



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:32 PM UTC

PDB ID : 9ESI / pdb_00009esi
EMDB ID : EMD-19942
Title : Structure of a B-state intermediate committed to discard (Bd-II state)
Authors : Soni, K.; Wild, K.; Sinning, I.
Deposited on : 2024-03-26
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

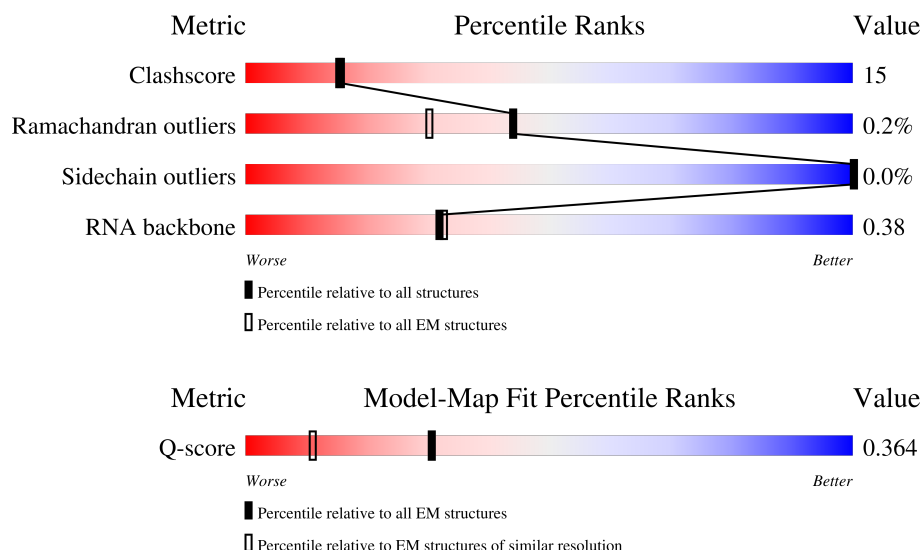
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	e	384	14% 34% 9% 57%
2	p	299	12% 13% 7% 80%
3	2	186	7% 5% 5% 87%

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Mol	Chain	Length	Quality of chain
4	5	120	
5	A	2363	
6	B	984	
7	C	340	
8	D	97	
9	E	147	
10	F	117	
11	G	115	
12	H	84	
13	I	78	
14	J	77	
15	K	473	
16	L	557	
17	M	354	
18	N	1284	
19	O	146	
20	P	388	
21	Q	265	
22	R	674	
23	S	488	
23	T	488	
23	U	488	
23	V	488	
24	W	757	
25	X	790	

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Mol	Chain	Length	Quality of chain
26	Y	229	
27	Z	187	
28	a	558	
29	b	293	
30	c	887	
31	d	155	
32	m	797	
33	n	361	
34	y	534	
35	z	647	
36	r	346	
37	q	56	
38	6	99	
39	1	29	
40	f	22	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 98220 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 Stress response protein bis1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	e	166	Total	C	N	O	S	0	0
			1329	838	221	268	2		

- Molecule 2 is a protein called Protein saf4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	p	60	Total	C	N	O	0	0
			487	304	89	94		

- Molecule 3 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	24	Total	C	N	O	P	0	0
			500	224	79	173	24		

- Molecule 4 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	102	Total	C	N	O	P	0	0
			2149	963	358	726	102		

- Molecule 5 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1986	Total	C	N	O	S	0	0
			16424	10532	2887	2938	67		

- Molecule 6 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	918	Total	C	N	O	S	0	0
			7298	4650	1251	1362	35		

- Molecule 7 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	301	Total	C	N	O	S	0	0
			2328	1460	415	442	11		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	96	Total	C	N	O	S	0	0
			760	470	147	136	7		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	97	Total	C	N	O	S	0	0
			726	462	129	130	5		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	81	Total	C	N	O	S	0	0
			638	407	109	118	4		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	102	Total	C	N	O	S	0	0
			819	516	150	149	4		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	80	Total	C	N	O	S	0	0
			652	422	113	115	2		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	73	Total	C	N	O	S	0	0
			574	373	95	104	2		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	73	Total	C	N	O	S	0	0
			573	366	98	108	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	391	Total	C	N	O	S	0	0
			3053	1925	551	563	14		

- Molecule 16 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	246	Total	C	N	O	S	0	0
			1954	1221	364	363	6		

- Molecule 17 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	234	Total	C	N	O	S	0	0
			1818	1131	329	343	15		

- Molecule 18 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	1284	Total	C	N	O	S	0	0
			10461	6715	1732	1969	45		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	144	Total	C	N	O	S	0	0
			1176	733	216	214	13		

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	271	Total	C	N	O	S	0	0
			2178	1354	397	416	11		

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	90	Total	C	N	O	S	0	0
			752	467	146	138	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	603	Total	C	N	O	S	0	0
			5108	3280	892	913	23		

- Molecule 23 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	132	Total	C	N	O	S	0	0
			1055	664	181	207	3		
23	T	134	Total	C	N	O	S	0	0
			1069	671	183	212	3		
23	U	430	Total	C	N	O	S	0	0
			2870	1806	492	563	9		
23	V	131	Total	C	N	O	S	0	0
			1044	655	180	206	3		

- Molecule 24 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	498	Total	C	N	O	S	0	0
			4126	2577	750	788	11		

- Molecule 25 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	654	Total	C	N	O	S	0	0
			5467	3534	918	996	19		

- Molecule 26 is a protein called Pre-mRNA-splicing factor syf2.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	98	Total	C	N	O	0	0
			845	522	157	166		

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	155	Total	C	N	O	S	0	0
			1232	766	220	243	3		

- Molecule 28 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	152	Total	C	N	O	S	0	0
			1035	644	185	205	1		

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	104	Total	C	N	O	S	0	0
			822	503	148	169	2		

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf22.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	204	Total	C	N	O	S	0	0
			1678	1071	280	315	12		

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase ppil.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	154	Total	C	N	O	S	0	0
			1179	750	202	223	4		

- Molecule 32 is a protein called G-patch domain-containing protein C1486.03.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	m	461	Total	C	N	O	S	0	0
			3813	2488	616	693	16		

- Molecule 33 is a protein called Uncharacterized protein C17A2.08c.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	n	30	Total	C	N	O	S	0	0
			248	153	44	50	1		

- Molecule 34 is a protein called Uncharacterized protein C20H4.06c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	y	200	Total	C	N	O	S	0	0
			1606	1000	279	323	4		

- Molecule 35 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	626	Total	C	N	O	S	0	0
			4980	3193	835	933	19		

- Molecule 36 is a protein called UNK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	r	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 37 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	q	56	Total	C	N	O	0	0
			295	182	57	56		

- Molecule 38 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	6	92	Total	C	N	O	P	0	0
			1970	882	365	631	92		

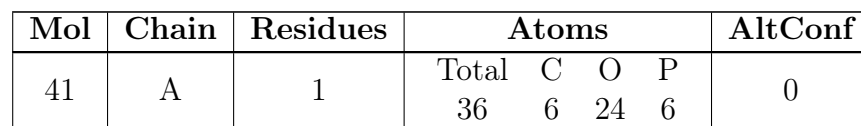
- Molecule 39 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1	29	Total	C	N	O	P	0	0
			605	272	91	213	29		

- Molecule 40 is a protein called UNK3.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	f	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).



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- The image displays the chemical structure of Guanosine Triphosphate (GTP). It consists of a guanine base (a purine ring system with an amino group at C2) linked to a ribose sugar, which is in turn linked to a chain of three phosphate groups. The structure is labeled with atom names (N1, N3, N7, C2, C4, C5, C6, C8, O6, O8, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100) and bond types (single, double, triple, aromatic, coordinate). The structure is shown in a 3D representation with wedge and dash bonds indicating stereochemistry.

Mol	Chain	Residues	Atoms					AltConf
42	B	1	Total 32	C 10	N 5	O 14	P 3	0

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- WORLD WIDE
PDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms		AltConf
43	B	1	Total 1	Mg 1	0
43	6	3	Total 3	Mg 3	0

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
44	M	2	Total 2	Zn 2	0
44	O	3	Total 3	Zn 3	0
44	P	1	Total 1	Zn 1	0

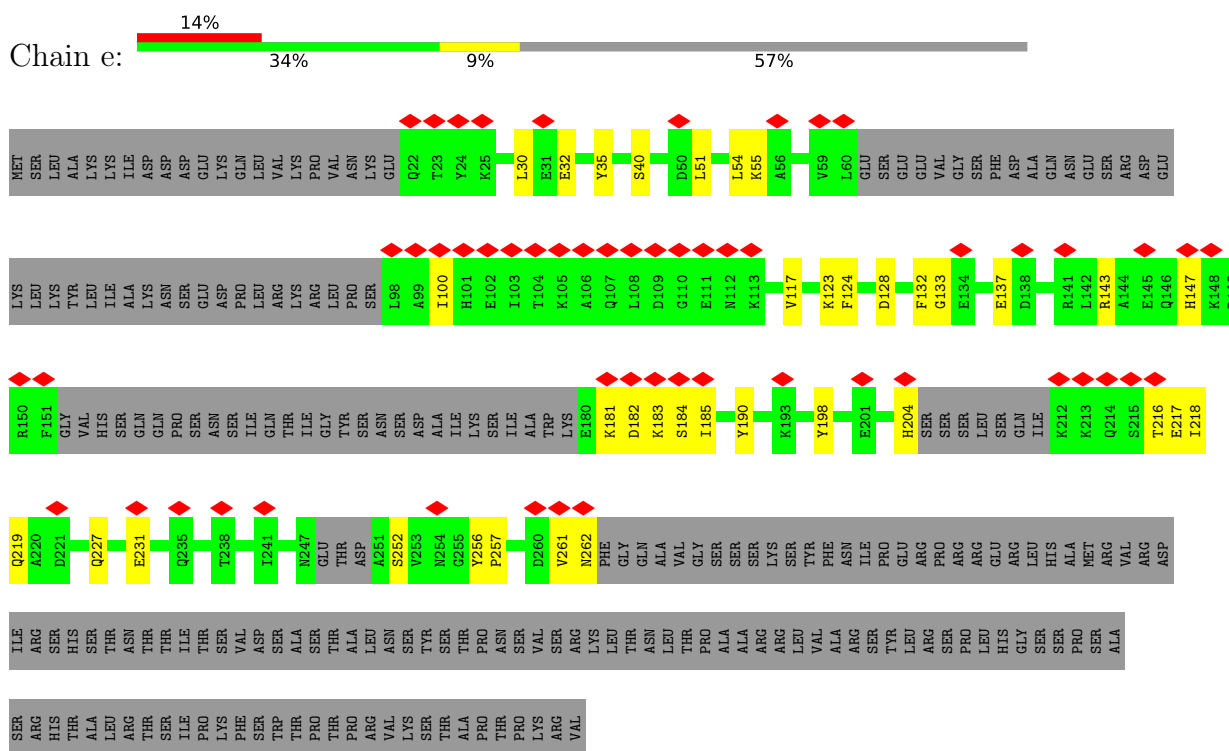
- Molecule 45 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
45	6	1	Total 1	K 1	0

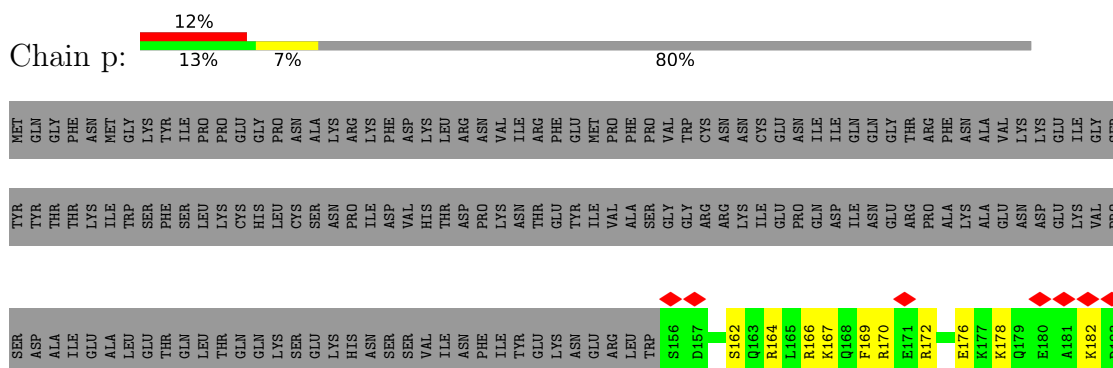
3 Residue-property plots

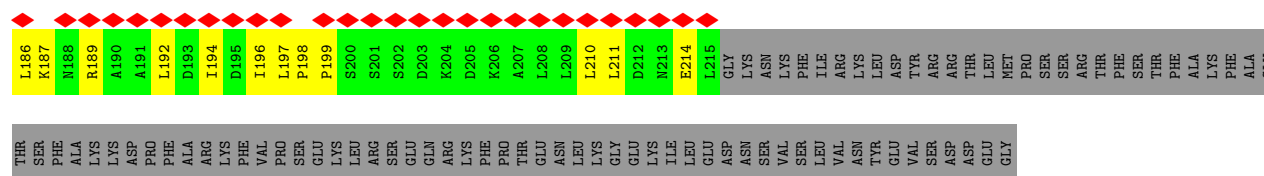
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Stress response protein bis1

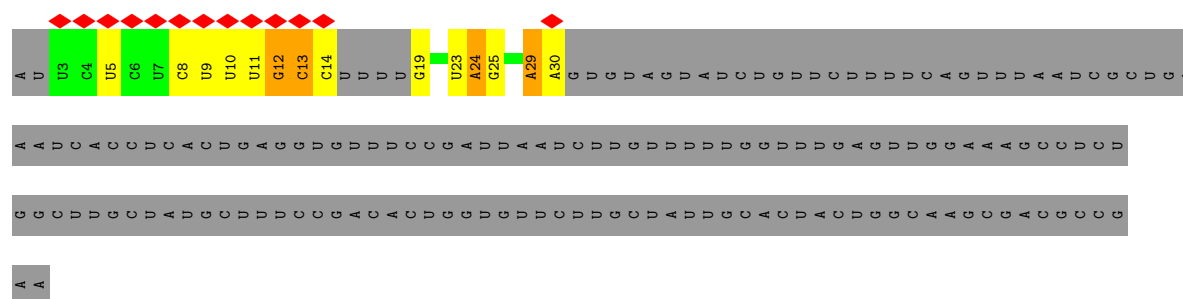


• Molecule 2: Protein saf4

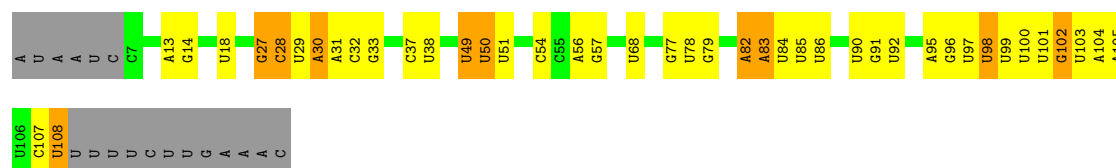




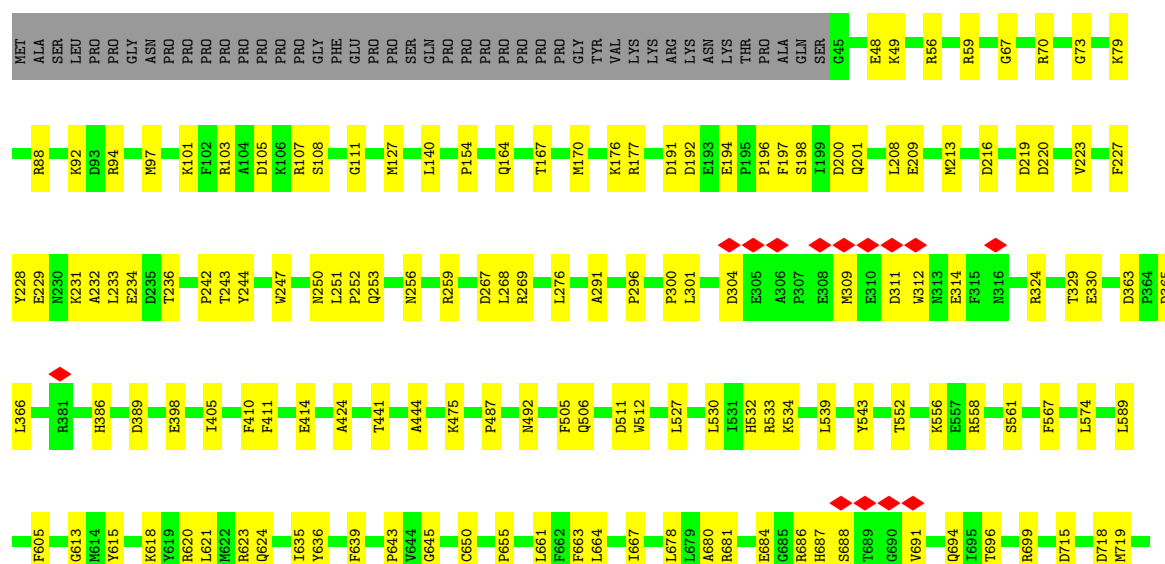
• Molecule 3: U2snRNA



• Molecule 4: U5snRNA

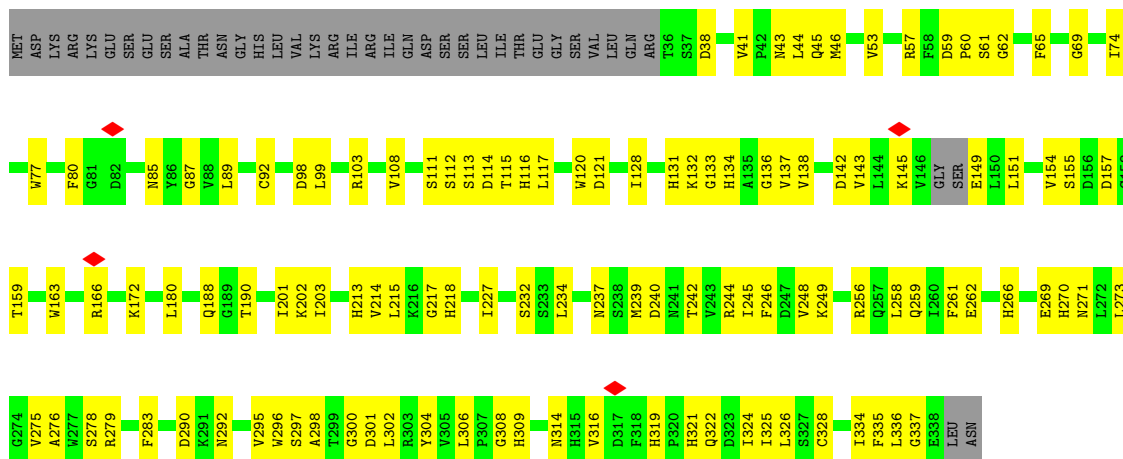


• Molecule 5: Pre-mRNA-splicing factor spp42



ILE	P1993	A1933	I1873	H1736	A1658	G1583	E1430	K1286	D1142	N984	K876	E722
GLU	N1994	T1934	R1874	S1737	Y1659	I1584	D1431	W1287	N1145	L986	G877	R725
LYS	L1995	E1935	S1875	A1738	K1660	M1586	E1432	L1291	N1150	T986	R878	Q726
GLY	D1996	P1936	L1876	W1661	W1661	H1587	D1434	M1295	K1153	D987	Q883	Q727
ARG	D1997	Q1937	P1877	N1662	N1662	G1588	S1435	T1296	K1153	V988	R884	K728
GLU	Q1998	P1937	P1878	S1663	S1663	G1588	W1436	Y1297	K1153	S1005	R885	I732
ASN	Q1999	V1939	P1879	R1665	R1665	T1592	D1437	Y1298	M1168	K1006	E886	I732
ALA	W2000	L1940	E1879	P1666	P1666	K1593	R1438	Y1299	R1176	V1011	H898	W746
GLN	L2001	F1941	E1880	L1669	L1669	L1594	G1439	E1300	R1176	L1016	I747	W746
THR	L2002	Q1881	Q1881	K1747	K1747	S1596	G1439	E1300	R1176	L1016	I747	P748
ALA	V2003	P1882	P1882	P1748	P1748	L1597	G1439	E1300	R1176	L1016	I747	P748
VAL	V2003	R1883	R1883	L1749	L1749	L1597	G1439	E1300	R1176	L1016	I747	P748
THR	E2004	Q1884	Q1884	L1750	L1750	L1597	G1439	E1300	R1176	L1016	I747	P748
THR	P2005	L1885	L1885	Q1751	Q1751	L1597	G1439	E1300	R1176	L1016	I747	P748
LYS	P2006	K1886	K1886	Q1752	Q1752	L1597	G1439	E1300	R1176	L1016	I747	P748
THR	L2007	L1887	L1887	S1753	S1753	L1597	G1439	E1300	R1176	L1016	I747	P748
THR	L2007	W1947	W1947	W1754	W1754	L1597	G1439	E1300	R1176	L1016	I747	P748
ASN	R2008	L1948	L1948	M1757	M1757	L1597	G1439	E1300	R1176	L1016	I747	P748
VAL	D2009	Q1949	Q1949	N1678	N1678	L1597	G1439	E1300	R1176	L1016	I747	P748
HIS	L2010	S1950	S1950	T1679	T1679	L1597	G1439	E1300	R1176	L1016	I747	P748
GLY	L2011	V1951	V1951	P1762	P1762	L1597	G1439	E1300	R1176	L1016	I747	P748
ASP	L2012	G1891	G1891	A1763	A1763	L1597	G1439	E1300	R1176	L1016	I747	P748
MET	L2012	M1892	M1892	R1770	R1770	L1597	G1439	E1300	R1176	L1016	I747	P748
VAL	L2014	L1893	L1893	F1834	F1834	L1597	G1439	E1300	R1176	L1016	I747	P748
THR	Y2015	T1895	T1895	N1835	N1835	L1597	G1439	E1300	R1176	L1016	I747	P748
THR	A2016	P1896	P1896	P1836	P1836	L1597	G1439	E1300	R1176	L1016	I747	P748
THR	K2017	A1956	A1956	P1837	P1837	L1597	G1439	E1300	R1176	L1016	I747	P748
ALA	K2018	F1957	F1957	T1838	T1838	L1597	G1439	E1300	R1176	L1016	I747	P748
TYR	N2019	S1958	S1958	G1839	G1839	L1597	G1439	E1300	R1176	L1016	I747	P748
GLU	N2020	R1959	R1959	Q1840	Q1840	L1597	G1439	E1300	R1176	L1016	I747	P748
ASN	N2021	L1960	L1960	Y1786	Y1786	L1597	G1439	E1300	R1176	L1016	I747	P748
GLY	L2021	I1961	I1961	Y1787	Y1787	L1597	G1439	E1300	R1176	L1016	I747	P748
LYS	N2022	L1962	L1962	S1788	S1788	L1597	G1439	E1300	R1176	L1016	I747	P748
PHE	V2023	I1963	I1963	S1789	S1789	L1597	G1439	E1300	R1176	L1016	I747	P748
SER	A2024	L1964	L1964	N1791	N1791	L1597	G1439	E1300	R1176	L1016	I747	P748
LYS	S2025	A1965	A1965	Y1792	Y1792	L1597	G1439	E1300	R1176	L1016	I747	P748
THR	L2026	A1966	A1966	Y1793	Y1793	L1597	G1439	E1300	R1176	L1016	I747	P748
GLU	T2027	L1967	L1967	Y1711	Y1711	L1597	G1439	E1300	R1176	L1016	I747	P748
TRP	N2028	M1968	M1968	K1707	K1707	L1597	G1439	E1300	R1176	L1016	I747	P748
ARG	S2029	V1969	V1969	Y1714	Y1714	L1597	G1439	E1300	R1176	L1016	I747	P748
ASN	E2030	M1970	M1970	A1715	A1715	L1597	G1439	E1300	R1176	L1016	I747	P748
ALA	VAL	T1971	T1971	Q1716	Q1716	L1597	G1439	E1300	R1176	L1016	I747	P748
ILE	ARG	E1972	E1972	S1717	S1717	L1597	G1439	E1300	R1176	L1016	I747	P748
SER	ASP	L1973	L1973	M1718	M1718	L1597	G1439	E1300	R1176	L1016	I747	P748
SER	ILE	T1974	T1974	Y1719	Y1719	L1597	G1439	E1300	R1176	L1016	I747	P748
ILE	ILE	Q1914	Q1914	P1720	P1720	L1597	G1439	E1300	R1176	L1016	I747	P748
SER	LEU	L1915	L1915	S1721	S1721	L1597	G1439	E1300	R1176	L1016	I747	P748
LEU	PRO	P1916	P1916	P1722	P1722	L1597	G1439	E1300	R1176	L1016	I747	P748
GLY	LEU	L1976	L1976	T1723	T1723	L1597	G1439	E1300	R1176	L1016	I747	P748
LEU	MET	I1977	I1977	G1724	G1724	L1597	G1439	E1300	R1176	L1016	I747	P748
ARG	THR	L1978	L1978	W1725	W1725	L1597	G1439	E1300	R1176	L1016	I747	P748
THR	ILE	Q1918	Q1918	V1804	V1804	L1597	G1439	E1300	R1176	L1016	I747	P748
LYS	THR	A1919	A1919	I1727	I1727	L1597	G1439	E1300	R1176	L1016	I747	P748
ALA	ALA	I1920	I1920	D1805	D1805	L1597	G1439	E1300	R1176	L1016	I747	P748
PRO	PRO	P1980	P1980	D1806	D1806	L1597	G1439	E1300	R1176	L1016	I747	P748
SER	LEU	D1981	D1981	T1807	T1807	L1597	G1439	E1300	R1176	L1016	I747	P748
GLN	GLN	K1982	K1982	N1808	N1808	L1597	G1439	E1300	R1176	L1016	I747	P748
ARG	ARG	S1983	S1983	V1809	V1809	L1597	G1439	E1300	R1176	L1016	I747	P748
GLN	GLN	K1984	K1984	Y1810	Y1810	L1597	G1439	E1300	R1176	L1016	I747	P748
GLN	GLN	I1985	I1985	R1811	R1811	L1597	G1439	E1300	R1176	L1016	I747	P748
ILE	ALA	T1986	T1986	V1812	V1812	L1597	G1439	E1300	R1176	L1016	I747	P748
ALA	GLU	K1987	K1987			L1597	G1439	E1300	R1176	L1016	I747	P748
GLU		E1988	E1988			L1597	G1439	E1300	R1176	L1016	I747	P748
		N1989	N1989			L1597	G1439	E1300	R1176	L1016	I747	P748
		H1990	H1990			L1597	G1439	E1300	R1176	L1016	I747	P748
		V1991	V1991			L1597	G1439	E1300	R1176	L1016	I747	P748
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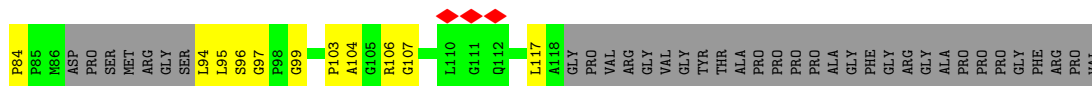
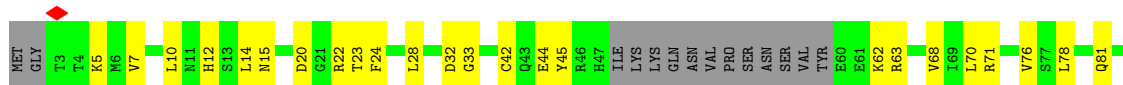




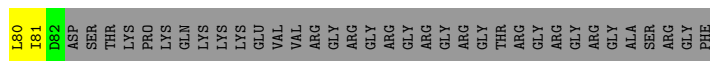
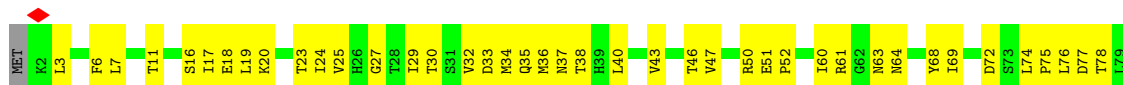
- Molecule 8: Small nuclear ribonucleoprotein Sm D3



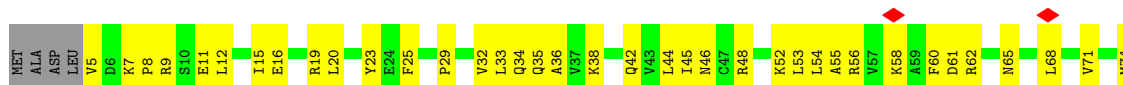
- Molecule 9: Small nuclear ribonucleoprotein-associated protein B

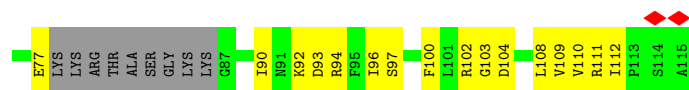


- Molecule 10: Small nuclear ribonucleoprotein Sm D1



- Molecule 11: Small nuclear ribonucleoprotein Sm D2





- Molecule 12: Small nuclear ribonucleoprotein E



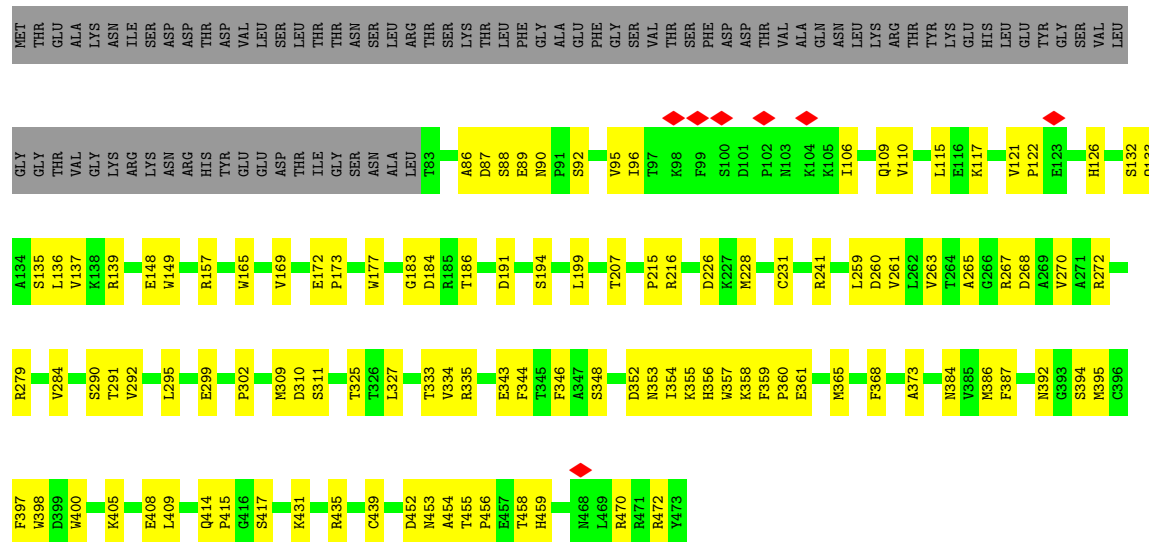
- Molecule 13: Small nuclear ribonucleoprotein F



- Molecule 14: Small nuclear ribonucleoprotein G



- Molecule 15: Pre-mRNA-splicing factor prp5



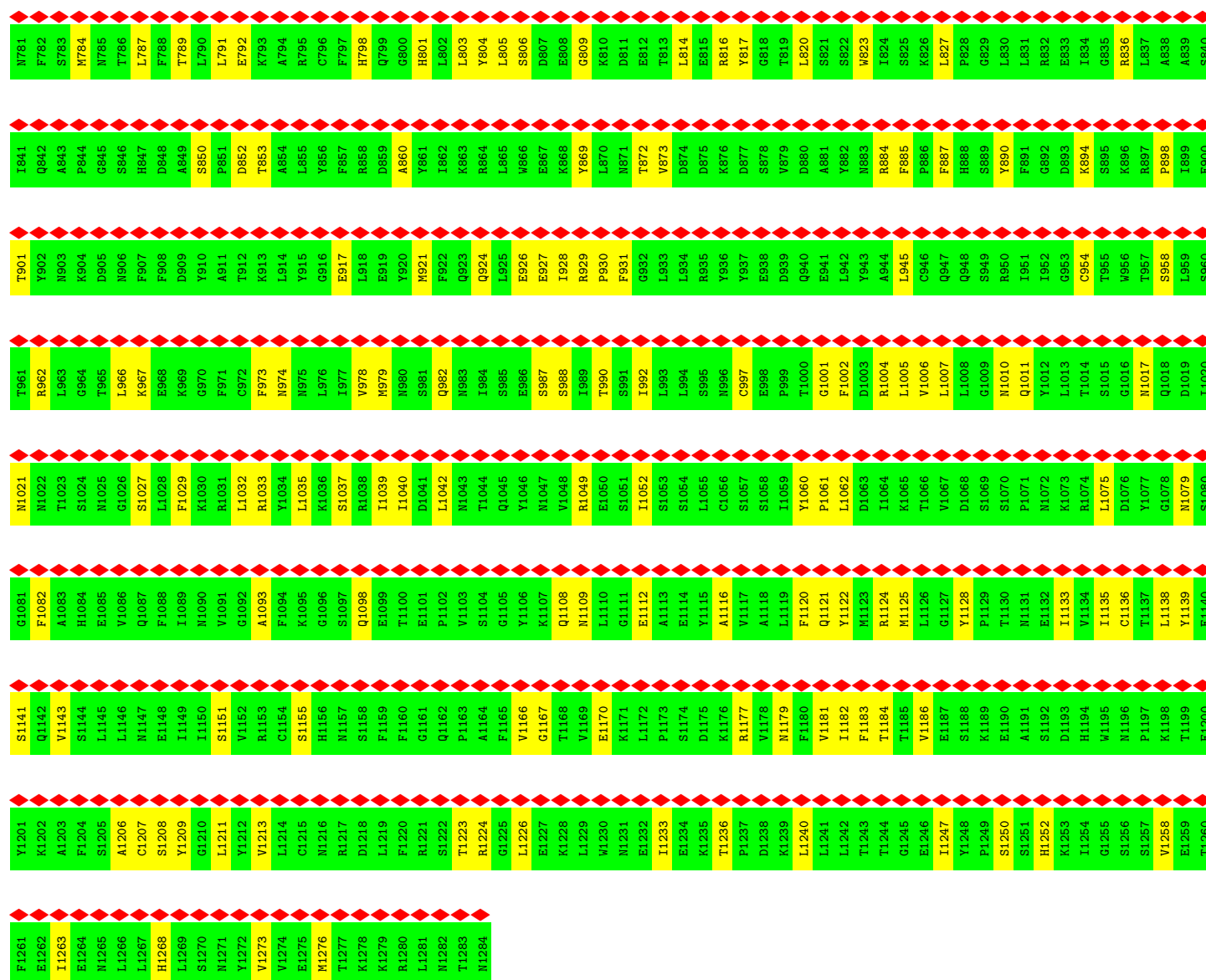
- Molecule 16: Pre-mRNA-processing protein 45



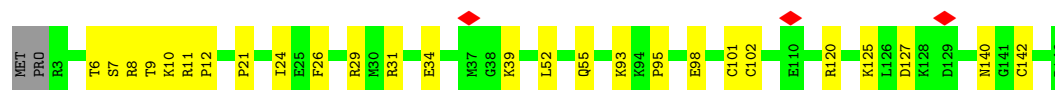
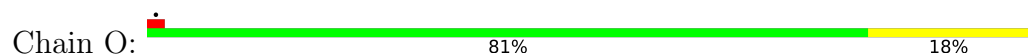
● Molecule 18: Pre-mRNA-splicing factor cwf11



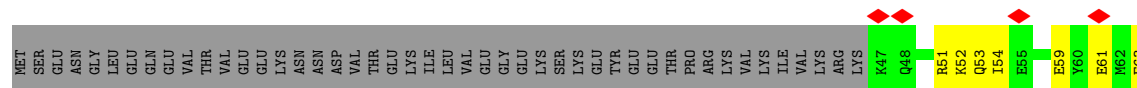
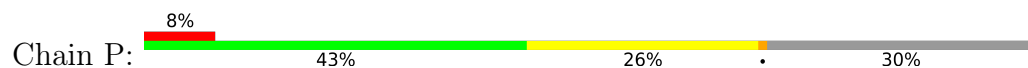
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R723	N663	P603	L543	F483	T423	F483	V303	H243	P183	M123	W63	L3
L724	S664	K604	H544	F484	A424	Y364	Y304	P244	S184	I124	Q64	Y4
Y725	T665	Q605	G545	V485	I425	A365	H305	V245	I185	Q125	R65	K5
T726	V666	L606	N546	T486	Q426	L366	L306	T246	V186	F126	V66	N6
Y727	A667	K607	A547	S487	Y427	K367	Q307	E247	E187	I127	N67	K7
N728	R668	F608	L548	V488	L428	V368	L308	D248	K188	T128	T68	K8
D729	N669	N609	D549	A489	S429	D369	T309	S249	F189	L129	E69	K9
K730	L670	F610	P550	P490	L430	F370	L310	C250	P190	C130	M70	Q10
Q731	F671	A611	L551	P491	S431	E371	F311	F251	F189	F131	S71	I11
L732	N672	L612	E552	Q492	F432	F372	S312	Y252	H192	Q132	L72	I12
E733	T673	V613	G553	L493	L373	L373	D313	T253	N193	F133	N73	N13
S734	V674	L614	V554	G494	H434	K374	F314	A254	L194	S134	H74	Y14
I735	E675	S615	T555	Q495	R435	N375	Q315	L255	L195	I75	I75	A15
L736	Q676	P616	D556	V496	Q436	V376	K316	R256	S196	N136	N76	N16
R737	L677	E617	F557	L497	Q437	F377	K316	M257	E197	L77	L77	S17
G738	Q678	A618	T558	P498	S438	I378	L318	S258	W198	K138	T78	N18
S739	S679	N619	T559	Q499	K439	N379	G319	L259	I199	L139	C79	W19
Q740	V680	K620	A560	F500	A440	T380	D320	Y260	H200	R140	M80	Q20
P741	L681	Y621	T561	V501	Y441	Y381	L321	Y261	S201	L81	Q21	Q21
G742	P682	W622	I562	K502	X442	D382	V322	D262	L202	L142	L82	N22
L743	N683	L623	C563	C503	F443	R383	F323	S263	L203	L142	L82	E23
T744	C684	D624	N564	Q504	L444	T384	C324	N264	I204	Y144	Y84	Q24
M745	H685	L625	D565	M505	L445	E265	T325	E265	K205	Q145	K85	V25
V746	V686	N626	D566	G506	L446	L386	Q326	L266	S206	L146	S86	E26
Y747	P687	L627	V567	L507	R447	V387	S328	F267	I207	T147	K87	F27
G748	S688	L628	G568	S508	S448	N388	S328	K268	S208	N148	Y88	Q28
P749	N689	W629	M569	R509	L449	D389	L329	K269	Y209	I149	E89	Q29
T750	L690	S630	F570	P510	Y450	Y390	Q330	M270	A210	S150	Y90	T30
R751	S691	L631	Q571	G511	A451	D391	Q331	T271	Q211	I151	I91	M31
G752	T692	L632	S572	P512	E452	E392	R332	D272	L152	L152	T92	L32
L753	N693	N633	D573	F513	L453	I393	Q333	D273	N153	W93	Q33	Q33
K754	S694	R634	M574	H514	L454	I394	K334	L274	K214	S154	D94	C34
H755	L695	A635	Q575	S515	N455	N395	L335	N275	Q215	L155	L95	I35
V756	L696	K636	S576	A516	F456	F396	E336	Y276	E216	D156	I96	L36
L757	P697	E637	S577	L517	S457	T397	E337	V277	A217	N157	D97	E37
G758	K698	F638	S578	R518	E458	L398	T338	L278	K218	L158	E98	A38
F699	P699	D579	D579	D519	Q459	K399	T339	K279	V219	D159	N99	V39
Y700	K760	N640	N580	L520	Y460	D400	S340	F280	T220	K160	R100	V40
T701	K641	W641	K581	K521	R461	V401	F341	P281	P221	V161	F101	I41
N702	L762	F642	S582	N522	R462	L402	L342	F282	L222	K162	Q102	S42
Q703	E643	T583	L583	S523	L463	S523	S343	D283	L223	Y163	L103	K43
W704	N584	D644	N584	L524	S464	E404	F344	N284	A224	L164	F104	D44
L705	K705	L645	V585	K525	L465	R405	N345	T285	I225	L165	F105	A45
I706	F646	F646	Y586	S526	K466	S406	S346	R286	I226	H166	E106	K46
S707	L647	P647	L587	P527	N467	V407	L347	G287	N227	D167	K107	Q47
A708	S588	S588	L587	F528	N467	M408	K348	N288	M228	S168	V108	V48
T709	F649	F649	T469	L529	T469	D409	S349	E289	S229	S169	I109	L49
W710	G650	G650	K470	C530	K470	Q410	L350	Y290	L230	S170	E110	S50
N711	T651	T651	N471	L531	N471	E411	C351	E291	V231	L171	V111	L51
D772	Y592	Y592	L472	I532	L472	N412	S352	K292	L232	T172	S112	L52
R773	H593	D653	T473	Y533	T473	S413	K353	E293	L233	K173	L113	H53
T774	S594	I654	K474	I534	K474	L414	C354	Q294	S234	A174	S114	E54
L775	R715	L595	D475	S535	D475	T415	Y355	K295	A235	F175	L115	L55
V776	H716	A596	N476	K536	N476	N416	L356	I296	F236	D176	N116	K56
G777	F717	P657	F477	N417	F477	Y417	R357	T297	P237	S177	L117	L57
L778	L178	L598	F478	H538	F478	F418	T358	N298	T238	Y178	S118	F58
S779	L719	N659	S479	E539	L419	L419	S359	D299	R239	K179	E119	E59
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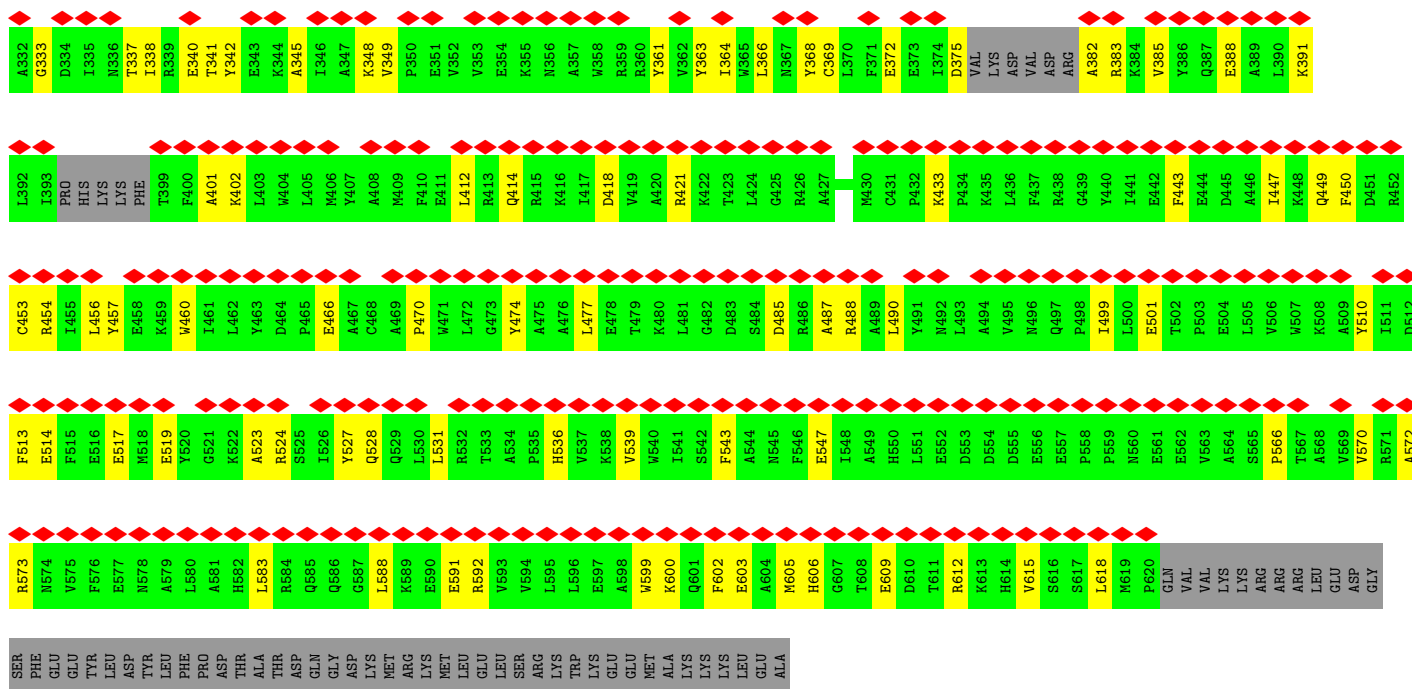
• Molecule 19: Pre-mRNA-splicing factor cwf14



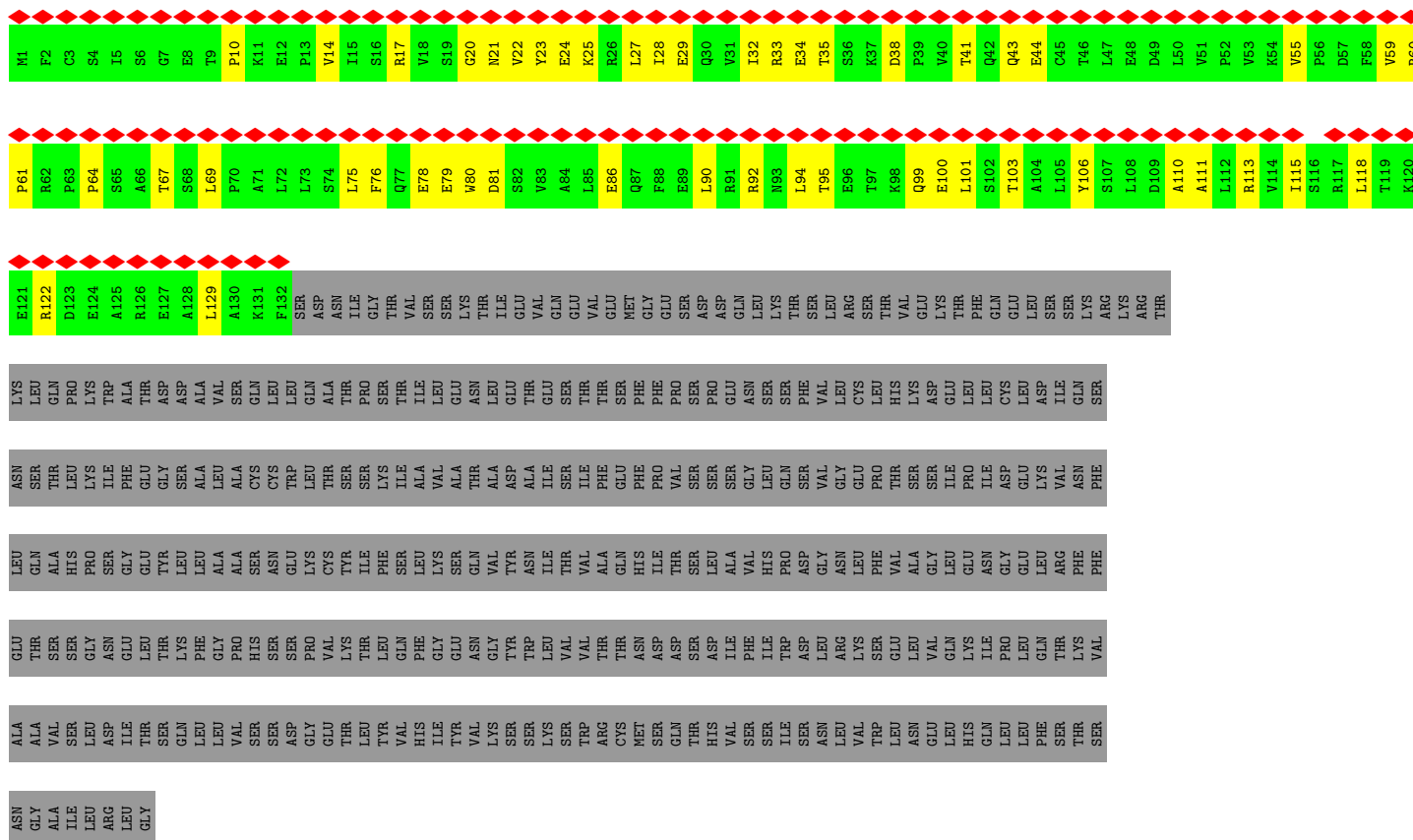
• Molecule 20: Pre-mRNA-splicing factor cwf2



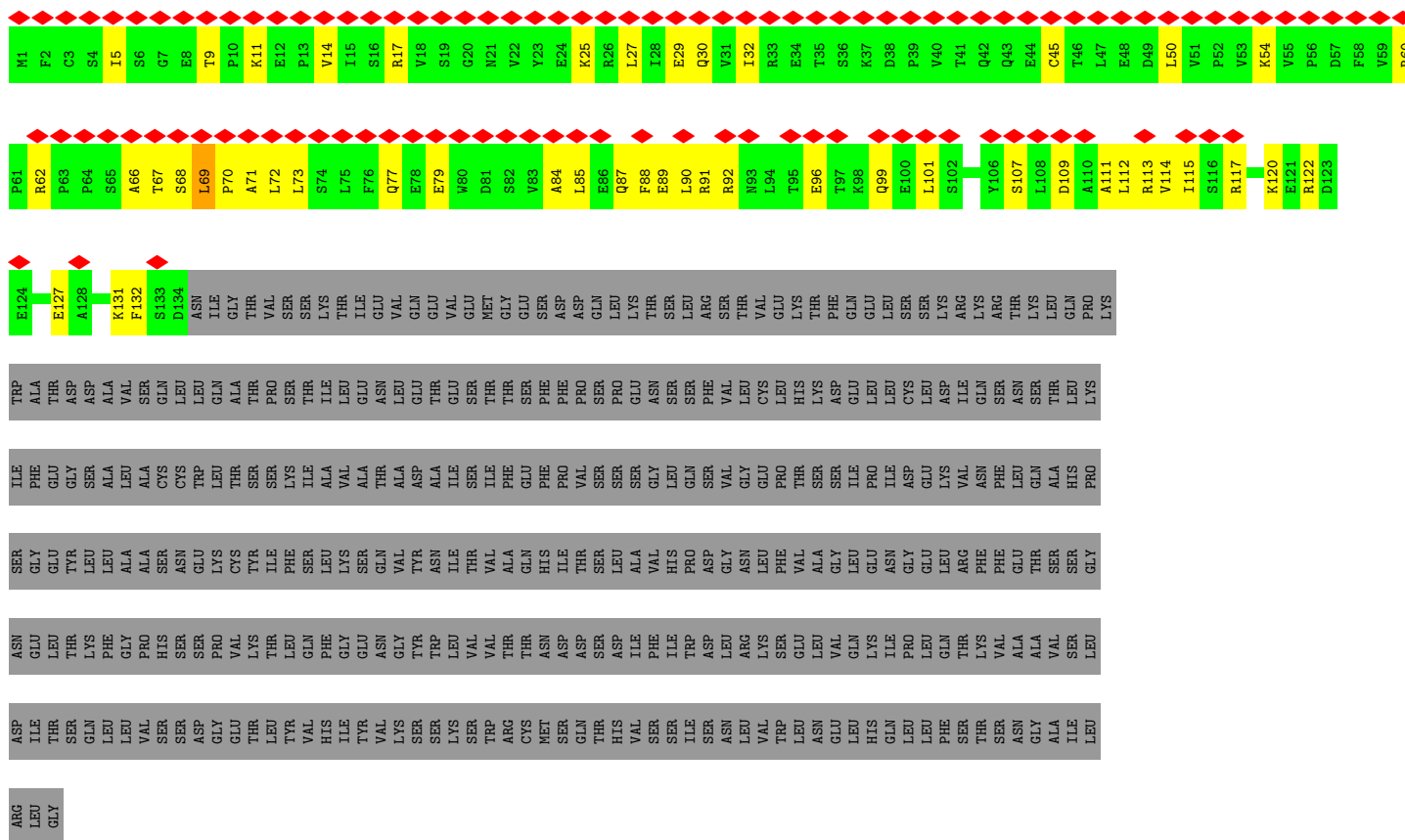




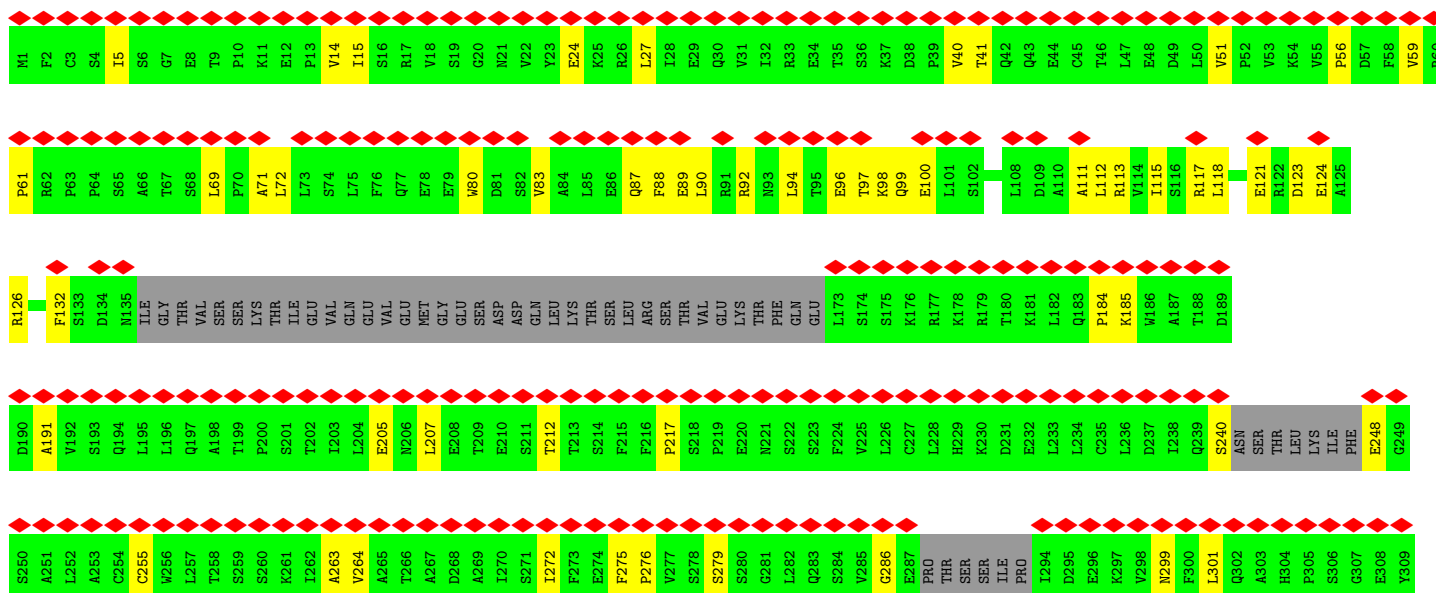
• Molecule 23: Pre-mRNA-processing factor 19



Chain T:

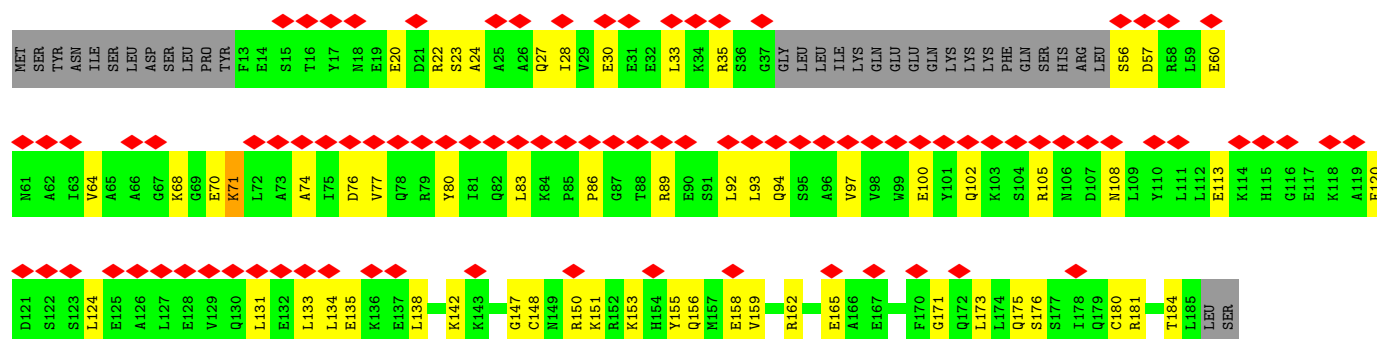


Chain U: 80% 68% 20%

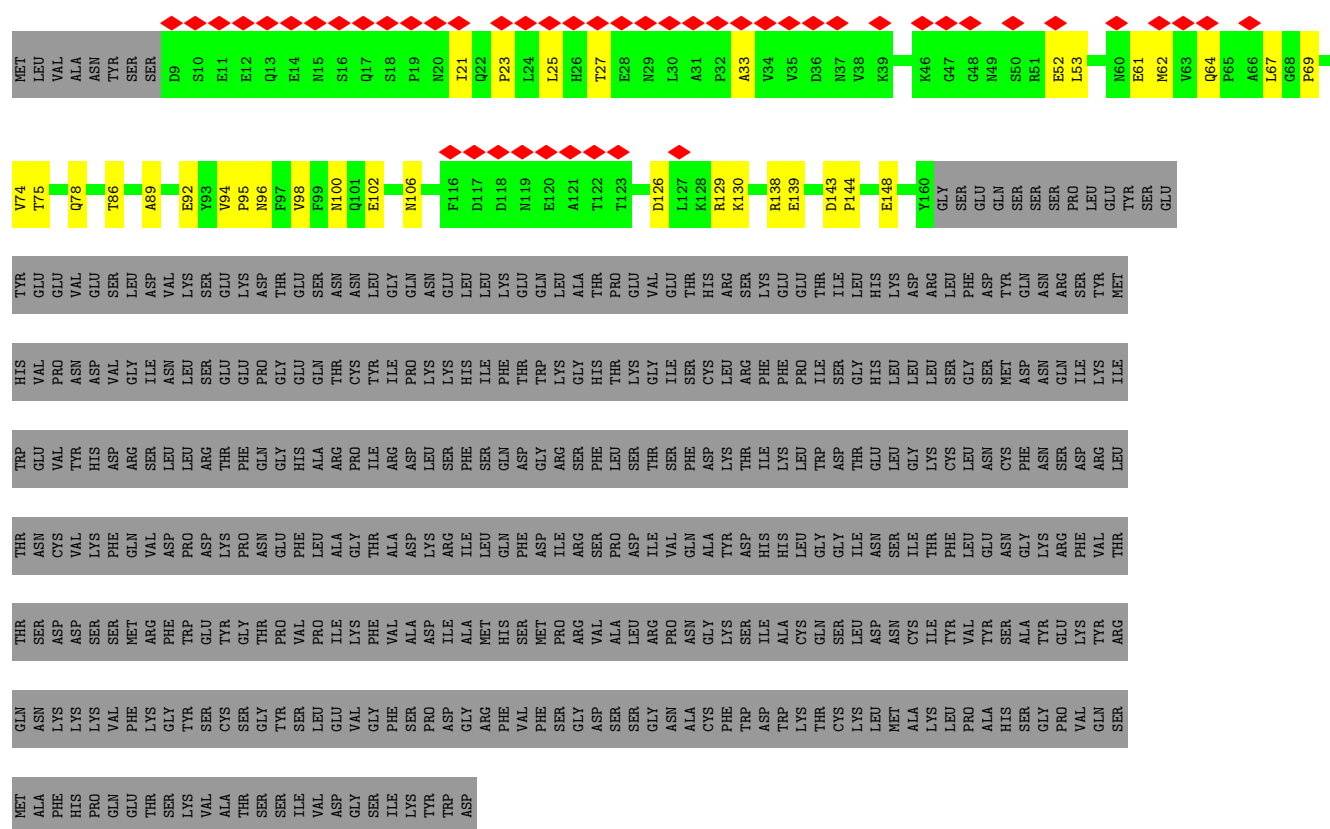




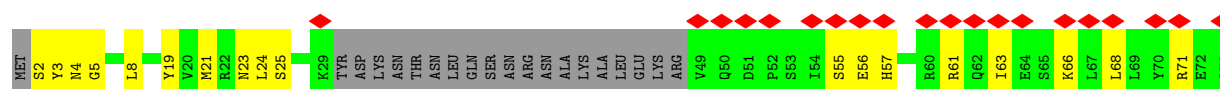


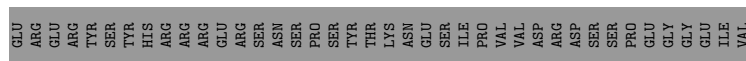


• Molecule 28: Pre-mRNA-processing factor 17



• Molecule 29: Pre-mRNA-splicing factor cwf21





ASP	LEU	SER	TYR	ASN	ARG	GLN	TYR	SER	PRO	VAL	LEU	GLY	ASP	ARG	ASN	SER	GLY	LEU	TYR	LYS	VAL	SER	ARG	LYS	ASN	GLU	SER	ASN	LEU	THR	TYR	LYS	ARG	LEU	THR	TYR	LYS	GLN	PRO	ALA	ASP
PRO	TRP	LEU	ARG	GLY	VAL	ASP	GLY	GLY	LEU	TYR	LYS	ASP	ARG	ASN	SER	GLY	LEU	TYR	LYS	VAL	SER	ARG	LYS	ASN	GLU	SER	ASN	LEU	THR	TYR	LYS	ARG	LEU	THR	TYR	LYS	GLN	PRO	ALA	ASP	

- Molecule 31: Peptidyl-prolyl cis-trans isomerase *ppi1*



- Molecule 32: G-patch domain-containing protein C1486.03



MET	GLN	ASN	GLU	TYR	VAL	ASP	MET	ASN	SER	SER	SER	GLU	ASP	SER	GLY	ASP	SER	ILE	LEU	GLU	GLY	GLY	ARG	LEU	ARG	ARG	PRO	SER	SER	PHE	ARG	GLY	GLN	GLN	LYS	GLU	GLU	ARG	ASP	ASP	MET	MET	LEU	GLY	ILE	PHE	GLY	GLU	GLU	GLU	GLU	ASP	GLU	ASP	GLY	PHE	HIS	ASN	SER	GLY	ILE	GLY	SER	ALA	ARG
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ASP GLU GLU HIS THR VAL LYS GLN LYS PRO PRO LEU ARG GLU LYS LYS LYS LYS PRO PRO LEU LYS SER SER SER GLU GLU ILE SER LYS ASP MET ASP GLY TYR ASN PRO ARG PHE LEU ALA SER SER LEU ASP THR LYS ILE ASP ALA SER LEU ASP THR LYS

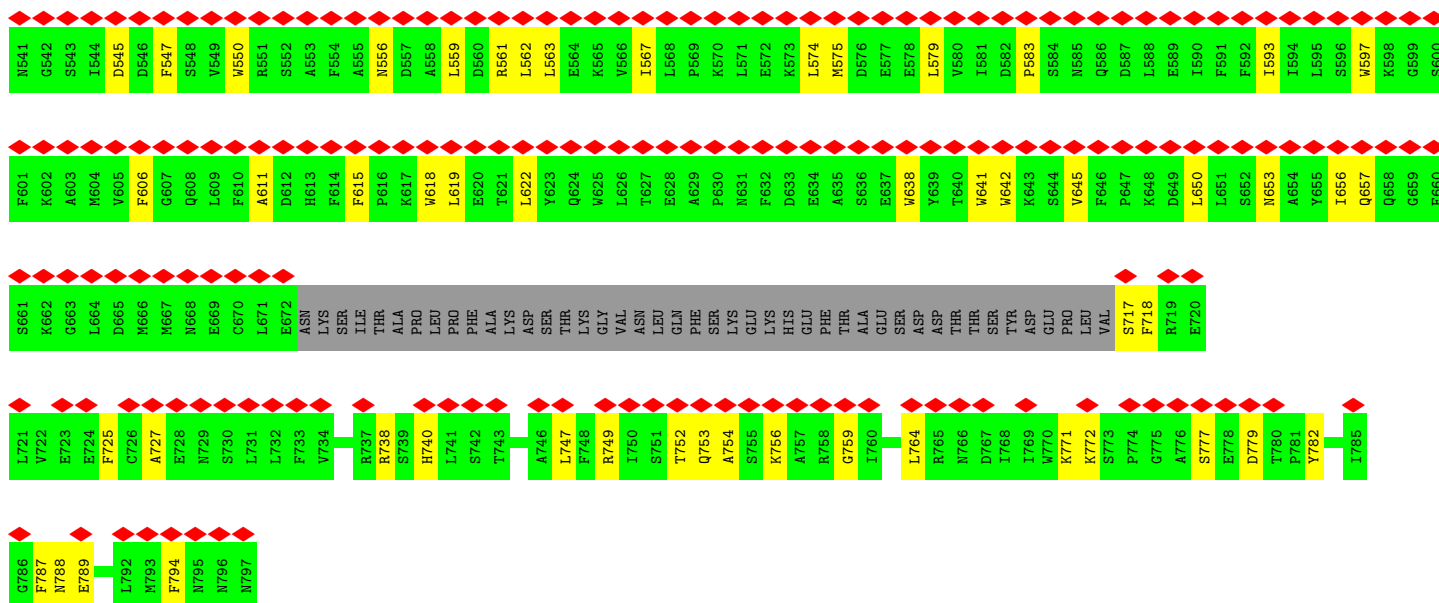
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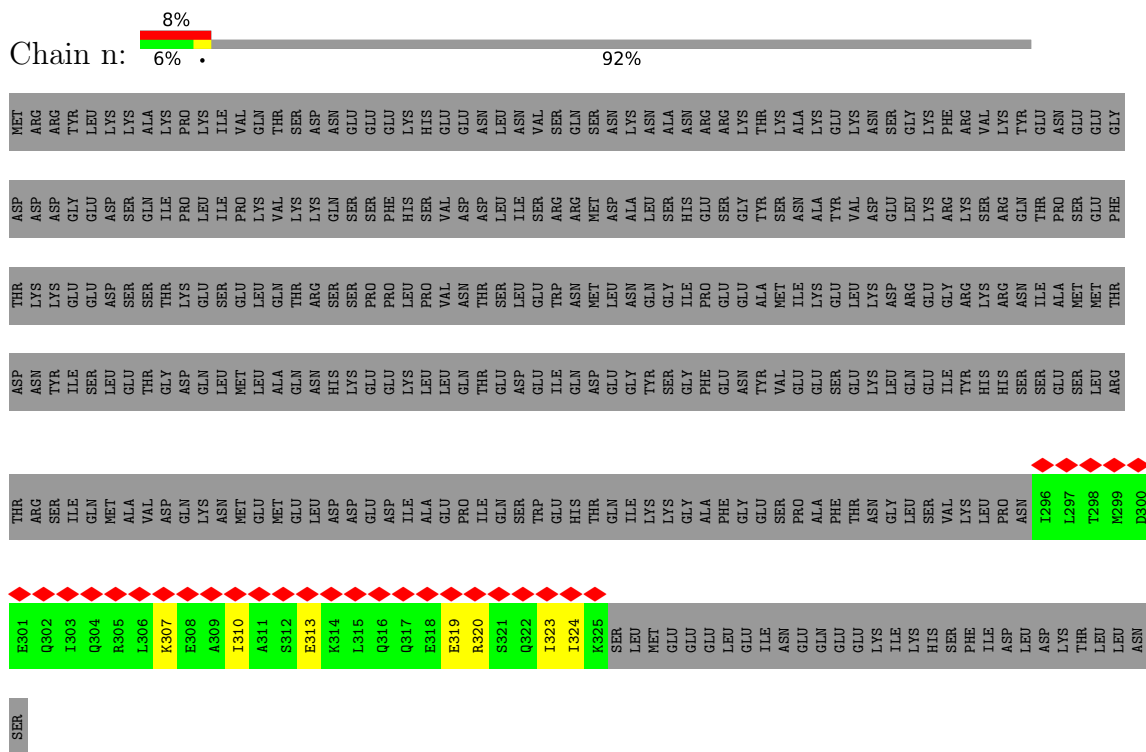
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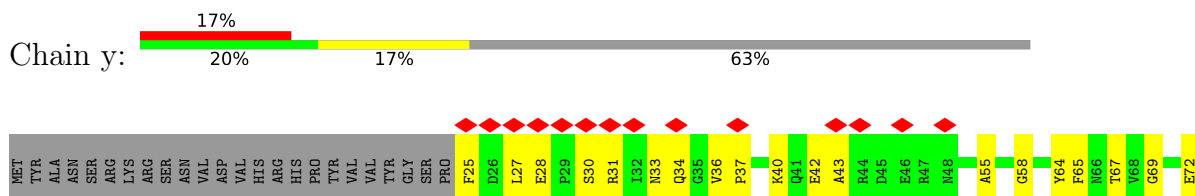
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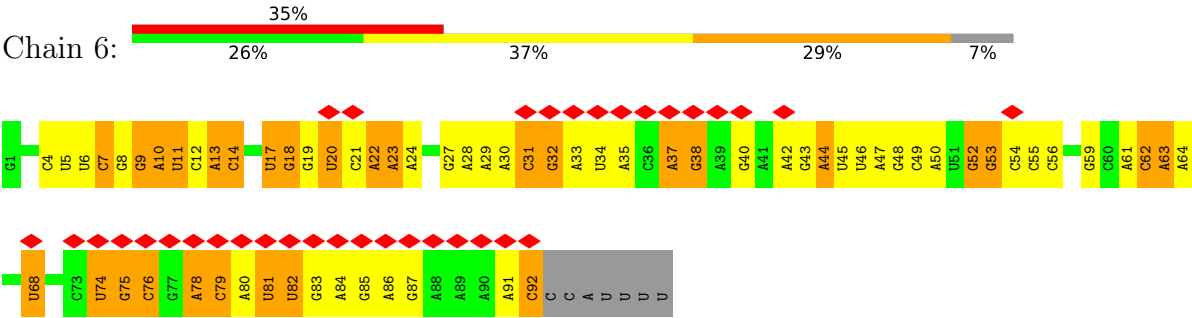
- Molecule 33: Uncharacterized protein C17A2.08c



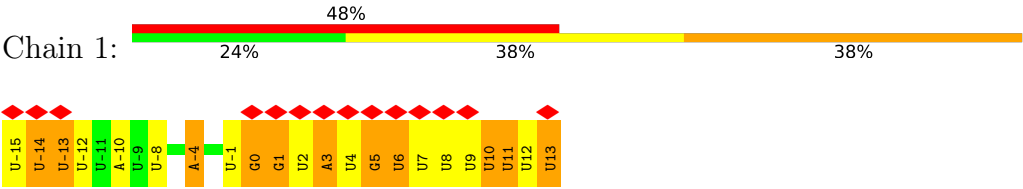
- Molecule 34: Uncharacterized protein C20H4.06c



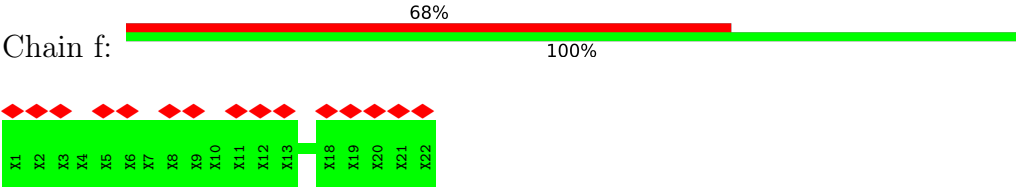




● Molecule 39: pre-mRNA



● Molecule 40: UNK3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72631	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	37.664	Depositor
Minimum map value	-23.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.904	Depositor
Recommended contour level	3.2	Depositor
Map size (Å)	460.32, 460.32, 460.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

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

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	e	0.24	0/1354	0.43	0/1831
2	p	0.18	0/491	0.43	0/654
3	2	0.24	0/554	0.29	0/856
4	5	0.44	0/2397	0.33	0/3727
5	A	0.45	0/16857	0.46	2/22848 (0.0%)
6	B	0.42	0/7459	0.44	0/10117
7	C	0.28	0/2376	0.41	0/3216
8	D	0.40	0/772	0.40	0/1038
9	E	0.30	0/737	0.46	0/993
10	F	0.31	0/646	0.57	0/875
11	G	0.25	0/829	0.47	0/1111
12	H	0.29	0/662	0.47	0/894
13	I	0.28	0/585	0.60	0/794
14	J	0.37	0/578	0.46	0/774
15	K	0.47	0/3130	0.49	0/4251
16	L	0.32	0/1991	0.46	0/2684
17	M	0.25	0/1841	0.44	0/2468
18	N	0.13	0/10690	0.33	0/14463
19	O	0.40	0/1199	0.48	0/1609
20	P	0.33	0/2222	0.57	1/2991 (0.0%)
21	Q	0.36	0/767	0.46	0/1028
22	R	0.26	0/5235	0.45	0/7067
23	S	0.20	0/1072	0.50	0/1453
23	T	0.19	0/1086	0.43	0/1472
23	U	0.14	0/2897	0.37	0/3914
23	V	0.19	0/1060	0.50	0/1437
24	W	0.25	0/4187	0.52	3/5613 (0.1%)
25	X	0.17	0/5599	0.44	0/7566
26	Y	0.16	0/857	0.41	0/1138
27	Z	0.20	0/1244	0.47	0/1667
28	a	0.28	0/1055	0.44	0/1443
29	b	0.27	0/829	0.38	0/1111

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	c	0.40	0/1711	0.49	0/2312
31	d	0.24	0/1206	0.43	0/1636
32	m	0.15	0/3916	0.36	0/5300
33	n	0.12	0/247	0.31	0/327
34	y	0.26	0/1641	0.58	0/2211
35	z	0.19	0/5079	0.41	0/6875
37	q	0.23	0/32	0.19	0/43
38	6	0.22	0/2207	0.36	0/3438
39	1	0.33	0/673	0.47	0/1043
All	All	0.31	0/99970	0.44	6/136288 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	Q	0	1
24	W	0	3
35	z	0	1
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	130	PRO	CA-N-CD	-6.83	102.43	112.00
24	W	626	THR	CA-C-N	-6.03	112.44	120.63
24	W	626	THR	C-N-CA	-6.03	112.44	120.63
5	A	1043	LYS	CB-CA-C	-5.86	109.80	116.54
5	A	978	TRP	CB-CG-CD2	-5.34	119.32	126.80
20	P	263	GLU	N-CA-CB	5.02	117.59	110.16

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	Q	223	ARG	Sidechain
24	W	533	ARG	Sidechain
24	W	537	ARG	Sidechain
24	W	657	TYR	Peptide

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Mol	Chain	Res	Type	Group
35	z	326	ARG	Sidechain

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	e	1329	0	1293	41	0
2	p	487	0	515	23	0
3	2	500	0	257	17	0
4	5	2149	0	1085	36	0
5	A	16424	0	16380	403	0
6	B	7298	0	7336	175	0
7	C	2328	0	2276	95	0
8	D	760	0	776	22	0
9	E	726	0	750	40	0
10	F	638	0	682	42	0
11	G	819	0	845	63	0
12	H	652	0	680	33	0
13	I	574	0	591	49	0
14	J	573	0	602	19	0
15	K	3053	0	3011	95	0
16	L	1954	0	1991	79	0
17	M	1818	0	1822	64	0
18	N	10461	0	10412	246	0
19	O	1176	0	1167	23	0
20	P	2178	0	2101	110	0
21	Q	752	0	729	25	0
22	R	5108	0	5024	200	0
23	S	1055	0	1075	58	0
23	T	1069	0	1084	48	0
23	U	2870	0	2403	79	0
23	V	1044	0	1066	71	0
24	W	4126	0	4148	185	0
25	X	5467	0	5372	211	0
26	Y	845	0	842	39	0
27	Z	1232	0	1242	58	0
28	a	1035	0	837	34	0
29	b	822	0	820	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	1678	0	1659	62	0
31	d	1179	0	1169	38	0
32	m	3813	0	3794	90	0
33	n	248	0	262	8	0
34	y	1606	0	1502	94	0
35	z	4980	0	5047	178	0
36	r	335	0	79	10	0
37	q	295	0	85	0	0
38	6	1970	0	994	52	0
39	1	605	0	302	14	0
40	f	110	0	29	0	0
41	A	36	0	6	0	0
42	B	32	0	12	4	0
43	6	3	0	0	0	0
43	B	1	0	0	0	0
44	M	2	0	0	0	0
44	O	3	0	0	0	0
44	P	1	0	0	0	0
45	6	1	0	0	0	0
All	All	98220	0	94154	2803	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 15.

All (2803) 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)
20:P:82:MET:HG2	38:6:32:G:H21	1.06	1.18
35:z:379:GLU:HG3	35:z:384:ASN:ND2	1.58	1.18
20:P:82:MET:HG2	38:6:32:G:N2	1.63	1.11
35:z:379:GLU:CG	35:z:384:ASN:HD21	1.68	1.06
20:P:118:LEU:HD11	20:P:153:ARG:NH2	1.71	1.04
34:y:171:ASN:OD1	35:z:338:ILE:HG13	1.60	1.00
27:Z:153:LYS:HD3	27:Z:156:GLN:HE21	1.26	1.00
20:P:85:ASP:HB2	20:P:88:LYS:HB2	1.41	0.99
25:X:490:GLU:HG3	25:X:494:GLY:HA3	1.43	0.99
35:z:379:GLU:HG3	35:z:384:ASN:HD21	0.84	0.97
20:P:82:MET:CG	38:6:32:G:N2	2.28	0.97
23:S:122:ARG:HH21	23:V:114:VAL:HG13	1.28	0.97
25:X:621:THR:HA	25:X:624:ARG:HE	1.30	0.96
35:z:568:LYS:HA	35:z:571:LYS:HG2	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:285:HIS:O	22:R:289:GLN:HB2	1.66	0.95
24:W:537:ARG:HH11	24:W:577:PHE:HB2	1.32	0.94
1:e:204:HIS:HB3	6:B:76:GLN:HB2	1.50	0.94
24:W:207:ILE:HG12	24:W:209:ILE:H	1.34	0.93
30:c:520:GLU:HA	30:c:567:PRO:HG3	1.51	0.93
35:z:371:TYR:HA	35:z:374:MET:HE3	1.53	0.91
1:e:40:SER:OG	16:L:301:GLN:NE2	2.03	0.91
24:W:155:MET:HG2	24:W:159:GLU:HG3	1.54	0.90
20:P:82:MET:CG	38:6:32:G:H21	1.86	0.89
24:W:536:ILE:HG22	24:W:537:ARG:H	1.36	0.88
23:S:122:ARG:HH22	23:V:115:ILE:HD13	1.38	0.88
20:P:118:LEU:HD11	20:P:153:ARG:HH21	1.37	0.87
23:S:110:ALA:HA	23:S:113:ARG:HE	1.40	0.87
18:N:206:SER:HB3	18:N:225:ILE:HD13	1.56	0.87
20:P:150:CYS:SG	20:P:224:GLN:NE2	2.49	0.86
16:L:115:GLU:HG2	16:L:116:LEU:HD12	1.59	0.84
24:W:192:ARG:HH12	24:W:196:LEU:HB2	1.42	0.84
17:M:82:SER:O	20:P:147:ASN:ND2	2.09	0.84
16:L:191:GLN:HE21	28:a:86:THR:HG23	1.42	0.84
5:A:1723:THR:OG1	5:A:1741:ASN:OD1	1.96	0.84
32:m:653:ASN:O	32:m:657:GLN:NE2	2.10	0.84
17:M:60:ARG:NH1	19:O:127:ASP:OD2	2.10	0.83
5:A:1665:ARG:HE	5:A:1666:PRO:HD2	1.44	0.83
23:T:69:LEU:HD12	23:T:71:ALA:H	1.42	0.83
14:J:8:ASP:OD1	14:J:10:LYS:NZ	2.11	0.82
23:S:122:ARG:HE	23:V:114:VAL:HG22	1.41	0.82
5:A:1605:LEU:HD22	5:A:1770:ARG:HH11	1.42	0.82
2:p:197:LEU:O	25:X:722:ARG:NH1	2.11	0.81
10:F:40:LEU:HB3	10:F:43:VAL:HG11	1.63	0.81
25:X:68:TRP:HE1	25:X:104:LEU:HD23	1.42	0.81
1:e:183:LYS:HG2	1:e:184:SER:H	1.45	0.81
7:C:203:ILE:HD11	7:C:215:LEU:HG	1.63	0.81
5:A:1757:ILE:HG23	5:A:1761:ASN:HD21	1.45	0.81
1:e:256:TYR:HE2	30:c:595:ALA:HA	1.46	0.80
12:H:82:GLN:NE2	14:J:57:ILE:O	2.14	0.80
1:e:217:GLU:OE2	21:Q:233:ASN:ND2	2.15	0.80
30:c:562:ASP:OD1	30:c:564:ASN:ND2	2.14	0.80
11:G:7:LYS:HB2	11:G:20:LEU:HD21	1.64	0.80
35:z:387:MET:HE2	35:z:415:HIS:HB3	1.64	0.79
22:R:118:ARG:HG3	26:Y:165:VAL:HG11	1.64	0.79
28:a:62:MET:HA	28:a:64:GLN:HE21	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:285:HIS:O	22:R:289:GLN:CB	2.30	0.79
5:A:1604:HIS:HB3	5:A:1607:GLN:HE21	1.47	0.79
17:M:102:LEU:HD23	17:M:103:VAL:HG23	1.62	0.79
2:p:192:LEU:HD11	2:p:194:ILE:HG22	1.65	0.78
7:C:297:SER:OG	7:C:301:ASP:OD1	2.01	0.78
18:N:665:ILE:HD11	18:N:740:GLN:HG2	1.64	0.78
24:W:537:ARG:HD2	24:W:577:PHE:CG	2.19	0.78
24:W:242:ASP:HA	24:W:249:LYS:HZ1	1.46	0.78
23:S:92:ARG:HH21	23:V:5:ILE:HG12	1.47	0.78
24:W:192:ARG:NH1	24:W:196:LEU:HB2	1.98	0.78
22:R:121:ASN:ND2	24:W:237:ASP:O	2.17	0.78
22:R:265:LYS:NZ	22:R:283:TYR:OH	2.16	0.78
24:W:176:LYS:HG3	38:6:42:A:H5''	1.66	0.78
8:D:64:SER:HA	9:E:71:ARG:HH21	1.50	0.77
5:A:1609:ILE:HG12	5:A:1763:ALA:HB1	1.67	0.77
20:P:96:ARG:NH1	20:P:97:CYS:O	2.16	0.77
17:M:47:CYS:SG	17:M:121:GLN:NE2	2.57	0.77
21:Q:46:GLU:OE1	21:Q:49:ARG:NH2	2.18	0.77
20:P:259:GLN:NE2	20:P:263:GLU:OE2	2.16	0.77
23:T:122:ARG:HH22	23:U:121:GLU:HB3	1.48	0.77
23:U:191:ALA:HB3	23:U:485:LEU:HB3	1.66	0.77
35:z:412:PRO:HB2	35:z:415:HIS:HD2	1.49	0.77
18:N:634:ARG:NH2	18:N:997:CYS:SG	2.58	0.77
5:A:1762:PRO:HB3	34:y:94:ILE:HD13	1.67	0.77
5:A:1602:ARG:HE	5:A:1770:ARG:NH2	1.83	0.77
5:A:1691:ARG:NH2	5:A:1697:SER:O	2.16	0.77
5:A:1736:HIS:ND1	5:A:1758:MET:SD	2.58	0.77
24:W:725:LEU:HD13	27:Z:159:VAL:HG21	1.67	0.77
24:W:245:ASN:HB2	24:W:248:GLU:HB2	1.67	0.76
7:C:306:LEU:HD13	9:E:106:ARG:HE	1.50	0.76
17:M:63:LYS:NZ	38:6:22:A:OP2	2.17	0.76
32:m:539:ILE:HD11	32:m:574:LEU:HD13	1.64	0.76
5:A:1817:THR:HG22	5:A:1818:PHE:H	1.50	0.76
22:R:17:GLN:NE2	24:W:151:ASP:OD1	2.18	0.76
24:W:246:PHE:HA	24:W:249:LYS:HG2	1.67	0.76
25:X:538:GLU:HA	25:X:541:VAL:HG12	1.67	0.76
5:A:1630:ILE:O	34:y:83:ARG:NH2	2.19	0.76
16:L:208:GLU:O	38:6:18:G:N1	2.19	0.76
5:A:1602:ARG:HE	5:A:1770:ARG:HH21	1.32	0.76
24:W:259:ASN:OD1	24:W:262:ARG:NH2	2.19	0.76
22:R:292:ASP:OD2	22:R:298:SER:OG	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:200:ASP:OD1	19:O:31:ARG:NH1	2.19	0.75
20:P:118:LEU:HD21	20:P:153:ARG:HH21	1.51	0.75
23:S:90:LEU:HB2	23:V:90:LEU:HD11	1.68	0.75
24:W:509:GLU:HA	24:W:512:ILE:HB	1.68	0.75
17:M:237:PRO:HB2	17:M:255:LYS:HD3	1.68	0.75
22:R:281:LYS:O	22:R:285:HIS:ND1	2.20	0.75
1:e:132:PHE:HE1	24:W:68:LYS:HG3	1.51	0.75
15:K:106:ILE:HG12	15:K:109:GLN:HG2	1.69	0.75
18:N:279:LYS:NZ	18:N:382:ASP:O	2.18	0.75
5:A:231:LYS:HB3	5:A:244:TYR:CE2	2.22	0.75
5:A:1576:GLN:HB3	5:A:1585:MET:HE1	1.69	0.74
8:D:17:THR:HG22	8:D:27:ARG:HD2	1.68	0.74
5:A:1282:LYS:HG2	34:y:208:ASN:HD21	1.51	0.74
5:A:1660:LYS:NZ	5:A:1661:TRP:O	2.20	0.74
18:N:778:SER:HB2	18:N:979:MET:HE3	1.68	0.74
5:A:1616:ASP:OD2	5:A:1761:ASN:ND2	2.21	0.74
5:A:1972:GLU:HG3	5:A:1975:LYS:HE2	1.69	0.74
35:z:605:VAL:O	35:z:609:LYS:NZ	2.20	0.74
22:R:88:ARG:HB3	24:W:225:ILE:HD12	1.70	0.74
23:V:99:GLN:NE2	36:r:230:UNK:O	2.21	0.74
18:N:694:SER:HB3	18:N:713:SER:HB3	1.69	0.73
20:P:147:ASN:OD1	20:P:148:VAL:N	2.21	0.73
10:F:77:ASP:OD1	11:G:58:LYS:NZ	2.20	0.73
18:N:306:LEU:HD23	18:N:329:LEU:HD23	1.68	0.73
5:A:191:ASP:OD1	5:A:192:ASP:N	2.21	0.73
15:K:290:SER:HB2	15:K:309:MET:HB3	1.69	0.73
18:N:772:ASP:HB2	18:N:974:ASN:HB2	1.70	0.73
18:N:988:SER:O	18:N:992:ILE:HD12	1.87	0.73
25:X:262:GLN:HA	25:X:265:ILE:HD12	1.71	0.73
5:A:1888:THR:HG22	5:A:1915:LEU:HB2	1.71	0.73
6:B:182:THR:O	6:B:183:HIS:ND1	2.20	0.73
10:F:46:THR:HG22	10:F:52:PRO:HB3	1.69	0.73
22:R:44:ASP:N	22:R:47:GLU:OE2	2.19	0.73
5:A:59:ARG:NH1	38:6:11:U:OP1	2.22	0.73
18:N:226:ILE:HG23	18:N:274:LEU:HD12	1.70	0.73
22:R:375:ASP:OD1	22:R:382:ALA:N	2.22	0.73
23:V:106:TYR:HB2	24:W:568:ILE:HG13	1.71	0.73
30:c:569:LEU:HD22	30:c:572:LEU:HD12	1.70	0.73
20:P:118:LEU:CD1	20:P:153:ARG:HH21	2.01	0.73
24:W:531:ILE:HG12	24:W:537:ARG:CZ	2.19	0.73
5:A:1430:GLU:HA	5:A:1433:GLU:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:176:LYS:NZ	5:A:645:GLY:O	2.23	0.72
18:N:801:HIS:NE2	18:N:927:GLU:OE2	2.21	0.72
24:W:203:LYS:HA	24:W:207:ILE:HB	1.70	0.72
6:B:585:LYS:NZ	6:B:586:ASP:O	2.23	0.72
5:A:1635:LYS:HB2	5:A:1653:ILE:HG22	1.72	0.72
25:X:599:GLU:OE1	25:X:608:SER:OG	2.08	0.72
7:C:203:ILE:HB	7:C:213:HIS:HD2	1.54	0.72
5:A:1236:GLY:HA2	5:A:1300:GLU:HG3	1.72	0.72
18:N:307:GLN:NE2	18:N:322:VAL:O	2.23	0.72
28:a:106:ASN:HD22	28:a:106:ASN:C	1.94	0.72
16:L:210:ASP:HB3	16:L:213:GLU:HG2	1.70	0.72
18:N:1179:ASN:HA	18:N:1208:SER:HB2	1.70	0.72
23:T:70:PRO:HA	23:T:73:LEU:HG	1.70	0.71
24:W:749:ASP:HA	24:W:752:ARG:HE	1.54	0.71
7:C:259:GLN:NE2	7:C:298:ALA:O	2.22	0.71
17:M:110:ASP:OD1	17:M:111:ILE:HD12	1.90	0.71
22:R:84:LYS:NZ	22:R:87:ALA:HB3	2.04	0.71
35:z:187:SER:HA	35:z:195:VAL:HG21	1.72	0.71
6:B:204:ASP:OD1	6:B:205:MET:N	2.22	0.71
16:L:191:GLN:HE22	17:M:23:CYS:HA	1.56	0.71
23:U:383:PHE:HD1	23:U:390:LEU:HD22	1.54	0.71
25:X:108:MET:HE3	25:X:110:VAL:HB	1.71	0.71
25:X:271:GLU:OE1	25:X:274:ARG:NH1	2.24	0.71
34:y:127:ASP:H	34:y:131:ARG:HH21	1.39	0.71
12:H:9:MET:HE3	14:J:34:TYR:H	1.56	0.71
23:S:129:LEU:HD22	23:V:125:ALA:HB2	1.73	0.71
1:e:51:LEU:HD13	16:L:305:GLU:HG2	1.73	0.71
15:K:86:ALA:O	22:R:259:ARG:NH1	2.22	0.71
6:B:814:GLN:HA	6:B:817:ARG:HD3	1.71	0.71
25:X:139:LEU:HD13	25:X:147:ILE:HG23	1.73	0.71
32:m:638:TRP:NE1	32:m:642:TRP:HE1	1.89	0.71
34:y:136:ARG:NH1	34:y:142:GLU:OE2	2.24	0.71
38:6:34:U:H2'	38:6:35:A:H8	1.56	0.71
5:A:1020:MET:HG2	5:A:1066:PHE:CZ	2.26	0.70
10:F:32:VAL:HG23	10:F:38:THR:HG22	1.73	0.70
34:y:42:GLU:HG2	34:y:43:ALA:H	1.56	0.70
6:B:254:ILE:HD13	6:B:597:MET:HE1	1.70	0.70
18:N:1273:VAL:HA	18:N:1276:MET:HE2	1.73	0.70
5:A:1725:VAL:HA	5:A:1740:GLY:HA3	1.74	0.70
20:P:118:LEU:CD1	20:P:153:ARG:NH2	2.51	0.70
20:P:122:ARG:HG2	20:P:124:MET:HE1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1684:TYR:HB2	5:A:1724:GLY:HA2	1.74	0.70
6:B:741:LEU:H	29:b:66:LYS:HG2	1.55	0.70
29:b:23:ASN:ND2	30:c:427:GLU:OE2	2.23	0.70
12:H:35:ASP:OD1	12:H:36:ILE:HD12	1.92	0.70
20:P:209:SER:OG	20:P:210:ARG:NH1	2.24	0.70
5:A:220:ASP:HA	5:A:256:ASN:HD21	1.57	0.70
18:N:529:LEU:HD11	18:N:611:ALA:HB1	1.74	0.70
5:A:680:ALA:O	5:A:684:GLU:HB2	1.92	0.70
16:L:163:LYS:O	16:L:167:GLN:NE2	2.24	0.70
6:B:245:GLU:HB3	6:B:248:MET:HE2	1.74	0.70
18:N:357:ARG:HH21	18:N:361:PRO:HD3	1.57	0.70
5:A:1542:LEU:HD23	5:A:1546:GLN:HB3	1.73	0.69
26:Y:118:ARG:NH2	38:6:82:U:OP1	2.26	0.69
2:p:186:LEU:HA	2:p:189:ARG:HE	1.57	0.69
5:A:1429:LEU:HD12	5:A:1430:GLU:H	1.57	0.69
8:D:2:SER:OG	9:E:32:ASP:OD2	2.09	0.69
22:R:333:GLY:O	22:R:337:THR:OG1	2.09	0.69
3:2:29:A:OP1	5:A:884:ARG:NH2	2.25	0.69
5:A:1582:THR:HG22	5:A:1584:ILE:H	1.57	0.69
6:B:534:GLU:OE1	32:m:772:LYS:NZ	2.23	0.69
5:A:1185:ARG:HE	21:Q:229:VAL:HG11	1.56	0.69
5:A:1809:VAL:HG11	5:A:1861:ALA:HB1	1.75	0.69
5:A:1874:ARG:NH2	5:A:1902:ASP:OD2	2.26	0.69
18:N:926:GLU:HG3	25:X:137:ARG:HH21	1.57	0.69
22:R:294:LEU:O	22:R:298:SER:OG	2.11	0.69
24:W:537:ARG:NH1	24:W:577:PHE:HB2	2.07	0.69
35:z:162:LEU:HA	35:z:165:ILE:HG22	1.73	0.69
1:e:190:TYR:OH	5:A:750:LYS:NZ	2.25	0.69
18:N:225:ILE:HA	18:N:228:MET:HE2	1.75	0.69
5:A:164:GLN:NE2	5:A:227:PHE:O	2.23	0.69
1:e:216:THR:HG22	21:Q:234:THR:HA	1.74	0.69
23:U:336:ILE:HA	23:U:352:LEU:HA	1.73	0.69
25:X:584:PRO:HD2	25:X:587:PHE:HB2	1.75	0.69
25:X:668:ALA:HB2	25:X:683:ILE:HD11	1.73	0.69
35:z:318:VAL:HG12	35:z:363:PHE:HB2	1.75	0.69
21:Q:223:ARG:C	21:Q:225:TRP:H	2.00	0.69
35:z:319:ASP:OD1	35:z:350:ARG:NH1	2.25	0.69
2:p:196:ILE:HG23	25:X:722:ARG:HD3	1.74	0.69
5:A:1296:THR:HG21	5:A:1489:TRP:CE3	2.28	0.69
16:L:191:GLN:NE2	17:M:24:GLU:OE1	2.26	0.69
35:z:428:VAL:HG13	35:z:429:LEU:HD12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1629:GLN:HA	5:A:1657:ALA:HA	1.75	0.68
7:C:103:ARG:HD3	7:C:145:LYS:HA	1.75	0.68
11:G:42:GLN:HG2	11:G:56:ARG:HH12	1.58	0.68
17:M:24:GLU:OE1	17:M:24:GLU:N	2.26	0.68
30:c:558:GLU:OE1	30:c:558:GLU:N	2.26	0.68
35:z:131:ILE:HG21	35:z:161:VAL:HG11	1.75	0.68
23:U:357:LEU:HB2	23:U:371:PHE:HB2	1.75	0.68
25:X:139:LEU:HD22	25:X:147:ILE:HG12	1.75	0.68
10:F:51:GLU:N	10:F:51:GLU:OE1	2.26	0.68
18:N:93:TRP:O	18:N:138:LYS:NZ	2.27	0.68
20:P:268:ASN:HA	20:P:271:LYS:HE3	1.75	0.68
31:d:7:GLN:OE1	31:d:12:LYS:NZ	2.27	0.68
5:A:1749:LEU:HD12	5:A:1752:GLN:HE21	1.58	0.68
38:6:47:A:H5''	38:6:47:A:H8	1.58	0.68
15:K:106:ILE:HG21	15:K:137:VAL:HA	1.76	0.68
17:M:88:GLN:NE2	17:M:131:TYR:OH	2.27	0.68
34:y:79:TRP:O	34:y:80:LYS:HD3	1.93	0.68
5:A:681:ARG:NH2	38:6:59:G:OP2	2.27	0.68
5:A:1589:LYS:HG3	39:1:-4:A:H5'	1.75	0.68
22:R:289:GLN:HA	25:X:538:GLU:OE2	1.93	0.68
30:c:515:ASP:OD2	30:c:559:ARG:NH2	2.26	0.68
5:A:1700:ILE:HD12	5:A:1730:ASP:HB2	1.75	0.68
5:A:1798:ASN:O	5:A:1801:GLN:HG2	1.93	0.68
17:M:148:GLU:HG3	20:P:282:LEU:HD21	1.75	0.68
22:R:418:ASP:OD1	22:R:421:ARG:NH1	2.26	0.68
31:d:28:ASN:OD1	31:d:29:PHE:N	2.27	0.68
17:M:91:LEU:HD13	17:M:95:LEU:HD22	1.74	0.68
19:O:140:ASN:O	28:a:138:ARG:NH2	2.27	0.68
5:A:1892:MET:HE2	5:A:1896:LEU:HD21	1.76	0.68
9:E:12:HIS:CD2	9:E:84:PRO:HG3	2.29	0.68
7:C:271:ASN:ND2	7:C:314:ASN:OD1	2.26	0.67
17:M:243:CYS:SG	17:M:244:SER:N	2.66	0.67
27:Z:102:GLN:OE1	27:Z:105:ARG:NH1	2.27	0.67
5:A:1844:LYS:HE2	5:A:1872:LEU:HD21	1.76	0.67
7:C:74:ILE:HB	7:C:89:LEU:HB2	1.76	0.67
11:G:61:ASP:OD1	11:G:62:ARG:N	2.27	0.67
13:I:23:ARG:NH1	13:I:29:GLU:OE1	2.26	0.67
17:M:26:CYS:SG	17:M:82:SER:OG	2.52	0.67
20:P:198:TRP:HE1	20:P:230:MET:HE3	1.59	0.67
22:R:338:ILE:HG23	22:R:340:GLU:H	1.59	0.67
23:V:108:LEU:HB2	24:W:600:CYS:SG	2.35	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:417:SER:OG	21:Q:248:ASN:ND2	2.27	0.67
5:A:984:ASN:ND2	5:A:1243:ASN:OD1	2.27	0.67
18:N:53:HIS:O	18:N:1224:ARG:NH1	2.27	0.67
24:W:202:LEU:HG	24:W:207:ILE:HA	1.75	0.67
5:A:1374:ILE:O	29:b:23:ASN:ND2	2.28	0.67
20:P:190:ILE:HG22	20:P:193:ARG:HH22	1.57	0.67
21:Q:223:ARG:O	21:Q:225:TRP:N	2.27	0.67
30:c:472:CYS:SG	30:c:516:SER:HB3	2.35	0.67
7:C:43:ASN:HD21	9:E:106:ARG:HH11	1.42	0.67
32:m:489:VAL:HG22	32:m:504:LEU:HD11	1.75	0.67
5:A:1976:LEU:HA	5:A:1979:ARG:HG2	1.77	0.67
20:P:98:VAL:HG12	20:P:101:ARG:HH11	1.60	0.67
22:R:337:THR:OG1	22:R:342:TYR:OH	2.06	0.67
23:V:112:LEU:HD21	24:W:600:CYS:HB2	1.76	0.67
5:A:1416:LYS:NZ	5:A:1431:ASP:O	2.27	0.67
24:W:130:PRO:O	24:W:134:LEU:N	2.27	0.67
30:c:578:ALA:O	30:c:582:ARG:NH2	2.26	0.67
24:W:743:GLU:HG3	27:Z:173:LEU:HD11	1.75	0.66
25:X:420:PRO:O	25:X:471:SER:OG	2.13	0.66
7:C:149:GLU:OE1	7:C:166:ARG:NH2	2.28	0.66
25:X:97:CYS:SG	25:X:100:ARG:NH2	2.69	0.66
23:T:62:ARG:NH1	23:T:66:ALA:O	2.28	0.66
34:y:117:ASN:HD22	35:z:593:ILE:HG13	1.60	0.66
5:A:1020:MET:HG2	5:A:1066:PHE:HZ	1.61	0.66
29:b:76:GLU:OE2	29:b:117:LYS:NZ	2.26	0.66
34:y:144:MET:HE3	34:y:145:LEU:HD22	1.77	0.66
35:z:80:ARG:HB2	35:z:83:VAL:HB	1.78	0.66
11:G:25:PHE:HZ	11:G:62:ARG:HA	1.60	0.66
20:P:53:GLN:NE2	20:P:102:ASP:OD1	2.28	0.66
23:V:98:LYS:HE2	24:W:535:LEU:HB2	1.76	0.66
30:c:579:ARG:HA	30:c:582:ARG:HE	1.60	0.66
10:F:35:GLN:OE1	10:F:37:ASN:ND2	2.28	0.66
12:H:23:HIS:O	12:H:41:GLN:NE2	2.28	0.66
20:P:118:LEU:HA	20:P:151:PHE:CE2	2.31	0.66
34:y:171:ASN:ND2	35:z:623:GLU:OE2	2.28	0.66
35:z:239:ILE:HD11	35:z:296:ARG:HH11	1.61	0.66
35:z:245:GLY:HA3	35:z:324:LYS:CE	2.25	0.66
5:A:56:ARG:NH2	38:6:10:A:OP1	2.21	0.66
6:B:583:ASN:ND2	6:B:583:ASN:O	2.29	0.66
17:M:178:ALA:HA	17:M:182:ALA:HB3	1.77	0.66
23:S:61:PRO:HG2	24:W:697:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:112:LEU:HD23	23:U:113:ARG:HE	1.61	0.66
23:U:272:ILE:HD13	23:U:301:LEU:HD13	1.77	0.66
5:A:251:LEU:HD21	5:A:424:ALA:HB2	1.78	0.66
5:A:962:TRP:NE1	5:A:1072:ASP:OD2	2.22	0.66
19:O:21:PRO:O	19:O:24:ILE:HG22	1.96	0.66
21:Q:55:GLU:CD	21:Q:59:ARG:HH21	2.04	0.66
23:V:111:ALA:O	23:V:115:ILE:HG12	1.97	0.66
24:W:174:GLN:HB3	24:W:179:LYS:HE3	1.77	0.66
5:A:103:ARG:NH1	38:6:20:U:O3'	2.28	0.65
5:A:1685:TRP:O	5:A:1725:VAL:N	2.27	0.65
6:B:724:PRO:HG2	6:B:727:ARG:HG3	1.78	0.65
23:S:17:ARG:HD3	23:T:17:ARG:HG3	1.76	0.65
18:N:73:ASN:HA	18:N:76:ASN:HD21	1.61	0.65
18:N:628:LEU:HD11	18:N:987:SER:HB2	1.79	0.65
27:Z:64:VAL:O	27:Z:68:LYS:HG2	1.96	0.65
5:A:1629:GLN:HE22	5:A:1661:TRP:CD1	2.14	0.65
21:Q:223:ARG:HB2	21:Q:226:ASP:OD1	1.96	0.65
32:m:505:HIS:HA	32:m:508:ILE:HG22	1.79	0.65
5:A:873:TYR:CE1	5:A:883:GLN:HG2	2.30	0.65
35:z:310:THR:HA	35:z:356:ARG:HH12	1.61	0.65
5:A:1689:GLN:HE22	5:A:1726:LEU:HD21	1.61	0.65
25:X:191:TRP:HB3	25:X:225:LEU:HD13	1.76	0.65
5:A:1666:PRO:HD3	5:A:1741:ASN:HD21	1.62	0.65
6:B:713:ASP:OD2	6:B:736:TYR:OH	2.14	0.65
20:P:264:GLU:O	20:P:268:ASN:ND2	2.29	0.65
5:A:969:GLU:HB2	5:A:973:LEU:HB3	1.79	0.65
18:N:1060:TYR:CE2	18:N:1062:LEU:HB2	2.31	0.65
25:X:511:ILE:HG13	25:X:512:ALA:H	1.62	0.65
31:d:20:GLU:HG2	31:d:21:HIS:HD2	1.62	0.65
5:A:108:SER:OG	16:L:213:GLU:OE2	2.14	0.65
11:G:45:ILE:HG12	11:G:109:VAL:HG12	1.77	0.65
34:y:210:ASP:OD1	34:y:211:GLY:N	2.29	0.65
5:A:1135:ARG:NH1	21:Q:223:ARG:HD2	2.13	0.64
15:K:89:GLU:OE2	22:R:259:ARG:NE	2.30	0.64
23:V:80:TRP:HB3	27:Z:100:GLU:CD	2.22	0.64
27:Z:83:LEU:HD23	27:Z:94:GLN:HE22	1.62	0.64
30:c:528:THR:OG1	30:c:531:ASP:OD1	2.14	0.64
34:y:125:ILE:HG13	34:y:131:ARG:HD3	1.78	0.64
20:P:289:LYS:O	20:P:293:ARG:NH1	2.30	0.64
22:R:44:ASP:OD1	22:R:45:LEU:N	2.26	0.64
24:W:530:VAL:HG23	24:W:531:ILE:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:z:423:LEU:HB3	35:z:429:LEU:HD13	1.78	0.64
5:A:414:GLU:OE2	6:B:407:HIS:NE2	2.22	0.64
9:E:117:LEU:O	16:L:185:ARG:NH2	2.26	0.64
22:R:47:GLU:HA	22:R:50:GLU:HG3	1.78	0.64
24:W:262:ARG:O	24:W:266:MET:HG2	1.97	0.64
32:m:556:ASN:O	32:m:561:ARG:NH1	2.30	0.64
34:y:160:PHE:O	34:y:164:TYR:N	2.30	0.64
17:M:38:GLU:OE2	17:M:55:ARG:NH1	2.31	0.64
18:N:226:ILE:HG21	18:N:270:MET:HG3	1.79	0.64
23:U:321:PHE:O	23:U:324:LYS:N	2.30	0.64
5:A:1490:GLN:HE21	5:A:1492:ASN:HD22	1.46	0.64
7:C:62:GLY:O	7:C:319:HIS:NE2	2.29	0.64
9:E:12:HIS:NE2	9:E:84:PRO:HG3	2.12	0.64
11:G:108:LEU:HD11	13:I:30:TYR:HE2	1.62	0.64
18:N:401:VAL:HG22	18:N:446:LEU:HD11	1.78	0.64
20:P:82:MET:SD	38:6:32:G:N2	2.70	0.64
23:V:66:ALA:HB1	27:Z:60:GLU:HG2	1.79	0.64
24:W:176:LYS:NZ	38:6:42:A:OP1	2.27	0.64
25:X:645:ARG:O	25:X:649:GLU:HG3	1.97	0.64
3:2:19:G:H22	38:6:50:A:H2	1.45	0.64
5:A:208:LEU:O	19:O:8:ARG:NH1	2.29	0.64
5:A:1803:PHE:HB2	5:A:1834:PHE:HB3	1.80	0.64
18:N:930:PRO:HD3	25:X:137:ARG:NH1	2.13	0.64
22:R:284:THR:HG21	22:R:306:LEU:HD22	1.79	0.64
35:z:547:VAL:HG22	35:z:557:THR:HG21	1.79	0.64
18:N:314:PHE:HB3	18:N:318:LEU:HG	1.80	0.64
22:R:201:HIS:O	22:R:206:ASN:ND2	2.30	0.64
24:W:536:ILE:O	24:W:537:ARG:HB2	1.97	0.64
24:W:537:ARG:O	24:W:539:SER:N	2.30	0.64
6:B:90:ASP:HB3	15:K:157:ARG:HG3	1.80	0.63
6:B:227:VAL:HG11	6:B:254:ILE:HD12	1.79	0.63
23:T:77:GLN:NE2	27:Z:74:ALA:O	2.31	0.63
24:W:203:LYS:HB3	24:W:207:ILE:HD12	1.79	0.63
25:X:321:SER:O	25:X:325:HIS:ND1	2.21	0.63
29:b:24:LEU:HB3	30:c:431:HIS:HD1	1.63	0.63
35:z:245:GLY:HA3	35:z:324:LYS:HD2	1.79	0.63
35:z:428:VAL:HG23	35:z:440:GLY:HA2	1.80	0.63
5:A:952:GLU:OE2	5:A:955:ARG:NH2	2.22	0.63
27:Z:64:VAL:HG23	27:Z:68:LYS:HZ3	1.63	0.63
35:z:62:LEU:HB2	35:z:67:TRP:CD1	2.33	0.63
18:N:715:ARG:NH1	18:N:767:ASP:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:98:GLU:OE1	19:O:98:GLU:N	2.31	0.63
20:P:177:TYR:HD1	20:P:214:PHE:HE1	1.45	0.63
22:R:48:LEU:HD13	24:W:257:ILE:HG23	1.79	0.63
23:S:100:GLU:OE1	23:V:97:THR:OG1	2.15	0.63
25:X:510:LYS:HZ3	26:Y:83:ILE:HB	1.64	0.63
5:A:1656:LEU:HA	5:A:1683:LYS:HD2	1.80	0.63
20:P:251:ASN:ND2	39:1:13:U:OP1	2.31	0.63
1:e:219:GLN:HE21	21:Q:232:ARG:HD3	1.62	0.63
5:A:1185:ARG:NE	21:Q:229:VAL:HG11	2.13	0.63
11:G:55:ALA:HB2	11:G:71:VAL:HA	1.80	0.63
15:K:405:LYS:HD3	15:K:408:GLU:HG2	1.80	0.63
35:z:608:GLU:N	35:z:608:GLU:OE1	2.31	0.63
5:A:1835:ASN:HB2	5:A:1840:GLN:H	1.63	0.63
12:H:80:LEU:HD21	14:J:60:VAL:HG13	1.81	0.63
20:P:117:CYS:SG	20:P:135:HIS:HD2	2.11	0.63
23:S:24:GLU:OE2	23:S:27:LEU:N	2.31	0.63
23:V:88:PHE:O	23:V:92:ARG:HG2	1.97	0.63
24:W:260:GLY:O	24:W:264:ASN:ND2	2.31	0.63
2:p:172:ARG:NH1	24:W:63:ARG:HH11	1.97	0.63
6:B:777:LYS:HA	6:B:780:ILE:HG22	1.81	0.63
7:C:217:GLY:O	7:C:244:ARG:NH1	2.32	0.63
10:F:68:TYR:HB2	11:G:100:PHE:HB3	1.81	0.63
23:U:83:VAL:HG22	23:U:87:GLN:HE21	1.64	0.63
23:U:420:VAL:HG13	23:U:438:GLU:HB2	1.81	0.63
7:C:308:GLY:HA3	9:E:106:ARG:HG2	1.79	0.63
22:R:42:ILE:HG23	22:R:47:GLU:HG2	1.79	0.63
24:W:247:ARG:O	24:W:251:GLU:HB2	1.99	0.63
24:W:672:CYS:HA	24:W:675:LEU:HG	1.81	0.63
32:m:296:LYS:NZ	33:n:313:GLU:HG3	2.13	0.63
11:G:8:PRO:HD2	11:G:9:ARG:HH12	1.64	0.63
18:N:199:ILE:O	18:N:203:LEU:HD12	1.99	0.63
18:N:369:ASP:H	18:N:372:PHE:HB3	1.63	0.63
23:U:255:CYS:HB3	23:U:264:VAL:HG23	1.81	0.63
32:m:511:TRP:O	32:m:515:LEU:N	2.31	0.63
35:z:245:GLY:HA3	35:z:324:LYS:NZ	2.14	0.63
36:r:222:UNK:O	36:r:226:UNK:N	2.31	0.63
25:X:437:MET:SD	25:X:438:GLU:HG3	2.39	0.62
11:G:44:LEU:HD13	11:G:54:LEU:HD12	1.81	0.62
24:W:509:GLU:O	24:W:513:GLN:HG3	1.99	0.62
25:X:108:MET:HG3	25:X:110:VAL:HG12	1.80	0.62
5:A:1429:LEU:O	5:A:1430:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:26:TRP:HZ3	13:I:69:ASN:HD22	1.47	0.62
18:N:160:LYS:NZ	18:N:248:ASP:OD1	2.27	0.62
22:R:256:GLU:OE1	22:R:259:ARG:NH1	2.32	0.62
35:z:210:LEU:HB3	35:z:363:PHE:HD1	1.62	0.62
23:T:11:LYS:HD3	23:T:60:ARG:HH22	1.64	0.62
3:2:5:U:O2	38:6:87:G:N2	2.21	0.62
5:A:196:PRO:HD3	5:A:543:TYR:CE2	2.35	0.62
5:A:873:TYR:HE1	5:A:883:GLN:HG2	1.65	0.62
11:G:55:ALA:HB3	11:G:68:LEU:HD12	1.81	0.62
18:N:1183:PHE:HB3	18:N:1213:VAL:HG22	1.82	0.62
21:Q:55:GLU:OE1	21:Q:59:ARG:NH2	2.30	0.62
28:a:126:ASP:O	28:a:130:LYS:HG3	2.00	0.62
38:6:53:G:O2'	38:6:55:C:OP1	2.17	0.62
5:A:986:THR:HG22	5:A:1244:ARG:HH22	1.65	0.62
25:X:513:THR:H	25:X:544:PHE:HZ	1.47	0.62
25:X:581:GLU:OE1	25:X:581:GLU:N	2.33	0.62
6:B:85:TYR:HB3	6:B:89:VAL:HG21	1.80	0.62
24:W:240:GLU:HB2	24:W:244:GLN:HB3	1.82	0.62
36:r:242:UNK:O	36:r:244:UNK:N	2.33	0.62
6:B:769:ASP:HB2	6:B:772:VAL:HB	1.80	0.62
18:N:836:ARG:NH2	18:N:890:TYR:O	2.30	0.62
18:N:929:ARG:HE	25:X:137:ARG:NH2	1.97	0.62
5:A:935:ASP:HB3	5:A:938:GLU:HG3	1.82	0.62
5:A:1354:MET:O	5:A:1354:MET:HG3	2.00	0.62
18:N:562:ILE:HA	18:N:585:VAL:HG22	1.81	0.62
35:z:387:MET:SD	35:z:387:MET:N	2.67	0.62
1:e:32:GLU:OE2	2:p:170:ARG:NH2	2.33	0.62
6:B:189:ARG:NH2	6:B:652:ASP:OD2	2.33	0.62
6:B:938:ALA:HB3	6:B:943:LEU:HD23	1.81	0.62
20:P:63:GLU:O	20:P:66:GLN:NE2	2.27	0.62
24:W:537:ARG:C	24:W:539:SER:H	2.06	0.62
25:X:512:ALA:HB2	26:Y:83:ILE:HG13	1.82	0.62
23:U:342:HIS:HE1	23:U:344:ASP:HB2	1.65	0.61
24:W:40:THR:OG1	24:W:43:GLN:OE1	2.18	0.61
18:N:872:THR:O	18:N:884:ARG:NH1	2.34	0.61
23:S:100:GLU:HA	23:S:103:THR:HG22	1.82	0.61
24:W:207:ILE:HG12	24:W:209:ILE:N	2.11	0.61
27:Z:131:LEU:O	27:Z:135:GLU:HG2	2.01	0.61
32:m:449:TRP:HE1	32:m:457:ALA:HB2	1.64	0.61
5:A:694:GLN:O	5:A:699:ARG:NH2	2.24	0.61
5:A:1654:LEU:HD12	5:A:1720:PRO:HG2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:111:SER:OG	7:C:138:VAL:HG13	2.00	0.61
18:N:480:LEU:HD21	18:N:483:PHE:HB2	1.83	0.61
30:c:576:ASP:HB3	30:c:603:TYR:CZ	2.35	0.61
6:B:532:ASP:OD2	32:m:738:ARG:NH2	2.33	0.61
11:G:29:PRO:HG3	13:I:36:SER:O	2.00	0.61
13:I:26:TRP:CZ3	13:I:69:ASN:ND2	2.69	0.61
32:m:317:SER:HA	32:m:320:PHE:HB2	1.82	0.61
7:C:155:SER:OG	7:C:157:ASP:OD1	2.18	0.61
23:S:60:ARG:CZ	24:W:701:TRP:HD1	2.13	0.61
24:W:174:GLN:O	24:W:179:LYS:NZ	2.29	0.61
25:X:87:HIS:HB2	25:X:91:PHE:HE1	1.66	0.61
32:m:431:GLU:O	32:m:435:MET:HG2	2.00	0.61
34:y:132:GLU:HG2	34:y:133:PHE:CD1	2.35	0.61
2:p:162:SER:OG	2:p:166:ARG:NH1	2.34	0.61
7:C:85:ASN:HB3	9:E:97:GLY:HA3	1.82	0.61
24:W:737:SER:O	24:W:741:GLN:HG2	2.01	0.61
25:X:219:TRP:HE1	25:X:256:LEU:HD22	1.66	0.61
35:z:317:VAL:HG23	35:z:354:ALA:HB2	1.82	0.61
6:B:628:TYR:OH	6:B:657:ASP:OD2	2.14	0.61
23:V:99:GLN:HE22	36:r:231:UNK:HA	1.66	0.61
24:W:131:ASN:HA	24:W:134:LEU:HB3	1.82	0.61
34:y:30:SER:O	34:y:33:ASN:ND2	2.33	0.61
6:B:146:VAL:HG12	6:B:154:LYS:HB2	1.82	0.61
25:X:592:TYR:OH	25:X:618:LYS:HE3	2.01	0.61
35:z:241:VAL:HG21	35:z:300:PHE:HD1	1.65	0.61
5:A:1762:PRO:HB2	34:y:97:ILE:HD11	1.82	0.61
5:A:1828:ASN:OD1	5:A:1848:THR:OG1	2.15	0.61
11:G:109:VAL:HG22	13:I:64:LEU:HB3	1.83	0.61
12:H:78:ILE:H	12:H:78:ILE:HD12	1.65	0.61
25:X:398:ARG:HH22	25:X:437:MET:HA	1.65	0.61
26:Y:137:GLU:OE1	26:Y:137:GLU:N	2.29	0.61
29:b:128:VAL:HA	29:b:131:TYR:HD2	1.66	0.61
30:c:541:LYS:O	30:c:545:GLN:HG3	2.00	0.61
31:d:6:LEU:HB2	31:d:13:ILE:HB	1.82	0.61
6:B:505:TYR:OH	6:B:552:ARG:NH1	2.34	0.60
7:C:115:THR:HG22	7:C:136:GLY:O	2.00	0.60
18:N:492:GLN:O	25:X:248:ARG:NH2	2.34	0.60
25:X:286:THR:HG21	25:X:289:ASN:HB2	1.83	0.60
19:O:11:ARG:HG2	19:O:12:PRO:HD2	1.82	0.60
31:d:92:ASN:ND2	31:d:115:LYS:O	2.33	0.60
5:A:978:TRP:CD1	5:A:1214:MET:HE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:m:545:ASP:OD2	32:m:550:TRP:NE1	2.33	0.60
11:G:32:VAL:O	11:G:111:ARG:NH2	2.34	0.60
5:A:127:MET:HE1	5:A:605:PHE:HZ	1.66	0.60
22:R:84:LYS:HZ1	22:R:87:ALA:HB3	1.66	0.60
24:W:141:PRO:HB2	24:W:146:LEU:HD21	1.84	0.60
24:W:159:GLU:HA	24:W:162:MET:HG2	1.81	0.60
28:a:67:LEU:HA	31:d:93:ALA:HB2	1.82	0.60
3:2:24:A:H5'	3:2:25:G:H5''	1.83	0.60
5:A:1307:GLU:N	5:A:1307:GLU:OE1	2.34	0.60
6:B:221:VAL:HG21	6:B:912:GLN:HB3	1.82	0.60
7:C:295:VAL:HB	7:C:304:TYR:HB2	1.83	0.60
24:W:537:ARG:HH11	24:W:577:PHE:CB	2.11	0.60
25:X:467:ASP:O	25:X:475:ARG:NH2	2.34	0.60
25:X:543:LEU:HD13	26:Y:83:ILE:HD11	1.82	0.60
28:a:64:GLN:OE1	31:d:62:ARG:NH1	2.31	0.60
30:c:417:TYR:HB2	30:c:449:MET:HE2	1.82	0.60
31:d:23:PRO:O	31:d:27:GLN:HG3	2.02	0.60
32:m:439:LYS:NZ	32:m:479:ASP:OD2	2.26	0.60
4:5:68:U:O4	5:A:492:ASN:ND2	2.33	0.60
5:A:1660:LYS:HZ1	5:A:1681:THR:N	2.00	0.60
8:D:37:MET:HE1	9:E:71:ARG:HD2	1.82	0.60
18:N:495:GLN:O	25:X:248:ARG:NH2	2.34	0.60
3:2:23:U:OP1	5:A:797:LYS:NZ	2.34	0.60
12:H:75:GLY:O	14:J:63:ARG:NH1	2.34	0.60
20:P:118:LEU:CD2	20:P:153:ARG:HH21	2.14	0.60
32:m:284:MET:O	32:m:288:ARG:HG2	2.02	0.60
34:y:138:ASP:OD1	34:y:141:GLY:HA3	2.01	0.60
12:H:31:PHE:O	14:J:22:ASN:ND2	2.31	0.60
22:R:485:ASP:OD1	22:R:488:ARG:NH1	2.35	0.60
23:S:110:ALA:HA	23:S:113:ARG:NE	2.15	0.60
29:b:68:LEU:HG	29:b:127:LEU:HD22	1.84	0.60
30:c:519:TRP:HZ3	30:c:560:LEU:HD22	1.67	0.60
1:e:143:ARG:NH2	16:L:281:ASP:OD1	2.35	0.59
5:A:635:ILE:O	5:A:639:PHE:HB2	2.02	0.59
5:A:722:GLU:OE1	5:A:722:GLU:N	2.34	0.59
5:A:1966:ALA:HB1	5:A:2007:LEU:HD22	1.84	0.59
17:M:170:LEU:HG	17:M:171:LYS:HE3	1.84	0.59
18:N:751:ARG:NH2	18:N:1206:ALA:O	2.35	0.59
20:P:69:GLN:NE2	20:P:80:GLY:O	2.35	0.59
35:z:497:SER:HA	35:z:500:PHE:CD2	2.37	0.59
5:A:1358:LEU:HD22	29:b:21:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1400:GLU:OE1	30:c:462:LYS:NZ	2.35	0.59
16:L:127:LEU:HA	16:L:130:ARG:HG3	1.83	0.59
20:P:214:PHE:HZ	39:1:10:U:H1'	1.66	0.59
22:R:112:GLU:OE2	22:R:116:LYS:HE2	2.02	0.59
23:S:55:VAL:HG11	27:Z:133:LEU:HD21	1.82	0.59
24:W:531:ILE:HG12	24:W:537:ARG:NH2	2.17	0.59
25:X:534:PHE:O	25:X:538:GLU:HG2	2.02	0.59
32:m:650:LEU:HB3	32:m:656:ILE:HD12	1.84	0.59
1:e:133:GLY:O	1:e:137:GLU:HG3	2.02	0.59
6:B:767:ASP:HB3	6:B:770:LYS:HE3	1.85	0.59
23:S:38:ASP:N	23:S:43:GLN:O	2.35	0.59
35:z:319:ASP:HB3	35:z:364:ARG:HG2	1.83	0.59
22:R:46:GLU:OE2	24:W:199:ARG:NH2	2.34	0.59
22:R:248:ALA:O	22:R:252:ILE:HG12	2.03	0.59
32:m:449:TRP:O	32:m:484:ARG:NH2	2.35	0.59
35:z:457:LEU:O	35:z:460:ASN:ND2	2.35	0.59
2:p:169:PHE:CZ	24:W:67:GLU:HB3	2.38	0.59
5:A:1514:PHE:O	5:A:1517:THR:OG1	2.20	0.59
15:K:117:LYS:HG3	22:R:225:GLN:NE2	2.18	0.59
24:W:514:GLU:O	24:W:518:GLU:N	2.35	0.59
24:W:514:GLU:HG2	24:W:521:ARG:HH22	1.68	0.59
31:d:112:LEU:HG	31:d:116:HIS:HD2	1.68	0.59
32:m:718:PHE:HE2	32:m:764:LEU:HD22	1.67	0.59
5:A:1295:MET:SD	5:A:1354:MET:HE2	2.42	0.59
5:A:1639:HIS:HE1	5:A:1718:MET:HE1	1.67	0.59
6:B:250:ASN:O	6:B:254:ILE:HG12	2.02	0.59
7:C:245:ILE:HG23	7:C:258:LEU:HB2	1.85	0.59
17:M:38:GLU:OE1	17:M:38:GLU:N	2.36	0.59
18:N:224:ALA:HA	18:N:418:PHE:CE1	2.38	0.59
22:R:488:ARG:NH2	22:R:517:GLU:OE1	2.35	0.59
16:L:191:GLN:NE2	28:a:86:THR:HG23	2.15	0.59
18:N:230:LEU:HD21	18:N:274:LEU:HA	1.85	0.59
23:T:84:ALA:HB1	27:Z:68:LYS:HE3	1.85	0.59
25:X:503:TYR:HA	25:X:506:VAL:HG12	1.83	0.59
3:2:13:C:O2'	5:A:725:ARG:NH2	2.35	0.59
5:A:1943:LEU:O	5:A:1992:TRP:NE1	2.35	0.59
22:R:412:LEU:HD13	22:R:443:PHE:HE1	1.67	0.59
24:W:677:ASN:OD1	24:W:678:ARG:N	2.36	0.59
5:A:1873:ILE:O	5:A:1881:GLN:NE2	2.36	0.59
18:N:214:LYS:HE3	18:N:259:LEU:HD12	1.85	0.59
20:P:93:SER:N	20:P:232:HIS:O	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:98:VAL:HG12	20:P:101:ARG:NH1	2.17	0.59
5:A:94:ARG:NH2	5:A:105:ASP:OD2	2.35	0.59
5:A:1095:LEU:HD22	5:A:1110:LEU:HD22	1.83	0.59
20:P:150:CYS:SG	20:P:221:ALA:HA	2.43	0.59
20:P:163:MET:HB3	20:P:245:TRP:HB2	1.83	0.59
23:S:69:LEU:HD22	23:U:80:TRP:HD1	1.68	0.59
23:S:75:LEU:O	23:S:78:GLU:HG3	2.03	0.59
23:U:385:GLU:OE2	23:U:430:GLN:N	2.36	0.59
14:J:21:LEU:HB2	14:J:25:ARG:HB2	1.84	0.58
15:K:110:VAL:HG11	22:R:199:VAL:HG22	1.84	0.58
18:N:333:GLN:O	18:N:336:GLU:HG2	2.03	0.58
18:N:393:ILE:HD11	18:N:435:ARG:HH21	1.67	0.58
24:W:518:GLU:O	24:W:522:LEU:N	2.33	0.58
27:Z:162:ARG:O	27:Z:165:GLU:HG3	2.03	0.58
30:c:565:LEU:HB3	30:c:567:PRO:HD2	1.84	0.58
5:A:1605:LEU:O	5:A:1609:ILE:HG13	2.03	0.58
18:N:852:ASP:OD1	18:N:929:ARG:NH1	2.35	0.58
18:N:929:ARG:HE	25:X:137:ARG:CZ	2.17	0.58
22:R:70:MET:HE3	22:R:100:ASP:HB3	1.83	0.58
5:A:746:ASN:OD1	5:A:808:LYS:NZ	2.34	0.58
11:G:104:ASP:HA	13:I:66:ARG:HH12	1.68	0.58
18:N:153:ASN:HB2	18:N:178:TYR:HE2	1.68	0.58
18:N:1060:TYR:HE2	18:N:1062:LEU:HB2	1.68	0.58
22:R:111:ILE:HG21	22:R:127:PHE:CZ	2.39	0.58
23:U:71:ALA:HB2	23:V:61:PRO:HG2	1.86	0.58
30:c:440:GLU:OE1	30:c:440:GLU:N	2.35	0.58
6:B:371:GLN:HE22	6:B:373:LEU:HB2	1.68	0.58
6:B:473:ILE:H	6:B:473:ILE:HD12	1.69	0.58
18:N:15:ALA:O	18:N:20:GLY:N	2.37	0.58
23:U:71:ALA:HB1	23:V:63:PRO:HD3	1.85	0.58
32:m:749:ARG:HE	32:m:759:GLY:HA3	1.68	0.58
6:B:791:GLY:N	6:B:796:GLU:O	2.33	0.58
18:N:746:VAL:HG22	18:N:1040:ILE:HD12	1.85	0.58
24:W:65:GLU:OE2	24:W:89:ARG:NH2	2.36	0.58
25:X:457:ALA:H	25:X:505:ARG:HH22	1.52	0.58
34:y:179:TYR:CZ	35:z:217:GLU:HG3	2.39	0.58
2:p:164:ARG:HB3	24:W:105:LEU:HD21	1.84	0.58
7:C:157:ASP:OD1	7:C:159:THR:HG22	2.03	0.58
28:a:75:THR:H	28:a:78:GLN:NE2	2.01	0.58
32:m:749:ARG:HH21	32:m:759:GLY:HA3	1.68	0.58
35:z:466:HIS:CE1	35:z:560:ARG:HH22	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:48:GLU:HG2	5:A:49:LYS:HD3	1.85	0.58
5:A:1272:LEU:O	5:A:1322:ARG:NH2	2.36	0.58
5:A:1800:ILE:HG12	5:A:1837:ARG:HG2	1.85	0.58
9:E:76:VAL:HA	10:F:64:ASN:ND2	2.18	0.58
13:I:60:LEU:HB3	13:I:63:ILE:HD11	1.86	0.58
23:U:342:HIS:CE1	23:U:344:ASP:HB2	2.38	0.58
26:Y:164:HIS:O	26:Y:168:LEU:HD23	2.04	0.58
5:A:911:MET:O	5:A:912:ARG:NH1	2.33	0.58
9:E:14:LEU:HD23	9:E:78:LEU:HD12	1.85	0.58
18:N:224:ALA:HA	18:N:418:PHE:HE1	1.69	0.58
22:R:127:PHE:O	22:R:131:VAL:HG22	2.03	0.58
22:R:186:GLU:OE2	22:R:189:ARG:HD2	2.03	0.58
23:T:67:THR:HG22	27:Z:108:ASN:HB2	1.86	0.58
24:W:700:ALA:HB1	27:Z:134:LEU:HD22	1.84	0.58
5:A:88:ARG:HG2	5:A:92:LYS:NZ	2.19	0.58
5:A:987:ASP:O	5:A:1123:ARG:NH2	2.37	0.58
23:U:379:LYS:H	23:U:394:THR:HA	1.69	0.58
23:V:55:VAL:HG22	23:V:56:PRO:HD2	1.84	0.58
23:V:101:LEU:O	23:V:105:LEU:HG	2.04	0.58
24:W:200:ARG:HA	24:W:203:LYS:HG2	1.85	0.58
31:d:17:LEU:HD23	31:d:26:CYS:HB2	1.86	0.58
33:n:320:ARG:O	33:n:324:ILE:HG12	2.03	0.58
5:A:191:ASP:HB3	5:A:194:GLU:HG2	1.84	0.58
5:A:296:PRO:HB3	5:A:475:LYS:HB2	1.84	0.58
6:B:710:ILE:HD12	6:B:710:ILE:H	1.69	0.58
18:N:751:ARG:NH1	18:N:1207:CYS:O	2.36	0.58
24:W:508:ARG:O	24:W:512:ILE:N	2.34	0.58
25:X:414:GLU:O	25:X:418:HIS:ND1	2.28	0.58
35:z:540:LEU:O	35:z:543:ARG:HG3	2.02	0.58
35:z:573:LEU:HD22	35:z:577:PHE:HE1	1.67	0.58
23:U:347:LEU:HA	23:U:362:THR:H	1.69	0.57
35:z:74:ILE:HB	35:z:119:ILE:HA	1.86	0.57
5:A:1429:LEU:C	5:A:1431:ASP:H	2.12	0.57
18:N:745:MET:HE3	18:N:1029:PHE:HD1	1.69	0.57
25:X:500:ARG:HA	25:X:500:ARG:CZ	2.34	0.57
30:c:588:PHE:CD2	30:c:596:LEU:HD11	2.39	0.57
5:A:48:GLU:OE1	5:A:48:GLU:N	2.27	0.57
6:B:90:ASP:OD2	15:K:157:ARG:NH1	2.37	0.57
6:B:178:ARG:HB3	6:B:181:ASP:OD2	2.04	0.57
6:B:225:ASP:HB3	6:B:629:PRO:HB2	1.86	0.57
6:B:703:VAL:HG12	6:B:803:PHE:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:108:LEU:HD11	13:I:30:TYR:CE2	2.39	0.57
18:N:560:ALA:HB2	18:N:587:LEU:HD12	1.85	0.57
22:R:241:GLU:O	22:R:245:ILE:HG12	2.05	0.57
23:S:80:TRP:CZ2	23:U:69:LEU:HB3	2.39	0.57
27:Z:24:ALA:O	27:Z:28:ILE:HG12	2.04	0.57
1:e:181:LYS:NZ	1:e:182:ASP:O	2.36	0.57
6:B:154:LYS:NZ	42:B:1001:GTP:O2G	2.37	0.57
18:N:1122:TYR:HD1	18:N:1276:MET:HE1	1.69	0.57
26:Y:91:GLN:OE1	26:Y:94:ARG:NH2	2.37	0.57
26:Y:178:ARG:NH1	38:6:81:U:OP2	2.37	0.57
34:y:144:MET:HE2	35:z:417:MET:SD	2.44	0.57
23:U:89:GLU:O	23:U:92:ARG:HG2	2.03	0.57
35:z:282:ASP:OD1	35:z:283:GLU:N	2.37	0.57
5:A:1410:TRP:HH2	5:A:1446:LEU:HD21	1.70	0.57
5:A:1969:VAL:HG12	5:A:1970:ASN:OD1	2.04	0.57
7:C:283:PHE:HD1	7:C:297:SER:HA	1.69	0.57
15:K:133:GLN:OE1	22:R:199:VAL:HG13	2.04	0.57
25:X:141:VAL:HG12	25:X:142:THR:HG23	1.86	0.57
32:m:534:LEU:HD13	32:m:567:ILE:HD11	1.86	0.57
39:1:-1:U:H5'	39:1:0:G:H5''	1.86	0.57
6:B:793:LEU:HD11	6:B:948:LEU:HD11	1.87	0.57
6:B:823:ILE:HG13	6:B:824:PRO:HD3	1.85	0.57
15:K:267:ARG:HG3	15:K:291:THR:HG22	1.87	0.57
15:K:344:PHE:HB2	16:L:140:LYS:HD3	1.86	0.57
22:R:609:GLU:HA	22:R:612:ARG:HD2	1.87	0.57
35:z:344:LYS:O	35:z:348:ILE:HD12	2.04	0.57
1:e:183:LYS:HG2	1:e:184:SER:N	2.17	0.57
5:A:728:LYS:NZ	16:L:249:TRP:O	2.37	0.57
5:A:863:VAL:O	5:A:867:GLU:HG3	2.05	0.57
7:C:151:LEU:HB2	7:C:163:TRP:HB2	1.87	0.57
15:K:226:ASP:OD1	15:K:228:MET:HG2	2.05	0.57
23:S:14:VAL:HG11	23:S:28:ILE:HG21	1.85	0.57
31:d:8:THR:HG23	31:d:11:GLY:H	1.70	0.57
4:5:96:G:C5	12:H:48:PHE:HE2	2.23	0.57
5:A:250:ASN:HB2	5:A:253:GLN:HG3	1.87	0.57
20:P:214:PHE:HE2	39:1:11:U:C6	2.22	0.57
22:R:9:LYS:NZ	35:z:257:GLU:OE2	2.38	0.57
22:R:158:ARG:NH1	22:R:186:GLU:OE2	2.37	0.57
5:A:1447:PHE:O	34:y:227:TYR:HD1	1.88	0.57
16:L:289:ALA:HA	24:W:75:LEU:HD22	1.86	0.56
18:N:59:GLU:OE1	18:N:85:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:183:ARG:HD3	26:Y:125:PRO:HG3	1.85	0.56
22:R:302:ASP:HA	22:R:305:ARG:HG2	1.87	0.56
25:X:637:LEU:HD23	25:X:638:ASN:H	1.69	0.56
30:c:487:LYS:NZ	30:c:491:GLU:OE1	2.38	0.56
32:m:788:ASN:OD1	32:m:789:GLU:N	2.38	0.56
18:N:917:GLU:O	18:N:921:MET:HG2	2.05	0.56
18:N:958:SER:O	18:N:962:ARG:NH1	2.37	0.56
21:Q:252:ARG:HH11	21:Q:252:ARG:HG3	1.69	0.56
1:e:257:PRO:O	30:c:601:ARG:NH2	2.39	0.56
5:A:539:LEU:HD11	5:A:561:SER:HB2	1.88	0.56
5:A:687:HIS:NE2	16:L:219:HIS:HB2	2.20	0.56
5:A:1239:ASN:HB3	5:A:1248:ARG:HD3	1.86	0.56
6:B:872:LEU:HD21	6:B:888:LEU:HD13	1.87	0.56
23:S:111:ALA:O	23:S:115:ILE:HG12	2.05	0.56
25:X:227:VAL:HG21	25:X:259:TYR:HD1	1.70	0.56
27:Z:60:GLU:O	27:Z:64:VAL:HG22	2.04	0.56
30:c:486:PHE:CD2	30:c:521:VAL:HB	2.41	0.56
35:z:464:CYS:SG	35:z:568:LYS:HD2	2.45	0.56
5:A:718:ASP:OD2	15:K:335:ARG:NH1	2.39	0.56
5:A:1654:LEU:HD21	5:A:1656:LEU:HG	1.87	0.56
5:A:1917:PHE:HD1	5:A:1920:ILE:HD11	1.71	0.56
7:C:283:PHE:CD1	7:C:297:SER:HA	2.41	0.56
15:K:346:PHE:HD1	15:K:359:PHE:CE1	2.24	0.56
15:K:352:ASP:OD1	15:K:353:ASN:N	2.38	0.56
23:S:20:GLY:O	23:S:21:ASN:ND2	2.38	0.56
24:W:521:ARG:O	24:W:524:LYS:HG2	2.05	0.56
25:X:98:PHE:HD1	25:X:111:ILE:HG23	1.71	0.56
31:d:32:LEU:HD11	31:d:37:TYR:CE1	2.40	0.56
5:A:1639:HIS:CE1	5:A:1718:MET:HE1	2.40	0.56
7:C:77:TRP:HH2	9:E:99:GLY:HA3	1.71	0.56
18:N:25:VAL:O	18:N:65:ARG:NH2	2.38	0.56
22:R:55:LYS:O	22:R:58:GLU:HG2	2.06	0.56
24:W:257:ILE:O	24:W:261:ILE:HG12	2.05	0.56
5:A:932:TYR:HB2	5:A:1056:GLY:HA3	1.87	0.56
5:A:1684:TYR:HA	5:A:1723:THR:O	2.06	0.56
6:B:162:VAL:HG21	6:B:179:TYR:CD2	2.41	0.56
22:R:281:LYS:C	22:R:285:HIS:HD1	2.14	0.56
23:S:43:GLN:NE2	23:S:44:GLU:OE1	2.39	0.56
23:S:80:TRP:CH2	23:U:69:LEU:HB3	2.41	0.56
35:z:211:PHE:CD2	35:z:368:GLU:HG3	2.40	0.56
35:z:401:ASN:HB2	35:z:404:GLN:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:678:GLU:HG2	6:B:793:LEU:HB3	1.88	0.56
15:K:358:LYS:NZ	15:K:361:GLU:OE2	2.39	0.56
18:N:748:GLY:HA3	18:N:1042:LEU:HD12	1.88	0.56
18:N:1116:ALA:HB1	18:N:1182:ILE:HD12	1.87	0.56
20:P:136:ARG:HH12	20:P:139:LYS:HG2	1.70	0.56
23:S:94:LEU:HD13	23:V:90:LEU:HD23	1.88	0.56
24:W:132:SER:O	24:W:135:ARG:HG2	2.05	0.56
35:z:249:ILE:O	35:z:253:ILE:HG12	2.05	0.56
35:z:621:GLU:HG2	35:z:626:ILE:HG13	1.87	0.56
2:p:167:LYS:HD3	2:p:170:ARG:NH1	2.20	0.56
2:p:176:GLU:OE1	24:W:63:ARG:NH1	2.38	0.56
5:A:1892:MET:O	5:A:1895:PRO:HD2	2.04	0.56
6:B:953:ARG:NE	6:B:959:GLU:OE2	2.23	0.56
7:C:328:CYS:HA	7:C:334:ILE:HG22	1.88	0.56
16:L:122:ARG:NH2	16:L:130:ARG:O	2.39	0.56
16:L:319:LYS:HD3	16:L:322:GLN:HE21	1.69	0.56
20:P:89:SER:O	20:P:90:GLN:C	2.48	0.56
24:W:507:ASP:N	25:X:529:TYR:O	2.38	0.56
35:z:163:LYS:NZ	35:z:189:PHE:O	2.23	0.56
35:z:393:PHE:O	35:z:397:LEU:HG	2.05	0.56
20:P:292:ASN:HD21	20:P:293:ARG:HH11	1.54	0.56
24:W:149:LEU:HD13	35:z:261:ILE:HG21	1.86	0.56
25:X:178:ILE:HA	25:X:181:TYR:CE1	2.40	0.56
38:6:74:U:H4'	38:6:75:G:OP1	2.05	0.56
5:A:140:LEU:HD12	5:A:506:GLN:O	2.06	0.56
5:A:1423:GLN:HG3	5:A:1425:ARG:HG2	1.87	0.56
6:B:336:ALA:O	6:B:340:ILE:HG12	2.05	0.56
6:B:657:ASP:HA	6:B:661:LEU:HD23	1.88	0.56
11:G:25:PHE:CE1	11:G:60:PHE:HE1	2.23	0.56
15:K:183:GLY:HA2	15:K:207:THR:HG23	1.88	0.56
18:N:332:ARG:NH1	18:N:379:ASN:OD1	2.27	0.56
18:N:411:GLU:OE1	18:N:1021:ASN:ND2	2.39	0.56
35:z:143:VAL:HB	35:z:172:PHE:HZ	1.71	0.56
38:6:38:G:O2'	39:1:3:A:N6	2.38	0.56
7:C:98:ASP:OD1	7:C:99:LEU:N	2.39	0.55
10:F:61:ARG:HH21	10:F:63:ASN:HD22	1.54	0.55
17:M:46:ILE:HG23	17:M:113:ARG:HE	1.71	0.55
18:N:306:LEU:HD13	18:N:381:TYR:OH	2.06	0.55
22:R:20:ALA:N	24:W:15:GLU:OE2	2.38	0.55
23:S:38:ASP:OD2	23:S:41:THR:OG1	2.23	0.55
27:Z:153:LYS:HD3	27:Z:156:GLN:NE2	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1635:LYS:NZ	5:A:1636:GLU:O	2.37	0.55
6:B:706:LEU:HD23	6:B:710:ILE:HB	1.88	0.55
7:C:269:GLU:OE1	7:C:269:GLU:N	2.35	0.55
18:N:741:PRO:HA	18:N:1004:ARG:HG2	1.88	0.55
23:T:25:LYS:O	23:T:29:GLU:HG2	2.05	0.55
23:T:27:LEU:O	23:T:30:GLN:HG2	2.06	0.55
25:X:448:ARG:HH12	25:X:498:THR:HG21	1.71	0.55
25:X:680:ALA:O	25:X:684:TYR:HD1	1.89	0.55
6:B:267:LEU:HB3	6:B:319:VAL:HG22	1.88	0.55
15:K:344:PHE:CE2	15:K:360:PRO:HD3	2.42	0.55
18:N:299:ASP:HB3	18:N:383:ARG:HH12	1.71	0.55
22:R:294:LEU:HD23	22:R:298:SER:HB3	1.89	0.55
23:S:103:THR:HA	23:S:106:TYR:CE2	2.42	0.55
28:a:106:ASN:C	28:a:106:ASN:ND2	2.65	0.55
5:A:664:LEU:HA	5:A:667:ILE:HG22	1.89	0.55
5:A:1841:LEU:N	5:A:1941:PHE:O	2.39	0.55
7:C:218:HIS:CE1	7:C:244:ARG:HG3	2.41	0.55
10:F:19:LEU:HD21	10:F:60:ILE:HD12	1.87	0.55
13:I:12:LEU:HD12	13:I:41:MET:HE2	1.86	0.55
16:L:188:PRO:HB3	17:M:24:GLU:OE2	2.06	0.55
20:P:196:ALA:HA	20:P:201:ILE:HD11	1.89	0.55
22:R:121:ASN:HA	22:R:124:ARG:HG2	1.88	0.55
22:R:237:GLU:HG2	22:R:238:PHE:HD1	1.71	0.55
5:A:1660:LYS:HZ1	5:A:1680:THR:C	2.14	0.55
16:L:205:VAL:HG23	17:M:36:THR:HG22	1.88	0.55
18:N:522:ASN:HA	18:N:525:LYS:HE3	1.87	0.55
22:R:50:GLU:CD	22:R:54:ARG:HH21	2.15	0.55
24:W:739:MET:SD	24:W:742:ILE:HD11	2.46	0.55
32:m:779:ASP:N	32:m:779:ASP:OD1	2.39	0.55
5:A:1801:GLN:HE22	5:A:1883:ARG:HB2	1.71	0.55
15:K:184:ASP:OD1	15:K:186:THR:OG1	2.21	0.55
23:T:115:ILE:HG22	23:U:115:ILE:HD11	1.89	0.55
9:E:23:THR:HB	9:E:45:TYR:HB2	1.89	0.55
10:F:78:THR:O	10:F:81:ILE:HG22	2.06	0.55
23:U:342:HIS:CD2	23:U:343:PRO:HD2	2.40	0.55
25:X:627:ILE:HA	25:X:630:VAL:HG22	1.89	0.55
25:X:681:ARG:O	25:X:685:ILE:HD12	2.06	0.55
27:Z:150:ARG:HE	28:a:33:ALA:HA	1.70	0.55
32:m:296:LYS:HZ3	33:n:313:GLU:HG3	1.71	0.55
15:K:96:ILE:HG21	22:R:228:LEU:HB3	1.88	0.55
18:N:52:LEU:HD22	18:N:57:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:694:ARG:NH2	25:X:728:GLN:OE1	2.40	0.55
27:Z:138:LEU:O	27:Z:142:LYS:HG2	2.07	0.55
29:b:134:GLN:O	29:b:138:GLU:HG2	2.07	0.55
6:B:149:HIS:CG	6:B:150:LEU:H	2.24	0.55
10:F:61:ARG:HH21	10:F:63:ASN:ND2	2.04	0.55
10:F:72:ASP:OD1	11:G:97:SER:OG	2.24	0.55
16:L:289:ALA:O	16:L:293:GLU:HG2	2.07	0.55
18:N:663:ASN:O	18:N:740:GLN:NE2	2.37	0.55
20:P:127:GLU:HG2	20:P:131:CYS:HB2	1.88	0.55
27:Z:89:ARG:HA	27:Z:92:LEU:HD13	1.89	0.55
34:y:65:PHE:H	34:y:67:THR:HG22	1.70	0.55
35:z:59:PRO:HA	35:z:62:LEU:CD2	2.36	0.55
5:A:1434:ASP:OD1	5:A:1435:SER:N	2.39	0.55
17:M:232:PHE:HD1	17:M:235:TYR:HD2	1.54	0.55
18:N:498:PRO:HG2	18:N:589:PRO:HB3	1.88	0.55
4:5:49:U:H2'	4:5:50:U:C6	2.41	0.54
16:L:91:LEU:HD12	16:L:92:ALA:H	1.72	0.54
29:b:134:GLN:HA	29:b:137:LYS:HE2	1.89	0.54
32:m:611:ALA:HA	32:m:615:PHE:HD2	1.72	0.54
34:y:127:ASP:N	34:y:131:ARG:HH21	2.04	0.54
35:z:107:ILE:HG13	35:z:110:ASP:HB3	1.88	0.54
7:C:85:ASN:HD22	9:E:99:GLY:H	1.55	0.54
7:C:154:VAL:HB	7:C:180:LEU:HB2	1.88	0.54
11:G:44:LEU:HB3	11:G:110:VAL:CG2	2.38	0.54
12:H:49:MET:HE2	14:J:63:ARG:HD2	1.88	0.54
17:M:42:GLN:HB2	17:M:53:ILE:HD11	1.89	0.54
18:N:850:SER:O	18:N:853:THR:OG1	2.23	0.54
20:P:311:ASP:OD1	20:P:312:LEU:N	2.40	0.54
32:m:515:LEU:HD23	32:m:519:ALA:HA	1.88	0.54
35:z:216:THR:OG1	35:z:222:SER:OG	2.21	0.54
35:z:229:ASN:O	35:z:233:THR:OG1	2.25	0.54
1:e:227:GLN:NE2	1:e:231:GLU:OE2	2.37	0.54
5:A:1714:ASP:OD2	5:A:1716:GLN:NE2	2.40	0.54
6:B:206:LYS:HE3	8:D:9:HIS:CD2	2.41	0.54
12:H:41:GLN:HB2	12:H:54:ASP:HB2	1.88	0.54
12:H:41:GLN:O	12:H:54:ASP:N	2.40	0.54
18:N:252:TYR:OH	18:N:256:ARG:NH1	2.40	0.54
18:N:696:LEU:N	18:N:711:THR:O	2.36	0.54
23:T:109:ASP:O	23:T:113:ARG:HG3	2.08	0.54
24:W:132:SER:OG	24:W:135:ARG:NH1	2.40	0.54
24:W:521:ARG:O	24:W:524:LYS:NZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:445:ASP:HB2	25:X:449:LYS:NZ	2.23	0.54
27:Z:64:VAL:HG23	27:Z:68:LYS:NZ	2.22	0.54
35:z:170:ASN:O	35:z:173:ARG:NH1	2.40	0.54
5:A:620:ARG:HD3	5:A:623:ARG:NH2	2.23	0.54
5:A:810:GLU:OE2	5:A:814:GLN:NE2	2.32	0.54
11:G:93:ASP:OD1	11:G:94:ARG:N	2.38	0.54
15:K:109:GLN:HA	15:K:133:GLN:NE2	2.23	0.54
23:T:112:LEU:HA	23:T:115:ILE:HG12	1.90	0.54
25:X:635:VAL:HG11	25:X:644:THR:HG22	1.90	0.54
31:d:3:ASN:HD22	31:d:155:LEU:HG	1.70	0.54
32:m:452:GLN:NE2	32:m:502:ASP:OD1	2.40	0.54
38:6:52:G:H2'	38:6:53:G:C8	2.42	0.54
5:A:67:GLY:HA3	5:A:70:ARG:HD2	1.88	0.54
17:M:232:PHE:CE2	17:M:252:VAL:HG11	2.43	0.54
18:N:1151:SER:HA	18:N:1155:SER:HB3	1.90	0.54
20:P:118:LEU:HA	20:P:151:PHE:CZ	2.43	0.54
24:W:536:ILE:HG22	24:W:537:ARG:N	2.16	0.54
25:X:243:ARG:NH1	25:X:279:GLU:OE1	2.38	0.54
25:X:637:LEU:HD23	25:X:638:ASN:N	2.22	0.54
35:z:423:LEU:HD22	35:z:428:VAL:HG11	1.89	0.54
4:5:29:U:H4'	4:5:30:A:H5'	1.89	0.54
5:A:1268:ILE:HG21	5:A:1315:CYS:HB2	1.90	0.54
5:A:1663:VAL:HG11	5:A:1741:ASN:HB3	1.88	0.54
5:A:1799:GLN:HA	34:y:133:PHE:CD2	2.42	0.54
6:B:701:MET:HE2	6:B:805:LEU:HD13	1.88	0.54
6:B:739:ASP:OD2	29:b:66:LYS:HD3	2.08	0.54
11:G:42:GLN:HB2	11:G:112:ILE:HB	1.90	0.54
18:N:151:ILE:HG12	18:N:245:VAL:HG21	1.89	0.54
35:z:392:LEU:HD11	35:z:450:ALA:HB2	1.89	0.54
2:p:211:LEU:HD21	25:X:713:PRO:HB3	1.89	0.54
5:A:1653:ILE:HD11	5:A:1686:ILE:HB	1.89	0.54
13:I:52:VAL:O	13:I:55:VAL:HG22	2.08	0.54
18:N:798:HIS:NE2	18:N:924:GLN:HG2	2.23	0.54
20:P:268:ASN:O	20:P:272:LYS:NZ	2.39	0.54
34:y:138:ASP:OD2	35:z:417:MET:HE2	2.08	0.54
35:z:243:LEU:HD12	35:z:249:ILE:HD13	1.89	0.54
3:2:30:A:C5	34:y:37:PRO:HD2	2.42	0.54
5:A:216:ASP:HB3	5:A:219:ASP:HB3	1.90	0.54
5:A:1063:ILE:HA	5:A:1066:PHE:CE1	2.42	0.54
18:N:777:LEU:O	18:N:979:MET:N	2.40	0.54
23:V:105:LEU:O	23:V:108:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:485:TYR:O	25:X:489:LEU:HG	2.07	0.54
5:A:365:ASP:OD1	5:A:366:LEU:N	2.41	0.54
5:A:862:LEU:HD22	5:A:901:LEU:HG	1.90	0.54
17:M:84:MET:HB2	20:P:146:ALA:HB3	1.90	0.54
18:N:8:LYS:HE3	18:N:51:LEU:HD13	1.89	0.54
18:N:73:ASN:HA	18:N:76:ASN:ND2	2.23	0.54
18:N:485:VAL:HG22	18:N:503:CYS:SG	2.48	0.54
23:U:399:ASP:HB2	23:U:414:ILE:O	2.08	0.54
25:X:541:VAL:HG21	25:X:553:TRP:CE2	2.43	0.54
25:X:577:GLU:HA	25:X:580:LEU:HG	1.89	0.54
32:m:358:ASP:N	32:m:358:ASP:OD1	2.41	0.54
34:y:31:ARG:NH2	35:z:497:SER:OG	2.41	0.54
35:z:245:GLY:HA3	35:z:324:LYS:CD	2.37	0.54
5:A:869:LEU:HD23	5:A:886:GLU:OE2	2.08	0.54
15:K:92:SER:HA	15:K:95:VAL:HG12	1.89	0.54
16:L:237:PRO:HD3	22:R:136:ARG:HH12	1.73	0.54
22:R:248:ALA:HA	22:R:263:ILE:HD11	1.90	0.54
22:R:261:ARG:O	22:R:265:LYS:HG2	2.08	0.54
22:R:599:TRP:CH2	22:R:615:VAL:HG22	2.43	0.54
23:V:118:LEU:HD21	23:V:122:ARG:NH1	2.23	0.54
5:A:363:ASP:N	5:A:363:ASP:OD1	2.41	0.53
5:A:635:ILE:HD11	5:A:655:PRO:HG2	1.89	0.53
7:C:46:MET:HB3	7:C:334:ILE:HG13	1.88	0.53
18:N:773:ARG:HB2	18:N:973:PHE:HA	1.90	0.53
20:P:213:ALA:C	20:P:214:PHE:HD1	2.15	0.53
24:W:159:GLU:OE1	24:W:159:GLU:N	2.38	0.53
5:A:1622:ASP:OD2	34:y:86:ASN:ND2	2.41	0.53
7:C:325:ILE:HG22	7:C:337:GLY:HA3	1.91	0.53
30:c:512:LEU:HD22	30:c:519:TRP:CD1	2.43	0.53
9:E:95:LEU:HD12	9:E:96:SER:N	2.23	0.53
10:F:7:LEU:HB3	10:F:32:VAL:HG11	1.91	0.53
12:H:18:LYS:O	12:H:22:GLN:HG2	2.09	0.53
12:H:82:GLN:HE22	14:J:57:ILE:HD12	1.74	0.53
18:N:58:PHE:HA	18:N:62:LEU:HG	1.90	0.53
23:V:10:PRO:HG2	23:V:13:PRO:HG3	1.89	0.53
23:V:30:GLN:NE2	23:V:34:GLU:OE2	2.30	0.53
24:W:594:ASN:O	24:W:598:GLU:HG3	2.08	0.53
31:d:27:GLN:O	31:d:31:THR:HG22	2.09	0.53
35:z:153:LEU:HD12	35:z:382:ILE:HG13	1.90	0.53
35:z:367:THR:HG22	35:z:369:LYS:H	1.72	0.53
5:A:636:TYR:HE1	5:A:650:CYS:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:102:ARG:HH11	11:G:104:ASP:HB2	1.74	0.53
16:L:202:ILE:HD12	17:M:19:PHE:CZ	2.43	0.53
18:N:836:ARG:HH22	18:N:894:LYS:HB2	1.74	0.53
23:S:29:GLU:HG3	23:S:33:ARG:HH21	1.72	0.53
35:z:225:GLU:OE2	35:z:229:ASN:ND2	2.41	0.53
35:z:456:LEU:O	35:z:459:SER:OG	2.25	0.53
38:6:6:U:O2'	38:6:7:C:O5'	2.24	0.53
4:5:77:G:OP1	19:O:93:LYS:NZ	2.39	0.53
15:K:148:GLU:OE1	15:K:148:GLU:N	2.42	0.53
16:L:183:TYR:OH	28:a:96:ASN:OD1	2.13	0.53
18:N:399:LYS:HA	18:N:402:LEU:HD12	1.89	0.53
18:N:666:TYR:HB2	18:N:768:THR:HA	1.90	0.53
22:R:302:ASP:O	22:R:305:ARG:HG2	2.09	0.53
23:U:14:VAL:HG12	23:U:51:VAL:HB	1.89	0.53
24:W:236:TYR:CD1	26:Y:156:VAL:HG13	2.44	0.53
24:W:623:PHE:CZ	24:W:627:TYR:CZ	2.96	0.53
25:X:238:VAL:O	25:X:242:PHE:HD2	1.92	0.53
34:y:114:SER:O	35:z:643:TYR:OH	2.22	0.53
5:A:978:TRP:HZ2	5:A:1112:THR:HB	1.73	0.53
6:B:242:ASP:CG	6:B:271:LYS:HD2	2.33	0.53
17:M:238:LEU:O	17:M:255:LYS:NZ	2.41	0.53
18:N:737:ARG:HD3	18:N:1040:ILE:HD11	1.90	0.53
25:X:398:ARG:NH2	25:X:437:MET:HA	2.23	0.53
5:A:715:ASP:O	5:A:719:MET:HG2	2.08	0.53
11:G:45:ILE:HB	11:G:53:LEU:HB2	1.91	0.53
20:P:177:TYR:HD1	20:P:214:PHE:CE1	2.25	0.53
20:P:316:ASP:OD1	20:P:317:GLY:N	2.33	0.53
22:R:59:PHE:HD2	22:R:76:TYR:CD1	2.27	0.53
25:X:84:PRO:HG2	25:X:122:GLN:HG2	1.89	0.53
38:6:37:A:O2'	38:6:38:G:OP1	2.27	0.53
15:K:89:GLU:OE1	15:K:89:GLU:N	2.42	0.53
18:N:240:ARG:HA	18:N:284:ASN:HB3	1.91	0.53
18:N:686:VAL:HG13	18:N:690:LEU:HD13	1.91	0.53
18:N:809:GLY:HA2	18:N:814:LEU:HD12	1.90	0.53
20:P:213:ALA:O	20:P:214:PHE:HD1	1.91	0.53
6:B:821:GLN:HG3	32:m:727:ALA:HB1	1.91	0.53
15:K:344:PHE:HE2	15:K:360:PRO:HD3	1.73	0.53
18:N:264:ASN:HB3	18:N:267:PHE:HB3	1.91	0.53
18:N:360:PHE:HB3	18:N:366:ILE:HD12	1.89	0.53
19:O:26:PHE:HE1	19:O:55:GLN:HG2	1.74	0.53
23:T:69:LEU:HB2	23:T:70:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:90:LEU:HD13	23:U:90:LEU:HD22	1.89	0.53
23:U:117:ARG:HG3	23:U:118:LEU:N	2.24	0.53
23:V:5:ILE:HD11	23:V:23:TYR:HD1	1.74	0.53
5:A:1856:ARG:HD2	5:A:1856:ARG:O	2.09	0.53
6:B:249:ILE:HB	6:B:849:GLU:OE1	2.08	0.53
7:C:41:VAL:HG11	9:E:103:PRO:HB3	1.91	0.53
7:C:46:MET:HE2	7:C:77:TRP:CH2	2.44	0.53
13:I:26:TRP:HZ3	13:I:69:ASN:ND2	2.07	0.53
24:W:743:GLU:OE2	27:Z:176:SER:OG	2.25	0.53
5:A:386:HIS:CE1	6:B:311:ARG:HG3	2.45	0.52
5:A:1080:ARG:NH1	5:A:1083:GLU:OE1	2.34	0.52
5:A:1576:GLN:HG2	5:A:1587:HIS:CE1	2.43	0.52
7:C:314:ASN:N	7:C:328:CYS:O	2.40	0.52
18:N:749:PRO:HA	18:N:1010:ASN:HD22	1.73	0.52
20:P:181:ILE:HG13	20:P:183:PRO:HD3	1.91	0.52
22:R:70:MET:O	22:R:74:MET:HG2	2.09	0.52
24:W:47:ARG:HB2	24:W:144:GLU:OE1	2.09	0.52
29:b:57:HIS:O	29:b:61:ARG:HG3	2.09	0.52
39:1:0:G:H1'	39:1:1:G:OP2	2.09	0.52
6:B:930:ILE:HG22	6:B:932:PRO:HD3	1.91	0.52
11:G:7:LYS:N	11:G:8:PRO:HD3	2.24	0.52
16:L:275:ASP:HB3	16:L:277:ARG:HH11	1.74	0.52
16:L:289:ALA:HA	24:W:75:LEU:CD2	2.39	0.52
32:m:434:MET:O	32:m:439:LYS:N	2.39	0.52
32:m:447:LYS:NZ	32:m:480:ASP:OD1	2.40	0.52
5:A:921:PHE:HD2	5:A:928:LEU:HB3	1.73	0.52
6:B:575:LYS:NZ	6:B:625:ASN:O	2.41	0.52
18:N:307:GLN:HG3	18:N:311:PHE:CZ	2.44	0.52
18:N:823:TRP:HE1	18:N:931:PHE:HE2	1.57	0.52
24:W:704:LEU:HD21	24:W:708:ARG:HH21	1.73	0.52
25:X:470:LEU:O	25:X:475:ARG:NE	2.39	0.52
25:X:497:GLU:CD	25:X:497:GLU:H	2.17	0.52
30:c:417:TYR:HB2	30:c:449:MET:CE	2.39	0.52
38:6:49:C:OP2	38:6:68:U:O2'	2.23	0.52
5:A:1960:LEU:HA	5:A:1963:ILE:HD12	1.91	0.52
6:B:140:ASP:OD1	6:B:208:LYS:NZ	2.40	0.52
7:C:53:VAL:O	7:C:314:ASN:ND2	2.38	0.52
7:C:113:SER:HA	7:C:137:VAL:HG13	1.91	0.52
10:F:11:THR:HA	10:F:29:ILE:HD11	1.91	0.52
11:G:46:ASN:HB3	11:G:52:LYS:NZ	2.24	0.52
11:G:90:ILE:HG13	11:G:92:LYS:HZ3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:982:GLN:O	18:N:1027:SER:OG	2.25	0.52
18:N:1143:VAL:HG13	18:N:1166:VAL:HG12	1.91	0.52
24:W:537:ARG:HG3	24:W:538:PRO:CD	2.40	0.52
25:X:597:ASP:O	25:X:601:LYS:HG2	2.09	0.52
38:6:13:A:O2'	38:6:14:C:OP1	2.28	0.52
5:A:312:TRP:CD1	5:A:314:GLU:H	2.27	0.52
5:A:1150:ASN:O	5:A:1176:ARG:NH2	2.43	0.52
5:A:1406:SER:HA	5:A:1439:GLY:HA2	1.90	0.52
18:N:213:GLU:OE1	18:N:218:LYS:HD2	2.10	0.52
18:N:318:LEU:HB2	18:N:322:VAL:HG23	1.92	0.52
18:N:449:LEU:HD13	18:N:557:PHE:HZ	1.75	0.52
22:R:215:GLU:OE2	22:R:253:ARG:NE	2.42	0.52
23:S:118:LEU:O	23:S:122:ARG:HD3	2.10	0.52
24:W:262:ARG:HA	24:W:265:GLU:CD	2.35	0.52
30:c:579:ARG:HA	30:c:582:ARG:HH21	1.75	0.52
4:5:38:U:P	5:A:623:ARG:HH21	2.33	0.52
4:5:100:U:C2	10:F:35:GLN:NE2	2.76	0.52
6:B:370:LYS:O	6:B:370:LYS:NZ	2.27	0.52
15:K:373:ALA:HB1	15:K:392:ASN:HD21	1.75	0.52
18:N:137:GLU:HA	18:N:140:ARG:HG3	1.90	0.52
18:N:787:LEU:O	18:N:791:LEU:HG	2.09	0.52
22:R:524:ARG:HG2	22:R:543:PHE:HE1	1.75	0.52
23:T:88:PHE:O	23:T:92:ARG:HG2	2.10	0.52
27:Z:27:GLN:HA	27:Z:30:GLU:HG3	1.91	0.52
31:d:52:ILE:HD11	31:d:106:LEU:HD11	1.92	0.52
32:m:362:VAL:HG11	32:m:429:HIS:CE1	2.45	0.52
32:m:718:PHE:CE2	32:m:764:LEU:HD22	2.44	0.52
5:A:874:SER:OG	5:A:876:LYS:NZ	2.28	0.52
6:B:916:ASP:OD2	6:B:917:HIS:ND1	2.38	0.52
20:P:106:THR:HG23	20:P:108:ALA:H	1.75	0.52
25:X:96:ASP:O	25:X:99:GLU:HG3	2.10	0.52
25:X:490:GLU:OE2	25:X:499:THR:OG1	2.27	0.52
28:a:69:PRO:HD3	31:d:53:GLN:OE1	2.10	0.52
5:A:1548:SER:O	5:A:1552:GLN:HG2	2.10	0.52
7:C:121:ASP:HB2	7:C:128:ILE:HD11	1.91	0.52
15:K:346:PHE:HD1	15:K:359:PHE:HE1	1.57	0.52
18:N:18:ASN:HA	18:N:25:VAL:HG21	1.92	0.52
18:N:117:LEU:HD11	18:N:205:LYS:HB3	1.92	0.52
22:R:116:LYS:HZ1	26:Y:172:ILE:HG22	1.74	0.52
32:m:488:ALA:HA	32:m:491:LYS:HE3	1.92	0.52
32:m:535:SER:OG	32:m:536:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1286:LYS:HG3	34:y:213:GLU:OE1	2.10	0.52
6:B:179:TYR:O	6:B:180:THR:OG1	2.19	0.52
6:B:960:ASP:OD1	6:B:961:VAL:N	2.42	0.52
15:K:231:CYS:HB3	15:K:241:ARG:HB2	1.92	0.52
16:L:92:ALA:HB1	16:L:102:ASP:H	1.75	0.52
17:M:84:MET:HG2	20:P:147:ASN:HB3	1.91	0.52
18:N:1177:ARG:NH2	18:N:1209:TYR:OH	2.43	0.52
25:X:263:TYR:CZ	25:X:267:ILE:HD11	2.45	0.52
32:m:300:ILE:HD11	33:n:310:ILE:HD12	1.92	0.52
32:m:362:VAL:HG11	32:m:429:HIS:ND1	2.25	0.52
35:z:412:PRO:HB2	35:z:415:HIS:CD2	2.39	0.52
5:A:1256:VAL:HG22	5:A:1298:TYR:CD1	2.45	0.52
6:B:105:ILE:HD11	15:K:199:LEU:CD2	2.40	0.52
13:I:30:TYR:CE1	13:I:50:GLU:HG2	2.45	0.52
17:M:75:ARG:HG3	17:M:75:ARG:HH11	1.74	0.52
30:c:409:LEU:O	30:c:413:ARG:HG3	2.10	0.52
38:6:47:A:H5''	38:6:47:A:C8	2.44	0.52
4:5:18:U:OP1	5:A:243:THR:OG1	2.24	0.51
5:A:389:ASP:N	5:A:389:ASP:OD1	2.43	0.51
5:A:754:LEU:HD12	5:A:755:PRO:HD2	1.91	0.51
5:A:1238:TRP:NE1	5:A:1300:GLU:OE2	2.40	0.51
5:A:1410:TRP:CH2	5:A:1446:LEU:HD21	2.46	0.51
7:C:203:ILE:HB	7:C:213:HIS:CD2	2.40	0.51
9:E:107:GLY:HA2	28:a:52:GLU:H	1.74	0.51
15:K:172:GLU:HG2	15:K:177:TRP:CE2	2.45	0.51
18:N:256:ARG:HG3	18:N:261:TYR:CZ	2.45	0.51
20:P:117:CYS:HB2	20:P:120:PHE:HB3	1.91	0.51
23:V:11:LYS:O	23:V:55:VAL:HG21	2.09	0.51
24:W:258:GLU:O	24:W:262:ARG:HD3	2.09	0.51
25:X:445:ASP:HB2	25:X:449:LYS:HZ3	1.76	0.51
27:Z:171:GLY:O	27:Z:175:GLN:HG2	2.10	0.51
30:c:480:SER:HA	30:c:483:GLU:OE1	2.10	0.51
5:A:750:LYS:HG2	16:L:279:LEU:HD22	1.90	0.51
8:D:70:ILE:HD13	9:E:68:VAL:HG22	1.92	0.51
18:N:39:VAL:HG22	18:N:48:VAL:HG11	1.92	0.51
18:N:739:SER:HA	18:N:765:LEU:HD21	1.92	0.51
20:P:85:ASP:HB2	20:P:88:LYS:CB	2.28	0.51
22:R:84:LYS:HZ3	22:R:87:ALA:HB3	1.73	0.51
22:R:573:ARG:HG3	22:R:602:PHE:HE2	1.74	0.51
23:T:96:GLU:HA	23:T:99:GLN:HG2	1.92	0.51
25:X:537:TYR:HB3	25:X:556:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:119:LEU:HD13	29:b:122:ALA:HB3	1.91	0.51
35:z:271:VAL:HG23	35:z:297:LYS:HA	1.92	0.51
5:A:167:THR:HG21	5:A:228:TYR:OH	2.10	0.51
5:A:1642:LYS:HG3	5:A:1650:CYS:SG	2.51	0.51
5:A:1848:THR:HA	5:A:1851:TRP:HE3	1.74	0.51
6:B:114:ILE:HG21	6:B:661:LEU:HD11	1.91	0.51
6:B:195:SER:HB3	6:B:226:GLU:HB3	1.93	0.51
6:B:396:THR:HG23	6:B:427:LEU:HG	1.92	0.51
6:B:861:TYR:OH	6:B:874:ASP:OD2	2.20	0.51
7:C:239:MET:HE1	7:C:270:HIS:CD2	2.45	0.51
16:L:324:LYS:HE2	32:m:513:PRO:HA	1.92	0.51
18:N:460:TYR:CD1	18:N:472:LEU:HD21	2.45	0.51
5:A:1669:LEU:HD13	5:A:1738:ALA:HB3	1.93	0.51
8:D:17:THR:HA	8:D:26:TYR:O	2.10	0.51
16:L:124:LEU:HD11	16:L:234:LEU:HD22	1.91	0.51
23:S:122:ARG:NH2	23:V:114:VAL:HG13	2.10	0.51
25:X:419:VAL:HB	25:X:421:TYR:CE1	2.46	0.51
25:X:429:GLN:HA	25:X:432:ILE:HG12	1.92	0.51
26:Y:127:TYR:HE2	26:Y:167:ARG:HH12	1.58	0.51
31:d:88:LEU:HD11	31:d:102:PHE:CD2	2.45	0.51
32:m:593:ILE:O	32:m:597:TRP:HD1	1.94	0.51
35:z:430:ASP:OD1	35:z:434:ASN:N	2.40	0.51
35:z:474:ILE:HD12	35:z:480:VAL:HG11	1.93	0.51
35:z:606:LEU:HA	35:z:609:LYS:HG2	1.93	0.51
15:K:241:ARG:HG3	15:K:279:ARG:HD3	1.92	0.51
15:K:346:PHE:HB3	15:K:359:PHE:CE1	2.45	0.51
21:Q:223:ARG:C	21:Q:225:TRP:N	2.65	0.51
22:R:118:ARG:HG3	26:Y:165:VAL:CG1	2.38	0.51
24:W:574:ASN:OD1	24:W:575:TYR:N	2.43	0.51
25:X:448:ARG:NH2	25:X:494:GLY:HA2	2.25	0.51
30:c:557:VAL:O	30:c:561:HIS:HB2	2.11	0.51
35:z:144:ILE:HG23	35:z:175:VAL:HB	1.92	0.51
5:A:92:LYS:HE3	19:O:34:GLU:HB3	1.92	0.51
5:A:1568:ARG:NE	5:A:1696:ASP:OD2	2.31	0.51
5:A:1602:ARG:NE	5:A:1770:ARG:HH21	2.07	0.51
6:B:823:ILE:CG1	6:B:824:PRO:HD3	2.41	0.51
8:D:17:THR:OG1	8:D:70:ILE:HB	2.11	0.51
14:J:28:TYR:CE2	14:J:54:LYS:HE3	2.46	0.51
18:N:776:VAL:HG12	18:N:979:MET:HE2	1.92	0.51
18:N:1017:ASN:ND2	18:N:1170:GLU:OE2	2.44	0.51
20:P:149:ASP:OD1	20:P:224:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:114:VAL:HG12	23:U:115:ILE:HD12	1.91	0.51
25:X:289:ASN:O	25:X:292:ILE:HG22	2.11	0.51
34:y:164:TYR:OH	35:z:329:ASN:OD1	2.19	0.51
38:6:84:A:H2'	38:6:85:G:C8	2.45	0.51
5:A:1605:LEU:HD22	5:A:1770:ARG:NH1	2.20	0.51
18:N:216:GLU:HG2	18:N:260:TYR:CD1	2.45	0.51
18:N:502:LYS:HE3	18:N:584:ASN:HB3	1.93	0.51
23:S:122:ARG:NH2	23:V:115:ILE:HD13	2.17	0.51
25:X:555:LEU:O	25:X:559:LYS:HG2	2.09	0.51
34:y:164:TYR:HE2	35:z:330:PRO:HD2	1.75	0.51
4:5:101:U:H3	11:G:65:ASN:HD21	1.57	0.51
5:A:1834:PHE:HA	5:A:1841:LEU:HD23	1.93	0.51
5:A:1897:GLU:HA	5:A:1900:LEU:HB2	1.93	0.51
7:C:319:HIS:HB2	7:C:324:ILE:HB	1.93	0.51
10:F:47:VAL:HB	10:F:50:ARG:HB2	1.93	0.51
18:N:413:SER:OG	18:N:416:ASN:ND2	2.38	0.51
19:O:95:PRO:HA	19:O:98:GLU:OE2	2.10	0.51
24:W:220:ASP:O	24:W:222:ASN:N	2.44	0.51
25:X:193:GLU:O	25:X:197:GLN:HG2	2.11	0.51
25:X:278:TYR:HE1	25:X:332:ILE:HD13	1.75	0.51
30:c:409:LEU:HD11	30:c:445:GLU:HG3	1.92	0.51
31:d:3:ASN:HD21	31:d:14:LEU:HD11	1.74	0.51
5:A:965:PRO:HD2	5:A:1462:VAL:HG22	1.92	0.51
5:A:971:PRO:HB3	5:A:1215:THR:HG21	1.93	0.51
12:H:60:ASP:OD1	12:H:61:ALA:N	2.35	0.51
15:K:216:ARG:NH2	15:K:260:ASP:OD1	2.43	0.51
16:L:217:PHE:CZ	17:M:50:PRO:HG3	2.46	0.51
18:N:652:PRO:HB2	18:N:1037:SER:HA	1.92	0.51
25:X:144:HIS:HB2	25:X:148:TRP:CD1	2.46	0.51
25:X:183:GLU:O	25:X:187:LYS:HG2	2.11	0.51
25:X:719:GLU:O	25:X:722:ARG:HB3	2.11	0.51
2:p:214:GLU:CD	25:X:708:ILE:HG22	2.36	0.51
4:5:49:U:H2'	4:5:50:U:H6	1.76	0.51
5:A:410:PHE:HE2	6:B:338:LEU:CD2	2.24	0.51
5:A:1762:PRO:HB3	34:y:94:ILE:HA	1.92	0.51
7:C:115:THR:HG22	7:C:136:GLY:C	2.36	0.51
7:C:240:ASP:OD1	7:C:242:THR:OG1	2.27	0.51
10:F:29:ILE:HA	10:F:40:LEU:HD23	1.93	0.51
11:G:32:VAL:HG23	11:G:33:LEU:HD22	1.93	0.51
18:N:789:THR:OG1	18:N:816:ARG:NH2	2.44	0.51
20:P:131:CYS:SG	20:P:132:GLU:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:122:ARG:HH11	23:V:118:LEU:HD22	1.76	0.51
25:X:103:ILE:HG22	25:X:104:LEU:HD22	1.92	0.51
25:X:417:THR:HG22	25:X:430:VAL:HG11	1.93	0.51
35:z:136:LEU:O	35:z:169:ARG:HD2	2.11	0.51
5:A:1035:LYS:HG3	5:A:1057:LEU:HD13	1.92	0.50
5:A:1986:THR:HG22	5:A:1993:PRO:HA	1.93	0.50
6:B:180:THR:HG22	6:B:549:ALA:HB2	1.91	0.50
10:F:76:LEU:O	10:F:80:LEU:HD23	2.10	0.50
15:K:354:ILE:HB	15:K:368:PHE:HB2	1.93	0.50
17:M:171:LYS:NZ	17:M:174:ARG:HD3	2.26	0.50
18:N:483:PHE:HE1	18:N:505:MET:HE3	1.75	0.50
18:N:1108:GLN:HE21	18:N:1141:SER:HB2	1.76	0.50
22:R:85:GLU:O	22:R:86:PHE:HD1	1.94	0.50
22:R:174:TRP:O	22:R:178:ILE:HG12	2.11	0.50
22:R:603:GLU:HG3	22:R:615:VAL:HG21	1.93	0.50
23:S:60:ARG:NH1	24:W:701:TRP:HB3	2.26	0.50
23:U:59:VAL:HG23	23:U:61:PRO:HD3	1.91	0.50
28:a:67:LEU:O	28:a:67:LEU:HD23	2.11	0.50
35:z:59:PRO:HG2	35:z:121:TYR:OH	2.11	0.50
4:5:97:U:H1'	14:J:65:ASN:HB2	1.94	0.50
6:B:231:MET:HE1	6:B:257:HIS:ND1	2.26	0.50
7:C:44:LEU:HD23	7:C:336:LEU:HD12	1.93	0.50
13:I:50:GLU:OE2	13:I:52:VAL:HB	2.11	0.50
18:N:751:ARG:HH12	18:N:1208:SER:HA	1.77	0.50
23:T:122:ARG:NH2	23:U:121:GLU:OE1	2.44	0.50
24:W:196:LEU:HD21	24:W:200:ARG:HH21	1.75	0.50
25:X:631:LEU:O	25:X:635:VAL:HG23	2.10	0.50
32:m:449:TRP:HZ2	32:m:456:LYS:HB2	1.76	0.50
38:6:55:C:H2'	38:6:56:C:O4'	2.11	0.50
5:A:197:PHE:CE2	5:A:589:LEU:HD21	2.45	0.50
5:A:1018:ARG:HG3	16:L:295:LEU:HD13	1.93	0.50
5:A:1603:SER:O	5:A:1605:LEU:N	2.44	0.50
5:A:1666:PRO:HD3	5:A:1741:ASN:ND2	2.24	0.50
6:B:404:LEU:O	6:B:408:LEU:HG	2.12	0.50
15:K:270:VAL:HG11	15:K:284:VAL:HG13	1.93	0.50
16:L:186:TYR:HD1	28:a:89:ALA:HB2	1.77	0.50
22:R:447:ILE:HG22	22:R:449:GLN:HG2	1.92	0.50
23:T:127:GLU:O	23:T:131:LYS:HG2	2.12	0.50
25:X:154:TYR:O	25:X:158:ILE:HG22	2.12	0.50
31:d:3:ASN:ND2	31:d:14:LEU:HD11	2.26	0.50
5:A:1495:ARG:HG3	34:y:218:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:455:THR:OG1	15:K:458:THR:OG1	2.14	0.50
17:M:69:ILE:HG23	17:M:84:MET:HE1	1.93	0.50
23:S:59:VAL:O	24:W:701:TRP:NE1	2.45	0.50
24:W:238:THR:HG23	24:W:241:GLU:HB3	1.93	0.50
25:X:398:ARG:NH2	25:X:436:GLU:OE1	2.37	0.50
31:d:28:ASN:O	31:d:32:LEU:HB2	2.11	0.50
35:z:143:VAL:HB	35:z:172:PHE:CZ	2.47	0.50
1:e:182:ASP:HB2	16:L:239:ARG:HH21	1.77	0.50
5:A:898:HIS:HB2	35:z:217:GLU:OE1	2.11	0.50
5:A:1099:ASP:N	5:A:1099:ASP:OD1	2.43	0.50
5:A:1371:ASP:OD1	5:A:1371:ASP:N	2.45	0.50
5:A:1490:GLN:NE2	5:A:1492:ASN:HD22	2.07	0.50
9:E:44:GLU:OE1	9:E:63:ARG:NE	2.38	0.50
10:F:33:ASP:OD1	10:F:34:MET:N	2.44	0.50
22:R:61:ASP:OD1	22:R:62:ALA:N	2.44	0.50
30:c:545:GLN:O	30:c:549:GLU:OE1	2.30	0.50
32:m:619:LEU:HD23	32:m:622:LEU:HD12	1.93	0.50
38:6:59:G:N2	38:6:62:C:OP2	2.31	0.50
8:D:27:ARG:HB3	8:D:45:SER:OG	2.12	0.50
9:E:15:ASN:ND2	9:E:81:GLN:HE21	2.10	0.50
10:F:69:ILE:HD12	11:G:96:ILE:HG21	1.94	0.50
15:K:346:PHE:HB3	15:K:359:PHE:HE1	1.76	0.50
22:R:186:GLU:HG3	22:R:188:GLU:OE2	2.12	0.50
25:X:98:PHE:CD1	25:X:111:ILE:HG23	2.46	0.50
35:z:145:LEU:HD11	35:z:162:LEU:HD22	1.94	0.50
35:z:162:LEU:HD23	35:z:174:LEU:HD22	1.94	0.50
5:A:405:ILE:HG22	6:B:346:ILE:HD13	1.93	0.50
5:A:1190:LEU:HD12	5:A:1191:THR:HG22	1.92	0.50
13:I:71:LEU:HD22	13:I:72:TRP:CD1	2.46	0.50
17:M:79:CYS:SG	17:M:80:CYS:N	2.85	0.50
18:N:745:MET:HE1	18:N:1007:LEU:HD12	1.93	0.50
18:N:898:PRO:HG2	18:N:901:THR:HG23	1.93	0.50
20:P:175:THR:HB	20:P:216:THR:HG23	1.92	0.50
20:P:178:VAL:HG23	20:P:243:VAL:HG22	1.93	0.50
23:U:388:TYR:HA	23:U:405:LEU:HD22	1.92	0.50
25:X:707:GLU:OE1	25:X:720:MET:HE3	2.12	0.50
32:m:725:PHE:CZ	32:m:787:PHE:HB3	2.47	0.50
5:A:810:GLU:OE2	5:A:813:ARG:NH2	2.42	0.50
9:E:20:ASP:OD2	9:E:22:ARG:NH2	2.45	0.50
15:K:173:PRO:HG3	15:K:215:PRO:HA	1.92	0.50
17:M:107:PRO:O	17:M:113:ARG:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:245:ILE:HD11	22:R:279:LEU:HA	1.92	0.50
22:R:460:TRP:CE2	22:R:470:PRO:HG3	2.46	0.50
24:W:600:CYS:HA	24:W:603:LEU:HG	1.93	0.50
35:z:325:GLN:O	35:z:337:LEU:HD12	2.12	0.50
35:z:497:SER:HA	35:z:500:PHE:CE2	2.47	0.50
7:C:232:SER:HB2	7:C:249:LYS:HE3	1.93	0.50
9:E:106:ARG:O	28:a:53:LEU:N	2.44	0.50
11:G:42:GLN:OE1	11:G:56:ARG:NH1	2.45	0.50
12:H:80:LEU:HD23	12:H:81:ILE:N	2.26	0.50
15:K:346:PHE:CD1	15:K:359:PHE:HE1	2.29	0.50
22:R:107:TRP:O	22:R:111:ILE:HG12	2.12	0.50
23:V:40:VAL:HG23	23:V:41:THR:HG23	1.92	0.50
24:W:6:GLY:HA2	24:W:43:GLN:HE22	1.77	0.50
26:Y:155:TRP:HA	26:Y:158:ASN:OD1	2.11	0.50
5:A:696:THR:OG1	38:6:64:A:OP1	2.21	0.49
5:A:1233:LEU:O	30:c:466:LEU:HD11	2.12	0.49
7:C:278:SER:OG	7:C:283:PHE:HB2	2.12	0.49
10:F:20:LYS:HB2	10:F:64:ASN:HA	1.94	0.49
13:I:21:LEU:HD11	13:I:29:GLU:HB2	1.93	0.49
18:N:191:LEU:O	18:N:195:LEU:HG	2.12	0.49
18:N:592:TYR:OH	18:N:602:ARG:NH1	2.42	0.49
23:U:476:LEU:H	23:U:488:GLY:C	2.20	0.49
25:X:68:TRP:NE1	25:X:104:LEU:HD23	2.21	0.49
32:m:547:PHE:HA	32:m:550:TRP:HD1	1.77	0.49
34:y:92:MET:HE3	34:y:96:ASP:HB2	1.94	0.49
5:A:411:PHE:HB2	6:B:391:LYS:HD2	1.93	0.49
5:A:1815:HIS:HB2	5:A:1823:THR:HB	1.94	0.49
8:D:89:VAL:HG12	8:D:91:LEU:HG	1.92	0.49
18:N:493:ILE:HD12	25:X:202:LEU:HD11	1.94	0.49
18:N:745:MET:HE3	18:N:1029:PHE:CD1	2.46	0.49
25:X:703:TRP:O	25:X:707:GLU:HG3	2.11	0.49
28:a:61:GLU:O	28:a:62:MET:HE2	2.12	0.49
6:B:531:GLU:HA	32:m:756:LYS:HD2	1.95	0.49
15:K:356:HIS:CD2	15:K:365:MET:HE2	2.48	0.49
23:T:5:ILE:HA	23:U:88:PHE:CD1	2.47	0.49
23:V:86:GLU:O	23:V:89:GLU:HG2	2.12	0.49
24:W:198:LYS:O	24:W:201:GLU:HG3	2.12	0.49
24:W:510:ARG:NE	24:W:510:ARG:O	2.45	0.49
25:X:265:ILE:HG12	25:X:300:PHE:CE1	2.47	0.49
38:6:49:C:H2'	38:6:50:A:O4'	2.13	0.49
4:5:56:A:O2'	4:5:57:G:H5''	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:492:VAL:HG22	6:B:508:ALA:HB2	1.94	0.49
6:B:501:ALA:HB2	6:B:661:LEU:HD12	1.94	0.49
11:G:111:ARG:HD2	13:I:62:GLU:OE2	2.12	0.49
15:K:89:GLU:OE1	22:R:259:ARG:HG2	2.12	0.49
15:K:392:ASN:OD1	15:K:394:SER:OG	2.22	0.49
23:T:67:THR:HG21	27:Z:105:ARG:HG3	1.93	0.49
23:V:106:TYR:OH	23:V:113:ARG:NH1	2.45	0.49
24:W:266:MET:HA	24:W:269:GLU:HG2	1.93	0.49
24:W:537:ARG:CG	24:W:538:PRO:HD2	2.43	0.49
25:X:585:PRO:HB3	25:X:619:VAL:HA	1.94	0.49
34:y:25:PHE:CE2	34:y:27:LEU:HA	2.48	0.49
35:z:543:ARG:O	35:z:547:VAL:HG23	2.12	0.49
5:A:1282:LYS:NZ	34:y:214:ASP:OD2	2.39	0.49
9:E:5:LYS:HE2	10:F:30:THR:HG21	1.94	0.49
9:E:32:ASP:OD1	9:E:33:GLY:N	2.45	0.49
23:U:24:GLU:HB3	23:U:27:LEU:HD12	1.94	0.49
23:U:361:GLU:HB3	23:U:364:SER:OG	2.12	0.49
23:V:102:SER:HA	23:V:105:LEU:HD12	1.95	0.49
32:m:308:GLY:HA2	32:m:311:MET:HG2	1.94	0.49
35:z:625:GLN:HB2	35:z:627:PHE:CE1	2.47	0.49
35:z:628:VAL:HG23	35:z:631:ILE:HD11	1.93	0.49
38:6:34:U:H2'	38:6:35:A:C8	2.43	0.49
5:A:1461:ARG:NH1	5:A:1479:TRP:O	2.45	0.49
6:B:752:ASP:OD2	6:B:789:ARG:NH2	2.43	0.49
22:R:388:GLU:O	22:R:391:LYS:HG2	2.12	0.49
25:X:251:ASP:OD1	25:X:251:ASP:N	2.45	0.49
34:y:143:LYS:HA	34:y:146:LYS:HD2	1.93	0.49
39:1:0:G:O2'	39:1:1:G:OP1	2.31	0.49
5:A:324:ARG:HG3	6:B:892:ILE:HG13	1.94	0.49
5:A:839:TRP:CZ2	5:A:843:ARG:HD2	2.47	0.49
7:C:61:SER:O	7:C:321:HIS:NE2	2.46	0.49
11:G:15:ILE:H	11:G:15:ILE:HD12	1.77	0.49
11:G:74:MET:N	11:G:74:MET:SD	2.86	0.49
13:I:15:LEU:HD23	13:I:15:LEU:O	2.12	0.49
14:J:21:LEU:HD21	14:J:62:ILE:HD13	1.94	0.49
15:K:268:ASP:OD2	15:K:272:ARG:NH1	2.45	0.49
22:R:302:ASP:OD1	22:R:303:LYS:N	2.46	0.49
22:R:599:TRP:CZ3	22:R:615:VAL:HG22	2.48	0.49
23:U:69:LEU:HD21	23:V:75:LEU:HB2	1.94	0.49
25:X:457:ALA:HB3	25:X:505:ARG:HH12	1.78	0.49
25:X:599:GLU:O	25:X:603:GLY:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:z:268:GLN:OE1	35:z:296:ARG:NE	2.38	0.49
1:e:32:GLU:O	1:e:35:TYR:N	2.46	0.49
5:A:1595:ILE:HG12	34:y:55:ALA:HB2	1.94	0.49
6:B:951:THR:HG22	6:B:955:LYS:HD2	1.95	0.49
7:C:266:HIS:CD2	7:C:273:LEU:HD12	2.48	0.49
10:F:27:GLY:HA3	10:F:43:VAL:HG12	1.95	0.49
17:M:235:TYR:HB3	17:M:263:ALA:HB2	1.94	0.49
18:N:629:VAL:HA	18:N:632:LEU:HD23	1.94	0.49
22:R:104:ILE:H	22:R:104:ILE:HD12	1.77	0.49
22:R:237:GLU:HG2	22:R:238:PHE:CD1	2.48	0.49
22:R:287:GLU:HB3	22:R:302:ASP:OD2	2.12	0.49
22:R:488:ARG:HG2	22:R:513:PHE:HE2	1.78	0.49
23:U:15:ILE:HD13	23:V:53:VAL:HG23	1.94	0.49
35:z:131:ILE:HG12	35:z:137:LEU:HD11	1.94	0.49
35:z:153:LEU:HD13	35:z:382:ILE:HA	1.95	0.49
5:A:1671:ASP:OD1	5:A:1671:ASP:N	2.42	0.49
17:M:150:ARG:HH12	20:P:263:GLU:HB2	1.77	0.49
18:N:929:ARG:HB3	25:X:137:ARG:HH12	1.77	0.49
22:R:84:LYS:HA	24:W:253:ASP:OD1	2.13	0.49
22:R:154:ILE:HA	22:R:157:CYS:SG	2.52	0.49
22:R:291:GLY:HA3	25:X:535:LYS:NZ	2.28	0.49
23:U:96:GLU:O	23:U:100:GLU:HG2	2.13	0.49
23:U:351:GLY:HA2	23:U:357:LEU:HA	1.95	0.49
24:W:529:GLN:O	24:W:530:VAL:HG22	2.13	0.49
25:X:572:THR:O	25:X:575:LEU:HG	2.13	0.49
34:y:223:PRO:HD2	34:y:225:MET:HE1	1.93	0.49
35:z:242:PHE:HE2	35:z:306:GLU:HG3	1.78	0.49
35:z:491:ASP:HA	35:z:494:VAL:HG22	1.95	0.49
5:A:1567:ASN:HB2	5:A:1593:LEU:HD21	1.95	0.49
5:A:1747:LYS:HB3	5:A:1748:PRO:HD3	1.95	0.49
6:B:570:ASP:N	6:B:570:ASP:OD1	2.44	0.49
6:B:600:SER:HB3	6:B:644:PHE:HB3	1.95	0.49
13:I:15:LEU:HD21	13:I:20:VAL:HG11	1.95	0.49
20:P:98:VAL:H	20:P:101:ARG:HH12	1.60	0.49
25:X:192:ASN:ND2	25:X:232:HIS:O	2.33	0.49
35:z:355:GLY:HA2	35:z:358:MET:O	2.13	0.49
5:A:613:GLY:HA2	5:A:615:TYR:CE2	2.48	0.48
6:B:694:ASN:OD1	6:B:696:LYS:HG2	2.13	0.48
16:L:241:VAL:O	16:L:245:GLU:HB2	2.13	0.48
18:N:77:LEU:HD12	18:N:80:MET:SD	2.53	0.48
20:P:83:ARG:HD3	38:6:31:C:C4	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:300:VAL:HG13	22:R:304:ARG:CZ	2.43	0.48
23:T:32:ILE:HD11	23:T:45:CYS:HB3	1.95	0.48
23:U:299:ASN:N	23:U:313:ALA:O	2.46	0.48
25:X:263:TYR:O	25:X:267:ILE:HG13	2.13	0.48
25:X:621:THR:HA	25:X:624:ARG:NE	2.14	0.48
6:B:287:TYR:OH	6:B:357:GLY:HA2	2.13	0.48
6:B:740:LEU:HD23	6:B:744:ARG:HG3	1.95	0.48
11:G:44:LEU:HD13	11:G:54:LEU:CD1	2.43	0.48
20:P:82:MET:HG2	38:6:32:G:C2	2.41	0.48
20:P:93:SER:OG	20:P:233:GLN:OE1	2.31	0.48
24:W:696:LYS:HG3	27:Z:131:LEU:HB2	1.95	0.48
25:X:230:PRO:HB3	25:X:263:TYR:CD1	2.48	0.48
4:5:27:G:O2'	4:5:28:C:OP2	2.28	0.48
5:A:1684:TYR:CB	5:A:1724:GLY:HA2	2.42	0.48
5:A:1970:ASN:ND2	5:A:2014:ASP:OD2	2.46	0.48
6:B:757:ASN:OD1	6:B:788:THR:OG1	2.32	0.48
13:I:49:GLU:HG3	13:I:56:LYS:HD3	1.96	0.48
18:N:529:LEU:HD12	18:N:530:CYS:H	1.79	0.48
18:N:1112:GLU:OE2	18:N:1184:THR:HB	2.13	0.48
22:R:21:GLU:CD	22:R:21:GLU:H	2.21	0.48
24:W:657:TYR:CE2	27:Z:92:LEU:HD23	2.48	0.48
34:y:92:MET:HE2	34:y:97:ILE:HG23	1.95	0.48
5:A:234:GLU:HG3	5:A:242:PRO:HA	1.94	0.48
5:A:1268:ILE:HD13	5:A:1271:ILE:HD12	1.95	0.48
5:A:1492:ASN:ND2	34:y:220:LEU:HG	2.29	0.48
11:G:90:ILE:HG13	11:G:92:LYS:NZ	2.27	0.48
16:L:111:HIS:NE2	16:L:229:PRO:O	2.43	0.48
18:N:666:TYR:CE1	18:N:696:LEU:HD13	2.47	0.48
18:N:798:HIS:HD1	18:N:801:HIS:H	1.61	0.48
18:N:805:LEU:HB2	18:N:954:CYS:HB3	1.96	0.48
18:N:1121:GLN:O	18:N:1125:MET:HG2	2.14	0.48
20:P:261:ARG:HH12	20:P:265:ARG:HH21	1.61	0.48
22:R:54:ARG:HA	22:R:57:LYS:HE3	1.94	0.48
22:R:147:MET:HE3	22:R:148:GLU:OE1	2.13	0.48
23:S:129:LEU:CD2	23:V:125:ALA:HB2	2.43	0.48
27:Z:97:VAL:HA	27:Z:100:GLU:OE2	2.13	0.48
5:A:1584:ILE:HD13	5:A:1597:LEU:HD13	1.95	0.48
6:B:922:PRO:HG2	6:B:943:LEU:HD12	1.95	0.48
10:F:18:GLU:HG3	10:F:24:ILE:HG13	1.94	0.48
15:K:470:ARG:HH12	15:K:472:ARG:HD2	1.79	0.48
16:L:191:GLN:NE2	17:M:23:CYS:HA	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:256:THR:HG23	17:M:259:SER:H	1.78	0.48
18:N:202:LEU:HD23	18:N:228:MET:HE1	1.96	0.48
23:U:191:ALA:O	23:U:485:LEU:N	2.46	0.48
25:X:589:LYS:NZ	25:X:623:ASP:O	2.45	0.48
28:a:96:ASN:O	28:a:100:ASN:ND2	2.46	0.48
1:e:204:HIS:CB	6:B:76:GLN:HB2	2.33	0.48
4:5:100:U:H4'	4:5:101:U:H5'	1.94	0.48
5:A:309:MET:HG3	5:A:311:ASP:H	1.78	0.48
5:A:1182:ILE:HD13	5:A:1185:ARG:HH11	1.78	0.48
6:B:601:VAL:HB	6:B:844:PRO:HG3	1.95	0.48
6:B:684:SER:HB3	6:B:702:VAL:HG23	1.96	0.48
13:I:25:LYS:HE2	13:I:68:ASN:O	2.14	0.48
18:N:70:MET:HG3	18:N:74:HIS:ND1	2.28	0.48
18:N:321:LEU:HD13	18:N:338:ILE:HA	1.96	0.48
21:Q:240:ASP:OD1	21:Q:240:ASP:N	2.44	0.48
22:R:322:TRP:HD1	22:R:325:LEU:HB2	1.79	0.48
24:W:710:ASN:OD1	24:W:711:LEU:N	2.46	0.48
26:Y:95:LYS:HE2	26:Y:121:ARG:HH22	1.77	0.48
32:m:575:MET:HE2	32:m:579:LEU:HD13	1.94	0.48
35:z:561:LEU:HD12	35:z:562:PRO:HD2	1.95	0.48
35:z:611:THR:HG21	35:z:633:LYS:HB2	1.96	0.48
3:2:12:G:H2'	3:2:13:C:H4'	1.96	0.48
4:5:96:G:N2	13:I:41:MET:HG3	2.29	0.48
6:B:154:LYS:HG2	42:B:1001:GTP:O1B	2.14	0.48
11:G:8:PRO:HD2	11:G:9:ARG:NH1	2.27	0.48
18:N:445:LEU:HB2	18:N:621:TYR:HB3	1.95	0.48
18:N:690:LEU:HD21	18:N:695:LEU:HD21	1.95	0.48
22:R:111:ILE:HD13	22:R:126:LEU:HD23	1.96	0.48
31:d:2:ALA:HB1	31:d:17:LEU:HB2	1.96	0.48
35:z:250:GLU:HA	35:z:253:ILE:HG12	1.94	0.48
5:A:127:MET:HE1	5:A:605:PHE:CZ	2.47	0.48
5:A:1624:GLU:OE2	5:A:1627:SER:OG	2.31	0.48
5:A:1638:ILE:HD12	5:A:1642:LYS:HE3	1.95	0.48
13:I:34:LEU:H	13:I:34:LEU:HD23	1.78	0.48
15:K:117:LYS:C	22:R:225:GLN:HE22	2.21	0.48
17:M:232:PHE:HE2	17:M:252:VAL:HG11	1.78	0.48
19:O:10:LYS:HD2	19:O:11:ARG:N	2.28	0.48
22:R:105:PRO:HG3	38:6:78:A:C8	2.49	0.48
22:R:280:TYR:HB3	22:R:306:LEU:CD1	2.44	0.48
22:R:453:CYS:HA	22:R:456:LEU:HD12	1.96	0.48
25:X:511:ILE:HG13	25:X:512:ALA:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:703:TRP:CZ2	25:X:720:MET:HB2	2.48	0.48
3:2:30:A:H2	34:y:40:LYS:HD2	1.78	0.48
5:A:329:THR:HG23	29:b:4:ASN:H	1.78	0.48
5:A:942:ASP:OD1	5:A:1035:LYS:NZ	2.47	0.48
5:A:959:PHE:HB3	5:A:963:VAL:HG21	1.94	0.48
5:A:1817:THR:HG22	5:A:1818:PHE:N	2.23	0.48
6:B:933:LYS:HZ1	6:B:935:LEU:HB2	1.79	0.48
18:N:58:PHE:CD2	18:N:62:LEU:HD11	2.49	0.48
18:N:449:LEU:HD13	18:N:557:PHE:CZ	2.49	0.48
20:P:184:THR:O	20:P:187:ILE:HG23	2.13	0.48
25:X:287:VAL:O	25:X:291:THR:HG23	2.14	0.48
25:X:624:ARG:HA	25:X:627:ILE:HG22	1.96	0.48
32:m:278:ARG:NH2	33:n:324:ILE:O	2.47	0.48
35:z:34:LEU:HD21	35:z:61:PHE:HD2	1.77	0.48
35:z:379:GLU:OE2	35:z:384:ASN:OD1	2.31	0.48
35:z:393:PHE:CE2	35:z:397:LEU:HD11	2.49	0.48
5:A:511:ASP:OD1	5:A:512:TRP:N	2.47	0.48
5:A:527:LEU:HD22	5:A:567:PHE:CE1	2.49	0.48
5:A:1689:GLN:N	5:A:1689:GLN:OE1	2.47	0.48
11:G:5:VAL:HG12	11:G:23:TYR:CD2	2.48	0.48
15:K:115:LEU:HD23	15:K:115:LEU:H	1.79	0.48
20:P:296:LYS:HG3	20:P:297:LEU:N	2.29	0.48
22:R:224:ARG:O	22:R:228:LEU:HG	2.13	0.48
23:U:123:ASP:OD1	23:U:124:GLU:N	2.47	0.48
35:z:456:LEU:HD22	35:z:468:ILE:HG22	1.95	0.48
3:2:9:U:H2'	3:2:10:U:H6	1.79	0.47
5:A:1011:VAL:HG11	5:A:1053:LEU:HD12	1.96	0.47
5:A:1153:LYS:HE3	5:A:1196:GLU:HA	1.96	0.47
5:A:1436:TRP:CE2	5:A:1444:ASN:ND2	2.82	0.47
6:B:776:VAL:HA	6:B:779:TYR:CE1	2.49	0.47
12:H:31:PHE:HA	12:H:79:THR:OG1	2.14	0.47
15:K:384:ASN:HB3	15:K:400:TRP:HB3	1.95	0.47
18:N:761:LEU:HD21	18:N:1006:VAL:HG21	1.96	0.47
20:P:174:TYR:CE2	20:P:220:GLU:HG2	2.49	0.47
22:R:111:ILE:O	22:R:115:MET:HG2	2.14	0.47
24:W:259:ASN:HA	24:W:262:ARG:HE	1.79	0.47
25:X:448:ARG:HH21	25:X:494:GLY:HA2	1.79	0.47
25:X:498:THR:HG22	25:X:501:LYS:NZ	2.28	0.47
3:2:14:C:H2'	38:6:76:C:C4	2.48	0.47
5:A:1215:THR:OG1	5:A:1216:GLY:N	2.45	0.47
7:C:114:ASP:O	7:C:115:THR:OG1	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:45:TYR:HE1	9:E:62:LYS:HE3	1.78	0.47
15:K:132:SER:O	15:K:136:LEU:HD12	2.14	0.47
18:N:421:GLN:OE1	18:N:440:ALA:HB2	2.14	0.47
18:N:519:ASP:O	18:N:523:SER:N	2.47	0.47
18:N:926:GLU:HG3	25:X:137:ARG:NH2	2.27	0.47
22:R:151:LEU:HD12	26:Y:160:PRO:HG3	1.96	0.47
23:S:115:ILE:HD11	23:V:111:ALA:HB2	1.95	0.47
34:y:120:ASP:O	34:y:121:THR:HG23	2.15	0.47
35:z:425:LEU:HD12	35:z:579:ARG:NH2	2.29	0.47
2:p:178:LYS:NZ	2:p:182:LYS:HB2	2.30	0.47
6:B:132:PHE:HZ	6:B:553:LEU:HB3	1.79	0.47
6:B:569:VAL:O	6:B:569:VAL:HG13	2.14	0.47
15:K:191:ASP:OD2	15:K:194:SER:OG	2.26	0.47
15:K:259:LEU:HB2	15:K:261:VAL:HG12	1.96	0.47
18:N:149:ILE:HG13	18:N:152:LEU:HD12	1.96	0.47
18:N:945:LEU:HD13	18:N:966:LEU:HD21	1.97	0.47
22:R:289:GLN:O	25:X:539:ARG:NH2	2.47	0.47
23:S:23:TYR:CG	23:S:28:ILE:HD13	2.50	0.47
25:X:574:ASP:HA	25:X:577:GLU:CD	2.39	0.47
32:m:322:VAL:HB	32:m:325:ALA:HB2	1.96	0.47
4:5:102:G:C5	10:F:20:LYS:NZ	2.81	0.47
6:B:356:TRP:CG	6:B:357:GLY:H	2.33	0.47
18:N:219:VAL:HG12	18:N:223:LEU:HG	1.94	0.47
18:N:410:GLN:O	18:N:413:SER:OG	2.31	0.47
19:O:26:PHE:CE1	19:O:55:GLN:HG2	2.49	0.47
20:P:261:ARG:O	20:P:264:GLU:HG3	2.14	0.47
32:m:296:LYS:O	32:m:300:ILE:HG12	2.13	0.47
38:6:86:A:H2'	38:6:87:G:C8	2.48	0.47
5:A:1460:TRP:CD1	5:A:1460:TRP:H	2.32	0.47
5:A:1963:ILE:O	5:A:1967:LEU:HG	2.15	0.47
7:C:188:GLN:OE1	7:C:190:THR:HG22	2.15	0.47
7:C:290:ASP:OD2	7:C:292:ASN:ND2	2.35	0.47
11:G:42:GLN:CG	11:G:56:ARG:HH12	2.27	0.47
18:N:1223:THR:HB	18:N:1226:LEU:HD12	1.97	0.47
22:R:84:LYS:HZ3	22:R:88:ARG:H	1.62	0.47
22:R:158:ARG:O	22:R:162:GLU:HG2	2.15	0.47
23:T:85:LEU:O	23:T:89:GLU:HG2	2.15	0.47
7:C:103:ARG:NE	7:C:145:LYS:O	2.47	0.47
7:C:232:SER:O	7:C:248:VAL:N	2.44	0.47
11:G:44:LEU:HB3	11:G:110:VAL:HG23	1.96	0.47
18:N:634:ARG:HD2	18:N:967:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:6:THR:O	19:O:9:THR:OG1	2.28	0.47
20:P:209:SER:HG	20:P:210:ARG:NH1	2.12	0.47
23:U:5:ILE:HB	23:U:27:LEU:HD13	1.97	0.47
23:V:88:PHE:O	23:V:91:ARG:HG2	2.14	0.47
25:X:472:PRO:HA	25:X:475:ARG:HB2	1.96	0.47
32:m:435:MET:O	32:m:439:LYS:HB3	2.14	0.47
32:m:494:PRO:HD3	32:m:533:ILE:HD13	1.95	0.47
34:y:125:ILE:CG1	34:y:131:ARG:HD3	2.45	0.47
34:y:174:TYR:HE1	35:z:220:VAL:HG12	1.79	0.47
35:z:241:VAL:HG12	35:z:318:VAL:CG2	2.45	0.47
5:A:398:GLU:HG3	12:H:6:GLN:HE22	1.79	0.47
5:A:624:GLN:HG2	5:A:663:PHE:HB2	1.97	0.47
5:A:1490:GLN:NE2	5:A:1492:ASN:HB2	2.29	0.47
5:A:1799:GLN:OE1	5:A:1954:TYR:OH	2.22	0.47
6:B:608:PRO:HD3	6:B:617:LEU:HD22	1.97	0.47
6:B:700:THR:HG23	6:B:806:MET:HB2	1.96	0.47
6:B:852:ALA:HB1	6:B:856:SER:HB2	1.96	0.47
11:G:77:GLU:OE2	11:G:92:LYS:NZ	2.47	0.47
15:K:149:TRP:CE2	15:K:456:PRO:HA	2.50	0.47
15:K:327:LEU:HD23	15:K:357:TRP:CE2	2.50	0.47
15:K:414:GLN:HB2	15:K:415:PRO:HD2	1.97	0.47
17:M:142:ASN:O	17:M:146:LYS:HG2	2.14	0.47
18:N:240:ARG:HE	18:N:285:THR:HA	1.79	0.47
18:N:566:ASP:OD2	18:N:584:ASN:N	2.27	0.47
18:N:745:MET:HB2	18:N:1039:ILE:HD12	1.96	0.47
18:N:777:LEU:HD23	18:N:978:VAL:HG13	1.95	0.47
20:P:99:ILE:HG23	20:P:103:SER:OG	2.15	0.47
20:P:187:ILE:HA	20:P:190:ILE:HG12	1.95	0.47
22:R:10:ASN:CG	24:W:153:ILE:HB	2.40	0.47
22:R:258:GLU:HA	22:R:261:ARG:HG2	1.97	0.47
22:R:536:HIS:HB3	22:R:539:VAL:HG23	1.97	0.47
23:T:69:LEU:HB2	23:T:70:PRO:HD2	1.97	0.47
23:T:87:GLN:O	23:T:91:ARG:HG2	2.15	0.47
24:W:627:TYR:O	24:W:628:SER:C	2.56	0.47
25:X:252:GLN:HB2	25:X:255:LYS:NZ	2.29	0.47
25:X:610:SER:HA	25:X:613:GLU:HG2	1.95	0.47
29:b:8:LEU:H	29:b:8:LEU:HD23	1.79	0.47
32:m:753:GLN:HG3	32:m:754:ALA:H	1.79	0.47
34:y:64:TYR:O	34:y:65:PHE:CD1	2.68	0.47
35:z:456:LEU:HD11	35:z:469:LEU:HA	1.96	0.47
5:A:1826:PRO:HG3	5:A:1857:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:26:TYR:HD2	8:D:44:ILE:HG21	1.80	0.47
18:N:1011:GLN:HE21	18:N:1033:ARG:HD3	1.80	0.47
22:R:338:ILE:O	22:R:341:THR:HG22	2.13	0.47
23:T:68:SER:N	23:T:72:LEU:HD23	2.30	0.47
31:d:45:ARG:HB3	31:d:53:GLN:HB3	1.97	0.47
32:m:302:ARG:HG2	32:m:348:PHE:HD2	1.80	0.47
35:z:412:PRO:CB	35:z:415:HIS:HD2	2.23	0.47
1:e:30:LEU:HD21	1:e:100:ILE:HG21	1.97	0.47
5:A:1594:LYS:O	5:A:1598:ILE:HG12	2.15	0.47
6:B:490:MET:HG2	6:B:510:VAL:HA	1.97	0.47
15:K:87:ASP:HA	22:R:259:ARG:NH1	2.30	0.47
18:N:333:GLN:O	18:N:337:GLU:OE1	2.33	0.47
19:O:101:CYS:SG	19:O:102:CYS:N	2.87	0.47
20:P:63:GLU:HG3	20:P:78:TRP:CH2	2.50	0.47
21:Q:54:ARG:HE	21:Q:54:ARG:HB2	1.60	0.47
23:T:127:GLU:CD	24:W:738:LYS:HZ1	2.21	0.47
23:V:91:ARG:HH12	23:V:92:ARG:HH11	1.63	0.47
23:V:106:TYR:HD1	23:V:109:ASP:HB2	1.79	0.47
25:X:541:VAL:HG21	25:X:553:TRP:NE1	2.30	0.47
26:Y:153:LEU:HD13	31:d:131:ARG:NH1	2.29	0.47
29:b:25:SER:O	29:b:25:SER:OG	2.31	0.47
35:z:162:LEU:O	35:z:166:LEU:HD23	2.14	0.47
35:z:306:GLU:O	35:z:353:ARG:NH1	2.48	0.47
6:B:559:VAL:HG12	6:B:560:ALA:N	2.30	0.47
6:B:760:ARG:HH21	6:B:804:ARG:HD3	1.79	0.47
10:F:17:ILE:HB	10:F:25:VAL:CG2	2.44	0.47
11:G:104:ASP:HA	13:I:66:ARG:NH1	2.30	0.47
15:K:149:TRP:HH2	15:K:454:ALA:HA	1.80	0.47
15:K:267:ARG:HG3	15:K:291:THR:CG2	2.44	0.47
20:P:63:GLU:HG3	20:P:78:TRP:CZ2	2.50	0.47
22:R:84:LYS:NZ	22:R:88:ARG:H	2.13	0.47
24:W:519:LYS:O	24:W:523:ALA:N	2.47	0.47
25:X:167:TYR:CE2	25:X:188:LEU:HD22	2.50	0.47
32:m:547:PHE:HA	32:m:550:TRP:CD1	2.49	0.47
32:m:618:TRP:CZ2	32:m:622:LEU:HD11	2.50	0.47
2:p:187:LYS:HB2	2:p:192:LEU:HB3	1.97	0.46
5:A:803:THR:HG23	5:A:921:PHE:CD1	2.50	0.46
5:A:906:ARG:HB3	5:A:906:ARG:NH1	2.30	0.46
5:A:1996:ASP:N	5:A:1999:GLN:OE1	2.27	0.46
10:F:23:THR:OG1	10:F:46:THR:O	2.23	0.46
15:K:435:ARG:NE	21:Q:61:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:292:ASN:ND2	20:P:293:ARG:HH11	2.13	0.46
23:S:64:PRO:HG3	23:T:9:THR:HG21	1.96	0.46
23:S:95:THR:O	23:S:99:GLN:HG3	2.14	0.46
23:V:16:SER:HB3	23:V:20:GLY:HA2	1.97	0.46
23:V:91:ARG:NH1	23:V:92:ARG:HH11	2.14	0.46
24:W:685:SER:HB3	27:Z:120:PHE:CZ	2.50	0.46
26:Y:116:TYR:O	26:Y:120:ILE:HG12	2.15	0.46
34:y:72:GLU:CD	34:y:72:GLU:H	2.24	0.46
35:z:76:CYS:O	35:z:121:TYR:HA	2.14	0.46
5:A:111:GLY:HA3	16:L:214:PRO:HD3	1.97	0.46
5:A:530:LEU:HD21	5:A:678:LEU:HD21	1.96	0.46
5:A:552:THR:HB	34:y:65:PHE:HD2	1.80	0.46
5:A:1659:TYR:HB2	5:A:1661:TRP:CZ2	2.51	0.46
13:I:28:GLN:OE1	13:I:28:GLN:N	2.48	0.46
17:M:69:ILE:HD11	17:M:74:ALA:HB2	1.97	0.46
18:N:551:LEU:H	18:N:551:LEU:HD23	1.80	0.46
18:N:715:ARG:NH1	18:N:768:THR:O	2.46	0.46
23:U:83:VAL:O	23:U:87:GLN:HG2	2.15	0.46
23:V:106:TYR:HB3	24:W:564:MET:SD	2.55	0.46
24:W:158:ASP:OD1	24:W:159:GLU:N	2.48	0.46
25:X:584:PRO:HB2	25:X:586:GLU:OE1	2.15	0.46
26:Y:183:THR:HG23	26:Y:184:LYS:HG2	1.97	0.46
32:m:279:ARG:HB3	32:m:283:LYS:HE3	1.96	0.46
35:z:497:SER:HA	35:z:500:PHE:HD2	1.80	0.46
35:z:582:ALA:HB1	35:z:590:TYR:HB3	1.97	0.46
1:e:261:VAL:HG13	1:e:262:ASN:H	1.80	0.46
4:5:96:G:H21	13:I:41:MET:HG3	1.81	0.46
5:A:1427:LEU:HB3	34:y:233:ILE:HD11	1.97	0.46
18:N:1011:GLN:HG2	18:N:1029:PHE:HE2	1.80	0.46
20:P:177:TYR:HD2	20:P:244:ARG:HB2	1.80	0.46
22:R:454:ARG:HG2	22:R:474:TYR:HE1	1.79	0.46
22:R:487:ALA:HA	22:R:490:LEU:HD12	1.97	0.46
24:W:236:TYR:HD1	26:Y:156:VAL:HG13	1.81	0.46
25:X:463:ILE:HG23	25:X:470:LEU:HD22	1.96	0.46
32:m:285:GLU:O	32:m:289:VAL:HG23	2.15	0.46
35:z:330:PRO:HG3	35:z:415:HIS:CE1	2.51	0.46
4:5:96:G:C5	12:H:48:PHE:CE2	3.03	0.46
5:A:208:LEU:HG	5:A:209:GLU:H	1.80	0.46
5:A:681:ARG:HE	5:A:686:ARG:HH22	1.64	0.46
5:A:718:ASP:OD1	15:K:333:THR:HG22	2.15	0.46
5:A:1214:MET:HG2	5:A:1215:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:183:HIS:O	6:B:187:ARG:HG2	2.16	0.46
6:B:715:GLU:OE2	6:B:799:ARG:NH2	2.49	0.46
7:C:57:ARG:HG2	7:C:57:ARG:HH11	1.80	0.46
12:H:33:GLN:HG2	12:H:36:ILE:HD13	1.98	0.46
13:I:49:GLU:HB2	13:I:56:LYS:HZ2	1.79	0.46
20:P:159:TYR:OH	20:P:173:ASN:ND2	2.47	0.46
22:R:324:ASP:O	22:R:327:LYS:HG2	2.16	0.46
24:W:514:GLU:HA	24:W:517:ALA:HB3	1.97	0.46
25:X:500:ARG:HA	25:X:500:ARG:NH1	2.30	0.46
28:a:64:GLN:HA	31:d:62:ARG:NH1	2.30	0.46
30:c:427:GLU:OE1	30:c:470:ARG:NH1	2.48	0.46
32:m:777:SER:OG	32:m:779:ASP:OD1	2.24	0.46
35:z:268:GLN:HE22	35:z:296:ARG:HH21	1.63	0.46
1:e:218:ILE:HG23	21:Q:230:VAL:HG12	1.97	0.46
4:5:82:A:HO2'	4:5:83:A:H8	1.57	0.46
13:I:7:ASN:HB2	13:I:10:PRO:HD2	1.98	0.46
17:M:148:GLU:OE1	17:M:148:GLU:HA	2.16	0.46
19:O:39:LYS:HD2	19:O:39:LYS:O	2.15	0.46
20:P:52:LYS:HD3	20:P:54:ILE:O	2.16	0.46
22:R:273:ARG:NH1	22:R:309:GLU:OE1	2.48	0.46
23:U:356:GLU:HA	23:U:372:GLY:HA2	1.96	0.46
24:W:242:ASP:OD1	24:W:243:ARG:N	2.46	0.46
25:X:358:ARG:HH12	25:X:362:LEU:HB2	1.79	0.46
25:X:599:GLU:HG2	25:X:603:GLY:HA3	1.97	0.46
32:m:278:ARG:HH21	33:n:324:ILE:HA	1.80	0.46
2:p:169:PHE:HD1	2:p:172:ARG:HH22	1.62	0.46
5:A:267:ASP:N	5:A:267:ASP:OD1	2.46	0.46
5:A:1432:LEU:HD12	5:A:1447:PHE:CZ	2.51	0.46
7:C:112:SER:O	7:C:138:VAL:HG12	2.15	0.46
11:G:12:LEU:HD23	11:G:16:GLU:CB	2.46	0.46
11:G:34:GLN:O	11:G:38:LYS:HG3	2.15	0.46
13:I:30:TYR:HE1	13:I:50:GLU:HG2	1.79	0.46
17:M:258:SER:O	17:M:262:ILE:HG23	2.16	0.46
18:N:405:ARG:NH1	18:N:548:LEU:O	2.48	0.46
22:R:275:LYS:HA	22:R:277:MET:HE1	1.96	0.46
24:W:196:LEU:HD21	24:W:200:ARG:NH2	2.30	0.46
25:X:573:ARG:HG3	25:X:574:ASP:N	2.30	0.46
25:X:717:VAL:HA	25:X:720:MET:HE2	1.98	0.46
26:Y:118:ARG:HH11	26:Y:121:ARG:HH11	1.64	0.46
28:a:23:PRO:O	28:a:27:THR:N	2.43	0.46
30:c:593:LEU:O	30:c:595:ALA:N	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:m:358:ASP:HB2	32:m:429:HIS:HB3	1.98	0.46
32:m:505:HIS:NE2	32:m:506:HIS:CE1	2.84	0.46
33:n:307:LYS:O	33:n:310:ILE:HG22	2.16	0.46
34:y:179:TYR:OH	35:z:217:GLU:OE2	2.32	0.46
5:A:300:PRO:O	5:A:301:LEU:HB3	2.16	0.46
5:A:1315:CYS:HA	5:A:1318:LYS:HG2	1.97	0.46
5:A:1378:ARG:HD2	29:b:8:LEU:HD22	1.98	0.46
7:C:57:ARG:HD2	7:C:99:LEU:O	2.16	0.46
22:R:289:GLN:C	25:X:539:ARG:HH12	2.24	0.46
23:S:10:PRO:HG3	23:S:22:VAL:HG12	1.98	0.46
23:V:71:ALA:O	23:V:75:LEU:HG	2.16	0.46
25:X:458:PRO:HG2	25:X:461:SER:HB3	1.98	0.46
26:Y:165:VAL:O	26:Y:169:VAL:HG23	2.16	0.46
5:A:1669:LEU:HD11	5:A:1750:ILE:HD11	1.97	0.46
6:B:631:SER:HA	6:B:644:PHE:O	2.16	0.46
13:I:22:VAL:HG12	13:I:73:VAL:HG22	1.98	0.46
17:M:168:GLN:NE2	17:M:169:ILE:HG23	2.30	0.46
18:N:520:LEU:HD22	18:N:524:ILE:HD11	1.97	0.46
18:N:974:ASN:ND2	18:N:1001:GLY:O	2.47	0.46
22:R:93:PHE:CD2	22:R:110:TYR:HD1	2.34	0.46
22:R:363:TYR:O	22:R:366:LEU:HG	2.16	0.46
23:U:94:LEU:HG	23:U:98:LYS:HE3	1.98	0.46
23:V:25:LYS:O	23:V:29:GLU:HG2	2.15	0.46
32:m:559:LEU:O	32:m:563:LEU:HG	2.16	0.46
34:y:116:ILE:H	35:z:643:TYR:HH	1.60	0.46
34:y:124:PRO:HB3	34:y:138:ASP:HB2	1.98	0.46
35:z:392:LEU:HD22	35:z:444:SER:HA	1.97	0.46
5:A:177:ARG:HD3	5:A:643:PRO:HB2	1.96	0.46
5:A:1556:ARG:HG2	5:A:1592:THR:HG23	1.97	0.46
5:A:1657:ALA:O	5:A:1683:LYS:NZ	2.49	0.46
5:A:1892:MET:O	5:A:1896:LEU:HG	2.16	0.46
6:B:584:LEU:HD23	6:B:585:LYS:O	2.16	0.46
6:B:628:TYR:O	6:B:631:SER:OG	2.28	0.46
6:B:812:PRO:O	6:B:817:ARG:NH2	2.49	0.46
6:B:832:SER:OG	6:B:966:TYR:O	2.33	0.46
9:E:62:LYS:HA	9:E:62:LYS:HD2	1.75	0.46
11:G:110:VAL:HG12	13:I:63:ILE:HD13	1.98	0.46
15:K:169:VAL:HB	15:K:439:CYS:SG	2.56	0.46
15:K:472:ARG:HD2	15:K:472:ARG:HA	1.77	0.46
16:L:180:ASP:OD1	16:L:180:ASP:N	2.47	0.46
18:N:14:TYR:HB3	18:N:31:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:53:HIS:CE1	18:N:85:LYS:HG2	2.51	0.46
18:N:561:THR:O	18:N:586:TYR:N	2.47	0.46
18:N:869:TYR:CE1	18:N:873:VAL:HG21	2.51	0.46
22:R:41:ASN:OD1	24:W:267:GLU:HG3	2.16	0.46
22:R:194:TYR:O	22:R:198:VAL:HG22	2.15	0.46
22:R:300:VAL:O	22:R:304:ARG:HD3	2.16	0.46
23:V:106:TYR:HB2	24:W:568:ILE:CG1	2.45	0.46
26:Y:183:THR:HA	38:6:79:C:C5	2.51	0.46
32:m:335:GLN:N	32:m:336:PRO:HD2	2.31	0.46
34:y:125:ILE:HD11	34:y:130:LEU:C	2.41	0.46
35:z:191:GLY:O	35:z:195:VAL:HG22	2.16	0.46
4:5:107:C:O2'	4:5:108:U:H5'	2.16	0.46
5:A:1747:LYS:O	5:A:1751:GLN:HG3	2.16	0.46
6:B:848:VAL:HG12	6:B:913:MET:HG2	1.98	0.46
14:J:10:LYS:HE2	14:J:10:LYS:HB2	1.72	0.46
15:K:355:LYS:HB2	15:K:357:TRP:CH2	2.51	0.46
18:N:1240:LEU:HB3	18:N:1263:ILE:HB	1.98	0.46
24:W:537:ARG:HG3	24:W:538:PRO:HD2	1.98	0.46
25:X:468:GLU:HA	25:X:475:ARG:HH22	1.81	0.46
25:X:526:GLU:OE2	25:X:527:ASN:ND2	2.49	0.46
32:m:512:LEU:HB2	32:m:513:PRO:HD3	1.97	0.46
32:m:534:LEU:HA	32:m:537:TRP:HB2	1.97	0.46
2:p:199:PRO:HD3	25:X:722:ARG:HH22	1.80	0.45
5:A:1438:ARG:HG2	30:c:458:ARG:HH21	1.80	0.45
6:B:97:ASP:OD2	15:K:199:LEU:HA	2.16	0.45
9:E:24:PHE:HB3	9:E:42:CYS:SG	2.56	0.45
11:G:38:LYS:HB3	11:G:38:LYS:HE3	1.83	0.45
16:L:142:SER:OG	16:L:143:ASP:N	2.42	0.45
18:N:1124:ARG:NH1	18:N:1128:TYR:O	2.49	0.45
20:P:61:GLU:O	20:P:61:GLU:HG2	2.16	0.45
23:U:99:GLN:OE1	24:W:712:THR:OG1	2.18	0.45
25:X:703:TRP:HZ2	25:X:720:MET:HB2	1.81	0.45
30:c:585:ILE:O	30:c:589:THR:HG23	2.16	0.45
5:A:1479:TRP:CD1	5:A:1479:TRP:H	2.33	0.45
6:B:933:LYS:NZ	6:B:935:LEU:HB2	2.31	0.45
18:N:529:LEU:HD12	18:N:530:CYS:N	2.30	0.45
24:W:97:ARG:NH1	24:W:100:LYS:HE2	2.31	0.45
26:Y:92:ARG:HH22	38:6:92:C:H5'	1.81	0.45
31:d:10:LEU:CD2	31:d:147:LEU:HD11	2.46	0.45
34:y:165:ASP:O	34:y:169:LEU:HG	2.15	0.45
5:A:1746:MET:HE1	5:A:1749:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1825:LYS:HE2	5:A:1848:THR:HG21	1.99	0.45
6:B:520:LYS:HE2	6:B:540:HIS:NE2	2.30	0.45
6:B:813:GLU:OE2	6:B:815:ILE:HB	2.16	0.45
19:O:101:CYS:HB3	19:O:142:CYS:SG	2.56	0.45
23:U:389:TRP:O	23:U:390:LEU:HD23	2.17	0.45
25:X:573:ARG:O	25:X:577:GLU:OE1	2.34	0.45
28:a:21:ILE:O	28:a:25:LEU:N	2.45	0.45
30:c:509:ALA:HB2	30:c:543:MET:HG3	1.99	0.45
35:z:383:LEU:O	35:z:383:LEU:HD23	2.16	0.45
1:e:204:HIS:CD2	6:B:76:GLN:H	2.34	0.45
5:A:1664:SER:O	5:A:1741:ASN:ND2	2.50	0.45
5:A:1803:PHE:HB3	5:A:1805:ASP:OD1	2.17	0.45
6:B:325:ASP:HB2	42:B:1001:GTP:C5	2.52	0.45
6:B:406:LYS:HB3	6:B:406:LYS:HE3	1.80	0.45
7:C:57:ARG:HG2	7:C:57:ARG:NH1	2.31	0.45
8:D:70:ILE:CD1	9:E:68:VAL:HG22	2.46	0.45
11:G:35:GLN:HG2	11:G:111:ARG:HH22	1.81	0.45
20:P:119:TYR:HD2	38:6:23:A:C6	2.34	0.45
24:W:530:VAL:HG23	24:W:531:ILE:H	1.81	0.45
25:X:448:ARG:NH1	25:X:498:THR:HG21	2.32	0.45
31:d:90:MET:HG2	31:d:119:PHE:CE1	2.51	0.45
34:y:98:MET:HE3	34:y:102:ASP:HB3	1.98	0.45
1:e:204:HIS:CE1	6:B:70:VAL:HG21	2.52	0.45
1:e:256:TYR:CE2	30:c:595:ALA:HA	2.37	0.45
5:A:985:LEU:HB2	5:A:988:VAL:HB	1.98	0.45
5:A:1416:LYS:HA	5:A:1419:GLU:HG3	1.98	0.45
5:A:1955:THR:O	5:A:1959:ARG:HG2	2.16	0.45
6:B:466:ILE:HG12	6:B:590:ILE:O	2.15	0.45
7:C:53:VAL:HG23	7:C:328:CYS:SG	2.57	0.45
7:C:227:ILE:HD11	7:C:248:VAL:HG21	1.98	0.45
15:K:470:ARG:NH1	15:K:472:ARG:HD2	2.31	0.45
16:L:124:LEU:CD1	16:L:234:LEU:HD22	2.46	0.45
16:L:159:LYS:HB2	16:L:159:LYS:HE2	1.75	0.45
16:L:331:LEU:HD13	32:m:513:PRO:HG2	1.99	0.45
18:N:638:PHE:HE1	18:N:990:THR:HG23	1.80	0.45
18:N:670:LEU:HG	18:N:732:LEU:HD22	1.99	0.45
22:R:146:TYR:CE1	22:R:150:MET:HE3	2.52	0.45
23:S:79:GLU:OE1	23:S:80:TRP:HD1	1.99	0.45
24:W:135:ARG:HG3	24:W:136:PHE:CD2	2.51	0.45
24:W:244:GLN:HG2	24:W:245:ASN:HD22	1.81	0.45
24:W:545:LYS:HG2	36:r:233:UNK:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:640:LEU:O	24:W:640:LEU:HD23	2.16	0.45
25:X:144:HIS:HB2	25:X:148:TRP:NE1	2.31	0.45
25:X:434:TRP:HA	25:X:437:MET:HG3	1.98	0.45
26:Y:140:LYS:O	26:Y:142:ARG:HD3	2.17	0.45
28:a:143:ASP:OD1	28:a:144:PRO:HD2	2.17	0.45
34:y:31:ARG:HA	35:z:493:PHE:HE2	1.81	0.45
35:z:256:ILE:HG13	35:z:300:PHE:HZ	1.80	0.45
35:z:302:THR:OG1	35:z:303:ASN:N	2.48	0.45
4:5:27:G:N3	4:5:27:G:H2'	2.32	0.45
6:B:726:LYS:HD3	6:B:726:LYS:N	2.31	0.45
7:C:239:MET:HA	7:C:266:HIS:ND1	2.31	0.45
10:F:75:PRO:HB2	10:F:78:THR:OG1	2.16	0.45
13:I:15:LEU:HD21	13:I:20:VAL:CG1	2.46	0.45
13:I:21:LEU:HD12	13:I:30:TYR:O	2.16	0.45
13:I:26:TRP:CH2	13:I:69:ASN:ND2	2.84	0.45
16:L:299:GLU:OE1	16:L:303:ARG:NH2	2.50	0.45
17:M:109:ASN:OD1	17:M:112:ASN:HB2	2.15	0.45
17:M:111:ILE:O	17:M:114:GLU:HG3	2.17	0.45
18:N:860:ALA:HA	25:X:103:ILE:HG12	1.99	0.45
20:P:51:ARG:HH21	20:P:101:ARG:HG3	1.82	0.45
20:P:75:TYR:O	20:P:77:LYS:N	2.50	0.45
23:S:55:VAL:HG11	27:Z:133:LEU:CD2	2.47	0.45
23:T:111:ALA:O	23:T:115:ILE:HG23	2.16	0.45
23:U:371:PHE:HE1	27:Z:35:ARG:HA	1.81	0.45
25:X:503:TYR:O	25:X:507:PHE:HD2	1.99	0.45
34:y:164:TYR:OH	35:z:331:TYR:HD2	1.99	0.45
1:e:256:TYR:HB3	30:c:601:ARG:HH22	1.82	0.45
5:A:247:TRP:HD1	5:A:441:THR:HG23	1.81	0.45
5:A:819:LYS:HA	5:A:819:LYS:HD3	1.74	0.45
5:A:1617:LEU:O	5:A:1621:LEU:HD23	2.16	0.45
12:H:28:ILE:HG23	12:H:78:ILE:HG23	1.99	0.45
22:R:257:TYR:CE1	22:R:290:PHE:CD2	3.04	0.45
25:X:202:LEU:HB2	25:X:218:ILE:HG21	1.98	0.45
25:X:661:LYS:HA	25:X:664:CYS:HB2	1.99	0.45
35:z:240:LEU:HB3	35:z:317:VAL:HG22	1.99	0.45
4:5:96:G:C4	12:H:48:PHE:CE2	3.04	0.45
5:A:906:ARG:HH22	24:W:140:GLU:HB2	1.82	0.45
5:A:1727:ILE:HG22	5:A:1738:ALA:HB2	1.99	0.45
6:B:828:ARG:HE	6:B:828:ARG:HB3	1.52	0.45
7:C:142:ASP:OD1	7:C:143:VAL:N	2.50	0.45
8:D:57:ASP:OD1	8:D:58:GLN:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:36:MET:HE3	11:G:102:ARG:HG3	1.98	0.45
17:M:39:PRO:HA	17:M:52:THR:HG22	1.98	0.45
17:M:116:PHE:HE1	17:M:120:GLN:HE21	1.65	0.45
18:N:256:ARG:HG3	18:N:261:TYR:CE2	2.52	0.45
19:O:120:ARG:HH11	19:O:142:CYS:HB3	1.81	0.45
25:X:238:VAL:HG13	25:X:242:PHE:CD2	2.52	0.45
31:d:74:ASP:OD1	31:d:74:ASP:N	2.48	0.45
34:y:64:TYR:O	34:y:65:PHE:HD1	1.99	0.45
35:z:109:PHE:CG	35:z:542:ILE:HD13	2.51	0.45
35:z:241:VAL:HG21	35:z:300:PHE:CD1	2.49	0.45
35:z:241:VAL:CG2	35:z:300:PHE:HD1	2.29	0.45
35:z:336:LYS:HB3	35:z:621:GLU:OE1	2.17	0.45
5:A:229:GLU:HB2	5:A:232:ALA:HA	1.98	0.45
5:A:843:ARG:NH2	5:A:1086:GLY:O	2.40	0.45
5:A:904:ILE:O	5:A:908:LEU:HD13	2.16	0.45
5:A:1686:ILE:HG12	5:A:1725:VAL:HB	1.98	0.45
6:B:179:TYR:CE1	6:B:550:ARG:HD2	2.52	0.45
6:B:229:ALA:HB3	6:B:230:PRO:HD3	1.99	0.45
7:C:45:GLN:HB2	9:E:104:ALA:HB3	1.99	0.45
10:F:16:SER:HB3	10:F:69:ILE:HB	1.99	0.45
12:H:29:TRP:N	12:H:29:TRP:CD1	2.83	0.45
15:K:452:ASP:N	15:K:452:ASP:OD1	2.50	0.45
16:L:311:ILE:O	16:L:314:GLN:HG3	2.17	0.45
18:N:326:GLN:HG3	25:X:271:GLU:HG2	1.98	0.45
18:N:737:ARG:HH11	18:N:1040:ILE:HD11	1.82	0.45
22:R:345:ALA:O	22:R:349:VAL:HG13	2.16	0.45
23:S:61:PRO:CG	24:W:697:ILE:HD11	2.44	0.45
23:U:126:ARG:HG2	23:U:126:ARG:HH11	1.82	0.45
25:X:246:ILE:HA	25:X:256:LEU:HD12	1.99	0.45
25:X:286:THR:HG22	25:X:287:VAL:N	2.31	0.45
26:Y:124:LYS:HG3	26:Y:127:TYR:OH	2.16	0.45
32:m:369:LEU:HA	32:m:372:PRO:HD2	1.99	0.45
35:z:239:ILE:HA	35:z:316:TYR:O	2.17	0.45
35:z:580:ASN:O	35:z:615:MET:HG2	2.17	0.45
11:G:103:GLY:O	13:I:66:ARG:NH1	2.50	0.45
19:O:125:LYS:HE3	19:O:125:LYS:HB3	1.78	0.45
20:P:294:LYS:N	20:P:294:LYS:HD2	2.32	0.45
25:X:588:SER:HB2	25:X:592:TYR:CE2	2.52	0.45
27:Z:181:ARG:O	27:Z:184:THR:OG1	2.32	0.45
32:m:740:HIS:HB2	32:m:747:LEU:HD11	1.99	0.45
5:A:783:ARG:HG2	5:A:788:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:95:LEU:HD12	9:E:96:SER:H	1.81	0.44
11:G:46:ASN:OD1	11:G:108:LEU:HB2	2.16	0.44
18:N:266:LEU:HD11	18:N:419:LEU:HD11	1.99	0.44
18:N:1032:LEU:HD23	18:N:1035:LEU:HD12	1.99	0.44
22:R:150:MET:HG3	26:Y:168:LEU:HD21	1.99	0.44
25:X:288:ARG:O	25:X:291:THR:OG1	2.23	0.44
25:X:401:GLU:OE1	25:X:437:MET:HE2	2.16	0.44
25:X:534:PHE:HA	25:X:537:TYR:HD2	1.81	0.44
28:a:62:MET:O	28:a:64:GLN:HG2	2.17	0.44
34:y:64:TYR:HB2	34:y:69:GLY:O	2.17	0.44
35:z:428:VAL:HG13	35:z:429:LEU:CD1	2.45	0.44
1:e:30:LEU:HD11	1:e:124:PHE:HD1	1.83	0.44
5:A:532:HIS:C	5:A:534:LYS:H	2.24	0.44
5:A:533:ARG:HG2	5:A:533:ARG:O	2.17	0.44
6:B:701:MET:SD	6:B:803:PHE:HB3	2.57	0.44
10:F:24:ILE:O	10:F:46:THR:OG1	2.30	0.44
18:N:251:PHE:CE2	18:N:255:LEU:HD11	2.53	0.44
18:N:488:VAL:HG21	18:N:602:ARG:HH12	1.82	0.44
18:N:1136:CYS:HA	18:N:1167:GLY:O	2.17	0.44
22:R:189:ARG:NH1	26:Y:147:TYR:HB3	2.32	0.44
22:R:369:CYS:HA	22:R:372:GLU:HG2	2.00	0.44
23:U:217:PRO:HG3	23:U:479:THR:HG21	1.99	0.44
25:X:355:TRP:O	25:X:359:VAL:HG23	2.17	0.44
25:X:357:ARG:HD3	25:X:360:LYS:HD2	1.99	0.44
26:Y:117:ASN:O	26:Y:121:ARG:HG3	2.18	0.44
35:z:241:VAL:CG2	35:z:300:PHE:HA	2.47	0.44
6:B:717:GLY:HA2	6:B:754:ARG:NH1	2.32	0.44
10:F:68:TYR:HD2	11:G:100:PHE:CD1	2.35	0.44
23:U:272:ILE:O	23:U:286:GLY:N	2.50	0.44
30:c:540:LEU:HD12	30:c:544:PHE:HE2	1.83	0.44
34:y:158:SER:HB3	35:z:412:PRO:HG3	1.99	0.44
34:y:171:ASN:HD22	35:z:623:GLU:CD	2.23	0.44
38:6:33:A:H2'	38:6:34:U:C6	2.52	0.44
4:5:102:G:C4	10:F:20:LYS:NZ	2.85	0.44
5:A:79:LYS:NZ	5:A:505:PHE:O	2.30	0.44
5:A:1153:LYS:HD3	5:A:1153:LYS:N	2.31	0.44
5:A:1629:GLN:NE2	5:A:1657:ALA:HB2	2.32	0.44
5:A:1887:VAL:HG11	5:A:1892:MET:CG	2.48	0.44
6:B:387:GLU:O	6:B:391:LYS:HG3	2.17	0.44
6:B:576:THR:HG21	6:B:594:ILE:HG12	1.99	0.44
6:B:699:ILE:HG13	6:B:808:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:14:LEU:HD13	9:E:28:LEU:HB2	1.98	0.44
22:R:83:GLN:HA	24:W:256:ILE:HG21	1.99	0.44
23:S:103:THR:HA	23:S:106:TYR:CZ	2.53	0.44
28:a:92:GLU:HG2	28:a:94:VAL:HG23	1.99	0.44
29:b:3:TYR:HB3	39:1:-10:A:C2	2.52	0.44
32:m:383:TYR:HA	32:m:386:LEU:HD12	1.99	0.44
38:6:44:A:H2'	38:6:45:U:C6	2.52	0.44
4:5:77:G:H2'	4:5:78:U:O4'	2.18	0.44
16:L:235:HIS:O	22:R:136:ARG:HG3	2.17	0.44
18:N:206:SER:CB	18:N:225:ILE:HD13	2.39	0.44
18:N:473:THR:HG22	18:N:477:PHE:O	2.17	0.44
18:N:1181:VAL:HG12	18:N:1207:CYS:HB2	1.98	0.44
22:R:327:LYS:HG3	22:R:328:LEU:HD22	1.99	0.44
23:S:76:PHE:HE1	23:T:72:LEU:HB3	1.83	0.44
24:W:640:LEU:HA	24:W:643:TYR:HB2	1.99	0.44
25:X:263:TYR:CE1	25:X:267:ILE:HD11	2.52	0.44
25:X:265:ILE:HG12	25:X:300:PHE:HE1	1.83	0.44
25:X:281:MET:HE3	25:X:293:ILE:HG21	2.00	0.44
29:b:123:ASP:HA	29:b:126:ILE:HG22	1.98	0.44
30:c:470:ARG:O	30:c:474:LEU:HG	2.18	0.44
31:d:94:GLY:O	31:d:115:LYS:HD3	2.16	0.44
35:z:315:VAL:O	35:z:354:ALA:HB1	2.17	0.44
4:5:50:U:H2'	4:5:51:U:C6	2.52	0.44
5:A:574:LEU:HD12	5:A:574:LEU:HA	1.87	0.44
7:C:108:VAL:N	7:C:120:TRP:O	2.40	0.44
11:G:71:VAL:HG22	11:G:96:ILE:O	2.18	0.44
19:O:6:THR:HG21	19:O:8:ARG:NH1	2.33	0.44
22:R:175:MET:O	22:R:179:ARG:HG3	2.17	0.44
22:R:188:GLU:H	22:R:188:GLU:CD	2.24	0.44
22:R:189:ARG:HH12	26:Y:147:TYR:HB3	1.81	0.44
23:T:92:ARG:NH2	23:T:96:GLU:OE2	2.50	0.44
24:W:640:LEU:HD23	24:W:644:GLU:HG3	2.00	0.44
34:y:95:ASP:OD1	34:y:103:ARG:HD3	2.18	0.44
35:z:144:ILE:HG12	35:z:175:VAL:HB	2.00	0.44
35:z:503:GLU:HB2	35:z:507:ILE:HD12	1.98	0.44
1:e:147:HIS:CE1	16:L:279:LEU:HA	2.53	0.44
5:A:688:SER:O	5:A:691:VAL:HG22	2.18	0.44
5:A:978:TRP:NE1	5:A:1214:MET:HE1	2.33	0.44
5:A:1674:ASP:OD1	5:A:1674:ASP:N	2.43	0.44
10:F:6:PHE:CE1	10:F:80:LEU:HD22	2.53	0.44
16:L:185:ARG:HA	16:L:201:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:461:ARG:HH22	18:N:550:PRO:HB3	1.82	0.44
22:R:48:LEU:O	22:R:52:GLN:HG3	2.17	0.44
22:R:303:LYS:HZ1	25:X:574:ASP:CG	2.21	0.44
22:R:528:GLN:HA	22:R:531:LEU:HB2	2.00	0.44
24:W:183:ARG:O	24:W:187:LEU:HD23	2.18	0.44
25:X:573:ARG:O	25:X:576:PHE:HB2	2.17	0.44
25:X:628:TYR:HE2	25:X:655:LEU:HD22	1.83	0.44
31:d:13:ILE:HD11	31:d:128:VAL:HB	1.99	0.44
35:z:613:TRP:CD1	35:z:636:SER:HG	2.35	0.44
5:A:556:LYS:HA	5:A:556:LYS:HD3	1.71	0.44
5:A:1685:TRP:HE3	5:A:1721:SER:HB2	1.83	0.44
6:B:273:ASP:OD1	6:B:323:SER:OG	2.25	0.44
6:B:756:THR:HG23	6:B:799:ARG:HA	1.98	0.44
6:B:848:VAL:HG12	6:B:913:MET:CG	2.47	0.44
15:K:348:SER:HG	15:K:357:TRP:HZ3	1.63	0.44
18:N:1060:TYR:CD1	18:N:1061:PRO:HD2	2.53	0.44
18:N:1247:ILE:O	18:N:1250:SER:OG	2.28	0.44
22:R:231:ILE:HG13	22:R:232:ASP:N	2.33	0.44
22:R:514:GLU:HB2	22:R:523:ALA:HB2	1.99	0.44
23:S:14:VAL:HG13	23:S:23:TYR:HB2	1.99	0.44
23:T:101:LEU:HD11	23:U:100:GLU:HB2	2.00	0.44
23:T:107:SER:HA	27:Z:33:LEU:HD21	1.99	0.44
31:d:39:ASP:OD1	31:d:151:LYS:HA	2.18	0.44
31:d:71:LYS:HA	31:d:98:ASN:O	2.17	0.44
32:m:752:THR:HB	32:m:794:PHE:CD2	2.52	0.44
34:y:144:MET:SD	35:z:420:LEU:HD13	2.58	0.44
6:B:812:PRO:HD2	6:B:817:ARG:HH22	1.82	0.44
15:K:86:ALA:C	22:R:259:ARG:HH22	2.26	0.44
18:N:668:ARG:O	18:N:760:LYS:NZ	2.46	0.44
23:T:132:PHE:CZ	23:U:132:PHE:HB3	2.53	0.44
27:Z:76:ASP:OD1	27:Z:77:VAL:N	2.48	0.44
28:a:95:PRO:HG2	28:a:98:VAL:HG12	1.99	0.44
31:d:5:GLU:OE2	31:d:14:LEU:HD13	2.18	0.44
31:d:88:LEU:HD12	31:d:103:PHE:O	2.18	0.44
34:y:144:MET:O	34:y:147:ASN:HB3	2.17	0.44
35:z:245:GLY:CA	35:z:324:LYS:HD2	2.44	0.44
38:6:5:U:H1'	38:6:9:G:N2	2.33	0.44
4:5:96:G:N2	13:I:39:SER:O	2.46	0.43
5:A:1576:GLN:HG2	5:A:1587:HIS:ND1	2.32	0.43
5:A:1969:VAL:HG11	5:A:2011:ILE:HA	1.99	0.43
6:B:252:THR:O	6:B:256:LYS:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:59:ASP:OD1	7:C:60:PRO:HD2	2.17	0.43
7:C:87:GLY:HA3	9:E:94:LEU:HD11	1.99	0.43
7:C:92:CYS:SG	7:C:112:SER:OG	2.58	0.43
8:D:6:LYS:HD2	8:D:90:PRO:HG2	2.00	0.43
11:G:29:PRO:HG2	13:I:42:ASN:O	2.17	0.43
15:K:398:TRP:CZ3	15:K:405:LYS:HB2	2.53	0.43
17:M:32:TYR:CE2	28:a:102:GLU:OE1	2.71	0.43
18:N:642:PHE:O	18:N:646:PHE:HB2	2.17	0.43
18:N:827:LEU:HB2	18:N:928:ILE:HG21	1.98	0.43
18:N:1233:ILE:O	18:N:1236:THR:OG1	2.34	0.43
20:P:118:LEU:CD1	20:P:151:PHE:HE2	2.31	0.43
22:R:289:GLN:O	25:X:539:ARG:NH1	2.50	0.43
22:R:401:ALA:CB	22:R:433:LYS:HD2	2.48	0.43
22:R:547:GLU:HB2	22:R:572:ALA:HB2	1.99	0.43
22:R:570:VAL:HA	22:R:573:ARG:HD2	2.00	0.43
23:S:17:ARG:NH1	23:T:17:ARG:HA	2.33	0.43
23:T:127:GLU:OE1	24:W:738:LYS:NZ	2.40	0.43
24:W:511:ARG:O	24:W:515:ARG:HG2	2.18	0.43
27:Z:180:CYS:O	27:Z:184:THR:HG23	2.19	0.43
32:m:346:VAL:HG23	32:m:347:GLU:OE1	2.18	0.43
35:z:49:HIS:O	35:z:54:LYS:NZ	2.51	0.43
35:z:219:TYR:O	35:z:223:ALA:N	2.46	0.43
35:z:575:ASP:HA	35:z:642:TYR:CZ	2.53	0.43
5:A:101:LYS:HB2	5:A:101:LYS:HE3	1.81	0.43
5:A:873:TYR:HE1	5:A:883:GLN:HE21	1.65	0.43
5:A:1107:PRO:HG2	21:Q:225:TRP:CE3	2.53	0.43
5:A:1451:ARG:NH1	34:y:228:ASP:OD2	2.40	0.43
5:A:1754:MET:HE2	5:A:1757:ILE:HD12	1.99	0.43
7:C:276:ALA:HB2	7:C:316:VAL:O	2.18	0.43
9:E:68:VAL:HG12	9:E:70:LEU:HD22	1.99	0.43
16:L:221:LYS:HE3	38:6:54:C:H4'	2.00	0.43
18:N:51:LEU:O	18:N:55:LEU:HD13	2.18	0.43
18:N:1263:ILE:HA	18:N:1268:HIS:ND1	2.33	0.43
22:R:43:THR:N	22:R:47:GLU:OE2	2.51	0.43
22:R:342:TYR:HB3	22:R:368:TYR:CE1	2.53	0.43
23:V:112:LEU:HD13	24:W:596:GLU:HB3	2.00	0.43
24:W:730:GLU:O	24:W:734:ILE:HG12	2.18	0.43
25:X:252:GLN:HB2	25:X:255:LYS:HZ2	1.83	0.43
25:X:398:ARG:HA	25:X:398:ARG:HD3	1.70	0.43
25:X:528:ALA:HA	25:X:530:PHE:CZ	2.53	0.43
25:X:532:ASP:HA	25:X:535:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:660:VAL:HA	25:X:663:MET:HE3	2.00	0.43
28:a:74:VAL:HA	28:a:78:GLN:HE21	1.83	0.43
30:c:520:GLU:CA	30:c:567:PRO:HG3	2.37	0.43
30:c:587:TYR:O	30:c:591:ILE:HG12	2.18	0.43
35:z:347:ALA:HB1	35:z:364:ARG:HH11	1.82	0.43
35:z:549:PHE:O	35:z:552:LYS:HB3	2.18	0.43
1:e:54:LEU:CD2	16:L:308:TYR:HB3	2.49	0.43
4:5:32:C:C5	5:A:487:PRO:HB2	2.54	0.43
4:5:104:A:O2'	11:G:48:ARG:HB3	2.17	0.43
5:A:107:ARG:NH1	16:L:213:GLU:OE1	2.51	0.43
5:A:1080:ARG:HD2	5:A:1080:ARG:HA	1.80	0.43
5:A:1360:PRO:HB2	5:A:1374:ILE:HD12	2.01	0.43
6:B:498:THR:HG22	6:B:499:VAL:H	1.84	0.43
16:L:202:ILE:HD12	17:M:19:PHE:HZ	1.83	0.43
16:L:217:PHE:CE1	17:M:50:PRO:HG3	2.53	0.43
16:L:325:GLU:O	16:L:328:LEU:HG	2.17	0.43
18:N:292:LYS:O	18:N:296:ILE:HG12	2.19	0.43
22:R:412:LEU:HD13	22:R:443:PHE:CE1	2.50	0.43
23:S:34:GLU:OE2	23:S:35:THR:HG22	2.17	0.43
24:W:678:ARG:CZ	27:Z:113:GLU:HG3	2.48	0.43
30:c:526:ARG:HA	30:c:571:GLY:HA3	1.99	0.43
30:c:529:GLU:HA	30:c:532:THR:HG22	2.00	0.43
5:A:558:ARG:HG2	5:A:558:ARG:HH11	1.84	0.43
7:C:202:LYS:HG2	7:C:214:VAL:HG12	2.01	0.43
7:C:306:LEU:HD13	9:E:106:ARG:NE	2.27	0.43
12:H:11:PRO:HG2	12:H:14:ASN:OD1	2.19	0.43
17:M:17:VAL:O	17:M:17:VAL:HG12	2.18	0.43
22:R:85:GLU:O	22:R:86:PHE:CD1	2.71	0.43
22:R:101:SER:OG	22:R:133:GLN:OE1	2.32	0.43
22:R:268:ILE:HD13	22:R:268:ILE:HA	1.87	0.43
22:R:460:TRP:CD2	22:R:470:PRO:HG3	2.53	0.43
23:T:54:LYS:HA	23:T:54:LYS:HD2	1.80	0.43
23:T:68:SER:H	23:T:72:LEU:HD23	1.83	0.43
23:V:33:ARG:HH12	23:V:47:LEU:HD21	1.84	0.43
23:V:66:ALA:CB	27:Z:60:GLU:HG2	2.48	0.43
24:W:627:TYR:O	24:W:630:LEU:N	2.51	0.43
25:X:192:ASN:OD1	25:X:232:HIS:NE2	2.52	0.43
32:m:454:SER:HB3	32:m:510:PRO:HG2	2.00	0.43
5:A:1168:MET:HG3	5:A:1206:ASP:HB3	2.00	0.43
6:B:329:CYS:SG	6:B:442:PHE:HB2	2.58	0.43
6:B:494:LYS:C	6:B:495:LEU:HD12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:663:SER:O	6:B:663:SER:OG	2.34	0.43
6:B:767:ASP:HB3	6:B:770:LYS:CE	2.48	0.43
6:B:861:TYR:CE1	6:B:871:VAL:HG21	2.53	0.43
7:C:326:LEU:HD12	7:C:326:LEU:HA	1.79	0.43
15:K:299:GLU:OE1	15:K:299:GLU:N	2.51	0.43
16:L:163:LYS:HE3	16:L:163:LYS:HB3	1.87	0.43
17:M:172:GLU:OE1	17:M:172:GLU:N	2.50	0.43
18:N:1002:PHE:HZ	18:N:1005:LEU:HD13	1.83	0.43
23:S:100:GLU:OE2	23:S:101:LEU:HD12	2.19	0.43
23:T:122:ARG:NH1	23:U:121:GLU:OE1	2.51	0.43
23:U:112:LEU:HD22	27:Z:22:ARG:HH11	1.84	0.43
23:U:442:VAL:O	23:U:454:CYS:HB3	2.18	0.43
25:X:695:VAL:O	25:X:695:VAL:HG12	2.17	0.43
30:c:526:ARG:HB2	30:c:531:ASP:OD2	2.18	0.43
32:m:531:SER:HB2	32:m:562:LEU:HD11	1.98	0.43
35:z:103:CYS:HA	35:z:119:ILE:O	2.18	0.43
35:z:236:PRO:HA	35:z:296:ARG:NH2	2.34	0.43
35:z:516:PHE:CD1	35:z:536:LEU:HD13	2.54	0.43
36:r:338:UNK:O	36:r:342:UNK:N	2.52	0.43
5:A:1449:LYS:HD3	5:A:1449:LYS:HA	1.86	0.43
6:B:149:HIS:CG	6:B:150:LEU:N	2.87	0.43
7:C:249:LYS:H	7:C:256:ARG:NH2	2.17	0.43
8:D:50:ASP:OD1	8:D:51:GLY:N	2.52	0.43
14:J:73:LEU:O	14:J:73:LEU:HD12	2.19	0.43
18:N:803:LEU:HD22	18:N:945:LEU:HD21	2.00	0.43
18:N:885:PHE:CZ	18:N:887:PHE:HB2	2.54	0.43
18:N:1139:TYR:HE2	18:N:1186:VAL:HB	1.84	0.43
22:R:10:ASN:OD1	24:W:153:ILE:HB	2.18	0.43
22:R:524:ARG:HA	22:R:527:TYR:HD2	1.83	0.43
23:S:86:GLU:O	23:S:90:LEU:HG	2.18	0.43
24:W:155:MET:CG	24:W:159:GLU:HG3	2.34	0.43
24:W:261:ILE:O	24:W:265:GLU:OE1	2.37	0.43
25:X:75:ARG:HB3	25:X:94:VAL:HG22	2.00	0.43
25:X:557:LEU:HD22	25:X:576:PHE:HE1	1.83	0.43
25:X:608:SER:O	25:X:612:LEU:HD23	2.19	0.43
30:c:554:LYS:O	30:c:557:VAL:HG22	2.18	0.43
35:z:59:PRO:HA	35:z:62:LEU:HD23	1.99	0.43
5:A:821:GLY:HA2	16:L:288:PHE:CE2	2.54	0.43
5:A:1757:ILE:HG23	5:A:1761:ASN:ND2	2.23	0.43
7:C:261:PHE:HE1	7:C:300:GLY:HA2	1.84	0.43
9:E:7:VAL:O	9:E:10:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:32:GLU:OE1	14:J:22:ASN:ND2	2.52	0.43
16:L:176:GLN:OE1	16:L:177:GLN:N	2.52	0.43
17:M:44:CYS:HB3	17:M:47:CYS:HB2	2.01	0.43
18:N:4:TYR:CZ	18:N:8:LYS:HD2	2.54	0.43
18:N:76:ASN:O	18:N:80:MET:HG2	2.18	0.43
18:N:533:TYR:HB2	18:N:608:PHE:HA	2.00	0.43
19:O:29:ARG:HB2	19:O:52:LEU:HD21	2.01	0.43
22:R:310:LYS:O	22:R:313:LYS:HG2	2.18	0.43
23:U:185:LYS:HB3	23:U:488:GLY:O	2.19	0.43
23:U:276:PRO:HG2	23:U:279:SER:HB2	2.00	0.43
23:V:21:ASN:HB3	23:V:23:TYR:CE2	2.54	0.43
23:V:81:ASP:OD2	27:Z:93:LEU:HD11	2.18	0.43
24:W:507:ASP:OD2	25:X:563:ARG:NH2	2.52	0.43
25:X:708:ILE:HG13	25:X:709:ARG:N	2.34	0.43
30:c:409:LEU:HD21	30:c:413:ARG:HH21	1.83	0.43
32:m:505:HIS:ND1	32:m:545:ASP:OD2	2.50	0.43
35:z:28:THR:HG23	35:z:31:ARG:HH21	1.83	0.43
35:z:244:SER:O	35:z:324:LYS:HG3	2.18	0.43
35:z:473:SER:OG	35:z:543:ARG:HB3	2.19	0.43
35:z:503:GLU:HA	35:z:633:LYS:HE3	2.00	0.43
35:z:609:LYS:HD3	35:z:609:LYS:N	2.33	0.43
39:1:-14:U:H3'	39:1:-13:U:H5''	2.01	0.43
1:e:261:VAL:HG13	1:e:262:ASN:N	2.33	0.43
4:5:32:C:C4	5:A:487:PRO:HB2	2.54	0.43
5:A:1034:ALA:HB2	24:W:78:THR:HB	2.01	0.43
5:A:1657:ALA:HB3	5:A:1682:ASN:OD1	2.19	0.43
6:B:396:THR:HG21	6:B:428:LEU:HD23	2.00	0.43
7:C:131:HIS:HB3	7:C:163:TRP:CE3	2.54	0.43
7:C:261:PHE:HB3	7:C:296:TRP:CZ2	2.54	0.43
9:E:76:VAL:HA	10:F:64:ASN:HD21	1.82	0.43
16:L:186:TYR:N	16:L:200:ARG:O	2.40	0.43
18:N:279:LYS:HZ3	18:N:383:ARG:HA	1.83	0.43
22:R:166:LYS:HE2	22:R:166:LYS:HB3	1.92	0.43
22:R:600:LYS:HA	22:R:615:VAL:HG11	2.00	0.43
23:U:56:PRO:HB3	23:V:2:PHE:HD2	1.82	0.43
24:W:251:GLU:OE1	24:W:255:LYS:HE3	2.19	0.43
25:X:431:TRP:HZ3	25:X:450:LEU:HD22	1.84	0.43
25:X:634:LYS:HA	25:X:634:LYS:HD2	1.77	0.43
30:c:519:TRP:CZ3	30:c:560:LEU:HD22	2.50	0.43
32:m:394:ASN:O	32:m:398:SER:OG	2.28	0.43
32:m:772:LYS:HB3	32:m:782:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:z:387:MET:CE	35:z:415:HIS:HB3	2.43	0.43
35:z:495:ALA:HB1	35:z:529:ASN:HA	2.01	0.43
5:A:250:ASN:HB3	5:A:252:PRO:HD2	2.01	0.43
5:A:661:LEU:HD23	5:A:661:LEU:HA	1.83	0.43
6:B:195:SER:HA	6:B:216:ASP:O	2.18	0.43
7:C:234:LEU:N	7:C:246:PHE:O	2.35	0.43
18:N:120:VAL:O	18:N:120:VAL:HG12	2.18	0.43
22:R:54:ARG:O	22:R:57:LYS:HG2	2.18	0.43
22:R:450:PHE:HA	22:R:453:CYS:HB2	2.01	0.43
23:S:122:ARG:NH1	23:V:118:LEU:HD22	2.33	0.43
24:W:530:VAL:O	24:W:534:ASP:N	2.52	0.43
33:n:319:GLU:O	33:n:323:ILE:HG12	2.18	0.43
35:z:585:GLN:CD	35:z:591:LYS:HG2	2.44	0.43
5:A:821:GLY:HA3	16:L:285:ASN:HD22	1.83	0.43
5:A:1659:TYR:HB2	5:A:1661:TRP:CH2	2.54	0.43
5:A:1663:VAL:O	5:A:1679:THR:OG1	2.22	0.43
5:A:1900:LEU:HG	5:A:1908:ILE:HD11	2.00	0.43
6:B:356:TRP:CE3	6:B:356:TRP:HA	2.54	0.43
8:D:60:TYR:HB2	14:J:12:TYR:HE2	1.84	0.43
8:D:64:SER:HA	9:E:71:ARG:NH2	2.26	0.43
15:K:135:SER:O	15:K:139:ARG:HG3	2.18	0.43
17:M:138:ALA:O	17:M:141:ARG:HG2	2.19	0.43
20:P:52:LYS:HE3	20:P:52:LYS:HB3	1.83	0.43
24:W:247:ARG:O	24:W:251:GLU:CB	2.65	0.43
25:X:513:THR:HG23	25:X:513:THR:O	2.18	0.43
25:X:520:TYR:CD2	25:X:536:ILE:HG12	2.54	0.43
29:b:19:TYR:HA	39:l:-10:A:O2'	2.18	0.43
35:z:342:ILE:HD13	35:z:350:ARG:NH1	2.34	0.43
1:e:185:ILE:HG23	15:K:373:ALA:HA	2.01	0.42
5:A:1303:ILE:HD12	30:c:424:VAL:HG13	2.01	0.42
5:A:1364:LEU:HD23	29:b:5:GLY:O	2.19	0.42
5:A:1890:LYS:NZ	5:A:1912:GLU:HG2	2.34	0.42
6:B:850:VAL:HG13	6:B:901:LEU:HD21	2.01	0.42
7:C:279:ARG:HH21	7:C:322:GLN:C	2.26	0.42
10:F:74:LEU:HD12	10:F:74:LEU:O	2.19	0.42
13:I:67:CYS:O	13:I:70:VAL:HG22	2.19	0.42
15:K:122:PRO:HA	15:K:126:HIS:HB2	2.01	0.42
15:K:302:PRO:HD2	15:K:359:PHE:HB3	2.00	0.42
17:M:73:CYS:C	17:M:75:ARG:H	2.27	0.42
18:N:257:MET:HE2	18:N:375:ASN:CB	2.49	0.42
18:N:743:LEU:HD21	18:N:1032:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:56:ALA:O	21:Q:59:ARG:HG2	2.19	0.42
22:R:85:GLU:C	22:R:86:PHE:CD1	2.97	0.42
22:R:573:ARG:HG3	22:R:602:PHE:CE2	2.54	0.42
23:S:67:THR:HA	23:T:79:GLU:OE1	2.19	0.42
24:W:537:ARG:HD2	24:W:577:PHE:CD1	2.52	0.42
24:W:699:HIS:HA	24:W:702:LYS:HE2	2.01	0.42
24:W:703:ALA:O	24:W:707:GLU:HG2	2.19	0.42
25:X:223:SER:O	25:X:227:VAL:HG23	2.19	0.42
25:X:682:LEU:HD23	25:X:682:LEU:HA	1.68	0.42
27:Z:148:CYS:O	27:Z:151:LYS:HG2	2.17	0.42
34:y:182:ASP:OD1	34:y:183:ASP:N	2.52	0.42
34:y:222:ALA:HA	34:y:225:MET:SD	2.59	0.42
1:e:128:ASP:OD2	2:p:166:ARG:HD2	2.18	0.42
2:p:167:LYS:HD3	2:p:170:ARG:HH12	1.84	0.42
4:5:82:A:O2'	4:5:83:A:H8	2.01	0.42
5:A:223:VAL:O	5:A:227:PHE:HB2	2.18	0.42
5:A:942:ASP:CG	5:A:1035:LYS:HZ3	2.27	0.42
5:A:1437:ASP:OD1	5:A:1437:ASP:N	2.46	0.42
6:B:438:PHE:O	6:B:440:VAL:N	2.52	0.42
6:B:794:CYS:SG	6:B:795:ASP:N	2.92	0.42
15:K:310:ASP:O	15:K:311:SER:OG	2.23	0.42
15:K:346:PHE:CD1	15:K:359:PHE:CE1	3.04	0.42
17:M:227:LYS:HD3	17:M:230:LYS:NZ	2.34	0.42
18:N:306:LEU:O	18:N:309:THR:OG1	2.28	0.42
18:N:671:PHE:HE1	18:N:680:VAL:HG21	1.84	0.42
18:N:1049:ARG:HG2	18:N:1075:LEU:HD22	2.02	0.42
20:P:184:THR:OG1	20:P:186:ASP:OD1	2.30	0.42
23:V:1:MET:HE1	23:V:13:PRO:HG2	1.99	0.42
25:X:292:ILE:HA	25:X:295:ASP:OD2	2.19	0.42
26:Y:142:ARG:HD3	26:Y:142:ARG:H	1.84	0.42
28:a:139:GLU:OE1	28:a:139:GLU:N	2.41	0.42
34:y:31:ARG:HE	35:z:494:VAL:HG12	1.83	0.42
5:A:768:SER:HB2	15:K:165:TRP:CZ2	2.54	0.42
5:A:919:ILE:HD13	5:A:932:TYR:CE2	2.54	0.42
5:A:1538:LYS:HE2	34:y:206:VAL:O	2.18	0.42
5:A:1707:LYS:HE2	5:A:1711:TYR:CZ	2.54	0.42
6:B:520:LYS:HD2	6:B:538:VAL:HG13	2.01	0.42
15:K:263:VAL:HG12	15:K:295:LEU:HD21	2.01	0.42
18:N:734:SER:HB2	18:N:746:VAL:HG21	2.01	0.42
18:N:1135:ILE:HG13	18:N:1182:ILE:HD11	2.00	0.42
20:P:259:GLN:O	20:P:263:GLU:OE1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:583:LEU:HD13	22:R:592:ARG:HA	2.01	0.42
23:U:405:LEU:HD23	23:U:405:LEU:H	1.84	0.42
32:m:717:SER:OG	32:m:718:PHE:N	2.52	0.42
34:y:124:PRO:HA	34:y:137:ASP:HB3	2.01	0.42
34:y:128:PRO:HD3	34:y:155:PHE:CE1	2.54	0.42
35:z:434:ASN:OD1	35:z:435:LEU:N	2.51	0.42
35:z:534:GLN:O	35:z:537:ARG:HG2	2.18	0.42
2:p:176:GLU:CD	24:W:63:ARG:HH12	2.26	0.42
5:A:868:ARG:HH11	5:A:1463:ARG:HD2	1.84	0.42
5:A:1635:LYS:HE2	5:A:1652:ASP:OD1	2.19	0.42
5:A:1856:ARG:HD3	5:A:1859:GLN:HB3	2.01	0.42
6:B:247:VAL:O	6:B:877:ARG:NH2	2.50	0.42
7:C:237:ASN:HB2	7:C:275:VAL:HG13	2.01	0.42
11:G:36:ALA:HB2	11:G:111:ARG:HH21	1.83	0.42
11:G:110:VAL:HG12	13:I:63:ILE:CD1	2.50	0.42
20:P:251:ASN:HB2	20:P:254:SER:HB3	2.01	0.42
22:R:77:GLY:O	22:R:81:LEU:HB2	2.19	0.42
22:R:361:TYR:HA	22:R:364:ILE:HG22	2.01	0.42
22:R:466:GLU:HG2	22:R:499:ILE:HG22	2.00	0.42
23:U:240:SER:O	23:U:248:GLU:N	2.53	0.42
23:V:16:SER:H	23:V:20:GLY:HA2	1.84	0.42
23:V:73:LEU:HD11	27:Z:80:TYR:HE2	1.84	0.42
24:W:537:ARG:CG	24:W:538:PRO:CD	2.97	0.42
27:Z:155:TYR:O	27:Z:158:GLU:HG3	2.19	0.42
29:b:124:VAL:HA	29:b:127:LEU:HD12	2.01	0.42
30:c:586:ASN:OD1	30:c:587:TYR:N	2.53	0.42
32:m:497:LYS:NZ	32:m:545:ASP:OD1	2.48	0.42
35:z:379:GLU:HB2	35:z:383:LEU:HD22	2.01	0.42
3:2:30:A:C6	34:y:37:PRO:HD2	2.54	0.42
4:5:84:U:H2'	4:5:85:U:C6	2.53	0.42
5:A:154:PRO:O	5:A:444:ALA:N	2.51	0.42
5:A:291:ALA:N	29:b:2:SER:O	2.40	0.42
7:C:132:LYS:HG2	7:C:133:GLY:N	2.35	0.42
7:C:279:ARG:NE	7:C:321:HIS:O	2.53	0.42
12:H:28:ILE:HG12	12:H:81:ILE:HD13	2.01	0.42
18:N:869:TYR:O	18:N:873:VAL:HB	2.19	0.42
20:P:292:ASN:OD1	20:P:293:ARG:NH1	2.52	0.42
22:R:466:GLU:HB3	22:R:501:GLU:HG3	2.00	0.42
24:W:237:ASP:OD2	24:W:239:SER:HB3	2.19	0.42
24:W:542:GLN:NE2	24:W:569:SER:O	2.49	0.42
25:X:548:VAL:HA	25:X:551:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:584:PRO:CD	25:X:587:PHE:HB2	2.48	0.42
38:6:17:U:O2'	38:6:18:G:OP2	2.34	0.42
2:p:169:PHE:CE2	24:W:67:GLU:HB3	2.53	0.42
5:A:107:ARG:NH2	16:L:215:PRO:O	2.52	0.42
5:A:1219:VAL:HG22	5:A:1254:ILE:HD13	2.02	0.42
6:B:330:PHE:CG	6:B:335:PHE:HE1	2.38	0.42
6:B:942:ASP:OD1	6:B:942:ASP:N	2.49	0.42
7:C:134:HIS:ND1	7:C:155:SER:OG	2.53	0.42
14:J:22:ASN:O	14:J:25:ARG:HD3	2.19	0.42
16:L:216:LYS:HE3	16:L:216:LYS:HB3	1.81	0.42
16:L:237:PRO:HD3	22:R:136:ARG:NH1	2.33	0.42
18:N:803:LEU:HG	18:N:820:LEU:HD11	2.00	0.42
20:P:120:PHE:HB2	20:P:135:HIS:CD2	2.55	0.42
23:U:72:LEU:HD12	23:V:63:PRO:HG2	2.00	0.42
24:W:197:GLN:OE1	24:W:200:ARG:NE	2.50	0.42
25:X:254:GLY:CA	25:X:293:ILE:HD11	2.50	0.42
25:X:455:VAL:HA	25:X:476:LEU:HD21	2.01	0.42
30:c:541:LYS:HG3	30:c:591:ILE:HD12	2.00	0.42
32:m:606:PHE:CE2	32:m:650:LEU:HD11	2.55	0.42
34:y:159:PRO:O	34:y:163:TYR:HD1	2.03	0.42
34:y:160:PHE:HB2	35:z:383:LEU:CD2	2.49	0.42
35:z:442:GLN:HG2	35:z:553:PHE:CE1	2.55	0.42
3:2:14:C:H2'	38:6:76:C:C5	2.54	0.42
5:A:1287:TRP:CZ2	5:A:1291:LEU:HD22	2.54	0.42
6:B:739:ASP:CG	29:b:66:LYS:HD3	2.45	0.42
6:B:846:TYR:CE1	6:B:891:VAL:HG22	2.54	0.42
12:H:46:ASP:OD1	12:H:46:ASP:N	2.52	0.42
15:K:387:PHE:HE1	15:K:395:MET:HE3	1.83	0.42
16:L:111:HIS:C	16:L:113:HIS:H	2.27	0.42
18:N:256:ARG:HA	18:N:261:TYR:CD1	2.55	0.42
20:P:91:VAL:O	20:P:92:LYS:C	2.62	0.42
20:P:178:VAL:HG21	20:P:195:PHE:HZ	1.85	0.42
22:R:310:LYS:HA	22:R:313:LYS:HE3	2.01	0.42
22:R:510:TYR:O	22:R:513:PHE:HB3	2.20	0.42
23:S:69:LEU:HD22	23:U:80:TRP:CD1	2.53	0.42
23:U:207:LEU:HD22	23:U:212:THR:O	2.19	0.42
25:X:186:CYS:HA	25:X:191:TRP:CZ3	2.55	0.42
25:X:357:ARG:HA	25:X:360:LYS:HG2	2.01	0.42
25:X:648:TYR:HE1	25:X:663:MET:HB2	1.85	0.42
30:c:475:SER:OG	30:c:476:ARG:N	2.53	0.42
34:y:142:GLU:O	34:y:146:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:398:GLU:HG3	12:H:6:GLN:NE2	2.35	0.42
5:A:1153:LYS:NZ	5:A:1198:THR:O	2.53	0.42
5:A:2025:SER:HB3	5:A:2028:ASN:ND2	2.35	0.42
6:B:752:ASP:N	6:B:785:GLN:OE1	2.30	0.42
11:G:5:VAL:HG21	11:G:19:ARG:NH1	2.34	0.42
18:N:211:GLN:NE2	18:N:367:LYS:HB2	2.35	0.42
20:P:124:MET:HE3	20:P:124:MET:HB3	1.85	0.42
22:R:42:ILE:HG21	22:R:48:LEU:HB2	2.01	0.42
23:T:67:THR:HB	27:Z:105:ARG:HA	2.01	0.42
24:W:696:LYS:HE3	27:Z:131:LEU:HA	2.00	0.42
25:X:105:LEU:HD12	25:X:108:MET:HB3	2.01	0.42
25:X:272:LYS:HA	25:X:272:LYS:HD2	1.85	0.42
25:X:428:ALA:O	25:X:432:ILE:HG23	2.20	0.42
27:Z:56:SER:OG	27:Z:57:ASP:N	2.48	0.42
34:y:183:ASP:HA	34:y:186:GLN:HE22	1.85	0.42
35:z:463:GLY:HA2	35:z:559:GLN:OE1	2.19	0.42
1:e:55:LYS:HA	16:L:308:TYR:CD2	2.55	0.42
4:5:85:U:H2'	4:5:86:U:C6	2.55	0.42
5:A:732:ILE:HD13	5:A:758:ILE:HD12	2.02	0.42
5:A:1016:LEU:O	5:A:1020:MET:HG3	2.19	0.42
6:B:325:ASP:HB2	42:B:1001:GTP:C6	2.55	0.42
13:I:25:LYS:HA	13:I:71:LEU:HD12	2.01	0.42
16:L:100:ALA:HB1	26:Y:150:ALA:O	2.18	0.42
18:N:1052:ILE:HG13	18:N:1211:LEU:HD22	2.02	0.42
18:N:1093:ALA:HB2	18:N:1098:GLN:NE2	2.34	0.42
18:N:1098:GLN:O	18:N:1109:ASN:ND2	2.52	0.42
22:R:349:VAL:HB	22:R:361:TYR:HE1	1.85	0.42
22:R:450:PHE:CE1	22:R:477:LEU:HD11	2.54	0.42
23:V:61:PRO:O	23:V:62:ARG:HG2	2.20	0.42
23:V:94:LEU:HA	23:V:97:THR:HG22	2.02	0.42
24:W:567:LEU:O	24:W:571:ASP:N	2.49	0.42
25:X:238:VAL:HG13	25:X:242:PHE:CE2	2.55	0.42
25:X:420:PRO:HA	25:X:473:GLN:HG3	2.02	0.42
25:X:447:ALA:O	25:X:451:ILE:HG12	2.20	0.42
25:X:520:TYR:CE1	25:X:524:LEU:HB2	2.55	0.42
30:c:454:ASN:ND2	30:c:507:PHE:HB2	2.34	0.42
32:m:322:VAL:HG12	32:m:324:GLU:H	1.83	0.42
32:m:771:LYS:HE2	32:m:771:LYS:HB3	1.71	0.42
36:r:232:UNK:C	36:r:234:UNK:H	2.32	0.42
38:6:85:G:H2'	38:6:86:A:C8	2.55	0.42
1:e:123:LYS:HB2	1:e:123:LYS:HE2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:30:A:H62	34:y:37:PRO:HB2	1.85	0.42
5:A:1005:SER:O	5:A:1006:LYS:HD3	2.20	0.42
5:A:1429:LEU:C	5:A:1431:ASP:N	2.77	0.42
5:A:1440:ILE:HD13	5:A:1440:ILE:HA	1.73	0.42
7:C:262:GLU:O	7:C:296:TRP:HZ2	2.03	0.42
11:G:9:ARG:NE	11:G:9:ARG:HA	2.35	0.42
12:H:10:ILE:O	12:H:10:ILE:HG13	2.20	0.42
16:L:184:ILE:O	16:L:201:ILE:HA	2.19	0.42
17:M:110:ASP:OD1	17:M:111:ILE:N	2.53	0.42
18:N:679:SER:OG	18:N:729:ASP:OD2	2.28	0.42
20:P:97:CYS:SG	20:P:98:VAL:N	2.93	0.42
22:R:292:ASP:OD1	22:R:295:GLY:HA2	2.20	0.42
22:R:605:MET:HE2	22:R:606:HIS:CE1	2.55	0.42
23:S:25:LYS:HA	23:S:25:LYS:HD2	1.92	0.42
23:U:99:GLN:NE2	23:U:99:GLN:HA	2.34	0.42
23:U:405:LEU:HG	23:U:406:ARG:HD2	2.01	0.42
24:W:155:MET:HG2	24:W:155:MET:O	2.19	0.42
24:W:537:ARG:HD2	24:W:577:PHE:CD2	2.55	0.42
24:W:675:LEU:HD11	27:Z:105:ARG:HH21	1.84	0.42
25:X:260:LEU:HD12	25:X:263:TYR:HD2	1.84	0.42
27:Z:24:ALA:O	27:Z:27:GLN:HG3	2.20	0.42
32:m:641:TRP:O	32:m:645:VAL:HG23	2.19	0.42
1:e:117:VAL:HB	5:A:827:ASP:OD1	2.19	0.41
5:A:170:MET:SD	5:A:213:MET:HE1	2.60	0.41
5:A:1660:LYS:NZ	5:A:1681:THR:O	2.53	0.41
5:A:1687:ASP:OD1	5:A:1726:LEU:HA	2.20	0.41
6:B:702:VAL:HG13	6:B:804:ARG:HE	1.84	0.41
7:C:172:LYS:HB2	7:C:172:LYS:HE2	1.91	0.41
8:D:19:GLU:HB3	8:D:25:THR:HG22	2.02	0.41
11:G:42:GLN:O	11:G:112:ILE:N	2.32	0.41
15:K:431:LYS:HA	15:K:431:LYS:HD3	1.79	0.41
16:L:281:ASP:OD2	16:L:283:GLU:OE1	2.37	0.41
17:M:301:LEU:O	17:M:305:VAL:N	2.53	0.41
18:N:671:PHE:CE1	18:N:732:LEU:HD13	2.55	0.41
18:N:792:GLU:OE1	18:N:817:TYR:HB2	2.20	0.41
22:R:147:MET:O	22:R:151:LEU:HD23	2.20	0.41
24:W:240:GLU:O	24:W:242:ASP:N	2.53	0.41
32:m:583:PRO:HG3	32:m:638:TRP:CZ2	2.55	0.41
34:y:110:LYS:HG3	34:y:112:TYR:HE1	1.85	0.41
35:z:553:PHE:HB2	35:z:555:ILE:HG12	2.01	0.41
5:A:197:PHE:CZ	5:A:589:LEU:HD21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:970:PRO:HB2	5:A:972:PRO:HD2	2.02	0.41
5:A:1549:GLY:HA3	34:y:58:GLY:O	2.21	0.41
5:A:1973:LYS:NZ	5:A:1976:LEU:HD22	2.34	0.41
6:B:311:ARG:NH2	6:B:315:GLU:OE2	2.53	0.41
7:C:65:PHE:CD2	7:C:326:LEU:HD21	2.55	0.41
8:D:65:HIS:CE1	14:J:68:ILE:HD13	2.55	0.41
11:G:11:GLU:N	11:G:12:LEU:HD12	2.35	0.41
12:H:21:GLN:OE1	12:H:21:GLN:HA	2.20	0.41
12:H:72:LEU:HD11	13:I:8:PRO:HB3	2.02	0.41
15:K:387:PHE:CE1	15:K:395:MET:HE3	2.55	0.41
18:N:606:LEU:HD12	18:N:606:LEU:HA	1.94	0.41
18:N:823:TRP:CZ2	18:N:928:ILE:HG13	2.56	0.41
18:N:1252:HIS:CG	18:N:1258:VAL:HG21	2.55	0.41
24:W:48:TRP:CE2	24:W:53:ASP:HB3	2.55	0.41
25:X:624:ARG:O	25:X:627:ILE:HG22	2.20	0.41
34:y:36:VAL:O	34:y:36:VAL:HG23	2.20	0.41
34:y:154:ASP:OD1	34:y:154:ASP:N	2.50	0.41
35:z:364:ARG:HD2	35:z:366:TYR:OH	2.20	0.41
5:A:1222:LEU:HD12	5:A:1223:PRO:HD2	2.02	0.41
5:A:1538:LYS:HD2	34:y:206:VAL:HG22	2.02	0.41
6:B:371:GLN:NE2	6:B:373:LEU:H	2.18	0.41
6:B:860:ILE:HG12	6:B:901:LEU:HD11	2.01	0.41
10:F:17:ILE:HD11	10:F:68:TYR:HE1	1.85	0.41
10:F:36:MET:HG3	10:F:36:MET:O	2.20	0.41
13:I:16:ILE:HG13	13:I:35:GLN:HA	2.02	0.41
13:I:31:LYS:O	13:I:48:ALA:HA	2.20	0.41
13:I:45:LEU:HB2	13:I:63:ILE:HB	2.02	0.41
15:K:87:ASP:HA	22:R:259:ARG:HH12	1.85	0.41
15:K:343:GLU:OE1	15:K:400:TRP:NE1	2.53	0.41
16:L:319:LYS:HA	16:L:322:GLN:NE2	2.35	0.41
18:N:140:ARG:HB2	18:N:144:TYR:CE2	2.55	0.41
18:N:480:LEU:CD1	18:N:505:MET:HB2	2.51	0.41
20:P:127:GLU:CG	20:P:131:CYS:HB2	2.49	0.41
22:R:322:TRP:O	22:R:326:LEU:HD23	2.20	0.41
22:R:402:LYS:HE2	22:R:402:LYS:HB2	1.90	0.41
22:R:566:PRO:O	22:R:570:VAL:HG23	2.19	0.41
23:V:2:PHE:O	23:V:22:VAL:HG21	2.20	0.41
23:V:23:TYR:HB2	23:V:28:ILE:HD11	2.03	0.41
24:W:510:ARG:CZ	24:W:513:GLN:HE22	2.32	0.41
25:X:454:ALA:O	25:X:476:LEU:HD21	2.21	0.41
29:b:55:SER:OG	29:b:56:GLU:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:y:31:ARG:HA	35:z:493:PHE:CE2	2.55	0.41
3:2:30:A:N3	3:2:30:A:H2'	2.34	0.41
5:A:330:GLU:OE1	5:A:330:GLU:N	2.51	0.41
5:A:1391:ASN:ND2	5:A:1393:TYR:HB3	2.35	0.41
6:B:222:ASP:HB3	6:B:650:TYR:HB2	2.02	0.41
7:C:237:ASN:HB2	7:C:275:VAL:CG1	2.50	0.41
15:K:88:SER:C	15:K:90:ASN:H	2.28	0.41
15:K:344:PHE:CE2	15:K:359:PHE:HB2	2.56	0.41
17:M:88:GLN:OE1	17:M:133:SER:HB2	2.20	0.41
20:P:52:LYS:HD3	20:P:54:ILE:C	2.45	0.41
22:R:122:HIS:O	22:R:126:LEU:HD13	2.20	0.41
22:R:192:GLY:O	22:R:196:ARG:HG3	2.19	0.41
22:R:277:MET:O	22:R:281:LYS:HG2	2.20	0.41
23:V:81:ASP:O	23:V:85:LEU:HG	2.20	0.41
25:X:398:ARG:HH21	25:X:436:GLU:CD	2.27	0.41
25:X:495:THR:O	25:X:499:THR:OG1	2.23	0.41
26:Y:131:ASP:OD1	26:Y:132:LYS:N	2.54	0.41
28:a:61:GLU:OE1	28:a:61:GLU:N	2.47	0.41
28:a:126:ASP:OD1	28:a:129:ARG:NH1	2.54	0.41
30:c:573:PHE:CZ	30:c:596:LEU:HD13	2.55	0.41
30:c:594:GLY:O	30:c:597:THR:HG22	2.18	0.41
34:y:150:TRP:CE2	34:y:152:GLY:HA3	2.55	0.41
35:z:426:LEU:HG	35:z:454:LYS:HD2	2.01	0.41
5:A:220:ASP:OD1	5:A:259:ARG:NH2	2.42	0.41
5:A:946:ASP:OD1	5:A:950:TRP:HD1	2.03	0.41
5:A:1234:LYS:HA	5:A:1234:LYS:HD2	1.87	0.41
5:A:1781:GLU:O	5:A:1782:PRO:C	2.63	0.41
6:B:725:GLN:NE2	6:B:744:ARG:O	2.53	0.41
7:C:296:TRP:CD1	7:C:302:LEU:HA	2.55	0.41
18:N:58:PHE:HB3	18:N:85:LYS:NZ	2.36	0.41
22:R:59:PHE:CD2	22:R:76:TYR:HA	2.55	0.41
22:R:307:GLN:HA	22:R:310:LYS:HG2	2.03	0.41
23:T:91:ARG:HH11	23:U:90:LEU:HD12	1.85	0.41
23:V:106:TYR:HA	23:V:109:ASP:HB2	2.02	0.41
24:W:529:GLN:HA	24:W:532:GLN:HB2	2.02	0.41
27:Z:20:GLU:OE2	27:Z:23:SER:OG	2.38	0.41
27:Z:70:GLU:O	27:Z:71:LYS:HB2	2.19	0.41
27:Z:147:GLY:HA2	27:Z:150:ARG:NH1	2.36	0.41
32:m:379:TRP:CD1	32:m:380:LYS:HG3	2.55	0.41
34:y:82:SER:C	34:y:84:ASN:H	2.27	0.41
2:p:198:PRO:O	25:X:725:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:19:G:H5'	16:L:261:PRO:HG2	2.03	0.41
5:A:268:LEU:O	5:A:269:ARG:HG2	2.20	0.41
5:A:1282:LYS:CG	34:y:208:ASN:HD21	2.26	0.41
6:B:707:GLU:HG2	6:B:708:LYS:H	1.85	0.41
7:C:43:ASN:HD21	9:E:106:ARG:HD2	1.85	0.41
7:C:201:ILE:HB	7:C:215:LEU:HB2	2.03	0.41
17:M:69:ILE:CG2	17:M:84:MET:HE1	2.50	0.41
18:N:72:LEU:O	18:N:76:ASN:ND2	2.53	0.41
18:N:193:ASN:HB3	18:N:197:ARG:HH12	1.85	0.41
20:P:82:MET:O	20:P:83:ARG:C	2.63	0.41
20:P:108:ALA:HB2	20:P:132:GLU:C	2.44	0.41
22:R:134:LEU:HB3	22:R:137:VAL:HG12	2.03	0.41
23:U:80:TRP:HA	23:U:83:VAL:HG12	2.01	0.41
24:W:132:SER:HA	24:W:135:ARG:CZ	2.51	0.41
28:a:98:VAL:O	28:a:102:GLU:HG3	2.20	0.41
29:b:131:TYR:O	29:b:134:GLN:HG3	2.21	0.41
34:y:31:ARG:O	34:y:34:GLN:HG2	2.20	0.41
35:z:464:CYS:SG	35:z:561:LEU:HD13	2.61	0.41
35:z:585:GLN:CG	35:z:591:LYS:HG2	2.51	0.41
5:A:276:LEU:HD23	5:A:276:LEU:HA	1.88	0.41
5:A:532:HIS:O	5:A:533:ARG:HB3	2.20	0.41
5:A:1142:ASP:OD2	5:A:1145:ASN:HA	2.19	0.41
7:C:116:HIS:C	7:C:117:LEU:HD12	2.46	0.41
12:H:27:SER:HB3	12:H:82:GLN:HB3	2.03	0.41
15:K:121:VAL:HG13	15:K:121:VAL:O	2.20	0.41
16:L:101:VAL:HG13	16:L:103:TYR:CE1	2.56	0.41
17:M:167:LYS:O	17:M:170:LEU:HB3	2.20	0.41
20:P:59:GLU:HG2	20:P:61:GLU:OE2	2.20	0.41
20:P:214:PHE:CE2	39:1:11:U:C6	3.05	0.41
22:R:383:ARG:HH22	22:R:414:GLN:HG3	1.86	0.41
26:Y:95:LYS:HE2	26:Y:121:ARG:NH2	2.35	0.41
31:d:29:PHE:HD2	31:d:119:PHE:HE2	1.67	0.41
35:z:281:VAL:O	35:z:285:MET:HG2	2.21	0.41
5:A:198:SER:OG	5:A:201:GLN:HG2	2.21	0.41
5:A:876:LYS:HG3	5:A:878:ARG:H	1.86	0.41
5:A:911:MET:HE2	5:A:914:PHE:CD2	2.56	0.41
5:A:1428:THR:HA	34:y:230:SER:HA	2.03	0.41
6:B:460:LYS:HA	6:B:460:LYS:HD2	1.79	0.41
7:C:306:LEU:HD12	7:C:306:LEU:O	2.21	0.41
8:D:91:LEU:HB3	8:D:92:PRO:HD2	2.01	0.41
13:I:19:PRO:HA	13:I:32:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:143:ASP:O	16:L:147:GLN:HG2	2.20	0.41
18:N:427:TYR:HD1	18:N:432:PHE:CD2	2.38	0.41
18:N:456:PHE:HB2	18:N:477:PHE:CE1	2.56	0.41
20:P:127:GLU:OE1	20:P:127:GLU:N	2.53	0.41
20:P:261:ARG:HH12	20:P:265:ARG:NH2	2.18	0.41
22:R:88:ARG:HB3	24:W:225:ILE:CD1	2.45	0.41
22:R:296:VAL:O	22:R:300:VAL:HG23	2.20	0.41
23:T:117:ARG:HA	23:T:120:LYS:NZ	2.36	0.41
23:U:205:GLU:HA	23:U:217:PRO:HA	2.03	0.41
23:U:342:HIS:CE1	23:U:344:ASP:H	2.38	0.41
24:W:71:HIS:NE2	24:W:75:LEU:HD11	2.36	0.41
24:W:159:GLU:CD	24:W:160:LYS:H	2.29	0.41
24:W:530:VAL:HG23	24:W:531:ILE:N	2.35	0.41
24:W:536:ILE:CG2	24:W:537:ARG:H	2.17	0.41
25:X:230:PRO:HB3	25:X:263:TYR:HD1	1.86	0.41
29:b:71:ARG:HH12	29:b:126:ILE:HG13	1.86	0.41
2:p:210:LEU:O	2:p:214:GLU:HG3	2.21	0.41
4:5:95:A:C6	13:I:40:TYR:HD2	2.38	0.41
5:A:97:MET:HE3	5:A:97:MET:HB3	1.93	0.41
5:A:615:TYR:OH	5:A:1574:GLY:HA2	2.21	0.41
5:A:851:PRO:HA	5:A:852:PRO:HD3	1.97	0.41
5:A:1037:ASN:ND2	5:A:1049:ASN:O	2.47	0.41
5:A:1185:ARG:HE	21:Q:229:VAL:CG1	2.31	0.41
5:A:1272:LEU:HA	5:A:1272:LEU:HD23	1.74	0.41
5:A:1635:LYS:HE2	5:A:1652:ASP:HA	2.01	0.41
5:A:1646:MET:N	5:A:1646:MET:SD	2.94	0.41
5:A:1654:LEU:C	5:A:1655:LEU:HD22	2.46	0.41
5:A:1973:LYS:HA	5:A:1973:LYS:HD2	1.92	0.41
6:B:153:GLY:HA3	6:B:270:ASN:HD22	1.86	0.41
6:B:682:ASP:OD1	6:B:683:THR:N	2.54	0.41
7:C:143:VAL:HG12	7:C:151:LEU:HD22	2.02	0.41
7:C:309:HIS:CE1	7:C:335:PHE:CD2	3.09	0.41
10:F:40:LEU:HB3	10:F:43:VAL:CG1	2.41	0.41
11:G:35:GLN:HG2	11:G:111:ARG:NH2	2.35	0.41
11:G:52:LYS:HB2	11:G:74:MET:SD	2.61	0.41
12:H:80:LEU:CD2	14:J:60:VAL:HG13	2.49	0.41
13:I:42:ASN:HB3	13:I:67:CYS:HB3	2.02	0.41
15:K:386:MET:HE2	15:K:386:MET:HB3	1.95	0.41
16:L:139:GLU:OE1	16:L:139:GLU:HA	2.21	0.41
18:N:81:LEU:HA	18:N:81:LEU:HD23	1.82	0.41
18:N:155:LEU:HD22	18:N:160:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:342:LEU:HB3	18:N:347:LEU:HG	2.02	0.41
20:P:119:TYR:CD2	38:6:23:A:C6	3.09	0.41
20:P:136:ARG:NH1	20:P:139:LYS:HG2	2.34	0.41
20:P:183:PRO:HD2	20:P:187:ILE:HG22	2.03	0.41
22:R:116:LYS:NZ	26:Y:172:ILE:HG22	2.35	0.41
22:R:189:ARG:HE	22:R:189:ARG:HB3	1.62	0.41
22:R:278:GLU:O	22:R:282:GLU:OE1	2.39	0.41
22:R:322:TRP:CZ2	22:R:348:LYS:HE3	2.55	0.41
22:R:453:CYS:HB3	22:R:457:TYR:CZ	2.56	0.41
22:R:588:LEU:HB3	22:R:591:GLU:HB2	2.02	0.41
23:S:78:GLU:HA	23:S:81:ASP:OD2	2.21	0.41
23:T:73:LEU:HD22	23:V:73:LEU:HD13	2.03	0.41
23:U:94:LEU:O	23:U:97:THR:HG22	2.21	0.41
23:U:263:ALA:O	23:U:275:PHE:N	2.54	0.41
23:V:23:TYR:CD2	23:V:28:ILE:HD11	2.56	0.41
23:V:91:ARG:NE	36:r:237:UNK:O	2.54	0.41
25:X:81:HIS:CE1	25:X:82:LEU:HD22	2.55	0.41
25:X:219:TRP:HE1	25:X:256:LEU:CD2	2.33	0.41
25:X:292:ILE:HA	25:X:292:ILE:HD12	1.94	0.41
30:c:414:LYS:HE2	30:c:414:LYS:HB2	1.85	0.41
30:c:490:TYR:HE1	30:c:540:LEU:HD21	1.86	0.41
30:c:576:ASP:HB3	30:c:603:TYR:CE1	2.56	0.41
31:d:32:LEU:HD11	31:d:37:TYR:HE1	1.83	0.41
35:z:306:GLU:HA	35:z:353:ARG:CZ	2.51	0.41
35:z:310:THR:HA	35:z:356:ARG:NH1	2.30	0.41
39:1:-15:U:H2'	39:1:-14:U:H5''	2.03	0.41
1:e:198:TYR:CE1	5:A:748:PRO:HB3	2.55	0.41
1:e:204:HIS:HD2	6:B:76:GLN:H	1.67	0.41
5:A:70:ARG:NH1	5:A:73:GLY:O	2.53	0.41
5:A:366:LEU:HD23	5:A:366:LEU:HA	1.88	0.41
5:A:1654:LEU:O	5:A:1655:LEU:HD22	2.21	0.41
6:B:190:VAL:O	6:B:190:VAL:HG12	2.20	0.41
15:K:149:TRP:HZ2	15:K:459:HIS:HB2	1.86	0.41
15:K:265:ALA:HB1	15:K:292:VAL:HB	2.03	0.41
16:L:183:TYR:HB2	28:a:92:GLU:O	2.21	0.41
18:N:134:SER:O	18:N:140:ARG:HB3	2.21	0.41
18:N:480:LEU:HD23	18:N:608:PHE:O	2.20	0.41
18:N:745:MET:HB3	18:N:1029:PHE:HE1	1.85	0.41
18:N:784:MET:HE3	18:N:784:MET:HB2	1.78	0.41
23:U:111:ALA:O	23:U:115:ILE:HG12	2.20	0.41
24:W:20:ALA:HB1	24:W:32:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:248:GLU:HA	24:W:251:GLU:HB3	2.03	0.41
24:W:541:THR:O	24:W:545:LYS:HD3	2.21	0.41
24:W:560:LEU:HG	24:W:561:LEU:HG	2.02	0.41
24:W:654:GLU:HG2	27:Z:86:PRO:HB3	2.03	0.41
24:W:675:LEU:HD21	27:Z:105:ARG:NH2	2.34	0.41
26:Y:161:ASP:OD1	26:Y:164:HIS:ND1	2.35	0.41
27:Z:94:GLN:HA	27:Z:97:VAL:HG22	2.03	0.41
27:Z:120:PHE:CZ	27:Z:124:LEU:HD11	2.56	0.41
31:d:70:ASP:OD1	31:d:70:ASP:N	2.54	0.41
32:m:359:SER:HA	32:m:362:VAL:HG12	2.03	0.41
34:y:160:PHE:CD2	35:z:415:HIS:NE2	2.90	0.41
35:z:140:TYR:O	35:z:169:ARG:NH1	2.43	0.41
4:5:98:U:N3	8:D:38:ASN:OD1	2.53	0.40
5:A:304:ASP:OD1	5:A:304:ASP:N	2.55	0.40
5:A:1600:ILE:O	5:A:1770:ARG:HD3	2.21	0.40
6:B:488:LEU:O	6:B:580:VAL:HA	2.21	0.40
6:B:838:SER:O	6:B:838:SER:OG	2.32	0.40
7:C:53:VAL:HA	7:C:69:GLY:HA3	2.03	0.40
15:K:397:PHE:HE1	15:K:409:LEU:HD12	1.86	0.40
15:K:453:ASN:O	15:K:455:THR:HG23	2.20	0.40
18:N:1017:ASN:HD22	18:N:1170:GLU:CD	2.29	0.40
18:N:1079:ASN:HB3	18:N:1082:PHE:HB2	2.02	0.40
18:N:1138:LEU:HG	18:N:1183:PHE:CZ	2.55	0.40
19:O:29:ARG:NH1	28:a:148:GLU:OE2	2.52	0.40
20:P:59:GLU:CD	20:P:59:GLU:H	2.29	0.40
20:P:77:LYS:HE3	20:P:77:LYS:HB3	1.75	0.40
22:R:372:GLU:OE2	22:R:385:VAL:HB	2.21	0.40
22:R:457:TYR:CD2	22:R:474:TYR:HD1	2.39	0.40
23:U:352:LEU:N	23:U:356:GLU:O	2.49	0.40
23:V:86:GLU:O	23:V:90:LEU:HG	2.21	0.40
23:V:99:GLN:HE22	36:r:230:UNK:C	2.33	0.40
24:W:21:VAL:HG11	24:W:48:TRP:CH2	2.56	0.40
24:W:161:GLU:O	24:W:165:GLU:HG3	2.21	0.40
25:X:574:ASP:HA	25:X:577:GLU:OE2	2.22	0.40
30:c:540:LEU:HD12	30:c:544:PHE:CE2	2.57	0.40
36:r:243:UNK:O	36:r:247:UNK:N	2.54	0.40
1:e:252:SER:HA	1:e:257:PRO:HA	2.03	0.40
5:A:233:LEU:HB3	5:A:236:THR:OG1	2.20	0.40
5:A:618:LYS:O	5:A:621:LEU:HD13	2.22	0.40
6:B:522:LYS:HD2	6:B:582:ASP:HA	2.03	0.40
7:C:188:GLN:HE22	7:C:190:THR:HG22	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:334:VAL:O	15:K:334:VAL:HG13	2.22	0.40
18:N:257:MET:HE2	18:N:375:ASN:HB2	2.02	0.40
20:P:52:LYS:HG2	20:P:126:SER:HA	2.03	0.40
22:R:517:GLU:C	22:R:519:GLU:H	2.30	0.40
22:R:599:TRP:HH2	22:R:618:LEU:HD12	1.86	0.40
23:T:14:VAL:HB	23:T:50:LEU:HB2	2.02	0.40
23:T:14:VAL:HG11	23:T:50:LEU:HD13	2.03	0.40
23:U:40:VAL:HG12	23:U:41:THR:HG23	2.03	0.40
24:W:237:ASP:CG	24:W:239:SER:HB3	2.46	0.40
25:X:172:GLN:NE2	25:X:173:VAL:HG13	2.37	0.40
25:X:414:GLU:HG2	25:X:418:HIS:CE1	2.56	0.40
29:b:63:ILE:HD12	29:b:63:ILE:HA	1.92	0.40
31:d:150:ILE:HG13	31:d:151:LYS:N	2.36	0.40
32:m:575:MET:HG3	32:m:579:LEU:HB3	2.03	0.40
34:y:145:LEU:HD12	34:y:150:TRP:HB2	2.02	0.40
34:y:215:GLN:N	34:y:215:GLN:OE1	2.54	0.40
35:z:273:LEU:HD13	35:z:287:VAL:HA	2.02	0.40
35:z:332:THR:HG22	35:z:596:LYS:NZ	2.36	0.40
39:1:5:G:H2'	39:1:6:U:C6	2.56	0.40
5:A:1495:ARG:HG3	34:y:218:TYR:CD1	2.56	0.40
5:A:1596:SER:O	5:A:1600:ILE:HG12	2.21	0.40
5:A:1735:MET:H	5:A:1735:MET:HG2	1.78	0.40
6:B:464:SER:OG	6:B:465:TYR:N	2.54	0.40
6:B:657:ASP:O	6:B:661:LEU:HB2	2.22	0.40
8:D:40:GLN:HG2	8:D:60:TYR:CD2	2.56	0.40
19:O:6:THR:HG22	19:O:7:SER:N	2.35	0.40
23:S:75:LEU:HA	23:S:78:GLU:HG3	2.03	0.40
23:S:90:LEU:CD1	23:V:86:GLU:HG2	2.51	0.40
25:X:687:GLY:C	25:X:689:GLN:H	2.29	0.40
26:Y:173:LYS:HB3	26:Y:173:LYS:HE2	1.78	0.40
29:b:23:ASN:C	29:b:25:SER:H	2.29	0.40
32:m:515:LEU:HG	32:m:519:ALA:N	2.36	0.40
3:2:8:C:H2'	3:2:9:U:C6	2.56	0.40
5:A:1135:ARG:NH1	21:Q:226:ASP:OD2	2.54	0.40
5:A:1892:MET:HE3	5:A:1892:MET:HB2	1.89	0.40
6:B:423:ASP:HB2	6:B:426:PRO:CG	2.50	0.40
6:B:706:LEU:HD21	6:B:758:ILE:CD1	2.51	0.40
10:F:3:LEU:O	10:F:3:LEU:HD23	2.21	0.40
15:K:325:THR:OG1	16:L:116:LEU:HD23	2.20	0.40
18:N:1120:PHE:HD1	18:N:1133:ILE:HG21	1.85	0.40
21:Q:50:LYS:HA	21:Q:50:LYS:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:74:MET:HG2	22:R:74:MET:H	1.77	0.40
22:R:133:GLN:HB3	22:R:134:LEU:HD12	2.03	0.40
22:R:310:LYS:HE3	22:R:310:LYS:HB3	1.77	0.40
22:R:599:TRP:CH2	22:R:618:LEU:HD12	2.57	0.40
23:U:94:LEU:HA	23:U:97:THR:HG22	2.04	0.40
24:W:156:ASP:CG	24:W:157:GLU:H	2.29	0.40
24:W:252:ALA:HA	24:W:255:LYS:HG2	2.02	0.40
24:W:597:ILE:O	24:W:601:ARG:HG2	2.22	0.40
27:Z:153:LYS:HD3	27:Z:153:LYS:HA	1.90	0.40
30:c:583:PHE:HA	30:c:586:ASN:ND2	2.36	0.40
32:m:344:LEU:HB3	32:m:345:PRO:HD3	2.04	0.40
32:m:505:HIS:HB3	32:m:550:TRP:CE2	2.57	0.40
35:z:470:SER:O	35:z:474:ILE:HG12	2.22	0.40
1:e:219:GLN:NE2	21:Q:232:ARG:HD3	2.31	0.40
1:e:256:TYR:HA	1:e:257:PRO:HD3	1.93	0.40
4:5:51:U:O2'	38:6:63:A:H8	2.04	0.40
4:5:96:G:C6	13:I:40:TYR:CE1	3.10	0.40
6:B:224:VAL:HG11	6:B:253:ARG:NH2	2.36	0.40
6:B:569:VAL:HG22	6:B:573:ILE:HD11	2.03	0.40
6:B:692:THR:OG1	6:B:697:ASN:HB2	2.21	0.40
7:C:38:ASP:HB2	7:C:80:PHE:CE1	2.57	0.40
7:C:85:ASN:ND2	9:E:99:GLY:H	2.19	0.40
10:F:7:LEU:HD21	11:G:100:PHE:CE2	2.56	0.40
13:I:20:VAL:HG12	13:I:75:GLU:C	2.46	0.40
15:K:133:GLN:O	15:K:137:VAL:HG12	2.21	0.40
16:L:91:LEU:HD23	31:d:131:ARG:NH2	2.37	0.40
16:L:200:ARG:NH2	17:M:28:GLY:O	2.43	0.40
18:N:83:LEU:HD23	18:N:129:LEU:HD13	2.03	0.40
18:N:335:LEU:HB3	18:N:378:ILE:HG12	2.03	0.40
18:N:542:LEU:HD23	18:N:542:LEU:HA	1.93	0.40
18:N:804:TYR:CZ	18:N:806:SER:HB3	2.57	0.40
23:S:28:ILE:O	23:S:32:ILE:HG12	2.21	0.40
23:U:401:PHE:HB2	23:U:403:TRP:HZ3	1.86	0.40
24:W:512:ILE:HD13	24:W:512:ILE:HA	2.00	0.40
25:X:246:ILE:HD13	25:X:257:TRP:CZ2	2.57	0.40
25:X:342:ASP:OD1	25:X:345:LEU:HD12	2.22	0.40
25:X:641:VAL:O	25:X:644:THR:HG23	2.21	0.40
26:Y:128:GLU:HB3	26:Y:132:LYS:NZ	2.37	0.40
27:Z:57:ASP:N	27:Z:57:ASP:OD1	2.54	0.40
30:c:469:GLU:HA	30:c:472:CYS:SG	2.61	0.40
34:y:127:ASP:O	34:y:131:ARG:HG2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:6:13:A:HO2'	38:6:14:C:P	2.44	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	e	156/384 (41%)	146 (94%)	10 (6%)	0	100	100
2	p	58/299 (19%)	55 (95%)	3 (5%)	0	100	100
5	A	1984/2363 (84%)	1893 (95%)	90 (4%)	1 (0%)	48	78
6	B	916/984 (93%)	867 (95%)	49 (5%)	0	100	100
7	C	297/340 (87%)	278 (94%)	19 (6%)	0	100	100
8	D	94/97 (97%)	93 (99%)	1 (1%)	0	100	100
9	E	91/147 (62%)	88 (97%)	3 (3%)	0	100	100
10	F	79/117 (68%)	73 (92%)	6 (8%)	0	100	100
11	G	98/115 (85%)	92 (94%)	6 (6%)	0	100	100
12	H	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
13	I	71/78 (91%)	68 (96%)	3 (4%)	0	100	100
14	J	71/77 (92%)	68 (96%)	3 (4%)	0	100	100
15	K	389/473 (82%)	359 (92%)	30 (8%)	0	100	100
16	L	242/557 (43%)	226 (93%)	14 (6%)	2 (1%)	16	47
17	M	222/354 (63%)	215 (97%)	7 (3%)	0	100	100
18	N	1282/1284 (100%)	1261 (98%)	21 (2%)	0	100	100
19	O	142/146 (97%)	136 (96%)	6 (4%)	0	100	100
20	P	265/388 (68%)	247 (93%)	17 (6%)	1 (0%)	30	61
21	Q	86/265 (32%)	82 (95%)	3 (4%)	1 (1%)	10	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	R	597/674 (89%)	585 (98%)	11 (2%)	1 (0%)	43	73
23	S	130/488 (27%)	121 (93%)	9 (7%)	0	100	100
23	T	132/488 (27%)	127 (96%)	4 (3%)	1 (1%)	16	47
23	U	414/488 (85%)	399 (96%)	15 (4%)	0	100	100
23	V	129/488 (26%)	118 (92%)	11 (8%)	0	100	100
24	W	488/757 (64%)	450 (92%)	33 (7%)	5 (1%)	12	41
25	X	642/790 (81%)	608 (95%)	33 (5%)	1 (0%)	43	73
26	Y	94/229 (41%)	89 (95%)	4 (4%)	1 (1%)	11	39
27	Z	151/187 (81%)	145 (96%)	5 (3%)	1 (1%)	18	49
28	a	150/558 (27%)	138 (92%)	12 (8%)	0	100	100
29	b	98/293 (33%)	92 (94%)	6 (6%)	0	100	100
30	c	202/887 (23%)	194 (96%)	8 (4%)	0	100	100
31	d	152/155 (98%)	138 (91%)	14 (9%)	0	100	100
32	m	455/797 (57%)	447 (98%)	7 (2%)	1 (0%)	43	73
33	n	28/361 (8%)	27 (96%)	1 (4%)	0	100	100
34	y	196/534 (37%)	168 (86%)	25 (13%)	3 (2%)	8	32
35	z	624/647 (96%)	611 (98%)	12 (2%)	1 (0%)	43	73
37	q	3/56 (5%)	3 (100%)	0	0	100	100
All	All	11306/17429 (65%)	10784 (95%)	502 (4%)	20 (0%)	44	73

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	Y	144	VAL
34	y	115	LYS
23	T	69	LEU
24	W	536	ILE
5	A	1115	ILE
16	L	131	LEU
21	Q	224	ARG
20	P	90	GLN
22	R	87	ALA
24	W	538	PRO
27	Z	71	LYS
32	m	321	THR
35	z	437	ASP

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Mol	Chain	Res	Type
24	W	221	TYR
16	L	112	GLU
25	X	83	ASN
24	W	537	ARG
24	W	530	VAL
34	y	127	ASP
34	y	28	GLU

5.3.2 Protein sidechains [i](#)

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	e	149/346 (43%)	149 (100%)	0	100	100
2	p	56/274 (20%)	56 (100%)	0	100	100
5	A	1798/2138 (84%)	1798 (100%)	0	100	100
6	B	821/881 (93%)	821 (100%)	0	100	100
7	C	257/292 (88%)	257 (100%)	0	100	100
8	D	85/86 (99%)	85 (100%)	0	100	100
9	E	80/118 (68%)	80 (100%)	0	100	100
10	F	76/102 (74%)	76 (100%)	0	100	100
11	G	91/101 (90%)	91 (100%)	0	100	100
12	H	73/76 (96%)	73 (100%)	0	100	100
13	I	64/69 (93%)	64 (100%)	0	100	100
14	J	63/67 (94%)	63 (100%)	0	100	100
15	K	333/405 (82%)	333 (100%)	0	100	100
16	L	211/477 (44%)	211 (100%)	0	100	100
17	M	198/306 (65%)	198 (100%)	0	100	100
18	N	1188/1188 (100%)	1188 (100%)	0	100	100
19	O	130/132 (98%)	130 (100%)	0	100	100
20	P	231/340 (68%)	231 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	Q	79/240 (33%)	79 (100%)	0	100	100
22	R	532/597 (89%)	532 (100%)	0	100	100
23	S	121/443 (27%)	121 (100%)	0	100	100
23	T	123/443 (28%)	123 (100%)	0	100	100
23	U	222/443 (50%)	220 (99%)	2 (1%)	70	80
23	V	120/443 (27%)	120 (100%)	0	100	100
24	W	443/656 (68%)	443 (100%)	0	100	100
25	X	586/707 (83%)	586 (100%)	0	100	100
26	Y	94/214 (44%)	94 (100%)	0	100	100
27	Z	132/163 (81%)	132 (100%)	0	100	100
28	a	79/496 (16%)	79 (100%)	0	100	100
29	b	95/275 (34%)	95 (100%)	0	100	100
30	c	188/816 (23%)	188 (100%)	0	100	100
31	d	128/129 (99%)	128 (100%)	0	100	100
32	m	425/719 (59%)	425 (100%)	0	100	100
33	n	28/335 (8%)	28 (100%)	0	100	100
34	y	173/478 (36%)	173 (100%)	0	100	100
35	z	564/585 (96%)	564 (100%)	0	100	100
37	q	2/2 (100%)	2 (100%)	0	100	100
All	All	10038/15582 (64%)	10036 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	U	184	PRO
23	U	415	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	e	147	HIS
1	e	204	HIS
1	e	219	GLN
5	A	253	GLN

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Mol	Chain	Res	Type
5	A	256	ASN
5	A	402	ASN
5	A	522	GLN
5	A	640	ASN
5	A	1027	ASN
5	A	1065	GLN
5	A	1134	GLN
5	A	1387	HIS
5	A	1391	ASN
5	A	1444	ASN
5	A	1452	HIS
5	A	1490	GLN
5	A	1511	HIS
5	A	1544	ASN
5	A	1576	GLN
5	A	1587	HIS
5	A	1607	GLN
5	A	1639	HIS
5	A	1752	GLN
6	B	213	GLN
6	B	343	HIS
6	B	497	ASN
6	B	503	ASN
6	B	596	HIS
6	B	733	GLN
6	B	821	GLN
7	C	40	ASN
7	C	139	ASN
7	C	191	GLN
7	C	213	HIS
7	C	322	GLN
9	E	11	ASN
9	E	81	GLN
10	F	37	ASN
10	F	64	ASN
11	G	40	HIS
12	H	33	GLN
12	H	82	GLN
15	K	459	HIS
16	L	113	HIS
16	L	191	GLN
16	L	301	GLN

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Mol	Chain	Res	Type
16	L	322	GLN
17	M	81	GLN
17	M	88	GLN
17	M	134	GLN
18	N	580	ASN
18	N	584	ASN
18	N	659	ASN
18	N	731	GLN
18	N	747	ASN
18	N	1045	GLN
18	N	1047	ASN
18	N	1108	GLN
19	O	35	ASN
20	P	111	ASN
20	P	156	HIS
20	P	224	GLN
20	P	268	ASN
20	P	287	ASN
20	P	323	ASN
21	Q	68	GLN
22	R	22	GLN
22	R	187	ASN
22	R	225	GLN
22	R	289	GLN
22	R	307	GLN
22	R	367	ASN
22	R	529	GLN
22	R	545	ASN
23	S	21	ASN
23	S	99	GLN
23	U	342	HIS
23	V	99	GLN
24	W	28	GLN
24	W	172	ASN
24	W	195	HIS
24	W	222	ASN
24	W	699	HIS
25	X	81	HIS
25	X	117	GLN
25	X	441	HIS
26	Y	98	GLN
27	Z	94	GLN

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Mol	Chain	Res	Type
27	Z	154	HIS
27	Z	156	GLN
30	c	442	GLN
30	c	561	HIS
31	d	3	ASN
31	d	82	HIS
31	d	101	GLN
31	d	116	HIS
32	m	766	ASN
34	y	117	ASN
34	y	208	ASN
35	z	108	GLN
35	z	111	HIS
35	z	289	ASN
35	z	384	ASN
35	z	415	HIS
35	z	451	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	22/186 (11%)	5 (22%)	0
38	6	91/99 (91%)	44 (48%)	7 (7%)
39	1	28/29 (96%)	19 (67%)	2 (7%)
4	5	101/120 (84%)	22 (21%)	2 (1%)
All	All	242/434 (55%)	90 (37%)	11 (4%)

All (90) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	11	U
3	2	12	G
3	2	13	C
3	2	24	A
3	2	29	A
4	5	13	A
4	5	14	G
4	5	27	G
4	5	28	C
4	5	30	A
4	5	31	A

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Mol	Chain	Res	Type
4	5	33	G
4	5	37	C
4	5	50	U
4	5	54	C
4	5	79	G
4	5	82	A
4	5	83	A
4	5	90	U
4	5	91	G
4	5	92	U
4	5	98	U
4	5	99	U
4	5	102	G
4	5	103	U
4	5	105	A
4	5	108	U
38	6	4	C
38	6	7	C
38	6	8	G
38	6	9	G
38	6	10	A
38	6	11	U
38	6	12	C
38	6	14	C
38	6	18	G
38	6	19	G
38	6	20	U
38	6	21	C
38	6	22	A
38	6	23	A
38	6	24	A
38	6	27	G
38	6	28	A
38	6	29	A
38	6	30	A
38	6	31	C
38	6	32	G
38	6	38	G
38	6	40	G
38	6	43	G
38	6	44	A
38	6	46	U

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Mol	Chain	Res	Type
38	6	48	G
38	6	52	G
38	6	53	G
38	6	61	A
38	6	62	C
38	6	63	A
38	6	68	U
38	6	74	U
38	6	75	G
38	6	76	C
38	6	78	A
38	6	79	C
38	6	80	A
38	6	81	U
38	6	82	U
38	6	83	G
38	6	91	A
38	6	92	C
39	1	-14	U
39	1	-13	U
39	1	-12	U
39	1	-8	U
39	1	-4	A
39	1	0	G
39	1	1	G
39	1	2	U
39	1	3	A
39	1	4	U
39	1	5	G
39	1	6	U
39	1	7	U
39	1	8	U
39	1	9	U
39	1	10	U
39	1	11	U
39	1	12	U
39	1	13	U

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	5	27	G

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Mol	Chain	Res	Type
4	5	49	U
38	6	13	A
38	6	17	U
38	6	29	A
38	6	30	A
38	6	37	A
38	6	52	G
38	6	74	U
39	1	0	G
39	1	1	G

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 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
42	GTP	B	1001	43	33,34,34	1.01	1 (3%)	50,54,54	1.59	9 (18%)
41	IHP	A	2401	-	36,36,36	1.58	13 (36%)	60,60,60	1.52	12 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	B	1001	43	-	0/22/38/38	0/3/3/3
41	IHP	A	2401	-	-	3/30/54/54	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	A	2401	IHP	P1-O31	-2.54	1.45	1.54
41	A	2401	IHP	P3-O33	-2.43	1.45	1.54
41	A	2401	IHP	P6-O46	-2.42	1.45	1.54
41	A	2401	IHP	P5-O45	-2.40	1.45	1.54
41	A	2401	IHP	P3-O43	-2.40	1.45	1.54
41	A	2401	IHP	P4-O34	-2.36	1.46	1.54
41	A	2401	IHP	P1-O11	2.34	1.63	1.59
41	A	2401	IHP	P6-O36	-2.31	1.46	1.54
41	A	2401	IHP	P1-O41	-2.29	1.46	1.54
41	A	2401	IHP	P5-O35	-2.28	1.46	1.54
41	A	2401	IHP	P4-O44	-2.28	1.46	1.54
42	B	1001	GTP	C5-N7	-2.28	1.34	1.39
41	A	2401	IHP	P2-O42	-2.27	1.46	1.54
41	A	2401	IHP	P2-O32	-2.20	1.46	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	B	1001	GTP	C5-C4-N3	-5.02	120.39	128.39
42	B	1001	GTP	C2-N3-C4	4.58	120.19	112.30
42	B	1001	GTP	C2-N1-C6	-3.32	119.09	125.11
42	B	1001	GTP	N9-C4-N3	3.29	132.54	125.95
41	A	2401	IHP	C5-C6-C1	3.17	117.38	110.43
41	A	2401	IHP	O11-P1-O21	-3.09	98.32	109.33
42	B	1001	GTP	N9-C8-N7	-2.98	107.88	113.40
42	B	1001	GTP	C5-C6-N1	2.85	120.51	113.25
41	A	2401	IHP	C6-C1-C2	2.80	116.58	110.43
41	A	2401	IHP	O41-P1-O31	2.61	117.60	107.80
41	A	2401	IHP	C6-C5-C4	2.61	116.14	110.43
42	B	1001	GTP	C8-N7-C5	2.61	108.90	104.26
42	B	1001	GTP	O6-C6-C5	-2.57	119.74	126.53
41	A	2401	IHP	O12-P2-O22	-2.30	101.13	109.33
41	A	2401	IHP	C3-C2-C1	2.21	115.27	110.43
41	A	2401	IHP	O41-P1-O11	-2.14	97.49	105.85
42	B	1001	GTP	O3G-PG-O3B	2.06	111.55	104.64
41	A	2401	IHP	O15-P5-O25	-2.03	102.10	109.33
41	A	2401	IHP	O44-P4-O34	2.03	115.40	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	A	2401	IHP	O42-P2-O32	2.02	115.37	107.80
41	A	2401	IHP	O11-C1-C2	2.02	113.05	108.76

There are no chirality outliers.

All (3) torsion outliers are listed below:

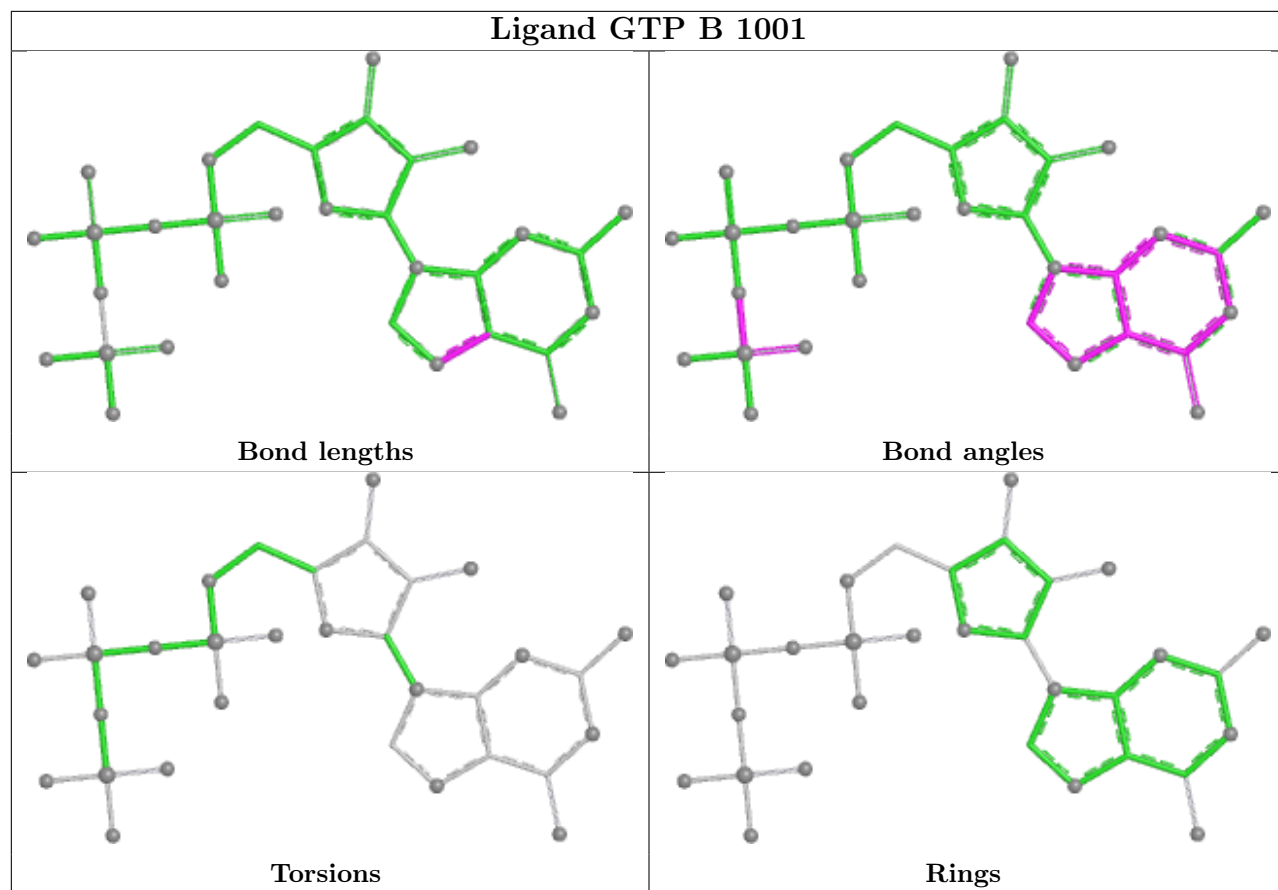
Mol	Chain	Res	Type	Atoms
41	A	2401	IHP	C1-O11-P1-O41
41	A	2401	IHP	C5-O15-P5-O35
41	A	2401	IHP	C6-O16-P6-O26

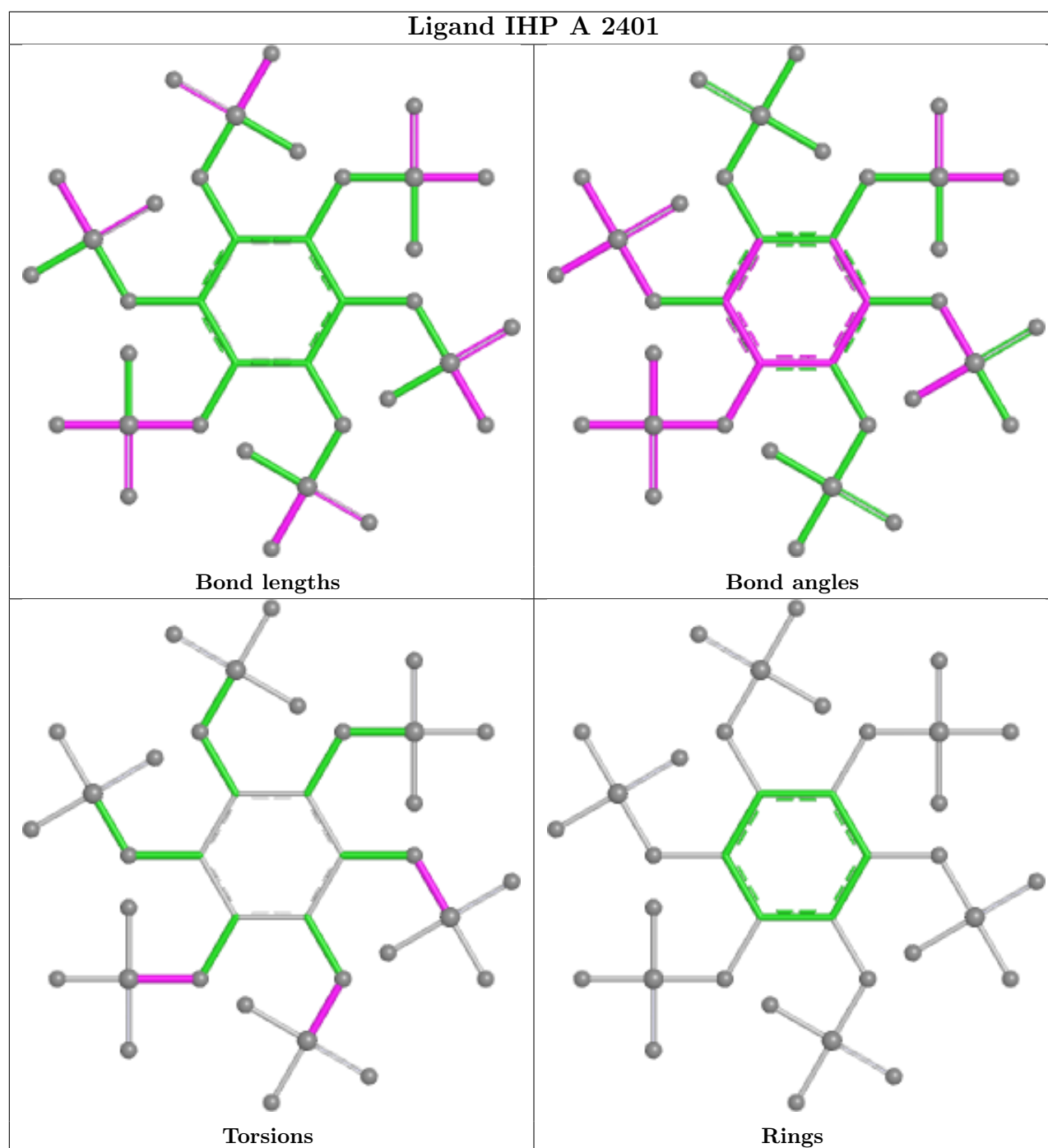
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	B	1001	GTP	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

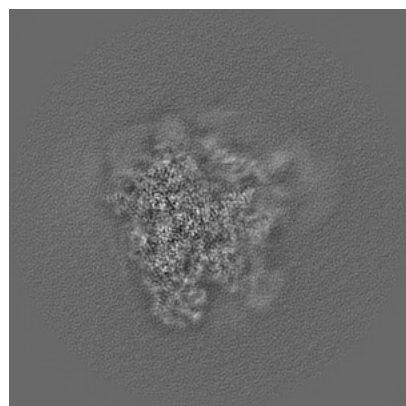
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19942. These allow visual inspection of the internal detail of the map and identification of artifacts.

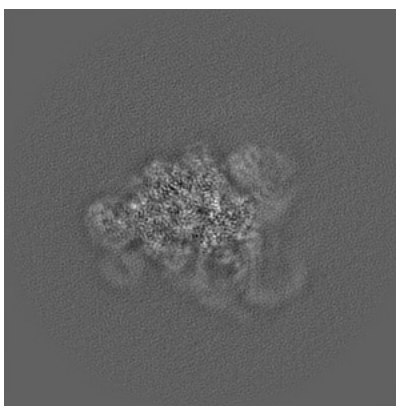
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

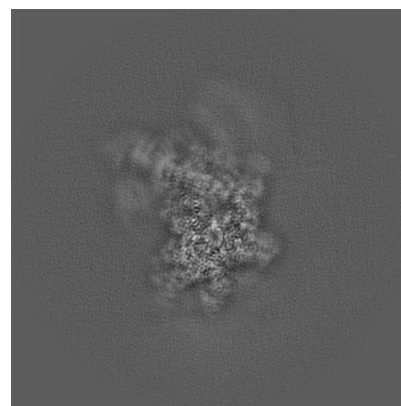
6.1.1 Primary map



X

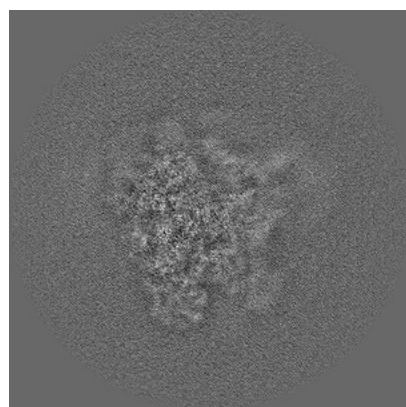


Y

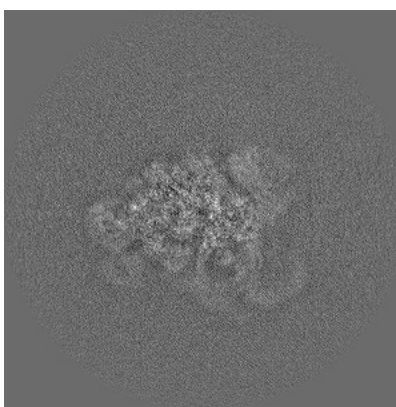


Z

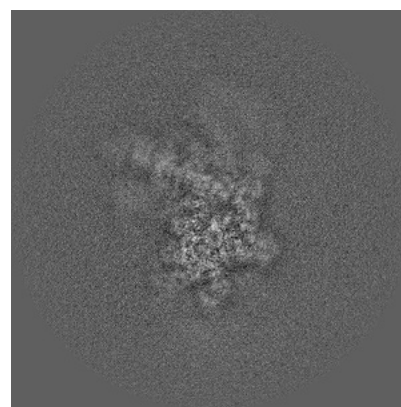
6.1.2 Raw map



X



Y

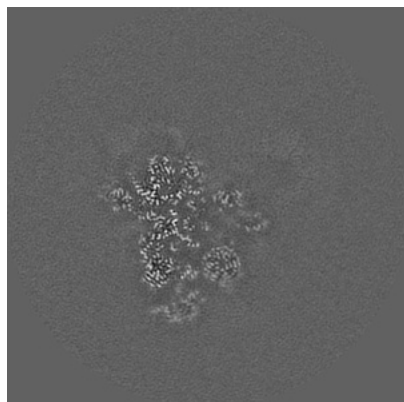


Z

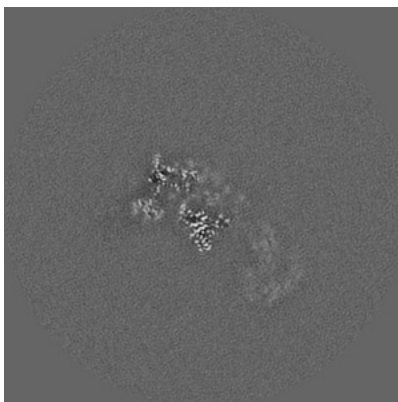
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

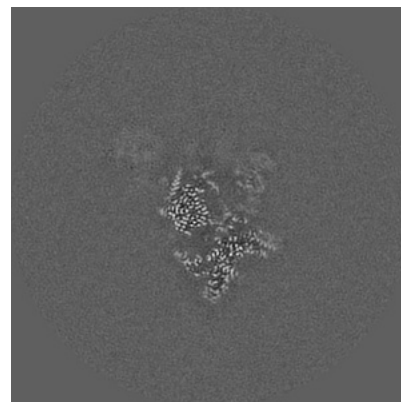
6.2.1 Primary map



X Index: 280

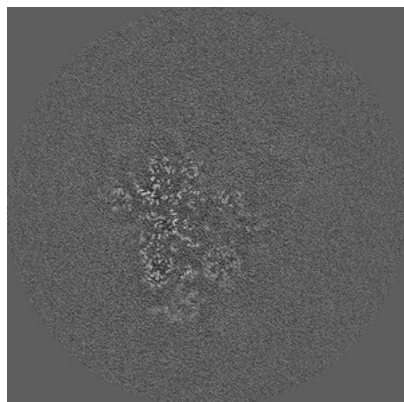


Y Index: 280

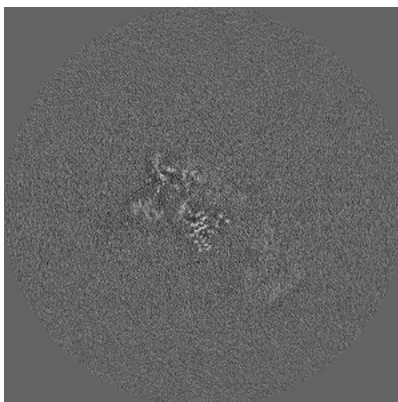


Z Index: 280

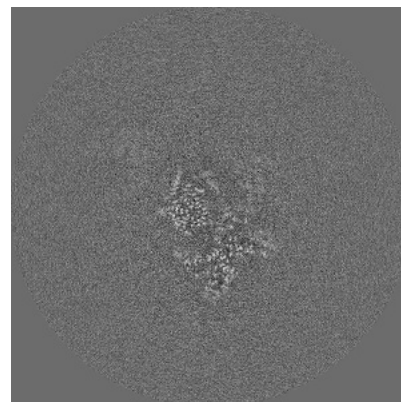
6.2.2 Raw map



X Index: 280



Y Index: 280

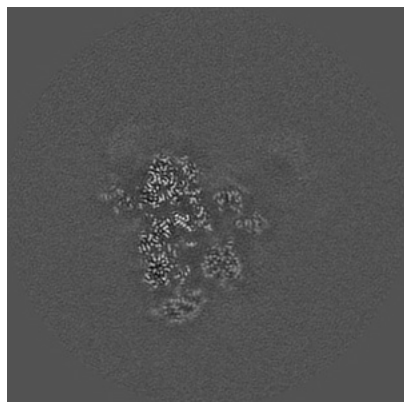


Z Index: 280

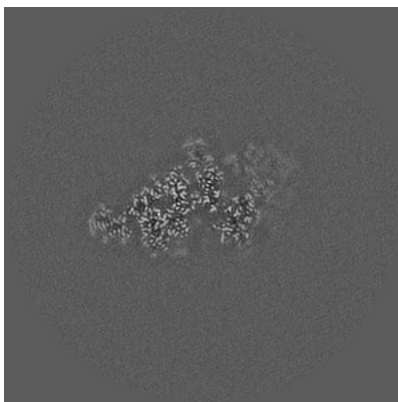
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

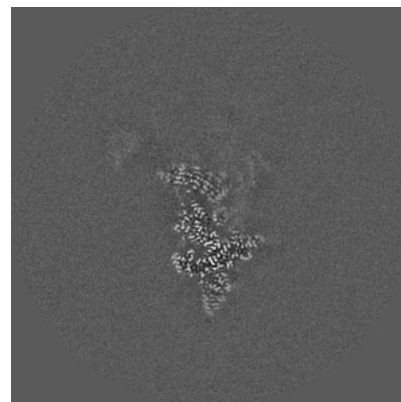
6.3.1 Primary map



X Index: 276

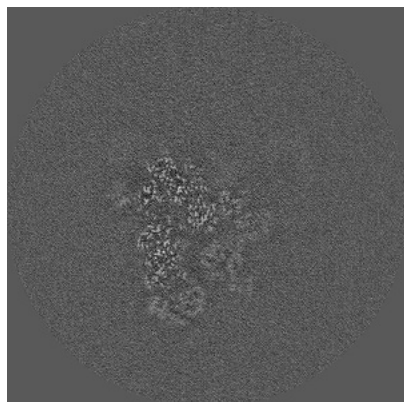


Y Index: 219

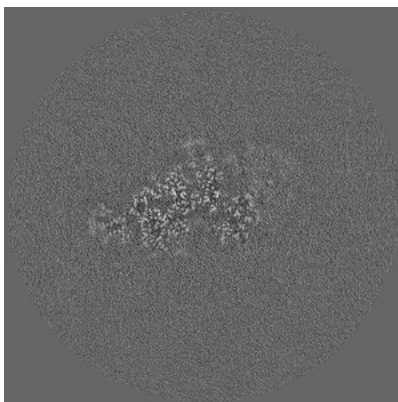


Z Index: 295

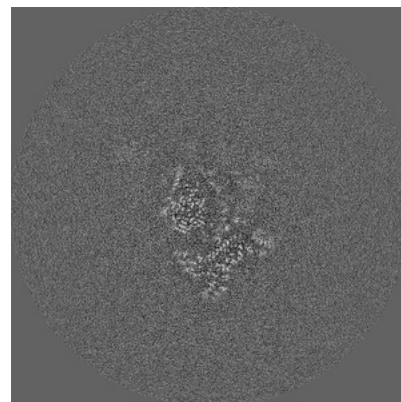
6.3.2 Raw map



X Index: 269



Y Index: 219

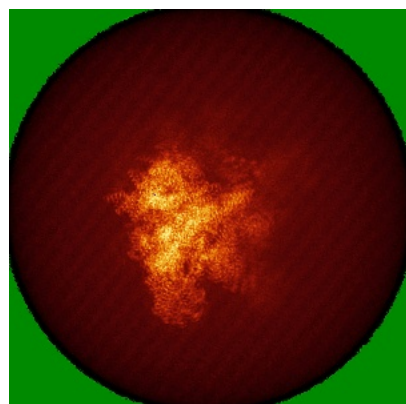


Z Index: 282

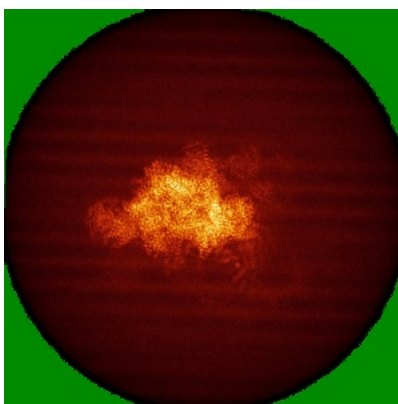
The images above show the largest variance slices of the map in three orthogonal directions.

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

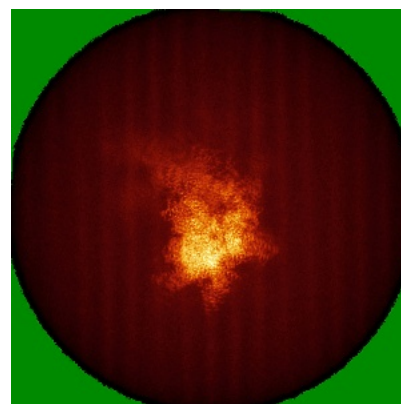
6.4.1 Primary map



X

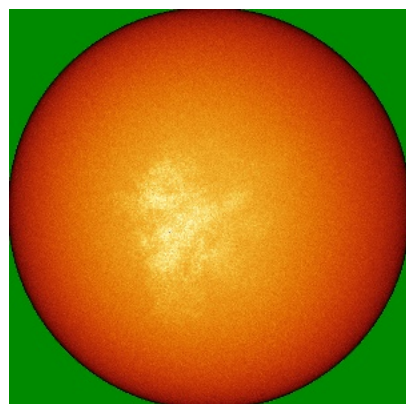


Y

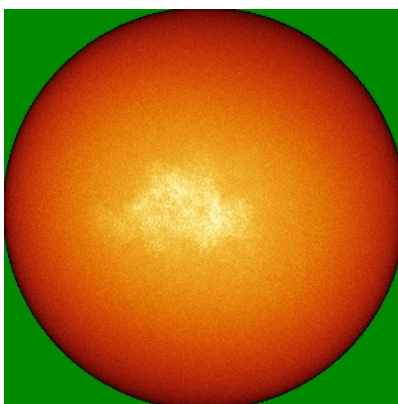


Z

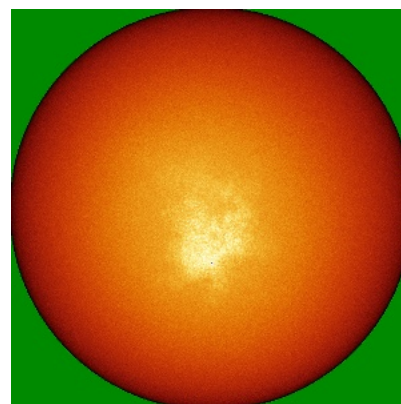
6.4.2 Raw map



X



Y

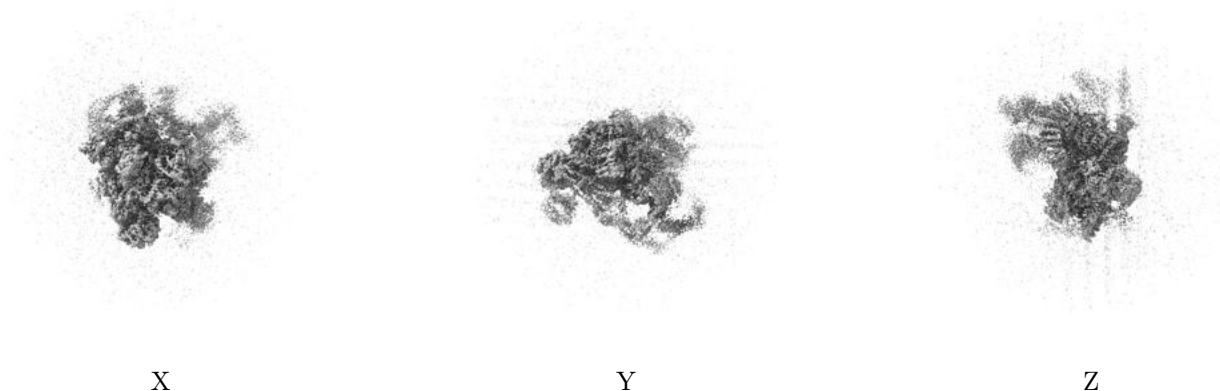


Z

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

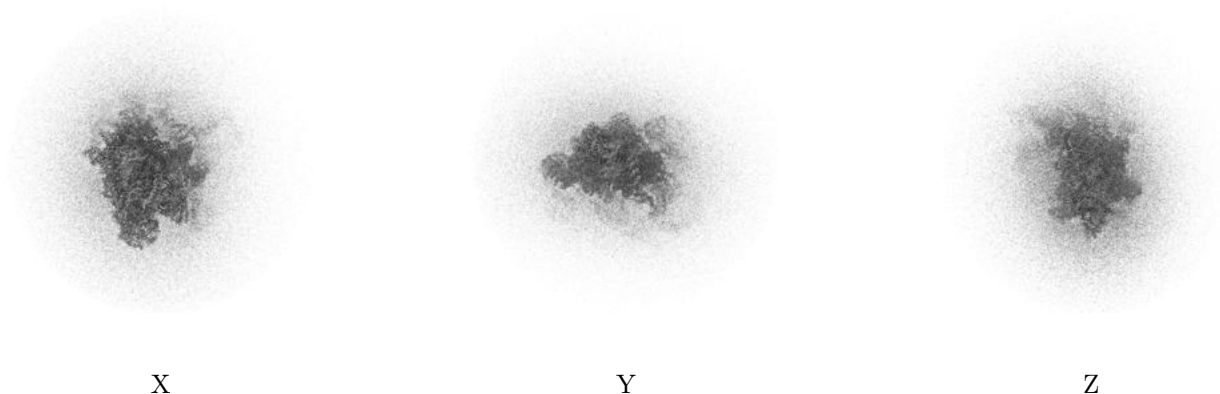
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

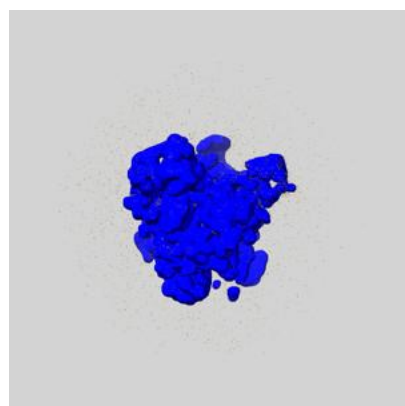
6.6 Mask visualisation [i](#)

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

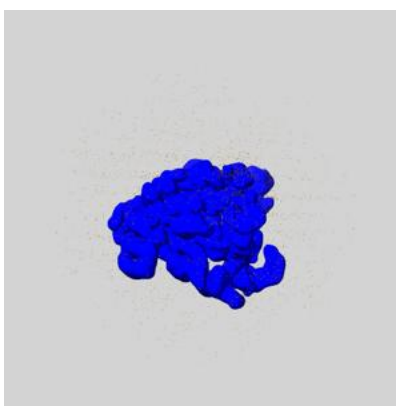
A mask typically either:

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

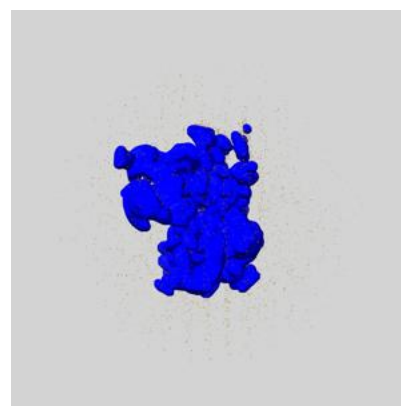
6.6.1 emd_19942_msk_1.map [i](#)



X



Y

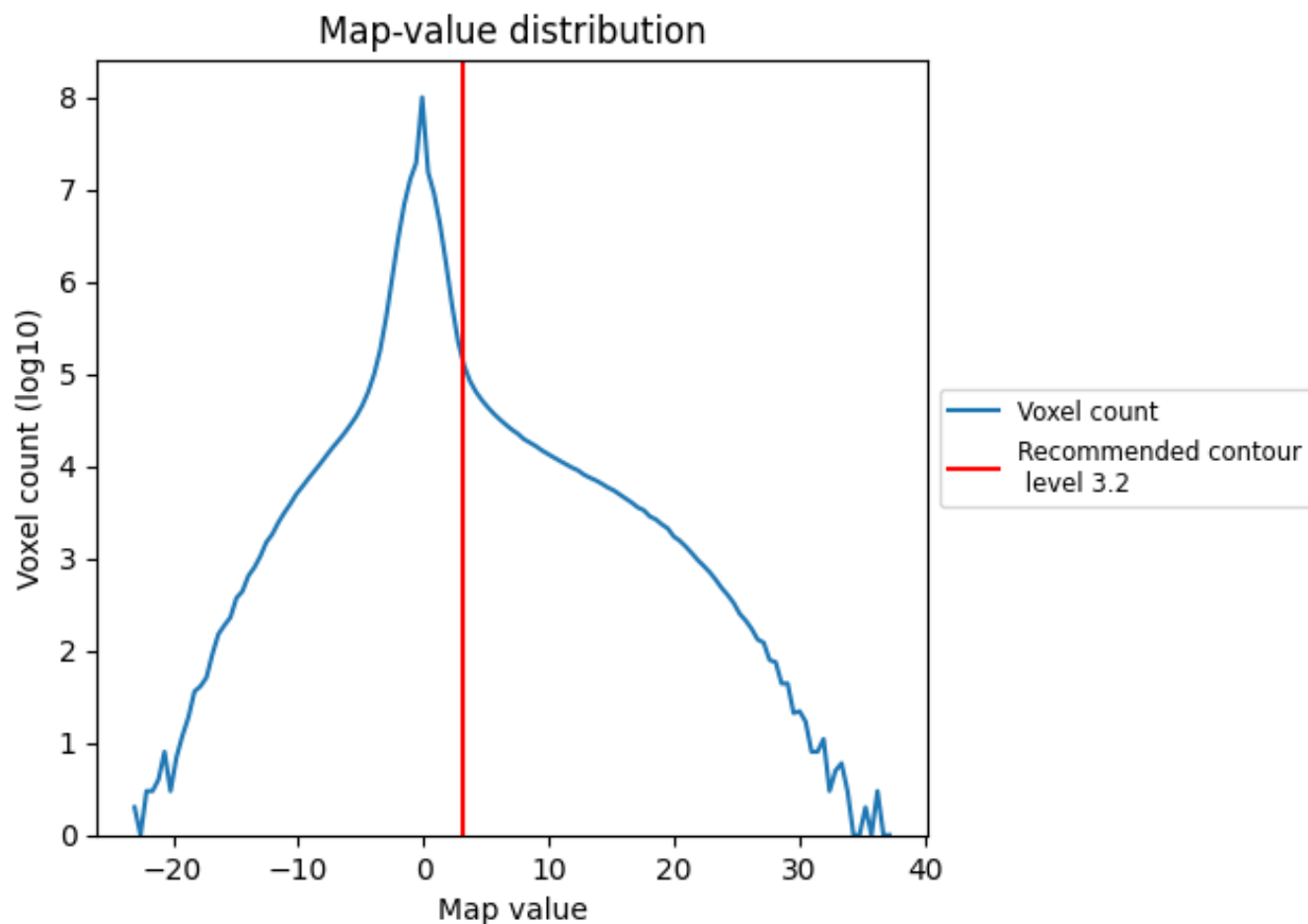


Z

7 Map analysis [i](#)

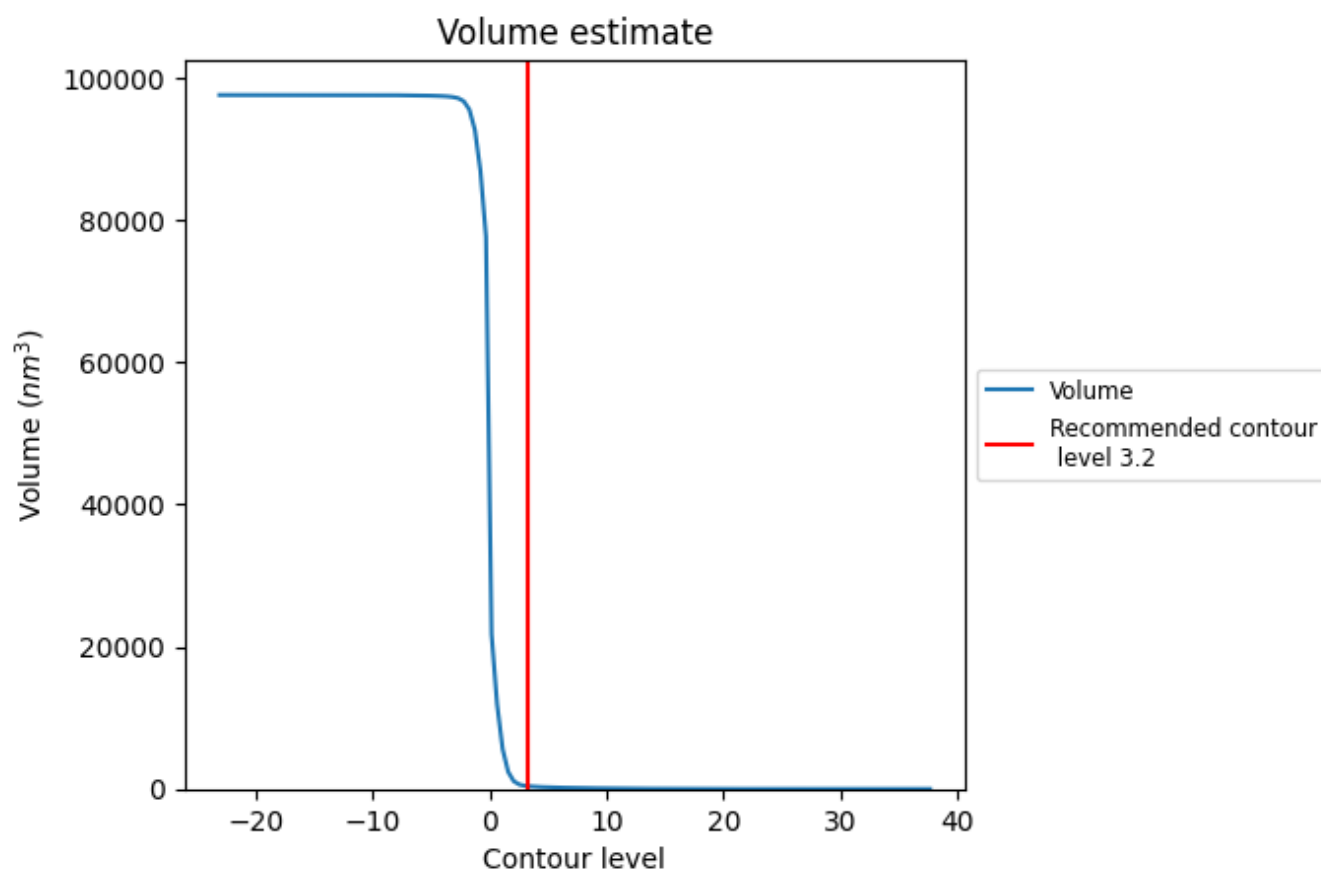
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

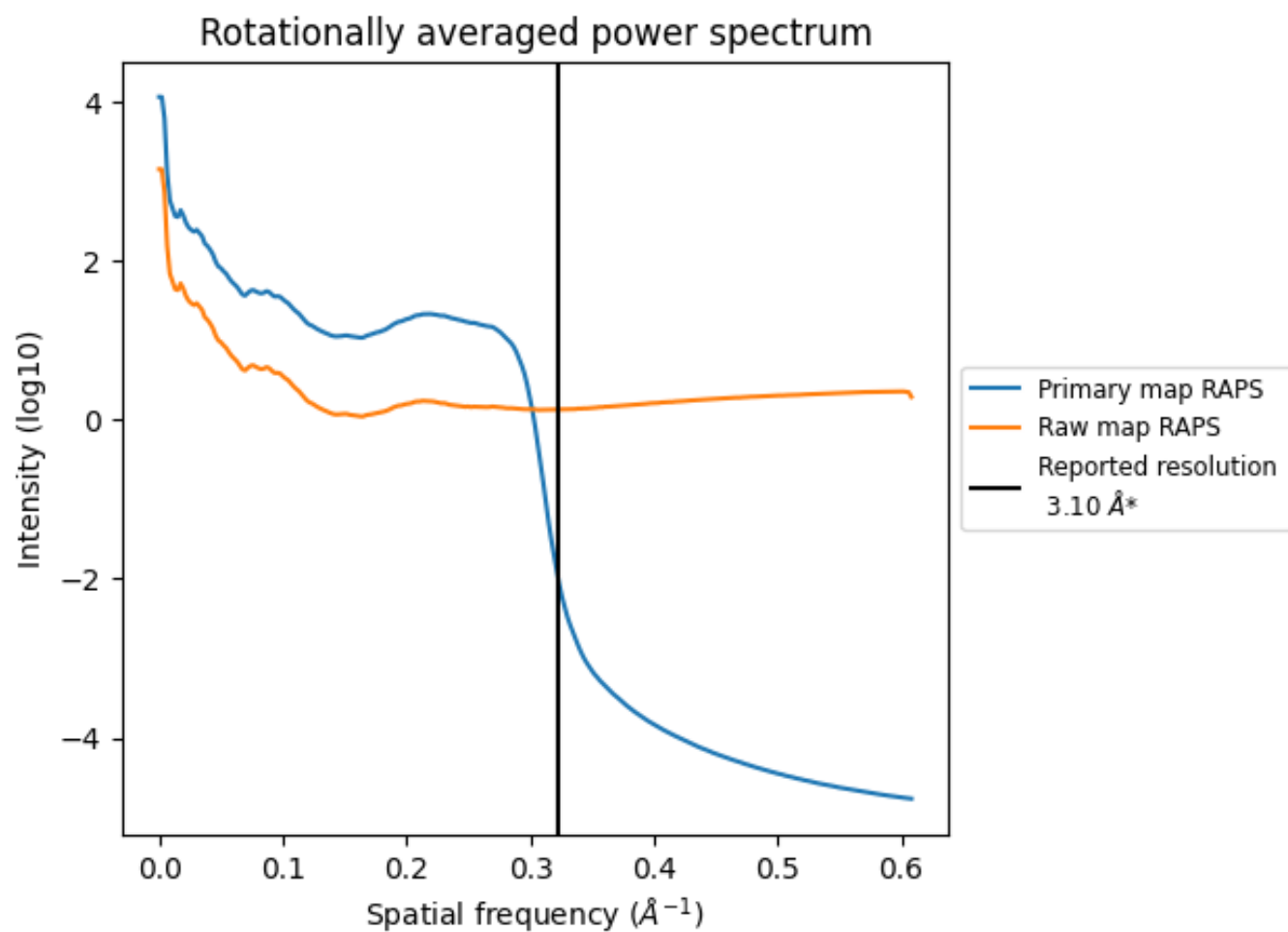
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm³; this corresponds to an approximate mass of 375 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 ⓘ

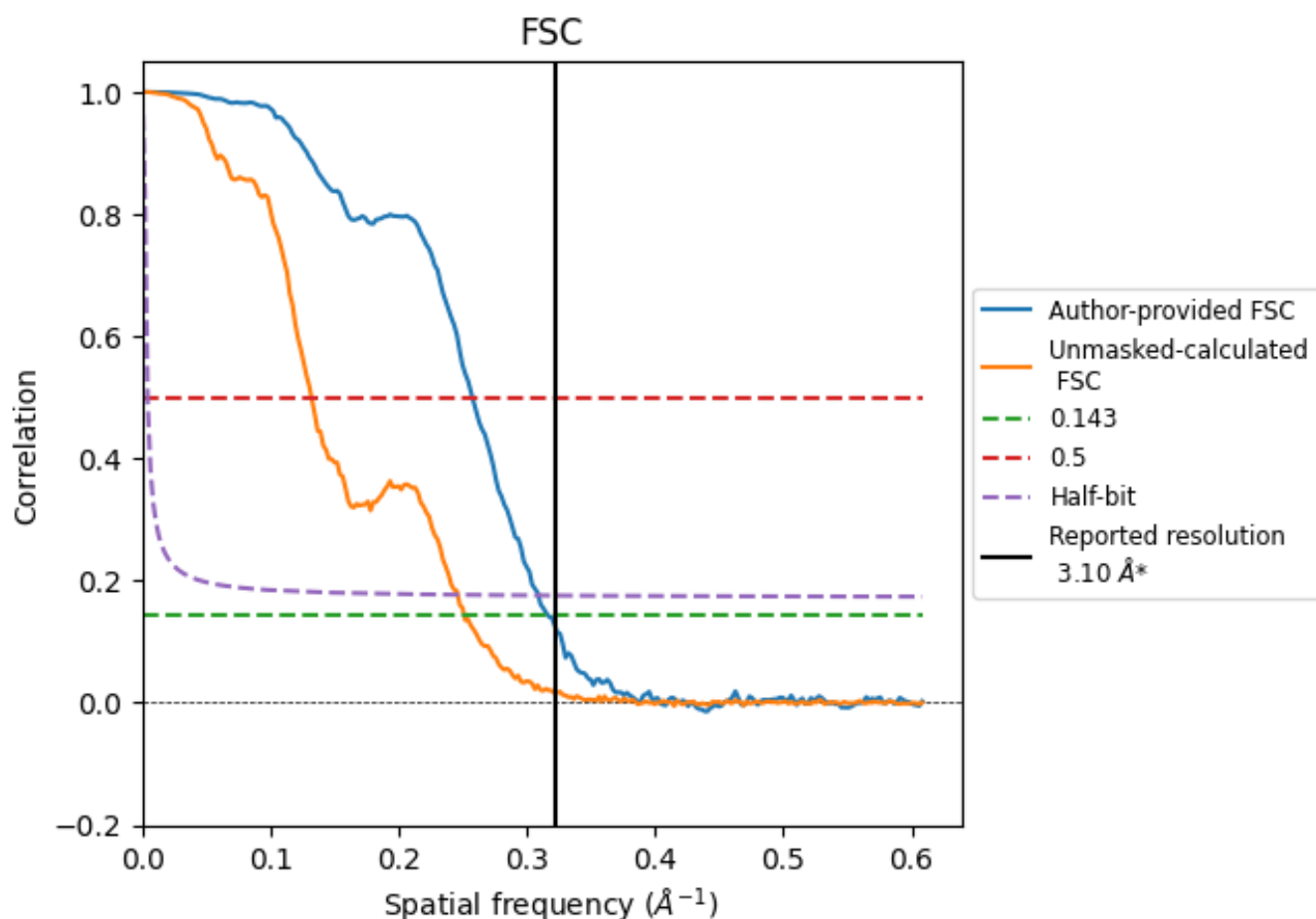


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

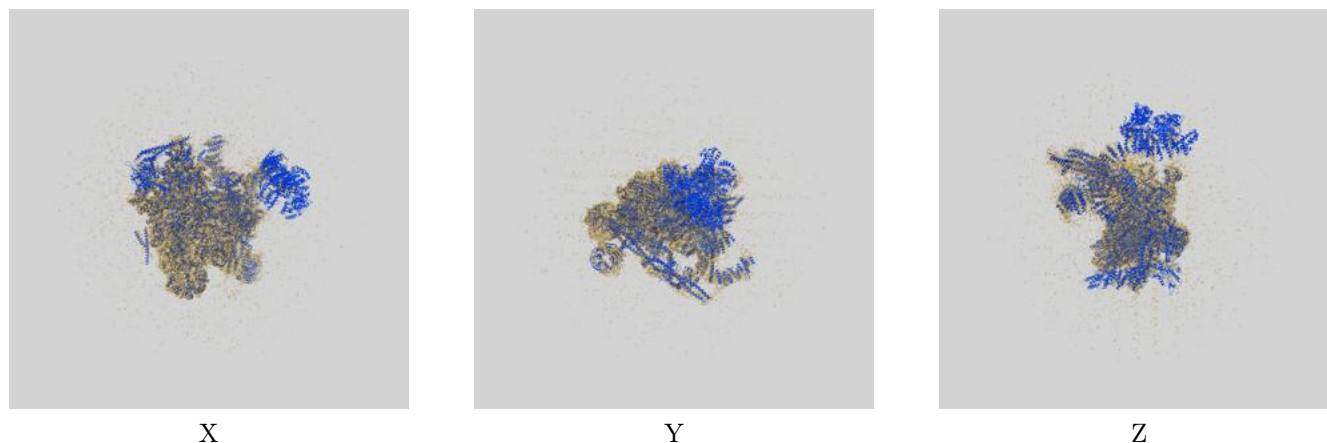
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.16	3.88	3.24
Unmasked-calculated*	3.98	7.58	4.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

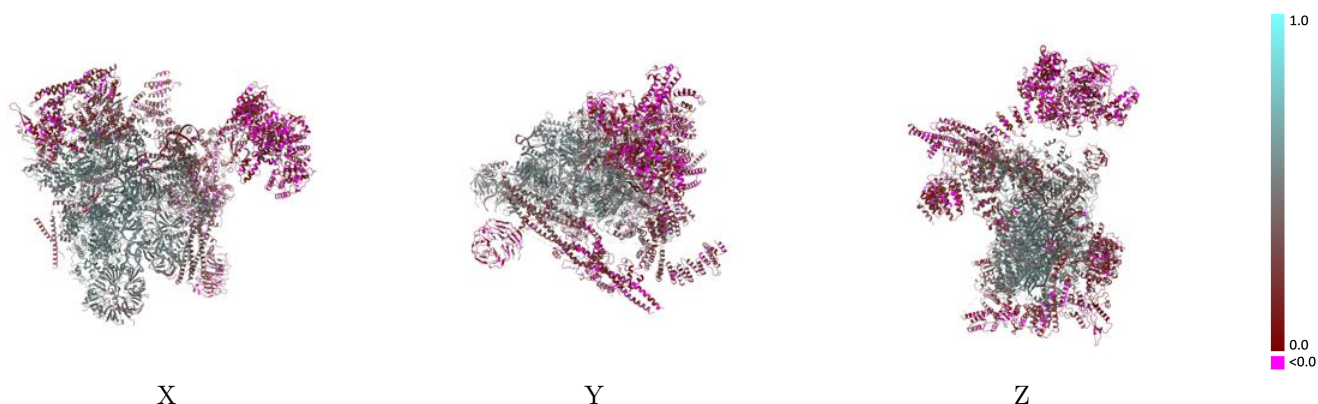
This section contains information regarding the fit between EMDB map EMD-19942 and PDB model 9ESI. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



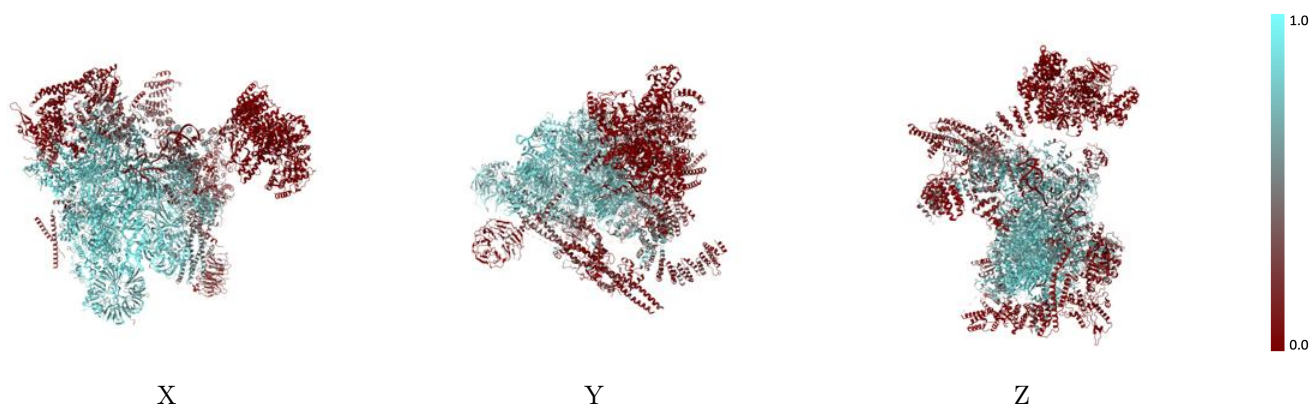
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



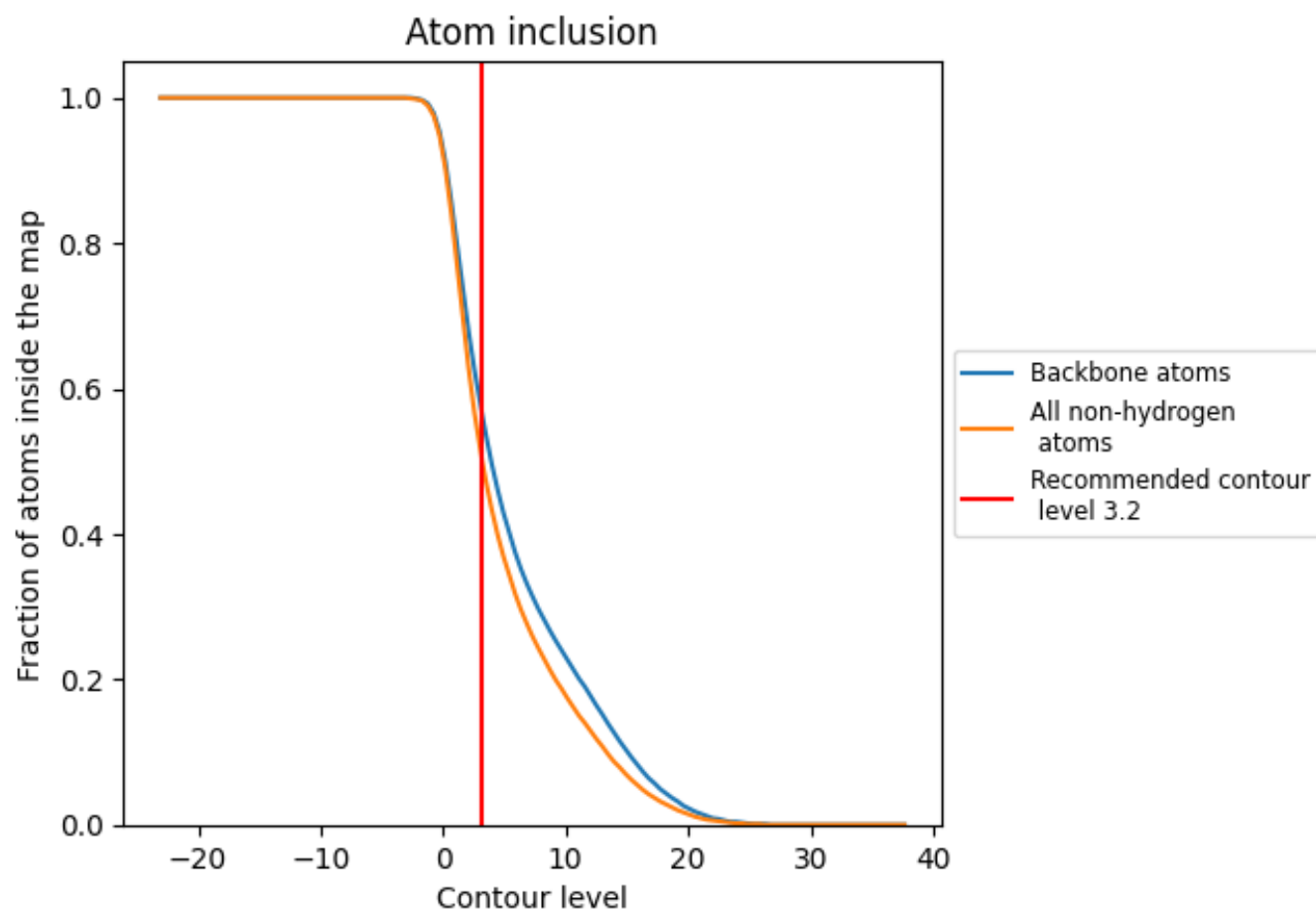
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 50% 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 (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4990	 0.3640
1	 0.5170	 0.4200
2	 0.4320	 0.3200
5	 0.9380	 0.5360
6	 0.5180	 0.4060
A	 0.7590	 0.4960
B	 0.8490	 0.5310
C	 0.7990	 0.5030
D	 0.8680	 0.5490
E	 0.7970	 0.5080
F	 0.7330	 0.4680
G	 0.7130	 0.4240
H	 0.7930	 0.5050
I	 0.7390	 0.4490
J	 0.8260	 0.5340
K	 0.8780	 0.5480
L	 0.7030	 0.4700
M	 0.4680	 0.3830
N	 0.0050	 0.1040
O	 0.8500	 0.5400
P	 0.6750	 0.4450
Q	 0.7790	 0.5310
R	 0.4450	 0.3280
S	 0.0530	 0.1340
T	 0.2000	 0.2100
U	 0.1300	 0.1600
V	 0.0770	 0.1340
W	 0.4690	 0.3200
X	 0.1770	 0.1980
Y	 0.1780	 0.3150
Z	 0.3780	 0.2660
a	 0.6470	 0.4370
b	 0.3050	 0.3220
c	 0.8220	 0.5050
d	 0.7110	 0.4720



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Chain	Atom inclusion	Q-score
e	 0.4730	 0.4550
f	 0.3910	 0.3230
m	 0.0830	 0.1860
n	 0.0210	 0.1600
p	 0.3440	 0.3510
q	 0.3880	 0.4780
r	 0.3490	 0.2780
y	 0.4500	 0.3500
z	 0.2880	 0.2760