



Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 02:52 AM EDT

PDB ID : 6AVO / pdb_00006avo
EMDB ID : EMD-7010
Title : Cryo-EM structure of human immunoproteasome with a novel noncompetitive inhibitor that selectively inhibits activated lymphocytes
Authors : Li, H.; Santos, R.; Bai, L.
Deposited on : 2017-09-04
Resolution : 3.80 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:

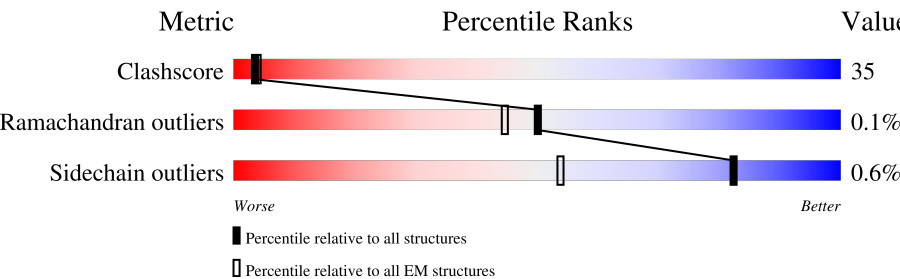
EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	199	
1	F	199	
2	B	234	
2	E	234	
3	C	204	
3	D	204	
4	G	263	
4	L	263	

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Mol	Chain	Length	Quality of chain
5	H	241	
5	M	241	
6	I	248	
6	N	248	
7	J	255	
7	Q	255	
8	K	246	
8	R	246	
9	O	261	
9	Z	261	
10	P	234	
10	b	234	
11	S	213	
11	X	213	
12	T	201	
12	V	201	
13	U	205	
13	Y	205	
14	W	219	
14	a	219	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 47715 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 Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	199	Total	C	N	O	S	0	0
			1493	939	254	291	9		
1	F	199	Total	C	N	O	S	0	0
			1493	939	254	291	9		

- Molecule 2 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	219	Total	C	N	O	S	0	0
			1609	1010	286	305	8		
2	E	219	Total	C	N	O	S	0	0
			1609	1010	286	305	8		

- Molecule 3 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	201	Total	C	N	O	S	0	0
			1563	977	273	298	15		
3	D	201	Total	C	N	O	S	0	0
			1563	977	273	298	15		

- Molecule 4 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	234	Total	C	N	O	S	1	0
			1817	1140	324	342	11		
4	L	234	Total	C	N	O	S	3	0
			1841	1153	332	345	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	233	Total	C	N	O	S	0	0
			1753	1100	289	353	11		
5	M	233	Total	C	N	O	S	0	0
			1748	1100	292	345	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	232	Total	C	N	O	S	2	0
			1749	1092	312	340	5		
6	N	232	Total	C	N	O	S	0	0
			1754	1098	309	342	5		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	239	Total	C	N	O	S	4	0
			1888	1198	325	353	12		
7	Q	239	Total	C	N	O	S	1	0
			1851	1175	314	350	12		

- Molecule 8 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	240	Total	C	N	O	S	2	0
			1850	1172	313	352	13		
8	R	240	Total	C	N	O	S	1	0
			1817	1149	304	350	14		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	240	Total	C	N	O	S	2	0
			1843	1168	313	351	11		
9	Z	240	Total	C	N	O	S	2	0
			1860	1182	320	347	11		

- Molecule 10 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	230	Total	C	N	O	S	0	0
			1741	1111	293	331	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	230	Total	C	N	O	S	3	0
			1788	1145	301	336	6		

- Molecule 11 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	213	Total	C	N	O	S	1	0
			1642	1041	280	310	11		
11	X	213	Total	C	N	O	S	2	0
			1636	1038	277	310	11		

- Molecule 12 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	196	Total	C	N	O	S	2	0
			1567	1006	266	285	10		
12	V	196	Total	C	N	O	S	3	0
			1581	1015	270	286	10		

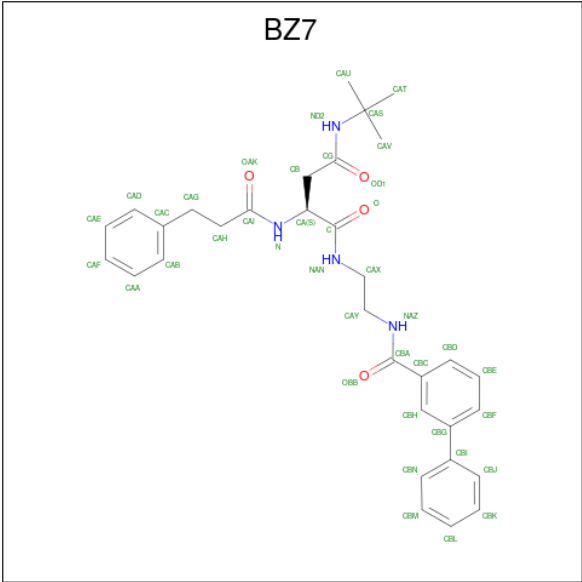
- Molecule 13 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	204	Total	C	N	O	S	2	0
			1599	1018	267	295	19		
13	Y	204	Total	C	N	O	S	2	0
			1604	1022	268	294	20		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	216	Total	C	N	O	S	1	0
			1692	1067	291	322	12		
14	a	216	Total	C	N	O	S	1	0
			1684	1062	290	320	12		

- Molecule 15 is N 1 -{2-[(1,1'-biphenyl)-3-carbonyl]amino}ethyl}-N 4 -tert-butyl-N 2 -(3-phenylpropanoyl)-L-aspartamide (CCD ID: BZ7) (formula: C₃₂H₃₈N₄O₄).

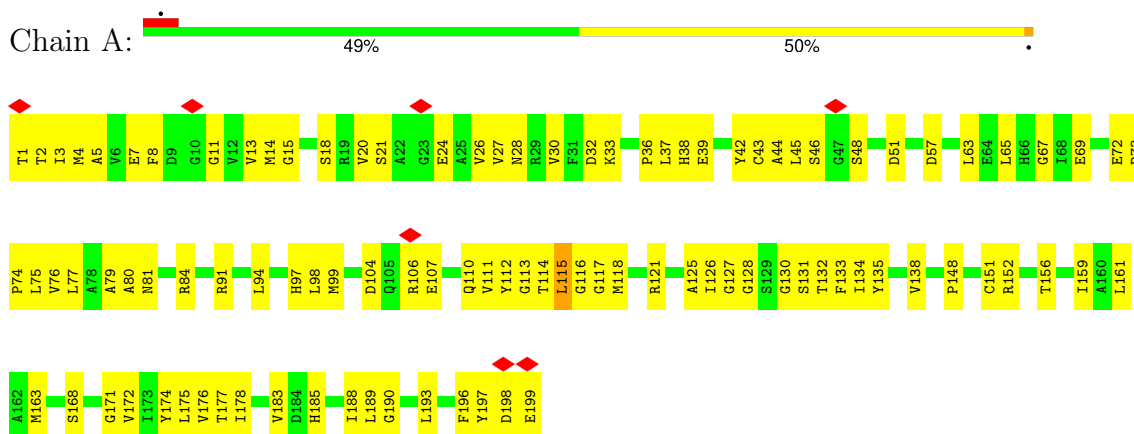


Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	N	O	0
			40	32	4	4	
15	D	1	Total	C	N	O	0
			40	32	4	4	

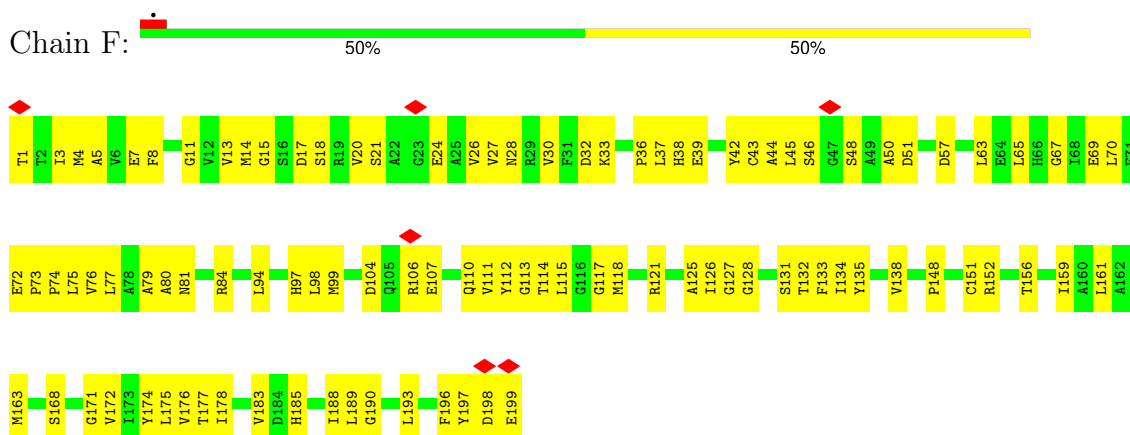
3 Residue-property plots

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.

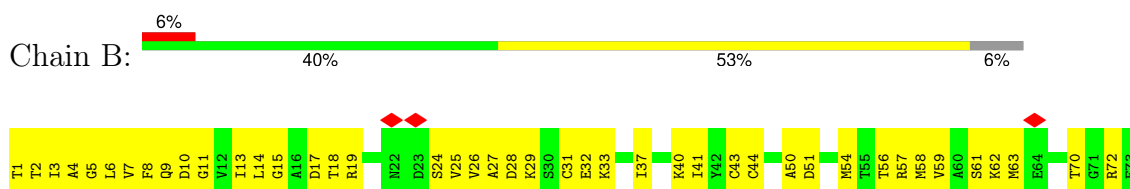
• Molecule 1: Proteasome subunit beta type-9

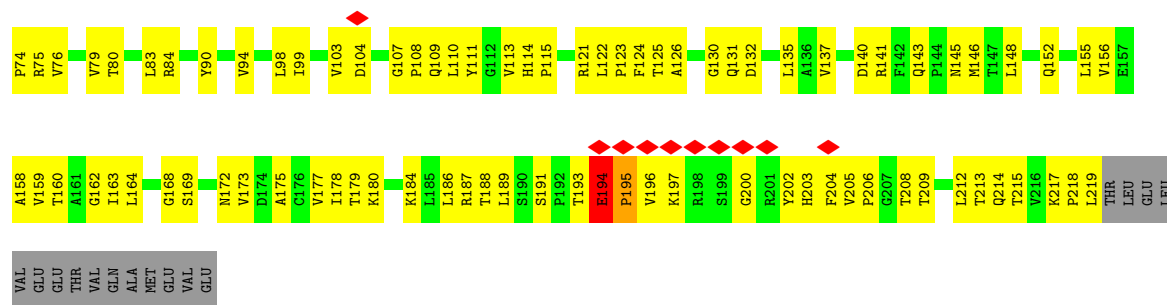


• Molecule 1: Proteasome subunit beta type-9

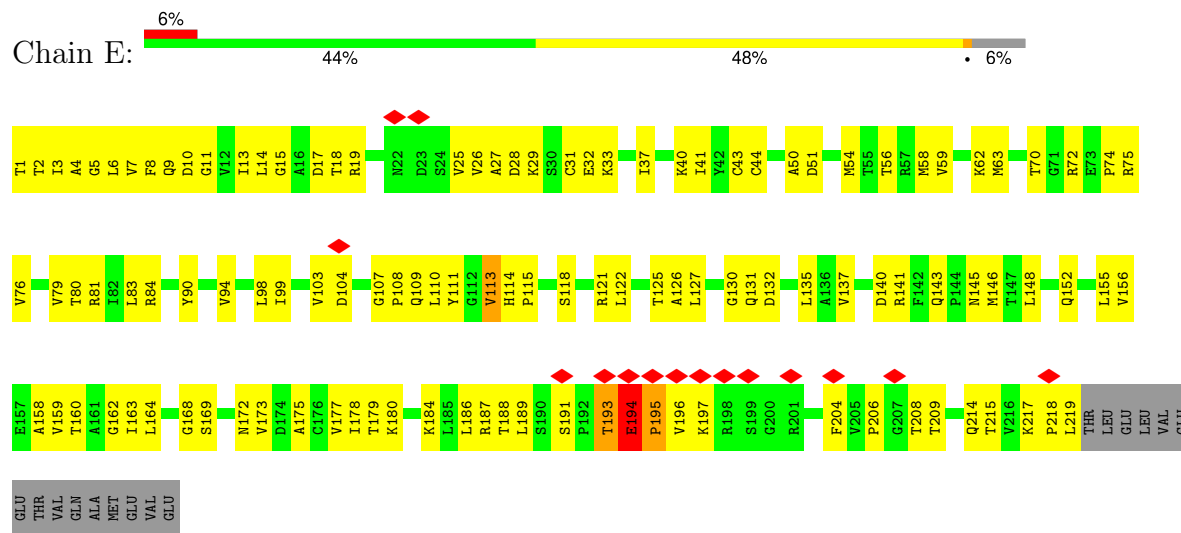


• Molecule 2: Proteasome subunit beta type-10





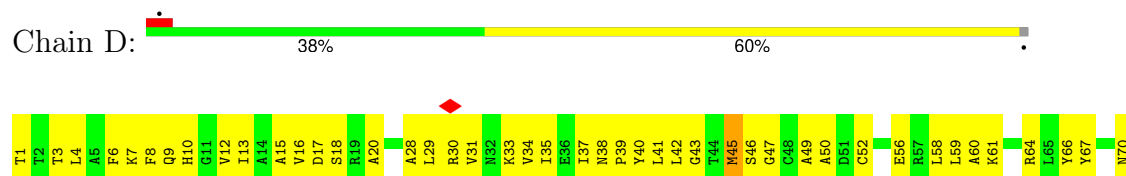
• Molecule 2: Proteasome subunit beta type-10

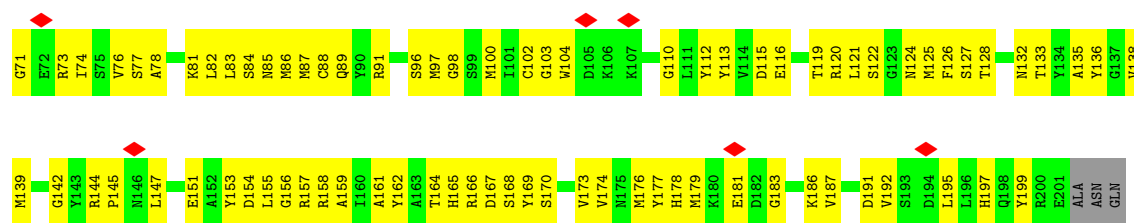


• Molecule 3: Proteasome subunit beta type-8

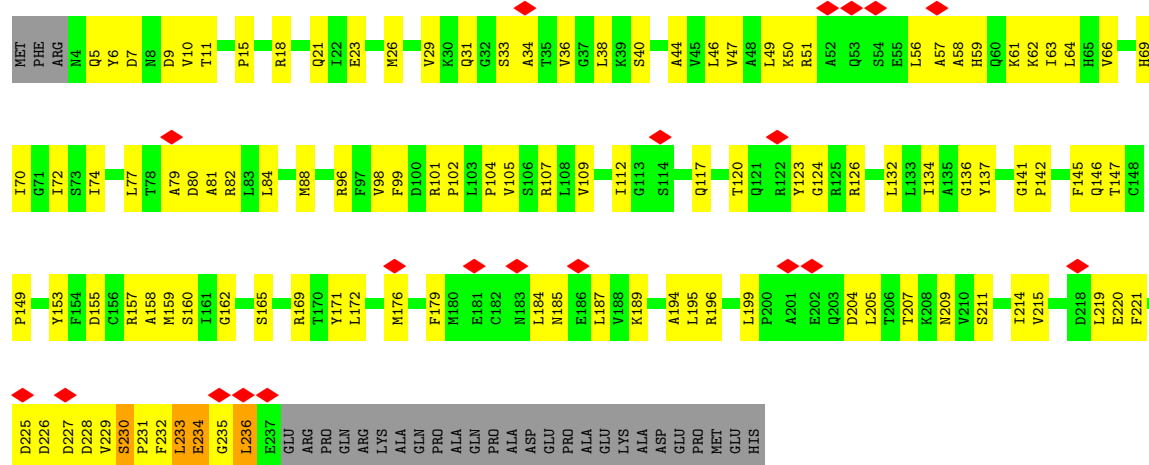


• Molecule 3: Proteasome subunit beta type-8

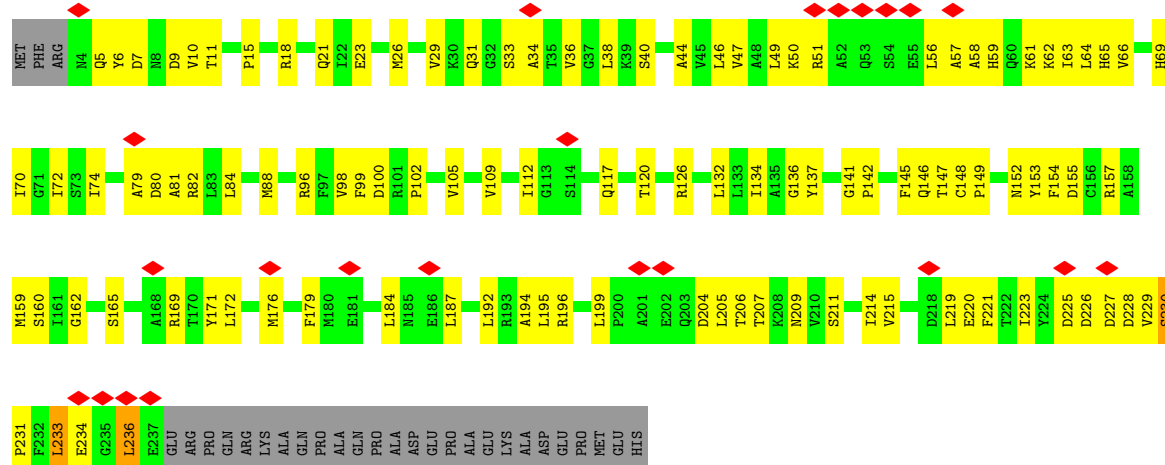




• Molecule 4: Proteasome subunit alpha type-1

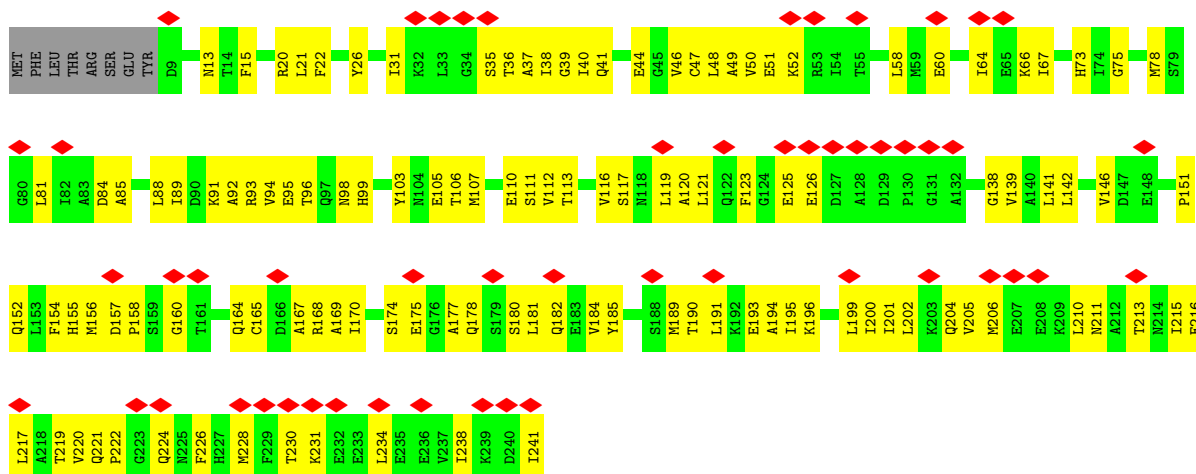


• Molecule 4: Proteasome subunit alpha type-1

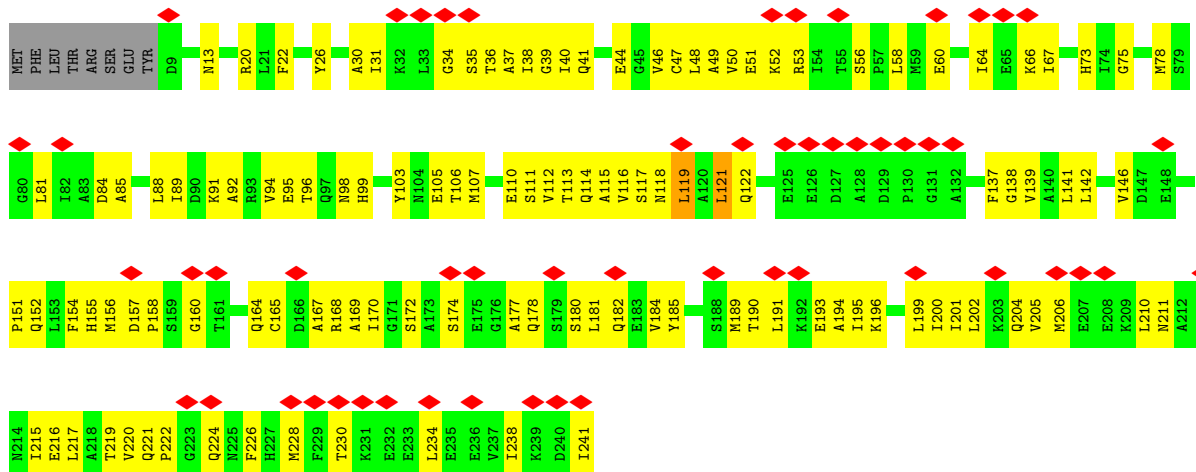


• Molecule 5: Proteasome subunit alpha type-5

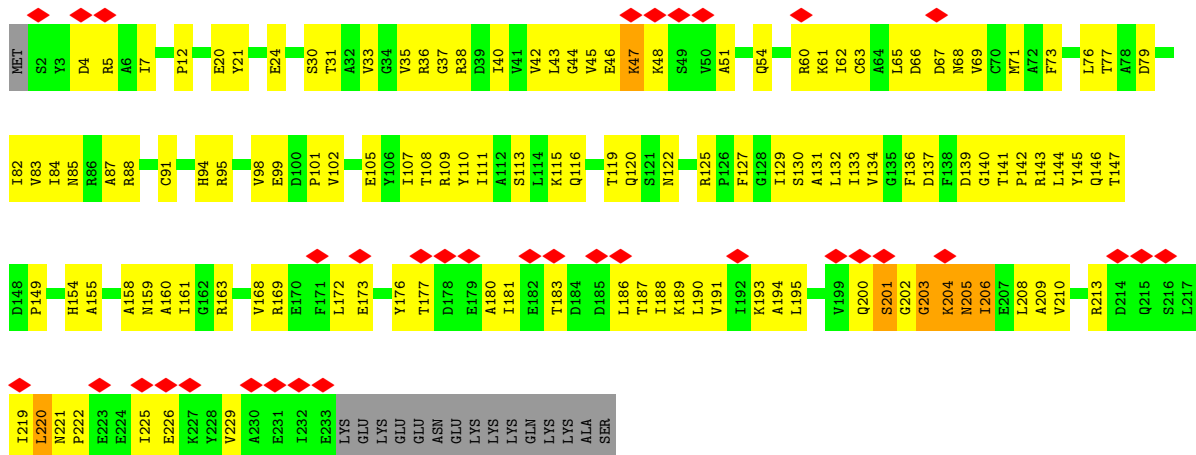




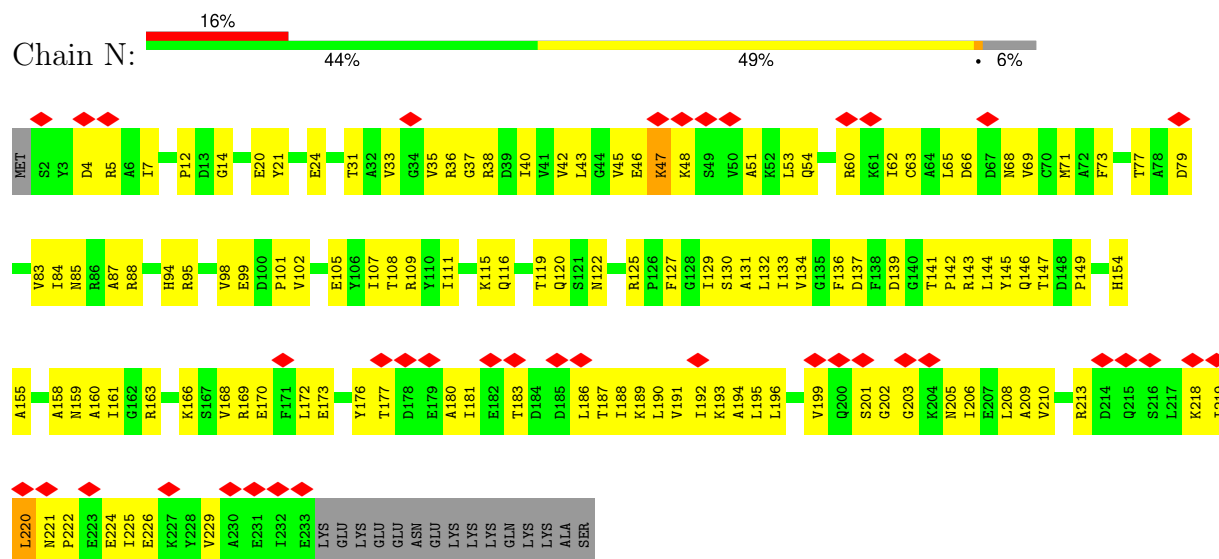
• Molecule 5: Proteasome subunit alpha type-5



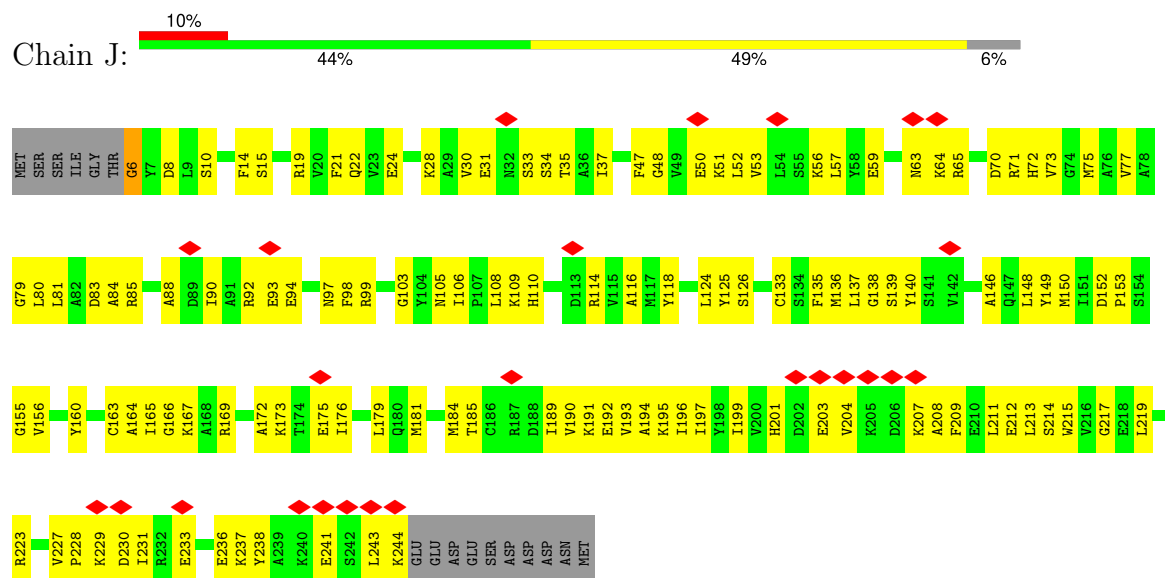
• Molecule 6: Proteasome subunit alpha type-7



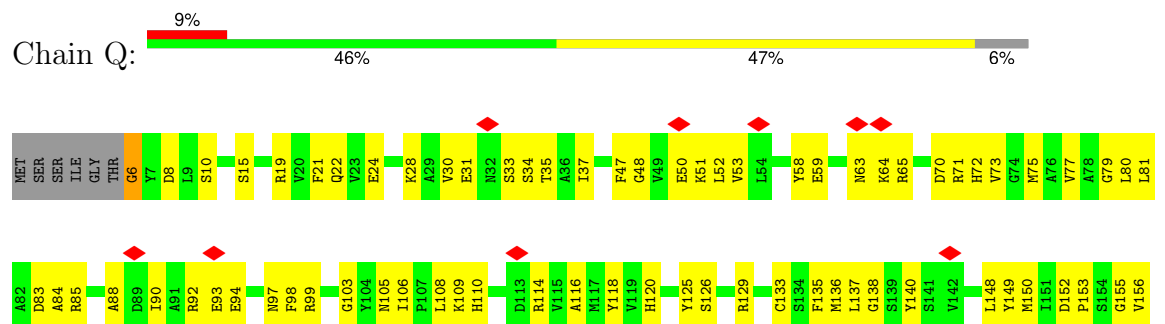
- Molecule 6: Proteasome subunit alpha type-7

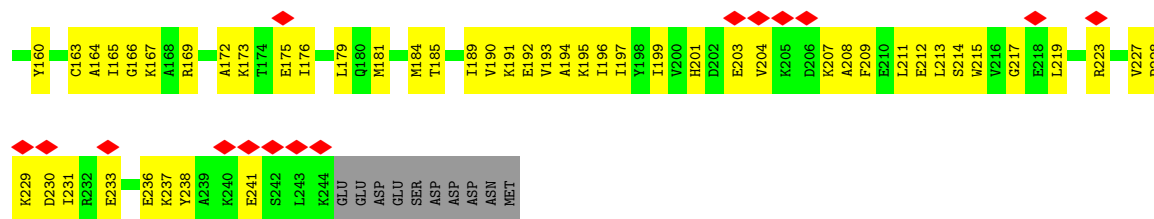


- Molecule 7: Proteasome subunit alpha type-3

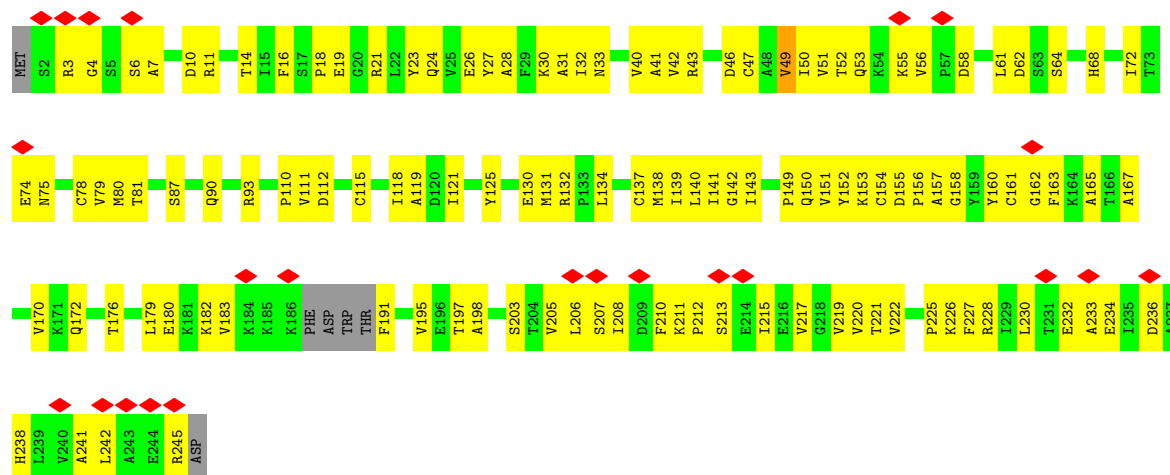


- Molecule 7: Proteasome subunit alpha type-3

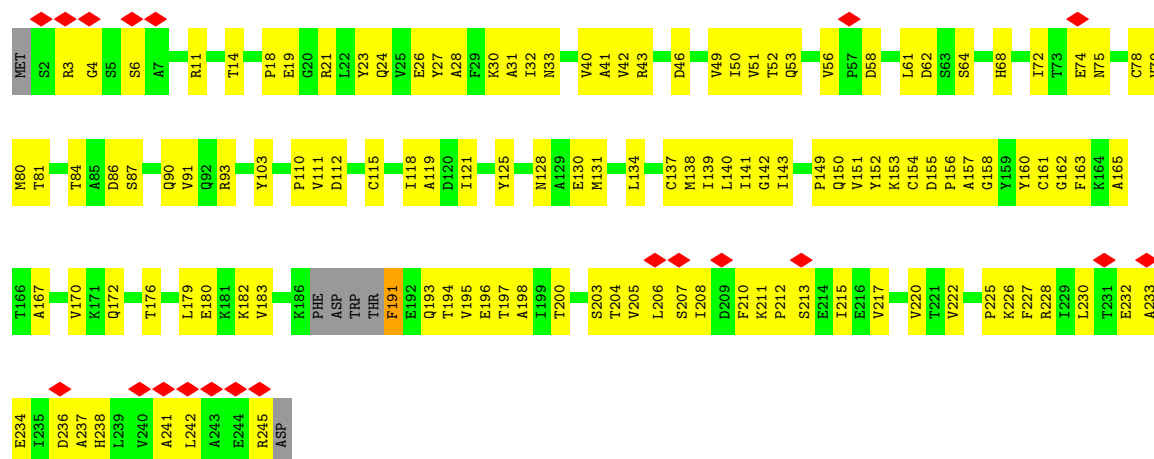




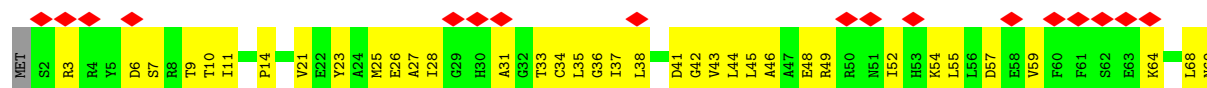
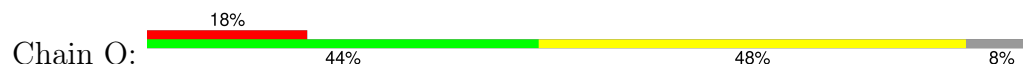
• Molecule 8: Proteasome subunit alpha type-6

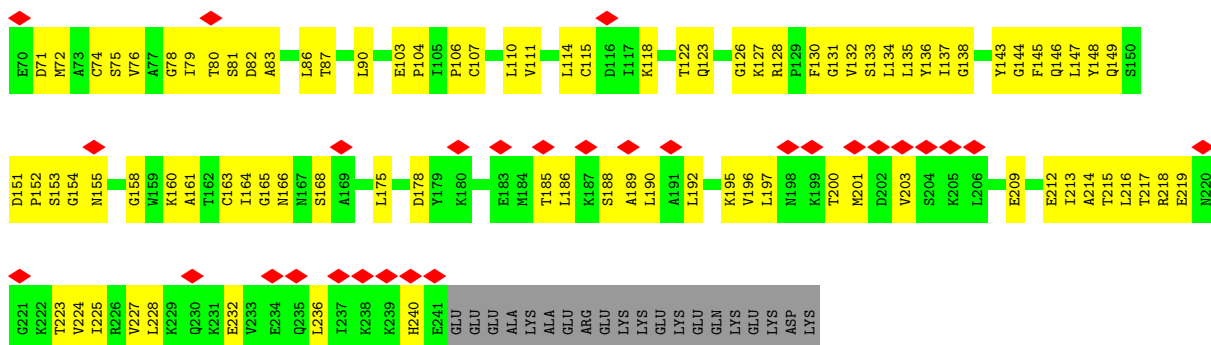


• Molecule 8: Proteasome subunit alpha type-6

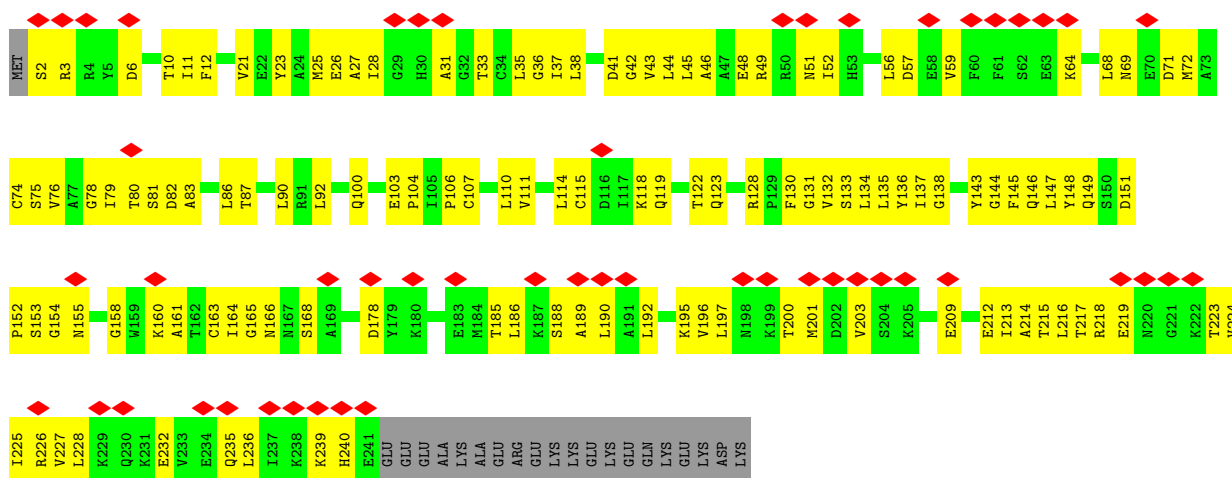
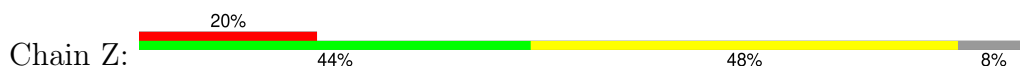


• Molecule 9: Proteasome subunit alpha type-4

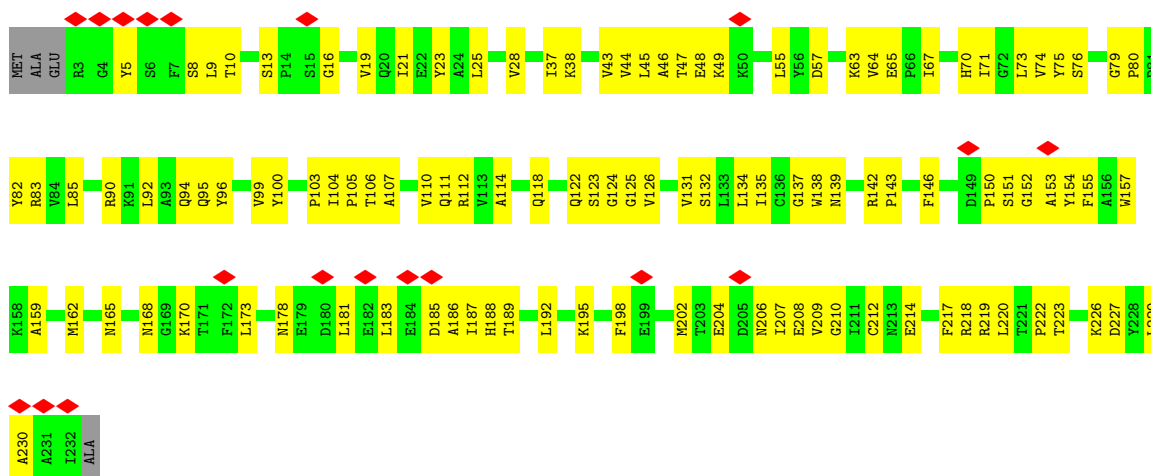




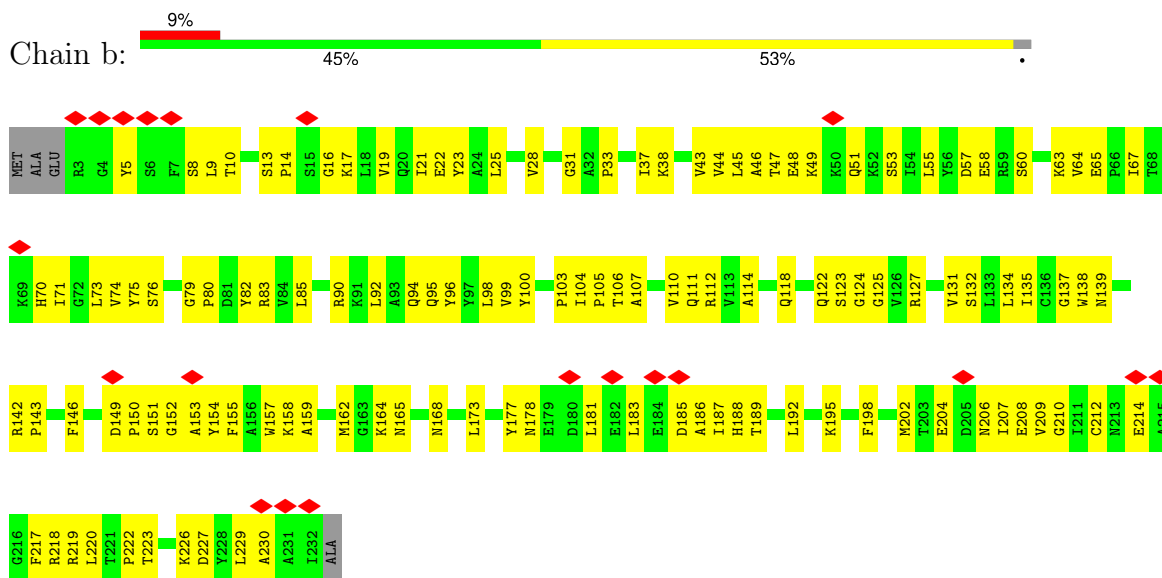
• Molecule 9: Proteasome subunit alpha type-4



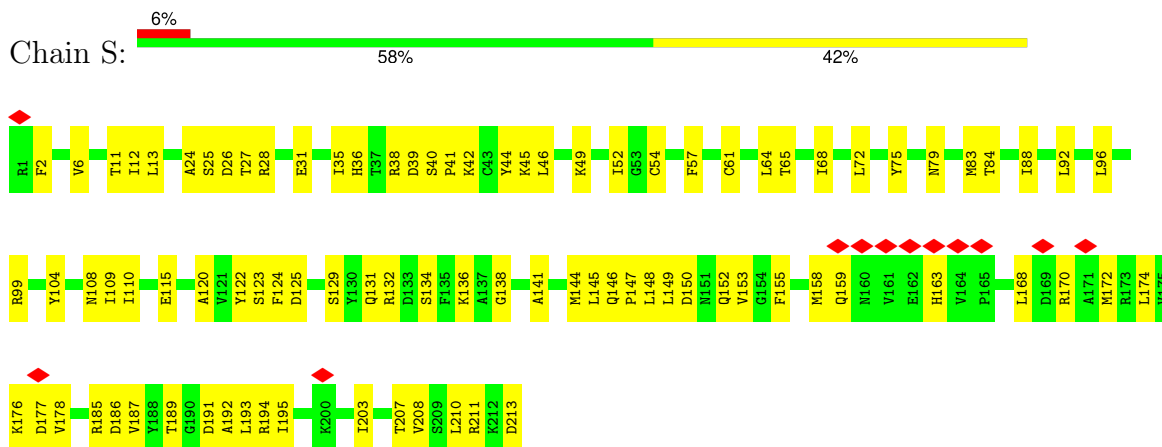
• Molecule 10: Proteasome subunit alpha type-2



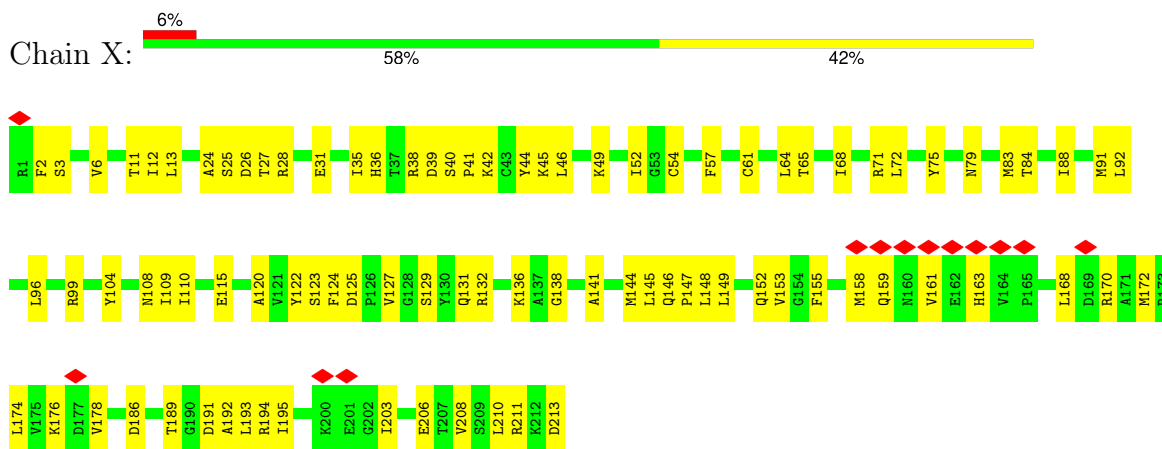
• Molecule 10: Proteasome subunit alpha type-2



• Molecule 11: Proteasome subunit beta type-1

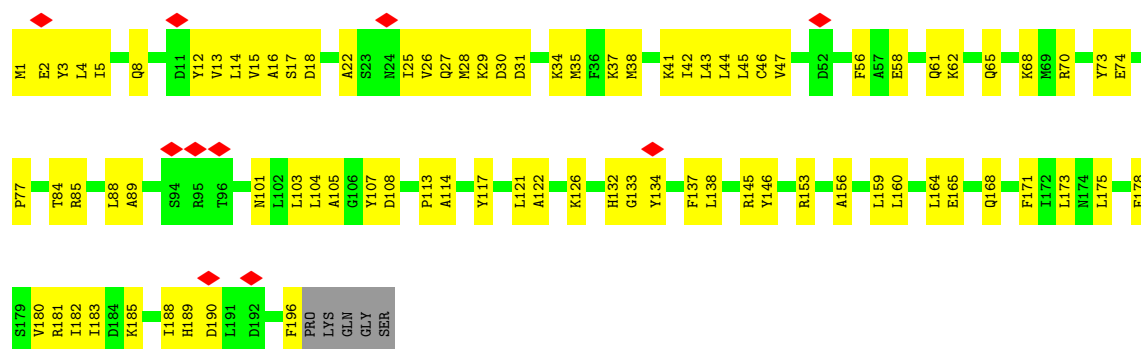


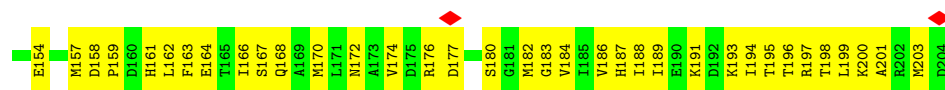
• Molecule 11: Proteasome subunit beta type-1



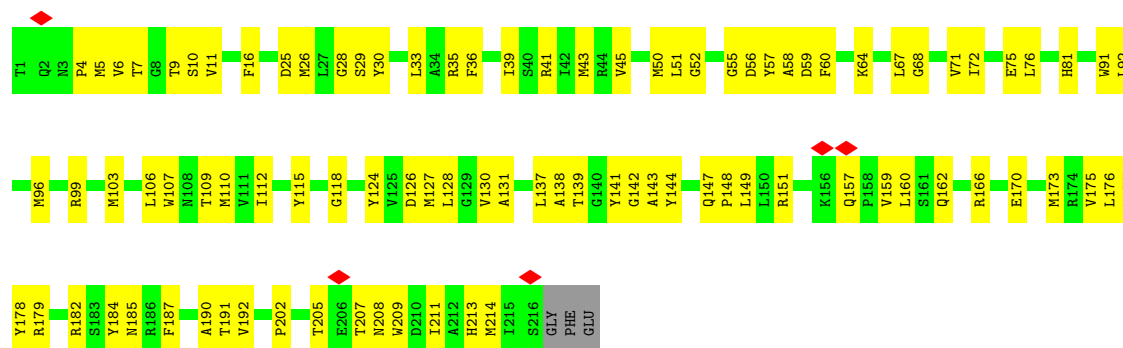
• Molecule 12: Proteasome subunit beta type-2



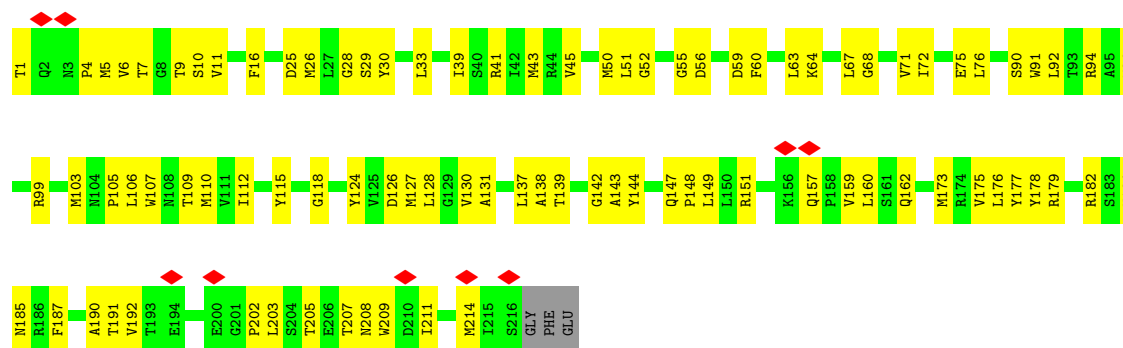




• Molecule 14: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75017	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0383	Depositor
Map size (Å)	307.2, 307.2, 307.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BZ7

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/1521	0.57	0/2062
1	F	0.41	0/1521	0.57	0/2062
2	B	0.40	0/1635	0.56	0/2222
2	E	0.40	0/1635	0.56	0/2222
3	C	0.41	0/1596	0.58	0/2152
3	D	0.41	0/1596	0.58	0/2152
4	G	0.37	0/1853	0.55	0/2510
4	L	0.36	0/1882	0.55	0/2548
5	H	0.32	0/1780	0.52	0/2412
5	M	0.32	0/1775	0.53	0/2401
6	I	0.39	0/1780	0.68	0/2422
6	N	0.34	0/1779	0.64	0/2420
7	J	0.37	0/1935	0.52	0/2605
7	Q	0.37	0/1889	0.52	0/2549
8	K	0.38	0/1886	0.56	0/2549
8	R	0.38	0/1850	0.55	0/2507
9	O	0.34	0/1879	0.50	0/2544
9	Z	0.34	0/1896	0.50	0/2562
10	P	0.39	0/1778	0.54	0/2419
10	b	0.38	0/1833	0.53	0/2489
11	S	0.41	0/1675	0.59	0/2257
11	X	0.40	0/1672	0.59	0/2257
12	T	0.39	0/1606	0.58	0/2174
12	V	0.39	0/1620	0.57	0/2191
13	U	0.42	0/1630	0.61	0/2197
13	Y	0.42	0/1639	0.58	0/2208
14	W	0.44	0/1728	0.58	0/2339
14	a	0.44	0/1720	0.58	0/2330
All	All	0.38	0/48589	0.56	0/65762

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
6	I	0	8
6	N	0	2
7	J	0	1
7	Q	0	1
9	O	0	2
9	Z	0	2
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	I	201	SER	Peptide
6	I	202	GLY	Peptide
6	I	203	GLY	Peptide
6	I	204	LYS	Peptide
6	I	205	ASN	Peptide
6	I	220	LEU	Peptide
6	I	47	LYS	Peptide
7	J	6	GLY	Peptide
6	N	220	LEU	Peptide
6	N	47	LYS	Peptide
9	O	203	VAL	Peptide
9	O	52	ILE	Peptide
7	Q	6	GLY	Peptide
9	Z	203	VAL	Peptide
9	Z	52	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1493	0	1458	111	0
1	F	1493	0	1458	111	0
2	B	1609	0	1646	157	0
2	E	1609	0	1646	140	0
3	C	1563	0	1512	137	0
3	D	1563	0	1512	151	0
4	G	1817	0	1788	129	0
4	L	1841	0	1810	140	0
5	H	1753	0	1704	122	0
5	M	1748	0	1722	146	0
6	I	1749	0	1672	165	0
6	N	1754	0	1691	208	0
7	J	1888	0	1882	125	0
7	Q	1851	0	1814	118	0
8	K	1850	0	1860	139	0
8	R	1817	0	1776	129	0
9	O	1843	0	1814	140	0
9	Z	1860	0	1864	147	0
10	P	1741	0	1683	109	0
10	b	1788	0	1761	129	0
11	S	1642	0	1635	113	0
11	X	1636	0	1625	107	0
12	T	1567	0	1566	116	0
12	V	1581	0	1586	117	0
13	U	1599	0	1621	115	0
13	Y	1604	0	1634	140	0
14	W	1692	0	1670	96	0
14	a	1684	0	1655	87	0
15	C	40	0	0	16	0
15	D	40	0	0	18	0
All	All	47715	0	47065	3318	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 35.

All (3318) 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)
6:N:203:GLY:HA2	6:N:229:VAL:CG2	1.28	1.56
6:N:46:GLU:HA	6:N:206:ILE:CG2	1.37	1.49
6:N:47:LYS:N	6:N:206:ILE:HG22	1.25	1.43
6:N:46:GLU:C	6:N:206:ILE:HG22	1.44	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:208:LEU:HD23	6:I:209:ALA:N	1.33	1.42
6:N:203:GLY:CA	6:N:229:VAL:HG21	1.49	1.39
8:R:193:GLN:CB	8:R:196:GLU:OE1	1.72	1.36
8:R:193:GLN:HB3	8:R:196:GLU:OE1	1.19	1.34
6:I:43:LEU:O	6:I:208:LEU:CG	1.74	1.33
6:I:208:LEU:CD2	6:I:209:ALA:H	1.40	1.33
6:N:46:GLU:CA	6:N:206:ILE:CG2	2.08	1.30
6:N:199:VAL:HG21	6:N:206:ILE:CD1	1.68	1.22
6:N:195:LEU:CD2	6:N:206:ILE:HD12	1.68	1.22
6:N:46:GLU:CA	6:N:206:ILE:HG22	1.67	1.21
6:N:60:ARG:NH1	6:N:219:ILE:HD13	1.57	1.20
6:N:203:GLY:C	6:N:229:VAL:HG21	1.64	1.20
6:I:208:LEU:CD2	6:I:209:ALA:O	1.90	1.20
6:N:46:GLU:HA	6:N:206:ILE:HG21	1.19	1.17
6:N:203:GLY:HA2	6:N:229:VAL:CB	1.76	1.16
6:N:203:GLY:CA	6:N:229:VAL:CG2	2.11	1.14
8:K:161:CYS:SG	8:K:163:PHE:CZ	2.41	1.14
6:N:47:LYS:N	6:N:206:ILE:CG2	2.13	1.12
4:G:79:ALA:HB3	5:H:121:LEU:HD12	1.31	1.11
5:M:91:LYS:NZ	5:M:119:LEU:HD21	1.66	1.10
6:N:203:GLY:HA2	6:N:229:VAL:CG1	1.81	1.10
6:N:195:LEU:HD22	6:N:206:ILE:HD12	1.10	1.10
6:I:43:LEU:O	6:I:208:LEU:HG	0.94	1.09
12:T:25:ILE:HG13	12:T:26:VAL:HG13	1.33	1.09
4:G:229:VAL:O	4:G:233:LEU:HB2	1.51	1.09
8:R:193:GLN:HB3	8:R:196:GLU:CD	1.75	1.09
6:N:199:VAL:HG21	6:N:206:ILE:HD13	1.20	1.09
8:K:32:ILE:CD1	8:K:137:CYS:SG	2.41	1.08
6:N:199:VAL:CG2	6:N:206:ILE:HD13	1.82	1.08
4:G:229:VAL:HG23	4:G:233:LEU:HD12	1.35	1.08
12:V:25:ILE:HG13	12:V:26:VAL:HG13	1.33	1.07
6:I:208:LEU:HD21	6:I:209:ALA:O	1.55	1.06
5:M:114:GLN:O	5:M:118:ASN:OD1	1.74	1.06
2:B:197:LYS:H	2:B:197:LYS:HD3	1.19	1.05
6:N:203:GLY:CA	6:N:229:VAL:HG11	1.85	1.05
8:R:141:ILE:HG22	8:R:151:VAL:HG12	1.39	1.04
2:E:195:PRO:HG2	11:X:211:ARG:HG2	1.40	1.04
2:E:197:LYS:H	2:E:197:LYS:HD3	1.20	1.04
3:D:3:THR:HG23	3:D:16:VAL:HG12	1.40	1.03
6:N:203:GLY:O	6:N:229:VAL:HG21	1.58	1.03
4:G:229:VAL:CG2	4:G:233:LEU:HD12	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:203:GLY:HA3	6:N:229:VAL:HG11	1.41	1.02
3:C:40:TYR:HB2	3:C:179:MET:HE1	1.42	1.01
2:E:194:GLU:H	2:E:195:PRO:CD	1.73	1.01
6:N:203:GLY:CA	6:N:229:VAL:CG1	2.39	1.01
3:D:40:TYR:HB2	3:D:179:MET:HE1	1.42	1.01
8:K:141:ILE:HG22	8:K:151:VAL:HG12	1.39	1.00
4:G:189:LYS:NZ	4:G:234:GLU:CD	2.19	1.00
5:M:41:GLN:HA	5:M:46:VAL:HG12	1.44	1.00
3:C:3:THR:HG23	3:C:16:VAL:HG12	1.40	0.99
2:B:194:GLU:H	2:B:195:PRO:CD	1.74	0.99
6:N:60:ARG:HH12	6:N:219:ILE:HD13	1.12	0.99
8:K:49[A]:VAL:HG21	8:K:195:VAL:HG22	1.43	0.99
5:H:41:GLN:HA	5:H:46:VAL:HG12	1.44	0.99
2:E:195:PRO:HG2	11:X:211:ARG:CG	1.93	0.98
3:C:133:THR:HG21	12:V:25:ILE:HD11	1.46	0.98
4:G:176:MET:HE1	7:J:56:LYS:HB3	1.42	0.98
11:S:148:LEU:HD23	11:S:178:VAL:HG12	1.47	0.97
1:A:4:MET:HG3	1:A:126:ILE:HG22	1.45	0.96
8:R:193:GLN:HB2	8:R:196:GLU:OE1	1.64	0.96
11:X:148:LEU:HD23	11:X:178:VAL:HG12	1.47	0.96
6:N:203:GLY:HA2	6:N:229:VAL:HG21	1.03	0.96
4:L:50:LYS:O	4:L:59:HIS:HB3	1.65	0.96
6:N:195:LEU:CD2	6:N:206:ILE:CD1	2.43	0.95
1:F:4:MET:HG3	1:F:126:ILE:HG22	1.45	0.95
6:I:208:LEU:HD23	6:I:209:ALA:CA	1.96	0.94
5:M:92:ALA:HB2	5:M:116:VAL:HG21	1.47	0.94
8:K:32:ILE:HD11	8:K:137:CYS:SG	2.06	0.94
5:M:91:LYS:HG2	5:M:119:LEU:HD11	1.50	0.94
6:I:208:LEU:HD23	6:I:209:ALA:H	0.84	0.94
6:I:208:LEU:CG	6:I:209:ALA:H	1.78	0.94
4:G:189:LYS:NZ	4:G:234:GLU:OE1	1.99	0.93
6:N:46:GLU:CA	6:N:206:ILE:HG21	1.83	0.92
11:S:45:LYS:HE3	11:S:203:ILE:HD12	1.51	0.92
3:C:33:LYS:O	3:C:45:MET:HG3	1.67	0.92
6:N:60:ARG:HH12	6:N:219:ILE:CD1	1.80	0.92
2:E:194:GLU:H	2:E:195:PRO:HD3	1.35	0.92
3:C:49:ALA:HB2	15:C:301:BZ7:CBH	1.99	0.92
6:N:46:GLU:HA	6:N:206:ILE:CB	1.99	0.91
3:C:31:VAL:HG11	15:C:301:BZ7:CBJ	1.99	0.91
3:D:35:ILE:HB	3:D:45:MET:HE2	1.53	0.91
3:D:49:ALA:HB1	15:D:301:BZ7:CBN	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:26:VAL:HG12	12:V:138:LEU:HD11	1.52	0.91
11:X:45:LYS:HE3	11:X:203:ILE:HD12	1.51	0.91
6:I:208:LEU:HD23	6:I:209:ALA:C	1.95	0.91
6:N:195:LEU:HD22	6:N:206:ILE:CD1	2.00	0.91
5:M:178:GLN:HG3	5:M:182:GLN:HE22	1.36	0.91
10:P:57:ASP:HB3	8:R:162:GLY:HA3	1.53	0.90
2:B:194:GLU:H	2:B:195:PRO:HD3	1.37	0.90
8:K:49[B]:VAL:HG22	8:K:219:VAL:HG12	1.53	0.90
8:K:49[A]:VAL:HG23	8:K:219:VAL:HG12	1.51	0.90
5:M:91:LYS:NZ	5:M:119:LEU:HD11	1.87	0.90
5:H:178:GLN:HG3	5:H:182:GLN:HE22	1.36	0.89
6:I:208:LEU:HD23	6:I:209:ALA:O	1.69	0.89
12:V:85:ARG:HH21	13:Y:60:GLN:HB2	1.35	0.89
9:Z:216:LEU:HD12	9:Z:225:ILE:HG12	1.55	0.88
2:E:137:VAL:HG21	2:E:158:ALA:HA	1.53	0.88
6:N:47:LYS:H	6:N:206:ILE:HG22	1.37	0.87
10:P:37:ILE:HG12	10:P:159:ALA:HB1	1.54	0.87
12:T:85:ARG:HH21	13:U:60:GLN:HB2	1.38	0.87
2:B:9:GLN:HG2	2:B:145:ASN:HD22	1.38	0.87
6:I:42:VAL:HG13	6:I:208:LEU:CD2	2.04	0.87
3:D:31:VAL:HG11	15:D:301:BZ7:CBK	2.05	0.87
2:B:137:VAL:HG21	2:B:158:ALA:HA	1.53	0.86
4:G:74:ILE:HG21	4:G:81:ALA:HB1	1.57	0.86
4:G:189:LYS:HZ2	4:G:234:GLU:CD	1.81	0.86
10:P:105:PRO:HA	10:P:139:ASN:HD21	1.40	0.86
2:E:194:GLU:N	2:E:195:PRO:CD	2.36	0.86
10:b:37:ILE:HG12	10:b:159:ALA:HB1	1.54	0.86
4:L:227:ASP:O	4:L:230:SER:OG	1.92	0.86
6:I:203:GLY:HA3	6:I:205:ASN:HB2	1.56	0.86
6:N:203:GLY:HA2	6:N:229:VAL:HG22	1.52	0.86
4:G:196:ARG:HH12	4:G:236:LEU:HB3	1.39	0.86
10:b:207:ILE:HD11	10:b:229:LEU:HD21	1.56	0.86
11:X:27:THR:HB	11:X:40:SER:H	1.41	0.86
15:D:301:BZ7:NAZ	15:D:301:BZ7:O	2.09	0.85
2:B:194:GLU:N	2:B:195:PRO:CD	2.36	0.85
9:O:216:LEU:HD12	9:O:225:ILE:HG12	1.55	0.85
15:C:301:BZ7:O	15:C:301:BZ7:NAZ	2.10	0.85
2:E:9:GLN:HG2	2:E:145:ASN:HD22	1.38	0.85
10:P:207:ILE:HD11	10:P:229:LEU:HD21	1.57	0.85
7:J:109:LYS:HA	7:J:149:TYR:HE2	1.42	0.84
3:D:31:VAL:HG11	15:D:301:BZ7:CBJ	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:74:ILE:HG21	4:L:81:ALA:HB1	1.57	0.84
3:C:164:THR:HG22	3:C:170:SER:HB3	1.58	0.84
5:M:49:ALA:HB2	5:M:217:LEU:HD13	1.60	0.84
3:D:164:THR:HG22	3:D:170:SER:HB3	1.58	0.84
6:N:60:ARG:NH1	6:N:219:ILE:CD1	2.37	0.84
10:b:105:PRO:HA	10:b:139:ASN:HD21	1.40	0.84
7:Q:109:LYS:HA	7:Q:149:TYR:HE2	1.42	0.83
11:S:27:THR:HB	11:S:40:SER:H	1.41	0.83
3:D:28:ALA:HB2	11:S:131:GLN:HE22	1.43	0.83
4:G:49:LEU:HG	4:G:195:LEU:HD21	1.60	0.83
5:H:49:ALA:HB2	5:H:217:LEU:HD13	1.60	0.83
4:L:49:LEU:HG	4:L:195:LEU:HD21	1.60	0.83
6:N:196:LEU:CD2	6:N:202:GLY:HA3	2.09	0.82
4:L:26:MET:HG2	4:L:149:PRO:HD2	1.61	0.82
12:T:8:GLN:HE21	12:T:113:PRO:HG2	1.44	0.82
4:G:26:MET:HG2	4:G:149:PRO:HD2	1.61	0.82
8:K:161:CYS:SG	8:K:163:PHE:CE2	2.69	0.82
3:D:33:LYS:O	3:D:45:MET:HG3	1.79	0.82
2:E:84:ARG:NH1	1:F:57:ASP:OD2	2.13	0.82
6:I:42:VAL:HG12	6:I:208:LEU:HD11	1.60	0.82
4:G:227:ASP:O	4:G:230:SER:OG	1.98	0.82
4:L:230:SER:HB2	4:L:231:PRO:HD3	1.61	0.82
4:L:229:VAL:O	4:L:233:LEU:HB2	1.80	0.82
5:M:105:GLU:OE2	11:S:75:TYR:OH	1.97	0.82
1:A:198:ASP:OD1	14:a:184:TYR:OH	1.96	0.81
3:D:7:LYS:HB3	3:D:12:VAL:HG22	1.61	0.81
6:N:108:THR:HG21	6:N:145:TYR:HB3	1.62	0.81
1:F:135:TYR:HE2	14:a:33:LEU:HD21	1.45	0.81
9:O:54:LYS:HG3	9:O:55:LEU:H	1.46	0.81
6:I:108:THR:HG21	6:I:145:TYR:HB3	1.62	0.81
1:A:106:ARG:HD3	1:A:107:GLU:HG2	1.61	0.81
5:H:40:ILE:HG12	5:H:167:ALA:HB1	1.62	0.81
8:R:193:GLN:O	8:R:195:VAL:N	2.13	0.81
2:B:215:THR:HG23	13:Y:196:THR:HB	1.62	0.81
9:O:68:LEU:HD11	9:O:74:CYS:HB3	1.63	0.81
9:Z:90:LEU:HD21	9:Z:114:LEU:HB2	1.63	0.81
6:N:46:GLU:C	6:N:206:ILE:CG2	2.33	0.80
3:C:7:LYS:HB3	3:C:12:VAL:HG22	1.61	0.80
2:E:9:GLN:HE21	2:E:145:ASN:HB3	1.45	0.80
5:M:91:LYS:NZ	5:M:119:LEU:CD2	2.44	0.80
8:R:80[A]:MET:HG3	8:R:87:SER:HB3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ARG:HD3	1:F:107:GLU:HG2	1.61	0.80
6:I:30:SER:HB2	6:I:61:LYS:HE2	1.63	0.80
2:B:9:GLN:HE21	2:B:145:ASN:HB3	1.45	0.80
2:E:63:MET:HG3	2:E:79:VAL:HG22	1.64	0.80
7:Q:52:LEU:HD23	7:Q:209:PHE:HB3	1.63	0.80
2:B:63:MET:HG3	2:B:79:VAL:HG22	1.64	0.79
5:H:52:LYS:NZ	5:H:64:ILE:O	2.15	0.79
4:L:51:ARG:O	4:L:59:HIS:HA	1.82	0.79
8:R:160:TYR:O	8:R:161:CYS:SG	2.39	0.79
12:V:8:GLN:HE21	12:V:113:PRO:HG2	1.44	0.79
4:G:189:LYS:HZ1	4:G:234:GLU:CD	1.90	0.79
5:M:52:LYS:NZ	5:M:64:ILE:O	2.15	0.79
5:H:92:ALA:HB2	5:H:116:VAL:HG21	1.64	0.79
3:D:120:ARG:NH2	6:N:99:GLU:OE2	2.16	0.79
14:W:25:ASP:HA	14:W:187:PHE:HA	1.64	0.79
5:M:40:ILE:HG12	5:M:167:ALA:HB1	1.63	0.79
9:O:90:LEU:HD21	9:O:114:LEU:HB2	1.63	0.79
9:Z:68:LEU:HD11	9:Z:74:CYS:HB3	1.63	0.79
6:I:43:LEU:O	6:I:208:LEU:CD1	2.30	0.79
9:O:42:GLY:HA3	9:O:217:THR:HG22	1.65	0.79
8:R:165:ALA:HB1	8:R:179:LEU:HD13	1.65	0.79
8:K:32:ILE:HD13	8:K:137:CYS:SG	2.21	0.79
8:K:165:ALA:HB1	8:K:179:LEU:HD13	1.65	0.79
13:U:7:GLY:HA2	13:U:140:THR:HG21	1.65	0.79
4:G:196:ARG:NH1	4:G:236:LEU:HB3	1.97	0.78
6:N:199:VAL:HG21	6:N:206:ILE:HD11	1.62	0.78
2:B:209:THR:HG21	13:Y:167:SER:HB3	1.66	0.78
4:G:66:VAL:HG21	4:G:72:ILE:HG23	1.66	0.78
6:N:132:LEU:HG	6:N:161:ILE:HD13	1.66	0.78
7:J:52:LEU:HD23	7:J:209:PHE:HB3	1.63	0.78
4:L:50:LYS:C	4:L:59:HIS:HB3	2.09	0.78
6:N:195:LEU:HB3	6:N:199:VAL:CG2	2.14	0.78
1:A:152:ARG:NH1	1:A:177:THR:OG1	2.16	0.78
6:N:36:ARG:HG3	6:N:142:PRO:HB2	1.66	0.78
4:L:66:VAL:HG21	4:L:72:ILE:HG23	1.66	0.77
9:Z:42:GLY:HA3	9:Z:217:THR:HG22	1.65	0.77
6:I:36:ARG:HG3	6:I:142:PRO:HB2	1.66	0.77
1:A:115:LEU:HD12	1:A:116:GLY:N	2.00	0.77
3:C:49:ALA:HB1	15:C:301:BZ7:CBN	2.14	0.77
6:I:42:VAL:HG13	6:I:208:LEU:HD21	1.66	0.77
3:D:157:ARG:O	3:D:161:ALA:HB2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:208:LEU:CD2	6:I:209:ALA:N	2.15	0.77
5:M:91:LYS:HZ3	5:M:119:LEU:HD21	1.49	0.77
13:Y:7:GLY:HA2	13:Y:140:THR:HG21	1.65	0.77
3:C:125:MET:HE3	3:C:139:MET:HE2	1.67	0.77
3:C:157:ARG:O	3:C:161:ALA:HB2	1.85	0.77
6:N:195:LEU:HD23	6:N:206:ILE:CD1	2.15	0.77
9:O:76:VAL:HG11	9:O:83:ALA:HB1	1.67	0.77
14:a:25:ASP:HA	14:a:187:PHE:HA	1.64	0.77
3:C:168:SER:OG	13:U:26:ARG:NH2	2.18	0.77
8:K:50:ILE:HG23	8:K:141:ILE:HD13	1.66	0.77
2:B:209:THR:OG1	13:Y:168:GLN:NE2	2.18	0.77
3:D:121:LEU:HD22	12:T:29:LYS:HD3	1.67	0.77
8:R:50:ILE:HG23	8:R:141:ILE:HD13	1.66	0.77
2:E:204:PHE:CD2	13:U:168:GLN:HG3	2.19	0.77
1:F:1:THR:N	1:F:168:SER:O	2.18	0.77
4:L:33:SER:HB3	4:L:51:ARG:HG3	1.67	0.77
5:H:189:MET:HE2	5:H:194:ALA:HA	1.67	0.76
11:X:27:THR:HG22	11:X:41:PRO:HA	1.67	0.76
2:B:27:ALA:O	11:S:185:ARG:NH1	2.18	0.76
3:D:125:MET:HE3	3:D:139:MET:HE2	1.67	0.76
3:D:31:VAL:CG1	15:D:301:BZ7:CBK	2.64	0.76
3:D:40:TYR:HB3	3:D:183:GLY:HA2	1.68	0.76
6:I:132:LEU:HG	6:I:161:ILE:HD13	1.66	0.76
6:N:47:LYS:CB	6:N:205:ASN:OD1	2.33	0.76
10:P:55:LEU:HD22	8:R:165:ALA:HB3	1.67	0.76
5:M:47:CYS:HA	5:M:219:THR:HG22	1.66	0.76
1:F:152:ARG:NH1	1:F:177:THR:OG1	2.16	0.76
5:M:189:MET:HE2	5:M:194:ALA:HA	1.67	0.76
8:R:205:VAL:HG23	8:R:206:LEU:HD12	1.68	0.76
1:A:1:THR:N	1:A:168:SER:O	2.18	0.76
10:b:74:VAL:HG12	10:b:134:LEU:HB2	1.66	0.76
4:G:51:ARG:O	4:G:59:HIS:HA	1.86	0.76
9:O:81:SER:HB2	10:P:118:GLN:HG3	1.68	0.76
6:N:203:GLY:O	6:N:229:VAL:CG2	2.34	0.75
8:K:53:GLN:HE21	8:K:206:LEU:HD21	1.49	0.75
11:S:27:THR:HG22	11:S:41:PRO:HA	1.67	0.75
2:B:59:VAL:HG21	2:B:83:LEU:HD23	1.69	0.75
2:E:59:VAL:HG21	2:E:83:LEU:HD23	1.69	0.75
5:H:47:CYS:HA	5:H:219:THR:HG22	1.66	0.75
3:C:40:TYR:HB3	3:C:183:GLY:HA2	1.68	0.75
4:G:126:ARG:HB3	5:H:13:ASN:HB3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:HE2	14:W:33:LEU:HD21	1.52	0.75
10:P:74:VAL:HG12	10:P:134:LEU:HB2	1.66	0.75
12:T:38:MET:O	12:T:65:GLN:NE2	2.20	0.75
11:X:123:SER:HB3	11:X:136:LYS:HG2	1.67	0.75
5:H:191:LEU:HD23	5:H:221:GLN:HE21	1.52	0.75
8:K:49[B]:VAL:HG21	8:K:195:VAL:HG22	1.67	0.75
14:W:185:ASN:OD1	14:W:205:THR:N	2.19	0.75
6:N:195:LEU:HD23	6:N:206:ILE:HD12	1.66	0.75
4:L:206:THR:O	4:L:233:LEU:HD11	1.87	0.74
8:R:53:GLN:HE21	8:R:206:LEU:HD21	1.50	0.74
1:F:198:ASP:OD1	14:W:184:TYR:OH	2.05	0.74
8:K:205:VAL:HG23	8:K:206:LEU:HD12	1.68	0.74
12:V:168:GLN:NE2	12:V:175:LEU:O	2.20	0.74
14:W:50:MET:HE2	14:W:192:VAL:HG12	1.67	0.74
9:Z:76:VAL:HG11	9:Z:83:ALA:HB1	1.67	0.74
11:S:123:SER:HB3	11:S:136:LYS:HG2	1.67	0.74
12:T:168:GLN:NE2	12:T:175:LEU:O	2.20	0.74
3:D:1:THR:N	3:D:169:TYR:O	2.20	0.74
2:B:187:ARG:HG3	2:B:188:THR:HG23	1.68	0.74
8:K:115:CYS:HB2	8:K:140:LEU:HD12	1.70	0.74
5:M:191:LEU:HD23	5:M:221:GLN:HE21	1.52	0.74
12:V:35:MET:HG2	12:V:45:LEU:HG	1.70	0.74
13:U:33:MET:HE2	13:U:182:MET:HE2	1.70	0.73
12:V:38:MET:O	12:V:65:GLN:NE2	2.20	0.73
4:L:9:ASP:OD1	9:O:3:ARG:NH2	2.21	0.73
4:L:33:SER:OG	4:L:62:LYS:NZ	2.21	0.73
7:J:48:GLY:HA2	7:J:213:LEU:HD23	1.70	0.73
11:X:49:LYS:NZ	11:X:115:GLU:OE2	2.21	0.73
14:a:50:MET:HE2	14:a:192:VAL:HG12	1.67	0.73
8:K:47:CYS:HB3	8:K:221:THR:HG22	1.69	0.73
4:L:31:GLN:O	4:L:51:ARG:NH2	2.21	0.73
4:L:196:ARG:HB2	4:L:205:LEU:HD11	1.68	0.73
11:S:49:LYS:NZ	11:S:115:GLU:OE2	2.21	0.73
2:E:19:ARG:HG3	2:E:26:VAL:HG13	1.70	0.73
5:M:67:ILE:HB	5:M:228:MET:HE1	1.70	0.73
14:a:185:ASN:OD1	14:a:205:THR:N	2.19	0.73
3:D:35:ILE:HB	3:D:45:MET:CE	2.18	0.73
4:G:196:ARG:HB2	4:G:205:LEU:HD11	1.68	0.73
5:M:91:LYS:HG2	5:M:119:LEU:CD1	2.18	0.73
2:E:187:ARG:HG3	2:E:188:THR:HG23	1.68	0.73
2:B:19:ARG:HG3	2:B:26:VAL:HG13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:THR:N	3:C:169:TYR:O	2.21	0.73
13:Y:33:MET:HE2	13:Y:182:MET:HE2	1.71	0.73
4:G:185:ASN:O	4:G:189:LYS:HG2	1.89	0.72
9:Z:81:SER:HB2	10:b:118:GLN:HG3	1.70	0.72
3:D:133:THR:HB	12:V:138:LEU:HD23	1.70	0.72
6:I:85[B]:ASN:OD1	12:V:70:ARG:NH1	2.19	0.72
7:Q:48:GLY:HA2	7:Q:213:LEU:HD23	1.70	0.72
12:T:4:LEU:HD22	12:T:45:LEU:HD23	1.70	0.72
12:T:13:VAL:HG11	12:T:105:ALA:HB1	1.70	0.72
12:V:4:LEU:HD22	12:V:45:LEU:HD23	1.70	0.72
2:B:15:GLY:HA3	2:B:155:LEU:HD21	1.72	0.72
10:b:110:VAL:HG22	10:b:135:ILE:HD12	1.71	0.72
5:H:67:ILE:HB	5:H:228:MET:HE1	1.70	0.72
6:N:221:ASN:ND2	6:N:224:GLU:OE1	2.22	0.72
8:R:115:CYS:HB2	8:R:140:LEU:HD12	1.70	0.72
9:O:185:THR:N	9:O:188:SER:OG	2.23	0.72
12:T:35:MET:HG2	12:T:45:LEU:HG	1.70	0.72
8:K:80:MET:HE2	8:K:87:SER:HA	1.72	0.72
5:M:91:LYS:CG	5:M:119:LEU:HD11	2.20	0.72
9:Z:37:ILE:HG12	9:Z:161:ALA:HB1	1.72	0.72
2:B:114:HIS:HB3	2:B:115:PRO:HD2	1.70	0.72
2:B:197:LYS:HD3	2:B:197:LYS:N	2.01	0.72
13:U:62:VAL:HG21	13:U:104:THR:HG21	1.71	0.72
12:V:13:VAL:HG11	12:V:105:ALA:HB1	1.70	0.72
6:N:47:LYS:H	6:N:206:ILE:HA	1.54	0.72
10:P:110:VAL:HG22	10:P:135:ILE:HD12	1.71	0.72
12:T:35:MET:HE2	12:T:45:LEU:HD21	1.72	0.72
6:I:69:VAL:HG11	6:I:107:ILE:HG21	1.72	0.72
14:a:10:SER:OG	14:a:142:GLY:N	2.20	0.72
4:L:58:ALA:HB2	5:M:164:GLN:OE1	1.90	0.71
6:N:69:VAL:HG11	6:N:107:ILE:HG21	1.71	0.71
6:N:88:ARG:HH11	12:T:70:ARG:HA	1.52	0.71
5:M:91:LYS:HZ1	5:M:119:LEU:HD21	1.52	0.71
9:O:37:ILE:HG12	9:O:161:ALA:HB1	1.72	0.71
9:Z:36:GLY:HA3	9:Z:45:LEU:HD23	1.71	0.71
8:K:217:VAL:HG11	8:K:230:LEU:HD12	1.72	0.71
9:O:36:GLY:HA3	9:O:45:LEU:HD23	1.71	0.71
12:T:1:MET:SD	12:T:2:GLU:N	2.60	0.71
12:T:164:LEU:HD13	12:T:178:PHE:HD2	1.55	0.71
9:Z:185:THR:N	9:Z:188:SER:OG	2.23	0.71
2:B:195:PRO:HG2	11:S:211:ARG:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:68:LYS:HD3	12:T:74:GLU:HG2	1.72	0.71
2:E:15:GLY:HA3	2:E:155:LEU:HD21	1.71	0.71
2:B:164:LEU:O	11:S:38:ARG:NH2	2.22	0.71
3:C:45:MET:HB3	3:C:52:CYS:HB3	1.71	0.71
15:D:301:BZ7:CAV	11:S:131:GLN:CD	2.64	0.71
8:R:143:ILE:HD13	8:R:149:PRO:HA	1.72	0.71
2:B:197:LYS:H	2:B:197:LYS:CD	2.01	0.71
12:T:85:ARG:HH22	13:U:57:THR:HA	1.55	0.71
13:Y:62:VAL:HG21	13:Y:104:THR:HG21	1.71	0.71
5:H:60:GLU:OE2	6:I:36:ARG:NH2	2.24	0.71
6:I:83:VAL:HG21	6:I:129:ILE:HD11	1.73	0.71
8:K:143:ILE:HD13	8:K:149:PRO:HA	1.72	0.71
4:L:126:ARG:HB3	5:M:13:ASN:HB3	1.73	0.71
12:V:164:LEU:HD13	12:V:178:PHE:HD2	1.55	0.71
3:C:120:ARG:NH2	6:I:99:GLU:OE2	2.24	0.70
8:R:217:VAL:HG11	8:R:230:LEU:HD12	1.72	0.70
8:R:220:VAL:HG12	8:R:227:PHE:HA	1.73	0.70
5:H:121:LEU:HD23	5:H:123:PHE:HE1	1.56	0.70
13:U:13:MET:HE3	13:U:162:LEU:HD12	1.72	0.70
13:U:112:ASP:OD2	13:U:115:THR:N	2.23	0.70
9:Z:235:GLN:HG3	9:Z:239:LYS:HE2	1.74	0.70
2:E:114:HIS:HB3	2:E:115:PRO:HD2	1.70	0.70
5:M:60:GLU:OE2	6:N:36:ARG:NH2	2.24	0.70
13:U:8:GLY:HA2	13:U:24:ASP:OD2	1.92	0.70
12:V:35:MET:HE2	12:V:45:LEU:HD21	1.72	0.70
6:N:83:VAL:HG21	6:N:129:ILE:HD11	1.73	0.70
3:C:69:ARG:HA	5:H:93:ARG:NH1	2.05	0.70
13:U:9:ALA:HB1	13:U:145:MET:HE1	1.74	0.70
14:W:25:ASP:O	14:W:41:ARG:NH2	2.25	0.70
2:E:19:ARG:HD3	2:E:26:VAL:HG22	1.74	0.70
8:K:220:VAL:HG12	8:K:227:PHE:HA	1.72	0.69
3:D:165:HIS:HE1	13:Y:203:MET:HE3	1.57	0.69
2:E:195:PRO:HG2	11:X:211:ARG:HG3	1.73	0.69
9:O:111:VAL:HG22	9:O:136:TYR:CD2	2.27	0.69
12:V:68:LYS:HD3	12:V:74:GLU:HG2	1.73	0.69
3:C:174:VAL:HG23	3:C:192:VAL:HG22	1.74	0.69
13:Y:8:GLY:HA3	13:Y:40:LYS:NZ	2.08	0.69
14:a:25:ASP:O	14:a:41:ARG:NH2	2.25	0.69
8:R:49:VAL:HG21	8:R:195:VAL:HG22	1.73	0.69
4:G:215:VAL:HB	4:G:221:PHE:HD1	1.57	0.69
6:N:46:GLU:CB	6:N:206:ILE:HG21	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:8:GLY:HA3	13:U:40:LYS:NZ	2.07	0.69
13:Y:9:ALA:HB1	13:Y:145:MET:HE1	1.74	0.69
3:D:174:VAL:HG23	3:D:192:VAL:HG22	1.74	0.69
1:F:152:ARG:HH11	1:F:177:THR:HG1	1.40	0.69
14:W:10:SER:OG	14:W:142:GLY:N	2.20	0.69
9:Z:111:VAL:HG22	9:Z:136:TYR:CD2	2.27	0.69
2:E:148:LEU:HD11	2:E:177:VAL:HG11	1.75	0.69
2:E:204:PHE:HD2	13:U:168:GLN:HG3	1.57	0.69
12:T:41:LYS:NZ	12:T:185:LYS:O	2.26	0.69
3:D:70:ASN:OD1	6:N:109:ARG:NH2	2.24	0.69
5:M:195:ILE:HG23	5:M:217:LEU:HD21	1.74	0.69
12:V:41:LYS:NZ	12:V:185:LYS:O	2.26	0.68
13:Y:8:GLY:HA2	13:Y:24:ASP:OD2	1.92	0.68
13:Y:89:MET:HE2	10:b:100:TYR:HE1	1.58	0.68
3:D:45:MET:HB3	3:D:52:CYS:HB3	1.75	0.68
8:R:80[A]:MET:HE2	8:R:91:VAL:HG23	1.76	0.68
4:G:165:SER:OG	4:G:169:ARG:NH1	2.26	0.68
6:I:43:LEU:HD21	6:I:134:VAL:HG11	1.74	0.68
4:L:184:LEU:HD11	4:L:214:ILE:HD13	1.75	0.68
3:C:112:TYR:HE1	3:C:122:SER:HB2	1.59	0.68
4:G:84:LEU:HD23	4:G:132:LEU:HD11	1.75	0.68
6:I:204:LYS:N	6:I:205:ASN:O	2.25	0.68
5:M:26:TYR:CD1	6:N:12:PRO:HA	2.28	0.68
2:B:19:ARG:HD3	2:B:26:VAL:HG22	1.74	0.68
1:F:81:ASN:ND2	7:Q:103:GLY:HA3	2.08	0.68
13:Y:141:CYS:HB3	13:Y:177:ASP:OD2	1.94	0.68
2:B:1:THR:N	2:B:168:GLY:O	2.27	0.68
2:B:148:LEU:HD11	2:B:177:VAL:HG11	1.75	0.68
6:N:42:VAL:HG21	6:N:188:ILE:HG12	1.76	0.68
7:Q:160:TYR:CE1	8:R:61:LEU:HD23	2.29	0.68
3:C:138:VAL:CG2	3:C:159:ALA:HA	2.24	0.68
3:D:138:VAL:HG21	3:D:159:ALA:HA	1.76	0.68
2:E:1:THR:N	2:E:168:GLY:O	2.27	0.68
6:I:203:GLY:HA3	6:I:205:ASN:CB	2.24	0.68
6:I:208:LEU:CG	6:I:209:ALA:N	2.52	0.68
2:B:44:CYS:HB2	2:B:99:ILE:HG23	1.76	0.68
1:F:37:LEU:HD11	1:F:43:CYS:HB3	1.76	0.68
5:H:195:ILE:HG23	5:H:217:LEU:HD21	1.74	0.68
4:L:215:VAL:HB	4:L:221:PHE:HD1	1.57	0.68
3:D:112:TYR:HE1	3:D:122:SER:HB2	1.59	0.67
6:I:31:THR:OG1	6:I:163:ARG:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:165:SER:OG	4:L:169:ARG:NH1	2.26	0.67
5:M:111:SER:OG	11:S:79:ASN:OD1	2.04	0.67
6:N:43:LEU:HD21	6:N:134:VAL:HG11	1.75	0.67
8:K:62:ASP:OD2	8:K:64:SER:OG	2.11	0.67
10:P:73:LEU:CD2	10:P:135:ILE:HG12	2.24	0.67
3:D:138:VAL:CG2	3:D:159:ALA:HA	2.24	0.67
2:E:51:ASP:OD2	13:U:98:ARG:NH2	2.24	0.67
4:G:184:LEU:HD11	4:G:214:ILE:HD13	1.76	0.67
6:I:42:VAL:HG13	6:I:208:LEU:HD22	1.76	0.67
8:K:21:ARG:NH2	8:K:26:GLU:OE1	2.28	0.67
8:K:165:ALA:HB3	10:b:55:LEU:HD22	1.76	0.67
4:L:88:MET:HG2	4:L:112:ILE:HD11	1.76	0.67
6:N:7:ILE:HG23	9:O:11:ILE:HG22	1.76	0.67
9:O:34:CYS:HG	9:O:75:SER:HG	1.22	0.67
14:a:5:MET:HE3	14:a:30:TYR:HE1	1.59	0.67
10:b:73:LEU:CD2	10:b:135:ILE:HG12	2.24	0.67
3:C:138:VAL:HG21	3:C:159:ALA:HA	1.76	0.67
3:C:157:ARG:O	3:C:161:ALA:CB	2.43	0.67
10:b:31:GLY:O	10:b:164:LYS:HG2	1.95	0.67
2:B:213:THR:HB	13:Y:198:THR:OG1	1.94	0.67
4:G:88:MET:HG2	4:G:112:ILE:HD11	1.76	0.67
6:I:225:ILE:O	6:I:229:VAL:HG23	1.95	0.67
6:N:46:GLU:HG3	6:N:206:ILE:HG21	1.76	0.67
7:Q:120:HIS:NE2	8:R:86:ASP:OD1	2.23	0.67
9:Z:57:ASP:OD2	10:b:38:LYS:HE2	1.95	0.67
14:a:25:ASP:OD1	14:a:41:ARG:NH2	2.28	0.67
5:H:38:ILE:HD11	5:H:177:ALA:HB1	1.77	0.67
5:M:38:ILE:HD11	5:M:177:ALA:HB1	1.77	0.67
6:N:225:ILE:O	6:N:229:VAL:HG23	1.95	0.67
8:R:21:ARG:NH2	8:R:26:GLU:OE1	2.28	0.67
13:U:141:CYS:HB3	13:U:177:ASP:OD2	1.94	0.67
1:A:63:LEU:HD21	1:A:79:ALA:HA	1.77	0.67
1:F:63:LEU:HD21	1:F:79:ALA:HA	1.77	0.67
6:N:146:GLN:OE1	6:N:159:ASN:ND2	2.28	0.67
2:E:44:CYS:HB2	2:E:99:ILE:HG23	1.76	0.67
4:G:50:LYS:HB3	4:G:59:HIS:CB	2.25	0.67
5:H:37:ALA:HB2	5:H:50:VAL:HG23	1.77	0.67
8:K:53:GLN:NE2	8:K:206:LEU:HD21	2.10	0.67
6:N:189:LYS:O	6:N:193:LYS:CB	2.43	0.67
13:Y:112:ASP:OD2	13:Y:115:THR:N	2.23	0.67
14:a:143:ALA:HA	14:a:147:GLN:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:LEU:HG	13:Y:200:LYS:HB2	1.76	0.67
2:E:194:GLU:N	2:E:195:PRO:HD2	2.10	0.67
8:K:158:GLY:O	10:b:83:ARG:NH2	2.27	0.67
14:W:5:MET:HE3	14:W:30:TYR:HE1	1.59	0.67
10:b:8:SER:OG	10:b:122:GLN:O	2.13	0.67
1:A:37:LEU:HD11	1:A:43:CYS:HB3	1.76	0.66
4:L:84:LEU:HD23	4:L:132:LEU:HD11	1.75	0.66
11:S:96:LEU:HD11	11:S:108:ASN:HD22	1.60	0.66
4:L:229:VAL:O	4:L:233:LEU:N	2.28	0.66
1:A:4:MET:CG	1:A:126:ILE:HG22	2.23	0.66
6:I:42:VAL:HG21	6:I:188:ILE:HG12	1.76	0.66
5:M:56:SER:OG	6:N:173:GLU:OE2	2.10	0.66
9:O:44:LEU:HD22	9:O:190:LEU:HD22	1.77	0.66
10:P:67:ILE:HD11	10:P:73:LEU:HD12	1.77	0.66
3:D:96:SER:HA	3:D:116:GLU:OE1	1.96	0.66
3:D:157:ARG:O	3:D:161:ALA:CB	2.43	0.66
2:E:194:GLU:H	2:E:195:PRO:HD2	1.60	0.66
8:K:41:ALA:HB2	8:K:50:ILE:HG22	1.78	0.66
6:I:203:GLY:CA	6:I:205:ASN:HB2	2.25	0.66
6:N:195:LEU:HB3	6:N:206:ILE:CD1	2.26	0.66
9:Z:72:MET:HE1	9:Z:110:LEU:HD23	1.77	0.66
1:A:97:HIS:NE2	1:A:99:MET:HE2	2.11	0.66
2:B:40:LYS:NZ	2:B:104:ASP:OD1	2.28	0.66
1:F:80:ALA:O	1:F:84:ARG:HB2	1.96	0.66
6:I:43:LEU:C	6:I:208:LEU:CD1	2.68	0.66
6:N:221:ASN:N	6:N:222:PRO:HD3	2.11	0.66
8:R:53:GLN:NE2	8:R:206:LEU:HD21	2.10	0.66
10:b:67:ILE:HD11	10:b:73:LEU:HD12	1.77	0.66
1:A:80:ALA:O	1:A:84:ARG:HB2	1.96	0.66
3:D:35:ILE:CB	3:D:45:MET:HE2	2.25	0.66
2:E:40:LYS:NZ	2:E:104:ASP:OD1	2.28	0.66
6:I:146:GLN:OE1	6:I:159:ASN:ND2	2.28	0.66
6:I:189:LYS:O	6:I:193:LYS:CB	2.43	0.66
2:B:194:GLU:N	2:B:195:PRO:HD2	2.09	0.66
1:F:97:HIS:NE2	1:F:99:MET:HE2	2.11	0.66
14:W:25:ASP:OD1	14:W:41:ARG:NH2	2.28	0.66
1:A:91:ARG:HH12	14:W:58:ALA:HB3	1.60	0.66
1:F:51:ASP:HB3	1:F:94:LEU:HD22	1.78	0.66
14:W:143:ALA:HA	14:W:147:GLN:HB2	1.76	0.66
2:B:6:LEU:HD11	2:B:146:MET:HE1	1.78	0.66
6:I:33:VAL:HB	6:I:195:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:91:LYS:NZ	5:M:119:LEU:CD1	2.59	0.66
8:R:62:ASP:OD2	8:R:64:SER:OG	2.11	0.66
2:B:51:ASP:HB3	2:B:94:VAL:HG13	1.78	0.65
2:E:156:VAL:HG21	2:E:189:LEU:HD12	1.78	0.65
9:O:54:LYS:HE2	10:P:170:LYS:HE2	1.78	0.65
10:P:110:VAL:HG22	10:P:135:ILE:CD1	2.26	0.65
8:R:41:ALA:HB2	8:R:50:ILE:HG22	1.78	0.65
12:T:38:MET:HE3	12:T:44:LEU:HB3	1.79	0.65
9:Z:44:LEU:HB3	9:Z:215:THR:HG22	1.78	0.65
5:M:37:ALA:HB2	5:M:50:VAL:HG23	1.77	0.65
6:N:210:VAL:N	6:N:218:LYS:O	2.26	0.65
2:B:215:THR:CG2	13:Y:196:THR:HB	2.26	0.65
2:E:197:LYS:H	2:E:197:LYS:CD	2.02	0.65
2:E:197:LYS:HD3	2:E:197:LYS:N	2.02	0.65
9:O:44:LEU:HB3	9:O:215:THR:HG22	1.78	0.65
12:T:8:GLN:NE2	12:T:113:PRO:HG2	2.12	0.65
10:b:110:VAL:HG22	10:b:135:ILE:CD1	2.26	0.65
2:B:51:ASP:OD2	13:Y:98:ARG:NH2	2.22	0.65
2:E:51:ASP:HB3	2:E:94:VAL:HG13	1.78	0.65
4:G:33:SER:OG	4:G:62:LYS:NZ	2.21	0.65
4:L:79:ALA:HB3	5:M:121:LEU:HD12	1.78	0.65
6:N:46:GLU:CG	6:N:206:ILE:HG21	2.26	0.65
12:V:38:MET:HE3	12:V:44:LEU:HB3	1.79	0.65
1:A:46:SER:OG	1:A:97:HIS:HB3	1.97	0.65
10:P:8:SER:OG	10:P:122:GLN:O	2.13	0.65
12:T:138:LEU:HD11	12:V:26:VAL:HG12	1.78	0.65
11:X:26:ASP:OD2	11:X:189:THR:HA	1.96	0.65
1:A:51:ASP:HB3	1:A:94:LEU:HD22	1.78	0.65
3:C:96:SER:HA	3:C:116:GLU:OE1	1.96	0.65
2:E:6:LEU:HD11	2:E:146:MET:HE1	1.78	0.65
2:E:122:LEU:HD11	2:E:125:THR:HB	1.78	0.65
8:K:49[B]:VAL:HG21	8:K:195:VAL:CG2	2.27	0.65
8:K:176:THR:HG23	10:b:55:LEU:HD12	1.78	0.65
4:L:176:MET:HA	4:L:179:PHE:CE2	2.32	0.65
11:X:96:LEU:HD11	11:X:108:ASN:HD22	1.60	0.65
14:a:92:LEU:HD22	14:a:112:ILE:HD11	1.78	0.65
3:C:33:LYS:O	3:C:45:MET:CG	2.42	0.65
6:I:35:VAL:HG12	6:I:158:ALA:HB1	1.79	0.65
6:N:195:LEU:HB3	6:N:199:VAL:HG23	1.78	0.65
13:U:44:MET:HE3	13:U:66:LEU:HD23	1.79	0.65
3:C:17:ASP:OD1	3:C:33:LYS:NZ	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:33:VAL:HB	6:N:195:LEU:HD11	1.78	0.65
10:b:38:LYS:HD2	10:b:143:PRO:HG2	1.79	0.65
2:B:195:PRO:HG2	11:S:211:ARG:CG	2.26	0.64
8:K:162:GLY:HA3	10:b:57:ASP:HB3	1.78	0.64
14:W:91:TRP:HE3	14:W:92:LEU:HD12	1.62	0.64
2:E:193:THR:HG21	11:X:211:ARG:CZ	2.27	0.64
2:B:122:LEU:HD11	2:B:125:THR:HB	1.78	0.64
2:B:156:VAL:HG21	2:B:189:LEU:HD12	1.78	0.64
9:O:72:MET:HE1	9:O:110:LEU:HD23	1.77	0.64
9:Z:213:ILE:HB	9:Z:228:LEU:HD12	1.79	0.64
3:D:6:PHE:CE1	3:D:13:ILE:HD11	2.33	0.64
2:E:208:THR:HA	11:X:159:GLN:HB2	1.78	0.64
8:K:241:ALA:O	8:K:245:ARG:NH1	2.30	0.64
5:M:39:GLY:HA3	5:M:48:LEU:HD23	1.78	0.64
9:O:44:LEU:CD2	9:O:190:LEU:HD22	2.27	0.64
8:R:241:ALA:O	8:R:245:ARG:NH1	2.30	0.64
2:E:28:ASP:HB2	13:U:130:MET:SD	2.37	0.64
9:O:218:ARG:NH1	9:O:223:THR:OG1	2.31	0.64
9:Z:44:LEU:HD22	9:Z:190:LEU:HD22	1.77	0.64
2:B:194:GLU:H	2:B:195:PRO:HD2	1.59	0.64
2:B:204:PHE:CZ	11:S:158:MET:HE2	2.33	0.64
4:G:176:MET:HA	4:G:179:PHE:CE2	2.32	0.64
5:H:39:GLY:HA3	5:H:48:LEU:HD23	1.78	0.64
9:O:213:ILE:HB	9:O:228:LEU:HD12	1.79	0.64
7:Q:28:LYS:HA	7:Q:31:GLU:HG2	1.80	0.64
14:a:72:ILE:O	14:a:76:LEU:HG	1.98	0.64
4:G:56:LEU:HD13	5:H:167:ALA:HB3	1.79	0.64
10:P:38:LYS:HD2	10:P:143:PRO:HG2	1.80	0.64
14:W:92:LEU:HD22	14:W:112:ILE:HD11	1.78	0.64
9:Z:44:LEU:CD2	9:Z:190:LEU:HD22	2.27	0.64
9:Z:218:ARG:NH1	9:Z:223:THR:OG1	2.31	0.64
1:F:46:SER:OG	1:F:97:HIS:HB3	1.97	0.64
6:N:35:VAL:HG12	6:N:158:ALA:HB1	1.79	0.64
13:Y:44:MET:HE3	13:Y:66:LEU:HD23	1.79	0.64
14:a:96:MET:CE	14:a:127:MET:HA	2.28	0.64
9:Z:72:MET:HG2	9:Z:138:GLY:HA3	1.79	0.64
4:L:50:LYS:HB3	4:L:59:HIS:CB	2.27	0.64
8:R:182:LYS:HD3	8:R:197:THR:HG23	1.80	0.64
11:S:26:ASP:OD2	11:S:189:THR:HA	1.96	0.64
3:C:6:PHE:CE1	3:C:13:ILE:HD11	2.33	0.63
6:N:31:THR:OG1	6:N:163:ARG:O	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:111:VAL:HG21	9:O:148:TYR:HD2	1.63	0.63
7:Q:34:SER:OG	7:Q:65:ARG:NH1	2.28	0.63
13:Y:17:ASN:HA	13:Y:118:PRO:HG3	1.79	0.63
3:D:17:ASP:OD1	3:D:33:LYS:NZ	2.28	0.63
1:F:126:ILE:HD11	1:F:135:TYR:CD1	2.34	0.63
6:I:7:ILE:HG23	9:Z:11:ILE:HG22	1.79	0.63
6:I:87:ALA:HB2	6:I:111:ILE:HD11	1.79	0.63
9:O:72:MET:HG2	9:O:138:GLY:HA3	1.78	0.63
15:C:301:BZ7:CAV	11:X:131:GLN:CD	2.71	0.63
7:J:53:VAL:HG12	7:J:208:ALA:O	1.98	0.63
6:N:53:LEU:HD13	9:O:161:ALA:O	1.98	0.63
12:V:8:GLN:NE2	12:V:113:PRO:HG2	2.11	0.63
1:F:135:TYR:CE2	14:a:33:LEU:HD21	2.32	0.63
4:G:47:VAL:HG12	4:G:195:LEU:HD22	1.80	0.63
7:Q:50:GLU:OE2	7:Q:201:HIS:ND1	2.26	0.63
12:T:121:LEU:HD12	13:U:5:TYR:CE2	2.34	0.63
3:C:7:LYS:CB	3:C:12:VAL:HG22	2.27	0.63
3:D:97:MET:H	3:D:116:GLU:HB3	1.64	0.63
4:L:47:VAL:HG12	4:L:195:LEU:HD22	1.80	0.63
5:M:91:LYS:HZ3	5:M:119:LEU:HD11	1.59	0.63
6:N:87:ALA:HB2	6:N:111:ILE:HD11	1.79	0.63
9:O:33:THR:OG1	9:O:163:CYS:SG	2.57	0.63
10:P:21:ILE:HG21	10:P:151:SER:HB3	1.81	0.63
10:P:45:LEU:O	10:P:210:GLY:N	2.23	0.63
14:W:96:MET:CE	14:W:127:MET:HA	2.28	0.63
2:B:17:ASP:OD1	2:B:33:LYS:NZ	2.31	0.63
3:C:97:MET:H	3:C:116:GLU:HB3	1.64	0.63
2:E:17:ASP:OD1	2:E:33:LYS:NZ	2.31	0.63
4:G:82:ARG:NH2	5:H:160:GLY:O	2.32	0.63
7:J:28:LYS:HA	7:J:31:GLU:HG2	1.80	0.63
5:M:91:LYS:HZ2	5:M:119:LEU:HD11	1.63	0.63
6:N:203:GLY:CA	6:N:229:VAL:HG22	2.19	0.63
9:Z:33:THR:OG1	9:Z:163:CYS:SG	2.57	0.63
1:A:126:ILE:HD11	1:A:135:TYR:CD1	2.34	0.63
3:C:31:VAL:CG1	15:C:301:BZ7:CBK	2.76	0.63
1:F:18:SER:OG	1:F:172:VAL:N	2.27	0.63
4:L:18[B]:ARG:HG2	4:L:23:GLU:OE2	1.98	0.63
2:E:44:CYS:HB2	2:E:99:ILE:CG2	2.29	0.63
2:E:107:GLY:O	2:E:109:GLN:HG3	1.98	0.63
2:E:206:PRO:HA	13:U:164:GLU:OE2	1.98	0.63
6:I:42:VAL:HG12	6:I:208:LEU:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:74:GLU:O	8:R:226:LYS:HA	1.99	0.63
8:R:80[A]:MET:HE2	8:R:91:VAL:CG2	2.29	0.63
12:T:16:ALA:HB2	12:T:160:LEU:HD21	1.81	0.63
9:Z:111:VAL:HG21	9:Z:148:TYR:HD2	1.63	0.63
2:B:44:CYS:HB2	2:B:99:ILE:CG2	2.29	0.62
2:B:152:GLN:HE21	2:B:189:LEU:HD21	1.64	0.62
8:K:74:GLU:O	8:K:226:LYS:HA	1.99	0.62
5:M:48:LEU:O	5:M:217:LEU:HD12	1.99	0.62
9:O:48:GLU:HG3	9:O:201:MET:HE3	1.81	0.62
7:J:33:SER:HB2	7:J:79:GLY:HA2	1.80	0.62
13:Y:33:MET:HE2	13:Y:182:MET:CE	2.30	0.62
3:C:125:MET:CE	3:C:139:MET:HE2	2.30	0.62
3:D:7:LYS:CB	3:D:12:VAL:HG22	2.27	0.62
3:D:88:CYS:O	3:D:91:ARG:HG3	1.99	0.62
1:F:115:LEU:O	1:F:118:MET:HG2	1.99	0.62
4:G:50:LYS:CB	4:G:59:HIS:CB	2.77	0.62
6:N:192:ILE:HD11	6:N:208:LEU:HD23	1.81	0.62
7:Q:53:VAL:HG12	7:Q:208:ALA:O	1.98	0.62
9:Z:111:VAL:HG22	9:Z:136:TYR:HD2	1.64	0.62
14:a:91:TRP:HE3	14:a:92:LEU:HD12	1.62	0.62
7:J:6:GLY:HA2	7:J:8:ASP:H	1.65	0.62
1:F:152:ARG:HG3	1:F:175:LEU:HD13	1.82	0.62
8:R:217:VAL:CG1	8:R:230:LEU:HD12	2.29	0.62
3:D:58:LEU:HD12	3:D:61:LYS:HE3	1.82	0.62
1:F:20:VAL:HG22	1:F:28:ASN:HB3	1.82	0.62
4:G:61:LYS:HE3	4:G:64:LEU:HD21	1.81	0.62
5:H:48:LEU:O	5:H:217:LEU:HD12	1.99	0.62
8:K:41:ALA:CB	8:K:50:ILE:HG22	2.29	0.62
4:L:18[A]:ARG:HD2	4:L:23:GLU:OE2	1.99	0.62
6:N:46:GLU:HA	6:N:206:ILE:HB	1.80	0.62
11:S:123:SER:CB	11:S:136:LYS:HG2	2.30	0.62
11:X:27:THR:OG1	11:X:192:ALA:HB3	2.00	0.62
13:Y:11:MET:HE3	13:Y:170:MET:SD	2.40	0.62
1:A:18:SER:OG	1:A:172:VAL:N	2.26	0.62
2:B:63:MET:CE	2:B:74:PRO:HB3	2.30	0.62
8:R:41:ALA:CB	8:R:50:ILE:HG22	2.29	0.62
10:b:21:ILE:HG21	10:b:151:SER:HB3	1.81	0.62
1:A:190:GLY:HA2	1:A:193:LEU:HD13	1.81	0.62
3:C:58:LEU:HD12	3:C:61:LYS:HE3	1.82	0.62
15:D:301:BZ7:CAV	11:S:131:GLN:NE2	2.62	0.62
8:K:217:VAL:CG1	8:K:230:LEU:HD12	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:41:GLN:NE2	5:M:151:PRO:O	2.32	0.62
2:B:107:GLY:O	2:B:109:GLN:HG3	1.98	0.62
3:C:88:CYS:O	3:C:91:ARG:HG3	1.99	0.62
8:K:182:LYS:HD3	8:K:197:THR:HG23	1.80	0.62
7:Q:19:ARG:NE	7:Q:24:GLU:OE2	2.31	0.62
8:R:110:PRO:HB2	8:R:112:ASP:OD1	2.00	0.62
14:W:72:ILE:O	14:W:76:LEU:HG	1.98	0.62
5:H:202:LEU:HA	5:H:205:VAL:HG22	1.82	0.62
9:O:111:VAL:HG22	9:O:136:TYR:HD2	1.64	0.62
13:Y:49:TYR:HD2	13:Y:189:ILE:HD11	1.64	0.62
1:A:42:TYR:HD2	1:A:176:VAL:HG21	1.65	0.61
2:E:164:LEU:O	11:X:38:ARG:NH2	2.32	0.61
5:H:41:GLN:NE2	5:H:151:PRO:O	2.32	0.61
9:O:44:LEU:CB	9:O:215:THR:HG22	2.30	0.61
7:Q:6:GLY:HA2	7:Q:8:ASP:H	1.65	0.61
13:U:49:TYR:HD2	13:U:189:ILE:HD11	1.64	0.61
1:F:42:TYR:HD2	1:F:176:VAL:HG21	1.65	0.61
1:F:190:GLY:HA2	1:F:193:LEU:HD13	1.81	0.61
8:K:110:PRO:HB2	8:K:112:ASP:OD1	2.00	0.61
7:Q:137:LEU:O	7:Q:148:LEU:HD12	2.00	0.61
8:R:80[B]:MET:HG3	8:R:87:SER:HB3	1.80	0.61
11:S:27:THR:OG1	11:S:192:ALA:HB3	2.00	0.61
10:b:212:CYS:HB2	10:b:217:PHE:HD1	1.65	0.61
3:D:77:SER:HA	3:D:112:TYR:HE2	1.65	0.61
6:I:40:ILE:HD11	6:I:210:VAL:HG13	1.82	0.61
5:M:202:LEU:HA	5:M:205:VAL:HG22	1.82	0.61
6:N:33:VAL:HG22	6:N:160:ALA:CB	2.30	0.61
11:S:145:LEU:HD22	11:S:178:VAL:HB	1.83	0.61
13:Y:122:SER:HB3	13:Y:136:VAL:HB	1.81	0.61
9:Z:28:ILE:HD11	9:Z:132:VAL:N	2.16	0.61
9:Z:111:VAL:HG21	9:Z:148:TYR:CD2	2.35	0.61
10:b:207:ILE:CD1	10:b:229:LEU:HD21	2.30	0.61
1:A:77:LEU:HA	1:A:112:TYR:HE2	1.66	0.61
4:G:229:VAL:HG21	4:G:233:LEU:HD12	1.78	0.61
9:O:28:ILE:HD11	9:O:132:VAL:N	2.16	0.61
13:U:33:MET:HE2	13:U:182:MET:CE	2.29	0.61
12:V:1[A]:MET:H3	12:V:173:LEU:HD13	1.64	0.61
11:X:123:SER:CB	11:X:136:LYS:HG2	2.30	0.61
9:Z:48:GLU:HG3	9:Z:201:MET:HE3	1.81	0.61
9:Z:90:LEU:HD21	9:Z:114:LEU:HD22	1.82	0.61
2:E:63:MET:CE	2:E:74:PRO:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:50:LYS:O	4:G:59:HIS:CB	2.48	0.61
13:U:11:MET:HE3	13:U:170:MET:SD	2.40	0.61
14:a:124:TYR:HE1	14:a:139:THR:HG22	1.66	0.61
3:D:125:MET:CE	3:D:139:MET:HE2	2.30	0.61
10:P:212:CYS:HB2	10:P:217:PHE:HD1	1.65	0.61
12:T:182:ILE:CG2	12:T:189:HIS:HB2	2.31	0.61
3:D:49:ALA:CB	15:D:301:BZ7:CBN	2.75	0.61
1:F:4:MET:CG	1:F:126:ILE:HG22	2.23	0.61
6:N:132:LEU:HD11	6:N:161:ILE:HG23	1.82	0.61
7:Q:33:SER:HB2	7:Q:79:GLY:HA2	1.80	0.61
12:V:182:ILE:CG2	12:V:189:HIS:HB2	2.31	0.61
1:A:20:VAL:HG22	1:A:28:ASN:HB3	1.82	0.61
1:A:152:ARG:HG3	1:A:175:LEU:HD13	1.81	0.61
2:E:4:ALA:HA	2:E:126:ALA:HA	1.83	0.61
8:K:157:ALA:O	10:b:80:PRO:HG2	2.01	0.61
12:V:16:ALA:HB2	12:V:160:LEU:HD21	1.81	0.61
12:V:16:ALA:HB2	12:V:180:VAL:HG22	1.83	0.61
14:a:127:MET:HG3	14:a:128:LEU:HG	1.83	0.61
10:b:209:VAL:CG1	10:b:220:LEU:HD12	2.31	0.61
3:C:77:SER:HA	3:C:112:TYR:HE2	1.65	0.61
3:D:40:TYR:HB3	3:D:183:GLY:CA	2.30	0.61
9:O:90:LEU:HD21	9:O:114:LEU:HD22	1.82	0.61
9:O:111:VAL:HG21	9:O:148:TYR:CD2	2.35	0.61
13:U:55:LEU:O	13:U:59:VAL:HG23	2.01	0.61
14:W:124:TYR:HE1	14:W:139:THR:HG22	1.66	0.61
13:Y:92:ASN:HD22	10:b:99:VAL:HG13	1.65	0.61
2:B:76:VAL:HG12	2:B:104:ASP:OD2	2.01	0.61
6:I:210:VAL:O	6:I:218:LYS:N	2.28	0.61
7:J:37:ILE:HD11	7:J:193:VAL:HG13	1.81	0.61
6:N:208:LEU:HD12	6:N:209:ALA:N	2.16	0.61
13:Y:163:PHE:O	13:Y:167:SER:OG	2.11	0.61
9:Z:44:LEU:CB	9:Z:215:THR:HG22	2.30	0.61
5:H:111:SER:OG	11:X:79:ASN:OD1	2.06	0.60
6:I:71:MET:HB3	6:I:133:ILE:HG12	1.83	0.60
11:S:150:ASP:OD2	13:Y:176:ARG:NE	2.22	0.60
13:U:122:SER:HB3	13:U:136:VAL:HB	1.81	0.60
3:C:40:TYR:CB	3:C:179:MET:HE1	2.25	0.60
2:E:152:GLN:HE21	2:E:189:LEU:HD21	1.64	0.60
6:I:33:VAL:HG22	6:I:160:ALA:CB	2.30	0.60
6:I:63:CYS:HB3	6:I:88:ARG:HH21	1.65	0.60
7:J:19:ARG:NE	7:J:24:GLU:OE2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:152[A]:ASN:OD1	7:Q:85:ARG:NH1	2.29	0.60
7:Q:37:ILE:HD11	7:Q:193:VAL:HG13	1.81	0.60
7:Q:75:MET:HE3	7:Q:135:PHE:CD2	2.36	0.60
3:D:40:TYR:CB	3:D:179:MET:HE1	2.25	0.60
2:E:76:VAL:HG12	2:E:104:ASP:OD2	2.01	0.60
1:F:77:LEU:HA	1:F:112:TYR:HE2	1.66	0.60
7:J:34:SER:OG	7:J:65:ARG:NH1	2.28	0.60
10:b:45:LEU:O	10:b:210:GLY:N	2.24	0.60
6:I:46:GLU:O	6:I:48:LYS:HA	2.02	0.60
7:J:137:LEU:O	7:J:148:LEU:HD12	2.00	0.60
3:C:16:VAL:HG21	3:C:34:VAL:HG23	1.83	0.60
4:G:230:SER:HB2	4:G:231:PRO:HD3	1.83	0.60
5:M:91:LYS:HZ2	5:M:119:LEU:CD1	2.15	0.60
11:X:145:LEU:HD22	11:X:178:VAL:HB	1.83	0.60
6:I:208:LEU:CD2	6:I:209:ALA:C	2.63	0.60
6:I:210:VAL:N	6:I:218:LYS:O	2.26	0.60
8:K:161:CYS:SG	8:K:163:PHE:HZ	2.14	0.60
6:N:46:GLU:O	6:N:48:LYS:HA	2.02	0.60
13:Y:55:LEU:O	13:Y:59:VAL:HG23	2.01	0.60
1:F:36:PRO:HB3	1:F:42:TYR:HE1	1.67	0.60
4:G:72:ILE:HG22	4:G:134:ILE:HG12	1.84	0.60
4:G:107:ARG:NH2	14:W:81:HIS:O	2.35	0.60
7:J:228:PRO:HG2	7:J:231:ILE:HD12	1.83	0.60
4:L:61:LYS:HE3	4:L:64:LEU:HD21	1.84	0.60
9:O:107:CYS:O	9:O:111:VAL:HG23	2.02	0.60
11:X:141:ALA:HB2	11:X:186:ASP:OD2	2.01	0.60
13:Y:148:MET:HE2	13:Y:172:ASN:HB2	1.83	0.60
3:C:40:TYR:HB3	3:C:183:GLY:CA	2.30	0.60
7:J:75:MET:HE3	7:J:135:PHE:CD2	2.36	0.60
7:J:80:LEU:HD23	7:J:83:ASP:OD2	2.02	0.60
7:J:229:LYS:NZ	7:J:233:GLU:OE2	2.19	0.60
6:N:199:VAL:HG11	6:N:206:ILE:HG12	1.84	0.60
7:Q:228:PRO:HG2	7:Q:231:ILE:HD12	1.83	0.60
9:Z:107:CYS:O	9:Z:111:VAL:HG23	2.02	0.60
10:b:138:TRP:CD1	10:b:214:GLU:HA	2.37	0.60
1:A:11:GLY:HA3	1:A:178:ILE:O	2.02	0.60
1:A:114:THR:HA	1:A:118:MET:O	2.02	0.60
2:B:4:ALA:HA	2:B:126:ALA:HA	1.83	0.60
3:C:70:ASN:OD1	6:I:109:ARG:NH2	2.35	0.60
4:G:26:MET:HA	4:G:149:PRO:HG2	1.84	0.60
6:I:132:LEU:HD11	6:I:161:ILE:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:212:PRO:O	8:K:232:GLU:HG3	2.02	0.60
10:P:209:VAL:CG1	10:P:220:LEU:HD12	2.31	0.60
8:R:212:PRO:O	8:R:232:GLU:HG3	2.02	0.60
11:S:141:ALA:HB2	11:S:186:ASP:OD2	2.01	0.60
1:A:81:ASN:ND2	7:J:103:GLY:HA3	2.17	0.60
4:G:184:LEU:HD11	4:G:214:ILE:HG21	1.83	0.60
7:J:150:MET:HG3	7:J:163:CYS:SG	2.42	0.60
4:L:50:LYS:CB	4:L:59:HIS:HB3	2.32	0.60
4:L:196:ARG:NH1	4:L:236:LEU:O	2.34	0.60
6:N:71:MET:HB3	6:N:133:ILE:HG12	1.83	0.60
12:T:16:ALA:HB2	12:T:180:VAL:HG22	1.83	0.60
9:Z:57:ASP:HB2	10:b:157:TRP:C	2.27	0.60
3:D:28:ALA:CB	11:S:131:GLN:HE22	2.13	0.59
2:E:81:ARG:HD3	8:R:103:TYR:O	2.02	0.59
6:I:43:LEU:C	6:I:208:LEU:HD11	2.27	0.59
6:N:195:LEU:CB	6:N:206:ILE:HD11	2.33	0.59
9:O:136:TYR:O	9:O:147:LEU:HD12	2.02	0.59
12:V:121:LEU:O	13:Y:57:THR:HB	2.02	0.59
1:F:67:GLY:HA2	1:F:74:PRO:HG3	1.85	0.59
4:L:57:ALA:HA	5:M:165:CYS:HA	1.83	0.59
4:L:72:ILE:HG22	4:L:134:ILE:HG12	1.84	0.59
14:W:11:VAL:O	14:W:138:ALA:HA	2.03	0.59
4:G:10:VAL:HG13	4:G:11:THR:HG23	1.84	0.59
4:G:228:ASP:O	4:G:231:PRO:HD2	2.02	0.59
6:I:88:ARG:HH11	12:V:70:ARG:HA	1.67	0.59
4:L:229:VAL:CG2	4:L:233:LEU:HD12	2.32	0.59
6:N:40:ILE:HD11	6:N:210:VAL:HG13	1.82	0.59
7:Q:150:MET:HG3	7:Q:163:CYS:SG	2.42	0.59
1:A:197:TYR:CZ	1:A:199:GLU:HB2	2.37	0.59
2:B:28:ASP:OD1	2:B:29:LYS:N	2.35	0.59
1:F:11:GLY:HA3	1:F:178:ILE:O	2.02	0.59
1:A:67:GLY:HA2	1:A:74:PRO:HG3	1.84	0.59
2:B:40:LYS:HD2	2:B:41:ILE:HG13	1.84	0.59
2:E:43:CYS:SG	2:E:98:LEU:HD22	2.42	0.59
1:F:8:PHE:HE1	1:F:13:VAL:HG23	1.66	0.59
6:I:220:LEU:HB2	6:I:225:ILE:HD11	1.84	0.59
8:R:208:ILE:HD12	8:R:210:PHE:HE1	1.67	0.59
10:b:47:THR:HB	10:b:74:VAL:HG21	1.83	0.59
2:B:131:GLN:O	2:B:135:LEU:HB2	2.03	0.59
3:C:134:TYR:HE1	12:T:137:PHE:HA	1.67	0.59
5:H:168:ARG:HD2	5:H:178:GLN:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:178:TYR:OH	14:a:208:ASN:N	2.26	0.59
1:A:8:PHE:HE1	1:A:13:VAL:HG23	1.66	0.59
3:D:16:VAL:HG21	3:D:34:VAL:HG23	1.83	0.59
1:F:197:TYR:CZ	1:F:199:GLU:HB2	2.37	0.59
6:N:68:ASN:OD1	6:N:69:VAL:HG23	2.03	0.59
10:P:47:THR:HB	10:P:74:VAL:HG21	1.83	0.59
12:V:2:GLU:HA	12:V:18:ASP:OD2	2.03	0.59
14:W:127:MET:HG3	14:W:128:LEU:HG	1.83	0.59
1:A:115:LEU:HD12	1:A:115:LEU:C	2.27	0.59
10:P:138:TRP:CD1	10:P:214:GLU:HA	2.37	0.59
7:Q:37:ILE:C	7:Q:136:MET:HE1	2.28	0.59
13:U:148:MET:HE2	13:U:172:ASN:HB2	1.83	0.59
9:Z:69:ASN:OD1	9:Z:71:ASP:N	2.31	0.59
1:A:189:LEU:HD22	14:a:209:TRP:HB2	1.85	0.59
2:B:25:VAL:HG13	11:S:144:MET:HE1	1.83	0.59
2:B:132:ASP:CG	14:a:144:TYR:HB3	2.28	0.59
2:E:28:ASP:OD1	2:E:29:LYS:N	2.35	0.59
1:F:24:GLU:HG3	14:W:182:ARG:HG2	1.85	0.59
1:F:42:TYR:OH	1:F:183:VAL:HG11	2.03	0.59
4:L:155:ASP:OD2	7:Q:59:GLU:HG3	2.03	0.59
5:M:168:ARG:HD2	5:M:178:GLN:OE1	2.03	0.59
10:P:57:ASP:HB3	8:R:162:GLY:CA	2.30	0.59
9:Z:136:TYR:O	9:Z:147:LEU:HD12	2.02	0.59
1:F:156:THR:OG1	1:F:175:LEU:HD11	2.03	0.59
5:H:113:THR:O	5:H:117:SER:HB3	2.03	0.59
7:J:50:GLU:OE2	7:J:201:HIS:ND1	2.26	0.59
4:L:26:MET:HA	4:L:149:PRO:HG2	1.84	0.59
6:N:47:LYS:HA	6:N:205:ASN:C	2.27	0.59
10:P:99:VAL:HG13	13:U:92:ASN:HD22	1.67	0.59
12:V:182:ILE:HG22	12:V:189:HIS:HB2	1.85	0.59
3:C:31:VAL:CG1	15:C:301:BZ7:CBJ	2.80	0.58
1:F:114:THR:HA	1:F:118:MET:O	2.02	0.58
8:K:53:GLN:OE1	8:K:55:LYS:HE3	2.03	0.58
5:M:47:CYS:CA	5:M:219:THR:HG22	2.33	0.58
6:N:199:VAL:HG22	6:N:206:ILE:HD13	1.80	0.58
10:P:198:PHE:HB2	10:P:202:MET:HE3	1.85	0.58
7:Q:90:ILE:HG13	7:Q:118:TYR:CE2	2.38	0.58
1:F:3:ILE:HD13	1:F:45:LEU:O	2.03	0.58
1:F:133:PHE:CZ	14:W:33:LEU:HD13	2.38	0.58
6:N:88:ARG:NH1	12:T:70:ARG:HA	2.18	0.58
10:P:28:VAL:HG11	10:P:132:SER:OG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:25:ASP:HA	14:a:187:PHE:CA	2.33	0.58
1:A:3:ILE:HD13	1:A:45:LEU:O	2.04	0.58
3:D:154:ASP:O	3:D:158:ARG:HG2	2.03	0.58
8:K:43:ARG:NH1	8:K:149:PRO:O	2.37	0.58
8:K:208:ILE:HD12	8:K:210:PHE:HE1	1.67	0.58
4:L:184:LEU:HD11	4:L:214:ILE:HG21	1.84	0.58
13:Y:19:VAL:HG13	13:Y:118:PRO:HB3	1.85	0.58
1:A:36:PRO:HB3	1:A:42:TYR:HE1	1.67	0.58
2:B:43:CYS:SG	2:B:98:LEU:HD22	2.42	0.58
3:C:164:THR:HG22	3:C:170:SER:CB	2.33	0.58
3:D:45:MET:HB3	3:D:52:CYS:CB	2.34	0.58
2:E:131:GLN:O	2:E:135:LEU:HB2	2.03	0.58
1:F:99:MET:SD	1:F:113:GLY:HA2	2.44	0.58
4:G:124:GLY:HA3	5:H:126:GLU:CD	2.29	0.58
6:N:85:ASN:OD1	12:T:70:ARG:NH1	2.37	0.58
11:S:146:GLN:HB3	11:S:147:PRO:HD3	1.86	0.58
14:W:178:TYR:OH	14:W:208:ASN:N	2.26	0.58
9:Z:28:ILE:HD13	9:Z:133:SER:OG	2.03	0.58
2:E:148:LEU:HD11	2:E:177:VAL:CG1	2.33	0.58
5:H:47:CYS:CA	5:H:219:THR:HG22	2.33	0.58
6:I:47:LYS:CB	6:I:205:ASN:HA	2.33	0.58
6:N:195:LEU:CB	6:N:206:ILE:CD1	2.82	0.58
7:Q:80:LEU:HD23	7:Q:83:ASP:OD2	2.02	0.58
13:U:19:VAL:HG13	13:U:118:PRO:HB3	1.85	0.58
2:B:148:LEU:HD11	2:B:177:VAL:CG1	2.32	0.58
4:G:196:ARG:HB2	4:G:205:LEU:CD1	2.34	0.58
6:I:68:ASN:OD1	6:I:69:VAL:HG23	2.03	0.58
4:L:50:LYS:CB	4:L:59:HIS:CB	2.81	0.58
12:T:2:GLU:HG2	12:T:34:LYS:HE2	1.86	0.58
3:C:154:ASP:O	3:C:158:ARG:HG2	2.03	0.58
3:D:81:LYS:HD3	6:N:99:GLU:OE2	2.04	0.58
2:E:40:LYS:HD2	2:E:41:ILE:HG13	1.84	0.58
7:J:90:ILE:HG13	7:J:118:TYR:CE2	2.38	0.58
12:V:2:GLU:HG2	12:V:34:LYS:HE2	1.86	0.58
14:W:25:ASP:HA	14:W:187:PHE:CA	2.33	0.58
14:W:50:MET:HE2	14:W:192:VAL:CG1	2.34	0.58
9:Z:118:LYS:O	9:Z:122:THR:HG23	2.03	0.58
3:C:35:ILE:HB	3:C:45:MET:CE	2.34	0.58
8:K:50:ILE:CG2	8:K:141:ILE:HD13	2.31	0.58
9:O:118:LYS:O	9:O:122:THR:HG23	2.03	0.58
14:a:11:VAL:O	14:a:138:ALA:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:28:VAL:HG11	10:b:132:SER:OG	2.03	0.58
1:A:42:TYR:OH	1:A:183:VAL:HG11	2.03	0.58
4:L:10:VAL:HG13	4:L:11:THR:HG23	1.84	0.58
8:R:50:ILE:CG2	8:R:141:ILE:HD13	2.31	0.58
13:U:154:GLU:H	13:U:157:MET:HE2	1.68	0.58
11:X:146:GLN:HB3	11:X:147:PRO:HD3	1.86	0.58
10:b:48:GLU:HG3	10:b:198:PHE:CE1	2.39	0.58
1:A:1:THR:HA	1:A:33:LYS:NZ	2.19	0.58
1:A:97:HIS:HE1	14:W:35:ARG:HH22	1.50	0.58
5:H:189:MET:HE2	5:H:194:ALA:CA	2.34	0.58
4:L:56:LEU:HD13	5:M:167:ALA:HB3	1.85	0.58
4:L:79:ALA:HB3	5:M:121:LEU:CD1	2.33	0.58
6:N:35:VAL:HG12	6:N:158:ALA:CB	2.34	0.58
8:R:228:ARG:HH12	8:R:230:LEU:HD23	1.69	0.58
14:a:50:MET:HE2	14:a:192:VAL:CG1	2.34	0.58
1:A:156:THR:OG1	1:A:175:LEU:HD11	2.03	0.57
3:D:47:GLY:O	15:D:301:BZ7:CBA	2.52	0.57
4:L:225:ASP:N	4:L:228:ASP:HB2	2.19	0.57
6:N:137:ASP:OD2	6:N:143:ARG:NE	2.36	0.57
11:S:176:LYS:HE2	11:S:208:VAL:HG21	1.86	0.57
12:T:182:ILE:HG22	12:T:189:HIS:HB2	1.85	0.57
2:B:18:THR:OG1	2:B:172:ASN:N	2.37	0.57
3:C:6:PHE:HA	3:C:124:ASN:O	2.04	0.57
3:C:53:GLN:NE2	15:C:301:BZ7:CBM	2.67	0.57
1:F:80:ALA:HB3	1:F:112:TYR:HD2	1.69	0.57
6:I:125:ARG:HE	9:Z:123:GLN:HA	1.69	0.57
9:O:31:ALA:HB2	9:O:78:GLY:HA2	1.85	0.57
8:R:43:ARG:NH1	8:R:149:PRO:O	2.37	0.57
12:T:1:MET:HE1	12:T:133:GLY:CA	2.34	0.57
12:V:43:LEU:HG	12:V:183:ILE:HD11	1.86	0.57
1:A:36:PRO:HB3	1:A:42:TYR:CE1	2.40	0.57
1:F:24:GLU:HB3	14:W:141:TYR:CE2	2.38	0.57
1:F:26:VAL:HG22	14:W:179:ARG:O	2.05	0.57
5:H:48:LEU:O	5:H:217:LEU:HA	2.04	0.57
8:K:228:ARG:HH12	8:K:230:LEU:HD23	1.69	0.57
5:M:189:MET:HE2	5:M:194:ALA:CA	2.34	0.57
6:N:115:LYS:O	6:N:119:THR:HG23	2.04	0.57
9:O:28:ILE:HD13	9:O:133:SER:OG	2.04	0.57
11:S:28:ARG:NE	11:S:191:ASP:OD2	2.25	0.57
12:T:164:LEU:HD22	12:T:178:PHE:CE2	2.39	0.57
10:b:178:ASN:OD1	10:b:181:LEU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:198:PHE:HB2	10:b:202:MET:HE3	1.85	0.57
2:B:14:LEU:O	2:B:175:ALA:HA	2.04	0.57
2:E:14:LEU:O	2:E:175:ALA:HA	2.04	0.57
4:G:207:THR:O	4:G:226:ASP:HA	2.04	0.57
6:I:158:ALA:CB	6:I:172:LEU:HD13	2.34	0.57
7:J:37:ILE:C	7:J:136:MET:HE1	2.28	0.57
6:N:158:ALA:CB	6:N:172:LEU:HD13	2.34	0.57
6:N:195:LEU:HB3	6:N:199:VAL:HG21	1.83	0.57
7:Q:64:LYS:NZ	7:Q:212:GLU:OE2	2.38	0.57
11:X:158:MET:SD	11:X:161:VAL:HG21	2.44	0.57
1:A:99:MET:SD	1:A:113:GLY:HA2	2.44	0.57
3:C:18:SER:HG	3:C:173:VAL:H	1.51	0.57
6:I:35:VAL:HG12	6:I:158:ALA:CB	2.34	0.57
4:L:196:ARG:HB2	4:L:205:LEU:CD1	2.34	0.57
8:R:153:LYS:O	8:R:160:TYR:HA	2.04	0.57
1:A:37:LEU:HD11	1:A:43:CYS:SG	2.45	0.57
2:B:25:VAL:CG1	11:S:144:MET:HE1	2.34	0.57
2:B:59:VAL:HG21	2:B:83:LEU:CD2	2.35	0.57
2:B:63:MET:HE3	2:B:74:PRO:HB3	1.86	0.57
3:D:47:GLY:O	15:D:301:BZ7:NAZ	2.37	0.57
3:D:103:GLY:C	3:D:179:MET:HE2	2.30	0.57
1:F:3:ILE:HD12	1:F:44:ALA:CB	2.35	0.57
1:F:36:PRO:HB3	1:F:42:TYR:CE1	2.40	0.57
6:I:42:VAL:CG1	6:I:208:LEU:CD1	2.82	0.57
2:E:37:ILE:HB	2:E:41:ILE:O	2.05	0.57
1:F:37:LEU:HD11	1:F:43:CYS:SG	2.45	0.57
8:K:33:ASN:OD1	8:K:170:VAL:HA	2.05	0.57
13:U:13:MET:HE3	13:U:162:LEU:CD1	2.34	0.57
12:V:38:MET:HE3	12:V:44:LEU:CB	2.35	0.57
9:Z:27:ALA:HB2	10:b:16:GLY:O	2.04	0.57
10:b:105:PRO:HA	10:b:139:ASN:ND2	2.17	0.57
3:D:40:TYR:OH	3:D:73:ARG:HG2	2.05	0.57
6:I:187:THR:O	6:I:190:LEU:HB3	2.05	0.57
4:L:230:SER:CB	4:L:231:PRO:HD3	2.33	0.57
12:T:2:GLU:HA	12:T:18:ASP:OD2	2.03	0.57
12:T:3:TYR:OH	12:T:5:ILE:HD12	2.05	0.57
12:T:26:VAL:HG11	12:V:138:LEU:HD21	1.85	0.57
12:V:3:TYR:OH	12:V:5:ILE:HD12	2.05	0.57
12:V:114:ALA:HB1	12:V:126:LYS:HE2	1.87	0.57
9:Z:31:ALA:HB2	9:Z:78:GLY:HA2	1.85	0.57
2:B:111:TYR:HE1	2:B:121:ARG:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:ALA:HB2	3:C:176:MET:HE2	1.86	0.57
3:D:9:GLN:HG2	3:D:145:PRO:O	2.05	0.57
6:I:115:LYS:O	6:I:119:THR:HG23	2.04	0.57
12:V:164:LEU:HD22	12:V:178:PHE:CE2	2.39	0.57
3:C:40:TYR:OH	3:C:73:ARG:HG2	2.05	0.57
2:E:59:VAL:HG21	2:E:83:LEU:CD2	2.35	0.57
5:H:220:VAL:HG22	5:H:226:PHE:HA	1.87	0.57
6:I:43:LEU:HD11	6:I:134:VAL:HG22	1.87	0.57
8:K:18:PRO:HA	10:b:23:TYR:CE1	2.40	0.57
8:K:47:CYS:CB	8:K:221:THR:HG22	2.33	0.57
4:L:38:LEU:HG	4:L:187:LEU:HD11	1.87	0.57
12:T:85:ARG:NH1	12:T:89:ALA:HB2	2.20	0.57
14:W:177:TYR:CE2	14:W:207:THR:HG21	2.40	0.57
9:Z:49:ARG:HD3	9:Z:212:GLU:CD	2.30	0.57
1:A:188:ILE:HG22	1:A:193:LEU:HD12	1.87	0.56
2:B:156:VAL:O	2:B:160:THR:OG1	2.23	0.56
3:D:6:PHE:HA	3:D:124:ASN:O	2.04	0.56
3:D:15:ALA:HB2	3:D:176:MET:HE2	1.86	0.56
3:D:18:SER:HG	3:D:173:VAL:H	1.51	0.56
2:E:13:ILE:HD12	2:E:177:VAL:HG22	1.87	0.56
4:G:225:ASP:N	4:G:228:ASP:HB2	2.19	0.56
6:I:137:ASP:OD2	6:I:143:ARG:NE	2.36	0.56
8:K:47:CYS:HB3	8:K:221:THR:HA	1.87	0.56
5:M:48:LEU:O	5:M:217:LEU:HA	2.04	0.56
5:M:169:ALA:O	5:M:174:SER:HB2	2.05	0.56
10:P:48:GLU:HG3	10:P:198:PHE:CE1	2.39	0.56
12:T:35:MET:HE2	12:T:45:LEU:CD2	2.35	0.56
13:Y:32:GLN:O	13:Y:34:VAL:HG23	2.05	0.56
9:Z:133:SER:C	9:Z:134:LEU:HD12	2.31	0.56
1:A:3:ILE:HD12	1:A:44:ALA:CB	2.35	0.56
3:D:40:TYR:CB	3:D:183:GLY:HA2	2.35	0.56
2:E:63:MET:HE3	2:E:74:PRO:HB3	1.86	0.56
5:H:120:ALA:HB1	5:H:158:PRO:O	2.05	0.56
8:K:220:VAL:HG13	8:K:227:PHE:HD1	1.70	0.56
6:N:65:LEU:HD11	6:N:71:MET:SD	2.45	0.56
9:O:35:LEU:HB3	9:O:163:CYS:CB	2.35	0.56
10:P:207:ILE:CD1	10:P:229:LEU:HD21	2.30	0.56
13:U:32:GLN:O	13:U:34:VAL:HG23	2.05	0.56
13:Y:122:SER:C	13:Y:123:LEU:HD12	2.30	0.56
13:Y:154:GLU:H	13:Y:157:MET:HE2	1.68	0.56
2:B:13:ILE:HD12	2:B:177:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ILE:HB	2:B:41:ILE:O	2.05	0.56
3:C:9:GLN:HG2	3:C:145:PRO:O	2.05	0.56
3:C:81:LYS:HD3	3:C:120:ARG:HH22	1.70	0.56
2:E:14:LEU:HB3	2:E:44:CYS:SG	2.46	0.56
1:F:1:THR:HA	1:F:33:LYS:NZ	2.19	0.56
1:F:188:ILE:HG22	1:F:193:LEU:HD12	1.87	0.56
6:I:65:LEU:HD11	6:I:71:MET:SD	2.45	0.56
8:K:179:LEU:O	8:K:183:VAL:HG22	2.06	0.56
4:L:33:SER:CB	4:L:51:ARG:HG3	2.34	0.56
4:L:50:LYS:O	4:L:59:HIS:CB	2.48	0.56
4:L:65[B]:HIS:CE1	4:L:223:ILE:HD12	2.40	0.56
6:N:47:LYS:HA	6:N:205:ASN:O	2.05	0.56
6:N:187:THR:O	6:N:190:LEU:HB3	2.05	0.56
10:P:178:ASN:OD1	10:P:181:LEU:HB2	2.05	0.56
8:R:33:ASN:OD1	8:R:170:VAL:HA	2.05	0.56
12:T:43:LEU:HG	12:T:183:ILE:HD11	1.86	0.56
13:U:122:SER:C	13:U:123:LEU:HD12	2.30	0.56
13:U:148:MET:HE2	13:U:172:ASN:CB	2.35	0.56
12:V:164:LEU:HD13	12:V:178:PHE:CD2	2.39	0.56
11:X:211:ARG:NH2	11:X:213:ASP:OD2	2.38	0.56
2:B:14:LEU:HB3	2:B:44:CYS:SG	2.46	0.56
3:C:133:THR:HB	12:T:138:LEU:HD23	1.86	0.56
6:I:7:ILE:CG2	9:Z:11:ILE:HG22	2.35	0.56
8:K:153:LYS:O	8:K:160:TYR:HA	2.05	0.56
5:M:91:LYS:CD	5:M:119:LEU:HD11	2.36	0.56
12:T:18:ASP:HA	12:T:178:PHE:CD1	2.41	0.56
12:T:114:ALA:HB1	12:T:126:LYS:HE2	1.87	0.56
11:X:168:LEU:O	11:X:172:MET:HG2	2.06	0.56
14:a:45:VAL:CG1	14:a:71:VAL:HG11	2.35	0.56
1:A:80:ALA:HB3	1:A:112:TYR:HD2	1.69	0.56
3:D:35:ILE:N	3:D:45:MET:HE3	2.21	0.56
8:K:137:CYS:SG	8:K:156:PRO:HD3	2.45	0.56
7:Q:184:MET:HB2	7:Q:189:ILE:HD11	1.86	0.56
12:T:38:MET:HE3	12:T:44:LEU:CB	2.35	0.56
13:Y:43:PRO:HB3	13:Y:49:TYR:CE1	2.40	0.56
3:C:31:VAL:HG13	15:C:301:BZ7:CBK	2.36	0.56
3:C:40:TYR:CB	3:C:183:GLY:HA2	2.35	0.56
3:C:42:LEU:HB3	3:C:102:CYS:HB2	1.88	0.56
3:C:113:TYR:HE1	3:C:128:THR:HG22	1.71	0.56
13:U:111:LEU:HD23	13:U:118:PRO:HA	1.88	0.56
9:Z:35:LEU:HB3	9:Z:163:CYS:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:49:ARG:NH1	9:Z:212:GLU:OE2	2.39	0.56
2:B:37:ILE:HD11	2:B:56:THR:OG1	2.06	0.56
3:D:87:MET:HE2	3:D:97:MET:HB3	1.88	0.56
2:E:37:ILE:HD11	2:E:56:THR:OG1	2.06	0.56
6:I:51:ALA:O	6:I:54:GLN:N	2.28	0.56
4:L:50:LYS:O	4:L:59:HIS:ND1	2.39	0.56
11:S:211:ARG:NH2	11:S:213:ASP:OD2	2.38	0.56
12:T:58:GLU:O	12:T:62:LYS:HG2	2.06	0.56
14:W:45:VAL:CG1	14:W:71:VAL:HG11	2.35	0.56
13:Y:16:LYS:CB	13:Y:158:ASP:HA	2.35	0.56
13:Y:148:MET:HE2	13:Y:172:ASN:CB	2.35	0.56
9:Z:134:LEU:HB3	9:Z:136:TYR:CE1	2.41	0.56
3:C:134:TYR:CE1	12:T:137:PHE:HA	2.40	0.56
2:E:111:TYR:HE1	2:E:121:ARG:HB2	1.69	0.56
4:L:207:THR:O	4:L:226:ASP:HA	2.04	0.56
6:N:125:ARG:HE	9:O:123:GLN:HA	1.70	0.56
9:O:49:ARG:HD3	9:O:212:GLU:CD	2.29	0.56
9:O:133:SER:C	9:O:134:LEU:HD12	2.31	0.56
13:U:43:PRO:HB3	13:U:49:TYR:CE1	2.40	0.56
12:V:85:ARG:NH1	12:V:89:ALA:HB2	2.20	0.56
11:X:176:LYS:HE2	11:X:208:VAL:HG21	1.86	0.56
13:Y:189:ILE:HA	13:Y:194:ILE:CD1	2.36	0.56
9:Z:226:ARG:HH12	9:Z:228:LEU:HD23	1.70	0.56
2:B:219:LEU:HD13	13:Y:194:ILE:HG12	1.88	0.56
3:D:42:LEU:HB3	3:D:102:CYS:HB2	1.88	0.56
4:L:96:ARG:NH1	4:L:102:PRO:HG3	2.21	0.56
4:L:207:THR:HA	4:L:233:LEU:CD1	2.36	0.56
5:M:51:GLU:OE1	5:M:206:MET:HG2	2.06	0.56
6:N:195:LEU:O	6:N:199:VAL:HG23	2.06	0.56
9:O:37:ILE:HG12	9:O:161:ALA:CB	2.36	0.56
11:S:168:LEU:O	11:S:172:MET:HG2	2.06	0.56
12:V:16:ALA:CB	12:V:160:LEU:HD21	2.36	0.56
13:Y:111:LEU:HD23	13:Y:118:PRO:HA	1.88	0.56
13:Y:170:MET:O	13:Y:174:VAL:HG22	2.06	0.56
14:a:177:TYR:CE2	14:a:207:THR:HG21	2.40	0.56
2:E:204:PHE:CE2	13:U:168:GLN:HG3	2.40	0.56
7:J:184:MET:HB2	7:J:189:ILE:HD11	1.86	0.56
4:L:58:ALA:N	5:M:164:GLN:O	2.30	0.56
4:L:206:THR:C	4:L:233:LEU:HD11	2.31	0.56
5:M:40:ILE:HG12	5:M:167:ALA:CB	2.34	0.56
6:N:43:LEU:HD11	6:N:134:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:196:LEU:HD22	6:N:202:GLY:HA3	1.88	0.56
9:O:134:LEU:HB3	9:O:136:TYR:CE1	2.41	0.56
10:P:100:TYR:HE1	13:U:89:MET:HE2	1.71	0.56
13:U:81:ILE:HD11	13:U:85:THR:HG22	1.88	0.56
13:U:170:MET:O	13:U:174:VAL:HG22	2.06	0.56
12:V:18:ASP:HA	12:V:178:PHE:CD1	2.41	0.56
12:V:58:GLU:O	12:V:62:LYS:HG2	2.06	0.56
3:C:81:LYS:HD3	3:C:120:ARG:NH2	2.21	0.55
3:D:81:LYS:HD3	3:D:120:ARG:HH22	1.70	0.55
3:D:113:TYR:HE1	3:D:128:THR:HG22	1.71	0.55
4:G:38:LEU:HG	4:G:187:LEU:HD11	1.87	0.55
7:J:64:LYS:NZ	7:J:212:GLU:OE2	2.37	0.55
4:L:59:HIS:CD2	4:L:59:HIS:H	2.22	0.55
6:N:206:ILE:O	6:N:206:ILE:HG13	2.04	0.55
14:W:60:PHE:CE2	14:W:64:LYS:HD2	2.41	0.55
14:a:147:GLN:HB3	14:a:148:PRO:HD3	1.87	0.55
10:b:33:PRO:HG3	10:b:164:LYS:HB2	1.87	0.55
10:b:92:LEU:HD13	10:b:112:ARG:HB3	1.88	0.55
10:b:181:LEU:HD21	10:b:186:ALA:HA	1.88	0.55
2:B:208:THR:HA	11:S:159:GLN:O	2.05	0.55
3:D:49:ALA:HB2	15:D:301:BZ7:CBH	2.35	0.55
3:D:128:THR:O	3:D:132:ASN:HB3	2.06	0.55
4:G:96:ARG:NH1	4:G:102:PRO:HG3	2.21	0.55
8:K:42:VAL:HG12	8:K:165:ALA:HB1	1.89	0.55
6:N:108:THR:HG21	6:N:145:TYR:CB	2.36	0.55
8:R:220:VAL:HG13	8:R:227:PHE:HD1	1.70	0.55
14:W:147:GLN:HB3	14:W:148:PRO:HD3	1.87	0.55
11:X:6:VAL:HG12	11:X:57:PHE:CE1	2.42	0.55
9:Z:219:GLU:OE1	9:Z:224:VAL:HG21	2.06	0.55
10:b:96:TYR:CE2	10:b:104:ILE:HA	2.42	0.55
1:A:7:GLU:OE2	1:A:121:ARG:NH2	2.37	0.55
1:A:42:TYR:CD2	1:A:176:VAL:HG21	2.41	0.55
5:H:40:ILE:HG12	5:H:167:ALA:CB	2.34	0.55
5:H:58:LEU:HD13	6:I:158:ALA:O	2.06	0.55
6:I:108:THR:HG21	6:I:145:TYR:CB	2.36	0.55
6:I:110:TYR:O	6:I:113:SER:OG	2.16	0.55
7:J:30:VAL:HG22	7:J:133[A]:CYS:HA	1.87	0.55
5:M:91:LYS:O	5:M:95:GLU:HG2	2.06	0.55
9:O:86:LEU:HD21	9:O:130:PHE:CD2	2.41	0.55
11:S:6:VAL:HG12	11:S:57:PHE:CE1	2.42	0.55
13:Y:81:ILE:HD11	13:Y:85:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:MET:HB3	3:C:52:CYS:CB	2.35	0.55
3:C:103:GLY:C	3:C:179:MET:HE2	2.30	0.55
2:E:40:LYS:HZ3	2:E:103:VAL:C	2.14	0.55
1:F:7:GLU:OE2	1:F:121:ARG:NH2	2.37	0.55
6:N:53:LEU:HD11	9:O:175:LEU:HB3	1.88	0.55
9:O:90:LEU:CD2	9:O:114:LEU:HB2	2.36	0.55
10:P:110:VAL:HG21	10:P:146:PHE:CD2	2.42	0.55
11:X:13:LEU:HD12	11:X:136:LYS:O	2.07	0.55
13:Y:16:LYS:HB2	13:Y:158:ASP:HA	1.87	0.55
9:Z:59:VAL:HG22	10:b:142:ARG:HH12	1.71	0.55
14:a:50:MET:SD	14:a:190:ALA:HB1	2.47	0.55
14:a:60:PHE:CE2	14:a:64:LYS:HD2	2.42	0.55
6:I:40:ILE:HD11	6:I:210:VAL:CG1	2.37	0.55
4:L:146:GLN:OE1	4:L:159:MET:HG2	2.06	0.55
6:N:51:ALA:O	6:N:54:GLN:N	2.28	0.55
6:N:77:THR:OG1	9:O:155:ASN:OD1	2.23	0.55
8:R:179:LEU:O	8:R:183:VAL:HG22	2.06	0.55
12:T:16:ALA:CB	12:T:160:LEU:HD21	2.36	0.55
1:A:97:HIS:C	1:A:98:LEU:HD12	2.32	0.55
2:E:159:VAL:HG11	2:E:173:VAL:HG23	1.89	0.55
4:G:146:GLN:OE1	4:G:159:MET:HG2	2.06	0.55
8:K:206:LEU:HD23	8:K:208:ILE:HD12	1.89	0.55
5:M:220:VAL:HG22	5:M:226:PHE:HA	1.87	0.55
9:O:49:ARG:NH1	9:O:212:GLU:OE2	2.39	0.55
7:Q:30:VAL:HG22	7:Q:133[A]:CYS:HA	1.88	0.55
12:V:4:LEU:HG	12:V:47:VAL:HG11	1.88	0.55
9:Z:232:GLU:O	9:Z:236:LEU:HG	2.06	0.55
2:E:18:THR:OG1	2:E:172:ASN:N	2.37	0.55
6:N:40:ILE:HD11	6:N:210:VAL:CG1	2.37	0.55
13:U:189:ILE:HA	13:U:194:ILE:CD1	2.36	0.55
13:Y:141:CYS:HB2	13:Y:144:GLN:OE1	2.07	0.55
1:A:126:ILE:HD11	1:A:135:TYR:CE1	2.42	0.55
1:F:72:GLU:CG	1:F:73:PRO:HD2	2.37	0.55
4:G:49:LEU:HD13	4:G:199:LEU:HD21	1.88	0.55
6:I:43:LEU:HD21	6:I:134:VAL:CG1	2.37	0.55
8:K:40:VAL:HG22	8:K:167:ALA:HB2	1.89	0.55
6:N:192:ILE:O	6:N:196:LEU:HG	2.07	0.55
6:N:195:LEU:HB3	6:N:206:ILE:HD11	1.88	0.55
10:P:92:LEU:HD13	10:P:112:ARG:HB3	1.89	0.55
10:P:96:TYR:CE2	10:P:104:ILE:HA	2.42	0.55
9:Z:86:LEU:HD21	9:Z:130:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:110:VAL:HG21	10:b:146:PHE:CD2	2.42	0.55
10:b:188:HIS:NE2	10:b:192:LEU:HD11	2.22	0.55
3:D:81:LYS:HD3	3:D:120:ARG:NH2	2.21	0.55
1:F:26:VAL:CG2	14:W:179:ARG:HD3	2.37	0.55
5:H:91:LYS:O	5:H:95:GLU:HG2	2.06	0.55
9:O:69:ASN:OD1	9:O:71:ASP:N	2.31	0.55
1:A:72:GLU:CG	1:A:73:PRO:HD2	2.37	0.55
2:B:75:ARG:HA	2:B:104:ASP:OD1	2.07	0.55
3:D:121:LEU:HD22	12:T:29:LYS:CD	2.37	0.55
1:F:37:LEU:HD11	1:F:43:CYS:CB	2.36	0.55
1:F:76:VAL:HB	1:F:110:GLN:OE1	2.07	0.55
6:I:71:MET:SD	6:I:84:ILE:HG12	2.47	0.55
6:N:71:MET:SD	6:N:84:ILE:HG12	2.47	0.55
9:O:107:CYS:HB2	9:O:146:GLN:OE1	2.06	0.55
10:P:181:LEU:HD21	10:P:186:ALA:HA	1.88	0.55
8:R:40:VAL:HG22	8:R:167:ALA:HB2	1.89	0.55
8:R:206:LEU:HD23	8:R:208:ILE:HD12	1.89	0.55
9:Z:46:ALA:HB1	9:Z:197:LEU:HD11	1.89	0.55
1:A:15:GLY:HA2	1:A:175:LEU:HD23	1.89	0.54
2:B:40:LYS:HZ3	2:B:103:VAL:C	2.15	0.54
3:C:153:TYR:OH	3:C:178:HIS:ND1	2.39	0.54
2:E:137:VAL:CG2	2:E:158:ALA:HA	2.33	0.54
1:F:42:TYR:CD2	1:F:176:VAL:HG21	2.41	0.54
4:G:47:VAL:HG12	4:G:195:LEU:CD2	2.37	0.54
8:K:46:ASP:O	8:K:222:VAL:HG23	2.07	0.54
4:L:74:ILE:CG2	4:L:81:ALA:HB1	2.35	0.54
9:O:219:GLU:OE1	9:O:224:VAL:HG21	2.06	0.54
11:S:13:LEU:HD12	11:S:136:LYS:O	2.06	0.54
13:U:22:ALA:O	13:U:41:ILE:HD11	2.07	0.54
14:W:50:MET:SD	14:W:190:ALA:HB1	2.47	0.54
14:W:92:LEU:HD23	14:W:110:MET:CE	2.37	0.54
11:X:84:THR:HG22	11:X:115:GLU:OE2	2.07	0.54
3:C:128:THR:O	3:C:132:ASN:HB3	2.06	0.54
3:D:58:LEU:CD1	3:D:61:LYS:HE3	2.37	0.54
3:D:164:THR:HG22	3:D:170:SER:CB	2.33	0.54
9:O:232:GLU:O	9:O:236:LEU:HG	2.06	0.54
10:P:25:LEU:HD21	10:P:150:PRO:HD2	1.89	0.54
10:P:188:HIS:O	10:P:192:LEU:HG	2.07	0.54
12:T:18:ASP:HA	12:T:178:PHE:HD1	1.72	0.54
12:V:18:ASP:HA	12:V:178:PHE:HD1	1.72	0.54
14:W:151:ARG:NH1	11:X:35:ILE:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:22:ALA:O	13:Y:41:ILE:HD11	2.07	0.54
9:Z:37:ILE:HG12	9:Z:161:ALA:CB	2.36	0.54
9:Z:107:CYS:HB2	9:Z:146:GLN:OE1	2.06	0.54
14:a:99:ARG:HH12	14:a:106:LEU:HD21	1.73	0.54
10:b:188:HIS:O	10:b:192:LEU:HG	2.07	0.54
1:A:76:VAL:HB	1:A:110:GLN:OE1	2.08	0.54
2:E:75:ARG:HA	2:E:104:ASP:OD1	2.07	0.54
4:G:207:THR:HA	4:G:233:LEU:CD1	2.37	0.54
5:H:51:GLU:OE1	5:H:206:MET:HG2	2.06	0.54
4:L:126:ARG:NH2	5:M:121:LEU:HD22	2.21	0.54
8:R:42:VAL:HG12	8:R:165:ALA:HB1	1.89	0.54
9:Z:37:ILE:HG23	9:Z:161:ALA:HB2	1.89	0.54
14:a:115:TYR:CZ	14:a:118:GLY:HA2	2.43	0.54
10:b:158:LYS:HB3	10:b:177:TYR:CE2	2.43	0.54
4:G:34:ALA:HA	4:G:162:GLY:HA3	1.89	0.54
6:I:105:GLU:HA	6:I:145:TYR:HE2	1.73	0.54
7:J:175:GLU:HG3	7:J:196:ILE:HG12	1.89	0.54
5:M:41:GLN:NE2	5:M:152:GLN:HA	2.23	0.54
11:S:84:THR:HG22	11:S:115:GLU:OE2	2.07	0.54
11:S:170:ARG:O	11:S:174:LEU:HD23	2.06	0.54
12:T:101:ASN:HB3	12:T:132:HIS:CD2	2.42	0.54
13:U:141:CYS:HB2	13:U:144:GLN:OE1	2.07	0.54
14:W:115:TYR:CZ	14:W:118:GLY:HA2	2.43	0.54
9:Z:51:ASN:HB3	9:Z:56:LEU:HD13	1.89	0.54
14:a:92:LEU:HD23	14:a:110:MET:CE	2.37	0.54
3:C:58:LEU:CD1	3:C:61:LYS:HE3	2.37	0.54
3:D:144:ARG:O	3:D:147:LEU:HG	2.08	0.54
1:F:15:GLY:HA2	1:F:175:LEU:HD23	1.89	0.54
4:L:49:LEU:HD13	4:L:199:LEU:HD21	1.88	0.54
6:N:7:ILE:CG2	9:O:11:ILE:HG22	2.37	0.54
10:P:80:PRO:HG2	8:R:157:ALA:O	2.08	0.54
10:P:85:LEU:HD12	10:P:131:VAL:HG21	1.88	0.54
12:V:35:MET:HE2	12:V:45:LEU:CD2	2.35	0.54
11:X:170:ARG:O	11:X:174:LEU:HD23	2.06	0.54
1:A:26:VAL:HG22	14:a:179:ARG:O	2.07	0.54
1:A:37:LEU:HD11	1:A:43:CYS:CB	2.36	0.54
2:B:137:VAL:CG2	2:B:158:ALA:HA	2.33	0.54
3:C:76:VAL:HG11	3:C:110:GLY:O	2.07	0.54
1:F:97:HIS:C	1:F:98:LEU:HD12	2.32	0.54
1:F:126:ILE:HD11	1:F:135:TYR:CE1	2.42	0.54
5:M:119:LEU:N	5:M:119:LEU:HD23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:26:MET:SD	14:W:202:PRO:HB3	2.48	0.54
9:Z:10:THR:HB	9:Z:123:GLN:O	2.08	0.54
9:Z:115:CYS:HB3	9:Z:154:GLY:O	2.08	0.54
14:a:26:MET:SD	14:a:202:PRO:HB3	2.48	0.54
2:B:159:VAL:HG11	2:B:173:VAL:HG23	1.89	0.54
2:E:118:SER:HB3	1:F:50:ALA:HB2	1.89	0.54
5:H:60:GLU:HB2	6:I:155:ALA:HB3	1.90	0.54
9:O:46:ALA:HB1	9:O:197:LEU:HD11	1.89	0.54
9:O:115:CYS:HB3	9:O:154:GLY:O	2.08	0.54
8:R:46:ASP:O	8:R:222:VAL:HG23	2.08	0.54
11:X:13:LEU:HD11	11:X:149:LEU:CD1	2.38	0.54
1:A:127:GLY:O	1:A:131:SER:HB3	2.08	0.54
3:D:132:ASN:OD1	3:D:133:THR:HG23	2.08	0.54
1:F:26:VAL:HG22	14:W:179:ARG:HA	1.90	0.54
4:G:9:ASP:OD1	9:Z:3:ARG:NH2	2.41	0.54
4:G:58:ALA:HB2	5:H:164:GLN:OE1	2.07	0.54
5:H:216:GLU:HB3	5:H:228:MET:SD	2.48	0.54
6:I:158:ALA:HB1	6:I:172:LEU:HD13	1.89	0.54
4:L:148:CYS:HB3	4:L:149:PRO:CD	2.37	0.54
6:N:63:CYS:SG	6:N:84:ILE:HD13	2.47	0.54
6:N:158:ALA:HB1	6:N:172:LEU:HD13	1.89	0.54
6:N:210:VAL:O	6:N:218:LYS:N	2.28	0.54
6:N:226:GLU:HA	6:N:229:VAL:CG2	2.38	0.54
9:O:37:ILE:HG23	9:O:161:ALA:HB2	1.89	0.54
10:P:28:VAL:HG13	10:P:76:SER:O	2.08	0.54
14:W:99:ARG:HH12	14:W:106:LEU:HD21	1.73	0.54
4:G:58:ALA:HB3	5:H:164:GLN:O	2.08	0.54
4:G:63:ILE:HD12	4:G:211:SER:OG	2.08	0.54
5:H:35:SER:HB3	5:H:51:GLU:HG3	1.90	0.54
8:K:206:LEU:HD23	8:K:208:ILE:CD1	2.38	0.54
4:L:215:VAL:HB	4:L:221:PHE:CD1	2.41	0.54
6:N:134:VAL:HG12	6:N:144:LEU:HD13	1.90	0.54
12:V:101:ASN:HB3	12:V:132:HIS:CD2	2.42	0.54
9:Z:235:GLN:O	9:Z:239:LYS:HG3	2.08	0.54
14:a:25:ASP:HA	14:a:187:PHE:CB	2.38	0.54
3:C:87:MET:HE2	3:C:97:MET:HB3	1.88	0.54
3:C:113:TYR:O	3:C:120:ARG:HA	2.08	0.54
3:C:128:THR:C	3:C:132:ASN:HB3	2.33	0.54
3:D:128:THR:C	3:D:132:ASN:HB3	2.33	0.54
1:F:127:GLY:O	1:F:131:SER:HB3	2.07	0.54
5:H:142:LEU:HD23	5:H:155:HIS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:166:LYS:O	6:N:170:GLU:HG2	2.08	0.54
10:P:65:GLU:HB3	10:P:90:ARG:HH11	1.72	0.54
13:U:141:CYS:O	13:U:145:MET:HE2	2.08	0.54
14:W:25:ASP:HA	14:W:187:PHE:CB	2.38	0.54
14:W:178:TYR:HE1	14:W:207:THR:HB	1.73	0.54
13:Y:17:ASN:HA	13:Y:118:PRO:CG	2.38	0.54
14:a:91:TRP:CE3	14:a:92:LEU:HD12	2.43	0.54
14:a:96:MET:HE3	14:a:127:MET:HA	1.90	0.54
10:b:111:GLN:HG2	10:b:154:TYR:OH	2.08	0.54
3:C:121:LEU:HD22	12:V:29:LYS:HD3	1.89	0.53
3:C:127:SER:O	3:C:132:ASN:HB2	2.08	0.53
3:D:76:VAL:HG11	3:D:110:GLY:O	2.08	0.53
2:E:122:LEU:CD1	2:E:125:THR:HB	2.37	0.53
1:F:70:LEU:CD2	7:Q:110:HIS:HB2	2.37	0.53
4:L:34:ALA:HA	4:L:162:GLY:HA3	1.89	0.53
4:L:47:VAL:HG12	4:L:195:LEU:CD2	2.37	0.53
4:L:229:VAL:HG21	4:L:233:LEU:HD12	1.89	0.53
5:M:216:GLU:HB3	5:M:228:MET:SD	2.48	0.53
7:Q:175:GLU:HG3	7:Q:196:ILE:HG12	1.89	0.53
10:b:37:ILE:HG12	10:b:159:ALA:CB	2.35	0.53
10:b:65:GLU:HB3	10:b:90:ARG:HH11	1.73	0.53
6:I:134:VAL:HG12	6:I:144:LEU:HD13	1.90	0.53
8:K:16:PHE:CE2	10:b:127:ARG:HD2	2.43	0.53
9:O:46:ALA:HB2	9:O:213:ILE:HG12	1.90	0.53
12:T:43:LEU:CG	12:T:183:ILE:HD11	2.39	0.53
12:T:164:LEU:HD13	12:T:178:PHE:CD2	2.39	0.53
12:V:43:LEU:CG	12:V:183:ILE:HD11	2.39	0.53
14:W:91:TRP:CE3	14:W:92:LEU:HD12	2.43	0.53
13:Y:27:PHE:HB2	13:Y:38:PHE:CB	2.39	0.53
10:b:44:VAL:CG2	10:b:187:ILE:HG12	2.39	0.53
10:b:107:ALA:O	10:b:111:GLN:HG3	2.08	0.53
1:A:8:PHE:HB3	1:A:151:CYS:SG	2.49	0.53
3:D:127:SER:O	3:D:132:ASN:HB2	2.08	0.53
5:H:91:LYS:HG2	5:H:119:LEU:HD11	1.89	0.53
6:I:43:LEU:H	6:I:208:LEU:HD21	1.73	0.53
6:I:226:GLU:HA	6:I:229:VAL:CG2	2.38	0.53
7:J:192:GLU:O	7:J:196:ILE:HG13	2.09	0.53
5:M:142:LEU:HD23	5:M:155:HIS:HA	1.90	0.53
10:P:107:ALA:O	10:P:111:GLN:HG3	2.08	0.53
8:R:206:LEU:HD23	8:R:208:ILE:CD1	2.38	0.53
11:S:13:LEU:HD11	11:S:149:LEU:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:14:LYS:NZ	13:U:133:ASP:HA	2.24	0.53
12:V:140:LEU:HD12	13:Y:32:GLN:HE21	1.73	0.53
9:Z:90:LEU:CD2	9:Z:114:LEU:HB2	2.36	0.53
2:B:208:THR:O	11:S:159:GLN:N	2.41	0.53
5:H:41:GLN:NE2	5:H:152:GLN:HA	2.23	0.53
7:J:15:SER:HB3	7:J:21:PHE:CE2	2.43	0.53
8:K:3:ARG:N	8:K:19:GLU:OE2	2.41	0.53
4:L:63:ILE:HD12	4:L:211:SER:OG	2.08	0.53
10:P:105:PRO:HA	10:P:139:ASN:ND2	2.17	0.53
8:R:3:ARG:N	8:R:19:GLU:OE2	2.41	0.53
8:R:208:ILE:HB	8:R:210:PHE:CE1	2.43	0.53
14:W:51:LEU:HD11	14:W:92:LEU:HD21	1.90	0.53
14:W:96:MET:HE3	14:W:127:MET:HA	1.90	0.53
9:Z:37:ILE:O	9:Z:43:VAL:HG13	2.08	0.53
10:b:74:VAL:CG1	10:b:134:LEU:HB2	2.35	0.53
10:b:85:LEU:HD12	10:b:131:VAL:HG21	1.89	0.53
3:C:3:THR:HG22	3:C:100:MET:CE	2.39	0.53
3:C:132:ASN:OD1	3:C:133:THR:HG23	2.08	0.53
7:J:190:VAL:HG21	7:J:215:TRP:CZ3	2.43	0.53
6:N:43:LEU:HD21	6:N:134:VAL:CG1	2.37	0.53
9:O:10:THR:HB	9:O:123:GLN:O	2.08	0.53
7:Q:15:SER:HB3	7:Q:21:PHE:CE2	2.43	0.53
12:T:1:MET:N	12:T:173:LEU:HD13	2.24	0.53
12:T:12:TYR:OH	12:T:156:ALA:HB2	2.09	0.53
13:U:148:MET:SD	11:X:147:PRO:HB2	2.48	0.53
14:W:126:ASP:OD1	14:W:130:VAL:HB	2.09	0.53
10:b:28:VAL:HG13	10:b:76:SER:O	2.08	0.53
2:B:122:LEU:CD1	2:B:125:THR:HB	2.37	0.53
1:F:26:VAL:CG2	14:W:179:ARG:HA	2.38	0.53
6:I:115:LYS:HE2	6:I:129:ILE:HD11	1.91	0.53
7:J:71:ARG:HB2	7:J:223:ARG:CD	2.38	0.53
8:K:212:PRO:C	8:K:232:GLU:HG3	2.33	0.53
4:L:49:LEU:HA	4:L:209:ASN:O	2.09	0.53
5:M:58:LEU:HD21	6:N:172:LEU:O	2.08	0.53
6:N:105:GLU:HA	6:N:145:TYR:HE2	1.73	0.53
6:N:115:LYS:HE2	6:N:129:ILE:HD11	1.91	0.53
9:O:83:ALA:O	9:O:87:THR:HG23	2.09	0.53
9:O:190:LEU:HD11	9:O:228:LEU:HD11	1.90	0.53
7:Q:71:ARG:HB2	7:Q:223:ARG:CD	2.38	0.53
11:S:148:LEU:HD22	13:Y:151:SER:OG	2.08	0.53
12:T:4:LEU:HG	12:T:47:VAL:HG11	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:141:CYS:O	13:Y:145:MET:HE2	2.08	0.53
9:Z:83:ALA:O	9:Z:87:THR:HG23	2.09	0.53
2:B:212:LEU:HG	13:Y:200:LYS:CB	2.38	0.53
3:D:3:THR:HG22	3:D:100:MET:CE	2.39	0.53
1:F:14:MET:HE2	1:F:44:ALA:HB2	1.91	0.53
4:L:229:VAL:O	4:L:233:LEU:CB	2.53	0.53
6:N:47:LYS:H	6:N:206:ILE:CA	2.20	0.53
9:O:45:LEU:O	9:O:213:ILE:HA	2.09	0.53
3:C:113:TYR:HB2	3:C:126:PHE:CE2	2.44	0.53
3:D:165:HIS:ND1	13:Y:203:MET:O	2.35	0.53
7:J:72:HIS:CE1	7:J:105:ASN:HB3	2.44	0.53
4:L:49:LEU:HG	4:L:195:LEU:CD2	2.36	0.53
7:Q:70:ASP:OD2	7:Q:99:ARG:NH2	2.41	0.53
12:T:27:GLN:OE1	12:T:30:ASP:HB3	2.09	0.53
11:X:31:GLU:HB3	11:X:36:HIS:HE2	1.74	0.53
14:a:51:LEU:HD11	14:a:92:LEU:HD21	1.90	0.53
10:b:25:LEU:HD21	10:b:150:PRO:HD2	1.89	0.53
2:B:6:LEU:HD21	2:B:146:MET:HE3	1.91	0.53
6:I:45:VAL:HG13	6:I:62:ILE:HD11	1.91	0.53
7:J:77:VAL:HG11	7:J:84:ALA:HB1	1.91	0.53
8:K:80:MET:HG3	8:K:87:SER:HB3	1.91	0.53
10:P:74:VAL:CG1	10:P:134:LEU:HB2	2.35	0.53
10:P:111:GLN:HG2	10:P:154:TYR:OH	2.08	0.53
8:R:42:VAL:HG12	8:R:165:ALA:CB	2.39	0.53
11:S:31:GLU:HB3	11:S:36:HIS:HE2	1.74	0.53
12:T:1:MET:HE1	12:T:134:TYR:H	1.73	0.53
13:Y:14:LYS:NZ	13:Y:133:ASP:HA	2.24	0.53
10:b:67:ILE:HD11	10:b:73:LEU:CD1	2.39	0.53
2:B:1:THR:N	2:B:169:SER:OG	2.21	0.53
1:F:8:PHE:HB3	1:F:151:CYS:SG	2.49	0.53
4:G:31:GLN:OE1	5:H:20:ARG:NE	2.42	0.53
4:G:49:LEU:HA	4:G:209:ASN:O	2.09	0.53
6:I:200:GLN:O	6:I:205:ASN:ND2	2.42	0.53
7:J:81:LEU:HD12	7:J:85:ARG:NH1	2.24	0.53
8:K:42:VAL:HG12	8:K:165:ALA:CB	2.39	0.53
8:K:208:ILE:HB	8:K:210:PHE:CE1	2.43	0.53
8:K:212:PRO:HB2	8:K:232:GLU:HG3	1.91	0.53
6:N:132:LEU:HD11	6:N:161:ILE:HG12	1.91	0.53
9:O:37:ILE:O	9:O:43:VAL:HG13	2.08	0.53
9:Z:46:ALA:HB2	9:Z:213:ILE:HG12	1.90	0.53
2:E:15:GLY:CA	2:E:155:LEU:HD21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:GLU:HG3	1:F:73:PRO:HD2	1.91	0.52
6:I:63:CYS:HB3	6:I:88:ARG:NH2	2.24	0.52
8:K:4:GLY:N	8:K:19:GLU:OE2	2.41	0.52
6:N:195:LEU:HD23	6:N:206:ILE:HD13	1.92	0.52
7:Q:72:HIS:CE1	7:Q:105:ASN:HB3	2.44	0.52
11:S:148:LEU:CD2	11:S:178:VAL:HG12	2.32	0.52
13:Y:3:MET:SD	13:Y:103:TYR:HB3	2.49	0.52
9:Z:128:ARG:HD3	10:b:10:THR:O	2.09	0.52
3:C:132:ASN:OD1	3:C:133:THR:N	2.43	0.52
3:C:144:ARG:O	3:C:147:LEU:HG	2.08	0.52
3:D:153:TYR:HH	3:D:178:HIS:HD1	1.57	0.52
3:D:191:ASP:OD1	3:D:192:VAL:N	2.43	0.52
4:G:74:ILE:HG22	4:G:132:LEU:CD2	2.39	0.52
6:I:87:ALA:CB	6:I:111:ILE:HD11	2.39	0.52
7:J:70:ASP:OD2	7:J:99:ARG:NH2	2.41	0.52
4:L:74:ILE:HG22	4:L:132:LEU:CD2	2.39	0.52
7:Q:140:TYR:CG	7:Q:217:GLY:HA2	2.45	0.52
8:R:212:PRO:C	8:R:232:GLU:HG3	2.33	0.52
12:T:103:LEU:HD23	12:T:117:TYR:HA	1.91	0.52
13:Y:10:VAL:HG12	13:Y:23:ALA:CB	2.40	0.52
10:b:209:VAL:HG12	10:b:220:LEU:HD12	1.91	0.52
1:A:14:MET:HE2	1:A:44:ALA:HB2	1.91	0.52
3:C:191:ASP:OD1	3:C:192:VAL:N	2.43	0.52
4:G:69:HIS:O	4:G:136:GLY:HA2	2.09	0.52
9:O:68:LEU:HD11	9:O:74:CYS:CB	2.38	0.52
7:Q:192:GLU:O	7:Q:196:ILE:HG13	2.09	0.52
12:T:16:ALA:CB	12:T:180:VAL:HG22	2.40	0.52
13:U:3:MET:SD	13:U:103:TYR:HB3	2.49	0.52
12:V:181:ARG:NE	12:V:190:ASP:OD1	2.41	0.52
1:A:163:MET:HE1	1:A:171:GLY:O	2.09	0.52
3:D:52:CYS:SG	3:D:97:MET:HG2	2.50	0.52
4:G:66:VAL:CG2	4:G:72:ILE:HG23	2.39	0.52
7:J:215:TRP:CE3	7:J:227:VAL:HG22	2.44	0.52
4:L:66:VAL:CG2	4:L:72:ILE:HG23	2.39	0.52
4:L:109:VAL:HG21	4:L:145:PHE:CG	2.45	0.52
11:X:193:LEU:HB3	11:X:208:VAL:HB	1.92	0.52
14:a:178:TYR:HE1	14:a:207:THR:HB	1.73	0.52
2:B:24:SER:O	11:S:187:VAL:HG22	2.09	0.52
2:B:70:THR:O	2:B:72:ARG:HG3	2.10	0.52
3:D:113:TYR:O	3:D:120:ARG:HA	2.09	0.52
3:D:132:ASN:OD1	3:D:133:THR:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:77:LEU:HD11	5:H:15:PHE:HE1	1.75	0.52
4:G:215:VAL:HB	4:G:221:PHE:CD1	2.41	0.52
7:J:75:MET:HE2	7:J:77:VAL:CG1	2.39	0.52
4:L:56:LEU:HD22	5:M:185:TYR:CD2	2.45	0.52
5:M:35:SER:HB3	5:M:51:GLU:HG3	1.90	0.52
5:M:180:SER:O	5:M:184:VAL:HG22	2.10	0.52
7:Q:81:LEU:HD12	7:Q:85:ARG:NH1	2.24	0.52
7:Q:190:VAL:HG21	7:Q:215:TRP:CZ3	2.43	0.52
9:Z:190:LEU:HD11	9:Z:228:LEU:HD11	1.91	0.52
1:A:72:GLU:HG3	1:A:73:PRO:HD2	1.91	0.52
2:E:70:THR:O	2:E:72:ARG:HG3	2.10	0.52
5:M:50:VAL:HG11	5:M:66:LYS:HB2	1.92	0.52
10:P:44:VAL:CG2	10:P:187:ILE:HG12	2.38	0.52
8:R:11:ARG:HG2	8:R:23:TYR:HD2	1.75	0.52
13:U:125:LEU:HD23	13:U:125:LEU:H	1.75	0.52
12:V:4:LEU:HD13	12:V:45:LEU:HB3	1.91	0.52
12:V:171:PHE:CE2	12:V:173:LEU:HB2	2.45	0.52
11:X:28:ARG:NE	11:X:191:ASP:OD2	2.25	0.52
9:Z:45:LEU:O	9:Z:213:ILE:HA	2.09	0.52
9:Z:80:THR:HB	10:b:153:ALA:HB2	1.90	0.52
14:a:211:ILE:HA	14:a:214:MET:SD	2.50	0.52
2:E:156:VAL:O	2:E:160:THR:OG1	2.23	0.52
4:G:33:SER:HG	4:G:62:LYS:HZ2	1.50	0.52
6:I:132:LEU:HD11	6:I:161:ILE:HG12	1.91	0.52
8:K:119:ALA:HB1	8:K:158:GLY:O	2.10	0.52
4:L:69:HIS:O	4:L:136:GLY:HA2	2.09	0.52
6:N:33:VAL:HG21	6:N:168:VAL:HG11	1.91	0.52
10:P:67:ILE:HD11	10:P:73:LEU:CD1	2.39	0.52
13:Y:7:GLY:HA2	13:Y:140:THR:CG2	2.38	0.52
14:a:162:GLN:NE2	14:a:191:THR:HG21	2.25	0.52
2:B:15:GLY:CA	2:B:155:LEU:HD21	2.39	0.52
1:F:8:PHE:CE2	1:F:148:PRO:HG3	2.45	0.52
1:F:163:MET:HE1	1:F:171:GLY:O	2.09	0.52
7:J:243:LEU:O	7:J:244:LYS:HG3	2.09	0.52
7:Q:75:MET:HE2	7:Q:77:VAL:CG1	2.39	0.52
7:Q:77:VAL:HG11	7:Q:84:ALA:HB1	1.91	0.52
8:R:4:GLY:N	8:R:19:GLU:OE2	2.41	0.52
13:U:27:PHE:HB2	13:U:38:PHE:CB	2.39	0.52
12:V:12:TYR:OH	12:V:156:ALA:HB2	2.09	0.52
13:Y:195:THR:HG21	13:Y:197:ARG:CZ	2.40	0.52
14:a:126:ASP:OD1	14:a:130:VAL:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:79:GLY:O	10:b:82:TYR:HB3	2.10	0.52
1:A:8:PHE:CE2	1:A:148:PRO:HG3	2.45	0.52
2:B:99:ILE:HD12	2:B:125:THR:HG23	1.92	0.52
3:D:113:TYR:HB2	3:D:126:PHE:CE2	2.44	0.52
2:E:6:LEU:HD21	2:E:146:MET:HE3	1.91	0.52
5:H:125:GLU:HG3	5:H:126:GLU:CD	2.35	0.52
5:M:47:CYS:CB	5:M:219:THR:HG22	2.40	0.52
10:P:79:GLY:O	10:P:82:TYR:HB3	2.10	0.52
14:W:211:ILE:HA	14:W:214:MET:SD	2.50	0.52
9:Z:49:ARG:NH2	9:Z:209:GLU:HA	2.25	0.52
3:C:52:CYS:SG	3:C:97:MET:HG2	2.50	0.52
1:F:3:ILE:HD12	1:F:44:ALA:HB3	1.92	0.52
5:H:47:CYS:CB	5:H:219:THR:HG22	2.40	0.52
6:I:33:VAL:HG21	6:I:168:VAL:HG11	1.91	0.52
9:O:59:VAL:HG22	10:P:142:ARG:HH22	1.74	0.52
10:P:48:GLU:HG3	10:P:198:PHE:HE1	1.75	0.52
10:P:155:PHE:HB2	10:P:157:TRP:HE1	1.75	0.52
7:Q:15:SER:HB3	7:Q:21:PHE:HE2	1.74	0.52
12:T:44:LEU:HG	12:T:46[B]:CYS:SG	2.50	0.52
13:U:95:TYR:CE1	13:U:98:ARG:HD3	2.45	0.52
1:A:128:GLY:O	1:A:131:SER:OG	2.28	0.51
3:C:60:ALA:O	3:C:64:ARG:HG2	2.10	0.51
3:C:66:TYR:CD2	3:C:74:ILE:HB	2.45	0.51
3:D:162:TYR:CE2	12:V:145:ARG:HA	2.45	0.51
4:G:176:MET:CE	7:J:56:LYS:HB3	2.29	0.51
5:H:31:ILE:HD11	5:H:138:GLY:C	2.35	0.51
8:K:11:ARG:HG2	8:K:23:TYR:HD2	1.75	0.51
4:L:50:LYS:HB3	4:L:59:HIS:HB2	1.91	0.51
6:N:45:VAL:HG13	6:N:62:ILE:HD11	1.91	0.51
8:R:119:ALA:HB1	8:R:158:GLY:O	2.10	0.51
8:R:212:PRO:HB2	8:R:232:GLU:HG3	1.91	0.51
13:U:195:THR:HG21	13:U:197:ARG:CZ	2.40	0.51
13:Y:95:TYR:CE1	13:Y:98:ARG:HD3	2.45	0.51
9:Z:214:ALA:HB2	9:Z:227:VAL:HG22	1.92	0.51
10:b:48:GLU:HG3	10:b:198:PHE:HE1	1.75	0.51
3:D:166:ARG:HD3	13:Y:33:MET:HE3	1.91	0.51
1:F:8:PHE:CE1	1:F:13:VAL:HG23	2.44	0.51
4:G:5:GLN:OE1	4:G:5:GLN:N	2.43	0.51
4:G:64:LEU:HD12	4:G:72:ILE:HD11	1.92	0.51
4:G:74:ILE:CG2	4:G:81:ALA:HB1	2.35	0.51
4:G:109:VAL:HG21	4:G:145:PHE:CG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:172:LEU:O	4:L:176:MET:HB3	2.11	0.51
5:M:31:ILE:HD11	5:M:138:GLY:C	2.35	0.51
6:N:71:MET:HE3	6:N:131:ALA:HB1	1.92	0.51
6:N:87:ALA:CB	6:N:111:ILE:HD11	2.39	0.51
6:N:192:ILE:HD11	6:N:208:LEU:CD2	2.39	0.51
9:O:135:LEU:HD11	9:O:164:ILE:HG12	1.93	0.51
12:V:103:LEU:HD23	12:V:117:TYR:HA	1.91	0.51
14:W:162:GLN:NE2	14:W:191:THR:HG21	2.25	0.51
10:b:73:LEU:HD23	10:b:135:ILE:HG12	1.92	0.51
1:A:135:TYR:CE2	14:W:33:LEU:HD21	2.40	0.51
2:E:11:GLY:HA2	2:E:108:PRO:CG	2.41	0.51
8:K:130:GLU:HA	10:b:5:TYR:HE2	1.74	0.51
8:R:80[A]:MET:CG	8:R:87:SER:HB3	2.38	0.51
11:S:13:LEU:N	11:S:24:ALA:O	2.44	0.51
13:U:10:VAL:HG12	13:U:23:ALA:CB	2.40	0.51
14:a:149:LEU:HD11	14:a:175:VAL:HG21	1.92	0.51
10:b:134:LEU:HD21	10:b:162:MET:HE3	1.92	0.51
1:A:3:ILE:HD12	1:A:44:ALA:HB3	1.92	0.51
1:A:161:LEU:HG	1:A:196:PHE:CE2	2.46	0.51
5:H:44:GLU:O	5:H:222:PRO:HD3	2.10	0.51
5:H:180:SER:O	5:H:184:VAL:HG22	2.10	0.51
4:L:50:LYS:HB3	4:L:59:HIS:HB3	1.90	0.51
4:L:64:LEU:HD12	4:L:72:ILE:HD11	1.92	0.51
4:L:230:SER:HB2	4:L:231:PRO:CD	2.36	0.51
5:M:35:SER:HB2	5:M:66:LYS:NZ	2.25	0.51
11:X:148:LEU:CD2	11:X:178:VAL:HG12	2.32	0.51
2:B:124:PHE:HE1	14:a:211:ILE:HG21	1.75	0.51
2:B:194:GLU:OE1	2:B:194:GLU:HA	2.10	0.51
1:F:161:LEU:HG	1:F:196:PHE:CE2	2.46	0.51
7:J:140:TYR:CG	7:J:217:GLY:HA2	2.45	0.51
7:J:228:PRO:CG	7:J:231:ILE:HD12	2.41	0.51
8:K:112:ASP:HB3	8:K:152:TYR:HE2	1.76	0.51
6:N:202:GLY:O	6:N:229:VAL:HG13	2.10	0.51
7:Q:215:TRP:CE3	7:Q:227:VAL:HG22	2.44	0.51
8:R:93:ARG:CZ	8:R:121:ILE:HD13	2.41	0.51
11:X:12:ILE:HG13	11:X:109:ILE:HD12	1.92	0.51
3:D:60:ALA:O	3:D:64:ARG:HG2	2.10	0.51
3:D:158:ARG:HD3	3:D:199:TYR:CE2	2.46	0.51
6:I:76:LEU:HD11	9:Z:12:PHE:HE1	1.76	0.51
7:J:15:SER:HB3	7:J:21:PHE:HE2	1.74	0.51
7:Q:215:TRP:CZ3	7:Q:227:VAL:HG13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:12:ILE:HG13	11:S:109:ILE:HD12	1.92	0.51
13:U:7:GLY:HA2	13:U:140:THR:CG2	2.38	0.51
12:V:1[B]:MET:H1	12:V:173:LEU:HD13	1.76	0.51
12:V:16:ALA:CB	12:V:180:VAL:HG22	2.39	0.51
2:B:18:THR:HG1	2:B:172:ASN:N	2.09	0.51
3:D:66:TYR:CD2	3:D:74:ILE:HB	2.45	0.51
2:E:9:GLN:HG2	2:E:145:ASN:ND2	2.17	0.51
2:E:99:ILE:HD12	2:E:125:THR:HG23	1.92	0.51
1:F:176:VAL:HG12	1:F:185:HIS:HA	1.93	0.51
4:G:18:ARG:NE	4:G:23:GLU:OE2	2.42	0.51
5:H:213:THR:HG22	5:H:231:LYS:NZ	2.25	0.51
6:I:5:ARG:HG3	9:Z:6:ASP:OD2	2.10	0.51
7:J:215:TRP:CZ3	7:J:227:VAL:HG13	2.46	0.51
4:L:6:TYR:CD2	4:L:15:PRO:HD3	2.46	0.51
4:L:154:PHE:CD2	7:Q:58:TYR:HE1	2.29	0.51
6:N:84:ILE:O	6:N:88:ARG:HG3	2.11	0.51
9:O:49:ARG:NH2	9:O:209:GLU:HA	2.25	0.51
10:P:209:VAL:HG12	10:P:220:LEU:HD12	1.91	0.51
7:Q:228:PRO:CG	7:Q:231:ILE:HD12	2.41	0.51
13:U:142:ALA:HA	13:U:145:MET:HE3	1.92	0.51
11:X:13:LEU:N	11:X:24:ALA:O	2.44	0.51
2:B:61:SER:HB2	10:b:98:LEU:HD21	1.91	0.51
3:D:4:LEU:HD13	3:D:139:MET:SD	2.51	0.51
5:H:50:VAL:HG11	5:H:66:LYS:HB2	1.92	0.51
6:I:183:THR:HG23	6:I:186:LEU:H	1.76	0.51
7:J:175:GLU:CG	7:J:196:ILE:HG12	2.41	0.51
9:O:38:LEU:HD12	9:O:43:VAL:HG22	1.93	0.51
10:P:64:VAL:HB	10:P:208:GLU:OE2	2.10	0.51
7:Q:175:GLU:CG	7:Q:196:ILE:HG12	2.41	0.51
10:b:64:VAL:HB	10:b:208:GLU:OE2	2.10	0.51
10:b:114:ALA:HB1	10:b:152:GLY:O	2.11	0.51
2:B:1:THR:HA	2:B:33:LYS:NZ	2.25	0.51
2:B:80:THR:HG21	2:B:111:TYR:CE2	2.46	0.51
3:D:133:THR:O	3:D:136:TYR:HB2	2.11	0.51
3:D:167:ASP:OD1	3:D:168:SER:N	2.44	0.51
2:E:80:THR:HG21	2:E:111:TYR:CE2	2.46	0.51
4:G:6:TYR:CD2	4:G:15:PRO:HD3	2.46	0.51
5:H:35:SER:HB2	5:H:66:LYS:NZ	2.26	0.51
6:I:33:VAL:HG22	6:I:160:ALA:HB2	1.93	0.51
8:K:183:VAL:HG12	8:K:191:PHE:CE2	2.45	0.51
4:L:40:SER:HA	4:L:179:PHE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:44:GLU:O	5:M:222:PRO:HD3	2.10	0.51
10:P:83:ARG:NH2	8:R:158:GLY:O	2.44	0.51
10:P:134:LEU:HD21	10:P:162:MET:HE3	1.92	0.51
7:Q:214:SER:HA	7:Q:227:VAL:HG23	1.93	0.51
7:Q:219:LEU:H	7:Q:219:LEU:HD23	1.76	0.51
8:R:151:VAL:HG23	8:R:163:PHE:HB2	1.93	0.51
11:S:193:LEU:HB3	11:S:208:VAL:HB	1.92	0.51
9:Z:135:LEU:HD11	9:Z:164:ILE:HG12	1.92	0.51
14:a:96:MET:HE1	14:a:106:LEU:O	2.11	0.51
2:B:212:LEU:HG	13:Y:200:LYS:CA	2.41	0.51
3:C:53:GLN:OE1	11:X:129:SER:HA	2.11	0.51
3:C:133:THR:O	3:C:136:TYR:HB2	2.11	0.51
7:J:160:TYR:HD2	7:J:163:CYS:HB2	1.75	0.51
7:J:214:SER:HA	7:J:227:VAL:HG23	1.93	0.51
8:K:93:ARG:CZ	8:K:121:ILE:HD13	2.41	0.51
8:K:151:VAL:HG23	8:K:163:PHE:HB2	1.93	0.51
4:L:5:GLN:OE1	4:L:5:GLN:N	2.43	0.51
6:N:47:LYS:H	6:N:206:ILE:CG2	2.06	0.51
6:N:145:TYR:HD1	6:N:155:ALA:HA	1.76	0.51
10:P:114:ALA:HB1	10:P:152:GLY:O	2.11	0.51
12:T:4:LEU:HD13	12:T:45:LEU:HB3	1.92	0.51
14:W:149:LEU:HD11	14:W:175:VAL:HG21	1.92	0.51
2:B:9:GLN:HG2	2:B:145:ASN:ND2	2.17	0.50
2:B:11:GLY:HA2	2:B:108:PRO:CG	2.41	0.50
3:C:158:ARG:HD3	3:C:199:TYR:CE2	2.46	0.50
1:F:14:MET:CE	1:F:44:ALA:HB2	2.41	0.50
1:F:171:GLY:HA2	14:W:209:TRP:CH2	2.46	0.50
6:I:84:ILE:O	6:I:88:ARG:HG3	2.11	0.50
5:M:38:ILE:HG12	5:M:169:ALA:HA	1.93	0.50
9:O:128:ARG:HD3	10:P:10:THR:O	2.11	0.50
9:O:214:ALA:HB2	9:O:227:VAL:HG22	1.92	0.50
7:Q:190:VAL:HG13	7:Q:213:LEU:HD13	1.94	0.50
7:Q:195:LYS:HE2	7:Q:199:ILE:HD11	1.92	0.50
12:V:85:ARG:HH22	13:Y:57:THR:HA	1.75	0.50
14:W:96:MET:HE1	14:W:106:LEU:O	2.11	0.50
13:Y:108:ILE:HB	13:Y:121:CYS:SG	2.51	0.50
3:C:31:VAL:HG11	15:C:301:BZ7:CBK	2.38	0.50
3:D:153:TYR:OH	3:D:178:HIS:ND1	2.39	0.50
2:E:1:THR:HA	2:E:33:LYS:NZ	2.25	0.50
4:G:172:LEU:O	4:G:176:MET:HB3	2.11	0.50
5:H:49:ALA:HB2	5:H:217:LEU:CD1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:105:GLU:OE2	11:X:75:TYR:OH	2.24	0.50
6:I:21:TYR:O	6:I:24:GLU:HB2	2.11	0.50
6:I:71:MET:HE3	6:I:131:ALA:HB1	1.92	0.50
7:Q:75:MET:HE3	7:Q:135:PHE:CG	2.46	0.50
12:T:171:PHE:CE2	12:T:173:LEU:HB2	2.45	0.50
13:U:108:ILE:HB	13:U:121:CYS:SG	2.51	0.50
13:Y:92:ASN:ND2	10:b:99:VAL:HG13	2.27	0.50
10:b:63:LYS:HE3	10:b:75:TYR:CZ	2.46	0.50
1:A:14:MET:CE	1:A:44:ALA:HB2	2.41	0.50
2:B:204:PHE:HD2	13:Y:168:GLN:HG3	1.76	0.50
4:G:157:ARG:NH1	4:G:176:MET:SD	2.84	0.50
7:J:70:ASP:HA	14:W:76:LEU:HD21	1.92	0.50
7:J:75:MET:HE3	7:J:135:PHE:CG	2.46	0.50
6:N:33:VAL:HG22	6:N:160:ALA:HB2	1.93	0.50
9:O:132:VAL:HG12	9:O:134:LEU:HD11	1.94	0.50
8:R:112:ASP:HB3	8:R:152:TYR:HE2	1.76	0.50
10:b:155:PHE:HB2	10:b:157:TRP:HE1	1.75	0.50
1:A:176:VAL:HG12	1:A:185:HIS:HA	1.93	0.50
3:D:133:THR:HG21	12:T:25:ILE:HD11	1.94	0.50
7:J:190:VAL:HG13	7:J:213:LEU:HD13	1.93	0.50
7:Q:160:TYR:HD2	7:Q:163:CYS:HB2	1.75	0.50
8:R:80[A]:MET:HE1	8:R:138:MET:SD	2.51	0.50
13:U:23:ALA:HB2	13:U:41:ILE:HD11	1.93	0.50
9:Z:132:VAL:HG12	9:Z:134:LEU:HD11	1.94	0.50
1:A:77:LEU:HD23	1:A:112:TYR:CE2	2.46	0.50
3:C:4:LEU:HD13	3:C:139:MET:SD	2.51	0.50
3:D:125:MET:CE	3:D:139:MET:HB3	2.42	0.50
2:E:195:PRO:CG	11:X:211:ARG:HG2	2.27	0.50
5:H:110:GLU:HA	5:H:154:PHE:HE2	1.77	0.50
6:I:37:GLY:HA2	6:I:181:ILE:HD12	1.94	0.50
7:J:70:ASP:OD1	7:J:71:ARG:N	2.44	0.50
8:K:80:MET:HE2	8:K:87:SER:CA	2.41	0.50
8:K:176:THR:O	8:K:180:GLU:HG3	2.12	0.50
6:N:43:LEU:O	6:N:208:LEU:HB2	2.12	0.50
6:N:208:LEU:CD1	6:N:209:ALA:N	2.74	0.50
6:N:220:LEU:HB3	6:N:221:ASN:C	2.36	0.50
10:P:37:ILE:HG12	10:P:159:ALA:CB	2.35	0.50
10:P:142:ARG:HD3	10:P:143:PRO:O	2.11	0.50
13:U:14:LYS:HA	13:U:19:VAL:HG12	1.94	0.50
13:Y:35:THR:HG22	13:Y:37:ASP:H	1.77	0.50
9:Z:38:LEU:HD12	9:Z:43:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:130:PHE:O	9:Z:152:PRO:HB3	2.12	0.50
1:A:8:PHE:CE1	1:A:13:VAL:HG23	2.45	0.50
3:C:125:MET:CE	3:C:139:MET:HB3	2.42	0.50
9:O:90:LEU:HD21	9:O:114:LEU:CB	2.37	0.50
12:T:181:ARG:NE	12:T:190:ASP:OD1	2.41	0.50
14:W:43:MET:SD	14:W:64:LYS:HG2	2.52	0.50
13:Y:14:LYS:HA	13:Y:19:VAL:HG12	1.94	0.50
13:Y:125:LEU:HD23	13:Y:125:LEU:H	1.75	0.50
2:B:5:GLY:HA3	2:B:110:LEU:HD21	1.93	0.50
2:B:208:THR:HA	11:S:159:GLN:HB2	1.93	0.50
3:C:133:THR:HB	12:T:138:LEU:CD2	2.42	0.50
3:C:133:THR:CG2	12:V:25:ILE:HD11	2.30	0.50
2:E:25:VAL:HG13	11:X:144:MET:HE1	1.93	0.50
1:F:77:LEU:HD23	1:F:112:TYR:CE2	2.46	0.50
4:G:107:ARG:NH2	14:W:81:HIS:HB2	2.27	0.50
5:H:38:ILE:HG12	5:H:169:ALA:HA	1.93	0.50
5:H:146:VAL:HG22	5:H:151:PRO:HA	1.93	0.50
6:I:134:VAL:HG12	6:I:144:LEU:CD1	2.42	0.50
7:J:179:LEU:HB2	7:J:181:MET:HE3	1.94	0.50
9:O:41:ASP:OD1	9:O:186:LEU:HB2	2.12	0.50
10:P:73:LEU:HD23	10:P:135:ILE:HG12	1.92	0.50
7:Q:37:ILE:CD1	7:Q:193:VAL:HG13	2.41	0.50
12:T:114:ALA:CB	12:T:126:LYS:HE2	2.42	0.50
12:V:12:TYR:HA	12:V:183:ILE:O	2.11	0.50
12:V:107:TYR:CE1	12:V:113:PRO:HD3	2.47	0.50
13:Y:142:ALA:HA	13:Y:145:MET:HE3	1.92	0.50
14:a:43:MET:SD	14:a:64:LYS:HG2	2.52	0.50
6:I:42:VAL:CG1	6:I:208:LEU:HD11	2.35	0.50
6:I:145:TYR:HD1	6:I:155:ALA:HA	1.76	0.50
4:L:50:LYS:CB	4:L:59:HIS:HB2	2.41	0.50
6:N:21:TYR:O	6:N:24:GLU:HB2	2.11	0.50
12:V:114:ALA:CB	12:V:126:LYS:HE2	2.42	0.50
9:Z:41:ASP:OD1	9:Z:186:LEU:HB2	2.12	0.50
2:B:202:TYR:OH	11:S:174:LEU:HD13	2.12	0.50
4:G:40:SER:HA	4:G:179:PHE:O	2.11	0.50
4:G:49:LEU:HG	4:G:195:LEU:CD2	2.36	0.50
5:H:85:ALA:O	5:H:89:ILE:HG12	2.12	0.50
7:J:37:ILE:CD1	7:J:193:VAL:HG13	2.41	0.50
4:L:157:ARG:NH1	4:L:176:MET:SD	2.84	0.50
10:P:63:LYS:HE3	10:P:75:TYR:CZ	2.46	0.50
8:R:115:CYS:SG	8:R:154:CYS:HB3	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:64:LEU:HD21	11:X:108:ASN:HD21	1.76	0.50
13:Y:27:PHE:HB2	13:Y:38:PHE:HB2	1.94	0.50
5:H:91:LYS:HZ2	5:H:119:LEU:HD21	1.77	0.49
4:L:148:CYS:HB3	4:L:149:PRO:HD2	1.94	0.49
5:M:85:ALA:O	5:M:89:ILE:HG12	2.12	0.49
6:N:183:THR:HG23	6:N:186:LEU:H	1.76	0.49
11:S:64:LEU:HD21	11:S:108:ASN:HD21	1.76	0.49
13:Y:27:PHE:HB2	13:Y:38:PHE:CG	2.47	0.49
9:Z:21:VAL:O	9:Z:25[B]:MET:HG2	2.12	0.49
10:b:142:ARG:HD3	10:b:143:PRO:O	2.11	0.49
1:A:133:PHE:CZ	14:a:33:LEU:HD13	2.47	0.49
3:C:167:ASP:OD1	3:C:168:SER:N	2.44	0.49
6:I:88:ARG:NH1	12:V:70:ARG:HA	2.27	0.49
7:J:164:ALA:O	7:J:169[A]:ARG:HG3	2.12	0.49
7:J:219:LEU:HD23	7:J:219:LEU:H	1.76	0.49
7:J:230:ASP:OD1	7:J:231:ILE:N	2.45	0.49
5:M:155:HIS:HD2	5:M:168:ARG:HG2	1.77	0.49
12:T:5:ILE:HG22	12:T:16:ALA:O	2.13	0.49
12:T:107:TYR:CE1	12:T:113:PRO:HD3	2.47	0.49
13:U:27:PHE:HB2	13:U:38:PHE:CG	2.47	0.49
14:W:124:TYR:HB2	14:W:137:LEU:HD13	1.93	0.49
5:H:38:ILE:HG12	5:H:169:ALA:CB	2.42	0.49
8:K:115:CYS:SG	8:K:154:CYS:HB3	2.52	0.49
4:L:33:SER:HB3	4:L:51:ARG:CG	2.40	0.49
4:L:57:ALA:CB	5:M:165:CYS:SG	3.01	0.49
9:O:143:TYR:HB2	9:O:146:GLN:NE2	2.28	0.49
10:P:195:LYS:HA	10:P:202:MET:HE3	1.95	0.49
8:R:143:ILE:CD1	8:R:149:PRO:HA	2.42	0.49
11:S:149:LEU:O	11:S:153:VAL:HB	2.12	0.49
13:U:35:THR:HG22	13:U:37:ASP:H	1.76	0.49
13:Y:23:ALA:HB2	13:Y:41:ILE:HD11	1.93	0.49
9:Z:72:MET:CE	9:Z:110:LEU:HD23	2.41	0.49
10:b:64:VAL:HA	10:b:73:LEU:O	2.11	0.49
15:C:301:BZ7:CAV	11:X:131:GLN:NE2	2.74	0.49
4:G:207:THR:HB	4:G:226:ASP:O	2.12	0.49
5:M:58:LEU:HD21	6:N:172:LEU:C	2.37	0.49
11:X:193:LEU:HD21	11:X:195:ILE:HD11	1.94	0.49
9:Z:143:TYR:HB2	9:Z:146:GLN:NE2	2.28	0.49
9:Z:192:LEU:O	9:Z:195:LYS:HB3	2.12	0.49
10:b:158:LYS:HD3	10:b:177:TYR:HE2	1.76	0.49
2:B:111:TYR:CE1	2:B:121:ARG:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:215:THR:CG2	13:U:196:THR:HB	2.43	0.49
5:M:38:ILE:HG12	5:M:169:ALA:CB	2.42	0.49
6:N:134:VAL:HG12	6:N:144:LEU:CD1	2.42	0.49
7:Q:230:ASP:OD1	7:Q:231:ILE:N	2.45	0.49
8:R:176:THR:O	8:R:180:GLU:HG3	2.12	0.49
11:S:174:LEU:O	11:S:178:VAL:HG22	2.12	0.49
12:T:12:TYR:HA	12:T:183:ILE:O	2.11	0.49
9:Z:178:ASP:OD2	9:Z:195:LYS:NZ	2.35	0.49
3:C:33:LYS:O	3:C:45:MET:SD	2.70	0.49
1:F:189:LEU:HD21	14:W:213:HIS:CE1	2.48	0.49
4:G:189:LYS:NZ	4:G:234:GLU:OE2	2.35	0.49
5:H:155:HIS:HD2	5:H:168:ARG:HG2	1.77	0.49
8:K:118:ILE:HG13	8:K:138:MET:HE1	1.93	0.49
8:K:152:TYR:CE1	8:K:162:GLY:HA2	2.48	0.49
6:N:95:ARG:NH1	6:N:101:PRO:HB3	2.27	0.49
9:O:192:LEU:O	9:O:195:LYS:HB3	2.12	0.49
11:S:125:ASP:OD1	11:S:129:SER:HB3	2.13	0.49
11:S:193:LEU:HD21	11:S:195:ILE:HD11	1.95	0.49
9:Z:226:ARG:NH1	9:Z:228:LEU:HD23	2.28	0.49
2:E:193:THR:HG21	11:X:211:ARG:NH2	2.28	0.49
1:F:20:VAL:HG23	1:F:27:VAL:HG23	1.95	0.49
5:H:51:GLU:HA	5:H:215:ILE:HG22	1.95	0.49
7:J:195:LYS:HE2	7:J:199:ILE:HD11	1.92	0.49
4:L:207:THR:HB	4:L:226:ASP:O	2.12	0.49
9:O:130:PHE:O	9:O:152:PRO:HB3	2.12	0.49
9:O:132:VAL:HG12	9:O:134:LEU:CD1	2.43	0.49
10:P:64:VAL:HA	10:P:73:LEU:O	2.11	0.49
11:S:72:LEU:HD23	11:S:83:MET:SD	2.53	0.49
12:T:18:ASP:HB2	12:T:175:LEU:HD22	1.94	0.49
9:Z:132:VAL:HG12	9:Z:134:LEU:CD1	2.43	0.49
5:M:146:VAL:HG22	5:M:151:PRO:HA	1.93	0.49
9:O:81:SER:CB	10:P:118:GLN:HG3	2.42	0.49
10:P:165:ASN:OD1	10:P:168:ASN:HB2	2.13	0.49
13:U:22:ALA:HB1	13:U:170:MET:HG3	1.93	0.49
11:X:72:LEU:HD23	11:X:83:MET:SD	2.53	0.49
13:Y:22:ALA:HB1	13:Y:170:MET:HG3	1.93	0.49
14:a:124:TYR:HB2	14:a:137:LEU:HD13	1.93	0.49
10:b:25:LEU:CD2	10:b:150:PRO:HD2	2.43	0.49
2:B:114:HIS:HB3	2:B:115:PRO:CD	2.42	0.49
3:D:144:ARG:CZ	3:D:147:LEU:HD23	2.43	0.49
4:L:66:VAL:HB	4:L:70:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:110:GLU:HA	5:M:154:PHE:HE2	1.76	0.49
7:Q:229:LYS:NZ	7:Q:233:GLU:OE2	2.19	0.49
11:X:54:CYS:HB3	11:X:61:CYS:SG	2.53	0.49
13:Y:6:ASN:HA	13:Y:28:GLY:O	2.13	0.49
7:J:71:ARG:HB2	7:J:223:ARG:HD3	1.95	0.49
5:M:49:ALA:HB2	5:M:217:LEU:CD1	2.38	0.49
10:P:25:LEU:CD2	10:P:150:PRO:HD2	2.43	0.49
10:P:126:VAL:HG12	8:R:128:ASN:HD22	1.78	0.49
8:R:152:TYR:CE1	8:R:162:GLY:HA2	2.47	0.49
11:S:12:ILE:HG22	11:S:25:SER:HB3	1.94	0.49
12:T:168:GLN:HG3	12:T:196:PHE:CG	2.48	0.49
12:V:5:ILE:HG22	12:V:16:ALA:O	2.13	0.49
12:V:15:VAL:HB	12:V:45:LEU:HD21	1.95	0.49
11:X:125:ASP:OD1	11:X:129:SER:HB3	2.13	0.49
11:X:174:LEU:O	11:X:178:VAL:HG22	2.12	0.49
10:b:165:ASN:OD1	10:b:168:ASN:HB2	2.13	0.49
1:A:57:ASP:OD2	2:B:84:ARG:NH1	2.36	0.48
6:I:95:ARG:NH1	6:I:101:PRO:HB3	2.27	0.48
7:J:51:LYS:NZ	7:J:212:GLU:OE1	2.39	0.48
6:N:46:GLU:CG	6:N:206:ILE:CG2	2.91	0.48
6:N:145:TYR:CD1	6:N:155:ALA:HA	2.48	0.48
9:O:72:MET:CE	9:O:110:LEU:HD23	2.41	0.48
7:Q:71:ARG:HB2	7:Q:223:ARG:HD3	1.95	0.48
12:V:168:GLN:HG3	12:V:196:PHE:CG	2.48	0.48
11:X:12:ILE:HG22	11:X:25:SER:HB3	1.94	0.48
11:X:99:ARG:HG3	11:X:104:TYR:CE2	2.48	0.48
9:Z:56:LEU:HD23	10:b:157:TRP:CE3	2.48	0.48
9:Z:165:GLY:N	9:Z:168:SER:OG	2.46	0.48
1:A:91:ARG:NH1	14:W:58:ALA:HB3	2.27	0.48
2:B:214:GLN:HE22	13:Y:197:ARG:CD	2.26	0.48
3:C:6:PHE:CD1	3:C:139:MET:HE3	2.48	0.48
3:C:144:ARG:CZ	3:C:147:LEU:HD23	2.43	0.48
2:E:111:TYR:CE1	2:E:121:ARG:HB2	2.47	0.48
4:G:56:LEU:CD1	5:H:181:LEU:HB3	2.43	0.48
4:G:204:ASP:OD1	4:G:205:LEU:N	2.47	0.48
5:M:177:ALA:HB2	5:M:205:VAL:HG11	1.94	0.48
5:M:210:LEU:HD23	5:M:211:ASN:N	2.28	0.48
9:O:165:GLY:N	9:O:168:SER:OG	2.46	0.48
7:Q:179:LEU:HB2	7:Q:181:MET:HE3	1.94	0.48
8:R:118:ILE:HG13	8:R:138:MET:HE1	1.93	0.48
8:R:233:ALA:O	8:R:236:ASP:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:27:PHE:HB2	13:U:38:PHE:HB2	1.94	0.48
13:U:66:LEU:HD13	13:U:90:VAL:HG22	1.95	0.48
12:V:1[A]:MET:HE3	12:V:2:GLU:N	2.28	0.48
12:V:18:ASP:HB2	12:V:175:LEU:HD22	1.94	0.48
13:Y:29:ILE:HG22	13:Y:30:GLN:H	1.78	0.48
10:b:123:SER:OG	10:b:124:GLY:N	2.46	0.48
2:E:5:GLY:HA3	2:E:110:LEU:HD21	1.93	0.48
2:E:194:GLU:OE1	2:E:194:GLU:HA	2.09	0.48
4:G:232:PHE:N	4:G:232:PHE:CD2	2.81	0.48
12:T:1:MET:HE1	12:T:133:GLY:HA2	1.94	0.48
12:V:37:LYS:HG3	12:V:188:ILE:CD1	2.44	0.48
10:b:195:LYS:HA	10:b:202:MET:HE3	1.95	0.48
2:E:195:PRO:CG	11:X:211:ARG:CG	2.81	0.48
5:H:190:THR:O	5:H:193:GLU:HB2	2.14	0.48
6:I:145:TYR:CD1	6:I:155:ALA:HA	2.48	0.48
7:Q:116:ALA:HB1	7:Q:155:GLY:O	2.14	0.48
13:U:29:ILE:HG22	13:U:30:GLN:H	1.78	0.48
12:V:107:TYR:HE1	12:V:113:PRO:HD3	1.78	0.48
13:Y:13[A]:MET:HE2	13:Y:166:ILE:HB	1.96	0.48
5:H:26:TYR:CD1	6:I:12:PRO:HA	2.49	0.48
5:H:142:LEU:HG	5:H:170:ILE:HD13	1.95	0.48
7:J:193:VAL:HA	7:J:196:ILE:HD12	1.95	0.48
7:J:203:GLU:HG2	7:J:204:VAL:N	2.28	0.48
8:K:212:PRO:HB2	8:K:232:GLU:CG	2.44	0.48
4:L:88:MET:HE3	4:L:112:ILE:HD11	1.95	0.48
8:R:80[B]:MET:HE2	8:R:87:SER:O	2.13	0.48
8:R:167:ALA:O	8:R:172:GLN:HG3	2.14	0.48
8:R:212:PRO:HB2	8:R:232:GLU:CG	2.44	0.48
13:U:3:MET:HE2	13:U:105:GLU:OE2	2.13	0.48
13:Y:8:GLY:HA3	13:Y:40:LYS:HZ2	1.77	0.48
13:Y:183:GLY:H	13:Y:201:ALA:HB3	1.79	0.48
1:A:20:VAL:HG23	1:A:27:VAL:HG23	1.95	0.48
3:C:138:VAL:HG23	3:C:159:ALA:HA	1.96	0.48
4:L:36:VAL:HG22	4:L:160:SER:CB	2.44	0.48
4:L:49:LEU:HD13	4:L:199:LEU:HD11	1.95	0.48
6:N:35:VAL:HA	6:N:158:ALA:HB2	1.96	0.48
9:O:111:VAL:HG22	9:O:136:TYR:CE2	2.48	0.48
10:P:126:VAL:HG12	8:R:128:ASN:ND2	2.28	0.48
8:R:79:VAL:CG1	8:R:139:ILE:HB	2.44	0.48
11:S:2:PHE:CZ	14:a:105:PRO:HG3	2.47	0.48
13:U:13:MET:HE2	13:U:166:ILE:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:1[A]:MET:HE1	12:V:133:GLY:HA3	1.94	0.48
13:Y:3:MET:HE2	13:Y:105:GLU:OE2	2.13	0.48
3:D:87:MET:SD	3:D:97:MET:HE3	2.54	0.48
4:G:66:VAL:HB	4:G:70:ILE:O	2.13	0.48
7:J:14:PHE:CE2	8:K:132:ARG:HD2	2.49	0.48
8:K:180:GLU:HG2	10:b:53:SER:OG	2.14	0.48
8:K:233:ALA:O	8:K:236:ASP:HB3	2.13	0.48
6:N:37:GLY:HA2	6:N:181:ILE:HD12	1.94	0.48
9:O:42:GLY:CA	9:O:217:THR:HG22	2.40	0.48
7:Q:172:ALA:O	7:Q:176:ILE:HG13	2.13	0.48
11:S:148:LEU:HD22	13:Y:151:SER:CB	2.44	0.48
2:B:179:THR:HG22	2:B:180:LYS:H	1.79	0.48
2:B:214:GLN:NE2	13:Y:197:ARG:HG2	2.28	0.48
1:F:112:TYR:CE1	1:F:121:ARG:HB2	2.49	0.48
4:G:57:ALA:CB	5:H:165:CYS:SG	3.02	0.48
8:K:11:ARG:HG2	8:K:23:TYR:CD2	2.49	0.48
5:M:52:LYS:NZ	5:M:216:GLU:OE2	2.46	0.48
6:N:202:GLY:O	6:N:229:VAL:CG1	2.61	0.48
10:P:5:TYR:HE2	8:R:130:GLU:HA	1.78	0.48
8:R:203:SER:O	8:R:207:SER:N	2.44	0.48
11:S:99:ARG:HG3	11:S:104:TYR:CE2	2.48	0.48
9:Z:46:ALA:CB	9:Z:213:ILE:HG12	2.43	0.48
14:a:51:LEU:HD23	14:a:52:GLY:N	2.29	0.48
1:A:112:TYR:CE1	1:A:121:ARG:HB2	2.49	0.48
1:A:115:LEU:O	1:A:118:MET:HG2	2.14	0.48
2:B:206:PRO:HA	13:Y:164:GLU:OE2	2.13	0.48
2:E:179:THR:HG22	2:E:180:LYS:H	1.79	0.48
4:G:36:VAL:HG22	4:G:160:SER:CB	2.44	0.48
7:J:109:LYS:HA	7:J:149:TYR:CE2	2.34	0.48
7:J:172:ALA:O	7:J:176:ILE:HG13	2.13	0.48
10:P:123:SER:OG	10:P:124:GLY:N	2.46	0.48
7:Q:163:CYS:SG	7:Q:164:ALA:N	2.87	0.48
7:Q:203:GLU:HG2	7:Q:204:VAL:N	2.28	0.48
13:U:193:LYS:O	13:U:194:ILE:HD13	2.14	0.48
11:X:149:LEU:O	11:X:153:VAL:HB	2.12	0.48
13:Y:66:LEU:HD13	13:Y:90:VAL:HG22	1.95	0.48
14:a:138:ALA:O	14:a:143:ALA:HB2	2.14	0.48
2:B:61:SER:CB	10:b:98:LEU:HD21	2.44	0.48
3:C:53:GLN:HE21	15:C:301:BZ7:CBM	2.25	0.48
2:E:184:LYS:HG3	2:E:186:LEU:HD12	1.95	0.48
2:E:193:THR:HB	11:X:211:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:229:VAL:O	4:G:233:LEU:N	2.47	0.48
5:H:52:LYS:NZ	5:H:216:GLU:OE2	2.46	0.48
5:H:177:ALA:HB2	5:H:205:VAL:HG11	1.95	0.48
5:H:210:LEU:HD23	5:H:211:ASN:N	2.28	0.48
6:I:77:THR:OG1	9:Z:155:ASN:OD1	2.31	0.48
8:K:143:ILE:CD1	8:K:149:PRO:HA	2.42	0.48
8:K:228:ARG:HH22	8:K:230:LEU:HD21	1.79	0.48
5:M:190:THR:O	5:M:193:GLU:HB2	2.14	0.48
9:O:46:ALA:CB	9:O:213:ILE:HG12	2.43	0.48
7:Q:193:VAL:HA	7:Q:196:ILE:HD12	1.95	0.48
8:R:228:ARG:HH22	8:R:230:LEU:HD21	1.79	0.48
11:S:72:LEU:HD21	11:S:88:ILE:HG12	1.96	0.48
11:S:92:LEU:HD23	11:S:110:ILE:HD11	1.96	0.48
13:U:6:ASN:HA	13:U:28:GLY:O	2.13	0.48
12:V:103:LEU:HG	12:V:132:HIS:HE1	1.79	0.48
14:W:5:MET:HE3	14:W:30:TYR:CE1	2.46	0.48
14:a:96:MET:SD	14:a:106:LEU:HB2	2.54	0.48
10:b:17:LYS:HG2	10:b:22:GLU:OE2	2.14	0.48
2:B:172:ASN:OD1	2:B:191:SER:HA	2.14	0.47
4:G:126:ARG:HH11	5:H:15:PHE:HZ	1.62	0.47
5:H:40:ILE:HG23	5:H:167:ALA:HB2	1.96	0.47
5:H:88:LEU:HD22	5:H:116:VAL:CG1	2.43	0.47
7:J:163:CYS:SG	7:J:164:ALA:N	2.87	0.47
8:K:79:VAL:CG1	8:K:139:ILE:HB	2.44	0.47
5:M:113:THR:O	5:M:117:SER:CB	2.62	0.47
9:O:114:LEU:HD23	9:O:136:TYR:OH	2.14	0.47
11:S:54:CYS:HB3	11:S:61:CYS:SG	2.53	0.47
11:S:174:LEU:O	11:S:178:VAL:HG13	2.14	0.47
12:T:15:VAL:HB	12:T:45:LEU:HD21	1.95	0.47
12:T:37:LYS:HG3	12:T:188:ILE:CD1	2.44	0.47
12:V:171:PHE:HE2	12:V:173:LEU:HB2	1.79	0.47
11:X:72:LEU:HD21	11:X:88:ILE:HG12	1.96	0.47
3:D:6:PHE:CD1	3:D:139:MET:HE3	2.48	0.47
3:D:115:ASP:OD1	3:D:116:GLU:N	2.47	0.47
5:H:155:HIS:CD2	5:H:168:ARG:HG2	2.49	0.47
6:I:5:ARG:HH22	9:Z:2:SER:HG	1.56	0.47
6:I:60:ARG:HH12	6:I:219:ILE:HD13	1.79	0.47
7:J:30:VAL:HG22	7:J:133[B]:CYS:HA	1.96	0.47
7:J:70:ASP:OD1	7:J:71:ARG:HD3	2.15	0.47
7:J:116:ALA:HB1	7:J:155:GLY:O	2.14	0.47
5:M:51:GLU:HA	5:M:215:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:142:LEU:HG	5:M:170:ILE:HD13	1.95	0.47
5:M:155:HIS:CD2	5:M:168:ARG:HG2	2.49	0.47
10:P:64:VAL:O	10:P:219:ARG:HD3	2.14	0.47
14:a:5:MET:HE3	14:a:30:TYR:CE1	2.46	0.47
2:B:32:GLU:OE2	2:B:187:ARG:NH1	2.47	0.47
3:C:112:TYR:CE1	3:C:122:SER:HB2	2.45	0.47
3:D:85:ASN:O	3:D:89:GLN:HG3	2.14	0.47
2:E:32:GLU:OE2	2:E:187:ARG:NH1	2.47	0.47
7:J:110:HIS:O	7:J:114:ARG:HG2	2.14	0.47
5:M:73:HIS:CE1	5:M:106:THR:HB	2.49	0.47
7:Q:185:THR:O	7:Q:189:ILE:HG12	2.14	0.47
8:R:11:ARG:HG2	8:R:23:TYR:CD2	2.49	0.47
11:S:38:ARG:NH1	11:S:191:ASP:OD1	2.48	0.47
11:S:96:LEU:HD11	11:S:108:ASN:ND2	2.27	0.47
13:U:186:VAL:N	13:U:197:ARG:O	2.46	0.47
10:b:9:LEU:HG	10:b:125:GLY:HA2	1.96	0.47
1:A:159:ILE:O	1:A:163:MET:HG3	2.15	0.47
2:B:184:LYS:HG3	2:B:186:LEU:HD12	1.95	0.47
3:C:162:TYR:HE2	12:T:145:ARG:HA	1.80	0.47
15:D:301:BZ7:CAV	11:S:131:GLN:HG2	2.44	0.47
2:E:58:MET:HE3	2:E:62:LYS:HE3	1.96	0.47
1:F:197:TYR:OH	1:F:199:GLU:HB2	2.15	0.47
4:G:96:ARG:CZ	4:G:102:PRO:HG3	2.44	0.47
6:I:169:ARG:O	6:I:173:GLU:HG3	2.14	0.47
7:J:6:GLY:HA2	7:J:8:ASP:OD1	2.14	0.47
4:L:204:ASP:OD1	4:L:205:LEU:N	2.47	0.47
7:Q:10:SER:OG	7:Q:126:SER:HA	2.14	0.47
12:T:103:LEU:HG	12:T:132:HIS:HE1	1.79	0.47
14:W:138:ALA:O	14:W:143:ALA:HB2	2.14	0.47
9:Z:114:LEU:HD23	9:Z:136:TYR:OH	2.14	0.47
3:C:87:MET:SD	3:C:97:MET:HE3	2.54	0.47
4:G:49:LEU:HD13	4:G:199:LEU:HD11	1.95	0.47
4:G:229:VAL:O	4:G:233:LEU:CB	2.43	0.47
6:I:94:HIS:CG	6:I:102:VAL:HG12	2.50	0.47
6:N:4:ASP:HA	6:N:122:ASN:HB3	1.96	0.47
6:N:5:ARG:HG3	9:O:6:ASP:OD2	2.14	0.47
7:Q:6:GLY:HA2	7:Q:8:ASP:OD1	2.14	0.47
8:R:130:GLU:OE1	8:R:130:GLU:N	2.44	0.47
12:V:123:ALA:HB2	13:Y:56:ALA:HB3	1.96	0.47
14:W:51:LEU:HD23	14:W:52:GLY:N	2.29	0.47
9:Z:56:LEU:HD23	10:b:157:TRP:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:223:THR:O	10:b:226:LYS:HB3	2.15	0.47
1:A:152:ARG:HH11	1:A:177:THR:HG1	1.51	0.47
2:B:11:GLY:HA2	2:B:108:PRO:HG3	1.97	0.47
3:C:85:ASN:O	3:C:89:GLN:HG3	2.14	0.47
3:D:133:THR:HB	12:V:138:LEU:CD2	2.43	0.47
1:F:159:ILE:O	1:F:163:MET:HG3	2.15	0.47
8:K:162:GLY:HA3	10:b:60:SER:HB3	1.97	0.47
8:K:167:ALA:O	8:K:172:GLN:HG3	2.14	0.47
9:O:33:THR:HB	9:O:166:ASN:O	2.15	0.47
10:P:185:ASP:O	10:P:189:THR:HG23	2.15	0.47
8:R:79:VAL:HG13	8:R:139:ILE:HB	1.96	0.47
12:T:103:LEU:HG	12:T:132:HIS:CE1	2.50	0.47
12:T:107:TYR:HE1	12:T:113:PRO:HD3	1.78	0.47
13:U:8:GLY:HA3	13:U:40:LYS:HZ3	1.76	0.47
13:U:27:PHE:HB3	13:U:35:THR:HB	1.97	0.47
13:Y:21:ILE:HG22	13:Y:187:HIS:HB2	1.95	0.47
3:C:115:ASP:OD1	3:C:116:GLU:N	2.47	0.47
3:D:42:LEU:HD11	3:D:177:TYR:CD2	2.50	0.47
2:E:114:HIS:HB3	2:E:115:PRO:CD	2.41	0.47
1:F:128:GLY:O	1:F:131:SER:OG	2.28	0.47
4:G:158:ALA:O	7:J:57:LEU:HD13	2.15	0.47
4:G:225:ASP:O	4:G:228:ASP:N	2.48	0.47
5:H:195:ILE:CG2	5:H:217:LEU:HD21	2.44	0.47
7:J:28:LYS:HG2	7:J:31:GLU:OE2	2.15	0.47
7:J:51:LYS:HD2	7:J:63:ASN:O	2.15	0.47
8:K:161:CYS:O	8:K:163:PHE:CD2	2.67	0.47
4:L:96:ARG:CZ	4:L:102:PRO:HG3	2.44	0.47
4:L:176:MET:HA	4:L:179:PHE:CD2	2.49	0.47
4:L:225:ASP:O	4:L:228:ASP:N	2.48	0.47
6:N:73:PHE:HA	6:N:130:SER:O	2.15	0.47
6:N:94:HIS:CG	6:N:102:VAL:HG12	2.50	0.47
6:N:169:ARG:O	6:N:173:GLU:HG3	2.14	0.47
6:N:176:TYR:OH	6:N:181:ILE:HD13	2.15	0.47
10:P:46:ALA:HA	10:P:208:GLU:O	2.15	0.47
10:P:223:THR:O	10:P:226:LYS:HB3	2.15	0.47
7:Q:70:ASP:OD1	7:Q:71:ARG:HD3	2.15	0.47
7:Q:181:MET:SD	7:Q:181:MET:N	2.87	0.47
11:S:35:ILE:HB	14:a:151:ARG:HH12	1.79	0.47
12:T:22:ALA:HB1	12:V:172:ILE:HD12	1.97	0.47
14:W:96:MET:SD	14:W:106:LEU:HB2	2.54	0.47
9:Z:148:TYR:HD1	9:Z:158:GLY:HA2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:GLY:C	3:C:176:MET:HE1	2.40	0.47
3:C:177:TYR:CE1	3:C:186:LYS:HG3	2.50	0.47
3:D:43:GLY:HA2	3:D:100:MET:O	2.15	0.47
3:D:78:ALA:HB2	6:N:98:VAL:HG13	1.96	0.47
2:E:11:GLY:HA2	2:E:108:PRO:HG3	1.97	0.47
4:G:176:MET:HA	4:G:179:PHE:CD2	2.49	0.47
6:I:4:ASP:HA	6:I:122:ASN:HB3	1.96	0.47
7:J:185:THR:O	7:J:189:ILE:HG12	2.14	0.47
8:K:18:PRO:HA	10:b:23:TYR:CD1	2.49	0.47
8:K:162:GLY:CA	10:b:57:ASP:HB3	2.44	0.47
4:L:105:VAL:HG21	4:L:136:GLY:HA3	1.97	0.47
9:O:25[B]:MET:HA	9:O:25[B]:MET:HE3	1.97	0.47
10:P:9:LEU:HG	10:P:125:GLY:HA2	1.96	0.47
11:S:31:GLU:OE1	11:S:36:HIS:NE2	2.47	0.47
12:T:4:LEU:HD11	12:T:47:VAL:HG13	1.96	0.47
12:T:171:PHE:HE2	12:T:173:LEU:HB2	1.79	0.47
12:T:173:LEU:HD23	12:V:173:LEU:HD23	1.97	0.47
13:U:120:ILE:HD12	13:U:136:VAL:HG13	1.96	0.47
12:V:175:LEU:HB3	12:V:178:PHE:HE1	1.80	0.47
9:Z:111:VAL:HG22	9:Z:136:TYR:CE2	2.48	0.47
3:D:31:VAL:HG22	11:S:131:GLN:OE1	2.15	0.47
3:D:177:TYR:CE1	3:D:186:LYS:HG3	2.50	0.47
2:E:18:THR:HG1	2:E:172:ASN:N	2.11	0.47
6:I:35:VAL:HA	6:I:158:ALA:HB2	1.95	0.47
7:J:215:TRP:CE2	7:J:219:LEU:HD11	2.50	0.47
4:L:109:VAL:HG22	4:L:134:ILE:HD12	1.97	0.47
5:M:40:ILE:HG23	5:M:167:ALA:HB2	1.96	0.47
9:O:106:PRO:HG2	12:T:73:TYR:OH	2.15	0.47
7:Q:30:VAL:HG22	7:Q:133[B]:CYS:HA	1.97	0.47
7:Q:51:LYS:HD2	7:Q:63:ASN:O	2.15	0.47
7:Q:110:HIS:O	7:Q:114:ARG:HG2	2.14	0.47
12:T:35:MET:HB2	12:T:181:ARG:NH1	2.29	0.47
13:Y:193:LYS:O	13:Y:194:ILE:HD13	2.14	0.47
1:A:197:TYR:OH	1:A:199:GLU:HB2	2.15	0.47
15:C:301:BZ7:CAE	11:X:127:VAL:HG11	2.45	0.47
3:D:138:VAL:HG23	3:D:159:ALA:HA	1.96	0.47
3:D:174:VAL:HG23	3:D:192:VAL:CG2	2.43	0.47
1:F:15:GLY:HA2	1:F:174:TYR:O	2.15	0.47
4:G:105:VAL:HG21	4:G:136:GLY:HA3	1.97	0.47
7:J:181:MET:N	7:J:181:MET:SD	2.87	0.47
4:L:69:HIS:CE1	4:L:102:PRO:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:105:VAL:HG12	4:L:145:PHE:CE2	2.50	0.47
4:L:219:LEU:HG	4:L:220:GLU:O	2.15	0.47
5:M:91:LYS:HZ3	5:M:119:LEU:CD2	2.21	0.47
9:O:145:PHE:CZ	9:O:218:ARG:HG2	2.50	0.47
11:S:92:LEU:CD2	11:S:110:ILE:HD11	2.45	0.47
11:X:92:LEU:HD23	11:X:110:ILE:HD11	1.96	0.47
11:X:174:LEU:O	11:X:178:VAL:HG13	2.14	0.47
9:Z:33:THR:HB	9:Z:166:ASN:O	2.15	0.47
9:Z:143:TYR:HB2	9:Z:146:GLN:HE21	1.80	0.47
10:b:185:ASP:O	10:b:189:THR:HG23	2.15	0.47
1:A:24:GLU:HG3	14:a:182:ARG:HG2	1.97	0.46
2:B:58:MET:HE3	2:B:62:LYS:HE3	1.96	0.46
3:C:43:GLY:HA2	3:C:100:MET:O	2.15	0.46
2:E:90:TYR:HD2	2:E:94:VAL:HG21	1.80	0.46
1:F:38:HIS:CD2	1:F:39:GLU:H	2.33	0.46
4:G:36:VAL:HG22	4:G:160:SER:OG	2.15	0.46
4:G:69:HIS:CE1	4:G:102:PRO:HB3	2.50	0.46
4:G:229:VAL:HG23	4:G:233:LEU:CD1	2.24	0.46
5:H:73:HIS:CE1	5:H:106:THR:HB	2.49	0.46
7:J:10:SER:OG	7:J:126:SER:HA	2.14	0.46
7:J:150:MET:HE1	7:J:169[B]:ARG:HH22	1.80	0.46
10:P:23:TYR:CE1	8:R:18:PRO:HA	2.50	0.46
7:Q:211:LEU:HD23	7:Q:236:GLU:CG	2.46	0.46
8:R:118:ILE:HG21	8:R:138:MET:CE	2.45	0.46
12:V:35:MET:HB2	12:V:181:ARG:NH1	2.30	0.46
11:X:38:ARG:NH1	11:X:191:ASP:OD1	2.48	0.46
11:X:92:LEU:CD2	11:X:110:ILE:HD11	2.45	0.46
9:Z:145:PHE:CZ	9:Z:218:ARG:HG2	2.50	0.46
10:b:64:VAL:O	10:b:219:ARG:HD3	2.14	0.46
3:D:29:LEU:HD22	13:Y:176:ARG:NH1	2.30	0.46
2:E:152:GLN:NE2	2:E:189:LEU:HD21	2.29	0.46
2:E:172:ASN:OD1	2:E:191:SER:HA	2.14	0.46
1:F:48:SER:HB3	1:F:51:ASP:HB2	1.98	0.46
4:G:57:ALA:HA	5:H:165:CYS:HA	1.97	0.46
6:I:176:TYR:OH	6:I:181:ILE:HD13	2.15	0.46
8:K:79:VAL:HG13	8:K:139:ILE:HB	1.96	0.46
5:M:30:ALA:HB2	6:N:14:GLY:CA	2.46	0.46
9:O:35:LEU:HB3	9:O:163:CYS:HB2	1.97	0.46
11:S:11:THR:HG23	11:S:138:GLY:O	2.16	0.46
13:Y:120:ILE:HD12	13:Y:136:VAL:HG13	1.96	0.46
14:a:7:THR:HA	14:a:55:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:PHE:CE2	3:C:10:HIS:HB2	2.51	0.46
3:D:8:PHE:CE2	3:D:10:HIS:HB2	2.51	0.46
4:G:7:ASP:O	4:G:21:GLN:NE2	2.48	0.46
6:I:73:PHE:HA	6:I:130:SER:O	2.15	0.46
7:Q:215:TRP:CE2	7:Q:219:LEU:HD11	2.50	0.46
11:S:145:LEU:CD2	11:S:178:VAL:HB	2.45	0.46
13:U:184:VAL:HB	13:U:199:LEU:HB2	1.97	0.46
12:V:4:LEU:HD11	12:V:47:VAL:HG13	1.96	0.46
13:Y:184:VAL:HB	13:Y:199:LEU:HB2	1.97	0.46
9:Z:28:ILE:HG21	9:Z:133:SER:OG	2.16	0.46
1:A:48:SER:HB3	1:A:51:ASP:HB2	1.98	0.46
6:I:33:VAL:CG2	6:I:168:VAL:HG11	2.46	0.46
6:I:127:PHE:O	6:I:149:PRO:HB3	2.15	0.46
5:M:195:ILE:CG2	5:M:217:LEU:HD21	2.44	0.46
9:O:143:TYR:HB2	9:O:146:GLN:HE21	1.80	0.46
7:Q:70:ASP:OD1	7:Q:71:ARG:N	2.44	0.46
7:Q:109:LYS:HA	7:Q:149:TYR:CE2	2.34	0.46
13:U:21:ILE:HG22	13:U:187:HIS:HB2	1.95	0.46
11:X:11:THR:HG23	11:X:138:GLY:O	2.16	0.46
13:Y:189:ILE:HA	13:Y:194:ILE:HD12	1.98	0.46
2:B:28:ASP:OD2	2:B:31:CYS:HB3	2.16	0.46
2:B:90:TYR:HD2	2:B:94:VAL:HG21	1.80	0.46
3:D:112:TYR:CE1	3:D:122:SER:HB2	2.45	0.46
5:H:84:ASP:HB2	5:H:139:VAL:HG23	1.98	0.46
4:L:69:HIS:CD2	4:L:70:ILE:HG13	2.50	0.46
11:S:46:LEU:HG	11:S:52:ILE:HG22	1.97	0.46
12:T:2:GLU:CG	12:T:34:LYS:HE2	2.45	0.46
13:U:50:ILE:HG23	13:U:50:ILE:O	2.16	0.46
13:U:159:PRO:O	13:U:162:LEU:HB3	2.16	0.46
13:U:183:GLY:H	13:U:201:ALA:HB3	1.79	0.46
12:V:43:LEU:HD12	12:V:183:ILE:HD11	1.97	0.46
13:Y:159:PRO:O	13:Y:162:LEU:HB3	2.16	0.46
9:Z:214:ALA:HA	9:Z:227:VAL:HA	1.98	0.46
1:A:28:ASN:ND2	1:A:30:VAL:H	2.13	0.46
2:B:212:LEU:HD21	13:Y:200:LYS:HG3	1.98	0.46
3:C:46:SER:HB3	3:C:98:GLY:O	2.16	0.46
3:C:192:VAL:O	3:C:195:LEU:HB2	2.15	0.46
3:D:31:VAL:HG21	15:D:301:BZ7:CBK	2.46	0.46
4:G:88:MET:HE3	4:G:112:ILE:HD11	1.95	0.46
4:G:105:VAL:HG12	4:G:145:PHE:CE2	2.50	0.46
11:S:35:ILE:O	14:a:151:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:103:LEU:HG	12:V:132:HIS:CE1	2.50	0.46
13:Y:186:VAL:N	13:Y:197:ARG:O	2.46	0.46
9:Z:35:LEU:HB3	9:Z:163:CYS:HB2	1.97	0.46
2:B:3:ILE:HD12	2:B:99:ILE:HG22	1.97	0.46
3:C:56:GLU:O	3:C:59:LEU:HB3	2.16	0.46
1:F:65:LEU:O	1:F:69:GLU:HG3	2.16	0.46
4:G:84:LEU:O	4:G:88:MET:HG3	2.16	0.46
8:K:14:THR:HG22	8:K:24:GLN:HB2	1.98	0.46
8:K:56:VAL:HG13	8:K:61:LEU:HB2	1.98	0.46
8:K:203:SER:O	8:K:207:SER:N	2.44	0.46
6:N:132:LEU:HG	6:N:161:ILE:CD1	2.41	0.46
9:O:103:GLU:HB2	9:O:104:PRO:HD2	1.97	0.46
12:T:175:LEU:HB3	12:T:178:PHE:HE1	1.80	0.46
13:U:65:ARG:O	13:U:68:PHE:HB3	2.16	0.46
14:W:103:MET:HE1	11:X:2:PHE:HD2	1.81	0.46
13:Y:3:MET:HE2	13:Y:105:GLU:CD	2.41	0.46
10:b:106:THR:O	10:b:110:VAL:HG23	2.16	0.46
1:A:15:GLY:HA2	1:A:174:TYR:O	2.15	0.46
2:B:28:ASP:HB2	13:Y:130:MET:SD	2.55	0.46
2:B:208:THR:HG22	11:S:159:GLN:O	2.15	0.46
3:D:192:VAL:O	3:D:195:LEU:HB2	2.15	0.46
3:D:197:HIS:CE1	13:Y:200:LYS:HZ2	2.33	0.46
1:F:189:LEU:HD22	14:W:209:TRP:HB2	1.96	0.46
4:G:109:VAL:HG12	4:G:153:TYR:CG	2.51	0.46
4:G:109:VAL:HG22	4:G:134:ILE:HD12	1.97	0.46
7:J:37:ILE:HG12	7:J:197:ILE:HD11	1.98	0.46
7:J:94:GLU:OE2	7:J:114:ARG:HG3	2.15	0.46
4:L:109:VAL:HG12	4:L:153:TYR:CG	2.51	0.46
5:M:110:GLU:CA	5:M:154:PHE:HE2	2.29	0.46
5:M:169:ALA:C	5:M:174:SER:HB2	2.41	0.46
6:N:46:GLU:HG3	6:N:199:VAL:HG22	1.98	0.46
6:N:105:GLU:HA	6:N:145:TYR:CE2	2.51	0.46
9:O:148:TYR:HD1	9:O:158:GLY:HA2	1.80	0.46
8:R:112:ASP:HA	8:R:152:TYR:CE2	2.51	0.46
11:S:92:LEU:HD23	11:S:124:PHE:CE2	2.51	0.46
12:V:43:LEU:CD1	12:V:183:ILE:HD11	2.46	0.46
11:X:120:ALA:HB2	11:X:132:ARG:NH2	2.31	0.46
9:Z:151:ASP:HB2	9:Z:152:PRO:CD	2.46	0.46
10:b:37:ILE:HG23	10:b:159:ALA:HB2	1.98	0.46
10:b:46:ALA:HA	10:b:208:GLU:O	2.15	0.46
10:b:90:ARG:O	10:b:94:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:GLN:O	2:B:146:MET:HG3	2.16	0.46
2:B:214:GLN:HE22	13:Y:197:ARG:NE	2.13	0.46
3:C:174:VAL:HG23	3:C:192:VAL:CG2	2.43	0.46
3:D:50:ALA:HB2	11:S:129:SER:HB2	1.96	0.46
5:H:110:GLU:CA	5:H:154:PHE:HE2	2.29	0.46
4:L:36:VAL:HG22	4:L:160:SER:OG	2.15	0.46
5:M:196:LYS:O	5:M:200:ILE:HG13	2.16	0.46
6:N:43:LEU:HD11	6:N:134:VAL:CG2	2.46	0.46
9:O:49:ARG:HH21	9:O:209:GLU:HA	1.81	0.46
9:O:79:ILE:HG21	9:O:82:ASP:OD2	2.16	0.46
9:O:144:GLY:O	9:O:146:GLN:HG3	2.16	0.46
7:Q:237:LYS:O	7:Q:241:GLU:HG3	2.16	0.46
8:R:14:THR:HG22	8:R:24:GLN:HB2	1.98	0.46
8:R:130:GLU:OE2	8:R:131:MET:HE1	2.16	0.46
11:S:11:THR:N	11:S:26:ASP:OD1	2.49	0.46
12:T:43:LEU:HD12	12:T:183:ILE:HD11	1.97	0.46
13:U:50:ILE:HD13	13:U:66:LEU:CD2	2.45	0.46
12:V:146:TYR:HB2	12:V:159:LEU:HD13	1.98	0.46
14:W:7:THR:HA	14:W:55:GLY:O	2.16	0.46
11:X:92:LEU:HD23	11:X:124:PHE:CE2	2.51	0.46
13:Y:27:PHE:HB3	13:Y:35:THR:HB	1.97	0.46
13:Y:50:ILE:HG23	13:Y:50:ILE:O	2.16	0.46
14:a:67:LEU:HD13	14:a:91:TRP:CZ3	2.51	0.46
10:b:45:LEU:N	10:b:210:GLY:O	2.42	0.46
1:A:132:THR:HG23	1:A:133:PHE:CE1	2.51	0.46
3:C:18:SER:HG	3:C:173:VAL:N	2.14	0.46
4:G:69:HIS:CD2	4:G:70:ILE:HG13	2.50	0.46
4:G:155:ASP:OD2	7:J:59:GLU:HG3	2.15	0.46
8:K:58:ASP:HB3	8:K:61:LEU:HG	1.98	0.46
5:M:221:GLN:HB2	5:M:224:GLN:HB3	1.98	0.46
6:N:208:LEU:HD12	6:N:208:LEU:C	2.41	0.46
10:P:8:SER:HA	10:P:123:SER:O	2.16	0.46
10:P:13:SER:HB3	10:P:19:VAL:HG13	1.98	0.46
8:R:58:ASP:HB3	8:R:61:LEU:HG	1.98	0.46
12:T:13:VAL:HG11	12:T:105:ALA:CB	2.43	0.46
12:V:140:LEU:CD1	13:Y:32:GLN:HE21	2.28	0.46
11:X:145:LEU:CD2	11:X:178:VAL:HB	2.45	0.46
13:Y:18:CYS:HA	13:Y:189:ILE:O	2.16	0.46
9:Z:35:LEU:HD23	9:Z:163:CYS:SG	2.56	0.46
9:Z:49:ARG:HH21	9:Z:209:GLU:HA	1.81	0.46
10:b:65:GLU:HB3	10:b:90:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:HIS:CD2	1:A:39:GLU:H	2.33	0.45
3:D:46:SER:HB3	3:D:98:GLY:O	2.16	0.45
4:G:98:VAL:HG12	4:G:99:PHE:CD1	2.51	0.45
4:G:219:LEU:HG	4:G:220:GLU:O	2.15	0.45
5:H:110:GLU:HA	5:H:154:PHE:CE2	2.51	0.45
6:I:82:ILE:HG13	9:Z:119:GLN:OE1	2.15	0.45
6:I:137:ASP:O	6:I:140:GLY:N	2.39	0.45
7:J:106:ILE:HD11	7:J:110:HIS:HD2	1.81	0.45
7:J:211:LEU:HD23	7:J:236:GLU:CG	2.45	0.45
6:N:33:VAL:CG2	6:N:168:VAL:HG11	2.46	0.45
6:N:127:PHE:O	6:N:149:PRO:HB3	2.15	0.45
10:P:37:ILE:HG23	10:P:159:ALA:HB2	1.98	0.45
7:Q:94:GLU:OE2	7:Q:114:ARG:HG3	2.15	0.45
7:Q:195:LYS:HG2	7:Q:199:ILE:CD1	2.46	0.45
14:W:68:GLY:HA2	14:W:71:VAL:HG22	1.98	0.45
14:a:157:GLN:HG2	14:a:159:VAL:O	2.16	0.45
2:B:76:VAL:HG11	2:B:109:GLN:HB2	1.99	0.45
3:C:42:LEU:HD11	3:C:177:TYR:CD2	2.50	0.45
2:E:3:ILE:HD12	2:E:99:ILE:HG22	1.97	0.45
2:E:143:GLN:O	2:E:146:MET:HG3	2.16	0.45
2:E:193:THR:HG21	11:X:213:ASP:CG	2.41	0.45
1:F:99:MET:SD	1:F:125:ALA:HB1	2.57	0.45
5:H:196:LYS:O	5:H:200:ILE:HG13	2.16	0.45
8:K:118:ILE:HG21	8:K:138:MET:CE	2.45	0.45
6:N:37:GLY:O	6:N:142:PRO:HG3	2.16	0.45
9:O:35:LEU:HD23	9:O:163:CYS:SG	2.56	0.45
9:O:151:ASP:HB2	9:O:152:PRO:CD	2.46	0.45
10:P:90:ARG:O	10:P:94:GLN:HG2	2.16	0.45
7:Q:33:SER:OG	7:Q:34:SER:N	2.49	0.45
8:R:111:VAL:HG21	8:R:142:GLY:HA3	1.99	0.45
12:T:121:LEU:O	13:U:57:THR:HB	2.16	0.45
11:X:31:GLU:OE1	11:X:36:HIS:NE2	2.47	0.45
11:X:46:LEU:HG	11:X:52:ILE:HG22	1.97	0.45
9:Z:59:VAL:HG22	10:b:142:ARG:HH22	1.82	0.45
1:A:75:LEU:CD2	1:A:104:ASP:HB2	2.46	0.45
1:A:99:MET:SD	1:A:125:ALA:HB1	2.57	0.45
2:B:13:ILE:HG12	2:B:155:LEU:HD13	1.99	0.45
6:I:43:LEU:HD11	6:I:134:VAL:CG2	2.46	0.45
7:J:33:SER:OG	7:J:34:SER:N	2.49	0.45
7:J:195:LYS:HG2	7:J:199:ILE:CD1	2.46	0.45
4:L:7:ASP:O	4:L:21:GLN:NE2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:34:GLY:O	5:M:172:SER:HB3	2.17	0.45
6:N:115:LYS:NZ	6:N:129:ILE:HG13	2.31	0.45
10:P:70:HIS:CE1	10:P:103:PRO:HB3	2.51	0.45
7:Q:28:LYS:HG2	7:Q:31:GLU:OE2	2.15	0.45
7:Q:31:GLU:O	7:Q:167:LYS:HA	2.17	0.45
7:Q:37:ILE:HG12	7:Q:197:ILE:HD11	1.98	0.45
7:Q:75:MET:HE2	7:Q:77:VAL:HG12	1.98	0.45
8:R:56:VAL:HG13	8:R:61:LEU:HB2	1.98	0.45
12:T:146:TYR:HB2	12:T:159:LEU:HD13	1.98	0.45
13:U:48:LEU:HD21	13:U:86:LEU:HD22	1.99	0.45
13:U:151:SER:CB	11:X:148:LEU:HD22	2.46	0.45
11:X:11:THR:N	11:X:26:ASP:OD1	2.49	0.45
9:Z:38:LEU:N	9:Z:160:LYS:O	2.31	0.45
9:Z:49:ARG:HD3	9:Z:212:GLU:HG3	1.99	0.45
9:Z:68:LEU:HD11	9:Z:74:CYS:CB	2.38	0.45
9:Z:144:GLY:O	9:Z:146:GLN:HG3	2.16	0.45
10:b:70:HIS:CE1	10:b:103:PRO:HB3	2.51	0.45
3:D:38:ASN:HD22	3:D:41:LEU:HD12	1.81	0.45
3:D:40:TYR:HB2	3:D:179:MET:CE	2.29	0.45
3:D:156:GLY:C	3:D:176:MET:HE1	2.40	0.45
1:F:75:LEU:CD2	1:F:104:ASP:HB2	2.46	0.45
4:G:126:ARG:HD2	5:H:21:LEU:HD21	1.98	0.45
7:J:237:LYS:O	7:J:241:GLU:HG3	2.16	0.45
8:K:72:ILE:CG1	8:K:78:CYS:HB2	2.47	0.45
8:K:210:PHE:CD2	8:K:215:ILE:HG21	2.52	0.45
9:O:25[B]:MET:SD	9:O:152:PRO:HD2	2.57	0.45
9:O:35:LEU:HB3	9:O:163:CYS:SG	2.57	0.45
7:Q:37:ILE:HD13	7:Q:196:ILE:CG2	2.45	0.45
8:R:72:ILE:CG1	8:R:78:CYS:HB2	2.47	0.45
8:R:210:PHE:CD2	8:R:215:ILE:HG21	2.52	0.45
12:V:5:ILE:CG2	12:V:16:ALA:HB3	2.47	0.45
12:V:77:PRO:HD2	12:V:108:ASP:HB2	1.98	0.45
12:V:175:LEU:HB3	12:V:178:PHE:CE1	2.52	0.45
11:X:96:LEU:HD11	11:X:108:ASN:ND2	2.27	0.45
13:Y:50:ILE:HD13	13:Y:66:LEU:CD2	2.45	0.45
9:Z:79:ILE:HG21	9:Z:82:ASP:OD2	2.16	0.45
3:C:38:ASN:HD22	3:C:41:LEU:HD12	1.81	0.45
3:D:30:ARG:HH12	11:S:134:SER:H	1.65	0.45
3:D:56:GLU:O	3:D:59:LEU:HB3	2.16	0.45
6:I:37:GLY:O	6:I:142:PRO:HG3	2.16	0.45
5:M:75:GLY:HA3	5:M:226:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:127:LYS:HD2	10:P:122:GLN:O	2.16	0.45
11:S:120:ALA:HB2	11:S:132:ARG:NH2	2.31	0.45
12:T:4:LEU:HD23	12:T:17:SER:HB3	1.98	0.45
13:U:3:MET:HE2	13:U:105:GLU:CD	2.41	0.45
13:U:189:ILE:HA	13:U:194:ILE:HD12	1.98	0.45
12:V:2:GLU:CG	12:V:34:LYS:HE2	2.45	0.45
9:Z:44:LEU:HD21	9:Z:189:ALA:C	2.42	0.45
9:Z:92[B]:LEU:HA	9:Z:92[B]:LEU:HD12	1.41	0.45
3:D:142:GLY:O	3:D:155:LEU:HD22	2.17	0.45
3:D:162:TYR:HE2	12:V:145:ARG:HA	1.79	0.45
5:H:75:GLY:HA3	5:H:226:PHE:CE1	2.52	0.45
5:H:191:LEU:CD2	5:H:221:GLN:HE21	2.26	0.45
7:J:37:ILE:HD13	7:J:196:ILE:CG2	2.45	0.45
7:J:85:ARG:O	7:J:88:ALA:HB3	2.17	0.45
8:K:130:GLU:OE1	8:K:130:GLU:N	2.44	0.45
8:K:176:THR:HG23	10:b:55:LEU:CD1	2.44	0.45
4:L:98:VAL:HG12	4:L:99:PHE:CD1	2.51	0.45
6:N:226:GLU:O	6:N:229:VAL:HB	2.16	0.45
9:O:44:LEU:HD21	9:O:189:ALA:C	2.42	0.45
13:Y:104:THR:C	13:Y:106:PRO:HD3	2.41	0.45
9:Z:35:LEU:HB3	9:Z:163:CYS:SG	2.57	0.45
14:a:99:ARG:NH1	14:a:106:LEU:HD21	2.32	0.45
10:b:70:HIS:CD2	10:b:71:ILE:HG13	2.52	0.45
2:B:2:THR:HG21	2:B:162:GLY:HA3	1.99	0.45
3:D:77:SER:HA	3:D:112:TYR:CE2	2.50	0.45
2:E:76:VAL:HG11	2:E:109:GLN:HB2	1.99	0.45
2:E:126:ALA:HB3	2:E:135:LEU:CD2	2.47	0.45
1:F:28:ASN:ND2	1:F:30:VAL:H	2.13	0.45
8:K:213:SER:HB3	8:K:232:GLU:OE2	2.16	0.45
4:L:44:ALA:HB2	4:L:142:PRO:HB3	1.98	0.45
4:L:126:ARG:HH21	5:M:121:LEU:HD22	1.81	0.45
9:O:28:ILE:HG21	9:O:133:SER:OG	2.16	0.45
7:Q:85:ARG:O	7:Q:88:ALA:HB3	2.17	0.45
11:S:68:ILE:HD11	11:S:92:LEU:HD13	1.99	0.45
13:U:104:THR:C	13:U:106:PRO:HD3	2.41	0.45
12:V:4:LEU:HD23	12:V:17:SER:HB3	1.98	0.45
11:X:145:LEU:HD21	11:X:178:VAL:O	2.17	0.45
13:Y:65:ARG:O	13:Y:68:PHE:HB3	2.16	0.45
9:Z:103:GLU:HB2	9:Z:104:PRO:HD2	1.97	0.45
2:E:13:ILE:HG12	2:E:155:LEU:HD13	1.99	0.45
2:E:27:ALA:HB1	13:U:130:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:28:ASP:OD2	2:E:31:CYS:HB3	2.16	0.45
7:J:31:GLU:O	7:J:167:LYS:HA	2.17	0.45
8:K:52:THR:HG23	8:K:53:GLN:O	2.17	0.45
8:K:112:ASP:HA	8:K:152:TYR:CE2	2.51	0.45
4:L:84:LEU:O	4:L:88:MET:HG3	2.16	0.45
6:N:53:LEU:HD11	9:O:175:LEU:CB	2.46	0.45
6:N:132:LEU:CD1	6:N:161:ILE:HG12	2.47	0.45
10:P:65:GLU:HB3	10:P:90:ARG:NH1	2.31	0.45
11:S:12:ILE:CD1	11:S:109:ILE:HD12	2.47	0.45
14:W:67:LEU:HD13	14:W:91:TRP:CZ3	2.51	0.45
9:Z:90:LEU:HD21	9:Z:114:LEU:CB	2.37	0.45
1:A:20:VAL:CG2	1:A:28:ASN:HB3	2.47	0.45
1:A:65:LEU:O	1:A:69:GLU:HG3	2.16	0.45
1:A:80:ALA:CB	1:A:112:TYR:HD2	2.29	0.45
3:C:178:HIS:HB2	3:C:187:VAL:HG21	1.99	0.45
1:F:75:LEU:HD23	1:F:104:ASP:HB2	1.98	0.45
1:F:132:THR:HG23	1:F:133:PHE:CE1	2.51	0.45
6:I:20:GLU:O	6:I:24:GLU:HG2	2.17	0.45
6:I:115:LYS:NZ	6:I:129:ILE:HG13	2.31	0.45
7:J:8:ASP:O	7:J:22:GLN:NE2	2.50	0.45
6:N:63:CYS:HB3	6:N:88:ARG:NH2	2.32	0.45
9:O:145:PHE:HZ	9:O:218:ARG:HG2	1.82	0.45
10:P:99:VAL:HG13	13:U:92:ASN:ND2	2.32	0.45
10:P:106:THR:O	10:P:110:VAL:HG23	2.16	0.45
11:S:12:ILE:HD11	11:S:109:ILE:HD12	1.99	0.45
12:T:165:GLU:HG2	12:T:196:PHE:HE1	1.81	0.45
14:W:4:PRO:HB2	14:W:7:THR:CG2	2.46	0.45
2:B:126:ALA:HB3	2:B:135:LEU:CD2	2.47	0.45
2:B:218:PRO:C	2:B:219:LEU:HD12	2.42	0.45
3:C:1:THR:HG23	3:C:33:LYS:HZ2	1.81	0.45
3:C:17:ASP:O	3:C:33:LYS:HD2	2.17	0.45
1:F:80:ALA:CB	1:F:112:TYR:HD2	2.29	0.45
6:I:132:LEU:HG	6:I:161:ILE:CD1	2.41	0.45
6:I:145:TYR:HE1	6:I:155:ALA:HB2	1.82	0.45
7:J:70:ASP:HA	14:W:76:LEU:CD2	2.47	0.45
8:K:90:GLN:HG3	8:K:134:LEU:HD13	1.99	0.45
8:K:111:VAL:HG21	8:K:142:GLY:HA3	1.98	0.45
9:O:21:VAL:HG11	9:O:153:SER:HB3	1.98	0.45
11:S:12:ILE:HD12	11:S:109:ILE:HB	1.99	0.45
12:T:43:LEU:CD1	12:T:183:ILE:HD11	2.46	0.45
12:T:68:LYS:HA	12:T:73:TYR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:18:CYS:HA	13:U:189:ILE:O	2.16	0.45
14:W:157:GLN:HG2	14:W:159:VAL:O	2.16	0.45
11:X:12:ILE:HD11	11:X:109:ILE:HD12	1.99	0.45
13:Y:48:LEU:HD21	13:Y:86:LEU:HD22	1.99	0.45
9:Z:21:VAL:HG11	9:Z:153:SER:HB3	1.98	0.45
9:Z:59:VAL:CG2	10:b:142:ARG:HH12	2.28	0.45
9:Z:145:PHE:HZ	9:Z:218:ARG:HG2	1.82	0.45
10:b:8:SER:HA	10:b:123:SER:O	2.16	0.45
10:b:13:SER:HB3	10:b:19:VAL:HG13	1.98	0.45
1:A:106:ARG:CD	1:A:107:GLU:HG2	2.41	0.44
3:C:142:GLY:O	3:C:155:LEU:HD22	2.17	0.44
6:I:132:LEU:CD1	6:I:161:ILE:HG12	2.47	0.44
7:J:75:MET:HE2	7:J:77:VAL:HG12	1.98	0.44
7:J:179:LEU:CD2	7:J:192:GLU:HG2	2.47	0.44
5:M:60:GLU:HB2	6:N:155:ALA:HB3	1.98	0.44
9:O:38:LEU:HD12	9:O:43:VAL:CG2	2.48	0.44
9:O:76:VAL:CG1	9:O:83:ALA:HB1	2.44	0.44
9:O:214:ALA:HA	9:O:227:VAL:HA	1.98	0.44
8:R:112:ASP:CB	8:R:152:TYR:HE2	2.29	0.44
8:R:213:SER:HB3	8:R:232:GLU:OE2	2.16	0.44
12:T:146:TYR:CB	12:T:159:LEU:HD13	2.47	0.44
14:W:99:ARG:NH1	14:W:106:LEU:HD21	2.32	0.44
11:X:64:LEU:HD21	11:X:96:LEU:HD21	2.00	0.44
11:X:64:LEU:CD2	11:X:108:ASN:HD21	2.31	0.44
9:Z:42:GLY:CA	9:Z:217:THR:HG22	2.41	0.44
1:A:132:THR:HG23	1:A:133:PHE:CD1	2.52	0.44
5:H:125:GLU:HG3	5:H:126:GLU:OE2	2.17	0.44
6:I:43:LEU:O	6:I:208:LEU:CD2	2.57	0.44
4:L:137:TYR:HE1	4:L:141:GLY:HA2	1.83	0.44
5:M:84:ASP:HB2	5:M:139:VAL:HG23	1.98	0.44
5:M:110:GLU:HA	5:M:154:PHE:CE2	2.51	0.44
9:O:46:ALA:CB	9:O:197:LEU:HD11	2.47	0.44
9:O:90:LEU:HD11	9:O:136:TYR:OH	2.18	0.44
12:T:5:ILE:CG2	12:T:16:ALA:HB3	2.47	0.44
12:V:165:GLU:HG2	12:V:196:PHE:HE1	1.81	0.44
14:a:4:PRO:HB2	14:a:7:THR:CG2	2.46	0.44
14:a:68:GLY:HA2	14:a:71:VAL:HG22	1.98	0.44
1:A:75:LEU:HD23	1:A:104:ASP:HB2	1.98	0.44
3:D:17:ASP:O	3:D:33:LYS:HD2	2.17	0.44
3:D:157:ARG:N	3:D:176:MET:HE1	2.33	0.44
2:E:217:LYS:HD3	2:E:218:PRO:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:218:PRO:C	2:E:219:LEU:HD12	2.42	0.44
4:G:50:LYS:HB2	4:G:59:HIS:CB	2.46	0.44
4:G:104:PRO:HB3	14:W:81:HIS:CE1	2.52	0.44
4:G:132:LEU:HB2	4:G:147:THR:OG1	2.17	0.44
6:I:226:GLU:O	6:I:229:VAL:HB	2.16	0.44
5:M:241:ILE:HG22	5:M:241:ILE:OXT	2.17	0.44
9:O:165:GLY:O	9:O:168:SER:OG	2.29	0.44
10:P:70:HIS:CD2	10:P:71:ILE:HG13	2.52	0.44
10:P:155:PHE:HB2	10:P:157:TRP:NE1	2.32	0.44
12:V:164:LEU:HD22	12:V:178:PHE:CD2	2.53	0.44
14:W:16:PHE:HB2	14:W:160:LEU:O	2.17	0.44
9:Z:81:SER:CB	10:b:118:GLN:HG3	2.45	0.44
14:a:92:LEU:CD2	14:a:112:ILE:HD11	2.47	0.44
10:b:155:PHE:HB2	10:b:157:TRP:NE1	2.33	0.44
2:B:206:PRO:HA	13:Y:164:GLU:CD	2.43	0.44
3:C:157:ARG:N	3:C:176:MET:HE1	2.32	0.44
2:E:156:VAL:HG21	2:E:189:LEU:CD1	2.46	0.44
5:H:22:PHE:HB3	5:H:26:TYR:HE2	1.83	0.44
5:H:199:LEU:HD11	5:H:215:ILE:HD12	2.00	0.44
4:L:82:ARG:NH2	5:M:160:GLY:O	2.48	0.44
6:N:20:GLU:O	6:N:24:GLU:HG2	2.17	0.44
10:P:204:GLU:HB2	10:P:222:PRO:O	2.18	0.44
7:Q:8:ASP:O	7:Q:22:GLN:NE2	2.50	0.44
8:R:228:ARG:NH1	8:R:230:LEU:HD23	2.32	0.44
12:T:77:PRO:HD2	12:T:108:ASP:HB2	1.98	0.44
12:V:29:LYS:NZ	12:V:31:ASP:OD1	2.32	0.44
12:V:86:ARG:HG3	9:Z:100:GLN:HA	1.98	0.44
12:V:146:TYR:CB	12:V:159:LEU:HD13	2.47	0.44
11:X:12:ILE:CD1	11:X:109:ILE:HD12	2.47	0.44
11:X:176:LYS:HE2	11:X:208:VAL:CG2	2.48	0.44
9:Z:196:VAL:O	9:Z:200:THR:HG23	2.17	0.44
14:a:16:PHE:HB2	14:a:160:LEU:O	2.17	0.44
1:A:73:PRO:HA	1:A:74:PRO:HD3	1.83	0.44
1:A:115:LEU:HD22	14:W:35:ARG:NH1	2.33	0.44
3:C:8:PHE:HE2	3:C:10:HIS:HB2	1.83	0.44
2:E:132:ASP:HB3	14:W:144:TYR:HB3	1.99	0.44
4:G:44:ALA:HB2	4:G:142:PRO:HB3	1.98	0.44
5:H:221:GLN:HB2	5:H:224:GLN:HB3	1.98	0.44
7:J:98:PHE:CE2	7:J:106:ILE:HA	2.53	0.44
8:K:112:ASP:CB	8:K:152:TYR:HE2	2.29	0.44
8:K:130:GLU:OE2	8:K:131:MET:HE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:98:VAL:HA	14:a:94:ARG:HG3	1.99	0.44
4:L:132:LEU:HB2	4:L:147:THR:OG1	2.17	0.44
6:N:141:THR:HG23	6:N:142:PRO:HD2	2.00	0.44
8:R:27:TYR:O	8:R:30:LYS:HB2	2.17	0.44
8:R:90:GLN:HG3	8:R:134:LEU:HD13	1.99	0.44
11:S:45:LYS:CE	11:S:203:ILE:HD12	2.37	0.44
11:S:145:LEU:HD21	11:S:178:VAL:O	2.17	0.44
11:S:176:LYS:HE2	11:S:208:VAL:CG2	2.47	0.44
12:T:164:LEU:HD22	12:T:178:PHE:CD2	2.53	0.44
12:V:13:VAL:HG11	12:V:105:ALA:CB	2.43	0.44
12:V:37:LYS:HE3	12:V:188:ILE:HD12	2.00	0.44
9:Z:38:LEU:HD12	9:Z:43:VAL:CG2	2.48	0.44
9:Z:90:LEU:CD2	9:Z:114:LEU:HD22	2.48	0.44
10:b:204:GLU:HB2	10:b:222:PRO:O	2.18	0.44
2:B:83:LEU:HD22	2:B:98:LEU:CD1	2.48	0.44
2:B:99:ILE:CD1	2:B:125:THR:HG23	2.48	0.44
15:C:301:BZ7:CAV	11:X:131:GLN:HG2	2.47	0.44
2:E:2:THR:HG21	2:E:162:GLY:HA3	1.99	0.44
4:L:58:ALA:CB	5:M:164:GLN:OE1	2.63	0.44
6:N:116:GLN:O	6:N:119:THR:OG1	2.33	0.44
6:N:130:SER:HA	6:N:147:THR:O	2.17	0.44
6:N:145:TYR:HA	6:N:154:HIS:O	2.18	0.44
9:O:196:VAL:O	9:O:200:THR:HG23	2.17	0.44
10:P:55:LEU:HD12	8:R:176:THR:HG23	2.00	0.44
12:T:4:LEU:HD23	12:T:17:SER:CB	2.48	0.44
11:X:64:LEU:CD2	11:X:96:LEU:HD21	2.48	0.44
10:b:76:SER:OG	10:b:162:MET:HG3	2.18	0.44
2:B:152:GLN:NE2	2:B:189:LEU:HD21	2.29	0.44
3:C:40:TYR:HB2	3:C:179:MET:CE	2.29	0.44
3:D:8:PHE:HE2	3:D:10:HIS:HB2	1.83	0.44
15:D:301:BZ7:CAV	11:S:131:GLN:CG	2.96	0.44
2:E:179:THR:HG22	2:E:180:LYS:N	2.33	0.44
1:F:132:THR:HG23	1:F:133:PHE:CD1	2.52	0.44
5:H:88:LEU:HD13	5:H:141:LEU:HD11	2.00	0.44
6:I:130:SER:HA	6:I:147:THR:O	2.17	0.44
6:I:191:VAL:HG11	6:I:208:LEU:CD1	2.47	0.44
6:I:200:GLN:O	6:I:201:SER:HB2	2.18	0.44
8:K:28:ALA:O	8:K:31:ALA:N	2.46	0.44
8:K:228:ARG:NH1	8:K:230:LEU:HD23	2.32	0.44
4:L:18[A]:ARG:HE	4:L:18[A]:ARG:HB2	1.64	0.44
9:O:90:LEU:CD2	9:O:114:LEU:HD22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:227:ASP:O	10:P:230:ALA:HB3	2.18	0.44
8:R:141:ILE:HA	8:R:150:GLN:O	2.18	0.44
12:T:175:LEU:HB3	12:T:178:PHE:CE1	2.52	0.44
13:U:50:ILE:HG13	13:U:108:ILE:HG12	2.00	0.44
12:V:56:PHE:CZ	12:V:84:THR:HG23	2.53	0.44
9:Z:23:TYR:CD1	10:b:14:PRO:HA	2.51	0.44
2:B:179:THR:HG22	2:B:180:LYS:N	2.33	0.44
3:C:144:ARG:NH1	3:C:151:GLU:OE1	2.51	0.44
3:C:162:TYR:CE2	12:T:145:ARG:HA	2.53	0.44
3:D:4:LEU:HA	3:D:127:SER:HA	2.00	0.44
3:D:144:ARG:NH1	3:D:151:GLU:OE1	2.51	0.44
4:G:137:TYR:HE1	4:G:141:GLY:HA2	1.83	0.44
6:I:45:VAL:HG22	6:I:62:ILE:HD11	2.00	0.44
7:J:211:LEU:HB3	7:J:236:GLU:OE2	2.18	0.44
5:M:22:PHE:HB3	5:M:26:TYR:HE2	1.83	0.44
5:M:107:MET:HE2	5:M:111:SER:C	2.43	0.44
6:N:145:TYR:HE1	6:N:155:ALA:HB2	1.82	0.44
9:O:82:ASP:HB2	9:O:132:VAL:HG21	2.00	0.44
10:P:45:LEU:N	10:P:210:GLY:O	2.42	0.44
11:S:64:LEU:CD2	11:S:96:LEU:HD21	2.48	0.44
11:X:12:ILE:HD12	11:X:109:ILE:HB	1.99	0.44
11:X:46:LEU:HD11	11:X:52:ILE:HB	1.99	0.44
13:Y:70:LEU:HD11	13:Y:81:ILE:CG2	2.48	0.44
13:Y:134:ASP:OD1	13:Y:135:PHE:N	2.51	0.44
9:Z:90:LEU:HD11	9:Z:136:TYR:OH	2.18	0.44
1:A:21:SER:HA	1:A:26:VAL:HA	2.00	0.44
2:B:50:ALA:O	2:B:54:MET:HG2	2.18	0.44
3:C:38:ASN:ND2	3:C:41:LEU:HD12	2.33	0.44
3:D:20:ALA:HB2	15:D:301:BZ7:CBJ	2.47	0.44
5:H:52:LYS:HE2	5:H:216:GLU:HG3	2.00	0.44
5:H:107:MET:HE2	5:H:111:SER:C	2.43	0.44
7:J:124:LEU:O	8:K:131:MET:HA	2.18	0.44
5:M:115:ALA:O	5:M:118:ASN:OD1	2.34	0.44
7:Q:106:ILE:HD11	7:Q:110:HIS:HD2	1.81	0.44
13:Y:50:ILE:HG13	13:Y:108:ILE:HG12	2.00	0.44
13:Y:163:PHE:CE1	13:Y:197:ARG:HD2	2.53	0.44
14:a:124:TYR:CE1	14:a:139:THR:HG22	2.51	0.44
2:B:203:HIS:HE1	13:Y:161:HIS:ND1	2.16	0.43
3:C:115:ASP:CB	3:C:119:THR:HB	2.48	0.43
2:E:99:ILE:CD1	2:E:125:THR:HG23	2.48	0.43
2:E:193:THR:CG2	11:X:213:ASP:CG	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:44:GLY:CA	6:I:208:LEU:HD12	2.48	0.43
6:I:116:GLN:O	6:I:119:THR:OG1	2.33	0.43
6:I:141:THR:HG23	6:I:142:PRO:HD2	2.00	0.43
7:Q:98:PHE:CE2	7:Q:106:ILE:HA	2.53	0.43
11:S:64:LEU:HD21	11:S:96:LEU:HD21	2.00	0.43
12:T:1:MET:CE	12:T:134:TYR:H	2.31	0.43
12:V:27[A]:GLN:CD	12:V:30:ASP:HB3	2.43	0.43
14:W:59:ASP:HB3	14:W:106:LEU:HD22	2.00	0.43
9:Z:23:TYR:CE1	10:b:14:PRO:HA	2.52	0.43
14:a:59:ASP:HB3	14:a:106:LEU:HD22	2.00	0.43
14:a:71:VAL:O	14:a:75:GLU:HG3	2.18	0.43
2:B:217:LYS:HD3	2:B:218:PRO:O	2.17	0.43
3:C:41:LEU:HG	3:C:73:ARG:HH22	1.83	0.43
3:D:18:SER:OG	3:D:173:VAL:HG22	2.18	0.43
5:H:85:ALA:N	5:H:139:VAL:HG21	2.34	0.43
6:I:38:ARG:O	6:I:213:ARG:NH2	2.51	0.43
6:I:145:TYR:HA	6:I:154:HIS:O	2.18	0.43
7:J:108:LEU:HD11	7:J:137:LEU:HD13	2.00	0.43
8:K:141:ILE:HA	8:K:150:GLN:O	2.18	0.43
4:L:58:ALA:HB3	5:M:164:GLN:HB3	1.99	0.43
4:L:229:VAL:HG23	4:L:233:LEU:HD12	1.99	0.43
6:N:202:GLY:C	6:N:229:VAL:HG13	2.43	0.43
9:O:27:ALA:HB2	10:P:16:GLY:O	2.17	0.43
11:S:46:LEU:HD11	11:S:52:ILE:HB	1.99	0.43
12:V:68:LYS:HA	12:V:73:TYR:O	2.17	0.43
11:X:45:LYS:CE	11:X:203:ILE:HD12	2.37	0.43
10:b:149[B]:ASP:HB2	10:b:150:PRO:HD2	2.00	0.43
2:B:200:GLY:HA3	11:S:177:ASP:OD2	2.18	0.43
3:D:37:ILE:HG23	3:D:60:ALA:HA	2.00	0.43
2:E:50:ALA:O	2:E:54:MET:HG2	2.18	0.43
1:F:106:ARG:CD	1:F:107:GLU:HG2	2.41	0.43
4:G:80:ASP:OD1	4:G:126:ARG:NH2	2.47	0.43
7:J:35:THR:HA	7:J:165:ILE:O	2.19	0.43
5:M:191:LEU:CD2	5:M:221:GLN:HE21	2.26	0.43
9:O:135:LEU:HD23	9:O:149:GLN:HA	2.01	0.43
10:P:95:GLN:O	10:P:99:VAL:HG23	2.18	0.43
7:Q:179:LEU:CD2	7:Q:192:GLU:HG2	2.47	0.43
12:T:4:LEU:HG	12:T:47:VAL:CG1	2.49	0.43
13:U:163:PHE:CE1	13:U:197:ARG:HD2	2.53	0.43
14:W:71:VAL:O	14:W:75:GLU:HG3	2.18	0.43
11:X:68:ILE:HD11	11:X:92:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:158:ASP:HB2	13:Y:159:PRO:CD	2.49	0.43
10:b:51:GLN:NE2	10:b:58[B]:GLU:OE2	2.44	0.43
3:C:37:ILE:HG23	3:C:60:ALA:HA	2.00	0.43
3:D:31:VAL:CG2	15:D:301:BZ7:CBK	2.96	0.43
5:H:37:ALA:HB2	5:H:50:VAL:CG2	2.46	0.43
7:J:93:GLU:HG2	7:J:97:ASN:ND2	2.33	0.43
7:J:191:LYS:O	7:J:194:ALA:HB3	2.18	0.43
8:K:50:ILE:HG13	8:K:50:ILE:O	2.18	0.43
8:K:75:ASN:OD1	8:K:225:PRO:HB2	2.19	0.43
5:M:41:GLN:CD	5:M:152:GLN:HA	2.44	0.43
6:N:66:ASP:CG	6:N:95:ARG:HH21	2.26	0.43
9:O:49:ARG:HD3	9:O:212:GLU:HG3	1.99	0.43
7:Q:203:GLU:O	7:Q:207:LYS:HG2	2.18	0.43
11:X:192:ALA:O	11:X:210:LEU:HD12	2.19	0.43
13:Y:107:VAL:HB	13:Y:136:VAL:HG21	2.00	0.43
10:b:204:GLU:O	10:b:222:PRO:HB3	2.19	0.43
10:b:212:CYS:HB2	10:b:217:PHE:CD1	2.50	0.43
2:B:8:PHE:HB2	2:B:146:MET:O	2.19	0.43
2:B:214:GLN:HE22	13:Y:197:ARG:HG2	1.83	0.43
3:C:4:LEU:HA	3:C:127:SER:HA	2.00	0.43
3:D:178:HIS:HB2	3:D:187:VAL:HG21	1.99	0.43
2:E:83:LEU:HD22	2:E:98:LEU:CD1	2.48	0.43
2:E:214:GLN:HE22	13:U:197:ARG:HG2	1.83	0.43
5:H:201:ILE:O	5:H:204:GLN:HB2	2.18	0.43
7:J:191:LYS:HD2	7:J:238:TYR:CD2	2.54	0.43
8:K:27:TYR:O	8:K:30:LYS:HB2	2.17	0.43
5:M:201:ILE:O	5:M:204:GLN:HB2	2.18	0.43
9:O:64:LYS:O	9:O:75:SER:HA	2.18	0.43
7:Q:35:THR:HA	7:Q:166:GLY:HA3	2.01	0.43
8:R:118:ILE:HG21	8:R:138:MET:HE1	2.01	0.43
13:U:158:ASP:HB2	13:U:159:PRO:CD	2.49	0.43
12:V:42:ILE:HG23	12:V:104:LEU:HD21	2.01	0.43
1:A:28:ASN:ND2	1:A:30:VAL:O	2.52	0.43
15:C:301:BZ7:N	11:X:125:ASP:OD2	2.51	0.43
3:D:18:SER:HG	3:D:173:VAL:N	2.14	0.43
2:E:132:ASP:CG	14:W:144:TYR:HB3	2.44	0.43
5:H:41:GLN:CD	5:H:152:GLN:HA	2.44	0.43
7:J:88:ALA:O	7:J:92:ARG:HG3	2.19	0.43
5:M:52:LYS:HE2	5:M:216:GLU:HG3	2.00	0.43
8:R:52:THR:HG23	8:R:53:GLN:O	2.17	0.43
8:R:151:VAL:HG23	8:R:151:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:2:PHE:HD2	14:a:103:MET:HE1	1.82	0.43
12:T:37:LYS:HE3	12:T:188:ILE:HD12	2.00	0.43
13:U:9:ALA:HB1	13:U:145:MET:CE	2.46	0.43
13:Y:14:LYS:HD2	13:Y:133:ASP:O	2.19	0.43
9:Z:46:ALA:CB	9:Z:197:LEU:HD11	2.47	0.43
10:b:73:LEU:HD21	10:b:135:ILE:HG12	2.00	0.43
2:B:6:LEU:HD23	2:B:7:VAL:N	2.34	0.43
3:C:172:GLY:HA2	13:U:202:ARG:NH2	2.34	0.43
3:D:113:TYR:CZ	12:T:28:MET:HE1	2.53	0.43
1:F:28:ASN:ND2	1:F:30:VAL:O	2.52	0.43
4:G:123:TYR:CE2	9:Z:2:SER:HB3	2.54	0.43
6:I:46:GLU:HA	6:I:206:ILE:CB	2.48	0.43
6:I:136:PHE:CE2	6:I:213:ARG:HA	2.54	0.43
7:J:70:ASP:CG	7:J:99:ARG:HH22	2.26	0.43
8:K:225:PRO:HG2	8:K:226:LYS:HD3	2.01	0.43
5:M:26:TYR:CE1	6:N:12:PRO:HA	2.54	0.43
5:M:88:LEU:HD13	5:M:141:LEU:HD11	2.00	0.43
5:M:199:LEU:HD11	5:M:215:ILE:HD12	2.00	0.43
12:T:85:ARG:NH1	12:T:122:ALA:HB1	2.34	0.43
9:Z:64:LYS:O	9:Z:75:SER:HA	2.19	0.43
14:a:9:THR:HG22	14:a:25:ASP:OD1	2.18	0.43
14:a:56:ASP:HB2	14:a:107:TRP:HB3	2.01	0.43
1:A:42:TYR:CZ	1:A:183:VAL:HG11	2.54	0.43
2:E:1:THR:N	2:E:169:SER:OG	2.21	0.43
2:E:58:MET:CE	2:E:62:LYS:HE3	2.48	0.43
4:G:109:VAL:HG21	4:G:145:PHE:CD2	2.54	0.43
4:G:230:SER:N	4:G:231:PRO:CD	2.81	0.43
6:I:105:GLU:HA	6:I:145:TYR:CE2	2.51	0.43
7:J:125:TYR:HE1	8:K:131:MET:HE3	1.82	0.43
7:J:203:GLU:O	7:J:207:LYS:HG2	2.18	0.43
8:K:161:CYS:O	8:K:163:PHE:CE2	2.71	0.43
5:M:81:LEU:HD12	5:M:138:GLY:HA3	2.01	0.43
5:M:85:ALA:N	5:M:139:VAL:HG21	2.34	0.43
5:M:157:ASP:HB2	5:M:158:PRO:HD2	2.01	0.43
6:N:98:VAL:O	6:N:99:GLU:HB2	2.19	0.43
10:P:138:TRP:NE1	10:P:214:GLU:HA	2.34	0.43
7:Q:108:LEU:HD11	7:Q:137:LEU:HD13	1.99	0.43
11:S:125:ASP:CG	11:S:129:SER:HB3	2.44	0.43
12:T:56:PHE:CZ	12:T:84:THR:HG23	2.53	0.43
14:W:9:THR:HG22	14:W:25:ASP:OD1	2.18	0.43
10:b:227:ASP:O	10:b:230:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:127:SER:OG	3:D:135:ALA:HB3	2.19	0.43
2:E:8:PHE:HE2	2:E:10:ASP:HB2	1.84	0.43
1:F:21:SER:HA	1:F:26:VAL:HA	2.00	0.43
1:F:26:VAL:HG23	14:W:179:ARG:HH11	1.84	0.43
5:H:99:HIS:CE1	5:H:103:TYR:HD2	2.37	0.43
6:I:35:VAL:HA	6:I:158:ALA:CB	2.49	0.43
7:J:28:LYS:HA	7:J:31:GLU:CG	2.47	0.43
7:J:81:LEU:O	7:J:81:LEU:HD13	2.19	0.43
8:K:118:ILE:HG21	8:K:138:MET:HE1	2.01	0.43
8:K:141:ILE:O	8:K:141:ILE:HG13	2.19	0.43
4:L:192:LEU:HD13	4:L:236:LEU:HD21	1.99	0.43
6:N:35:VAL:HA	6:N:158:ALA:CB	2.49	0.43
10:P:76:SER:OG	10:P:162:MET:HG3	2.18	0.43
10:P:204:GLU:O	10:P:222:PRO:HB3	2.19	0.43
7:Q:88:ALA:O	7:Q:92:ARG:HG3	2.19	0.43
7:Q:93:GLU:HG2	7:Q:97:ASN:ND2	2.33	0.43
7:Q:211:LEU:HB3	7:Q:236:GLU:OE2	2.18	0.43
12:T:42:ILE:HG23	12:T:104:LEU:HD21	2.01	0.43
13:U:48:LEU:HD21	13:U:86:LEU:CD2	2.49	0.43
11:X:125:ASP:CG	11:X:129:SER:HB3	2.44	0.43
9:Z:38:LEU:HD11	9:Z:145:PHE:C	2.44	0.43
14:a:177:TYR:CE1	14:a:185:ASN:HB2	2.54	0.43
10:b:85:LEU:HD23	10:b:85:LEU:HA	1.87	0.43
10:b:138:TRP:NE1	10:b:214:GLU:HA	2.34	0.43
10:b:165:ASN:OD1	10:b:168:ASN:ND2	2.52	0.43
1:A:77:LEU:O	1:A:77:LEU:HD22	2.19	0.43
3:C:153:TYR:HH	3:C:178:HIS:HD1	1.57	0.43
3:D:115:ASP:CB	3:D:119:THR:HB	2.48	0.43
4:G:58:ALA:N	5:H:164:GLN:O	2.41	0.43
5:H:156:MET:HG2	5:H:157:ASP:N	2.34	0.43
6:I:31:THR:HB	6:I:46:GLU:OE1	2.19	0.43
7:J:64:LYS:HG2	7:J:212:GLU:OE2	2.19	0.43
4:L:206:THR:O	4:L:233:LEU:CD1	2.64	0.43
4:L:207:THR:HA	4:L:233:LEU:HD13	1.99	0.43
6:N:45:VAL:HG22	6:N:62:ILE:HD11	2.00	0.43
6:N:136:PHE:CE2	6:N:213:ARG:HA	2.54	0.43
11:S:64:LEU:CD2	11:S:108:ASN:HD21	2.31	0.43
9:Z:135:LEU:HD23	9:Z:149:GLN:HA	2.01	0.43
3:C:18:SER:OG	3:C:173:VAL:HG22	2.18	0.42
3:D:38:ASN:ND2	3:D:41:LEU:HD12	2.33	0.42
3:D:113:TYR:CE1	3:D:128:THR:HG22	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:151:VAL:HG23	8:K:151:VAL:O	2.18	0.42
5:M:36:THR:O	5:M:51:GLU:HG2	2.19	0.42
7:Q:28:LYS:HA	7:Q:31:GLU:CG	2.47	0.42
11:S:27:THR:HG22	11:S:41:PRO:CA	2.45	0.42
13:U:134:ASP:OD1	13:U:135:PHE:N	2.51	0.42
9:Z:82:ASP:HB2	9:Z:132:VAL:HG21	2.00	0.42
10:b:37:ILE:HD11	10:b:173:LEU:CD2	2.49	0.42
10:b:37:ILE:HD11	10:b:173:LEU:HD21	2.01	0.42
2:E:8:PHE:HB2	2:E:146:MET:O	2.19	0.42
2:E:140:ASP:HB3	2:E:141:ARG:HD2	2.00	0.42
1:F:134:ILE:O	1:F:138:VAL:HG22	2.19	0.42
5:H:91:LYS:HG2	5:H:119:LEU:CD1	2.49	0.42
6:I:66:ASP:CG	6:I:95:ARG:HH21	2.26	0.42
7:J:35:THR:HA	7:J:166:GLY:HA3	2.01	0.42
8:K:49[B]:VAL:CG2	8:K:219:VAL:HG12	2.36	0.42
4:L:31:GLN:OE1	5:M:20:ARG:NE	2.53	0.42
10:P:37:ILE:HD11	10:P:173:LEU:CD2	2.49	0.42
7:Q:191:LYS:O	7:Q:194:ALA:HB3	2.18	0.42
8:R:155:ASP:HB2	8:R:156:PRO:CD	2.49	0.42
13:U:47:ARG:NH2	13:U:191:LYS:O	2.52	0.42
12:V:88:LEU:HD13	12:V:88:LEU:O	2.19	0.42
9:Z:235:GLN:CG	9:Z:239:LYS:HE2	2.47	0.42
10:b:106:THR:OG1	10:b:137:GLY:HA3	2.19	0.42
1:A:118:MET:SD	14:W:36:PHE:HE2	2.42	0.42
2:B:54:MET:HG3	13:Y:95:TYR:CE1	2.54	0.42
2:B:58:MET:CE	2:B:62:LYS:HE3	2.48	0.42
3:D:1:THR:CB	3:D:33:LYS:HZ3	2.31	0.42
3:D:31:VAL:HG13	15:D:301:BZ7:CBK	2.49	0.42
3:D:104:TRP:CE2	3:D:181:GLU:HG3	2.55	0.42
1:F:20:VAL:CG2	1:F:28:ASN:HB3	2.47	0.42
4:G:230:SER:CB	4:G:231:PRO:HD3	2.47	0.42
6:I:30:SER:HB2	6:I:61:LYS:CE	2.43	0.42
6:I:191:VAL:O	6:I:194:ALA:HB3	2.18	0.42
8:K:68:HIS:O	8:K:79:VAL:HA	2.19	0.42
5:M:137:PHE:HD1	6:N:120:GLN:HE22	1.65	0.42
9:O:9:THR:OG1	9:O:126:GLY:O	2.37	0.42
10:P:106:THR:OG1	10:P:137:GLY:HA3	2.19	0.42
7:Q:179:LEU:HD21	7:Q:192:GLU:HG2	2.02	0.42
8:R:50:ILE:O	8:R:50:ILE:HG13	2.18	0.42
8:R:200:THR:O	8:R:204:THR:OG1	2.31	0.42
12:T:88:LEU:O	12:T:88:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:177:TYR:CE1	14:W:185:ASN:HB2	2.54	0.42
11:X:24:ALA:HA	11:X:194:ARG:O	2.19	0.42
11:X:42:LYS:HB3	11:X:54:CYS:O	2.19	0.42
13:Y:26:ARG:HB2	13:Y:182:MET:HB2	2.01	0.42
9:Z:90:LEU:CG	9:Z:114:LEU:HD22	2.49	0.42
14:a:173:MET:SD	14:a:176:LEU:HD12	2.59	0.42
2:B:140:ASP:HB3	2:B:141:ARG:HD2	2.00	0.42
2:E:159:VAL:O	2:E:163:ILE:HG13	2.19	0.42
4:G:137:TYR:CE1	4:G:141:GLY:HA2	2.54	0.42
5:H:46:VAL:O	5:H:219:THR:HA	2.19	0.42
5:H:238:ILE:O	5:H:241:ILE:N	2.52	0.42
6:I:42:VAL:CG1	6:I:208:LEU:HD21	2.45	0.42
6:I:76:LEU:HD11	9:Z:12:PHE:CE1	2.55	0.42
6:I:98:VAL:O	6:I:99:GLU:HB2	2.19	0.42
7:J:152:ASP:OD1	7:J:156:VAL:HG12	2.19	0.42
8:K:208:ILE:HD12	8:K:210:PHE:CE1	2.52	0.42
5:M:99:HIS:CE1	5:M:103:TYR:HD2	2.37	0.42
6:N:31:THR:HB	6:N:46:GLU:OE1	2.19	0.42
6:N:33:VAL:HG22	6:N:160:ALA:HB1	2.00	0.42
6:N:60:ARG:CZ	6:N:219:ILE:CD1	2.96	0.42
6:N:105:GLU:HG2	6:N:109:ARG:NH1	2.35	0.42
6:N:191:VAL:O	6:N:194:ALA:HB3	2.18	0.42
9:O:90:LEU:HD21	9:O:114:LEU:CD2	2.50	0.42
9:O:90:LEU:CG	9:O:114:LEU:HD22	2.49	0.42
7:Q:81:LEU:O	7:Q:81:LEU:HD13	2.19	0.42
13:Y:19:VAL:CG1	13:Y:118:PRO:HB3	2.48	0.42
13:Y:48:LEU:HD21	13:Y:86:LEU:CD2	2.49	0.42
2:B:8:PHE:HE2	2:B:10:ASP:HB2	1.84	0.42
1:F:42:TYR:CZ	1:F:183:VAL:HG11	2.54	0.42
5:H:36:THR:O	5:H:51:GLU:HG2	2.19	0.42
5:M:46:VAL:O	5:M:219:THR:HA	2.19	0.42
10:P:85:LEU:HD23	10:P:85:LEU:HA	1.87	0.42
7:Q:28:LYS:CA	7:Q:31:GLU:HG2	2.48	0.42
7:Q:125:TYR:HE1	8:R:131:MET:HE3	1.85	0.42
8:R:141:ILE:HG13	8:R:141:ILE:O	2.19	0.42
8:R:211:LYS:HB3	8:R:212:PRO:HD2	2.01	0.42
12:T:85:ARG:NH2	13:U:57:THR:HA	2.30	0.42
13:U:14:LYS:HD2	13:U:133:ASP:O	2.18	0.42
13:U:18:CYS:SG	13:U:159:PRO:HG3	2.60	0.42
13:U:107:VAL:HB	13:U:136:VAL:HG21	2.01	0.42
14:W:124:TYR:O	14:W:131:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:12:ILE:CG1	11:X:109:ILE:HD12	2.50	0.42
11:X:27:THR:HG22	11:X:41:PRO:CA	2.45	0.42
13:Y:16:LYS:HB3	13:Y:158:ASP:HA	2.01	0.42
13:Y:18:CYS:SG	13:Y:159:PRO:HG3	2.60	0.42
2:B:214:GLN:CD	13:Y:197:ARG:HG2	2.45	0.42
3:C:127:SER:OG	3:C:135:ALA:HB3	2.19	0.42
3:D:41:LEU:HG	3:D:73:ARG:HH22	1.83	0.42
2:E:6:LEU:HD23	2:E:7:VAL:N	2.34	0.42
4:G:117:GLN:O	4:G:120:THR:OG1	2.30	0.42
5:H:50:VAL:HG12	5:H:67:ILE:CD1	2.50	0.42
7:J:160:TYR:CE1	8:K:61:LEU:HD23	2.54	0.42
7:J:169[A]:ARG:HG2	7:J:173:LYS:HE3	2.01	0.42
7:Q:64:LYS:HG2	7:Q:212:GLU:OE2	2.19	0.42
7:Q:191:LYS:HD2	7:Q:238:TYR:CD2	2.54	0.42
11:S:12:ILE:CG1	11:S:109:ILE:HD12	2.50	0.42
12:V:4:LEU:HD23	12:V:17:SER:CB	2.48	0.42
14:a:45:VAL:HG12	14:a:71:VAL:HG11	2.01	0.42
14:a:124:TYR:O	14:a:131:ALA:HA	2.19	0.42
10:b:38:LYS:HD2	10:b:143:PRO:CG	2.49	0.42
10:b:95:GLN:O	10:b:99:VAL:HG23	2.19	0.42
1:A:134:ILE:O	1:A:138:VAL:HG22	2.19	0.42
3:C:112:TYR:HD1	3:C:122:SER:HA	1.85	0.42
5:H:154:PHE:HD1	5:H:164:GLN:HA	1.85	0.42
6:I:33:VAL:HG22	6:I:160:ALA:HB1	2.00	0.42
6:I:134:VAL:HA	6:I:143:ARG:O	2.20	0.42
6:I:177:THR:O	6:I:180:ALA:HB3	2.20	0.42
7:J:179:LEU:HD21	7:J:192:GLU:HG2	2.02	0.42
5:M:50:VAL:HG12	5:M:67:ILE:CD1	2.50	0.42
5:M:91:LYS:HZ3	5:M:119:LEU:CD1	2.29	0.42
7:Q:195:LYS:O	7:Q:199:ILE:HG13	2.19	0.42
14:W:56:ASP:HB2	14:W:107:TRP:HB3	2.01	0.42
14:W:173:MET:SD	14:W:176:LEU:HD12	2.59	0.42
11:X:176:LYS:NZ	11:X:206:GLU:OE2	2.41	0.42
14:a:28:GLY:HA3	14:a:39:ILE:HD11	2.01	0.42
2:B:10:ASP:HB3	2:B:179:THR:HG23	2.02	0.42
4:G:56:LEU:HD22	5:H:185:TYR:CD2	2.55	0.42
8:K:208:ILE:HB	8:K:210:PHE:CD1	2.55	0.42
4:L:230:SER:CB	4:L:231:PRO:CD	2.97	0.42
6:N:36:ARG:CG	6:N:142:PRO:HB2	2.44	0.42
9:O:76:VAL:HG21	9:O:83:ALA:HB1	2.02	0.42
10:P:37:ILE:HD11	10:P:173:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:73:LEU:HD21	10:P:135:ILE:HG12	2.00	0.42
8:R:75:ASN:OD1	8:R:225:PRO:HB2	2.19	0.42
8:R:208:ILE:HB	8:R:210:PHE:CD1	2.55	0.42
13:U:58:ASP:OD2	13:U:103:TYR:N	2.35	0.42
12:V:4:LEU:HG	12:V:47:VAL:CG1	2.49	0.42
13:Y:26:ARG:HD2	13:Y:182:MET:HG2	2.02	0.42
13:Y:183:GLY:N	13:Y:201:ALA:HB3	2.35	0.42
9:Z:82:ASP:HB2	9:Z:132:VAL:CG2	2.50	0.42
2:B:103:VAL:CG2	2:B:178:ILE:HG22	2.50	0.42
2:B:132:ASP:OD2	14:a:144:TYR:HB3	2.19	0.42
1:F:77:LEU:O	1:F:77:LEU:HD22	2.19	0.42
1:F:163:MET:HE1	1:F:193:LEU:HD21	2.02	0.42
5:H:78:MET:HB3	5:H:141:LEU:HD23	2.02	0.42
8:K:50:ILE:CG2	8:K:141:ILE:HG21	2.50	0.42
8:K:80:MET:CE	8:K:87:SER:HA	2.43	0.42
5:M:96:THR:HG22	5:M:112:VAL:HG22	2.02	0.42
5:M:202:LEU:HA	5:M:205:VAL:CG2	2.50	0.42
5:M:230:THR:O	5:M:234:LEU:HG	2.20	0.42
9:O:38:LEU:HD11	9:O:145:PHE:C	2.44	0.42
7:Q:35:THR:HA	7:Q:165:ILE:O	2.19	0.42
11:S:6:VAL:HG12	11:S:57:PHE:HE1	1.84	0.42
11:S:44:TYR:O	11:S:52:ILE:HG22	2.20	0.42
11:S:192:ALA:O	11:S:210:LEU:HD12	2.19	0.42
13:U:70:LEU:HD11	13:U:81:ILE:CG2	2.48	0.42
12:V:14:LEU:HD11	12:V:180:VAL:CG1	2.50	0.42
12:V:85:ARG:NH1	12:V:122:ALA:HB1	2.34	0.42
12:V:145:ARG:HG3	12:V:146:TYR:CD1	2.55	0.42
13:Y:9:ALA:HB1	13:Y:145:MET:CE	2.46	0.42
9:Z:134:LEU:HB3	9:Z:136:TYR:HE1	1.83	0.42
2:B:1:THR:HA	2:B:17:ASP:OD2	2.20	0.42
2:B:19:ARG:HD3	2:B:26:VAL:CG2	2.47	0.42
2:B:214:GLN:OE1	13:Y:197:ARG:HG2	2.20	0.42
3:D:42:LEU:O	3:D:102:CYS:N	2.45	0.42
2:E:1:THR:HG23	2:E:33:LYS:HZ3	1.84	0.42
5:H:81:LEU:HD12	5:H:138:GLY:HA3	2.01	0.42
7:J:72:HIS:O	7:J:139[A]:SER:HB2	2.20	0.42
7:J:228:PRO:HD2	7:J:231:ILE:HD12	2.01	0.42
5:M:91:LYS:HZ2	5:M:119:LEU:CD2	2.28	0.42
7:Q:72:HIS:CD2	7:Q:73:VAL:HG23	2.54	0.42
7:Q:152:ASP:HB2	7:Q:153:PRO:CD	2.49	0.42
7:Q:152:ASP:OD1	7:Q:156:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:50:ILE:CG2	8:R:141:ILE:HG21	2.50	0.42
8:R:68:HIS:O	8:R:79:VAL:HA	2.19	0.42
14:W:28:GLY:HA3	14:W:39:ILE:HD11	2.01	0.42
11:X:45:LYS:HG3	11:X:203:ILE:CD1	2.50	0.42
13:Y:20:ALA:HB2	13:Y:188:ILE:HD13	2.02	0.42
14:a:109:THR:HA	14:a:126:ASP:HA	2.02	0.42
1:A:32:ASP:HA	1:A:174:TYR:CE2	2.55	0.41
2:B:159:VAL:O	2:B:163:ILE:HG13	2.19	0.41
3:C:104:TRP:CE2	3:C:181:GLU:HG3	2.55	0.41
2:E:103:VAL:CG2	2:E:178:ILE:HG22	2.50	0.41
1:F:63:LEU:HD21	1:F:79:ALA:CA	2.49	0.41
5:H:234:LEU:O	5:H:238:ILE:HG13	2.20	0.41
6:I:176:TYR:HE1	6:I:181:ILE:HG21	1.85	0.41
7:J:72:HIS:CD2	7:J:73:VAL:HG23	2.54	0.41
4:L:109:VAL:HG21	4:L:145:PHE:CD2	2.54	0.41
5:M:156:MET:HG2	5:M:157:ASP:N	2.34	0.41
6:N:95:ARG:NH2	6:N:101:PRO:HB3	2.35	0.41
9:O:82:ASP:HB2	9:O:132:VAL:CG2	2.50	0.41
10:P:165:ASN:OD1	10:P:168:ASN:ND2	2.52	0.41
11:S:44:TYR:CD2	11:S:65:THR:HG21	2.54	0.41
12:T:145:ARG:HG3	12:T:146:TYR:CD1	2.55	0.41
13:U:26:ARG:HD2	13:U:182:MET:HG2	2.02	0.41
11:X:6:VAL:HG12	11:X:57:PHE:HE1	1.84	0.41
13:Y:47:ARG:NH2	13:Y:191:LYS:O	2.52	0.41
2:B:212:LEU:HD21	13:Y:200:LYS:CG	2.50	0.41
3:C:104:TRP:CE2	3:C:181:GLU:HA	2.55	0.41
3:C:115:ASP:HB2	3:C:119:THR:HB	2.02	0.41
2:E:114:HIS:CE1	2:E:127:LEU:HD11	2.55	0.41
6:I:120:GLN:O	6:I:120:GLN:HG2	2.20	0.41
6:I:221[B]:ASN:HA	6:I:222:PRO:HD3	1.60	0.41
7:J:152:ASP:HB2	7:J:153:PRO:CD	2.49	0.41
8:K:125:TYR:CE2	8:K:134:LEU:HG	2.55	0.41
8:K:155:ASP:HB2	8:K:156:PRO:CD	2.49	0.41
8:K:211:LYS:HB3	8:K:212:PRO:HD2	2.01	0.41
4:L:33:SER:HG	4:L:62:LYS:HZ2	1.57	0.41
4:L:206:THR:C	4:L:233:LEU:CD1	2.93	0.41
6:N:95:ARG:CZ	6:N:101:PRO:HB3	2.51	0.41
6:N:220:LEU:HA	6:N:221:ASN:CB	2.49	0.41
10:P:183:LEU:O	10:P:186:ALA:HB3	2.20	0.41
10:P:218:ARG:NH1	10:P:220:LEU:HD23	2.35	0.41
7:Q:228:PRO:HD2	7:Q:231:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:28:ALA:O	8:R:31:ALA:N	2.46	0.41
8:R:191:PHE:HD1	8:R:191:PHE:HA	1.70	0.41
8:R:206:LEU:HD22	8:R:210:PHE:CZ	2.55	0.41
11:S:39:ASP:OD1	11:S:41:PRO:HD3	2.20	0.41
12:T:29:LYS:NZ	12:T:31:ASP:OD1	2.32	0.41
13:U:26:ARG:HB2	13:U:182:MET:HB2	2.01	0.41
9:Z:135:LEU:HG	9:Z:164:ILE:CD1	2.50	0.41
14:a:63:LEU:HD23	14:a:63:LEU:HA	1.88	0.41
1:A:84:ARG:HD3	1:A:117:GLY:O	2.21	0.41
1:A:152:ARG:CZ	1:A:152:ARG:HB2	2.49	0.41
1:A:163:MET:HE1	1:A:193:LEU:HD21	2.01	0.41
2:B:51:ASP:HB3	2:B:94:VAL:CG1	2.48	0.41
2:E:99:ILE:HG23	2:E:99:ILE:O	2.21	0.41
1:F:20:VAL:O	1:F:27:VAL:HG22	2.20	0.41
1:F:32:ASP:HA	1:F:174:TYR:CD2	2.56	0.41
5:H:157:ASP:HB2	5:H:158:PRO:HD2	2.01	0.41
5:H:169:ALA:O	5:H:174:SER:HB2	2.20	0.41
6:I:137:ASP:HB2	6:I:139:ASP:OD1	2.21	0.41
8:K:6:SER:OG	8:K:11:ARG:HG3	2.20	0.41
8:K:32:ILE:HG23	8:K:81:THR:HG22	2.02	0.41
4:L:26:MET:O	4:L:29:VAL:HG22	2.20	0.41
5:M:154:PHE:HD1	5:M:164:GLN:HA	1.85	0.41
6:N:134:VAL:HA	6:N:143:ARG:O	2.20	0.41
9:O:28:ILE:HD11	9:O:131:GLY:C	2.45	0.41
9:O:135:LEU:HG	9:O:164:ILE:CD1	2.50	0.41
7:Q:70:ASP:CG	7:Q:99:ARG:HH22	2.26	0.41
7:Q:228:PRO:HB2	7:Q:230:ASP:OD1	2.20	0.41
14:W:45:VAL:HG12	14:W:71:VAL:HG11	2.01	0.41
9:Z:28:ILE:HD11	9:Z:131:GLY:C	2.45	0.41
9:Z:51:ASN:HB3	9:Z:56:LEU:CD1	2.51	0.41
9:Z:86:LEU:HD22	9:Z:114:LEU:HD11	2.02	0.41
10:b:183:LEU:O	10:b:186:ALA:HB3	2.20	0.41
10:b:218:ARG:NH1	10:b:220:LEU:HD23	2.35	0.41
3:C:38:ASN:HB3	3:C:39:PRO:HD2	2.02	0.41
15:C:301:BZ7:CAE	11:X:127:VAL:CG1	2.98	0.41
3:D:38:ASN:HB3	3:D:39:PRO:HD2	2.02	0.41
2:E:140:ASP:C	2:E:141:ARG:HD2	2.46	0.41
2:E:175:ALA:O	2:E:186:LEU:HB2	2.20	0.41
1:F:32:ASP:HA	1:F:174:TYR:CE2	2.55	0.41
1:F:84:ARG:HD3	1:F:117:GLY:O	2.21	0.41
1:F:152:ARG:CZ	1:F:152:ARG:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:67:ASP:OD1	12:V:69:MET:HE1	2.20	0.41
6:I:220:LEU:CB	6:I:225:ILE:HD11	2.51	0.41
7:J:73:VAL:HA	7:J:138:GLY:O	2.21	0.41
4:L:6:TYR:CE2	4:L:15:PRO:HD3	2.55	0.41
5:M:88:LEU:HD22	5:M:116:VAL:HG13	2.02	0.41
7:Q:73:VAL:HA	7:Q:138:GLY:O	2.21	0.41
11:S:24:ALA:HA	11:S:194:ARG:O	2.19	0.41
11:S:152:GLN:HB2	11:S:174:LEU:HD11	2.02	0.41
13:U:20:ALA:HB2	13:U:188:ILE:HD13	2.02	0.41
13:U:43:PRO:HB3	13:U:49:TYR:HE1	1.84	0.41
13:U:69:ARG:HD3	13:U:93:LEU:HD12	2.03	0.41
14:W:162:GLN:HE21	14:W:191:THR:HG21	1.85	0.41
11:X:122:TYR:HA	11:X:131:GLN:O	2.20	0.41
14:a:6:VAL:HA	14:a:29:SER:O	2.21	0.41
14:a:92:LEU:HD23	14:a:110:MET:HE3	2.02	0.41
1:A:20:VAL:O	1:A:27:VAL:HG22	2.20	0.41
2:B:54:MET:HG3	13:Y:95:TYR:CD1	2.56	0.41
2:B:99:ILE:HG23	2:B:99:ILE:O	2.21	0.41
3:C:87:MET:HE2	3:C:116:GLU:HA	2.03	0.41
2:E:83:LEU:HD13	2:E:98:LEU:CD1	2.51	0.41
1:F:18:SER:OG	1:F:172:VAL:HG22	2.21	0.41
7:J:37:ILE:HD13	7:J:196:ILE:HG21	2.02	0.41
7:J:195:LYS:O	7:J:199:ILE:HG13	2.20	0.41
8:K:40:VAL:HG22	8:K:167:ALA:CB	2.51	0.41
8:K:206:LEU:HD22	8:K:210:PHE:CZ	2.55	0.41
5:M:78:MET:HB3	5:M:141:LEU:HD23	2.02	0.41
9:O:23:TYR:O	9:O:26:GLU:HB2	2.20	0.41
8:R:125:TYR:CE2	8:R:134:LEU:HG	2.55	0.41
11:S:145:LEU:HD23	11:S:145:LEU:HA	1.90	0.41
14:W:124:TYR:CE1	14:W:139:THR:HG22	2.51	0.41
11:X:44:TYR:CD2	11:X:65:THR:HG21	2.54	0.41
13:Y:108:ILE:O	13:Y:120:ILE:HA	2.21	0.41
1:A:1:THR:HG23	1:A:33:LYS:HZ3	1.84	0.41
2:B:83:LEU:HD13	2:B:98:LEU:CD1	2.51	0.41
2:B:175:ALA:O	2:B:186:LEU:HB2	2.20	0.41
3:C:58:LEU:HG	3:C:86:MET:HE1	2.03	0.41
3:D:112:TYR:HD1	3:D:122:SER:HA	1.85	0.41
3:D:115:ASP:HB2	3:D:119:THR:HB	2.02	0.41
2:E:187:ARG:O	2:E:188:THR:OG1	2.38	0.41
8:K:7:ALA:N	8:K:10:ASP:OD2	2.43	0.41
4:L:137:TYR:CE1	4:L:141:GLY:HA2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:46:GLU:HG3	6:N:206:ILE:CG2	2.46	0.41
6:N:129:ILE:HG13	6:N:129:ILE:O	2.20	0.41
6:N:137:ASP:HB2	6:N:139:ASP:OD1	2.20	0.41
9:O:38:LEU:N	9:O:160:LYS:O	2.31	0.41
9:O:55:LEU:HD23	9:O:55:LEU:HA	1.89	0.41
7:Q:211:LEU:HD23	7:Q:236:GLU:HG2	2.02	0.41
12:T:160:LEU:O	12:T:164:LEU:HG	2.20	0.41
11:X:44:TYR:O	11:X:52:ILE:HG22	2.20	0.41
3:D:58:LEU:HG	3:D:86:MET:HE1	2.03	0.41
3:D:126:PHE:HD1	3:D:126:PHE:HA	1.73	0.41
5:H:94:VAL:HG12	5:H:98:ASN:ND2	2.36	0.41
5:H:96:THR:HG22	5:H:112:VAL:HG22	2.02	0.41
4:L:11:THR:HA	7:Q:129:ARG:HD3	2.03	0.41
4:L:100:ASP:HB2	14:a:90:SER:OG	2.21	0.41
6:N:38:ARG:O	6:N:213:ARG:NH2	2.51	0.41
9:O:86:LEU:HD23	9:O:86:LEU:HA	1.85	0.41
10:P:38:LYS:HG3	10:P:43:VAL:HG22	2.03	0.41
10:P:49:LYS:HB2	10:P:206:ASN:HA	2.02	0.41
8:R:160:TYR:C	8:R:161:CYS:SG	3.02	0.41
12:V:13:VAL:CG1	12:V:105:ALA:HB1	2.46	0.41
11:X:68:ILE:HD11	11:X:92:LEU:CD1	2.51	0.41
13:Y:29:ILE:HG22	13:Y:30:GLN:N	2.36	0.41
13:Y:158:ASP:HB2	13:Y:159:PRO:HD2	2.03	0.41
9:Z:195:LYS:HA	9:Z:240:HIS:CE1	2.56	0.41
4:G:26:MET:O	4:G:29:VAL:HG22	2.20	0.41
5:H:40:ILE:HD11	5:H:181:LEU:CD2	2.51	0.41
5:H:230:THR:O	5:H:234:LEU:HG	2.20	0.41
6:I:105:GLU:HG2	6:I:109:ARG:NH1	2.35	0.41
6:I:129:ILE:HG13	6:I:129:ILE:O	2.20	0.41
7:J:47:PHE:O	7:J:213:LEU:HA	2.21	0.41
8:K:182:LYS:HG2	8:K:191:PHE:HE1	1.85	0.41
8:K:238:HIS:O	8:K:242:LEU:HG	2.21	0.41
4:L:80:ASP:OD1	4:L:126:ARG:NH2	2.47	0.41
5:M:191:LEU:HD12	5:M:191:LEU:HA	1.88	0.41
6:N:79:ASP:CG	6:N:125:ARG:HH22	2.29	0.41
6:N:177:THR:O	6:N:180:ALA:HB3	2.20	0.41
10:P:195:LYS:HZ1	10:P:202:MET:HB2	1.84	0.41
7:Q:47:PHE:O	7:Q:213:LEU:HA	2.21	0.41
11:S:42:LYS:HB3	11:S:54:CYS:O	2.19	0.41
11:S:92:LEU:HD12	11:S:92:LEU:HA	1.79	0.41
12:T:14:LEU:HD11	12:T:180:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:104:LEU:HD23	12:T:104:LEU:O	2.21	0.41
13:U:14:LYS:HZ1	13:U:133:ASP:HA	1.86	0.41
11:X:39:ASP:OD1	11:X:41:PRO:HD3	2.20	0.41
13:Y:16:LYS:C	13:Y:18:CYS:N	2.78	0.41
9:Z:49:ARG:CD	9:Z:212:GLU:HG3	2.51	0.41
2:B:2:THR:OG1	2:B:130:GLY:HA3	2.21	0.41
3:C:104:TRP:CZ2	3:C:181:GLU:HG3	2.56	0.41
3:D:67:TYR:O	3:D:71:GLY:HA2	2.21	0.41
3:D:104:TRP:CE2	3:D:181:GLU:HA	2.55	0.41
2:E:1:THR:HA	2:E:17:ASP:OD2	2.20	0.41
2:E:209:THR:HG21	13:U:167:SER:HB3	2.02	0.41
1:F:13:VAL:HA	1:F:176:VAL:O	2.21	0.41
1:F:20:VAL:HG23	1:F:27:VAL:CG2	2.51	0.41
4:G:80:ASP:CG	4:G:126:ARG:HH22	2.29	0.41
5:H:189:MET:HE2	5:H:194:ALA:N	2.36	0.41
6:I:95:ARG:NH2	6:I:101:PRO:HB3	2.35	0.41
7:J:28:LYS:HA	7:J:31:GLU:CD	2.46	0.41
8:K:230:LEU:HD22	8:K:234:GLU:OE1	2.21	0.41
4:L:46:LEU:HD23	4:L:46:LEU:HA	1.90	0.41
4:L:58:ALA:HB3	5:M:164:GLN:O	2.20	0.41
4:L:171:TYR:CD2	4:L:194:ALA:HB2	2.56	0.41
5:M:94:VAL:HG12	5:M:98:ASN:ND2	2.36	0.41
5:M:157:ASP:HB2	5:M:158:PRO:CD	2.50	0.41
5:M:180:SER:HB3	5:M:201:ILE:HG12	2.03	0.41
5:M:189:MET:HE2	5:M:194:ALA:N	2.36	0.41
5:M:189:MET:CE	5:M:194:ALA:HA	2.45	0.41
6:N:176:TYR:HE1	6:N:181:ILE:HG21	1.86	0.41
6:N:195:LEU:HB2	6:N:206:ILE:HD11	2.03	0.41
6:N:221:ASN:N	6:N:222:PRO:CD	2.82	0.41
9:O:54:LYS:CG	9:O:55:LEU:H	2.25	0.41
9:O:178:ASP:OD2	9:O:195:LYS:NZ	2.35	0.41
8:R:6:SER:OG	8:R:11:ARG:HG3	2.20	0.41
8:R:193:GLN:C	8:R:195:VAL:N	2.79	0.41
8:R:205:VAL:HG23	8:R:206:LEU:CD1	2.46	0.41
11:S:6:VAL:HG12	11:S:57:PHE:CD1	2.56	0.41
11:S:45:LYS:HG3	11:S:203:ILE:CD1	2.50	0.41
11:S:122:TYR:HA	11:S:131:GLN:O	2.20	0.41
11:S:152:GLN:CB	11:S:174:LEU:HD11	2.51	0.41
12:T:44:LEU:C	12:T:45:LEU:HD12	2.46	0.41
13:U:20:ALA:HA	13:U:187:HIS:O	2.21	0.41
13:U:49:TYR:CD2	13:U:189:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:44:LEU:C	12:V:45:LEU:HD12	2.46	0.41
14:W:92:LEU:HD23	14:W:110:MET:HE3	2.02	0.41
14:W:109:THR:HA	14:W:126:ASP:HA	2.02	0.41
14:W:151:ARG:HH12	11:X:35:ILE:HB	1.86	0.41
11:X:152:GLN:CB	11:X:174:LEU:HD11	2.51	0.41
13:Y:69:ARG:HD3	13:Y:93:LEU:HD12	2.03	0.41
9:Z:76:VAL:HG21	9:Z:83:ALA:HB1	2.02	0.41
9:Z:137:ILE:O	9:Z:137:ILE:HG13	2.21	0.41
14:a:109:THR:O	14:a:139:THR:HG21	2.21	0.41
10:b:149[B]:ASP:HB2	10:b:150:PRO:CD	2.51	0.41
1:A:63:LEU:HD21	1:A:79:ALA:CA	2.49	0.41
3:C:67:TYR:O	3:C:71:GLY:HA2	2.21	0.41
3:D:82:LEU:CD2	3:D:86:MET:HE3	2.51	0.41
2:E:90:TYR:CD2	2:E:94:VAL:HG21	2.55	0.41
1:F:5:ALA:HB3	1:F:111:VAL:HG11	2.03	0.41
1:F:36:PRO:HA	1:F:42:TYR:HD1	1.86	0.41
1:F:172:VAL:HB	1:F:188:ILE:O	2.21	0.41
6:I:176:TYR:CE1	6:I:181:ILE:HG21	2.56	0.41
6:I:208:LEU:HG	6:I:209:ALA:H	1.77	0.41
5:M:191:LEU:O	5:M:194:ALA:HB3	2.21	0.41
5:M:199:LEU:HD13	5:M:199:LEU:HA	1.97	0.41
6:N:51:ALA:O	6:N:53:LEU:N	2.54	0.41
9:O:57:ASP:OD2	10:P:38:LYS:HE2	2.21	0.41
9:O:137:ILE:O	9:O:137:ILE:HG13	2.21	0.41
10:P:195:LYS:HE2	10:P:202:MET:SD	2.61	0.41
7:Q:137:LEU:O	7:Q:148:LEU:HA	2.21	0.41
8:R:238:HIS:O	8:R:242:LEU:HG	2.21	0.41
14:W:6:VAL:HA	14:W:29:SER:O	2.21	0.41
11:X:6:VAL:HG12	11:X:57:PHE:CD1	2.56	0.41
1:A:118:MET:HE3	14:W:57:TYR:CE2	2.56	0.40
1:A:172:VAL:HB	1:A:188:ILE:O	2.21	0.40
1:A:189:LEU:HD22	14:a:209:TRP:CB	2.51	0.40
2:B:90:TYR:CD2	2:B:94:VAL:HG21	2.55	0.40
2:B:103:VAL:HG23	2:B:178:ILE:HG22	2.03	0.40
2:B:219:LEU:CD1	13:Y:194:ILE:HG12	2.50	0.40
3:D:33:LYS:O	3:D:45:MET:CG	2.60	0.40
3:D:81:LYS:O	3:D:84:SER:HB3	2.21	0.40
2:E:2:THR:OG1	2:E:130:GLY:HA3	2.21	0.40
2:E:63:MET:HG3	2:E:79:VAL:CG2	2.44	0.40
4:G:6:TYR:CE2	4:G:15:PRO:HD3	2.55	0.40
6:I:79:ASP:CG	6:I:125:ARG:HH22	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:221[A]:ASN:HA	6:I:222:PRO:HD3	1.59	0.40
7:J:137:LEU:O	7:J:148:LEU:HA	2.21	0.40
7:J:228:PRO:HB2	7:J:230:ASP:OD1	2.20	0.40
5:M:234:LEU:O	5:M:238:ILE:HG13	2.20	0.40
6:N:21:TYR:CE1	9:O:14:PRO:HA	2.55	0.40
7:Q:156:VAL:CG2	8:R:84:THR:HG21	2.51	0.40
8:R:32:ILE:HG23	8:R:81:THR:HG22	2.02	0.40
11:S:122:TYR:HB3	11:S:124:PHE:HE1	1.87	0.40
12:V:73:TYR:OH	9:Z:106:PRO:HG2	2.20	0.40
14:W:9:THR:OG1	14:W:10:SER:N	2.52	0.40
11:X:155:PHE:CD2	11:X:163:HIS:HA	2.57	0.40
9:Z:23:TYR:O	9:Z:26:GLU:HB2	2.20	0.40
14:a:1:THR:HG21	14:a:59:ASP:OD2	2.21	0.40
14:a:203:LEU:HD23	14:a:203:LEU:HA	1.89	0.40
10:b:181:LEU:CD2	10:b:186:ALA:HA	2.51	0.40
2:B:205:VAL:O	2:B:208:THR:HG23	2.21	0.40
3:D:47:GLY:O	15:D:301:BZ7:CBC	2.69	0.40
2:E:98:LEU:HB2	2:E:113:VAL:HG13	2.04	0.40
2:E:103:VAL:HG23	2:E:178:ILE:HG22	2.03	0.40
6:I:95:ARG:CZ	6:I:101:PRO:HB3	2.51	0.40
7:J:211:LEU:HD23	7:J:236:GLU:HG2	2.02	0.40
8:K:130:GLU:HA	10:b:5:TYR:CE2	2.55	0.40
5:M:37:ALA:HB2	5:M:50:VAL:CG2	2.46	0.40
5:M:40:ILE:HD11	5:M:181:LEU:CD2	2.51	0.40
5:M:58:LEU:HD11	6:N:173:GLU:N	2.37	0.40
9:O:46:ALA:HB1	9:O:197:LEU:CD1	2.50	0.40
8:R:51:VAL:CG1	8:R:198:ALA:HB1	2.51	0.40
8:R:234:GLU:O	8:R:237:ALA:HB3	2.22	0.40
13:U:29:ILE:HG22	13:U:30:GLN:N	2.36	0.40
13:U:47:ARG:HD3	13:U:111:LEU:HD12	2.03	0.40
9:Z:148:TYR:CD1	9:Z:158:GLY:HA2	2.56	0.40
1:A:5:ALA:HB3	1:A:111:VAL:HG11	2.03	0.40
1:A:126:ILE:HG21	1:A:126:ILE:HD13	1.87	0.40
3:C:59:LEU:HD22	3:C:83:LEU:HB2	2.03	0.40
4:G:46:LEU:HD23	4:G:46:LEU:HA	1.90	0.40
4:G:171:TYR:HD2	4:G:194:ALA:HB2	1.86	0.40
5:H:48:LEU:C	5:H:217:LEU:HD12	2.46	0.40
5:H:191:LEU:O	5:H:194:ALA:HB3	2.21	0.40
6:I:91:CYS:SG	6:I:107:ILE:HD13	2.62	0.40
4:L:80:ASP:CG	4:L:126:ARG:HH22	2.29	0.40
5:M:48:LEU:C	5:M:217:LEU:HD12	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:169:ARG:O	7:Q:173:LYS:HG3	2.22	0.40
8:R:50:ILE:HG23	8:R:141:ILE:HG21	2.03	0.40
11:S:68:ILE:HD11	11:S:92:LEU:CD1	2.51	0.40
11:S:155:PHE:CD2	11:S:163:HIS:HA	2.57	0.40
11:S:193:LEU:O	11:S:207:THR:HA	2.21	0.40
12:V:46:CYS:SG	12:V:53:THR:HA	2.61	0.40
12:V:153:ARG:O	12:V:156:ALA:HB3	2.22	0.40
12:V:160:LEU:O	12:V:164:LEU:HG	2.20	0.40
14:W:166:ARG:O	14:W:170:GLU:HG3	2.22	0.40
13:Y:20:ALA:HA	13:Y:187:HIS:O	2.21	0.40
13:Y:44:MET:HG2	13:Y:50:ILE:HG22	2.03	0.40
13:Y:47:ARG:HD3	13:Y:111:LEU:HD12	2.03	0.40
9:Z:46:ALA:HB1	9:Z:197:LEU:CD1	2.50	0.40
9:Z:86:LEU:HA	9:Z:86:LEU:HD23	1.86	0.40
2:B:9:GLN:HG3	2:B:145:ASN:HA	2.03	0.40
2:B:54:MET:SD	2:B:57:ARG:NH2	2.87	0.40
3:C:81:LYS:O	3:C:84:SER:HB3	2.21	0.40
2:E:10:ASP:HB3	2:E:179:THR:HG23	2.02	0.40
2:E:19:ARG:HD3	2:E:26:VAL:CG2	2.47	0.40
2:E:148:LEU:O	2:E:148:LEU:HD23	2.22	0.40
1:F:17:ASP:OD1	1:F:33:LYS:NZ	2.54	0.40
4:G:171:TYR:CD2	4:G:194:ALA:HB2	2.56	0.40
5:H:195:ILE:O	5:H:199:LEU:HD23	2.22	0.40
6:I:45:VAL:HG23	6:I:45:VAL:O	2.21	0.40
8:K:51:VAL:CG1	8:K:198:ALA:HB1	2.51	0.40
4:L:117:GLN:O	4:L:120:THR:OG1	2.30	0.40
5:M:118:ASN:O	5:M:122:GLN:HG3	2.21	0.40
6:N:176:TYR:CE1	6:N:181:ILE:HG21	2.56	0.40
9:O:49:ARG:NE	9:O:212:GLU:HG3	2.36	0.40
9:O:148:TYR:CD1	9:O:158:GLY:HA2	2.56	0.40
7:Q:28:LYS:HA	7:Q:31:GLU:CD	2.46	0.40
12:T:44:LEU:HD13	12:T:104:LEU:HD12	2.04	0.40
12:T:61:GLN:O	12:T:65:GLN:HG2	2.21	0.40
13:U:108:ILE:O	13:U:120:ILE:HA	2.21	0.40
13:U:158:ASP:HB2	13:U:159:PRO:HD2	2.03	0.40
12:V:61:GLN:O	12:V:65:GLN:HG2	2.21	0.40
10:b:44:VAL:HG23	10:b:187:ILE:HG12	2.04	0.40
1:A:2:THR:OG1	1:A:130:GLY:HA3	2.22	0.40
1:A:18:SER:OG	1:A:172:VAL:HG22	2.21	0.40
1:A:20:VAL:HG23	1:A:27:VAL:CG2	2.51	0.40
2:B:123:PRO:HB3	14:a:214:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:ASP:C	2:B:141:ARG:HD2	2.46	0.40
2:B:148:LEU:O	2:B:148:LEU:HD23	2.22	0.40
3:C:35:ILE:N	3:C:45:MET:HE3	2.36	0.40
3:C:82:LEU:CD2	3:C:86:MET:HE3	2.51	0.40
3:D:59:LEU:HD22	3:D:83:LEU:HB2	2.03	0.40
5:H:157:ASP:HB2	5:H:158:PRO:CD	2.51	0.40
7:J:33:SER:O	7:J:167:LYS:HB3	2.21	0.40
4:L:199:LEU:HD23	4:L:199:LEU:HA	1.92	0.40
5:M:35:SER:HA	5:M:53:ARG:NH2	2.37	0.40
6:N:196:LEU:HD21	6:N:202:GLY:HA3	1.96	0.40
9:O:49:ARG:CD	9:O:212:GLU:HG3	2.51	0.40
9:O:80:THR:HB	10:P:153:ALA:HB2	2.04	0.40
9:O:195:LYS:HA	9:O:240:HIS:CE1	2.56	0.40
10:P:38:LYS:HD2	10:P:143:PRO:CG	2.49	0.40
10:P:181:LEU:CD2	10:P:186:ALA:HA	2.51	0.40
7:Q:28:LYS:C	7:Q:31:GLU:HG2	2.47	0.40
7:Q:37:ILE:HD13	7:Q:196:ILE:HG21	2.02	0.40
8:R:230:LEU:HD22	8:R:234:GLU:OE1	2.21	0.40
12:T:153:ARG:O	12:T:156:ALA:HB3	2.22	0.40
13:U:183:GLY:N	13:U:201:ALA:HB3	2.35	0.40
12:V:1[A]:MET:HE1	12:V:133:GLY:CA	2.52	0.40
12:V:88:LEU:HD12	12:V:122:ALA:HB2	2.03	0.40
12:V:142:ILE:HD11	12:V:166:GLU:HG2	2.04	0.40
11:X:12:ILE:CD1	11:X:109:ILE:HB	2.51	0.40
11:X:71:ARG:HB3	11:X:91:MET:SD	2.62	0.40
13:Y:24:ASP:OD2	13:Y:180:SER:HB3	2.22	0.40
14:a:9:THR:OG1	14:a:10:SER:N	2.52	0.40
10:b:38:LYS:HG3	10:b:43:VAL:HG22	2.03	0.40
10:b:49:LYS:HB2	10:b:206:ASN:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/199 (99%)	183 (93%)	14 (7%)	0	100	100
1	F	197/199 (99%)	183 (93%)	14 (7%)	0	100	100
2	B	217/234 (93%)	183 (84%)	32 (15%)	2 (1%)	14	45
2	E	217/234 (93%)	184 (85%)	31 (14%)	2 (1%)	14	45
3	C	199/204 (98%)	179 (90%)	20 (10%)	0	100	100
3	D	199/204 (98%)	180 (90%)	19 (10%)	0	100	100
4	G	233/263 (89%)	214 (92%)	18 (8%)	1 (0%)	30	63
4	L	235/263 (89%)	217 (92%)	18 (8%)	0	100	100
5	H	231/241 (96%)	209 (90%)	22 (10%)	0	100	100
5	M	231/241 (96%)	210 (91%)	21 (9%)	0	100	100
6	I	232/248 (94%)	203 (88%)	28 (12%)	1 (0%)	30	63
6	N	230/248 (93%)	204 (89%)	26 (11%)	0	100	100
7	J	241/255 (94%)	222 (92%)	19 (8%)	0	100	100
7	Q	238/255 (93%)	219 (92%)	19 (8%)	0	100	100
8	K	238/246 (97%)	218 (92%)	20 (8%)	0	100	100
8	R	237/246 (96%)	215 (91%)	21 (9%)	1 (0%)	30	63
9	O	240/261 (92%)	223 (93%)	17 (7%)	0	100	100
9	Z	240/261 (92%)	223 (93%)	17 (7%)	0	100	100
10	P	228/234 (97%)	211 (92%)	17 (8%)	0	100	100
10	b	231/234 (99%)	214 (93%)	17 (7%)	0	100	100
11	S	212/213 (100%)	188 (89%)	24 (11%)	0	100	100
11	X	213/213 (100%)	189 (89%)	24 (11%)	0	100	100
12	T	196/201 (98%)	179 (91%)	17 (9%)	0	100	100
12	V	196/201 (98%)	177 (90%)	19 (10%)	0	100	100
13	U	204/205 (100%)	190 (93%)	14 (7%)	0	100	100
13	Y	204/205 (100%)	189 (93%)	14 (7%)	1 (0%)	25	58
14	W	215/219 (98%)	190 (88%)	25 (12%)	0	100	100
14	a	215/219 (98%)	190 (88%)	25 (12%)	0	100	100
All	All	6166/6446 (96%)	5586 (91%)	572 (9%)	8 (0%)	50	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	I	206	ILE
8	R	194	THR
2	B	195	PRO
2	E	195	PRO
4	G	235	GLY
2	E	194	GLU
2	B	194	GLU
13	Y	17	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	153/153 (100%)	152 (99%)	1 (1%)	81	86
1	F	153/153 (100%)	153 (100%)	0	100	100
2	B	171/185 (92%)	167 (98%)	4 (2%)	45	63
2	E	171/185 (92%)	167 (98%)	4 (2%)	45	63
3	C	164/166 (99%)	163 (99%)	1 (1%)	84	88
3	D	164/166 (99%)	163 (99%)	1 (1%)	84	88
4	G	194/224 (87%)	188 (97%)	6 (3%)	35	56
4	L	198/224 (88%)	194 (98%)	4 (2%)	50	68
5	H	188/203 (93%)	187 (100%)	1 (0%)	86	90
5	M	187/203 (92%)	185 (99%)	2 (1%)	70	79
6	I	175/211 (83%)	175 (100%)	0	100	100
6	N	178/211 (84%)	177 (99%)	1 (1%)	84	88
7	J	199/212 (94%)	199 (100%)	0	100	100
7	Q	192/212 (91%)	192 (100%)	0	100	100
8	K	201/210 (96%)	199 (99%)	2 (1%)	73	80
8	R	192/210 (91%)	190 (99%)	2 (1%)	73	80
9	O	191/221 (86%)	189 (99%)	2 (1%)	73	80
9	Z	194/221 (88%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	P	176/191 (92%)	176 (100%)	0	100	100
10	b	185/191 (97%)	185 (100%)	0	100	100
11	S	175/178 (98%)	175 (100%)	0	100	100
11	X	175/178 (98%)	173 (99%)	2 (1%)	70	79
12	T	166/171 (97%)	166 (100%)	0	100	100
12	V	167/171 (98%)	165 (99%)	2 (1%)	67	77
13	U	173/174 (99%)	173 (100%)	0	100	100
13	Y	175/174 (101%)	174 (99%)	1 (1%)	84	88
14	W	180/181 (99%)	180 (100%)	0	100	100
14	a	178/181 (98%)	178 (100%)	0	100	100
All	All	5015/5360 (94%)	4979 (99%)	36 (1%)	82	86

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
2	B	113	VAL
2	B	193	THR
2	B	194	GLU
2	B	196	VAL
3	C	45	MET
3	D	45	MET
2	E	113	VAL
2	E	193	THR
2	E	194	GLU
2	E	196	VAL
4	G	101[A]	ARG
4	G	101[B]	ARG
4	G	230	SER
4	G	233	LEU
4	G	234	GLU
4	G	236	LEU
5	H	175	GLU
8	K	49[A]	VAL
8	K	49[B]	VAL
4	L	230	SER
4	L	233	LEU
4	L	234	GLU

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Mol	Chain	Res	Type
4	L	236	LEU
5	M	119	LEU
5	M	121	LEU
6	N	201	SER
9	O	7[A]	SER
9	O	7[B]	SER
8	R	137	CYS
8	R	191	PHE
12	V	1[A]	MET
12	V	1[B]	MET
11	X	3[A]	SER
11	X	3[B]	SER
13	Y	16	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	38	HIS
2	B	9	GLN
2	B	66	HIS
2	B	93	HIS
2	B	114	HIS
2	B	145	ASN
2	B	152	GLN
2	B	203	HIS
2	B	214	GLN
3	C	9	GLN
3	D	9	GLN
3	D	197	HIS
2	E	9	GLN
2	E	66	HIS
2	E	93	HIS
2	E	114	HIS
2	E	145	ASN
2	E	152	GLN
1	F	28	ASN
1	F	38	HIS
4	G	65	HIS
4	G	143	HIS
5	H	73	HIS
5	H	99	HIS

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Mol	Chain	Res	Type
5	H	221	GLN
5	H	224	GLN
6	I	92	GLN
7	J	97	ASN
7	J	110	HIS
8	K	68	HIS
8	K	100	ASN
8	K	128	ASN
4	L	143	HIS
5	M	98	ASN
5	M	99	HIS
5	M	221	GLN
5	M	224	GLN
6	N	92	GLN
9	O	102	GLN
9	O	109	GLN
9	O	149	GLN
9	O	240	HIS
10	P	101	GLN
10	P	108	GLN
7	Q	97	ASN
7	Q	110	HIS
7	Q	143	ASN
8	R	53	GLN
8	R	68	HIS
8	R	100	ASN
8	R	128	ASN
11	S	108	ASN
11	S	131	GLN
11	S	157	ASN
11	S	163	HIS
12	T	55	GLN
12	T	65	GLN
12	T	82	ASN
12	T	132	HIS
12	T	174	ASN
13	U	92	ASN
13	U	172	ASN
12	V	82	ASN
12	V	132	HIS
12	V	174	ASN
14	W	47	ASN

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Mol	Chain	Res	Type
14	W	69	GLN
14	W	89	HIS
14	W	162	GLN
14	W	213	HIS
11	X	108	ASN
11	X	151	ASN
11	X	163	HIS
13	Y	32	GLN
13	Y	92	ASN
13	Y	168	GLN
9	Z	40	ASN
9	Z	102	GLN
9	Z	109	GLN
9	Z	149	GLN
9	Z	235	GLN
9	Z	240	HIS
14	a	2	GLN
14	a	81	HIS
14	a	89	HIS
14	a	162	GLN
14	a	213	HIS
10	b	101	GLN
10	b	108	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
15	BZ7	C	301	-	42,42,42	2.94	13 (30%)	56,56,56	1.18	3 (5%)
15	BZ7	D	301	-	42,42,42	2.94	14 (33%)	56,56,56	1.18	3 (5%)

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
15	BZ7	C	301	-	-	16/37/37/37	0/3/3/3
15	BZ7	D	301	-	-	16/37/37/37	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	301	BZ7	CAE-CAD	8.32	1.53	1.38
15	D	301	BZ7	CAE-CAD	8.31	1.53	1.38
15	D	301	BZ7	CAB-CAC	7.25	1.53	1.38
15	C	301	BZ7	CAB-CAC	7.22	1.53	1.38
15	D	301	BZ7	CAF-CAA	6.80	1.53	1.38
15	C	301	BZ7	CAF-CAA	6.77	1.53	1.38
15	D	301	BZ7	CG-ND2	6.72	1.45	1.34
15	C	301	BZ7	CG-ND2	6.70	1.45	1.34
15	D	301	BZ7	CAI-N	5.51	1.45	1.34
15	C	301	BZ7	CAI-N	5.49	1.45	1.34
15	D	301	BZ7	CBA-NAZ	5.33	1.45	1.33
15	C	301	BZ7	CBA-NAZ	5.32	1.45	1.33
15	D	301	BZ7	C-NAN	5.11	1.45	1.33
15	C	301	BZ7	C-NAN	5.08	1.45	1.33
15	D	301	BZ7	CAA-CAB	-3.98	1.32	1.38
15	C	301	BZ7	CAA-CAB	-3.95	1.32	1.38
15	C	301	BZ7	CAD-CAC	-3.46	1.32	1.38
15	D	301	BZ7	CAD-CAC	-3.45	1.32	1.38
15	D	301	BZ7	CAF-CAE	-2.83	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	301	BZ7	CAF-CAE	-2.78	1.32	1.38
15	D	301	BZ7	O-C	-2.32	1.18	1.23
15	C	301	BZ7	O-C	-2.32	1.19	1.23
15	C	301	BZ7	OD1-CG	-2.20	1.18	1.23
15	C	301	BZ7	OAK-CAI	-2.20	1.18	1.23
15	D	301	BZ7	OAK-CAI	-2.19	1.18	1.23
15	D	301	BZ7	OD1-CG	-2.15	1.19	1.23
15	D	301	BZ7	CAS-ND2	-2.01	1.45	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	301	BZ7	CAS-ND2-CG	-4.82	119.97	126.14
15	C	301	BZ7	CAS-ND2-CG	-4.81	119.97	126.14
15	D	301	BZ7	CB-CG-ND2	3.35	120.01	115.87
15	C	301	BZ7	CB-CG-ND2	3.31	119.96	115.87
15	C	301	BZ7	CAH-CAI-N	2.35	120.01	115.86
15	D	301	BZ7	CAH-CAI-N	2.33	119.97	115.86

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	301	BZ7	CBF-CBG-CBI-CBJ
15	C	301	BZ7	CBH-CBG-CBI-CBN
15	D	301	BZ7	CBF-CBG-CBI-CBJ
15	D	301	BZ7	CBH-CBG-CBI-CBN
15	C	301	BZ7	CBF-CBG-CBI-CBN
15	C	301	BZ7	CBH-CBG-CBI-CBJ
15	D	301	BZ7	CBF-CBG-CBI-CBN
15	D	301	BZ7	CBH-CBG-CBI-CBJ
15	D	301	BZ7	CAY-CAX-NAN-C
15	C	301	BZ7	NAZ-CBA-CBC-CBD
15	C	301	BZ7	CAY-CAX-NAN-C
15	C	301	BZ7	OBB-CBA-CBC-CBD
15	D	301	BZ7	NAZ-CBA-CBC-CBD
15	D	301	BZ7	OBB-CBA-CBC-CBD
15	C	301	BZ7	NAZ-CBA-CBC-CBH
15	C	301	BZ7	OBB-CBA-CBC-CBH
15	D	301	BZ7	OBB-CBA-CBC-CBH
15	D	301	BZ7	NAZ-CBA-CBC-CBH
15	C	301	BZ7	N-CA-CB-CG

Continued on next page...

Continued from previous page...

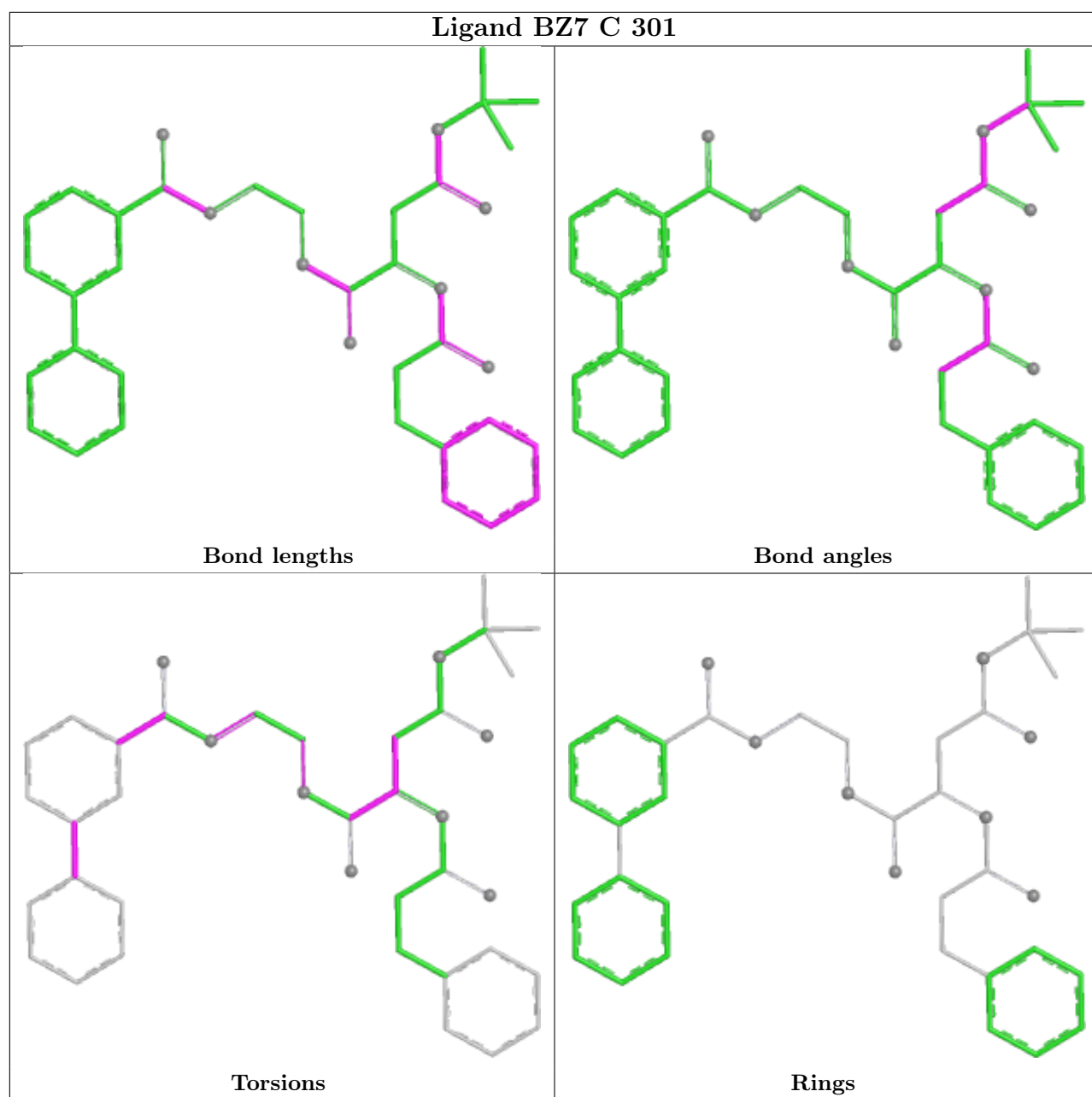
Mol	Chain	Res	Type	Atoms
15	D	301	BZ7	N-CA-CB-CG
15	C	301	BZ7	CAX-CAY-NAZ-CBA
15	C	301	BZ7	C-CA-CB-CG
15	D	301	BZ7	C-CA-CB-CG
15	D	301	BZ7	CAX-CAY-NAZ-CBA
15	D	301	BZ7	NAN-C-CA-N
15	C	301	BZ7	NAN-C-CA-N
15	C	301	BZ7	O-C-CA-N
15	D	301	BZ7	O-C-CA-N
15	D	301	BZ7	O-C-CA-CB
15	C	301	BZ7	O-C-CA-CB
15	D	301	BZ7	NAN-C-CA-CB
15	C	301	BZ7	NAN-C-CA-CB

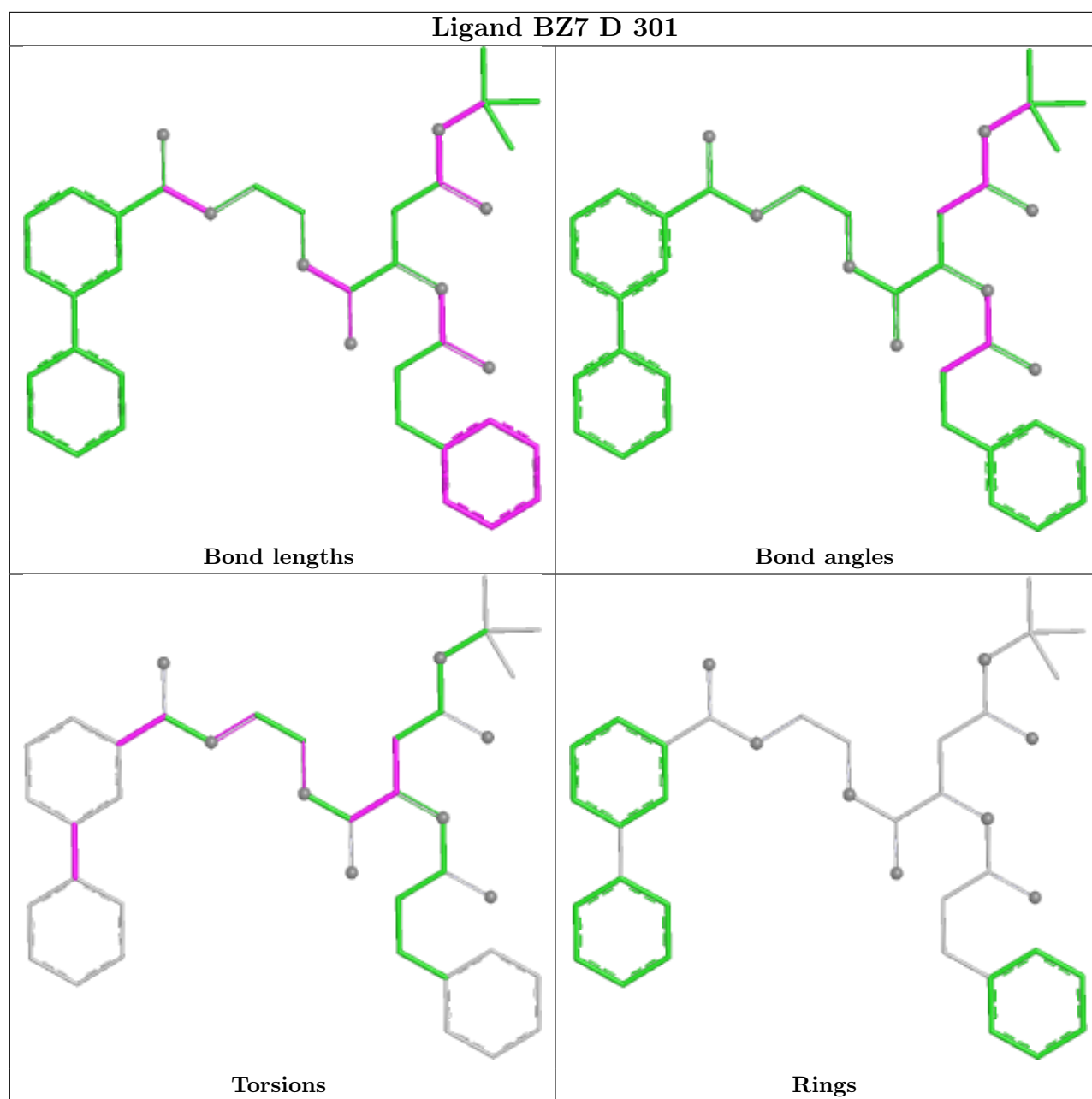
There are no ring outliers.

2 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	301	BZ7	16	0
15	D	301	BZ7	18	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.

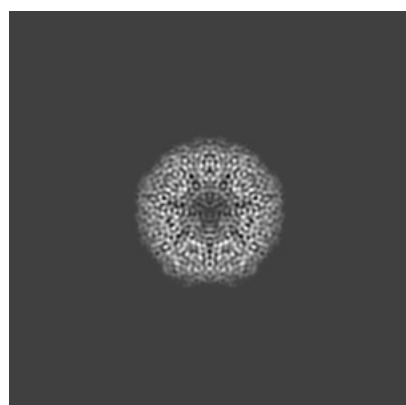
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7010. These allow visual inspection of the internal detail of the map and identification of artifacts.

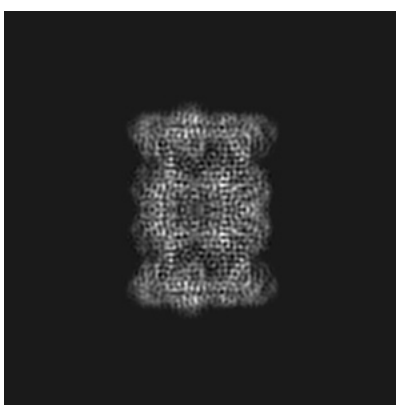
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

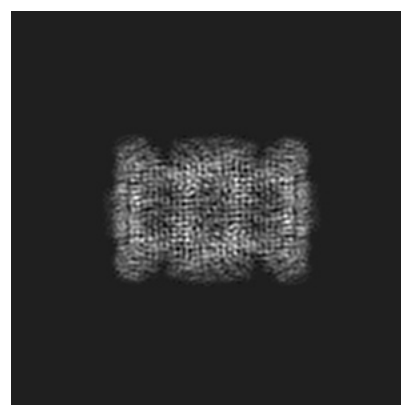
6.1.1 Primary map



X



Y

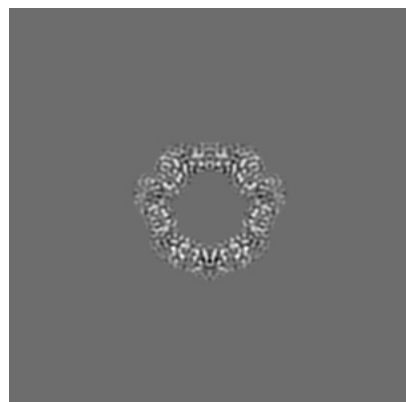


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128

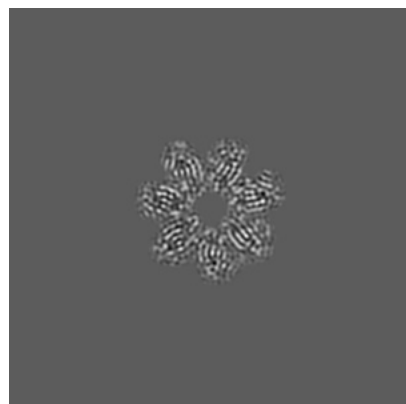


Z Index: 128

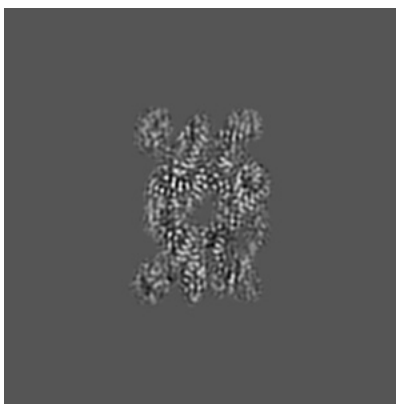
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 144



Y Index: 106

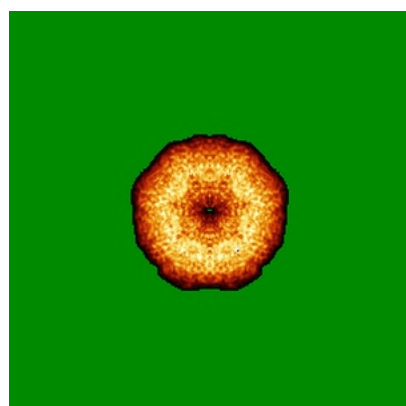


Z Index: 105

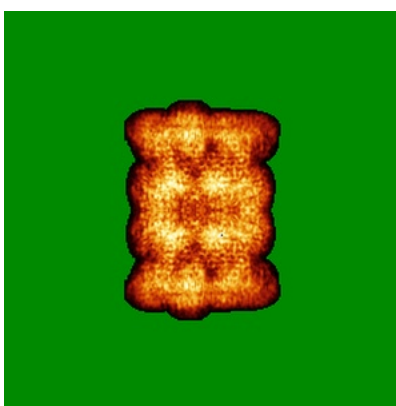
The images above show the largest variance slices of the map in three orthogonal directions.

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

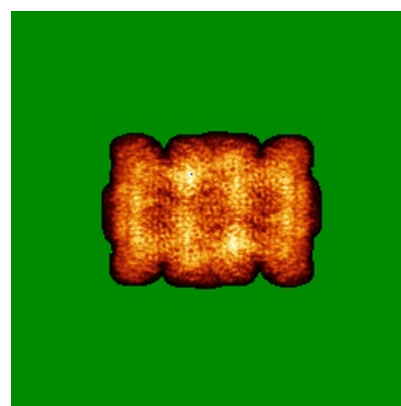
6.4.1 Primary map



X



Y

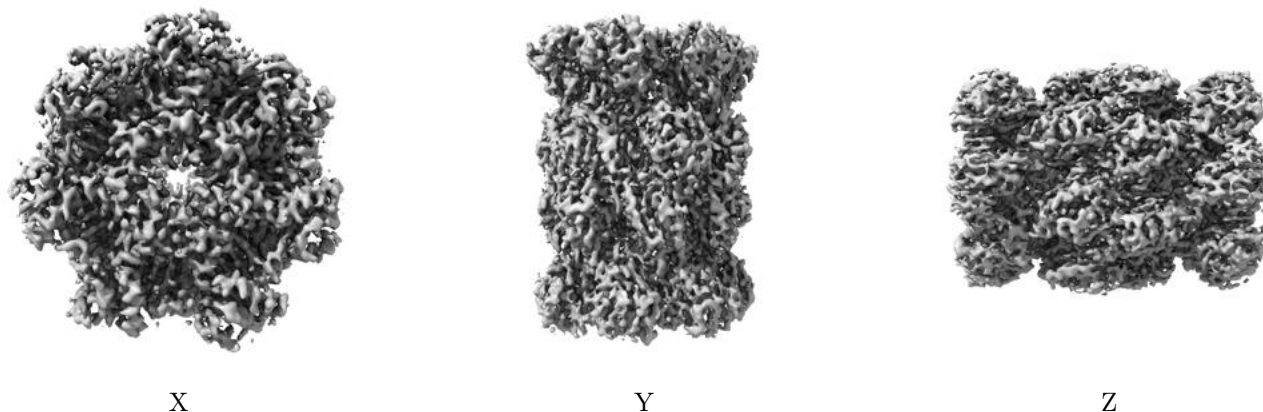


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0383. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

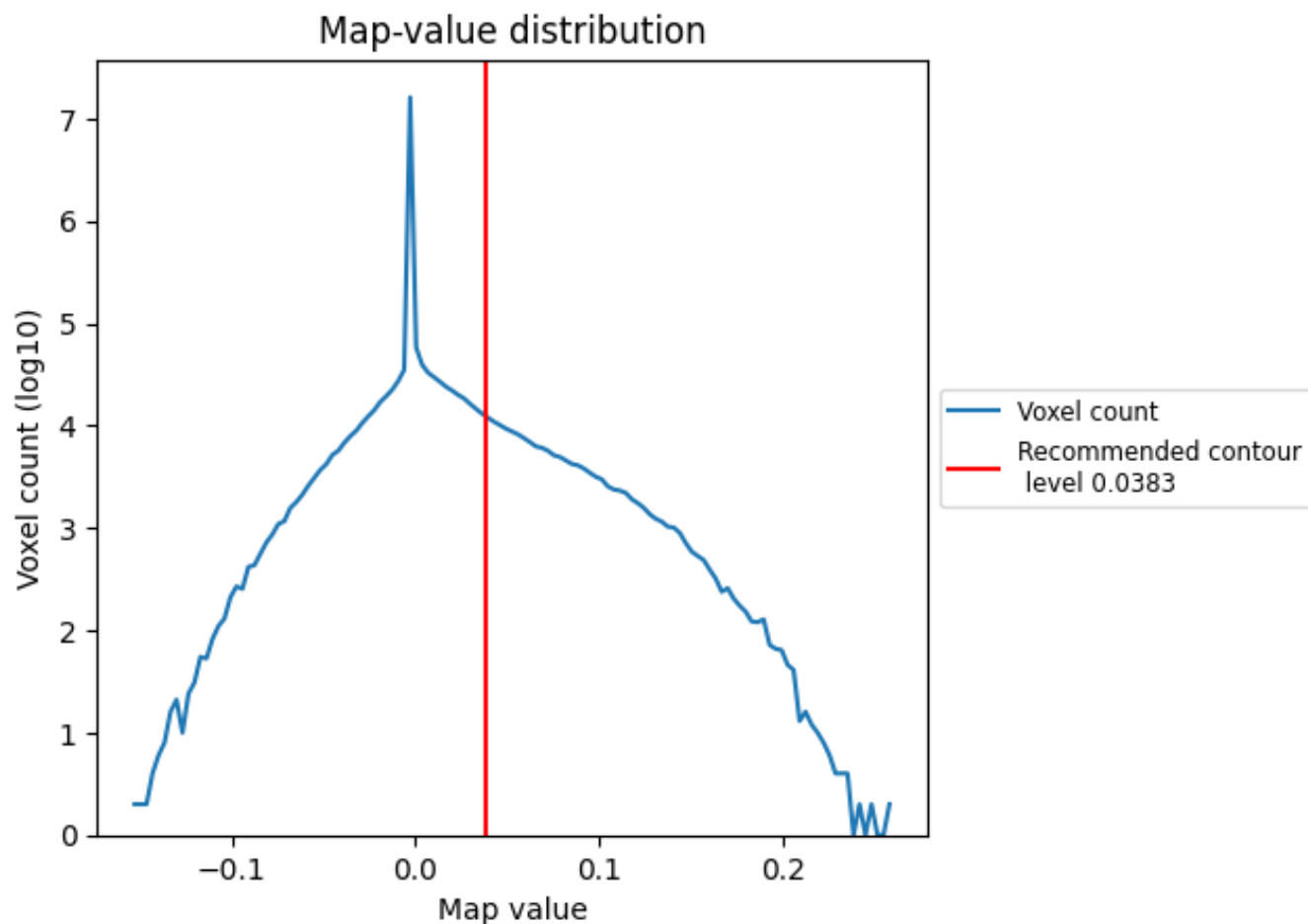
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

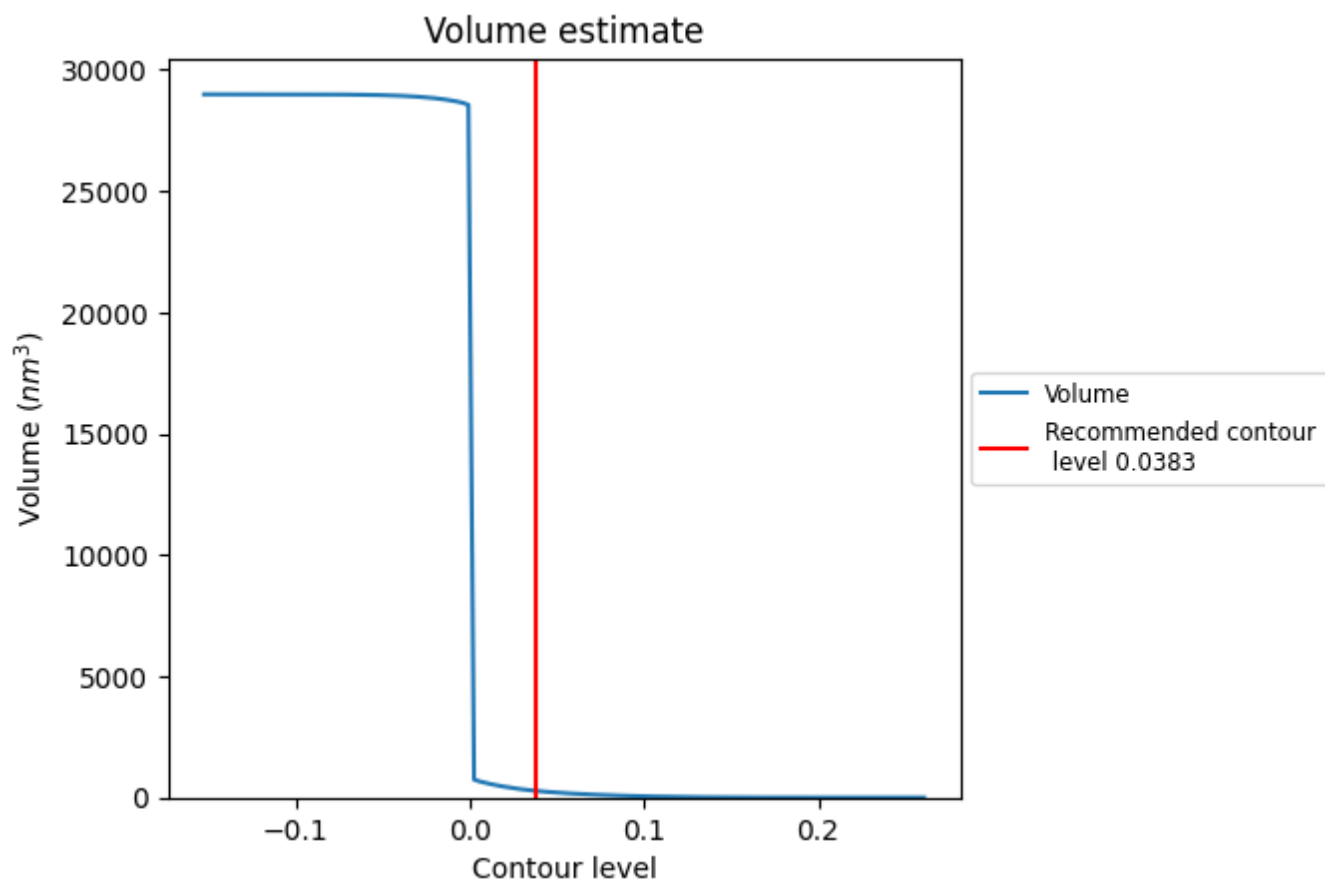
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

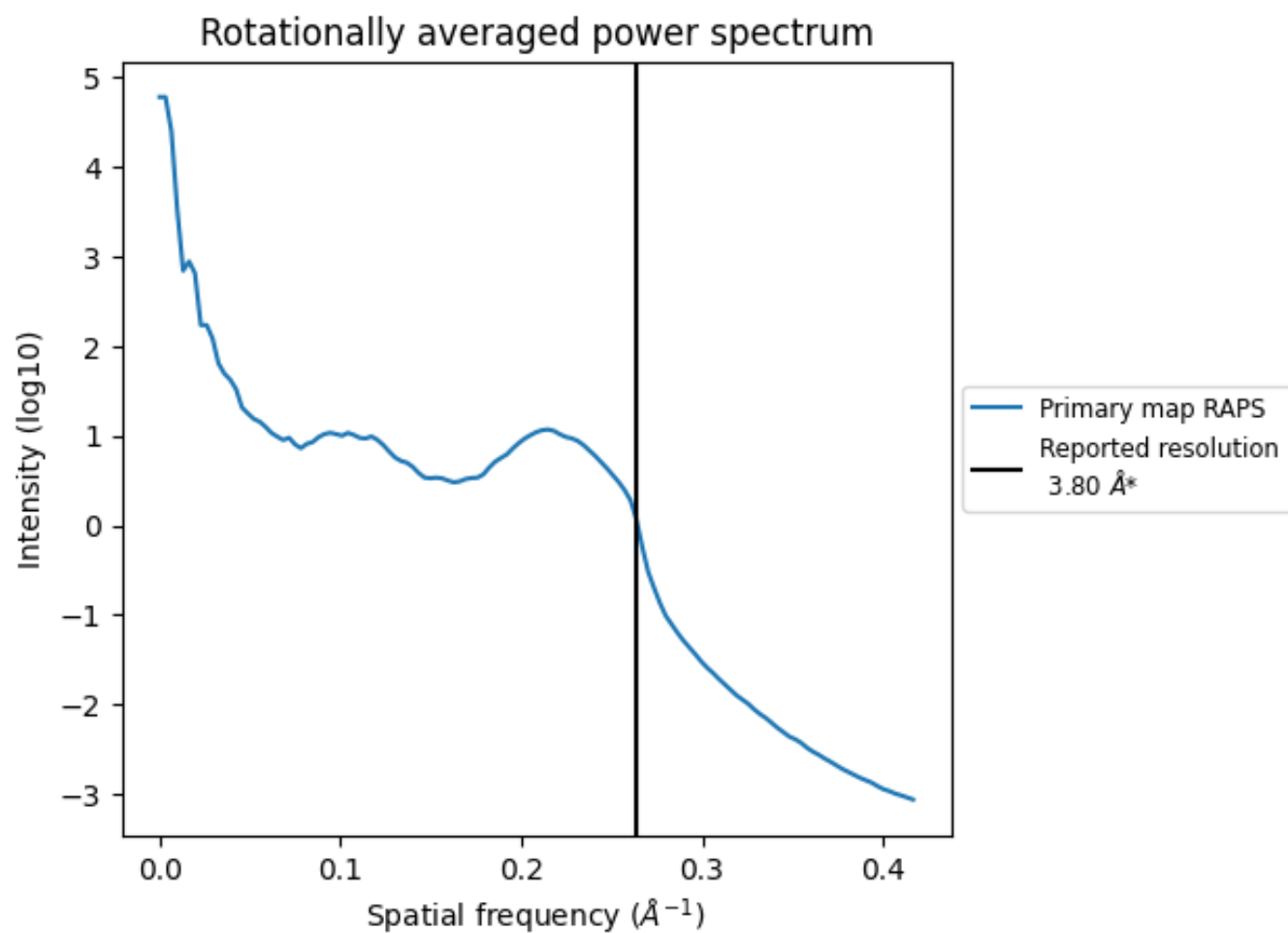
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm³; this corresponds to an approximate mass of 247 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 0.263 Å⁻¹

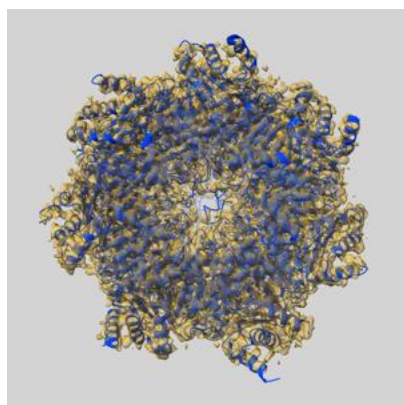
8 Fourier-Shell correlation

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

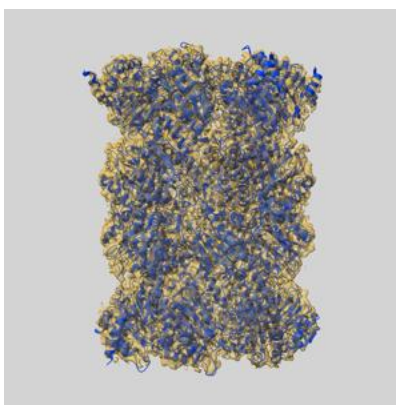
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7010 and PDB model 6AVO. Per-residue inclusion information can be found in section 3 on page 8.

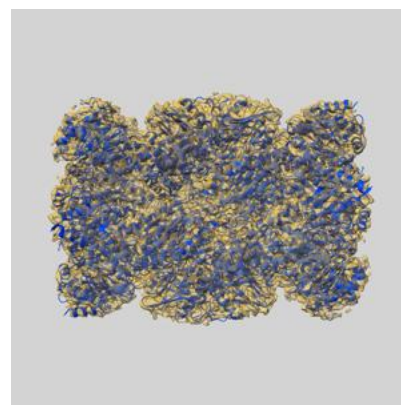
9.1 Map-model overlay [i](#)



X



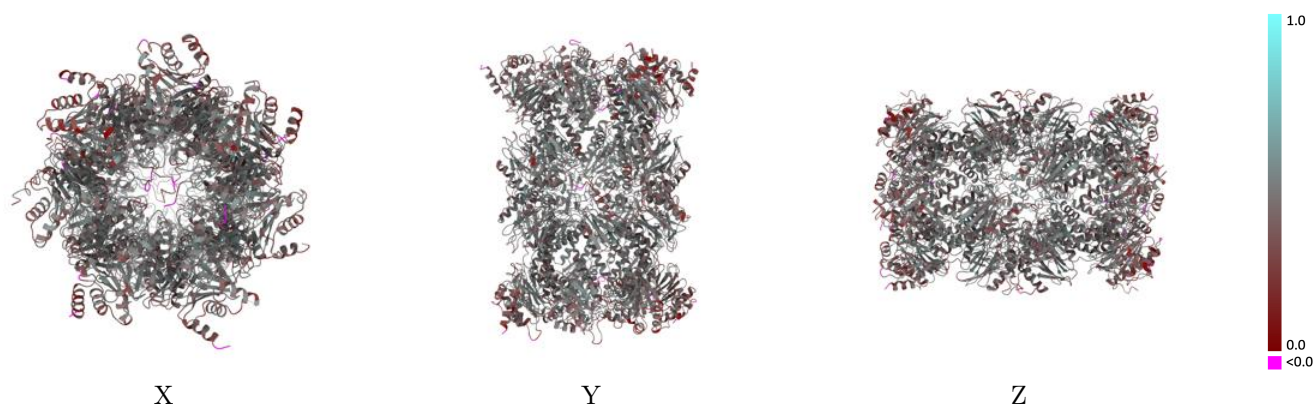
Y



Z

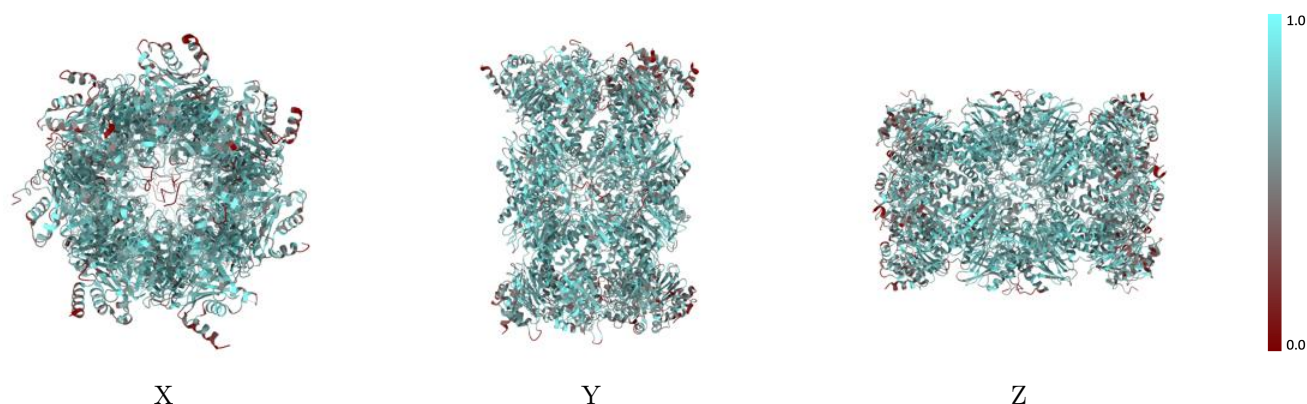
The images above show the 3D surface view of the map at the recommended contour level 0.0383 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



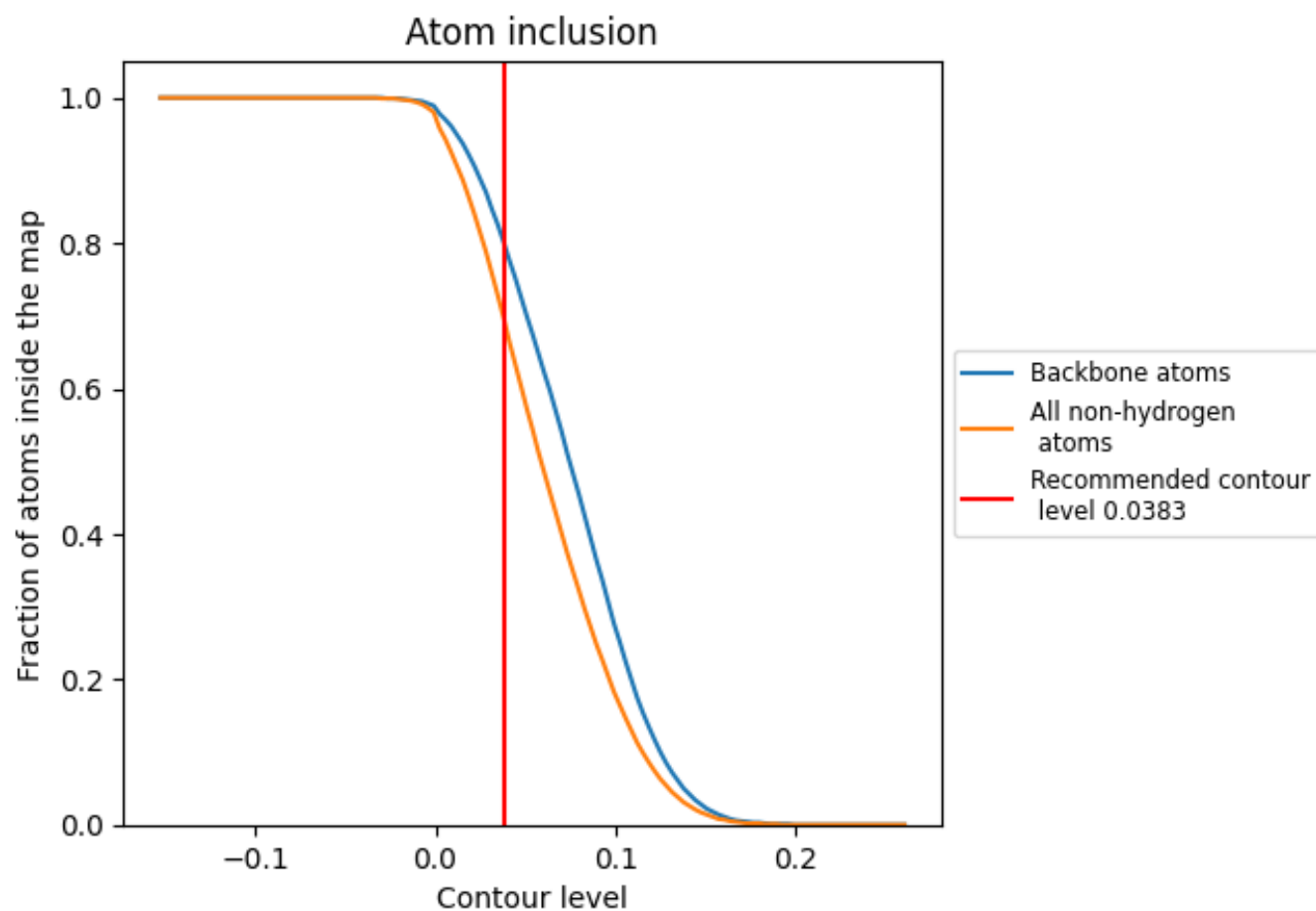
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0383).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0383) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6940	 0.4310
A	 0.7410	 0.4580
B	 0.7110	 0.4360
C	 0.7810	 0.4510
D	 0.7670	 0.4470
E	 0.7030	 0.4390
F	 0.7430	 0.4620
G	 0.6810	 0.4290
H	 0.5670	 0.3760
I	 0.6380	 0.4070
J	 0.6770	 0.4190
K	 0.6810	 0.4260
L	 0.6800	 0.4280
M	 0.5700	 0.3790
N	 0.6330	 0.4050
O	 0.6120	 0.4020
P	 0.6980	 0.4290
Q	 0.6770	 0.4190
R	 0.6960	 0.4290
S	 0.7250	 0.4570
T	 0.7250	 0.4380
U	 0.7600	 0.4650
V	 0.7260	 0.4410
W	 0.7600	 0.4620
X	 0.7270	 0.4590
Y	 0.7450	 0.4630
Z	 0.6110	 0.3960
a	 0.7650	 0.4620
b	 0.6980	 0.4290

