



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 03:49 PM UTC

PDB ID : 8HE5 / pdb_00008he5
EMDB ID : EMD-34685
Title : RNA polymerase II elongation complex bound with Rad26 and Elf1, stalled at SHL(-3.5) of the nucleosome
Authors : Osumi, K.; Kujirai, T.; Ehara, H.; Kinoshita, C.; Saotome, M.; Kagawa, W.; Sekine, S.; Takizawa, Y.; Kurumizaka, H.
Deposited on : 2022-11-07
Resolution : 6.95 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:

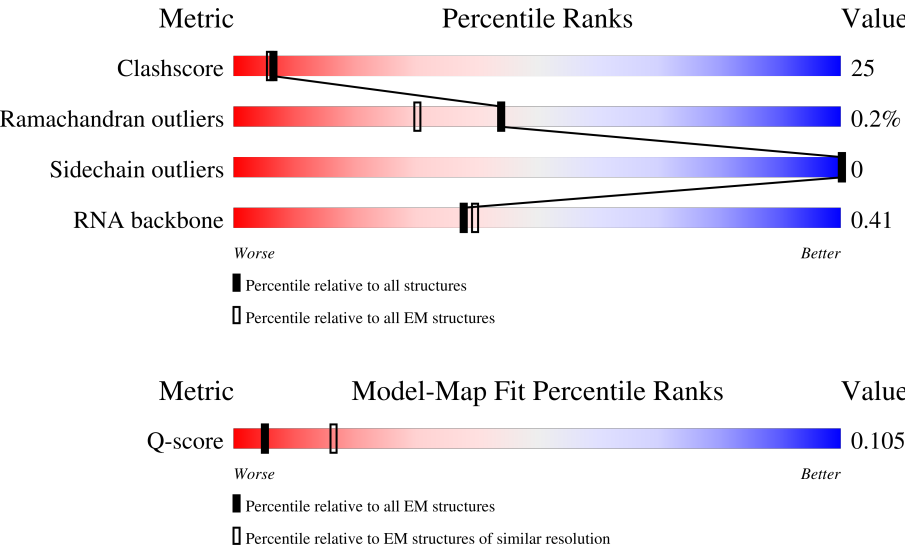
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.95 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	454 (6.45 - 7.41)

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	A	1743	35% 46% 19%
2	B	1227	44% 50% 6%
3	C	304	41% 45% 13%

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Mol	Chain	Length	Quality of chain
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	M	113	
14	N	198	
15	O	1094	
16	P	16	
17	T	198	
18	a	139	
18	e	139	
19	b	106	
19	f	106	
20	c	133	
20	g	133	
21	d	129	
21	h	129	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 48360 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1412	Total	C	N	O	S	0	0
			11123	7014	1938	2101	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9228	5816	1630	1724	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	64	Total	C	N	O	S	0	0
			505	318	82	99	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP C4QZ45
M	-1	PRO	-	expression tag	UNP C4QZ45
M	0	GLY	-	expression tag	UNP C4QZ45

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	142	Total	C	N	O	P	0	0
			2922	1385	526	869	142		

- Molecule 15 is a protein called DNA repair protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	516	Total	C	N	O	S	0	0
			4206	2710	739	744	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	GLY	-	expression tag	UNP F2QSG0
O	-4	PRO	-	expression tag	UNP F2QSG0
O	-3	LEU	-	expression tag	UNP F2QSG0
O	-2	GLY	-	expression tag	UNP F2QSG0
O	-1	SER	-	expression tag	UNP F2QSG0
O	0	HIS	-	expression tag	UNP F2QSG0

- Molecule 16 is a RNA chain called RNA (5'-R(P*GP*UP*UP*UP*UP*CP*GP*UP*UP*GP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	16	Total	C	N	O	P	0	0
			329	147	42	124	16		

- Molecule 17 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	154	Total	C	N	O	P	0	0
			3144	1489	605	897	153		

- Molecule 18 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
18	e	97	Total	C	N	O	S	0	0
			800	503	155	138	4		

- Molecule 19 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
19	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 20 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	c	103	Total	C	N	O	0	0
			796	502	155	139		
20	g	105	Total	C	N	O	0	0
			810	511	158	141		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908

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Chain	Residue	Modelled	Actual	Comment	Reference
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

- Molecule 21 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
21	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-3	GLY	-	expression tag	UNP P06899
d	-2	SER	-	expression tag	UNP P06899
d	-1	HIS	-	expression tag	UNP P06899
h	-3	GLY	-	expression tag	UNP P06899
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Zn	0
			2	2	
22	B	1	Total	Zn	0
			1	1	
22	C	1	Total	Zn	0
			1	1	
22	I	2	Total	Zn	0
			2	2	
22	J	1	Total	Zn	0
			1	1	
22	L	1	Total	Zn	0
			1	1	
22	M	1	Total	Zn	0
			1	1	

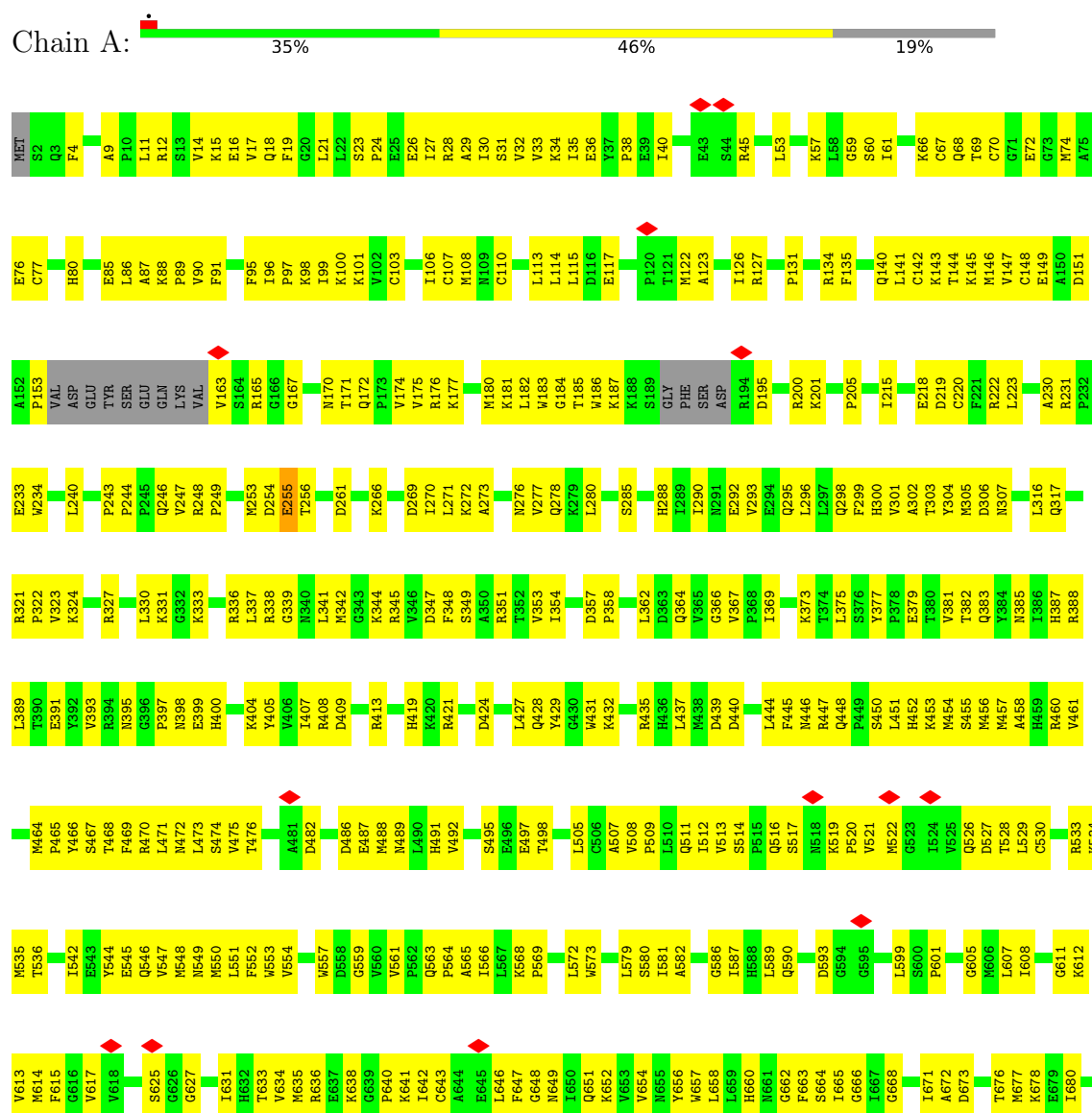
- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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.

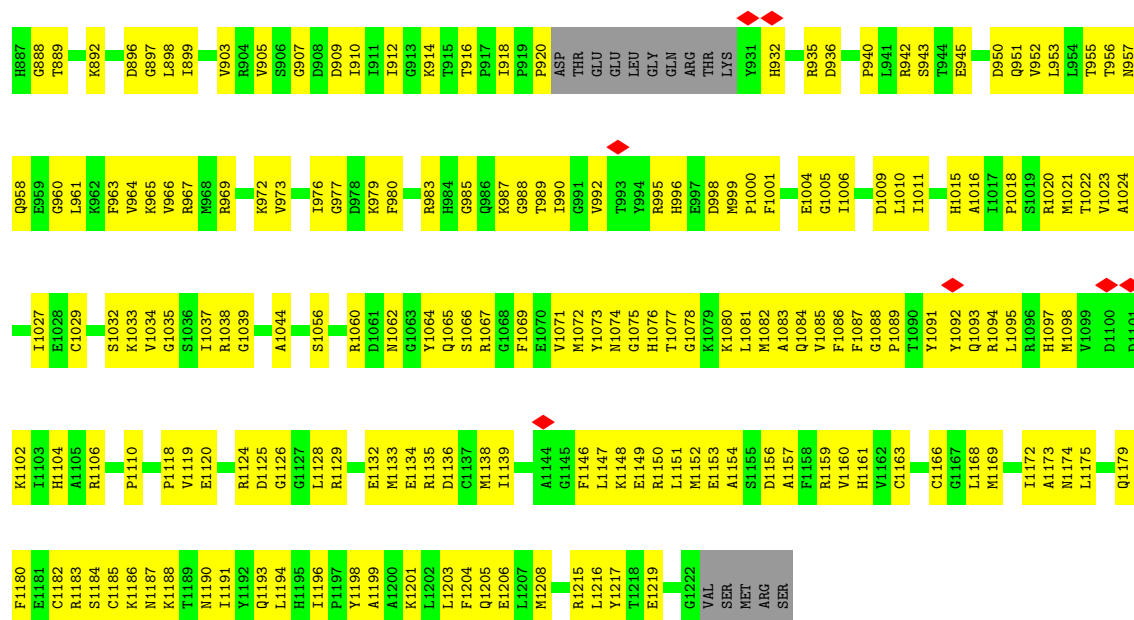
• Molecule 1: DNA-directed RNA polymerase subunit



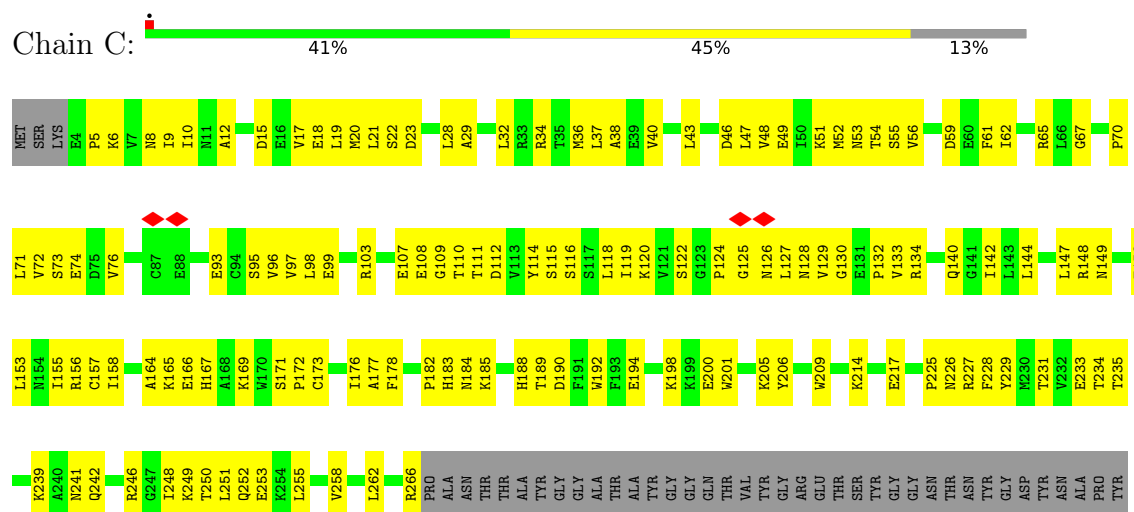


Chain B:

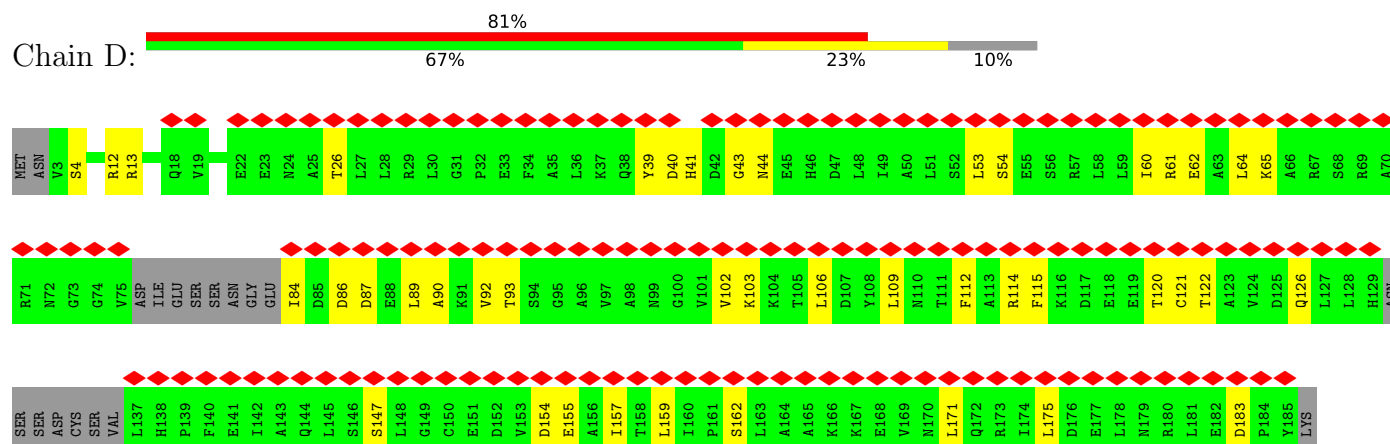


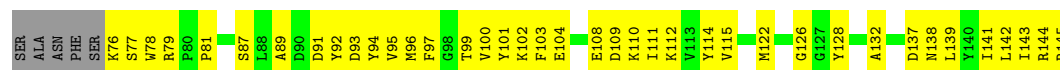


- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

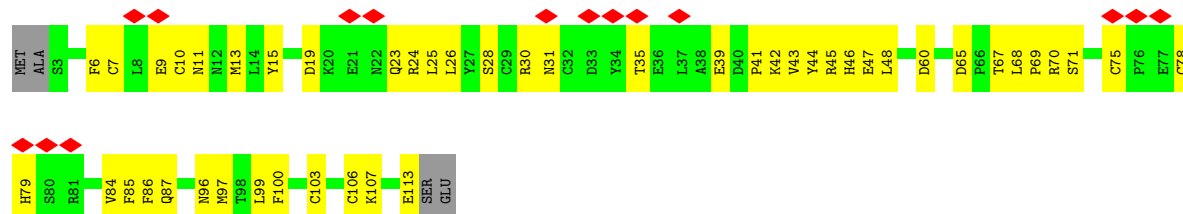


- Molecule 4: RNA polymerase II subunit B32

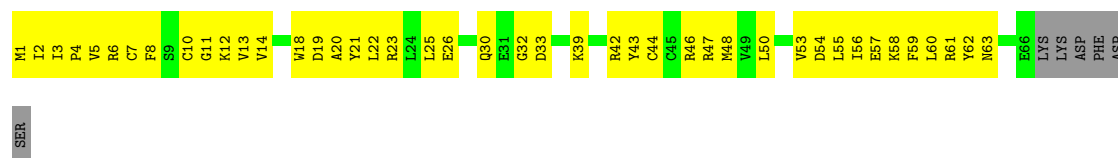




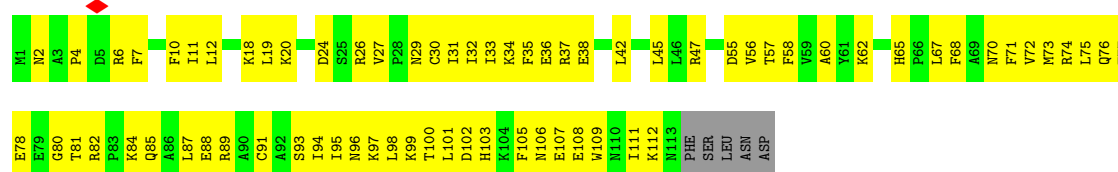
• Molecule 9: DNA-directed RNA polymerase subunit



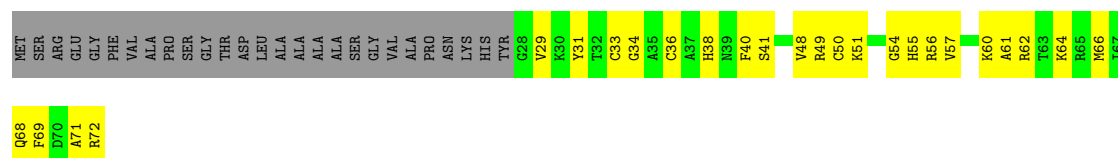
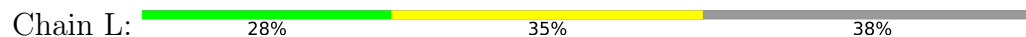
• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



• Molecule 11: RNA polymerase II subunit B12.5



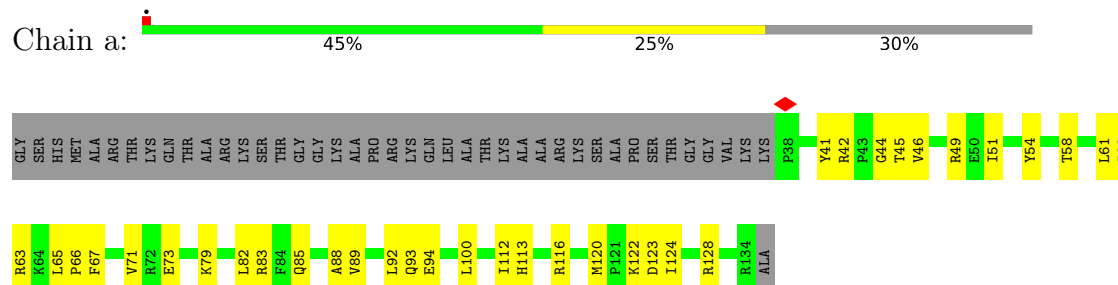
• Molecule 12: RNA polymerase subunit ABC10-alpha



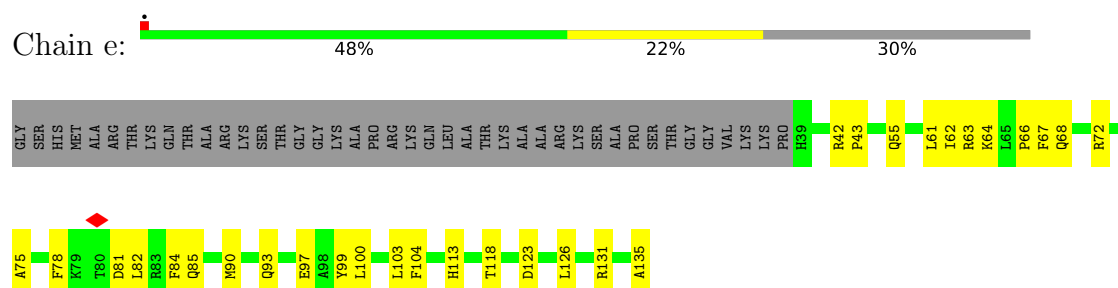
• Molecule 13: Transcription elongation factor 1 homolog



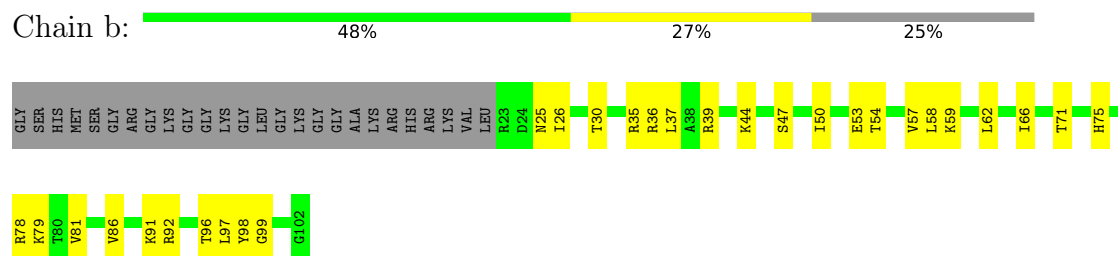
- Molecule 18: Histone H3.1



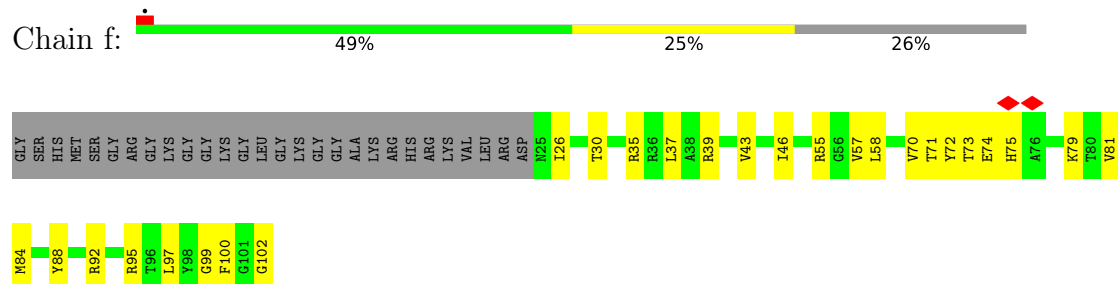
- Molecule 18: Histone H3.1



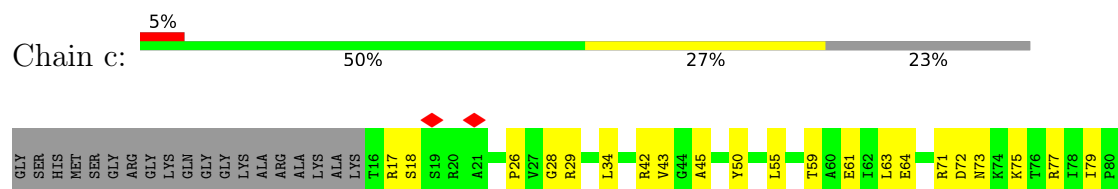
- Molecule 19: Histone H4

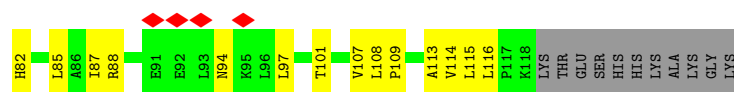


- Molecule 19: Histone H4



- Molecule 20: Histone H2A type 1-B/E

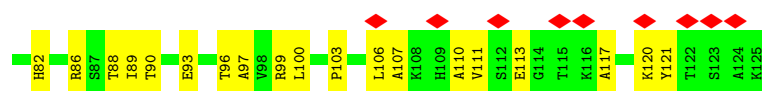
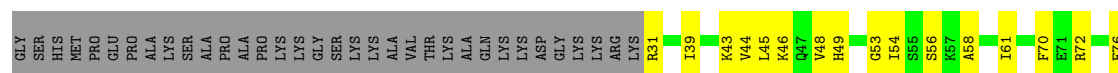




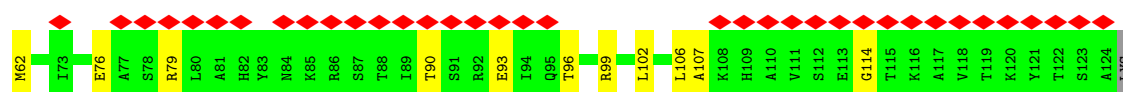
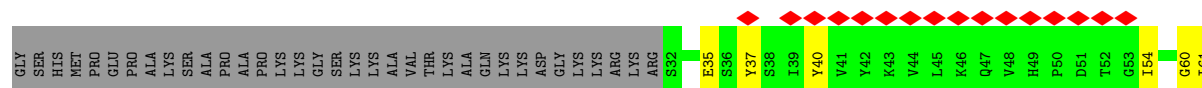
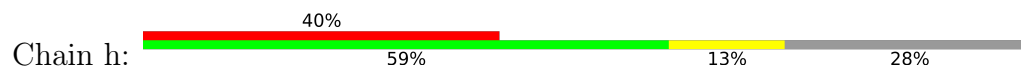
- Molecule 20: Histone H2A type 1-B/E



- Molecule 21: Histone H2B type 1-J



- Molecule 21: Histone H2B type 1-J



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.008	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00519	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.17	0/11329	0.48	3/15310 (0.0%)
2	B	0.17	0/9407	0.49	2/12685 (0.0%)
3	C	0.16	0/2139	0.44	0/2895
4	D	0.11	0/1326	0.32	0/1788
5	E	0.20	0/1772	0.53	3/2385 (0.1%)
6	F	0.14	0/687	0.38	0/931
7	G	0.13	0/1353	0.38	0/1837
8	H	0.17	0/1069	0.46	0/1444
9	I	0.13	0/934	0.37	0/1257
10	J	0.17	0/554	0.53	0/742
11	K	0.18	0/953	0.43	0/1291
12	L	0.18	0/365	0.57	0/484
13	M	0.18	0/513	0.45	2/693 (0.3%)
14	N	0.18	0/3273	0.36	0/5053
15	O	0.18	0/4301	0.59	3/5818 (0.1%)
16	P	0.09	0/363	0.17	0/561
17	T	0.18	0/3533	0.33	0/5444
18	a	0.11	0/813	0.27	0/1090
18	e	0.14	0/811	0.37	0/1086
19	b	0.11	0/645	0.28	0/862
19	f	0.13	0/626	0.30	0/837
20	c	0.12	0/806	0.35	0/1089
20	g	0.10	0/820	0.25	0/1107
21	d	0.12	0/757	0.32	0/1015
21	h	0.10	0/736	0.26	0/990
All	All	0.16	0/49885	0.44	13/68694 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	984	THR	CA-C-N	6.82	124.53	120.24
1	A	984	THR	C-N-CA	6.82	124.53	120.24
5	E	63	PRO	CA-C-N	-6.81	110.82	120.49
5	E	63	PRO	C-N-CA	-6.81	110.82	120.49
1	A	526	GLN	CB-CA-C	-6.51	109.08	116.63
15	O	473	ARG	CB-CA-C	-6.27	109.33	116.54
2	B	31	VAL	N-CA-C	-5.93	107.35	113.10
15	O	435	VAL	N-CA-C	-5.71	107.20	113.43
13	M	59	PRO	CA-N-CD	-5.59	104.17	112.00
13	M	59	PRO	N-CD-CG	-5.56	94.86	103.20
5	E	126	VAL	N-CA-C	-5.09	106.48	111.77
2	B	868	ILE	N-CA-C	-5.08	107.78	111.90
15	O	472	ILE	N-CA-C	-5.04	107.64	111.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1228	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11123	0	11147	779	0
2	B	9228	0	9232	585	0
3	C	2098	0	2057	150	0
4	D	1314	0	1314	29	0
5	E	1740	0	1754	138	0
6	F	677	0	693	40	0
7	G	1324	0	1342	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1052	0	1050	79	0
9	I	917	0	866	54	0
10	J	545	0	560	51	0
11	K	932	0	944	85	0
12	L	359	0	359	29	0
13	M	505	0	495	16	0
14	N	2922	0	1602	71	0
15	O	4206	0	4285	179	0
16	P	329	0	165	10	0
17	T	3144	0	1717	96	0
18	a	801	0	839	36	0
18	e	800	0	836	36	0
19	b	638	0	676	29	0
19	f	619	0	659	28	0
20	c	796	0	848	33	0
20	g	810	0	866	19	0
21	d	746	0	771	33	0
21	h	725	0	745	17	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	C	1	0	0	0	0
22	I	2	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	M	1	0	0	0	0
23	A	1	0	0	0	0
All	All	48360	0	45822	2286	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 (2286) 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)
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	1.91	1.09
2:B:245:MET:HE1	2:B:354:LEU:H	1.26	1.00
1:A:839:GLN:NE2	2:B:1133:MET:SD	2.46	0.88
10:J:20:ALA:HA	10:J:23:ARG:HE	1.37	0.88
1:A:528:THR:HA	1:A:654:VAL:HG11	1.56	0.87
1:A:1157:ASP:OD2	1:A:1241:ARG:NH2	2.07	0.87
2:B:554:TRP:HE1	2:B:593:MET:HE3	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:64:GLU:HA	21:d:49:HIS:HE1	1.41	0.85
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.61	0.83
3:C:110:THR:HA	3:C:147:LEU:O	1.79	0.83
3:C:9:ILE:HG12	3:C:19:LEU:HG	1.60	0.83
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.59	0.82
2:B:886:LYS:HD3	2:B:888:GLY:H	1.44	0.82
8:H:79:ARG:HD3	11:K:57:THR:HB	1.61	0.81
15:O:323:VAL:HG12	15:O:324:GLY:H	1.43	0.81
1:A:546:GLN:HG2	1:A:550:MET:HE2	1.63	0.81
1:A:1339:LEU:HD22	1:A:1384:LEU:HG	1.63	0.81
10:J:7:CYS:HB3	10:J:11:GLY:H	1.45	0.81
2:B:209:SER:HA	2:B:397:LYS:HG3	1.62	0.80
2:B:605:GLU:HG3	2:B:625:ARG:HH22	1.47	0.80
10:J:1:MET:HA	10:J:54:ASP:HA	1.63	0.80
2:B:60:GLN:HE21	2:B:429:ILE:HG12	1.47	0.79
1:A:107:CYS:CB	1:A:110:CYS:SG	2.70	0.79
2:B:784:ASN:OD1	2:B:788:ARG:NH1	2.15	0.79
2:B:805:LYS:O	2:B:1044:ALA:N	2.15	0.78
1:A:301:VAL:HG12	1:A:305:MET:HE1	1.66	0.78
1:A:1286:TYR:HB2	1:A:1310:GLU:HB3	1.66	0.77
1:A:636:ARG:NH1	1:A:880:GLU:OE1	2.16	0.77
3:C:73:SER:HA	3:C:129:VAL:HG12	1.65	0.77
8:H:79:ARG:NH1	11:K:76:GLN:OE1	2.18	0.77
3:C:47:LEU:HB2	3:C:158:ILE:HB	1.66	0.77
15:O:578:LYS:HD2	15:O:783:ILE:HG12	1.67	0.77
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.67	0.76
18:e:75:ALA:HB1	18:e:82:LEU:HD11	1.67	0.76
1:A:1137:GLN:HG3	1:A:1285:VAL:HB	1.68	0.76
2:B:985:GLY:O	2:B:1020:ARG:NH2	2.18	0.76
2:B:1084:GLN:OE1	3:C:189:THR:OG1	2.04	0.76
5:E:27:TYR:HA	5:E:63:PRO:HA	1.67	0.76
1:A:568:LYS:HG2	1:A:569:PRO:HA	1.68	0.75
1:A:475:VAL:HA	1:A:522:MET:HE2	1.68	0.75
3:C:65:ARG:HH12	10:J:4:PRO:HA	1.51	0.75
1:A:712:ARG:NH2	9:I:87:GLN:OE1	2.17	0.75
2:B:398:ARG:HE	2:B:622:ASP:HB3	1.52	0.75
2:B:1168:LEU:HD22	2:B:1208:MET:HE1	1.66	0.75
1:A:1029:ALA:HB3	1:A:1032:ARG:HE	1.52	0.75
2:B:353:LEU:O	2:B:367:LYS:NZ	2.18	0.75
2:B:802:PRO:HG2	2:B:805:LYS:HD3	1.67	0.75
6:F:97:ARG:NH2	6:F:106:PRO:O	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ILE:HG13	5:E:166:ARG:HE	1.50	0.75
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.33	0.75
2:B:497:ARG:NH2	2:B:524:GLN:O	2.19	0.74
18:a:62:ILE:O	18:a:93:GLN:NE2	2.20	0.74
1:A:899:TYR:O	1:A:1031:ARG:NH1	2.20	0.74
20:c:55:LEU:HD11	21:d:70:PHE:HB2	1.69	0.74
1:A:533:ARG:NH1	1:A:746:GLN:O	2.19	0.74
2:B:105:ARG:O	2:B:965:LYS:NZ	2.21	0.74
3:C:10:ILE:HD11	3:C:20:MET:HE3	1.69	0.74
1:A:516:GLN:NE2	1:A:1365:TYR:O	2.20	0.74
2:B:918:ILE:HD11	2:B:935:ARG:HB2	1.68	0.74
1:A:243:PRO:O	1:A:248:ARG:NH1	2.20	0.74
2:B:290:LEU:O	2:B:294:CYS:N	2.21	0.74
2:B:998:ASP:HB3	2:B:1076:HIS:HE1	1.53	0.74
2:B:1159:ARG:HA	2:B:1194:LEU:O	1.86	0.74
1:A:769:GLN:HB3	1:A:820:ALA:HB2	1.70	0.74
3:C:262:LEU:HD21	11:K:87:LEU:HD23	1.69	0.74
1:A:18:GLN:NE2	1:A:19:PHE:O	2.20	0.74
1:A:867:PHE:HE2	5:E:209:SER:HA	1.51	0.73
1:A:1153:GLU:HA	9:I:45:ARG:HA	1.68	0.73
6:F:133:VAL:HG22	6:F:147:GLY:HA2	1.69	0.73
11:K:99:LYS:O	11:K:103:HIS:ND1	2.20	0.73
15:O:335:LYS:HB3	15:O:494:LEU:HD12	1.69	0.73
1:A:331:LYS:NZ	17:T:56:DC:O5'	2.21	0.73
3:C:147:LEU:HD21	3:C:153:LEU:HD23	1.69	0.73
5:E:93:ARG:HA	5:E:122:MET:HE1	1.70	0.73
5:E:110:ILE:HG13	5:E:134:PHE:HB2	1.71	0.73
2:B:111:TYR:HB2	2:B:195:VAL:HB	1.70	0.73
2:B:750:GLY:H	2:B:753:ALA:HB3	1.53	0.73
2:B:771:SER:O	2:B:775:LYS:NZ	2.21	0.73
2:B:847:ASP:OD2	2:B:995:ARG:NH1	2.22	0.73
1:A:1125:GLU:OE1	1:A:1132:LYS:NZ	2.21	0.73
2:B:818:PRO:HG3	10:J:53:VAL:HG21	1.71	0.72
3:C:65:ARG:NH2	10:J:3:ILE:O	2.22	0.72
20:c:64:GLU:HA	21:d:49:HIS:CE1	2.24	0.72
1:A:344:LYS:HG2	2:B:1135:ARG:HH22	1.53	0.72
1:A:447:ARG:O	1:A:450:SER:OG	2.06	0.72
1:A:897:ARG:NH2	1:A:1035:GLU:OE1	2.23	0.72
11:K:45:LEU:HD21	11:K:94:ILE:HG21	1.72	0.72
2:B:290:LEU:HD13	9:I:6:PHE:HE2	1.54	0.72
1:A:330:LEU:HD21	2:B:1206:GLU:HG3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:THR:OG1	5:E:139:LEU:O	2.04	0.72
2:B:490:ARG:NH2	2:B:531:ASN:OD1	2.23	0.72
2:B:586:PRO:HG2	2:B:610:ARG:HH21	1.53	0.72
1:A:176:ARG:NH2	1:A:185:THR:OG1	2.23	0.71
11:K:108:GLU:HA	11:K:111:ILE:HG12	1.72	0.71
5:E:67:ALA:O	5:E:71:TYR:N	2.23	0.71
5:E:198:ILE:HG23	5:E:206:ARG:HD3	1.72	0.71
8:H:5:LEU:HG	8:H:61:ASN:HD22	1.54	0.71
18:e:62:ILE:HD11	19:f:37:LEU:HD11	1.72	0.71
1:A:373:LYS:NZ	1:A:397:PRO:O	2.23	0.71
3:C:107:GLU:O	3:C:148:ARG:NH1	2.22	0.71
1:A:846:LEU:HD22	1:A:849:ILE:HD11	1.70	0.71
1:A:1112:ASN:HD21	1:A:1116:PRO:HG3	1.54	0.71
2:B:413:LEU:HB3	2:B:446:ILE:HG13	1.71	0.71
2:B:475:VAL:HG21	17:T:66:DC:H5''	1.72	0.71
1:A:1172:VAL:HG11	1:A:1241:ARG:NH1	2.05	0.70
12:L:62:ARG:O	12:L:64:LYS:NZ	2.23	0.70
15:O:748:THR:O	15:O:777:GLN:NE2	2.22	0.70
1:A:1280:PRO:O	1:A:1315:ASN:ND2	2.23	0.70
1:A:366:GLY:HA3	1:A:470:ARG:HB2	1.72	0.70
1:A:1168:ASP:OD2	1:A:1196:ARG:NE	2.22	0.70
1:A:1194:LEU:HD11	1:A:1241:ARG:HE	1.56	0.70
5:E:42:ARG:NH2	5:E:48:SER:O	2.24	0.70
1:A:590:GLN:HE21	1:A:607:LEU:HD13	1.57	0.70
1:A:1004:GLY:HA3	1:A:1009:ILE:HD13	1.73	0.70
1:A:517:SER:OG	1:A:1365:TYR:O	2.09	0.70
2:B:107:ARG:NH2	2:B:956:THR:OG1	2.25	0.70
1:A:866:GLN:NE2	1:A:1376:ASP:OD2	2.24	0.70
2:B:766:ARG:NH2	2:B:985:GLY:O	2.23	0.70
2:B:641:ASN:HD21	2:B:646:ARG:HA	1.56	0.70
7:G:152:THR:HA	7:G:157:ILE:HG22	1.74	0.70
18:a:113:HIS:NE2	18:e:123:ASP:OD1	2.21	0.70
1:A:1397:THR:O	1:A:1402:ARG:NH2	2.25	0.69
3:C:248:ILE:O	3:C:252:GLN:HG3	1.91	0.69
5:E:108:ILE:HG22	5:E:132:GLU:HB2	1.74	0.69
9:I:78:CYS:SG	9:I:103:CYS:CB	2.80	0.69
1:A:774:LYS:HG2	1:A:775:ARG:H	1.57	0.69
3:C:164:ALA:HB2	3:C:171:SER:HA	1.75	0.69
11:K:10:PHE:HA	11:K:37:ARG:HB3	1.74	0.69
17:T:16:DA:H4'	17:T:17:DA:H5'	1.73	0.69
1:A:1314:ILE:HG21	1:A:1337:GLU:HG3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:LYS:NZ	2:B:689:TYR:OH	2.21	0.69
2:B:709:THR:HG21	2:B:735:HIS:HA	1.73	0.69
2:B:898:LEU:HD21	2:B:964:VAL:HG21	1.73	0.69
3:C:74:GLU:O	3:C:246:ARG:NH2	2.26	0.69
8:H:109:ASP:HA	8:H:128:TYR:HB2	1.74	0.69
20:c:113:ALA:HA	20:c:116:LEU:HD23	1.75	0.69
1:A:535:MET:HE2	1:A:657:TRP:HB3	1.72	0.69
1:A:296:LEU:HA	1:A:299:PHE:CE1	2.28	0.69
3:C:116:SER:HA	3:C:134:ARG:HH21	1.58	0.69
5:E:42:ARG:HD2	5:E:46:CYS:HB2	1.73	0.69
7:G:153:ASP:O	7:G:155:ASN:N	2.24	0.69
2:B:573:ILE:HG12	2:B:617:PHE:HB3	1.75	0.68
14:N:-73:DT:H3	17:T:73:DA:H61	1.39	0.68
15:O:804:GLN:O	15:O:808:ASN:HB2	1.92	0.68
1:A:851:VAL:HG22	1:A:857:THR:HG22	1.74	0.68
2:B:1196:ILE:HD11	2:B:1201:LYS:HE3	1.76	0.68
5:E:176:ARG:O	5:E:211:ARG:NH1	2.25	0.68
10:J:47:ARG:HA	10:J:50:LEU:HB3	1.75	0.68
1:A:349:SER:HB2	2:B:1128:LEU:HD22	1.74	0.68
1:A:454:MET:HG2	1:A:521:VAL:HG11	1.75	0.68
15:O:710:ASP:HA	15:O:740:VAL:HG11	1.74	0.68
14:N:31:DT:H3	17:T:-31:DA:H61	1.40	0.68
17:T:-34:DG:H3'	21:d:86:ARG:HE	1.58	0.68
1:A:468:THR:O	1:A:470:ARG:NH1	2.26	0.68
3:C:266:ARG:NH2	11:K:88:GLU:OE2	2.26	0.68
6:F:138:LEU:HD11	6:F:144:GLU:HG3	1.75	0.68
1:A:440:ASP:N	1:A:461:VAL:O	2.26	0.68
1:A:985:ILE:HG23	1:A:1030:THR:HG21	1.75	0.68
1:A:914:ILE:HA	1:A:981:SER:H	1.57	0.68
1:A:983:LEU:HD12	1:A:1041:ARG:HD3	1.75	0.68
2:B:178:VAL:HG22	2:B:182:LYS:HZ3	1.58	0.68
2:B:325:PHE:O	2:B:329:ARG:NH1	2.27	0.68
2:B:505:ARG:NH1	2:B:526:CYS:O	2.23	0.68
5:E:25:ARG:HH12	5:E:154:ARG:HB2	1.57	0.67
15:O:648:ALA:HB2	15:O:690:ARG:HH22	1.59	0.67
1:A:840:ARG:NH2	17:T:59:DC:O3'	2.27	0.67
1:A:886:THR:O	1:A:941:ARG:NH1	2.26	0.67
15:O:340:ILE:HG13	15:O:371:GLU:HG3	1.74	0.67
15:O:362:ALA:HA	15:O:365:LEU:HG	1.76	0.67
15:O:623:LYS:HE2	15:O:630:LEU:HG	1.76	0.67
9:I:78:CYS:SG	9:I:103:CYS:HB3	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:120:MET:SD	18:a:122:LYS:NZ	2.62	0.67
1:A:61:ILE:HD11	1:A:249:PRO:HB3	1.76	0.67
1:A:254:ASP:OD1	17:T:69:DC:N4	2.27	0.67
1:A:280:LEU:HD11	1:A:293:VAL:HB	1.76	0.67
1:A:1172:VAL:HG11	1:A:1241:ARG:HH11	1.59	0.67
2:B:562:TYR:OH	2:B:572:ARG:NH1	2.26	0.67
3:C:20:MET:SD	3:C:227:ARG:NH2	2.63	0.67
14:N:37:DC:O2	17:T:-37:DG:N2	2.19	0.67
15:O:680:MET:HE3	15:O:684:LEU:HG	1.76	0.67
1:A:57:LYS:O	1:A:69:THR:OG1	2.12	0.67
2:B:979:LYS:NZ	2:B:980:PHE:O	2.28	0.67
15:O:326:ILE:HG12	15:O:493:ILE:HD12	1.77	0.67
1:A:107:CYS:HB3	1:A:110:CYS:SG	2.34	0.67
10:J:7:CYS:CB	10:J:10:CYS:SG	2.82	0.67
1:A:336:ARG:NH2	2:B:1199:ALA:O	2.28	0.67
3:C:124:PRO:HG2	3:C:127:LEU:HD22	1.77	0.66
18:a:123:ASP:OD1	18:e:113:HIS:NE2	2.21	0.66
1:A:1159:ASP:O	1:A:1243:ARG:NH2	2.28	0.66
1:A:1210:THR:OG1	1:A:1213:GLN:OE1	2.13	0.66
1:A:1296:ASP:N	1:A:1300:GLU:O	2.26	0.66
2:B:1187:ASN:HD21	2:B:1190:ASN:HB3	1.59	0.66
7:G:34:VAL:HG22	7:G:45:ILE:HG21	1.75	0.66
2:B:627:TYR:HB2	2:B:689:TYR:HB3	1.77	0.66
6:F:85:LEU:HD13	6:F:128:ARG:HH22	1.58	0.66
2:B:809:MET:SD	2:B:815:ARG:NH1	2.68	0.66
3:C:206:TYR:HA	3:C:209:TRP:HD1	1.60	0.66
1:A:1194:LEU:HD13	1:A:1241:ARG:HH21	1.60	0.66
2:B:71:ILE:HD11	2:B:125:THR:HB	1.77	0.66
2:B:704:PRO:HA	2:B:707:LEU:HD13	1.77	0.66
5:E:12:TRP:NE1	5:E:36:GLN:O	2.27	0.66
1:A:513:VAL:HA	1:A:520:PRO:HA	1.77	0.66
15:O:450:ARG:HH12	15:O:454:LYS:HE3	1.60	0.66
1:A:548:MET:HA	1:A:551:LEU:HD12	1.76	0.66
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.60	0.66
14:N:58:DC:OP1	20:c:77:ARG:N	2.28	0.66
1:A:45:ARG:NH1	2:B:920:PRO:O	2.29	0.66
3:C:52:MET:HA	12:L:62:ARG:HH22	1.61	0.66
1:A:1145:LEU:HD22	1:A:1274:ILE:HB	1.78	0.66
2:B:108:ASN:O	2:B:958:GLN:NE2	2.28	0.65
2:B:595:ASP:OD1	2:B:598:ARG:NH2	2.22	0.65
2:B:1106:ARG:NH1	2:B:1125:ASP:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:NZ	14:N:-50:DT:OP1	2.28	0.65
1:A:113:LEU:O	1:A:165:ARG:NH1	2.29	0.65
1:A:498:THR:HG21	2:B:1149:GLU:HG2	1.79	0.65
3:C:98:LEU:HB2	3:C:157:CYS:HB2	1.78	0.65
1:A:151:ASP:HB3	1:A:163:VAL:HG23	1.79	0.65
1:A:545:GLU:OE2	11:K:47:ARG:NH1	2.29	0.65
1:A:758:ASN:O	1:A:762:MET:HG3	1.96	0.65
2:B:628:ARG:HH12	2:B:743:ILE:H	1.43	0.65
14:N:-37:DG:H2''	14:N:-36:DG:C8	2.32	0.65
14:N:28:DA:H61	17:T:-28:DT:H3	1.43	0.65
1:A:691:VAL:HG22	1:A:719:VAL:HG13	1.77	0.65
1:A:878:GLN:HG2	1:A:1058:SER:HA	1.79	0.65
15:O:455:HIS:O	15:O:459:ARG:NH2	2.29	0.65
1:A:327:ARG:HG3	1:A:1409:VAL:HG11	1.78	0.65
1:A:367:VAL:HG21	1:A:461:VAL:HG22	1.78	0.65
2:B:950:ASP:OD2	2:B:967:ARG:NH2	2.29	0.65
1:A:452:HIS:HD2	1:A:454:MET:HB2	1.62	0.65
1:A:891:ASP:N	1:A:1298:SER:O	2.29	0.65
1:A:968:ASN:OD1	1:A:971:GLN:NE2	2.30	0.65
2:B:204:ILE:N	2:B:472:VAL:O	2.29	0.65
3:C:111:THR:HB	3:C:147:LEU:HB2	1.77	0.65
3:C:49:GLU:OE1	3:C:156:ARG:NH2	2.30	0.65
3:C:177:ALA:HB3	3:C:231:THR:HB	1.78	0.65
4:D:171:LEU:HD23	4:D:175:LEU:HD23	1.79	0.65
1:A:780:PHE:HB2	1:A:783:ARG:HG2	1.77	0.65
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.78	0.65
6:F:90:ARG:HD3	6:F:125:LEU:HD21	1.78	0.65
15:O:625:CYS:O	15:O:653:LYS:NZ	2.29	0.65
1:A:458:ALA:HB3	1:A:507:ALA:HA	1.79	0.65
1:A:723:LEU:HB2	1:A:775:ARG:HH22	1.61	0.65
1:A:1152:THR:OG1	9:I:46:HIS:O	2.14	0.65
1:A:1218:ILE:HA	1:A:1221:VAL:HG12	1.79	0.65
2:B:1016:ALA:O	2:B:1020:ARG:N	2.27	0.65
8:H:91:ASP:O	8:H:144:ARG:NH1	2.30	0.64
15:O:755:ILE:HG13	15:O:785:ARG:HH11	1.62	0.64
17:T:-37:DG:H4'	17:T:-36:DT:H5'	1.80	0.64
1:A:838:ILE:HG12	1:A:1104:LYS:HZ2	1.61	0.64
8:H:102:LYS:HG3	8:H:114:TYR:HB2	1.79	0.64
1:A:464:MET:O	1:A:470:ARG:NH2	2.31	0.64
1:A:841:ARG:HH12	1:A:1107:LEU:HB3	1.61	0.64
3:C:9:ILE:H	11:K:108:GLU:CD	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:54:SER:O	8:H:145:ARG:NH1	2.30	0.64
15:O:606:ARG:O	15:O:609:GLN:NE2	2.30	0.64
18:e:81:ASP:O	19:f:79:LYS:NZ	2.30	0.64
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.79	0.64
2:B:480:THR:HG23	2:B:483:SER:H	1.62	0.64
3:C:103:ARG:HG2	3:C:152:GLU:HG2	1.80	0.64
1:A:1165:ILE:HG22	1:A:1167:GLU:H	1.61	0.64
2:B:229:ALA:HB2	2:B:378:LEU:HB2	1.78	0.64
17:T:-13:DA:OP1	18:a:63:ARG:NH1	2.31	0.64
20:g:112:GLN:H	20:g:115:LEU:HD12	1.62	0.64
1:A:437:LEU:HD21	1:A:461:VAL:HG21	1.79	0.64
1:A:516:GLN:HE21	1:A:1366:VAL:HG22	1.63	0.64
1:A:1106:ILE:HG23	1:A:1351:LEU:HD11	1.79	0.64
15:O:329:ASP:HB3	15:O:566:ARG:HB2	1.80	0.64
3:C:184:ASN:ND2	3:C:189:THR:O	2.29	0.63
14:N:-46:DT:O2	17:T:47:DG:N2	2.32	0.63
11:K:82:ARG:HB2	11:K:85:GLN:HG2	1.80	0.63
15:O:626:ASN:O	15:O:651:SER:OG	2.15	0.63
1:A:1163:THR:HB	1:A:1241:ARG:HH12	1.62	0.63
2:B:413:LEU:HD23	2:B:446:ILE:HA	1.78	0.63
2:B:634:GLU:OE2	2:B:646:ARG:NE	2.30	0.63
5:E:46:CYS:HA	5:E:52:PRO:HA	1.81	0.63
11:K:65:HIS:HE1	11:K:67:LEU:HD12	1.64	0.63
15:O:517:ARG:HH11	15:O:562:TYR:HE2	1.46	0.63
1:A:1423:ASP:HB2	1:A:1425:ARG:HD2	1.80	0.63
2:B:19:THR:O	2:B:22:SER:OG	2.15	0.63
8:H:5:LEU:HD11	8:H:61:ASN:HB3	1.81	0.63
1:A:19:PHE:O	2:B:1215:ARG:NH2	2.26	0.63
1:A:514:SER:HB3	1:A:521:VAL:HG12	1.79	0.63
1:A:951:ASN:HB2	1:A:1293:SER:HB3	1.81	0.63
1:A:1149:THR:HB	9:I:48:LEU:HD22	1.79	0.63
1:A:1190:GLN:HB2	1:A:1245:ILE:HG12	1.81	0.63
2:B:301:GLN:OE1	2:B:385:ARG:NH2	2.32	0.63
8:H:55:LEU:HD13	8:H:145:ARG:HA	1.78	0.63
15:O:623:LYS:NZ	17:T:74:DA:OP1	2.26	0.63
2:B:1033:LYS:HE2	2:B:1088:GLY:HA3	1.81	0.63
15:O:369:CYS:SG	15:O:373:HIS:NE2	2.72	0.63
1:A:1118:LEU:HD11	1:A:1315:ASN:H	1.63	0.63
2:B:1075:GLY:O	3:C:34:ARG:NH1	2.32	0.63
3:C:51:LYS:NZ	3:C:99:GLU:OE2	2.32	0.63
14:N:32:DG:O6	17:T:-33:DA:N6	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:255:ARG:HE	15:O:377:PRO:HA	1.64	0.63
2:B:189:ASP:OD1	2:B:478:ARG:NH1	2.32	0.63
2:B:802:PRO:HB3	2:B:1091:TYR:CD2	2.34	0.63
11:K:71:PHE:HE1	11:K:73:MET:HB2	1.63	0.63
1:A:122:MET:HE2	1:A:141:LEU:HB2	1.79	0.62
1:A:1462:PRO:HD3	7:G:19:GLY:HA3	1.81	0.62
2:B:607:SER:OG	2:B:691:ASP:OD2	2.17	0.62
15:O:760:TRP:HE3	15:O:799:ARG:HH22	1.47	0.62
1:A:12:ARG:HH22	7:G:10:ILE:HG13	1.63	0.62
1:A:1033:ILE:O	1:A:1038:ARG:N	2.30	0.62
3:C:93:GLU:HA	3:C:124:PRO:HG3	1.81	0.62
7:G:23:ASN:O	7:G:26:LEU:HB2	1.99	0.62
7:G:101:ALA:HB3	7:G:108:VAL:HB	1.81	0.62
8:H:101:TYR:CZ	8:H:114:TYR:HB3	2.33	0.62
1:A:719:VAL:HG12	1:A:775:ARG:NH1	2.15	0.62
1:A:1395:ALA:HB3	1:A:1402:ARG:HD3	1.79	0.62
2:B:106:LEU:HD13	12:L:57:VAL:HG11	1.81	0.62
8:H:11:THR:O	8:H:13:GLN:NE2	2.32	0.62
15:O:556:LYS:O	15:O:560:SER:HB2	1.99	0.62
8:H:39:THR:O	8:H:122:MET:HA	1.99	0.62
2:B:204:ILE:O	2:B:206:GLN:NE2	2.32	0.62
2:B:735:HIS:HB3	9:I:70:ARG:HG2	1.81	0.62
2:B:1000:PRO:HB2	2:B:1072:MET:HB3	1.81	0.62
8:H:111:ILE:HG12	8:H:128:TYR:HA	1.80	0.62
21:d:117:ALA:HA	21:d:120:LYS:HE2	1.79	0.62
1:A:881:ARG:HB2	1:A:955:ASN:HD21	1.65	0.62
2:B:27:GLU:OE1	2:B:679:SER:N	2.29	0.62
2:B:556:MET:HE1	2:B:589:LEU:HD22	1.80	0.62
2:B:953:LEU:HD23	2:B:965:LYS:HD2	1.82	0.62
8:H:12:VAL:O	8:H:52:ASP:N	2.29	0.62
11:K:29:ASN:ND2	11:K:78:GLU:O	2.29	0.62
1:A:108:MET:HG3	1:A:186:TRP:HE1	1.63	0.62
8:H:102:LYS:HE3	8:H:114:TYR:CG	2.34	0.62
15:O:661:LEU:HD23	15:O:704:PHE:HZ	1.64	0.62
1:A:122:MET:O	1:A:126:ILE:HG12	1.99	0.62
2:B:935:ARG:NH2	16:P:-1:U:O2	2.33	0.62
11:K:78:GLU:HG3	11:K:80:GLY:H	1.64	0.62
15:O:323:VAL:HG12	15:O:324:GLY:N	2.15	0.62
15:O:576:PRO:HD3	15:O:777:GLN:HB3	1.81	0.62
1:A:582:ALA:HB1	1:A:649:ASN:HB3	1.82	0.62
2:B:107:ARG:NH2	2:B:957:ASN:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:572:ARG:HB2	2:B:616:GLU:HG2	1.82	0.62
2:B:1219:GLU:HG2	4:D:12:ARG:HH21	1.64	0.62
15:O:347:HIS:HB2	15:O:352:LEU:HD12	1.81	0.62
8:H:59:LEU:HD22	8:H:139:LEU:HD21	1.80	0.61
9:I:60:ASP:HA	9:I:107:LYS:HD2	1.81	0.61
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.35	0.61
15:O:627:HIS:CE1	15:O:683:ILE:HG13	2.34	0.61
1:A:353:VAL:O	1:A:469:PHE:N	2.33	0.61
1:A:747:MET:HE1	2:B:1015:HIS:CD2	2.35	0.61
1:A:1193:TRP:CD1	1:A:1259:GLU:HB2	2.35	0.61
8:H:92:TYR:CD2	8:H:144:ARG:HG3	2.35	0.61
1:A:23:SER:HB3	1:A:234:TRP:CE2	2.35	0.61
1:A:536:THR:HB	1:A:617:VAL:HG13	1.82	0.61
1:A:801:VAL:HA	1:A:813:GLU:HG2	1.80	0.61
1:A:858:ARG:HG2	1:A:864:ILE:HG12	1.82	0.61
1:A:867:PHE:N	5:E:207:TYR:OH	2.33	0.61
15:O:673:LEU:HB3	15:O:735:LEU:HG	1.82	0.61
1:A:711:LEU:HD23	9:I:97:MET:H	1.65	0.61
1:A:989:ILE:HG22	1:A:993:ARG:HH21	1.66	0.61
1:A:1389:ARG:NH1	17:T:56:DC:O3'	2.34	0.61
5:E:92:MET:HE2	5:E:123:ILE:HG12	1.81	0.61
1:A:1194:LEU:CD1	1:A:1241:ARG:HE	2.13	0.61
3:C:48:VAL:O	12:L:69:PHE:N	2.33	0.61
3:C:241:ASN:HA	11:K:105:PHE:HZ	1.63	0.61
5:E:18:VAL:O	5:E:21:MET:HB2	2.00	0.61
14:N:58:DC:H5'	20:c:77:ARG:HE	1.65	0.61
1:A:569:PRO:HD2	8:H:46:MET:HE2	1.83	0.61
1:A:1331:TYR:CE1	1:A:1350:SER:HB2	2.35	0.61
2:B:641:ASN:HA	2:B:644:GLU:HB2	1.81	0.61
3:C:49:GLU:HG2	3:C:156:ARG:HB3	1.80	0.61
18:a:112:ILE:HD13	20:g:112:GLN:HG3	1.83	0.61
2:B:617:PHE:CZ	2:B:619:ILE:HD11	2.36	0.61
2:B:645:LEU:HG	2:B:707:LEU:HD21	1.83	0.61
5:E:157:ASP:O	5:E:161:SER:HB3	2.01	0.61
7:G:44:TYR:OH	7:G:157:ILE:O	2.19	0.61
15:O:356:VAL:HB	15:O:441:VAL:HG22	1.83	0.61
18:e:72:ARG:HH21	18:e:84:PHE:H	1.49	0.61
1:A:1391:GLY:HA2	1:A:1394:ARG:HD2	1.81	0.61
2:B:51:TRP:NE1	2:B:80:GLY:O	2.31	0.61
2:B:268:VAL:HG12	2:B:330:GLY:HA2	1.83	0.61
5:E:155:LEU:HD12	5:E:194:VAL:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:55:DA:H2"	17:T:56:DC:H5"	1.82	0.61
1:A:491:HIS:HB3	2:B:1150:ARG:HH21	1.65	0.60
1:A:1344:ILE:HG13	1:A:1379:THR:HB	1.82	0.60
2:B:210:ALA:H	2:B:397:LYS:HA	1.66	0.60
1:A:421:ARG:HB2	1:A:424:ASP:HB2	1.83	0.60
1:A:586:GLY:O	1:A:638:LYS:NZ	2.28	0.60
2:B:18:TRP:O	2:B:811:TYR:OH	2.17	0.60
15:O:647:SER:HB3	15:O:650:LYS:HD3	1.82	0.60
1:A:32:VAL:HG11	1:A:80:HIS:HB3	1.83	0.60
1:A:215:ILE:HG23	1:A:219:ASP:HB3	1.82	0.60
1:A:466:TYR:HE2	11:K:67:LEU:HD13	1.66	0.60
3:C:183:HIS:HB2	3:C:185:LYS:HG3	1.83	0.60
3:C:251:LEU:HD22	11:K:98:LEU:HD11	1.82	0.60
2:B:304:GLU:OE1	9:I:46:HIS:NE2	2.33	0.60
11:K:29:ASN:ND2	11:K:81:THR:O	2.34	0.60
1:A:844:LYS:HZ3	1:A:1405:PHE:HB2	1.65	0.60
2:B:91:GLU:OE1	2:B:97:HIS:ND1	2.32	0.60
2:B:628:ARG:NH1	2:B:629:PRO:O	2.33	0.60
2:B:786:ASN:OD1	2:B:967:ARG:NH2	2.34	0.60
5:E:7:ILE:HG23	5:E:10:ARG:HH21	1.66	0.60
7:G:27:ARG:NH2	7:G:54:ILE:O	2.35	0.60
10:J:6:ARG:HG2	10:J:11:GLY:HA2	1.83	0.60
1:A:1039:LEU:HD22	1:A:1043:ALA:HB1	1.83	0.60
5:E:169:LEU:HD22	5:E:173:GLN:HB3	1.83	0.60
8:H:102:LYS:HZ2	8:H:104:GLU:HB2	1.65	0.60
15:O:486:LEU:O	15:O:491:ARG:NH2	2.35	0.60
1:A:447:ARG:NH1	1:A:448:GLN:O	2.33	0.60
6:F:101:ILE:HG23	6:F:117:PRO:HB3	1.83	0.60
15:O:545:VAL:O	15:O:549:TYR:N	2.33	0.60
18:a:124:ILE:HD11	19:b:50:ILE:HG23	1.83	0.60
1:A:388:ARG:HH22	1:A:435:ARG:HH11	1.48	0.60
1:A:1115:THR:O	1:A:1333:ASN:ND2	2.35	0.60
2:B:605:GLU:O	2:B:625:ARG:NH1	2.35	0.60
2:B:979:LYS:HG3	2:B:1095:LEU:HD23	1.82	0.60
2:B:1067:ARG:NH2	3:C:200:GLU:OE1	2.35	0.60
5:E:71:TYR:OH	5:E:154:ARG:O	2.15	0.60
15:O:480:SER:O	15:O:485:GLN:NE2	2.33	0.60
18:e:62:ILE:O	18:e:93:GLN:NE2	2.35	0.60
2:B:889:THR:OG1	2:B:909:ASP:OD1	2.19	0.60
11:K:77:THR:OG1	11:K:81:THR:O	2.13	0.60
1:A:1331:TYR:HE1	1:A:1350:SER:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:HIS:HA	9:I:113:GLU:HG3	1.83	0.59
1:A:764:ALA:O	1:A:807:ARG:NH2	2.35	0.59
1:A:464:MET:HG2	1:A:465:PRO:HD2	1.84	0.59
1:A:779:GLY:HA3	2:B:509:ASN:HB2	1.84	0.59
1:A:1327:SER:HB2	5:E:141:VAL:HG11	1.84	0.59
2:B:264:THR:OG1	2:B:271:ASP:OD1	2.16	0.59
3:C:148:ARG:HD3	10:J:60:LEU:HB3	1.82	0.59
10:J:7:CYS:HB3	10:J:10:CYS:SG	2.41	0.59
14:N:-23:DT:OP1	18:e:72:ARG:NH2	2.34	0.59
1:A:316:LEU:HA	1:A:322:PRO:HA	1.84	0.59
1:A:694:ILE:HG22	1:A:715:PHE:HD1	1.66	0.59
8:H:93:ASP:OD2	8:H:145:ARG:N	2.36	0.59
8:H:100:VAL:N	8:H:137:ASP:O	2.34	0.59
1:A:1351:LEU:HD23	1:A:1375:VAL:HG12	1.84	0.59
5:E:80:GLU:OE2	5:E:98:ARG:NH1	2.35	0.59
1:A:676:THR:HB	1:A:737:ASN:HD22	1.67	0.59
2:B:12:ILE:HG13	2:B:645:LEU:HD12	1.84	0.59
2:B:479:TYR:HA	2:B:792:MET:HE1	1.84	0.59
2:B:686:VAL:HG23	2:B:687:ILE:HG13	1.84	0.59
2:B:702:MET:HB3	2:B:727:LYS:HE2	1.84	0.59
2:B:1149:GLU:OE2	2:B:1150:ARG:NH1	2.36	0.59
1:A:1446:VAL:HG22	6:F:132:LEU:HD12	1.84	0.59
12:L:33:CYS:HB2	12:L:50:CYS:SG	2.42	0.59
19:f:92:ARG:HG3	21:h:79:ARG:HH22	1.68	0.59
1:A:388:ARG:NH2	1:A:435:ARG:HH11	2.01	0.59
1:A:492:VAL:C	2:B:1150:ARG:HH22	2.10	0.59
1:A:638:LYS:HB3	1:A:642:ILE:HG13	1.85	0.59
1:A:768:GLN:HA	1:A:800:PHE:HA	1.85	0.59
2:B:849:GLY:HA2	2:B:852:ARG:HE	1.68	0.59
15:O:736:LEU:HD22	15:O:738:THR:HG22	1.84	0.59
1:A:1152:THR:O	9:I:46:HIS:N	2.27	0.59
7:G:23:ASN:OD1	7:G:27:ARG:NH1	2.35	0.59
11:K:91:CYS:O	11:K:95:ILE:HG12	2.03	0.59
14:N:-7:DG:H4'	14:N:-6:DG:H5'	1.84	0.59
15:O:677:THR:HA	17:T:75:DC:H5''	1.85	0.59
1:A:497:GLU:HB3	6:F:92:ARG:HH22	1.68	0.59
1:A:783:ARG:NH1	9:I:67:THR:OG1	2.36	0.59
1:A:803:ASN:HB2	1:A:809:LEU:HD13	1.84	0.59
1:A:1395:ALA:O	1:A:1402:ARG:NH1	2.36	0.59
2:B:862:GLN:HB2	2:B:963:PHE:HD1	1.67	0.59
3:C:192:TRP:O	3:C:201:TRP:NE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:155:LEU:HD22	5:E:159:GLU:HB3	1.84	0.59
5:E:202:GLU:HG2	5:E:203:THR:HG23	1.84	0.59
15:O:534:VAL:HG13	15:O:544:GLN:HG2	1.85	0.59
1:A:331:LYS:HD2	1:A:1407:GLU:HA	1.85	0.58
1:A:806:LEU:HA	2:B:1023:VAL:HG11	1.85	0.58
4:D:115:PHE:HB3	4:D:120:THR:HG23	1.85	0.58
8:H:103:PHE:HZ	8:H:132:ALA:HA	1.67	0.58
1:A:699:GLN:HB2	9:I:99:LEU:HD13	1.84	0.58
2:B:327:GLY:HA3	2:B:341:ARG:HG2	1.84	0.58
4:D:92:VAL:HG13	4:D:93:THR:HG23	1.85	0.58
1:A:348:PHE:HA	1:A:375:LEU:HD22	1.86	0.58
1:A:440:ASP:HA	1:A:460:ARG:HB3	1.85	0.58
2:B:554:TRP:NE1	2:B:593:MET:HE3	2.13	0.58
2:B:792:MET:HG2	2:B:855:PHE:HE1	1.67	0.58
2:B:979:LYS:HZ1	2:B:987:LYS:HB2	1.68	0.58
5:E:25:ARG:NH1	5:E:154:ARG:HB2	2.18	0.58
15:O:678:ARG:NH2	17:T:76:DG:OP2	2.34	0.58
2:B:91:GLU:OE1	12:L:56:ARG:NH2	2.36	0.58
6:F:90:ARG:NH2	6:F:153:VAL:HA	2.18	0.58
8:H:30:SER:HB3	8:H:36:ILE:HB	1.86	0.58
18:e:131:ARG:O	20:g:99:ARG:NH2	2.36	0.58
1:A:26:GLU:OE2	2:B:1184:SER:OG	2.18	0.58
1:A:439:ASP:OD1	1:A:440:ASP:N	2.37	0.58
3:C:6:LYS:O	3:C:22:SER:N	2.34	0.58
13:M:47:LEU:HB3	13:M:56:PHE:HB3	1.86	0.58
15:O:627:HIS:CE1	15:O:630:LEU:HB2	2.38	0.58
20:c:42:ARG:HG3	21:d:88:THR:HG23	1.84	0.58
1:A:1114:LYS:HG3	1:A:1115:THR:HG23	1.85	0.58
1:A:1194:LEU:HD11	1:A:1241:ARG:HB3	1.84	0.58
2:B:992:VAL:HG23	11:K:67:LEU:HD21	1.86	0.58
2:B:1074:ASN:O	2:B:1078:GLY:N	2.31	0.58
4:D:87:ASP:OD1	4:D:103:LYS:NZ	2.37	0.58
1:A:148:CYS:HB2	1:A:172:GLN:HG2	1.85	0.58
1:A:533:ARG:NH1	1:A:749:SER:OG	2.37	0.58
1:A:712:ARG:HG2	9:I:97:MET:HB2	1.85	0.58
1:A:787:HIS:ND1	2:B:700:ILE:O	2.36	0.58
1:A:897:ARG:NE	1:A:897:ARG:O	2.36	0.58
1:A:1000:PHE:O	1:A:1056:GLN:NE2	2.34	0.58
2:B:172:LEU:HA	2:B:175:LEU:HD12	1.86	0.58
2:B:473:SER:O	2:B:474:GLN:NE2	2.36	0.58
8:H:36:ILE:HD13	8:H:126:GLY:HA3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:O	2:B:1217:TYR:N	2.36	0.58
1:A:900:VAL:HG21	1:A:930:LEU:HD13	1.85	0.58
1:A:948:VAL:HG11	1:A:1019:LEU:HD21	1.85	0.58
2:B:19:THR:HG21	2:B:656:GLN:HG3	1.85	0.58
2:B:799:PRO:HD2	10:J:1:MET:N	2.18	0.58
2:B:883:LEU:HD21	2:B:918:ILE:HG13	1.86	0.58
6:F:82:THR:O	6:F:136:ARG:NH1	2.31	0.58
6:F:84:TYR:HB3	6:F:154:ASP:HB2	1.86	0.58
9:I:7:CYS:HB3	9:I:11:ASN:H	1.69	0.58
1:A:341:LEU:HB3	1:A:1432:MET:HG2	1.84	0.58
1:A:364:GLN:HG2	1:A:460:ARG:HB2	1.85	0.58
14:N:53:DC:H42	17:T:-53:DG:H1	1.51	0.58
19:b:98:TYR:HB3	21:h:61:ILE:HA	1.85	0.58
19:f:72:TYR:OH	21:h:79:ARG:NH2	2.37	0.58
1:A:113:LEU:HG	1:A:115:LEU:H	1.68	0.58
1:A:762:MET:HG2	2:B:1021:MET:HG3	1.85	0.58
1:A:1029:ALA:H	1:A:1032:ARG:HH21	1.50	0.58
3:C:156:ARG:HH11	3:C:158:ILE:HG12	1.69	0.58
11:K:98:LEU:HA	11:K:101:LEU:HD12	1.86	0.58
1:A:568:LYS:NZ	8:H:92:TYR:O	2.27	0.57
1:A:857:THR:O	1:A:865:ILE:N	2.37	0.57
1:A:38:PRO:HG3	1:A:271:LEU:HG	1.85	0.57
6:F:85:LEU:HD23	6:F:90:ARG:NE	2.18	0.57
1:A:364:GLN:NE2	1:A:440:ASP:OD1	2.38	0.57
1:A:381:VAL:HG21	1:A:427:LEU:HB3	1.85	0.57
1:A:896:LYS:O	1:A:1031:ARG:NH2	2.37	0.57
1:A:1104:LYS:HE2	1:A:1104:LYS:HA	1.84	0.57
2:B:341:ARG:NH2	13:M:75:ASP:OD1	2.37	0.57
2:B:476:LEU:HD11	2:B:484:THR:HG23	1.85	0.57
2:B:987:LYS:HG2	2:B:1020:ARG:HH22	1.70	0.57
2:B:1034:VAL:HG13	2:B:1038:ARG:HH11	1.70	0.57
3:C:54:THR:OG1	3:C:152:GLU:N	2.36	0.57
15:O:263:ARG:NH2	15:O:277:GLU:O	2.37	0.57
1:A:34:LYS:NZ	1:A:85:GLU:H	2.01	0.57
1:A:266:LYS:NZ	1:A:324:LYS:O	2.34	0.57
1:A:516:GLN:O	1:A:1367:ASN:N	2.36	0.57
1:A:557:TRP:O	11:K:26:ARG:NH1	2.38	0.57
1:A:1192:PRO:O	1:A:1243:ARG:NH1	2.37	0.57
2:B:31:VAL:HG11	2:B:166:ARG:NH2	2.19	0.57
1:A:17:VAL:HG22	2:B:1216:LEU:HD23	1.86	0.57
1:A:53:LEU:O	1:A:248:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:THR:HG22	1:A:307:ASN:HA	1.86	0.57
1:A:1211:MET:HG3	1:A:1238:LEU:HB3	1.86	0.57
2:B:551:LEU:HD11	2:B:619:ILE:HG13	1.86	0.57
3:C:96:VAL:HG11	3:C:130:GLY:HA3	1.85	0.57
4:D:62:GLU:HA	4:D:65:LYS:HG2	1.86	0.57
14:N:-57:DT:H1'	14:N:-56:DG:H5'	1.86	0.57
1:A:269:ASP:O	1:A:272:LYS:HG3	2.04	0.57
1:A:445:PHE:CB	1:A:457:MET:O	2.53	0.57
1:A:533:ARG:HH22	1:A:746:GLN:HB3	1.69	0.57
1:A:551:LEU:HD23	1:A:581:ILE:HG21	1.85	0.57
1:A:853:TYR:HB3	6:F:81:THR:HG21	1.85	0.57
1:A:1123:ASP:O	1:A:1127:ALA:N	2.28	0.57
2:B:86:ARG:NH2	2:B:170:CYS:O	2.35	0.57
7:G:137:ILE:HG23	7:G:143:VAL:HG11	1.87	0.57
15:O:382:VAL:HG23	15:O:388:GLY:HA3	1.84	0.57
3:C:10:ILE:HD13	3:C:18:GLU:HG2	1.87	0.57
3:C:20:MET:HE1	3:C:209:TRP:CD2	2.39	0.57
15:O:607:ILE:HG12	15:O:612:ARG:HB2	1.86	0.57
1:A:834:GLU:HA	1:A:837:TYR:HD1	1.69	0.57
17:T:61:DA:H2'	17:T:62:DA:H8	1.70	0.57
1:A:1145:LEU:HA	1:A:1148:VAL:HG22	1.86	0.57
2:B:557:GLU:HB2	2:B:582:ILE:HB	1.87	0.57
11:K:12:LEU:HD22	11:K:18:LYS:HG3	1.87	0.57
11:K:95:ILE:O	11:K:99:LYS:HG2	2.05	0.57
1:A:428:GLN:NE2	1:A:429:TYR:O	2.38	0.57
1:A:464:MET:HE3	1:A:470:ARG:HE	1.70	0.57
2:B:630:LEU:HD12	2:B:690:VAL:HG21	1.87	0.57
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.87	0.57
1:A:710:THR:O	1:A:714:SER:N	2.32	0.56
1:A:1441:THR:HB	6:F:92:ARG:HG2	1.86	0.56
2:B:99:MET:HE1	2:B:111:TYR:HA	1.86	0.56
2:B:575:VAL:O	2:B:578:VAL:HG12	2.05	0.56
7:G:81:PRO:HD2	7:G:157:ILE:HD11	1.87	0.56
1:A:351:ARG:NH2	1:A:448:GLN:OE1	2.38	0.56
1:A:635:MET:HE1	1:A:640:PRO:HA	1.87	0.56
14:N:-81:DG:H22	17:T:81:DC:H42	1.52	0.56
15:O:721:LEU:HA	15:O:724:VAL:HG12	1.87	0.56
1:A:453:LYS:HG3	1:A:511:GLN:HE22	1.70	0.56
1:A:509:PRO:HB3	1:A:640:PRO:HB2	1.87	0.56
1:A:530:CYS:HA	1:A:750:ALA:HB1	1.86	0.56
1:A:706:LYS:HB2	1:A:709:MET:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:VAL:HG23	1:A:914:ILE:HG23	1.87	0.56
1:A:1211:MET:HE1	1:A:1231:SER:N	2.20	0.56
2:B:337:ARG:O	2:B:341:ARG:HB2	2.04	0.56
2:B:1172:ILE:HG22	2:B:1179:GLN:HE22	1.71	0.56
15:O:579:SER:HB3	15:O:782:THR:HG22	1.85	0.56
1:A:837:TYR:HA	1:A:840:ARG:HD2	1.87	0.56
1:A:891:ASP:H	1:A:1299:GLY:HA3	1.71	0.56
1:A:1097:THR:HG23	1:A:1102:ARG:HD3	1.86	0.56
1:A:1214:VAL:HG13	1:A:1276:LEU:HD21	1.88	0.56
2:B:112:SER:OG	2:B:160:LYS:HG2	2.05	0.56
2:B:166:ARG:NH1	2:B:190:MET:SD	2.78	0.56
3:C:140:GLN:NE2	10:J:19:ASP:OD2	2.38	0.56
6:F:134:ILE:HD13	6:F:151:LEU:HD23	1.87	0.56
1:A:834:GLU:HA	1:A:837:TYR:CD1	2.41	0.56
1:A:963:ARG:NH2	1:A:967:GLN:OE1	2.34	0.56
1:A:1154:ILE:O	9:I:43:VAL:N	2.32	0.56
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.87	0.56
5:E:25:ARG:NH1	5:E:154:ARG:HH11	2.03	0.56
1:A:407:ILE:HB	1:A:432:LYS:HB2	1.87	0.56
1:A:409:ASP:H	1:A:431:TRP:CD1	2.24	0.56
15:O:664:TRP:HZ3	15:O:754:ILE:HD11	1.69	0.56
15:O:794:GLU:O	15:O:798:HIS:ND1	2.29	0.56
1:A:16:GLU:HB3	1:A:1421:LEU:HD11	1.88	0.56
1:A:883:THR:HG22	1:A:955:ASN:HB2	1.87	0.56
2:B:786:ASN:O	2:B:967:ARG:NH1	2.30	0.56
14:N:-55:DT:H3	17:T:55:DA:H61	1.52	0.56
14:N:2:DG:H2''	14:N:3:DC:H5'	1.87	0.56
1:A:672:ALA:HB3	1:A:677:MET:HE3	1.88	0.56
1:A:981:SER:HA	1:A:1038:ARG:HH21	1.71	0.56
2:B:568:THR:O	2:B:615:ARG:NH1	2.38	0.56
8:H:77:SER:OG	8:H:79:ARG:NH2	2.39	0.56
20:c:63:LEU:HD22	21:d:45:LEU:HD13	1.86	0.56
1:A:302:ALA:O	1:A:306:ASP:N	2.25	0.56
1:A:1193:TRP:HB3	1:A:1263:LEU:HD22	1.88	0.56
2:B:285:PRO:HB2	9:I:11:ASN:HD22	1.71	0.56
2:B:489:ARG:NH2	2:B:533:SER:O	2.38	0.56
5:E:174:LEU:O	5:E:176:ARG:NH1	2.39	0.56
15:O:449:LEU:HD23	15:O:482:THR:HB	1.88	0.56
15:O:646:GLY:HA2	15:O:683:ILE:HD12	1.88	0.56
17:T:-43:DT:OP1	20:c:17:ARG:N	2.37	0.56
1:A:1065:MET:HG2	2:B:1139:ILE:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:LEU:O	1:A:1149:THR:N	2.38	0.56
2:B:89:MET:HB3	2:B:99:MET:HB2	1.86	0.56
2:B:597:ARG:HH21	2:B:689:TYR:HB2	1.69	0.56
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.87	0.56
5:E:81:PHE:CD1	5:E:110:ILE:HB	2.41	0.56
5:E:81:PHE:HE1	5:E:110:ILE:HD13	1.69	0.56
1:A:231:ARG:HB2	1:A:234:TRP:CG	2.41	0.55
1:A:347:ASP:H	2:B:1154:ALA:HB1	1.71	0.55
3:C:43:LEU:HD22	3:C:129:VAL:HB	1.87	0.55
5:E:13:ARG:HB3	5:E:140:VAL:O	2.07	0.55
9:I:28:SER:HB2	9:I:35:THR:HG23	1.88	0.55
1:A:445:PHE:CD2	1:A:488:MET:HE2	2.41	0.55
1:A:498:THR:HB	2:B:1146:PHE:HD1	1.72	0.55
2:B:373:TYR:OH	2:B:377:ARG:NH2	2.39	0.55
2:B:632:ILE:HD11	2:B:688:GLU:HB3	1.87	0.55
4:D:40:ASP:OD2	4:D:44:ASN:ND2	2.39	0.55
5:E:54:ARG:HG3	5:E:112:GLN:HE21	1.71	0.55
14:N:17:DA:H2	17:T:-16:DT:H3	1.53	0.55
15:O:308:GLN:HA	15:O:338:GLN:HE21	1.71	0.55
17:T:5:DC:H4'	17:T:6:DC:H5'	1.88	0.55
21:h:102:LEU:HD22	21:h:106:LEU:HD23	1.88	0.55
1:A:1025:ARG:O	1:A:1032:ARG:NH2	2.39	0.55
1:A:1140:ILE:HG22	1:A:1282:ILE:HG21	1.88	0.55
2:B:38:PHE:O	2:B:41:PHE:HB3	2.07	0.55
8:H:6:PHE:HB3	8:H:59:LEU:HB2	1.87	0.55
8:H:79:ARG:HH12	11:K:58:PHE:HB2	1.69	0.55
15:O:803:LYS:HD3	15:O:806:LEU:HD12	1.88	0.55
17:T:8:DC:OP2	19:f:35:ARG:NH2	2.34	0.55
1:A:514:SER:N	1:A:519:LYS:O	2.37	0.55
1:A:1157:ASP:OD1	1:A:1158:PRO:HD2	2.07	0.55
15:O:583:LEU:HD11	15:O:786:LEU:HD13	1.89	0.55
1:A:724:ASN:O	1:A:727:ARG:HG2	2.07	0.55
1:A:951:ASN:OD1	1:A:952:GLY:N	2.39	0.55
3:C:37:LEU:HG	3:C:176:ILE:HD12	1.89	0.55
5:E:21:MET:HE1	5:E:186:TYR:CD2	2.41	0.55
15:O:725:PHE:HB2	15:O:731:TYR:HE2	1.71	0.55
18:e:135:ALA:HB3	20:g:91:GLU:HG3	1.87	0.55
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.40	0.55
1:A:1116:PRO:HB2	1:A:1313:GLY:HA2	1.88	0.55
1:A:1269:HIS:NE2	1:A:1273:LEU:HD22	2.21	0.55
2:B:288:GLU:N	2:B:288:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:LYS:HD2	3:C:188:HIS:HB2	1.89	0.55
2:B:1156:ASP:OD2	2:B:1199:ALA:N	2.30	0.55
5:E:170:LYS:HD3	5:E:172:SER:H	1.72	0.55
21:d:45:LEU:HA	21:d:48:VAL:HG22	1.88	0.55
20:g:83:LEU:HD13	21:h:62:MET:HE3	1.87	0.55
1:A:18:GLN:O	2:B:1215:ARG:N	2.33	0.55
1:A:601:PRO:HA	8:H:25:ARG:HH21	1.72	0.55
3:C:10:ILE:HD11	3:C:20:MET:HB2	1.88	0.55
8:H:47:PHE:CD2	8:H:94:TYR:HB2	2.42	0.55
1:A:472:ASN:ND2	1:A:651:GLN:OE1	2.40	0.55
1:A:508:VAL:HB	1:A:509:PRO:HD3	1.89	0.55
1:A:1120:VAL:HG13	1:A:1325:VAL:HG13	1.89	0.55
2:B:951:GLN:OE1	2:B:967:ARG:NH1	2.40	0.55
3:C:156:ARG:NH1	3:C:158:ILE:HG12	2.22	0.55
3:C:190:ASP:OD1	3:C:192:TRP:N	2.38	0.55
7:G:93:ASN:O	7:G:100:PHE:N	2.38	0.55
11:K:30:CYS:HB2	11:K:76:GLN:HG3	1.88	0.55
1:A:529:LEU:HD23	1:A:752:SER:HA	1.89	0.55
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	1.88	0.55
3:C:148:ARG:HB2	10:J:60:LEU:HD22	1.89	0.55
3:C:166:GLU:O	12:L:72:ARG:NH2	2.40	0.55
4:D:4:SER:OG	7:G:8:SER:O	2.24	0.55
6:F:79:ARG:NH1	6:F:145:ASP:O	2.39	0.55
7:G:60:ARG:NH1	7:G:69:GLU:OE2	2.40	0.55
18:a:94:GLU:HG2	20:g:103:ALA:HA	1.89	0.55
1:A:219:ASP:HA	1:A:222:ARG:HG2	1.89	0.55
1:A:925:GLU:HA	1:A:928:LYS:HE3	1.88	0.55
2:B:955:THR:HA	12:L:48:VAL:HG11	1.87	0.55
7:G:91:VAL:HA	7:G:101:ALA:HA	1.89	0.55
8:H:56:THR:HB	8:H:144:ARG:HB2	1.89	0.55
8:H:99:THR:HA	8:H:138:ASN:HA	1.88	0.55
1:A:327:ARG:NH2	1:A:1410:GLU:OE2	2.33	0.54
1:A:636:ARG:NH2	1:A:878:GLN:O	2.40	0.54
1:A:1296:ASP:OD1	1:A:1297:GLU:N	2.41	0.54
2:B:554:TRP:O	2:B:583:HIS:NE2	2.36	0.54
3:C:249:LYS:NZ	11:K:102:ASP:OD2	2.38	0.54
15:O:465:ILE:HD13	15:O:492:VAL:HB	1.89	0.54
21:d:82:HIS:NE2	20:g:37:GLY:O	2.36	0.54
1:A:444:LEU:HB3	1:A:491:HIS:HB2	1.89	0.54
2:B:358:THR:HG21	2:B:363:PHE:HB2	1.89	0.54
2:B:987:LYS:H	2:B:1020:ARG:HH22	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:LYS:HB2	3:C:188:HIS:HB3	1.89	0.54
3:C:96:VAL:HG21	3:C:129:VAL:HG23	1.89	0.54
7:G:34:VAL:HG13	7:G:35:GLU:HG2	1.89	0.54
15:O:755:ILE:HG13	15:O:785:ARG:NH1	2.21	0.54
18:a:79:LYS:HB3	18:a:82:LEU:HD11	1.89	0.54
1:A:446:ASN:HB3	1:A:489:ASN:HB2	1.90	0.54
2:B:998:ASP:HB3	2:B:1076:HIS:CE1	2.39	0.54
2:B:1065:GLN:OE1	2:B:1069:PHE:N	2.36	0.54
18:a:51:ILE:HG13	19:b:39:ARG:HD2	1.89	0.54
3:C:28:LEU:HD21	11:K:101:LEU:HD11	1.89	0.54
17:T:-44:DA:H3'	20:c:28:GLY:HA3	1.90	0.54
1:A:740:ASP:HA	1:A:745:LYS:HE2	1.90	0.54
2:B:532:LEU:HD21	2:B:538:ILE:HD11	1.89	0.54
3:C:46:ASP:HA	3:C:169:LYS:HZ2	1.72	0.54
3:C:235:THR:HB	10:J:13:VAL:HG23	1.89	0.54
11:K:96:ASN:OD1	11:K:97:LYS:N	2.39	0.54
15:O:478:ASP:HA	15:O:481:LEU:HD12	1.90	0.54
20:g:32:ARG:NH1	21:h:35:GLU:OE2	2.40	0.54
1:A:535:MET:HE1	1:A:654:VAL:HA	1.89	0.54
2:B:996:HIS:HA	2:B:999:MET:HE3	1.90	0.54
1:A:533:ARG:HH12	1:A:746:GLN:C	2.15	0.54
1:A:1104:LYS:HZ3	1:A:1107:LEU:HD22	1.73	0.54
2:B:77:ILE:HG21	2:B:119:MET:HE2	1.90	0.54
2:B:355:PRO:HB2	2:B:359:GLN:HE21	1.73	0.54
5:E:54:ARG:HH11	5:E:81:PHE:HB3	1.73	0.54
6:F:146:TRP:CE3	6:F:151:LEU:HD13	2.43	0.54
11:K:55:ASP:O	11:K:78:GLU:N	2.39	0.54
15:O:326:ILE:HG23	15:O:493:ILE:HB	1.90	0.54
1:A:60:SER:O	1:A:246:GLN:NE2	2.41	0.54
1:A:1155:TYR:OH	1:A:1167:GLU:OE1	2.25	0.54
1:A:1160:PRO:O	1:A:1243:ARG:NE	2.40	0.54
3:C:49:GLU:HB2	12:L:66:MET:SD	2.48	0.54
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.90	0.54
1:A:447:ARG:HH11	1:A:448:GLN:H	1.56	0.54
1:A:1076:GLU:O	1:A:1080:GLN:NE2	2.22	0.54
2:B:776:GLN:HG3	2:B:1095:LEU:HD11	1.90	0.54
5:E:186:TYR:HD1	5:E:187:LEU:HD23	1.72	0.54
10:J:44:CYS:O	10:J:47:ARG:HD3	2.08	0.54
15:O:672:LEU:HB2	15:O:753:VAL:HG22	1.88	0.54
17:T:-13:DA:H5''	19:b:30:THR:HG21	1.89	0.54
1:A:244:PRO:HG2	1:A:247:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:ILE:HG21	1:A:1373:LEU:HD21	1.89	0.54
2:B:1072:MET:HB2	2:B:1081:LEU:HD12	1.90	0.54
3:C:12:ALA:HA	3:C:17:VAL:HG12	1.90	0.54
3:C:148:ARG:HG3	3:C:149:ASN:H	1.73	0.54
5:E:85:PRO:HA	5:E:112:GLN:HB2	1.90	0.54
15:O:358:VAL:HG22	15:O:465:ILE:HB	1.89	0.54
2:B:215:GLN:N	2:B:230:GLU:O	2.35	0.53
2:B:335:GLY:H	13:M:74:ILE:HD13	1.72	0.53
10:J:43:TYR:HA	10:J:46:ARG:HB2	1.89	0.53
21:d:89:ILE:HG23	21:d:93:GLU:HB2	1.90	0.53
1:A:495:SER:O	1:A:498:THR:OG1	2.24	0.53
1:A:856:THR:HG1	1:A:858:ARG:HE	1.56	0.53
1:A:938:VAL:O	1:A:942:LYS:HG3	2.08	0.53
1:A:1201:ARG:HH22	1:A:1210:THR:HA	1.72	0.53
1:A:1424:CYS:HA	1:A:1429:GLU:HG2	1.90	0.53
2:B:316:ILE:HG21	2:B:322:ALA:HB2	1.90	0.53
3:C:120:LYS:NZ	3:C:128:ASN:OD1	2.40	0.53
5:E:76:THR:H	5:E:105:SER:HB3	1.72	0.53
9:I:44:TYR:HB3	9:I:46:HIS:CE1	2.43	0.53
14:N:-57:DT:H3	17:T:57:DA:H61	1.56	0.53
1:A:270:ILE:HD11	1:A:304:TYR:HB2	1.90	0.53
1:A:549:ASN:HA	11:K:60:ALA:HB1	1.90	0.53
1:A:668:GLY:HA2	1:A:671:ILE:HG12	1.91	0.53
1:A:1295:PRO:HA	1:A:1301:TYR:HA	1.90	0.53
2:B:74:ARG:NH2	2:B:126:SER:OG	2.42	0.53
2:B:314:PHE:HE1	9:I:31:ASN:HB2	1.73	0.53
2:B:478:ARG:NH1	2:B:782:LEU:HD11	2.22	0.53
3:C:70:PRO:HG2	3:C:133:VAL:HB	1.88	0.53
5:E:184:ALA:HA	5:E:189:LEU:HD12	1.90	0.53
5:E:196:LYS:HE2	5:E:198:ILE:HG13	1.89	0.53
15:O:427:ARG:O	15:O:427:ARG:NH1	2.41	0.53
2:B:265:LEU:O	2:B:268:VAL:HG22	2.09	0.53
2:B:366:ARG:HG3	2:B:559:LEU:HD12	1.90	0.53
2:B:786:ASN:HA	2:B:967:ARG:HH22	1.73	0.53
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.49	0.53
1:A:668:GLY:HA3	2:B:1067:ARG:HD2	1.90	0.53
1:A:720:SER:HA	1:A:775:ARG:NH2	2.23	0.53
2:B:230:GLU:HB2	2:B:246:GLN:HG3	1.90	0.53
2:B:859:TYR:OH	2:B:945:GLU:OE1	2.27	0.53
3:C:262:LEU:HD13	11:K:88:GLU:HG3	1.91	0.53
4:D:159:LEU:HD13	7:G:144:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:117:PRO:O	5:E:121:LYS:HG2	2.09	0.53
8:H:78:TRP:CH2	8:H:81:PRO:HD3	2.44	0.53
17:T:60:DA:H2'	17:T:61:DA:C8	2.43	0.53
20:c:88:ARG:NH1	20:c:94:ASN:OD1	2.41	0.53
1:A:149:GLU:HG3	1:A:153:PRO:HG3	1.91	0.53
1:A:838:ILE:CG1	1:A:1104:LYS:HZ2	2.21	0.53
1:A:870:GLY:O	5:E:203:THR:OG1	2.16	0.53
1:A:1152:THR:HG21	1:A:1271:LEU:HD21	1.90	0.53
2:B:307:LYS:HZ2	9:I:13:MET:HE2	1.73	0.53
5:E:134:PHE:CZ	5:E:185:ARG:HB3	2.43	0.53
9:I:75:CYS:O	9:I:79:HIS:ND1	2.41	0.53
13:M:21:THR:OG1	13:M:34:VAL:O	2.27	0.53
15:O:323:VAL:HG11	15:O:514:PHE:CD1	2.43	0.53
15:O:635:ALA:O	15:O:639:SER:OG	2.21	0.53
16:P:2:U:H2'	16:P:3:U:C6	2.43	0.53
1:A:307:ASN:ND2	1:A:323:VAL:O	2.31	0.53
1:A:1140:ILE:HG12	1:A:1322:VAL:HG21	1.90	0.53
2:B:848:ARG:HH21	10:J:6:ARG:NH1	2.07	0.53
8:H:17:ASN:OD1	8:H:44:ASN:ND2	2.42	0.53
15:O:275:GLU:HG3	15:O:276:GLU:H	1.73	0.53
1:A:607:LEU:O	1:A:614:MET:N	2.37	0.53
1:A:1101:PRO:O	1:A:1105:GLU:HG3	2.08	0.53
1:A:1155:TYR:HB2	1:A:1194:LEU:HD23	1.91	0.53
1:A:1237:LYS:HE3	1:A:1239:ILE:HD11	1.91	0.53
1:A:1347:THR:HG21	1:A:1384:LEU:HD21	1.91	0.53
2:B:1029:CYS:O	2:B:1033:LYS:HG3	2.08	0.53
11:K:31:ILE:HG21	11:K:84:LYS:HE3	1.91	0.53
20:c:34:LEU:HD13	20:c:43:VAL:HG11	1.90	0.53
20:g:78:ILE:HB	21:h:54:ILE:HG13	1.90	0.53
1:A:88:LYS:HG2	1:A:89:PRO:HD2	1.90	0.53
1:A:277:VAL:HA	1:A:280:LEU:HD12	1.90	0.53
1:A:377:TYR:HD2	1:A:435:ARG:HE	1.56	0.53
1:A:1026:ALA:C	1:A:1032:ARG:HH22	2.16	0.53
2:B:452:TYR:O	2:B:456:THR:OG1	2.20	0.53
3:C:95:SER:OG	3:C:158:ILE:HG23	2.09	0.53
4:D:61:ARG:NH1	4:D:86:ASP:OD1	2.41	0.53
6:F:84:TYR:O	6:F:136:ARG:NH2	2.37	0.53
1:A:747:MET:HE2	2:B:1018:PRO:HG3	1.90	0.53
1:A:982:ASP:O	1:A:1041:ARG:NH2	2.31	0.53
1:A:1118:LEU:HB2	1:A:1311:THR:OG1	2.08	0.53
1:A:1229:MET:HE3	1:A:1231:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:GLY:O	1:A:1347:THR:OG1	2.22	0.53
2:B:957:ASN:ND2	2:B:961:LEU:HB2	2.24	0.53
2:B:1160:VAL:HB	2:B:1169:MET:SD	2.49	0.53
11:K:95:ILE:O	11:K:99:LYS:NZ	2.42	0.53
15:O:678:ARG:NH1	15:O:712:THR:OG1	2.42	0.53
15:O:739:ARG:HG3	17:T:76:DG:H4'	1.91	0.53
19:b:35:ARG:O	19:b:39:ARG:HG2	2.08	0.53
1:A:457:MET:HE2	1:A:508:VAL:HG13	1.91	0.52
1:A:1165:ILE:HD11	9:I:41:PRO:HD2	1.91	0.52
1:A:1381:ARG:HH21	5:E:175:PRO:HA	1.73	0.52
2:B:452:TYR:CE2	2:B:458:ASN:HB2	2.44	0.52
4:D:154:ASP:OD1	4:D:155:GLU:N	2.43	0.52
9:I:103:CYS:N	9:I:106:CYS:SG	2.80	0.52
15:O:664:TRP:HB3	15:O:669:HIS:HB2	1.91	0.52
1:A:248:ARG:O	1:A:248:ARG:HG2	2.09	0.52
1:A:762:MET:HA	1:A:805:TYR:HB2	1.90	0.52
1:A:1390:HIS:CD2	14:N:-53:DT:H5''	2.44	0.52
2:B:413:LEU:HD21	2:B:449:GLY:HA3	1.91	0.52
10:J:56:ILE:HG13	10:J:60:LEU:HG	1.91	0.52
11:K:55:ASP:OD1	11:K:89:ARG:NH2	2.42	0.52
13:M:73:TRP:NE1	13:M:77:CYS:SG	2.82	0.52
18:a:61:LEU:HD22	19:b:36:ARG:HB3	1.90	0.52
2:B:272:ILE:HD13	2:B:326:ILE:HG12	1.91	0.52
3:C:225:PRO:HB2	3:C:228:PHE:CZ	2.44	0.52
11:K:24:ASP:HB2	11:K:32:ILE:HG12	1.91	0.52
14:N:35:DT:H1'	14:N:36:DA:C4	2.44	0.52
20:c:101:THR:HG23	19:f:97:LEU:HD13	1.91	0.52
1:A:123:ALA:O	1:A:127:ARG:HG2	2.09	0.52
2:B:621:THR:HA	2:B:625:ARG:HE	1.73	0.52
7:G:25:TYR:O	7:G:28:GLU:HG3	2.09	0.52
15:O:646:GLY:HA2	15:O:683:ILE:HG23	1.91	0.52
20:c:45:ALA:HB1	21:d:121:TYR:HE2	1.74	0.52
2:B:64:HIS:HB2	2:B:71:ILE:HG21	1.91	0.52
12:L:49:ARG:NH2	12:L:54:GLY:O	2.42	0.52
15:O:290:LEU:HB3	15:O:294:TYR:HD2	1.75	0.52
17:T:56:DC:H2''	17:T:57:DA:H2'	1.91	0.52
1:A:498:THR:HG22	2:B:1146:PHE:HA	1.91	0.52
1:A:534:LYS:HE2	1:A:663:PHE:HB2	1.91	0.52
4:D:90:ALA:HB2	4:D:106:LEU:HD12	1.91	0.52
5:E:65:PRO:HA	5:E:68:LEU:HB2	1.91	0.52
6:F:111:ILE:HD12	6:F:120:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:24:ASP:OD2	11:K:74:ARG:NH2	2.42	0.52
17:T:61:DA:H2'	17:T:62:DA:C8	2.45	0.52
20:c:59:THR:HG23	21:d:44:VAL:HG11	1.91	0.52
1:A:17:VAL:HB	1:A:1422:ASP:HB3	1.91	0.52
1:A:454:MET:HA	1:A:511:GLN:HE21	1.74	0.52
1:A:874:LEU:O	1:A:1369:ARG:NH1	2.43	0.52
1:A:1376:ASP:O	1:A:1380:SER:N	2.43	0.52
2:B:60:GLN:HB2	2:B:73:LYS:HB3	1.92	0.52
2:B:329:ARG:NH2	13:M:68:ASP:OD2	2.43	0.52
9:I:44:TYR:HB3	9:I:46:HIS:HE1	1.75	0.52
1:A:292:GLU:O	1:A:295:GLN:HG3	2.09	0.52
1:A:564:PRO:HD2	8:H:78:TRP:CD1	2.45	0.52
1:A:1029:ALA:H	1:A:1032:ARG:NH2	2.08	0.52
2:B:415:ARG:HE	2:B:419:ARG:NH1	2.08	0.52
4:D:114:ARG:NH2	4:D:147:SER:O	2.43	0.52
5:E:109:PHE:N	5:E:132:GLU:O	2.31	0.52
15:O:550:LYS:HA	15:O:553:VAL:HG12	1.92	0.52
1:A:131:PRO:O	1:A:134:ARG:HG2	2.10	0.52
1:A:720:SER:HA	1:A:775:ARG:CZ	2.39	0.52
1:A:1287:MET:HE3	1:A:1307:TRP:CD2	2.45	0.52
2:B:83:TYR:N	2:B:116:TYR:O	2.40	0.52
9:I:87:GLN:NE2	9:I:96:ASN:O	2.42	0.52
15:O:259:TRP:CH2	15:O:278:TRP:HB3	2.44	0.52
15:O:627:HIS:NE2	15:O:683:ILE:HG13	2.25	0.52
15:O:806:LEU:HD23	15:O:809:LYS:HZ3	1.75	0.52
1:A:149:GLU:O	1:A:165:ARG:NE	2.42	0.52
1:A:358:PRO:O	1:A:652:LYS:NZ	2.32	0.52
1:A:869:TYR:O	1:A:873:GLY:N	2.39	0.52
2:B:33:GLN:HG3	2:B:538:ILE:HD13	1.90	0.52
11:K:102:ASP:OD2	11:K:106:ASN:ND2	2.41	0.52
1:A:95:PHE:O	1:A:99:ILE:N	2.43	0.51
1:A:445:PHE:HB2	1:A:457:MET:O	2.10	0.51
1:A:466:TYR:CE2	11:K:67:LEU:HD13	2.44	0.51
1:A:723:LEU:HB3	1:A:800:PHE:CD1	2.45	0.51
1:A:1150:SER:HB3	1:A:1200:ASP:HB2	1.91	0.51
1:A:1195:LEU:HD23	1:A:1242:CYS:HB2	1.92	0.51
1:A:1390:HIS:O	1:A:1394:ARG:N	2.43	0.51
2:B:210:ALA:HB2	2:B:398:ARG:HG2	1.90	0.51
2:B:215:GLN:HB3	2:B:217:PHE:CZ	2.45	0.51
2:B:595:ASP:HA	2:B:598:ARG:HE	1.75	0.51
2:B:766:ARG:HH22	2:B:987:LYS:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.45	0.51
2:B:1001:PHE:CE2	3:C:178:PHE:HB3	2.45	0.51
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.42	0.51
2:B:1182:CYS:O	2:B:1186:LYS:N	2.43	0.51
5:E:45:ILE:HG23	5:E:57:MET:HB2	1.92	0.51
9:I:69:PRO:O	9:I:84:VAL:HG12	2.10	0.51
1:A:419:HIS:NE2	1:A:421:ARG:HG3	2.26	0.51
1:A:664:SER:OG	1:A:665:ILE:N	2.44	0.51
1:A:838:ILE:HG12	1:A:841:ARG:HH21	1.74	0.51
2:B:412:ILE:HG22	2:B:416:LYS:NZ	2.24	0.51
3:C:248:ILE:HG21	11:K:102:ASP:HB2	1.91	0.51
5:E:36:GLN:HG2	5:E:41:PHE:HB2	1.91	0.51
1:A:505:LEU:HD11	6:F:88:TYR:HA	1.92	0.51
1:A:816:PHE:O	1:A:819:MET:HB2	2.10	0.51
1:A:1156:TYR:HD1	1:A:1193:TRP:HA	1.76	0.51
2:B:179:ASP:HA	2:B:182:LYS:HE2	1.92	0.51
2:B:349:LEU:HD13	2:B:353:LEU:HD22	1.92	0.51
4:D:41:HIS:CD2	7:G:73:LYS:HE3	2.45	0.51
8:H:110:LYS:HA	8:H:126:GLY:O	2.10	0.51
9:I:106:CYS:SG	9:I:107:LYS:N	2.83	0.51
14:N:5:DT:H2"	14:N:6:DA:C8	2.45	0.51
18:e:84:PHE:HA	19:f:81:VAL:HB	1.91	0.51
1:A:255:GLU:OE2	16:P:0:C:N4	2.44	0.51
1:A:783:ARG:NH2	1:A:788:PHE:O	2.41	0.51
2:B:101:PRO:HG3	2:B:111:TYR:CE1	2.45	0.51
2:B:166:ARG:NH2	2:B:190:MET:HB3	2.24	0.51
2:B:627:TYR:HA	2:B:690:VAL:O	2.10	0.51
2:B:744:HIS:HB3	2:B:747:MET:HG2	1.93	0.51
2:B:833:TYR:O	2:B:838:SER:OG	2.28	0.51
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.92	0.51
5:E:92:MET:HE3	5:E:96:CYS:SG	2.50	0.51
15:O:376:TRP:HD1	15:O:379:LEU:HG	1.75	0.51
19:f:88:TYR:OH	19:f:102:GLY:O	2.26	0.51
1:A:12:ARG:NH2	7:G:10:ILE:HG13	2.25	0.51
1:A:89:PRO:HG2	1:A:205:PRO:HB2	1.92	0.51
1:A:288:HIS:NE2	1:A:292:GLU:OE2	2.44	0.51
1:A:375:LEU:HB3	1:A:492:VAL:HG21	1.92	0.51
1:A:790:LYS:NZ	9:I:67:THR:OG1	2.42	0.51
1:A:1015:ASN:O	5:E:204:SER:HB2	2.11	0.51
2:B:1037:ILE:O	10:J:46:ARG:NH2	2.44	0.51
4:D:90:ALA:HB1	4:D:102:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:MET:HG3	1:A:298:GLN:HG2	1.91	0.51
1:A:739:LYS:HG2	1:A:742:ASN:HB2	1.93	0.51
1:A:990:HIS:CE1	1:A:993:ARG:HH22	2.29	0.51
2:B:108:ASN:HA	2:B:198:GLY:HA3	1.93	0.51
2:B:608:ILE:HG13	2:B:619:ILE:HD12	1.93	0.51
2:B:778:MET:SD	2:B:779:GLY:N	2.84	0.51
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.93	0.51
15:O:653:LYS:HE2	15:O:756:TYR:CZ	2.45	0.51
1:A:512:ILE:O	1:A:521:VAL:N	2.35	0.51
1:A:564:PRO:HB3	1:A:573:TRP:CE2	2.45	0.51
1:A:1204:MET:HA	1:A:1204:MET:HE3	1.91	0.51
1:A:1460:TYR:CD1	6:F:106:PRO:HB3	2.46	0.51
2:B:531:ASN:ND2	2:B:532:LEU:O	2.43	0.51
2:B:532:LEU:HD23	2:B:536:SER:HB2	1.92	0.51
2:B:784:ASN:HB3	10:J:62:TYR:CZ	2.45	0.51
1:A:29:ALA:HB1	2:B:1184:SER:HA	1.92	0.51
1:A:379:GLU:OE1	1:A:388:ARG:NH2	2.44	0.51
1:A:723:LEU:HD13	1:A:800:PHE:CG	2.46	0.51
1:A:1001:VAL:HG23	1:A:1013:GLN:HE22	1.75	0.51
1:A:1098:LEU:HD13	1:A:1361:PHE:HB2	1.92	0.51
2:B:498:ASP:HB2	14:N:-57:DT:O4'	2.11	0.51
2:B:846:ILE:O	2:B:852:ARG:NH2	2.44	0.51
15:O:472:ILE:HA	15:O:479:ILE:HG21	1.93	0.51
1:A:766:VAL:HB	1:A:801:VAL:HG11	1.92	0.51
2:B:326:ILE:HD13	2:B:349:LEU:HD21	1.91	0.51
3:C:239:LYS:HB2	3:C:242:GLN:HG3	1.93	0.51
12:L:60:LYS:NZ	12:L:61:ALA:O	2.40	0.51
13:M:56:PHE:CZ	13:M:58:ALA:HB2	2.46	0.51
14:N:-50:DT:H2''	14:N:-49:DG:C8	2.46	0.51
1:A:140:GLN:HA	1:A:143:LYS:HD3	1.93	0.51
1:A:321:ARG:CZ	16:P:4:G:H4'	2.40	0.51
1:A:351:ARG:NH1	17:T:62:DA:H5'	2.26	0.51
2:B:28:LYS:HZ3	2:B:678:TRP:HE1	1.59	0.51
2:B:1132:GLU:HA	2:B:1135:ARG:HG3	1.92	0.51
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.44	0.51
5:E:3:ASP:OD1	5:E:6:ARG:NH2	2.44	0.51
1:A:66:LYS:HD2	1:A:72:GLU:HA	1.93	0.50
1:A:818:ALA:HA	2:B:764:SER:OG	2.11	0.50
1:A:846:LEU:HD21	1:A:1377:VAL:HG11	1.93	0.50
1:A:1348:ARG:HD2	5:E:199:ARG:NH2	2.26	0.50
2:B:789:MET:HG3	2:B:965:LYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:170:LYS:NZ	5:E:171:GLU:OE2	2.43	0.50
17:T:-5:DA:H3'	18:a:42:ARG:HH21	1.75	0.50
18:e:103:LEU:HD22	19:f:57:VAL:HG11	1.92	0.50
1:A:98:LYS:HZ3	1:A:1414:GLU:HA	1.75	0.50
1:A:680:ILE:HD13	1:A:764:ALA:HA	1.94	0.50
1:A:828:THR:O	1:A:832:THR:HG23	2.11	0.50
2:B:956:THR:HG23	12:L:48:VAL:HB	1.93	0.50
3:C:255:LEU:HB2	11:K:95:ILE:HD11	1.92	0.50
5:E:115:ILE:HB	5:E:120:ASN:HD21	1.77	0.50
5:E:177:ILE:O	5:E:213:CYS:HA	2.11	0.50
6:F:112:GLU:N	6:F:114:GLU:OE1	2.41	0.50
17:T:57:DA:HI'	17:T:58:DG:C8	2.46	0.50
1:A:467:SER:OG	11:K:2:ASN:ND2	2.44	0.50
1:A:1300:GLU:OE1	1:A:1300:GLU:N	2.41	0.50
1:A:1346:ALA:HB2	5:E:149:VAL:HG22	1.92	0.50
2:B:377:ARG:NH2	2:B:616:GLU:OE2	2.44	0.50
2:B:444:THR:HG1	2:B:447:THR:HG1	1.59	0.50
2:B:838:SER:HA	2:B:989:THR:O	2.11	0.50
2:B:1060:ARG:NH1	2:B:1066:SER:H	2.09	0.50
5:E:82:CYS:SG	5:E:87:VAL:HG22	2.52	0.50
5:E:144:THR:HA	5:E:149:VAL:HG11	1.92	0.50
5:E:152:HIS:ND1	5:E:183:VAL:HG21	2.25	0.50
14:N:-79:DG:H2'	14:N:-78:DG:C8	2.46	0.50
1:A:989:ILE:HG22	1:A:993:ARG:HE	1.77	0.50
2:B:30:LEU:HD21	2:B:489:ARG:HD2	1.93	0.50
2:B:534:LEU:HD12	2:B:747:MET:HA	1.93	0.50
2:B:963:PHE:HE2	2:B:965:LYS:HE3	1.77	0.50
3:C:97:VAL:N	3:C:122:SER:OG	2.26	0.50
20:c:73:ASN:HD22	20:c:82:HIS:CD2	2.30	0.50
2:B:1035:GLY:O	2:B:1039:GLY:N	2.42	0.50
4:D:183:ASP:OD1	4:D:183:ASP:N	2.44	0.50
11:K:31:ILE:HD13	11:K:84:LYS:HE3	1.93	0.50
20:c:81:ARG:HE	20:c:85:LEU:HD11	1.77	0.50
19:f:75:HIS:CG	21:h:96:THR:HG21	2.47	0.50
1:A:1401:MET:SD	1:A:1428:SER:OG	2.69	0.50
1:A:1452:LEU:HD22	6:F:131:PRO:HA	1.94	0.50
2:B:701:ALA:HB3	2:B:741:CYS:HB2	1.93	0.50
3:C:21:LEU:HD21	11:K:101:LEU:HD22	1.94	0.50
9:I:86:PHE:O	9:I:100:PHE:N	2.45	0.50
14:N:-81:DG:H22	17:T:81:DC:N4	2.09	0.50
15:O:763:SER:O	15:O:766:VAL:HG12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:71:ARG:NH1	20:c:72:ASP:OD1	2.44	0.50
1:A:819:MET:HE1	2:B:508:HIS:C	2.37	0.50
1:A:858:ARG:HG2	1:A:864:ILE:HA	1.92	0.50
1:A:970:GLN:HA	1:A:975:LEU:HD23	1.94	0.50
2:B:22:SER:HA	2:B:25:PHE:CD1	2.47	0.50
2:B:225:ILE:HG23	2:B:248:LYS:HB2	1.94	0.50
8:H:13:GLN:NE2	8:H:29:ILE:HG22	2.26	0.50
9:I:71:SER:HB3	9:I:85:PHE:HE1	1.76	0.50
11:K:93:SER:O	11:K:97:LYS:HG2	2.11	0.50
1:A:780:PHE:HE1	1:A:785:LEU:HD23	1.77	0.50
1:A:1367:ASN:OD1	1:A:1368:TYR:N	2.45	0.50
2:B:896:ASP:OD1	2:B:898:LEU:HB2	2.12	0.50
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.47	0.50
7:G:29:LYS:HA	7:G:32:THR:HG22	1.92	0.50
13:M:28:CYS:HB3	13:M:52:CYS:HB3	1.94	0.50
21:d:54:ILE:HG13	21:d:58:ALA:HB3	1.92	0.50
1:A:184:GLY:O	1:A:200:ARG:HA	2.11	0.50
1:A:542:ILE:HG22	1:A:547:VAL:HG23	1.94	0.50
1:A:775:ARG:NH1	1:A:798:LYS:HZ3	2.10	0.50
1:A:1345:GLU:OE2	5:E:199:ARG:NE	2.45	0.50
1:A:1447:MET:HB2	7:G:59:GLY:O	2.12	0.50
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.93	0.50
2:B:418:THR:HB	2:B:419:ARG:HH11	1.77	0.50
12:L:38:HIS:HE1	12:L:51:LYS:HB2	1.77	0.50
15:O:371:GLU:HB2	15:O:375:TRP:CD1	2.47	0.50
18:a:113:HIS:CD2	18:e:126:LEU:HD22	2.47	0.50
1:A:1194:LEU:O	1:A:1263:LEU:HD21	2.12	0.49
2:B:848:ARG:HG2	10:J:6:ARG:HB3	1.94	0.49
3:C:115:SER:HB3	3:C:142:ILE:HB	1.94	0.49
10:J:43:TYR:HA	10:J:46:ARG:HD3	1.94	0.49
12:L:31:TYR:N	12:L:40:PHE:O	2.33	0.49
14:N:22:DT:O4	17:T:-23:DC:N4	2.43	0.49
15:O:312:VAL:HG13	15:O:342:PHE:HB2	1.93	0.49
1:A:345:ARG:CZ	2:B:1120:GLU:HB2	2.42	0.49
1:A:723:LEU:HD12	1:A:775:ARG:NH1	2.26	0.49
1:A:931:ASN:O	1:A:934:TYR:N	2.45	0.49
1:A:1033:ILE:HD13	1:A:1037:PHE:CZ	2.46	0.49
1:A:1209:LEU:HG	1:A:1277:ARG:HD2	1.94	0.49
2:B:119:MET:SD	2:B:437:LEU:HD21	2.51	0.49
2:B:522:GLU:O	2:B:526:CYS:N	2.45	0.49
2:B:848:ARG:HH21	10:J:6:ARG:HH12	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:ALA:O	8:H:110:LYS:NZ	2.44	0.49
1:A:1006:ASN:H	1:A:1009:ILE:HD12	1.77	0.49
1:A:1320:MET:HE1	5:E:141:VAL:HB	1.94	0.49
1:A:1348:ARG:NE	1:A:1376:ASP:OD1	2.40	0.49
1:A:1378:MET:SD	1:A:1384:LEU:HD22	2.52	0.49
2:B:552:GLU:HA	2:B:556:MET:HG2	1.94	0.49
2:B:848:ARG:NH1	10:J:8:PHE:O	2.43	0.49
2:B:883:LEU:HB3	2:B:932:HIS:CE1	2.47	0.49
2:B:1156:ASP:HB2	2:B:1198:TYR:HB3	1.93	0.49
3:C:214:LYS:HB2	3:C:217:GLU:HB2	1.94	0.49
5:E:61:ALA:HB3	5:E:77:LEU:HB3	1.94	0.49
15:O:560:SER:HB3	15:O:561:PRO:HD3	1.95	0.49
15:O:688:LEU:O	15:O:692:ASN:ND2	2.45	0.49
18:a:116:ARG:NH2	18:a:123:ASP:OD1	2.42	0.49
18:e:63:ARG:CZ	18:e:66:PRO:HG2	2.42	0.49
18:e:104:PHE:HE2	19:f:37:LEU:HB3	1.77	0.49
1:A:351:ARG:HA	1:A:488:MET:O	2.12	0.49
1:A:854:ASP:OD2	1:A:856:THR:OG1	2.25	0.49
1:A:1156:TYR:HB3	9:I:25:LEU:HD13	1.93	0.49
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.95	0.49
3:C:205:LYS:HE3	3:C:206:TYR:CE2	2.47	0.49
4:D:60:ILE:HG21	4:D:109:LEU:HD13	1.95	0.49
9:I:65:ASP:HB3	9:I:68:LEU:HD23	1.94	0.49
10:J:57:GLU:OE2	10:J:58:LYS:NZ	2.44	0.49
1:A:174:VAL:HB	1:A:185:THR:HB	1.94	0.49
1:A:379:GLU:OE1	1:A:435:ARG:NH1	2.46	0.49
1:A:547:VAL:HG21	1:A:573:TRP:CD2	2.47	0.49
1:A:566:ILE:HB	1:A:572:LEU:HB2	1.93	0.49
1:A:719:VAL:HG12	1:A:775:ARG:HH12	1.77	0.49
1:A:787:HIS:NE2	2:B:742:GLU:OE1	2.45	0.49
1:A:881:ARG:HB2	1:A:955:ASN:ND2	2.26	0.49
10:J:18:TRP:O	10:J:22:LEU:HG	2.13	0.49
17:T:56:DC:H2''	17:T:57:DA:H5'	1.95	0.49
19:f:84:MET:HE2	19:f:84:MET:N	2.28	0.49
1:A:1348:ARG:HE	1:A:1376:ASP:CG	2.19	0.49
2:B:73:LYS:HG3	2:B:125:THR:HG22	1.93	0.49
2:B:1149:GLU:O	2:B:1153:GLU:HG3	2.12	0.49
3:C:47:LEU:HB3	12:L:68:GLN:NE2	2.26	0.49
3:C:74:GLU:HB3	3:C:242:GLN:HE22	1.78	0.49
5:E:93:ARG:HE	5:E:97:LEU:HG	1.78	0.49
10:J:56:ILE:HD12	10:J:59:PHE:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:26:ARG:HB3	11:K:74:ARG:HH21	1.78	0.49
14:N:-53:DT:H2''	14:N:-52:DC:C6	2.48	0.49
15:O:648:ALA:HA	15:O:654:MET:HG3	1.94	0.49
15:O:791:SER:OG	15:O:793:GLU:OE1	2.27	0.49
1:A:24:PRO:HA	1:A:27:ILE:HD12	1.94	0.49
1:A:253:MET:O	16:P:1:G:N2	2.44	0.49
1:A:568:LYS:NZ	8:H:89:ALA:O	2.27	0.49
1:A:666:GLY:HA3	2:B:1069:PHE:CZ	2.48	0.49
1:A:802:GLU:OE1	1:A:802:GLU:N	2.45	0.49
1:A:966:ILE:HD11	1:A:1028:LEU:HD21	1.93	0.49
1:A:1042:ASP:O	1:A:1046:TRP:HE3	1.96	0.49
1:A:1100:VAL:O	1:A:1104:LYS:HG2	2.12	0.49
2:B:103:GLU:OE2	12:L:56:ARG:NH1	2.46	0.49
2:B:660:ASP:HB2	2:B:675:VAL:C	2.38	0.49
2:B:1097:HIS:O	2:B:1098:MET:HE2	2.13	0.49
3:C:8:ASN:OD1	3:C:20:MET:HB3	2.13	0.49
3:C:48:VAL:HG23	12:L:71:ALA:HB2	1.95	0.49
1:A:96:ILE:HG23	1:A:182:LEU:HD11	1.95	0.49
1:A:296:LEU:O	1:A:300:HIS:ND1	2.34	0.49
1:A:762:MET:HE2	2:B:1021:MET:HB2	1.95	0.49
1:A:1065:MET:HG3	1:A:1068:VAL:HB	1.94	0.49
1:A:1127:ALA:HB1	1:A:1306:LEU:HB3	1.95	0.49
2:B:181:TYR:CZ	10:J:61:ARG:HD2	2.47	0.49
2:B:824:ILE:O	2:B:1009:ASP:N	2.46	0.49
2:B:879:ARG:HA	2:B:885:LEU:HD11	1.94	0.49
14:N:32:DG:H2''	14:N:33:DT:H5'	1.94	0.49
20:g:87:ILE:HD12	20:g:97:LEU:HD12	1.95	0.49
1:A:379:GLU:HG2	1:A:389:LEU:HD11	1.93	0.49
1:A:755:SER:N	1:A:758:ASN:OD1	2.45	0.49
1:A:850:MET:HB3	1:A:1439:MET:HE1	1.94	0.49
2:B:459:TRP:CD1	2:B:472:VAL:HB	2.48	0.49
5:E:212:ILE:HG12	5:E:214:LEU:HG	1.95	0.49
7:G:13:LEU:HD23	7:G:22:MET:HE3	1.93	0.49
8:H:8:ASP:OD1	8:H:9:ILE:N	2.46	0.49
1:A:336:ARG:HH21	2:B:1203:LEU:HB2	1.77	0.49
1:A:559:GLY:HA3	11:K:26:ARG:HG2	1.95	0.49
2:B:233:SER:HB3	2:B:245:MET:HE3	1.95	0.49
2:B:1038:ARG:NH1	2:B:1062:ASN:OD1	2.46	0.49
2:B:1148:LYS:O	2:B:1152:MET:N	2.46	0.49
3:C:125:GLY:HA2	3:C:126:ASN:HA	1.57	0.49
3:C:167:HIS:CD2	12:L:72:ARG:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:THR:HG23	5:E:119:ALA:H	1.77	0.49
8:H:9:ILE:O	8:H:31:THR:N	2.40	0.49
10:J:30:GLN:NE2	10:J:32:GLY:H	2.11	0.49
1:A:551:LEU:HB3	1:A:557:TRP:CD2	2.48	0.48
1:A:673:ASP:HB2	1:A:737:ASN:HD21	1.77	0.48
2:B:82:ILE:HG22	2:B:117:LEU:HD13	1.94	0.48
2:B:275:VAL:HG11	2:B:310:ILE:HD13	1.94	0.48
3:C:182:PRO:HD2	3:C:185:LYS:HZ1	1.77	0.48
12:L:33:CYS:SG	12:L:34:GLY:N	2.85	0.48
15:O:308:GLN:OE1	15:O:338:GLN:NE2	2.46	0.48
15:O:521:LEU:HB3	15:O:522:PRO:HD3	1.94	0.48
17:T:17:DA:H5"	18:e:63:ARG:HE	1.78	0.48
18:a:83:ARG:O	19:b:81:VAL:N	2.46	0.48
2:B:292:HIS:CE1	2:B:368:THR:HB	2.48	0.48
2:B:590:VAL:HG21	2:B:610:ARG:HD2	1.95	0.48
3:C:166:GLU:C	11:K:6:ARG:HE	2.21	0.48
1:A:40:ILE:HG22	1:A:53:LEU:HB2	1.95	0.48
1:A:86:LEU:HD21	1:A:240:LEU:HD23	1.94	0.48
1:A:330:LEU:C	1:A:338:ARG:HH22	2.21	0.48
1:A:1258:GLU:HG3	9:I:30:ARG:HH22	1.77	0.48
1:A:1266:ILE:O	1:A:1270:MET:HG3	2.13	0.48
2:B:23:ALA:O	2:B:26:GLU:HG3	2.13	0.48
2:B:200:GLU:OE1	2:B:478:ARG:NH2	2.46	0.48
2:B:522:GLU:CD	2:B:524:GLN:HE22	2.21	0.48
2:B:1004:GLU:OE1	2:B:1064:TYR:OH	2.22	0.48
2:B:1166:CYS:HA	4:D:13:ARG:HB2	1.94	0.48
3:C:124:PRO:O	3:C:127:LEU:HB2	2.13	0.48
7:G:93:ASN:OD1	7:G:94:VAL:N	2.47	0.48
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.77	0.48
15:O:313:GLN:O	15:O:313:GLN:NE2	2.44	0.48
17:T:9:DG:H5"	18:e:43:PRO:HA	1.95	0.48
1:A:147:VAL:HG23	1:A:171:THR:HG22	1.95	0.48
1:A:809:LEU:HD21	1:A:813:GLU:HG3	1.95	0.48
1:A:1100:VAL:HA	1:A:1103:LEU:HD12	1.95	0.48
2:B:227:HIS:CE1	2:B:382:ALA:HA	2.49	0.48
2:B:597:ARG:NH1	2:B:606:VAL:O	2.46	0.48
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.46	0.48
3:C:56:VAL:HG23	10:J:56:ILE:HD11	1.95	0.48
8:H:89:ALA:HB1	8:H:95:VAL:HG21	1.95	0.48
15:O:491:ARG:HB2	15:O:513:ILE:HA	1.95	0.48
17:T:27:DG:H2"	17:T:28:DG:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASN:ND2	2:B:1134:GLU:HG2	2.28	0.48
2:B:248:LYS:NZ	2:B:271:ASP:OD1	2.44	0.48
4:D:115:PHE:HB2	4:D:121:CYS:SG	2.54	0.48
5:E:54:ARG:HA	5:E:57:MET:HE3	1.95	0.48
5:E:65:PRO:HA	5:E:68:LEU:HD12	1.95	0.48
15:O:262:LYS:HA	15:O:265:GLN:HE21	1.78	0.48
15:O:513:ILE:HG13	15:O:514:PHE:N	2.28	0.48
15:O:678:ARG:HA	15:O:681:LEU:HD12	1.94	0.48
15:O:806:LEU:HD23	15:O:809:LYS:NZ	2.27	0.48
19:f:39:ARG:NH1	19:f:43:VAL:O	2.47	0.48
1:A:11:LEU:HB2	2:B:1193:GLN:HE21	1.79	0.48
1:A:117:GLU:OE2	1:A:127:ARG:NH2	2.35	0.48
1:A:550:MET:O	1:A:554:VAL:N	2.46	0.48
1:A:761:GLN:HB3	1:A:805:TYR:HE2	1.77	0.48
1:A:783:ARG:NH2	1:A:786:PRO:O	2.47	0.48
1:A:804:SER:OG	1:A:807:ARG:NE	2.45	0.48
1:A:844:LYS:NZ	1:A:1405:PHE:HB2	2.29	0.48
1:A:1029:ALA:O	1:A:1033:ILE:HG12	2.14	0.48
1:A:1267:GLU:O	1:A:1271:LEU:HG	2.14	0.48
1:A:1381:ARG:C	5:E:176:ARG:HB2	2.39	0.48
2:B:852:ARG:HG3	2:B:973:VAL:HG22	1.96	0.48
11:K:60:ALA:O	11:K:73:MET:HG2	2.14	0.48
18:a:58:THR:HG21	20:g:81:ARG:HB2	1.96	0.48
18:e:75:ALA:HA	18:e:78:PHE:HD2	1.77	0.48
1:A:373:LYS:HZ1	1:A:398:ASN:HA	1.78	0.48
1:A:452:HIS:CD2	1:A:454:MET:HB2	2.45	0.48
1:A:455:SER:O	1:A:456:MET:HE2	2.14	0.48
1:A:587:ILE:HA	1:A:964:ARG:HH22	1.79	0.48
1:A:715:PHE:HZ	1:A:793:PHE:HB3	1.78	0.48
1:A:890:SER:O	1:A:894:PHE:N	2.29	0.48
1:A:971:GLN:NE2	1:A:972:ILE:HG12	2.28	0.48
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.05	0.48
7:G:5:LYS:HD3	7:G:78:VAL:HG22	1.96	0.48
15:O:336:THR:O	15:O:340:ILE:HG12	2.12	0.48
15:O:549:TYR:CE1	15:O:814:PRO:HG2	2.49	0.48
15:O:552:ALA:O	15:O:556:LYS:HD3	2.14	0.48
15:O:689:GLU:HG3	15:O:706:PHE:HZ	1.78	0.48
19:f:26:ILE:HG13	19:f:55:ARG:HD3	1.96	0.48
2:B:115:VAL:O	2:B:157:HIS:HD2	1.96	0.48
2:B:117:LEU:HB3	2:B:158:ILE:HD11	1.95	0.48
2:B:395:GLY:HA3	2:B:693:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480:THR:O	2:B:483:SER:OG	2.18	0.48
2:B:860:MET:HG2	2:B:965:LYS:HG2	1.94	0.48
4:D:112:PHE:O	4:D:114:ARG:NH1	2.47	0.48
14:N:-9:DC:H2''	14:N:-8:DG:N7	2.28	0.48
15:O:624:ILE:HD12	15:O:628:PRO:HA	1.95	0.48
1:A:15:LYS:N	2:B:1217:TYR:O	2.43	0.48
1:A:296:LEU:HD12	1:A:299:PHE:CZ	2.48	0.48
1:A:357:ASP:HB2	1:A:470:ARG:HB3	1.95	0.48
1:A:680:ILE:O	1:A:684:ILE:HG12	2.13	0.48
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.48	0.48
5:E:155:LEU:HD11	5:E:210:TYR:CD2	2.48	0.48
8:H:17:ASN:ND2	8:H:24:SER:HB3	2.29	0.48
8:H:63:LEU:HD11	8:H:87:SER:HB2	1.96	0.48
14:N:-3:DA:OP1	18:e:118:THR:N	2.45	0.48
15:O:462:GLY:O	15:O:488:THR:OG1	2.26	0.48
1:A:146:MET:N	1:A:146:MET:SD	2.86	0.48
2:B:355:PRO:O	2:B:359:GLN:NE2	2.47	0.48
2:B:396:LYS:C	2:B:397:LYS:HD3	2.39	0.48
2:B:840:ILE:HD12	2:B:992:VAL:HG12	1.96	0.48
3:C:95:SER:OG	3:C:158:ILE:HD12	2.14	0.48
3:C:241:ASN:OD1	3:C:242:GLN:N	2.47	0.48
8:H:92:TYR:CG	8:H:142:LEU:HB3	2.49	0.48
14:N:-81:DG:N7	15:O:714:SER:HB2	2.29	0.48
15:O:329:ASP:HB2	15:O:335:LYS:HE2	1.95	0.48
17:T:-8:DC:H2'	17:T:-7:DG:C8	2.49	0.48
1:A:28:ARG:HA	1:A:31:SER:HB3	1.95	0.47
1:A:330:LEU:O	1:A:338:ARG:NH1	2.43	0.47
1:A:790:LYS:HB2	9:I:69:PRO:HD3	1.96	0.47
2:B:328:ARG:HB2	2:B:329:ARG:NH1	2.29	0.47
2:B:892:LYS:HB3	2:B:899:ILE:HG22	1.94	0.47
2:B:1071:VAL:HG22	2:B:1084:GLN:HG3	1.94	0.47
2:B:1203:LEU:HA	2:B:1206:GLU:OE2	2.14	0.47
11:K:71:PHE:CE1	11:K:73:MET:HB2	2.47	0.47
13:M:49:CYS:HB3	13:M:54:LEU:H	1.79	0.47
15:O:671:THR:HG22	15:O:733:VAL:HG22	1.96	0.47
16:P:1:G:H2'	16:P:2:U:C6	2.49	0.47
17:T:30:DT:H4'	21:d:31:ARG:HD3	1.96	0.47
21:h:90:THR:OG1	21:h:93:GLU:OE1	2.22	0.47
1:A:769:GLN:HG3	1:A:817:HIS:HA	1.96	0.47
2:B:1065:GLN:HG3	3:C:201:TRP:CZ3	2.50	0.47
2:B:1106:ARG:HH12	2:B:1110:PRO:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:ARG:HD2	5:E:187:LEU:C	2.39	0.47
7:G:79:TRP:HZ3	7:G:104:GLY:HA3	1.77	0.47
12:L:29:VAL:HG13	12:L:60:LYS:HE2	1.95	0.47
15:O:737:THR:O	15:O:739:ARG:N	2.39	0.47
16:P:2:U:H2'	16:P:3:U:H6	1.79	0.47
17:T:20:DG:H2''	17:T:21:DC:O5'	2.14	0.47
1:A:697:LYS:O	1:A:702:GLU:N	2.47	0.47
1:A:886:THR:HB	1:A:941:ARG:HD3	1.97	0.47
1:A:1105:GLU:OE1	1:A:1113:ILE:HB	2.13	0.47
2:B:249:LEU:HD13	2:B:261:ILE:HG12	1.95	0.47
3:C:262:LEU:HB3	11:K:88:GLU:OE2	2.13	0.47
5:E:25:ARG:CZ	5:E:187:LEU:HD22	2.44	0.47
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.95	0.47
9:I:39:GLU:OE1	9:I:39:GLU:N	2.47	0.47
14:N:-47:DC:O2	17:T:48:DG:N2	2.47	0.47
14:N:-46:DT:H2''	14:N:-45:DG:C8	2.50	0.47
17:T:64:DA:H2''	17:T:65:DA:H5''	1.96	0.47
20:g:85:LEU:HD23	20:g:108:LEU:HD23	1.96	0.47
1:A:301:VAL:O	1:A:304:TYR:HB3	2.15	0.47
1:A:748:VAL:HG21	1:A:759:ILE:HD11	1.96	0.47
1:A:1009:ILE:HG13	5:E:166:ARG:NE	2.24	0.47
1:A:1037:PHE:CE2	1:A:1039:LEU:HG	2.49	0.47
2:B:83:TYR:OH	2:B:118:ASP:OD2	2.23	0.47
2:B:590:VAL:HG12	2:B:617:PHE:CE1	2.49	0.47
4:D:40:ASP:OD1	4:D:44:ASN:N	2.47	0.47
5:E:155:LEU:HA	5:E:159:GLU:OE1	2.14	0.47
12:L:33:CYS:CB	12:L:36:CYS:SG	2.97	0.47
17:T:1:DT:H2'	17:T:2:DG:C8	2.49	0.47
17:T:46:DA:H2''	17:T:47:DG:C8	2.49	0.47
19:f:35:ARG:HD3	19:f:46:ILE:HD12	1.95	0.47
1:A:344:LYS:HG2	2:B:1135:ARG:NH2	2.26	0.47
1:A:351:ARG:HE	1:A:487:GLU:HG3	1.80	0.47
1:A:1006:ASN:OD1	1:A:1007:GLU:N	2.48	0.47
1:A:1157:ASP:HB3	1:A:1243:ARG:HH22	1.79	0.47
2:B:621:THR:HA	2:B:625:ARG:HH21	1.78	0.47
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	1.96	0.47
2:B:805:LYS:HD2	2:B:809:MET:HE2	1.95	0.47
8:H:63:LEU:HD11	8:H:89:ALA:H	1.79	0.47
14:N:-19:DG:H2''	14:N:-18:DG:H5'	1.97	0.47
15:O:331:MET:HE2	15:O:774:ARG:HH12	1.78	0.47
17:T:-5:DA:H2''	17:T:-4:DC:C5	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:e:61:LEU:N	18:e:97:GLU:OE2	2.48	0.47
18:e:78:PHE:HB3	19:f:70:VAL:HG11	1.97	0.47
1:A:458:ALA:O	1:A:508:VAL:HG23	2.14	0.47
1:A:687:ALA:CB	1:A:726:ALA:HB2	2.44	0.47
2:B:182:LYS:HA	10:J:63:ASN:HD21	1.79	0.47
2:B:281:LEU:HA	2:B:346:LYS:NZ	2.30	0.47
2:B:862:GLN:HG2	2:B:863:GLU:O	2.15	0.47
3:C:115:SER:N	3:C:142:ILE:O	2.47	0.47
3:C:153:LEU:HD12	3:C:155:ILE:HD11	1.96	0.47
5:E:77:LEU:HD11	5:E:108:ILE:HG23	1.97	0.47
8:H:26:ILE:O	8:H:39:THR:HA	2.15	0.47
12:L:33:CYS:CB	12:L:50:CYS:SG	3.03	0.47
14:N:-8:DG:H2''	14:N:-7:DG:C8	2.49	0.47
15:O:263:ARG:HH21	15:O:280:LYS:HB2	1.80	0.47
15:O:596:GLU:O	15:O:600:ARG:HG2	2.14	0.47
17:T:23:DA:H2'	17:T:24:DA:C5	2.50	0.47
17:T:76:DG:H2''	17:T:77:DG:C8	2.48	0.47
1:A:95:PHE:O	1:A:99:ILE:HG13	2.15	0.47
1:A:658:LEU:O	1:A:662:GLY:N	2.48	0.47
1:A:738:LEU:HD22	1:A:742:ASN:HD21	1.80	0.47
1:A:887:ILE:HG23	1:A:945:ARG:HG2	1.96	0.47
2:B:78:ARG:NH1	2:B:79:PHE:O	2.47	0.47
2:B:821:GLN:HB2	2:B:851:PHE:CZ	2.50	0.47
2:B:910:ILE:HG13	2:B:940:PRO:HB3	1.95	0.47
3:C:20:MET:HE2	3:C:229:TYR:CD1	2.48	0.47
3:C:252:GLN:HE21	11:K:98:LEU:HB3	1.78	0.47
5:E:14:SER:HA	5:E:139:LEU:O	2.14	0.47
5:E:152:HIS:CD2	5:E:197:ILE:HG23	2.50	0.47
5:E:178:GLN:HG2	5:E:181:ASP:N	2.30	0.47
8:H:10:PHE:HA	8:H:30:SER:HA	1.97	0.47
14:N:-53:DT:O2	17:T:54:DG:N2	2.48	0.47
14:N:28:DA:OP1	19:b:79:LYS:N	2.47	0.47
19:b:47:SER:HB3	19:b:50:ILE:HG12	1.96	0.47
21:d:110:ALA:HA	21:d:113:GLU:HG2	1.97	0.47
20:g:112:GLN:HB2	20:g:115:LEU:HG	1.96	0.47
1:A:142:CYS:HA	1:A:145:LYS:NZ	2.30	0.47
1:A:547:VAL:HA	1:A:550:MET:HE3	1.97	0.47
1:A:1075:GLY:O	1:A:1079:THR:HG23	2.15	0.47
2:B:398:ARG:NH2	2:B:620:PHE:HB3	2.30	0.47
2:B:1033:LYS:HG2	2:B:1089:PRO:HD2	1.97	0.47
5:E:21:MET:SD	5:E:186:TYR:HA	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HA	1:A:177:LYS:HE3	1.97	0.47
1:A:220:CYS:SG	1:A:231:ARG:NH1	2.86	0.47
1:A:220:CYS:SG	1:A:231:ARG:NH2	2.81	0.47
1:A:535:MET:HE1	1:A:654:VAL:HG22	1.96	0.47
1:A:569:PRO:CD	8:H:46:MET:HE2	2.43	0.47
1:A:868:LEU:HD13	1:A:1002:LEU:HD11	1.97	0.47
1:A:1228:VAL:HG12	1:A:1242:CYS:SG	2.55	0.47
2:B:631:PHE:HB3	2:B:645:LEU:CD2	2.45	0.47
3:C:67:GLY:O	3:C:169:LYS:HB2	2.15	0.47
6:F:90:ARG:NE	6:F:154:ASP:O	2.48	0.47
11:K:34:LYS:HZ3	11:K:70:ASN:HB2	1.79	0.47
13:M:15:ILE:HG13	14:N:-47:DC:C5	2.50	0.47
14:N:28:DA:H3'	19:b:78:ARG:HG2	1.95	0.47
17:T:-50:DC:H2''	17:T:-49:DG:H5''	1.96	0.47
20:c:73:ASN:HD22	20:c:82:HIS:HD2	1.63	0.47
19:f:70:VAL:O	19:f:74:GLU:HG2	2.15	0.47
20:g:50:TYR:CD1	21:h:114:GLY:HA3	2.50	0.47
1:A:369:ILE:HD11	1:A:400:HIS:HB2	1.96	0.47
1:A:608:ILE:HG13	1:A:613:VAL:HG22	1.97	0.47
1:A:854:ASP:OD1	1:A:855:GLY:N	2.48	0.47
1:A:1428:SER:HA	1:A:1431:VAL:HG22	1.97	0.47
2:B:20:VAL:HG13	2:B:678:TRP:HZ3	1.80	0.47
2:B:977:GLY:H	2:B:990:ILE:HB	1.79	0.47
5:E:67:ALA:HA	5:E:70:LYS:HB3	1.95	0.47
5:E:178:GLN:OE1	5:E:178:GLN:N	2.31	0.47
10:J:58:LYS:HD3	10:J:61:ARG:HH12	1.80	0.47
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.97	0.47
15:O:274:ASP:OD1	15:O:275:GLU:N	2.48	0.47
15:O:475:PRO:HD3	15:O:508:SER:HB2	1.97	0.47
17:T:-34:DG:H3'	21:d:86:ARG:NE	2.28	0.47
1:A:631:ILE:O	1:A:635:MET:HG2	2.15	0.46
1:A:1172:VAL:HG12	1:A:1229:MET:SD	2.54	0.46
1:A:1289:LYS:NZ	1:A:1305:GLU:HB3	2.30	0.46
2:B:762:ASN:ND2	2:B:1022:THR:OG1	2.48	0.46
2:B:783:THR:OG1	10:J:62:TYR:OH	2.24	0.46
2:B:789:MET:HE1	2:B:951:GLN:OE1	2.15	0.46
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.80	0.46
2:B:857:ARG:HD3	2:B:942:ARG:HE	1.80	0.46
2:B:869:SER:HB3	15:O:636:LYS:NZ	2.31	0.46
12:L:50:CYS:HB3	12:L:55:HIS:H	1.79	0.46
15:O:455:HIS:HB2	15:O:459:ARG:HH22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:-14:DA:H2"	17:T:-13:DA:C8	2.50	0.46
18:a:41:TYR:CG	18:a:42:ARG:N	2.84	0.46
1:A:382:THR:HG23	1:A:385:ASN:HD21	1.80	0.46
1:A:451:LEU:HD13	1:A:1079:THR:HG21	1.96	0.46
1:A:807:ARG:HD2	2:B:722:THR:HG22	1.96	0.46
1:A:1291:LYS:HG3	1:A:1303:ASN:HB3	1.97	0.46
1:A:1425:ARG:H	1:A:1425:ARG:HD3	1.80	0.46
2:B:214:VAL:HG11	2:B:377:ARG:HD2	1.96	0.46
2:B:235:LEU:HD21	2:B:359:GLN:HE22	1.80	0.46
2:B:805:LYS:HD2	2:B:809:MET:HG3	1.98	0.46
2:B:957:ASN:CG	2:B:961:LEU:H	2.23	0.46
5:E:95:PHE:O	5:E:99:ILE:HG12	2.15	0.46
15:O:678:ARG:N	17:T:75:DC:OP1	2.47	0.46
1:A:90:VAL:HB	1:A:298:GLN:HE22	1.79	0.46
1:A:339:GLY:HA2	2:B:1129:ARG:HH22	1.81	0.46
1:A:569:PRO:HD3	8:H:93:ASP:O	2.15	0.46
1:A:680:ILE:HG23	1:A:730:ALA:HB1	1.97	0.46
1:A:730:ALA:HB1	1:A:764:ALA:HB1	1.97	0.46
2:B:100:PHE:CD2	2:B:172:LEU:HD11	2.51	0.46
2:B:398:ARG:HB3	2:B:624:GLY:HA3	1.97	0.46
5:E:183:VAL:O	5:E:187:LEU:N	2.45	0.46
8:H:108:GLU:HG2	8:H:109:ASP:N	2.30	0.46
10:J:23:ARG:HA	10:J:26:GLU:CD	2.40	0.46
15:O:740:VAL:HG23	17:T:77:DG:OP2	2.16	0.46
1:A:542:ILE:HG21	1:A:550:MET:HE1	1.98	0.46
1:A:815:PHE:HE2	2:B:509:ASN:HA	1.81	0.46
2:B:99:MET:HE1	2:B:111:TYR:HD1	1.80	0.46
2:B:233:SER:OG	2:B:356:HIS:ND1	2.31	0.46
2:B:810:GLU:HA	2:B:815:ARG:NH1	2.31	0.46
2:B:839:MET:HE1	2:B:988:GLY:O	2.15	0.46
3:C:36:MET:HA	3:C:40:VAL:HG23	1.98	0.46
15:O:507:TRP:CE3	15:O:521:LEU:HD13	2.50	0.46
17:T:-35:DA:H2"	17:T:-34:DG:C8	2.49	0.46
18:a:100:LEU:HD22	19:b:54:THR:HG23	1.96	0.46
19:b:71:THR:HG23	21:d:99:ARG:NH1	2.30	0.46
19:b:91:LYS:HA	19:b:96:THR:OG1	2.16	0.46
1:A:103:CYS:HB3	1:A:175:VAL:HG11	1.97	0.46
1:A:303:THR:HA	1:A:306:ASP:C	2.41	0.46
1:A:395:ASN:HB3	1:A:399:GLU:OE2	2.15	0.46
1:A:445:PHE:CE2	1:A:471:LEU:HD21	2.49	0.46
1:A:652:LYS:HD3	1:A:652:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:VAL:HG12	2:B:326:ILE:HD11	1.97	0.46
2:B:283:VAL:HG11	2:B:292:HIS:CE1	2.51	0.46
2:B:1146:PHE:O	2:B:1149:GLU:HG3	2.16	0.46
5:E:135:GLN:HG3	5:E:137:SER:H	1.81	0.46
13:M:32:ASN:O	13:M:51:LYS:NZ	2.38	0.46
14:N:26:DA:H2''	14:N:27:DG:C8	2.50	0.46
18:a:54:TYR:CE2	19:b:36:ARG:HG2	2.51	0.46
18:e:64:LYS:O	18:e:68:GLN:HB2	2.16	0.46
1:A:306:ASP:OD1	1:A:327:ARG:HD3	2.15	0.46
1:A:487:GLU:HB3	2:B:1102:LYS:HD2	1.97	0.46
1:A:507:ALA:HB1	1:A:509:PRO:HD2	1.97	0.46
1:A:852:HIS:NE2	1:A:858:ARG:HB2	2.30	0.46
1:A:1328:SER:HA	5:E:146:HIS:HA	1.98	0.46
2:B:425:MET:O	2:B:429:ILE:HB	2.15	0.46
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	1.98	0.46
14:N:-81:DG:H2'	14:N:-81:DG:N3	2.31	0.46
17:T:51:DC:N4	17:T:52:DG:O6	2.49	0.46
1:A:891:ASP:N	1:A:1299:GLY:HA3	2.31	0.46
2:B:219:LYS:HG2	2:B:225:ILE:HB	1.96	0.46
2:B:825:VAL:HG21	2:B:1092:TYR:CE2	2.51	0.46
2:B:842:ASN:HA	2:B:999:MET:HE1	1.98	0.46
5:E:170:LYS:H	5:E:173:GLN:HB2	1.81	0.46
8:H:91:ASP:HB3	8:H:144:ARG:HH12	1.81	0.46
14:N:64:DG:H1	17:T:-64:DC:H42	1.63	0.46
15:O:719:GLN:O	15:O:723:ASP:N	2.48	0.46
1:A:884:ILE:HG13	1:A:1023:LEU:HD13	1.97	0.46
2:B:1024:ALA:HA	2:B:1027:ILE:HD12	1.97	0.46
3:C:40:VAL:HB	3:C:172:PRO:HG3	1.97	0.46
3:C:98:LEU:HD13	3:C:120:LYS:HA	1.98	0.46
7:G:54:ILE:HG23	7:G:74:TYR:HB3	1.98	0.46
10:J:12:LYS:HZ3	10:J:39:LYS:HD2	1.80	0.46
11:K:26:ARG:HH21	11:K:74:ARG:NE	2.13	0.46
13:M:58:ALA:HB3	13:M:69:ILE:HD13	1.98	0.46
16:P:3:U:H2'	16:P:4:G:O4'	2.15	0.46
1:A:91:PHE:CE1	1:A:205:PRO:HG3	2.51	0.46
1:A:106:ILE:HD13	1:A:215:ILE:HD11	1.97	0.46
1:A:387:HIS:O	1:A:391:GLU:HG2	2.16	0.46
1:A:1140:ILE:HD11	1:A:1322:VAL:HG11	1.97	0.46
2:B:206:GLN:HE21	2:B:472:VAL:HG13	1.80	0.46
2:B:279:ARG:HA	2:B:284:VAL:HA	1.98	0.46
2:B:559:LEU:HD22	2:B:579:TRP:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:177:ILE:HG23	5:E:213:CYS:HA	1.97	0.46
6:F:114:GLU:HB3	6:F:119:GLN:HB2	1.97	0.46
11:K:84:LYS:H	11:K:84:LYS:HD2	1.81	0.46
14:N:-17:DT:H2'	14:N:-16:DT:C2	2.51	0.46
15:O:751:ASN:O	15:O:781:VAL:HA	2.15	0.46
20:c:26:PRO:HG2	20:c:29:ARG:HB2	1.98	0.46
1:A:33:VAL:HG13	1:A:35:ILE:HD11	1.98	0.46
1:A:67:CYS:HB3	1:A:70:CYS:SG	2.56	0.46
1:A:364:GLN:HG3	1:A:460:ARG:NH2	2.30	0.46
1:A:762:MET:HE1	2:B:1018:PRO:HA	1.97	0.46
1:A:884:ILE:HD11	1:A:958:LEU:HD11	1.98	0.46
1:A:1145:LEU:HD21	1:A:1270:MET:O	2.16	0.46
1:A:1211:MET:HE1	1:A:1231:SER:H	1.81	0.46
2:B:792:MET:HG2	2:B:855:PHE:CE1	2.49	0.46
6:F:90:ARG:HH22	6:F:153:VAL:HA	1.81	0.46
10:J:19:ASP:N	10:J:19:ASP:OD1	2.46	0.46
14:N:-23:DT:H6	14:N:-23:DT:H2'	1.65	0.46
15:O:365:LEU:HD22	15:O:383:ILE:HD11	1.98	0.46
15:O:672:LEU:HD13	15:O:674:PHE:CZ	2.50	0.46
1:A:697:LYS:HA	1:A:702:GLU:HB2	1.98	0.45
1:A:1104:LYS:NZ	1:A:1107:LEU:HD22	2.31	0.45
2:B:72:ASN:ND2	2:B:128:ASP:OD2	2.50	0.45
2:B:202:VAL:O	2:B:473:SER:HA	2.16	0.45
2:B:995:ARG:HG3	2:B:996:HIS:H	1.81	0.45
3:C:20:MET:HE2	3:C:229:TYR:CE1	2.51	0.45
3:C:194:GLU:N	3:C:200:GLU:OE2	2.47	0.45
3:C:206:TYR:HA	3:C:209:TRP:CD1	2.46	0.45
1:A:74:MET:HE1	1:A:246:GLN:HG3	1.98	0.45
1:A:115:LEU:HG	1:A:145:LYS:HE3	1.98	0.45
1:A:1155:TYR:HA	9:I:42:LYS:HA	1.96	0.45
3:C:53:ASN:H	12:L:62:ARG:NH1	2.14	0.45
3:C:169:LYS:NZ	12:L:72:ARG:HB3	2.31	0.45
10:J:12:LYS:HD2	10:J:39:LYS:HZ2	1.82	0.45
15:O:308:GLN:O	15:O:312:VAL:HG23	2.17	0.45
19:b:53:GLU:O	19:b:57:VAL:HG23	2.15	0.45
1:A:354:ILE:HD11	1:A:486:ASP:HB2	1.99	0.45
1:A:389:LEU:O	1:A:393:VAL:HG23	2.17	0.45
1:A:867:PHE:N	5:E:207:TYR:HH	2.15	0.45
1:A:1007:GLU:HA	1:A:1010:LYS:HE3	1.98	0.45
2:B:799:PRO:HD2	10:J:1:MET:H3	1.80	0.45
1:A:14:VAL:HG11	2:B:1216:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PHE:HE2	1:A:471:LEU:HD21	1.81	0.45
1:A:627:GLY:C	1:A:881:ARG:HH12	2.24	0.45
1:A:1151:ALA:HA	9:I:47:GLU:HA	1.98	0.45
2:B:784:ASN:HB2	2:B:787:VAL:HG22	1.99	0.45
5:E:189:LEU:HD11	5:E:195:VAL:HG21	1.98	0.45
11:K:73:MET:SD	11:K:75:LEU:HB2	2.56	0.45
15:O:383:ILE:HA	15:O:443:ILE:HB	1.99	0.45
15:O:491:ARG:HD2	15:O:512:PHE:CE1	2.52	0.45
15:O:513:ILE:HG13	15:O:514:PHE:H	1.82	0.45
21:d:72:ARG:O	21:d:76:GLU:HG2	2.16	0.45
1:A:546:GLN:HG3	1:A:656:TYR:HE1	1.80	0.45
4:D:39:TYR:HB3	4:D:43:GLY:HA2	1.98	0.45
11:K:36:GLU:HB3	11:K:37:ARG:NH1	2.31	0.45
14:N:14:DT:H1'	14:N:15:DT:H5'	1.98	0.45
15:O:706:PHE:HA	15:O:733:VAL:O	2.16	0.45
15:O:753:VAL:HB	15:O:783:ILE:HD13	1.99	0.45
21:d:103:PRO:O	21:d:107:ALA:N	2.31	0.45
18:e:63:ARG:HH22	19:f:30:THR:HG21	1.81	0.45
19:f:75:HIS:NE2	21:h:93:GLU:HG3	2.32	0.45
20:g:87:ILE:HD13	20:g:93:LEU:HD13	1.99	0.45
1:A:4:PHE:HB3	2:B:1159:ARG:HH22	1.82	0.45
1:A:465:PRO:HB2	11:K:4:PRO:HD3	1.99	0.45
1:A:533:ARG:HG3	1:A:750:ALA:HA	1.97	0.45
2:B:1174:ASN:HB3	2:B:1179:GLN:HG3	1.98	0.45
6:F:79:ARG:HD2	6:F:144:GLU:HB3	1.99	0.45
11:K:27:VAL:HG23	11:K:30:CYS:HB2	1.99	0.45
14:N:-57:DT:H3	17:T:57:DA:N6	2.14	0.45
17:T:-47:DT:H1'	17:T:-46:DC:C2	2.52	0.45
1:A:680:ILE:HG12	1:A:730:ALA:HB1	1.99	0.45
1:A:1014:GLN:O	1:A:1018:SER:OG	2.29	0.45
1:A:1116:PRO:O	1:A:1313:GLY:N	2.49	0.45
2:B:30:LEU:HD21	2:B:489:ARG:HH11	1.81	0.45
2:B:111:TYR:N	2:B:195:VAL:O	2.37	0.45
2:B:324:ASP:OD2	2:B:338:ARG:NH2	2.49	0.45
2:B:830:TYR:OH	2:B:1074:ASN:ND2	2.49	0.45
2:B:1083:ALA:HA	3:C:190:ASP:OD2	2.16	0.45
5:E:28:PHE:N	5:E:62:ASN:O	2.50	0.45
8:H:8:ASP:OD1	8:H:30:SER:OG	2.32	0.45
9:I:24:ARG:HH22	9:I:41:PRO:HD3	1.81	0.45
15:O:634:HIS:O	15:O:638:ARG:HG2	2.17	0.45
17:T:23:DA:H2'	17:T:24:DA:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:29:DA:H2"	17:T:30:DT:C5	2.51	0.45
1:A:87:ALA:HB2	1:A:278:GLN:HG3	1.98	0.45
1:A:180:MET:HG2	1:A:181:LYS:HG2	1.97	0.45
1:A:814:PHE:CE1	2:B:760:ASP:HA	2.52	0.45
1:A:899:TYR:N	1:A:1031:ARG:HH11	2.14	0.45
2:B:25:PHE:HA	2:B:29:GLY:H	1.82	0.45
2:B:56:LEU:HG	2:B:422:TYR:CZ	2.51	0.45
2:B:354:LEU:HD13	2:B:357:ILE:HD12	1.98	0.45
2:B:786:ASN:HA	2:B:967:ARG:NH2	2.32	0.45
5:E:37:SER:OG	5:E:39:GLU:OE2	2.29	0.45
10:J:14:VAL:HG11	10:J:48:MET:HE3	1.99	0.45
10:J:33:ASP:OD1	10:J:33:ASP:N	2.49	0.45
15:O:276:GLU:HB3	15:O:278:TRP:CE2	2.51	0.45
15:O:340:ILE:HG13	15:O:371:GLU:CG	2.45	0.45
18:a:88:ALA:HB1	19:b:86:VAL:HG21	1.99	0.45
20:c:107:VAL:HG22	20:c:108:LEU:H	1.82	0.45
1:A:536:THR:OG1	1:A:579:LEU:HD11	2.17	0.45
1:A:643:CYS:HA	1:A:646:LEU:HG	1.98	0.45
1:A:934:TYR:HA	1:A:937:LEU:HD12	1.99	0.45
2:B:314:PHE:CE1	9:I:31:ASN:HB2	2.52	0.45
2:B:486:SER:O	2:B:490:ARG:NH1	2.50	0.45
2:B:1104:HIS:CE1	2:B:1125:ASP:HA	2.52	0.45
2:B:1160:VAL:HG21	2:B:1201:LYS:NZ	2.31	0.45
3:C:108:GLU:HA	3:C:148:ARG:HH22	1.82	0.45
3:C:209:TRP:HB3	3:C:227:ARG:NH2	2.32	0.45
7:G:22:MET:HE2	7:G:70:PHE:CE2	2.52	0.45
15:O:578:LYS:HD3	15:O:781:VAL:O	2.16	0.45
15:O:670:LYS:HB3	15:O:725:PHE:CZ	2.52	0.45
20:g:26:PRO:HG3	21:h:40:TYR:CZ	2.52	0.45
1:A:26:GLU:O	1:A:30:ILE:HD12	2.16	0.45
1:A:101:LYS:HB3	1:A:135:PHE:CE2	2.51	0.45
1:A:1113:ILE:HD11	1:A:1333:ASN:ND2	2.32	0.45
1:A:1229:MET:HE2	1:A:1241:ARG:HG3	1.98	0.45
1:A:1430:ASN:O	1:A:1434:GLY:N	2.50	0.45
1:A:1433:LEU:HD21	2:B:1204:PHE:HZ	1.82	0.45
2:B:95:THR:O	2:B:97:HIS:ND1	2.50	0.45
2:B:200:GLU:CD	2:B:478:ARG:HH21	2.25	0.45
2:B:822:ASN:O	10:J:47:ARG:NH2	2.50	0.45
2:B:1159:ARG:NH2	2:B:1175:LEU:HD21	2.32	0.45
5:E:3:ASP:O	5:E:6:ARG:HG3	2.17	0.45
8:H:10:PHE:CE2	8:H:38:LEU:HB2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:59:DA:OP2	20:c:75:LYS:NZ	2.50	0.45
20:c:61:GLU:O	20:c:64:GLU:HG3	2.17	0.45
1:A:408:ARG:HG3	1:A:431:TRP:CE2	2.52	0.44
1:A:553:TRP:CE2	11:K:62:LYS:HB2	2.51	0.44
1:A:563:GLN:HB3	8:H:97:PHE:CE2	2.51	0.44
1:A:919:ASP:O	1:A:923:ASP:HB2	2.17	0.44
1:A:1211:MET:HB2	1:A:1238:LEU:HD13	1.99	0.44
2:B:628:ARG:HH22	2:B:743:ILE:N	2.15	0.44
2:B:835:GLN:O	2:B:838:SER:OG	2.35	0.44
3:C:23:ASP:OD1	3:C:226:ASN:ND2	2.40	0.44
4:D:64:LEU:HB3	4:D:89:LEU:HD22	1.99	0.44
14:N:44:DT:H2"	14:N:45:DT:C6	2.52	0.44
15:O:507:TRP:CH2	15:O:521:LEU:HB2	2.52	0.44
15:O:625:CYS:HB3	15:O:788:ILE:HD12	1.98	0.44
15:O:658:LYS:HG2	15:O:687:PHE:HZ	1.81	0.44
15:O:760:TRP:O	15:O:799:ARG:NH2	2.51	0.44
1:A:727:ARG:HA	1:A:765:CYS:SG	2.57	0.44
2:B:283:VAL:HG11	2:B:292:HIS:HE1	1.82	0.44
2:B:323:LEU:HD21	2:B:346:LYS:HE2	1.97	0.44
2:B:1172:ILE:HD11	2:B:1183:ARG:HE	1.82	0.44
3:C:15:ASP:OD1	3:C:234:THR:OG1	2.34	0.44
3:C:47:LEU:HB3	12:L:68:GLN:HE21	1.82	0.44
7:G:44:TYR:HE2	7:G:106:LEU:HD23	1.82	0.44
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.98	0.44
15:O:555:LEU:O	15:O:559:ILE:HG12	2.17	0.44
18:e:72:ARG:NH2	18:e:84:PHE:H	2.12	0.44
1:A:605:GLY:HA3	1:A:615:PHE:HE1	1.81	0.44
1:A:656:TYR:O	1:A:660:HIS:ND1	2.35	0.44
1:A:709:MET:HG2	1:A:714:SER:OG	2.16	0.44
1:A:841:ARG:NH2	1:A:1104:LYS:HZ3	2.16	0.44
1:A:1152:THR:HG22	1:A:1197:LEU:HB2	1.99	0.44
2:B:20:VAL:HG11	2:B:631:PHE:CE1	2.52	0.44
2:B:476:LEU:HD12	2:B:487:HIS:ND1	2.33	0.44
2:B:594:ARG:HG2	2:B:598:ARG:NE	2.32	0.44
2:B:839:MET:HE1	2:B:988:GLY:C	2.43	0.44
2:B:1039:GLY:HA2	10:J:50:LEU:HD22	1.99	0.44
5:E:81:PHE:CE1	5:E:110:ILE:HB	2.53	0.44
14:N:-74:DT:H2"	14:N:-73:DT:C6	2.52	0.44
20:c:87:ILE:HD12	20:c:97:LEU:HD12	1.98	0.44
19:f:71:THR:HG22	21:h:96:THR:OG1	2.17	0.44
1:A:21:LEU:H	1:A:230:ALA:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:MET:HG3	1:A:511:GLN:HB3	1.99	0.44
2:B:99:MET:HE1	2:B:111:TYR:CD1	2.52	0.44
2:B:400:ASP:CG	2:B:404:PRO:HB2	2.42	0.44
2:B:489:ARG:NH2	2:B:531:ASN:HD21	2.15	0.44
2:B:515:VAL:HG21	2:B:530:LYS:HD2	1.99	0.44
2:B:1147:LEU:O	2:B:1151:LEU:HG	2.18	0.44
18:e:100:LEU:HD11	19:f:58:LEU:HD13	1.99	0.44
20:g:81:ARG:NH1	20:g:107:VAL:O	2.42	0.44
1:A:89:PRO:O	1:A:205:PRO:HG2	2.18	0.44
1:A:709:MET:O	1:A:714:SER:OG	2.36	0.44
1:A:735:GLU:HA	1:A:738:LEU:HG	1.99	0.44
1:A:830:VAL:HG22	2:B:500:LYS:HZ2	1.83	0.44
1:A:962:LEU:HD12	1:A:1027:ARG:HG3	2.00	0.44
2:B:208:ARG:NH1	2:B:469:ARG:HH12	2.15	0.44
2:B:649:LYS:HE2	2:B:653:ARG:HH22	1.81	0.44
2:B:907:GLY:HA3	2:B:943:SER:O	2.17	0.44
3:C:48:VAL:HB	12:L:69:PHE:HB2	1.99	0.44
8:H:92:TYR:HA	8:H:144:ARG:HG2	2.00	0.44
10:J:1:MET:HE3	10:J:55:LEU:HD12	2.00	0.44
10:J:21:TYR:O	10:J:25:LEU:HG	2.17	0.44
19:b:99:GLY:HA2	21:h:60:GLY:C	2.42	0.44
20:c:50:TYR:OH	21:d:111:VAL:HA	2.18	0.44
20:c:114:VAL:HG23	20:c:115:LEU:HG	2.00	0.44
1:A:231:ARG:HB2	1:A:234:TRP:CD1	2.53	0.44
1:A:231:ARG:HB3	1:A:233:GLU:OE1	2.17	0.44
1:A:466:TYR:CE1	2:B:976:ILE:HD12	2.53	0.44
1:A:945:ARG:NE	1:A:1301:TYR:OH	2.41	0.44
2:B:338:ARG:N	13:M:75:ASP:OD1	2.51	0.44
2:B:557:GLU:OE1	2:B:567:HIS:NE2	2.51	0.44
5:E:7:ILE:HG23	5:E:10:ARG:NH2	2.30	0.44
10:J:1:MET:HB3	10:J:55:LEU:HB2	1.99	0.44
11:K:19:LEU:HD12	11:K:35:PHE:HE1	1.82	0.44
20:c:109:PRO:HA	18:e:55:GLN:HG2	2.00	0.44
18:e:63:ARG:HG3	18:e:66:PRO:HD2	1.99	0.44
1:A:70:CYS:HB2	2:B:1173:ALA:O	2.18	0.44
1:A:397:PRO:HB2	1:A:404:LYS:HD3	1.99	0.44
1:A:547:VAL:HG21	1:A:573:TRP:CG	2.53	0.44
1:A:580:SER:OG	1:A:612:LYS:HA	2.18	0.44
1:A:738:LEU:HD22	1:A:742:ASN:ND2	2.33	0.44
1:A:883:THR:HB	1:A:954:HIS:NE2	2.33	0.44
1:A:1198:GLU:HA	1:A:1239:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:GLU:HA	2:B:367:LYS:HG3	2.00	0.44
2:B:491:THR:OG1	2:B:530:LYS:O	2.30	0.44
2:B:550:PHE:CD2	2:B:602:ILE:HG12	2.51	0.44
2:B:1074:ASN:OD1	2:B:1077:THR:N	2.51	0.44
5:E:98:ARG:O	5:E:101:GLU:HG2	2.18	0.44
5:E:181:ASP:OD1	5:E:182:PRO:HD2	2.17	0.44
14:N:21:DG:H2'	14:N:22:DT:H71	1.98	0.44
18:a:46:VAL:HG13	18:a:49:ARG:HH12	1.82	0.44
21:d:61:ILE:HG13	19:f:99:GLY:HA2	1.99	0.44
1:A:270:ILE:CD1	1:A:304:TYR:HB2	2.46	0.44
1:A:565:ALA:HB1	8:H:96:MET:HE3	1.99	0.44
1:A:943:PHE:HA	1:A:947:ILE:HD13	2.00	0.44
1:A:1149:THR:HA	1:A:1199:LEU:HD23	2.00	0.44
1:A:1348:ARG:HB2	1:A:1379:THR:HG21	2.00	0.44
2:B:157:HIS:NE2	2:B:159:GLY:O	2.50	0.44
2:B:520:THR:OG1	2:B:527:GLY:N	2.30	0.44
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.44
15:O:672:LEU:HD13	15:O:674:PHE:HZ	1.83	0.44
17:T:-34:DG:H2''	17:T:-33:DA:N7	2.32	0.44
17:T:37:DC:H2''	17:T:38:DA:C8	2.53	0.44
19:b:92:ARG:NE	21:d:76:GLU:OE2	2.50	0.44
1:A:141:LEU:O	1:A:144:THR:OG1	2.33	0.44
1:A:285:SER:HB2	1:A:290:ILE:HG13	2.00	0.44
1:A:407:ILE:N	1:A:432:LYS:O	2.38	0.44
1:A:843:VAL:HG11	2:B:1136:ASP:OD2	2.17	0.44
2:B:63:GLN:NE2	2:B:69:ASP:OD2	2.51	0.44
2:B:490:ARG:HH21	2:B:531:ASN:CG	2.25	0.44
2:B:572:ARG:HH12	2:B:615:ARG:NE	2.16	0.44
2:B:579:TRP:CZ2	2:B:582:ILE:HD11	2.53	0.44
2:B:647:ILE:HG13	2:B:651:HIS:HB2	2.00	0.44
2:B:648:THR:O	2:B:652:ILE:HG12	2.18	0.44
2:B:796:LEU:HD23	2:B:799:PRO:HA	2.00	0.44
3:C:32:LEU:HB3	3:C:36:MET:HE1	1.99	0.44
7:G:38:CYS:SG	7:G:39:THR:N	2.91	0.44
12:L:31:TYR:HD2	12:L:41:SER:HA	1.83	0.44
14:N:-28:DC:H42	17:T:28:DG:H1	1.66	0.44
15:O:255:ARG:HG2	15:O:377:PRO:HB3	2.00	0.44
15:O:719:GLN:HA	15:O:722:VAL:HB	1.99	0.44
21:d:76:GLU:HB2	21:d:97:ALA:HB1	1.99	0.44
1:A:338:ARG:HA	1:A:342:MET:HG2	1.99	0.43
1:A:589:LEU:HD21	1:A:633:THR:HG21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:ILE:HA	1:A:634:VAL:HG12	2.00	0.43
1:A:691:VAL:HG11	1:A:795:PRO:HG3	2.00	0.43
1:A:709:MET:HG3	1:A:713:GLU:OE1	2.17	0.43
1:A:822:ARG:HD3	2:B:507:LEU:H	1.83	0.43
1:A:968:ASN:HA	1:A:971:GLN:HE21	1.83	0.43
1:A:1437:ALA:O	1:A:1442:GLY:HA3	2.18	0.43
2:B:77:ILE:HG13	2:B:121:LYS:HD3	2.00	0.43
2:B:357:ILE:HG12	2:B:578:VAL:HG23	2.00	0.43
2:B:559:LEU:HD22	2:B:579:TRP:CE2	2.53	0.43
2:B:1150:ARG:HA	2:B:1154:ALA:HB3	2.00	0.43
5:E:196:LYS:HE3	5:E:208:ALA:HA	2.00	0.43
15:O:244:ILE:HB	15:O:373:HIS:CD2	2.51	0.43
19:b:26:ILE:HD13	19:b:59:LYS:HD2	2.00	0.43
1:A:147:VAL:HG23	1:A:171:THR:HA	2.00	0.43
1:A:218:GLU:HG3	1:A:222:ARG:HH11	1.83	0.43
1:A:608:ILE:HA	1:A:613:VAL:HA	1.99	0.43
1:A:699:GLN:HA	9:I:97:MET:O	2.18	0.43
1:A:775:ARG:HH11	1:A:798:LYS:HZ3	1.63	0.43
1:A:981:SER:HA	1:A:1038:ARG:NH2	2.32	0.43
1:A:985:ILE:N	1:A:986:PRO:HD2	2.32	0.43
1:A:1102:ARG:O	1:A:1106:ILE:HG12	2.18	0.43
1:A:1415:ALA:O	1:A:1419:ALA:N	2.51	0.43
2:B:42:MET:HE1	2:B:163:ILE:HD12	1.99	0.43
2:B:588:MET:SD	2:B:589:LEU:N	2.91	0.43
2:B:1187:ASN:ND2	2:B:1190:ASN:HB3	2.28	0.43
8:H:93:ASP:N	8:H:143:ILE:O	2.29	0.43
17:T:4:DC:H2"	17:T:5:DC:OP2	2.18	0.43
18:a:41:TYR:CD2	18:a:45:THR:HB	2.53	0.43
1:A:148:CYS:HB3	1:A:170:ASN:O	2.19	0.43
1:A:482:ASP:HA	2:B:836:GLU:CG	2.48	0.43
1:A:768:GLN:HG2	1:A:775:ARG:HH21	1.82	0.43
1:A:967:GLN:NE2	1:A:970:GLN:OE1	2.51	0.43
1:A:1009:ILE:HG13	5:E:166:ARG:HH21	1.83	0.43
1:A:1316:LEU:O	1:A:1320:MET:HB2	2.18	0.43
2:B:458:ASN:HA	2:B:469:ARG:O	2.18	0.43
2:B:469:ARG:HH21	2:B:494:PRO:HG3	1.83	0.43
2:B:535:LEU:HD13	2:B:743:ILE:HD12	2.00	0.43
2:B:695:GLU:HA	2:B:698:ILE:HG12	2.01	0.43
2:B:848:ARG:NH2	10:J:10:CYS:O	2.50	0.43
2:B:872:GLU:CD	2:B:914:LYS:HD3	2.43	0.43
7:G:56:VAL:HG12	7:G:72:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:246:ASP:OD1	15:O:255:ARG:NH1	2.38	0.43
15:O:514:PHE:CE2	15:O:517:ARG:HB2	2.52	0.43
17:T:3:DT:H2''	17:T:4:DC:H5'	2.01	0.43
18:a:67:PHE:HE1	19:b:58:LEU:HD11	1.83	0.43
20:c:79:ILE:HG12	20:c:82:HIS:CE1	2.53	0.43
1:A:1118:LEU:HD21	1:A:1314:ILE:HG12	2.00	0.43
1:A:1260:ASP:OD2	9:I:44:TYR:OH	2.34	0.43
1:A:1452:LEU:O	1:A:1455:SER:OG	2.32	0.43
2:B:41:PHE:CE2	2:B:46:ILE:HD11	2.53	0.43
2:B:229:ALA:HB1	2:B:374:MET:SD	2.59	0.43
2:B:756:ILE:HD11	2:B:770:GLN:HE21	1.83	0.43
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.59	0.43
5:E:8:ILE:HD13	5:E:42:ARG:HD3	1.99	0.43
5:E:134:PHE:HA	5:E:185:ARG:HH22	1.83	0.43
15:O:371:GLU:HA	15:O:374:ARG:HG2	1.99	0.43
17:T:8:DC:P	19:f:35:ARG:HH12	2.41	0.43
1:A:36:GLU:C	1:A:271:LEU:HD21	2.44	0.43
1:A:183:TRP:HA	1:A:201:LYS:O	2.18	0.43
1:A:520:PRO:O	1:A:625:SER:HB3	2.19	0.43
1:A:666:GLY:HA3	2:B:1069:PHE:CE1	2.53	0.43
1:A:1061:HIS:CE1	6:F:87:LYS:H	2.37	0.43
2:B:33:GLN:OE1	2:B:33:GLN:N	2.48	0.43
2:B:288:GLU:OE1	9:I:11:ASN:ND2	2.51	0.43
2:B:476:LEU:HA	2:B:487:HIS:CE1	2.53	0.43
2:B:634:GLU:CD	2:B:646:ARG:HE	2.23	0.43
5:E:57:MET:HE3	5:E:57:MET:HB3	1.87	0.43
14:N:-22:DG:H1'	14:N:-21:DG:C8	2.53	0.43
15:O:556:LYS:O	15:O:560:SER:CB	2.66	0.43
17:T:5:DC:H1'	17:T:6:DC:C2	2.54	0.43
18:a:94:GLU:HB3	19:b:97:LEU:HD21	2.01	0.43
1:A:333:LYS:HD2	17:T:58:DG:OP2	2.18	0.43
1:A:362:LEU:HD22	1:A:647:PHE:HD2	1.83	0.43
1:A:473:LEU:O	1:A:476:THR:OG1	2.26	0.43
1:A:580:SER:OG	1:A:612:LYS:HD2	2.19	0.43
1:A:593:ASP:HB2	1:A:605:GLY:H	1.81	0.43
1:A:769:GLN:OE1	1:A:817:HIS:ND1	2.40	0.43
1:A:785:LEU:HB2	1:A:788:PHE:CD2	2.54	0.43
1:A:1358:VAL:O	1:A:1361:PHE:HB3	2.18	0.43
2:B:872:GLU:OE1	2:B:916:THR:OG1	2.32	0.43
2:B:963:PHE:HE2	2:B:965:LYS:CE	2.32	0.43
5:E:150:PRO:HG2	5:E:152:HIS:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-4:DG:N2	17:T:5:DC:O2	2.52	0.43
14:N:53:DC:N4	17:T:-53:DG:H1	2.17	0.43
15:O:383:ILE:HG22	15:O:388:GLY:HA2	2.01	0.43
15:O:582:VAL:HG13	15:O:785:ARG:HB2	1.99	0.43
19:b:75:HIS:CG	21:d:96:THR:HG21	2.54	0.43
1:A:317:GLN:N	1:A:321:ARG:O	2.43	0.43
1:A:369:ILE:HD11	1:A:400:HIS:CB	2.49	0.43
1:A:1287:MET:HE3	1:A:1307:TRP:CE3	2.53	0.43
1:A:1387:ILE:O	1:A:1387:ILE:HG22	2.19	0.43
5:E:45:ILE:HD12	5:E:57:MET:HB2	2.00	0.43
8:H:102:LYS:HE3	8:H:114:TYR:CD1	2.53	0.43
14:N:-79:DG:O6	17:T:78:DC:N4	2.52	0.43
15:O:297:PRO:HB3	15:O:348:TYR:CE1	2.54	0.43
15:O:326:ILE:HG13	15:O:513:ILE:HD13	2.00	0.43
1:A:57:LYS:HA	1:A:68:GLN:HB2	2.01	0.43
1:A:551:LEU:HD22	1:A:557:TRP:NE1	2.34	0.43
1:A:761:GLN:HB3	1:A:805:TYR:CE2	2.53	0.43
1:A:1019:LEU:HD12	5:E:203:THR:C	2.44	0.43
2:B:286:ASP:HA	2:B:289:ILE:HD12	2.00	0.43
2:B:866:PHE:CZ	2:B:916:THR:HG23	2.53	0.43
2:B:1069:PHE:HB2	3:C:201:TRP:HH2	1.84	0.43
3:C:5:PRO:HD2	11:K:100:THR:HG21	2.00	0.43
3:C:61:PHE:O	3:C:65:ARG:HG3	2.19	0.43
3:C:262:LEU:HD11	11:K:87:LEU:HG	2.00	0.43
5:E:197:ILE:HB	5:E:209:SER:OG	2.19	0.43
13:M:45:GLY:O	13:M:57:GLN:NE2	2.38	0.43
15:O:246:ASP:CG	15:O:255:ARG:HH12	2.26	0.43
15:O:256:LEU:HD11	15:O:278:TRP:CZ3	2.54	0.43
21:h:76:GLU:O	21:h:79:ARG:HG2	2.19	0.43
1:A:408:ARG:HG3	1:A:431:TRP:CZ2	2.54	0.43
1:A:717:GLY:C	1:A:721:ARG:HE	2.27	0.43
1:A:785:LEU:HD23	1:A:785:LEU:HA	1.81	0.43
2:B:111:TYR:OH	2:B:170:CYS:SG	2.64	0.43
2:B:305:MET:O	2:B:308:PRO:HD2	2.18	0.43
2:B:632:ILE:HA	2:B:740:HIS:CD2	2.54	0.43
2:B:935:ARG:NH1	2:B:936:ASP:HB3	2.33	0.43
3:C:120:LYS:HZ1	3:C:128:ASN:HA	1.84	0.43
5:E:64:THR:HB	5:E:66:GLU:OE1	2.19	0.43
8:H:46:MET:SD	8:H:94:TYR:HE1	2.42	0.43
11:K:31:ILE:HG13	11:K:33:ILE:HD11	2.00	0.43
14:N:19:DC:H6	14:N:19:DC:H2'	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:26:DG:H4'	17:T:27:DG:H5'	2.00	0.43
17:T:52:DG:H2''	17:T:53:DA:C8	2.53	0.43
17:T:62:DA:C2'	17:T:63:DA:H5'	2.49	0.43
1:A:691:VAL:O	1:A:695:ILE:HG13	2.19	0.43
1:A:799:GLY:HA2	1:A:816:PHE:CD2	2.53	0.43
1:A:824:GLY:O	1:A:828:THR:HG23	2.19	0.43
1:A:994:ASP:O	1:A:998:LYS:HG2	2.18	0.43
1:A:1143:THR:HG22	1:A:1276:LEU:HB2	2.01	0.43
1:A:1292:VAL:HG11	1:A:1306:LEU:HD12	2.01	0.43
1:A:1352:TYR:HE1	1:A:1356:LEU:HD12	1.84	0.43
1:A:1367:ASN:OD1	1:A:1369:ARG:HG2	2.19	0.43
2:B:290:LEU:HD13	9:I:6:PHE:CE2	2.44	0.43
2:B:544:SER:O	2:B:548:ILE:HG12	2.18	0.43
2:B:597:ARG:NE	2:B:604:PRO:O	2.44	0.43
2:B:987:LYS:HG2	2:B:1020:ARG:NH2	2.32	0.43
3:C:183:HIS:HB2	3:C:185:LYS:CG	2.49	0.43
5:E:9:SER:HB2	5:E:13:ARG:NH1	2.34	0.43
8:H:13:GLN:HE21	8:H:29:ILE:HG22	1.83	0.43
15:O:259:TRP:CD1	15:O:377:PRO:HG2	2.54	0.43
15:O:658:LYS:HG2	15:O:687:PHE:CZ	2.53	0.43
18:a:62:ILE:HG13	19:b:37:LEU:HD11	2.01	0.43
21:d:90:THR:N	21:d:93:GLU:OE1	2.52	0.43
1:A:810:THR:HG23	1:A:813:GLU:H	1.84	0.42
2:B:9:ASP:HA	2:B:648:THR:HB	2.01	0.42
2:B:22:SER:HA	2:B:25:PHE:HD1	1.83	0.42
2:B:273:PRO:HD2	2:B:276:ILE:HD12	2.01	0.42
2:B:642:LYS:HE2	2:B:737:THR:HG22	2.01	0.42
5:E:170:LYS:HD3	5:E:171:GLU:HG3	1.99	0.42
7:G:163:ILE:O	7:G:163:ILE:HG22	2.20	0.42
8:H:8:ASP:HB3	8:H:10:PHE:HE1	1.84	0.42
11:K:107:GLU:O	11:K:111:ILE:HG23	2.19	0.42
15:O:362:ALA:HB3	17:T:78:DC:H5'	2.00	0.42
15:O:595:TYR:O	15:O:599:LEU:HB2	2.19	0.42
15:O:639:SER:HA	15:O:645:TYR:CD2	2.54	0.42
17:T:-36:DT:H2''	17:T:-35:DA:N7	2.34	0.42
21:d:45:LEU:O	21:d:49:HIS:N	2.43	0.42
18:e:100:LEU:HD11	19:f:58:LEU:HD22	2.01	0.42
20:g:29:ARG:HD2	21:h:37:TYR:HE2	1.84	0.42
1:A:830:VAL:HG12	1:A:834:GLU:OE2	2.19	0.42
1:A:1400:LEU:HD21	1:A:1432:MET:HE3	2.01	0.42
2:B:177:GLU:O	2:B:181:TYR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:ILE:H	3:C:10:ILE:HD12	1.83	0.42
15:O:718:ARG:O	15:O:721:LEU:HG	2.20	0.42
15:O:777:GLN:NE2	15:O:778:LYS:HG2	2.34	0.42
18:a:89:VAL:HA	18:a:92:LEU:HD12	2.01	0.42
20:c:61:GLU:HA	20:c:64:GLU:HG3	2.00	0.42
1:A:1447:MET:HE1	6:F:135:ARG:HE	1.84	0.42
2:B:356:HIS:HD2	2:B:578:VAL:HB	1.83	0.42
2:B:478:ARG:HH11	2:B:782:LEU:HD11	1.84	0.42
2:B:645:LEU:HD23	2:B:645:LEU:HA	1.78	0.42
2:B:806:THR:O	2:B:809:MET:HB3	2.19	0.42
5:E:54:ARG:HG3	5:E:112:GLN:NE2	2.33	0.42
5:E:171:GLU:O	5:E:212:ILE:HD13	2.20	0.42
6:F:76:LYS:HA	6:F:79:ARG:HG3	2.02	0.42
9:I:19:ASP:O	9:I:23:GLN:N	2.48	0.42
11:K:45:LEU:HG	11:K:94:ILE:HD13	2.01	0.42
14:N:38:DG:H2"	14:N:39:DA:H8	1.84	0.42
14:N:65:DA:H2"	14:N:66:DT:H72	2.02	0.42
15:O:315:LEU:HD21	15:O:327:LEU:HD22	2.00	0.42
15:O:722:VAL:O	15:O:726:ASN:ND2	2.52	0.42
18:a:67:PHE:CZ	19:b:62:LEU:HD21	2.54	0.42
18:e:62:ILE:HG21	18:e:67:PHE:HB2	2.01	0.42
1:A:587:ILE:O	1:A:611:GLY:N	2.51	0.42
1:A:801:VAL:HG12	1:A:803:ASN:H	1.83	0.42
1:A:880:GLU:O	1:A:957:PRO:HA	2.19	0.42
2:B:91:GLU:OE2	2:B:91:GLU:N	2.40	0.42
2:B:398:ARG:HH22	2:B:620:PHE:HB3	1.84	0.42
2:B:464:LYS:HD2	2:B:464:LYS:O	2.19	0.42
2:B:788:ARG:C	2:B:789:MET:HE2	2.44	0.42
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.54	0.42
3:C:65:ARG:CZ	10:J:5:VAL:HG23	2.49	0.42
5:E:58:SER:HA	5:E:79:VAL:O	2.18	0.42
5:E:126:VAL:O	5:E:126:VAL:HG12	2.19	0.42
11:K:55:ASP:HB2	11:K:78:GLU:HG2	2.01	0.42
14:N:70:DG:H2"	14:N:71:DA:C8	2.54	0.42
15:O:739:ARG:HA	15:O:739:ARG:HD2	1.76	0.42
18:e:85:GLN:N	19:f:81:VAL:O	2.53	0.42
1:A:77:CYS:SG	1:A:246:GLN:NE2	2.92	0.42
1:A:142:CYS:HA	1:A:145:LYS:HZ3	1.85	0.42
1:A:738:LEU:HD11	1:A:759:ILE:HD13	2.00	0.42
1:A:849:ILE:HG21	1:A:1373:LEU:HD11	2.00	0.42
1:A:1076:GLU:O	1:A:1079:THR:OG1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:LYS:HE2	1:A:1104:LYS:CA	2.48	0.42
1:A:1223:SER:OG	1:A:1224:ASP:N	2.50	0.42
2:B:850:LEU:HG	2:B:851:PHE:CD2	2.55	0.42
2:B:903:VAL:HG23	2:B:905:VAL:HG13	2.02	0.42
3:C:120:LYS:NZ	3:C:128:ASN:HA	2.34	0.42
5:E:2:GLU:OE1	5:E:2:GLU:N	2.52	0.42
6:F:81:THR:OG1	6:F:144:GLU:OE1	2.37	0.42
7:G:149:GLY:HA3	7:G:160:ILE:HD13	2.01	0.42
8:H:59:LEU:HD22	8:H:139:LEU:HD11	2.01	0.42
8:H:96:MET:HB3	8:H:141:ILE:CG2	2.49	0.42
10:J:14:VAL:HG11	10:J:48:MET:CE	2.49	0.42
13:M:17:GLN:NE2	14:N:-48:DC:H3'	2.34	0.42
15:O:369:CYS:HG	15:O:373:HIS:CD2	2.37	0.42
21:d:103:PRO:HD2	21:d:106:LEU:HD23	2.01	0.42
1:A:337:LEU:HD13	1:A:1404:SER:HA	2.01	0.42
1:A:842:LEU:HD11	1:A:1107:LEU:HD21	2.01	0.42
1:A:1359:ILE:HD13	1:A:1366:VAL:HB	2.00	0.42
2:B:18:TRP:HZ3	2:B:747:MET:HE3	1.84	0.42
2:B:38:PHE:CE2	2:B:42:MET:HE3	2.54	0.42
2:B:301:GLN:O	2:B:304:GLU:HG3	2.19	0.42
2:B:369:PHE:CE2	2:B:560:GLU:HG3	2.55	0.42
3:C:115:SER:HA	3:C:144:LEU:HD11	2.01	0.42
3:C:171:SER:OG	3:C:173:CYS:O	2.38	0.42
3:C:250:THR:O	3:C:253:GLU:HG3	2.20	0.42
5:E:115:ILE:HD12	5:E:120:ASN:HD21	1.85	0.42
14:N:-13:DA:H5''	18:e:63:ARG:CZ	2.50	0.42
1:A:19:PHE:HD2	1:A:1415:ALA:HB1	1.84	0.42
1:A:852:HIS:CD2	1:A:858:ARG:HD2	2.55	0.42
2:B:27:GLU:HB3	2:B:678:TRP:HB3	2.01	0.42
2:B:290:LEU:HD21	2:B:306:LEU:HD11	2.01	0.42
2:B:299:ASP:OD2	2:B:385:ARG:NH1	2.52	0.42
2:B:336:ILE:HD11	2:B:341:ARG:HG3	2.00	0.42
2:B:1160:VAL:HG11	2:B:1201:LYS:HD2	2.01	0.42
2:B:1204:PHE:CE2	2:B:1216:LEU:HD11	2.55	0.42
3:C:29:ALA:HB1	3:C:178:PHE:HE2	1.85	0.42
3:C:59:ASP:HA	3:C:62:ILE:HG12	2.02	0.42
3:C:73:SER:HB3	3:C:76:VAL:HB	2.01	0.42
5:E:55:LYS:HG3	5:E:56:LEU:HD12	2.02	0.42
5:E:115:ILE:HD13	5:E:133:THR:HG21	2.00	0.42
11:K:108:GLU:O	11:K:112:LYS:HB2	2.19	0.42
1:A:110:CYS:SG	1:A:167:GLY:HA2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:HA	1:A:234:TRP:CE3	2.54	0.42
1:A:672:ALA:HB1	1:A:737:ASN:ND2	2.35	0.42
1:A:732:ARG:O	1:A:736:MET:HG2	2.20	0.42
1:A:1065:MET:SD	1:A:1439:MET:HE2	2.59	0.42
1:A:1400:LEU:HD22	1:A:1429:GLU:CD	2.44	0.42
2:B:455:ALA:HB1	17:T:67:DA:H4'	2.01	0.42
2:B:503:LYS:HG2	2:B:504:PRO:HD3	2.02	0.42
2:B:639:LYS:O	2:B:642:LYS:HB3	2.20	0.42
2:B:805:LYS:CD	2:B:809:MET:HE2	2.50	0.42
4:D:154:ASP:HA	4:D:157:ILE:HG12	2.02	0.42
5:E:66:GLU:CD	5:E:66:GLU:H	2.27	0.42
8:H:109:ASP:O	8:H:110:LYS:HD2	2.20	0.42
11:K:35:PHE:HB3	11:K:38:GLU:HG3	2.00	0.42
15:O:578:LYS:NZ	15:O:769:ARG:HD3	2.35	0.42
17:T:-39:DT:H2''	17:T:-38:DC:C5	2.55	0.42
1:A:665:ILE:HD12	1:A:743:ASN:HB2	2.01	0.42
1:A:963:ARG:O	1:A:967:GLN:HG2	2.19	0.42
1:A:1262:MET:SD	1:A:1263:LEU:N	2.93	0.42
1:A:1287:MET:HG3	1:A:1307:TRP:CZ3	2.54	0.42
2:B:18:TRP:CZ3	2:B:747:MET:HE3	2.55	0.42
2:B:390:ASP:OD1	2:B:391:ARG:N	2.53	0.42
4:D:61:ARG:NH2	4:D:84:ILE:O	2.35	0.42
4:D:122:THR:O	4:D:126:GLN:OE1	2.37	0.42
8:H:57:VAL:HG22	8:H:143:ILE:HD12	2.01	0.42
10:J:7:CYS:HA	10:J:48:MET:SD	2.60	0.42
15:O:629:ASP:HB2	15:O:650:LYS:HZ2	1.85	0.42
17:T:8:DC:H2''	17:T:9:DG:C8	2.55	0.42
18:a:71:VAL:HG13	19:b:66:ILE:HD11	2.01	0.42
1:A:527:ASP:OD1	2:B:1015:HIS:HE1	2.02	0.42
1:A:599:LEU:HD21	8:H:39:THR:HG21	2.01	0.42
1:A:766:VAL:HG22	1:A:805:TYR:CE2	2.55	0.42
1:A:839:GLN:O	1:A:843:VAL:HG23	2.20	0.42
1:A:1129:ASP:OD1	1:A:1130:ILE:N	2.53	0.42
1:A:1258:GLU:HG3	9:I:30:ARG:NH2	2.34	0.42
2:B:118:ASP:HA	2:B:154:ASN:O	2.20	0.42
2:B:431:THR:HB	2:B:433:ARG:HG2	2.02	0.42
2:B:634:GLU:HG3	2:B:639:LYS:HD2	2.01	0.42
2:B:798:TYR:HB2	2:B:821:GLN:HE21	1.85	0.42
2:B:1182:CYS:HB3	2:B:1187:ASN:HB3	2.02	0.42
3:C:71:LEU:HD23	3:C:132:PRO:HA	2.02	0.42
3:C:241:ASN:HD22	11:K:109:TRP:NE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:92:TYR:CD1	8:H:142:LEU:HB3	2.55	0.42
15:O:629:ASP:H	15:O:650:LYS:HZ1	1.68	0.42
1:A:273:ALA:HA	1:A:276:ASN:HD22	1.85	0.41
1:A:509:PRO:HG2	1:A:641:LYS:NZ	2.35	0.41
2:B:60:GLN:HE22	2:B:432:ASP:CG	2.28	0.41
2:B:166:ARG:NH2	2:B:190:MET:O	2.53	0.41
2:B:484:THR:O	2:B:488:LEU:HG	2.20	0.41
11:K:20:LYS:HB3	11:K:34:LYS:HB3	2.02	0.41
15:O:475:PRO:HG3	15:O:507:TRP:HZ3	1.85	0.41
15:O:721:LEU:O	15:O:724:VAL:HG12	2.20	0.41
15:O:751:ASN:HB2	15:O:779:LYS:HZ2	1.85	0.41
20:c:18:SER:HA	20:c:26:PRO:HA	2.02	0.41
20:c:77:ARG:HG2	21:d:53:GLY:HA3	2.01	0.41
18:e:99:TYR:HA	19:f:95:ARG:HH22	1.84	0.41
1:A:4:PHE:HB3	2:B:1159:ARG:NH2	2.35	0.41
1:A:126:ILE:HD12	1:A:222:ARG:HB2	2.03	0.41
1:A:299:PHE:O	1:A:303:THR:HG23	2.20	0.41
1:A:473:LEU:HD12	1:A:474:SER:N	2.34	0.41
1:A:482:ASP:OD1	1:A:482:ASP:N	2.50	0.41
1:A:692:GLN:HA	1:A:695:ILE:HD12	2.02	0.41
1:A:752:SER:O	1:A:753:LYS:HE2	2.20	0.41
1:A:861:LEU:HD23	5:E:173:GLN:HG2	2.02	0.41
1:A:1117:ALA:N	1:A:1333:ASN:HD21	2.18	0.41
2:B:559:LEU:HD21	2:B:581:GLY:H	1.85	0.41
2:B:786:ASN:HB3	2:B:951:GLN:HE22	1.85	0.41
2:B:1119:VAL:HB	2:B:1124:ARG:NE	2.35	0.41
6:F:78:GLU:O	6:F:80:THR:HG23	2.20	0.41
9:I:71:SER:HB3	9:I:85:PHE:CE1	2.55	0.41
15:O:278:TRP:CD2	15:O:378:PRO:HB3	2.56	0.41
15:O:609:GLN:HE22	15:O:611:LYS:CB	2.33	0.41
15:O:627:HIS:CE1	15:O:630:LEU:HD13	2.55	0.41
17:T:34:DA:H2"	17:T:35:DC:C6	2.56	0.41
18:a:128:ARG:NH2	19:b:57:VAL:HG13	2.34	0.41
19:f:73:THR:OG1	19:f:81:VAL:HG22	2.20	0.41
1:A:114:LEU:HA	1:A:165:ARG:NH2	2.35	0.41
1:A:187:LYS:NZ	1:A:195:ASP:HB2	2.35	0.41
1:A:544:TYR:HD2	8:H:78:TRP:HZ3	1.68	0.41
1:A:715:PHE:CZ	1:A:793:PHE:HB3	2.56	0.41
1:A:852:HIS:HB3	6:F:139:PRO:HD3	2.02	0.41
1:A:1219:SER:OG	1:A:1228:VAL:HG21	2.21	0.41
2:B:409:LEU:HD23	2:B:450:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:490:ARG:HH21	2:B:531:ASN:HB2	1.86	0.41
2:B:897:GLY:O	2:B:912:ILE:HD12	2.20	0.41
3:C:5:PRO:HD3	11:K:97:LYS:NZ	2.35	0.41
3:C:112:ASP:HB3	3:C:114:TYR:CE2	2.55	0.41
3:C:118:LEU:HB2	3:C:132:PRO:HG3	2.02	0.41
5:E:57:MET:HE1	5:E:81:PHE:CD2	2.56	0.41
8:H:23:VAL:HA	8:H:42:ILE:O	2.20	0.41
9:I:15:TYR:CD2	9:I:30:ARG:HG2	2.55	0.41
17:T:25:DG:H4'	17:T:26:DG:H5'	2.02	0.41
19:b:71:THR:HG21	21:d:100:LEU:HG	2.01	0.41
1:A:108:MET:SD	1:A:170:ASN:HB3	2.60	0.41
1:A:601:PRO:HA	8:H:25:ARG:NH2	2.34	0.41
1:A:973:PHE:HB3	1:A:1040:ASN:HD21	1.85	0.41
1:A:1350:SER:HA	1:A:1353:LYS:HG2	2.02	0.41
2:B:14:THR:HG22	2:B:18:TRP:NE1	2.36	0.41
2:B:108:ASN:HB3	2:B:197:ASN:OD1	2.20	0.41
2:B:855:PHE:CZ	2:B:857:ARG:HB2	2.56	0.41
2:B:856:PHE:HB3	2:B:967:ARG:HE	1.85	0.41
2:B:952:VAL:HG13	2:B:966:VAL:HG22	2.02	0.41
2:B:1072:MET:HG2	2:B:1085:VAL:HB	2.02	0.41
5:E:16:ARG:O	5:E:20:GLU:HG3	2.20	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.95	0.41
14:N:-29:DT:H2''	14:N:-28:DC:C5	2.54	0.41
14:N:-16:DT:H4'	14:N:-15:DA:H5'	2.02	0.41
14:N:64:DG:H2''	14:N:65:DA:C8	2.55	0.41
15:O:466:LEU:HD13	15:O:512:PHE:CZ	2.56	0.41
1:A:473:LEU:HD22	2:B:835:GLN:OE1	2.20	0.41
1:A:778:PHE:HB3	1:A:783:ARG:N	2.35	0.41
1:A:870:GLY:HA3	1:A:1369:ARG:CZ	2.50	0.41
1:A:1009:ILE:HA	5:E:166:ARG:HH21	1.85	0.41
1:A:1372:ALA:HA	1:A:1375:VAL:HG22	2.02	0.41
2:B:17:CYS:SG	2:B:631:PHE:HE2	2.43	0.41
2:B:85:SER:O	2:B:113:SER:OG	2.28	0.41
2:B:365:THR:O	2:B:368:THR:OG1	2.26	0.41
2:B:827:ILE:CG2	2:B:1086:PHE:HB3	2.51	0.41
2:B:1060:ARG:NH2	2:B:1065:GLN:HA	2.36	0.41
4:D:53:LEU:HD13	4:D:114:ARG:HH22	1.85	0.41
5:E:183:VAL:HA	5:E:186:TYR:HB3	2.01	0.41
8:H:40:LEU:HD13	8:H:122:MET:HB2	2.03	0.41
10:J:12:LYS:HB2	10:J:42:ARG:NH2	2.35	0.41
11:K:7:PHE:HD2	11:K:11:ILE:HG13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:465:ILE:HG23	15:O:494:LEU:HD23	2.02	0.41
15:O:528:PHE:C	15:O:531:PRO:HD2	2.45	0.41
17:T:55:DA:C2'	17:T:56:DC:H5''	2.49	0.41
20:c:18:SER:OG	20:c:26:PRO:HB3	2.20	0.41
1:A:9:ALA:HB3	2:B:1193:GLN:HB3	2.02	0.41
1:A:344:LYS:HE2	2:B:1151:LEU:HD22	2.03	0.41
1:A:383:GLN:HA	1:A:429:TYR:CZ	2.55	0.41
1:A:542:ILE:HG21	1:A:550:MET:CE	2.50	0.41
1:A:735:GLU:OE1	1:A:756:PHE:HA	2.20	0.41
1:A:902:LEU:HG	1:A:927:GLN:OE1	2.20	0.41
1:A:909:ILE:HD11	1:A:913:VAL:HG21	2.02	0.41
1:A:1339:LEU:HA	1:A:1343:GLY:O	2.21	0.41
2:B:436:ASN:HB3	2:B:439:LEU:HD22	2.02	0.41
2:B:825:VAL:HA	2:B:1010:LEU:O	2.20	0.41
2:B:983:ARG:HG3	2:B:1093:GLN:HE22	1.86	0.41
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.49	0.41
2:B:1161:HIS:HE1	2:B:1175:LEU:HD11	1.86	0.41
8:H:24:SER:HB3	8:H:44:ASN:HD21	1.85	0.41
11:K:27:VAL:HG22	11:K:74:ARG:NH2	2.36	0.41
13:M:60:ILE:O	13:M:60:ILE:HG13	2.21	0.41
14:N:4:DG:H1'	14:N:5:DT:C2	2.56	0.41
15:O:246:ASP:HB2	15:O:381:VAL:O	2.19	0.41
15:O:256:LEU:HD11	15:O:278:TRP:HZ3	1.85	0.41
15:O:285:LYS:HD2	15:O:286:GLN:N	2.36	0.41
15:O:556:LYS:NZ	15:O:810:ILE:HG23	2.36	0.41
17:T:-26:DT:H2''	17:T:-25:DA:C8	2.56	0.41
17:T:-6:DT:H4'	17:T:-5:DA:H5'	2.03	0.41
1:A:599:LEU:HG	8:H:25:ARG:NH1	2.36	0.41
1:A:783:ARG:CZ	1:A:786:PRO:HA	2.51	0.41
1:A:852:HIS:ND1	6:F:139:PRO:HB3	2.35	0.41
1:A:857:THR:OG1	1:A:866:GLN:N	2.52	0.41
1:A:1155:TYR:O	1:A:1194:LEU:HB3	2.21	0.41
1:A:1285:VAL:HG11	1:A:1309:LEU:HB3	2.02	0.41
2:B:110:THR:HA	2:B:196:ILE:HA	2.02	0.41
2:B:543:PRO:O	2:B:546:PRO:HD2	2.21	0.41
2:B:804:ALA:HB3	2:B:983:ARG:HH22	1.85	0.41
3:C:99:GLU:HB3	3:C:119:ILE:HG13	2.02	0.41
3:C:251:LEU:CD2	11:K:98:LEU:HD11	2.49	0.41
3:C:258:VAL:HG21	11:K:42:LEU:HD21	2.02	0.41
5:E:135:GLN:O	5:E:139:LEU:HD23	2.21	0.41
14:N:-7:DG:O6	17:T:6:DC:N4	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:65:LEU:HB3	18:a:66:PRO:HD3	2.03	0.41
1:A:247:VAL:HG21	2:B:1205:GLN:NE2	2.35	0.41
1:A:850:MET:HE1	1:A:852:HIS:HA	2.03	0.41
1:A:945:ARG:NH2	1:A:1299:GLY:O	2.54	0.41
2:B:232:ARG:HD3	2:B:244:THR:HB	2.02	0.41
2:B:604:PRO:HB2	2:B:689:TYR:CE2	2.56	0.41
2:B:631:PHE:CE1	2:B:743:ILE:HG12	2.55	0.41
3:C:132:PRO:HG2	3:C:134:ARG:NH2	2.35	0.41
3:C:148:ARG:HD2	3:C:148:ARG:HA	1.95	0.41
3:C:198:LYS:HD2	3:C:198:LYS:HA	1.84	0.41
5:E:152:HIS:HB3	5:E:195:VAL:HG11	2.01	0.41
5:E:155:LEU:HD11	5:E:210:TYR:HD2	1.86	0.41
15:O:294:TYR:HB2	15:O:316:TRP:CZ2	2.55	0.41
15:O:514:PHE:CD2	15:O:517:ARG:HB2	2.56	0.41
18:a:94:GLU:CD	20:g:104:GLN:H	2.29	0.41
21:d:46:LYS:HA	21:d:46:LYS:HD3	1.90	0.41
18:e:90:MET:HE2	19:f:100:PHE:HZ	1.86	0.41
1:A:72:GLU:CB	1:A:76:GLU:HB3	2.51	0.41
1:A:80:HIS:H	1:A:244:PRO:HB3	1.85	0.41
1:A:248:ARG:HB2	1:A:261:ASP:CG	2.45	0.41
1:A:446:ASN:OD1	1:A:456:MET:HE1	2.20	0.41
1:A:551:LEU:HB3	1:A:557:TRP:CE3	2.56	0.41
1:A:561:VAL:HG12	8:H:79:ARG:HH21	1.85	0.41
1:A:678:LYS:HA	1:A:678:LYS:HE2	2.02	0.41
1:A:743:ASN:HA	1:A:746:GLN:HB2	2.02	0.41
1:A:1068:VAL:O	1:A:1072:GLN:HG3	2.21	0.41
1:A:1118:LEU:HD11	1:A:1315:ASN:N	2.32	0.41
1:A:1168:ASP:OD2	1:A:1239:ILE:HG21	2.20	0.41
1:A:1214:VAL:HG13	1:A:1276:LEU:CD2	2.51	0.41
1:A:1226:LEU:HB3	1:A:1242:CYS:HB3	2.02	0.41
1:A:1316:LEU:HD23	1:A:1341:VAL:HG21	2.02	0.41
2:B:23:ALA:O	2:B:678:TRP:HB2	2.21	0.41
2:B:38:PHE:HD2	2:B:167:SER:HB3	1.85	0.41
2:B:99:MET:CE	2:B:111:TYR:HA	2.50	0.41
2:B:233:SER:OG	2:B:354:LEU:HA	2.21	0.41
2:B:393:HIS:NE2	2:B:696:GLU:HG2	2.36	0.41
2:B:430:GLU:OE2	2:B:431:THR:HG23	2.21	0.41
2:B:605:GLU:HB2	2:B:627:TYR:CE2	2.56	0.41
2:B:631:PHE:HB2	2:B:741:CYS:O	2.21	0.41
2:B:634:GLU:HG3	2:B:641:ASN:HB3	2.02	0.41
2:B:1010:LEU:HD23	2:B:1011:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1180:PHE:O	2:B:1188:LYS:HA	2.21	0.41
3:C:10:ILE:HB	3:C:18:GLU:HG2	2.03	0.41
3:C:15:ASP:O	3:C:233:GLU:HA	2.20	0.41
3:C:109:GLY:H	3:C:148:ARG:NH1	2.18	0.41
5:E:164:LEU:HD23	5:E:164:LEU:HA	1.81	0.41
6:F:75:LEU:O	6:F:79:ARG:HG3	2.21	0.41
7:G:144:ARG:N	7:G:169:GLY:O	2.52	0.41
14:N:70:DG:H3'	18:e:42:ARG:HG3	2.01	0.41
15:O:705:LYS:HB3	15:O:731:TYR:HA	2.03	0.41
16:P:-3:U:H2'	16:P:-2:U:O4'	2.21	0.41
17:T:-54:DA:P	21:d:56:SER:H	2.44	0.41
17:T:-24:DG:H5''	18:a:85:GLN:HA	2.03	0.41
17:T:47:DG:H2''	17:T:48:DG:C8	2.55	0.41
18:a:44:GLY:HA3	19:b:44:LYS:HE3	2.03	0.41
1:A:333:LYS:HD2	17:T:58:DG:P	2.61	0.41
1:A:367:VAL:HB	1:A:461:VAL:HG13	2.01	0.41
1:A:801:VAL:HG22	1:A:813:GLU:HG3	2.03	0.41
1:A:1207:LYS:O	1:A:1277:ARG:NH1	2.54	0.41
2:B:354:LEU:HD11	2:B:371:LEU:HG	2.03	0.41
2:B:722:THR:HG22	2:B:722:THR:O	2.20	0.41
2:B:796:LEU:HG	2:B:798:TYR:H	1.86	0.41
2:B:798:TYR:HB2	2:B:821:GLN:NE2	2.36	0.41
2:B:957:ASN:OD1	2:B:960:GLY:N	2.53	0.41
2:B:1204:PHE:CZ	2:B:1216:LEU:HD21	2.56	0.41
3:C:55:SER:HB3	3:C:153:LEU:HD21	2.03	0.41
4:D:54:SER:HB3	4:D:121:CYS:SG	2.61	0.41
5:E:10:ARG:HG2	5:E:140:VAL:CG2	2.50	0.41
5:E:194:VAL:HG22	5:E:212:ILE:HA	2.03	0.41
8:H:112:LYS:HE3	8:H:114:TYR:CE1	2.56	0.41
14:N:13:DT:H5'	14:N:13:DT:C6	2.56	0.41
15:O:450:ARG:O	15:O:450:ARG:HG3	2.21	0.41
20:c:81:ARG:NH2	18:e:55:GLN:O	2.43	0.41
1:A:135:PHE:HB2	1:A:223:LEU:C	2.46	0.40
1:A:419:HIS:CD2	1:A:421:ARG:HG3	2.56	0.40
1:A:445:PHE:HB3	1:A:457:MET:O	2.22	0.40
1:A:859:ASN:OD1	1:A:863:ASP:N	2.54	0.40
1:A:1194:LEU:HA	1:A:1194:LEU:HD12	1.91	0.40
2:B:347:ASP:O	2:B:351:LYS:N	2.39	0.40
2:B:628:ARG:HG2	2:B:629:PRO:HD2	2.03	0.40
2:B:1001:PHE:HB2	2:B:1005:GLY:HA2	2.02	0.40
3:C:72:VAL:O	3:C:129:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:26:THR:O	4:D:162:SER:OG	2.37	0.40
7:G:121:TYR:CE2	7:G:123:PRO:HG3	2.56	0.40
9:I:87:GLN:HG2	9:I:99:LEU:HA	2.02	0.40
15:O:665:LYS:HE3	15:O:704:PHE:CD1	2.56	0.40
1:A:405:TYR:CD1	1:A:413:ARG:HB3	2.56	0.40
1:A:831:LYS:HA	1:A:834:GLU:OE2	2.21	0.40
1:A:867:PHE:CE2	5:E:209:SER:HA	2.42	0.40
1:A:1284:LYS:O	1:A:1312:ASP:N	2.45	0.40
1:A:1331:TYR:CE2	1:A:1333:ASN:HA	2.57	0.40
2:B:112:SER:HB3	2:B:160:LYS:NZ	2.36	0.40
2:B:400:ASP:OD1	2:B:404:PRO:HB2	2.22	0.40
2:B:661:ASP:OD1	2:B:661:ASP:N	2.52	0.40
2:B:1006:ILE:HG22	2:B:1087:PHE:HZ	1.87	0.40
3:C:53:ASN:H	12:L:62:ARG:HH12	1.67	0.40
3:C:165:LYS:NZ	11:K:10:PHE:HB3	2.36	0.40
3:C:167:HIS:HB3	3:C:169:LYS:HG2	2.02	0.40
5:E:20:GLU:OE1	5:E:142:ASN:ND2	2.51	0.40
5:E:57:MET:HE1	5:E:81:PHE:CG	2.56	0.40
6:F:85:LEU:HB3	6:F:90:ARG:HH21	1.86	0.40
14:N:-26:DC:H2'	14:N:-25:DC:C5	2.56	0.40
15:O:263:ARG:NH2	15:O:280:LYS:HB2	2.36	0.40
15:O:582:VAL:HG22	15:O:785:ARG:HG3	2.03	0.40
16:P:5:U:H2'	16:P:6:U:C6	2.56	0.40
1:A:254:ASP:O	1:A:256:THR:N	2.54	0.40
1:A:739:LYS:CG	1:A:742:ASN:HB2	2.50	0.40
1:A:1441:THR:HB	6:F:92:ARG:CG	2.51	0.40
2:B:505:ARG:NH2	2:B:524:GLN:O	2.51	0.40
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.21	0.40
2:B:1180:PHE:HB3	2:B:1191:ILE:HG21	2.04	0.40
5:E:21:MET:O	5:E:25:ARG:HG2	2.21	0.40
5:E:115:ILE:HG13	5:E:115:ILE:O	2.21	0.40
6:F:128:ARG:HD2	6:F:128:ARG:HA	1.82	0.40
7:G:106:LEU:HD13	7:G:159:ALA:HB3	2.03	0.40
8:H:76:LYS:HD2	8:H:76:LYS:O	2.20	0.40
11:K:82:ARG:NH2	11:K:84:LYS:HD3	2.37	0.40
11:K:85:GLN:HA	11:K:88:GLU:OE1	2.20	0.40
18:a:73:GLU:OE1	19:b:25:ASN:HB2	2.20	0.40
1:A:98:LYS:NZ	1:A:1414:GLU:HA	2.36	0.40
1:A:321:ARG:HG3	1:A:322:PRO:HD2	2.03	0.40
1:A:552:PHE:HE2	11:K:72:VAL:O	2.04	0.40
1:A:636:ARG:NH1	1:A:880:GLU:HB3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:GLY:O	1:A:652:LYS:HG2	2.20	0.40
1:A:1462:PRO:O	7:G:21:GLN:NE2	2.55	0.40
2:B:20:VAL:HG21	2:B:631:PHE:CZ	2.56	0.40
2:B:435:PHE:HE2	2:B:437:LEU:HD12	1.86	0.40
2:B:1082:MET:HE3	3:C:190:ASP:CA	2.52	0.40
2:B:1106:ARG:HE	2:B:1118:PRO:HB3	1.86	0.40
5:E:15:PHE:HZ	5:E:59:PHE:CD2	2.40	0.40
5:E:178:GLN:HA	5:E:214:LEU:O	2.21	0.40
8:H:33:ASN:OD1	8:H:33:ASN:N	2.54	0.40
9:I:10:CYS:SG	9:I:31:ASN:HB3	2.61	0.40
14:N:-4:DG:H2"	14:N:-3:DA:C8	2.57	0.40
1:A:547:VAL:O	1:A:551:LEU:HG	2.22	0.40
2:B:100:PHE:HD2	2:B:172:LEU:HD11	1.86	0.40
2:B:211:ALA:HB1	2:B:232:ARG:O	2.21	0.40
2:B:972:LYS:HG3	2:B:1094:ARG:HH12	1.87	0.40
5:E:18:VAL:HA	5:E:21:MET:HG2	2.03	0.40
5:E:44:LYS:HG3	5:E:45:ILE:HD13	2.03	0.40
9:I:9:GLU:HG2	9:I:10:CYS:N	2.37	0.40
9:I:26:LEU:HD13	9:I:35:THR:CG2	2.51	0.40
17:T:-13:DA:H5"	18:a:63:ARG:HH12	1.87	0.40
18:a:122:LYS:HG3	18:e:113:HIS:HE1	1.85	0.40
21:d:39:ILE:O	21:d:43:LYS:HG3	2.22	0.40
21:d:58:ALA:HA	21:d:61:ILE:HD12	2.04	0.40
21:h:99:ARG:HA	21:h:107:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1400/1743 (80%)	1313 (94%)	85 (6%)	2 (0%)	48 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1145/1227 (93%)	1068 (93%)	75 (7%)	2 (0%)	43	78
3	C	261/304 (86%)	247 (95%)	14 (5%)	0	100	100
4	D	162/186 (87%)	152 (94%)	10 (6%)	0	100	100
5	E	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
6	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	161 (95%)	7 (4%)	1 (1%)	21	59
8	H	129/145 (89%)	124 (96%)	5 (4%)	0	100	100
9	I	109/115 (95%)	100 (92%)	9 (8%)	0	100	100
10	J	64/72 (89%)	57 (89%)	6 (9%)	1 (2%)	7	38
11	K	111/118 (94%)	109 (98%)	2 (2%)	0	100	100
12	L	43/72 (60%)	38 (88%)	5 (12%)	0	100	100
13	M	62/113 (55%)	60 (97%)	2 (3%)	0	100	100
15	O	506/1094 (46%)	457 (90%)	45 (9%)	4 (1%)	16	54
18	a	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
18	e	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
19	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
19	f	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
20	c	101/133 (76%)	96 (95%)	5 (5%)	0	100	100
20	g	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
21	d	93/129 (72%)	90 (97%)	3 (3%)	0	100	100
21	h	91/129 (70%)	90 (99%)	1 (1%)	0	100	100
All	All	5186/6743 (77%)	4876 (94%)	300 (6%)	10 (0%)	44	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	62	ALA
15	O	306	ASP
15	O	718	ARG
1	A	255	GLU
7	G	154	VAL
15	O	483	CYS
10	J	2	ILE
15	O	323	VAL
1	A	960	VAL

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Mol	Chain	Res	Type
2	B	529	VAL

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	A	1225/1528 (80%)	1225 (100%)	0	100	100
2	B	1012/1077 (94%)	1012 (100%)	0	100	100
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	143/160 (89%)	143 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100
13	M	61/99 (62%)	61 (100%)	0	100	100
15	O	463/979 (47%)	463 (100%)	0	100	100
18	a	85/114 (75%)	85 (100%)	0	100	100
18	e	84/114 (74%)	84 (100%)	0	100	100
19	b	65/81 (80%)	65 (100%)	0	100	100
19	f	63/81 (78%)	63 (100%)	0	100	100
20	c	82/102 (80%)	82 (100%)	0	100	100
20	g	83/102 (81%)	83 (100%)	0	100	100
21	d	81/107 (76%)	81 (100%)	0	100	100
21	h	79/107 (74%)	79 (100%)	0	100	100
All	All	4609/5867 (79%)	4609 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	246	GLN
1	A	314	GLN
1	A	428	GLN
1	A	436	HIS
1	A	516	GLN
1	A	590	GLN
1	A	649	ASN
1	A	692	GLN
1	A	737	ASN
1	A	746	GLN
1	A	839	GLN
1	A	971	GLN
1	A	1112	ASN
1	A	1303	ASN
2	B	60	GLN
2	B	70	ASN
2	B	72	ASN
2	B	227	HIS
2	B	292	HIS
2	B	298	ASN
2	B	359	GLN
2	B	376	ASN
2	B	458	ASN
2	B	474	GLN
2	B	767	ASN
2	B	862	GLN
2	B	1076	HIS
2	B	1093	GLN
2	B	1117	GLN
2	B	1179	GLN
2	B	1195	HIS
4	D	179	ASN
5	E	4	ASN
5	E	113	ASN
5	E	120	ASN
7	G	14	HIS
7	G	24	GLN
8	H	13	GLN

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Mol	Chain	Res	Type
8	H	17	ASN
8	H	44	ASN
8	H	61	ASN
8	H	136	GLN
9	I	89	GLN
10	J	30	GLN
11	K	70	ASN
13	M	65	GLN
15	O	265	GLN
15	O	338	GLN
15	O	546	GLN
15	O	609	GLN
15	O	667	GLN
15	O	669	HIS
18	a	108	ASN
20	c	68	ASN
20	c	73	ASN
20	c	112	GLN
21	d	67	ASN
18	e	76	GLN
18	e	93	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	15/16 (93%)	5 (33%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	-4	U
16	P	-3	U
16	P	0	C
16	P	1	G
16	P	10	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

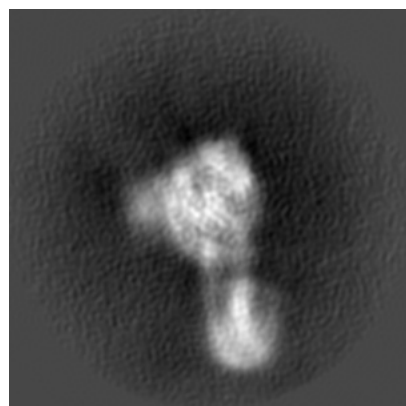
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34685. These allow visual inspection of the internal detail of the map and identification of artifacts.

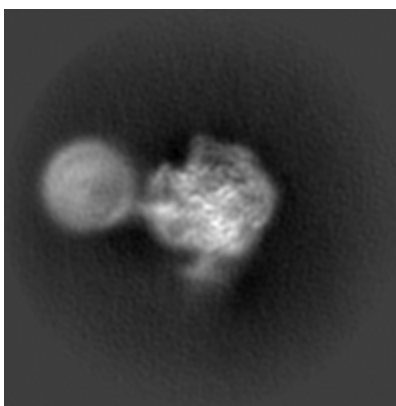
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

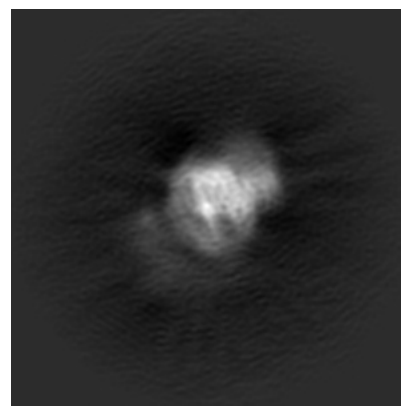
6.1.1 Primary map



X

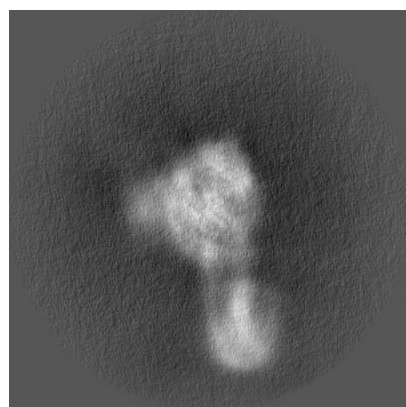


Y

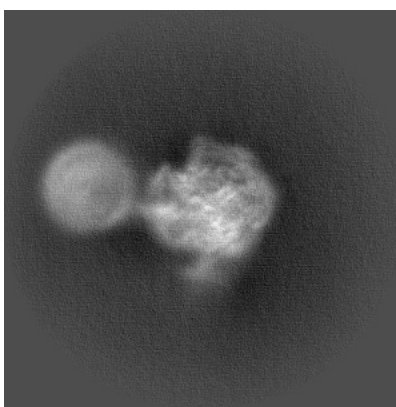


Z

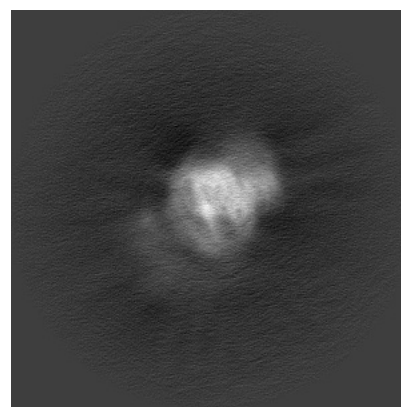
6.1.2 Raw map



X



Y

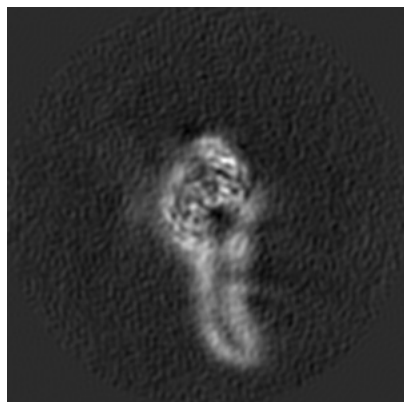


Z

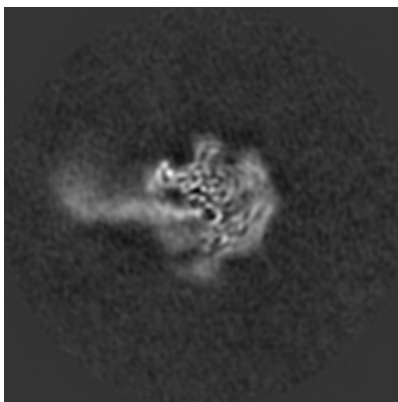
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

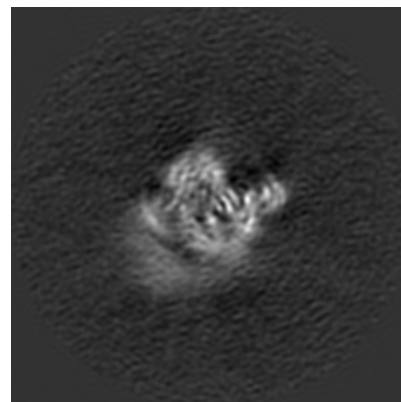
6.2.1 Primary map



X Index: 200

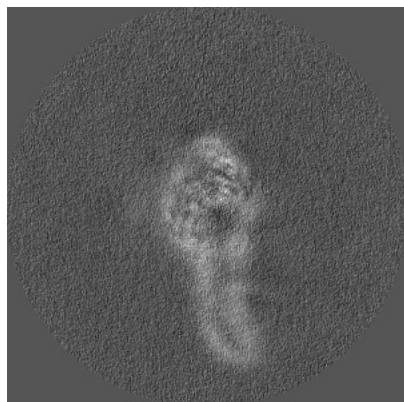


Y Index: 200

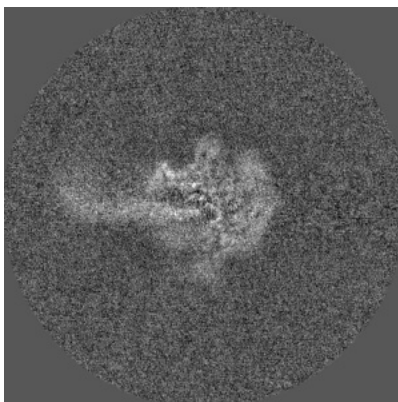


Z Index: 200

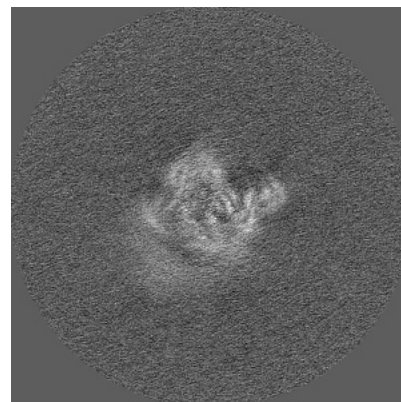
6.2.2 Raw map



X Index: 200



Y Index: 200

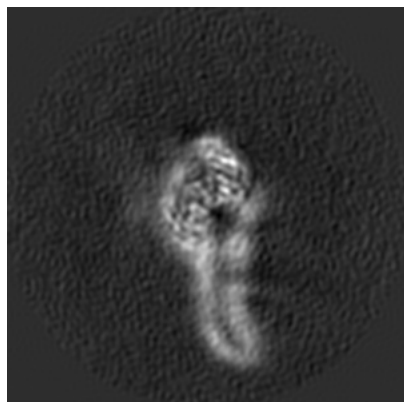


Z Index: 200

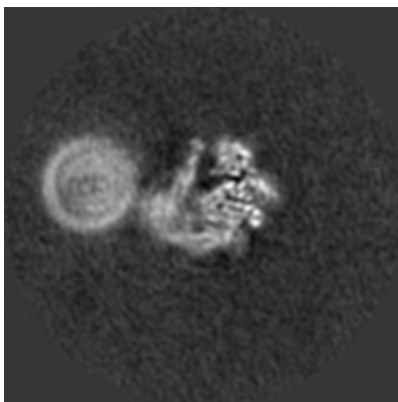
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

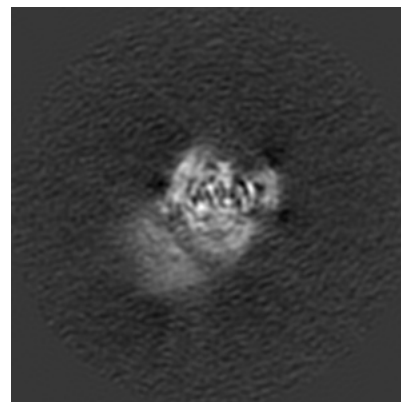
6.3.1 Primary map



X Index: 199

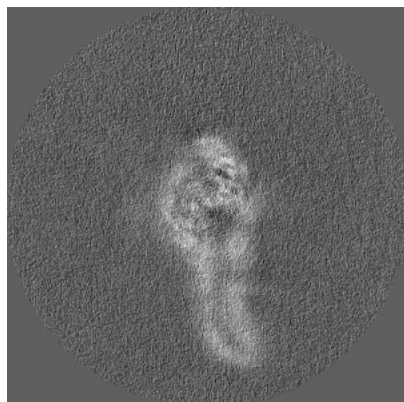


Y Index: 227

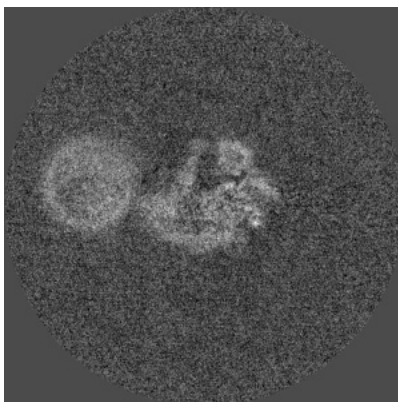


Z Index: 215

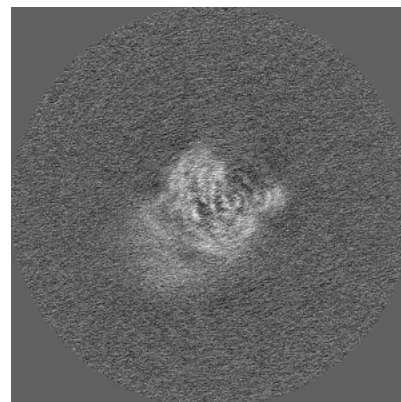
6.3.2 Raw map



X Index: 201



Y Index: 227

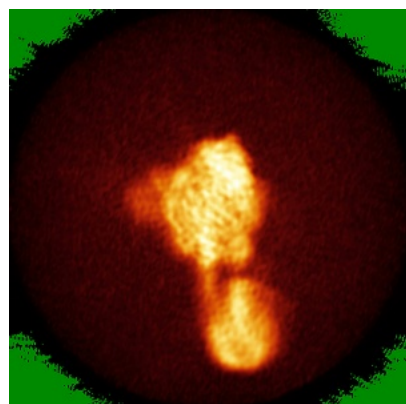


Z Index: 206

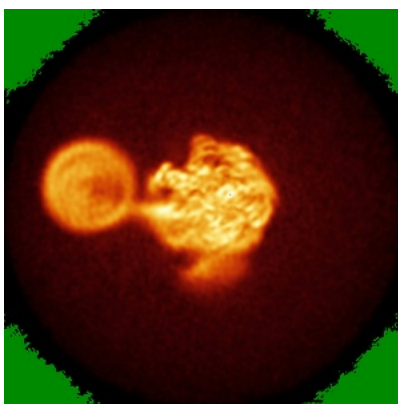
The images above show the largest variance slices of the map in three orthogonal directions.

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

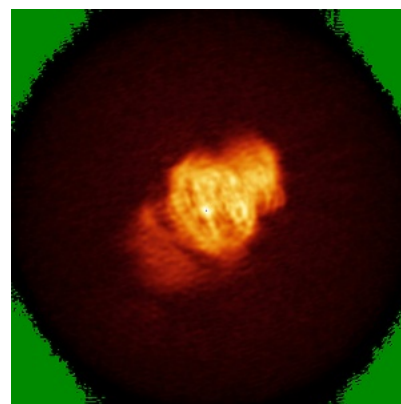
6.4.1 Primary map



X

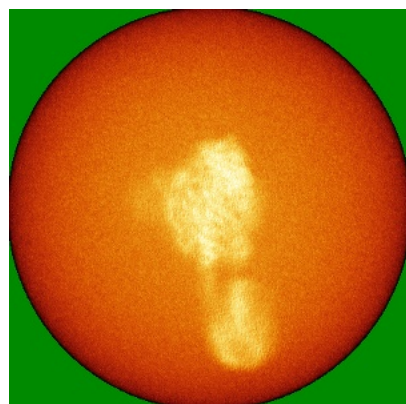


Y

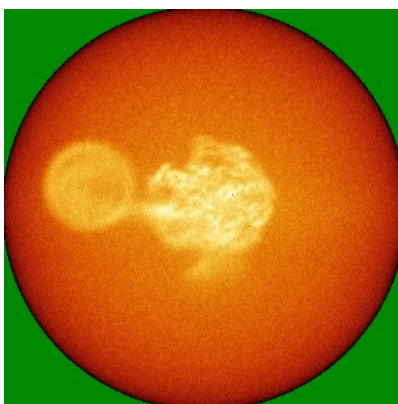


Z

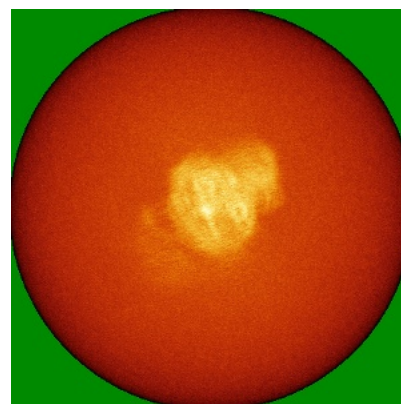
6.4.2 Raw map



X



Y



Z

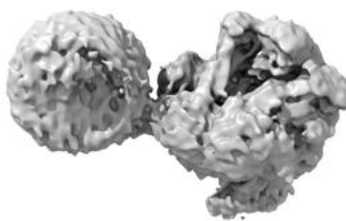
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

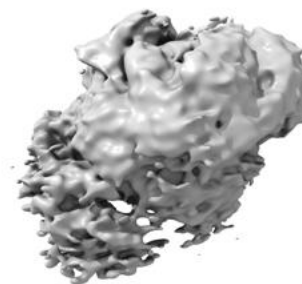
6.5.1 Primary map



X



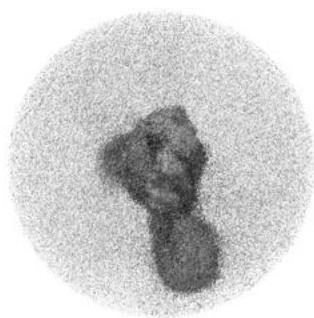
Y



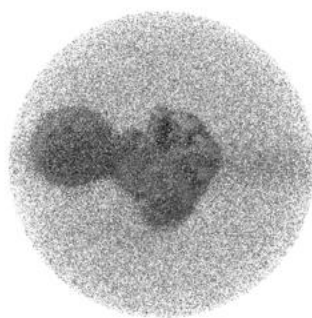
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00519. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

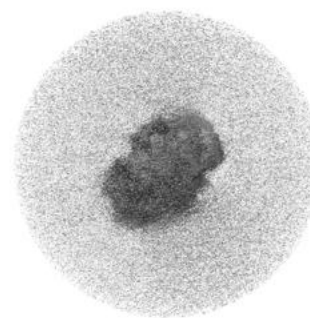
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

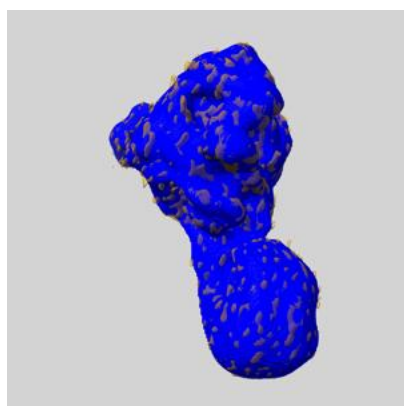
6.6 Mask visualisation [i](#)

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

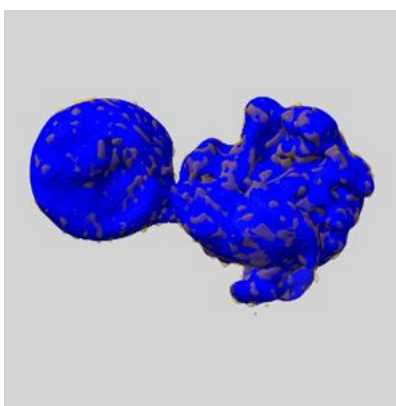
A mask typically either:

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

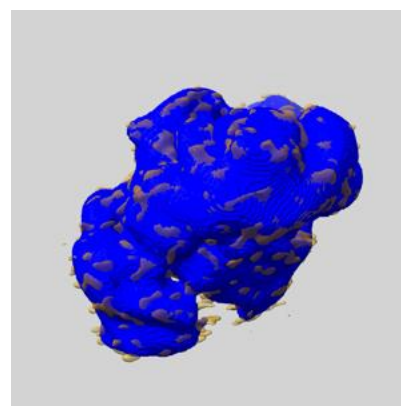
6.6.1 emd_34685_msk_1.map [i](#)



X

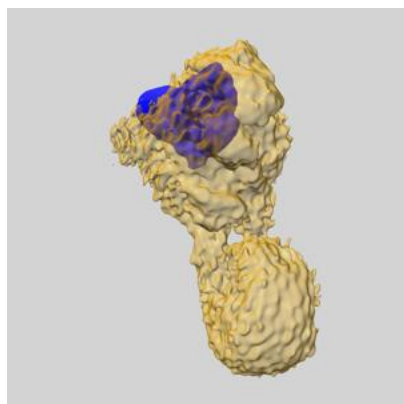


Y

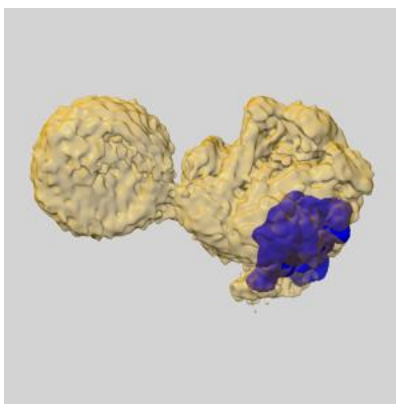


Z

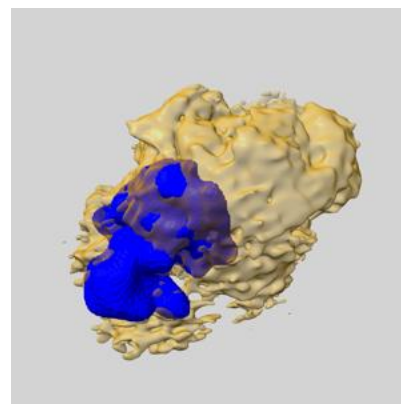
6.6.2 emd_34685_msk_2.map [i](#)



X

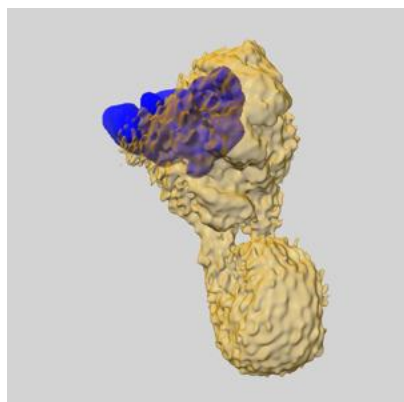


Y

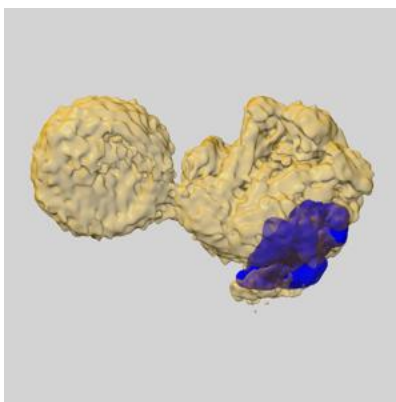


Z

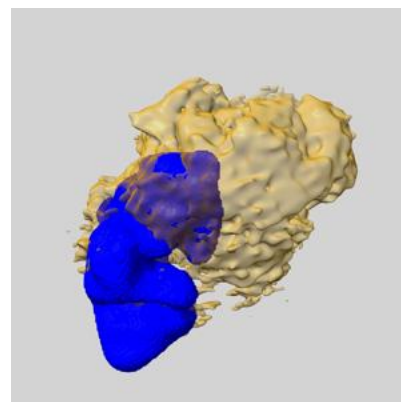
6.6.3 emd_34685_msk_3.map [i](#)



X



Y

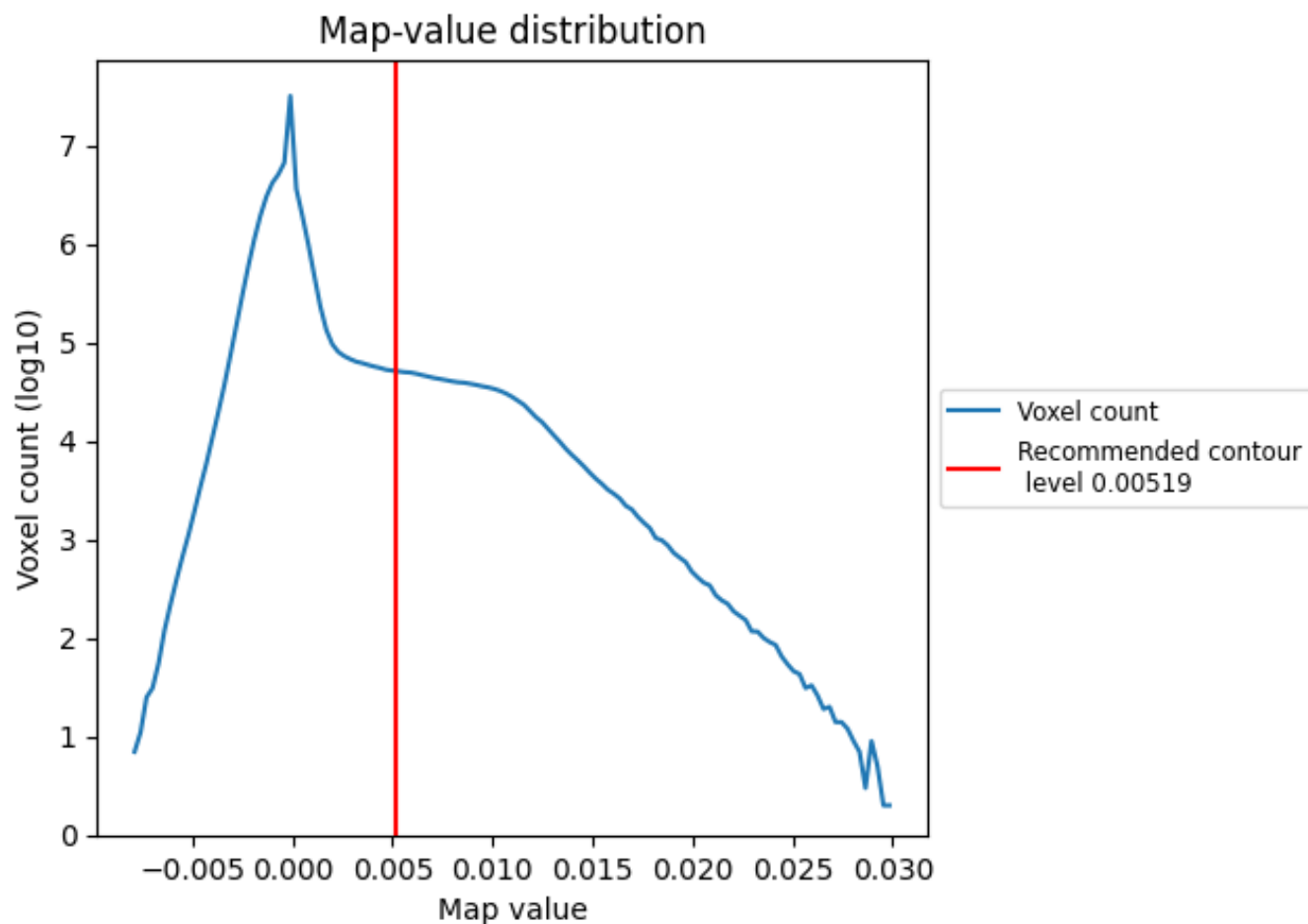


Z

7 Map analysis [i](#)

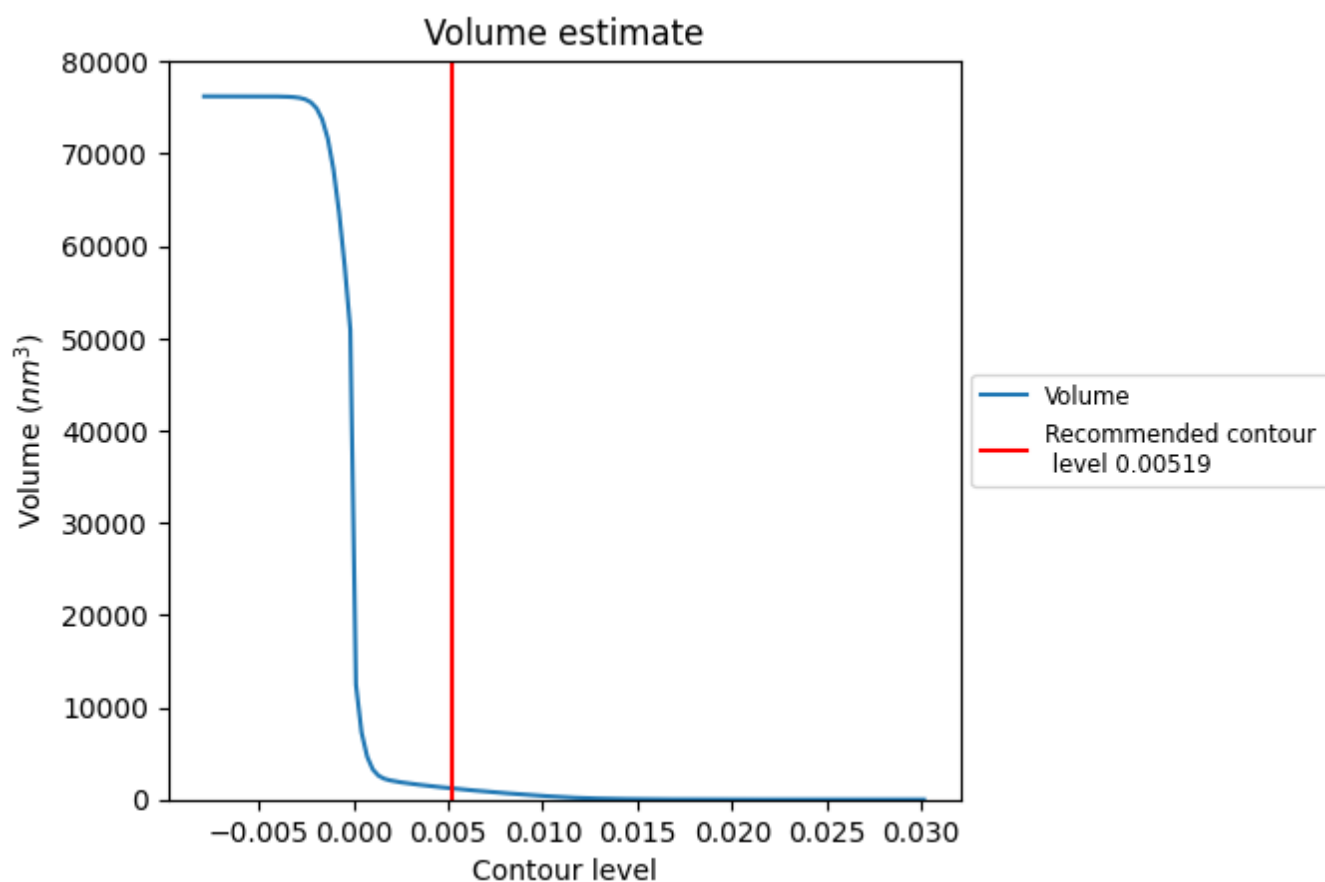
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

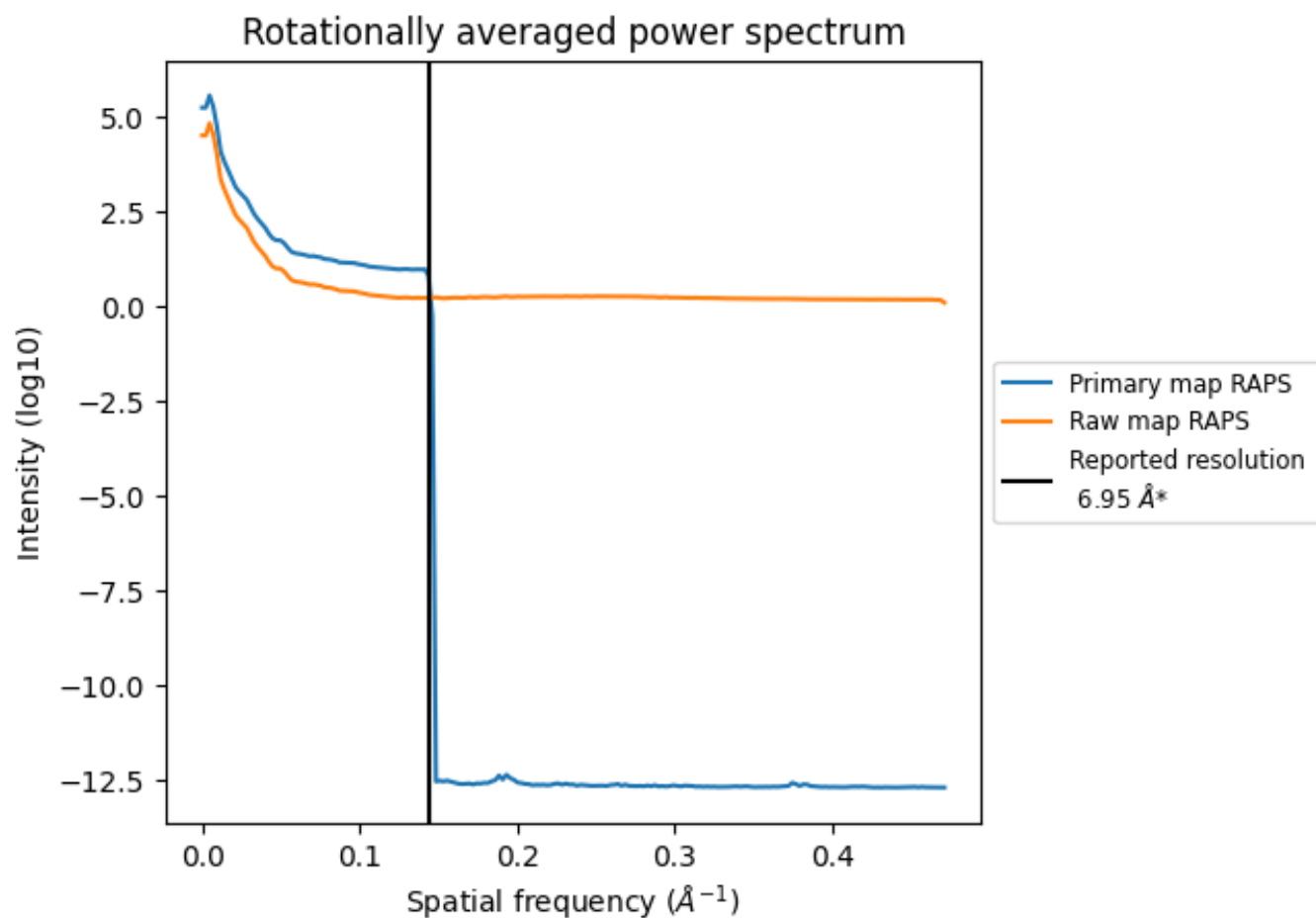
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1220 nm³; this corresponds to an approximate mass of 1102 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 ⓘ

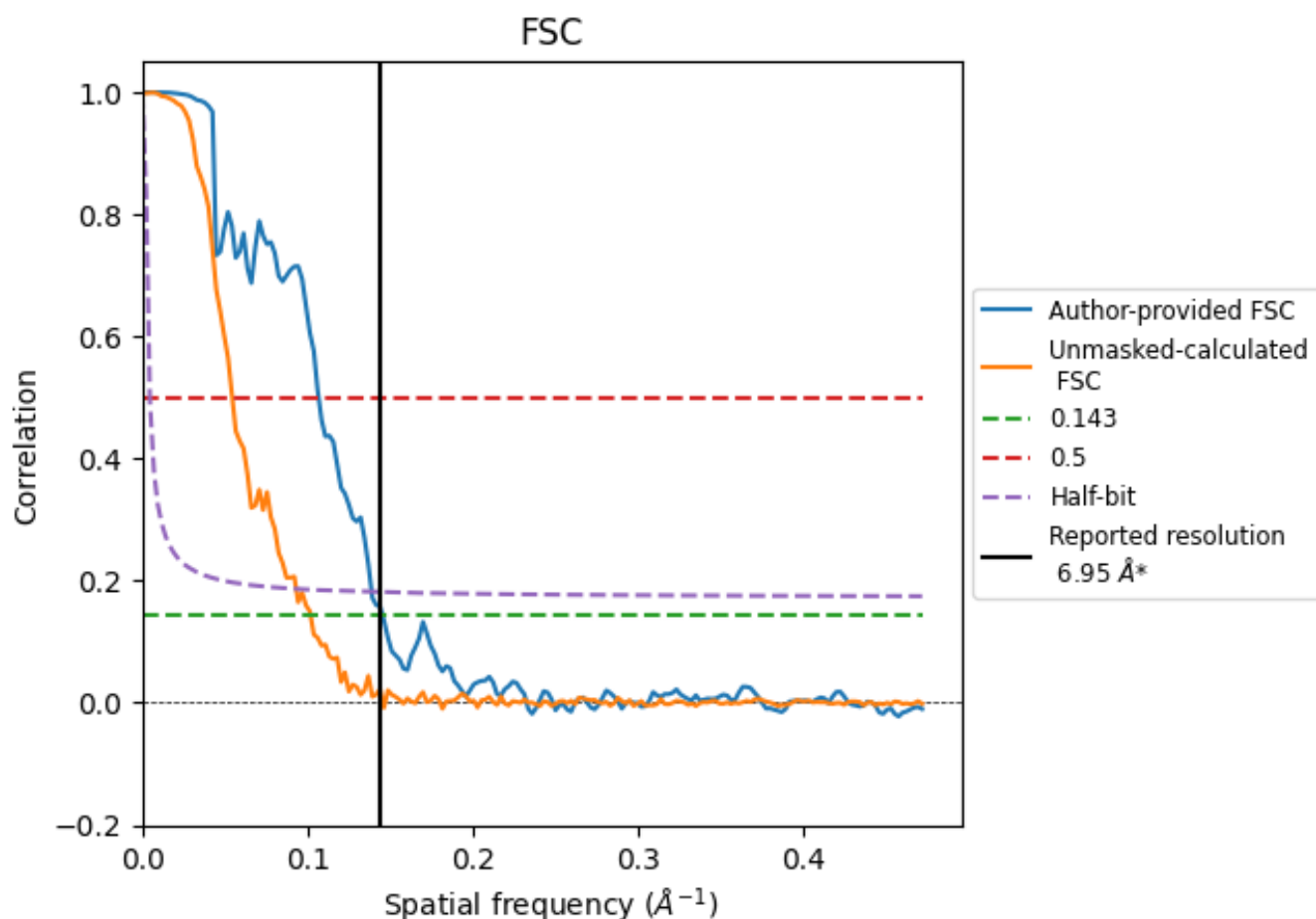


*Reported resolution corresponds to spatial frequency of 0.144 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.144 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

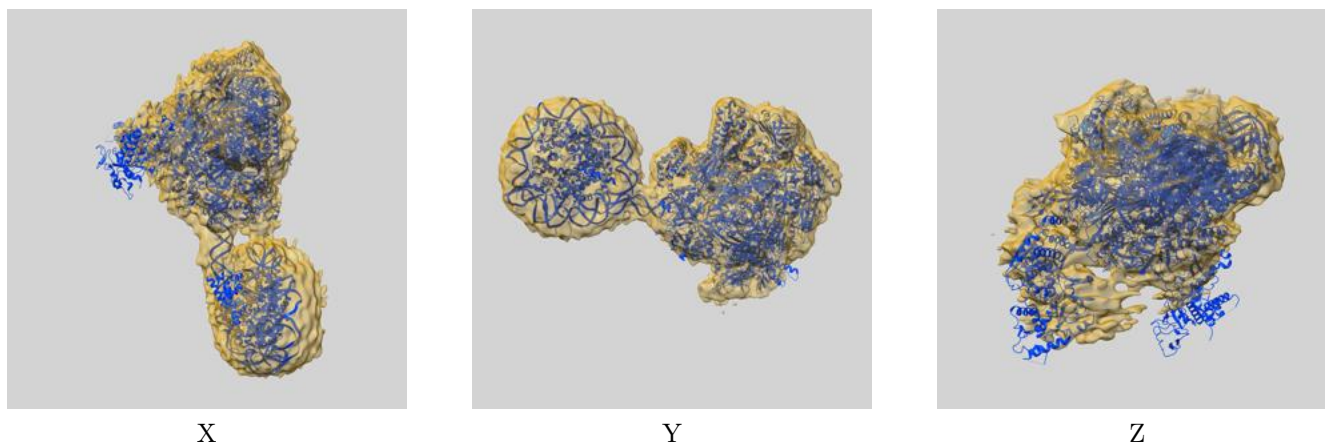
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.95	-	-
Author-provided FSC curve	6.88	9.37	7.21
Unmasked-calculated*	9.82	18.35	10.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.82 differs from the reported value 6.95 by more than 10 %

9 Map-model fit [i](#)

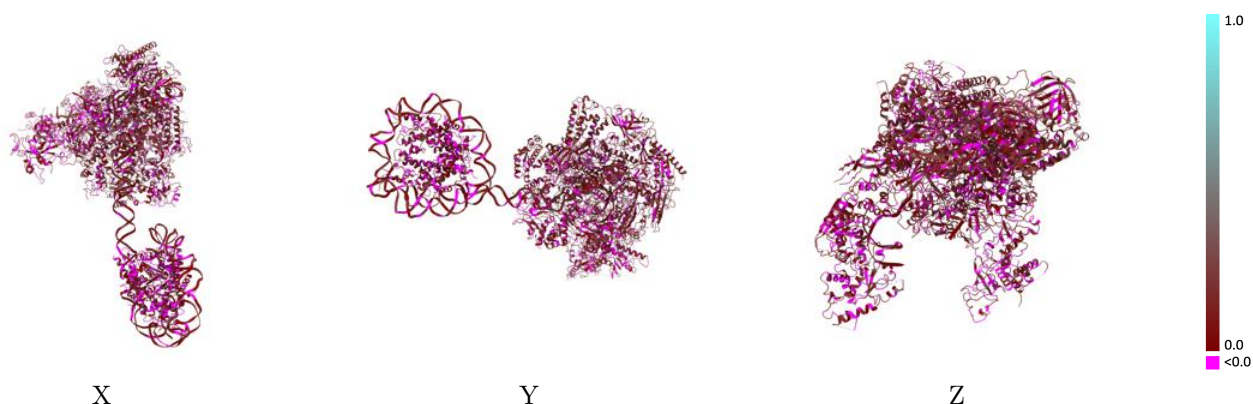
This section contains information regarding the fit between EMDB map EMD-34685 and PDB model 8HE5. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



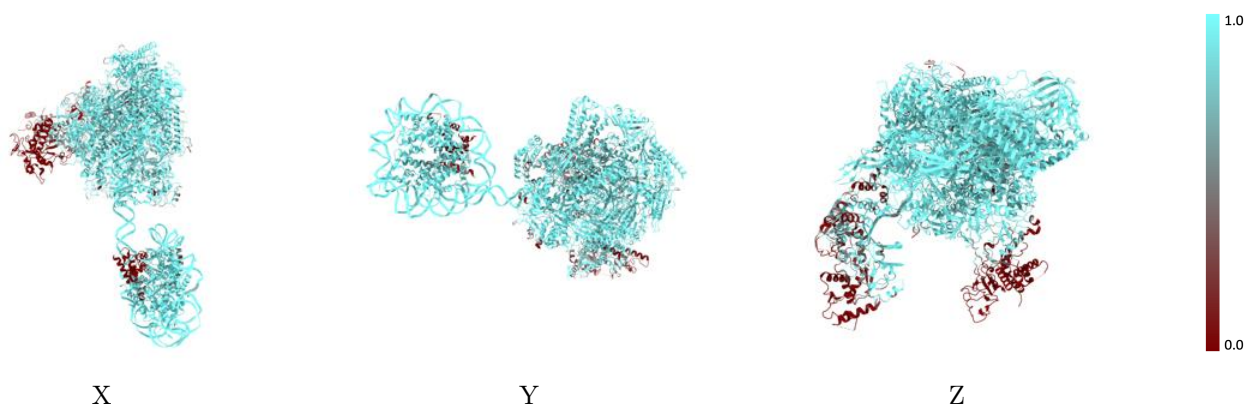
The images above show the 3D surface view of the map at the recommended contour level 0.00519 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



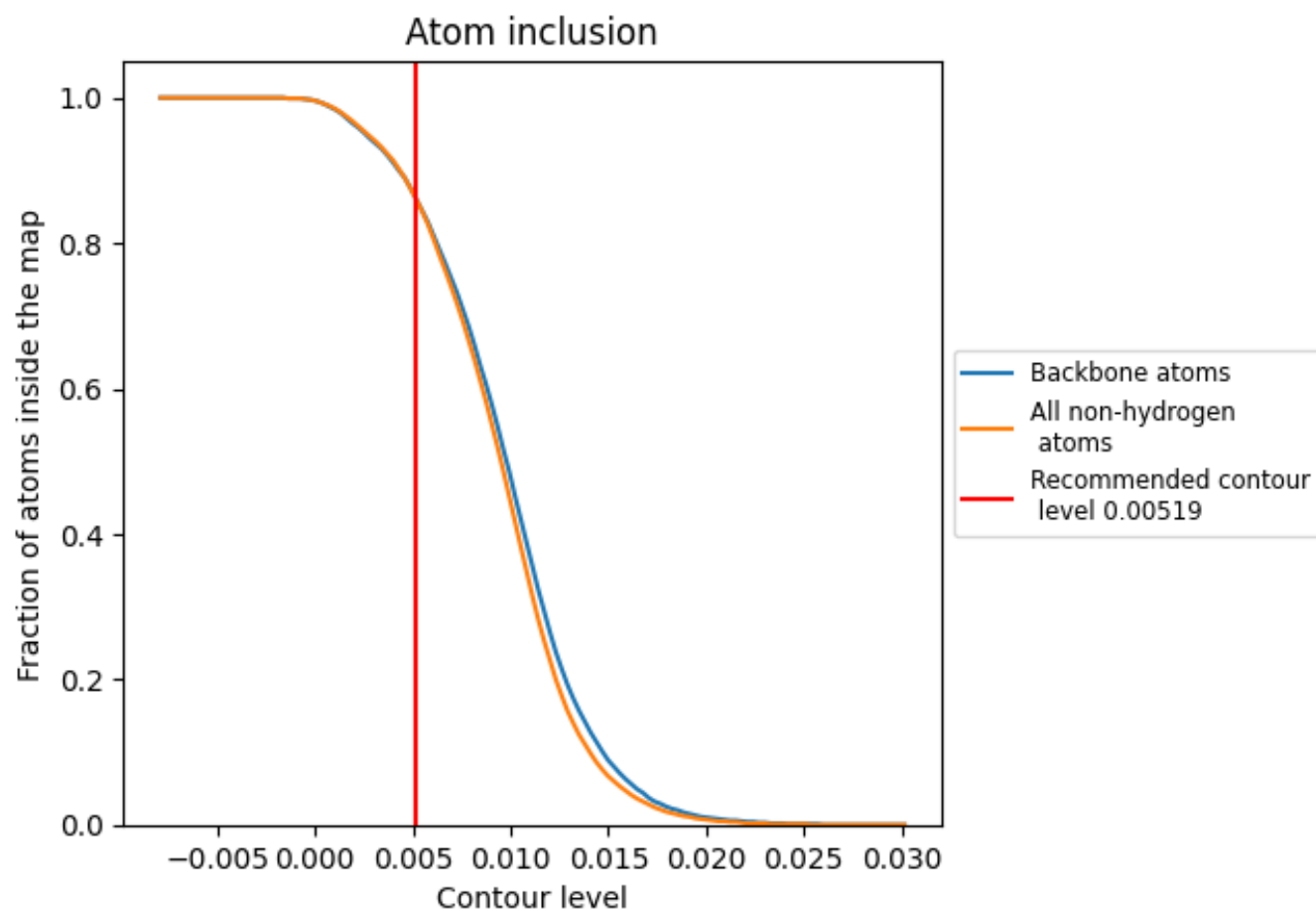
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00519).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.00519) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.1050
A	 0.9480	 0.1340
B	 0.9350	 0.1180
C	 0.9860	 0.1240
D	 0.1110	 0.0720
E	 0.9490	 0.1290
F	 0.9770	 0.1000
G	 0.3620	 0.0690
H	 0.9810	 0.1300
I	 0.8580	 0.0740
J	 0.9910	 0.1260
K	 0.9730	 0.1200
L	 1.0000	 0.1140
M	 0.8230	 0.1060
N	 0.9830	 0.1030
O	 0.5070	 0.0620
P	 0.9820	 0.1900
T	 0.9790	 0.1180
a	 0.9880	 0.0550
b	 1.0000	 0.0410
c	 0.9440	 0.0830
d	 0.8780	 0.0370
e	 0.9810	 0.0550
f	 0.9450	 0.0360
g	 0.5460	 0.0480
h	 0.4110	 0.0410

