:MET:HB3	1.98	0.44
15:X:481:LEU:HD22	15:X:510:ILE:HD11	1.99	0.44
16:Y:294:GLN:NE2	16:Y:310:GLN:O	2.49	0.44
16:Y:311:THR:O	16:Y:314:VAL:HG12	2.17	0.44
16:Y:329:GLN:NE2	16:Y:334:ARG:HB3	2.32	0.44
2:C:31:HIS:CD2	2:C:35:ARG:NH1	2.86	0.44
7:A:181:ARG:HH11	15:X:646:ASP:HB3	1.82	0.44
7:A:195:PRO:O	15:W:651:ASP:HB3	2.18	0.44
7:A:417:ARG:HH22	16:Y:479:ALA:HB2	1.82	0.44
7:A:502:LYS:O	7:A:506:THR:HG23	2.18	0.44
10:Q:141:TYR:HA	10:Q:144:GLN:HB2	2.00	0.44
12:T:413:HIS:ND1	12:T:414:TYR:HD1	2.15	0.44
5:I:138:DT:H2''	5:I:139:DA:C8	2.52	0.44
7:A:999:ASP:OD2	7:A:1264:PRO:HG3	2.18	0.44
7:A:1292:ARG:NE	7:A:1292:ARG:HA	2.33	0.44
9:P:215:LYS:HE3	9:P:216:LEU:HD21	1.97	0.44
10:Q:183:LEU:HD12	10:Q:189:HIS:O	2.16	0.44
10:Q:1802:ILE:HD12	16:Y:357:ILE:HD12	2.00	0.44
12:T:423:LYS:HA	12:T:426:SER:HB3	2.00	0.44
15:W:884:ILE:O	15:W:888:VAL:HG12	2.18	0.44
15:W:906:PHE:HE2	15:X:906:PHE:CE2	2.35	0.44
2:G:32:ARG:NH2	3:H:35:GLU:OE2	2.48	0.44
5:I:66:DC:N4	6:J:81:DC:H42	2.16	0.44
5:I:70:DC:N4	6:J:78:DG:H1	2.16	0.44
10:Q:278:ILE:O	10:Q:278:ILE:HG13	2.17	0.44
10:Q:1764:ILE:HD12	10:Q:1764:ILE:H	1.82	0.44
12:T:156:PHE:O	12:T:177:ASP:HB2	2.18	0.44
15:W:605:GLU:HA	15:W:608:LEU:HD12	2.00	0.44
16:Y:465:THR:O	17:Z:189:LYS:HE3	2.17	0.44
1:B:43:VAL:HG11	4:K:119:ILE:HD13	2.00	0.44
6:J:44:DA:H2''	6:J:45:DT:H71	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1099:VAL:HG13	7:A:1151:ILE:HG22	1.99	0.44
7:A:1300:ARG:NH2	7:A:1302:PRO:CG	2.80	0.44
8:N:177:THR:HG21	8:N:197:LEU:O	2.18	0.44
10:Q:38:PRO:HB3	10:Q:92:TYR:CE1	2.44	0.44
10:Q:433:CYS:SG	10:Q:1782:TYR:HB2	2.58	0.44
12:T:375:THR:HB	12:T:377:ARG:NH2	2.32	0.44
12:T:612:ARG:CZ	12:T:612:ARG:HA	2.48	0.44
14:V:296:LYS:O	14:V:299:SER:N	2.51	0.44
15:X:450:PHE:CD1	15:X:459:PRO:HB3	2.53	0.44
1:F:50:ILE:O	1:F:53:GLU:N	2.50	0.44
8:N:74:ALA:HA	8:N:77:VAL:HG22	1.99	0.44
9:P:297:THR:OG1	9:P:329:ILE:HA	2.18	0.44
10:Q:139:SER:OG	10:Q:142:LEU:HB2	2.17	0.44
10:Q:237:TRP:CE3	10:Q:318:LEU:HD23	2.53	0.44
10:Q:371:LYS:HD3	10:Q:406:HIS:NE2	2.32	0.44
10:Q:388:GLY:HA2	10:Q:391:ILE:HD11	1.99	0.44
12:T:176:MET:HG2	12:T:203:MET:HG2	1.99	0.44
14:V:192:ASP:H	14:V:193:MET:HE2	1.83	0.44
15:X:606:THR:O	15:X:610:LEU:HG	2.18	0.44
5:I:63:DG:C2	6:J:86:DG:N2	2.85	0.44
5:I:140:DC:H2''	5:I:141:DA:C8	2.53	0.44
6:J:41:DG:H1'	6:J:42:DT:H5'	1.99	0.44
6:J:56:DG:H4'	7:A:861:GLU:HG2	1.99	0.44
7:A:780:GLU:HG2	7:A:781:MET:N	2.32	0.44
7:A:877:TYR:HD1	7:A:905:ARG:HB2	1.82	0.44
7:A:976:LEU:HD23	7:A:977:LEU:N	2.33	0.44
9:P:124:PHE:CE1	9:P:132:MET:HE2	2.53	0.44
10:Q:40:VAL:HG22	10:Q:43:LYS:HE3	1.99	0.44
10:Q:158:TYR:HB2	10:Q:196:ASP:OD2	2.17	0.44
11:R:198:GLU:HA	11:R:201:LYS:HB3	1.99	0.44
16:Y:348:GLU:N	16:Y:360:ARG:HH22	2.15	0.44
4:K:82:LEU:HA	4:K:82:LEU:HD23	1.77	0.44
5:I:25:DG:C4	5:I:26:DC:C5	3.06	0.44
5:I:50:DG:H1	6:J:98:DC:N4	2.16	0.44
7:A:465:GLU:HA	7:A:468:ARG:HB3	1.99	0.44
7:A:764:TRP:CE2	7:A:768:LEU:HD11	2.53	0.44
7:A:889:HIS:CE1	7:A:923:ALA:HB2	2.53	0.44
7:A:1101:LEU:HD12	7:A:1102:PHE:H	1.83	0.44
12:T:163:PHE:CE1	18:a:1672:LEU:HD13	2.53	0.44
15:X:477:PRO:HB3	15:X:513:GLN:HE21	1.82	0.44
4:E:57:SER:HB2	4:E:59:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:100:LEU:HD23	4:E:100:LEU:HA	1.67	0.43
5:I:34:DG:H5'	5:I:34:DG:H8	1.82	0.43
5:I:39:DA:N6	6:J:109:DT:H3	2.16	0.43
7:A:757:TYR:HA	7:A:760:LYS:HB2	2.00	0.43
7:A:1311:PRO:HA	7:A:1314:ILE:HB	1.99	0.43
8:N:127:TRP:CZ3	8:N:192:ILE:HD12	2.52	0.43
9:P:156:GLY:O	9:P:303:THR:OG1	2.33	0.43
9:P:208:ILE:HD13	9:P:243:PRO:HD3	1.99	0.43
10:Q:138:VAL:HG23	10:Q:139:SER:H	1.82	0.43
10:Q:423:TYR:O	10:Q:427:GLU:HG3	2.17	0.43
12:T:423:LYS:O	12:T:427:ASP:N	2.41	0.43
14:V:213:MET:HA	14:V:217:MET:HE3	1.99	0.43
15:W:481:LEU:HD12	15:W:481:LEU:HA	1.81	0.43
15:X:887:LEU:HD21	17:Z:235:MET:SD	2.57	0.43
18:a:1659:HIS:C	18:a:1661:THR:H	2.26	0.43
2:C:100:VAL:HG11	1:F:98:TYR:CE2	2.53	0.43
6:J:45:DT:H2''	6:J:46:DC:C5	2.53	0.43
7:A:963:LEU:O	7:A:967:ARG:HG2	2.19	0.43
7:A:1082:PHE:CE1	7:A:1112:MET:HE1	2.53	0.43
8:N:162:ASN:HD22	8:N:349:ILE:CG2	2.31	0.43
8:N:172:SER:OG	8:N:354:ASN:HB2	2.18	0.43
10:Q:233:PHE:O	10:Q:236:PHE:HB3	2.19	0.43
10:Q:287:LEU:HD12	10:Q:324:PHE:HZ	1.82	0.43
10:Q:427:GLU:HG2	10:Q:1778:ASN:ND2	2.34	0.43
14:V:263:ILE:HG23	14:V:265:LYS:HZ2	1.82	0.43
15:W:928:LEU:HG	17:Z:266:PHE:HE1	1.83	0.43
15:X:512:TYR:HB3	15:X:513:GLN:OE1	2.17	0.43
17:Z:272:ARG:HH11	17:Z:276:LEU:HD13	1.83	0.43
4:K:94:GLU:HA	4:K:94:GLU:OE1	2.17	0.43
4:E:119:ILE:O	1:F:50:ILE:HD11	2.18	0.43
7:A:412:PHE:CE1	18:a:1598:PRO:HD3	2.53	0.43
7:A:1261:ASP:O	7:A:1263:VAL:HG23	2.18	0.43
7:A:1277:GLU:O	7:A:1280:PHE:HB2	2.18	0.43
8:N:120:VAL:N	8:N:148:ALA:O	2.50	0.43
10:Q:430:ASP:CG	10:Q:1783:SER:H	2.26	0.43
11:R:235:VAL:O	15:X:524:GLY:N	2.52	0.43
12:T:168:TYR:CE1	12:T:172:ILE:HD13	2.53	0.43
15:W:862:ALA:O	15:W:866:LEU:N	2.40	0.43
15:W:944:MET:SD	15:W:945:ARG:N	2.91	0.43
17:Z:244:GLU:HA	17:Z:247:GLN:CG	2.47	0.43
3:D:76:GLU:HG2	3:D:101:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:68:DG:H21	6:J:69:DG:N2	2.15	0.43
7:A:173:ASN:HD21	7:A:176:GLN:HB2	1.83	0.43
7:A:1311:PRO:N	7:A:1314:ILE:HD12	2.33	0.43
10:Q:59:GLY:HA2	10:Q:101:GLU:OE2	2.19	0.43
10:Q:270:PHE:HA	17:Z:195:ARG:NH1	2.32	0.43
10:Q:1797:LEU:HD22	10:Q:1815:LEU:HD11	2.00	0.43
14:V:261:ARG:HA	14:V:283:MET:H	1.82	0.43
4:K:46:VAL:HA	4:K:49:ARG:HG2	2.00	0.43
4:K:51:ILE:HG13	4:K:52:ARG:HD2	2.00	0.43
1:B:15:ALA:N	1:B:18:HIS:O	2.51	0.43
4:E:50:GLU:OE2	1:F:39:ARG:NE	2.44	0.43
7:A:468:ARG:HA	7:A:471:LYS:HD2	2.00	0.43
9:P:242:LEU:HD12	9:P:246:GLN:NE2	2.33	0.43
10:Q:381:LEU:HA	10:Q:381:LEU:HD23	1.84	0.43
10:Q:462:LEU:HD12	10:Q:465:VAL:HG11	1.99	0.43
11:R:234:GLN:C	15:X:523:MET:HE3	2.44	0.43
14:V:233:PHE:O	14:V:237:ILE:HG12	2.19	0.43
15:X:465:TYR:CD2	15:X:490:LEU:HD13	2.52	0.43
18:a:1636:ARG:HA	18:a:1667:TRP:CZ3	2.53	0.43
3:H:33:ARG:HG3	6:J:123:DC:H4'	2.00	0.43
7:A:448:ARG:HE	7:A:448:ARG:HB2	1.66	0.43
7:A:1073:LEU:HD23	7:A:1073:LEU:HA	1.88	0.43
7:A:1243:ARG:H	7:A:1243:ARG:HG3	1.48	0.43
9:P:109:PRO:HA	9:P:136:ILE:HD12	2.01	0.43
9:P:226:GLU:HB3	9:P:255:PHE:CE2	2.54	0.43
14:V:177:HIS:HA	14:V:180:ALA:HB3	1.99	0.43
15:W:919:ALA:O	15:W:922:TYR:HB3	2.18	0.43
15:X:443:ARG:HA	15:X:450:PHE:CE2	2.54	0.43
15:X:892:VAL:HG12	15:X:896:MET:HE2	2.01	0.43
15:X:905:HIS:HA	15:X:908:GLU:OE2	2.19	0.43
2:C:67:GLY:HA3	3:D:49:HIS:CD2	2.54	0.43
2:G:71:ARG:CB	2:G:71:ARG:HH11	2.31	0.43
6:J:26:DC:H6	6:J:26:DC:H2'	1.68	0.43
7:A:487:LYS:HE3	8:N:399:ILE:HD13	1.99	0.43
7:A:1292:ARG:O	7:A:1296:ARG:NH1	2.51	0.43
14:V:360:GLU:HA	14:V:363:LYS:HZ2	1.84	0.43
15:W:510:ILE:HA	15:W:510:ILE:HD13	1.83	0.43
15:W:909:LEU:HD21	16:Y:164:LYS:HE3	2.00	0.43
18:a:1681:ARG:HD3	18:a:1681:ARG:H	1.84	0.43
1:B:66:ILE:CD1	4:K:92:LEU:HD11	2.47	0.43
2:G:102:ILE:HG23	3:H:61:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:ARG:HH22	5:I:28:DC:H5''	1.84	0.43
5:I:33:DG:H2''	5:I:34:DG:H8	1.83	0.43
6:J:68:DG:H2''	6:J:69:DG:C8	2.54	0.43
7:A:472:HIS:O	7:A:475:TYR:HB2	2.19	0.43
7:A:768:LEU:HD23	7:A:768:LEU:HA	1.83	0.43
7:A:808:ILE:HD13	7:A:855:VAL:HG13	2.01	0.43
7:A:925:LEU:HA	7:A:928:LEU:HB2	2.00	0.43
7:A:929:LEU:HB2	7:A:933:PHE:HB2	2.00	0.43
7:A:1112:MET:HG3	7:A:1116:PHE:CE1	2.54	0.43
7:A:1304:LEU:O	7:A:1304:LEU:HG	2.18	0.43
7:A:1315:ILE:HG22	7:A:1316:LYS:HG3	1.99	0.43
8:N:89:LYS:HB2	8:N:94:GLU:CG	2.49	0.43
8:N:311:PRO:HG3	8:N:323:LEU:HA	2.01	0.43
9:P:201:THR:OG1	9:P:202:THR:N	2.50	0.43
9:P:242:LEU:HD12	9:P:246:GLN:HE22	1.84	0.43
10:Q:235:LYS:NZ	10:Q:238:LYS:HD2	2.34	0.43
12:T:212:LYS:O	12:T:214:GLU:N	2.52	0.43
12:T:429:ILE:HD13	17:Z:190:HIS:HB3	2.01	0.43
14:V:223:CYS:SG	14:V:228:LEU:HB2	2.59	0.43
15:X:878:ALA:O	15:X:882:ARG:HD2	2.18	0.43
4:E:123:ASP:OD1	4:K:113:HIS:NE2	2.51	0.43
5:I:58:DT:H1'	5:I:59:DA:C8	2.54	0.43
6:J:55:DG:C5	6:J:56:DG:C6	3.07	0.43
6:J:94:DG:C4	6:J:95:DG:C8	3.06	0.43
7:A:370:ARG:HG3	7:A:373:ARG:NH2	2.34	0.43
7:A:1113:GLU:HG3	7:A:1123:TYR:CE2	2.53	0.43
8:N:127:TRP:CZ2	8:N:194:LYS:HB2	2.53	0.43
8:N:138:GLU:O	8:N:142:GLU:N	2.46	0.43
9:P:151:ILE:HG22	9:P:164:PRO:HB3	2.01	0.43
10:Q:1792:ARG:HG2	10:Q:1792:ARG:HH11	1.83	0.43
14:V:367:ASP:O	14:V:370:ARG:HB3	2.19	0.43
15:W:615:MET:SD	15:W:615:MET:N	2.87	0.43
15:X:601:TRP:HH2	15:X:634:GLU:C	2.26	0.43
15:X:612:ALA:HB1	15:X:623:VAL:HG13	2.01	0.43
17:Z:244:GLU:O	17:Z:248:ILE:HG12	2.19	0.43
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.70	0.43
3:H:33:ARG:CG	6:J:123:DC:H4'	2.49	0.43
6:J:14:DA:H8	6:J:14:DA:H5''	1.82	0.43
7:A:546:LYS:HG2	7:A:550:LEU:CD2	2.49	0.43
7:A:906:ARG:NH2	7:A:928:LEU:O	2.51	0.43
7:A:928:LEU:HA	7:A:928:LEU:HD23	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:337:ASP:O	8:N:340:ILE:HG12	2.19	0.43
9:P:213:LYS:HA	9:P:217:CYS:SG	2.58	0.43
10:Q:43:LYS:CG	10:Q:77:ASN:HD22	2.20	0.43
10:Q:329:GLN:HG3	10:Q:369:PHE:CE1	2.54	0.43
10:Q:395:VAL:HG13	10:Q:400:TYR:OH	2.18	0.43
11:R:215:ASN:ND2	15:X:480:TYR:O	2.50	0.43
12:T:188:ASN:ND2	12:T:191:GLN:OE1	2.52	0.43
18:a:1633:ALA:HB1	18:a:1638:VAL:HG21	2.01	0.43
5:I:83:DG:N2	6:J:65:DC:N3	2.61	0.42
7:A:381:ARG:HE	7:A:385:LEU:HD21	1.83	0.42
9:P:204:ALA:O	9:P:207:GLU:HG2	2.19	0.42
10:Q:454:ILE:HD12	10:Q:454:ILE:HG23	1.76	0.42
10:Q:522:LYS:HB2	10:Q:522:LYS:HE3	1.83	0.42
15:W:469:MET:HE3	15:W:469:MET:HB2	1.71	0.42
15:W:903:LEU:HD13	15:X:902:LYS:NZ	2.34	0.42
15:X:877:ALA:HA	17:Z:224:MET:HE1	2.01	0.42
16:Y:479:ALA:HA	16:Y:482:TYR:HD2	1.83	0.42
6:J:13:DT:H6	6:J:13:DT:H2'	1.72	0.42
7:A:884:HIS:O	7:A:887:LYS:HG2	2.19	0.42
7:A:1303:ARG:HG2	7:A:1307:GLU:OE1	2.18	0.42
8:N:119:PRO:HG2	8:N:406:PHE:HZ	1.84	0.42
8:N:121:LEU:HD13	8:N:410:TRP:CH2	2.53	0.42
8:N:162:ASN:HD22	8:N:349:ILE:HG23	1.83	0.42
10:Q:427:GLU:HG2	10:Q:1778:ASN:HD22	1.83	0.42
12:T:143:LEU:HA	12:T:146:GLN:HE21	1.84	0.42
12:T:218:TYR:CE2	12:T:222:LYS:HB2	2.54	0.42
15:X:450:PHE:CE1	15:X:459:PRO:HB3	2.54	0.42
3:H:49:HIS:C	3:H:51:ASP:H	2.27	0.42
6:J:63:DC:H1'	6:J:64:DG:H5'	2.01	0.42
7:A:371:GLU:O	7:A:375:GLN:HG3	2.20	0.42
7:A:844:PHE:O	7:A:848:LEU:HG	2.19	0.42
9:P:103:VAL:O	9:P:132:MET:HA	2.19	0.42
9:P:117:GLU:O	9:P:121:GLN:HG3	2.19	0.42
10:Q:455:GLN:HG2	10:Q:462:LEU:HD22	2.00	0.42
11:R:257:LEU:H	11:R:261:GLN:HE21	1.68	0.42
12:T:402:LEU:HD21	12:T:413:HIS:HA	2.01	0.42
16:Y:455:TRP:CE2	17:Z:203:ILE:HD12	2.54	0.42
2:C:21:ALA:HB2	3:D:121:TYR:HB2	2.01	0.42
5:I:16:DG:C2	6:J:133:DA:C2	3.08	0.42
5:I:93:DC:H6	5:I:93:DC:H2'	1.65	0.42
7:A:1103:CYS:SG	7:A:1109:MET:HG3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1248:GLN:OE1	7:A:1248:GLN:HA	2.18	0.42
8:N:12:GLY:O	8:N:119:PRO:HD2	2.19	0.42
9:P:256:ARG:HA	9:P:259:GLU:OE2	2.18	0.42
12:T:236:ARG:HA	12:T:239[A]:SER:HB2	2.01	0.42
12:T:378:LEU:O	12:T:379:GLN:C	2.63	0.42
14:V:337:GLU:OE1	14:V:337:GLU:N	2.51	0.42
15:X:423:HIS:CG	15:X:424:ILE:N	2.87	0.42
15:X:440:ALA:HA	15:X:443:ARG:HG3	2.01	0.42
17:Z:233:SER:HA	17:Z:236:VAL:HG22	2.01	0.42
1:B:66:ILE:HD11	4:K:92:LEU:CD1	2.48	0.42
3:H:39:ILE:HD11	3:H:40:TYR:CZ	2.55	0.42
9:P:188:TYR:HA	9:P:191:LYS:HB2	2.00	0.42
9:P:332:PRO:O	9:P:335:ARG:HD3	2.19	0.42
10:Q:95:ARG:O	10:Q:95:ARG:HD2	2.19	0.42
10:Q:136:HIS:HE2	14:V:227:ASP:CG	2.26	0.42
10:Q:138:VAL:HG22	10:Q:143:ARG:HH21	1.84	0.42
11:R:210:PHE:CE2	15:X:485:ALA:HA	2.55	0.42
12:T:178:PHE:O	12:T:182:LYS:HG3	2.18	0.42
12:T:539:ALA:HA	12:T:542:PHE:HB3	2.01	0.42
14:V:186:LEU:HD22	14:V:205:THR:HG22	2.01	0.42
14:V:300:GLU:OE1	14:V:300:GLU:N	2.51	0.42
6:J:106:DG:H2"	6:J:107:DT:H5"	2.02	0.42
7:A:370:ARG:HG3	7:A:373:ARG:HH22	1.84	0.42
7:A:374:LEU:HD12	15:W:645:GLU:OE2	2.19	0.42
7:A:1052:PHE:O	7:A:1054:HIS:N	2.52	0.42
8:N:338:ILE:C	8:N:340:ILE:H	2.28	0.42
10:Q:309:ASN:HB3	10:Q:312:CYS:SG	2.60	0.42
10:Q:397:GLN:C	10:Q:399:SER:H	2.28	0.42
10:Q:454:ILE:C	10:Q:456:MET:N	2.78	0.42
11:R:265:TYR:CE2	11:R:267:LYS:HB2	2.55	0.42
12:T:157:SER:O	12:T:179:SER:HB3	2.20	0.42
12:T:560:GLN:O	12:T:564:LEU:HG	2.20	0.42
15:W:420:GLN:NE2	15:X:532:HIS:O	2.40	0.42
15:X:477:PRO:HB3	15:X:513:GLN:NE2	2.35	0.42
15:X:481:LEU:HB3	15:X:511:ASN:HD21	1.84	0.42
16:Y:296:LYS:HG3	16:Y:309:THR:OG1	2.20	0.42
4:K:100:LEU:HD23	4:K:100:LEU:HA	1.79	0.42
1:F:66:ILE:HA	1:F:66:ILE:HD13	1.83	0.42
6:J:132:DC:H2"	6:J:133:DA:C8	2.54	0.42
7:A:197:PRO:HB2	7:A:199:HIS:ND1	2.34	0.42
7:A:1017:LEU:O	7:A:1032:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1085:LEU:HA	7:A:1088:ILE:HG12	2.01	0.42
11:R:281:THR:HG22	18:a:1651:HIS:O	2.19	0.42
12:T:156:PHE:HZ	12:T:207:ALA:HB2	1.85	0.42
15:W:884:ILE:HD13	16:Y:137:ILE:HD12	2.02	0.42
15:X:905:HIS:HB3	17:Z:252:HIS:ND1	2.34	0.42
15:X:933:ALA:HA	15:X:936:MET:CE	2.50	0.42
16:Y:163:ARG:NH2	16:Y:167:ASP:OD2	2.33	0.42
6:J:125:DG:C5	6:J:126:DC:N4	2.88	0.42
7:A:412:PHE:HD2	15:W:639:PHE:HZ	1.68	0.42
7:A:941:GLN:OE1	7:A:944:ASN:HA	2.20	0.42
7:A:1219:LYS:O	7:A:1222:LEU:HB2	2.20	0.42
8:N:109:MET:HE3	8:N:110:HIS:NE2	2.34	0.42
10:Q:169:LEU:O	10:Q:173:VAL:HG23	2.19	0.42
10:Q:399:SER:O	10:Q:403:ILE:HG13	2.18	0.42
10:Q:466:LYS:CB	10:Q:521:GLU:HB2	2.44	0.42
10:Q:1763:PRO:O	10:Q:1766:LYS:HB2	2.20	0.42
11:R:225:TYR:O	11:R:234:GLN:N	2.33	0.42
12:T:376:GLY:C	12:T:378:LEU:HD22	2.44	0.42
14:V:283:MET:HE1	14:V:322:HIS:HB3	2.02	0.42
15:X:942:ALA:HA	15:X:945:ARG:NH1	2.34	0.42
16:Y:353:LYS:HE3	16:Y:355:SER:OG	2.20	0.42
4:K:93:GLN:O	4:K:97:GLU:HG2	2.20	0.42
19:M:319:UNK:O	19:M:323:UNK:N	2.53	0.42
5:I:128:DG:H2'	5:I:129:DT:H71	2.01	0.42
6:J:95:DG:C6	6:J:96:DT:C4	3.08	0.42
6:J:133:DA:N7	6:J:134:DC:N4	2.67	0.42
7:A:748:LEU:HD21	7:A:798:GLU:CG	2.48	0.42
9:P:9:VAL:HG23	9:P:340:TRP:CD1	2.55	0.42
9:P:334:GLU:OE2	9:P:334:GLU:N	2.51	0.42
10:Q:192:GLN:HB3	10:Q:194:GLU:CD	2.45	0.42
11:R:272:ASP:HA	11:R:275:ARG:NH2	2.35	0.42
12:T:162:ASP:HA	12:T:165:ALA:O	2.20	0.42
15:W:897:LYS:O	15:W:901:ILE:HG13	2.20	0.42
15:W:917:ARG:HH11	17:Z:255:LYS:NZ	2.18	0.42
15:X:606:THR:HA	15:X:609:LEU:HB3	2.01	0.42
16:Y:312:ARG:N	16:Y:313:PRO:HD2	2.35	0.42
16:Y:500:GLN:HA	16:Y:503:ARG:NH2	2.34	0.42
3:D:86:ARG:HG3	3:D:86:ARG:HH11	1.84	0.42
7:A:455:LYS:HE2	7:A:455:LYS:HA	2.01	0.42
7:A:500:LEU:O	7:A:504:VAL:HG23	2.20	0.42
7:A:757:TYR:HB2	7:A:979:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:196:ASP:O	10:Q:199:ILE:HG22	2.20	0.42
10:Q:310:ARG:N	10:Q:310:ARG:HD3	2.34	0.42
14:V:358:ASP:OD2	14:V:358:ASP:N	2.51	0.42
15:X:466:ARG:HG3	15:X:467:ASN:N	2.35	0.42
15:X:932:GLN:O	15:X:935:HIS:HB3	2.20	0.42
5:I:94:DG:C2	6:J:55:DG:C2	3.08	0.41
6:J:68:DG:H2''	6:J:69:DG:N7	2.35	0.41
6:J:102:DA:H2''	6:J:103:DG:C8	2.52	0.41
6:J:126:DC:H2''	6:J:127:DC:O5'	2.19	0.41
7:A:830:VAL:HG12	7:A:853:PHE:HA	2.02	0.41
7:A:1242:GLU:HA	7:A:1245:ALA:HB3	2.02	0.41
9:P:8:LEU:O	9:P:103:VAL:HA	2.19	0.41
9:P:213:LYS:HD2	9:P:306:TYR:OH	2.20	0.41
10:Q:36:LYS:HD3	14:V:156:MET:HE1	2.01	0.41
10:Q:325:ILE:HG23	10:Q:328:ARG:NH1	2.35	0.41
12:T:138:GLU:O	12:T:142:GLN:HG2	2.20	0.41
15:W:616:TYR:CE1	15:W:622:LYS:HE3	2.55	0.41
18:a:1635:ARG:NH1	18:a:1637:ASP:HB3	2.31	0.41
1:B:44:LYS:HB2	2:G:115:LEU:HD12	2.01	0.41
2:C:32:ARG:NH2	3:D:35:GLU:OE1	2.50	0.41
7:A:915:GLN:HA	7:A:1181:HIS:ND1	2.34	0.41
7:A:1198:GLU:CG	7:A:1275:ARG:HD3	2.49	0.41
8:N:396:GLY:O	8:N:399:ILE:HG22	2.20	0.41
9:P:116:ARG:HD2	9:P:371:HIS:CE1	2.56	0.41
9:P:283:MET:HE2	9:P:283:MET:HB3	1.93	0.41
10:Q:20:LEU:O	10:Q:23:LEU:HB3	2.20	0.41
10:Q:325:ILE:HG22	10:Q:329:GLN:NE2	2.32	0.41
10:Q:371:LYS:HE2	10:Q:371:LYS:HB2	1.85	0.41
10:Q:1770:LEU:O	10:Q:1774:LEU:HD23	2.20	0.41
14:V:216:GLU:OE2	14:V:242:ARG:NH1	2.42	0.41
14:V:240:ALA:O	14:V:244:GLN:HG3	2.20	0.41
14:V:376:ARG:HG2	14:V:376:ARG:NH1	2.34	0.41
15:W:438:VAL:HG13	15:W:443:ARG:NH2	2.35	0.41
15:X:537:THR:O	18:a:1625:SER:HB3	2.20	0.41
16:Y:416:GLU:O	16:Y:419:THR:OG1	2.29	0.41
17:Z:198:ARG:HH11	17:Z:201:ARG:HH21	1.67	0.41
5:I:47:DC:H2''	5:I:48:DT:C7	2.50	0.41
5:I:70:DC:H2''	5:I:71:DG:C8	2.56	0.41
5:I:95:DC:H2''	5:I:96:DC:O5'	2.20	0.41
7:A:1112:MET:HA	7:A:1112:MET:HE2	2.03	0.41
8:N:266:VAL:HG11	8:N:297:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:338:ILE:HA	8:N:341:ARG:HG3	2.01	0.41
11:R:280:ASN:HB3	15:W:619:ASP:CG	2.44	0.41
12:T:150:LYS:O	12:T:152:PRO:HD3	2.20	0.41
15:W:439:HIS:ND1	15:W:441:ILE:HG12	2.35	0.41
15:W:944:MET:SD	15:W:945:ARG:HG2	2.60	0.41
15:X:427:PRO:HG3	15:X:512:TYR:CE1	2.55	0.41
16:Y:501:GLN:HG3	16:Y:502:ARG:NH2	2.35	0.41
2:G:24:GLN:CD	3:H:47:GLN:HE22	2.28	0.41
5:I:144:DC:H6	5:I:144:DC:H2'	1.71	0.41
7:A:488:GLU:HA	7:A:491:ARG:HD2	2.02	0.41
7:A:1010:HIS:ND1	7:A:1018:LEU:HD11	2.36	0.41
10:Q:27:HIS:CE1	10:Q:32:SER:HB2	2.55	0.41
10:Q:132:ASN:CB	10:Q:135:GLN:HB2	2.50	0.41
10:Q:146:TYR:CE2	14:V:231:LEU:HD23	2.55	0.41
10:Q:307:ALA:N	10:Q:338:ILE:HD11	2.35	0.41
12:T:140:LEU:HD22	12:T:196:LEU:HD22	2.02	0.41
14:V:341:ARG:HD2	15:X:488:ARG:O	2.21	0.41
14:V:341:ARG:NH1	14:V:349:TRP:CD2	2.88	0.41
16:Y:498:LYS:O	16:Y:502:ARG:HG2	2.20	0.41
17:Z:251:ARG:NH1	17:Z:255:LYS:HG3	2.35	0.41
2:G:92:GLU:OE2	3:H:103:PRO:HG2	2.21	0.41
5:I:63:DG:H2''	5:I:64:DC:H5'	2.02	0.41
6:J:111:DC:C2	6:J:112:DG:C6	3.09	0.41
7:A:463:GLU:O	7:A:466:ARG:HG3	2.19	0.41
7:A:465:GLU:O	7:A:469:ARG:N	2.54	0.41
7:A:545:LYS:HE3	7:A:940:GLU:OE2	2.21	0.41
7:A:806:PHE:HD1	7:A:877:TYR:HB3	1.86	0.41
7:A:1054:HIS:HA	7:A:1057:GLU:HG2	2.03	0.41
9:P:216:LEU:HD12	9:P:250:ILE:HD11	2.01	0.41
11:R:272:ASP:OD2	12:T:161:THR:HG22	2.20	0.41
12:T:429:ILE:CD1	17:Z:190:HIS:HB3	2.51	0.41
12:T:605:ILE:HG22	12:T:606:VAL:HG12	2.03	0.41
12:T:606:VAL:HG22	12:T:607:SER:N	2.35	0.41
14:V:176:ILE:O	14:V:180:ALA:N	2.39	0.41
14:V:184:GLU:HA	14:V:209:ASN:HD22	1.84	0.41
15:X:924:ARG:HH22	16:Y:317:GLN:CD	2.29	0.41
16:Y:136:ARG:NH1	16:Y:140:LEU:HD11	2.36	0.41
3:D:105:GLU:OE2	3:D:109:HIS:CE1	2.74	0.41
5:I:70:DC:N3	6:J:78:DG:N2	2.66	0.41
6:J:81:DC:H2''	6:J:82:DG:C8	2.56	0.41
7:A:423:CYS:SG	16:Y:493:ARG:HB2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:821:GLU:OE2	7:A:821:GLU:HA	2.21	0.41
7:A:999:ASP:O	7:A:1080:GLY:HA3	2.20	0.41
7:A:1052:PHE:C	7:A:1053:GLN:HG3	2.44	0.41
10:Q:367:ASP:CB	10:Q:370:LEU:HD13	2.50	0.41
10:Q:1775:ILE:O	10:Q:1779:ILE:HG12	2.19	0.41
14:V:301:LEU:HD23	14:V:301:LEU:HA	1.79	0.41
15:W:457:LYS:HB2	15:W:457:LYS:HE2	1.91	0.41
15:X:927:LEU:O	15:X:931:ARG:N	2.44	0.41
16:Y:432:ASN:O	16:Y:436:THR:HG23	2.21	0.41
4:K:126:LEU:O	4:K:129:ARG:N	2.53	0.41
2:G:71:ARG:NH1	2:G:71:ARG:HB2	2.35	0.41
2:G:116:LEU:HD23	2:G:116:LEU:H	1.85	0.41
6:J:39:DG:C6	6:J:40:DA:C6	3.09	0.41
7:A:893:LEU:HD12	7:A:893:LEU:HA	1.87	0.41
7:A:941:GLN:HB2	7:A:944:ASN:HA	2.02	0.41
9:P:334:GLU:H	9:P:334:GLU:CD	2.28	0.41
10:Q:316:LEU:HA	10:Q:316:LEU:HD23	1.82	0.41
10:Q:1807:ALA:O	10:Q:1811:LEU:HD12	2.20	0.41
12:T:220:ALA:O	12:T:224:LEU:HB2	2.21	0.41
16:Y:455:TRP:HD1	16:Y:456:LEU:HD12	1.84	0.41
6:J:53:DG:C4	6:J:54:DC:C5	3.09	0.41
7:A:448:ARG:N	10:Q:1767:HIS:ND1	2.69	0.41
7:A:994:TYR:OH	7:A:1200:ARG:NH1	2.54	0.41
9:P:359:LYS:H	9:P:359:LYS:HG2	1.70	0.41
10:Q:310:ARG:O	10:Q:313:LEU:HB2	2.21	0.41
15:X:493:ASP:OD2	15:X:495:CYS:HB3	2.20	0.41
16:Y:145:GLN:HA	16:Y:148:MET:HG3	2.02	0.41
16:Y:291:GLN:HG3	16:Y:292:PRO:O	2.21	0.41
18:a:1604:LEU:O	18:a:1608:GLU:N	2.39	0.41
3:H:43:LYS:HB2	3:H:43:LYS:NZ	2.35	0.41
3:H:68:ASP:CG	3:H:72:ARG:HH21	2.29	0.41
5:I:33:DG:H2"	5:I:34:DG:C8	2.56	0.41
7:A:476:LEU:O	7:A:480:LEU:HG	2.20	0.41
7:A:1063:LEU:O	7:A:1063:LEU:HD23	2.20	0.41
7:A:1078:ALA:CA	7:A:1303:ARG:HH21	2.34	0.41
7:A:1193:ILE:HD12	22:A:1703:ADP:C8	2.56	0.41
8:N:333:VAL:HG21	8:N:345:TYR:CE1	2.55	0.41
10:Q:1794:GLU:OE2	10:Q:1818:LEU:HD21	2.21	0.41
11:R:266:TYR:O	11:R:266:TYR:CG	2.74	0.41
12:T:199:ASN:HB3	12:T:203:MET:HE3	2.02	0.41
12:T:219:LYS:O	12:T:223:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:402:LEU:HD23	12:T:402:LEU:H	1.86	0.41
14:V:339:ALA:HB1	15:X:465:TYR:CD2	2.56	0.41
15:W:620:TRP:HZ3	15:W:635:CYS:CB	2.34	0.41
17:Z:253:GLN:O	17:Z:257:ARG:HG2	2.21	0.41
2:C:58:LEU:HD23	2:C:58:LEU:HA	1.81	0.41
2:G:45:ALA:O	2:G:48:PRO:HD2	2.21	0.41
6:J:25:DG:C5	6:J:26:DC:C4	3.09	0.41
7:A:382:ILE:O	7:A:386:GLU:HG3	2.20	0.41
7:A:892:LYS:O	7:A:892:LYS:HG3	2.20	0.41
9:P:120:THR:HA	9:P:132:MET:HE1	2.03	0.41
12:T:550:THR:O	12:T:554:ARG:HD3	2.21	0.41
15:W:909:LEU:O	15:W:913:MET:N	2.48	0.41
15:W:915:ARG:O	15:W:918:GLU:HG2	2.21	0.41
15:X:888:VAL:HG12	17:Z:234:LEU:HD21	2.03	0.41
1:B:38:ALA:HB1	1:B:43:VAL:CG2	2.51	0.40
6:J:128:DT:H2"	6:J:129:DC:C5	2.57	0.40
7:A:172:PHE:O	7:A:172:PHE:CG	2.73	0.40
7:A:765:LEU:HB3	7:A:792:LEU:CD1	2.51	0.40
7:A:805:PRO:HG2	7:A:875:TRP:HA	2.02	0.40
7:A:941:GLN:HB2	7:A:944:ASN:N	2.34	0.40
7:A:1077:ARG:HH11	7:A:1077:ARG:HD2	1.75	0.40
8:N:325:VAL:HA	8:N:328:VAL:HB	2.02	0.40
8:N:389:ARG:HA	8:N:392:SER:HB3	2.03	0.40
10:Q:93:TYR:OH	10:Q:101:GLU:OE1	2.26	0.40
15:X:602:THR:HB	15:X:605:GLU:CB	2.51	0.40
15:X:893:GLU:OE2	15:X:897:LYS:HE3	2.21	0.40
4:E:46:VAL:HB	6:J:83:DT:P	2.61	0.40
5:I:46:DT:H2"	5:I:47:DC:C6	2.56	0.40
5:I:80:DC:H2"	5:I:81:DC:C6	2.56	0.40
6:J:51:DT:H2"	6:J:52:DG:C8	2.56	0.40
7:A:369:GLU:HG2	12:T:565:SER:CB	2.52	0.40
7:A:384:GLU:HA	7:A:387:ASN:HD21	1.85	0.40
7:A:461:LYS:O	7:A:465:GLU:HG3	2.21	0.40
7:A:751:ASN:HB2	7:A:824:LYS:O	2.21	0.40
7:A:813:SER:OG	7:A:1135:ARG:NH1	2.54	0.40
8:N:214:ASN:OD1	8:N:215:ILE:N	2.52	0.40
10:Q:299:GLU:O	10:Q:303:VAL:HG23	2.22	0.40
10:Q:447:VAL:O	10:Q:450:VAL:HB	2.21	0.40
14:V:299:SER:OG	14:V:300:GLU:OE1	2.40	0.40
14:V:368:GLN:O	14:V:372:THR:HG23	2.21	0.40
15:X:430:ALA:HA	15:X:432:TRP:NE1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:15:LYS:HG2	2:C:19:SER:OG	2.22	0.40
2:G:63:LEU:HD23	2:G:63:LEU:HA	1.77	0.40
2:G:119:LYS:HE2	2:G:119:LYS:HB3	1.86	0.40
5:I:47:DC:H2''	5:I:48:DT:H71	2.03	0.40
5:I:82:DC:H2''	5:I:83:DG:H5'	2.04	0.40
7:A:541:LEU:HB3	7:A:545:LYS:HZ1	1.85	0.40
7:A:886:MET:N	7:A:886:MET:SD	2.94	0.40
7:A:938:THR:O	7:A:940:GLU:N	2.53	0.40
7:A:1116:PHE:O	7:A:1120:GLY:N	2.55	0.40
7:A:1304:LEU:O	7:A:1306:GLU:N	2.54	0.40
8:N:193:VAL:CG2	8:N:332:SER:HB3	2.50	0.40
9:P:209:VAL:HA	9:P:212:ILE:HD12	2.04	0.40
12:T:236:ARG:HA	12:T:239[B]:SER:HB3	2.02	0.40
12:T:377:ARG:O	12:T:378:LEU:CG	2.64	0.40
15:W:438:VAL:HA	15:W:442:GLU:OE2	2.20	0.40
15:W:873:ALA:O	15:W:877:ALA:N	2.39	0.40
16:Y:358:PRO:HA	16:Y:361:LEU:HB2	2.03	0.40
1:B:38:ALA:HB1	1:B:43:VAL:HG21	2.03	0.40
5:I:16:DG:H2''	5:I:17:DC:H5'	2.03	0.40
5:I:18:DC:C2	5:I:19:DG:C5	3.09	0.40
5:I:116:DC:O2	6:J:32:DG:N2	2.54	0.40
6:J:91:DA:C4	6:J:92:DG:C5	3.10	0.40
7:A:922:TRP:CZ3	7:A:933:PHE:HE1	2.39	0.40
7:A:941:GLN:HB3	7:A:943:PHE:CE1	2.57	0.40
10:Q:93:TYR:CE2	10:Q:97:LEU:HB2	2.55	0.40
10:Q:161:LEU:HA	10:Q:161:LEU:HD23	1.84	0.40
10:Q:214:LEU:HG	14:V:177:HIS:CE1	2.57	0.40
10:Q:221:PHE:HB3	10:Q:225:TRP:CZ3	2.56	0.40
11:R:225:TYR:HB3	15:X:523:MET:HE2	2.04	0.40
11:R:279:LEU:HD13	15:W:620:TRP:HB2	2.04	0.40
14:V:212:LEU:HD13	14:V:212:LEU:HA	1.92	0.40
15:X:486:CYS:O	15:X:490:LEU:HG	2.22	0.40
15:X:876:LEU:HA	15:X:879:VAL:HG12	2.03	0.40
15:X:933:ALA:HA	15:X:936:MET:HE1	2.03	0.40
1:B:45:ARG:O	4:K:118:THR:HA	2.22	0.40
7:A:371:GLU:OE1	7:A:375:GLN:NE2	2.54	0.40
7:A:412:PHE:CD1	18:a:1598:PRO:HD3	2.56	0.40
7:A:457:GLU:HA	7:A:460:GLN:OE1	2.22	0.40
7:A:1300:ARG:NH1	7:A:1300:ARG:CB	2.84	0.40
9:P:90:PHE:CE1	9:P:103:VAL:HG11	2.55	0.40
10:Q:142:LEU:O	10:Q:145:SER:OG	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:465:TYR:HD2	15:X:490:LEU:HD22	1.85	0.40
18:a:1653:LEU:HD12	18:a:1666:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	85/103 (82%)	78 (92%)	7 (8%)	0	100	100
1	F	84/103 (82%)	81 (96%)	3 (4%)	0	100	100
2	C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
2	G	106/130 (82%)	103 (97%)	3 (3%)	0	100	100
3	D	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
3	H	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
4	E	93/136 (68%)	90 (97%)	3 (3%)	0	100	100
4	K	96/136 (71%)	91 (95%)	5 (5%)	0	100	100
7	A	797/1485 (54%)	714 (90%)	82 (10%)	1 (0%)	48	78
8	N	324/429 (76%)	300 (93%)	24 (7%)	0	100	100
9	P	309/375 (82%)	295 (96%)	14 (4%)	0	100	100
10	Q	490/870 (56%)	432 (88%)	56 (11%)	2 (0%)	30	59
11	R	90/514 (18%)	83 (92%)	7 (8%)	0	100	100
12	T	264/652 (40%)	236 (89%)	28 (11%)	0	100	100
14	V	234/385 (61%)	215 (92%)	19 (8%)	0	100	100
15	W	242/1214 (20%)	230 (95%)	12 (5%)	0	100	100
15	X	246/1214 (20%)	231 (94%)	15 (6%)	0	100	100
16	Y	239/529 (45%)	229 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Z	90/411 (22%)	88 (98%)	2 (2%)	0	100	100
18	a	90/1020 (9%)	75 (83%)	14 (16%)	1 (1%)	11	38
All	All	4166/10088 (41%)	3851 (92%)	311 (8%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	Q	455	GLN
10	Q	451	SER
18	a	1649	PRO
7	A	169	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	72/79 (91%)	72 (100%)	0	100	100
1	F	67/79 (85%)	67 (100%)	0	100	100
2	C	81/102 (79%)	81 (100%)	0	100	100
2	G	84/102 (82%)	84 (100%)	0	100	100
3	D	77/106 (73%)	77 (100%)	0	100	100
3	H	79/106 (74%)	79 (100%)	0	100	100
4	E	82/111 (74%)	82 (100%)	0	100	100
4	K	84/111 (76%)	84 (100%)	0	100	100
7	A	720/1303 (55%)	720 (100%)	0	100	100
8	N	287/364 (79%)	287 (100%)	0	100	100
9	P	270/318 (85%)	270 (100%)	0	100	100
10	Q	446/765 (58%)	446 (100%)	0	100	100
11	R	83/452 (18%)	83 (100%)	0	100	100
12	T	245/587 (42%)	245 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	V	214/346 (62%)	214 (100%)	0	100	100
15	W	216/1030 (21%)	216 (100%)	0	100	100
15	X	222/1030 (22%)	222 (100%)	0	100	100
16	Y	227/455 (50%)	227 (100%)	0	100	100
17	Z	86/361 (24%)	85 (99%)	1 (1%)	63	72
18	a	82/912 (9%)	82 (100%)	0	100	100
All	All	3724/8719 (43%)	3723 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
17	Z	232	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	GLN
3	D	47	GLN
3	D	109	HIS
1	F	27	GLN
2	G	68	ASN
2	G	73	ASN
2	G	89	ASN
3	H	47	GLN
3	H	67	ASN
7	A	176	GLN
7	A	387	ASN
7	A	415	GLN
7	A	470	GLN
7	A	477	ASN
7	A	508	HIS
7	A	515	GLN
7	A	736	HIS
7	A	756	GLN
7	A	771	ASN
7	A	817	ASN
7	A	944	ASN
7	A	1062	HIS
7	A	1164	ASN

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Mol	Chain	Res	Type
7	A	1195	GLN
8	N	128	ASN
8	N	145	ASN
8	N	277	GLN
8	N	327	HIS
8	N	370	GLN
9	P	246	GLN
9	P	263	GLN
10	Q	77	ASN
10	Q	353	HIS
10	Q	470	HIS
11	R	211	ASN
12	T	148	GLN
14	V	154	ASN
14	V	179	ASN
14	V	209	ASN
14	V	368	GLN
15	W	467	ASN
15	W	632	GLN
15	W	895	GLN
15	W	925	GLN
15	X	506	GLN
15	X	932	GLN
16	Y	169	GLN
16	Y	294	GLN
16	Y	344	GLN
16	Y	432	ASN
16	Y	472	ASN
16	Y	501	GLN
17	Z	197	GLN
17	Z	238	GLN
17	Z	268	ASN
18	a	1602	GLN
18	a	1606	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	BEF	A	1701	-	0,3,3	-	-	-		
22	ADP	A	1703	21	28,29,29	1.37	5 (17%)	43,45,45	1.90	10 (23%)

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
22	ADP	A	1703	21	-	7/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1703	ADP	C5-C4	4.57	1.47	1.39
22	A	1703	ADP	C5-C6	2.47	1.47	1.41
22	A	1703	ADP	C5-N7	-2.42	1.34	1.39
22	A	1703	ADP	C8-N7	2.19	1.35	1.31
22	A	1703	ADP	C4-N9	-2.01	1.33	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1703	ADP	C5-C4-N3	-5.69	118.88	126.72
22	A	1703	ADP	N3-C4-N9	4.64	135.07	127.17
22	A	1703	ADP	C2-N3-C4	3.54	120.48	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1703	ADP	C4-C5-N7	-3.28	106.83	110.58
22	A	1703	ADP	N3-C2-N1	-3.07	123.94	128.58
22	A	1703	ADP	C4-N9-C8	2.79	108.67	105.74
22	A	1703	ADP	C3'-C2'-C1'	2.57	106.33	101.46
22	A	1703	ADP	C5-N7-C8	2.37	107.18	103.45
22	A	1703	ADP	C2'-C1'-N9	-2.22	107.78	113.30
22	A	1703	ADP	O2A-PA-O1A	2.06	122.04	112.44

There are no chirality outliers.

All (7) torsion outliers are listed below:

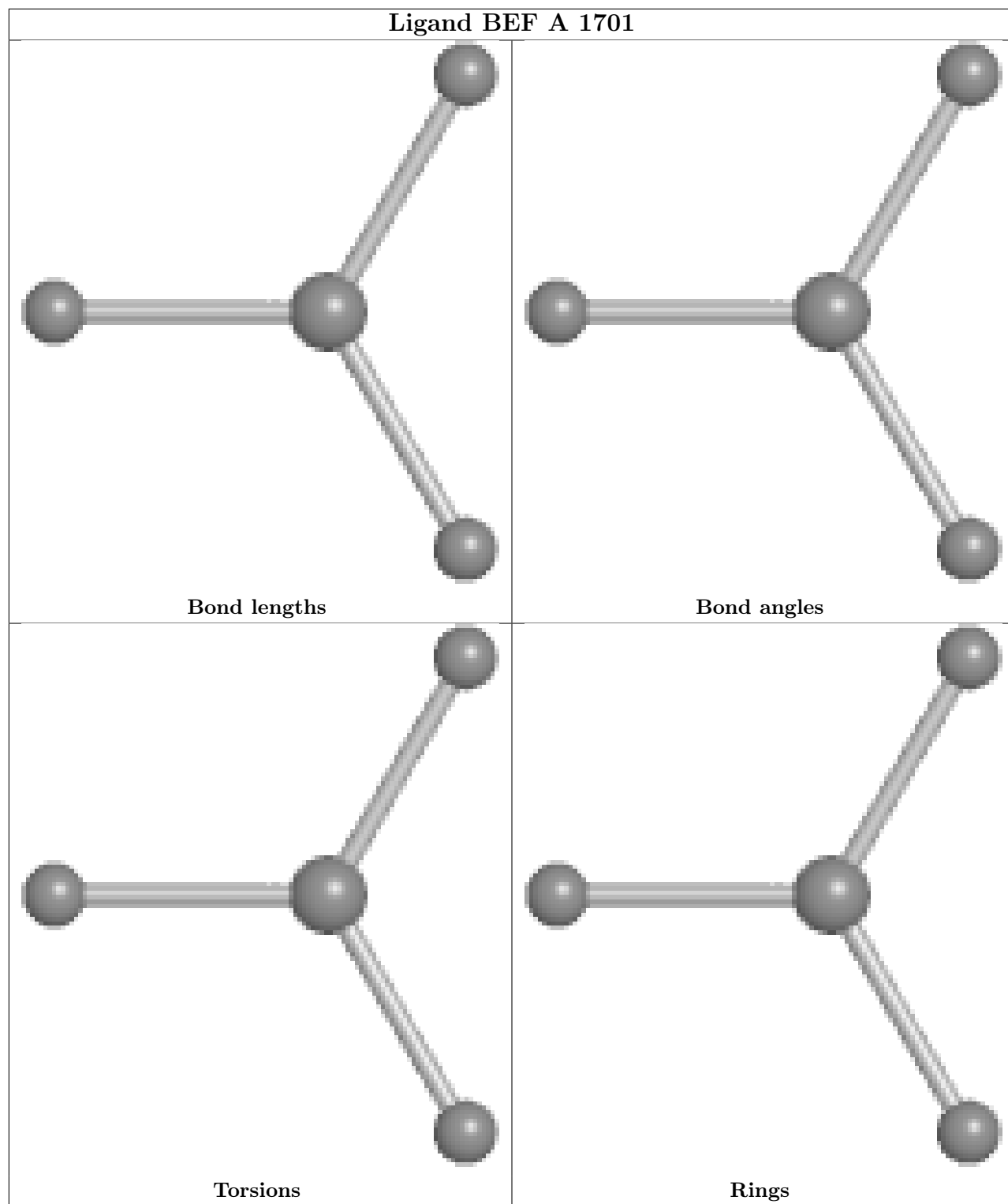
Mol	Chain	Res	Type	Atoms
22	A	1703	ADP	C5'-O5'-PA-O2A
22	A	1703	ADP	O4'-C4'-C5'-O5'
22	A	1703	ADP	C3'-C4'-C5'-O5'
22	A	1703	ADP	PB-O3A-PA-O1A
22	A	1703	ADP	C5'-O5'-PA-O1A
22	A	1703	ADP	C5'-O5'-PA-O3A
22	A	1703	ADP	PB-O3A-PA-O2A

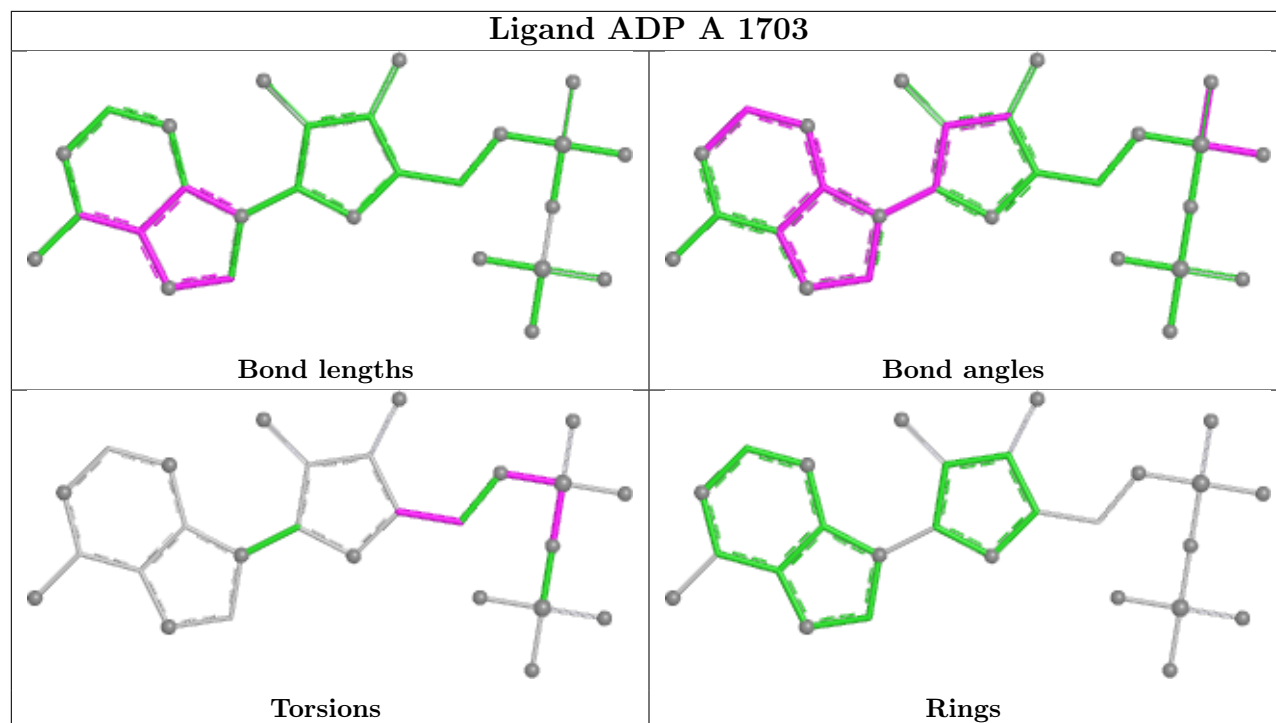
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1701	BEF	3	0
22	A	1703	ADP	11	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

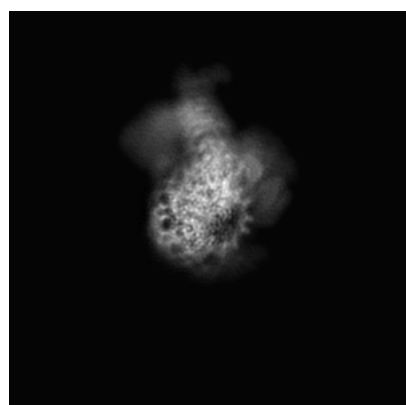
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31926. These allow visual inspection of the internal detail of the map and identification of artifacts.

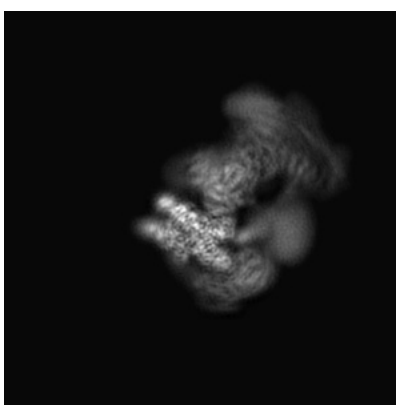
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

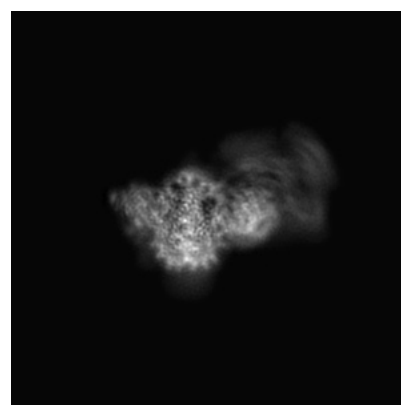
6.1.1 Primary map



X



Y

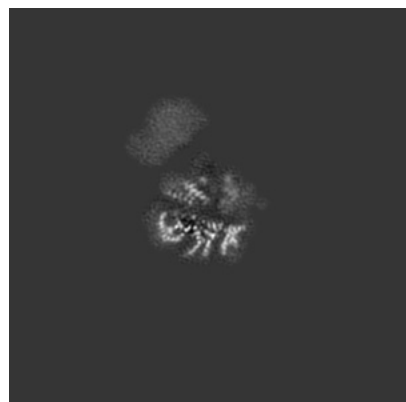


Z

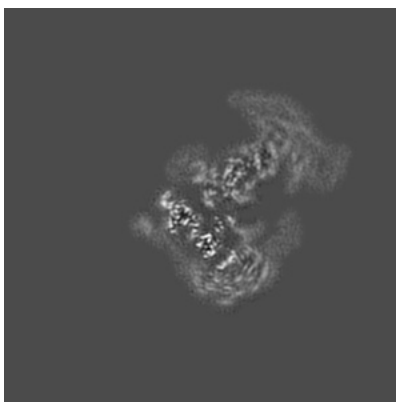
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180



Y Index: 180

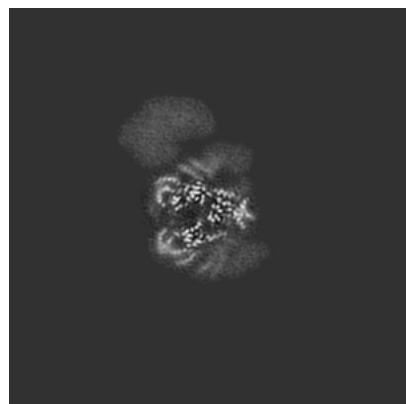


Z Index: 180

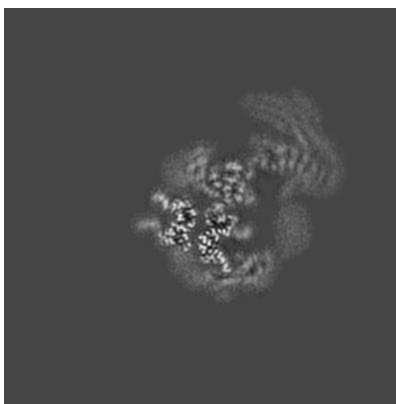
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

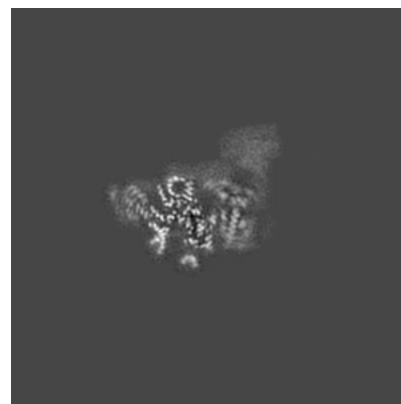
6.3.1 Primary map



X Index: 159



Y Index: 169

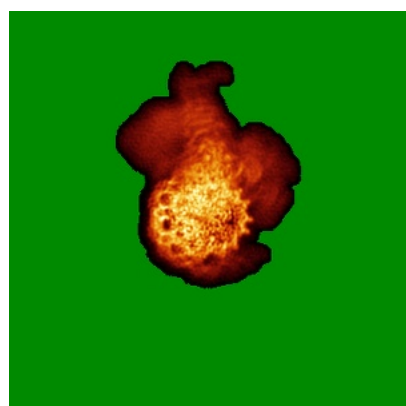


Z Index: 192

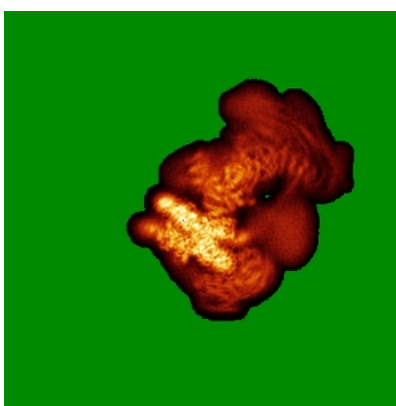
The images above show the largest variance slices of the map in three orthogonal directions.

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

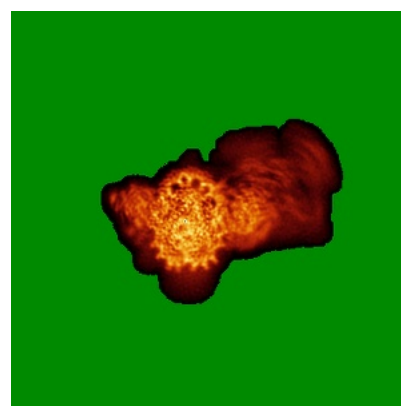
6.4.1 Primary map



X



Y

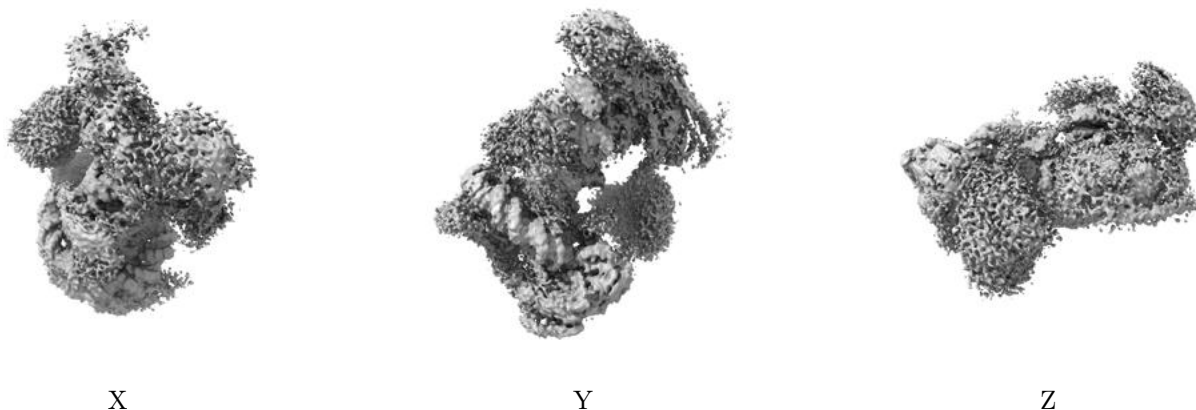


Z

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 0.0062. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

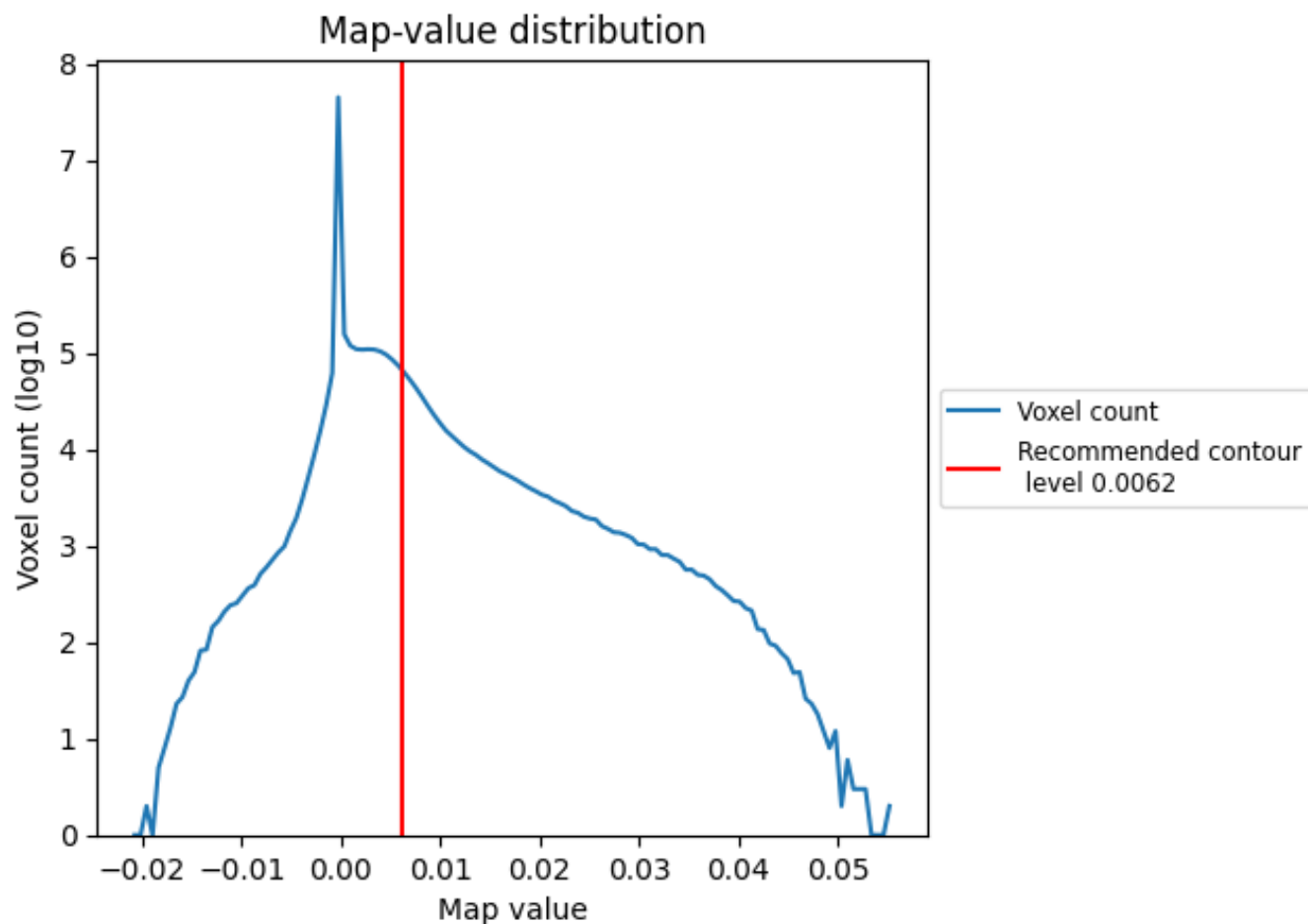
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

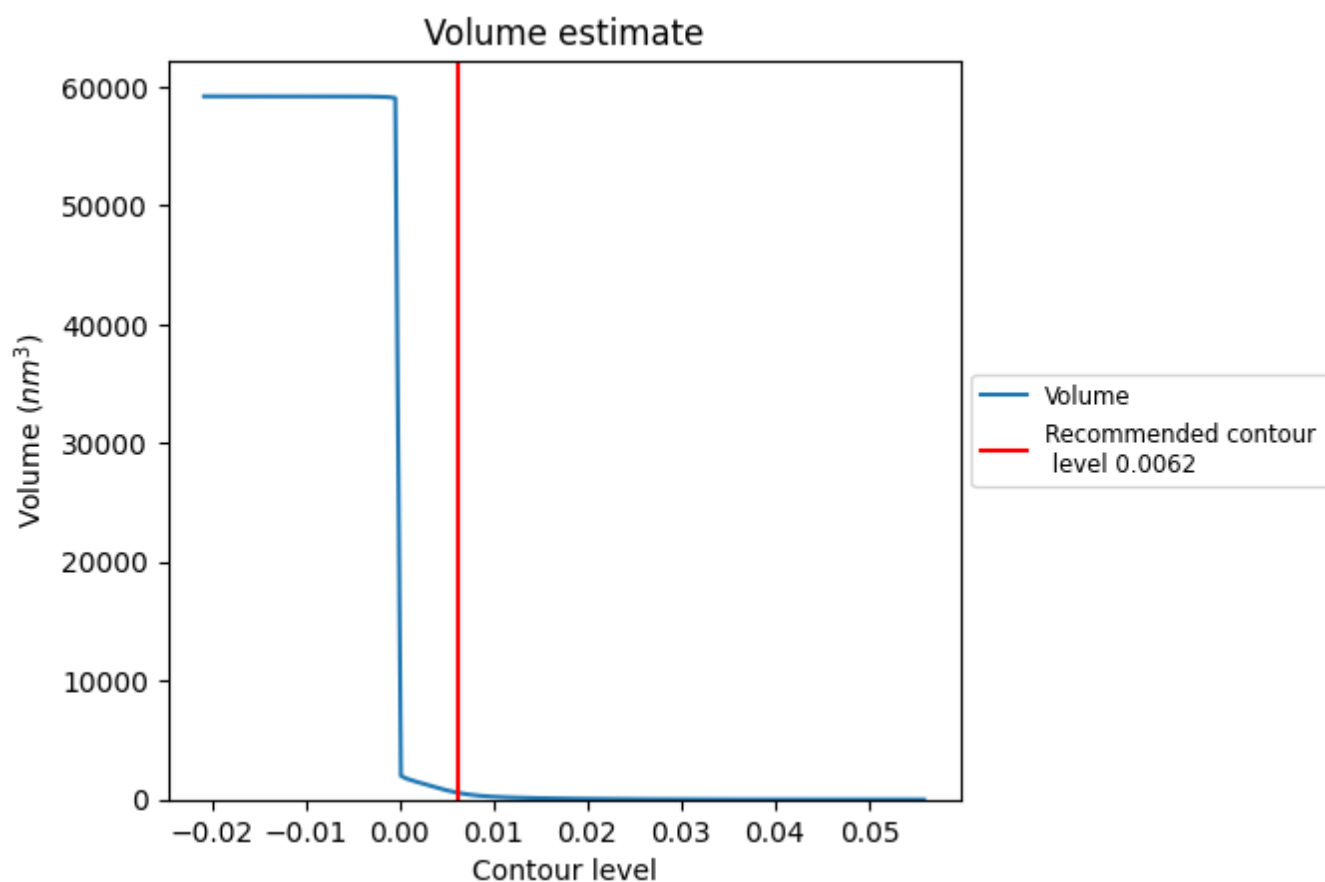
This section contains the results of statistical analysis of the map.

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.

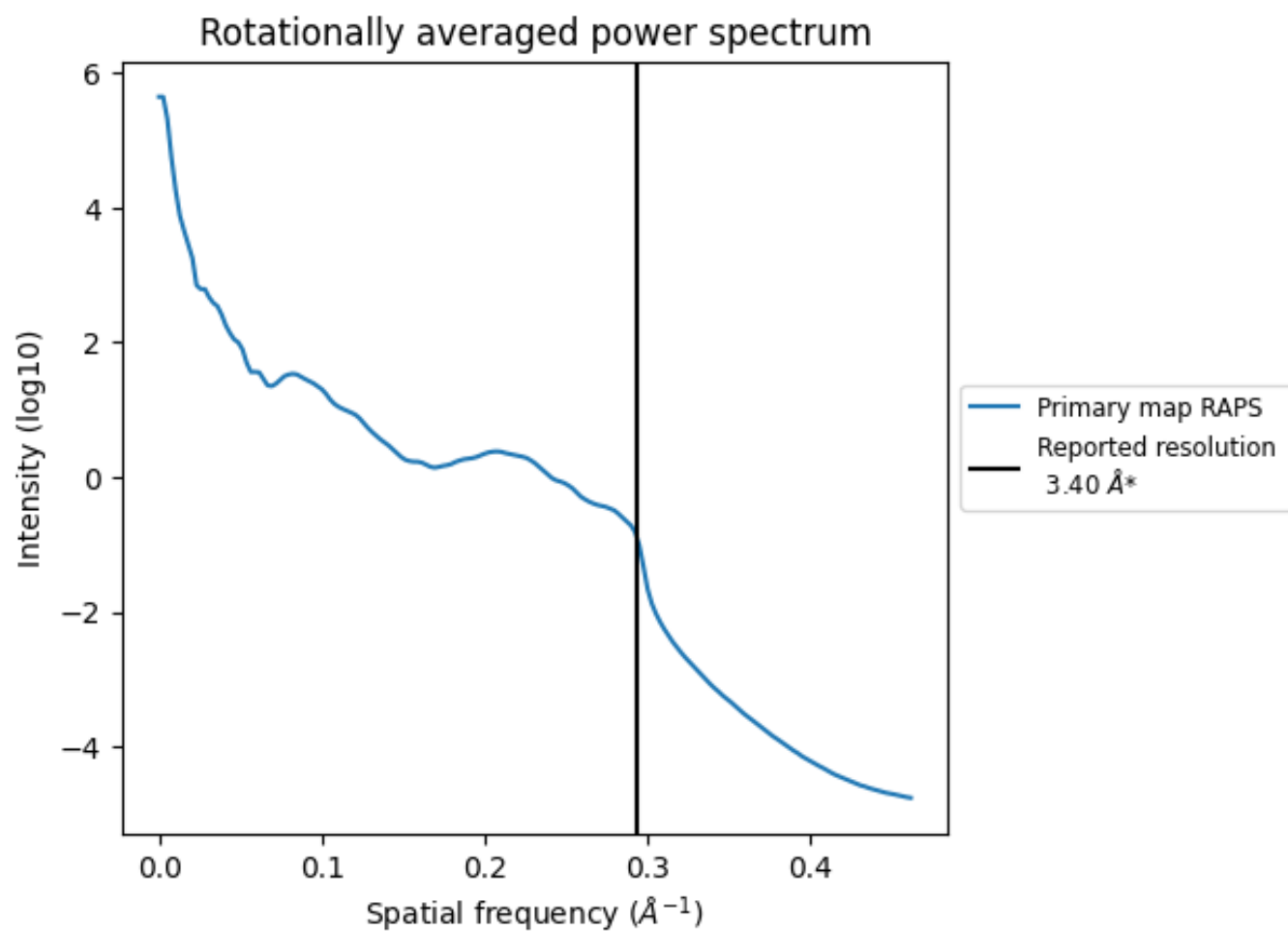
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 575 nm³; this corresponds to an approximate mass of 519 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 0.294 Å⁻¹

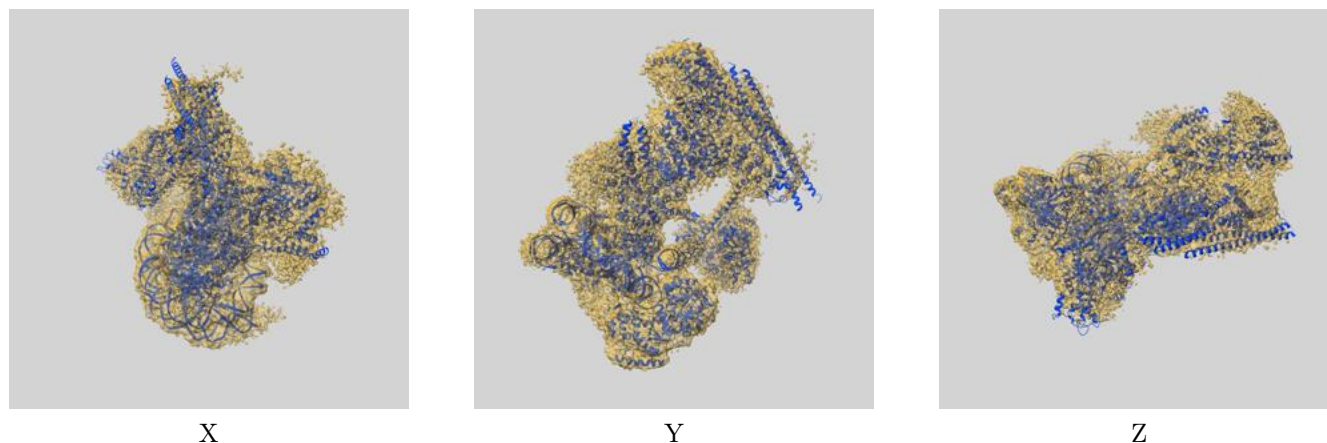
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

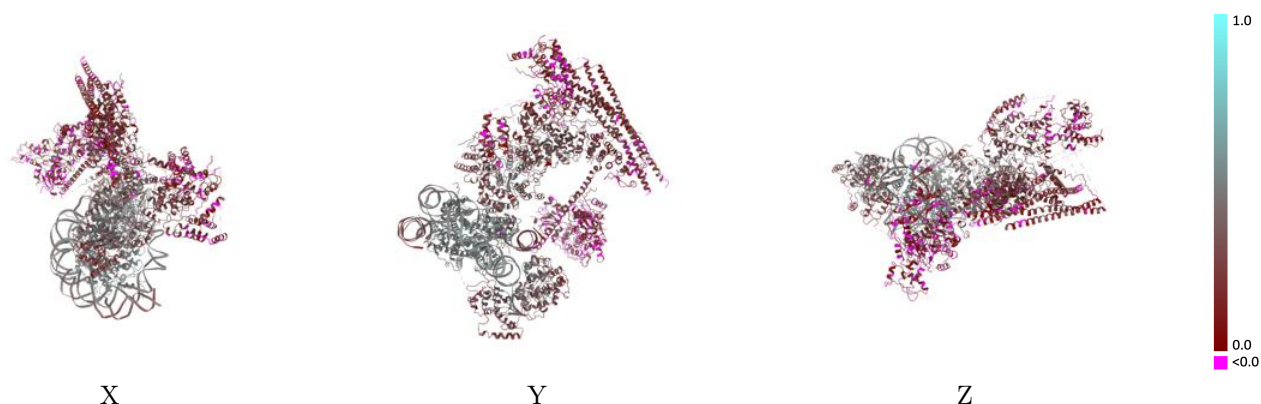
This section contains information regarding the fit between EMDB map EMD-31926 and PDB model 7VDV. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



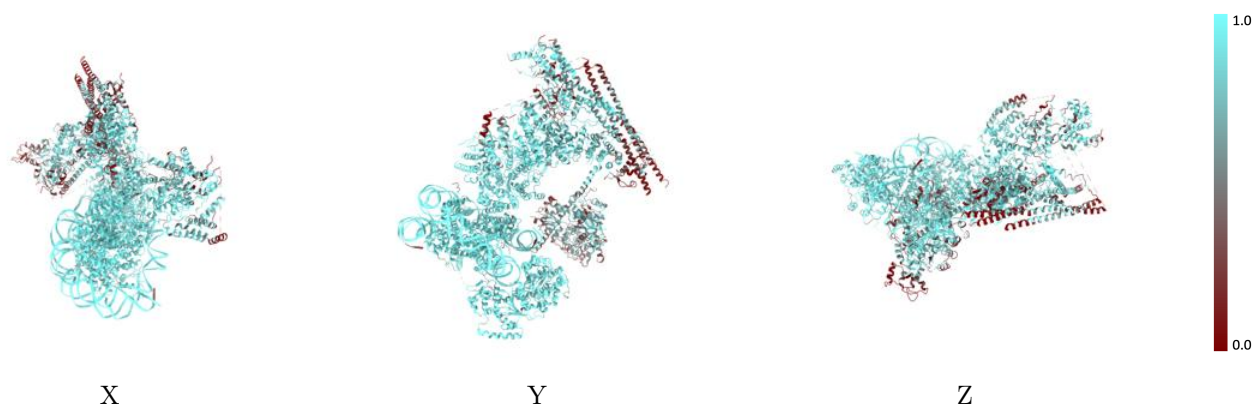
The images above show the 3D surface view of the map at the recommended contour level 0.0062 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



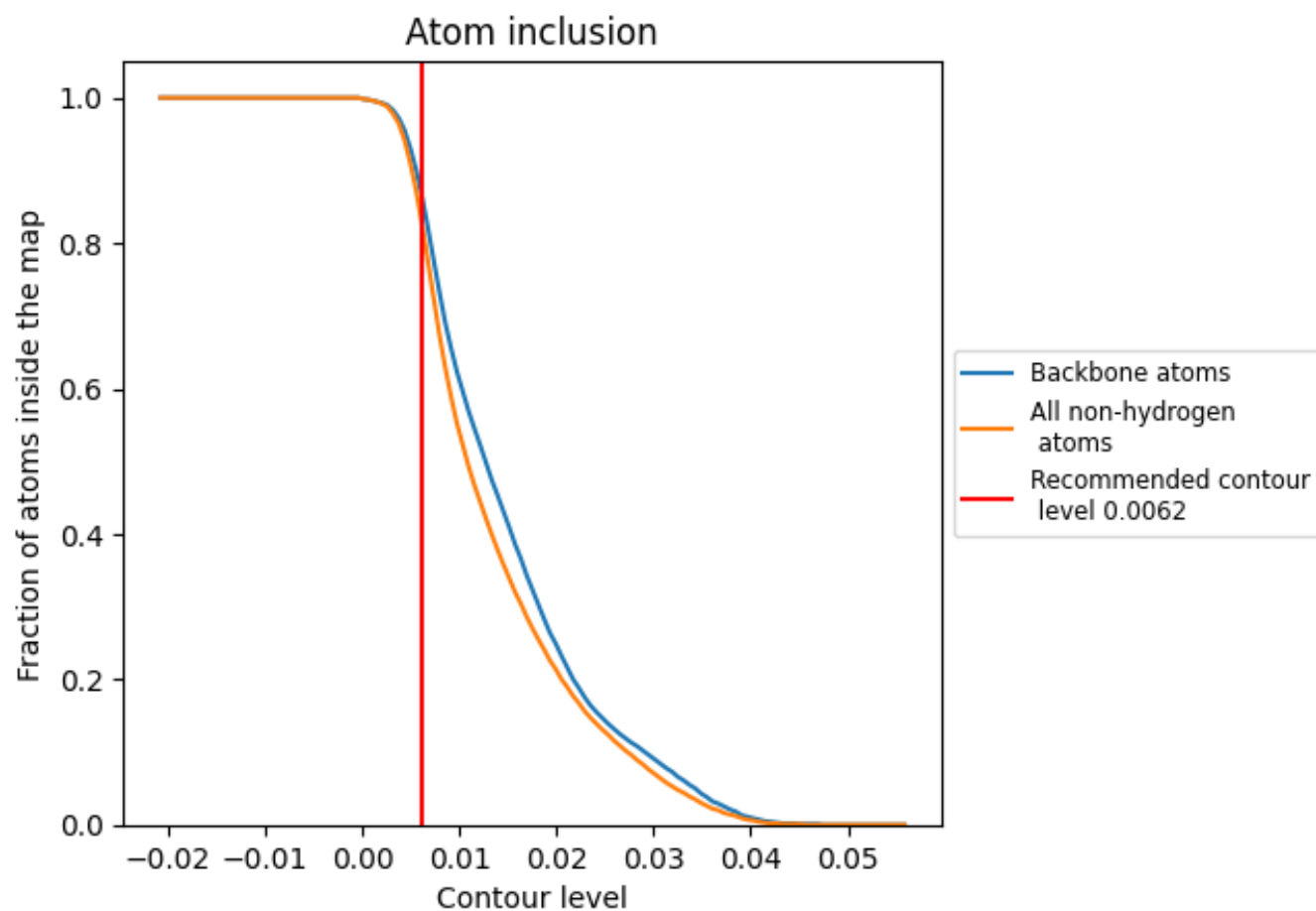
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0062).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.0062) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.3150
A	 0.8640	 0.3170
B	 0.9570	 0.5090
C	 0.9940	 0.5150
D	 0.9940	 0.5110
E	 0.9920	 0.5150
F	 0.9520	 0.5190
G	 0.9780	 0.5090
H	 0.9850	 0.5050
I	 0.9980	 0.4350
J	 0.9680	 0.4190
K	 0.9550	 0.4920
M	 0.7750	 0.1560
N	 0.6510	 0.1120
P	 0.4900	 0.1020
Q	 0.8730	 0.3070
R	 0.9730	 0.3480
T	 0.6500	 0.1690
U	 0.7710	 0.2360
V	 0.9660	 0.3910
W	 0.7650	 0.3070
X	 0.7280	 0.2340
Y	 0.5600	 0.1990
Z	 0.4600	 0.1730
a	 0.8380	 0.3010

