



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:20 PM UTC

PDB ID : 7EG8 / pdb_00007eg8
EMDB ID : EMD-31108
Title : TFIID-based core PIC on PUMA promoter
Authors : Chen, X.; Qi, Y.; Hou, H.; Wang, X.; Wu, Z.; Li, J.; Xu, Y.
Deposited on : 2021-03-24
Resolution : 7.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

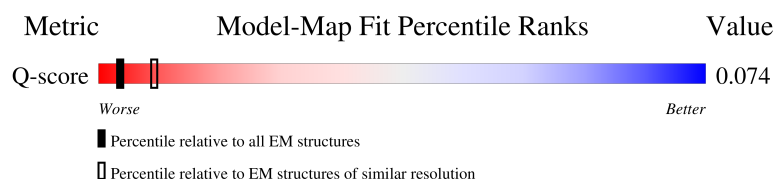
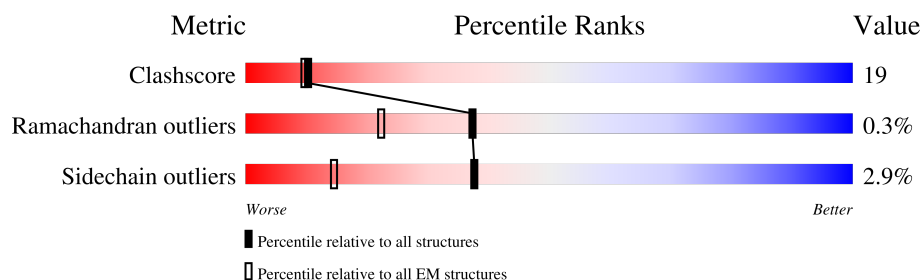
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	412 (6.90 - 7.90)

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

Mol	Chain	Length	Quality of chain
1	A	1872	31% 22% 9% . 68%
2	B	1199	70% 65% 14% . 20%
3	D	1085	13% 9% . . 85%
3	d	1085	15% 12% . 85%

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Mol	Chain	Length	Quality of chain
4	E	800	
4	e	800	
5	F	677	
5	f	677	
6	G	349	
7	H	310	
8	I	264	
8	i	264	
9	J	218	
9	j	218	
10	L	161	
10	l	161	
11	O	109	
12	P	339	
13	Q	376	
14	R	316	
15	S	517	
16	T	249	
17	X	85	
18	Y	85	
19	c	929	
20	k	211	
21	m	124	
22	o	1970	
23	p	1174	

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Mol	Chain	Length	Quality of chain
24	q	275	
25	r	142	
26	s	210	
27	t	127	
28	u	172	
29	v	150	
30	w	125	
31	x	67	
32	y	117	
33	z	58	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 82798 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 Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	602	Total	C	N	O	S	0	0
			4927	3142	858	899	28		

- Molecule 2 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	164	Total	C	N	O	S	0	0
			1366	851	256	255	4		
3	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	546	Total	C	N	O	S	0	0
			4364	2766	757	820	21		
4	e	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	404	Total	C	N	O	S	0	0
			3081	1954	537	572	18		
5	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	145	Total	C	N	O	S	0	0
			1180	748	217	211	4		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
8	i	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	89	Total	C	N	O	S	0	0
			709	457	114	134	4		
9	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	76	Total	C	N	O	S	0	0
			622	388	109	122	3		
10	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 11 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	97	Total	C	N	O	S	0	0
			771	491	133	145	2		

- Molecule 12 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	177	Total	C	N	O	S	0	0
			1412	918	249	238	7		

- Molecule 13 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	122	Total	C	N	O	S	0	0
			996	623	162	207	4		

- Molecule 14 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	251	Total	C	N	O	S	0	0
			1938	1214	344	363	17		

- Molecule 15 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	108	Total	C	N	O	S	0	0
			872	558	153	159	2		

- Molecule 16 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 17 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	85	Total	C	N	O	P	0	0
			1751	829	329	508	85		

- Molecule 18 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	85	Total	C	N	O	P	0	0
			1734	824	313	512	85		

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 21 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 22 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	1427	Total	C	N	O	S	0	0
			11308	7114	2023	2099	72		

- Molecule 23 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 27 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	t	79	Total	C	N	O	S	0	0
			635	406	108	116	5		

- Molecule 28 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	u	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 29 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	v	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 30 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 31 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	x	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 32 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	y	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 33 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	R	1	Total	Zn	0
			1	1	
34	o	2	Total	Zn	0
			2	2	
34	p	1	Total	Zn	0
			1	1	
34	q	1	Total	Zn	0
			1	1	
34	w	2	Total	Zn	0
			2	2	
34	x	1	Total	Zn	0
			1	1	
34	z	1	Total	Zn	0
			1	1	

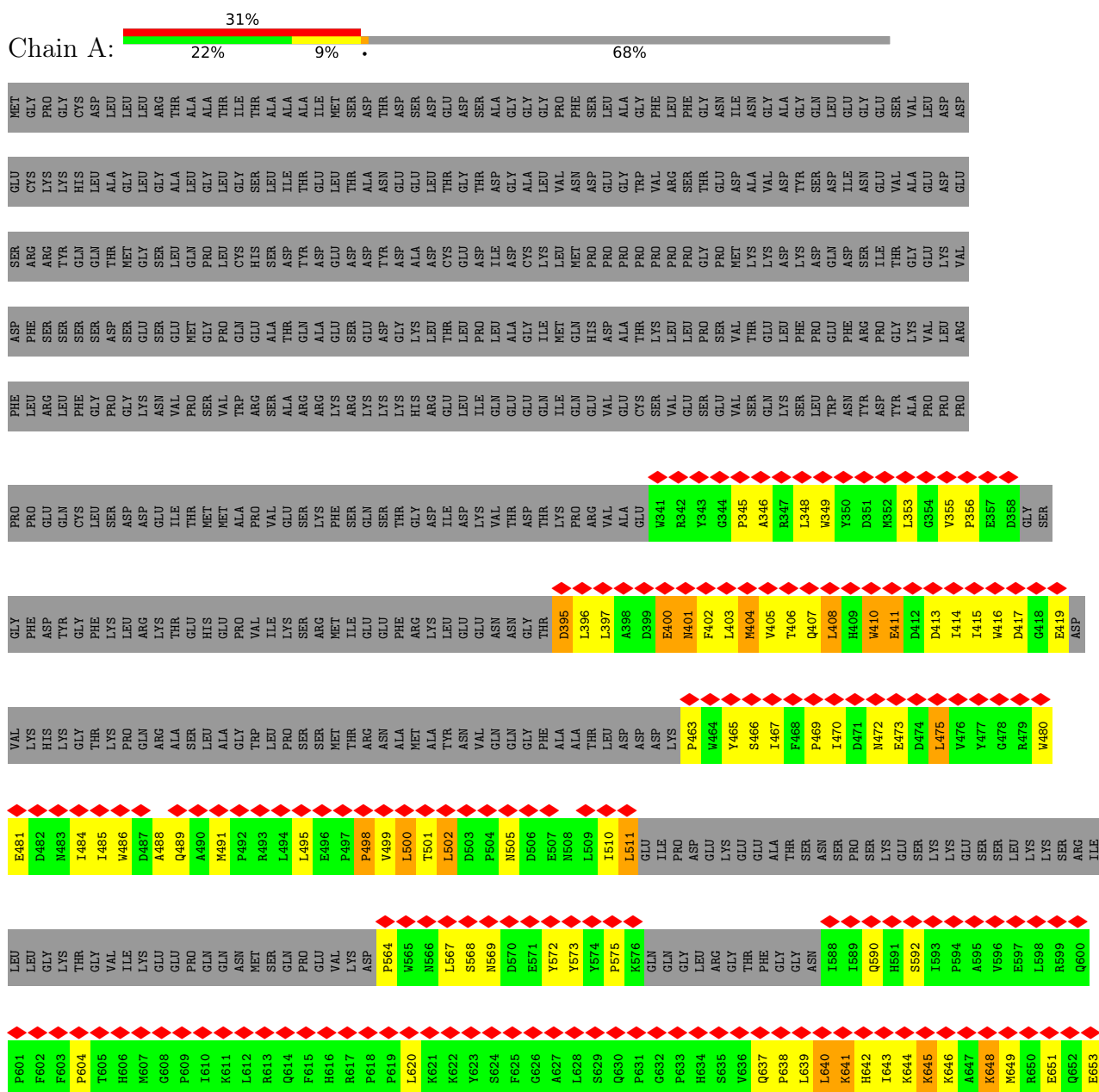
- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	o	1	Total	Mg	0
			1	1	

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: Transcription initiation factor TFIID subunit 1

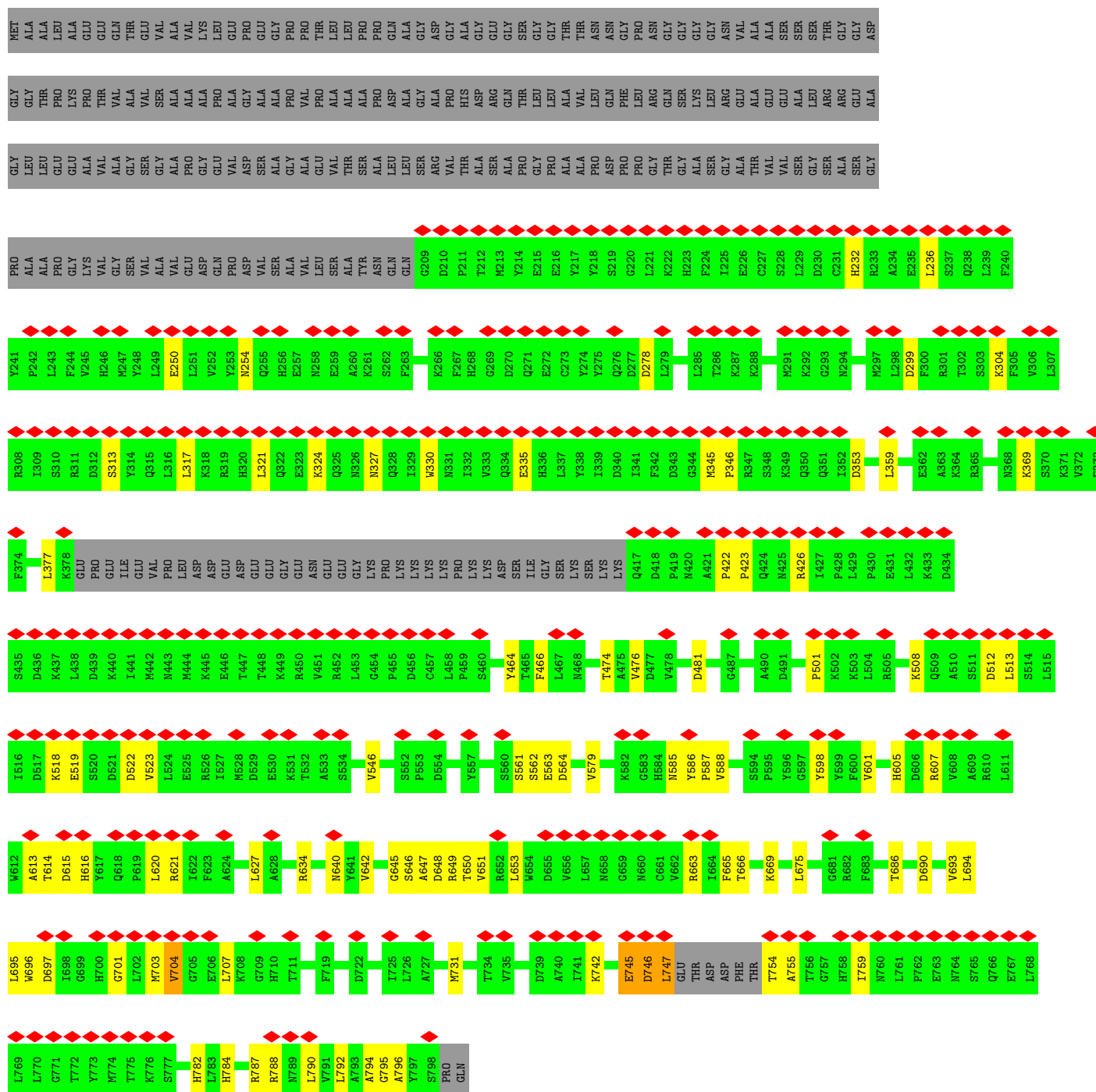


GLN	VAL	PHE	GLU	THR	VAL	CYS	E1204	ASN	S1084	E1024	S964	GLY	I843	V782	E861
ALA	ALA	ALA	F1205	HIS	GLY	GLY	F1205	HIS	T1085	V1025	Y965	GLU	R843	G783	M662
PHE	PHE	GLY	ILE	ASP	THR	ASP	I1026	ASP	ASP	L1026	V966	LYS	X844	Q784	F663
ILE	ILE	GLY	LYS	ASP	THR	ASP	D1027	THR	THR	D1027	K967	PHE	R845	Q785	F664
LEU	LEU	ALA	PHE	ASP	SER	SER	V1028	SER	SER	V1028	P968	ALA	R846	C786	M665
LEU	LEU	ALA	ALA	ASP	SER	SER	N1029	SER	SER	N1029	P969	PRO	K947	P787	M666
ASP	ASP	LEU	LEU	ALA	ALA	ALA	R1030	ASP	ASP	R1030	N970	GLU	K948	S728	T667
ASP	ASP	PHE	PHE	GLU	GLU	GLU	T1031	GLN	GLN	T1031	K971	GLU	C949	P729	P668
GLN	GLN	THR	THR	GLU	GLU	GLU	S1032	THR	THR	S1032	PRO	ASN	A850	F730	Q669
GLN	GLN	LYS	LYS	ASP	ASP	ASP	M1033	GLN	GLN	M1033	THR	GLU	D851	L731	D670
ASP	ASP	LYS	LYS	ASP	ASP	ASP	T1034	LYS	LYS	T1034	GLN	GLU	F852	G732	L671
ASP	ASP	GLY	GLY	ASP	ASP	ASP	E1035	ASP	ASP	E1035	GLN	GLU	K853	P733	T672
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN	GLY	GLY	GLN	PRO	GLY	R854	L734	G673
GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	GLY	GLY	ALA	THR	GLY	T855	H735	K674
GLY	GLY	GLY	GLY	GLY	GLY	GLY	ARG	ARG	GLY	ARG	LYS	GLY	G856	P736	D675
GLY	GLY	GLY	GLY	GLY	GLY	GLY	ARG	ARG	GLY	ARG	PRO	GLY	M857	Q737	G676
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO	GLN	D858	G738	D677
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO	GLN	S859	L739	L678
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	LYS	N860	L740	I679
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	LYS	N861	Q741	L680
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	THR	M862	A742	A881
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	N863	F743	E682
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	L864	E744	Y683
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	K865	N745	S684
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	S866	Q737	E685
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	N867	G738	E686
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	D867	L746	E687
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	F868	F748	N687
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	R869	R749	G688
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	L870	A750	P689
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	P871	P751	L690
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	T872	I752	M691
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	E873	Y753	M692
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	E874	L754	Q693
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	E875	H755	V694
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	I876	K756	G695
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	R877	M757	
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	A878	P758	T698
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GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	V880	T760	I700
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	S881	D761	K701
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	P882	P762	N702
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	E883	L763	Y703
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	Q884	I764	Y704
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	T951	I825	K705
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	G944	R826	R706
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	K945	M827	K707
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	C946	E828	P708
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	L947	R821	G709
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	L948	P822	K701
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	E949	R823	N702
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	V950	R824	Y703
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	T951	I825	Y704
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	G952	R826	K705
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	V953	M766	R706
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	A954	T767	K707
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	E1014	P768	P708
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	E1015	G770	G709
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	E1016	Y771	K710
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	I1017	Y772	D711
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	K1018	I773	P712
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	K1019	R774	G713
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	L1020	E775	A714
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	S1021	L776	P715
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	R1022	G776	D716
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	W1023	L777	C717
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR		V781	K718
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR			Y719
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR			G720
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR			E721

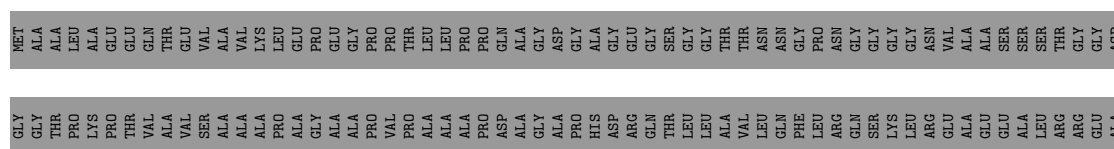
GLY	PRO	R963	Y901	ALA	GLN	VAL	LEU	SER	GLN	HIS	SER	LEU	ALA	PRO
PRO	GLY	E964	Y902	GLY	GLN	LEU	ALA	LEU	ARG	ALA	GLY	ALA	ALA	PRO
GLY	SER	R965	S903	ASN	GLN	SER	LEU	LEU	PRO	PRO	ALA	GLY	ASN	GLY
GLY	GLY	L966	H904	LEU	LEU	THR	THR	ARG	VAL	THR	THR	ALA	GLY	ALA
ALA	ALA	M967	A905	SER	ASN	GLN	GLN	LEU	ALA	THR	LEU	ALA	GLY	ALA
GLY	GLY	R968	T906	GLU	PRO	PRO	THR	LEU	SER	ALA	THR	ALA	GLY	ALA
GLY	SER	A969	Q907	GLU	LEU	THR	GLN	SER	ALA	PRO	THR	SER	SER	ALA
GLY	GLY	A970	Q908	SER	GLN	VAL	VAL	ASP	GLY	PRO	THR	ALA	GLY	PRO
PRO	PRO	L975	R909	ARG	VAL	GLY	GLY	SER	LYS	ARG	VAL	ALA	ALA	PRO
GLY	SER	SER	L910	ILE	VAL	VAL	VAL	ALA	GLN	PRO	LEU	SER	ALA	PRO
SER	ARG	ARG	L911	LEU	VAL	GLY	GLY	PHE	THR	ALA	MET	THR	PRO	ALA
VAL	VAL	SER	Q911	ALA	VAL	LYS	GLN	THR	ILE	THR	VAL	VAL	ALA	ALA
ARG	ARG	ARG	H912	THR	VAL	LYS	GLN	GLN	ALA	PRO	ARG	GLY	PRO	ALA
PRO	PRO	GLN	H913	ASN	GLY	PRO	GLY	GLN	ALA	THR	GLY	GLY	ALA	ALA
GLY	GLY	GLU	V914	SER	ALA	GLN	GLN	ALA	ALA	SER	PRO	GLN	ALA	PRO
ASP	ASP	ASP	V915	GLU	VAL	PRO	THR	SER	ASN	PRO	PRO	PRO	ALA	PRO
SER	SER	GLU	E915	LEU	LEU	THR	GLN	GLN	ASN	ALA	ALA	GLN	ALA	ALA
GLY	GLY	PRO	K916	VAL	VAL	VAL	VAL	VAL	VAL	PRO	VAL	SER	PRO	ALA
VAL	VAL	Q981	T917	GLY	THR	VAL	GLY	THR	LYS	PRO	GLY	GLY	GLY	ALA
THR	THR	L982	S918	LEU	LYS	ILE	PRO	PRO	PRO	ILE	PRO	GLY	GLY	ALA
PRO	PRO	R983	E919	THR	ALA	GLN	GLN	GLN	ASN	THR	THR	GLN	GLY	ALA
ARG	ARG	L984	T920	ARG	LEU	GLN	GLN	PRO	VAL	THR	ASN	VAL	GLY	ALA
GLN	GLN	K985	A921	SER	SER	ALA	PRO	THR	GLY	VAL	GLN	GLN	GLY	ALA
PHE	PHE	Q986	Q925	LYS	VAL	VAL	LYS	ASP	ASP	THR	ASP	GLN	GLN	ALA
THR	THR	K987	F926	ASP	ALA	PRO	PRO	GLY	THR	GLY	LYS	GLY	GLY	ALA
ARG	ARG	A988	S927	GLU	GLN	ALA	ALA	THR	ALA	THR	ALA	GLY	GLY	ALA
		R989	Y928	THR	GLN	ALA	ILE	LEU	LEU	ILE	ILE	PRO	PRO	ALA
		E990	K929	LYS	VAL	ARG	ARG	THR	THR	ALA	ARG	THR	PRO	ALA
		M991	D930	ALA	ALA	PRO	PRO	ALA	ASP	THR	ALA	THR	PRO	ALA
		Q992	D931	GLN	GLN	PRO	GLN	VAL	VAL	GLN	VAL	THR	PRO	ALA
		R993	D932	LYS	ASN	VAL	VAL	THR	THR	GLN	THR	GLY	ALA	ALA
		Q994	R933	ASN	LYS	THR	THR	SER	SER	ALA	THR	GLY	ALA	ALA
		E995	Y934	LEU	LYS	LEU	LEU	SER	ARG	ILE	PRO	GLY	ALA	ALA
		L996	E935	THR	GLY	THR	VAL	SER	LEU	THR	THR	LYS	GLY	ALA
		A997	Q936	GLU	PRO	GLN	GLN	TYR	ASN	THR	ASN	GLY	VAL	ALA
		Q998	O937	R880	GLY	THR	THR	ARG	GLY	THR	ASN	GLY	VAL	ALA
				R881	GLY	PRO	ARG	GLU	GLN	ILE	GLN	GLY	LYS	ALA
		Q1001	S938	T882	GLY	MET	THR	LEU	SER	ILE	GLN	GLY	ALA	ALA
		R1002	D939	L883	GLY	VAL	THR	ALA	ASN	LYS	GLN	LEU	ALA	ALA
		D1003	H940	SER	SER	ALA	GLY	GLY	SER	VAL	GLN	LEU	VAL	ALA
		A1004	R941	PHE	PHE	LEU	THR	SER	SER	THR	THR	ILE	VAL	ALA
		N1005	R941	ARG	ARG	ARG	THR	PRO	PRO	GLN	GLN	PRO	VAL	ALA
		L1006	A942	G886	ASP	ASP	ALA	GLN	GLN	ALA	GLN	GLN	VAL	ALA
		T1007	Q943	R887	ASP	ASP	ALA	GLN	TYR	ASN	ASN	GLN	GLN	ALA
		A1008	L944	R888	ASP	ASN	VAL	VAL	LEU	THR	VAL	LEU	ARG	ALA
		L1009	K945	H889	ILE	ARG	THR	SER	VAL	LYS	VAL	ARG	ARG	ALA
		A1010	F946	G890	ASN	ILE	SER	THR	VAL	GLN	LYS	VAL	VAL	ALA
		A1011	F947	T891	ASP	ASP	THR	GLN	PRO	GLN	LYS	VAL	VAL	ALA
	ILE	GLY	E948	T892	VAL	MET	ALA	PHE	THR	CYS	THR	THR	THR	ALA
	GLY	PRO	E949	R893	ALA	LEU	GLN	LEU	LEU	ASN	ASN	GLN	ALA	ALA
	PRO	ARG	Q949	E893	SER	THR	THR	ARG	PRO	THR	THR	GLN	GLN	ALA
	LYS	LYS	L950	L894	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
	ARG	ARG	D951	H895	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ALA
	ARG	ARG	Q952	F896	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
	LYS	LYS	H953	D897	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
	VAL	VAL	E954	V898	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
	ASP	ASP	K955	V899	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
	CYS	CYS	Q956	R899	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
	PRO	PRO	R957	S900	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
			K958		THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
			D959		THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
			E960		THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
			Q961		THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
			E962		THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA

Chain d:

[illegible]

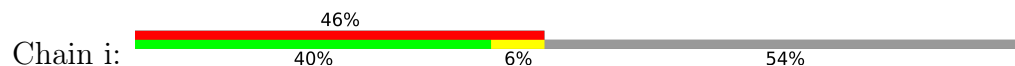
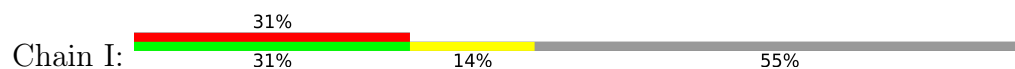


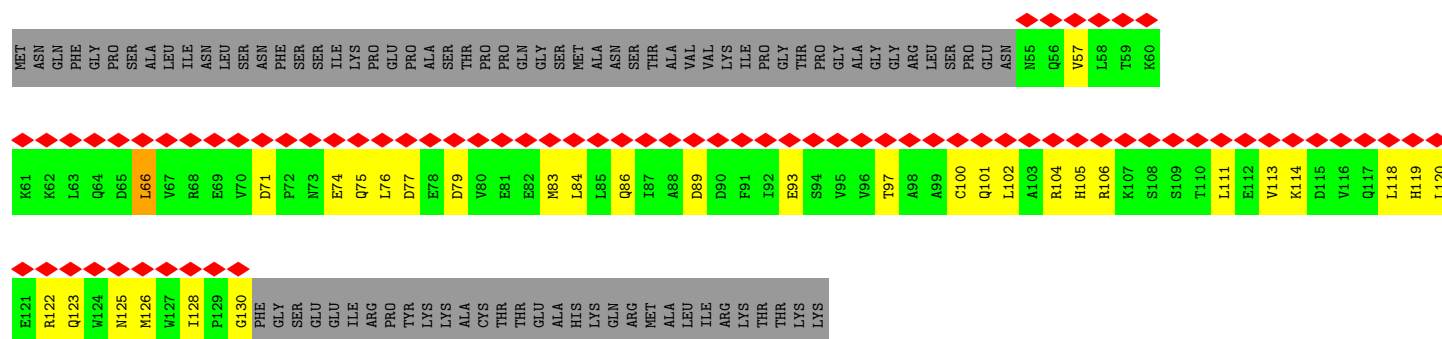
• Molecule 4: Transcription initiation factor TFIID subunit 5



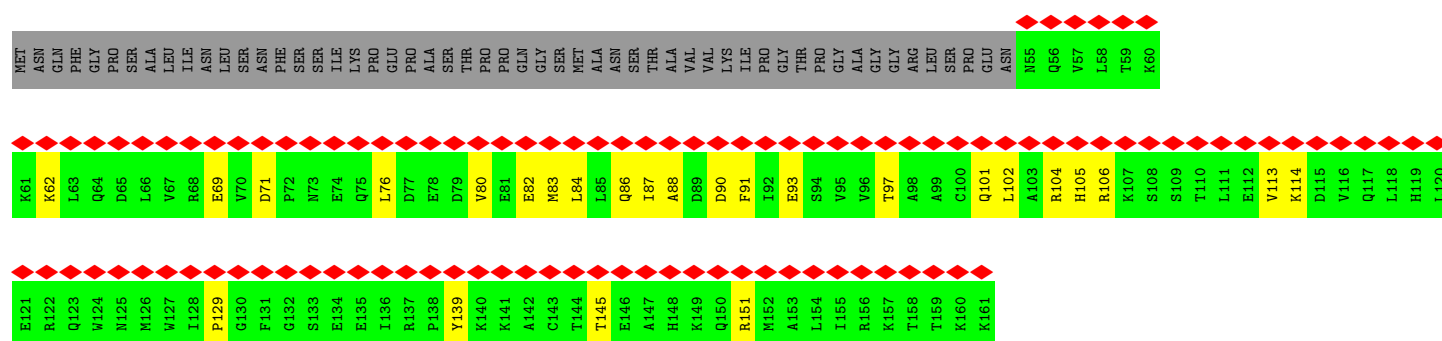


Chain H:

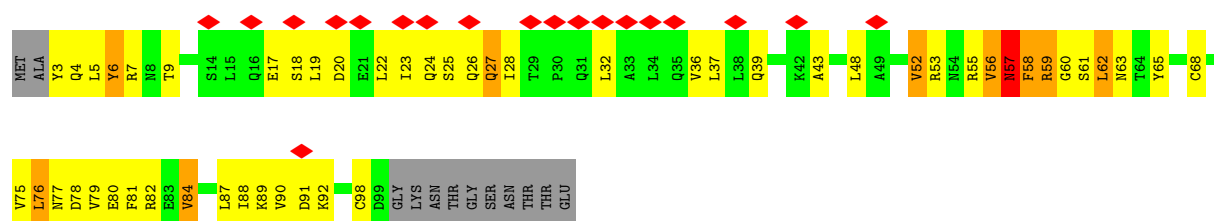




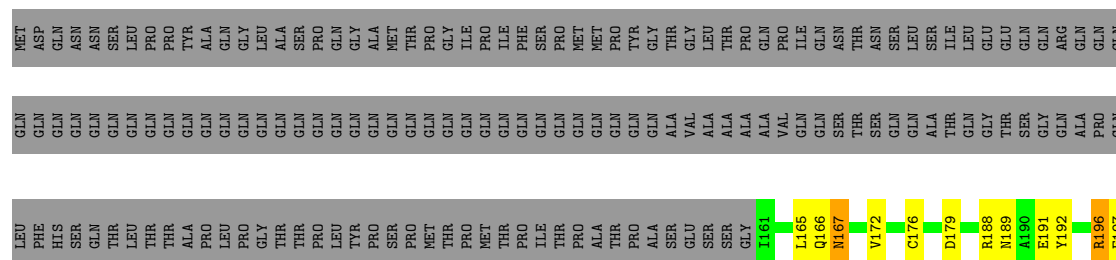
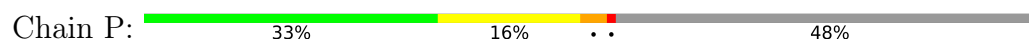
• Molecule 10: Transcription initiation factor TFIID subunit 12

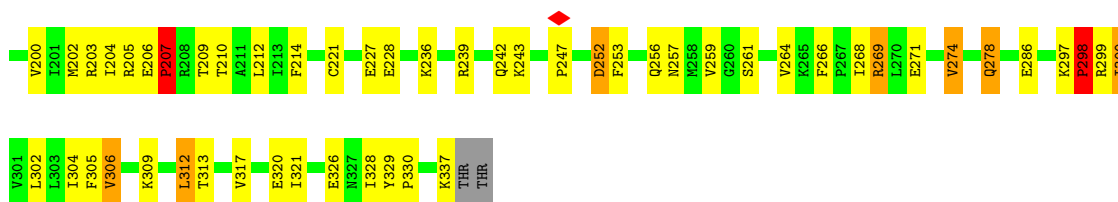


• Molecule 11: Transcription initiation factor IIA subunit 2

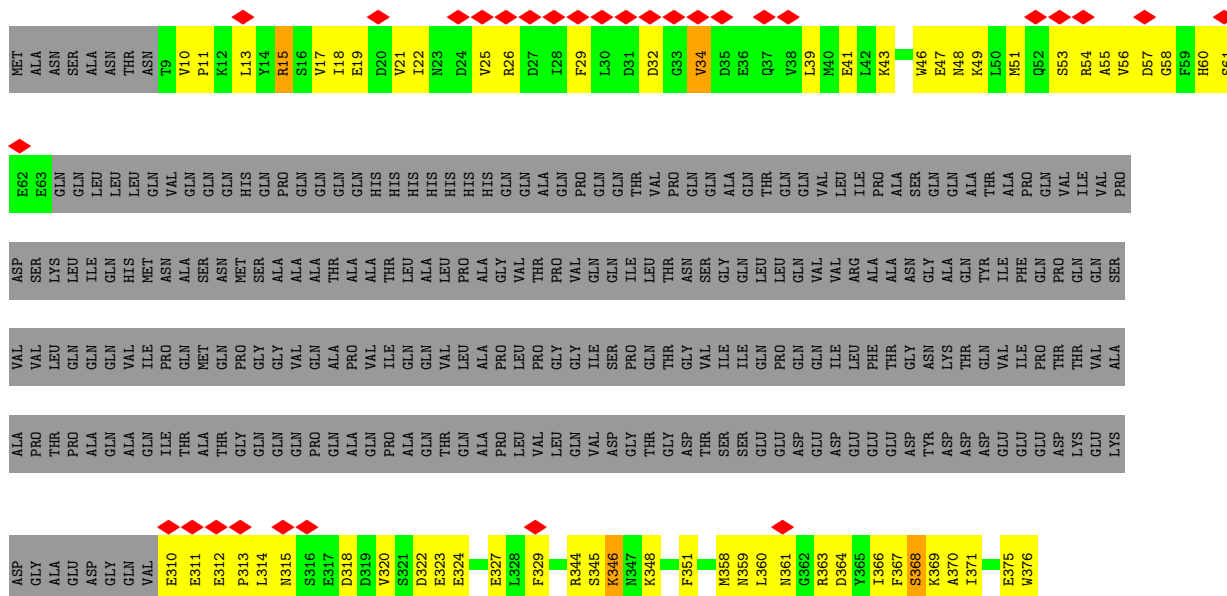


• Molecule 12: TATA-box-binding protein

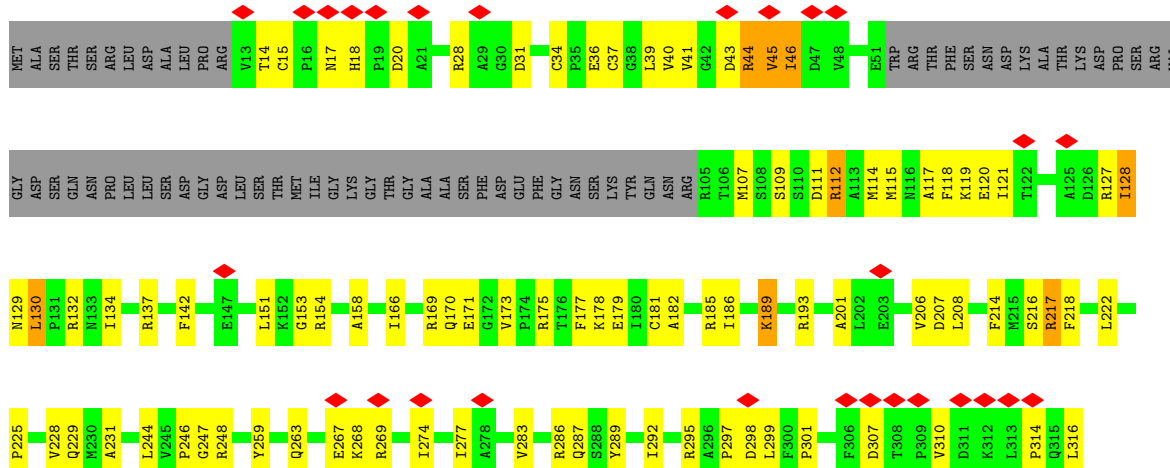




• Molecule 13: Transcription initiation factor IIA subunit 1

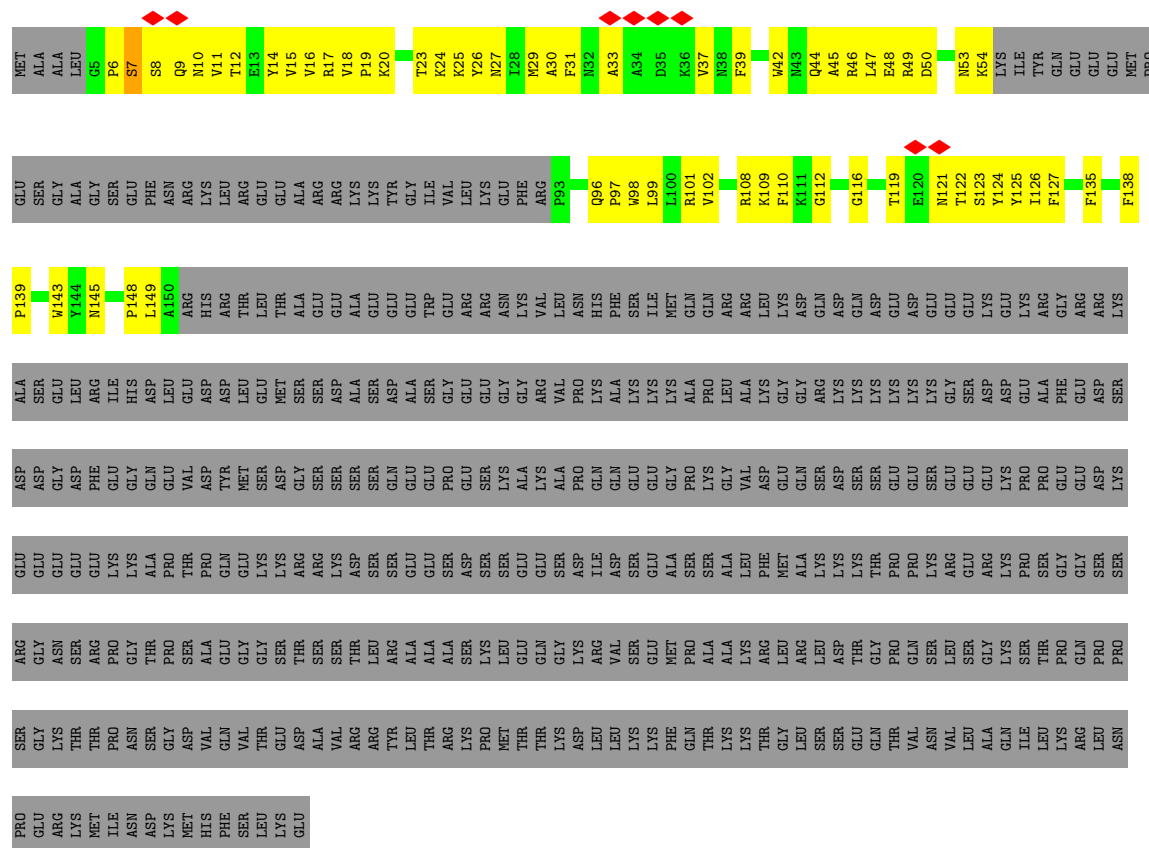


• Molecule 14: Transcription initiation factor IIB

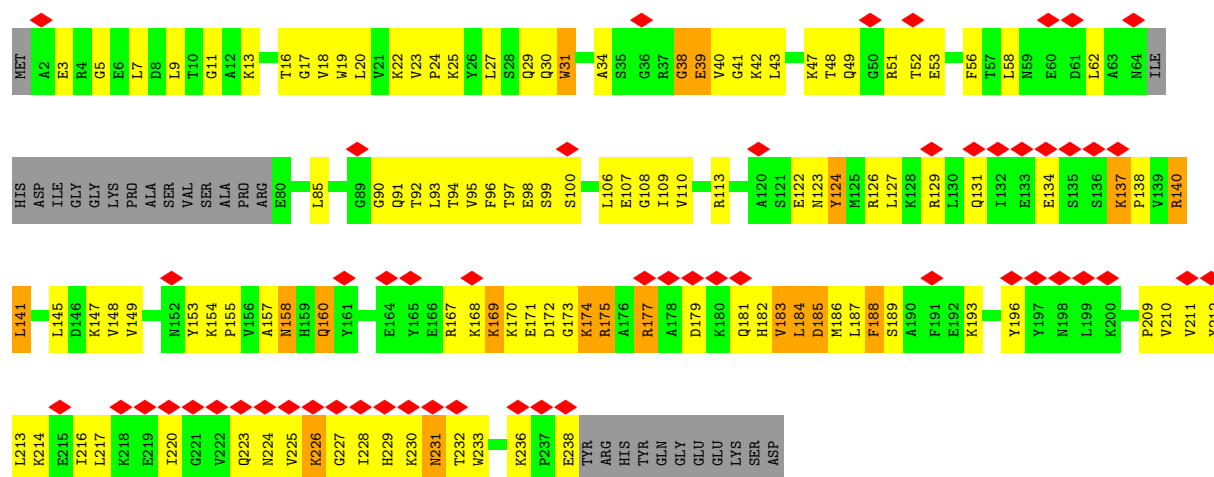


• Molecule 15: General transcription factor IIF subunit 1

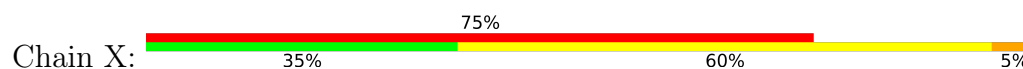




• Molecule 16: General transcription factor IIF subunit 2

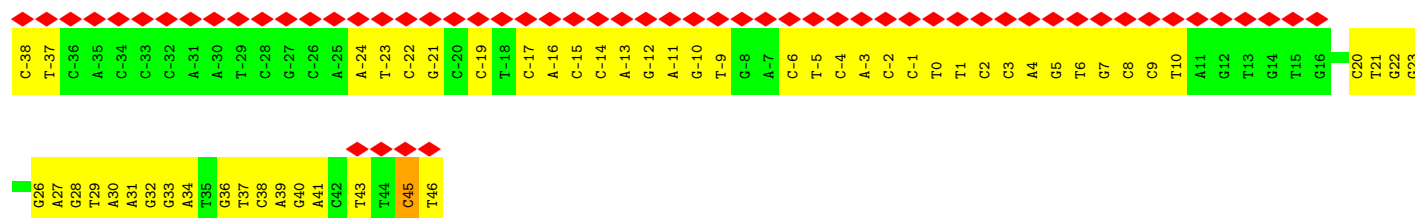


• Molecule 17: DNA (85-MER)

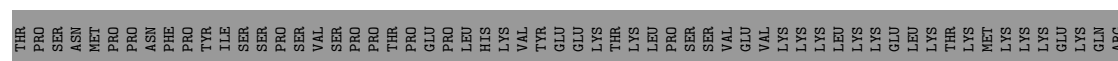
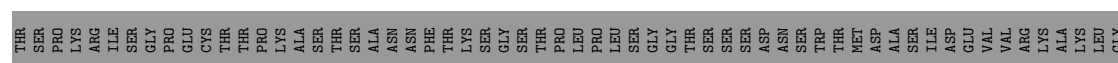
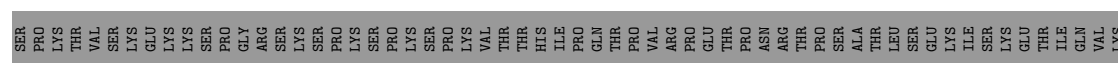
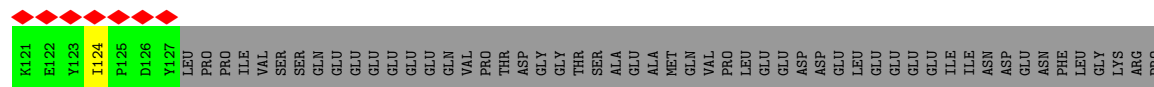
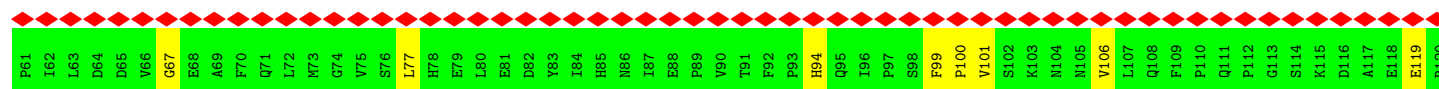


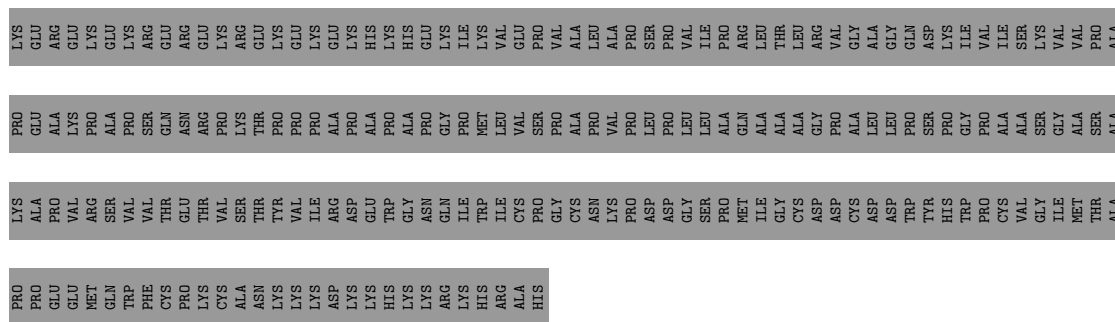


• Molecule 18: DNA (85-MER)

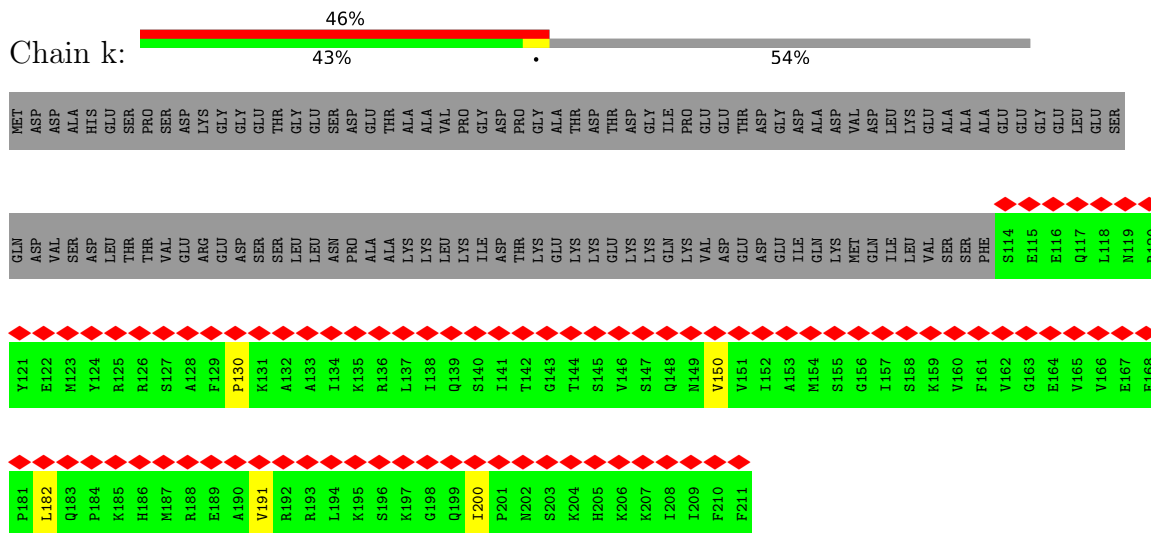


• Molecule 19: Transcription initiation factor TFIID subunit 3

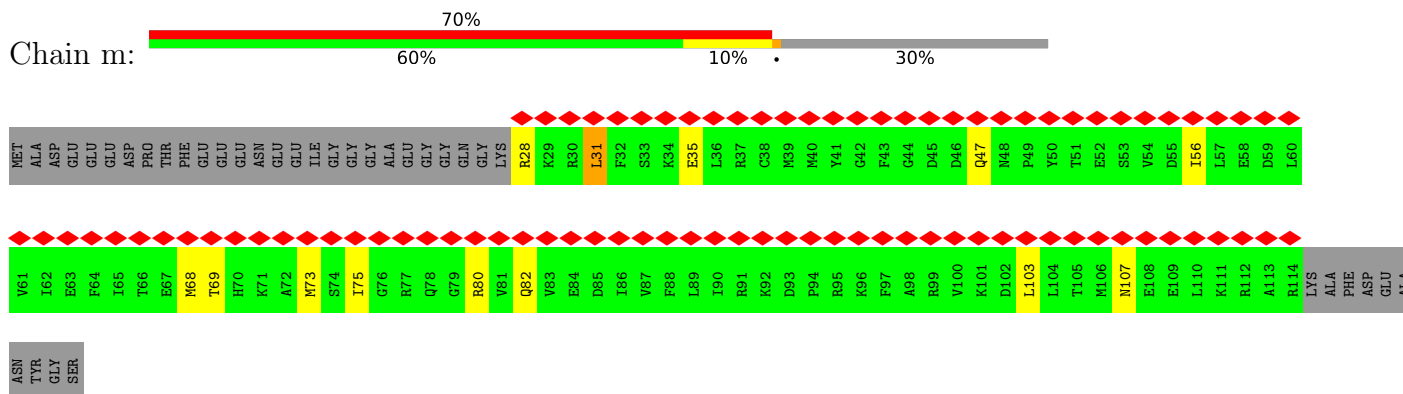




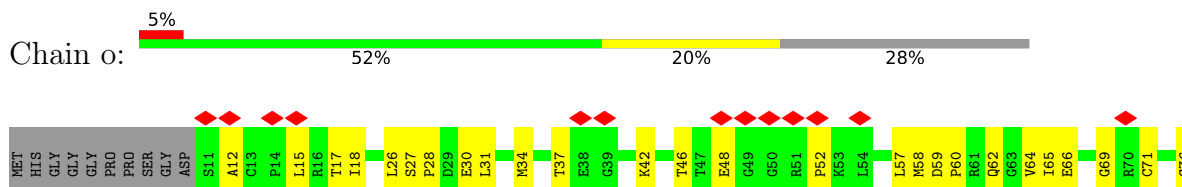
- Molecule 20: Transcription initiation factor TFIID subunit 11



- Molecule 21: Transcription initiation factor TFIID subunit 13

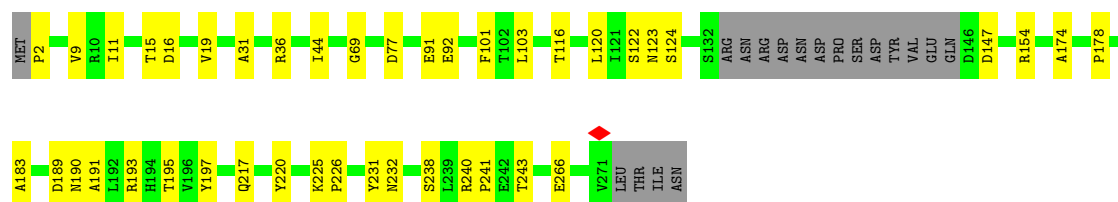


- Molecule 22: RPB1



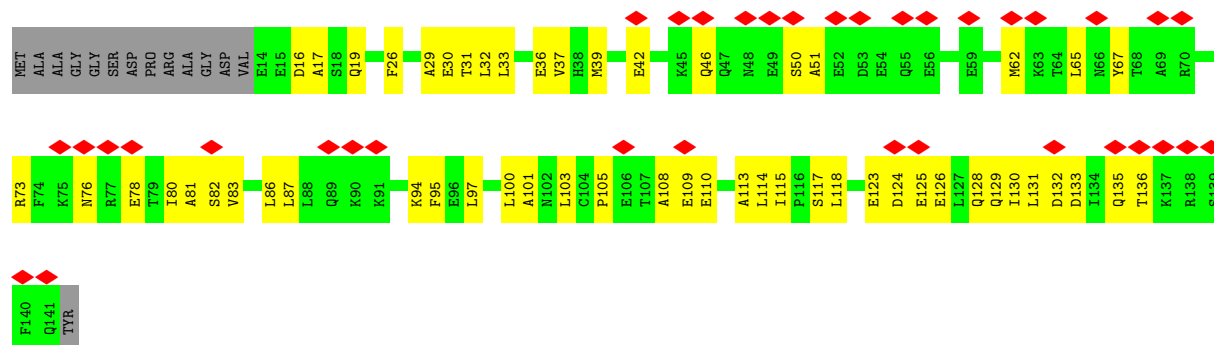


Chain q: 



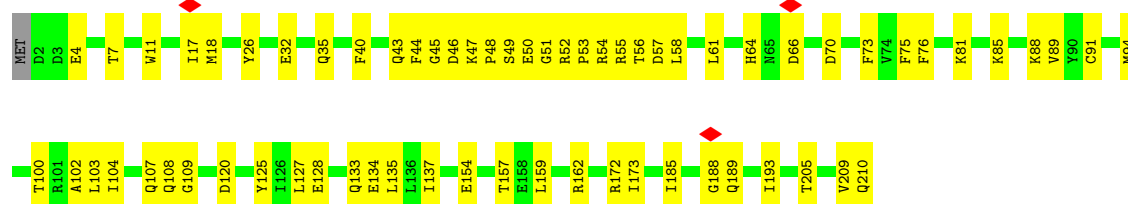
- Molecule 25: DNA-directed RNA polymerase II subunit RPB4

Chain r: 



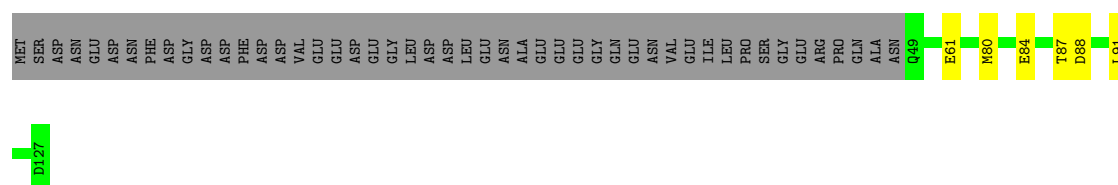
- Molecule 26: DNA-directed RNA polymerase II subunit E

Chain s: 



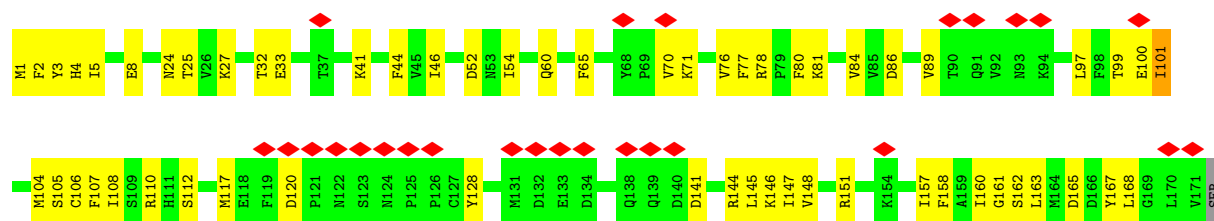
- Molecule 27: DNA-directed RNA polymerase II subunit F

Chain t: 



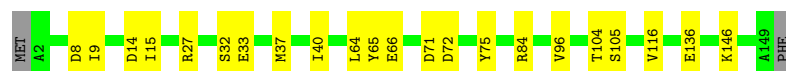
- Molecule 28: DNA-directed RNA polymerase II subunit RPB7

Chain u: 



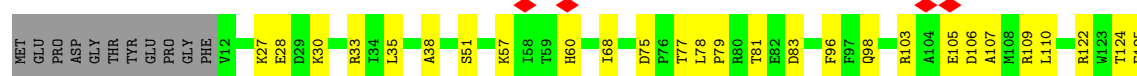
- Molecule 29: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v: 84% 15% .



- Molecule 30: DNA-directed RNA polymerase II subunit RPB9

Chain w: 70% 22% 9%



- Molecule 31: RPB10

Chain x: 82% 13% .



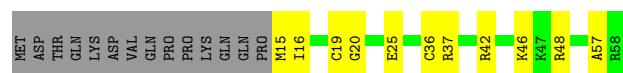
- Molecule 32: RNA_pol_L_2 domain-containing protein

Chain y: 85% 15%



- Molecule 33: RPB12

Chain z: 57% 19% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.689	Depositor
Minimum map value	-0.746	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.19	Depositor
Map size ($\text{\AA}$)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.70	0/5046	0.96	7/6810 (0.1%)
2	B	0.48	1/7993 (0.0%)	0.70	7/10836 (0.1%)
3	D	0.61	0/1379	0.92	5/1843 (0.3%)
3	d	0.25	0/1321	0.47	0/1772
4	E	0.34	0/4469	0.58	1/6050 (0.0%)
4	e	0.29	0/4433	0.53	0/6004
5	F	0.68	1/3139 (0.0%)	1.02	5/4264 (0.1%)
5	f	0.47	0/3140	0.80	6/4268 (0.1%)
6	G	0.68	0/1199	0.95	1/1612 (0.1%)
7	H	0.55	0/1673	0.80	3/2285 (0.1%)
8	I	0.33	0/981	0.54	1/1332 (0.1%)
8	i	0.21	0/989	0.40	0/1343
9	J	0.28	0/724	0.50	0/982
9	j	0.22	0/775	0.44	0/1049
10	L	0.49	0/630	0.86	1/852 (0.1%)
10	l	0.32	0/888	0.61	0/1194
11	O	0.73	0/781	1.19	8/1061 (0.8%)
12	P	0.93	0/1438	1.25	4/1935 (0.2%)
13	Q	0.58	0/1013	1.02	3/1366 (0.2%)
14	R	0.48	0/1966	1.04	9/2655 (0.3%)
15	S	0.35	0/896	0.79	0/1213
16	T	0.74	0/1817	1.15	9/2445 (0.4%)
17	X	0.39	0/1966	0.72	4/3034 (0.1%)
18	Y	0.37	0/1942	0.68	2/2993 (0.1%)
19	c	0.48	0/1035	0.67	0/1406
20	k	0.29	0/799	0.53	1/1070 (0.1%)
21	m	0.31	0/733	0.55	0/977
22	o	0.31	0/11516	0.53	2/15548 (0.0%)
23	p	0.31	0/9243	0.47	1/12475 (0.0%)
24	q	0.32	0/2102	0.44	0/2857
25	r	0.17	0/1019	0.45	0/1374
26	s	0.22	0/1751	0.47	0/2366

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	t	0.29	0/645	0.48	0/871
28	u	0.20	0/1365	0.45	0/1853
29	v	0.29	0/1207	0.47	0/1628
30	w	0.23	0/948	0.45	0/1284
31	x	0.36	0/516	0.44	0/696
32	y	0.31	0/956	0.47	0/1294
33	z	0.28	0/377	0.43	0/500
All	All	0.44	2/84810 (0.0%)	0.70	80/115397 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	ASN	C-O	-6.04	1.18	1.24
5	F	395	ARG	C-O	5.72	1.32	1.24

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	491	HIS	N-CA-C	-9.45	100.97	111.28
14	R	112	ARG	N-CA-C	-9.32	101.12	111.28
14	R	130	LEU	CA-C-N	9.13	129.21	119.90
14	R	130	LEU	C-N-CA	9.13	129.21	119.90
11	O	58	PHE	N-CA-C	9.11	120.26	108.24
5	f	149	PRO	O-C-N	9.08	125.49	121.31
3	D	993	GLN	N-CA-C	8.41	120.45	111.28
1	A	356	PRO	N-CA-C	7.90	124.79	114.68
7	H	163	PRO	N-CA-C	7.38	124.02	113.47
12	P	167	ASN	CB-CA-C	-7.37	96.59	109.86
11	O	62	LEU	N-CA-C	7.36	120.49	110.55
2	B	495	GLN	N-CA-C	-7.19	104.51	113.28
17	X	-35	DA	C4'-C3'-O3'	-7.15	99.27	110.00
1	A	715	PRO	N-CA-C	-7.13	100.05	111.03
5	F	271	VAL	N-CA-C	-7.05	106.13	112.90
22	o	1144	LEU	N-CA-C	7.01	118.72	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	k	180	PRO	N-CA-C	6.67	118.83	110.70
5	f	326	HIS	N-CA-C	-6.65	104.26	112.38
3	D	994	GLN	N-CA-C	6.63	118.51	111.28
1	A	396	LEU	N-CA-C	-6.61	104.96	113.16
5	f	319	LEU	N-CA-C	-6.57	103.95	112.68
14	R	45	VAL	N-CA-C	-6.51	106.33	113.43
1	A	641	LYS	N-CA-C	-6.41	104.15	112.23
7	H	114	SER	N-CA-C	-6.41	105.49	113.38
16	T	129	ARG	CA-C-N	6.39	128.84	120.28
16	T	129	ARG	C-N-CA	6.39	128.84	120.28
14	R	34	CYS	CA-C-N	6.29	126.03	119.05
14	R	34	CYS	C-N-CA	6.29	126.03	119.05
16	T	39	GLU	N-CA-C	-6.25	99.52	109.76
1	A	1205	PHE	CA-CB-CG	-6.17	107.63	113.80
18	Y	45	DC	C2'-C3'-O3'	-6.11	102.33	111.50
14	R	217	ARG	N-CA-C	6.09	117.92	111.28
17	X	19	DG	C2'-C3'-O3'	-6.03	102.46	111.50
8	I	87	PRO	O-C-N	-6.01	118.33	121.15
3	D	963	ARG	N-CA-C	-6.00	104.74	111.28
2	B	181	GLY	CA-C-O	-5.99	118.00	122.37
5	f	255	MET	N-CA-C	-5.99	104.81	114.09
17	X	21	DC	C2'-C3'-O3'	-5.97	102.54	111.50
14	R	44	ARG	N-CA-C	-5.95	105.60	112.86
13	Q	368	SER	N-CA-C	-5.87	105.21	112.90
23	p	823	PHE	CB-CA-C	-5.84	101.67	110.90
3	D	946	PHE	CA-CB-CG	5.82	119.62	113.80
16	T	188	PHE	N-CA-C	-5.81	105.03	111.36
5	F	316	GLN	CB-CA-C	5.71	120.10	110.79
12	P	298	PRO	N-CA-C	-5.66	100.81	112.47
5	F	324	ASP	N-CA-C	-5.65	105.21	111.71
2	B	583	GLU	CB-CA-C	-5.64	101.44	110.79
16	T	124	TYR	N-CA-C	5.63	117.41	111.28
5	f	150	PRO	N-CA-C	5.58	117.51	110.70
2	B	264	GLU	N-CA-C	-5.57	106.16	113.17
11	O	6	TYR	N-CA-C	5.53	119.12	112.93
14	R	307	ASP	N-CA-C	-5.50	106.93	113.97
16	T	157	ALA	N-CA-C	-5.49	100.23	109.07
3	D	1056	THR	CB-CA-C	5.47	118.75	109.84
16	T	183	VAL	O-C-N	5.46	127.57	121.94
22	o	1145	GLY	CA-C-O	-5.46	116.82	122.28
12	P	207	PRO	N-CA-C	-5.42	101.32	112.47
6	G	183	ILE	N-CA-C	-5.40	102.55	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	329	LEU	N-CA-C	-5.32	106.49	112.87
2	B	491	HIS	CB-CA-C	5.31	119.61	110.79
1	A	793	GLY	O-C-N	-5.29	116.48	121.77
16	T	31	TRP	N-CA-C	5.27	117.77	111.71
5	F	272	VAL	N-CA-C	-5.26	105.25	110.62
5	F	149	PRO	N-CA-C	5.24	117.10	110.70
12	P	205	ARG	CB-CA-C	-5.24	101.12	110.70
11	O	57	ASN	CA-C-O	-5.18	115.05	121.06
11	O	58	PHE	CB-CA-C	-5.15	101.55	112.78
11	O	27	GLN	CA-C-N	-5.12	114.13	122.57
11	O	27	GLN	C-N-CA	-5.12	114.13	122.57
10	L	66	LEU	N-CA-C	-5.11	105.79	111.36
7	H	220	THR	N-CA-C	-5.10	106.47	113.30
18	Y	43	DT	C2'-C3'-O3'	-5.10	103.85	111.50
13	Q	15	ARG	N-CA-C	-5.10	105.61	111.07
4	E	795	GLY	N-CA-C	5.08	125.23	113.18
1	A	498	PRO	N-CA-CB	5.08	108.58	103.25
13	Q	346	LYS	CB-CA-C	-5.08	110.74	116.63
17	X	-40	DC	C2'-C3'-O3'	-5.07	103.90	111.50
16	T	185	ASP	N-CA-C	-5.04	105.48	110.97
11	O	9	THR	N-CA-C	-5.04	101.76	109.41
2	B	541	ARG	CB-CA-C	-5.01	101.72	110.09

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	821	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4927	0	4869	327	0
2	B	7796	0	7751	216	0
3	D	1366	0	1390	154	0
3	d	1307	0	1318	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	4364	0	4244	103	0
4	e	4327	0	4197	47	0
5	F	3081	0	3014	429	0
5	f	3081	0	3012	89	0
6	G	1180	0	1235	59	0
7	H	1633	0	1621	236	0
8	I	959	0	968	206	0
8	i	967	0	977	46	0
9	J	709	0	710	101	0
9	j	759	0	759	17	0
10	L	622	0	620	117	0
10	l	876	0	891	81	0
11	O	771	0	763	185	0
12	P	1412	0	1506	105	0
13	Q	996	0	926	176	0
14	R	1938	0	1977	109	0
15	S	872	0	848	233	0
16	T	1788	0	1819	359	0
17	X	1751	0	954	96	0
18	Y	1734	0	956	99	0
19	c	1011	0	975	26	0
20	k	785	0	818	8	0
21	m	724	0	744	13	0
22	o	11308	0	11428	290	0
23	p	9062	0	9107	223	0
24	q	2059	0	2008	32	0
25	r	1005	0	964	65	0
26	s	1720	0	1737	50	0
27	t	635	0	665	5	0
28	u	1334	0	1333	70	0
29	v	1186	0	1147	14	0
30	w	927	0	859	19	0
31	x	507	0	523	7	0
32	y	937	0	959	13	0
33	z	372	0	379	10	0
34	R	1	0	0	0	0
34	o	2	0	0	0	0
34	p	1	0	0	0	0
34	q	1	0	0	0	0
34	w	2	0	0	0	0
34	x	1	0	0	0	0
34	z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	o	1	0	0	0	0
All	All	82798	0	80971	3113	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 19.

All (3113) 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)
16:T:124:TYR:CE1	23:p:596:ILE:HD13	1.22	1.67
5:F:47:ILE:HG21	8:I:19:MET:SD	1.09	1.65
16:T:124:TYR:CG	23:p:596:ILE:HD11	1.20	1.62
5:F:48:LYS:CG	8:I:22:ILE:HG23	1.17	1.60
8:I:60:HIS:CE1	10:L:118:LEU:CD2	1.84	1.59
16:T:124:TYR:CD1	23:p:596:ILE:CD1	1.80	1.59
5:F:47:ILE:CD1	8:I:19:MET:HE1	1.11	1.59
16:T:124:TYR:CD1	23:p:596:ILE:HD11	1.37	1.58
5:F:312:ILE:HG13	5:F:334:ALA:CB	1.11	1.57
11:O:88:ILE:HG21	13:Q:360:LEU:CB	1.27	1.55
16:T:124:TYR:CE2	23:p:596:ILE:HG12	1.03	1.55
5:F:15:PRO:CB	8:I:14:LYS:HZ1	1.15	1.55
11:O:22:LEU:CB	11:O:28:ILE:HG12	1.35	1.55
5:F:48:LYS:HG3	8:I:22:ILE:CG2	1.11	1.55
8:I:60:HIS:CE1	10:L:118:LEU:HD22	1.36	1.55
16:T:124:TYR:CZ	23:p:596:ILE:HG12	1.42	1.54
8:i:73:LEU:HD22	10:l:105:HIS:CE1	1.04	1.54
1:A:1169:ARG:CB	1:A:1181:ARG:NH1	1.69	1.54
15:S:8:SER:CB	16:T:49:GLN:HA	1.36	1.54
16:T:124:TYR:CE2	23:p:596:ILE:CG1	1.91	1.54
11:O:55:ARG:NH2	13:Q:369:LYS:CB	1.68	1.53
15:S:8:SER:HB3	16:T:49:GLN:CA	1.34	1.53
5:F:47:ILE:HD13	8:I:19:MET:CE	1.04	1.51
8:i:60:HIS:CE1	10:l:106:ARG:NH2	1.75	1.50
3:D:881:ARG:NH2	10:L:57:VAL:CG2	1.75	1.50
12:P:243:LYS:NZ	13:Q:318:ASP:HA	1.17	1.46
5:F:312:ILE:CG1	5:F:334:ALA:CB	1.90	1.46
8:i:73:LEU:CD2	10:l:105:HIS:CE1	1.95	1.45
5:F:211:ARG:HG2	7:H:165:TYR:CD2	1.51	1.45
11:O:53:ARG:CB	13:Q:368:SER:HA	1.46	1.44
5:F:47:ILE:CG2	8:I:19:MET:SD	2.03	1.42
10:L:106:ARG:HH11	10:L:114:LYS:NZ	1.00	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:881:ARG:NH2	10:L:57:VAL:HG22	1.15	1.42
5:F:211:ARG:CG	7:H:165:TYR:HD2	1.29	1.42
15:S:8:SER:O	16:T:48:THR:CA	1.69	1.40
16:T:124:TYR:CE1	23:p:596:ILE:CD1	1.92	1.40
10:L:106:ARG:NH1	10:L:114:LYS:HZ2	1.20	1.39
16:T:124:TYR:CZ	23:p:596:ILE:CG1	2.05	1.39
13:Q:47:GLU:OE2	13:Q:60:HIS:CE1	1.75	1.38
11:O:53:ARG:CB	13:Q:368:SER:CA	2.00	1.38
1:A:639:LEU:HD21	1:A:774:ARG:CG	1.55	1.37
11:O:88:ILE:CG2	13:Q:360:LEU:HB3	1.55	1.37
5:F:412:LEU:HD13	5:F:417:ARG:CD	1.55	1.36
10:L:106:ARG:HH12	10:L:114:LYS:CD	1.35	1.36
8:i:73:LEU:HD22	10:l:105:HIS:NE2	1.39	1.36
1:A:1169:ARG:CD	1:A:1181:ARG:HH11	1.37	1.35
5:F:71:ILE:HB	8:I:38:GLN:NE2	1.39	1.35
5:F:43:VAL:CG2	8:I:43:ALA:HB1	1.55	1.34
11:O:79:VAL:O	11:O:90:VAL:CG1	1.76	1.34
15:S:17:ARG:HG2	16:T:39:GLU:CG	1.55	1.33
5:F:68:THR:HG21	8:I:34:ARG:NH1	1.37	1.33
5:F:67:THR:HA	8:I:32:GLU:CD	1.53	1.33
5:F:15:PRO:CB	8:I:14:LYS:NZ	1.76	1.32
15:S:8:SER:HA	16:T:48:THR:O	1.23	1.32
5:F:312:ILE:CG1	5:F:334:ALA:HB1	1.53	1.31
5:F:211:ARG:CG	7:H:165:TYR:CD2	2.09	1.30
15:S:17:ARG:HG2	16:T:39:GLU:CB	1.61	1.30
5:F:370:TRP:CH2	5:F:406:VAL:HG11	1.65	1.30
12:P:243:LYS:HZ1	13:Q:318:ASP:CA	1.43	1.30
1:A:469:PRO:HA	7:H:166:ARG:NH1	1.44	1.30
1:A:1169:ARG:CG	1:A:1181:ARG:NH1	1.95	1.30
1:A:1190:VAL:CG2	6:G:162:VAL:HG13	1.61	1.30
11:O:22:LEU:CB	11:O:28:ILE:CG1	2.09	1.30
12:P:274:VAL:CG1	14:R:208:LEU:HD11	1.58	1.30
11:O:22:LEU:HB2	11:O:28:ILE:CD1	1.61	1.29
11:O:53:ARG:C	13:Q:368:SER:HB3	1.55	1.29
2:B:848:HIS:CD2	7:H:226:ALA:HB2	1.66	1.29
5:F:15:PRO:HB3	8:I:14:LYS:NZ	0.98	1.28
11:O:32:LEU:HD13	13:Q:32:ASP:OD2	1.28	1.28
11:O:53:ARG:CB	13:Q:367:PHE:C	2.05	1.28
4:E:615:ASP:OD1	8:I:114:ARG:HB3	1.34	1.27
2:B:762:ASP:OD1	2:B:768:PRO:HG3	1.29	1.27
4:E:694:LEU:HD13	4:E:703:MET:CE	1.64	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:87:HIS:HB3	9:J:212:LYS:NZ	1.49	1.26
10:L:101:GLN:O	10:L:105:HIS:CD2	1.88	1.26
10:L:106:ARG:NH1	10:L:114:LYS:HD2	1.47	1.26
8:i:73:LEU:CD2	10:l:105:HIS:NE2	1.95	1.26
3:D:881:ARG:HH21	10:L:57:VAL:CG1	1.50	1.25
5:F:312:ILE:CG1	5:F:334:ALA:HB3	1.59	1.25
11:O:55:ARG:CZ	13:Q:369:LYS:HB2	1.64	1.25
1:A:488:ALA:HB1	5:f:271:VAL:CG2	1.65	1.25
1:A:1169:ARG:CD	1:A:1181:ARG:NH1	2.00	1.25
15:S:18:VAL:C	16:T:38:GLY:O	1.78	1.25
16:T:124:TYR:CD1	23:p:596:ILE:HD13	1.57	1.25
10:l:101:GLN:O	10:l:105:HIS:CD2	1.90	1.25
11:O:88:ILE:CD1	13:Q:360:LEU:HB2	1.67	1.25
15:S:31:PHE:O	16:T:92:THR:N	1.69	1.25
5:F:412:LEU:CD1	5:F:417:ARG:HD2	1.67	1.24
5:F:370:TRP:CH2	5:F:406:VAL:CG1	2.20	1.24
3:D:891:ILE:CG2	10:L:111:LEU:HB2	1.65	1.24
5:F:219:GLU:CG	7:H:156:PRO:HB2	1.68	1.24
11:O:22:LEU:HB2	11:O:28:ILE:CG1	1.65	1.23
11:O:53:ARG:O	13:Q:368:SER:CB	1.83	1.23
2:B:848:HIS:NE2	7:H:225:THR:HG23	1.51	1.23
1:A:1185:VAL:CG1	1:A:1191:ILE:HG12	1.67	1.23
10:l:87:ILE:O	10:l:91:PHE:CD2	1.90	1.23
15:S:8:SER:O	16:T:48:THR:HA	1.08	1.22
10:L:106:ARG:NH1	10:L:114:LYS:NZ	1.81	1.21
17:X:-9:DG:N2	18:Y:9:DC:N3	1.85	1.21
5:F:68:THR:N	8:I:32:GLU:OE1	1.73	1.21
10:L:106:ARG:NH1	10:L:114:LYS:CD	1.98	1.21
12:P:188:ARG:NH1	13:Q:322:ASP:CG	1.98	1.21
8:i:60:HIS:ND1	10:l:106:ARG:NH2	1.78	1.21
11:O:88:ILE:HG23	13:Q:361:ASN:ND2	1.54	1.21
16:T:124:TYR:OH	23:p:596:ILE:HG23	1.41	1.20
11:O:55:ARG:HH12	13:Q:369:LYS:CE	1.55	1.20
5:F:213:ILE:HB	7:H:163:PRO:O	1.38	1.19
1:A:1185:VAL:CG1	1:A:1191:ILE:CG1	2.20	1.19
5:F:308:VAL:CB	5:F:337:VAL:HG11	1.73	1.19
11:O:53:ARG:CB	13:Q:367:PHE:O	1.91	1.19
15:S:15:VAL:CG1	16:T:39:GLU:OE2	1.89	1.19
4:E:694:LEU:CD1	4:E:703:MET:HE1	1.72	1.19
11:O:53:ARG:O	13:Q:368:SER:HB3	1.01	1.19
12:P:188:ARG:NH2	13:Q:323:GLU:O	1.75	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:THR:HG23	7:H:213:LEU:HD23	1.25	1.18
2:B:846:TYR:CD1	7:H:227:LEU:O	1.95	1.18
11:O:79:VAL:O	11:O:90:VAL:HG12	1.33	1.18
1:A:1169:ARG:HD3	1:A:1181:ARG:NH1	1.53	1.18
3:D:889:HIS:HA	10:L:104:ARG:NH2	1.57	1.18
1:A:564:PRO:HG2	2:B:744:PHE:CE2	1.79	1.18
8:i:60:HIS:CG	10:l:106:ARG:HH21	1.61	1.18
3:D:889:HIS:C	10:L:104:ARG:HH21	1.51	1.17
1:A:1169:ARG:CB	1:A:1181:ARG:CZ	2.22	1.17
5:F:335:ARG:HH11	5:F:382:GLU:HA	1.09	1.17
15:S:18:VAL:HG23	16:T:40:VAL:HG22	1.23	1.17
15:S:135:PHE:CE2	16:T:43:LEU:HD23	1.80	1.16
1:A:488:ALA:HB1	5:f:271:VAL:HG23	1.24	1.16
12:P:243:LYS:NZ	13:Q:318:ASP:CA	2.01	1.16
11:O:65:TYR:CE1	12:P:191:GLU:HG2	1.81	1.16
1:A:639:LEU:HD21	1:A:774:ARG:HG2	1.17	1.15
5:F:213:ILE:HG21	7:H:163:PRO:CB	1.75	1.15
5:F:213:ILE:HG21	7:H:163:PRO:HB3	1.15	1.15
5:F:14:LEU:HD13	8:I:15:ASP:OD1	1.47	1.15
5:F:71:ILE:CB	8:I:38:GLN:HE21	1.59	1.14
5:F:320:ARG:HD2	5:F:321:PRO:HD3	1.21	1.14
11:O:53:ARG:CB	13:Q:368:SER:N	2.07	1.14
12:P:214:PHE:HD2	17:X:-24:DG:H4'	1.08	1.14
15:S:17:ARG:CA	16:T:39:GLU:HA	1.78	1.14
15:S:18:VAL:HG23	16:T:40:VAL:CG2	1.74	1.14
1:A:1190:VAL:HG22	6:G:162:VAL:HG13	1.24	1.14
4:E:704:VAL:HG11	4:E:747:LEU:HG	1.26	1.14
5:F:316:GLN:NE2	5:F:320:ARG:HA	1.61	1.14
10:L:106:ARG:NH1	10:L:114:LYS:CE	2.10	1.14
4:E:696:TRP:CE3	4:E:703:MET:HB3	1.82	1.14
5:F:43:VAL:HG21	8:I:43:ALA:HB1	1.21	1.13
11:O:22:LEU:HB3	11:O:28:ILE:HG12	1.22	1.13
14:R:182:ALA:HB2	16:T:153:TYR:O	1.47	1.13
5:F:244:GLN:OE1	7:H:133:ALA:HB3	1.48	1.13
14:R:175:ARG:HH22	23:p:102:ASP:HA	0.99	1.13
3:D:881:ARG:HH21	10:L:57:VAL:HG13	1.06	1.12
5:F:43:VAL:CG2	8:I:43:ALA:CB	2.27	1.12
1:A:1165:LEU:HB2	1:A:1191:ILE:CG2	1.78	1.12
3:D:891:ILE:HG21	10:L:111:LEU:HD22	1.31	1.12
3:D:1083:PHE:HE2	4:E:585:ASN:ND2	1.47	1.12
11:O:65:TYR:HE1	12:P:191:GLU:CG	1.60	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:178:LYS:HB3	16:T:154:LYS:HB3	1.30	1.12
1:A:784:GLN:H	1:A:1073:GLN:NE2	1.48	1.12
5:F:51:ALA:CB	8:I:23:LEU:CD2	2.28	1.11
11:O:55:ARG:NH2	13:Q:369:LYS:HB2	1.44	1.11
1:A:639:LEU:CD2	1:A:774:ARG:HG2	1.81	1.11
12:P:274:VAL:HG11	14:R:208:LEU:HD11	1.22	1.11
15:S:18:VAL:HB	16:T:40:VAL:HG13	1.27	1.11
1:A:1169:ARG:HB3	1:A:1181:ARG:NH1	1.49	1.11
11:O:88:ILE:HD13	13:Q:360:LEU:HB2	1.13	1.10
1:A:638:PRO:CG	6:G:39:LEU:HD23	1.82	1.10
5:F:14:LEU:HD23	8:I:18:MET:HB3	1.23	1.10
1:A:1185:VAL:HG11	1:A:1191:ILE:HG12	1.33	1.10
2:B:846:TYR:C	7:H:226:ALA:O	1.93	1.10
11:O:17:GLU:HB2	13:Q:49:LYS:HZ3	1.03	1.10
8:i:73:LEU:HD22	10:l:105:HIS:ND1	1.66	1.10
5:F:15:PRO:HG3	8:I:14:LYS:HG3	1.11	1.09
11:O:65:TYR:CE1	12:P:191:GLU:CG	2.34	1.09
15:S:8:SER:O	16:T:48:THR:C	1.93	1.09
15:S:125:TYR:CE2	16:T:31:TRP:CE3	2.39	1.09
16:T:124:TYR:CG	23:p:596:ILE:CD1	2.11	1.09
1:A:573:TYR:HA	2:B:657:ARG:HD3	1.35	1.09
3:D:881:ARG:HH22	10:L:57:VAL:CG2	1.47	1.09
5:F:67:THR:HA	8:I:32:GLU:CG	1.81	1.09
11:O:88:ILE:HD12	13:Q:360:LEU:HD12	1.30	1.09
13:Q:47:GLU:OE2	13:Q:60:HIS:ND1	1.85	1.09
15:S:44:GLN:C	16:T:9:LEU:HD11	1.77	1.09
15:S:122:THR:HG22	16:T:24:PRO:HA	1.29	1.09
7:H:116:ARG:HD3	9:J:126:TYR:HE1	1.09	1.08
15:S:135:PHE:HE2	16:T:43:LEU:HD23	1.02	1.08
12:P:214:PHE:CD2	17:X:-24:DG:C4'	2.36	1.08
1:A:1165:LEU:HB2	1:A:1191:ILE:HG21	1.34	1.08
5:F:17:GLU:OE2	8:I:14:LYS:HE3	1.54	1.08
5:F:219:GLU:HG2	7:H:156:PRO:CB	1.82	1.08
11:O:88:ILE:CG2	13:Q:360:LEU:CB	2.17	1.08
16:T:124:TYR:CD2	23:p:596:ILE:CG1	2.36	1.07
16:T:124:TYR:CD2	23:p:596:ILE:HD11	1.87	1.07
1:A:575:PRO:HD3	2:B:608:ASN:HD22	0.98	1.07
1:A:753:TYR:CD2	1:A:1077:LEU:HB3	1.86	1.07
4:E:697:ASP:O	4:E:701:GLY:HA2	1.53	1.07
5:F:51:ALA:HB1	8:I:23:LEU:HD22	1.33	1.07
12:P:214:PHE:CD2	17:X:-24:DG:H4'	1.89	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:320:ARG:HD3	5:F:415:ILE:HB	1.34	1.07
5:F:90:GLU:OE1	9:J:208:GLY:O	1.70	1.07
5:F:89:GLN:CD	9:J:210:ASN:HD22	1.62	1.06
5:F:308:VAL:HG21	5:F:337:VAL:CG1	1.84	1.06
19:c:67:GLY:HA3	9:j:116:LEU:CD1	1.84	1.06
3:D:917:ILE:CD1	3:D:1058:VAL:HG21	1.84	1.06
5:F:43:VAL:HG22	8:I:43:ALA:HB1	1.35	1.06
5:F:370:TRP:CZ2	5:F:406:VAL:HG12	1.91	1.06
11:O:55:ARG:CZ	13:Q:369:LYS:CB	2.26	1.06
5:F:15:PRO:CG	8:I:14:LYS:HZ2	1.67	1.06
5:F:68:THR:CG2	8:I:34:ARG:NH1	2.18	1.06
14:R:175:ARG:NH2	23:p:102:ASP:HA	1.68	1.06
5:F:15:PRO:CG	8:I:14:LYS:HG3	1.85	1.06
7:H:111:ALA:O	9:J:126:TYR:CZ	2.10	1.05
7:H:116:ARG:HD3	9:J:126:TYR:CE1	1.91	1.05
15:S:125:TYR:CD2	16:T:31:TRP:HZ3	1.74	1.05
11:O:55:ARG:NH2	13:Q:369:LYS:HB3	1.47	1.05
1:A:486:TRP:HH2	5:f:358:THR:HB	1.17	1.05
1:A:1169:ARG:HB2	1:A:1181:ARG:NH1	1.69	1.05
5:F:68:THR:HG21	8:I:34:ARG:CZ	1.87	1.05
15:S:17:ARG:HG2	16:T:39:GLU:HB2	1.25	1.05
3:d:909:ARG:NE	10:l:91:PHE:CE1	2.23	1.05
11:O:23:ILE:HA	11:O:28:ILE:O	1.56	1.05
18:Y:9:DC:H2"	18:Y:10:DT:H71	1.37	1.05
10:L:106:ARG:HH11	10:L:114:LYS:CE	1.68	1.05
5:F:312:ILE:HG12	5:F:334:ALA:HB3	1.35	1.04
15:S:17:ARG:HA	16:T:39:GLU:HA	1.36	1.04
1:A:639:LEU:HD21	1:A:774:ARG:HG3	1.36	1.04
15:S:17:ARG:CG	16:T:39:GLU:HB2	1.88	1.04
17:X:-38:DG:N2	18:Y:39:DA:C6	2.25	1.04
1:A:1169:ARG:HB3	1:A:1181:ARG:CZ	1.81	1.04
15:S:18:VAL:N	16:T:38:GLY:O	1.89	1.04
3:D:889:HIS:CA	10:L:104:ARG:NH2	2.21	1.04
14:R:217:ARG:HH21	23:p:102:ASP:HB2	1.20	1.04
15:S:31:PHE:N	16:T:92:THR:O	1.88	1.04
1:A:575:PRO:HD3	2:B:608:ASN:ND2	1.73	1.03
12:P:214:PHE:CE2	17:X:-24:DG:O4'	2.11	1.03
15:S:8:SER:HA	16:T:48:THR:C	1.82	1.03
1:A:1169:ARG:HB2	1:A:1181:ARG:CZ	1.86	1.03
5:F:290:MET:SD	5:F:340:ILE:HG21	1.97	1.03
16:T:124:TYR:CZ	23:p:596:ILE:CD1	2.30	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:881:ARG:CG	10:L:57:VAL:HG11	1.87	1.03
11:O:79:VAL:O	11:O:90:VAL:HG13	1.54	1.03
15:S:45:ALA:CB	16:T:9:LEU:HD21	1.88	1.03
10:l:102:LEU:HA	10:l:105:HIS:HD2	1.18	1.03
1:A:1187:LYS:O	1:A:1191:ILE:HG13	1.59	1.03
5:F:67:THR:CA	8:I:32:GLU:CD	2.30	1.03
5:F:308:VAL:CG2	5:F:337:VAL:HG11	1.89	1.02
15:S:125:TYR:CE2	16:T:31:TRP:CZ3	2.48	1.02
1:A:1185:VAL:O	1:A:1191:ILE:HD11	1.58	1.01
5:F:14:LEU:HD13	8:I:15:ASP:CG	1.84	1.01
11:O:55:ARG:NH2	13:Q:369:LYS:C	2.18	1.01
15:S:18:VAL:HB	16:T:40:VAL:CG1	1.90	1.01
15:S:124:TYR:HE1	16:T:22:LYS:HG3	1.24	1.01
11:O:88:ILE:HG21	13:Q:360:LEU:HB2	1.26	1.01
1:A:639:LEU:HD13	1:A:643:ILE:HD11	1.42	1.01
11:O:17:GLU:CB	13:Q:49:LYS:HZ3	1.74	1.01
15:S:8:SER:CA	16:T:48:THR:C	2.33	1.01
2:B:735:ILE:CG2	7:H:176:ARG:NH1	2.24	1.01
3:D:917:ILE:HD12	3:D:1058:VAL:HG21	1.42	1.01
17:X:-35:DA:C2	18:Y:36:DG:N2	2.29	1.01
1:A:1198:ARG:NH1	6:G:181:TRP:CD2	2.28	1.00
4:E:615:ASP:OD1	8:I:114:ARG:CB	2.08	1.00
15:S:121:ASN:HA	16:T:25:LYS:HE2	1.42	1.00
16:T:140:ARG:HH22	23:p:89:GLU:HB3	1.24	1.00
10:l:87:ILE:O	10:l:91:PHE:HD2	1.36	1.00
15:S:31:PHE:HB2	16:T:92:THR:HB	1.00	1.00
5:F:211:ARG:HG3	7:H:165:TYR:CD2	1.96	1.00
15:S:124:TYR:CE1	16:T:22:LYS:HG3	1.97	0.99
18:Y:9:DC:H2"	18:Y:10:DT:C7	1.92	0.99
5:F:283:MET:SD	5:F:311:CYS:SG	2.60	0.99
5:F:308:VAL:HB	5:F:337:VAL:HG11	1.41	0.99
11:O:17:GLU:HB2	13:Q:49:LYS:NZ	1.77	0.99
11:O:22:LEU:HB2	11:O:28:ILE:HG12	1.23	0.99
1:A:575:PRO:HG3	2:B:610:GLU:HG2	1.41	0.99
16:T:147:LYS:HG3	16:T:148:VAL:H	1.24	0.99
15:S:17:ARG:CG	16:T:39:GLU:CG	2.40	0.99
14:R:154:ARG:NH1	18:Y:22:DG:H5"	1.76	0.99
15:S:8:SER:CA	16:T:48:THR:O	2.10	0.99
1:A:1185:VAL:HG12	1:A:1191:ILE:CG1	1.92	0.99
5:F:89:GLN:OE1	9:J:210:ASN:ND2	1.96	0.99
5:F:43:VAL:HG22	8:I:43:ALA:CB	1.91	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:45:ALA:HB3	16:T:9:LEU:HD21	1.42	0.98
16:T:124:TYR:CD2	23:p:596:ILE:HG12	1.95	0.98
8:I:60:HIS:CE1	10:L:118:LEU:HD21	1.98	0.98
11:O:65:TYR:HE1	12:P:191:GLU:HG2	1.15	0.98
1:A:1198:ARG:HH12	6:G:181:TRP:CG	1.81	0.98
3:D:1006:LEU:CD1	11:O:68:CYS:HB3	1.94	0.98
1:A:1016:GLU:HA	1:A:1019:LYS:HE3	1.42	0.98
2:B:848:HIS:CD2	7:H:226:ALA:CB	2.46	0.98
8:I:60:HIS:CE1	10:L:118:LEU:HD23	1.99	0.98
3:D:889:HIS:O	10:L:104:ARG:NH2	1.97	0.98
19:c:77:LEU:CD1	9:j:116:LEU:HD23	1.93	0.98
1:A:486:TRP:CH2	5:f:358:THR:HB	1.97	0.98
5:F:211:ARG:HB3	7:H:165:TYR:HE2	1.26	0.98
1:A:469:PRO:CA	7:H:166:ARG:NH1	2.27	0.98
11:O:55:ARG:NH2	13:Q:369:LYS:CA	2.27	0.97
12:P:188:ARG:NH1	13:Q:322:ASP:OD1	1.90	0.97
16:T:122:GLU:CD	16:T:126:ARG:HH11	1.72	0.97
5:F:48:LYS:HG3	8:I:22:ILE:HG21	1.44	0.97
13:Q:47:GLU:CD	13:Q:60:HIS:ND1	2.23	0.97
8:i:60:HIS:CE1	10:l:106:ARG:CZ	2.47	0.97
7:H:106:THR:OG1	9:J:161:LYS:NZ	1.98	0.97
12:P:257:ASN:HB2	17:X:-27:DT:H5"	1.45	0.97
4:E:696:TRP:HA	4:E:703:MET:HA	1.43	0.97
2:B:834:THR:HG23	7:H:213:LEU:CD2	1.95	0.96
5:F:71:ILE:HB	8:I:38:GLN:HE21	0.82	0.96
5:F:316:GLN:N	5:F:327:TRP:HH2	1.54	0.96
1:A:725:CYS:SG	1:A:725:CYS:O	2.22	0.96
11:O:22:LEU:HB3	11:O:28:ILE:CG1	1.80	0.96
5:F:15:PRO:HG3	8:I:14:LYS:CG	1.94	0.96
7:H:119:ILE:O	9:J:131:PRO:HG3	1.63	0.96
1:A:1190:VAL:HG22	6:G:162:VAL:CG1	1.96	0.96
5:F:370:TRP:CZ2	5:F:406:VAL:CG1	2.47	0.96
1:A:470:ILE:HD11	7:H:166:ARG:N	1.81	0.96
1:A:1016:GLU:OE1	1:A:1019:LYS:HE2	1.65	0.96
3:D:891:ILE:HG13	10:L:100:CYS:SG	2.05	0.96
10:L:93:GLU:O	10:L:97:THR:HG23	1.65	0.96
2:B:781:TYR:HB3	7:H:176:ARG:NH2	1.80	0.96
10:L:106:ARG:HH12	10:L:114:LYS:HD2	0.81	0.96
17:X:-46:DA:N1	18:Y:46:DT:N3	2.11	0.96
2:B:735:ILE:CG2	7:H:176:ARG:CZ	2.43	0.96
5:F:15:PRO:CG	8:I:14:LYS:NZ	2.26	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:53:ARG:C	13:Q:368:SER:CB	2.36	0.96
3:D:917:ILE:HD12	3:D:1058:VAL:HG11	1.46	0.96
1:A:564:PRO:HG2	2:B:744:PHE:CD2	2.00	0.95
3:D:881:ARG:HB2	10:L:57:VAL:CG1	1.96	0.95
3:D:901:TYR:CE1	10:L:128:ILE:HB	2.01	0.95
15:S:44:GLN:C	16:T:9:LEU:CD1	2.39	0.95
16:T:140:ARG:NH2	23:p:89:GLU:HB3	1.81	0.95
1:A:639:LEU:CD2	1:A:774:ARG:CG	2.43	0.95
4:E:615:ASP:CG	8:I:114:ARG:HB3	1.90	0.95
15:S:17:ARG:CG	16:T:39:GLU:CB	2.43	0.95
15:S:17:ARG:CB	16:T:39:GLU:HA	1.96	0.95
3:D:881:ARG:CB	10:L:57:VAL:HG11	1.96	0.95
15:S:44:GLN:HA	16:T:9:LEU:HD12	1.47	0.95
5:F:14:LEU:CD1	8:I:15:ASP:OD1	2.14	0.95
3:D:997:ALA:O	3:D:1001:GLN:HG3	1.65	0.95
5:F:66:LEU:HB3	8:I:31:TYR:HA	1.46	0.95
5:F:320:ARG:CD	5:F:321:PRO:HD3	1.96	0.95
4:E:598:TYR:CE1	8:I:114:ARG:HD3	2.02	0.95
15:S:17:ARG:HG2	16:T:39:GLU:HG3	1.46	0.95
2:B:310:ASP:CG	7:H:223:TYR:HE2	1.75	0.95
5:F:14:LEU:HD22	8:I:15:ASP:OD1	1.66	0.94
12:P:242:GLN:OE1	13:Q:315:ASN:HB2	1.67	0.94
15:S:17:ARG:CG	16:T:39:GLU:HG3	1.96	0.94
15:S:24:LYS:HA	16:T:98:GLU:O	1.66	0.94
3:D:891:ILE:HG22	10:L:111:LEU:HB2	1.48	0.94
15:S:31:PHE:HB2	16:T:92:THR:CB	1.96	0.94
14:R:185:ARG:HA	16:T:158:ASN:OD1	1.67	0.94
3:D:881:ARG:NH2	10:L:57:VAL:CG1	2.30	0.94
5:F:15:PRO:HG3	8:I:14:LYS:HZ2	1.32	0.94
1:A:638:PRO:HG3	6:G:39:LEU:HD23	1.46	0.94
8:i:60:HIS:CD2	10:l:106:ARG:NE	2.36	0.94
1:A:488:ALA:CB	5:f:271:VAL:HG23	1.98	0.94
1:A:1185:VAL:HG11	1:A:1191:ILE:CG1	1.93	0.94
3:D:898:VAL:HG22	10:L:113:VAL:HG23	1.50	0.94
15:S:31:PHE:CB	16:T:92:THR:HB	1.96	0.94
19:c:67:GLY:HA3	9:j:116:LEU:HD11	1.48	0.94
1:A:349:TRP:CZ2	5:f:262:PHE:CE1	2.55	0.94
2:B:848:HIS:HD2	7:H:226:ALA:HB2	1.23	0.93
5:F:316:GLN:N	5:F:327:TRP:CH2	2.36	0.93
11:O:22:LEU:HB3	11:O:28:ILE:HG23	1.50	0.93
3:D:901:TYR:CE1	10:L:128:ILE:O	2.21	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:125:TYR:CE2	16:T:31:TRP:HE3	1.86	0.93
1:A:639:LEU:HD11	1:A:774:ARG:HG2	1.48	0.93
11:O:22:LEU:HB3	11:O:28:ILE:CG2	1.99	0.93
5:F:48:LYS:HG2	8:I:22:ILE:HG23	1.51	0.93
4:E:621:ARG:NH2	8:I:104:LEU:HG	1.82	0.93
3:D:901:TYR:HE1	10:L:128:ILE:O	1.49	0.93
15:S:17:ARG:HA	16:T:39:GLU:CA	1.98	0.93
5:F:370:TRP:HH2	5:F:406:VAL:CG1	1.72	0.93
2:B:780:LYS:O	7:H:183:ARG:NH1	2.01	0.93
4:E:598:TYR:HE1	8:I:114:ARG:HD3	1.32	0.93
5:F:66:LEU:HD23	8:I:31:TYR:CB	1.98	0.93
11:O:32:LEU:CD1	13:Q:32:ASP:OD2	2.17	0.93
8:i:60:HIS:CD2	10:l:106:ARG:HE	1.86	0.93
5:F:213:ILE:HA	7:H:164:THR:O	1.68	0.92
7:H:118:VAL:HG21	9:J:127:THR:CG2	2.00	0.92
5:F:301:VAL:O	5:F:305:ILE:HG12	1.68	0.92
15:S:125:TYR:CD2	16:T:31:TRP:CZ3	2.58	0.92
5:F:52:GLN:HE21	8:I:26:MET:HB3	1.32	0.92
11:O:17:GLU:CB	13:Q:49:LYS:NZ	2.32	0.92
3:D:917:ILE:HD12	3:D:1058:VAL:CG2	2.00	0.92
5:F:71:ILE:HD11	8:I:35:VAL:HG13	1.52	0.91
15:S:44:GLN:CA	16:T:9:LEU:HD12	2.00	0.91
1:A:488:ALA:HB1	5:f:271:VAL:HG21	1.52	0.91
5:F:67:THR:HA	8:I:32:GLU:HG3	1.50	0.91
1:A:1185:VAL:CB	1:A:1191:ILE:HG12	1.99	0.91
11:O:76:LEU:HB3	11:O:79:VAL:HG21	1.51	0.91
5:F:320:ARG:HD2	5:F:321:PRO:CD	1.99	0.91
11:O:58:PHE:HZ	13:Q:358:MET:HE1	1.36	0.91
1:A:1169:ARG:HB3	1:A:1181:ARG:NH2	1.83	0.91
15:S:18:VAL:CB	16:T:40:VAL:HG13	2.00	0.91
3:D:889:HIS:HA	10:L:104:ARG:HH22	1.36	0.91
12:P:188:ARG:NH1	13:Q:322:ASP:OD2	2.01	0.91
5:F:320:ARG:HB2	5:F:415:ILE:HD12	1.50	0.91
1:A:465:TYR:CG	7:H:167:GLU:OE1	2.24	0.91
5:F:219:GLU:HG2	7:H:156:PRO:HB2	0.91	0.91
17:X:-38:DG:N2	18:Y:39:DA:N1	2.18	0.90
3:D:917:ILE:HD12	3:D:1058:VAL:CB	2.01	0.90
5:F:51:ALA:HB1	8:I:23:LEU:CD2	1.95	0.90
15:S:18:VAL:CG2	16:T:40:VAL:CG2	2.49	0.90
10:l:87:ILE:C	10:l:91:PHE:CD2	2.50	0.90
1:A:640:LEU:HD23	6:G:35:GLY:HA3	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:917:ILE:CD1	3:D:1058:VAL:HG11	2.00	0.90
1:A:1165:LEU:CB	1:A:1191:ILE:HG23	2.02	0.90
11:O:22:LEU:CA	11:O:28:ILE:HG12	2.00	0.90
11:O:60:GLY:HA2	11:O:79:VAL:HG13	1.51	0.90
1:A:1198:ARG:NH1	6:G:181:TRP:CG	2.39	0.90
11:O:88:ILE:HG21	13:Q:360:LEU:HB3	0.92	0.90
5:F:211:ARG:HG3	7:H:165:TYR:HD2	1.31	0.90
13:Q:55:ALA:O	13:Q:56:VAL:HG23	1.71	0.90
7:H:110:TYR:OH	9:J:160:GLN:HB3	1.70	0.90
15:S:23:THR:O	16:T:99:SER:HA	1.71	0.90
8:i:60:HIS:NE2	10:l:106:ARG:CZ	2.35	0.90
1:A:638:PRO:CB	6:G:39:LEU:HD23	2.01	0.90
1:A:495:LEU:HD13	5:f:268:ARG:NH2	1.87	0.89
5:F:308:VAL:CG2	5:F:337:VAL:CG1	2.49	0.89
15:S:24:LYS:HD3	16:T:97:THR:CB	2.03	0.89
5:F:87:HIS:HB3	9:J:212:LYS:HZ1	1.11	0.89
16:T:124:TYR:CD2	23:p:596:ILE:CD1	2.45	0.89
2:B:846:TYR:HD1	7:H:227:LEU:O	1.35	0.89
12:P:274:VAL:HG11	14:R:208:LEU:CD1	2.03	0.89
13:Q:47:GLU:CD	13:Q:60:HIS:CG	2.51	0.89
3:D:917:ILE:HB	3:D:1058:VAL:CG1	2.02	0.89
7:H:37:LEU:HD11	9:J:138:TYR:CE2	2.07	0.89
11:O:22:LEU:HD12	11:O:28:ILE:HD13	1.52	0.89
2:B:735:ILE:HG22	7:H:176:ARG:NH1	1.86	0.89
1:A:639:LEU:CD1	1:A:774:ARG:HG2	2.02	0.89
10:L:102:LEU:HA	10:L:105:HIS:HD2	1.36	0.89
5:F:87:HIS:HB3	9:J:212:LYS:HZ3	1.37	0.89
18:Y:9:DC:C2'	18:Y:10:DT:H71	2.03	0.89
3:D:889:HIS:C	10:L:104:ARG:NH2	2.31	0.89
5:F:66:LEU:HD23	8:I:31:TYR:HB2	1.54	0.89
5:F:48:LYS:CG	8:I:22:ILE:CG2	2.01	0.88
16:T:16:THR:HG21	16:T:107:GLU:O	1.73	0.88
2:B:846:TYR:O	7:H:226:ALA:O	1.84	0.88
15:S:8:SER:HB3	16:T:49:GLN:N	1.87	0.88
3:D:917:ILE:HD12	3:D:1058:VAL:CG1	2.02	0.88
8:I:60:HIS:ND1	10:L:118:LEU:CD2	2.37	0.88
8:i:73:LEU:HD22	10:l:105:HIS:CD2	2.08	0.88
1:A:484:ILE:HA	5:f:306:PRO:HB3	1.56	0.88
5:F:14:LEU:N	8:I:18:MET:HG2	1.89	0.88
11:O:88:ILE:CG2	13:Q:361:ASN:ND2	2.36	0.88
2:B:310:ASP:CG	7:H:223:TYR:CE2	2.50	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:31:PHE:O	16:T:91:GLN:HA	1.74	0.88
1:A:1169:ARG:HD3	1:A:1181:ARG:HH11	0.72	0.88
5:F:51:ALA:O	8:I:28:ILE:HD11	1.74	0.88
15:S:8:SER:C	16:T:48:THR:C	2.42	0.88
17:X:22:DG:N2	18:Y:-22:DC:O2	2.06	0.88
28:u:44:PHE:HB2	28:u:77:PHE:HB3	1.56	0.88
11:O:55:ARG:HH12	13:Q:369:LYS:HE2	1.39	0.88
12:P:243:LYS:CE	13:Q:318:ASP:HA	2.03	0.88
8:i:73:LEU:HD21	10:l:105:HIS:NE2	1.89	0.88
10:l:87:ILE:C	10:l:91:PHE:HD2	1.82	0.88
14:R:175:ARG:NH2	23:p:102:ASP:CA	2.37	0.87
5:F:211:ARG:HB3	7:H:165:TYR:CE2	2.08	0.87
5:F:312:ILE:HD11	5:F:334:ALA:C	1.99	0.87
4:E:694:LEU:HD13	4:E:703:MET:HE1	0.88	0.87
5:F:48:LYS:HE3	8:I:22:ILE:HG12	1.56	0.87
1:A:511:LEU:H	1:A:511:LEU:HD22	1.37	0.87
1:A:1016:GLU:OE1	1:A:1019:LYS:CE	2.23	0.87
11:O:18:SER:N	13:Q:49:LYS:HZ2	1.73	0.87
2:B:848:HIS:CE1	7:H:225:THR:HG23	2.09	0.87
11:O:58:PHE:CZ	13:Q:358:MET:HE1	2.10	0.87
15:S:135:PHE:CE2	16:T:43:LEU:CD2	2.57	0.87
1:A:1185:VAL:CG1	1:A:1191:ILE:HG13	2.05	0.87
5:F:370:TRP:CD1	5:F:416:ASP:HA	2.10	0.87
1:A:666:ARG:HH21	2:B:512:GLY:N	1.72	0.86
1:A:784:GLN:H	1:A:1073:GLN:HE22	0.89	0.86
3:D:881:ARG:NH2	10:L:57:VAL:CB	2.38	0.86
5:F:15:PRO:HB3	8:I:14:LYS:CE	2.05	0.86
11:O:22:LEU:CB	11:O:28:ILE:CD1	2.42	0.86
2:B:835:ARG:CD	7:H:187:GLU:OE2	2.23	0.86
5:F:335:ARG:NH1	5:F:382:GLU:HA	1.76	0.86
12:P:188:ARG:HH12	13:Q:322:ASP:CG	1.81	0.86
15:S:15:VAL:HG11	16:T:39:GLU:OE2	1.73	0.86
17:X:-13:DA:OP2	17:X:-13:DA:H3'	1.75	0.86
2:B:845:SER:O	7:H:226:ALA:O	1.92	0.86
11:O:88:ILE:HG23	13:Q:361:ASN:HD22	1.37	0.86
1:A:1165:LEU:HB2	1:A:1191:ILE:HG23	1.57	0.86
11:O:55:ARG:HH12	13:Q:369:LYS:CD	1.87	0.86
8:i:60:HIS:CE1	10:l:106:ARG:HH22	1.90	0.86
5:F:14:LEU:CD2	8:I:18:MET:HB3	2.04	0.86
11:O:55:ARG:NH1	13:Q:369:LYS:CE	2.37	0.86
2:B:847:ARG:C	7:H:226:ALA:HB1	2.00	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:22:LEU:CD1	11:O:28:ILE:HD13	2.06	0.86
1:A:638:PRO:HB3	6:G:39:LEU:CD2	2.05	0.85
5:F:71:ILE:HD11	8:I:35:VAL:HG22	1.57	0.85
18:Y:8:DC:H2"	18:Y:9:DC:C5	2.11	0.85
1:A:1185:VAL:HG12	1:A:1191:ILE:HG13	1.57	0.85
1:A:1190:VAL:HG23	6:G:162:VAL:HG13	1.57	0.85
7:H:111:ALA:HB1	9:J:126:TYR:CE2	2.11	0.85
1:A:784:GLN:N	1:A:1073:GLN:HE22	1.73	0.85
12:P:214:PHE:CD2	17:X:-24:DG:O4'	2.28	0.85
16:T:131:GLN:NE2	23:p:543:GLU:OE1	2.09	0.85
2:B:762:ASP:OD1	2:B:768:PRO:CG	2.21	0.85
5:F:211:ARG:HG2	7:H:165:TYR:HD2	0.80	0.85
2:B:835:ARG:HD3	7:H:187:GLU:HG3	1.58	0.85
5:F:87:HIS:CB	9:J:212:LYS:NZ	2.38	0.85
16:T:124:TYR:CZ	23:p:596:ILE:HD13	2.00	0.85
3:D:891:ILE:HG23	10:L:111:LEU:HB2	1.57	0.85
5:F:17:GLU:OE2	8:I:14:LYS:CE	2.25	0.85
5:F:71:ILE:CD1	8:I:35:VAL:HA	2.07	0.85
10:l:102:LEU:HA	10:l:105:HIS:CD2	2.08	0.85
22:o:108:ARG:HH12	22:o:191:ILE:HB	1.41	0.85
3:D:917:ILE:HB	3:D:1058:VAL:HG13	1.59	0.85
8:i:73:LEU:CD2	10:l:105:HIS:CD2	2.60	0.84
1:A:572:TYR:CD2	2:B:689:GLN:HB2	2.13	0.84
11:O:55:ARG:NH1	13:Q:369:LYS:CD	2.40	0.84
12:P:274:VAL:HG12	14:R:208:LEU:HD11	1.57	0.84
15:S:102:VAL:HB	15:S:108:ARG:HB3	1.59	0.84
8:i:61:ALA:HA	10:l:106:ARG:HG2	1.57	0.84
11:O:22:LEU:O	11:O:28:ILE:N	2.10	0.84
12:P:259:VAL:HG21	18:Y:28:DG:N2	1.92	0.84
15:S:18:VAL:CA	16:T:38:GLY:O	2.25	0.84
3:D:891:ILE:CG2	10:L:111:LEU:CB	2.54	0.84
1:A:465:TYR:CD1	7:H:167:GLU:OE1	2.30	0.84
5:F:51:ALA:HB2	8:I:23:LEU:HD21	1.58	0.84
15:S:125:TYR:HE2	16:T:31:TRP:CE3	1.96	0.84
1:A:1165:LEU:CB	1:A:1191:ILE:CG2	2.56	0.84
11:O:22:LEU:C	11:O:28:ILE:HG12	2.03	0.84
11:O:55:ARG:NH1	13:Q:369:LYS:HD3	1.93	0.84
16:T:49:GLN:N	16:T:49:GLN:OE1	2.08	0.84
2:B:735:ILE:HG21	7:H:176:ARG:NH1	1.92	0.84
2:B:310:ASP:OD1	7:H:223:TYR:CE2	2.32	0.83
5:F:14:LEU:CG	8:I:15:ASP:OD1	2.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:111:ALA:O	9:J:126:TYR:CE1	2.31	0.83
8:I:60:HIS:ND1	10:L:118:LEU:HD21	1.93	0.83
18:Y:9:DC:C2'	18:Y:10:DT:C7	2.55	0.83
3:D:901:TYR:HE1	10:L:128:ILE:C	1.85	0.83
1:A:486:TRP:HH2	5:f:358:THR:CB	1.89	0.83
5:F:370:TRP:CZ3	5:F:420:ALA:HB2	2.14	0.83
1:A:639:LEU:HD13	1:A:643:ILE:CD1	2.08	0.83
14:R:175:ARG:HH22	23:p:102:ASP:CA	1.86	0.83
19:c:77:LEU:HD13	9:j:116:LEU:HD23	1.61	0.83
8:i:73:LEU:CG	10:l:105:HIS:CE1	2.60	0.83
5:F:244:GLN:OE1	7:H:133:ALA:CB	2.26	0.83
11:O:22:LEU:HD13	11:O:28:ILE:HG21	1.59	0.83
25:r:113:ALA:HB1	28:u:165:ASP:OD1	1.78	0.83
1:A:666:ARG:NE	2:B:512:GLY:HA2	1.94	0.82
5:F:214:HIS:H	7:H:164:THR:HG22	1.43	0.82
4:E:704:VAL:HG11	4:E:747:LEU:CG	2.07	0.82
5:F:14:LEU:CD2	8:I:15:ASP:OD1	2.27	0.82
5:F:308:VAL:HG21	5:F:337:VAL:HG12	1.61	0.82
7:H:111:ALA:HB2	9:J:157:LEU:CD1	2.09	0.82
14:R:154:ARG:NH2	18:Y:22:DG:OP1	2.13	0.82
3:D:881:ARG:NH2	10:L:57:VAL:HG13	1.90	0.82
1:A:469:PRO:HA	7:H:166:ARG:HH11	1.41	0.82
1:A:753:TYR:CD2	1:A:1077:LEU:CB	2.61	0.82
11:O:62:LEU:HA	11:O:76:LEU:HD13	1.62	0.82
15:S:16:VAL:N	16:T:41:GLY:O	2.12	0.82
14:R:107:MET:SD	22:o:329:MET:HE1	2.20	0.82
5:F:15:PRO:CB	8:I:14:LYS:CE	2.58	0.81
10:L:101:GLN:C	10:L:105:HIS:CD2	2.57	0.81
5:f:447:ALA:HA	5:f:456:GLY:HA3	1.61	0.81
1:A:666:ARG:HE	2:B:512:GLY:HA2	1.43	0.81
11:O:65:TYR:HE1	12:P:191:GLU:HG3	1.43	0.81
3:D:936:GLN:HE21	3:D:936:GLN:H	1.28	0.81
5:F:211:ARG:CG	7:H:165:TYR:CE2	2.61	0.81
5:F:89:GLN:CD	9:J:210:ASN:ND2	2.38	0.81
7:H:73:GLY:HA3	9:J:142:ALA:HB3	1.60	0.81
16:T:124:TYR:CZ	23:p:596:ILE:CG2	2.64	0.81
11:O:27:GLN:NE2	13:Q:41:GLU:OE1	2.14	0.81
3:D:901:TYR:CE1	10:L:128:ILE:CB	2.63	0.81
5:F:48:LYS:CD	8:I:22:ILE:HG23	2.08	0.81
16:T:124:TYR:CZ	23:p:596:ILE:HG23	2.15	0.81
1:A:638:PRO:HB3	6:G:39:LEU:HD23	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:16:VAL:HB	16:T:56:PHE:HE1	1.46	0.81
19:c:67:GLY:HA3	9:j:116:LEU:HD13	1.60	0.81
1:A:569:ASN:CG	2:B:689:GLN:HA	2.04	0.81
10:L:71:ASP:HB2	10:L:74:GLU:HB2	1.61	0.81
10:l:101:GLN:C	10:l:105:HIS:CD2	2.59	0.81
5:F:80:VAL:CG1	8:I:45:ARG:HH12	1.93	0.81
5:F:322:ASP:C	5:F:324:ASP:H	1.86	0.81
11:O:22:LEU:HB2	11:O:28:ILE:HD11	1.61	0.81
25:r:103:LEU:HD21	28:u:84:VAL:HB	1.62	0.81
1:A:470:ILE:HD11	7:H:165:TYR:C	2.05	0.80
1:A:470:ILE:HD12	7:H:166:ARG:HB2	1.63	0.80
1:A:639:LEU:HD12	1:A:639:LEU:O	1.82	0.80
15:S:121:ASN:CA	16:T:25:LYS:HE2	2.10	0.80
4:E:747:LEU:HD22	4:E:747:LEU:H	1.44	0.80
8:I:132:LEU:HG	9:J:121:MET:HE2	1.61	0.80
1:A:564:PRO:CG	2:B:744:PHE:CE2	2.62	0.80
5:F:324:ASP:HA	5:F:327:TRP:HB3	1.62	0.80
13:Q:358:MET:HE2	13:Q:367:PHE:HD2	1.46	0.80
5:F:89:GLN:NE2	9:J:210:ASN:HD22	1.79	0.80
8:I:132:LEU:HG	9:J:121:MET:CE	2.12	0.80
3:D:881:ARG:HG2	10:L:57:VAL:HG11	1.62	0.80
3:D:905:ALA:O	10:L:126:MET:HE1	1.80	0.80
14:R:175:ARG:NH2	23:p:102:ASP:C	2.40	0.80
15:S:45:ALA:N	16:T:9:LEU:HD11	1.97	0.80
2:B:735:ILE:HG22	7:H:176:ARG:HH12	1.46	0.80
15:S:16:VAL:O	16:T:41:GLY:O	2.00	0.80
16:T:147:LYS:HG3	16:T:148:VAL:N	1.96	0.80
1:A:1185:VAL:C	1:A:1191:ILE:HD11	2.07	0.80
1:A:666:ARG:HH21	2:B:512:GLY:CA	1.94	0.80
1:A:950:VAL:HG11	1:A:1066:CYS:SG	2.22	0.80
15:S:121:ASN:O	16:T:25:LYS:HG3	1.82	0.79
16:T:122:GLU:OE2	16:T:123:ASN:O	2.00	0.79
12:P:243:LYS:HZ3	13:Q:318:ASP:CB	1.95	0.79
3:D:889:HIS:CA	10:L:104:ARG:HH21	1.87	0.79
3:D:991:MET:HE2	16:T:193:LYS:HZ1	1.48	0.79
10:l:102:LEU:CA	10:l:105:HIS:HD2	1.95	0.79
2:B:835:ARG:HD2	7:H:187:GLU:OE2	1.82	0.79
4:e:747:LEU:HD23	4:e:747:LEU:H	1.47	0.79
3:D:891:ILE:CG2	10:L:111:LEU:HD22	2.12	0.79
15:S:124:TYR:HE1	16:T:22:LYS:CG	1.95	0.79
3:D:966:LEU:HD11	3:D:981:GLN:NE2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:15:VAL:HG12	16:T:39:GLU:OE2	1.82	0.79
15:S:24:LYS:HB3	16:T:99:SER:HA	1.64	0.79
10:l:93:GLU:O	10:l:97:THR:HG23	1.83	0.79
4:E:704:VAL:HG12	4:E:759:ILE:HD13	1.65	0.79
5:F:370:TRP:HZ2	5:F:406:VAL:HG12	1.43	0.78
15:S:24:LYS:HD3	16:T:97:THR:HB	1.64	0.78
16:T:16:THR:O	16:T:109:ILE:HD12	1.83	0.78
5:F:47:ILE:CD1	8:I:19:MET:CE	1.97	0.78
5:F:80:VAL:HG11	8:I:42:PHE:CE1	2.19	0.78
11:O:88:ILE:HD13	13:Q:360:LEU:CB	2.05	0.78
5:F:71:ILE:HD11	8:I:35:VAL:CG1	2.13	0.78
14:R:154:ARG:HH12	18:Y:22:DG:H5"	1.46	0.78
3:d:1082:ALA:HB2	10:l:83:MET:HE2	1.62	0.78
3:D:881:ARG:NH2	10:L:57:VAL:HG21	1.91	0.78
14:R:129:ASN:HD22	23:p:99:TRP:CD1	2.01	0.78
14:R:217:ARG:NE	23:p:102:ASP:O	2.12	0.78
15:S:6:PRO:O	15:S:10:ASN:CB	2.31	0.78
15:S:124:TYR:OH	16:T:22:LYS:HE2	1.83	0.78
16:T:145:LEU:HG	23:p:92:TYR:HB3	1.65	0.78
2:B:781:TYR:HB3	7:H:176:ARG:HH21	1.46	0.78
3:D:891:ILE:HG21	10:L:111:LEU:CD2	2.11	0.78
5:F:274:ASN:ND2	5:F:316:GLN:HA	1.99	0.78
16:T:18:VAL:HG21	16:T:95:VAL:HG23	1.65	0.78
3:D:901:TYR:CD1	10:L:128:ILE:HG22	2.19	0.78
2:B:361:ARG:HD2	2:B:367:GLU:HB2	1.66	0.78
3:D:966:LEU:HD11	3:D:981:GLN:HE21	1.49	0.78
25:r:115:ILE:HG22	25:r:117:SER:H	1.49	0.78
13:Q:43:LYS:O	13:Q:47:GLU:HG3	1.84	0.77
15:S:17:ARG:HB3	16:T:39:GLU:HA	1.63	0.77
15:S:18:VAL:CG2	16:T:40:VAL:HG21	2.13	0.77
16:T:122:GLU:OE1	16:T:126:ARG:NH1	1.89	0.77
5:F:43:VAL:HG21	8:I:43:ALA:CB	2.04	0.77
25:r:73:ARG:HH12	28:u:144:ARG:HH12	1.31	0.77
5:F:47:ILE:HD13	8:I:19:MET:HE3	1.58	0.77
5:F:273:GLN:NE2	5:F:273:GLN:H	1.81	0.77
1:A:1185:VAL:HB	1:A:1191:ILE:HG12	1.66	0.77
16:T:124:TYR:OH	23:p:596:ILE:CG2	2.29	0.77
11:O:65:TYR:CE1	12:P:191:GLU:HG3	2.15	0.77
12:P:305:PHE:CZ	18:Y:30:DA:H2"	2.20	0.77
15:S:17:ARG:HG2	16:T:39:GLU:CD	2.08	0.77
22:o:461:GLN:HB2	22:o:462:PRO:HD3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:47:ILE:HD13	8:I:19:MET:SD	2.24	0.77
5:F:312:ILE:CD1	5:F:334:ALA:HB1	2.15	0.77
7:H:118:VAL:HG21	9:J:127:THR:HG23	1.67	0.77
11:O:22:LEU:HB3	11:O:28:ILE:CB	2.14	0.77
11:O:88:ILE:HD12	13:Q:360:LEU:CD1	2.10	0.77
12:P:243:LYS:HZ3	13:Q:318:ASP:HB2	1.48	0.77
15:S:50:ASP:HB3	15:S:97:PRO:HG2	1.66	0.77
14:R:18:HIS:HE1	14:R:37:CYS:SG	2.08	0.77
12:P:274:VAL:CG1	14:R:208:LEU:CD1	2.53	0.77
15:S:8:SER:OG	16:T:49:GLN:HA	1.84	0.77
15:S:31:PHE:O	16:T:91:GLN:CA	2.33	0.77
8:i:60:HIS:NE2	10:l:106:ARG:NH2	2.29	0.77
21:m:31:LEU:HD23	21:m:31:LEU:H	1.47	0.77
23:p:68:GLN:HB3	23:p:83:ARG:HB3	1.64	0.77
11:O:82:ARG:HE	11:O:87:LEU:HB2	1.49	0.76
1:A:666:ARG:NH2	2:B:512:GLY:HA2	1.98	0.76
14:R:109:SER:O	14:R:112:ARG:HG3	1.85	0.76
16:T:47:LYS:HG2	16:T:52:THR:HG23	1.67	0.76
15:S:23:THR:O	16:T:100:SER:N	2.19	0.76
5:F:14:LEU:CA	8:I:18:MET:HG2	2.15	0.76
5:F:71:ILE:CD1	8:I:35:VAL:HG13	2.15	0.76
12:P:259:VAL:CG2	18:Y:28:DG:N2	2.48	0.76
15:S:24:LYS:HD3	16:T:97:THR:OG1	1.86	0.76
15:S:31:PHE:O	16:T:91:GLN:C	2.28	0.76
8:i:60:HIS:O	10:l:106:ARG:NE	2.19	0.76
1:A:639:LEU:CG	1:A:774:ARG:HG2	2.16	0.76
7:H:102:PHE:CZ	9:J:158:ALA:HA	2.20	0.76
5:F:71:ILE:HD11	8:I:35:VAL:CG2	2.16	0.76
11:O:53:ARG:CA	13:Q:368:SER:HB3	2.15	0.76
15:S:19:PRO:HA	16:T:38:GLY:HA3	1.68	0.76
7:H:117:MET:O	9:J:129:THR:HA	1.84	0.76
15:S:18:VAL:CB	16:T:40:VAL:CG1	2.62	0.76
17:X:-35:DA:C2	18:Y:36:DG:C2	2.73	0.76
23:p:953:ASP:OD1	24:q:36:ARG:NH2	2.19	0.76
1:A:1016:GLU:CD	1:A:1019:LYS:CE	2.59	0.75
3:D:966:LEU:HD21	3:D:981:GLN:HE21	1.49	0.75
5:F:359:PHE:HB3	5:F:380:LEU:HG	1.68	0.75
5:F:429:LYS:O	5:F:433:PRO:HD2	1.85	0.75
8:i:73:LEU:HD22	10:l:105:HIS:CG	2.21	0.75
23:p:83:ARG:HG3	23:p:133:ILE:HG23	1.68	0.75
28:u:89:VAL:HG23	28:u:99:THR:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:248:ARG:NH2	18:Y:33:DG:OP2	2.18	0.75
15:S:121:ASN:HA	16:T:25:LYS:CE	2.16	0.75
7:H:36:THR:HG21	9:J:134:VAL:HG21	1.67	0.75
5:F:211:ARG:CB	7:H:165:TYR:HE2	2.00	0.75
11:O:7:ARG:CZ	11:O:37:LEU:HB3	2.17	0.75
17:X:-22:DC:O2	18:Y:22:DG:N2	2.19	0.75
1:A:1198:ARG:HH12	6:G:181:TRP:CD1	2.05	0.75
3:D:881:ARG:HH21	10:L:57:VAL:CB	1.98	0.75
5:F:66:LEU:HD23	8:I:31:TYR:HB3	1.68	0.75
11:O:88:ILE:HG21	13:Q:360:LEU:CA	2.16	0.75
12:P:243:LYS:HZ3	13:Q:318:ASP:CA	1.93	0.75
5:F:312:ILE:CD1	5:F:334:ALA:CB	2.64	0.75
16:T:225:VAL:C	16:T:227:GLY:H	1.94	0.75
10:I:76:LEU:HD13	10:I:84:LEU:HD12	1.67	0.75
22:O:319:ASP:HB2	22:O:340:LYS:HD3	1.68	0.75
3:D:1006:LEU:HD11	11:O:68:CYS:HB3	1.67	0.75
1:A:666:ARG:HH21	2:B:512:GLY:HA2	1.51	0.75
5:F:320:ARG:HD3	5:F:415:ILE:CB	2.15	0.75
12:P:188:ARG:HH11	13:Q:322:ASP:CG	1.69	0.75
1:A:1185:VAL:O	1:A:1191:ILE:CD1	2.33	0.74
2:B:276:LEU:HD11	7:H:228:LEU:HD23	1.69	0.74
5:F:211:ARG:CB	7:H:165:TYR:CE2	2.69	0.74
1:A:784:GLN:N	1:A:1073:GLN:NE2	2.32	0.74
11:O:22:LEU:HB2	11:O:28:ILE:HD13	1.67	0.74
11:O:55:ARG:NH2	13:Q:369:LYS:O	2.18	0.74
12:P:257:ASN:HB2	17:X:-27:DT:C5'	2.16	0.74
15:S:16:VAL:H	16:T:42:LYS:HA	1.49	0.74
2:B:835:ARG:HD3	7:H:187:GLU:CG	2.17	0.74
3:D:901:TYR:CE1	10:L:128:ILE:HG22	2.22	0.74
5:F:308:VAL:HG21	5:F:337:VAL:HG11	1.54	0.74
19:c:77:LEU:HD12	9:j:116:LEU:HD23	1.68	0.74
11:O:5:LEU:HD22	11:O:98:CYS:SG	2.27	0.74
4:E:359:LEU:HD12	4:E:359:LEU:O	1.87	0.74
5:F:71:ILE:HD11	8:I:35:VAL:CB	2.15	0.74
1:A:970:ASN:OD1	1:A:970:ASN:N	2.21	0.74
5:F:412:LEU:CD1	5:F:417:ARG:HB2	2.17	0.74
15:S:125:TYR:HD2	16:T:23:VAL:HG21	1.52	0.74
5:F:213:ILE:HD13	7:H:163:PRO:HB3	1.68	0.74
10:L:106:ARG:HH12	10:L:114:LYS:CG	2.00	0.74
11:O:88:ILE:HG22	13:Q:360:LEU:HB3	1.68	0.74
12:P:243:LYS:NZ	13:Q:318:ASP:CB	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:1125:LYS:HA	22:o:1128:ILE:HB	1.70	0.74
11:O:88:ILE:HB	13:Q:360:LEU:HD13	1.70	0.74
15:S:16:VAL:N	16:T:42:LYS:HA	2.02	0.74
1:A:470:ILE:CD1	7:H:166:ARG:N	2.51	0.74
5:F:87:HIS:CB	9:J:212:LYS:HZ3	1.98	0.74
5:F:412:LEU:HD13	5:F:417:ARG:CG	2.17	0.74
8:I:60:HIS:HE1	10:L:118:LEU:HD22	0.92	0.74
2:B:276:LEU:HD11	7:H:228:LEU:CD2	2.18	0.73
2:B:735:ILE:HG21	7:H:176:ARG:CZ	2.18	0.73
10:L:102:LEU:HA	10:L:105:HIS:CD2	2.21	0.73
15:S:18:VAL:CG2	16:T:40:VAL:CG1	2.66	0.73
22:o:606:HIS:HB3	22:o:626:THR:HG23	1.69	0.73
4:E:696:TRP:CE3	4:E:703:MET:CB	2.69	0.73
5:F:213:ILE:HG22	7:H:164:THR:O	1.87	0.73
22:o:334:ARG:NH1	22:o:335:PRO:O	2.20	0.73
8:i:60:HIS:CG	10:l:106:ARG:NH2	2.37	0.73
30:w:30:LYS:HA	30:w:33:ARG:HH21	1.53	0.73
1:A:1190:VAL:CG2	6:G:162:VAL:CG1	2.54	0.73
12:P:271:GLU:OE1	14:R:208:LEU:HD13	1.88	0.73
15:S:14:TYR:O	16:T:43:LEU:N	2.21	0.73
1:A:573:TYR:CD2	2:B:657:ARG:HA	2.24	0.73
5:F:322:ASP:O	5:F:324:ASP:N	2.21	0.73
15:S:15:VAL:HG13	16:T:39:GLU:OE2	1.87	0.73
1:A:950:VAL:HG21	1:A:1065:GLU:HG3	1.71	0.73
23:p:344:GLN:NE2	23:p:353:VAL:O	2.22	0.73
1:A:662:MET:SD	2:B:475:LYS:NZ	2.62	0.73
11:O:55:ARG:NH1	13:Q:369:LYS:CB	2.52	0.73
13:Q:29:PHE:HD2	13:Q:34:VAL:HG11	1.54	0.73
1:A:1019:LYS:HB2	1:A:1019:LYS:HZ2	1.52	0.72
5:F:342:LYS:HG3	5:F:352:GLN:CD	2.14	0.72
16:T:181:GLN:HE21	16:T:181:GLN:HA	1.52	0.72
25:r:108:ALA:HB2	25:r:128:GLN:HB2	1.71	0.72
3:D:891:ILE:HG22	10:L:111:LEU:CB	2.19	0.72
11:O:58:PHE:HB3	11:O:81:PHE:CE2	2.24	0.72
5:F:308:VAL:CG1	5:F:337:VAL:HG11	2.18	0.72
14:R:217:ARG:NH2	23:p:102:ASP:HB2	2.01	0.72
16:T:16:THR:CG2	16:T:107:GLU:O	2.38	0.72
30:w:81:THR:HG22	30:w:83:ASP:H	1.54	0.72
1:A:567:LEU:HD22	2:B:745:GLN:CG	2.19	0.72
5:F:66:LEU:O	8:I:32:GLU:HG3	1.88	0.72
22:o:1189:ASP:OD2	22:o:1258:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:256:GLN:HG3	17:X:-26:DC:H5''	1.71	0.72
1:A:666:ARG:HH21	2:B:512:GLY:H	1.35	0.72
1:A:1169:ARG:HB3	1:A:1181:ARG:HH22	1.52	0.72
3:D:955:LYS:O	3:D:955:LYS:NZ	2.23	0.72
4:E:697:ASP:O	4:E:701:GLY:CA	2.37	0.72
5:F:418:ILE:H	5:F:418:ILE:HD12	1.54	0.72
5:F:67:THR:HB	8:I:32:GLU:OE2	1.90	0.72
13:Q:55:ALA:O	13:Q:56:VAL:CG2	2.38	0.72
11:O:88:ILE:CD1	13:Q:360:LEU:CB	2.60	0.72
22:o:538:VAL:HG22	22:o:539:GLN:H	1.54	0.72
1:A:1197:ILE:HD12	6:G:166:VAL:CG1	2.20	0.72
2:B:846:TYR:C	7:H:226:ALA:C	2.52	0.72
1:A:572:TYR:CE2	2:B:689:GLN:HB2	2.25	0.71
7:H:111:ALA:HB2	9:J:157:LEU:HD11	1.72	0.71
23:p:274:ARG:HG2	23:p:279:VAL:HA	1.70	0.71
25:r:29:ALA:O	25:r:94:LYS:NZ	2.18	0.71
25:r:87:LEU:HD22	25:r:97:LEU:HB2	1.71	0.71
1:A:1019:LYS:HB2	1:A:1019:LYS:NZ	2.05	0.71
14:R:185:ARG:HG3	23:p:433:LEU:CD2	2.20	0.71
5:F:320:ARG:CD	5:F:415:ILE:HB	2.17	0.71
11:O:25:SER:C	11:O:27:GLN:H	1.98	0.71
14:R:185:ARG:HA	16:T:158:ASN:CG	2.14	0.71
5:F:14:LEU:HD13	8:I:15:ASP:OD2	1.91	0.71
7:H:110:TYR:CZ	9:J:160:GLN:HB3	2.26	0.71
15:S:39:PHE:HZ	16:T:92:THR:HG21	1.55	0.71
8:I:132:LEU:HD21	9:J:121:MET:HE1	1.72	0.71
2:B:241:PRO:HG2	2:B:496:MET:HE1	1.72	0.71
5:F:114:LEU:HD13	7:H:53:ALA:HB3	1.70	0.71
1:A:1193:ALA:HB3	6:G:166:VAL:HG21	1.70	0.71
5:F:81:GLU:C	5:F:83:LEU:H	1.99	0.71
15:S:45:ALA:HB3	16:T:9:LEU:CD2	2.19	0.71
22:o:60:PRO:HA	22:o:65:ILE:HD11	1.71	0.71
22:o:1166:LEU:HB3	22:o:1293:LEU:HA	1.73	0.71
3:D:901:TYR:CE1	10:L:128:ILE:CG2	2.73	0.71
16:T:16:THR:O	16:T:109:ILE:N	2.24	0.71
3:D:917:ILE:CB	3:D:1058:VAL:HG11	2.21	0.71
3:D:1085:LYS:HZ3	10:L:83:MET:HE1	1.55	0.71
5:F:213:ILE:CG2	7:H:163:PRO:CB	2.64	0.71
3:D:881:ARG:HB2	10:L:57:VAL:HG12	1.71	0.70
11:O:55:ARG:CZ	13:Q:369:LYS:HB3	2.08	0.70
15:S:24:LYS:CA	16:T:98:GLU:O	2.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:60:HIS:CD2	10:l:106:ARG:CZ	2.74	0.70
22:o:406:VAL:HG21	22:o:419:ILE:HD11	1.72	0.70
1:A:666:ARG:CZ	2:B:512:GLY:HA2	2.20	0.70
1:A:1189:ALA:HB2	6:G:154:LYS:HD3	1.72	0.70
5:F:329:LEU:O	5:F:329:LEU:HD23	1.91	0.70
5:F:335:ARG:NH1	5:F:382:GLU:CA	2.52	0.70
15:S:6:PRO:O	15:S:10:ASN:HB3	1.90	0.70
22:o:107:LEU:HD13	22:o:191:ILE:HD12	1.73	0.70
29:v:104:THR:HG22	29:v:105:SER:H	1.57	0.70
13:Q:18:ILE:HG12	13:Q:46:TRP:CH2	2.26	0.70
15:S:23:THR:O	16:T:99:SER:CA	2.38	0.70
5:F:66:LEU:CD2	8:I:31:TYR:HB3	2.22	0.70
5:F:412:LEU:HD13	5:F:417:ARG:HD2	0.74	0.70
15:S:126:ILE:HB	15:S:138:PHE:HB2	1.70	0.70
10:l:106:ARG:HH12	10:l:114:LYS:HG3	1.54	0.70
22:o:1102:MET:HE1	22:o:1124:LEU:HD13	1.74	0.70
23:p:133:ILE:HA	23:p:139:GLN:HE22	1.55	0.70
5:F:22:VAL:HG13	8:I:44:PHE:HE1	1.56	0.70
5:F:213:ILE:HB	7:H:163:PRO:C	2.15	0.70
7:H:93:ILE:HD13	9:J:155:ILE:HD11	1.72	0.70
12:P:300:ILE:HD11	12:P:320:GLU:HB3	1.73	0.70
15:S:30:ALA:HA	16:T:92:THR:O	1.92	0.70
14:R:297:PRO:HB3	14:R:310:VAL:HG21	1.73	0.70
7:H:66:GLN:HG3	9:J:138:TYR:CE1	2.25	0.70
1:A:575:PRO:HG3	2:B:610:GLU:CG	2.21	0.69
3:D:898:VAL:CG2	10:L:113:VAL:HG23	2.22	0.69
5:F:319:LEU:H	5:F:319:LEU:HD23	1.57	0.69
11:O:55:ARG:NH1	13:Q:369:LYS:NZ	2.40	0.69
16:T:196:TYR:HB2	16:T:232:THR:CG2	2.22	0.69
1:A:469:PRO:HA	7:H:166:ARG:CZ	2.21	0.69
3:D:917:ILE:CG1	3:D:1058:VAL:HG21	2.21	0.69
14:R:286:ARG:HG3	14:R:316:LEU:HG	1.74	0.69
15:S:121:ASN:O	16:T:25:LYS:HE2	1.92	0.69
5:F:312:ILE:HG13	5:F:334:ALA:HB1	0.70	0.69
5:F:412:LEU:HD11	5:F:417:ARG:HB2	1.75	0.69
20:k:191:VAL:HG13	20:k:200:ILE:HD13	1.74	0.69
28:u:1:MET:N	28:u:78:ARG:O	2.25	0.69
17:X:9:DG:H1	18:Y:9:DC:H42	1.40	0.69
3:D:917:ILE:HB	3:D:1058:VAL:HG11	1.75	0.69
5:F:100:GLY:O	8:I:34:ARG:NH2	2.26	0.69
7:H:119:ILE:HD13	9:J:129:THR:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:966:LEU:CD1	3:D:981:GLN:HG3	2.23	0.69
5:F:335:ARG:HD2	5:F:378:ALA:O	1.93	0.69
14:R:193:ARG:HH12	18:Y:23:DG:P	2.16	0.69
18:Y:-19:DC:OP2	18:Y:-19:DC:H6	1.74	0.69
1:A:568:SER:HB2	2:B:389:ASN:HB2	1.74	0.69
3:D:991:MET:HE2	16:T:193:LYS:NZ	2.08	0.69
5:F:71:ILE:HD12	8:I:35:VAL:HA	1.74	0.69
5:F:92:ILE:HG13	5:F:93:PRO:HD3	1.74	0.69
15:S:45:ALA:HB2	16:T:9:LEU:HD21	1.70	0.69
26:s:172:ARG:NH2	26:s:210:GLN:O	2.25	0.69
6:G:129:LYS:O	6:G:129:LYS:NZ	2.23	0.69
7:H:36:THR:CG2	9:J:134:VAL:HG21	2.22	0.69
17:X:-32:DC:H42	18:Y:32:DG:H1	1.39	0.69
25:r:80:ILE:HA	25:r:83:VAL:HG12	1.75	0.69
5:F:68:THR:OG1	8:I:32:GLU:OE1	2.05	0.69
17:X:-38:DG:C2	18:Y:39:DA:N1	2.60	0.69
3:d:909:ARG:NE	10:l:91:PHE:CZ	2.55	0.69
30:w:105:GLU:HG2	30:w:106:ASP:H	1.58	0.69
3:D:966:LEU:CD2	3:D:981:GLN:HE21	2.06	0.68
11:O:58:PHE:CD1	11:O:81:PHE:HD2	2.11	0.68
5:F:315:ARG:C	5:F:327:TRP:HH2	2.01	0.68
12:P:243:LYS:HZ1	13:Q:318:ASP:C	2.00	0.68
1:A:1187:LYS:O	1:A:1191:ILE:CG1	2.39	0.68
5:F:52:GLN:HG2	8:I:26:MET:HG3	1.74	0.68
11:O:18:SER:N	13:Q:49:LYS:NZ	2.40	0.68
11:O:55:ARG:HH12	13:Q:369:LYS:NZ	1.90	0.68
11:O:88:ILE:CG2	13:Q:360:LEU:HB2	2.03	0.68
15:S:44:GLN:CA	16:T:9:LEU:CD1	2.71	0.68
5:f:447:ALA:CA	5:f:456:GLY:HA3	2.23	0.68
16:T:18:VAL:HG21	16:T:95:VAL:CG2	2.23	0.68
3:D:966:LEU:CD1	3:D:981:GLN:HE21	2.07	0.68
3:D:966:LEU:C	3:D:966:LEU:HD23	2.17	0.68
3:D:1006:LEU:HD11	11:O:68:CYS:SG	2.34	0.68
4:E:426:ARG:HH11	4:E:640:ASN:HD22	1.42	0.68
12:P:189:ASN:CG	13:Q:376:TRP:HZ2	2.01	0.68
14:R:182:ALA:CB	16:T:153:TYR:O	2.36	0.68
22:o:1344:MET:HE2	26:s:134:GLU:HA	1.75	0.68
2:B:835:ARG:HD3	7:H:187:GLU:OE2	1.92	0.68
13:Q:311:GLU:OE1	13:Q:311:GLU:N	2.22	0.68
16:T:124:TYR:CZ	23:p:596:ILE:CB	2.77	0.68
1:A:495:LEU:HD13	5:f:268:ARG:CZ	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:848:HIS:CD2	7:H:226:ALA:CA	2.77	0.68
5:F:368:THR:HG22	5:F:373:ARG:HB2	1.76	0.68
22:o:1156:ASP:OD1	22:o:1157:ILE:N	2.27	0.68
25:r:17:ALA:HB3	28:u:81:LYS:O	1.93	0.68
1:A:567:LEU:HD22	2:B:745:GLN:HG2	1.76	0.67
1:A:1198:ARG:NH1	6:G:181:TRP:CE2	2.53	0.67
17:X:-9:DG:H22	18:Y:9:DC:N4	1.92	0.67
18:Y:9:DC:H2"	18:Y:10:DT:C5	2.29	0.67
23:p:320:PHE:O	23:p:324:ARG:NH1	2.27	0.67
3:D:881:ARG:CZ	10:L:57:VAL:CG2	2.69	0.67
1:A:969:PRO:HG3	17:X:21:DC:OP1	1.94	0.67
5:F:51:ALA:O	8:I:28:ILE:CD1	2.42	0.67
14:R:134:ILE:HG12	14:R:171:GLU:HG3	1.76	0.67
16:T:124:TYR:CE2	23:p:596:ILE:CD1	2.54	0.67
1:A:950:VAL:CG2	1:A:1065:GLU:HG3	2.24	0.67
11:O:22:LEU:CB	11:O:28:ILE:HD13	2.23	0.67
12:P:165:LEU:HD21	12:P:321:ILE:HG13	1.76	0.67
4:e:645:GLY:H	4:e:675:LEU:HD11	1.59	0.67
1:A:590:GLN:NE2	2:B:513:LYS:NZ	2.42	0.67
4:E:615:ASP:OD1	8:I:114:ARG:CA	2.41	0.67
5:F:67:THR:HA	8:I:32:GLU:OE2	1.91	0.67
5:F:274:ASN:HB2	5:F:317:LEU:H	1.58	0.67
12:P:243:LYS:NZ	13:Q:318:ASP:C	2.53	0.67
15:S:8:SER:O	16:T:49:GLN:N	2.26	0.67
7:H:111:ALA:HB2	9:J:157:LEU:HD13	1.76	0.67
15:S:8:SER:C	16:T:48:THR:CA	2.63	0.67
2:B:847:ARG:HA	7:H:226:ALA:HB1	1.76	0.67
11:O:80:GLU:HG2	11:O:89:LYS:HA	1.77	0.67
15:S:125:TYR:HD2	16:T:31:TRP:HZ3	1.37	0.67
22:o:95:PHE:HB2	22:o:311:GLN:HE22	1.59	0.67
22:o:811:ILE:HD12	30:w:79:PRO:HB3	1.74	0.67
22:o:1005:HIS:HD2	22:o:1007:ILE:HG12	1.59	0.67
2:B:310:ASP:OD2	7:H:223:TYR:HE2	1.77	0.67
3:D:1083:PHE:CE2	4:E:585:ASN:ND2	2.37	0.67
5:F:80:VAL:HG13	8:I:45:ARG:HH12	1.58	0.67
15:S:126:ILE:N	15:S:138:PHE:O	2.23	0.67
16:T:149:VAL:HG11	23:p:146:LYS:CD	2.25	0.67
5:F:319:LEU:HD23	5:F:319:LEU:N	2.10	0.67
8:I:60:HIS:NE2	10:L:118:LEU:CD2	2.54	0.67
13:Q:47:GLU:OE2	13:Q:60:HIS:CG	2.45	0.67
15:S:49:ARG:NH1	15:S:96:GLN:O	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:c:67:GLY:CA	9:j:116:LEU:HD11	2.25	0.67
3:D:966:LEU:HD21	3:D:981:GLN:NE2	2.10	0.66
12:P:204:ILE:HG13	12:P:207:PRO:HD2	1.78	0.66
15:S:16:VAL:HB	16:T:56:PHE:CE1	2.27	0.66
3:d:1082:ALA:HB2	10:l:83:MET:CE	2.25	0.66
22:o:922:PHE:H	22:o:1052:ARG:HH11	1.43	0.66
5:F:43:VAL:CG2	8:I:43:ALA:CA	2.73	0.66
7:H:111:ALA:HA	9:J:126:TYR:OH	1.95	0.66
23:p:249:LYS:HG2	23:p:252:ILE:HD11	1.77	0.66
30:w:109:ARG:NH2	30:w:125:GLU:O	2.28	0.66
1:A:463:PRO:HD3	5:F:222:LEU:HD13	1.76	0.66
5:F:324:ASP:HA	5:F:327:TRP:CB	2.25	0.66
15:S:27:ASN:HB2	16:T:96:PHE:CE1	2.30	0.66
23:p:1120:ASN:HD22	23:p:1145:GLN:HB2	1.60	0.66
25:r:73:ARG:NH2	28:u:86:ASP:OD2	2.28	0.66
5:F:90:GLU:CD	9:J:208:GLY:HA3	2.20	0.66
12:P:188:ARG:HH21	13:Q:324:GLU:HA	1.61	0.66
14:R:109:SER:HA	14:R:112:ARG:HD2	1.76	0.66
10:l:82:GLU:O	10:l:86:GLN:HG3	1.95	0.66
23:p:1022:LEU:HD12	23:p:1023:ARG:HG2	1.78	0.66
1:A:472:ASN:N	5:f:299:LYS:HZ3	1.93	0.66
1:A:1063:LYS:HD3	1:A:1063:LYS:C	2.21	0.66
4:E:694:LEU:HB3	4:E:703:MET:CE	2.26	0.66
5:F:213:ILE:CB	7:H:163:PRO:O	2.30	0.66
7:H:118:VAL:CG2	9:J:127:THR:HG23	2.25	0.66
11:O:57:ASN:O	11:O:57:ASN:ND2	2.28	0.66
22:o:626:THR:HG22	22:o:627:LYS:H	1.60	0.66
22:o:1345:ARG:HG2	26:s:133:GLN:NE2	2.10	0.66
2:B:402:ILE:HD12	2:B:455:LEU:HD12	1.77	0.66
5:F:80:VAL:HG11	8:I:42:PHE:HE1	1.58	0.66
14:R:43:ASP:O	22:o:79:THR:HG21	1.96	0.66
24:q:154:ARG:HD3	31:x:64:PRO:HD3	1.78	0.66
1:A:1169:ARG:HH22	6:G:169:LEU:HD22	1.61	0.66
5:F:46:ARG:HB3	8:I:42:PHE:HE2	1.60	0.66
7:H:108:PRO:HG3	9:J:119:PHE:CD2	2.30	0.66
7:H:111:ALA:CB	9:J:157:LEU:HD11	2.26	0.66
11:O:39:GLN:HG2	13:Q:25:VAL:HG12	1.76	0.66
15:S:121:ASN:C	16:T:25:LYS:HE2	2.20	0.66
1:A:349:TRP:HE1	5:f:262:PHE:HA	1.60	0.66
5:F:48:LYS:HE3	8:I:22:ILE:HA	1.77	0.66
5:F:113:ASP:HA	7:H:52:SER:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:-23:DC:O2	18:Y:23:DG:N2	2.18	0.66
2:B:847:ARG:CA	7:H:226:ALA:HB1	2.25	0.66
4:E:615:ASP:OD2	8:I:114:ARG:HG2	1.96	0.66
8:i:60:HIS:CD2	10:l:106:ARG:NH2	2.63	0.66
23:p:854:ILE:HD12	23:p:866:ILE:HG22	1.77	0.66
4:E:359:LEU:HD13	4:E:627:LEU:HD12	1.76	0.66
5:F:14:LEU:HA	8:I:18:MET:HG2	1.76	0.66
11:O:25:SER:OG	11:O:27:GLN:HB2	1.96	0.66
15:S:124:TYR:CE1	16:T:22:LYS:HE2	2.31	0.65
25:r:87:LEU:HD13	25:r:97:LEU:HD22	1.77	0.65
28:u:32:THR:OG1	28:u:33:GLU:OE1	2.14	0.65
11:O:3:TYR:C	11:O:5:LEU:H	2.04	0.65
23:p:690:CYS:SG	23:p:691:SER:N	2.69	0.65
26:s:51:GLY:O	26:s:54:ARG:NH2	2.29	0.65
5:F:67:THR:CB	8:I:32:GLU:OE2	2.45	0.65
2:B:431:LEU:HD22	2:B:431:LEU:H	1.61	0.65
7:H:102:PHE:CE1	9:J:158:ALA:O	2.49	0.65
7:H:107:LEU:HD11	9:J:157:LEU:C	2.21	0.65
16:T:148:VAL:HG13	23:p:125:TYR:OH	1.96	0.65
1:A:1190:VAL:CA	6:G:162:VAL:HG13	2.26	0.65
2:B:827:ARG:NE	7:H:211:PHE:HZ	1.95	0.65
5:F:101:GLY:HA3	8:I:34:ARG:NH2	2.12	0.65
5:F:329:LEU:HD23	5:F:329:LEU:C	2.21	0.65
11:O:19:LEU:HA	11:O:28:ILE:HD11	1.78	0.65
23:p:677:MET:H	23:p:682:LEU:HD12	1.62	0.65
26:s:17:ILE:HD11	26:s:135:LEU:HD13	1.78	0.65
3:D:1006:LEU:HD13	11:O:68:CYS:HB3	1.75	0.65
4:E:694:LEU:HB3	4:E:703:MET:HE3	1.79	0.65
4:E:788:ARG:O	7:H:145:HIS:HB2	1.96	0.65
13:Q:48:ASN:HA	13:Q:51:MET:HE2	1.78	0.65
16:T:137:LYS:O	16:T:137:LYS:HD3	1.96	0.65
2:B:159:LEU:HD23	2:B:159:LEU:H	1.62	0.65
7:H:108:PRO:HG3	9:J:119:PHE:CG	2.30	0.65
11:O:55:ARG:HH21	13:Q:369:LYS:C	1.93	0.65
15:S:8:SER:HB3	16:T:49:GLN:HA	0.66	0.65
24:q:15:THR:HG22	24:q:16:ASP:H	1.62	0.65
12:P:167:ASN:HD22	12:P:259:VAL:HB	1.62	0.65
24:q:19:VAL:HG23	24:q:241:PRO:HB2	1.79	0.65
4:E:614:THR:O	8:I:114:ARG:O	2.14	0.65
5:f:239:ARG:HD3	5:f:284:ARG:HH11	1.60	0.65
1:A:950:VAL:CG2	1:A:1065:GLU:CG	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:68:THR:N	8:I:32:GLU:CD	2.55	0.64
5:F:219:GLU:CB	7:H:156:PRO:HB2	2.26	0.64
12:P:278:GLN:CD	12:P:278:GLN:H	2.04	0.64
15:S:47:LEU:HB2	16:T:7:LEU:HD22	1.79	0.64
22:o:533:PRO:O	22:o:647:THR:OG1	2.15	0.64
1:A:1168:TYR:HB2	6:G:180:ARG:HB3	1.78	0.64
17:X:-36:DC:H2''	17:X:-35:DA:H5'	1.79	0.64
1:A:1189:ALA:CB	6:G:154:LYS:HD3	2.26	0.64
1:A:1190:VAL:HG21	6:G:165:GLU:OE1	1.97	0.64
4:E:615:ASP:OD1	8:I:114:ARG:C	2.41	0.64
12:P:305:PHE:CE1	18:Y:30:DA:H2''	2.32	0.64
16:T:31:TRP:HD1	16:T:62:LEU:HD21	1.62	0.64
5:F:312:ILE:HD11	5:F:335:ARG:N	2.11	0.64
23:p:313:GLU:HG3	23:p:316:VAL:HG12	1.80	0.64
1:A:411:GLU:HG2	5:F:358:THR:HG21	1.80	0.64
5:F:361:LYS:HA	5:F:364:VAL:HG22	1.79	0.64
5:f:320:ARG:NH1	5:f:320:ARG:HB3	2.12	0.64
1:A:349:TRP:NE1	5:f:262:PHE:CD1	2.66	0.64
4:E:359:LEU:HD11	4:E:648:ASP:HB2	1.80	0.64
7:H:132:LYS:HE2	7:H:134:LEU:H	1.62	0.64
13:Q:26:ARG:HH21	13:Q:39:LEU:HD23	1.61	0.64
15:S:125:TYR:CD2	16:T:23:VAL:HG21	2.32	0.64
16:T:225:VAL:C	16:T:227:GLY:N	2.55	0.64
28:u:101:ILE:HG23	28:u:104:MET:HB3	1.79	0.64
2:B:490:SER:HA	2:B:493:TRP:HB2	1.78	0.64
4:E:696:TRP:CZ3	4:E:703:MET:HB3	2.32	0.64
5:F:14:LEU:HB3	8:I:15:ASP:OD1	1.98	0.64
10:L:102:LEU:CA	10:L:105:HIS:HD2	2.08	0.64
11:O:55:ARG:HA	11:O:55:ARG:HE	1.62	0.64
13:Q:47:GLU:OE1	13:Q:60:HIS:ND1	2.30	0.64
2:B:947:GLU:HB2	2:B:988:PRO:HD2	1.80	0.64
5:F:213:ILE:HG21	7:H:163:PRO:HB2	1.76	0.64
7:H:69:ILE:HG21	9:J:138:TYR:HB2	1.79	0.64
1:A:484:ILE:CA	5:f:306:PRO:HB3	2.27	0.63
1:A:575:PRO:CD	2:B:608:ASN:HB2	2.28	0.63
3:D:901:TYR:CD1	10:L:128:ILE:CG2	2.80	0.63
3:D:881:ARG:HD3	10:L:57:VAL:CG1	2.29	0.63
3:D:881:ARG:CD	10:L:57:VAL:HG11	2.28	0.63
5:F:320:ARG:O	5:F:324:ASP:HB2	1.99	0.63
12:P:239:ARG:HB2	13:Q:314:LEU:HG	1.79	0.63
15:S:135:PHE:CD2	16:T:43:LEU:CD2	2.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:1146:GLN:HB3	22:o:1149:ARG:HH21	1.62	0.63
1:A:414:ILE:HG23	5:F:310:THR:HA	1.78	0.63
2:B:844:PRO:HB2	7:H:225:THR:O	1.98	0.63
10:l:106:ARG:NH1	10:l:114:LYS:HG3	2.13	0.63
25:r:26:PHE:CZ	28:u:78:ARG:HG3	2.33	0.63
4:E:745:GLU:OE1	4:E:745:GLU:HA	1.98	0.63
15:S:18:VAL:O	16:T:38:GLY:O	2.12	0.63
17:X:-35:DA:N3	18:Y:36:DG:N2	2.46	0.63
22:o:1323:THR:OG1	22:o:1325:ASP:OD1	2.15	0.63
5:F:68:THR:HG21	8:I:34:ARG:HH11	1.56	0.63
16:T:40:VAL:O	16:T:56:PHE:HZ	1.81	0.63
3:D:1006:LEU:HD11	11:O:68:CYS:CB	2.29	0.63
25:r:62:MET:HA	25:r:65:LEU:HB3	1.79	0.63
1:A:590:GLN:HE22	2:B:513:LYS:NZ	1.97	0.63
14:R:111:ASP:O	14:R:115:MET:HB2	1.99	0.63
10:l:101:GLN:O	10:l:105:HIS:CG	2.47	0.63
1:A:950:VAL:HG21	1:A:1065:GLU:CG	2.28	0.63
5:F:84:TYR:HB3	8:I:41:GLU:OE1	1.99	0.63
5:F:319:LEU:H	5:F:319:LEU:CD2	2.12	0.63
10:L:106:ARG:HH11	10:L:114:LYS:HZ2	0.63	0.63
15:S:20:LYS:HE3	16:T:34:ALA:O	1.99	0.63
16:T:196:TYR:HB2	16:T:232:THR:HG22	1.79	0.63
22:o:193:ARG:HA	22:o:198:LEU:HA	1.79	0.63
1:A:1169:ARG:CB	1:A:1181:ARG:NH2	2.52	0.62
8:i:73:LEU:HD13	10:l:105:HIS:CE1	2.34	0.62
23:p:311:ILE:HD11	23:p:317:ALA:HA	1.81	0.62
1:A:639:LEU:HG	1:A:773:ILE:O	1.99	0.62
17:X:-12:DC:H2"	17:X:-11:DT:H71	1.81	0.62
13:Q:47:GLU:OE2	13:Q:60:HIS:NE2	2.27	0.62
15:S:17:ARG:CA	16:T:39:GLU:HG3	2.30	0.62
23:p:407:MET:HE1	23:p:444:LEU:HG	1.81	0.62
1:A:575:PRO:CD	2:B:608:ASN:HD22	1.92	0.62
11:O:58:PHE:CG	11:O:81:PHE:HD2	2.17	0.62
15:S:17:ARG:CB	16:T:39:GLU:CA	2.75	0.62
12:P:259:VAL:CG2	18:Y:28:DG:H21	2.09	0.62
1:A:511:LEU:HD22	1:A:511:LEU:N	2.10	0.62
3:D:881:ARG:CZ	10:L:57:VAL:HG22	2.16	0.62
3:D:962:GLU:HA	3:D:965:ILE:HB	1.82	0.62
3:D:991:MET:CE	16:T:193:LYS:NZ	2.63	0.62
13:Q:15:ARG:HH21	13:Q:58:GLY:HA2	1.65	0.62
8:i:73:LEU:HD21	10:l:105:HIS:CD2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:327:ARG:NH2	22:o:336:LEU:O	2.29	0.62
1:A:355:VAL:O	1:A:355:VAL:HG23	1.97	0.62
2:B:583:GLU:CD	2:B:583:GLU:H	2.06	0.62
7:H:93:ILE:HD11	9:J:144:PHE:HZ	1.65	0.62
7:H:108:PRO:HA	9:J:119:PHE:CE1	2.34	0.62
14:R:153:GLY:HA3	18:Y:21:DT:H5"	1.81	0.62
14:R:173:VAL:HB	14:R:175:ARG:HH12	1.64	0.62
22:o:508:SER:OG	22:o:509:LEU:N	2.31	0.62
3:D:1083:PHE:HE2	4:E:585:ASN:HD21	0.72	0.62
5:F:316:GLN:CD	5:F:320:ARG:HA	2.24	0.62
14:R:297:PRO:HA	14:R:310:VAL:HG11	1.82	0.62
28:u:3:TYR:HB2	28:u:76:VAL:HG12	1.82	0.62
1:A:638:PRO:CD	6:G:39:LEU:HD23	2.29	0.62
12:P:259:VAL:HG23	18:Y:28:DG:H21	1.64	0.62
15:S:16:VAL:O	16:T:39:GLU:HG3	2.00	0.62
16:T:149:VAL:HG11	23:p:146:LYS:HD3	1.81	0.62
22:o:232:GLU:HA	22:o:235:VAL:HG12	1.80	0.62
1:A:480:TRP:CZ2	5:f:354:ARG:NH2	2.67	0.62
1:A:1198:ARG:HH12	6:G:181:TRP:CD2	1.57	0.62
23:p:82:PRO:HB3	23:p:134:LYS:HB3	1.81	0.62
28:u:151:ARG:HB3	28:u:158:PHE:HE1	1.65	0.62
2:B:158:GLY:HA2	2:B:188:PHE:HB3	1.81	0.61
2:B:735:ILE:CG2	7:H:176:ARG:NH2	2.62	0.61
16:T:183:VAL:HG12	16:T:187:LEU:HG	1.81	0.61
16:T:181:GLN:HA	16:T:181:GLN:NE2	2.15	0.61
22:o:27:SER:N	22:o:30:GLU:OE1	2.33	0.61
5:F:114:LEU:HD13	7:H:53:ALA:CB	2.29	0.61
15:S:24:LYS:CB	16:T:99:SER:HA	2.31	0.61
22:o:97:VAL:HA	22:o:100:LEU:HD23	1.81	0.61
22:o:330:GLN:HE22	22:o:336:LEU:HD11	1.65	0.61
5:F:71:ILE:CD1	8:I:35:VAL:HG22	2.30	0.61
5:F:213:ILE:CD1	7:H:163:PRO:HB3	2.30	0.61
12:P:189:ASN:ND2	13:Q:376:TRP:HZ2	1.99	0.61
22:o:125:LYS:O	22:o:129:ILE:HG12	2.01	0.61
22:o:1430:CYS:O	22:o:1435:THR:HG22	2.01	0.61
24:q:193:ARG:HD3	24:q:220:TYR:HD1	1.65	0.61
5:F:90:GLU:OE1	9:J:208:GLY:C	2.44	0.61
5:F:335:ARG:HD3	5:F:382:GLU:OE1	1.99	0.61
23:p:111:ASN:HD21	23:p:742:VAL:HG11	1.65	0.61
23:p:565:THR:HG21	23:p:580:PRO:HG3	1.83	0.61
4:E:519:GLU:HG3	4:E:519:GLU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:613:ALA:HB2	4:E:620:LEU:HD11	1.81	0.61
5:F:15:PRO:HG3	8:I:14:LYS:NZ	2.04	0.61
5:F:370:TRP:HB3	5:F:419:GLY:HA3	1.82	0.61
13:Q:56:VAL:HG12	13:Q:57:ASP:N	2.16	0.61
10:l:76:LEU:HD13	10:l:84:LEU:CD1	2.30	0.61
22:o:217:SER:OG	22:o:219:GLU:OE1	2.18	0.61
22:o:1177:TYR:OH	30:w:28:GLU:OE2	2.19	0.61
25:r:110:GLU:OE2	28:u:167:TYR:CG	2.53	0.61
11:O:57:ASN:H	11:O:57:ASN:HD22	1.48	0.61
24:q:36:ARG:HH12	32:y:40:HIS:HB2	1.66	0.61
2:B:873:LEU:HD12	7:H:201:GLN:NE2	2.16	0.61
5:F:370:TRP:CH2	5:F:420:ALA:HB2	2.36	0.61
7:H:192:ARG:NH1	7:H:209:SER:O	2.34	0.61
12:P:188:ARG:NH2	13:Q:323:GLU:C	2.56	0.61
15:S:24:LYS:HB3	16:T:99:SER:CA	2.29	0.61
22:o:108:ARG:NH2	22:o:191:ILE:O	2.33	0.61
22:o:136:GLN:HG3	22:o:139:LYS:HB3	1.83	0.61
28:u:24:ASN:HA	28:u:27:LYS:HG3	1.82	0.61
2:B:873:LEU:HD12	7:H:201:GLN:HE22	1.65	0.61
5:f:330:ARG:HH22	5:f:371:THR:HB	1.66	0.61
1:A:564:PRO:CG	2:B:744:PHE:CD2	2.82	0.61
1:A:639:LEU:HD11	1:A:774:ARG:CG	2.26	0.61
3:D:881:ARG:HD3	10:L:57:VAL:HG13	1.83	0.61
8:I:60:HIS:NE2	10:L:118:LEU:HD23	2.16	0.61
12:P:243:LYS:HZ1	13:Q:318:ASP:HA	0.59	0.61
16:T:183:VAL:O	16:T:187:LEU:N	2.29	0.61
17:X:-6:DA:C2	18:Y:7:DG:N2	2.68	0.61
4:E:501:PRO:HD3	7:H:149:HIS:HB3	1.83	0.60
19:c:67:GLY:CA	9:j:116:LEU:CD1	2.70	0.60
15:S:25:LYS:N	16:T:98:GLU:O	2.34	0.60
3:d:1082:ALA:CB	10:l:83:MET:HE2	2.32	0.60
5:f:219:GLU:OE1	5:f:219:GLU:N	2.26	0.60
1:A:410:TRP:HB2	5:F:306:PRO:HG3	1.83	0.60
16:T:20:LEU:O	16:T:113:ARG:HA	2.02	0.60
22:o:930:LEU:HG	22:o:939:VAL:HG23	1.83	0.60
1:A:485:ILE:CD1	5:f:268:ARG:HG2	2.32	0.60
1:A:753:TYR:CG	1:A:1077:LEU:HB3	2.36	0.60
1:A:1198:ARG:NH1	6:G:181:TRP:CD1	2.67	0.60
11:O:58:PHE:HB2	13:Q:371:ILE:O	2.02	0.60
17:X:-24:DG:OP2	17:X:-24:DG:H8	1.85	0.60
25:r:16:ASP:OD1	28:u:81:LYS:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:696:TRP:CZ3	4:E:703:MET:SD	2.95	0.60
19:c:18:CYS:O	19:c:23:TRP:HB2	2.01	0.60
3:d:884:GLU:HA	3:d:887:LYS:HE3	1.82	0.60
22:o:341:GLN:HA	22:o:344:LYS:HE3	1.82	0.60
2:B:846:TYR:CE1	7:H:227:LEU:O	2.54	0.60
3:D:916:LYS:HE2	3:D:1066:CYS:SG	2.41	0.60
5:F:52:GLN:HG2	8:I:26:MET:CG	2.32	0.60
5:F:370:TRP:CZ3	5:F:420:ALA:CB	2.85	0.60
11:O:5:LEU:HD13	11:O:98:CYS:SG	2.42	0.60
11:O:22:LEU:HD13	11:O:28:ILE:CG2	2.28	0.60
11:O:56:VAL:HG21	11:O:58:PHE:CE2	2.37	0.60
11:O:58:PHE:CG	11:O:81:PHE:CD2	2.90	0.60
16:T:188:PHE:N	16:T:188:PHE:HD1	2.00	0.60
22:o:853:LYS:NZ	22:o:1102:MET:O	2.30	0.60
5:F:48:LYS:HE3	8:I:22:ILE:CG1	2.31	0.60
7:H:93:ILE:HD11	9:J:144:PHE:CZ	2.36	0.60
15:S:18:VAL:HG21	16:T:40:VAL:HG21	1.83	0.60
16:T:223:GLN:H	16:T:223:GLN:CD	2.09	0.60
16:T:228:ILE:HG13	16:T:228:ILE:O	2.01	0.60
5:f:349:ASN:HB3	5:f:351:ILE:HG13	1.84	0.60
8:i:73:LEU:CD1	10:l:105:HIS:CE1	2.84	0.60
22:o:1005:HIS:CD2	22:o:1007:ILE:HG12	2.36	0.60
24:q:44:ILE:HD12	24:q:178:PRO:HB3	1.84	0.60
25:r:103:LEU:HD21	28:u:84:VAL:CB	2.32	0.60
30:w:35:LEU:HD12	30:w:51:SER:HA	1.83	0.60
2:B:328:ASN:HA	7:H:227:LEU:CD1	2.31	0.60
3:D:962:GLU:HG2	3:D:963:ARG:N	2.17	0.60
14:R:289:TYR:OH	14:R:314:PRO:O	2.17	0.60
15:S:9:GLN:O	15:S:9:GLN:HG2	2.01	0.60
15:S:39:PHE:CZ	16:T:92:THR:HG21	2.37	0.60
15:S:125:TYR:HE2	16:T:31:TRP:CZ3	2.11	0.60
17:X:-38:DG:H22	18:Y:38:DC:H42	1.48	0.60
1:A:484:ILE:HG12	5:f:306:PRO:HB3	1.84	0.60
3:D:958:LYS:O	3:D:958:LYS:HE2	2.02	0.60
12:P:274:VAL:HG11	14:R:208:LEU:HD21	1.82	0.60
14:R:28:ARG:HE	23:p:842:HIS:HE1	1.49	0.60
3:d:909:ARG:CZ	10:l:91:PHE:CE1	2.85	0.60
23:p:584:MET:HE3	23:p:605:ARG:HB2	1.83	0.60
1:A:470:ILE:CD1	7:H:166:ARG:HB2	2.32	0.60
2:B:431:LEU:C	2:B:431:LEU:HD23	2.26	0.60
3:D:873:LEU:HB3	3:D:878:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:40:VAL:HG11	9:J:130:ILE:HG12	1.84	0.60
14:R:181:CYS:HB3	16:T:155:PRO:O	2.01	0.60
15:S:124:TYR:HE1	16:T:22:LYS:CE	2.15	0.60
16:T:184:LEU:C	16:T:184:LEU:HD23	2.27	0.60
16:T:220:ILE:C	16:T:220:ILE:HD12	2.26	0.60
1:A:1190:VAL:CB	6:G:162:VAL:HG13	2.31	0.59
11:O:89:LYS:N	13:Q:361:ASN:HD21	2.00	0.59
12:P:214:PHE:CE2	17:X:-24:DG:C1'	2.84	0.59
13:Q:324:GLU:CD	13:Q:324:GLU:H	2.09	0.59
17:X:-35:DA:N1	18:Y:36:DG:C2	2.70	0.59
15:S:116:GLY:HA2	23:p:356:PHE:CD1	2.37	0.59
15:S:127:PHE:O	16:T:19:TRP:HB2	2.01	0.59
16:T:122:GLU:CD	16:T:123:ASN:H	2.10	0.59
8:i:73:LEU:HB2	10:l:105:HIS:HE1	1.66	0.59
25:r:16:ASP:HB3	25:r:19:GLN:HG2	1.83	0.59
3:D:1085:LYS:NZ	10:L:83:MET:CE	2.65	0.59
7:H:102:PHE:HZ	9:J:158:ALA:HA	1.65	0.59
1:A:1016:GLU:OE1	1:A:1019:LYS:HE3	2.02	0.59
8:I:56:ILE:HG21	10:L:122:ARG:HH21	1.68	0.59
8:I:132:LEU:CG	9:J:121:MET:CE	2.79	0.59
11:O:88:ILE:HD12	13:Q:360:LEU:HB2	1.77	0.59
5:F:14:LEU:HD22	8:I:15:ASP:O	2.02	0.59
11:O:58:PHE:CD2	13:Q:370:ALA:HB1	2.37	0.59
19:c:99:PHE:HB2	19:c:100:PRO:HD3	1.83	0.59
4:E:703:MET:O	4:E:703:MET:HG3	2.01	0.59
22:o:1129:ASN:ND2	22:o:1415:THR:HB	2.18	0.59
1:A:1190:VAL:HG22	6:G:162:VAL:HA	1.85	0.59
2:B:203:LYS:HD3	2:B:237:MET:HE3	1.83	0.59
5:F:68:THR:CB	8:I:34:ARG:NH1	2.65	0.59
11:O:22:LEU:C	11:O:28:ILE:H	2.09	0.59
15:S:16:VAL:CG2	16:T:43:LEU:HB2	2.33	0.59
15:S:17:ARG:CB	16:T:39:GLU:CB	2.81	0.59
15:S:46:ARG:NH2	16:T:3:GLU:OE1	2.32	0.59
22:o:18:ILE:HB	22:o:1462:GLN:HE22	1.68	0.59
1:A:1185:VAL:HG12	1:A:1191:ILE:CD1	2.32	0.59
5:F:369:PRO:O	5:F:373:ARG:N	2.32	0.59
11:O:17:GLU:HB3	13:Q:49:LYS:NZ	2.18	0.59
11:O:25:SER:C	11:O:27:GLN:N	2.59	0.59
11:O:75:VAL:HG21	13:Q:327:GLU:HG3	1.84	0.59
12:P:210:THR:HG21	18:Y:26:DG:H4'	1.85	0.59
15:S:102:VAL:O	15:S:108:ARG:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1085:LYS:HZ3	10:L:83:MET:CE	2.16	0.59
5:F:48:LYS:CE	8:I:22:ILE:HG12	2.30	0.59
5:F:319:LEU:HG	5:F:319:LEU:O	2.02	0.59
22:o:331:LYS:O	22:o:334:ARG:N	2.35	0.59
22:o:1030:SER:HB2	26:s:162:ARG:HE	1.67	0.59
3:D:1080:TYR:CD1	4:E:585:ASN:OD1	2.55	0.59
4:E:586:TYR:HB3	4:E:605:HIS:HB3	1.85	0.59
5:F:14:LEU:CB	8:I:15:ASP:OD1	2.50	0.59
22:o:1257:LEU:HD12	22:o:1259:ILE:HD11	1.85	0.59
13:Q:26:ARG:NH2	13:Q:39:LEU:CD2	2.65	0.58
1:A:1157:ASN:O	1:A:1159:SER:N	2.35	0.58
11:O:22:LEU:O	11:O:28:ILE:O	2.21	0.58
13:Q:15:ARG:HH21	13:Q:58:GLY:CA	2.15	0.58
22:o:17:THR:HG22	22:o:18:ILE:H	1.68	0.58
22:o:1230:GLN:HA	22:o:1233:GLU:CD	2.28	0.58
23:p:988:LYS:O	23:p:992:ASN:ND2	2.31	0.58
5:F:369:PRO:O	5:F:373:ARG:CB	2.52	0.58
19:c:21:LEU:HD12	19:c:21:LEU:C	2.29	0.58
2:B:848:HIS:NE2	7:H:226:ALA:N	2.51	0.58
5:F:44:SER:HB3	8:I:22:ILE:HD11	1.85	0.58
15:S:124:TYR:CE1	16:T:22:LYS:CE	2.87	0.58
21:m:31:LEU:HD23	21:m:31:LEU:N	2.16	0.58
25:r:16:ASP:OD2	28:u:81:LYS:HD3	2.03	0.58
1:A:1185:VAL:HB	1:A:1191:ILE:CG1	2.33	0.58
4:E:694:LEU:CD1	4:E:703:MET:CE	2.51	0.58
4:E:742:LYS:HA	4:E:745:GLU:HG2	1.85	0.58
15:S:26:TYR:CD1	16:T:97:THR:HG22	2.38	0.58
15:S:124:TYR:CZ	16:T:22:LYS:HE2	2.38	0.58
16:T:209:PRO:HG2	16:T:212:TYR:HB3	1.84	0.58
4:E:474:THR:OG1	4:E:546:VAL:O	2.19	0.58
11:O:25:SER:O	11:O:27:GLN:N	2.36	0.58
23:p:124:LEU:HD22	23:p:152:ILE:HD11	1.85	0.58
5:F:305:ILE:HB	5:F:306:PRO:HD3	1.83	0.58
5:F:320:ARG:N	5:F:321:PRO:HD2	2.18	0.58
15:S:18:VAL:CG2	16:T:40:VAL:HG11	2.33	0.58
17:X:7:DT:H2"	17:X:8:DC:C6	2.38	0.58
23:p:591:ARG:NH1	23:p:601:VAL:O	2.36	0.58
25:r:132:ASP:HA	25:r:135:GLN:HG2	1.84	0.58
1:A:1165:LEU:CG	1:A:1191:ILE:HG23	2.33	0.58
11:O:55:ARG:NH1	13:Q:369:LYS:HB3	2.18	0.58
14:R:129:ASN:HD22	23:p:99:TRP:HD1	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:-35:DA:C4	18:Y:36:DG:N2	2.72	0.58
23:p:820:LYS:HE3	23:p:826:GLU:HB2	1.85	0.58
1:A:662:MET:HE3	2:B:509:ASN:HB3	1.86	0.58
1:A:1190:VAL:HA	6:G:162:VAL:CG1	2.34	0.58
16:T:18:VAL:N	16:T:109:ILE:O	2.32	0.58
1:A:929:THR:HG22	1:A:954:ALA:HA	1.86	0.57
2:B:769:LYS:O	2:B:769:LYS:HG3	2.03	0.57
4:E:464:TYR:CE2	5:F:133:ALA:HB2	2.39	0.57
4:E:695:LEU:O	4:E:703:MET:HA	2.04	0.57
5:F:71:ILE:CG2	8:I:38:GLN:HE21	2.14	0.57
15:S:112:GLY:HA2	15:S:145:ASN:O	2.04	0.57
4:e:562:SER:OG	4:e:564:ASP:OD1	2.21	0.57
22:o:1242:ASP:HA	22:o:1262:MET:HE2	1.86	0.57
29:v:27:ARG:HD2	29:v:40:ILE:HG23	1.86	0.57
1:A:485:ILE:HD12	5:f:268:ARG:HG2	1.87	0.57
1:A:666:ARG:HE	2:B:512:GLY:CA	2.14	0.57
3:D:917:ILE:HG13	3:D:1058:VAL:HG21	1.86	0.57
25:r:132:ASP:O	25:r:136:THR:OG1	2.14	0.57
28:u:147:ILE:HG13	28:u:160:ILE:H	1.69	0.57
5:F:114:LEU:HB2	7:H:52:SER:N	2.18	0.57
14:R:169:ARG:NH1	14:R:207:ASP:O	2.38	0.57
1:A:1185:VAL:HB	1:A:1191:ILE:CD1	2.34	0.57
12:P:227:GLU:OE1	12:P:227:GLU:N	2.37	0.57
14:R:214:PHE:HB3	14:R:218:PHE:CE2	2.40	0.57
15:S:6:PRO:O	15:S:10:ASN:HB2	2.04	0.57
22:o:457:ILE:HD11	22:o:515:ILE:HD12	1.86	0.57
22:o:554:PHE:HB3	22:o:585:LEU:HD23	1.85	0.57
24:q:9:VAL:HG11	32:y:105:PHE:HD1	1.69	0.57
30:w:105:GLU:HG2	30:w:106:ASP:N	2.19	0.57
1:A:484:ILE:CG1	5:f:306:PRO:HB3	2.35	0.57
5:F:207:ARG:HD2	5:F:207:ARG:N	2.18	0.57
7:H:171:ASP:HB3	7:H:174:VAL:HG12	1.86	0.57
22:o:1184:THR:HG21	22:o:1190:GLN:HB2	1.85	0.57
26:s:11:TRP:NE1	26:s:35:GLN:O	2.33	0.57
1:A:1198:ARG:HH12	6:G:181:TRP:NE1	2.00	0.57
11:O:39:GLN:HG2	13:Q:25:VAL:CG1	2.35	0.57
15:S:45:ALA:N	16:T:9:LEU:CD1	2.64	0.57
19:c:12:VAL:HG23	5:f:118:ILE:HA	1.86	0.57
23:p:1046:THR:HG22	23:p:1047:TYR:H	1.70	0.57
25:r:78:GLU:HA	25:r:81:ALA:HB3	1.85	0.57
28:u:52:ASP:HB2	28:u:71:LYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:LEU:CD2	6:G:35:GLY:HA3	2.31	0.57
2:B:431:LEU:H	2:B:431:LEU:CD2	2.17	0.57
7:H:108:PRO:HA	9:J:119:PHE:CZ	2.40	0.57
11:O:76:LEU:HB3	11:O:79:VAL:CG2	2.30	0.57
12:P:167:ASN:HB2	12:P:259:VAL:H	1.70	0.57
24:q:31:ALA:O	24:q:231:TYR:OH	2.23	0.57
26:s:100:THR:HG23	26:s:125:TYR:H	1.69	0.57
15:S:126:ILE:O	15:S:138:PHE:N	2.34	0.57
28:u:89:VAL:HG12	28:u:141:ASP:HB2	1.87	0.57
10:L:119:HIS:NE2	10:L:123:GLN:OE1	2.38	0.57
11:O:53:ARG:CA	13:Q:368:SER:CA	2.80	0.57
5:f:320:ARG:CB	5:f:320:ARG:HH11	2.18	0.57
1:A:1165:LEU:HG	1:A:1191:ILE:HG23	1.85	0.57
2:B:735:ILE:HG23	7:H:176:ARG:NH2	2.20	0.57
11:O:58:PHE:HD2	13:Q:370:ALA:HB1	1.70	0.57
17:X:-40:DC:OP2	17:X:-40:DC:H2'	2.05	0.57
4:e:484:LEU:HD21	4:e:504:LEU:HD21	1.86	0.57
1:A:851:ASP:OD1	1:A:851:ASP:N	2.37	0.56
2:B:310:ASP:OD1	7:H:223:TYR:CD2	2.58	0.56
7:H:118:VAL:HG21	9:J:127:THR:HG21	1.82	0.56
8:I:132:LEU:HG	9:J:121:MET:SD	2.45	0.56
16:T:34:ALA:HB1	16:T:38:GLY:HA2	1.85	0.56
4:e:636:HIS:HD2	4:e:638:ASN:H	1.53	0.56
25:r:130:ILE:HA	25:r:133:ASP:HB2	1.86	0.56
2:B:560:TYR:CD2	2:B:581:ILE:HD11	2.39	0.56
5:F:67:THR:CA	8:I:32:GLU:HG3	2.29	0.56
5:F:71:ILE:HD11	8:I:35:VAL:HA	1.86	0.56
10:L:101:GLN:O	10:L:105:HIS:CG	2.52	0.56
11:O:56:VAL:HG21	11:O:58:PHE:CZ	2.40	0.56
18:Y:9:DC:H2'	18:Y:10:DT:C7	2.34	0.56
5:f:223:TYR:HD2	5:f:255:MET:HE1	1.71	0.56
1:A:402:PHE:HA	1:A:407:GLN:NE2	2.20	0.56
11:O:88:ILE:HB	13:Q:360:LEU:CD1	2.34	0.56
13:Q:55:ALA:C	13:Q:56:VAL:HG23	2.30	0.56
14:R:173:VAL:O	14:R:175:ARG:NH1	2.39	0.56
15:S:17:ARG:HB3	16:T:39:GLU:CA	2.33	0.56
15:S:19:PRO:N	16:T:38:GLY:O	2.34	0.56
16:T:30:GLN:HG2	16:T:62:LEU:HG	1.87	0.56
16:T:188:PHE:N	16:T:188:PHE:CD1	2.71	0.56
16:T:225:VAL:O	16:T:227:GLY:N	2.38	0.56
5:f:280:ILE:O	5:f:284:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:p:313:GLU:OE2	23:p:316:VAL:N	2.36	0.56
25:r:33:LEU:HD13	25:r:101:ALA:HB1	1.87	0.56
1:A:844:LYS:HZ3	17:X:31:DT:H71	1.69	0.56
3:D:1085:LYS:HZ2	10:L:83:MET:HE2	1.70	0.56
5:F:71:ILE:HB	8:I:38:GLN:HE22	1.59	0.56
7:H:73:GLY:HA3	9:J:142:ALA:CB	2.31	0.56
11:O:32:LEU:O	11:O:36:VAL:HG23	2.05	0.56
15:S:16:VAL:O	16:T:39:GLU:CG	2.54	0.56
16:T:31:TRP:CD1	16:T:62:LEU:HD21	2.39	0.56
25:r:16:ASP:CG	28:u:81:LYS:HD3	2.30	0.56
1:A:486:TRP:HH2	5:f:358:THR:CG2	2.18	0.56
5:F:43:VAL:HG22	8:I:43:ALA:HB2	1.83	0.56
15:S:135:PHE:CD2	16:T:43:LEU:HD22	2.40	0.56
8:i:60:HIS:NE2	10:l:106:ARG:NE	2.50	0.56
22:o:46:THR:HG22	22:o:57:LEU:HB2	1.87	0.56
23:p:625:LEU:HD13	23:p:675:LEU:HD21	1.88	0.56
24:q:2:PRO:HB3	32:y:54:PRO:HD2	1.87	0.56
1:A:355:VAL:O	1:A:355:VAL:CG2	2.54	0.56
1:A:564:PRO:HB2	2:B:744:PHE:CE2	2.41	0.56
3:D:917:ILE:CB	3:D:1058:VAL:CG1	2.78	0.56
22:o:691:ASP:OD2	22:o:765:ASN:ND2	2.32	0.56
5:F:368:THR:N	5:F:373:ARG:HH11	2.03	0.56
11:O:17:GLU:C	13:Q:49:LYS:NZ	2.63	0.56
12:P:188:ARG:NH2	13:Q:324:GLU:HA	2.20	0.56
12:P:203:ARG:NH2	13:Q:344:ARG:NH2	2.54	0.56
12:P:210:THR:HB	18:Y:27:DA:H5'	1.88	0.56
22:o:856:GLU:OE2	23:p:494:LYS:NZ	2.39	0.56
28:u:100:GLU:HG3	28:u:105:SER:HA	1.87	0.56
1:A:1190:VAL:HG22	6:G:162:VAL:CA	2.36	0.56
4:E:345:MET:HE3	4:E:346:PRO:HD2	1.87	0.56
5:F:412:LEU:CD1	5:F:417:ARG:CB	2.83	0.56
11:O:88:ILE:CD1	13:Q:360:LEU:HD12	2.21	0.56
15:S:47:LEU:HB3	16:T:7:LEU:HB2	1.87	0.56
18:Y:1:DT:H2''	18:Y:2:DC:C6	2.41	0.56
23:p:387:HIS:NE2	23:p:671:GLU:OE2	2.35	0.56
1:A:349:TRP:CE2	5:f:262:PHE:CD1	2.94	0.56
1:A:472:ASN:N	5:f:299:LYS:NZ	2.53	0.56
1:A:1016:GLU:CD	1:A:1019:LYS:HE3	2.30	0.56
2:B:61:ASN:O	2:B:130:VAL:HG23	2.06	0.56
3:D:958:LYS:HE2	3:D:958:LYS:C	2.31	0.56
4:E:561:SER:HB2	4:E:588:VAL:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:88:ILE:CB	13:Q:360:LEU:CB	2.84	0.56
14:R:154:ARG:CZ	18:Y:22:DG:H5''	2.34	0.56
5:f:253:TYR:O	5:f:254:GLN:HB3	2.06	0.56
22:o:460:ARG:HG2	22:o:461:GLN:H	1.69	0.56
26:s:56:THR:HG22	26:s:57:ASP:H	1.71	0.56
1:A:401:ASN:H	1:A:401:ASN:HD22	1.53	0.56
1:A:590:GLN:HE22	2:B:513:LYS:HZ3	1.54	0.56
3:D:905:ALA:O	10:L:126:MET:CE	2.51	0.56
7:H:111:ALA:HA	9:J:157:LEU:HD21	1.88	0.56
18:Y:-2:DC:H2''	18:Y:-1:DC:C6	2.41	0.56
22:o:1101:GLN:NE2	22:o:1389:ASP:OD2	2.39	0.56
23:p:627:ILE:HD11	23:p:663:GLU:HB2	1.88	0.56
28:u:107:PHE:O	28:u:161:GLY:N	2.28	0.56
1:A:480:TRP:CE2	5:f:354:ARG:NH2	2.74	0.55
3:D:991:MET:CE	16:T:193:LYS:HZ1	2.17	0.55
5:F:67:THR:CA	8:I:32:GLU:OE2	2.52	0.55
7:H:69:ILE:CG2	9:J:138:TYR:HB2	2.35	0.55
11:O:55:ARG:HA	11:O:55:ARG:NE	2.21	0.55
12:P:253:PHE:CD2	12:P:253:PHE:O	2.59	0.55
18:Y:8:DC:H2''	18:Y:9:DC:H5	1.70	0.55
23:p:357:CYS:HB2	23:p:360:LYS:HE2	1.89	0.55
23:p:666:ASP:OD1	23:p:667:THR:N	2.36	0.55
23:p:1136:GLU:HG2	23:p:1143:LYS:HE3	1.89	0.55
1:A:575:PRO:HD2	2:B:608:ASN:HB2	1.87	0.55
2:B:259:ASP:HB3	2:B:262:MET:O	2.06	0.55
4:E:790:LEU:HD13	7:H:146:ILE:HG12	1.87	0.55
5:F:43:VAL:HG23	8:I:43:ALA:HA	1.88	0.55
5:F:308:VAL:HB	5:F:337:VAL:CG1	2.26	0.55
14:R:193:ARG:NH1	18:Y:23:DG:OP2	2.37	0.55
8:i:73:LEU:CD1	10:l:105:HIS:NE2	2.69	0.55
23:p:570:ASN:ND2	23:p:616:THR:OG1	2.40	0.55
2:B:544:LEU:HD23	2:B:590:ILE:HD11	1.88	0.55
5:F:406:VAL:HG11	5:F:420:ALA:HB2	1.88	0.55
14:R:179:GLU:HG2	16:T:154:LYS:HZ3	1.71	0.55
16:T:122:GLU:HG3	16:T:123:ASN:O	2.06	0.55
16:T:184:LEU:HG	16:T:188:PHE:CZ	2.42	0.55
25:r:32:LEU:CD2	28:u:2:PHE:HB3	2.36	0.55
26:s:189:GLN:O	26:s:209:VAL:HG12	2.07	0.55
1:A:470:ILE:HG21	5:F:212:SER:OG	2.07	0.55
5:F:14:LEU:HA	8:I:18:MET:CB	2.37	0.55
5:F:213:ILE:CG2	7:H:163:PRO:HB3	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:82:ARG:HB2	11:O:87:LEU:HD13	1.88	0.55
14:R:17:ASN:OD1	14:R:18:HIS:ND1	2.39	0.55
15:S:17:ARG:HA	16:T:40:VAL:H	1.71	0.55
22:o:1150:ASP:OD2	22:o:1153:ARG:NH1	2.39	0.55
5:F:17:GLU:CD	8:I:14:LYS:HE3	2.30	0.55
5:F:412:LEU:C	5:F:414:ASN:H	2.14	0.55
13:Q:29:PHE:CD2	13:Q:34:VAL:HG11	2.39	0.55
14:R:214:PHE:O	14:R:218:PHE:HD2	1.89	0.55
22:o:1229:GLU:OE1	22:o:1229:GLU:N	2.38	0.55
1:A:414:ILE:HG21	5:F:313:VAL:HG22	1.89	0.55
5:F:55:LEU:HD13	8:I:28:ILE:HG23	1.88	0.55
5:F:114:LEU:HB2	7:H:52:SER:H	1.72	0.55
14:R:295:ARG:HG2	14:R:299:LEU:HG	1.86	0.55
15:S:8:SER:CB	16:T:49:GLN:CA	2.24	0.55
15:S:48:GLU:OE2	16:T:5:GLY:HA3	2.07	0.55
25:r:17:ALA:HB2	28:u:80:PHE:HB3	1.88	0.55
1:A:349:TRP:CZ2	5:f:262:PHE:CD1	2.95	0.55
5:F:265:GLU:OE2	5:F:265:GLU:HA	2.06	0.55
12:P:192:TYR:HB2	12:P:200:VAL:HG22	1.87	0.55
14:R:127:ARG:NH1	23:p:435:ILE:O	2.40	0.55
15:S:42:TRP:O	16:T:13:LYS:HD3	2.06	0.55
23:p:685:LYS:NZ	23:p:686:GLU:O	2.38	0.55
1:A:645:LYS:O	1:A:645:LYS:NZ	2.34	0.55
2:B:838:ASN:CG	7:H:214:ILE:HG13	2.32	0.55
5:F:71:ILE:HD11	8:I:35:VAL:CA	2.37	0.55
7:H:47:GLU:OE1	7:H:113:ARG:NH2	2.40	0.55
7:H:110:TYR:CE2	9:J:160:GLN:HB3	2.41	0.55
7:H:118:VAL:CG2	9:J:127:THR:CG2	2.80	0.55
25:r:100:LEU:HA	25:r:103:LEU:HB2	1.89	0.55
1:A:405:VAL:HA	1:A:410:TRP:HE1	1.71	0.55
7:H:40:VAL:HG21	9:J:130:ILE:HG23	1.88	0.55
11:O:43:ALA:CB	13:Q:21:VAL:HG22	2.37	0.55
11:O:90:VAL:HG22	11:O:92:LYS:H	1.71	0.55
15:S:24:LYS:CA	16:T:99:SER:HA	2.37	0.55
3:d:911:GLN:NE2	10:l:69:GLU:OE2	2.40	0.55
3:d:917:ILE:HD11	3:d:1063:LEU:HD13	1.87	0.55
22:o:728:THR:OG1	22:o:731:ASN:OD1	2.25	0.55
25:r:103:LEU:O	28:u:144:ARG:NH1	2.40	0.55
11:O:23:ILE:CA	11:O:28:ILE:O	2.43	0.54
13:Q:15:ARG:NH2	13:Q:58:GLY:HA3	2.22	0.54
14:R:111:ASP:O	14:R:115:MET:N	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:1218:ARG:HA	22:o:1221:MET:HB2	1.89	0.54
28:u:112:SER:HB2	28:u:163:LEU:H	1.72	0.54
3:D:966:LEU:HD13	3:D:981:GLN:HG3	1.88	0.54
14:R:225:PRO:HG2	14:R:228:VAL:HG23	1.90	0.54
15:S:119:THR:HG22	15:S:123:SER:HA	1.89	0.54
22:o:364:ARG:NH1	22:o:502:ASN:OD1	2.40	0.54
22:o:1365:ILE:HG23	22:o:1369:LEU:HD12	1.89	0.54
1:A:470:ILE:CG2	5:F:212:SER:OG	2.56	0.54
5:F:412:LEU:CD1	5:F:417:ARG:CG	2.81	0.54
4:e:368:ASN:ND2	4:e:701:GLY:HA3	2.23	0.54
22:o:139:LYS:HA	22:o:142:THR:HG22	1.89	0.54
1:A:466:SER:HA	5:F:221:GLN:NE2	2.23	0.54
4:E:278:ASP:OD2	4:E:649:ARG:NH2	2.40	0.54
5:F:418:ILE:HD12	5:F:418:ILE:N	2.20	0.54
15:S:110:PHE:CD1	15:S:148:PRO:HA	2.42	0.54
18:Y:31:DA:H8	18:Y:31:DA:H5"	1.72	0.54
8:i:73:LEU:HB2	10:l:105:HIS:CE1	2.42	0.54
22:o:1139:LEU:HD12	22:o:1139:LEU:O	2.06	0.54
2:B:571:LEU:HD21	2:B:619:MET:HE1	1.89	0.54
4:E:563:GLU:HG2	4:E:587:PRO:HG3	1.90	0.54
5:F:47:ILE:HG23	8:I:39:MET:SD	2.47	0.54
5:F:403:ILE:O	5:F:406:VAL:HG22	2.08	0.54
7:H:50:PHE:CZ	9:J:195:LEU:HB2	2.42	0.54
7:H:102:PHE:CZ	9:J:158:ALA:CA	2.91	0.54
12:P:176:CYS:SG	12:P:247:PRO:O	2.60	0.54
22:o:360:ASP:HB3	23:p:1062:ARG:HE	1.72	0.54
25:r:125:GLU:HA	25:r:128:GLN:HB3	1.90	0.54
4:E:645:GLY:H	4:E:675:LEU:HD11	1.73	0.54
5:F:51:ALA:CB	8:I:23:LEU:HD23	2.30	0.54
5:F:67:THR:C	8:I:32:GLU:OE1	2.47	0.54
13:Q:43:LYS:NZ	13:Q:60:HIS:HE1	2.06	0.54
15:S:24:LYS:CD	16:T:97:THR:HB	2.37	0.54
16:T:94:THR:HG22	16:T:109:ILE:HG23	1.90	0.54
19:c:67:GLY:CA	9:j:116:LEU:HD13	2.33	0.54
22:o:381:PRO:HB3	22:o:480:SER:HA	1.90	0.54
22:o:1375:ARG:NE	22:o:1403:ASP:OD1	2.40	0.54
22:o:1435:THR:OG1	22:o:1436:VAL:N	2.38	0.54
25:r:67:TYR:CZ	28:u:101:ILE:HG13	2.43	0.54
1:A:1190:VAL:CA	6:G:162:VAL:CG1	2.85	0.54
15:S:16:VAL:HG23	16:T:43:LEU:N	2.23	0.54
15:S:18:VAL:HG21	16:T:40:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:122:GLU:CD	16:T:126:ARG:NH1	2.49	0.54
25:r:73:ARG:HH12	28:u:144:ARG:NH1	2.02	0.54
1:A:638:PRO:HG3	6:G:39:LEU:CD2	2.30	0.54
2:B:629:ARG:NH1	2:B:658:ASP:OD2	2.37	0.54
3:D:881:ARG:CB	10:L:57:VAL:CG1	2.64	0.54
4:E:621:ARG:HH22	8:I:104:LEU:HG	1.68	0.54
4:E:696:TRP:CH2	4:E:703:MET:SD	3.00	0.54
15:S:17:ARG:HA	16:T:39:GLU:HG3	1.89	0.54
17:X:-38:DG:H22	18:Y:38:DC:N4	2.05	0.54
4:e:251:LEU:O	4:e:256:HIS:HB2	2.08	0.54
22:o:1287:CYS:HA	23:p:251:ALA:HB2	1.90	0.54
23:p:629:GLU:OE1	23:p:630:LYS:N	2.40	0.54
1:A:999:SER:O	1:A:1001:LYS:N	2.41	0.54
4:E:704:VAL:HA	4:E:759:ILE:HD11	1.89	0.54
5:F:308:VAL:HG11	5:F:337:VAL:HG11	1.88	0.54
7:H:107:LEU:HD11	9:J:157:LEU:HB3	1.90	0.54
16:T:30:GLN:NE2	16:T:62:LEU:O	2.27	0.54
4:e:610:ARG:HD3	4:e:619:PRO:HG3	1.89	0.54
22:o:1130:ILE:HD11	22:o:1405:MET:HE2	1.89	0.54
22:o:1374:VAL:HG11	22:o:1411:LEU:HD21	1.90	0.54
23:p:113:ALA:HA	23:p:118:LEU:HB2	1.89	0.54
2:B:248:SER:OG	2:B:322:MET:SD	2.65	0.54
2:B:846:TYR:CA	7:H:226:ALA:O	2.56	0.54
5:F:316:GLN:NE2	5:F:320:ARG:CA	2.54	0.54
11:O:19:LEU:O	11:O:28:ILE:HD11	2.08	0.54
15:S:24:LYS:HE2	16:T:99:SER:OG	2.07	0.54
5:f:390:THR:HG23	5:f:391:LEU:HD22	1.89	0.54
22:o:76:GLY:HA2	22:o:80:GLU:HG2	1.91	0.54
22:o:1212:LEU:HB2	22:o:1285:LEU:HD21	1.90	0.54
1:A:349:TRP:CZ2	5:f:262:PHE:CZ	2.96	0.53
7:H:73:GLY:C	9:J:142:ALA:HB1	2.32	0.53
13:Q:26:ARG:NH2	13:Q:39:LEU:HD23	2.23	0.53
14:R:179:GLU:HG2	16:T:154:LYS:NZ	2.24	0.53
16:T:124:TYR:CD2	23:p:596:ILE:HG13	2.39	0.53
17:X:2:DG:H2"	17:X:3:DT:C6	2.43	0.53
22:o:93:PRO:HG2	22:o:219:GLU:HG3	1.90	0.53
2:B:628:ILE:O	2:B:644:GLN:NE2	2.41	0.53
4:e:646:SER:OG	4:e:647:ALA:N	2.41	0.53
22:o:1345:ARG:HG2	26:s:133:GLN:HE22	1.73	0.53
23:p:242:ARG:HB2	23:p:254:GLN:HE21	1.74	0.53
25:r:42:GLU:O	25:r:46:GLN:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:123:GLU:HG2	25:r:126:GLU:HB2	1.90	0.53
5:F:368:THR:HB	5:F:373:ARG:CZ	2.38	0.53
14:R:111:ASP:O	14:R:115:MET:CB	2.55	0.53
16:T:34:ALA:CB	16:T:38:GLY:HA2	2.38	0.53
5:f:352:GLN:O	5:f:356:THR:OG1	2.25	0.53
22:o:1437:ASP:N	22:o:1437:ASP:OD1	2.41	0.53
28:u:8:GLU:HB3	28:u:71:LYS:HD2	1.89	0.53
1:A:567:LEU:HD22	2:B:745:GLN:NE2	2.23	0.53
2:B:66:ASN:HD21	2:B:119:PRO:HB3	1.73	0.53
5:F:214:HIS:N	7:H:164:THR:HG22	2.17	0.53
6:G:149:ARG:HG3	6:G:151:THR:HG23	1.90	0.53
22:o:101:VAL:O	22:o:104:MET:HG3	2.08	0.53
22:o:1118:THR:HG22	22:o:1123:ARG:HB2	1.90	0.53
25:r:132:ASP:OD1	25:r:135:GLN:NE2	2.41	0.53
1:A:472:ASN:HB2	5:f:299:LYS:HD3	1.90	0.53
3:D:881:ARG:CD	10:L:57:VAL:CG1	2.85	0.53
7:H:221:ILE:HG22	7:H:224:LEU:HD12	1.89	0.53
11:O:53:ARG:CA	13:Q:368:SER:CB	2.84	0.53
15:S:48:GLU:O	15:S:99:LEU:N	2.38	0.53
17:X:-10:DA:H2"	17:X:-9:DG:C8	2.44	0.53
18:Y:2:DC:H2"	18:Y:3:DC:C6	2.43	0.53
22:o:902:GLU:OE2	22:o:982:ASN:HB2	2.09	0.53
22:o:1313:GLN:HA	22:o:1332:GLN:HE21	1.74	0.53
28:u:110:ARG:HG3	28:u:117:MET:HE3	1.91	0.53
1:A:395:ASP:OD1	1:A:395:ASP:N	2.41	0.53
5:F:55:LEU:HD13	8:I:28:ILE:HG12	1.90	0.53
5:F:118:ILE:HA	7:H:39:VAL:HG13	1.91	0.53
5:F:433:PRO:HA	5:F:436:ALA:HB3	1.90	0.53
5:f:215:GLU:H	5:f:215:GLU:CD	2.17	0.53
5:f:283:MET:HG3	5:f:329:LEU:HD11	1.90	0.53
22:o:576:GLN:HA	29:v:75:TYR:HB2	1.91	0.53
7:H:118:VAL:CG2	9:J:127:THR:OG1	2.56	0.53
9:J:130:ILE:HG13	9:J:160:GLN:HE21	1.74	0.53
5:f:318:CYS:SG	5:f:326:HIS:HB3	2.49	0.53
1:A:662:MET:HE2	1:A:664:PHE:CE1	2.43	0.53
7:H:107:LEU:HD11	9:J:157:LEU:O	2.09	0.53
7:H:116:ARG:NH1	9:J:126:TYR:CE1	2.76	0.53
14:R:263:GLN:HA	14:R:268:LYS:HG2	1.91	0.53
18:Y:-1:DC:H2"	18:Y:0:DT:C6	2.44	0.53
18:Y:37:DT:H2"	18:Y:38:DC:H5"	1.90	0.53
22:o:1101:GLN:HE22	22:o:1391:SER:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:128:GLN:O	25:r:132:ASP:N	2.34	0.53
2:B:328:ASN:HA	7:H:227:LEU:HD11	1.90	0.53
2:B:345:CYS:HA	2:B:348:GLN:HE21	1.73	0.53
2:B:765:ASN:HD22	2:B:765:ASN:N	2.07	0.53
2:B:827:ARG:NE	7:H:211:PHE:CZ	2.75	0.53
2:B:848:HIS:CE1	7:H:225:THR:C	2.87	0.53
14:R:267:GLU:OE1	14:R:269:ARG:NH2	2.41	0.53
15:S:31:PHE:C	16:T:92:THR:H	2.04	0.53
3:d:963:ARG:NH2	3:d:964:GLU:OE2	2.42	0.53
1:A:569:ASN:ND2	2:B:689:GLN:HA	2.24	0.53
1:A:572:TYR:CE1	2:B:689:GLN:OE1	2.62	0.53
2:B:808:PRO:HA	2:B:864:ASN:HB3	1.90	0.53
3:D:966:LEU:CD1	3:D:981:GLN:CG	2.86	0.53
9:J:128:PRO:HB2	9:J:160:GLN:HE22	1.74	0.53
16:T:149:VAL:HG11	23:p:146:LYS:HD2	1.90	0.53
18:Y:5:DG:H2"	18:Y:6:DT:C6	2.44	0.53
4:e:747:LEU:HG	4:e:747:LEU:O	2.09	0.53
5:F:310:THR:C	5:F:312:ILE:H	2.17	0.52
9:J:137:TYR:OH	9:J:141:ARG:NH2	2.43	0.52
13:Q:312:GLU:HB2	13:Q:313:PRO:HD3	1.90	0.52
15:S:47:LEU:CB	16:T:7:LEU:HB2	2.39	0.52
16:T:175:ARG:HE	16:T:175:ARG:N	2.06	0.52
17:X:-9:DG:C6	18:Y:8:DC:N4	2.76	0.52
17:X:12:DC:H2"	17:X:13:DT:C6	2.44	0.52
22:o:400:ASP:N	22:o:400:ASP:OD1	2.41	0.52
22:o:1343:LEU:HB3	22:o:1364:GLU:OE2	2.09	0.52
1:A:844:LYS:HZ3	17:X:31:DT:C7	2.22	0.52
1:A:1015:GLU:O	1:A:1019:LYS:HG3	2.09	0.52
4:E:324:LYS:HG2	4:E:327:ASN:HD22	1.74	0.52
5:F:22:VAL:CG1	8:I:44:PHE:HE1	2.21	0.52
5:F:67:THR:C	8:I:32:GLU:CD	2.77	0.52
5:F:211:ARG:HG2	7:H:165:TYR:CE2	2.25	0.52
4:e:595:PRO:HD2	4:e:639:SER:HB3	1.91	0.52
5:f:447:ALA:O	5:f:453:GLY:HA2	2.09	0.52
26:s:94:MET:HE2	26:s:125:TYR:HD2	1.74	0.52
1:A:406:THR:C	5:F:354:ARG:HH22	2.17	0.52
2:B:66:ASN:OD1	2:B:187:ARG:NH1	2.43	0.52
2:B:152:LEU:HD23	2:B:155:PRO:HB3	1.91	0.52
2:B:529:VAL:HG11	2:B:560:TYR:HB2	1.91	0.52
5:F:76:LYS:HG3	5:F:96:PHE:HB3	1.91	0.52
5:F:80:VAL:HG12	8:I:45:ARG:HH12	1.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:17:ARG:CD	16:T:39:GLU:HB2	2.39	0.52
22:o:77:ASN:ND2	22:o:80:GLU:OE2	2.41	0.52
2:B:834:THR:CG2	7:H:213:LEU:HD23	2.17	0.52
3:D:931:ASP:HB3	8:I:130:LYS:HD2	1.92	0.52
4:E:423:PRO:HG2	4:E:426:ARG:HB2	1.92	0.52
5:F:52:GLN:NE2	8:I:26:MET:O	2.42	0.52
10:L:76:LEU:HD13	10:L:84:LEU:HD12	1.91	0.52
11:O:53:ARG:O	13:Q:368:SER:OG	2.27	0.52
13:Q:26:ARG:NH2	13:Q:39:LEU:HD21	2.24	0.52
17:X:15:DG:H2''	17:X:16:DT:C6	2.45	0.52
18:Y:-6:DC:H2''	18:Y:-5:DT:C6	2.45	0.52
18:Y:27:DA:H2'	18:Y:27:DA:OP2	2.08	0.52
22:o:911:PRO:O	22:o:963:ARG:NH2	2.42	0.52
1:A:639:LEU:CD1	1:A:643:ILE:HD11	2.27	0.52
3:D:943:GLN:HA	3:D:946:PHE:HB3	1.91	0.52
3:D:1056:THR:HG22	10:L:74:GLU:HG3	1.91	0.52
6:G:181:TRP:CE3	6:G:181:TRP:O	2.63	0.52
14:R:151:LEU:HD11	14:R:201:ALA:HB2	1.90	0.52
14:R:175:ARG:HH21	23:p:102:ASP:C	2.15	0.52
22:o:535:MET:O	22:o:669:TYR:OH	2.20	0.52
22:o:1177:TYR:CE1	22:o:1209:PRO:HB2	2.44	0.52
1:A:411:GLU:HB3	5:F:358:THR:HG21	1.91	0.52
2:B:835:ARG:HD3	7:H:187:GLU:CD	2.34	0.52
5:F:14:LEU:N	5:F:44:SER:HG	2.06	0.52
5:F:283:MET:HE1	5:F:308:VAL:HA	1.91	0.52
11:O:88:ILE:CB	13:Q:360:LEU:HB2	2.39	0.52
15:S:8:SER:CB	16:T:49:GLN:N	2.65	0.52
16:T:51:ARG:HG2	16:T:52:THR:N	2.24	0.52
24:q:190:ASN:O	24:q:193:ARG:NH1	2.42	0.52
33:z:36:CYS:SG	33:z:37:ARG:N	2.82	0.52
1:A:564:PRO:CB	2:B:744:PHE:CE2	2.92	0.52
2:B:937:THR:HG23	2:B:939:ASN:H	1.74	0.52
11:O:57:ASN:HD22	11:O:57:ASN:N	2.07	0.52
12:P:167:ASN:ND2	12:P:259:VAL:HB	2.24	0.52
15:S:46:ARG:HB2	15:S:101:ARG:HB2	1.91	0.52
19:c:33:LEU:HD13	9:j:197:MET:HE1	1.91	0.52
4:e:269:GLY:O	8:i:97:ARG:NH2	2.43	0.52
23:p:892:CYS:SG	23:p:893:SER:N	2.82	0.52
25:r:105:PRO:HG2	25:r:131:LEU:HD11	1.92	0.52
26:s:55:ARG:HH22	26:s:107:GLN:HG3	1.75	0.52
1:A:1197:ILE:HD12	6:G:166:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:243:LEU:HD21	5:F:284:ARG:HB3	1.92	0.52
5:F:273:GLN:H	5:F:273:GLN:CD	2.17	0.52
11:O:53:ARG:CB	13:Q:368:SER:CB	2.86	0.52
18:Y:9:DC:H2'	18:Y:10:DT:H73	1.91	0.52
3:d:943:GLN:NE2	4:e:509:GLN:O	2.41	0.52
4:e:423:PRO:HG2	4:e:426:ARG:HB2	1.91	0.52
5:f:320:ARG:NH1	5:f:320:ARG:CB	2.73	0.52
10:l:106:ARG:HD2	10:l:114:LYS:NZ	2.24	0.52
22:o:34:MET:HA	23:p:1138:ARG:HB3	1.92	0.52
22:o:220:ARG:O	22:o:224:ILE:HG13	2.10	0.52
23:p:134:LYS:O	23:p:135:GLU:HG3	2.10	0.52
4:E:304:LYS:NZ	4:E:335:GLU:O	2.42	0.52
4:E:747:LEU:HD22	4:E:747:LEU:N	2.20	0.52
5:F:55:LEU:CD1	8:I:28:ILE:HG23	2.40	0.52
5:F:71:ILE:CD1	8:I:35:VAL:CA	2.83	0.52
5:F:335:ARG:CZ	5:F:382:GLU:OE1	2.58	0.52
12:P:302:LEU:HD12	12:P:302:LEU:N	2.24	0.52
14:R:185:ARG:HG3	23:p:433:LEU:HD21	1.91	0.52
15:S:18:VAL:CG2	16:T:40:VAL:HG13	2.37	0.52
4:e:607:ARG:NH1	8:i:87:PRO:O	2.43	0.52
22:o:364:ARG:HH22	22:o:461:GLN:NE2	2.08	0.52
22:o:1124:LEU:O	22:o:1128:ILE:N	2.36	0.52
22:o:1192:TRP:HA	22:o:1195:VAL:HG22	1.92	0.52
28:u:46:ILE:HD11	28:u:77:PHE:HB2	1.92	0.52
30:w:96:PHE:HD2	30:w:110:LEU:HD11	1.75	0.52
1:A:510:ILE:HB	1:A:511:LEU:HD13	1.92	0.52
1:A:844:LYS:NZ	17:X:31:DT:C7	2.73	0.52
2:B:489:GLN:OE1	2:B:489:GLN:N	2.34	0.52
5:F:47:ILE:CD1	8:I:19:MET:HE3	2.23	0.52
5:F:328:ALA:HA	5:F:374:TYR:HE2	1.74	0.52
6:G:163:GLU:HG2	6:G:167:LYS:HE3	1.92	0.52
11:O:5:LEU:HD23	11:O:6:TYR:CZ	2.45	0.52
12:P:256:GLN:CG	17:X:-26:DC:H5''	2.38	0.52
14:R:218:PHE:HD1	14:R:277:ILE:HG22	1.74	0.52
17:X:-11:DT:H2'	17:X:-11:DT:OP2	2.10	0.52
22:o:365:THR:OG1	22:o:366:VAL:N	2.40	0.52
22:o:814:ASP:OD2	23:p:689:TYR:OH	2.17	0.52
25:r:73:ARG:NH1	28:u:144:ARG:HH12	2.06	0.52
26:s:64:HIS:HD2	26:s:66:ASP:H	1.58	0.52
14:R:185:ARG:CG	23:p:433:LEU:CD2	2.88	0.51
15:S:125:TYR:CZ	16:T:31:TRP:HE3	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:17:GLY:HA2	16:T:109:ILE:O	2.10	0.51
16:T:27:LEU:HD11	16:T:58:LEU:HD21	1.91	0.51
17:X:-5:DC:H2''	17:X:-4:DT:C6	2.45	0.51
10:l:101:GLN:HG2	10:l:104:ARG:HH11	1.75	0.51
25:r:115:ILE:HD12	25:r:118:LEU:HD12	1.91	0.51
2:B:847:ARG:HA	7:H:226:ALA:CB	2.40	0.51
2:B:847:ARG:HA	7:H:226:ALA:C	2.34	0.51
3:D:881:ARG:HH22	10:L:57:VAL:HG22	0.53	0.51
3:D:966:LEU:HD13	3:D:981:GLN:CG	2.40	0.51
5:F:52:GLN:NE2	8:I:26:MET:HB3	2.15	0.51
13:Q:18:ILE:HG23	13:Q:46:TRP:CZ3	2.44	0.51
15:S:124:TYR:CE1	16:T:22:LYS:CG	2.80	0.51
22:o:282:ASP:OD1	22:o:283:ILE:N	2.43	0.51
22:o:1288:ILE:O	22:o:1292:MET:HG2	2.10	0.51
25:r:36:GLU:HG3	25:r:39:MET:HE2	1.93	0.51
28:u:97:LEU:HB2	28:u:108:ILE:HB	1.91	0.51
2:B:656:GLU:HG2	2:B:661:ALA:HB3	1.93	0.51
4:E:232:HIS:HD1	4:E:313:SER:HG	1.55	0.51
4:E:653:LEU:HB2	4:E:663:ARG:HB2	1.91	0.51
11:O:89:LYS:H	13:Q:361:ASN:HD21	1.58	0.51
13:Q:18:ILE:O	13:Q:22:ILE:HG12	2.10	0.51
15:S:8:SER:HB3	16:T:49:GLN:CB	2.29	0.51
17:X:-42:DG:OP2	17:X:-42:DG:H2'	2.11	0.51
17:X:-13:DA:H3'	17:X:-13:DA:P	2.49	0.51
3:d:916:LYS:NZ	3:d:1070:GLU:OE2	2.42	0.51
22:o:631:GLU:HG3	22:o:992:LYS:HE3	1.91	0.51
1:A:1163:ARG:HB3	6:G:183:ILE:HG22	1.91	0.51
3:D:898:VAL:HG22	10:L:113:VAL:CG2	2.33	0.51
4:E:562:SER:OG	4:E:564:ASP:OD1	2.28	0.51
5:F:368:THR:H	5:F:373:ARG:NH1	2.09	0.51
5:F:370:TRP:NE1	5:F:416:ASP:CB	2.60	0.51
7:H:37:LEU:CD1	9:J:138:TYR:CE2	2.87	0.51
8:I:132:LEU:CG	9:J:121:MET:HE2	2.38	0.51
14:R:286:ARG:HH12	17:X:-38:DG:H8	1.58	0.51
15:S:16:VAL:C	16:T:39:GLU:HG3	2.35	0.51
16:T:16:THR:HB	16:T:108:GLY:HA2	1.93	0.51
23:p:230:ARG:HB2	23:p:231:PRO:HD3	1.92	0.51
1:A:828:GLU:HA	1:A:831:LYS:HB2	1.92	0.51
5:F:324:ASP:CA	5:F:327:TRP:HB3	2.35	0.51
5:F:367:LYS:O	5:F:367:LYS:HG2	2.11	0.51
11:O:78:ASP:HA	11:O:91:ASP:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:88:ILE:HG21	13:Q:360:LEU:C	2.35	0.51
15:S:135:PHE:HE2	16:T:43:LEU:CD2	1.92	0.51
17:X:11:DT:H2''	17:X:12:DC:C6	2.44	0.51
10:l:106:ARG:CD	10:l:114:LYS:NZ	2.74	0.51
22:o:1205:ALA:O	22:o:1206:ARG:NE	2.38	0.51
1:A:1019:LYS:NZ	1:A:1019:LYS:CB	2.73	0.51
2:B:276:LEU:HD11	7:H:228:LEU:HD21	1.92	0.51
3:D:891:ILE:CG2	10:L:111:LEU:CD2	2.82	0.51
3:D:897:ASP:OD2	10:L:130:GLY:O	2.29	0.51
16:T:93:LEU:HB2	16:T:110:VAL:HB	1.92	0.51
16:T:210:VAL:O	16:T:214:LYS:N	2.36	0.51
16:T:216:ILE:O	16:T:220:ILE:HG13	2.10	0.51
10:l:76:LEU:CD1	10:l:84:LEU:HD12	2.39	0.51
22:o:304:ALA:O	22:o:307:VAL:HG12	2.10	0.51
22:o:364:ARG:HH22	22:o:461:GLN:CD	2.17	0.51
33:z:16:ILE:HD11	33:z:25:GLU:HB3	1.93	0.51
1:A:666:ARG:NH2	2:B:512:GLY:H	2.05	0.51
5:F:51:ALA:HB1	8:I:28:ILE:HD12	1.92	0.51
7:H:32:ALA:O	7:H:36:THR:OG1	2.29	0.51
7:H:110:TYR:HD2	9:J:157:LEU:HD22	1.75	0.51
7:H:116:ARG:NH1	9:J:126:TYR:CD1	2.79	0.51
12:P:210:THR:HG21	18:Y:26:DG:O3'	2.11	0.51
23:p:888:THR:HG23	23:p:889:LYS:H	1.76	0.51
26:s:26:TYR:HD1	26:s:64:HIS:HA	1.75	0.51
26:s:46:ASP:OD1	26:s:52:ARG:NH2	2.44	0.51
2:B:159:LEU:HD23	2:B:159:LEU:N	2.25	0.51
2:B:735:ILE:HG23	7:H:176:ARG:CZ	2.38	0.51
3:D:936:GLN:H	3:D:936:GLN:NE2	2.03	0.51
5:F:42:GLU:OE2	8:I:46:TYR:HE2	1.94	0.51
11:O:22:LEU:C	11:O:28:ILE:CG1	2.82	0.51
13:Q:15:ARG:NH2	13:Q:58:GLY:CA	2.74	0.51
14:R:214:PHE:HB3	14:R:218:PHE:HE2	1.75	0.51
17:X:-35:DA:N1	18:Y:36:DG:N2	2.57	0.51
21:m:28:ARG:HH21	21:m:31:LEU:HD21	1.75	0.51
22:o:340:LYS:HG2	22:o:1436:VAL:HG11	1.93	0.51
25:r:110:GLU:O	25:r:114:LEU:N	2.39	0.51
25:r:110:GLU:CD	28:u:167:TYR:HB2	2.36	0.51
2:B:90:THR:O	2:B:968:ARG:NH2	2.43	0.51
4:E:324:LYS:O	4:E:327:ASN:ND2	2.44	0.51
8:I:132:LEU:CD2	9:J:121:MET:CE	2.89	0.51
12:P:271:GLU:OE1	14:R:208:LEU:CD1	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:17:ARG:HA	16:T:40:VAL:N	2.25	0.51
15:S:26:TYR:HD1	16:T:97:THR:HG22	1.75	0.51
1:A:1190:VAL:HG13	6:G:166:VAL:HG23	1.94	0.51
2:B:781:TYR:HB3	7:H:176:ARG:HH22	1.67	0.51
5:F:15:PRO:CG	8:I:14:LYS:CG	2.69	0.51
5:F:368:THR:HB	5:F:373:ARG:NH1	2.26	0.51
8:I:132:LEU:CD2	9:J:121:MET:HE1	2.41	0.51
12:P:259:VAL:HG11	18:Y:29:DT:C2	2.46	0.51
14:R:109:SER:C	14:R:112:ARG:HG3	2.36	0.51
14:R:231:ALA:HA	14:R:301:PRO:HG3	1.93	0.51
16:T:230:LYS:O	16:T:231:ASN:C	2.53	0.51
4:e:500:THR:HG22	4:e:502:LYS:H	1.76	0.51
23:p:132:VAL:HG22	23:p:140:LEU:HB3	1.93	0.51
29:v:65:TYR:O	29:v:66:GLU:HG2	2.11	0.51
1:A:472:ASN:HD22	5:f:299:LYS:HA	1.75	0.50
1:A:654:ARG:HB2	1:A:654:ARG:HH11	1.75	0.50
1:A:840:SER:HA	1:A:843:ARG:HE	1.77	0.50
3:D:998:GLN:HB3	3:D:1002:ARG:HH21	1.75	0.50
11:O:22:LEU:CB	11:O:28:ILE:CG2	2.83	0.50
12:P:203:ARG:HH21	13:Q:344:ARG:NH2	2.08	0.50
14:R:128:ILE:HG13	14:R:130:LEU:HG	1.92	0.50
19:c:21:LEU:HD12	19:c:21:LEU:O	2.11	0.50
22:o:141:LEU:HB2	22:o:236:LEU:O	2.11	0.50
22:o:191:ILE:HG12	22:o:200:ALA:HB2	1.93	0.50
1:A:466:SER:CB	5:F:221:GLN:HE22	2.24	0.50
1:A:659:GLY:H	2:B:475:LYS:HG2	1.76	0.50
5:F:322:ASP:C	5:F:324:ASP:N	2.49	0.50
11:O:56:VAL:HG23	11:O:57:ASN:N	2.25	0.50
25:r:31:THR:HA	28:u:2:PHE:O	2.11	0.50
2:B:827:ARG:CG	7:H:211:PHE:HZ	2.23	0.50
5:F:368:THR:N	5:F:373:ARG:NH1	2.58	0.50
7:H:50:PHE:CE1	9:J:195:LEU:HB2	2.47	0.50
11:O:88:ILE:CG1	13:Q:360:LEU:HB2	2.37	0.50
19:c:1:MET:HG3	5:f:126:PRO:HB3	1.94	0.50
22:o:66:GLU:HG2	22:o:69:GLY:H	1.76	0.50
22:o:104:MET:HA	22:o:107:LEU:HG	1.93	0.50
22:o:734:ARG:NH1	30:w:107:ALA:O	2.39	0.50
2:B:202:TRP:HB2	2:B:238:LEU:HB3	1.91	0.50
4:E:501:PRO:HD3	7:H:149:HIS:CB	2.40	0.50
15:S:17:ARG:HA	16:T:39:GLU:CG	2.41	0.50
1:A:567:LEU:HD22	2:B:745:GLN:HE21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:VAL:HG12	1:A:1191:ILE:HD11	1.94	0.50
5:F:81:GLU:C	5:F:83:LEU:N	2.63	0.50
5:F:257:PRO:O	5:F:261:THR:OG1	2.26	0.50
9:J:139:LEU:HB3	9:J:144:PHE:HB3	1.92	0.50
12:P:305:PHE:CZ	18:Y:30:DA:C2'	2.93	0.50
12:P:312:LEU:HD13	12:P:321:ILE:HG23	1.94	0.50
14:R:169:ARG:HD3	14:R:207:ASP:H	1.77	0.50
15:S:121:ASN:C	16:T:25:LYS:HG3	2.36	0.50
16:T:181:GLN:HE21	16:T:181:GLN:CA	2.17	0.50
16:T:184:LEU:HG	16:T:188:PHE:CE1	2.47	0.50
19:c:77:LEU:HD23	19:c:77:LEU:O	2.11	0.50
22:o:64:VAL:HG22	22:o:71:CYS:HB2	1.93	0.50
1:A:590:GLN:NE2	2:B:513:LYS:HZ2	2.09	0.50
3:D:965:ILE:HA	3:D:968:ARG:HH11	1.77	0.50
17:X:-11:DT:OP2	17:X:-11:DT:H6	1.95	0.50
18:Y:28:DG:H3'	18:Y:29:DT:H71	1.94	0.50
4:e:234:ALA:HB2	4:e:648:ASP:HB2	1.94	0.50
8:i:73:LEU:CB	10:l:105:HIS:CE1	2.94	0.50
1:A:639:LEU:CD1	1:A:643:ILE:CD1	2.86	0.50
1:A:1016:GLU:CD	1:A:1019:LYS:HE2	2.29	0.50
7:H:36:THR:HG21	9:J:134:VAL:CG2	2.38	0.50
12:P:207:PRO:HD2	12:P:207:PRO:O	2.11	0.50
17:X:-22:DC:N3	18:Y:22:DG:N2	2.56	0.50
4:e:650:THR:HG22	4:e:666:THR:HG22	1.93	0.50
24:q:193:ARG:HD3	24:q:220:TYR:CD1	2.47	0.50
25:r:110:GLU:OE2	28:u:167:TYR:CB	2.60	0.50
4:E:601:VAL:HG21	4:E:642:VAL:HG11	1.92	0.50
16:T:18:VAL:O	16:T:110:VAL:HA	2.12	0.50
16:T:137:LYS:HD3	16:T:137:LYS:C	2.37	0.50
18:Y:38:DC:H2''	18:Y:39:DA:H5'	1.93	0.50
22:o:1155:LYS:HA	22:o:1309:MET:HE1	1.92	0.50
23:p:359:THR:HG21	23:p:554:GLU:HG3	1.94	0.50
1:A:406:THR:HG22	5:F:350:ASN:HD22	1.76	0.50
1:A:484:ILE:HG12	5:f:306:PRO:CB	2.42	0.50
1:A:564:PRO:HB2	2:B:744:PHE:HE2	1.76	0.50
3:D:898:VAL:HG23	10:L:113:VAL:HB	1.94	0.50
4:E:693:VAL:HB	4:E:707:LEU:HB2	1.94	0.50
11:O:7:ARG:NH1	11:O:37:LEU:HD13	2.27	0.50
5:f:97:ALA:HB2	5:f:106:PHE:HE1	1.77	0.50
22:o:546:ARG:HD3	22:o:772:SER:HB3	1.93	0.50
22:o:1347:LEU:HB3	26:s:137:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:v:14:ASP:OD1	29:v:15:ILE:N	2.43	0.50
5:F:273:GLN:CD	5:F:273:GLN:N	2.70	0.49
11:O:53:ARG:C	13:Q:368:SER:N	2.70	0.49
13:Q:348:LYS:HZ2	13:Q:375:GLU:CD	2.20	0.49
4:e:693:VAL:HB	4:e:707:LEU:HB2	1.94	0.49
23:p:933:ASP:OD2	23:p:1050:ARG:NH2	2.41	0.49
25:r:103:LEU:HD21	28:u:84:VAL:CG1	2.41	0.49
2:B:274:LEU:HG	2:B:278:LYS:HE2	1.93	0.49
12:P:297:LYS:HB3	12:P:298:PRO:HD3	1.94	0.49
14:R:177:PHE:O	14:R:181:CYS:N	2.38	0.49
14:R:178:LYS:O	16:T:154:LYS:HA	2.12	0.49
4:e:586:TYR:HB3	4:e:605:HIS:HB3	1.94	0.49
1:A:564:PRO:HG2	2:B:744:PHE:CZ	2.40	0.49
2:B:328:ASN:HA	7:H:227:LEU:HD13	1.94	0.49
4:E:466:PHE:HB2	4:E:796:ALA:HA	1.94	0.49
4:E:651:VAL:HB	4:E:665:PHE:HB2	1.95	0.49
5:F:211:ARG:O	7:H:165:TYR:CE2	2.65	0.49
5:F:370:TRP:HH2	5:F:406:VAL:HG13	1.71	0.49
7:H:27:ASP:OD1	7:H:27:ASP:N	2.46	0.49
7:H:110:TYR:CE2	9:J:160:GLN:CB	2.95	0.49
14:R:117:ALA:O	14:R:121:ILE:N	2.45	0.49
21:m:69:THR:HG23	21:m:80:ARG:HE	1.77	0.49
23:p:563:ASP:OD1	23:p:563:ASP:N	2.45	0.49
23:p:830:GLU:OE2	23:p:870:THR:OG1	2.24	0.49
2:B:27:LYS:HE3	2:B:490:SER:HB3	1.95	0.49
2:B:598:ARG:HH11	2:B:619:MET:HE3	1.77	0.49
5:F:114:LEU:H	7:H:52:SER:HA	1.76	0.49
5:F:279:LEU:HD22	5:F:330:ARG:NH2	2.28	0.49
22:o:812:LYS:HG3	30:w:77:THR:O	2.12	0.49
23:p:497:LYS:HG3	23:p:498:PRO:HD3	1.94	0.49
28:u:99:THR:O	28:u:106:CYS:HB3	2.12	0.49
1:A:411:GLU:CG	5:F:358:THR:HG21	2.43	0.49
2:B:739:ASN:ND2	2:B:782:ASN:OD1	2.44	0.49
5:F:335:ARG:CD	5:F:382:GLU:OE1	2.60	0.49
11:O:20:ASP:HA	11:O:23:ILE:HD12	1.95	0.49
14:R:28:ARG:HH12	22:o:430:ARG:HE	1.61	0.49
24:q:189:ASP:O	24:q:191:ALA:N	2.41	0.49
26:s:188:GLY:N	26:s:210:GLN:OE1	2.45	0.49
1:A:654:ARG:HH22	6:G:80:ILE:HG22	1.77	0.49
2:B:559:LYS:HZ3	2:B:559:LYS:HB2	1.78	0.49
5:F:14:LEU:HA	8:I:18:MET:CG	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:126:TYR:HE2	9:J:157:LEU:HD11	1.77	0.49
11:O:53:ARG:C	13:Q:368:SER:CA	2.85	0.49
11:O:59:ARG:O	11:O:59:ARG:HG2	2.12	0.49
14:R:119:LYS:NZ	23:p:436:LYS:NZ	2.60	0.49
1:A:467:ILE:HG22	1:A:467:ILE:O	2.12	0.49
2:B:867:VAL:HG13	7:H:203:LEU:HB3	1.95	0.49
3:D:901:TYR:HE1	10:L:128:ILE:CB	2.17	0.49
4:E:634:ARG:HG3	4:E:675:LEU:HB2	1.94	0.49
15:S:18:VAL:N	16:T:39:GLU:HA	2.28	0.49
15:S:124:TYR:HD1	16:T:22:LYS:HA	1.77	0.49
16:T:141:LEU:O	23:p:90:GLN:NE2	2.42	0.49
22:o:132:LYS:HD2	22:o:133:SER:HB3	1.94	0.49
22:o:766:PHE:HB3	22:o:781:ILE:HD12	1.95	0.49
23:p:845:TYR:CD1	23:p:865:VAL:HG11	2.48	0.49
23:p:1119:CYS:SG	23:p:1120:ASN:N	2.85	0.49
29:v:8:ASP:OD1	29:v:9:ILE:N	2.39	0.49
1:A:569:ASN:HB3	1:A:572:TYR:HD2	1.78	0.49
1:A:950:VAL:HG23	1:A:1065:GLU:CG	2.41	0.49
4:E:754:THR:OG1	4:E:755:ALA:N	2.43	0.49
15:S:8:SER:CB	16:T:48:THR:C	2.84	0.49
16:T:127:LEU:CD2	23:p:547:GLU:OE1	2.61	0.49
3:d:909:ARG:NE	10:l:91:PHE:HE1	2.04	0.49
22:o:111:CYS:SG	22:o:114:CYS:HB3	2.53	0.49
22:o:860:ILE:HD12	22:o:1124:LEU:HD23	1.93	0.49
23:p:647:GLU:H	23:p:647:GLU:CD	2.19	0.49
26:s:64:HIS:CD2	26:s:66:ASP:H	2.31	0.49
3:D:901:TYR:CZ	10:L:128:ILE:HB	2.44	0.49
5:F:312:ILE:HG22	5:F:313:VAL:HG13	1.94	0.49
5:F:329:LEU:C	5:F:329:LEU:CD2	2.86	0.49
5:F:370:TRP:CZ3	5:F:420:ALA:CA	2.96	0.49
6:G:181:TRP:CD2	6:G:181:TRP:C	2.87	0.49
11:O:92:LYS:NZ	13:Q:329:PHE:HB2	2.28	0.49
12:P:259:VAL:HG21	18:Y:28:DG:C2	2.47	0.49
13:Q:47:GLU:OE2	13:Q:60:HIS:CD2	2.65	0.49
14:R:222:LEU:HD22	14:R:269:ARG:HG3	1.94	0.49
15:S:15:VAL:HA	16:T:42:LYS:CB	2.43	0.49
17:X:22:DG:C2	18:Y:-21:DG:N1	2.80	0.49
5:f:24:GLU:HG2	10:l:145:THR:HG21	1.93	0.49
5:f:39:LEU:HD22	8:i:47:VAL:HG13	1.94	0.49
22:o:1318:LYS:HD3	22:o:1330:ALA:HB1	1.94	0.49
26:s:56:THR:O	26:s:57:ASP:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:u:151:ARG:HB3	28:u:158:PHE:CE1	2.46	0.49
1:A:1014:GLU:O	1:A:1018:LYS:HB2	2.13	0.49
5:F:124:ARG:HA	7:H:123:PRO:O	2.12	0.49
6:G:94:MET:HE3	6:G:96:VAL:HG22	1.94	0.49
15:S:24:LYS:CD	16:T:97:THR:CB	2.86	0.49
23:p:513:GLU:CD	23:p:525:ASN:HD22	2.20	0.49
30:w:27:LYS:HD2	30:w:38:ALA:HB2	1.95	0.49
1:A:648:LYS:HE3	1:A:648:LYS:HB3	1.45	0.48
2:B:560:TYR:HD2	2:B:581:ILE:HD11	1.78	0.48
5:F:39:LEU:HD11	8:I:51:LEU:HD11	1.94	0.48
12:P:269:ARG:HG3	12:P:337:LYS:HE2	1.94	0.48
14:R:268:LYS:O	14:R:269:ARG:NH1	2.37	0.48
16:T:122:GLU:HA	16:T:126:ARG:NH1	2.28	0.48
17:X:22:DG:N2	18:Y:-21:DG:C2	2.81	0.48
4:e:439:ASP:OD1	4:e:555:ARG:NH2	2.44	0.48
22:o:1030:SER:HB2	26:s:162:ARG:NE	2.28	0.48
23:p:851:ASP:H	33:z:15:MET:HE1	1.78	0.48
24:q:183:ALA:HB3	24:q:232:ASN:HB3	1.95	0.48
25:r:26:PHE:CE2	28:u:78:ARG:HG3	2.48	0.48
1:A:824:ARG:HB3	1:A:863:VAL:HG12	1.95	0.48
2:B:135:TRP:HA	2:B:138:VAL:HG12	1.95	0.48
3:D:955:LYS:HA	3:D:955:LYS:HD2	1.56	0.48
6:G:48:HIS:HD2	6:G:54:GLY:HA2	1.78	0.48
8:I:56:ILE:HG21	10:L:122:ARG:NH2	2.27	0.48
16:T:148:VAL:CG1	23:p:125:TYR:OH	2.61	0.48
4:e:270:ASP:OD1	4:e:271:GLN:NE2	2.41	0.48
22:o:695:ASP:OD1	22:o:695:ASP:N	2.43	0.48
22:o:795:GLY:HA2	22:o:1108:HIS:NE2	2.28	0.48
22:o:1296:MET:CG	22:o:1298:LEU:HG	2.44	0.48
5:F:369:PRO:O	5:F:373:ARG:HB2	2.13	0.48
11:O:55:ARG:HE	11:O:55:ARG:CA	2.25	0.48
13:Q:359:ASN:HA	13:Q:363:ARG:O	2.14	0.48
14:R:295:ARG:NH2	14:R:298:ASP:OD2	2.46	0.48
16:T:18:VAL:HG23	16:T:110:VAL:HG22	1.94	0.48
4:e:724:GLU:OE1	4:e:789:ASN:ND2	2.46	0.48
22:o:59:ASP:HB3	22:o:62:GLN:HB2	1.95	0.48
22:o:896:LEU:HD13	22:o:980:PRO:HG3	1.96	0.48
23:p:311:ILE:HG13	23:p:316:VAL:HG13	1.93	0.48
3:D:998:GLN:HA	3:D:1001:GLN:CD	2.38	0.48
5:F:308:VAL:CG2	5:F:337:VAL:HG12	2.31	0.48
7:H:43:SER:CB	7:H:119:ILE:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:135:THR:HG22	7:H:135:THR:O	2.12	0.48
16:T:122:GLU:CG	16:T:123:ASN:N	2.76	0.48
23:p:910:THR:OG1	33:z:42:ARG:O	2.24	0.48
30:w:68:ILE:HG13	30:w:122:ARG:HD2	1.95	0.48
5:F:15:PRO:HG3	8:I:14:LYS:CD	2.44	0.48
13:Q:56:VAL:CG1	13:Q:57:ASP:N	2.76	0.48
14:R:107:MET:SD	22:o:329:MET:CE	2.97	0.48
14:R:119:LYS:HZ2	23:p:436:LYS:NZ	2.11	0.48
26:s:18:MET:HE2	26:s:32:GLU:HG2	1.95	0.48
3:D:1057:ARG:NH2	10:L:77:ASP:OD1	2.47	0.48
4:E:481:ASP:HB3	4:E:787:ARG:HH22	1.77	0.48
15:S:16:VAL:O	16:T:41:GLY:N	2.47	0.48
5:f:254:GLN:O	5:f:258:ARG:NH2	2.47	0.48
22:o:278:HIS:CD2	22:o:330:GLN:HE21	2.32	0.48
25:r:29:ALA:HB1	28:u:3:TYR:CG	2.48	0.48
26:s:85:LYS:HD2	26:s:88:LYS:HD2	1.96	0.48
1:A:927:VAL:O	1:A:933:ASN:ND2	2.44	0.48
2:B:570:GLU:HA	2:B:625:LEU:HA	1.95	0.48
12:P:299:ARG:C	12:P:300:ILE:HG12	2.39	0.48
13:Q:17:VAL:O	13:Q:21:VAL:HG23	2.14	0.48
14:R:244:LEU:HD11	14:R:295:ARG:HD3	1.95	0.48
15:S:49:ARG:HB3	15:S:96:GLN:HB3	1.96	0.48
20:k:173:CYS:SG	20:k:179:MET:O	2.72	0.48
20:k:191:VAL:HG13	20:k:200:ILE:CD1	2.42	0.48
22:o:795:GLY:HA3	22:o:1107:PHE:HD2	1.78	0.48
22:o:1312:PRO:HG3	22:o:1317:LYS:HB2	1.96	0.48
22:o:1391:SER:OG	22:o:1392:TYR:N	2.46	0.48
24:q:197:TYR:HD2	24:q:217:GLN:HE21	1.62	0.48
25:r:30:GLU:O	28:u:4:HIS:N	2.44	0.48
26:s:102:ALA:HB3	26:s:127:LEU:HG	1.95	0.48
26:s:103:LEU:HG	26:s:128:GLU:HB2	1.95	0.48
29:v:64:LEU:HB3	29:v:84:ARG:HB2	1.96	0.48
31:x:24:LEU:HB3	31:x:29:TYR:HD2	1.79	0.48
5:F:370:TRP:CG	5:F:416:ASP:HA	2.45	0.48
13:Q:43:LYS:HE2	13:Q:47:GLU:OE2	2.13	0.48
23:p:131:THR:HA	23:p:141:GLN:HA	1.95	0.48
32:y:114:GLU:OE1	32:y:114:GLU:N	2.40	0.48
1:A:349:TRP:HZ2	5:f:262:PHE:CE1	2.24	0.48
2:B:431:LEU:CD2	2:B:431:LEU:N	2.76	0.48
5:F:317:LEU:N	5:F:317:LEU:CD2	2.77	0.48
16:T:122:GLU:CB	16:T:126:ARG:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:228:ILE:O	16:T:229:HIS:C	2.56	0.48
4:e:651:VAL:HG13	4:e:665:PHE:HB2	1.95	0.48
22:o:278:HIS:HD2	22:o:330:GLN:HE21	1.61	0.48
22:o:460:ARG:HB2	22:o:501:MET:HE3	1.96	0.48
25:r:128:GLN:HA	25:r:131:LEU:HB2	1.95	0.48
27:t:88:ASP:HB3	27:t:91:LEU:HB2	1.95	0.48
1:A:1022:ARG:HE	1:A:1022:ARG:HB3	1.45	0.48
3:D:933:ARG:HB2	8:I:132:LEU:HD22	1.96	0.48
17:X:-21:DA:H2"	17:X:-20:DG:C8	2.49	0.48
17:X:-9:DG:H22	18:Y:9:DC:H42	1.58	0.48
4:e:747:LEU:H	4:e:747:LEU:CD2	2.22	0.48
22:o:408:ARG:HH21	22:o:412:GLN:HB3	1.79	0.48
22:o:1104:LEU:HG	22:o:1105:ASN:OD1	2.14	0.48
22:o:1206:ARG:O	22:o:1263:ASN:ND2	2.47	0.48
25:r:124:ASP:OD1	25:r:125:GLU:N	2.47	0.48
25:r:129:GLN:O	25:r:133:ASP:N	2.38	0.48
26:s:75:PHE:HB2	26:s:104:ILE:HG22	1.96	0.48
29:v:32:SER:HB3	29:v:37:MET:H	1.78	0.48
4:E:788:ARG:HB3	7:H:145:HIS:HA	1.96	0.47
5:F:81:GLU:HB3	5:F:83:LEU:HD13	1.96	0.47
11:O:60:GLY:HA2	11:O:79:VAL:CG1	2.35	0.47
15:S:15:VAL:HA	16:T:42:LYS:HA	1.95	0.47
15:S:44:GLN:O	16:T:9:LEU:HD11	2.11	0.47
22:o:52:PRO:HA	22:o:58:MET:HE1	1.96	0.47
22:o:753:GLY:O	22:o:757:GLN:HG2	2.13	0.47
24:q:9:VAL:HG11	32:y:105:PHE:CD1	2.48	0.47
32:y:5:PRO:HG2	32:y:8:GLU:HG3	1.96	0.47
1:A:349:TRP:HE1	5:f:262:PHE:CA	2.28	0.47
1:A:1204:GLU:OE1	1:A:1204:GLU:HA	2.14	0.47
2:B:636:VAL:HG23	2:B:638:ARG:HB3	1.96	0.47
3:D:1085:LYS:NZ	10:L:83:MET:HE1	2.24	0.47
4:E:746:ASP:OD1	4:E:746:ASP:N	2.30	0.47
5:F:47:ILE:CG1	8:I:19:MET:CE	2.86	0.47
5:F:51:ALA:C	8:I:28:ILE:HD11	2.37	0.47
11:O:17:GLU:CB	13:Q:49:LYS:HZ1	2.25	0.47
13:Q:18:ILE:HG12	13:Q:46:TRP:CZ2	2.48	0.47
16:T:188:PHE:O	16:T:189:SER:C	2.57	0.47
22:o:738:GLU:HA	22:o:741:VAL:HG12	1.95	0.47
22:o:842:GLY:O	22:o:845:GLU:HG3	2.14	0.47
22:o:1192:TRP:CZ2	22:o:1258:ARG:HD3	2.49	0.47
1:A:648:LYS:HG2	1:A:648:LYS:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ASN:ND2	2:B:320:ALA:O	2.35	0.47
2:B:848:HIS:NE2	7:H:225:THR:C	2.72	0.47
2:B:883:PHE:HA	7:H:222:PRO:HB3	1.96	0.47
2:B:953:LEU:HD12	2:B:979:PHE:HE2	1.79	0.47
5:F:317:LEU:N	5:F:317:LEU:HD23	2.29	0.47
5:F:318:CYS:HB3	5:F:319:LEU:HD23	1.96	0.47
5:F:415:ILE:O	5:F:415:ILE:HG12	2.14	0.47
16:T:30:GLN:O	16:T:62:LEU:HD11	2.15	0.47
17:X:-45:DG:H2''	17:X:-44:DA:C8	2.49	0.47
17:X:16:DT:H2''	17:X:17:DG:C8	2.49	0.47
18:Y:-11:DA:H2''	18:Y:-10:DG:C8	2.49	0.47
4:e:556:ASN:HA	4:e:572:LEU:HB2	1.96	0.47
22:o:1095:LEU:C	22:o:1098:PRO:HD2	2.39	0.47
22:o:1202:PHE:HZ	22:o:1262:MET:HG3	1.78	0.47
22:o:1242:ASP:O	22:o:1262:MET:N	2.41	0.47
23:p:371:ARG:NH1	23:p:609:GLU:OE1	2.47	0.47
5:F:15:PRO:HD2	8:I:15:ASP:HA	1.96	0.47
15:S:121:ASN:O	16:T:25:LYS:CE	2.61	0.47
18:Y:-24:DA:H2''	18:Y:-23:DT:H72	1.97	0.47
3:d:922:GLN:NE2	10:l:71:ASP:OD2	2.47	0.47
5:f:257:PRO:O	5:f:261:THR:OG1	2.31	0.47
22:o:286:ILE:HG13	22:o:289:GLN:HE21	1.79	0.47
22:o:875:TYR:OH	27:t:61:GLU:OE2	2.25	0.47
1:A:488:ALA:CB	5:f:271:VAL:CG2	2.59	0.47
1:A:1068:ARG:HD2	1:A:1068:ARG:C	2.39	0.47
5:F:51:ALA:HB2	8:I:23:LEU:CD2	2.11	0.47
5:F:58:MET:HG3	5:F:66:LEU:H	1.79	0.47
5:F:214:HIS:CB	7:H:164:THR:CG2	2.92	0.47
15:S:18:VAL:H	16:T:39:GLU:CA	2.26	0.47
22:o:1028:PRO:C	22:o:1030:SER:H	2.22	0.47
23:p:384:ASP:HB3	23:p:387:HIS:HB2	1.96	0.47
1:A:567:LEU:HA	2:B:745:GLN:NE2	2.30	0.47
2:B:329:LEU:HB3	2:B:342:THR:HG23	1.96	0.47
12:P:274:VAL:HG11	14:R:208:LEU:CD2	2.44	0.47
15:S:45:ALA:HB2	16:T:9:LEU:HD11	1.97	0.47
3:d:941:ARG:NH2	8:i:123:THR:O	2.48	0.47
4:e:720:SER:OG	4:e:721:ARG:N	2.46	0.47
22:o:229:SER:N	22:o:232:GLU:OE2	2.48	0.47
22:o:551:ARG:NH2	22:o:625:ASP:OD1	2.46	0.47
23:p:59:VAL:HG11	23:p:91:ILE:HD11	1.97	0.47
23:p:380:ARG:HG2	23:p:608:ARG:HH22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:p:809:VAL:HG22	23:p:810:PHE:H	1.80	0.47
31:x:3:ILE:HD12	31:x:4:PRO:HD2	1.95	0.47
1:A:573:TYR:HD2	2:B:657:ARG:C	2.23	0.47
1:A:642:HIS:C	1:A:642:HIS:CD2	2.92	0.47
3:D:966:LEU:HD11	3:D:981:GLN:HG3	1.97	0.47
3:D:998:GLN:HG2	16:T:182:HIS:HE1	1.80	0.47
4:E:321:LEU:HB3	4:E:330:TRP:HB2	1.97	0.47
5:F:214:HIS:H	7:H:164:THR:CG2	2.20	0.47
7:H:40:VAL:CG1	9:J:130:ILE:HG12	2.44	0.47
15:S:24:LYS:HA	16:T:99:SER:HA	1.96	0.47
15:S:109:LYS:HD2	15:S:149:LEU:HD23	1.97	0.47
16:T:124:TYR:CE1	23:p:596:ILE:CG2	2.95	0.47
16:T:147:LYS:O	23:p:94:SER:HB2	2.14	0.47
16:T:181:GLN:O	16:T:184:LEU:HB3	2.14	0.47
17:X:-14:DC:H2''	17:X:-13:DA:H5'	1.97	0.47
17:X:14:DG:H2''	17:X:15:DG:C8	2.50	0.47
17:X:23:DA:OP2	17:X:23:DA:H8	1.98	0.47
18:Y:-23:DT:H2''	18:Y:-22:DC:C6	2.50	0.47
19:c:26:VAL:HG23	9:j:195:LEU:HB3	1.96	0.47
3:d:1061:ARG:NH1	8:i:119:ARG:O	2.48	0.47
5:f:102:ARG:HD3	10:l:151:ARG:HG3	1.96	0.47
22:o:154:CYS:SG	22:o:184:CYS:HB3	2.55	0.47
22:o:267:GLN:HB3	23:p:890:ARG:HH22	1.79	0.47
22:o:692:SER:O	22:o:692:SER:OG	2.24	0.47
22:o:922:PHE:HB2	22:o:1052:ARG:HB2	1.97	0.47
22:o:946:ALA:O	22:o:950:ASN:ND2	2.47	0.47
22:o:1389:ASP:OD1	22:o:1389:ASP:N	2.38	0.47
23:p:260:LEU:HD22	23:p:347:MET:HE1	1.97	0.47
23:p:265:GLN:HG2	23:p:266:GLU:N	2.29	0.47
23:p:1137:CYS:HB3	23:p:1142:ASN:HB3	1.95	0.47
28:u:44:PHE:O	28:u:76:VAL:HA	2.15	0.47
29:v:136:GLU:OE1	29:v:136:GLU:N	2.48	0.47
5:F:424:GLN:O	5:F:428:LEU:HG	2.15	0.47
7:H:92:ASP:O	7:H:96:THR:OG1	2.32	0.47
11:O:58:PHE:HB3	11:O:81:PHE:HE2	1.77	0.47
11:O:79:VAL:N	11:O:90:VAL:O	2.48	0.47
15:S:42:TRP:CD1	15:S:102:VAL:HG11	2.50	0.47
17:X:3:DT:H2''	17:X:4:DG:C8	2.50	0.47
18:Y:27:DA:H2''	18:Y:28:DG:H5''	1.97	0.47
4:e:589:TRP:HB3	5:f:60:MET:HE3	1.96	0.47
22:o:221:VAL:HA	22:o:224:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:1184:THR:OG1	22:o:1189:ASP:OD1	2.31	0.47
23:p:773:PRO:HG3	31:x:53:VAL:HG11	1.96	0.47
26:s:107:GLN:HG2	26:s:108:GLN:OE1	2.15	0.47
3:D:1085:LYS:NZ	10:L:83:MET:HE2	2.27	0.47
5:F:44:SER:O	8:I:22:ILE:HD13	2.15	0.47
5:F:68:THR:H	8:I:32:GLU:CD	2.10	0.47
5:F:112:VAL:O	7:H:53:ALA:O	2.33	0.47
5:F:412:LEU:CD1	5:F:417:ARG:CD	2.50	0.47
8:I:63:LYS:NZ	8:I:69:ASP:OD1	2.47	0.47
8:I:119:ARG:NH1	8:I:120:TYR:OH	2.48	0.47
17:X:17:DG:H2"	17:X:18:DA:C8	2.50	0.47
22:o:859:TYR:CZ	22:o:863:ARG:HD2	2.50	0.47
26:s:61:LEU:HD12	26:s:73:PHE:HD2	1.79	0.47
26:s:120:ASP:OD1	26:s:120:ASP:N	2.44	0.47
1:A:575:PRO:HD3	2:B:608:ASN:HB2	1.95	0.47
4:E:299:ASP:OD2	4:E:607:ARG:NH2	2.38	0.47
5:F:427:LEU:HD12	5:F:427:LEU:HA	1.71	0.47
6:G:41:ASP:OD1	6:G:41:ASP:N	2.48	0.47
14:R:132:ARG:HB3	23:p:914:GLU:HB3	1.96	0.47
15:S:24:LYS:HB2	16:T:97:THR:HB	1.96	0.47
22:o:274:ASP:OD1	22:o:277:THR:N	2.29	0.47
23:p:898:THR:OG1	23:p:1079:SER:HA	2.15	0.47
1:A:469:PRO:N	7:H:166:ARG:HH12	2.13	0.46
1:A:473:GLU:CD	5:F:212:SER:HB2	2.41	0.46
3:D:881:ARG:CZ	10:L:57:VAL:HG21	2.42	0.46
5:F:48:LYS:HG2	8:I:22:ILE:CG2	2.24	0.46
5:F:52:GLN:HE21	8:I:26:MET:CB	2.18	0.46
7:H:118:VAL:HG22	9:J:127:THR:OG1	2.15	0.46
16:T:23:VAL:HG21	16:T:31:TRP:CZ3	2.50	0.46
5:f:330:ARG:NH1	5:f:371:THR:O	2.47	0.46
22:o:102:LYS:HZ2	22:o:1445:HIS:CE1	2.33	0.46
22:o:291:ARG:O	22:o:295:GLN:HB2	2.15	0.46
23:p:50:PHE:HA	23:p:54:SER:HB3	1.97	0.46
23:p:856:PRO:HG2	33:z:48:ARG:HA	1.96	0.46
28:u:146:LYS:O	28:u:162:SER:OG	2.27	0.46
31:x:10:CYS:SG	31:x:42:ARG:NE	2.86	0.46
1:A:1185:VAL:CB	1:A:1191:ILE:CG1	2.75	0.46
3:D:917:ILE:CG1	3:D:1058:VAL:HG11	2.45	0.46
5:F:290:MET:SD	5:F:340:ILE:CG2	2.88	0.46
14:R:15:CYS:HB2	14:R:18:HIS:O	2.15	0.46
15:S:29:MET:O	16:T:94:THR:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:30:ALA:HB1	16:T:91:GLN:HG2	1.97	0.46
16:T:51:ARG:NH1	16:T:53:GLU:HB2	2.30	0.46
17:X:-45:DG:N2	18:Y:45:DC:O2	2.33	0.46
4:e:474:THR:OG1	4:e:546:VAL:O	2.28	0.46
22:o:327:ARG:CZ	22:o:335:PRO:HB2	2.45	0.46
22:o:1166:LEU:HB2	22:o:1296:MET:HB2	1.97	0.46
28:u:97:LEU:HD11	28:u:128:TYR:HE2	1.80	0.46
29:v:96:VAL:HG22	29:v:116:VAL:HG22	1.96	0.46
1:A:349:TRP:CE2	5:f:262:PHE:CE1	3.01	0.46
1:A:653:GLU:HB3	1:A:662:MET:HE1	1.98	0.46
1:A:657:SER:O	2:B:475:LYS:HB3	2.15	0.46
3:D:898:VAL:CG2	10:L:113:VAL:HA	2.45	0.46
5:F:15:PRO:CB	8:I:14:LYS:HE3	2.42	0.46
6:G:173:ASP:OD2	6:G:179:THR:HG21	2.16	0.46
10:L:106:ARG:CD	10:L:114:LYS:HZ3	2.28	0.46
19:c:119:GLU:HG3	4:e:790:LEU:HD11	1.96	0.46
22:o:305:GLU:O	22:o:309:LEU:HD23	2.16	0.46
22:o:1177:TYR:HE1	22:o:1209:PRO:HB2	1.80	0.46
23:p:28:ILE:HD11	23:p:644:LYS:HB3	1.97	0.46
23:p:502:HIS:ND1	23:p:504:THR:OG1	2.33	0.46
23:p:625:LEU:HD12	23:p:665:ILE:HG13	1.97	0.46
26:s:70:ASP:OD1	26:s:70:ASP:N	2.49	0.46
28:u:112:SER:HB2	28:u:162:SER:HA	1.95	0.46
7:H:110:TYR:HD2	9:J:157:LEU:CD2	2.28	0.46
16:T:95:VAL:O	16:T:106:LEU:HD12	2.15	0.46
5:f:328:ALA:C	5:f:330:ARG:N	2.72	0.46
8:i:73:LEU:CD2	10:l:105:HIS:CG	2.92	0.46
22:o:565:MET:HE1	32:y:74:ARG:HB2	1.96	0.46
22:o:801:GLY:HA3	23:p:503:ASN:HB2	1.97	0.46
22:o:1128:ILE:HG23	22:o:1414:ILE:HD11	1.97	0.46
23:p:446:TYR:O	23:p:450:THR:HG22	2.16	0.46
1:A:410:TRP:CE3	1:A:411:GLU:HG3	2.50	0.46
2:B:564:LEU:HB2	2:B:581:ILE:HD13	1.97	0.46
5:F:213:ILE:CA	7:H:164:THR:O	2.51	0.46
11:O:56:VAL:HG22	13:Q:369:LYS:O	2.15	0.46
12:P:236:LYS:HG2	12:P:239:ARG:HH12	1.81	0.46
12:P:256:GLN:HA	12:P:256:GLN:OE1	2.16	0.46
15:S:17:ARG:C	16:T:39:GLU:HA	2.38	0.46
22:o:1121:VAL:N	22:o:1122:PRO:HD2	2.31	0.46
24:q:91:GLU:HG3	24:q:92:GLU:H	1.80	0.46
26:s:47:LYS:O	26:s:51:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:VAL:HG23	1:A:1065:GLU:HG2	1.97	0.46
2:B:848:HIS:CE1	7:H:225:THR:O	2.69	0.46
5:F:319:LEU:N	5:F:319:LEU:CD2	2.75	0.46
16:T:122:GLU:HB2	16:T:126:ARG:HD2	1.97	0.46
5:f:326:HIS:ND1	5:f:326:HIS:N	2.63	0.46
10:l:76:LEU:CD1	10:l:84:LEU:CD1	2.94	0.46
23:p:1119:CYS:HA	23:p:1146:ILE:HD13	1.98	0.46
24:q:193:ARG:NH2	24:q:217:GLN:OE1	2.49	0.46
25:r:94:LYS:HZ2	28:u:3:TYR:HE1	1.62	0.46
5:F:43:VAL:CG2	8:I:43:ALA:HA	2.44	0.46
5:F:112:VAL:HG11	7:H:55:LYS:HD3	1.98	0.46
7:H:116:ARG:CD	9:J:126:TYR:CE1	2.82	0.46
16:T:223:GLN:OE1	16:T:223:GLN:N	2.47	0.46
4:e:717:LEU:HD22	4:e:726:LEU:HD11	1.97	0.46
5:f:326:HIS:O	5:f:330:ARG:HG2	2.15	0.46
23:p:84:TYR:CD2	23:p:132:VAL:HG12	2.50	0.46
23:p:961:ILE:HD11	31:x:42:ARG:HD2	1.98	0.46
2:B:27:LYS:CE	2:B:490:SER:HB3	2.45	0.46
11:O:55:ARG:HH12	13:Q:369:LYS:HB3	1.80	0.46
15:S:24:LYS:CB	16:T:98:GLU:C	2.89	0.46
3:d:909:ARG:CZ	10:l:91:PHE:HE1	2.27	0.46
4:e:554:ASP:OD1	4:e:554:ASP:N	2.45	0.46
22:o:872:MET:HE1	22:o:1470:CYS:SG	2.55	0.46
23:p:371:ARG:HH22	23:p:380:ARG:HH22	1.63	0.46
23:p:1144:THR:HG21	28:u:41:LYS:HB2	1.98	0.46
2:B:568:VAL:HG22	2:B:628:ILE:HG23	1.98	0.46
2:B:766:LEU:HA	2:B:807:THR:HG21	1.96	0.46
3:D:905:ALA:CB	10:L:120:LEU:HD21	2.46	0.46
5:F:51:ALA:CB	8:I:23:LEU:HD22	2.04	0.46
14:R:181:CYS:CB	16:T:155:PRO:O	2.64	0.46
17:X:13:DT:H2"	17:X:14:DG:C8	2.50	0.46
5:f:327:TRP:O	5:f:330:ARG:HB2	2.15	0.46
10:l:83:MET:SD	10:l:86:GLN:OE1	2.74	0.46
22:o:1129:ASN:HD22	22:o:1413:ALA:HB1	1.80	0.46
23:p:1035:ARG:NH1	23:p:1036:LYS:O	2.48	0.46
24:q:123:ASN:OD1	24:q:124:SER:N	2.48	0.46
26:s:11:TRP:HB2	26:s:40:PHE:CD2	2.51	0.46
1:A:469:PRO:CA	7:H:166:ARG:HH12	2.24	0.46
4:E:324:LYS:HA	4:E:327:ASN:HB3	1.97	0.46
4:E:646:SER:OG	4:E:647:ALA:N	2.49	0.46
7:H:205:LYS:HA	7:H:205:LYS:HD3	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:7:SER:HA	16:T:47:LYS:HD3	1.98	0.46
5:f:58:MET:HE3	5:f:64:GLN:HA	1.98	0.46
22:o:111:CYS:SG	22:o:154:CYS:HB2	2.56	0.46
22:o:152:ASN:O	22:o:188:GLN:HG2	2.15	0.46
22:o:1342:SER:O	22:o:1346:VAL:HG23	2.16	0.46
22:o:1479:LYS:HE2	22:o:1482:TYR:HE1	1.80	0.46
23:p:276:LEU:HG	23:p:343:LEU:HD21	1.97	0.46
23:p:626:LEU:HD23	23:p:662:VAL:HG12	1.98	0.46
1:A:411:GLU:CB	5:F:358:THR:HG21	2.46	0.45
1:A:730:PHE:CD1	1:A:730:PHE:N	2.82	0.45
10:L:101:GLN:C	10:L:105:HIS:HD2	2.17	0.45
16:T:169:LYS:NZ	16:T:169:LYS:HA	2.31	0.45
5:f:317:LEU:HD12	5:f:329:LEU:HD23	1.98	0.45
20:k:182:LEU:HD23	20:k:182:LEU:HA	1.85	0.45
10:l:106:ARG:HH12	10:l:114:LYS:CG	1.82	0.45
22:o:1097:GLU:CG	22:o:1098:PRO:HD3	2.45	0.45
22:o:1230:GLN:O	22:o:1234:LYS:HG2	2.16	0.45
3:D:889:HIS:O	10:L:104:ARG:CZ	2.61	0.45
3:D:891:ILE:HG21	10:L:111:LEU:HB2	1.80	0.45
5:F:103:GLU:HB3	7:H:59:GLU:HG2	1.97	0.45
7:H:194:MET:HE2	7:H:194:MET:HB2	1.85	0.45
11:O:88:ILE:HG23	13:Q:361:ASN:CG	2.33	0.45
12:P:192:TYR:O	12:P:192:TYR:CG	2.65	0.45
12:P:252:ASP:OD1	12:P:252:ASP:N	2.49	0.45
15:S:45:ALA:CB	16:T:9:LEU:CD2	2.78	0.45
16:T:147:LYS:CG	16:T:148:VAL:N	2.66	0.45
22:o:198:LEU:HG	22:o:216:LEU:HB2	1.98	0.45
23:p:853:LEU:HB2	33:z:46:LYS:NZ	2.30	0.45
28:u:147:ILE:HA	28:u:160:ILE:O	2.16	0.45
2:B:71:ARG:HD3	2:B:73:TYR:CE1	2.51	0.45
2:B:848:HIS:CD2	7:H:226:ALA:HA	2.51	0.45
7:H:110:TYR:HH	9:J:160:GLN:HB3	1.77	0.45
7:H:115:GLN:H	7:H:115:GLN:HG3	1.58	0.45
13:Q:358:MET:HE2	13:Q:367:PHE:CD2	2.38	0.45
16:T:177:ARG:HD2	16:T:177:ARG:HA	1.52	0.45
18:Y:-15:DC:H2"	18:Y:-14:DC:C6	2.52	0.45
3:d:888:LYS:H	3:d:888:LYS:HG3	1.45	0.45
3:d:1084:LEU:HB3	8:i:99:ARG:HH21	1.81	0.45
9:j:176:MET:HE1	21:m:75:ILE:HD11	1.97	0.45
22:o:294:GLU:OE2	22:o:303:ILE:HG21	2.16	0.45
23:p:591:ARG:NH2	23:p:663:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:p:794:VAL:HG12	23:p:967:ILE:HG22	1.99	0.45
1:A:604:PRO:O	1:A:889:TYR:OH	2.34	0.45
3:D:1004:ALA:CB	11:O:4:GLN:HB2	2.47	0.45
5:F:90:GLU:OE2	9:J:208:GLY:HA3	2.16	0.45
5:F:214:HIS:HB3	7:H:164:THR:HG21	1.98	0.45
8:I:74:ALA:O	8:I:78:ARG:HB2	2.17	0.45
5:f:83:LEU:HD22	8:i:41:GLU:HG2	1.99	0.45
23:p:1141:ARG:HE	23:p:1143:LYS:HZ1	1.62	0.45
26:s:4:GLU:HA	26:s:7:THR:HG22	1.98	0.45
5:F:335:ARG:HH11	5:F:382:GLU:CA	1.99	0.45
5:F:335:ARG:NH1	5:F:430:HIS:NE2	2.62	0.45
12:P:203:ARG:NH2	13:Q:344:ARG:CZ	2.80	0.45
3:d:1080:TYR:OH	4:e:606:ASP:OD2	2.27	0.45
22:o:37:THR:O	22:o:87:HIS:HE1	1.98	0.45
22:o:511:THR:HG22	23:p:1101:GLN:HB3	1.98	0.45
22:o:584:PRO:O	22:o:585:LEU:HD12	2.16	0.45
24:q:240:ARG:HB2	24:q:243:THR:HG22	1.99	0.45
1:A:796:SER:H	1:A:799:ALA:HB3	1.81	0.45
3:D:901:TYR:CE2	10:L:120:LEU:HD22	2.52	0.45
4:E:784:HIS:HB3	4:E:792:LEU:HB2	1.99	0.45
14:R:111:ASP:O	14:R:115:MET:HG3	2.15	0.45
22:o:26:LEU:HD23	22:o:26:LEU:H	1.82	0.45
23:p:65:ILE:HD11	23:p:86:LEU:HD12	1.98	0.45
23:p:908:MET:HE3	23:p:910:THR:HG22	1.98	0.45
1:A:401:ASN:HD22	1:A:401:ASN:N	2.14	0.45
1:A:950:VAL:CG1	1:A:1066:CYS:SG	2.99	0.45
3:D:1003:ASP:N	3:D:1003:ASP:OD1	2.49	0.45
4:E:481:ASP:OD1	4:E:481:ASP:N	2.41	0.45
5:F:48:LYS:CE	8:I:22:ILE:HG23	2.45	0.45
5:F:324:ASP:O	5:F:328:ALA:N	2.40	0.45
14:R:121:ILE:HD11	14:R:142:PHE:HD2	1.81	0.45
15:S:16:VAL:C	16:T:41:GLY:O	2.59	0.45
15:S:17:ARG:CB	16:T:39:GLU:HB2	2.43	0.45
15:S:45:ALA:CB	16:T:9:LEU:HD11	2.46	0.45
18:Y:-10:DG:H2''	18:Y:-9:DT:C6	2.52	0.45
18:Y:-3:DA:H2''	18:Y:-2:DC:C6	2.52	0.45
22:o:261:ARG:HB3	22:o:276:LEU:HD11	1.99	0.45
25:r:29:ALA:HA	28:u:5:ILE:HG22	1.98	0.45
25:r:94:LYS:O	25:r:97:LEU:HG	2.17	0.45
1:A:844:LYS:NZ	17:X:31:DT:H71	2.31	0.45
2:B:184:ASN:ND2	2:B:184:ASN:N	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:18:VAL:CB	16:T:40:VAL:HG11	2.44	0.45
16:T:154:LYS:N	16:T:155:PRO:HD3	2.32	0.45
3:d:860:VAL:HA	21:m:47:GLN:HG2	1.98	0.45
22:o:191:ILE:HG12	22:o:200:ALA:CB	2.46	0.45
24:q:266:GLU:HG2	32:y:21:ILE:HG12	1.99	0.45
30:w:124:THR:OG1	30:w:125:GLU:N	2.49	0.45
1:A:405:VAL:HG21	5:F:301:VAL:CG1	2.46	0.45
1:A:475:LEU:HD23	1:A:480:TRP:HE1	1.82	0.45
1:A:573:TYR:OH	2:B:662:GLN:OE1	2.31	0.45
1:A:857:MET:HE3	1:A:858:ASP:H	1.81	0.45
3:D:1080:TYR:HD1	4:E:585:ASN:OD1	1.97	0.45
4:E:353:ASP:O	4:E:669:LYS:NZ	2.47	0.45
5:F:136:LEU:HD23	5:F:136:LEU:HA	1.76	0.45
5:F:310:THR:C	5:F:312:ILE:N	2.73	0.45
13:Q:367:PHE:C	13:Q:367:PHE:CD1	2.95	0.45
3:d:910:LEU:HD11	10:l:88:ALA:HB2	1.98	0.45
4:e:633:THR:O	4:e:634:ARG:NH2	2.45	0.45
5:f:149:PRO:HA	5:f:150:PRO:HD3	1.83	0.45
22:o:1248:ASN:ND2	22:o:1256:VAL:H	2.15	0.45
23:p:486:ASN:OD1	23:p:491:ARG:NH2	2.50	0.45
24:q:190:ASN:HD21	24:q:195:THR:HG23	1.81	0.45
1:A:572:TYR:CD1	2:B:689:GLN:CD	2.94	0.45
7:H:127:GLN:N	7:H:128:PRO:HD2	2.32	0.45
9:J:123:LEU:O	9:J:153:ARG:NH1	2.50	0.45
11:O:18:SER:H	13:Q:49:LYS:HZ2	1.59	0.45
12:P:228:GLU:OE1	12:P:228:GLU:HA	2.16	0.45
15:S:18:VAL:HB	16:T:40:VAL:HG11	1.90	0.45
28:u:76:VAL:HG22	28:u:77:PHE:H	1.81	0.45
28:u:89:VAL:HA	28:u:99:THR:HA	1.99	0.45
32:y:42:LEU:O	32:y:45:ILE:HG22	2.17	0.45
1:A:950:VAL:CG2	1:A:1065:GLU:HG2	2.47	0.44
2:B:559:LYS:HB2	2:B:559:LYS:NZ	2.31	0.44
2:B:827:ARG:CG	7:H:211:PHE:CZ	3.00	0.44
4:E:650:THR:HG22	4:E:666:THR:HG22	1.99	0.44
5:F:80:VAL:CG1	8:I:45:ARG:NH1	2.73	0.44
5:F:233:GLY:HA2	5:F:239:ARG:HE	1.82	0.44
5:F:332:PHE:CE2	5:F:336:LEU:HD11	2.52	0.44
5:F:350:ASN:OD1	5:F:350:ASN:N	2.50	0.44
8:I:38:GLN:HA	8:I:41:GLU:HB2	1.98	0.44
15:S:16:VAL:CA	16:T:41:GLY:O	2.64	0.44
16:T:11:GLY:HA3	16:T:106:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:1178:ASP:OD1	22:o:1185:VAL:HG23	2.17	0.44
22:o:1190:GLN:NE2	22:o:1194:ASN:HB2	2.32	0.44
22:o:1483:GLY:HA3	27:t:80:MET:HG2	1.98	0.44
23:p:329:GLY:HA3	23:p:335:ARG:HG3	1.98	0.44
23:p:463:ARG:HE	23:p:463:ARG:HB3	1.62	0.44
28:u:24:ASN:OD1	28:u:25:THR:N	2.50	0.44
1:A:404:MET:O	1:A:408:LEU:HB2	2.17	0.44
1:A:675:ASP:OD1	6:G:78:LYS:NZ	2.37	0.44
3:D:917:ILE:CG2	3:D:1058:VAL:HG11	2.46	0.44
5:F:335:ARG:HG2	5:F:382:GLU:CG	2.33	0.44
12:P:214:PHE:HE2	17:X:-24:DG:C1'	2.26	0.44
14:R:129:ASN:ND2	23:p:99:TRP:CD1	2.79	0.44
14:R:129:ASN:ND2	23:p:99:TRP:HD1	2.14	0.44
3:d:913:LEU:HD21	10:l:87:ILE:HD13	1.99	0.44
20:k:150:VAL:HG22	21:m:82:GLN:HB3	1.98	0.44
22:o:481:THR:O	22:o:483:ARG:NE	2.50	0.44
22:o:663:ASP:OD1	22:o:666:ARG:NH1	2.50	0.44
22:o:1030:SER:CB	26:s:162:ARG:HE	2.30	0.44
23:p:341:GLU:O	23:p:345:LYS:N	2.41	0.44
23:p:1108:PHE:HZ	23:p:1150:ARG:HG2	1.81	0.44
24:q:103:LEU:HD12	24:q:120:LEU:HD22	2.00	0.44
25:r:50:SER:OG	25:r:51:ALA:N	2.50	0.44
26:s:55:ARG:HA	26:s:58:LEU:HD12	1.98	0.44
26:s:94:MET:HE2	26:s:125:TYR:CD2	2.52	0.44
5:F:335:ARG:NE	5:F:382:GLU:OE1	2.48	0.44
5:F:426:LEU:C	5:F:426:LEU:HD23	2.42	0.44
7:H:44:LEU:HD11	9:J:160:GLN:HG2	1.99	0.44
13:Q:348:LYS:NZ	13:Q:375:GLU:CD	2.76	0.44
15:S:25:LYS:O	16:T:97:THR:HA	2.18	0.44
15:S:26:TYR:HB2	15:S:139:PRO:O	2.16	0.44
17:X:21:DC:H2'	17:X:21:DC:OP2	2.17	0.44
3:d:909:ARG:HH11	10:l:91:PHE:HZ	1.63	0.44
22:o:726:GLU:OE1	22:o:726:GLU:N	2.51	0.44
23:p:787:GLY:HA2	23:p:790:GLN:HE21	1.82	0.44
23:p:1142:ASN:ND2	23:p:1145:GLN:O	2.46	0.44
1:A:1185:VAL:CG1	1:A:1191:ILE:CD1	2.90	0.44
5:F:114:LEU:N	7:H:52:SER:HA	2.32	0.44
5:F:244:GLN:CD	7:H:133:ALA:HB3	2.36	0.44
5:F:366:GLU:OE1	5:F:366:GLU:HA	2.17	0.44
15:S:143:TRP:C	15:S:143:TRP:CD1	2.95	0.44
16:T:153:TYR:C	16:T:155:PRO:HD3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:-40:DC:O2	18:Y:40:DG:C2	2.71	0.44
17:X:-6:DA:H2''	17:X:-5:DC:C6	2.53	0.44
19:c:24:ASP:CB	9:j:192:LYS:HD2	2.48	0.44
5:f:219:GLU:H	5:f:219:GLU:CD	2.21	0.44
21:m:103:LEU:O	21:m:107:ASN:ND2	2.51	0.44
22:o:79:THR:OG1	22:o:80:GLU:OE1	2.34	0.44
23:p:458:LYS:NZ	23:p:461:GLN:HB3	2.33	0.44
26:s:88:LYS:HA	26:s:91:CYS:HB2	1.99	0.44
1:A:573:TYR:CD1	2:B:657:ARG:NH1	2.85	0.44
1:A:1182:CYS:O	1:A:1182:CYS:SG	2.75	0.44
2:B:69:GLN:NE2	2:B:156:LYS:O	2.47	0.44
2:B:431:LEU:HD23	2:B:431:LEU:O	2.17	0.44
3:D:950:LEU:HG	4:E:518:LYS:HD2	2.00	0.44
4:E:464:TYR:CD2	5:F:133:ALA:HB2	2.52	0.44
5:F:71:ILE:CB	8:I:38:GLN:NE2	2.32	0.44
12:P:278:GLN:OE1	12:P:278:GLN:N	2.49	0.44
13:Q:310:GLU:HB3	13:Q:313:PRO:CD	2.47	0.44
15:S:10:ASN:O	16:T:47:LYS:N	2.37	0.44
15:S:18:VAL:O	16:T:34:ALA:CB	2.66	0.44
17:X:1:DG:H2''	17:X:2:DG:C8	2.53	0.44
17:X:23:DA:N6	18:Y:-24:DA:N6	2.66	0.44
5:f:105:TYR:O	9:j:217:PHE:N	2.51	0.44
5:f:320:ARG:HH11	5:f:320:ARG:HB2	1.83	0.44
10:l:106:ARG:HD2	10:l:114:LYS:HZ1	1.82	0.44
24:q:77:ASP:OD1	24:q:77:ASP:N	2.46	0.44
30:w:75:ASP:HB3	30:w:78:LEU:HD12	1.99	0.44
1:A:486:TRP:CH2	5:f:358:THR:CG2	3.01	0.44
2:B:496:MET:HB2	2:B:496:MET:HE3	1.84	0.44
3:D:905:ALA:HB2	10:L:120:LEU:HD21	2.00	0.44
5:F:66:LEU:C	8:I:32:GLU:HG3	2.43	0.44
8:I:132:LEU:CD1	9:J:121:MET:SD	3.06	0.44
22:o:322:LEU:HD12	22:o:323:PRO:HD2	1.99	0.44
22:o:1286:ARG:NH2	23:p:251:ALA:O	2.50	0.44
23:p:371:ARG:NH2	23:p:380:ARG:HH22	2.16	0.44
25:r:32:LEU:HD23	28:u:2:PHE:HB3	1.99	0.44
1:A:345:PRO:HG3	1:A:500:LEU:HG	1.99	0.44
1:A:489:GLN:H	1:A:489:GLN:CD	2.25	0.44
1:A:567:LEU:CD2	2:B:745:GLN:HE21	2.30	0.44
2:B:367:GLU:OE2	2:B:371:LYS:NZ	2.40	0.44
4:E:613:ALA:HB3	4:E:616:HIS:HD2	1.83	0.44
5:F:14:LEU:CD2	8:I:15:ASP:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:116:ARG:HG3	7:H:116:ARG:O	2.16	0.44
14:R:18:HIS:CE1	14:R:37:CYS:SG	2.99	0.44
16:T:49:GLN:N	16:T:49:GLN:CD	2.73	0.44
17:X:5:DA:H2"	17:X:6:DG:C8	2.53	0.44
17:X:18:DA:H2"	17:X:19:DG:C8	2.53	0.44
18:Y:40:DG:H2"	18:Y:41:DA:C8	2.53	0.44
24:q:116:THR:HB	24:q:147:ASP:HB3	2.00	0.44
27:t:84:GLU:O	27:t:84:GLU:HG2	2.16	0.44
5:F:47:ILE:HG23	8:I:19:MET:SD	2.37	0.44
5:F:400:GLY:O	5:F:404:ARG:HG2	2.18	0.44
7:H:43:SER:HB2	7:H:119:ILE:HD11	1.99	0.44
11:O:17:GLU:C	13:Q:49:LYS:HZ1	2.25	0.44
15:S:33:ALA:H	16:T:90:GLY:C	2.25	0.44
22:o:277:THR:HA	22:o:280:LEU:HD12	2.00	0.44
22:o:346:LYS:HB2	22:o:351:ARG:HH21	1.82	0.44
22:o:460:ARG:HG2	22:o:461:GLN:N	2.32	0.44
23:p:526:LEU:H	23:p:526:LEU:HD23	1.83	0.44
23:p:628:VAL:HG22	23:p:633:LEU:HD23	2.00	0.44
25:r:109:GLU:O	25:r:113:ALA:N	2.49	0.44
26:s:154:GLU:O	26:s:157:THR:HG22	2.17	0.44
30:w:103:ARG:O	30:w:103:ARG:HD3	2.18	0.44
1:A:1197:ILE:CD1	6:G:166:VAL:CG1	2.94	0.44
3:D:1002:ARG:H	3:D:1002:ARG:HG2	1.43	0.44
4:E:250:GLU:O	4:E:254:ASN:ND2	2.50	0.44
7:H:73:GLY:CA	9:J:142:ALA:HB3	2.39	0.44
7:H:111:ALA:CB	9:J:126:TYR:CE2	2.93	0.44
11:O:7:ARG:NH2	11:O:37:LEU:HB3	2.33	0.44
15:S:54:LYS:HE2	15:S:54:LYS:HB2	1.84	0.44
18:Y:-14:DC:H2"	18:Y:-13:DA:C8	2.53	0.44
18:Y:6:DT:H2"	18:Y:7:DG:C8	2.53	0.44
22:o:17:THR:HG22	22:o:18:ILE:N	2.32	0.44
22:o:514:GLU:O	22:o:518:LEU:HB2	2.18	0.44
22:o:652:LEU:HD12	22:o:652:LEU:HA	1.87	0.44
23:p:551:GLU:OE1	23:p:551:GLU:N	2.45	0.44
23:p:849:ASP:HB3	33:z:15:MET:HE3	2.00	0.44
25:r:95:PHE:CE1	28:u:1:MET:HE3	2.53	0.44
33:z:19:CYS:SG	33:z:20:GLY:N	2.91	0.44
1:A:690:LEU:HD22	1:A:747:LEU:HD22	1.99	0.43
2:B:839:MET:HE1	2:B:843:LEU:HD13	2.00	0.43
4:E:696:TRP:HA	4:E:703:MET:CA	2.32	0.43
7:H:110:TYR:CD2	9:J:157:LEU:CD2	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:196:ARG:HD3	12:P:196:ARG:HA	1.81	0.43
4:e:504:LEU:HD23	4:e:504:LEU:HA	1.90	0.43
10:l:113:VAL:O	10:l:113:VAL:HG22	2.18	0.43
10:l:139:TYR:HD2	21:m:73:MET:HE3	1.83	0.43
22:o:260:VAL:O	22:o:342:ARG:NH2	2.50	0.43
22:o:784:VAL:HG22	23:p:978:ILE:HD11	1.99	0.43
23:p:840:MET:HB3	23:p:891:ASP:OD2	2.18	0.43
32:y:63:VAL:HG22	32:y:71:ILE:HG22	2.00	0.43
2:B:780:LYS:HA	7:H:183:ARG:HH12	1.83	0.43
3:D:964:GLU:O	3:D:968:ARG:HG2	2.18	0.43
16:T:145:LEU:HD21	23:p:92:TYR:CD2	2.53	0.43
17:X:-29:DA:H1'	17:X:-28:DC:C5	2.52	0.43
18:Y:20:DC:H2''	18:Y:21:DT:C5	2.53	0.43
19:c:28:LEU:HD23	19:c:28:LEU:HA	1.89	0.43
19:c:77:LEU:HD12	9:j:116:LEU:CD2	2.44	0.43
5:f:11:ASN:OD1	5:f:48:LYS:NZ	2.51	0.43
5:f:217:SER:H	5:f:220:GLN:HE21	1.65	0.43
22:o:111:CYS:SG	22:o:188:GLN:NE2	2.92	0.43
22:o:936:GLU:HA	22:o:939:VAL:HG12	2.00	0.43
22:o:1422:GLN:HB3	22:o:1424:THR:HG23	2.01	0.43
23:p:323:SER:OG	23:p:324:ARG:NH1	2.48	0.43
23:p:628:VAL:HG12	23:p:629:GLU:O	2.18	0.43
24:q:101:PHE:CE1	24:q:122:SER:HB3	2.53	0.43
25:r:125:GLU:O	25:r:129:GLN:N	2.40	0.43
1:A:400:GLU:HG3	1:A:401:ASN:N	2.32	0.43
1:A:489:GLN:H	1:A:489:GLN:NE2	2.15	0.43
1:A:1063:LYS:C	1:A:1063:LYS:CD	2.88	0.43
1:A:1065:GLU:OE1	1:A:1065:GLU:HA	2.19	0.43
5:F:15:PRO:HB2	8:I:14:LYS:HE3	2.00	0.43
14:R:185:ARG:HD2	16:T:160:GLN:HE22	1.82	0.43
16:T:177:ARG:CB	16:T:177:ARG:HH21	2.31	0.43
17:X:-15:DA:H2''	17:X:-14:DC:C6	2.53	0.43
19:c:101:VAL:HG22	5:f:127:LEU:HA	2.00	0.43
23:p:374:LEU:HD23	23:p:374:LEU:HA	1.85	0.43
1:A:414:ILE:HG21	5:F:313:VAL:CG2	2.47	0.43
1:A:1150:THR:HG21	6:G:150:LYS:NZ	2.32	0.43
1:A:1190:VAL:HG22	6:G:162:VAL:CB	2.46	0.43
5:F:14:LEU:HA	8:I:18:MET:HB3	2.00	0.43
10:L:93:GLU:O	10:L:97:THR:CG2	2.52	0.43
12:P:207:PRO:O	12:P:207:PRO:CD	2.65	0.43
16:T:210:VAL:HA	16:T:213:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:4:DA:H2''	18:Y:5:DG:C8	2.53	0.43
4:e:479:THR:OG1	4:e:481:ASP:O	2.33	0.43
22:o:910:LYS:N	22:o:911:PRO:HD2	2.33	0.43
22:o:1171:ALA:HB3	22:o:1215:GLU:HG3	2.00	0.43
22:o:1198:GLU:C	22:o:1200:PRO:HD3	2.43	0.43
23:p:256:ILE:HD11	23:p:373:LEU:HD21	2.00	0.43
23:p:799:SER:HB2	24:q:174:ALA:HB2	2.00	0.43
3:D:917:ILE:HG21	3:D:1058:VAL:HG11	2.00	0.43
5:F:68:THR:CG2	8:I:34:ARG:HH12	2.24	0.43
6:G:181:TRP:CD2	6:G:181:TRP:O	2.72	0.43
7:H:155:ASP:OD1	7:H:155:ASP:N	2.51	0.43
8:I:21:GLN:HE22	8:I:24:LYS:HE2	1.84	0.43
12:P:202:MET:HB2	12:P:202:MET:HE3	1.85	0.43
13:Q:366:ILE:HG22	13:Q:367:PHE:N	2.33	0.43
14:R:169:ARG:HD3	14:R:206:VAL:HB	2.00	0.43
16:T:174:LYS:HB3	16:T:174:LYS:HE3	1.50	0.43
19:c:124:ILE:HD11	5:f:133:ALA:HB1	2.00	0.43
22:o:434:LYS:NZ	22:o:437:ASP:HB3	2.34	0.43
22:o:917:GLU:O	22:o:921:ARG:HB2	2.17	0.43
22:o:927:GLU:HG3	22:o:927:GLU:O	2.18	0.43
22:o:1211:LEU:HD11	22:o:1258:ARG:NE	2.33	0.43
23:p:934:LYS:HZ1	23:p:942:LYS:HD2	1.84	0.43
28:u:2:PHE:HA	28:u:76:VAL:O	2.19	0.43
28:u:84:VAL:HA	28:u:145:LEU:O	2.18	0.43
5:F:50:ILE:O	5:F:54:ALA:N	2.47	0.43
5:F:90:GLU:OE1	9:J:208:GLY:HA3	2.18	0.43
7:H:59:GLU:HA	7:H:62:THR:HG22	1.99	0.43
12:P:304:ILE:HD12	12:P:304:ILE:N	2.34	0.43
14:R:189:LYS:H	14:R:189:LYS:HG2	1.40	0.43
18:Y:-13:DA:H2''	18:Y:-12:DG:C8	2.53	0.43
4:e:667:GLY:O	4:e:692:ARG:NH2	2.52	0.43
5:f:317:LEU:HG	5:f:330:ARG:HE	1.83	0.43
22:o:273:GLN:OE1	22:o:278:HIS:N	2.52	0.43
22:o:420:ILE:HD11	22:o:426:ARG:HH21	1.83	0.43
23:p:629:GLU:O	23:p:630:LYS:C	2.62	0.43
23:p:718:GLN:HG2	23:p:720:PRO:HD2	2.01	0.43
29:v:71:ASP:O	29:v:72:ASP:HB3	2.18	0.43
1:A:592:SER:OG	1:A:695:GLY:O	2.31	0.43
2:B:925:LYS:HA	2:B:925:LYS:HD3	1.78	0.43
5:F:48:LYS:HE3	8:I:22:ILE:CB	2.48	0.43
5:F:258:ARG:HD2	5:F:258:ARG:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:47:LEU:HG	15:S:98:TRP:CE3	2.53	0.43
16:T:23:VAL:HG13	16:T:27:LEU:HD23	2.01	0.43
17:X:-3:DG:H2"	17:X:-2:DG:C8	2.54	0.43
17:X:0:DA:H2"	17:X:1:DG:C8	2.53	0.43
5:f:447:ALA:CB	5:f:456:GLY:HA3	2.48	0.43
22:o:491:PRO:HG2	22:o:535:MET:HE2	2.01	0.43
25:r:76:ASN:O	25:r:80:ILE:HD12	2.19	0.43
2:B:781:TYR:CB	7:H:176:ARG:HH21	2.24	0.43
5:F:402:ARG:O	5:F:406:VAL:HG13	2.19	0.43
5:F:418:ILE:H	5:F:418:ILE:CD1	2.27	0.43
8:I:23:LEU:HD22	8:I:28:ILE:HD12	2.01	0.43
11:O:61:SER:H	11:O:79:VAL:HG22	1.83	0.43
12:P:306:VAL:HG21	14:R:246:PRO:HB2	2.00	0.43
15:S:124:TYR:OH	16:T:22:LYS:CE	2.60	0.43
16:T:122:GLU:HG3	16:T:123:ASN:N	2.34	0.43
19:c:21:LEU:HD11	19:c:23:TRP:CD1	2.54	0.43
8:i:45:ARG:HG3	9:j:212:LYS:HB3	2.01	0.43
8:i:73:LEU:HD13	10:l:105:HIS:NE2	2.33	0.43
25:r:73:ARG:CZ	28:u:86:ASP:OD2	2.66	0.43
1:A:469:PRO:N	7:H:166:ARG:NH1	2.66	0.43
1:A:575:PRO:HD3	2:B:608:ASN:CB	2.48	0.43
12:P:179:ASP:OD1	12:P:179:ASP:C	2.62	0.43
14:R:18:HIS:NE2	14:R:36:GLU:OE2	2.52	0.43
14:R:158:ALA:HA	14:R:186:ILE:HG13	2.01	0.43
17:X:-1:DA:H2"	17:X:0:DA:C8	2.54	0.43
18:Y:-12:DG:H2"	18:Y:-11:DA:C8	2.53	0.43
4:e:542:HIS:CE1	4:e:568:ARG:HG3	2.53	0.43
22:o:1312:PRO:O	22:o:1332:GLN:NE2	2.51	0.43
32:y:26:LYS:HG3	32:y:27:VAL:HG22	2.00	0.43
1:A:349:TRP:HZ2	5:f:262:PHE:CZ	2.36	0.43
2:B:339:THR:HB	2:B:340:PRO:HD3	2.01	0.43
2:B:831:GLU:OE1	2:B:835:ARG:NH2	2.52	0.43
5:F:215:GLU:O	5:F:254:GLN:NE2	2.39	0.43
7:H:111:ALA:O	9:J:126:TYR:OH	2.33	0.43
11:O:63:ASN:HB3	11:O:75:VAL:O	2.19	0.43
12:P:264:VAL:HG23	12:P:266:PHE:H	1.84	0.43
15:S:24:LYS:HB2	16:T:98:GLU:C	2.44	0.43
15:S:30:ALA:CA	16:T:92:THR:O	2.64	0.43
16:T:236:LYS:C	16:T:238:GLU:H	2.27	0.43
5:f:428:LEU:HD13	5:f:458:LEU:CB	2.49	0.43
8:i:16:ALA:HB2	8:i:40:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:404:GLU:HG3	22:o:407:ARG:NH2	2.34	0.43
22:o:1191:GLU:O	22:o:1195:VAL:HG13	2.19	0.43
22:o:1226:LEU:HA	22:o:1230:GLN:NE2	2.34	0.43
23:p:545:LEU:HD23	23:p:545:LEU:HA	1.83	0.43
29:v:32:SER:OG	29:v:33:GLU:N	2.52	0.43
4:E:369:LYS:HD3	4:E:369:LYS:HA	1.74	0.42
10:L:106:ARG:NH1	10:L:114:LYS:CG	2.71	0.42
15:S:29:MET:HB3	16:T:94:THR:OG1	2.19	0.42
15:S:143:TRP:NE1	15:S:145:ASN:OD1	2.37	0.42
3:d:871:THR:O	10:l:62:LYS:NZ	2.42	0.42
10:l:80:VAL:O	10:l:84:LEU:HG	2.19	0.42
22:o:863:ARG:HH21	22:o:1415:THR:HA	1.84	0.42
22:o:1180:ASN:HB3	22:o:1182:GLN:OE1	2.18	0.42
22:o:1429:LYS:HE2	22:o:1429:LYS:HA	2.01	0.42
25:r:103:LEU:O	28:u:144:ARG:CZ	2.67	0.42
1:A:1193:ALA:CB	6:G:166:VAL:HG21	2.42	0.42
1:A:1203:GLU:N	1:A:1203:GLU:OE2	2.52	0.42
2:B:414:LEU:HB2	2:B:523:VAL:HG13	1.99	0.42
2:B:859:ARG:HA	2:B:859:ARG:HD2	1.80	0.42
3:D:943:GLN:HG2	4:E:513:LEU:HB2	2.01	0.42
3:D:950:LEU:HD23	3:D:950:LEU:HA	1.87	0.42
10:L:106:ARG:HD2	10:L:114:LYS:NZ	2.34	0.42
12:P:261:SER:HB3	18:Y:29:DT:H4'	2.00	0.42
13:Q:351:PHE:CD1	13:Q:351:PHE:N	2.87	0.42
15:S:23:THR:O	16:T:99:SER:C	2.62	0.42
15:S:53:ASN:HB2	15:S:96:GLN:OE1	2.19	0.42
4:e:332:ILE:HA	4:e:336:HIS:HD2	1.84	0.42
22:o:28:PRO:HA	22:o:31:LEU:HB2	2.01	0.42
22:o:379:GLY:HA2	22:o:475:ARG:O	2.19	0.42
22:o:1028:PRO:O	22:o:1029:LEU:HB3	2.18	0.42
22:o:1146:GLN:HA	22:o:1149:ARG:HE	1.84	0.42
28:u:54:ILE:HG13	28:u:70:VAL:HG23	2.00	0.42
2:B:562:GLY:O	2:B:581:ILE:HG12	2.19	0.42
2:B:653:LEU:HG	2:B:684:ILE:HG13	2.00	0.42
2:B:875:LYS:NZ	2:B:906:GLU:OE2	2.45	0.42
4:E:731:MET:HE3	4:E:731:MET:HB3	1.91	0.42
5:F:401:GLU:C	5:F:401:GLU:CD	2.87	0.42
10:L:120:LEU:O	10:L:125:ASN:N	2.52	0.42
15:S:27:ASN:HB2	16:T:96:PHE:CZ	2.53	0.42
16:T:18:VAL:HG13	16:T:108:GLY:HA3	2.00	0.42
16:T:217:LEU:HD13	16:T:233:TRP:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:220:ILE:C	16:T:220:ILE:CD1	2.91	0.42
17:X:4:DG:H2''	17:X:5:DA:C8	2.54	0.42
18:Y:3:DC:H2''	18:Y:4:DA:C8	2.54	0.42
3:d:1078:LEU:HD21	10:l:90:ASP:OD2	2.19	0.42
22:o:350:VAL:HG13	22:o:351:ARG:HG3	2.01	0.42
22:o:1244:ASN:O	22:o:1259:ILE:HA	2.19	0.42
22:o:1361:ASP:OD1	22:o:1363:VAL:HG22	2.20	0.42
23:p:90:GLN:HG3	23:p:91:ILE:N	2.34	0.42
23:p:1046:THR:HG22	23:p:1047:TYR:N	2.32	0.42
26:s:49:SER:C	26:s:50:GLU:HG3	2.44	0.42
28:u:100:GLU:HA	28:u:106:CYS:H	1.82	0.42
1:A:727:THR:HG23	1:A:727:THR:O	2.19	0.42
2:B:219:ASP:OD1	2:B:219:ASP:N	2.52	0.42
5:F:67:THR:CB	8:I:32:GLU:CD	2.90	0.42
5:F:360:THR:O	5:F:364:VAL:HG22	2.18	0.42
16:T:224:ASN:HB3	16:T:226:LYS:HE2	2.01	0.42
4:e:504:LEU:HD22	4:e:575:PHE:HZ	1.85	0.42
22:o:48:GLU:OE1	22:o:48:GLU:N	2.52	0.42
22:o:330:GLN:O	22:o:331:LYS:HE2	2.20	0.42
22:o:1006:PRO:HB3	22:o:1051:SER:OG	2.20	0.42
22:o:1230:GLN:HB2	22:o:1234:LYS:NZ	2.34	0.42
23:p:36:GLU:OE1	23:p:653:TRP:HB3	2.20	0.42
23:p:110:PRO:HG2	23:p:163:LEU:HD11	2.00	0.42
23:p:143:GLN:N	23:p:143:GLN:OE1	2.52	0.42
23:p:334:LYS:HD3	23:p:334:LYS:HA	1.83	0.42
24:q:44:ILE:HD11	24:q:238:SER:CB	2.50	0.42
29:v:8:ASP:OD2	29:v:32:SER:OG	2.36	0.42
3:D:957:ARG:HD3	3:D:957:ARG:HA	1.56	0.42
5:F:312:ILE:HG22	5:F:313:VAL:CG1	2.49	0.42
13:Q:369:LYS:HB3	13:Q:369:LYS:HE2	1.71	0.42
15:S:121:ASN:O	16:T:25:LYS:CG	2.62	0.42
16:T:51:ARG:CG	16:T:52:THR:N	2.82	0.42
16:T:181:GLN:HE22	16:T:184:LEU:HD13	1.84	0.42
4:e:774:MET:HE2	4:e:774:MET:HB2	1.91	0.42
10:l:129:PRO:HB2	21:m:56:ILE:HG23	2.01	0.42
22:o:403:GLN:O	22:o:406:VAL:HG12	2.19	0.42
22:o:403:GLN:HA	22:o:406:VAL:HG12	2.01	0.42
22:o:1129:ASN:HD21	22:o:1415:THR:HB	1.85	0.42
24:q:69:GLY:HA3	33:z:57:ALA:HB1	2.01	0.42
1:A:637:GLN:HG2	6:G:40:LYS:HD2	2.00	0.42
1:A:899:LYS:HE3	1:A:899:LYS:HB2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:VAL:CB	1:A:1191:ILE:CD1	2.96	0.42
4:E:690:ASP:OD1	4:E:690:ASP:N	2.43	0.42
5:F:17:GLU:OE2	8:I:14:LYS:HE2	2.18	0.42
5:F:48:LYS:HE3	8:I:22:ILE:CA	2.47	0.42
5:F:90:GLU:C	5:F:92:ILE:H	2.27	0.42
5:F:213:ILE:CG2	7:H:164:THR:O	2.63	0.42
5:F:412:LEU:O	5:F:412:LEU:HG	2.19	0.42
7:H:111:ALA:HB1	9:J:126:TYR:HE2	1.78	0.42
12:P:188:ARG:HH21	13:Q:324:GLU:CA	2.29	0.42
13:Q:19:GLU:HA	13:Q:19:GLU:OE1	2.19	0.42
15:S:11:VAL:O	15:S:12:THR:HG23	2.18	0.42
16:T:25:LYS:O	16:T:29:GLN:N	2.45	0.42
16:T:179:ASP:HB3	16:T:182:HIS:HB3	2.01	0.42
17:X:-2:DG:H2"	17:X:-1:DA:C8	2.54	0.42
9:j:149:PRO:O	9:j:153:ARG:NH1	2.46	0.42
22:o:15:LEU:HA	23:p:1148:LEU:O	2.20	0.42
22:o:397:PHE:HB3	27:t:87:THR:HG23	2.02	0.42
22:o:1448:SER:OG	22:o:1449:ASP:N	2.52	0.42
23:p:341:GLU:HG2	23:p:342:VAL:N	2.35	0.42
23:p:912:ASN:HB3	23:p:918:PHE:CD1	2.54	0.42
24:q:15:THR:HG22	24:q:16:ASP:N	2.33	0.42
26:s:173:ILE:O	26:s:209:VAL:HA	2.19	0.42
3:D:953:ILE:HD12	3:D:953:ILE:HA	1.95	0.42
4:E:747:LEU:N	4:E:747:LEU:HD13	2.34	0.42
5:F:213:ILE:CG2	7:H:163:PRO:C	2.93	0.42
5:F:219:GLU:CD	5:F:219:GLU:C	2.86	0.42
5:F:335:ARG:NH1	5:F:381:ALA:C	2.78	0.42
11:O:5:LEU:CD2	11:O:98:CYS:SG	3.02	0.42
14:R:14:THR:N	14:R:20:ASP:HB3	2.34	0.42
17:X:-40:DC:O2	18:Y:40:DG:N1	2.53	0.42
22:o:12:ALA:HB3	23:p:1135:TYR:HE2	1.85	0.42
22:o:89:GLU:O	22:o:287:ASN:ND2	2.51	0.42
22:o:721:HIS:HE1	30:w:98:GLN:HE21	1.67	0.42
22:o:881:ASN:OD1	22:o:882:SER:N	2.40	0.42
22:o:1097:GLU:HG2	22:o:1098:PRO:HD3	2.00	0.42
23:p:109:MET:HB2	23:p:112:GLU:OE1	2.20	0.42
23:p:296:GLU:CD	23:p:296:GLU:H	2.27	0.42
23:p:368:MET:HE3	23:p:368:MET:HB2	1.85	0.42
23:p:516:GLU:HA	23:p:520:VAL:HG22	2.02	0.42
28:u:44:PHE:CZ	28:u:157:ILE:HB	2.54	0.42
1:A:998:LEU:HB3	1:A:1003:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:476:VAL:HB	4:E:782:HIS:HB2	2.01	0.42
11:O:7:ARG:NH1	11:O:37:LEU:HB3	2.35	0.42
15:S:6:PRO:O	15:S:10:ASN:N	2.53	0.42
16:T:181:GLN:NE2	16:T:181:GLN:CA	2.78	0.42
19:c:94:HIS:CD2	5:f:122:LEU:HD22	2.54	0.42
4:e:636:HIS:CD2	4:e:638:ASN:H	2.36	0.42
5:f:55:LEU:HD13	8:i:28:ILE:HG12	2.01	0.42
22:o:1248:ASN:HD21	22:o:1256:VAL:HB	1.84	0.42
28:u:168:LEU:H	28:u:168:LEU:HD23	1.85	0.42
29:v:146:LYS:HE2	29:v:146:LYS:HB2	1.86	0.42
1:A:925:ASP:N	1:A:925:ASP:OD1	2.52	0.42
2:B:594:SER:OG	2:B:595:LYS:N	2.51	0.42
4:E:377:LEU:HD21	4:E:422:PRO:HG2	2.00	0.42
4:E:508:LYS:HB3	4:E:512:ASP:HB2	2.02	0.42
5:F:370:TRP:CZ3	5:F:420:ALA:HA	2.55	0.42
5:F:388:ILE:HA	5:F:392:ILE:HG12	2.02	0.42
10:L:76:LEU:HD13	10:L:84:LEU:CD1	2.50	0.42
12:P:278:GLN:CD	12:P:278:GLN:N	2.76	0.42
12:P:329:TYR:N	12:P:330:PRO:HD2	2.35	0.42
14:R:154:ARG:NH2	18:Y:22:DG:P	2.93	0.42
15:S:17:ARG:CG	16:T:39:GLU:CD	2.85	0.42
15:S:37:VAL:HG11	15:S:42:TRP:CZ2	2.55	0.42
16:T:182:HIS:O	16:T:185:ASP:HB2	2.18	0.42
17:X:-27:DT:H3'	17:X:-27:DT:OP2	2.20	0.42
22:o:42:LYS:O	22:o:288:ASN:ND2	2.44	0.42
22:o:1005:HIS:O	22:o:1008:LYS:HB2	2.20	0.42
22:o:1018:LYS:HE3	22:o:1018:LYS:HB2	1.90	0.42
22:o:1098:PRO:O	22:o:1101:GLN:HG2	2.20	0.42
23:p:193:VAL:O	23:p:467:SER:HA	2.20	0.42
23:p:225:LEU:H	23:p:225:LEU:HD23	1.84	0.42
23:p:991:ALA:O	31:x:46:ARG:NE	2.53	0.42
24:q:11:ILE:HD11	32:y:109:ILE:HG22	2.02	0.42
1:A:413:ASP:O	1:A:414:ILE:C	2.63	0.42
1:A:500:LEU:HA	1:A:500:LEU:HD23	1.81	0.42
3:D:898:VAL:HG22	10:L:113:VAL:HA	2.02	0.42
4:E:579:VAL:CG2	8:I:115:LEU:HD22	2.50	0.42
5:F:320:ARG:NH2	5:F:414:ASN:C	2.78	0.42
11:O:27:GLN:HE22	13:Q:41:GLU:CD	2.28	0.42
11:O:77:ASN:O	11:O:79:VAL:HG23	2.19	0.42
13:Q:53:SER:O	13:Q:54:ARG:HB2	2.20	0.42
14:R:214:PHE:HA	14:R:217:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:18:VAL:H	16:T:39:GLU:HA	1.83	0.42
5:f:432:ALA:HB1	5:f:462:GLN:CB	2.49	0.42
22:o:1231:ILE:O	22:o:1235:ILE:HG12	2.20	0.42
25:r:82:SER:O	25:r:86:LEU:N	2.52	0.42
26:s:185:ILE:HG22	26:s:209:VAL:HG11	2.01	0.42
1:A:797:LYS:HD2	1:A:797:LYS:HA	1.63	0.41
1:A:931:PRO:O	1:A:935:THR:OG1	2.25	0.41
2:B:216:SER:OG	2:B:217:ASN:N	2.52	0.41
5:F:213:ILE:CB	7:H:163:PRO:C	2.90	0.41
12:P:212:LEU:HD21	18:Y:26:DG:H1'	2.01	0.41
17:X:-26:DC:H3'	17:X:-26:DC:P	2.60	0.41
17:X:6:DG:H2''	17:X:7:DT:C6	2.54	0.41
18:Y:7:DG:H2''	18:Y:8:DC:C6	2.55	0.41
20:k:179:MET:HB3	20:k:180:PRO:HD2	2.01	0.41
22:o:576:GLN:HG3	22:o:577:PRO:HD2	2.03	0.41
22:o:1130:ILE:HG23	22:o:1362:ILE:HD11	2.02	0.41
23:p:728:MET:HE2	23:p:942:LYS:HD3	2.02	0.41
25:r:36:GLU:OE1	25:r:36:GLU:N	2.53	0.41
1:A:825:ILE:HD12	1:A:830:ILE:HD11	2.01	0.41
2:B:464:ILE:HG12	2:B:513:LYS:HE2	2.02	0.41
2:B:544:LEU:HD22	2:B:625:LEU:HD22	2.02	0.41
3:D:891:ILE:HG21	10:L:111:LEU:CG	2.50	0.41
3:D:961:GLN:O	3:D:965:ILE:N	2.53	0.41
4:E:615:ASP:OD2	8:I:114:ARG:CG	2.66	0.41
4:E:696:TRP:CH2	4:E:703:MET:CE	3.03	0.41
5:F:43:VAL:HG21	8:I:43:ALA:CA	2.46	0.41
7:H:160:ILE:HD13	7:H:160:ILE:HA	1.93	0.41
11:O:22:LEU:CD1	11:O:28:ILE:HG21	2.41	0.41
14:R:216:SER:HA	14:R:229:GLN:NE2	2.35	0.41
15:S:110:PHE:HD1	15:S:148:PRO:HA	1.85	0.41
16:T:226:LYS:HA	16:T:226:LYS:HD3	1.83	0.41
18:Y:33:DG:H2'	18:Y:34:DA:C8	2.55	0.41
22:o:437:ASP:OD1	22:o:438:LEU:N	2.54	0.41
22:o:819:SER:O	22:o:819:SER:OG	2.38	0.41
23:p:267:VAL:HG12	23:p:268:PRO:O	2.20	0.41
23:p:634:LEU:HD23	23:p:634:LEU:HA	1.86	0.41
23:p:794:VAL:HG22	23:p:944:THR:O	2.20	0.41
1:A:638:PRO:HA	1:A:773:ILE:HG23	2.01	0.41
1:A:662:MET:HA	2:B:510:VAL:HA	2.02	0.41
1:A:1055:VAL:HG13	1:A:1056:ALA:H	1.85	0.41
2:B:62:ARG:H	2:B:62:ARG:HG2	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:898:VAL:CG2	10:L:113:VAL:CG2	2.96	0.41
5:F:231:CYS:HB3	5:F:285:MET:HE2	2.03	0.41
11:O:19:LEU:O	11:O:23:ILE:HG13	2.20	0.41
13:Q:43:LYS:HE2	13:Q:60:HIS:CE1	2.56	0.41
14:R:119:LYS:NZ	23:p:436:LYS:HZ2	2.17	0.41
16:T:140:ARG:NH2	23:p:89:GLU:CB	2.70	0.41
16:T:147:LYS:CG	16:T:148:VAL:H	2.04	0.41
3:d:1060:LEU:HD11	10:l:83:MET:HG3	2.03	0.41
21:m:80:ARG:HA	21:m:80:ARG:HD2	1.85	0.41
22:o:515:ILE:HD13	22:o:515:ILE:HA	1.90	0.41
22:o:1082:HIS:HA	22:o:1083:PRO:HD3	1.87	0.41
22:o:1204:VAL:HG23	22:o:1205:ALA:H	1.85	0.41
23:p:100:GLU:HG3	23:p:101:ARG:H	1.85	0.41
32:y:82:SER:OG	32:y:84:GLN:OE1	2.38	0.41
1:A:345:PRO:O	1:A:346:ALA:HB3	2.21	0.41
2:B:646:ASP:OD1	2:B:646:ASP:N	2.54	0.41
4:E:651:VAL:HG21	4:E:686:THR:HG21	2.01	0.41
5:F:66:LEU:HD22	8:I:31:TYR:HB3	2.01	0.41
16:T:158:ASN:HD22	16:T:158:ASN:N	2.18	0.41
18:Y:36:DG:H2''	18:Y:37:DT:C6	2.55	0.41
20:k:179:MET:HB3	20:k:180:PRO:CD	2.50	0.41
22:o:320:ASN:HB3	22:o:327:ARG:NE	2.35	0.41
23:p:957:THR:HG22	23:p:1028:LEU:CD2	2.50	0.41
23:p:1088:GLU:OE1	23:p:1091:ARG:NH1	2.53	0.41
25:r:37:VAL:HG21	28:u:2:PHE:CE2	2.55	0.41
26:s:85:LYS:O	26:s:89:VAL:N	2.46	0.41
2:B:735:ILE:HG22	7:H:176:ARG:CZ	2.33	0.41
3:D:1006:LEU:HD23	3:D:1006:LEU:HA	1.79	0.41
4:E:466:PHE:HE1	4:E:794:ALA:HB1	1.86	0.41
5:F:249:ASP:HB3	5:F:252:LEU:HB2	2.02	0.41
5:F:426:LEU:O	5:F:429:LYS:HG2	2.21	0.41
6:G:129:LYS:HA	6:G:129:LYS:HD2	1.76	0.41
11:O:19:LEU:CA	11:O:28:ILE:HD11	2.49	0.41
12:P:167:ASN:HD21	18:Y:28:DG:H1'	1.86	0.41
15:S:46:ARG:N	15:S:101:ARG:O	2.39	0.41
16:T:40:VAL:O	16:T:56:PHE:CZ	2.69	0.41
17:X:-22:DC:H42	18:Y:22:DG:H1	1.69	0.41
17:X:-6:DA:C2	18:Y:7:DG:C2	3.08	0.41
4:e:690:ASP:N	4:e:690:ASP:OD1	2.53	0.41
22:o:215:LEU:HD23	22:o:215:LEU:H	1.85	0.41
23:p:399:LEU:HD23	23:p:399:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:LEU:HD22	1:A:1012:VAL:HG21	2.01	0.41
2:B:203:LYS:HZ3	2:B:235:HIS:HB3	1.86	0.41
3:D:917:ILE:CD1	3:D:1058:VAL:CG2	2.67	0.41
3:D:966:LEU:HD11	3:D:981:GLN:CG	2.49	0.41
4:E:236:LEU:HD21	4:E:317:LEU:HB2	2.03	0.41
5:F:48:LYS:HE3	8:I:22:ILE:HG23	2.03	0.41
5:F:68:THR:CB	8:I:34:ARG:HH11	2.32	0.41
5:F:277:ALA:O	5:F:278:LEU:C	2.64	0.41
11:O:88:ILE:HD12	13:Q:360:LEU:CG	2.50	0.41
14:R:283:VAL:O	14:R:287:GLN:HG2	2.21	0.41
15:S:30:ALA:HB1	16:T:91:GLN:OE1	2.20	0.41
16:T:122:GLU:HA	16:T:126:ARG:HH11	1.84	0.41
18:Y:-4:DC:H2''	18:Y:-3:DA:C8	2.55	0.41
5:f:336:LEU:HD12	5:f:336:LEU:HA	1.88	0.41
22:o:140:ARG:HH12	22:o:235:VAL:HA	1.85	0.41
22:o:1158:LEU:HD22	22:o:1309:MET:HE3	2.02	0.41
23:p:847:LYS:NZ	23:p:864:ASP:OD2	2.43	0.41
26:s:48:PRO:HA	26:s:53:PRO:HG2	2.03	0.41
2:B:749:LEU:HA	2:B:752:THR:HG22	2.03	0.41
5:F:90:GLU:OE1	9:J:208:GLY:CA	2.69	0.41
5:F:90:GLU:O	5:F:92:ILE:N	2.54	0.41
10:L:106:ARG:CD	10:L:114:LYS:NZ	2.83	0.41
11:O:76:LEU:CB	11:O:79:VAL:HG21	2.35	0.41
13:Q:47:GLU:OE1	13:Q:60:HIS:CG	2.71	0.41
14:R:289:TYR:HA	14:R:292:ILE:HG12	2.03	0.41
17:X:-43:DA:H2''	17:X:-42:DG:C8	2.55	0.41
4:e:718:ARG:HD3	4:e:718:ARG:HA	1.77	0.41
5:f:220:GLN:H	5:f:220:GLN:HG2	1.72	0.41
22:o:1296:MET:HG2	22:o:1298:LEU:HG	2.01	0.41
23:p:502:HIS:CE1	23:p:504:THR:HG1	2.31	0.41
23:p:639:HIS:O	23:p:643:LEU:HB2	2.21	0.41
23:p:1021:HIS:HD2	23:p:1025:ASN:HB2	1.85	0.41
23:p:1119:CYS:SG	23:p:1121:LEU:HD23	2.61	0.41
28:u:120:ASP:OD1	28:u:120:ASP:N	2.42	0.41
1:A:638:PRO:HG3	6:G:39:LEU:HB3	2.03	0.41
1:A:794:PRO:O	1:A:795:ASN:C	2.64	0.41
2:B:885:ASP:HA	2:B:888:ILE:HG12	2.02	0.41
3:D:881:ARG:NH1	10:L:89:ASP:HA	2.35	0.41
13:Q:345:SER:O	13:Q:346:LYS:C	2.64	0.41
14:R:128:ILE:H	14:R:128:ILE:HG12	1.73	0.41
17:X:-4:DT:H2''	17:X:-3:DG:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:223:TYR:CD2	5:f:255:MET:HE1	2.52	0.41
5:f:402:ARG:HH22	5:f:403:ILE:HD12	1.85	0.41
20:k:130:PRO:HD3	21:m:35:GLU:HG2	2.02	0.41
22:o:200:ALA:N	22:o:214:ILE:O	2.54	0.41
22:o:355:MET:SD	22:o:355:MET:N	2.94	0.41
22:o:859:TYR:CE2	22:o:863:ARG:HD2	2.56	0.41
23:p:824:ASP:OD1	23:p:825:GLN:N	2.53	0.41
23:p:840:MET:HE2	23:p:891:ASP:OD2	2.20	0.41
1:A:502:LEU:O	5:F:208:LEU:HD22	2.21	0.41
1:A:620:LEU:HD11	1:A:766:ARG:HD3	2.02	0.41
1:A:1197:ILE:CD1	6:G:166:VAL:HG11	2.51	0.41
2:B:55:PRO:HB3	2:B:60:LEU:HD22	2.02	0.41
2:B:77:ILE:HG12	2:B:146:ILE:HG23	2.03	0.41
2:B:817:ARG:H	2:B:817:ARG:HG3	1.47	0.41
2:B:957:MET:O	2:B:968:ARG:NH1	2.53	0.41
3:D:995:GLU:H	3:D:995:GLU:HG3	1.66	0.41
4:E:615:ASP:CG	8:I:114:ARG:CB	2.76	0.41
5:F:126:PRO:CD	7:H:29:TYR:HA	2.51	0.41
5:F:374:TYR:CE1	5:F:422:HIS:HB3	2.56	0.41
6:G:74:MET:HE1	6:G:136:ILE:HD12	2.02	0.41
14:R:118:PHE:HA	14:R:121:ILE:HB	2.02	0.41
14:R:218:PHE:CD1	14:R:277:ILE:HG22	2.55	0.41
15:S:16:VAL:H	16:T:41:GLY:C	2.21	0.41
16:T:160:GLN:H	16:T:160:GLN:HG3	1.66	0.41
16:T:184:LEU:O	16:T:185:ASP:C	2.64	0.41
17:X:-22:DC:H2''	17:X:-21:DA:C8	2.56	0.41
17:X:-22:DC:N4	18:Y:22:DG:H1	2.18	0.41
17:X:-11:DT:H2''	17:X:-10:DA:C8	2.55	0.41
18:Y:-38:DC:H2''	18:Y:-37:DT:C6	2.56	0.41
22:o:448:ARG:NH1	22:o:451:CYS:SG	2.94	0.41
22:o:584:PRO:C	22:o:585:LEU:HD12	2.46	0.41
22:o:948:ILE:HG12	22:o:1007:ILE:HG21	2.02	0.41
22:o:1156:ASP:OD1	22:o:1156:ASP:C	2.64	0.41
22:o:1172:ASN:HD22	30:w:57:LYS:HE3	1.86	0.41
23:p:557:SER:HA	23:p:558:PRO:HD3	1.94	0.41
24:q:225:LYS:HG3	24:q:226:PRO:HD2	2.03	0.41
26:s:45:GLY:HA3	26:s:53:PRO:HD3	2.03	0.41
2:B:371:LYS:HA	2:B:371:LYS:HD3	1.87	0.41
5:F:233:GLY:CA	5:F:239:ARG:HE	2.34	0.41
7:H:87:GLN:HA	7:H:88:PRO:HD3	1.82	0.41
7:H:106:THR:CB	9:J:161:LYS:NZ	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:200:LEU:HD23	9:J:200:LEU:HA	1.95	0.41
13:Q:324:GLU:CD	13:Q:324:GLU:N	2.78	0.41
15:S:30:ALA:CB	16:T:93:LEU:HD23	2.50	0.41
4:e:620:LEU:HD13	8:i:104:LEU:HD22	2.03	0.41
22:o:689:ILE:CD1	23:p:985:LEU:HD22	2.51	0.41
22:o:1029:LEU:HD11	26:s:159:LEU:HD23	2.02	0.41
22:o:1375:ARG:NH1	22:o:1379:GLU:OE1	2.54	0.41
23:p:455:ASP:H	23:p:458:LYS:HB3	1.87	0.41
23:p:552:ASN:OD1	23:p:553:LEU:N	2.49	0.41
26:s:43:GLN:NE2	26:s:44:PHE:CZ	2.90	0.41
26:s:55:ARG:O	26:s:76:PHE:HB2	2.21	0.41
26:s:81:LYS:HA	26:s:109:GLY:O	2.21	0.41
1:A:725:CYS:SG	1:A:734:LEU:HD12	2.61	0.40
2:B:295:LEU:HD13	2:B:477:LEU:HD11	2.03	0.40
2:B:492:MET:HB2	2:B:492:MET:HE3	1.85	0.40
5:F:15:PRO:CD	8:I:14:LYS:HZ2	2.30	0.40
5:F:66:LEU:CD2	8:I:31:TYR:CB	2.79	0.40
5:F:295:LEU:H	5:F:295:LEU:HG	1.76	0.40
5:F:320:ARG:N	5:F:321:PRO:CD	2.83	0.40
5:F:350:ASN:O	5:F:354:ARG:NH1	2.54	0.40
13:Q:11:PRO:O	13:Q:15:ARG:HG2	2.21	0.40
18:Y:-17:DC:H2"	18:Y:-16:DA:C8	2.55	0.40
3:d:909:ARG:NH1	10:l:91:PHE:CE1	2.89	0.40
21:m:68:MET:HE3	21:m:68:MET:HB3	1.94	0.40
22:o:1428:MET:SD	22:o:1429:LYS:HG2	2.61	0.40
23:p:220:GLU:OE2	23:p:236:TRP:NE1	2.55	0.40
25:r:36:GLU:HA	25:r:39:MET:HE2	2.02	0.40
26:s:85:LYS:O	26:s:89:VAL:HG23	2.21	0.40
1:A:405:VAL:HB	5:F:302:HIS:HB3	2.03	0.40
1:A:511:LEU:N	1:A:511:LEU:HD13	2.36	0.40
2:B:267:HIS:HB3	2:B:277:LEU:HD11	2.04	0.40
4:E:564:ASP:OD1	4:E:564:ASP:N	2.51	0.40
5:F:65:LYS:HA	5:F:65:LYS:HD2	1.93	0.40
12:P:206:GLU:HB3	12:P:207:PRO:HD3	2.03	0.40
12:P:239:ARG:HB2	13:Q:314:LEU:CG	2.50	0.40
12:P:326:GLU:OE1	12:P:326:GLU:HA	2.21	0.40
13:Q:10:VAL:HG22	13:Q:366:ILE:HD11	2.02	0.40
13:Q:51:MET:HG2	13:Q:61:SER:HB3	0.90	0.40
15:S:18:VAL:O	16:T:38:GLY:C	2.64	0.40
16:T:187:LEU:HD23	16:T:187:LEU:HA	1.88	0.40
22:o:1068:LEU:O	22:o:1072:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:1164:THR:O	22:o:1298:LEU:HB2	2.21	0.40
22:o:1228:MET:SD	22:o:1255:LEU:HG	2.61	0.40
22:o:1428:MET:SD	22:o:1429:LYS:HE3	2.61	0.40
28:u:44:PHE:HZ	28:u:157:ILE:HB	1.85	0.40
28:u:60:GLN:NE2	28:u:65:PHE:HB2	2.36	0.40
30:w:60:HIS:O	30:w:60:HIS:ND1	2.54	0.40
2:B:102:ASN:OD1	2:B:102:ASN:N	2.54	0.40
3:D:965:ILE:HA	3:D:968:ARG:HD2	2.03	0.40
12:P:189:ASN:ND2	13:Q:376:TRP:CZ2	2.85	0.40
14:R:166:ILE:O	14:R:170:GLN:HG3	2.22	0.40
14:R:259:TYR:HD1	14:R:274:ILE:HD12	1.86	0.40
17:X:22:DG:N2	18:Y:-21:DG:N1	2.68	0.40
4:e:256:HIS:O	4:e:257:GLU:HB2	2.21	0.40
4:e:298:LEU:HD12	4:e:298:LEU:HA	1.98	0.40
22:o:102:LYS:O	22:o:106:VAL:HG13	2.22	0.40
22:o:635:LEU:HD12	22:o:635:LEU:HA	1.93	0.40
22:o:986:MET:HE2	22:o:1075:LYS:HD3	2.03	0.40
23:p:350:HIS:HD2	23:p:572:CYS:SG	2.45	0.40
26:s:193:ILE:HB	26:s:205:THR:HG23	2.03	0.40
33:z:15:MET:HB3	33:z:16:ILE:H	1.61	0.40
2:B:176:HIS:HE1	2:B:310:ASP:H	1.68	0.40
3:D:966:LEU:CD2	3:D:966:LEU:C	2.89	0.40
5:F:396:LEU:HA	5:F:399:GLU:CD	2.46	0.40
7:H:73:GLY:C	9:J:142:ALA:CB	2.94	0.40
16:T:124:TYR:CE1	23:p:596:ILE:HG21	2.56	0.40
17:X:-28:DC:H2''	17:X:-27:DT:H2'	2.03	0.40
5:f:83:LEU:HD11	8:i:42:PHE:HB2	2.03	0.40
22:o:486:LEU:HD21	23:p:790:GLN:HB2	2.04	0.40
22:o:1134:PRO:O	22:o:1137:PRO:HD3	2.22	0.40
22:o:1145:GLY:C	22:o:1147:SER:N	2.78	0.40
22:o:1486:ILE:HB	22:o:1487:PRO:HD3	2.03	0.40
1:A:659:GLY:N	2:B:475:LYS:HG2	2.35	0.40
2:B:180:CYS:HB2	2:B:313:TYR:HB2	2.04	0.40
2:B:937:THR:HG22	2:B:940:MET:HG3	2.03	0.40
5:F:214:HIS:CB	7:H:164:THR:HG21	2.51	0.40
5:F:396:LEU:HA	5:F:399:GLU:OE1	2.20	0.40
7:H:38:GLN:NE2	7:H:59:GLU:OE2	2.54	0.40
7:H:166:ARG:HA	7:H:166:ARG:HD2	1.87	0.40
11:O:6:TYR:CZ	11:O:48:LEU:CD1	3.05	0.40
15:S:8:SER:CB	16:T:48:THR:O	2.69	0.40
17:X:19:DG:H2''	17:X:20:DG:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:745:LEU:HD23	22:o:745:LEU:HA	1.85	0.40
22:o:1257:LEU:CD1	22:o:1259:ILE:HD11	2.51	0.40
23:p:214:LYS:HG3	23:p:215:TYR:CD1	2.57	0.40
23:p:968:ASN:OD1	23:p:969:PRO:HD2	2.21	0.40
23:p:980:HIS:O	23:p:980:HIS:ND1	2.55	0.40
28:u:81:LYS:HD2	28:u:148:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	584/1872 (31%)	544 (93%)	35 (6%)	5 (1%)	14	51
2	B	959/1199 (80%)	913 (95%)	46 (5%)	0	100	100
3	D	158/1085 (15%)	141 (89%)	17 (11%)	0	100	100
3	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
4	E	540/800 (68%)	503 (93%)	34 (6%)	3 (1%)	21	59
4	e	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
5	F	400/677 (59%)	373 (93%)	23 (6%)	4 (1%)	12	48
5	f	399/677 (59%)	377 (94%)	22 (6%)	0	100	100
6	G	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
7	H	207/310 (67%)	184 (89%)	19 (9%)	4 (2%)	6	32
8	I	118/264 (45%)	114 (97%)	4 (3%)	0	100	100
8	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
9	J	85/218 (39%)	82 (96%)	3 (4%)	0	100	100
9	j	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
10	L	74/161 (46%)	67 (90%)	7 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	l	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
11	O	95/109 (87%)	85 (90%)	7 (7%)	3 (3%)	3	21
12	P	175/339 (52%)	162 (93%)	11 (6%)	2 (1%)	11	46
13	Q	118/376 (31%)	110 (93%)	7 (6%)	1 (1%)	16	54
14	R	247/316 (78%)	235 (95%)	10 (4%)	2 (1%)	16	54
15	S	104/517 (20%)	102 (98%)	2 (2%)	0	100	100
16	T	218/249 (88%)	198 (91%)	15 (7%)	5 (2%)	5	28
19	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
20	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
21	m	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
22	o	1417/1970 (72%)	1306 (92%)	110 (8%)	1 (0%)	48	83
23	p	1128/1174 (96%)	1054 (93%)	74 (7%)	0	100	100
24	q	253/275 (92%)	226 (89%)	27 (11%)	0	100	100
25	r	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
26	s	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
27	t	77/127 (61%)	73 (95%)	4 (5%)	0	100	100
28	u	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
29	v	146/150 (97%)	133 (91%)	13 (9%)	0	100	100
30	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
31	x	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
32	y	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
33	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
All	All	9780/17897 (55%)	9122 (93%)	628 (6%)	30 (0%)	37	72

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1000	LEU
1	A	1158	SER
5	F	323	VAL
7	H	141	PRO
7	H	222	PRO
11	O	52	VAL
13	Q	320	VAL

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Mol	Chain	Res	Type
1	A	661	GLU
4	E	522	ASP
4	E	704	VAL
11	O	26	GLN
14	R	46	ILE
5	F	413	SER
12	P	207	PRO
16	T	173	GLY
16	T	231	ASN
5	F	64	GLN
5	F	439	ARG
11	O	84	VAL
16	T	226	LYS
22	o	583	ARG
1	A	640	LEU
7	H	134	LEU
7	H	164	THR
12	P	298	PRO
14	R	247	GLY
16	T	38	GLY
16	T	138	PRO
1	A	498	PRO
4	E	523	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	536/1665 (32%)	477 (89%)	59 (11%)	6	20
2	B	876/1083 (81%)	855 (98%)	21 (2%)	43	64
3	D	147/815 (18%)	113 (77%)	34 (23%)	1	5
3	d	146/815 (18%)	145 (99%)	1 (1%)	76	81
4	E	478/657 (73%)	475 (99%)	3 (1%)	78	83
4	e	475/657 (72%)	473 (100%)	2 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	320/574 (56%)	300 (94%)	20 (6%)	16	37
5	f	322/574 (56%)	310 (96%)	12 (4%)	30	51
6	G	133/322 (41%)	126 (95%)	7 (5%)	20	41
7	H	181/270 (67%)	170 (94%)	11 (6%)	17	38
8	I	106/235 (45%)	104 (98%)	2 (2%)	50	67
8	i	107/235 (46%)	107 (100%)	0	100	100
9	J	78/154 (51%)	78 (100%)	0	100	100
9	j	83/154 (54%)	83 (100%)	0	100	100
10	L	71/141 (50%)	67 (94%)	4 (6%)	19	40
10	l	98/141 (70%)	98 (100%)	0	100	100
11	O	84/98 (86%)	77 (92%)	7 (8%)	10	30
12	P	153/293 (52%)	134 (88%)	19 (12%)	4	16
13	Q	111/324 (34%)	108 (97%)	3 (3%)	39	61
14	R	213/268 (80%)	201 (94%)	12 (6%)	19	40
15	S	93/448 (21%)	92 (99%)	1 (1%)	65	76
16	T	196/218 (90%)	177 (90%)	19 (10%)	8	24
19	c	113/833 (14%)	111 (98%)	2 (2%)	51	68
20	k	87/182 (48%)	87 (100%)	0	100	100
21	m	80/106 (76%)	79 (99%)	1 (1%)	61	74
22	o	1257/1748 (72%)	1248 (99%)	9 (1%)	76	81
23	p	993/1027 (97%)	990 (100%)	3 (0%)	86	86
24	q	234/252 (93%)	234 (100%)	0	100	100
25	r	106/126 (84%)	106 (100%)	0	100	100
26	s	191/192 (100%)	191 (100%)	0	100	100
27	t	69/111 (62%)	69 (100%)	0	100	100
28	u	147/153 (96%)	146 (99%)	1 (1%)	76	81
29	v	129/131 (98%)	129 (100%)	0	100	100
30	w	103/112 (92%)	103 (100%)	0	100	100
31	x	53/56 (95%)	53 (100%)	0	100	100
32	y	106/106 (100%)	106 (100%)	0	100	100
33	z	41/55 (74%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8716/15331 (57%)	8463 (97%)	253 (3%)	38 58

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	LEU
1	A	353	LEU
1	A	395	ASP
1	A	397	LEU
1	A	400	GLU
1	A	401	ASN
1	A	403	LEU
1	A	404	MET
1	A	408	LEU
1	A	410	TRP
1	A	411	GLU
1	A	415	ILE
1	A	416	TRP
1	A	417	ASP
1	A	419	GLU
1	A	475	LEU
1	A	481	GLU
1	A	491	MET
1	A	499	VAL
1	A	500	LEU
1	A	501	THR
1	A	502	LEU
1	A	505	ASN
1	A	511	LEU
1	A	641	LYS
1	A	644	LYS
1	A	645	LYS
1	A	646	LYS
1	A	648	LYS
1	A	649	MET
1	A	651	GLU
1	A	654	ARG
1	A	655	GLN
1	A	667	THR
1	A	685	GLU
1	A	711	ASP
1	A	727	THR

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Mol	Chain	Res	Type
1	A	730	PHE
1	A	797	LYS
1	A	798	ARG
1	A	828	GLU
1	A	854	ARG
1	A	925	ASP
1	A	943	LYS
1	A	970	ASN
1	A	971	LYS
1	A	994	ASP
1	A	995	LEU
1	A	1019	LYS
1	A	1020	LEU
1	A	1022	ARG
1	A	1026	ILE
1	A	1029	VAL
1	A	1052	ARG
1	A	1054	SER
1	A	1064	GLU
1	A	1069	ILE
1	A	1165	LEU
1	A	1203	GLU
2	B	21	GLU
2	B	71	ARG
2	B	140	GLU
2	B	184	ASN
2	B	262	MET
2	B	266	THR
2	B	293	GLU
2	B	431	LEU
2	B	559	LYS
2	B	603	LYS
2	B	640	VAL
2	B	746	SER
2	B	771	VAL
2	B	816	VAL
2	B	817	ARG
2	B	818	THR
2	B	819	LEU
2	B	820	ASP
2	B	944	LEU
2	B	945	CYS

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Mol	Chain	Res	Type
2	B	987	LEU
3	D	873	LEU
3	D	893	GLU
3	D	929	LYS
3	D	932	ASP
3	D	933	ARG
3	D	936	GLN
3	D	938	SER
3	D	939	ASP
3	D	941	ARG
3	D	944	LEU
3	D	945	LYS
3	D	946	PHE
3	D	947	PHE
3	D	948	GLU
3	D	949	GLN
3	D	950	LEU
3	D	951	ASP
3	D	952	GLN
3	D	953	ILE
3	D	955	LYS
3	D	957	ARG
3	D	958	LYS
3	D	959	ASP
3	D	960	GLU
3	D	962	GLU
3	D	965	ILE
3	D	966	LEU
3	D	967	MET
3	D	968	ARG
3	D	998	GLN
3	D	1002	ARG
3	D	1003	ASP
3	D	1054	ARG
3	D	1056	THR
4	E	745	GLU
4	E	746	ASP
4	E	747	LEU
5	F	63	ARG
5	F	92	ILE
5	F	136	LEU
5	F	261	THR

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Mol	Chain	Res	Type
5	F	269	VAL
5	F	271	VAL
5	F	280	ILE
5	F	295	LEU
5	F	301	VAL
5	F	312	ILE
5	F	317	LEU
5	F	326	HIS
5	F	348	THR
5	F	354	ARG
5	F	397	GLN
5	F	406	VAL
5	F	408	ASP
5	F	411	VAL
5	F	415	ILE
5	F	427	LEU
6	G	41	ASP
6	G	129	LYS
6	G	131	ILE
6	G	143	VAL
6	G	181	TRP
6	G	182	GLU
6	G	183	ILE
7	H	115	GLN
7	H	132	LYS
7	H	135	THR
7	H	155	ASP
7	H	159	TYR
7	H	164	THR
7	H	203	LEU
7	H	205	LYS
7	H	217	ARG
7	H	219	PHE
7	H	221	ILE
8	I	78	ARG
8	I	90	ASP
10	L	66	LEU
10	L	75	GLN
10	L	79	ASP
10	L	86	GLN
11	O	24	GLN
11	O	52	VAL

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Mol	Chain	Res	Type
11	O	56	VAL
11	O	57	ASN
11	O	59	ARG
11	O	76	LEU
11	O	84	VAL
12	P	166	GLN
12	P	172	VAL
12	P	196	ARG
12	P	197	PHE
12	P	209	THR
12	P	221	CYS
12	P	252	ASP
12	P	268	ILE
12	P	269	ARG
12	P	274	VAL
12	P	278	GLN
12	P	286	GLU
12	P	300	ILE
12	P	306	VAL
12	P	309	LYS
12	P	312	LEU
12	P	313	THR
12	P	317	VAL
12	P	328	ILE
13	Q	13	LEU
13	Q	34	VAL
13	Q	364	ASP
14	R	31	ASP
14	R	39	LEU
14	R	40	VAL
14	R	41	VAL
14	R	44	ARG
14	R	45	VAL
14	R	46	ILE
14	R	114	MET
14	R	120	GLU
14	R	128	ILE
14	R	137	ARG
14	R	189	LYS
15	S	7	SER
16	T	85	LEU
16	T	134	GLU

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Mol	Chain	Res	Type
16	T	137	LYS
16	T	140	ARG
16	T	141	LEU
16	T	158	ASN
16	T	160	GLN
16	T	167	ARG
16	T	168	LYS
16	T	169	LYS
16	T	170	LYS
16	T	171	GLU
16	T	172	ASP
16	T	174	LYS
16	T	175	ARG
16	T	177	ARG
16	T	184	LEU
16	T	186	MET
16	T	211	VAL
19	c	24	ASP
19	c	106	VAL
3	d	888	LYS
4	e	546	VAL
4	e	579	VAL
5	f	253	TYR
5	f	261	THR
5	f	272	VAL
5	f	322	ASP
5	f	323	VAL
5	f	326	HIS
5	f	356	THR
5	f	366	GLU
5	f	408	ASP
5	f	411	VAL
5	f	412	LEU
5	f	421	ASP
21	m	31	LEU
22	o	192	ARG
22	o	579	ILE
22	o	581	LYS
22	o	883	ILE
22	o	1139	LEU
22	o	1420	ASN
22	o	1421	ARG

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Mol	Chain	Res	Type
22	o	1422	GLN
22	o	1423	ASP
23	p	438	ARG
23	p	841	ARG
23	p	914	GLU
28	u	101	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (172) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	ASN
1	A	489	GLN
1	A	569	ASN
1	A	590	GLN
1	A	630	GLN
1	A	637	GLN
1	A	693	GLN
1	A	702	ASN
1	A	795	ASN
1	A	860	ASN
1	A	896	GLN
1	A	1073	GLN
2	B	30	HIS
2	B	36	ASN
2	B	39	ASN
2	B	137	HIS
2	B	160	HIS
2	B	176	HIS
2	B	183	GLN
2	B	235	HIS
2	B	348	GLN
2	B	439	HIS
2	B	450	GLN
2	B	471	GLN
2	B	577	HIS
2	B	644	GLN
2	B	652	GLN
2	B	663	GLN
2	B	745	GLN
2	B	750	GLN
2	B	765	ASN
2	B	813	ASN

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Mol	Chain	Res	Type
2	B	864	ASN
2	B	882	HIS
2	B	908	GLN
2	B	912	ASN
2	B	963	HIS
3	D	875	GLN
3	D	912	ASN
3	D	925	ASN
3	D	936	GLN
3	D	943	GLN
3	D	981	GLN
3	D	1001	GLN
4	E	254	ASN
4	E	268	HIS
4	E	326	ASN
4	E	327	ASN
4	E	351	GLN
4	E	616	HIS
4	E	640	ASN
4	E	733	ASN
5	F	37	GLN
5	F	52	GLN
5	F	59	HIS
5	F	79	ASN
5	F	119	ASN
5	F	221	GLN
5	F	270	ASN
5	F	273	GLN
5	F	275	ASN
5	F	316	GLN
5	F	326	HIS
6	G	10	HIS
6	G	48	HIS
6	G	142	ASN
7	H	66	GLN
7	H	142	HIS
7	H	145	HIS
7	H	201	GLN
8	I	21	GLN
8	I	38	GLN
8	I	60	HIS
8	I	98	GLN

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Mol	Chain	Res	Type
9	J	160	GLN
9	J	173	HIS
9	J	210	ASN
10	L	105	HIS
10	L	117	GLN
11	O	8	ASN
11	O	13	ASN
11	O	27	GLN
11	O	31	GLN
11	O	57	ASN
12	P	167	ASN
12	P	189	ASN
12	P	193	ASN
13	Q	60	HIS
13	Q	352	HIS
13	Q	361	ASN
14	R	116	ASN
14	R	229	GLN
16	T	86	GLN
16	T	158	ASN
16	T	181	GLN
16	T	182	HIS
19	c	27	GLN
19	c	50	HIS
3	d	912	ASN
4	e	223	HIS
4	e	256	HIS
4	e	320	HIS
4	e	368	ASN
4	e	424	GLN
4	e	660	ASN
4	e	733	ASN
5	f	30	GLN
5	f	64	GLN
5	f	119	ASN
5	f	134	HIS
5	f	325	ASN
8	i	38	GLN
8	i	60	HIS
8	i	81	GLN
9	j	210	ASN
20	k	186	HIS

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Mol	Chain	Res	Type
20	k	205	HIS
10	l	73	ASN
10	l	105	HIS
21	m	107	ASN
22	o	62	GLN
22	o	123	ASN
22	o	278	HIS
22	o	289	GLN
22	o	296	ASN
22	o	311	GLN
22	o	330	GLN
22	o	372	ASN
22	o	507	GLN
22	o	590	GLN
22	o	620	HIS
22	o	721	HIS
22	o	731	ASN
22	o	739	ASN
22	o	809	HIS
22	o	913	ASN
22	o	950	ASN
22	o	1005	HIS
22	o	1230	GLN
22	o	1248	ASN
22	o	1332	GLN
22	o	1445	HIS
22	o	1462	GLN
23	p	56	GLN
23	p	68	GLN
23	p	111	ASN
23	p	254	GLN
23	p	287	HIS
23	p	370	HIS
23	p	525	ASN
23	p	537	GLN
23	p	570	ASN
23	p	741	HIS
23	p	755	GLN
23	p	777	ASN
23	p	842	HIS
23	p	1021	HIS
23	p	1094	GLN

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Mol	Chain	Res	Type
23	p	1117	HIS
23	p	1120	ASN
23	p	1160	GLN
25	r	19	GLN
25	r	129	GLN
26	s	22	HIS
26	s	132	GLN
26	s	133	GLN
28	u	60	GLN
29	v	130	ASN
29	v	131	ASN
30	w	45	GLN
32	y	29	ASN
32	y	89	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

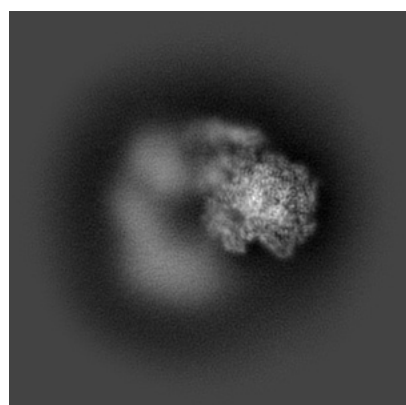
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31108. These allow visual inspection of the internal detail of the map and identification of artifacts.

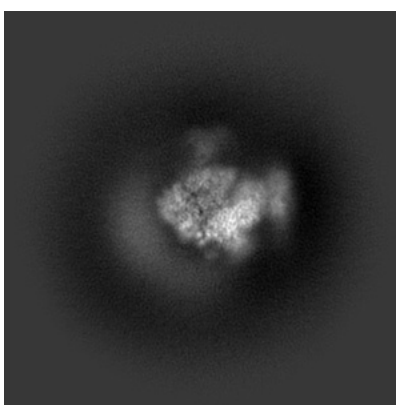
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

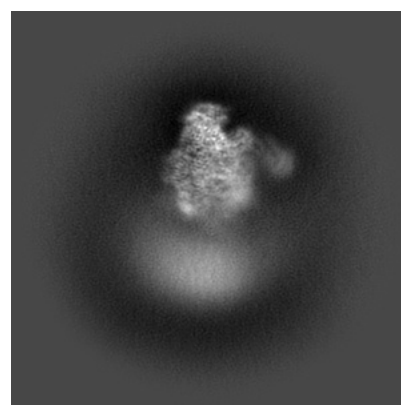
6.1.1 Primary map



X



Y

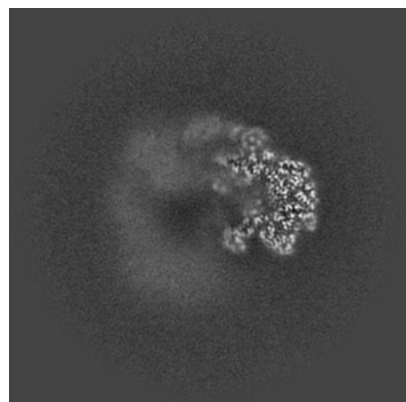


Z

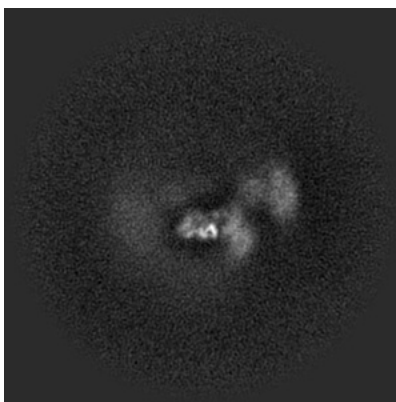
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

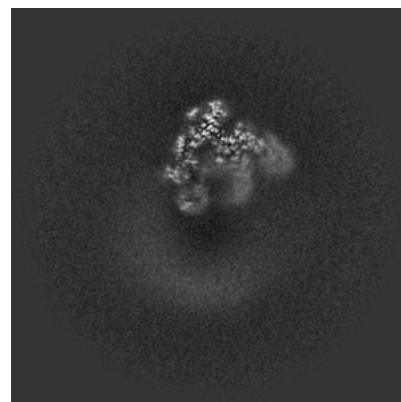
6.2.1 Primary map



X Index: 180



Y Index: 180

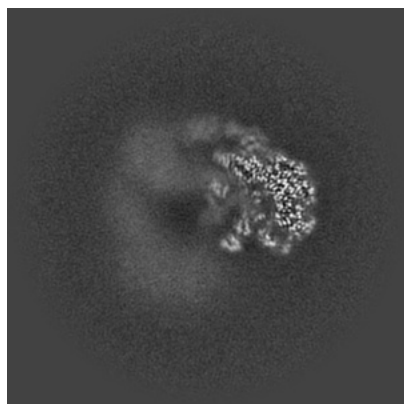


Z Index: 180

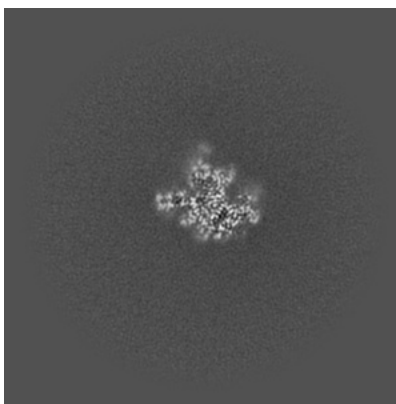
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

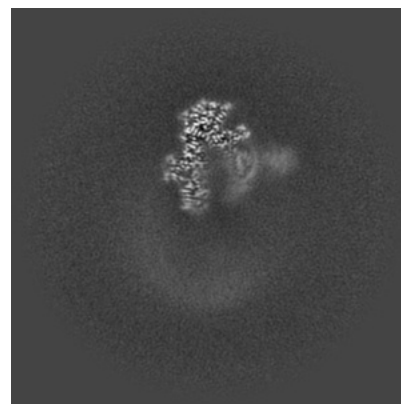
6.3.1 Primary map



X Index: 176



Y Index: 244

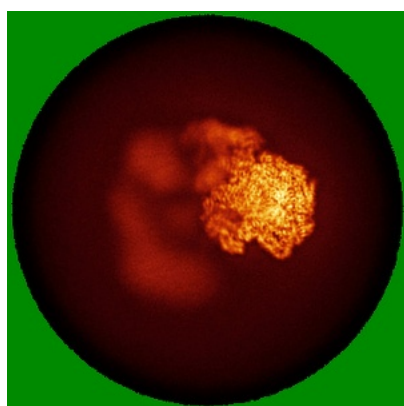


Z Index: 190

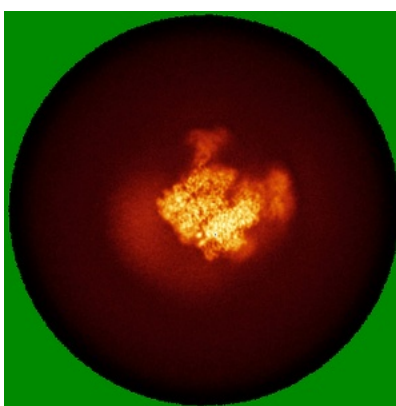
The images above show the largest variance slices of the map in three orthogonal directions.

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

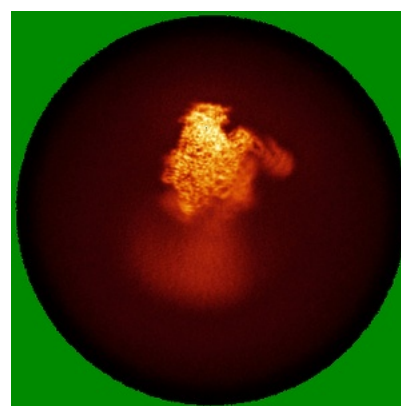
6.4.1 Primary map



X



Y

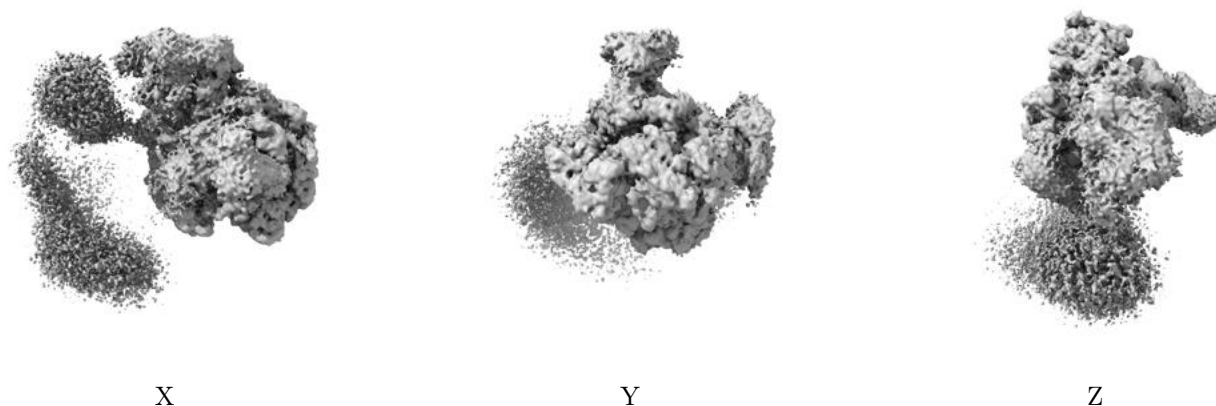


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

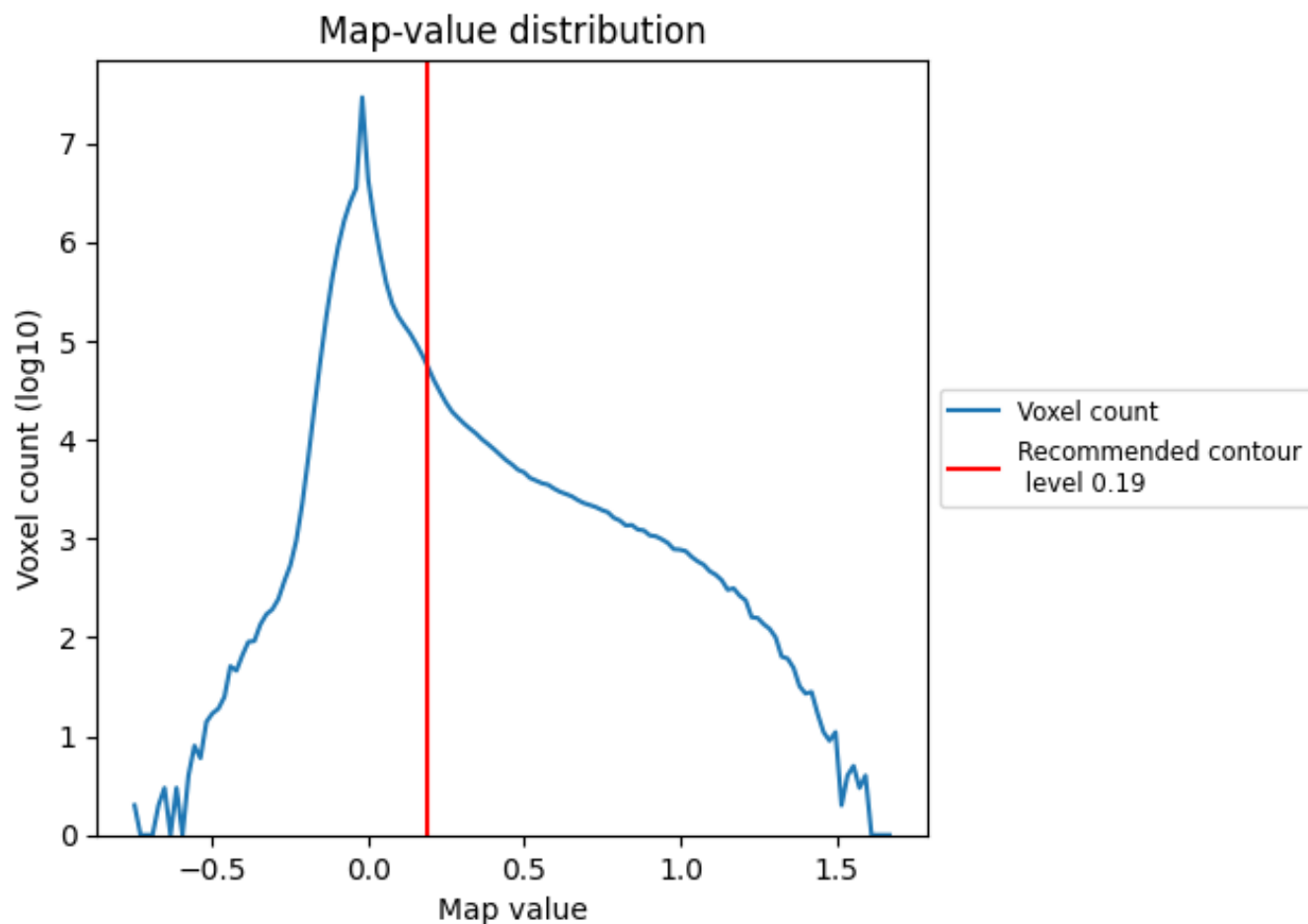
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

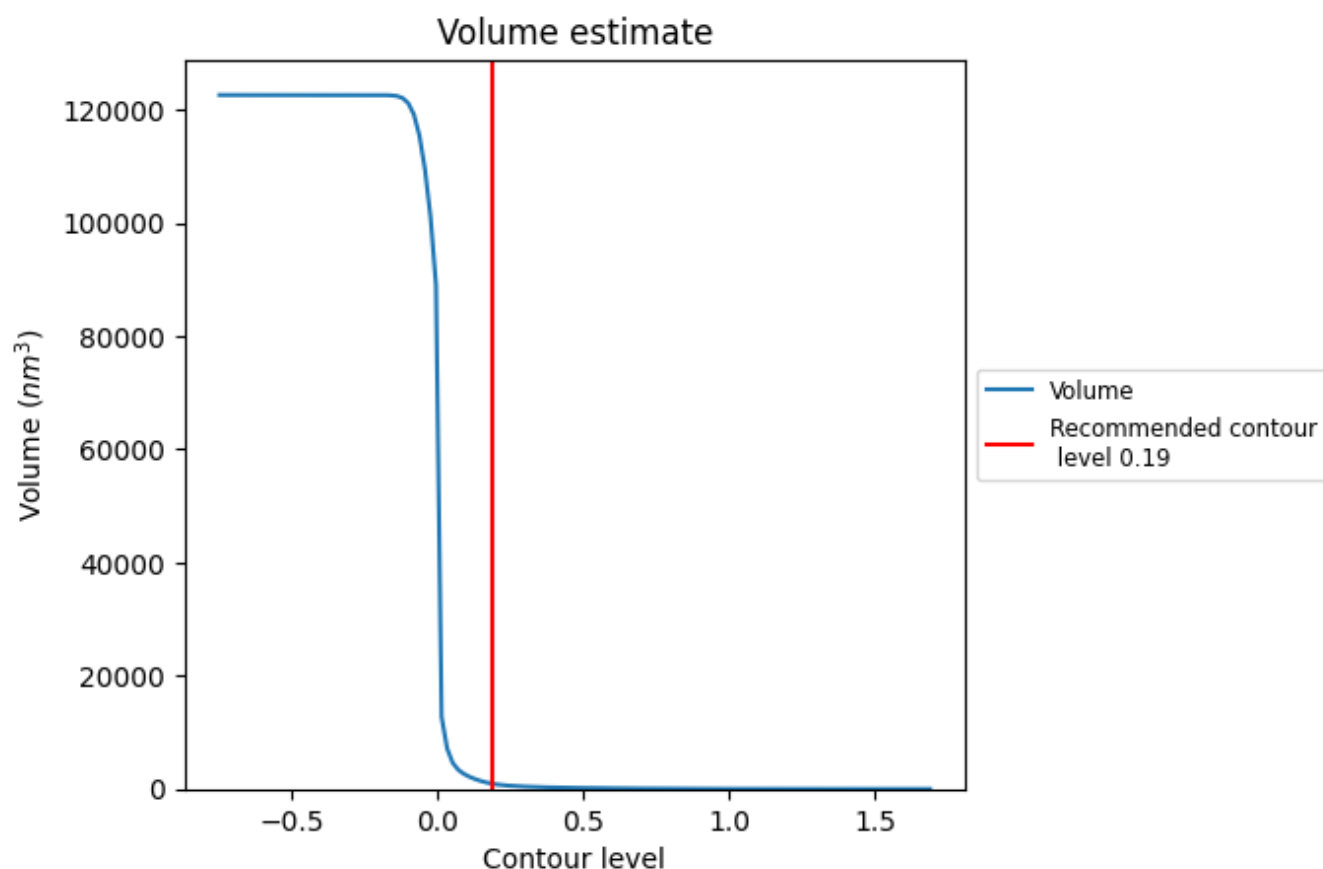
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

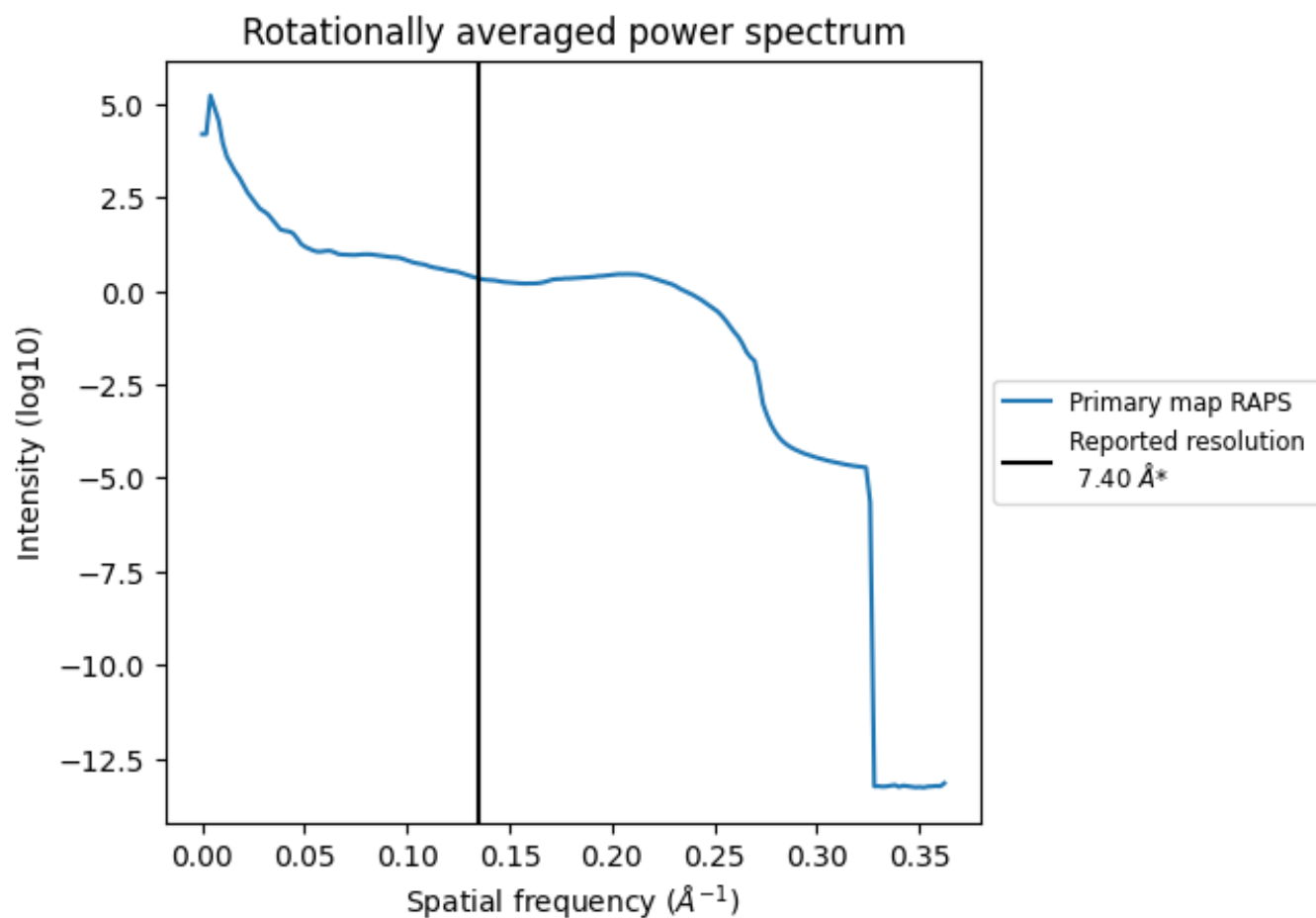
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 917 nm^3 ; this corresponds to an approximate mass of 828 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 0.135 Å⁻¹

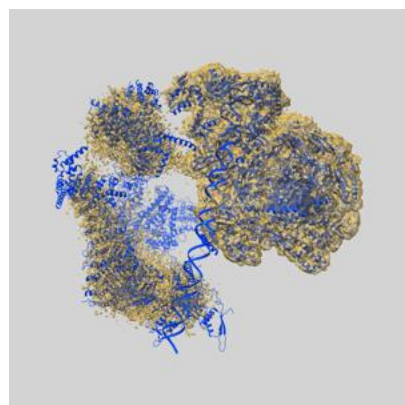
8 Fourier-Shell correlation

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

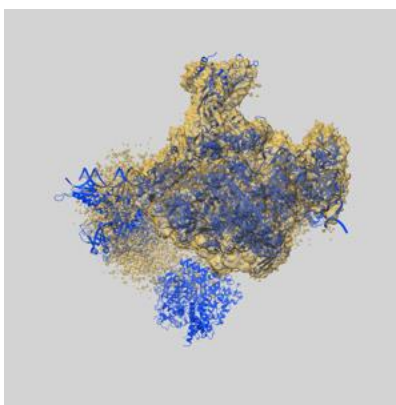
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31108 and PDB model 7EG8. Per-residue inclusion information can be found in section [3](#) on page [11](#).

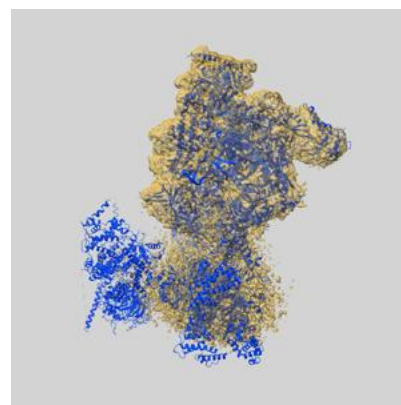
9.1 Map-model overlay [i](#)



X



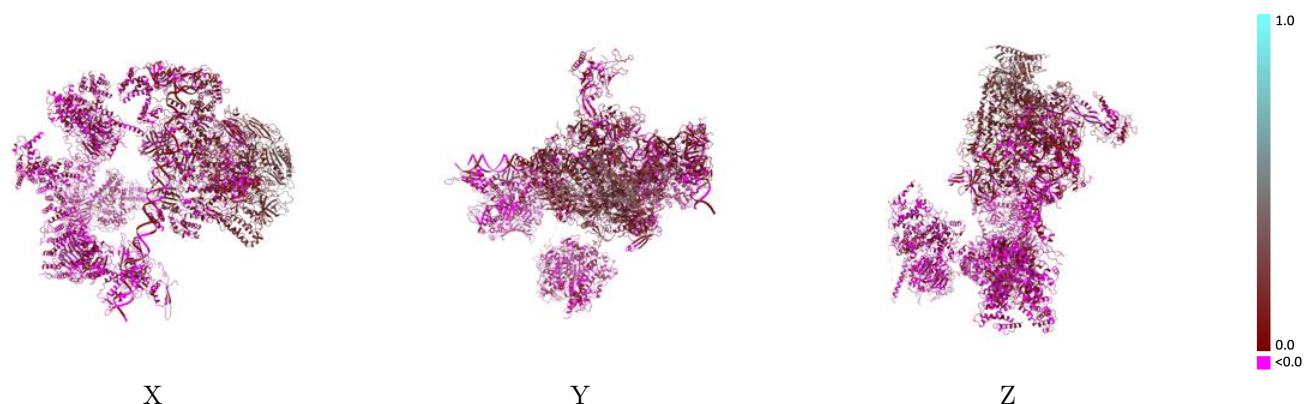
Y



Z

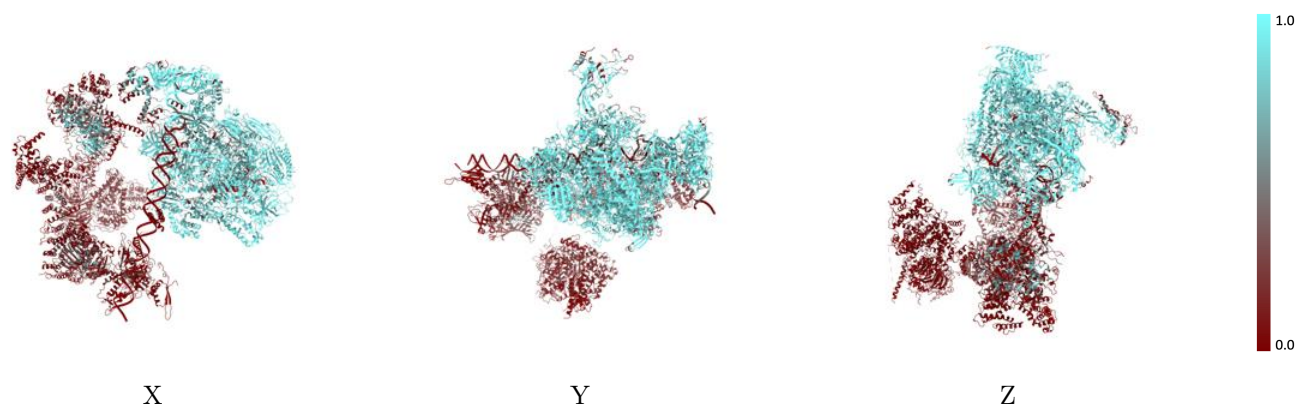
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



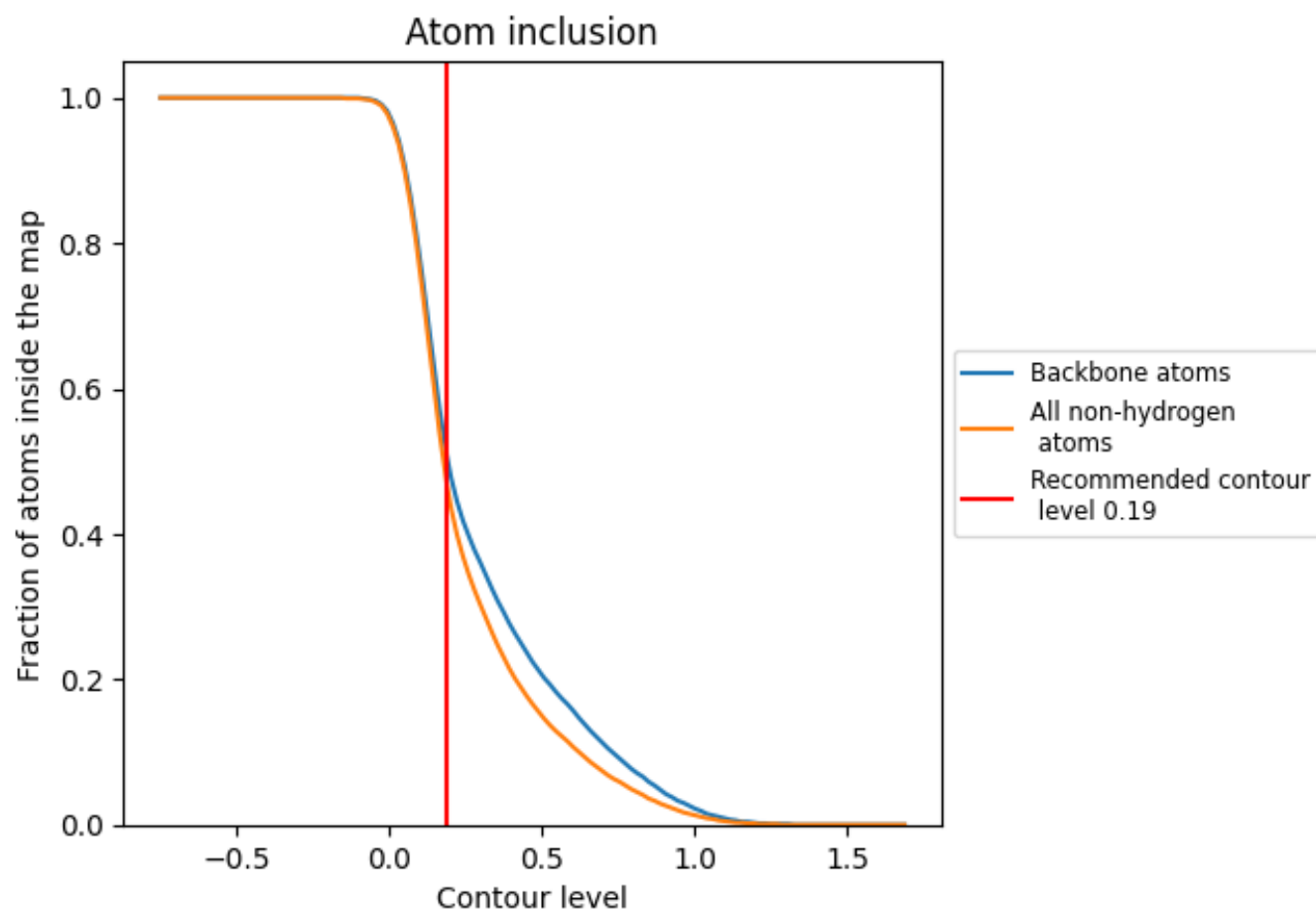
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 47% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4700	 0.0740
A	 0.0570	 -0.0030
B	 0.1580	 -0.0020
D	 0.1770	 0.0200
E	 0.4080	 0.0150
F	 0.1710	 0.0150
G	 0.0380	 0.0120
H	 0.2120	 0.0060
I	 0.3090	 0.0320
J	 0.3760	 0.0080
L	 0.0410	 0.0510
O	 0.7370	 0.0280
P	 0.9270	 0.0760
Q	 0.7070	 0.0260
R	 0.7950	 0.0950
S	 0.9090	 0.0710
T	 0.6790	 0.0610
X	 0.2470	 0.0420
Y	 0.2990	 0.0290
c	 0.0030	 -0.0170
d	 0.0000	 0.0130
e	 0.0070	 -0.0070
f	 0.0560	 0.0020
i	 0.0030	 0.0160
j	 0.0000	 0.0210
k	 0.0000	 -0.0100
l	 0.0010	 -0.0020
m	 0.0000	 -0.0130
o	 0.8420	 0.1510
p	 0.8460	 0.1660
q	 0.9570	 0.3080
r	 0.6830	 0.0570
s	 0.8600	 0.1060
t	 0.9290	 0.1960
u	 0.7780	 0.0630



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Chain	Atom inclusion	Q-score
v	 0.9500	 0.2600
w	 0.8880	 0.1830
x	 0.9310	 0.2950
y	 0.9290	 0.2800
z	 0.9580	 0.2160