Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 10:56 PM EDT

PDB ID	:	3SHJ
Title	:	Proteasome in complex with hydroxyurea derivative HU10
Authors	:	Gallastegui, N.; Beck, P.; Arciniega, M.; Hillebrand, S.; Huber, R.; Groll, M.
Deposited on	:	2011-06-16
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

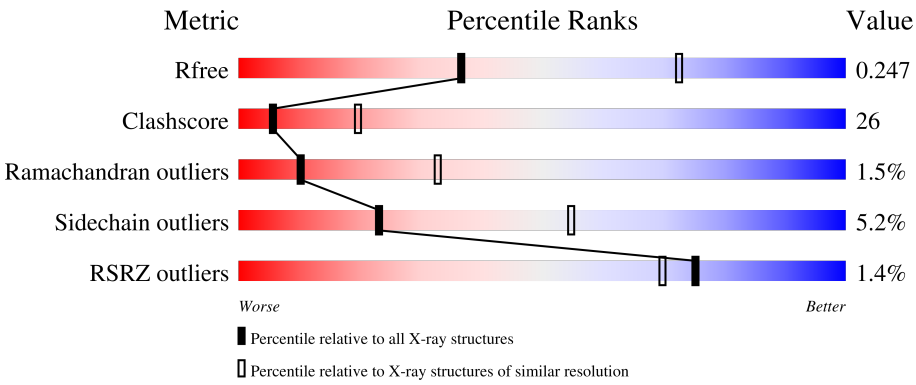
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	62% 36% •
1	O	250	2% 64% 34% •
2	B	244	2% 53% 41% 6%
2	P	244	2% 55% 39% 6%
3	C	241	2% 56% 41% •

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Mol	Chain	Length	Quality of chain
3	Q	241	7% 54% 42% •
4	D	242	2% 60% 36% •
4	R	242	3% 55% 40% •
5	E	233	% 49% 45% 6%
5	S	233	4% 51% 43% 6%
6	F	244	% 56% 41% •
6	T	244	59% 38% •
7	G	243	2% 56% 41% •
7	U	243	% 52% 44% •
8	H	222	55% 41% •
8	V	222	% 54% 41% 5%
9	I	204	61% 35% •
9	W	204	61% 36% •
10	J	198	% 58% 39% •
10	X	198	2% 56% 41% •
11	K	212	59% 39% •
11	Y	212	61% 36% •
12	L	222	54% 41% 5%
12	Z	222	% 55% 41% 5%
13	1	233	63% 34% •
13	M	233	59% 38% •
14	2	196	59% 38% •
14	N	196	67% 31% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MES	K	1(L)	-	X	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 50905 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	1905	1201	321	380	3	0	0	0
2	P	244	1905	1201	321	380	3	0	0	0

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	1891	1181	331	375	4	0	0	0
3	Q	241	1891	1181	331	375	4	0	0	0

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	242	1862	1162	314	379	7	0	0	0
4	R	242	1862	1162	314	379	7	0	0	0

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	233	1795	1129	312	350	4	0	0	0
5	S	233	1795	1129	312	350	4	0	0	0

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	244	1897	1205	330	358	4	0	0	0
6	T	244	1897	1205	330	358	4	0	0	0

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	243	1921	1221	322	370	8	0	0	0
7	U	243	1921	1221	322	370	8	0	0	0

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	222	1685	1061	293	324	7	0	0	0
8	V	222	1685	1061	293	324	7	0	0	0

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	1581	1010	258	305	8	0	0	0
9	W	204	1581	1010	258	305	8	0	0	0

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	198	1585	1005	269	305	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	198	1585	1005	269	305	6	0	0	0

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1644	1045	280	312	7	0	0	0
11	Y	212	1644	1045	280	312	7	0	0	0

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	222	1757	1115	303	335	4	0	0	0
12	Z	222	1757	1115	303	335	4	0	0	0

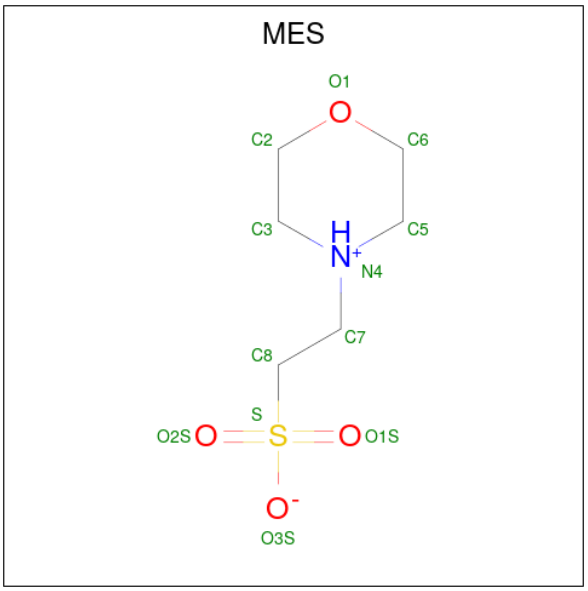
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	233	1824	1154	312	351	7	0	0	0
13	1	233	1824	1154	312	351	7	0	0	0

- Molecule 14 is a protein called Proteasome component PRE3.

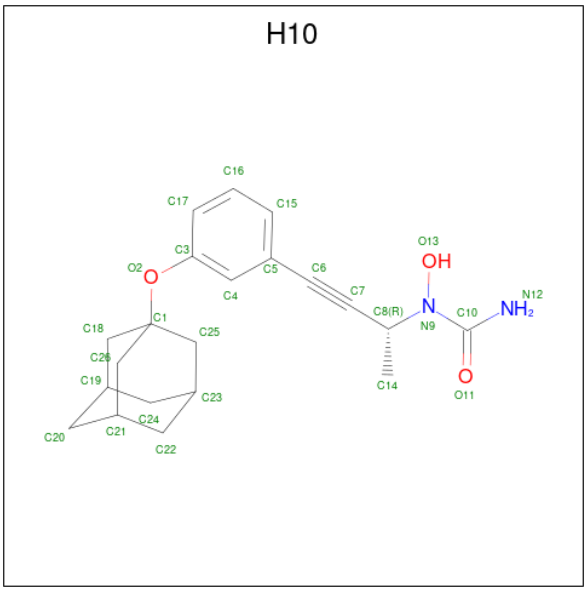
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	196	1512	955	250	300	7	0	0	0
14	2	196	1512	955	250	300	7	0	0	0

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
15	K	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
15	Y	1	12	6	1	4	1	0	0

- Molecule 16 is 1-hydroxy-1-[(2R)-4-{3-[(3S,5S,7S)-tricyclo[3.3.1.1 3,7]dec-1-yloxy]phenyl}but-3-yn-2-yl]urea (three-letter code: H10) (formula: $C_{21}H_{26}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
16	K	1	26	21	2	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
16	Y	1	26	21	2	3	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	A	49	49	49	0	0
17	B	36	36	36	0	0
17	C	37	37	37	0	0
17	D	36	36	36	0	0
17	E	23	23	23	0	0
17	F	47	47	47	0	0
17	G	58	58	58	0	0
17	H	46	46	46	0	0
17	I	65	65	65	0	0
17	J	48	48	48	0	0
17	K	49	49	49	0	0
17	L	58	58	58	0	0
17	M	66	66	66	0	0
17	N	56	56	56	0	0
17	O	30	30	30	0	0
17	P	29	29	29	0	0
17	Q	24	24	24	0	0
17	R	30	30	30	0	0

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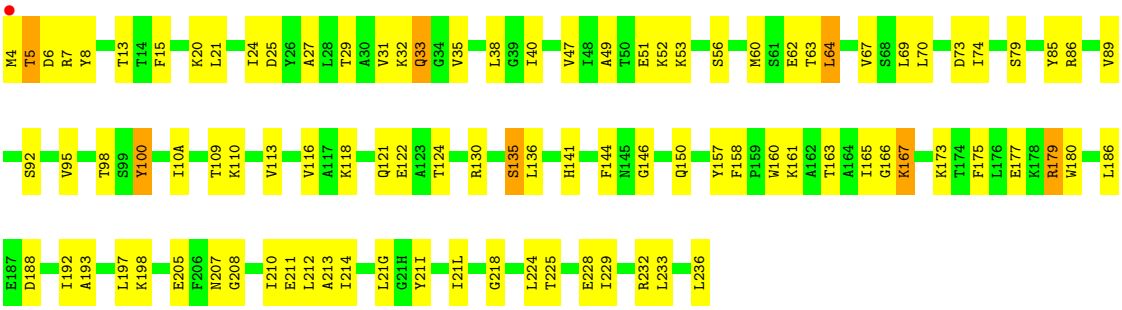
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	S	19	19	19	0	0
			Total	O		
17	T	38	38	38	0	0
			Total	O		
17	U	60	60	60	0	0
			Total	O		
17	V	42	42	42	0	0
			Total	O		
17	W	57	57	57	0	0
			Total	O		
17	X	48	48	48	0	0
			Total	O		
17	Y	50	50	50	0	0
			Total	O		
17	Z	50	50	50	0	0
			Total	O		
17	1	69	69	69	0	0
			Total	O		
17	2	61	61	61	0	0

3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

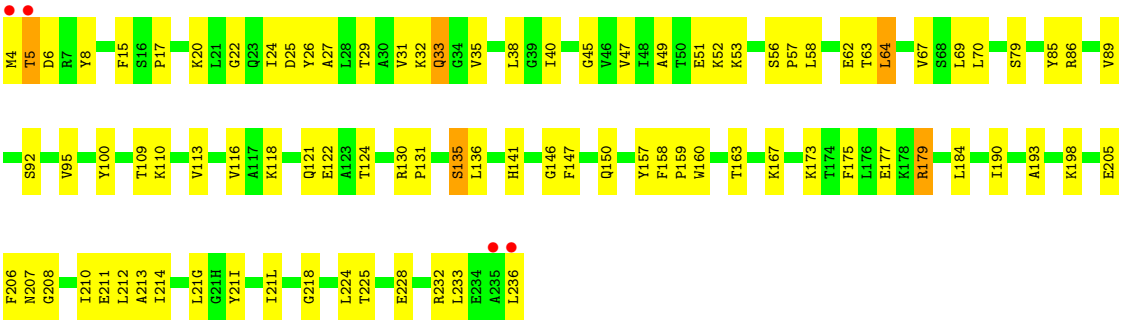
• Molecule 1: Proteasome component Y7

Chain A: 62% 36%



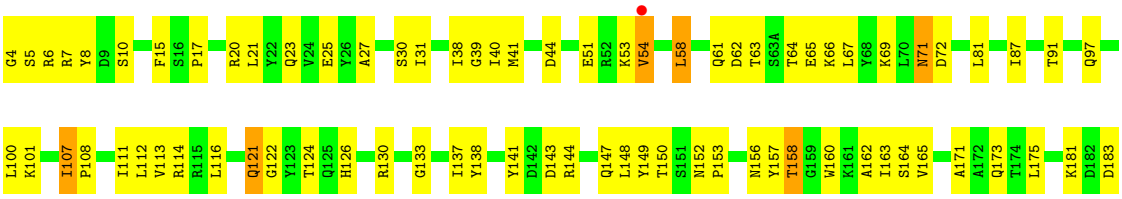
• Molecule 1: Proteasome component Y7

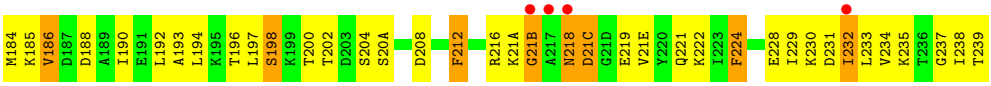
Chain O: 2% 64% 34%



• Molecule 2: Proteasome component Y13

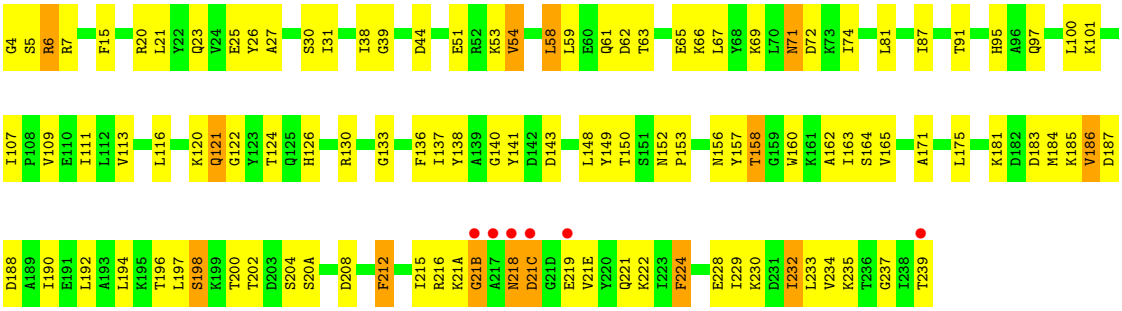
Chain B: 2% 53% 41% 6%





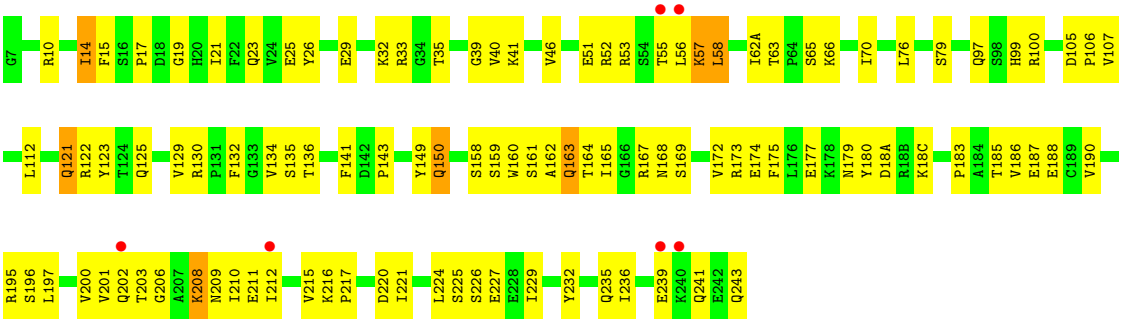
• Molecule 2: Proteasome component Y13

Chain P:



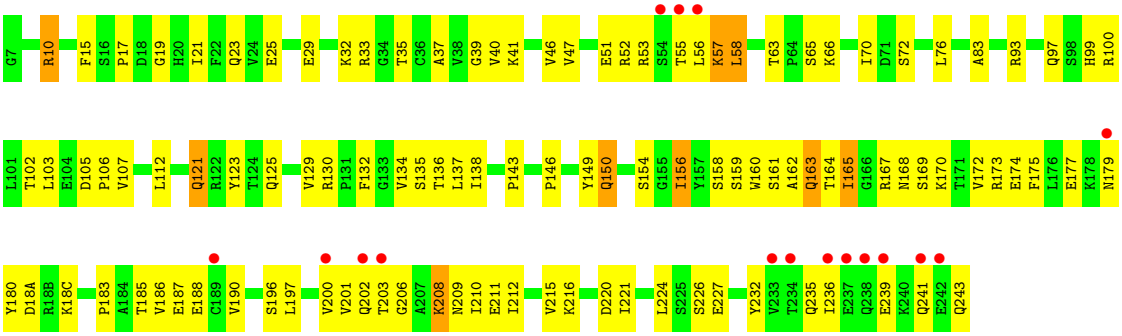
• Molecule 3: Proteasome component PRE6

Chain C:



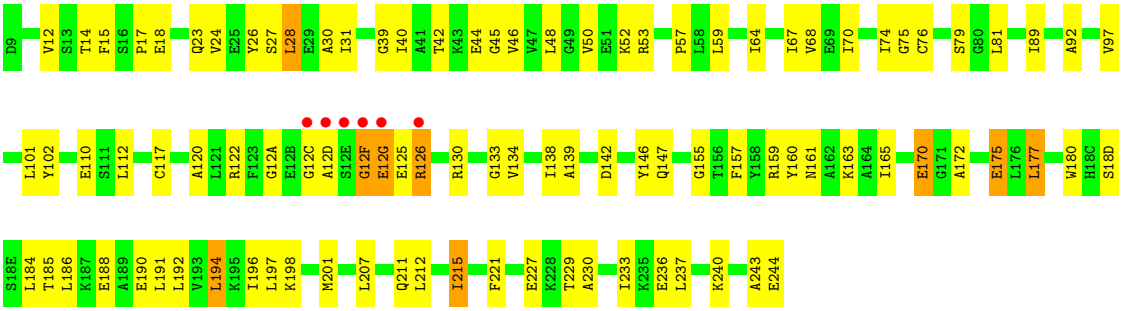
• Molecule 3: Proteasome component PRE6

Chain Q:



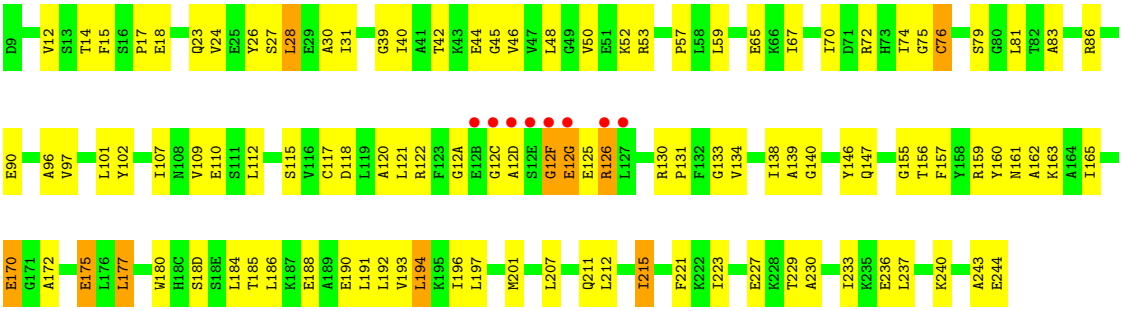
• Molecule 4: Proteasome component PUP2

Chain D:



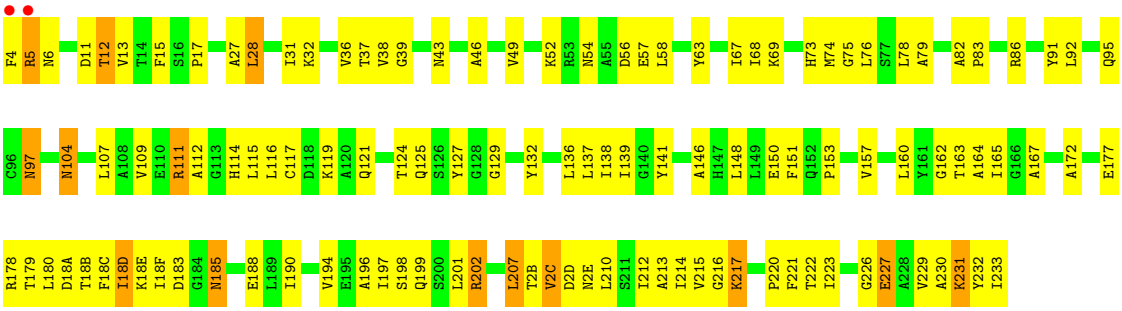
- Molecule 4: Proteasome component PUP2

Chain R:



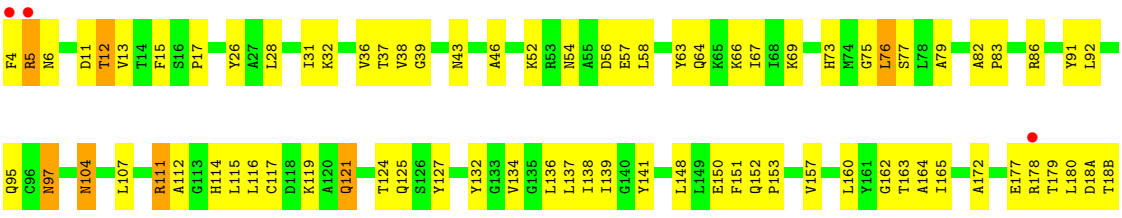
- Molecule 5: Proteasome component PRE5

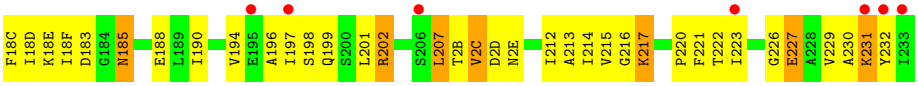
Chain E:



- Molecule 5: Proteasome component PRE5

Chain S:



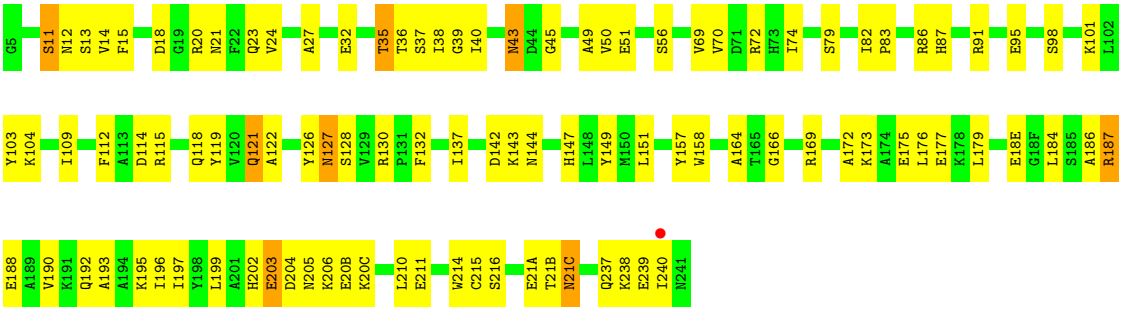


- Molecule 6: Proteasome component C1

Chain F:

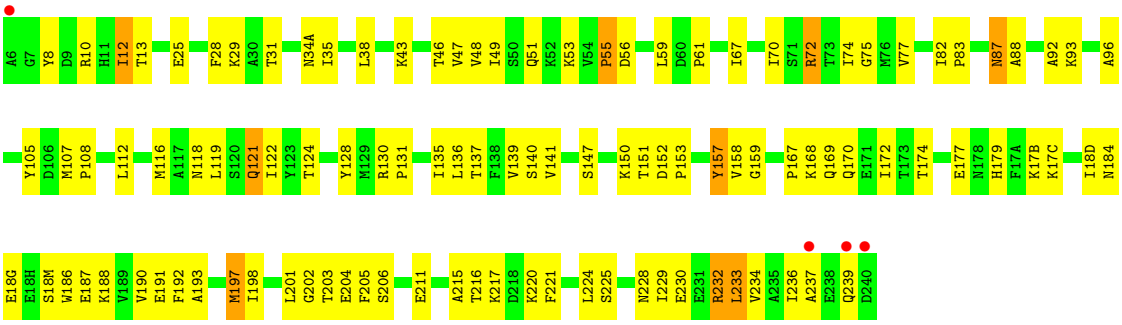
- Molecule 6: Proteasome component C1

Chain T:



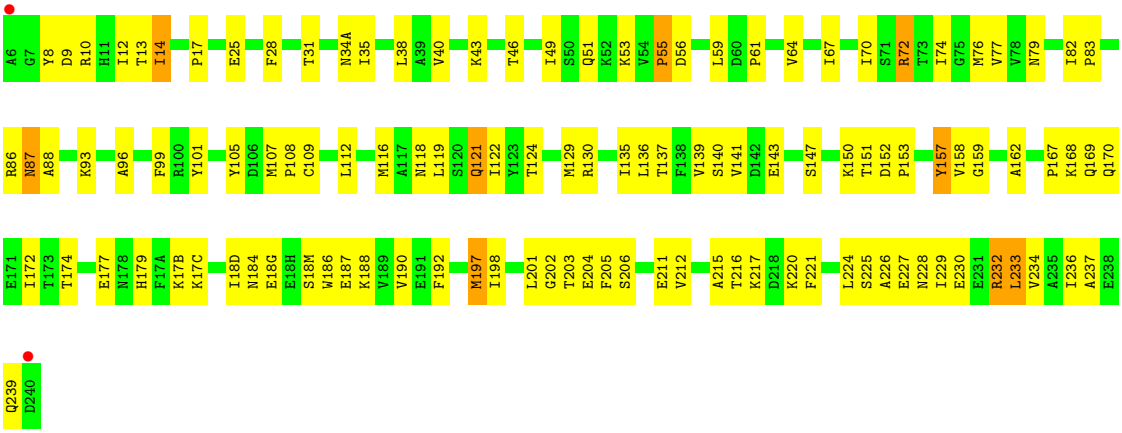
- Molecule 7: Proteasome component C7-alpha

Chain G:



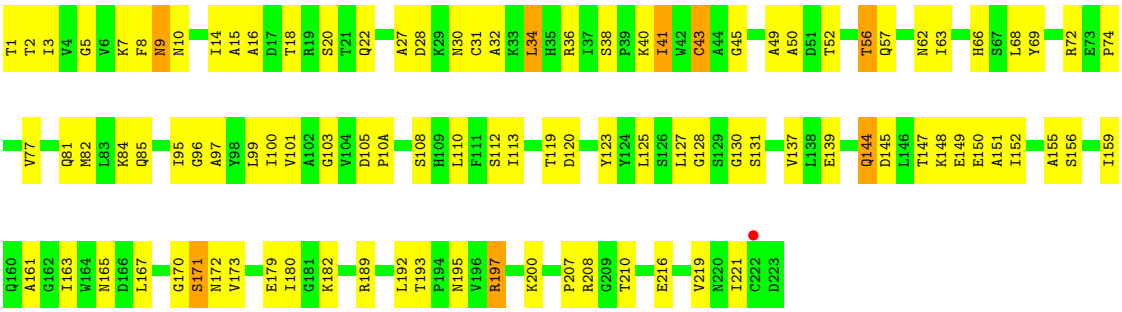
- Molecule 7: Proteasome component C7-alpha

Chain U:



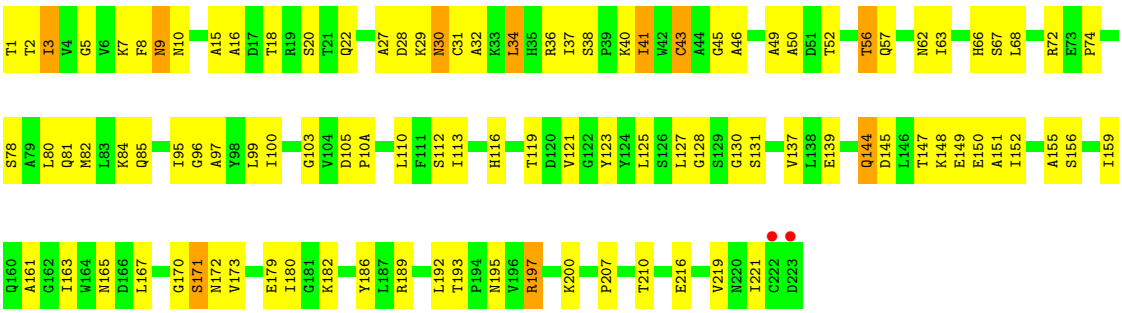
• Molecule 8: Proteasome component PUP1

Chain H:



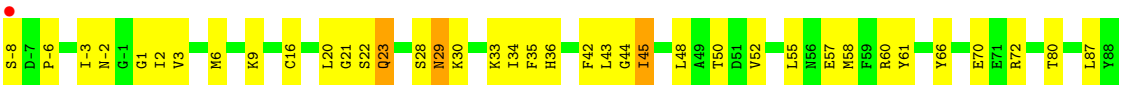
• Molecule 8: Proteasome component PUP1

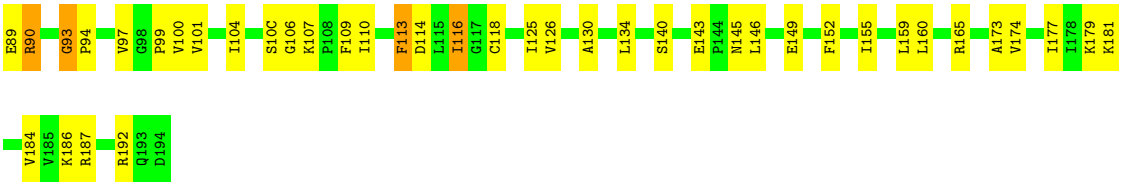
Chain V:



• Molecule 9: Proteasome component PUP3

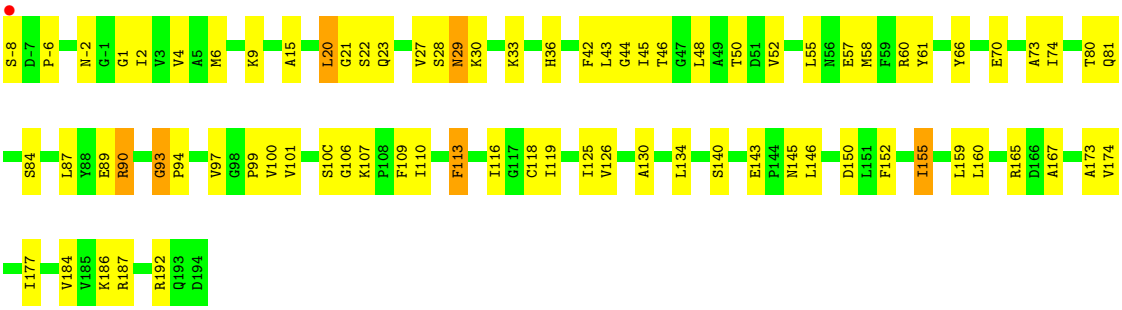
Chain I:





• Molecule 9: Proteasome component PUP3

Chain W:

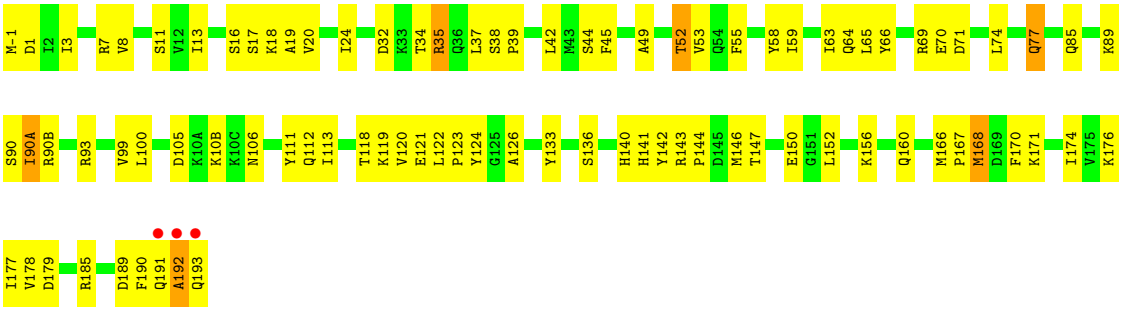


• Molecule 10: Proteasome component C11

Chain J:

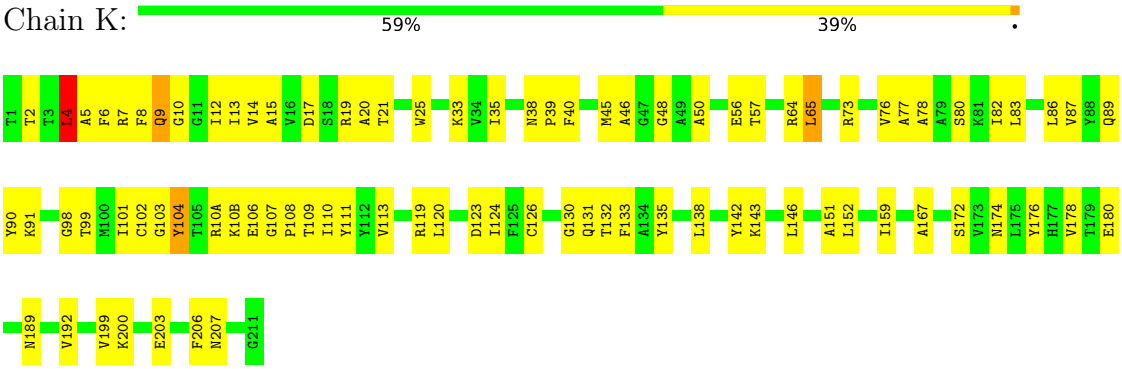
• Molecule 10: Proteasome component C11

Chain X:



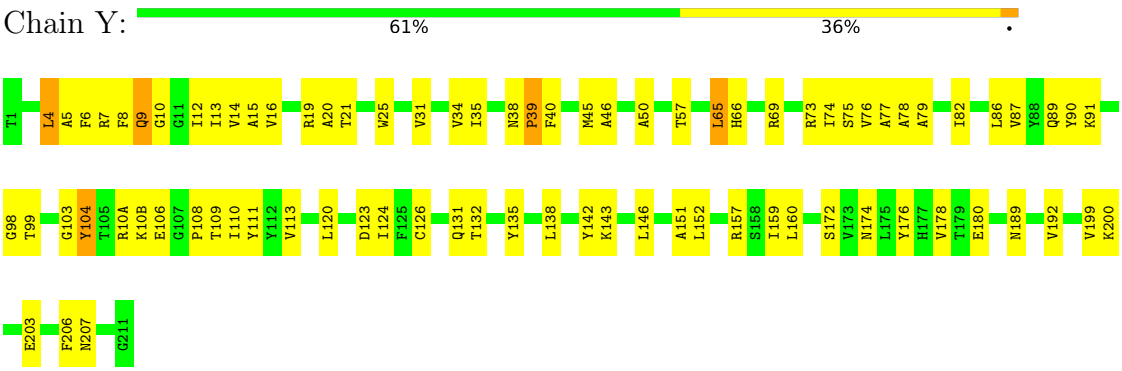
• Molecule 11: Proteasome component PRE2

Chain K:



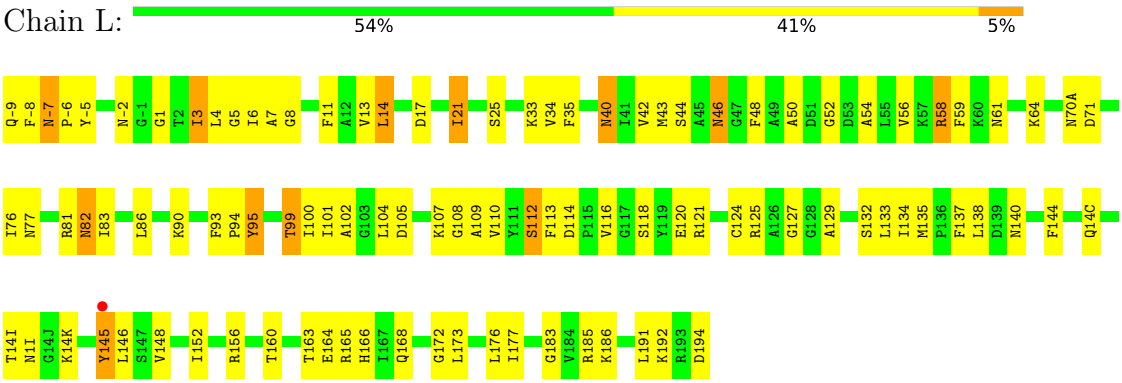
- Molecule 11: Proteasome component PRE2

Chain Y:



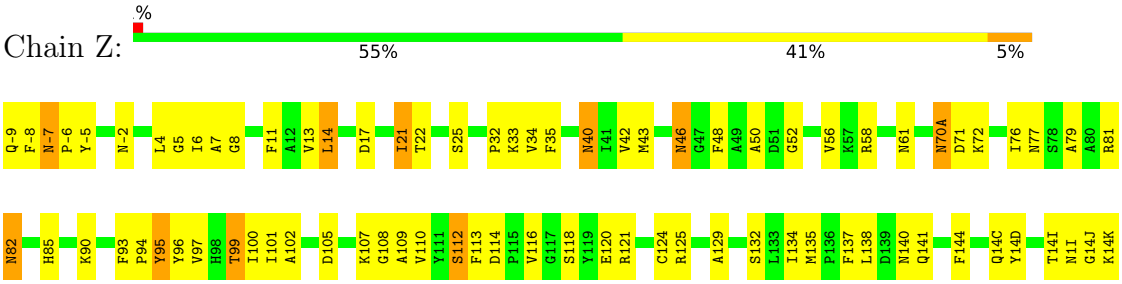
- Molecule 12: Proteasome component C5

Chain L:



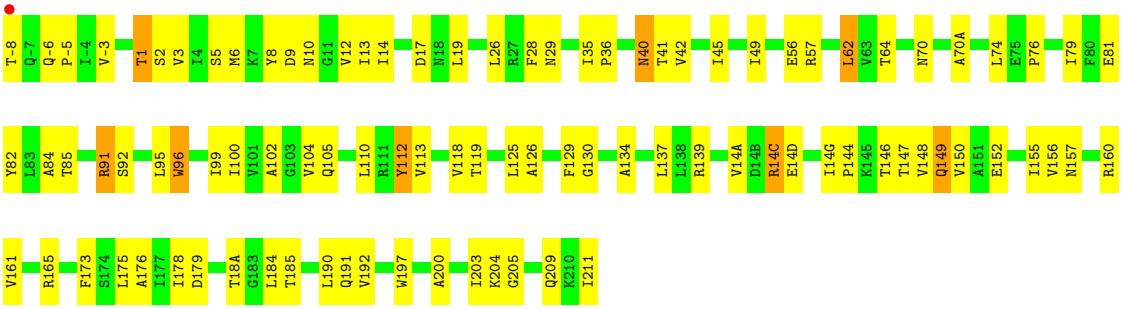
- Molecule 12: Proteasome component C5

Chain Z:



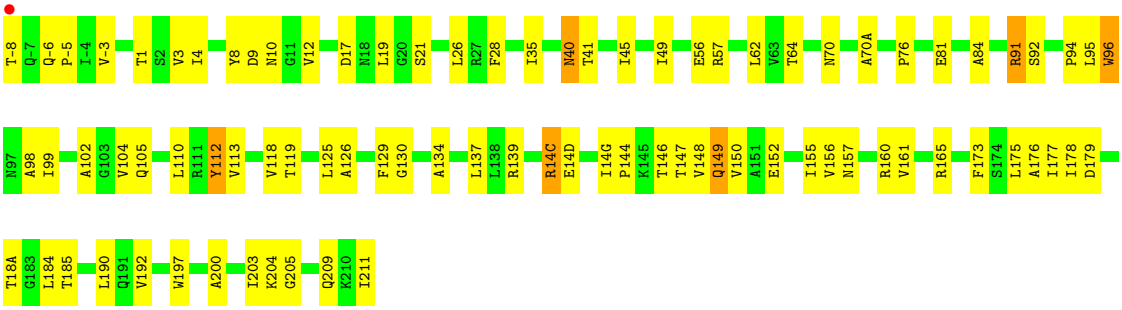
• Molecule 13: Proteasome component PRE4

Chain M:



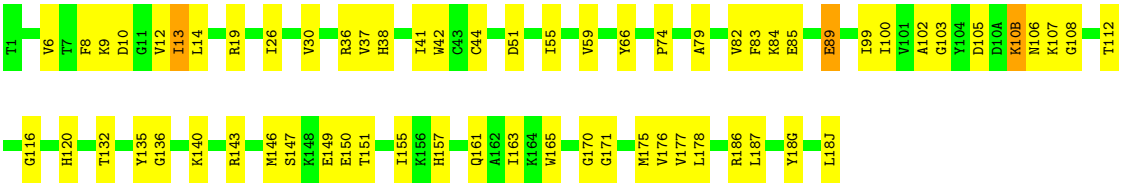
• Molecule 13: Proteasome component PRE4

Chain 1:



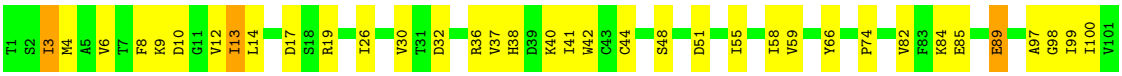
• Molecule 14: Proteasome component PRE3

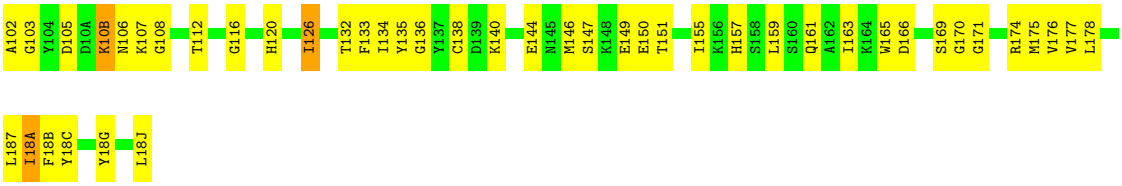
Chain N:



• Molecule 14: Proteasome component PRE3

Chain 2:




A102
G103
Y104
D105
D10A
K10B
N106
K107
G108
T112
G116
H120
I126
T132
F133
I134
Y135
G136
Y137
C138
D139
K140
E144
N145
M146
S147
K148
E149
E150
T151
I155
K156
H157
S158
L159
S160
Q161
A162
I163
K164
W165
D166
S169
G170
G171
R174
M175
V176
V177
L178
L187
I18A
F18B
Y18C
Y18G
L18J

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.12Å 300.56Å 144.06Å 90.00° 112.76° 90.00°	Depositor
Resolution (Å)	49.77 – 2.80 49.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (49.77-2.80) 92.3 (49.77-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.266 0.222 , 0.247	Depositor DCC
R_{free} test set	11760 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.853	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 59.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	50905	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: H10, MES

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	0.37	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.64	0/2642
2	B	0.37	0/1935	0.63	0/2618
2	P	0.38	0/1935	0.64	0/2618
3	C	0.36	0/1920	0.62	0/2598
3	Q	0.36	0/1920	0.62	0/2598
4	D	0.36	0/1887	0.64	0/2541
4	R	0.36	0/1887	0.64	0/2541
5	E	0.35	0/1823	0.60	0/2463
5	S	0.36	0/1823	0.61	0/2463
6	F	0.37	0/1937	0.61	0/2614
6	T	0.37	0/1937	0.62	0/2614
7	G	0.40	0/1959	0.63	0/2652
7	U	0.40	0/1959	0.63	0/2652
8	H	0.38	0/1716	0.66	0/2326
8	V	0.38	0/1716	0.66	0/2326
9	I	0.38	0/1611	0.67	0/2174
9	W	0.40	0/1611	0.68	0/2174
10	J	0.39	0/1613	0.66	0/2173
10	X	0.40	0/1613	0.66	0/2173
11	K	0.40	0/1681	0.66	1/2274 (0.0%)
11	Y	0.40	0/1681	0.65	0/2274
12	L	0.39	0/1795	0.67	1/2420 (0.0%)
12	Z	0.38	0/1795	0.67	1/2420 (0.0%)
13	1	0.39	0/1855	0.67	2/2514 (0.1%)
13	M	0.38	0/1855	0.66	1/2514 (0.0%)
14	2	0.40	0/1541	0.65	0/2087
14	N	0.40	0/1541	0.66	0/2087
All	All	0.38	0/50450	0.64	6/68192 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	95	LEU	N-CA-C	-5.85	95.22	111.00
13	1	95	LEU	N-CA-C	-5.76	95.44	111.00
12	L	95	TYR	N-CA-C	-5.49	96.17	111.00
12	Z	95	TYR	N-CA-C	-5.22	96.90	111.00
11	K	4	LEU	CA-CB-CG	5.07	126.95	115.30
13	1	98	ALA	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	99	0
1	O	1915	0	1926	89	0
2	B	1905	0	1901	117	0
2	P	1905	0	1901	116	0
3	C	1891	0	1900	121	0
3	Q	1891	0	1900	128	0
4	D	1862	0	1836	89	0
4	R	1862	0	1836	93	0
5	E	1795	0	1797	127	0
5	S	1795	0	1797	119	0
6	F	1897	0	1886	113	0
6	T	1897	0	1886	103	0
7	G	1921	0	1910	109	0
7	U	1921	0	1910	116	0
8	H	1685	0	1688	94	0
8	V	1685	0	1688	103	0
9	I	1581	0	1574	86	0
9	W	1581	0	1574	80	0
10	J	1585	0	1590	91	0
10	X	1585	0	1590	98	0
11	K	1644	0	1595	85	0
11	Y	1644	0	1595	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1757	0	1711	105	0
12	Z	1757	0	1711	102	0
13	1	1824	0	1832	81	0
13	M	1824	0	1832	87	0
14	2	1512	0	1481	80	0
14	N	1512	0	1481	61	0
15	K	12	0	13	0	0
15	Y	12	0	13	0	0
16	K	26	0	26	4	0
16	Y	26	0	26	7	0
17	1	69	0	0	9	0
17	2	61	0	0	5	0
17	A	49	0	0	3	0
17	B	36	0	0	3	0
17	C	37	0	0	6	0
17	D	36	0	0	4	0
17	E	23	0	0	5	0
17	F	47	0	0	4	0
17	G	58	0	0	5	0
17	H	46	0	0	2	0
17	I	65	0	0	3	0
17	J	48	0	0	4	0
17	K	49	0	0	4	0
17	L	58	0	0	5	0
17	M	66	0	0	5	0
17	N	56	0	0	4	0
17	O	30	0	0	2	0
17	P	29	0	0	4	0
17	Q	24	0	0	5	0
17	R	30	0	0	4	0
17	S	19	0	0	1	0
17	T	38	0	0	4	0
17	U	60	0	0	7	0
17	V	42	0	0	4	0
17	W	57	0	0	6	0
17	X	48	0	0	8	0
17	Y	50	0	0	3	0
17	Z	50	0	0	11	0
All	All	50905	0	49332	2529	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 26.

All (2529) 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)
8:H:15:ALA:HB3	8:H:159:ILE:HD11	1.25	1.17
2:P:74:ILE:HD11	2:P:109:VAL:HG22	1.12	1.10
7:U:9:ASP:HA	7:U:14:ILE:HD11	1.25	1.10
2:B:202:THR:HG22	2:B:204:SER:H	1.13	1.09
8:H:50:ALA:HB2	9:I:116:ILE:HD13	1.33	1.09
8:V:15:ALA:HB3	8:V:159:ILE:HD11	1.24	1.09
6:T:49:ALA:HB1	6:T:197:ILE:HD11	1.33	1.08
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.20	1.06
2:P:74:ILE:HD13	2:P:140:GLY:HA3	1.30	1.06
8:H:15:ALA:CB	8:H:159:ILE:HD11	1.86	1.06
4:R:74:ILE:HD11	4:R:109:VAL:HG22	1.11	1.06
7:G:96:ALA:HA	7:G:107:MET:HE2	1.37	1.06
6:T:49:ALA:CB	6:T:197:ILE:HD11	1.86	1.05
8:V:15:ALA:CB	8:V:159:ILE:HD11	1.84	1.05
2:P:202:THR:HG22	2:P:204:SER:H	1.11	1.05
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.21	1.02
5:S:38:VAL:HG23	5:S:197:ILE:HD13	1.38	1.02
7:U:96:ALA:HA	7:U:107:MET:HE2	1.41	1.02
2:B:107:ILE:HD13	2:B:108:PRO:O	1.60	1.02
5:E:49:VAL:HG13	5:E:212:ILE:CD1	1.89	1.01
7:U:12:ILE:HG13	7:U:14:ILE:HD12	1.39	1.01
11:Y:7:ARG:HG3	11:Y:12:ILE:CD1	1.92	1.00
1:A:21:LEU:HB3	1:A:24:ILE:HD13	1.42	0.99
3:Q:201:VAL:CG2	3:Q:210:ILE:HD11	1.93	0.98
1:A:177:GLU:HG2	2:B:58:LEU:CD2	1.93	0.98
13:1:40:ASN:H	13:1:40:ASN:HD22	1.10	0.98
5:E:49:VAL:HG13	5:E:212:ILE:HD11	1.41	0.98
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	0.98	0.98
9:I:177:ILE:HD12	9:I:187:ARG:HH12	1.23	0.97
3:C:70:ILE:HD13	3:C:112:LEU:HD11	1.45	0.96
8:H:50:ALA:CB	9:I:116:ILE:HD13	1.94	0.96
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	1.48	0.95
10:X:37:LEU:HB3	10:X:63:ILE:HD13	1.49	0.95
11:Y:6:PHE:HB2	11:Y:124:ILE:HD13	1.49	0.95
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.46	0.94
3:Q:201:VAL:HG21	3:Q:210:ILE:CD1	1.94	0.94
13:1:157:ASN:HD22	13:1:160:ARG:HH11	0.99	0.94
4:R:74:ILE:CD1	4:R:109:VAL:HG22	1.97	0.93
3:Q:70:ILE:HD13	3:Q:112:LEU:HD11	1.49	0.93
12:L:3:ILE:HD13	12:L:127:GLY:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ILE:HD12	2:B:112:LEU:HB2	1.47	0.93
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.04	0.92
8:H:128:GLY:O	8:H:131:SER:HB2	1.70	0.92
6:T:197:ILE:HD13	6:T:210:LEU:HD11	1.52	0.92
1:O:15:PHE:H	2:P:23:GLN:HE22	1.09	0.92
2:B:15:PHE:H	3:C:23:GLN:HE22	1.13	0.91
13:M:40:ASN:HD22	13:M:40:ASN:H	1.09	0.91
4:R:74:ILE:HD13	4:R:140:GLY:HA3	1.51	0.91
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.35	0.91
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.35	0.91
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.34	0.91
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.50	0.91
12:L:3:ILE:HD12	12:L:46:ASN:HB2	1.53	0.90
8:V:128:GLY:O	8:V:131:SER:HB2	1.71	0.90
14:2:17:ASP:HB3	14:2:163:ILE:HD11	1.54	0.90
14:2:18(A):ILE:HD13	14:2:18(B):PHE:N	1.86	0.90
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.15	0.89
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.74	0.88
8:V:221:ILE:HD11	9:W:184:VAL:HB	1.56	0.88
3:Q:154:SER:OG	3:Q:156:ILE:HD13	1.74	0.87
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.10	0.87
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.71	0.87
3:C:15:PHE:H	4:D:23:GLN:HE22	1.15	0.87
7:U:70:ILE:HD11	7:U:76:MET:HB2	1.56	0.87
12:L:83:ILE:HD13	12:L:86:LEU:HD12	1.57	0.86
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.40	0.86
9:I:44:GLY:C	9:I:45:ILE:HD12	1.95	0.86
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.39	0.86
4:D:28:LEU:HA	4:D:31:ILE:HD12	1.56	0.86
1:A:15:PHE:H	2:B:23:GLN:HE22	1.20	0.86
9:I:152:PHE:HB2	9:I:177:ILE:HD11	1.58	0.85
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.58	0.85
5:S:221:PHE:CE1	5:S:223:ILE:HD11	2.09	0.85
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.40	0.85
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.40	0.85
5:E:28:LEU:HA	5:E:31:ILE:HD13	1.58	0.85
10:J:2:ILE:HD13	10:J:130:SER:OG	1.76	0.85
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	1.92	0.85
2:P:194:LEU:HD11	2:P:232:ILE:HD13	1.59	0.85
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.57	0.85
6:F:38:ILE:HD12	6:F:40:ILE:HD11	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:74:ILE:CD1	2:P:109:VAL:HG22	2.02	0.85
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.58	0.85
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.41	0.84
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.42	0.84
4:R:28:LEU:HA	4:R:31:ILE:HD12	1.58	0.84
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.75	0.84
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.58	0.84
6:T:49:ALA:HB1	6:T:197:ILE:CD1	2.07	0.84
10:X:55:PHE:O	10:X:59:ILE:HD13	1.77	0.84
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.77	0.84
8:H:50:ALA:HB2	9:I:116:ILE:CD1	2.08	0.84
2:B:158:THR:HG22	3:C:63:THR:HG23	1.59	0.83
7:U:9:ASP:CA	7:U:14:ILE:HD11	2.07	0.83
1:A:177:GLU:HG2	2:B:58:LEU:HD21	1.59	0.83
1:O:179:ARG:HB3	1:O:179:ARG:HH11	1.42	0.83
3:Q:156:ILE:HD12	4:R:83:ALA:HB2	1.61	0.83
8:H:221:ILE:HD11	9:I:184:VAL:HB	1.59	0.83
2:B:194:LEU:HD11	2:B:232:ILE:HD13	1.59	0.83
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	1.92	0.83
11:Y:7:ARG:HG3	11:Y:12:ILE:HD11	1.58	0.83
2:P:202:THR:HG22	2:P:204:SER:N	1.94	0.82
14:2:163:ILE:HD13	14:2:169:SER:HB3	1.62	0.82
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.76	0.82
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.93	0.82
12:Z:134:ILE:HD12	12:Z:158:SER:HB3	1.61	0.82
5:E:213:ALA:HB2	5:E:223:ILE:HD12	1.60	0.82
5:S:15:PHE:H	6:T:23:GLN:HE22	1.26	0.82
9:W:4:VAL:HG13	9:W:155:ILE:HD11	1.62	0.81
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.16	0.81
3:C:163:GLN:NE2	3:C:164:THR:H	1.79	0.81
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.93	0.81
11:K:102:CYS:SG	11:K:110:ILE:HD12	2.20	0.81
4:R:74:ILE:HD11	4:R:109:VAL:CG2	2.04	0.81
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.16	0.81
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.61	0.81
5:E:15:PHE:H	6:F:23:GLN:HE22	1.27	0.81
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.25	0.80
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.29	0.80
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.25	0.80
5:S:213:ALA:HB2	5:S:223:ILE:HD12	1.62	0.80
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.62	0.80
13:1:40:ASN:HD22	13:1:40:ASN:N	1.74	0.80
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.62	0.80
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.64	0.79
12:L:21:ILE:HD12	8:V:167:LEU:CD1	2.12	0.79
12:L:3:ILE:HD12	12:L:46:ASN:CB	2.11	0.79
1:A:13:THR:HG21	1:A:24:ILE:HD11	1.63	0.79
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.63	0.79
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.65	0.79
7:G:121:GLN:O	7:G:124:THR:HB	1.83	0.79
3:Q:159:SER:HB2	17:Q:1140:HOH:O	1.83	0.79
14:N:13:ILE:HD13	14:N:177:VAL:HG13	1.63	0.79
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.26	0.78
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.64	0.78
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.64	0.78
12:L:100:ILE:HG13	12:L:112:SER:HB3	1.62	0.78
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.65	0.78
7:U:121:GLN:O	7:U:124:THR:HB	1.83	0.78
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.97	0.78
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.63	0.78
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.65	0.78
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.82	0.78
7:G:198:ILE:HG23	7:G:203:THR:O	1.84	0.78
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.98	0.78
1:O:47:VAL:HG21	1:O:190:ILE:HD13	1.66	0.78
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.84	0.77
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.64	0.77
11:K:12:ILE:HG21	11:K:110:ILE:HD11	1.64	0.77
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.67	0.77
13:M:40:ASN:HD22	13:M:40:ASN:N	1.75	0.77
7:U:217:LYS:HA	7:U:217:LYS:HE3	1.65	0.77
5:S:190:ILE:HD11	5:S:214:ILE:HD12	1.67	0.77
8:V:10:ASN:OD1	8:V:180:ILE:HD12	1.85	0.77
9:W:152:PHE:HD1	9:W:177:ILE:HD11	1.49	0.77
10:J:90(A):ILE:HD11	10:J:116:LEU:HD22	1.65	0.77
12:L:59:PHE:CD1	12:L:83:ILE:HD11	2.19	0.77
5:E:12:THR:HG21	5:E:124:THR:HA	1.66	0.77
14:2:144:GLU:HG2	17:2:1115:HOH:O	1.84	0.77
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.97	0.77
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.66	0.77
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.66	0.76
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.00	0.76
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.66	0.76
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.68	0.76
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.66	0.76
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.49	0.76
14:2:13:ILE:HD13	14:2:177:VAL:HG13	1.67	0.76
2:P:158:THR:HG22	3:Q:63:THR:HG23	1.66	0.76
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.67	0.76
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.01	0.76
6:T:237:GLN:O	6:T:240:ILE:HG22	1.86	0.76
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.69	0.75
4:R:76:CYS:HB2	4:R:138:ILE:HD13	1.67	0.75
8:V:52:THR:O	8:V:56:THR:HB	1.86	0.75
9:W:27:VAL:HG13	17:X:622:HOH:O	1.86	0.75
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.86	0.75
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.68	0.75
7:U:198:ILE:HG23	7:U:203:THR:O	1.86	0.75
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.69	0.75
10:X:156:LYS:O	10:X:160:GLN:HG3	1.85	0.75
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	2.00	0.75
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.69	0.75
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.68	0.74
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.87	0.74
8:V:15:ALA:CB	8:V:159:ILE:CD1	2.65	0.74
1:A:100:TYR:N	1:A:10(A):ILE:HD13	2.02	0.74
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.53	0.74
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	1.97	0.74
10:J:156:LYS:O	10:J:160:GLN:HG3	1.88	0.74
3:Q:65:SER:HB2	17:Q:303:HOH:O	1.87	0.74
2:B:107:ILE:CD1	2:B:108:PRO:O	2.33	0.74
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.00	0.74
5:S:12:THR:HG21	5:S:124:THR:HA	1.68	0.74
8:H:15:ALA:CB	8:H:159:ILE:CD1	2.65	0.74
12:L:166:HIS:HD2	12:L:168:GLN:H	1.35	0.74
13:1:14(C):ARG:HH11	13:1:14(C):ARG:HG3	1.52	0.74
5:S:38:VAL:HG23	5:S:197:ILE:CD1	2.15	0.74
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	2.01	0.74
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.53	0.73
2:B:202:THR:HG22	2:B:204:SER:N	1.96	0.73
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:45:ILE:HD12	9:I:45:ILE:N	2.03	0.73
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.52	0.73
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.53	0.73
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	1.87	0.73
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.01	0.73
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.69	0.73
9:I:114:ASP:OD2	9:I:116:ILE:HD12	1.88	0.73
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.89	0.73
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.71	0.73
9:W:119:ILE:HD12	9:W:119:ILE:H	1.53	0.73
11:Y:7:ARG:HG3	11:Y:12:ILE:HD13	1.70	0.73
4:R:72:ARG:HG3	17:R:1302:HOH:O	1.88	0.72
7:U:70:ILE:HD11	7:U:76:MET:CB	2.19	0.72
11:K:80:SER:HA	11:K:101:ILE:HD13	1.71	0.72
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.68	0.72
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.36	0.72
14:2:126:ILE:H	14:2:126:ILE:HD13	1.53	0.72
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.02	0.72
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.69	0.72
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.04	0.72
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.72	0.72
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.89	0.72
5:E:49:VAL:HA	5:E:212:ILE:HD13	1.72	0.72
1:O:47:VAL:CG2	1:O:190:ILE:HD13	2.20	0.72
5:S:36:VAL:HG13	5:S:197:ILE:HD11	1.70	0.72
3:C:185:THR:HG22	3:C:187:GLU:H	1.55	0.71
14:N:30:VAL:HG21	13:1:203:ILE:HD13	1.72	0.71
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.02	0.71
5:S:67:ILE:HG21	5:S:223:ILE:HD12	1.72	0.71
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.91	0.71
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.55	0.71
13:M:100:ILE:HD13	13:M:112:TYR:HB2	1.73	0.71
13:M:152:GLU:O	13:M:156:VAL:HG23	1.90	0.71
2:P:74:ILE:CD1	2:P:140:GLY:HA3	2.15	0.71
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.56	0.71
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.71	0.71
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.71	0.71
6:F:237:GLN:O	6:F:240:ILE:HG22	1.90	0.71
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.90	0.71
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.72	0.71
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:LYS:HG2	3:C:161:SER:O	1.89	0.71
5:E:67:ILE:HG21	5:E:223:ILE:HD12	1.73	0.71
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.39	0.71
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.39	0.71
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.72	0.71
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.26	0.71
4:R:121:LEU:N	17:R:853:HOH:O	2.23	0.71
10:X:90(A):ILE:HD13	10:X:90(A):ILE:O	1.91	0.71
1:O:121:GLN:O	1:O:124:THR:HB	1.91	0.70
6:T:193:ALA:O	6:T:197:ILE:HD12	1.90	0.70
4:R:76:CYS:CB	4:R:138:ILE:HD13	2.20	0.70
9:W:155:ILE:O	9:W:155:ILE:HD13	1.91	0.70
10:X:55:PHE:CE2	10:X:59:ILE:HD11	2.26	0.70
2:B:107:ILE:HD11	2:B:112:LEU:N	2.07	0.70
5:E:68:ILE:HD11	5:E:78:LEU:HD23	1.74	0.70
8:H:52:THR:O	8:H:56:THR:HB	1.91	0.70
10:J:90(A):ILE:CD1	10:J:116:LEU:HD22	2.21	0.70
4:D:70:ILE:HD12	4:D:92:ALA:HB3	1.73	0.70
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.06	0.70
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.89	0.70
12:Z:100:ILE:HG12	12:Z:112:SER:HB3	1.72	0.70
9:I:45:ILE:N	9:I:45:ILE:CD1	2.54	0.70
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.26	0.70
14:2:134:ILE:HD13	14:2:138:CYS:SG	2.31	0.70
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.07	0.70
7:G:49:ILE:CD1	7:G:193:ALA:HB1	2.22	0.70
13:M:149:GLN:NE2	13:M:149:GLN:H	1.90	0.70
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.27	0.70
5:E:97:ASN:HD21	12:L:61:ASN:ND2	1.90	0.70
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.73	0.70
10:J:59:ILE:O	10:J:63:ILE:HD13	1.90	0.70
6:T:79:SER:HA	17:T:1238:HOH:O	1.92	0.70
9:I:177:ILE:CD1	9:I:187:ARG:HH12	2.01	0.70
9:W:6:MET:HE3	9:W:155:ILE:HG12	1.73	0.70
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.72	0.69
7:U:14:ILE:HD13	7:U:14:ILE:H	1.57	0.69
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.73	0.69
10:J:24:ILE:HG13	10:X:133:TYR:OH	1.92	0.69
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.91	0.69
2:P:121:GLN:O	2:P:124:THR:HB	1.91	0.69
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:203:ILE:HD13	14:2:30:VAL:HG21	1.73	0.69
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	1.89	0.69
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.27	0.69
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.23	0.69
12:L:3:ILE:HD13	12:L:3:ILE:H	1.55	0.69
10:X:37:LEU:HD13	10:X:63:ILE:CD1	2.22	0.69
14:2:59:VAL:HG22	14:2:82:VAL:HG12	1.74	0.69
5:E:221:PHE:CZ	5:E:223:ILE:HD11	2.28	0.69
9:I:35:PHE:CE1	9:I:45:ILE:HD13	2.27	0.69
1:O:173:LYS:O	1:O:177:GLU:HG3	1.91	0.69
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.91	0.69
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.75	0.69
5:S:221:PHE:CZ	5:S:223:ILE:HD11	2.28	0.69
1:A:173:LYS:O	1:A:177:GLU:HG3	1.93	0.69
5:E:210:LEU:HD22	5:E:233:ILE:HD11	1.75	0.69
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.75	0.69
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.75	0.69
10:J:-1:MET:HG2	10:J:1:ASP:H	1.58	0.69
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.58	0.69
13:1:149:GLN:NE2	13:1:149:GLN:H	1.91	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.68
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.28	0.68
13:1:152:GLU:O	13:1:156:VAL:HG23	1.92	0.68
2:P:137:ILE:HD11	2:P:165:VAL:HG22	1.74	0.68
3:Q:15:PHE:CD1	3:Q:21:ILE:HD11	2.28	0.68
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.75	0.68
5:S:220:PRO:O	5:S:222:THR:HG23	1.94	0.68
6:F:54:ILE:HD11	6:F:209:GLU:HB2	1.76	0.68
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.29	0.68
3:C:185:THR:HB	3:C:188:GLU:HG2	1.75	0.68
5:E:97:ASN:ND2	12:L:61:ASN:HD21	1.90	0.68
6:F:173:LYS:O	6:F:177:GLU:HG3	1.94	0.68
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.73	0.68
2:P:74:ILE:HD11	2:P:109:VAL:CG2	2.07	0.68
12:L:173:LEU:HB2	12:L:191:LEU:HD11	1.76	0.68
1:O:15:PHE:N	2:P:23:GLN:HE22	1.89	0.68
6:F:49:ALA:HB2	6:F:212:ILE:HD12	1.74	0.68
8:H:172:ASN:HD22	8:H:193:THR:HA	1.59	0.68
12:L:3:ILE:CD1	12:L:127:GLY:O	2.42	0.68
8:V:41:ILE:HD12	8:V:103:GLY:HA3	1.75	0.68
14:N:186:ARG:HD3	17:N:933:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.07	0.67
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.76	0.67
17:C:247:HOH:O	10:J:68:ILE:HD13	1.93	0.67
12:L:177:ILE:HD13	12:L:185:ARG:NH2	2.09	0.67
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.23	0.67
7:G:135:ILE:HD13	7:G:152:ASP:HA	1.75	0.67
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.75	0.67
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.77	0.67
1:A:121:GLN:O	1:A:124:THR:HB	1.94	0.67
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.76	0.67
9:W:152:PHE:CD1	9:W:177:ILE:HD11	2.30	0.67
8:V:34:LEU:HB2	17:V:578:HOH:O	1.95	0.67
10:X:-1:MET:HG2	10:X:1:ASP:H	1.59	0.67
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.76	0.67
7:G:8:TYR:O	7:G:12:ILE:HD13	1.94	0.67
7:G:87:ASN:C	7:G:87:ASN:HD22	1.98	0.67
8:H:34:LEU:HB2	17:H:540:HOH:O	1.95	0.67
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.74	0.67
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.76	0.67
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.76	0.66
2:B:137:ILE:HD11	2:B:165:VAL:HG22	1.77	0.66
7:G:96:ALA:HA	7:G:107:MET:CE	2.22	0.66
7:G:135:ILE:HD13	7:G:153:PRO:HD3	1.77	0.66
5:S:207:LEU:HD23	5:S:207:LEU:H	1.60	0.66
7:U:96:ALA:HA	7:U:107:MET:CE	2.21	0.66
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.76	0.66
5:E:198:SER:HA	5:E:201:LEU:HG	1.76	0.66
12:L:21:ILE:HD12	8:V:167:LEU:HD11	1.76	0.66
12:Z:100:ILE:HD11	12:Z:125:ARG:HG3	1.77	0.66
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.76	0.66
1:A:110:LYS:HG2	17:A:285:HOH:O	1.94	0.66
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.60	0.66
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.26	0.66
4:R:50:VAL:HG22	4:R:67:ILE:HD11	1.76	0.66
14:2:155:ILE:HG22	14:2:175:MET:HE2	1.77	0.66
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.76	0.66
2:P:190:ILE:CG2	2:P:232:ILE:HD11	2.26	0.66
7:U:59:LEU:O	7:U:61:PRO:HD3	1.95	0.66
7:U:87:ASN:C	7:U:87:ASN:HD22	1.98	0.66
4:D:50:VAL:HG22	4:D:67:ILE:HD11	1.77	0.66
5:E:220:PRO:O	5:E:222:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:172:ASN:HD22	8:V:193:THR:HA	1.61	0.66
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.77	0.65
6:F:211:GLU:O	6:F:212:ILE:HD13	1.96	0.65
7:G:77:VAL:HG12	7:G:137:THR:HB	1.79	0.65
5:S:198:SER:HA	5:S:201:LEU:HG	1.76	0.65
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.76	0.65
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.97	0.65
10:X:69:ARG:HD2	17:X:553:HOH:O	1.95	0.65
4:D:142:ASP:HA	17:D:1309:HOH:O	1.95	0.65
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.78	0.65
13:1:35:ILE:CD1	13:1:56:GLU:HG3	2.26	0.65
10:J:-1:MET:HG2	10:J:1:ASP:N	2.12	0.65
3:Q:37:ALA:HB3	3:Q:165:ILE:HD11	1.77	0.65
11:K:109:THR:O	11:K:110:ILE:HD13	1.96	0.65
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	1.96	0.65
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.77	0.65
4:R:24:VAL:O	4:R:27:SER:HB3	1.97	0.65
5:S:67:ILE:CD1	5:S:77:SER:HB3	2.26	0.65
1:O:24:ILE:HD11	1:O:124:THR:OG1	1.95	0.65
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.77	0.65
10:J:147:THR:OG1	10:J:150:GLU:HG3	1.96	0.65
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.11	0.65
14:N:59:VAL:HG22	14:N:82:VAL:HG12	1.77	0.65
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.26	0.65
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.32	0.65
7:U:227:GLU:HG2	17:U:1255:HOH:O	1.94	0.65
8:V:148:LYS:O	8:V:152:ILE:HG12	1.97	0.65
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	1.97	0.65
1:A:197:LEU:CD2	1:A:210:ILE:HD12	2.27	0.65
5:E:177:GLU:OE1	6:F:56:SER:HB2	1.95	0.65
5:E:207:LEU:HD23	5:E:207:LEU:H	1.61	0.65
7:G:49:ILE:HD12	7:G:49:ILE:N	2.12	0.65
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.61	0.65
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.79	0.65
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.61	0.65
6:T:173:LYS:O	6:T:177:GLU:HG3	1.97	0.65
6:T:45:GLY:HA3	6:T:215:CYS:O	1.97	0.64
6:F:45:GLY:HA3	6:F:215:CYS:O	1.97	0.64
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	1.79	0.64
13:M:100:ILE:CD1	13:M:112:TYR:HB2	2.27	0.64
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.77	0.64
8:H:15:ALA:HB1	8:H:159:ILE:CD1	2.27	0.64
5:S:132:TYR:O	5:S:153:PRO:HB3	1.96	0.64
8:V:15:ALA:HB1	8:V:159:ILE:CD1	2.27	0.64
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.79	0.64
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	1.95	0.64
10:X:64:GLN:HA	17:X:665:HOH:O	1.97	0.64
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.33	0.64
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.98	0.64
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.78	0.64
3:C:15:PHE:N	4:D:23:GLN:HE22	1.93	0.64
7:G:186:TRP:O	7:G:190:VAL:HG23	1.98	0.64
7:U:12:ILE:CG1	7:U:14:ILE:HD12	2.24	0.64
7:G:59:LEU:O	7:G:61:PRO:HD3	1.97	0.64
10:J:168:MET:HE2	10:X:168:MET:HE2	1.80	0.64
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.95	0.64
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.79	0.64
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.62	0.64
13:1:35:ILE:HD12	13:1:45:ILE:HD12	1.80	0.64
14:2:17:ASP:CB	14:2:163:ILE:HD11	2.27	0.64
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.80	0.64
8:H:41:ILE:HD12	8:H:103:GLY:HA3	1.80	0.64
6:T:74:ILE:HG12	6:T:109:ILE:CD1	2.27	0.64
3:C:14:ILE:HD13	3:C:14:ILE:H	1.63	0.64
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.80	0.64
3:Q:170:LYS:HB2	17:Q:833:HOH:O	1.97	0.64
13:1:148:VAL:HG23	17:1:182:HOH:O	1.98	0.64
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.63	0.63
6:T:175:GLU:OE1	6:T:199:LEU:HD23	1.98	0.63
10:J:168:MET:HG2	10:X:168:MET:HE3	1.80	0.63
13:M:40:ASN:N	13:M:40:ASN:ND2	2.46	0.63
14:N:155:ILE:HG22	14:N:175:MET:HE2	1.79	0.63
10:X:147:THR:OG1	10:X:150:GLU:HG3	1.98	0.63
12:Z:173:LEU:HB2	12:Z:191:LEU:HD11	1.80	0.63
11:K:142:TYR:O	11:K:143:LYS:HD2	1.97	0.63
10:X:-1:MET:HG2	10:X:1:ASP:N	2.13	0.63
4:D:17:PRO:HD2	17:D:1171:HOH:O	1.99	0.63
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.79	0.63
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.80	0.63
11:Y:66:HIS:HA	17:Y:1210:HOH:O	1.97	0.63
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.34	0.63
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.12	0.63
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.34	0.63
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.80	0.63
10:J:32:ASP:OD2	10:J:34:THR:HG22	1.99	0.63
4:D:24:VAL:O	4:D:27:SER:HB3	1.99	0.63
4:D:102:TYR:O	12:L:81:ARG:HG3	1.99	0.63
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.80	0.63
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.12	0.63
7:U:186:TRP:O	7:U:190:VAL:HG23	1.98	0.63
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.79	0.63
8:V:81:GLN:O	8:V:85:GLN:HG3	1.99	0.63
5:E:18(D):ILE:O	5:E:18(D):ILE:HD13	1.98	0.63
5:E:213:ALA:HB2	5:E:223:ILE:CD1	2.29	0.63
11:K:143:LYS:HA	17:K:1394:HOH:O	1.98	0.63
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.28	0.63
14:2:18(A):ILE:HD12	14:2:18(C):TYR:CZ	2.34	0.63
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.34	0.62
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.79	0.62
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.46	0.62
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.80	0.62
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.81	0.62
14:2:163:ILE:CD1	14:2:169:SER:HB3	2.29	0.62
5:E:213:ALA:CB	5:E:223:ILE:CD1	2.77	0.62
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.30	0.62
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.81	0.62
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.64	0.62
12:L:3:ILE:CD1	12:L:46:ASN:HB2	2.29	0.62
13:M:74:LEU:HD13	13:M:79:ILE:HD11	1.81	0.62
5:S:67:ILE:HD13	5:S:77:SER:HB3	1.81	0.62
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.34	0.62
9:I:33:LYS:O	9:I:44:GLY:HA2	2.00	0.62
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.92	0.62
7:U:236:ILE:HG13	7:U:237:ALA:N	2.14	0.62
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.80	0.62
9:W:43:LEU:CD2	9:W:45:ILE:HD11	2.30	0.62
1:O:21(I):TYR:HE2	1:O:21(L):ILE:HD13	1.64	0.62
5:S:177:GLU:OE1	6:T:56:SER:HB2	2.00	0.62
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.14	0.62
1:A:197:LEU:HD23	1:A:210:ILE:HD12	1.82	0.62
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.81	0.62
11:Y:35:ILE:HD11	11:Y:45:MET:CE	2.29	0.62
9:I:159:LEU:HD21	9:I:173:ALA:HB1	1.80	0.62
9:I:177:ILE:HD12	9:I:187:ARG:NH1	2.06	0.62
12:L:3:ILE:HD13	12:L:3:ILE:N	2.14	0.62
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	1.99	0.62
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.30	0.62
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.63	0.62
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.81	0.62
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.80	0.62
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.35	0.62
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.35	0.62
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.64	0.62
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.63	0.62
5:E:194:VAL:O	5:E:197:ILE:HG22	2.00	0.62
7:G:77:VAL:CG1	7:G:137:THR:HB	2.30	0.62
9:I:114:ASP:HB2	17:I:851:HOH:O	1.99	0.62
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.64	0.62
12:Z:109:ALA:HA	17:Z:375:HOH:O	2.00	0.62
11:K:172:SER:HA	11:K:192:VAL:HG23	1.82	0.62
3:Q:37:ALA:HB3	3:Q:165:ILE:CD1	2.29	0.62
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.29	0.62
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.15	0.62
8:H:81:GLN:O	8:H:85:GLN:HG3	2.00	0.61
2:P:190:ILE:HG22	2:P:232:ILE:HD11	1.82	0.61
11:Y:172:SER:HA	11:Y:192:VAL:HG23	1.82	0.61
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.82	0.61
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.48	0.61
6:T:175:GLU:HB3	6:T:196:ILE:CD1	2.30	0.61
7:U:70:ILE:HD12	7:U:74:ILE:HG22	1.81	0.61
16:Y:2(I):H10:H22A	12:Z:125:ARG:NH2	2.15	0.61
12:Z:148:VAL:O	12:Z:152:ILE:HG12	1.98	0.61
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.65	0.61
7:G:225:SER:O	7:G:229:ILE:HG12	2.00	0.61
16:K:2(I):H10:H22A	12:L:125:ARG:NH2	2.15	0.61
7:U:35:ILE:HD11	7:U:53:LYS:HG3	1.82	0.61
7:U:77:VAL:HG12	7:U:137:THR:HB	1.82	0.61
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.30	0.61
2:P:143:ASP:OD2	10:X:10(B):LYS:HE2	2.01	0.61
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.65	0.61
9:W:4:VAL:CG1	9:W:155:ILE:HD11	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.34	0.61
5:E:132:TYR:O	5:E:153:PRO:HB3	1.99	0.61
10:J:112:GLN:NE2	10:J:126:ALA:H	1.99	0.61
14:N:30:VAL:CG2	13:1:203:ILE:HD13	2.31	0.61
4:R:102:TYR:O	12:Z:81:ARG:HG3	1.99	0.61
9:W:159:LEU:HD21	9:W:173:ALA:HB1	1.81	0.61
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.35	0.61
14:N:6:VAL:CG2	14:N:155:ILE:HD11	2.30	0.61
9:W:90:ARG:HA	9:W:90:ARG:HH11	1.65	0.61
11:K:133:PHE:HA	17:X:203:HOH:O	2.01	0.61
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.66	0.61
7:U:35:ILE:CD1	7:U:53:LYS:HG3	2.29	0.61
1:A:32:LYS:HG2	17:A:354:HOH:O	2.00	0.61
1:A:85:TYR:O	1:A:89:VAL:HG23	2.01	0.61
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.35	0.61
9:W:33:LYS:O	9:W:44:GLY:HA2	2.01	0.61
11:Y:199:VAL:O	11:Y:203:GLU:HB3	2.00	0.61
1:A:10(A):ILE:N	1:A:10(A):ILE:HD12	2.16	0.61
2:P:184:MET:HE3	2:P:188:ASP:HB3	1.82	0.61
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.31	0.61
8:H:77:VAL:HG22	17:H:258:HOH:O	2.01	0.61
10:J:133:TYR:OH	10:X:24:ILE:HG12	2.00	0.61
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.01	0.61
11:Y:6:PHE:HB2	11:Y:124:ILE:CD1	2.25	0.61
1:A:233:LEU:O	1:A:236:LEU:HB2	2.00	0.60
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.47	0.60
9:I:90:ARG:HA	9:I:90:ARG:HH11	1.65	0.60
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.65	0.60
13:M:200:ALA:HA	13:M:203:ILE:HD12	1.83	0.60
1:O:233:LEU:O	1:O:236:LEU:HB2	2.00	0.60
5:S:213:ALA:CB	5:S:223:ILE:CD1	2.78	0.60
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.31	0.60
8:V:37:ILE:HD11	8:V:43:CYS:HB2	1.82	0.60
1:A:69:LEU:HD23	1:A:69:LEU:C	2.22	0.60
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.82	0.60
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.81	0.60
3:C:186:VAL:O	3:C:190:VAL:HG23	2.01	0.60
8:H:148:LYS:O	8:H:152:ILE:HG12	2.01	0.60
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.16	0.60
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.36	0.60
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:101:LYS:HE2	13:1:57:ARG:HH22	1.66	0.60
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.31	0.60
7:G:96:ALA:CA	7:G:107:MET:HE2	2.23	0.60
9:W:6:MET:HE1	9:W:155:ILE:HA	1.83	0.60
11:Y:6:PHE:CB	11:Y:124:ILE:HD13	2.28	0.60
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.15	0.60
6:F:101:LYS:HE2	13:M:57:ARG:HH22	1.66	0.60
6:F:137:ILE:CD1	6:F:150:MET:HB2	2.31	0.60
7:G:48:VAL:C	7:G:49:ILE:HD12	2.22	0.60
8:V:15:ALA:HB1	8:V:159:ILE:HD11	1.78	0.60
10:X:112:GLN:NE2	10:X:126:ALA:H	2.00	0.60
14:N:83:PHE:CE1	14:N:99:ILE:HD13	2.36	0.60
1:O:21(I):TYR:CE2	1:O:21(L):ILE:HD13	2.37	0.60
10:X:52:THR:CG2	10:X:53:VAL:N	2.65	0.60
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.83	0.60
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.01	0.60
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.16	0.60
10:J:52:THR:CG2	10:J:53:VAL:N	2.64	0.60
4:R:186:LEU:O	4:R:190:GLU:HG3	2.01	0.60
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.83	0.60
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.84	0.60
6:F:101:LYS:HE2	13:M:57:ARG:NH2	2.17	0.60
6:F:229:LEU:HG	6:F:233:ILE:HD11	1.84	0.60
7:G:35:ILE:HD11	7:G:53:LYS:HG3	1.83	0.60
9:I:6:MET:CE	9:I:155:ILE:HA	2.31	0.60
14:2:126:ILE:HD13	14:2:126:ILE:N	2.17	0.60
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.32	0.60
7:G:35:ILE:CD1	7:G:53:LYS:HG3	2.32	0.60
4:R:177:LEU:HD13	5:S:58:LEU:HD11	1.84	0.60
7:U:70:ILE:CD1	7:U:76:MET:HB2	2.30	0.60
10:X:37:LEU:HB3	10:X:63:ILE:CD1	2.28	0.60
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.02	0.60
3:C:136:THR:O	3:C:150:GLN:HA	2.02	0.59
9:I:48:LEU:HG	9:I:50:THR:HG22	1.84	0.59
10:J:168:MET:HE3	10:X:168:MET:HG2	1.82	0.59
13:M:203:ILE:HD13	14:2:30:VAL:CG2	2.31	0.59
6:F:137:ILE:HD12	6:F:163:ALA:HB3	1.83	0.59
6:F:137:ILE:HD11	6:F:163:ALA:HB1	1.84	0.59
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.02	0.59
7:U:86:ARG:HD2	17:U:249:HOH:O	2.01	0.59
8:V:100:ILE:HD13	8:V:112:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:ILE:HG22	2:B:232:ILE:HD11	1.83	0.59
4:R:81:LEU:HB3	17:R:599:HOH:O	2.02	0.59
5:S:194:VAL:O	5:S:197:ILE:HG22	2.01	0.59
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.17	0.59
3:C:46:VAL:O	3:C:215:VAL:HG12	2.02	0.59
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.84	0.59
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.84	0.59
9:I:-3:ILE:HD12	9:I:48:LEU:HD13	1.85	0.59
9:I:35:PHE:HE1	9:I:45:ILE:HD13	1.66	0.59
5:S:213:ALA:HB2	5:S:223:ILE:CD1	2.30	0.59
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.03	0.59
7:G:43:LYS:HB2	7:G:18(G):GLU:O	2.02	0.59
14:N:13:ILE:CD1	14:N:177:VAL:HG13	2.32	0.59
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.02	0.59
4:R:28:LEU:HA	4:R:31:ILE:CD1	2.32	0.59
6:T:101:LYS:HE2	13:1:57:ARG:NH2	2.17	0.59
9:W:43:LEU:HD21	9:W:45:ILE:HD11	1.85	0.59
9:W:48:LEU:HG	9:W:50:THR:HG22	1.85	0.59
10:X:90(B):ARG:NH1	17:X:266:HOH:O	2.34	0.59
6:F:69:VAL:HG12	17:F:319:HOH:O	2.01	0.59
3:Q:136:THR:O	3:Q:150:GLN:HA	2.03	0.59
8:V:155:ALA:O	8:V:159:ILE:HD12	2.02	0.59
10:X:140:HIS:HD2	10:X:141:HIS:CE1	2.20	0.59
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.84	0.59
7:U:77:VAL:CG1	7:U:137:THR:HB	2.33	0.59
3:C:235:GLN:O	3:C:239:GLU:HG2	2.03	0.59
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.83	0.59
5:S:46:ALA:HB1	5:S:139:ILE:HB	1.85	0.59
8:V:219:VAL:O	8:V:221:ILE:HD12	2.02	0.59
3:C:57:LYS:O	3:C:58:LEU:HB2	2.03	0.59
3:C:163:GLN:HE21	3:C:164:THR:H	1.51	0.59
10:J:143:ARG:O	10:J:146:MET:HG3	2.03	0.59
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.37	0.59
14:N:42:TRP:HZ2	13:1:211:ILE:HD11	1.68	0.59
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.85	0.59
7:U:168:LYS:O	7:U:172:ILE:HG12	2.02	0.59
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.85	0.59
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.50	0.59
6:F:175:GLU:HB3	6:F:196:ILE:CD1	2.31	0.59
2:P:74:ILE:HD12	2:P:109:VAL:HG13	1.85	0.59
4:R:53:ARG:O	4:R:53:ARG:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.03	0.59
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.01	0.59
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.85	0.58
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.84	0.58
9:I:104:ILE:HD12	9:I:181:LYS:N	2.18	0.58
11:K:76:VAL:N	11:K:106:GLU:OE2	2.36	0.58
6:T:195:LYS:HZ2	6:T:196:ILE:HD13	1.67	0.58
9:W:6:MET:CE	9:W:155:ILE:HA	2.33	0.58
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.85	0.58
4:D:12(F):GLY:HA3	17:D:965:HOH:O	2.03	0.58
13:1:175:LEU:HD23	13:1:176:ALA:N	2.18	0.58
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.66	0.58
12:L:93:PHE:N	12:L:94:PRO:HD3	2.18	0.58
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.85	0.58
5:S:207:LEU:H	5:S:207:LEU:CD2	2.16	0.58
7:U:43:LYS:HB2	7:U:18(G):GLU:O	2.04	0.58
8:V:40:LYS:O	8:V:41:ILE:HD13	2.03	0.58
8:V:221:ILE:HD11	9:W:184:VAL:CB	2.32	0.58
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.18	0.58
11:K:7:ARG:HD2	11:K:108:PRO:O	2.03	0.58
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.34	0.58
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.19	0.58
12:Z:32:PRO:HD2	17:Z:1177:HOH:O	2.04	0.58
5:E:167:ALA:HB3	17:E:1131:HOH:O	2.03	0.58
7:G:8:TYR:C	7:G:10:ARG:H	2.06	0.58
2:B:184:MET:HE3	2:B:188:ASP:HB3	1.85	0.58
4:D:186:LEU:O	4:D:190:GLU:HG3	2.03	0.58
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.86	0.58
6:T:197:ILE:HD13	6:T:210:LEU:CD1	2.29	0.58
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.84	0.58
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.85	0.58
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.86	0.58
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	1.85	0.58
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.38	0.58
2:B:185:LYS:HD3	2:B:186:VAL:N	2.19	0.58
13:M:146:THR:HA	17:M:1069:HOH:O	2.04	0.58
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.52	0.58
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.84	0.58
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.86	0.58
2:P:74:ILE:HD13	2:P:140:GLY:CA	2.21	0.58
2:P:95:HIS:HB2	17:P:249:HOH:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.85	0.58
3:C:122:ARG:NH2	17:C:806:HOH:O	2.36	0.58
8:H:210:THR:HG21	12:Z:14(C):GLN:HG2	1.86	0.58
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.86	0.58
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.34	0.58
5:E:68:ILE:CD1	5:E:78:LEU:HD23	2.34	0.58
8:H:172:ASN:ND2	8:H:193:THR:HG22	2.19	0.58
12:Z:105:ASP:OD2	12:Z:107:LYS:HB2	2.04	0.58
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.86	0.58
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.85	0.57
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.02	0.57
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.86	0.57
8:H:219:VAL:O	8:H:221:ILE:HD12	2.04	0.57
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.84	0.57
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.85	0.57
11:K:199:VAL:O	11:K:203:GLU:HB3	2.03	0.57
12:L:105:ASP:OD2	12:L:107:LYS:HB2	2.04	0.57
1:O:69:LEU:C	1:O:69:LEU:HD23	2.24	0.57
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.39	0.57
2:P:185:LYS:HD3	2:P:186:VAL:N	2.19	0.57
3:Q:215:VAL:HG23	3:Q:221:ILE:HG13	1.86	0.57
14:2:14:LEU:O	14:2:175:MET:HA	2.04	0.57
4:D:70:ILE:CD1	4:D:89:ILE:HG23	2.34	0.57
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.69	0.57
6:F:49:ALA:CB	6:F:212:ILE:HD12	2.34	0.57
11:K:99:THR:HG22	11:K:113:VAL:O	2.04	0.57
14:N:14:LEU:O	14:N:175:MET:HA	2.03	0.57
5:E:213:ALA:CB	5:E:223:ILE:HD12	2.34	0.57
6:F:229:LEU:HG	6:F:233:ILE:CD1	2.33	0.57
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.05	0.57
11:K:25:TRP:CH2	12:L:132:SER:HA	2.40	0.57
8:V:18:THR:HG21	8:V:172:ASN:HB2	1.86	0.57
13:1:157:ASN:HB3	17:1:558:HOH:O	2.03	0.57
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.87	0.57
11:K:146:LEU:HD23	11:K:151:ALA:HA	1.87	0.57
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.05	0.57
1:O:15:PHE:H	2:P:23:GLN:NE2	1.92	0.57
1:O:212:LEU:HD23	1:O:213:ALA:N	2.19	0.57
13:1:14(D):GLU:O	13:1:14(G):ILE:HG13	2.05	0.57
5:E:46:ALA:HB1	5:E:139:ILE:HB	1.86	0.57
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:LEU:H	5:E:207:LEU:CD2	2.17	0.57
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.32	0.57
6:F:203:GLU:OE1	6:F:203:GLU:HA	2.03	0.57
3:Q:15:PHE:H	4:R:23:GLN:NE2	1.95	0.57
7:G:236:ILE:HD12	7:G:237:ALA:N	2.19	0.57
13:M:1:THR:HA	17:M:849:HOH:O	2.05	0.57
9:W:74:ILE:HB	17:W:517:HOH:O	2.04	0.57
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.34	0.57
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.86	0.57
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.70	0.57
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.87	0.57
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.86	0.57
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.20	0.57
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.86	0.57
3:Q:52:ARG:NH2	3:Q:211:GLU:HB3	2.20	0.57
6:T:186:ALA:O	6:T:190:VAL:HG23	2.04	0.57
7:U:96:ALA:CA	7:U:107:MET:HE2	2.27	0.57
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.20	0.57
8:H:155:ALA:O	8:H:159:ILE:HD12	2.04	0.57
9:I:6:MET:HE1	9:I:155:ILE:HA	1.85	0.57
9:I:152:PHE:HB2	9:I:177:ILE:CD1	2.31	0.57
13:M:100:ILE:HD11	13:M:112:TYR:HD1	1.70	0.57
13:M:211:ILE:HD11	14:2:42:TRP:HZ2	1.69	0.57
1:O:85:TYR:O	1:O:89:VAL:HG23	2.05	0.57
8:V:159:ILE:HD13	8:V:173:VAL:HG13	1.85	0.57
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.70	0.57
12:Z:163:THR:HB	17:Z:200:HOH:O	2.04	0.57
13:1:200:ALA:HA	13:1:203:ILE:HD12	1.86	0.57
10:J:185:ARG:HG2	10:J:185:ARG:HH11	1.69	0.57
12:L:-2:ASN:HA	12:L:21:ILE:O	2.05	0.57
2:P:113:VAL:HG22	2:P:138:TYR:CD2	2.40	0.57
10:X:143:ARG:O	10:X:146:MET:HG3	2.04	0.57
2:B:163:ILE:HG12	2:B:164:SER:N	2.20	0.56
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.87	0.56
7:U:158:VAL:HG22	7:U:159:GLY:N	2.20	0.56
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.86	0.56
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.87	0.56
7:G:158:VAL:HG22	7:G:159:GLY:N	2.20	0.56
10:J:76:PRO:HD2	17:J:296:HOH:O	2.06	0.56
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.03	0.56
14:2:13:ILE:HG13	14:2:151:THR:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD23	1:A:213:ALA:N	2.20	0.56
2:B:8:TYR:CD2	7:G:12:ILE:HD12	2.40	0.56
2:B:27:ALA:O	2:B:31:ILE:HG12	2.05	0.56
5:E:28:LEU:CA	5:E:31:ILE:HD13	2.33	0.56
6:F:87:HIS:HD2	6:F:132:PHE:HE2	1.53	0.56
6:F:137:ILE:HD13	6:F:150:MET:HB2	1.88	0.56
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.87	0.56
10:J:140:HIS:HD2	10:J:141:HIS:CE1	2.22	0.56
7:U:9:ASP:HA	7:U:14:ILE:CD1	2.18	0.56
2:B:71:ASN:ND2	2:B:72:ASP:H	2.04	0.56
3:C:52:ARG:NH2	3:C:211:GLU:HB3	2.20	0.56
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.85	0.56
13:M:17:ASP:HA	13:M:173:PHE:CB	2.35	0.56
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.88	0.56
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.07	0.56
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.88	0.56
4:D:117:CYS:HB3	4:D:155:GLY:O	2.05	0.56
5:E:4:PHE:CE1	5:E:17:PRO:HD2	2.41	0.56
3:Q:156:ILE:N	3:Q:156:ILE:CD1	2.68	0.56
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.35	0.56
6:T:121:GLN:NE2	17:T:385:HOH:O	2.38	0.56
14:2:163:ILE:HD12	14:2:170:GLY:N	2.20	0.56
7:G:136:LEU:O	7:G:150:LYS:HA	2.05	0.56
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.41	0.56
4:R:117:CYS:HB3	4:R:155:GLY:O	2.05	0.56
5:S:190:ILE:O	5:S:194:VAL:HG23	2.06	0.56
5:S:207:LEU:HD23	5:S:207:LEU:N	2.20	0.56
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.05	0.56
5:E:49:VAL:HG13	5:E:212:ILE:HD13	1.83	0.56
7:G:108:PRO:HB3	8:H:72:ARG:NH2	2.20	0.56
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.06	0.56
9:I:113:PHE:HA	9:I:118:CYS:O	2.06	0.56
12:L:3:ILE:CD1	12:L:46:ASN:CB	2.83	0.56
2:P:107:ILE:HG22	17:P:410:HOH:O	2.06	0.56
5:S:67:ILE:HG21	5:S:223:ILE:CD1	2.36	0.56
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.88	0.56
5:E:49:VAL:HG22	5:E:212:ILE:HD12	1.87	0.56
7:G:168:LYS:O	7:G:172:ILE:HG12	2.06	0.56
10:J:52:THR:HG23	10:J:53:VAL:N	2.21	0.56
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.40	0.56
4:R:39:GLY:O	4:R:40:ILE:HD13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.18	0.56
1:A:21:LEU:CB	1:A:24:ILE:HD13	2.26	0.56
3:C:70:ILE:CD1	3:C:112:LEU:HD11	2.30	0.56
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.99	0.56
7:G:74:ILE:HG21	7:G:112:LEU:HD23	1.88	0.56
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.53	0.56
8:H:200:LYS:HE3	9:I:140:SER:O	2.06	0.56
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.06	0.56
2:P:163:ILE:HG12	2:P:164:SER:N	2.20	0.56
3:Q:156:ILE:HD12	4:R:83:ALA:CB	2.36	0.56
5:E:58:LEU:HD12	5:E:58:LEU:N	2.21	0.56
6:F:186:ALA:O	6:F:190:VAL:HG23	2.06	0.56
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.88	0.56
9:W:87:LEU:HD11	9:W:99:PRO:HG2	1.88	0.56
4:D:28:LEU:HA	4:D:31:ILE:CD1	2.32	0.55
5:E:190:ILE:O	5:E:194:VAL:HG23	2.05	0.55
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.22	0.55
11:K:12:ILE:CG2	11:K:110:ILE:HD11	2.34	0.55
12:L:90:LYS:HE3	12:L:93:PHE:O	2.06	0.55
14:N:13:ILE:HG13	14:N:151:THR:HG21	1.87	0.55
7:U:140:SER:HA	7:U:215:ALA:HB1	1.88	0.55
9:W:113:PHE:HA	9:W:118:CYS:O	2.06	0.55
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.89	0.55
3:C:97:GLN:NE2	3:C:97:GLN:HA	2.21	0.55
6:F:210:LEU:HD11	6:F:212:ILE:HD11	1.88	0.55
8:H:18:THR:HG21	8:H:172:ASN:HB2	1.88	0.55
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.41	0.55
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.88	0.55
14:N:51:ASP:O	14:N:55:ILE:HG12	2.07	0.55
11:Y:12:ILE:HD12	11:Y:110:ILE:HD11	1.89	0.55
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.87	0.55
14:2:13:ILE:CD1	14:2:177:VAL:HG13	2.36	0.55
2:B:113:VAL:HG22	2:B:138:TYR:CD2	2.41	0.55
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.41	0.55
7:G:233:LEU:O	7:G:236:ILE:HG13	2.06	0.55
2:P:100:LEU:HG	9:W:60:ARG:NH2	2.22	0.55
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.75	0.55
14:2:37:VAL:CG2	14:2:41:ILE:HG22	2.36	0.55
8:H:18:THR:HB	8:H:30:ASN:HD22	1.72	0.55
11:K:102:CYS:CB	11:K:110:ILE:HD12	2.37	0.55
2:P:194:LEU:HD11	2:P:232:ILE:CD1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.88	0.55
6:T:203:GLU:HA	6:T:203:GLU:OE1	2.05	0.55
7:U:49:ILE:HD13	7:U:212:VAL:HG22	1.89	0.55
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.72	0.55
7:G:49:ILE:HD13	7:G:193:ALA:HB1	1.89	0.55
4:R:65:GLU:HA	17:R:750:HOH:O	2.06	0.55
12:Z:173:LEU:HG	12:Z:175:ILE:HD11	1.88	0.55
14:2:13:ILE:HD13	14:2:177:VAL:HG22	1.88	0.55
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.53	0.55
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.88	0.55
3:C:29:GLU:OE2	3:C:32:LYS:HE2	2.07	0.55
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.06	0.55
3:Q:125:GLN:NE2	17:Q:872:HOH:O	2.39	0.55
10:X:52:THR:HG23	10:X:53:VAL:N	2.22	0.55
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.42	0.55
10:J:11:SER:HB2	10:J:178:VAL:O	2.07	0.55
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.55	0.55
6:T:69:VAL:HG12	17:1:811:HOH:O	2.06	0.55
7:U:8:TYR:C	7:U:10:ARG:H	2.09	0.55
7:U:116:MET:HE3	17:U:431:HOH:O	2.06	0.55
8:V:18:THR:HB	8:V:30:ASN:HD22	1.72	0.55
13:1:12:VAL:HG21	13:1:102:ALA:HB1	1.88	0.55
3:C:33:ARG:HD2	17:C:565:HOH:O	2.07	0.55
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.07	0.55
7:G:135:ILE:CD1	7:G:153:PRO:HD3	2.36	0.55
9:I:87:LEU:HD11	9:I:99:PRO:HG2	1.88	0.55
12:L:59:PHE:CG	12:L:83:ILE:HD11	2.42	0.55
14:N:37:VAL:CG2	14:N:41:ILE:HG22	2.37	0.55
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.21	0.55
13:1:177:ILE:C	13:1:178:ILE:HD12	2.27	0.55
3:C:35:THR:HB	3:C:51:GLU:HG3	1.89	0.55
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.07	0.55
5:E:125:GLN:HB3	17:E:1296:HOH:O	2.07	0.55
13:M:175:LEU:HD23	13:M:176:ALA:N	2.21	0.55
2:P:224:PHE:HD2	2:P:224:PHE:N	2.05	0.55
3:Q:29:GLU:OE2	3:Q:32:LYS:HE2	2.07	0.55
1:A:13:THR:HG21	1:A:24:ILE:CD1	2.35	0.54
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.89	0.54
2:B:224:PHE:N	2:B:224:PHE:HD2	2.04	0.54
4:D:59:LEU:HD11	4:D:64:ILE:HD11	1.88	0.54
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:ILE:HG22	8:H:16:ALA:HB2	1.88	0.54
8:H:84:LYS:HG3	8:H:85:GLN:N	2.22	0.54
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.54	0.54
7:U:136:LEU:O	7:U:150:LYS:HA	2.05	0.54
2:B:114:ARG:NH1	10:J:70:GLU:OE2	2.37	0.54
2:B:224:PHE:N	2:B:224:PHE:CD2	2.76	0.54
6:F:12:ASN:HB3	6:F:127:ASN:HA	1.90	0.54
7:G:151:THR:HG22	7:G:157:TYR:CB	2.38	0.54
7:G:230:GLU:O	7:G:234:VAL:HG23	2.07	0.54
11:K:50:ALA:HB2	12:L:116:VAL:HG23	1.89	0.54
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.19	0.54
6:T:49:ALA:HB3	6:T:197:ILE:HD11	1.80	0.54
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.38	0.54
8:V:200:LYS:HE3	9:W:140:SER:O	2.08	0.54
9:W:15:ALA:HB3	9:W:155:ILE:CD1	2.37	0.54
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.07	0.54
8:H:113:ILE:HD12	8:H:113:ILE:N	2.22	0.54
5:S:201:LEU:O	5:S:202:ARG:HB2	2.08	0.54
6:T:87:HIS:HD2	6:T:132:PHE:HE2	1.54	0.54
7:U:55:PRO:HG2	7:U:56:ASP:H	1.73	0.54
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.89	0.54
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.28	0.54
5:E:111:ARG:HG2	5:E:111:ARG:NH1	2.23	0.54
12:L:145:TYR:CD1	12:L:146:LEU:N	2.75	0.54
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.90	0.54
7:U:143:GLU:HG2	17:U:928:HOH:O	2.07	0.54
8:V:84:LYS:HG3	8:V:85:GLN:N	2.23	0.54
8:V:100:ILE:HD13	8:V:112:SER:CB	2.38	0.54
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.07	0.54
5:E:68:ILE:N	5:E:68:ILE:HD12	2.23	0.54
7:G:87:ASN:C	7:G:87:ASN:ND2	2.61	0.54
7:G:140:SER:HA	7:G:215:ALA:HB1	1.89	0.54
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.42	0.54
6:T:119:TYR:O	6:T:122:ALA:HB3	2.08	0.54
9:W:9:LYS:HD3	9:W:145:ASN:HD22	1.71	0.54
10:X:58:TYR:CD2	10:X:59:ILE:HD12	2.43	0.54
11:Y:12:ILE:HD12	11:Y:110:ILE:CG1	2.37	0.54
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.89	0.54
14:N:10(B):LYS:C	14:N:10(B):LYS:HD3	2.28	0.54
2:P:87:ILE:O	2:P:91:THR:HG23	2.08	0.54
9:W:73:ALA:HB1	17:W:204:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:17:ASP:HA	13:1:173:PHE:CB	2.36	0.54
4:D:229:THR:HG22	4:D:233:ILE:HD11	1.90	0.54
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.90	0.54
7:G:172:ILE:HD11	7:G:201:LEU:CD2	2.38	0.54
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.08	0.54
6:T:72:ARG:HD2	13:1:64:THR:OG1	2.07	0.54
6:T:127:ASN:HD22	6:T:128:SER:N	2.05	0.54
10:X:185:ARG:HG2	10:X:185:ARG:HH11	1.73	0.54
3:C:39:GLY:O	3:C:162:ALA:HA	2.08	0.54
5:E:207:LEU:HD23	5:E:207:LEU:N	2.22	0.54
6:F:238:LYS:HZ2	6:F:239:GLU:HG3	1.73	0.54
14:N:41:ILE:HD13	14:N:79:ALA:HB2	1.90	0.54
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.37	0.54
4:R:243:ALA:O	4:R:244:GLU:HB2	2.08	0.54
7:U:226:ALA:HA	7:U:229:ILE:HD12	1.90	0.54
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.42	0.54
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.05	0.54
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.18	0.54
7:G:55:PRO:HG2	7:G:56:ASP:H	1.73	0.54
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.90	0.54
2:P:27:ALA:O	2:P:31:ILE:HG12	2.07	0.54
3:Q:97:GLN:NE2	3:Q:97:GLN:HA	2.22	0.54
9:W:43:LEU:HG	9:W:45:ILE:HD11	1.90	0.54
12:Z:76:ILE:HG22	17:Z:948:HOH:O	2.08	0.54
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.06	0.54
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.73	0.54
12:L:13:VAL:HG12	12:L:177:ILE:HG12	1.90	0.54
7:U:87:ASN:C	7:U:87:ASN:ND2	2.60	0.54
7:U:204:GLU:HG3	17:U:1284:HOH:O	2.07	0.54
10:X:44:SER:OG	10:X:100:LEU:HB2	2.07	0.54
1:A:49:ALA:HB2	1:A:212:LEU:HG	1.89	0.53
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.43	0.53
5:E:67:ILE:HG21	5:E:223:ILE:CD1	2.37	0.53
7:G:49:ILE:HD11	7:G:193:ALA:CB	2.39	0.53
7:G:116:MET:HE3	17:G:551:HOH:O	2.07	0.53
11:K:35:ILE:N	11:K:35:ILE:HD12	2.23	0.53
11:K:48:GLY:HA3	17:K:406:HOH:O	2.07	0.53
2:P:235:LYS:C	2:P:237:GLY:H	2.11	0.53
3:Q:39:GLY:O	3:Q:162:ALA:HA	2.08	0.53
3:Q:72:SER:O	3:Q:221:ILE:HD13	2.08	0.53
13:1:150:VAL:HG21	17:1:323:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.23	0.53
11:K:174:ASN:HD21	11:K:189:ASN:HB2	1.73	0.53
4:R:207:LEU:HD23	4:R:207:LEU:C	2.29	0.53
4:R:221:PHE:HE1	4:R:223:ILE:HD11	1.73	0.53
6:T:238:LYS:HZ2	6:T:239:GLU:HG3	1.74	0.53
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.89	0.53
2:B:15:PHE:N	3:C:23:GLN:HE22	1.96	0.53
5:E:210:LEU:HD22	5:E:233:ILE:CD1	2.38	0.53
8:H:40:LYS:O	8:H:41:ILE:HD13	2.09	0.53
8:H:159:ILE:HD13	8:H:173:VAL:HG13	1.89	0.53
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.91	0.53
1:O:35:VAL:HG11	1:O:51:GLU:HB3	1.89	0.53
1:O:47:VAL:HG23	1:O:212:LEU:HD21	1.89	0.53
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.07	0.53
7:U:74:ILE:HG21	7:U:112:LEU:HD23	1.89	0.53
8:V:37:ILE:HD13	8:V:41:ILE:HG22	1.91	0.53
9:W:100:VAL:HG13	9:W:125:ILE:HG21	1.89	0.53
5:E:74:MET:HE1	5:E:109:VAL:HA	1.91	0.53
6:F:195:LYS:HZ2	6:F:196:ILE:HD13	1.73	0.53
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.38	0.53
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.08	0.53
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.90	0.53
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.39	0.53
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.72	0.53
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.73	0.53
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.43	0.53
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.44	0.53
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.08	0.53
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.90	0.53
3:C:175:PHE:O	3:C:179:ASN:HB2	2.09	0.53
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.37	0.53
2:P:224:PHE:N	2:P:224:PHE:CD2	2.76	0.53
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.08	0.53
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.43	0.53
5:S:4:PHE:CE1	5:S:17:PRO:HD2	2.44	0.53
7:U:230:GLU:O	7:U:234:VAL:HG23	2.08	0.53
8:V:40:LYS:C	8:V:41:ILE:HD13	2.29	0.53
10:X:13:ILE:HG12	10:X:177:ILE:HD12	1.90	0.53
13:1:40:ASN:N	13:1:40:ASN:ND2	2.46	0.53
2:B:107:ILE:HD11	2:B:112:LEU:H	1.71	0.53
3:C:21:ILE:HD12	3:C:21:ILE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:243:ALA:O	4:D:244:GLU:HB2	2.08	0.53
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.43	0.53
11:K:35:ILE:HD13	11:K:56:GLU:OE1	2.09	0.53
11:K:86:LEU:O	11:K:89:GLN:HB2	2.08	0.53
12:L:177:ILE:CD1	12:L:185:ARG:NH2	2.72	0.53
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.89	0.53
2:P:71:ASN:ND2	2:P:72:ASP:H	2.06	0.53
3:Q:70:ILE:CD1	3:Q:112:LEU:HD11	2.32	0.53
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.72	0.53
1:A:144:PHE:CD2	9:I:72:ARG:HD2	2.43	0.53
1:A:212:LEU:HD22	1:A:224:LEU:HD12	1.90	0.53
10:J:77:GLN:NE2	10:J:77:GLN:C	2.61	0.53
11:K:200:LYS:HE3	11:K:206:PHE:O	2.08	0.53
4:R:17:PRO:HG3	5:S:26:TYR:CE2	2.44	0.53
5:S:15:PHE:H	6:T:23:GLN:NE2	2.03	0.53
12:Z:175:ILE:HD12	12:Z:175:ILE:N	2.23	0.53
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.90	0.53
4:D:138:ILE:N	4:D:138:ILE:HD12	2.24	0.53
5:E:15:PHE:H	6:F:23:GLN:NE2	2.04	0.53
8:H:40:LYS:C	8:H:41:ILE:HD13	2.29	0.53
10:J:167:PRO:CB	10:X:168:MET:HE1	2.39	0.53
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.69	0.53
6:T:74:ILE:HG12	6:T:109:ILE:HD13	1.91	0.53
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.89	0.53
8:V:3:ILE:HD11	8:V:127:LEU:CB	2.38	0.53
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.29	0.53
12:Z:114:ASP:HB2	12:Z:118:SER:OG	2.09	0.53
3:C:14:ILE:HD13	3:C:14:ILE:N	2.24	0.53
4:D:53:ARG:O	4:D:53:ARG:HG2	2.09	0.53
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.73	0.53
8:H:221:ILE:HD11	9:I:184:VAL:CB	2.34	0.53
9:I:-8:SER:O	9:I:-6:PRO:HD3	2.09	0.53
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.74	0.53
7:U:49:ILE:CD1	7:U:212:VAL:HG22	2.39	0.53
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.39	0.53
2:B:235:LYS:C	2:B:237:GLY:H	2.12	0.52
3:C:15:PHE:H	4:D:23:GLN:NE2	1.96	0.52
3:C:241:GLN:C	3:C:243:GLN:H	2.12	0.52
5:E:201:LEU:O	5:E:202:ARG:HB2	2.09	0.52
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.39	0.52
1:O:62:GLU:C	1:O:64:LEU:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:58:LEU:N	5:S:58:LEU:HD12	2.24	0.52
4:D:39:GLY:O	4:D:40:ILE:HD13	2.10	0.52
5:E:214:ILE:O	5:E:221:PHE:HA	2.10	0.52
9:I:9:LYS:HD3	9:I:145:ASN:HD22	1.74	0.52
14:N:9:LYS:O	14:N:107:LYS:HD3	2.09	0.52
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.91	0.52
2:P:101:LYS:NZ	10:X:85:GLN:HE22	2.08	0.52
4:R:215:ILE:HD13	4:R:215:ILE:C	2.30	0.52
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.91	0.52
9:W:29:ASN:ND2	9:W:29:ASN:H	2.08	0.52
10:J:168:MET:CE	10:X:168:MET:CE	2.87	0.52
12:L:114:ASP:HB2	12:L:118:SER:OG	2.09	0.52
6:T:35:THR:HG23	6:T:36:THR:N	2.24	0.52
7:U:101:TYR:OH	14:2:58:ILE:HD11	2.10	0.52
11:Y:76:VAL:N	11:Y:106:GLU:OE2	2.39	0.52
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.23	0.52
14:2:116:GLY:HA3	17:2:192:HOH:O	2.10	0.52
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.73	0.52
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.09	0.52
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.91	0.52
8:H:50:ALA:CB	9:I:116:ILE:CD1	2.76	0.52
9:I:93:GLY:N	9:I:94:PRO:CD	2.73	0.52
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.91	0.52
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.10	0.52
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.09	0.52
3:Q:241:GLN:C	3:Q:243:GLN:H	2.13	0.52
11:Y:12:ILE:HD12	11:Y:110:ILE:HG13	1.91	0.52
3:C:163:GLN:NE2	3:C:164:THR:N	2.55	0.52
5:E:138:ILE:HD12	5:E:138:ILE:N	2.23	0.52
8:H:95:ILE:O	8:H:97:ALA:N	2.41	0.52
1:O:110:LYS:HG2	17:O:376:HOH:O	2.10	0.52
3:Q:154:SER:CB	3:Q:156:ILE:HD13	2.38	0.52
3:Q:18(A):ASP:OD1	3:Q:18(C):LYS:HB2	2.10	0.52
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.43	0.52
10:X:52:THR:CG2	10:X:53:VAL:H	2.22	0.52
12:Z:-8:PHE:HB3	13:1:-8:THR:HG23	1.92	0.52
2:B:143:ASP:OD2	10:J:10(B):LYS:HE2	2.10	0.52
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.92	0.52
10:J:63:ILE:N	10:J:63:ILE:CD1	2.72	0.52
11:K:78:ALA:O	11:K:82:ILE:HG12	2.10	0.52
1:O:177:GLU:HG2	2:P:58:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.91	0.52
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.92	0.52
4:R:236:GLU:O	4:R:240:LYS:HG3	2.09	0.52
9:W:101:VAL:O	9:W:110:ILE:HA	2.09	0.52
10:X:11:SER:HB2	10:X:178:VAL:O	2.09	0.52
11:Y:35:ILE:HD11	11:Y:45:MET:HE3	1.91	0.52
13:1:91:ARG:HG3	13:1:92:SER:N	2.24	0.52
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.92	0.52
6:F:127:ASN:HD22	6:F:128:SER:N	2.08	0.52
6:F:137:ILE:HD11	6:F:150:MET:SD	2.49	0.52
8:H:101:VAL:HG12	8:H:113:ILE:HD11	1.91	0.52
9:I:22:SER:O	9:I:23:GLN:HB2	2.10	0.52
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.12	0.52
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.91	0.52
4:R:229:THR:HG22	4:R:233:ILE:HD11	1.91	0.52
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.92	0.52
8:V:144:GLN:O	8:V:145:ASP:HB2	2.09	0.52
10:J:13:ILE:HD12	10:J:13:ILE:N	2.25	0.52
5:S:138:ILE:HD12	5:S:138:ILE:N	2.24	0.52
5:S:214:ILE:O	5:S:221:PHE:HA	2.09	0.52
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.91	0.52
4:D:198:LYS:HG3	17:D:499:HOH:O	2.10	0.52
6:F:238:LYS:NZ	6:F:239:GLU:HG3	2.25	0.52
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.44	0.52
3:Q:33:ARG:CB	3:Q:33:ARG:NH1	2.73	0.52
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.39	0.52
13:1:-3:VAL:HG12	13:1:49:ILE:HG13	1.92	0.52
1:A:62:GLU:C	1:A:64:LEU:H	2.14	0.52
2:B:87:ILE:O	2:B:91:THR:HG23	2.10	0.52
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.92	0.52
8:H:144:GLN:O	8:H:145:ASP:HB2	2.09	0.52
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.92	0.52
13:M:113:VAL:HA	13:M:118:VAL:O	2.09	0.52
1:O:141:HIS:HA	1:O:146:GLY:O	2.10	0.52
2:P:185:LYS:O	2:P:188:ASP:N	2.42	0.52
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.75	0.52
7:U:192:PHE:C	7:U:192:PHE:CD1	2.83	0.52
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.92	0.52
12:Z:152:ILE:O	12:Z:156:ARG:HG3	2.09	0.52
13:1:113:VAL:HA	13:1:118:VAL:O	2.10	0.52
14:2:146:MET:CE	14:2:150:GLU:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.39	0.51
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.92	0.51
4:D:215:ILE:C	4:D:215:ILE:HD13	2.30	0.51
6:F:137:ILE:HD13	6:F:150:MET:CB	2.41	0.51
10:J:52:THR:CG2	10:J:53:VAL:H	2.23	0.51
10:J:133:TYR:HD1	17:Y:593:HOH:O	1.92	0.51
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.45	0.51
9:W:80:THR:HG1	9:W:109:PHE:HE2	1.58	0.51
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.92	0.51
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.45	0.51
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.10	0.51
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.92	0.51
5:E:137:LEU:CD2	5:E:150:GLU:HG3	2.41	0.51
9:I:104:ILE:HD12	9:I:179:LYS:C	2.30	0.51
11:K:12:ILE:HB	11:K:178:VAL:HB	1.91	0.51
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.08	0.51
12:L:129:ALA:HB1	12:L:166:HIS:CE1	2.45	0.51
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.92	0.51
7:U:172:ILE:HD11	7:U:201:LEU:CD2	2.40	0.51
6:T:12:ASN:HB3	6:T:127:ASN:HA	1.92	0.51
14:2:146:MET:HE3	17:2:774:HOH:O	2.10	0.51
1:A:21:LEU:HB3	1:A:24:ILE:CD1	2.28	0.51
10:J:44:SER:OG	10:J:100:LEU:HB2	2.10	0.51
11:K:4:LEU:CD2	11:K:15:ALA:HB3	2.41	0.51
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.76	0.51
5:S:79:ALA:HB3	5:S:165:ILE:HD12	1.93	0.51
5:S:137:LEU:CD2	5:S:150:GLU:HG3	2.40	0.51
6:T:115:ARG:HA	17:T:573:HOH:O	2.11	0.51
7:U:31:THR:HG21	7:U:135:ILE:HG13	1.93	0.51
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.75	0.51
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.91	0.51
1:A:35:VAL:HG11	1:A:51:GLU:HB3	1.91	0.51
4:D:207:LEU:C	4:D:207:LEU:HD23	2.31	0.51
13:M:130:GLY:O	13:M:134:ALA:HB3	2.10	0.51
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.93	0.51
5:S:46:ALA:O	5:S:139:ILE:HD12	2.11	0.51
6:T:87:HIS:HD2	6:T:132:PHE:CE2	2.29	0.51
9:W:119:ILE:HD12	9:W:119:ILE:N	2.22	0.51
11:Y:174:ASN:HD21	11:Y:189:ASN:HB2	1.75	0.51
12:Z:48:PHE:CZ	12:Z:50:ALA:HB3	2.46	0.51
13:1:21:SER:HB2	17:1:278:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.70	0.51
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.46	0.51
10:J:113:ILE:HA	10:J:118:THR:O	2.11	0.51
13:M:147:THR:OG1	13:M:150:VAL:HG23	2.11	0.51
10:X:166:MET:CE	10:X:168:MET:HB2	2.41	0.51
2:B:101:LYS:HG3	9:I:57:GLU:HB3	1.93	0.51
3:C:195:ARG:HD3	17:C:1019:HOH:O	2.10	0.51
8:H:3:ILE:CG1	8:H:100:ILE:HD12	2.38	0.51
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.76	0.51
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.44	0.51
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.10	0.51
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.93	0.51
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.10	0.51
6:T:13:SER:HB2	7:U:130:ARG:HD3	1.93	0.51
6:T:147:HIS:HD2	17:T:242:HOH:O	1.92	0.51
10:X:16:SER:HB2	17:X:1152:HOH:O	2.10	0.51
1:A:92:SER:OG	1:A:116:VAL:HG22	2.11	0.51
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.76	0.51
3:C:18(A):ASP:OD1	3:C:18(C):LYS:HB2	2.11	0.51
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.26	0.51
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.75	0.51
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.93	0.51
1:O:31:VAL:HG11	1:O:135:SER:HB2	1.91	0.51
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.93	0.51
3:Q:165:ILE:H	3:Q:165:ILE:HD13	1.75	0.51
5:S:185:ASN:OD1	5:S:188:GLU:HG2	2.11	0.51
11:Y:50:ALA:HB2	12:Z:116:VAL:HG23	1.91	0.51
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.41	0.51
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.46	0.51
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.73	0.51
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.31	0.51
13:M:70:ASN:ND2	13:M:70(A):ALA:HA	2.26	0.51
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.11	0.51
3:Q:165:ILE:HD13	3:Q:165:ILE:N	2.25	0.51
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.93	0.51
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.41	0.51
6:T:238:LYS:NZ	6:T:239:GLU:HG3	2.26	0.51
11:Y:4:LEU:CD2	11:Y:15:ALA:HB3	2.41	0.51
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.11	0.51
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.26	0.51
1:A:98:THR:O	1:A:10(A):ILE:HD11	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:ILE:HD12	6:F:40:ILE:N	2.26	0.51
8:H:108:SER:HB3	8:H:180:ILE:HD11	1.92	0.51
10:J:3:ILE:HG22	10:J:100:LEU:CD1	2.41	0.51
12:L:99:THR:C	12:L:100:ILE:HD12	2.30	0.51
12:L:135:MET:CE	9:W:165:ARG:NH2	2.74	0.51
14:N:13:ILE:HD13	14:N:177:VAL:HG22	1.93	0.51
2:P:121:GLN:NE2	17:P:462:HOH:O	2.43	0.51
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.26	0.51
7:U:151:THR:HG22	7:U:157:TYR:CB	2.41	0.51
8:V:32:ALA:HB1	17:V:578:HOH:O	2.11	0.51
8:V:147:THR:HG23	8:V:150:GLU:OE1	2.10	0.51
8:V:159:ILE:HD13	8:V:173:VAL:CG1	2.41	0.51
9:W:93:GLY:N	9:W:94:PRO:CD	2.73	0.51
11:Y:4:LEU:HD11	11:Y:159:ILE:HG12	1.93	0.51
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.64	0.51
13:1:70:ASN:ND2	13:1:70(A):ALA:HA	2.26	0.51
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.11	0.50
5:E:226:GLY:O	5:E:229:VAL:HG22	2.10	0.50
6:F:35:THR:HG23	6:F:36:THR:N	2.26	0.50
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.93	0.50
1:O:190:ILE:HD11	1:O:214:ILE:CG2	2.41	0.50
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.08	0.50
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.11	0.50
5:S:226:GLY:O	5:S:229:VAL:HG22	2.11	0.50
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.92	0.50
6:T:43:ASN:HD22	6:T:43:ASN:N	2.10	0.50
9:W:192:ARG:HD2	17:W:1258:HOH:O	2.10	0.50
10:X:35:ARG:O	10:X:42:LEU:HD12	2.11	0.50
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.11	0.50
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.93	0.50
5:E:185:ASN:OD1	5:E:188:GLU:HG2	2.10	0.50
10:J:168:MET:HE2	10:X:168:MET:CE	2.41	0.50
11:K:12:ILE:HD13	11:K:110:ILE:HD11	1.93	0.50
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.17	0.50
2:P:239:THR:HG22	2:P:239:THR:OXT	2.10	0.50
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.41	0.50
13:1:9:ASP:OD1	13:1:10:ASN:N	2.44	0.50
3:C:163:GLN:HE21	3:C:164:THR:N	2.09	0.50
5:E:36:VAL:HG22	5:E:37:THR:N	2.26	0.50
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.28	0.50
11:K:4:LEU:HD11	11:K:159:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:76:ILE:HG23	12:L:77:ASN:N	2.27	0.50
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.55	0.50
5:S:172:ALA:HB2	5:S:196:ALA:O	2.11	0.50
8:V:50:ALA:HB3	9:W:116:ILE:HD12	1.93	0.50
8:V:95:ILE:O	8:V:97:ALA:N	2.41	0.50
10:X:34:THR:CG2	10:X:176:LYS:NZ	2.75	0.50
12:Z:21:ILE:HB	12:Z:25:SER:O	2.11	0.50
1:A:60:MET:HE1	17:G:600:HOH:O	2.12	0.50
3:C:52:ARG:HH21	3:C:211:GLU:HB3	1.76	0.50
4:D:112:LEU:C	4:D:112:LEU:HD13	2.31	0.50
6:F:119:TYR:O	6:F:122:ALA:HB3	2.11	0.50
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.93	0.50
12:L:152:ILE:O	12:L:156:ARG:HG3	2.11	0.50
5:S:36:VAL:HG22	5:S:37:THR:N	2.26	0.50
8:V:172:ASN:ND2	8:V:193:THR:HA	2.25	0.50
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.75	0.50
5:E:18(C):PHE:HA	5:E:18(F):ILE:CD1	2.40	0.50
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.45	0.50
7:G:47:VAL:HG12	7:G:49:ILE:HD11	1.92	0.50
11:K:45:MET:SD	16:K:2(I):H10:H15	2.51	0.50
7:U:107:MET:HE3	7:U:112:LEU:HB2	1.93	0.50
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.46	0.50
10:X:13:ILE:HG12	10:X:177:ILE:CD1	2.42	0.50
11:Y:4:LEU:HD21	11:Y:15:ALA:HB3	1.94	0.50
13:1:19:LEU:HD12	13:1:28:PHE:O	2.12	0.50
9:I:152:PHE:CB	9:I:177:ILE:HD11	2.38	0.50
10:J:168:MET:CE	10:X:168:MET:HG2	2.42	0.50
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.94	0.50
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.12	0.50
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.41	0.50
9:W:177:ILE:HD12	9:W:177:ILE:N	2.27	0.50
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.75	0.50
10:J:166:MET:CE	10:J:168:MET:HB2	2.42	0.50
14:N:13:ILE:HG13	14:N:151:THR:CG2	2.41	0.50
5:S:73:HIS:HE1	5:S:107:LEU:O	1.94	0.50
7:U:108:PRO:HB3	8:V:72:ARG:NH2	2.25	0.50
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.46	0.50
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.60	0.50
2:B:181:LYS:HD2	2:B:183:ASP:OD1	2.12	0.50
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.42	0.50
9:I:80:THR:HG1	9:I:109:PHE:HE2	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.47	0.50
13:M:-3:VAL:HG12	13:M:49:ILE:HG13	1.93	0.50
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.41	0.50
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.92	0.50
5:S:139:ILE:CD1	5:S:215:VAL:HG12	2.42	0.50
17:V:1181:HOH:O	9:W:150:ASP:HA	2.11	0.50
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.12	0.50
3:C:35:THR:OG1	3:C:66:LYS:NZ	2.45	0.50
3:C:125:GLN:O	3:C:125:GLN:HG3	2.12	0.50
4:D:236:GLU:O	4:D:240:LYS:HG3	2.12	0.50
5:E:73:HIS:HE1	5:E:107:LEU:O	1.95	0.50
5:E:139:ILE:CD1	5:E:215:VAL:HG12	2.42	0.50
7:G:38:LEU:C	7:G:38:LEU:HD12	2.32	0.50
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.32	0.50
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.25	0.50
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.95	0.50
1:A:141:HIS:HA	1:A:146:GLY:O	2.11	0.49
4:D:70:ILE:HD13	4:D:89:ILE:HG23	1.94	0.49
17:E:1080:HOH:O	12:L:64:LYS:HE3	2.11	0.49
9:I:94:PRO:HA	17:I:205:HOH:O	2.12	0.49
14:N:38:HIS:HD2	17:N:1366:HOH:O	1.95	0.49
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.42	0.49
12:Z:76:ILE:HD13	12:Z:109:ALA:HB3	1.93	0.49
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.12	0.49
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.46	0.49
6:T:35:THR:O	6:T:166:GLY:HA3	2.12	0.49
11:Y:7:ARG:HA	11:Y:12:ILE:HD13	1.94	0.49
12:Z:85:HIS:HE1	17:Z:197:HOH:O	1.96	0.49
12:Z:99:THR:CG2	17:Z:231:HOH:O	2.60	0.49
1:A:47:VAL:HG23	1:A:212:LEU:HD21	1.94	0.49
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.21	0.49
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.93	0.49
9:I:101:VAL:O	9:I:110:ILE:HA	2.11	0.49
9:I:113:PHE:CD2	9:I:113:PHE:N	2.81	0.49
11:K:8:PHE:CE2	11:K:13:ILE:HG12	2.47	0.49
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.93	0.49
7:U:141:VAL:HG21	7:U:216:THR:HA	1.94	0.49
11:Y:74:ILE:HD11	11:Y:78:ALA:CB	2.42	0.49
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.93	0.49
2:B:107:ILE:HD12	2:B:112:LEU:CB	2.32	0.49
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:9:ASP:OD1	13:M:10:ASN:N	2.46	0.49
1:O:62:GLU:CD	1:O:62:GLU:H	2.15	0.49
3:Q:221:ILE:N	3:Q:221:ILE:HD12	2.27	0.49
4:R:172:ALA:HB1	4:R:196:ILE:HG21	1.94	0.49
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.23	0.49
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	1.95	0.49
6:F:109:ILE:CG2	6:F:147:HIS:HB2	2.41	0.49
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.95	0.49
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.94	0.49
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.18	0.49
5:S:179:THR:HG22	5:S:18(B):THR:HB	1.95	0.49
11:Y:8:PHE:CE2	11:Y:13:ILE:HG12	2.47	0.49
14:2:159:LEU:O	14:2:163:ILE:HG12	2.13	0.49
4:D:27:SER:O	4:D:31:ILE:HG13	2.13	0.49
5:E:54:ASN:ND2	5:E:56:ASP:O	2.45	0.49
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.40	0.49
7:G:47:VAL:HG12	7:G:49:ILE:HD12	1.94	0.49
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.25	0.49
12:L:17:ASP:HA	12:L:172:GLY:O	2.12	0.49
2:P:27:ALA:O	2:P:30:SER:HB3	2.13	0.49
7:U:38:LEU:C	7:U:38:LEU:HD12	2.33	0.49
7:U:217:LYS:HA	7:U:217:LYS:CE	2.41	0.49
9:W:22:SER:O	9:W:23:GLN:HB2	2.12	0.49
2:B:27:ALA:O	2:B:30:SER:HB3	2.12	0.49
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.94	0.49
7:G:192:PHE:C	7:G:192:PHE:CD1	2.85	0.49
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.95	0.49
10:J:168:MET:HG2	10:X:168:MET:CE	2.41	0.49
10:J:185:ARG:HG2	10:J:185:ARG:NH1	2.27	0.49
11:K:86:LEU:HD13	11:K:86:LEU:C	2.33	0.49
12:L:5:GLY:O	12:L:124:CYS:HA	2.12	0.49
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.12	0.49
10:X:3:ILE:HG22	10:X:100:LEU:CD1	2.43	0.49
14:2:9:LYS:O	14:2:107:LYS:HD3	2.13	0.49
14:2:13:ILE:HG13	14:2:151:THR:CG2	2.42	0.49
3:C:41:LYS:HD3	3:C:161:SER:HA	1.95	0.49
4:D:14:THR:HG22	4:D:15:PHE:N	2.27	0.49
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.76	0.49
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.95	0.49
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.94	0.49
1:O:92:SER:OG	1:O:116:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:NE2	3:Q:164:THR:N	2.58	0.49
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.95	0.49
11:Y:45:MET:SD	16:Y:2(I):H10:H15	2.53	0.49
2:B:107:ILE:HD13	2:B:107:ILE:C	2.33	0.49
5:E:179:THR:HG22	5:E:18(B):THR:HB	1.95	0.49
8:H:172:ASN:ND2	8:H:193:THR:HA	2.25	0.49
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.94	0.49
14:N:146:MET:CE	14:N:150:GLU:HB3	2.42	0.49
2:P:181:LYS:HD2	2:P:183:ASP:OD1	2.13	0.49
9:I:100:VAL:HG13	9:I:125:ILE:HG21	1.95	0.49
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.94	0.49
12:L:35:PHE:CD2	12:L:56:VAL:HG11	2.48	0.49
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.94	0.49
3:Q:137:LEU:HG	3:Q:165:ILE:HD12	1.95	0.49
6:T:74:ILE:HG12	6:T:109:ILE:HD11	1.95	0.49
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.48	0.49
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.94	0.49
13:1:130:GLY:O	13:1:134:ALA:HB3	2.12	0.49
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.27	0.48
12:L:1(I):ASN:HA	17:L:1110:HOH:O	2.12	0.48
2:P:196:THR:O	2:P:200:THR:HG23	2.13	0.48
3:Q:55:THR:HG22	3:Q:56:LEU:CD2	2.40	0.48
3:Q:97:GLN:HA	3:Q:97:GLN:HE21	1.77	0.48
4:R:112:LEU:HD13	4:R:112:LEU:C	2.34	0.48
9:W:113:PHE:CD2	9:W:113:PHE:N	2.81	0.48
10:X:113:ILE:HA	10:X:118:THR:O	2.12	0.48
12:Z:99:THR:HG23	17:Z:231:HOH:O	2.13	0.48
2:B:185:LYS:O	2:B:188:ASP:N	2.44	0.48
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.43	0.48
4:D:175:GLU:OE1	4:D:175:GLU:HA	2.13	0.48
5:E:210:LEU:CD2	5:E:233:ILE:HD11	2.41	0.48
7:U:17:PRO:HD3	17:U:584:HOH:O	2.14	0.48
17:A:242:HOH:O	8:H:69:TYR:HA	2.11	0.48
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.13	0.48
3:C:163:GLN:NE2	3:C:163:GLN:CA	2.75	0.48
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.94	0.48
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.95	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.94	0.48
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.43	0.48
4:R:27:SER:O	4:R:31:ILE:HG13	2.13	0.48
4:R:175:GLU:OE1	4:R:175:GLU:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:221:PHE:CE1	5:S:223:ILE:CD1	2.91	0.48
7:U:12:ILE:O	7:U:14:ILE:HD13	2.13	0.48
9:W:89:GLU:O	9:W:90:ARG:NH1	2.47	0.48
11:Y:20:ALA:HA	16:Y:2(I):H10:O11	2.13	0.48
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.47	0.48
13:1:94:PRO:HA	17:1:219:HOH:O	2.12	0.48
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.44	0.48
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.94	0.48
3:C:52:ARG:HD2	3:C:208:LYS:O	2.13	0.48
9:I:152:PHE:CD1	9:I:177:ILE:HD11	2.48	0.48
11:K:4:LEU:HD21	11:K:15:ALA:HB3	1.94	0.48
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.94	0.48
1:O:27:ALA:O	1:O:31:VAL:HG23	2.13	0.48
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.48	0.48
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.13	0.48
1:A:109:THR:O	1:A:113:VAL:HG23	2.14	0.48
6:F:49:ALA:CB	6:F:212:ILE:CD1	2.91	0.48
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.44	0.48
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.13	0.48
5:S:52:LYS:O	5:S:63:TYR:HD2	1.96	0.48
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.76	0.48
6:T:109:ILE:HG22	6:T:149:TYR:CE2	2.48	0.48
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.96	0.48
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.48	0.48
6:F:35:THR:O	6:F:166:GLY:HA3	2.14	0.48
17:G:248:HOH:O	8:H:82:MET:HA	2.14	0.48
9:I:29:ASN:ND2	9:I:29:ASN:H	2.11	0.48
10:J:24:ILE:HG13	10:J:24:ILE:O	2.13	0.48
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.95	0.48
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.96	0.48
2:B:8:TYR:CE2	7:G:12:ILE:HD12	2.48	0.48
2:B:194:LEU:HD11	2:B:232:ILE:CD1	2.36	0.48
2:B:237:GLY:O	2:B:238:ILE:HD13	2.14	0.48
5:E:46:ALA:O	5:E:139:ILE:HD12	2.13	0.48
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.95	0.48
5:E:79:ALA:HB3	5:E:165:ILE:HD12	1.94	0.48
14:2:174:ARG:HD2	17:2:307:HOH:O	2.14	0.48
1:A:32:LYS:HE2	1:A:32:LYS:CA	2.43	0.48
1:A:32:LYS:HA	1:A:32:LYS:CE	2.43	0.48
3:C:65:SER:HB2	17:C:274:HOH:O	2.13	0.48
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:62:LEU:HD13	13:M:79:ILE:CD1	2.43	0.48
1:O:24:ILE:HD13	1:O:131:PRO:CG	2.44	0.48
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.77	0.48
4:R:50:VAL:HG22	4:R:67:ILE:CD1	2.44	0.48
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.78	0.48
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.95	0.48
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.96	0.48
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.96	0.48
5:E:172:ALA:HB2	5:E:196:ALA:O	2.14	0.48
8:H:32:ALA:HB2	8:H:189:ARG:NH1	2.27	0.48
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.29	0.48
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.47	0.48
1:O:32:LYS:HA	1:O:32:LYS:CE	2.41	0.48
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.96	0.48
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.13	0.48
4:R:18:GLU:OE2	4:R:18:GLU:N	2.45	0.48
4:R:227:GLU:OE2	4:R:227:GLU:N	2.45	0.48
9:W:15:ALA:HB3	9:W:155:ILE:HD11	1.96	0.48
9:W:43:LEU:CG	9:W:45:ILE:HD11	2.42	0.48
11:Y:66:HIS:CG	11:Y:74:ILE:HD13	2.49	0.48
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.13	0.48
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.29	0.48
13:1:112:TYR:O	13:1:119:THR:HA	2.14	0.48
3:C:97:GLN:HA	3:C:97:GLN:HE21	1.77	0.48
3:C:173:ARG:O	3:C:177:GLU:HG3	2.13	0.48
1:O:32:LYS:HE2	1:O:32:LYS:CA	2.42	0.48
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.96	0.48
3:Q:35:THR:OG1	3:Q:66:LYS:NZ	2.45	0.48
8:V:37:ILE:HD11	8:V:43:CYS:CB	2.43	0.48
8:V:116:HIS:HB2	17:V:1297:HOH:O	2.12	0.48
10:X:11:SER:HB3	10:X:179:ASP:HB3	1.96	0.48
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.96	0.48
10:X:37:LEU:HD13	10:X:63:ILE:HD13	1.93	0.48
13:1:190:LEU:N	13:1:190:LEU:HD12	2.29	0.48
14:2:40:LYS:C	14:2:41:ILE:HD12	2.34	0.48
14:2:163:ILE:HD13	14:2:169:SER:CB	2.37	0.48
1:A:62:GLU:CD	1:A:62:GLU:H	2.16	0.47
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.96	0.47
7:G:70:ILE:HD12	7:G:92:ALA:HB3	1.96	0.47
11:K:200:LYS:HG3	11:K:206:PHE:HB2	1.96	0.47
14:N:6:VAL:O	14:N:12:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:132:THR:HA	14:N:135:TYR:HD2	1.79	0.47
13:1:14(C):ARG:HG3	13:1:14(C):ARG:NH1	2.26	0.47
14:2:103:GLY:HA2	14:2:178:LEU:HD23	1.96	0.47
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.95	0.47
1:A:15:PHE:N	2:B:23:GLN:HE22	2.00	0.47
2:B:239:THR:HG22	2:B:239:THR:OXT	2.13	0.47
4:D:70:ILE:HD12	4:D:92:ALA:CB	2.43	0.47
5:E:213:ALA:HB1	5:E:223:ILE:CD1	2.44	0.47
10:J:34:THR:CG2	10:J:176:LYS:NZ	2.77	0.47
1:O:52:LYS:HG3	1:O:211:GLU:HB2	1.96	0.47
3:Q:70:ILE:HD11	3:Q:76:LEU:HD13	1.96	0.47
3:Q:121:GLN:NE2	3:Q:121:GLN:C	2.67	0.47
6:T:127:ASN:HD22	6:T:127:ASN:N	2.11	0.47
13:1:147:THR:OG1	13:1:150:VAL:HG23	2.14	0.47
1:A:69:LEU:HD23	1:A:70:LEU:N	2.29	0.47
2:B:141:TYR:CD1	2:B:141:TYR:C	2.88	0.47
4:D:172:ALA:HB1	4:D:196:ILE:HG21	1.96	0.47
5:E:221:PHE:CE1	5:E:223:ILE:CD1	2.92	0.47
6:F:137:ILE:CD1	6:F:163:ALA:CB	2.92	0.47
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.13	0.47
7:G:8:TYR:O	7:G:12:ILE:CD1	2.60	0.47
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.14	0.47
10:X:77:GLN:C	10:X:77:GLN:NE2	2.68	0.47
6:F:43:ASN:N	6:F:43:ASN:HD22	2.11	0.47
6:F:203:GLU:O	6:F:206:LYS:HD2	2.14	0.47
8:H:5:GLY:HA3	8:H:110:LEU:HD11	1.96	0.47
9:I:43:LEU:HG	9:I:45:ILE:HD11	1.97	0.47
3:Q:163:GLN:HE21	3:Q:164:THR:N	2.13	0.47
4:R:230:ALA:HA	4:R:233:ILE:HD12	1.97	0.47
4:R:243:ALA:O	4:R:244:GLU:CB	2.62	0.47
8:V:32:ALA:HB2	8:V:189:ARG:NH1	2.30	0.47
8:V:170:GLY:O	8:V:171:SER:HB2	2.15	0.47
10:X:58:TYR:HD2	10:X:59:ILE:HD12	1.79	0.47
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.50	0.47
10:J:168:MET:HE1	10:X:167:PRO:CB	2.44	0.47
12:L:1:GLY:HA3	12:L:33:LYS:HZ2	1.80	0.47
14:N:120:HIS:HA	17:N:1107:HOH:O	2.15	0.47
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.15	0.47
6:T:203:GLU:O	6:T:206:LYS:HD2	2.13	0.47
10:X:34:THR:CG2	10:X:176:LYS:HZ2	2.27	0.47
11:Y:78:ALA:O	11:Y:82:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:THR:O	2:B:200:THR:HG23	2.14	0.47
4:D:243:ALA:O	4:D:244:GLU:CB	2.62	0.47
5:E:31:ILE:HD12	5:E:31:ILE:N	2.30	0.47
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.15	0.47
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.80	0.47
12:L:21:ILE:HD12	8:V:167:LEU:HD13	1.96	0.47
14:N:85:GLU:O	14:N:89:GLU:HB2	2.14	0.47
6:T:127:ASN:C	6:T:127:ASN:ND2	2.68	0.47
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.30	0.47
14:2:132:THR:HA	14:2:135:TYR:HD2	1.78	0.47
1:A:31:VAL:HG11	1:A:135:SER:HB2	1.97	0.47
1:A:100:TYR:CA	1:A:10(A):ILE:HD13	2.44	0.47
2:B:44:ASP:OD1	2:B:185:LYS:HE3	2.14	0.47
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.50	0.47
8:H:7:LYS:HG3	8:H:123:TYR:HA	1.96	0.47
9:I:43:LEU:HG	9:I:45:ILE:CD1	2.45	0.47
9:I:10(C):SER:C	9:I:107:LYS:H	2.17	0.47
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.67	0.47
14:N:6:VAL:HG21	14:N:155:ILE:HD11	1.97	0.47
1:O:4:MET:CG	1:O:5:THR:H	2.26	0.47
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.50	0.47
1:O:150:GLN:O	1:O:157:TYR:HA	2.15	0.47
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.44	0.47
5:S:28:LEU:HA	5:S:31:ILE:HD12	1.97	0.47
5:S:54:ASN:ND2	5:S:56:ASP:O	2.48	0.47
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.30	0.47
9:W:10(C):SER:C	9:W:107:LYS:H	2.18	0.47
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.96	0.47
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.45	0.47
12:Z:35:PHE:CD2	12:Z:56:VAL:HG11	2.50	0.47
14:2:19:ARG:HG3	14:2:26:ILE:HG23	1.97	0.47
2:B:15:PHE:H	3:C:23:GLN:NE2	1.95	0.47
2:B:229:ILE:O	2:B:233:LEU:HB2	2.15	0.47
6:F:127:ASN:HD22	6:F:127:ASN:N	2.11	0.47
11:Y:12:ILE:HD12	11:Y:110:ILE:CD1	2.44	0.47
12:Z:21:ILE:HG12	12:Z:22:THR:N	2.30	0.47
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.15	0.47
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.96	0.47
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.96	0.47
12:L:-8:PHE:HB3	13:M:-8:THR:HG23	1.97	0.47
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:100:ILE:HD11	8:V:127:LEU:HG	1.96	0.47
2:B:122:GLY:C	2:B:124:THR:H	2.18	0.47
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.96	0.47
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.77	0.47
10:J:69:ARG:HD2	17:J:514:HOH:O	2.15	0.47
11:K:20:ALA:HA	16:K:2(I):H10:O11	2.15	0.47
12:L:21:ILE:HB	12:L:25:SER:O	2.15	0.47
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.74	0.47
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.14	0.47
5:S:67:ILE:HD13	5:S:77:SER:CB	2.44	0.47
9:W:-8:SER:O	9:W:-6:PRO:HD3	2.15	0.47
12:Z:85:HIS:CE1	17:Z:197:HOH:O	2.68	0.47
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.53	0.46
3:C:159:SER:O	4:D:59:LEU:HD22	2.15	0.46
12:L:185:ARG:HB3	12:L:185:ARG:NH1	2.29	0.46
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.53	0.46
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.31	0.46
6:T:142:ASP:O	6:T:144:ASN:N	2.48	0.46
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.14	0.46
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.98	0.46
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.96	0.46
6:F:192:GLN:O	6:F:196:ILE:HG12	2.15	0.46
7:G:107:MET:HE3	7:G:112:LEU:HB2	1.98	0.46
7:G:234:VAL:O	7:G:237:ALA:HB3	2.15	0.46
2:P:229:ILE:O	2:P:233:LEU:HB2	2.15	0.46
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.50	0.46
12:Z:8:GLY:HA3	12:Z:11:PHE:CZ	2.51	0.46
12:Z:134:ILE:O	12:Z:137:PHE:HB3	2.15	0.46
1:A:27:ALA:O	1:A:31:VAL:HG23	2.15	0.46
3:C:158:SER:CB	4:D:59:LEU:HD21	2.45	0.46
4:D:227:GLU:OE2	4:D:227:GLU:N	2.46	0.46
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.30	0.46
7:G:118:ASN:O	7:G:122:ILE:HD13	2.15	0.46
7:G:141:VAL:HG21	7:G:216:THR:HA	1.96	0.46
13:M:3:VAL:O	13:M:126:ALA:HA	2.15	0.46
13:M:91:ARG:HG3	13:M:92:SER:N	2.29	0.46
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.96	0.46
5:S:67:ILE:HG21	5:S:213:ALA:HB2	1.97	0.46
6:T:127:ASN:HD22	6:T:127:ASN:C	2.19	0.46
7:U:225:SER:O	7:U:229:ILE:HG13	2.15	0.46
10:X:45:PHE:HB3	10:X:99:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:3:VAL:O	13:1:126:ALA:HA	2.15	0.46
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.51	0.46
12:L:163:THR:HG23	17:L:1264:HOH:O	2.15	0.46
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.31	0.46
5:S:15:PHE:N	6:T:23:GLN:HE22	2.04	0.46
5:S:69:LYS:HB3	17:S:528:HOH:O	2.16	0.46
7:U:87:ASN:HD22	7:U:88:ALA:N	2.14	0.46
1:A:24:ILE:H	1:A:24:ILE:HD12	1.81	0.46
3:C:57:LYS:HD2	3:C:58:LEU:N	2.30	0.46
3:C:167:ARG:O	3:C:168:ASN:HB2	2.16	0.46
5:E:52:LYS:O	5:E:63:TYR:HD2	1.98	0.46
7:G:31:THR:HG21	7:G:135:ILE:HG12	1.96	0.46
11:K:46:ALA:HB3	11:K:98:GLY:O	2.15	0.46
2:P:5:SER:O	2:P:7:ARG:N	2.49	0.46
2:P:141:TYR:CD1	2:P:141:TYR:C	2.88	0.46
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.45	0.46
4:R:170:GLU:OE1	4:R:170:GLU:N	2.49	0.46
7:U:70:ILE:HD12	7:U:74:ILE:CG2	2.43	0.46
8:V:7:LYS:HG3	8:V:123:TYR:HA	1.97	0.46
10:X:185:ARG:HG2	10:X:185:ARG:NH1	2.29	0.46
14:2:3:ILE:HD13	14:2:3:ILE:N	2.30	0.46
1:A:13:THR:CG2	1:A:24:ILE:CD1	2.94	0.46
2:B:41:MET:HE3	17:B:240:HOH:O	2.15	0.46
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.96	0.46
4:D:170:GLU:N	4:D:170:GLU:OE1	2.49	0.46
5:E:69:LYS:HB3	17:E:684:HOH:O	2.14	0.46
9:I:114:ASP:OD2	9:I:116:ILE:CD1	2.61	0.46
10:J:11:SER:HB3	10:J:179:ASP:HB3	1.96	0.46
13:M:184:LEU:HD23	13:M:185:THR:N	2.30	0.46
2:P:122:GLY:C	2:P:124:THR:H	2.19	0.46
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.50	0.46
4:R:14:THR:HG22	4:R:15:PHE:N	2.30	0.46
4:R:79:SER:HB3	4:R:165:ILE:HD12	1.96	0.46
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.81	0.46
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.50	0.46
11:Y:79:ALA:HA	11:Y:82:ILE:HD12	1.98	0.46
12:Z:8:GLY:O	12:Z:108:GLY:HA3	2.15	0.46
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.18	0.46
5:E:220:PRO:O	5:E:221:PHE:C	2.54	0.46
6:F:229:LEU:O	6:F:233:ILE:HD12	2.16	0.46
1:O:198:LYS:HE3	1:O:236:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.46	0.46
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.50	0.46
6:T:109:ILE:CG2	6:T:147:HIS:HB2	2.42	0.46
7:U:25:GLU:O	7:U:28:PHE:HB2	2.16	0.46
1:A:130:ARG:HH11	1:A:130:ARG:HG3	1.81	0.46
3:C:134:VAL:HG12	3:C:135:SER:N	2.30	0.46
4:D:68:VAL:HG21	4:D:89:ILE:HD13	1.97	0.46
7:G:49:ILE:CD1	7:G:193:ALA:CB	2.90	0.46
8:H:45:GLY:HA2	8:H:99:LEU:HD23	1.97	0.46
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.98	0.46
3:Q:215:VAL:HG13	3:Q:215:VAL:O	2.16	0.46
5:S:213:ALA:HB1	5:S:223:ILE:CD1	2.46	0.46
8:V:45:GLY:HA2	8:V:99:LEU:HD23	1.98	0.46
1:A:4:MET:CG	1:A:5:THR:H	2.25	0.46
2:B:100:LEU:HG	9:I:60:ARG:NH2	2.31	0.46
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.50	0.46
3:C:212:ILE:HD13	3:C:229:ILE:HG23	1.98	0.46
5:E:139:ILE:HD12	5:E:215:VAL:HG12	1.98	0.46
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.14	0.46
11:K:126:CYS:HB2	11:K:135:TYR:CZ	2.51	0.46
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.51	0.46
3:Q:93:ARG:HD2	17:Q:314:HOH:O	2.16	0.46
3:Q:159:SER:O	4:R:59:LEU:HD22	2.16	0.46
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.51	0.46
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.14	0.46
6:F:137:ILE:CD1	6:F:163:ALA:HB3	2.45	0.46
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.97	0.46
12:L:134:ILE:O	12:L:137:PHE:HB3	2.16	0.46
14:N:147:SER:OG	14:N:150:GLU:HG3	2.16	0.46
4:R:196:ILE:H	4:R:196:ILE:HD12	1.81	0.46
6:T:192:GLN:O	6:T:196:ILE:HG12	2.16	0.46
8:H:159:ILE:HD13	8:H:173:VAL:CG1	2.47	0.45
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.29	0.45
12:L:82:ASN:C	12:L:82:ASN:HD22	2.20	0.45
13:M:-6:GLN:O	13:M:-6:GLN:HG3	2.15	0.45
13:M:112:TYR:C	13:M:112:TYR:CD2	2.89	0.45
13:M:147:THR:HB	13:M:149:GLN:NE2	2.31	0.45
5:S:150:GLU:O	5:S:157:VAL:HA	2.16	0.45
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.79	0.45
7:U:18(M):SER:HB2	7:U:187:GLU:OE2	2.16	0.45
8:V:5:GLY:HA3	8:V:110:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:SER:HA	3:C:172:VAL:CG1	2.47	0.45
3:C:232:TYR:O	3:C:236:ILE:HG13	2.16	0.45
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.31	0.45
5:E:43:ASN:HB2	5:E:183:ASP:OD1	2.16	0.45
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.31	0.45
11:K:7:ARG:CG	11:K:108:PRO:HB2	2.40	0.45
11:K:12:ILE:HD13	11:K:110:ILE:CD1	2.45	0.45
12:L:140:ASN:O	12:L:144:PHE:HA	2.16	0.45
8:V:15:ALA:HB1	8:V:159:ILE:HD13	1.98	0.45
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.98	0.45
1:A:7:ARG:NH1	5:E:127:TYR:HD2	2.14	0.45
1:A:179:ARG:HH11	1:A:179:ARG:CB	2.22	0.45
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.98	0.45
9:I:89:GLU:O	9:I:90:ARG:NH1	2.48	0.45
9:I:192:ARG:HD3	17:I:1187:HOH:O	2.15	0.45
11:K:172:SER:CA	11:K:192:VAL:HG23	2.47	0.45
13:M:29:ASN:N	17:M:802:HOH:O	2.50	0.45
1:O:130:ARG:HH11	1:O:130:ARG:HG3	1.82	0.45
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.32	0.45
5:S:95:GLN:HG3	5:S:115:LEU:HD13	1.97	0.45
5:S:139:ILE:HG22	5:S:148:LEU:HD13	1.96	0.45
7:U:70:ILE:HA	7:U:93:LYS:HG2	1.99	0.45
10:X:52:THR:HG22	10:X:53:VAL:H	1.81	0.45
10:X:189:ASP:HA	10:X:191:GLN:OE1	2.16	0.45
14:2:85:GLU:O	14:2:89:GLU:HB2	2.15	0.45
1:A:52:LYS:HG3	1:A:211:GLU:HB2	1.96	0.45
2:B:107:ILE:CD1	2:B:112:LEU:H	2.28	0.45
4:D:12:VAL:HG23	4:D:12(A):GLY:HA2	1.98	0.45
5:E:15:PHE:N	6:F:23:GLN:HE22	2.05	0.45
10:J:45:PHE:HB3	10:J:99:VAL:HG12	1.97	0.45
10:J:52:THR:HG22	10:J:53:VAL:H	1.81	0.45
11:K:35:ILE:HD11	11:K:45:MET:HB2	1.99	0.45
2:P:228:GLU:O	2:P:232:ILE:HG22	2.17	0.45
2:P:235:LYS:C	2:P:237:GLY:N	2.69	0.45
3:Q:167:ARG:O	3:Q:168:ASN:HB2	2.16	0.45
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.46	0.45
5:S:38:VAL:HG12	5:S:39:GLY:N	2.31	0.45
7:U:18(D):ILE:O	7:U:18(G):GLU:N	2.49	0.45
7:U:234:VAL:O	7:U:237:ALA:HB3	2.16	0.45
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.17	0.45
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:167:LEU:HB3	12:Z:167:ILE:HD13	1.99	0.45
1:O:31:VAL:HG13	1:O:79:SER:O	2.16	0.45
2:P:138:TYR:HB2	2:P:149:TYR:HB2	1.98	0.45
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.46	0.45
3:Q:15:PHE:CD1	3:Q:21:ILE:CD1	2.99	0.45
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.28	0.45
7:U:139:VAL:HA	7:U:147:SER:O	2.16	0.45
7:U:197:MET:HG2	7:U:205:PHE:CE1	2.51	0.45
12:Z:6:ILE:HG12	12:Z:124:CYS:CB	2.47	0.45
12:Z:33:LYS:NZ	17:Z:754:HOH:O	2.49	0.45
12:Z:14(I):THR:O	12:Z:1(I):ASN:HB3	2.16	0.45
3:C:79:SER:HB2	3:C:165:ILE:HD12	1.98	0.45
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.51	0.45
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.99	0.45
8:H:36:ARG:HG3	8:H:38:SER:O	2.17	0.45
8:H:49:ALA:HB1	9:I:118:CYS:SG	2.56	0.45
12:L:11:PHE:CE1	12:L:148:VAL:HA	2.51	0.45
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.98	0.45
6:T:24:VAL:O	6:T:27:ALA:HB3	2.17	0.45
7:U:46:THR:HG21	7:U:139:VAL:HB	1.99	0.45
9:W:43:LEU:HG	9:W:45:ILE:CD1	2.47	0.45
9:W:80:THR:HG23	9:W:113:PHE:CE1	2.52	0.45
11:Y:7:ARG:CG	11:Y:108:PRO:HB2	2.38	0.45
13:1:178:ILE:HD12	13:1:178:ILE:N	2.32	0.45
14:2:132:THR:HA	14:2:135:TYR:CD2	2.52	0.45
1:A:197:LEU:HD21	1:A:210:ILE:HD12	1.99	0.45
2:B:21:LEU:O	2:B:25:GLU:HG2	2.16	0.45
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.64	0.45
11:K:6:PHE:HA	11:K:123:ASP:O	2.16	0.45
11:K:64:ARG:HD2	17:K:959:HOH:O	2.17	0.45
11:Y:7:ARG:CG	11:Y:12:ILE:HD11	2.39	0.45
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.81	0.45
14:2:107:LYS:HG2	14:2:108:GLY:H	1.82	0.45
14:2:18(A):ILE:HD12	14:2:18(C):TYR:CE2	2.52	0.45
1:A:38:LEU:C	1:A:38:LEU:HD12	2.36	0.45
2:B:97:GLN:NE2	17:B:246:HOH:O	2.49	0.45
2:B:171:ALA:O	2:B:175:LEU:HG	2.17	0.45
12:L:14(I):THR:O	12:L:1(I):ASN:HB3	2.16	0.45
1:O:212:LEU:HD23	1:O:212:LEU:C	2.37	0.45
3:Q:190:VAL:HG13	3:Q:212:ILE:HG21	1.99	0.45
11:Y:90:TYR:O	11:Y:91:LYS:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:157:ASN:ND2	17:1:905:HOH:O	2.45	0.45
4:D:50:VAL:HG22	4:D:67:ILE:CD1	2.44	0.45
6:F:109:ILE:HG22	6:F:149:TYR:CE2	2.52	0.45
6:F:142:ASP:O	6:F:144:ASN:N	2.50	0.45
7:G:25:GLU:O	7:G:28:PHE:HB2	2.17	0.45
13:M:19:LEU:HD12	13:M:28:PHE:O	2.17	0.45
14:N:103:GLY:HA2	14:N:178:LEU:HD23	1.99	0.45
1:O:69:LEU:HD23	1:O:70:LEU:N	2.32	0.45
10:X:185:ARG:NH1	17:X:730:HOH:O	2.50	0.45
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.52	0.45
2:B:235:LYS:C	2:B:237:GLY:N	2.70	0.45
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.81	0.45
5:E:38:VAL:HG12	5:E:39:GLY:N	2.32	0.45
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.82	0.45
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.16	0.45
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.52	0.45
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.99	0.45
2:P:111:ILE:HD11	10:X:70:GLU:HG2	1.99	0.45
2:P:224:PHE:HD2	2:P:224:PHE:H	1.65	0.45
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.17	0.45
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.52	0.45
4:R:197:LEU:O	4:R:201:MET:HG3	2.17	0.45
6:T:45:GLY:CA	6:T:215:CYS:O	2.65	0.45
1:A:212:LEU:HD23	1:A:212:LEU:C	2.37	0.44
1:A:224:LEU:HB2	1:A:229:ILE:HD11	1.98	0.44
3:C:55:THR:HG22	3:C:56:LEU:CD2	2.42	0.44
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.99	0.44
5:E:198:SER:HA	5:E:201:LEU:CG	2.47	0.44
6:F:49:ALA:HA	6:F:211:GLU:O	2.17	0.44
6:F:18(C):HIS:CE1	17:F:1343:HOH:O	2.70	0.44
7:G:18(M):SER:HB2	7:G:187:GLU:OE2	2.17	0.44
9:I:80:THR:HG23	9:I:113:PHE:CE1	2.52	0.44
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.99	0.44
11:K:109:THR:C	11:K:110:ILE:HD13	2.37	0.44
14:N:163:ILE:CG2	14:N:170:GLY:HA2	2.47	0.44
1:O:40:ILE:HD12	1:O:193:ALA:HB2	1.98	0.44
1:O:86:ARG:NE	7:U:118:ASN:HD21	2.13	0.44
2:P:44:ASP:OD1	2:P:185:LYS:HE3	2.16	0.44
3:Q:220:ASP:C	3:Q:221:ILE:HD12	2.37	0.44
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.57	0.44
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:29:ASN:C	9:W:29:ASN:HD22	2.21	0.44
11:Y:14:VAL:HB	11:Y:176:TYR:HB2	1.98	0.44
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.17	0.44
13:1:112:TYR:C	13:1:112:TYR:CD2	2.90	0.44
13:1:147:THR:HB	13:1:149:GLN:NE2	2.31	0.44
3:C:121:GLN:NE2	3:C:121:GLN:C	2.71	0.44
5:E:17:PRO:HA	6:F:26:TYR:CD2	2.52	0.44
6:F:45:GLY:CA	6:F:215:CYS:O	2.65	0.44
8:H:9:ASN:OD1	8:H:10:ASN:N	2.50	0.44
10:J:189:ASP:HA	10:J:191:GLN:OE1	2.18	0.44
12:L:35:PHE:HA	17:L:1224:HOH:O	2.17	0.44
3:Q:125:GLN:HB2	4:R:130:ARG:HG2	1.99	0.44
8:V:37:ILE:N	8:V:37:ILE:HD12	2.31	0.44
10:X:65:LEU:HD21	10:X:69:ARG:HH22	1.83	0.44
2:B:181:LYS:O	2:B:184:MET:HG3	2.18	0.44
5:E:91:TYR:CD1	5:E:119:LYS:HD2	2.52	0.44
6:F:127:ASN:HD22	6:F:127:ASN:C	2.20	0.44
6:F:127:ASN:C	6:F:127:ASN:ND2	2.69	0.44
7:G:8:TYR:C	7:G:10:ARG:N	2.70	0.44
9:I:29:ASN:C	9:I:29:ASN:HD22	2.20	0.44
10:J:35:ARG:O	10:J:42:LEU:HD12	2.17	0.44
10:J:66:TYR:CE2	10:J:74:LEU:HG	2.52	0.44
1:O:109:THR:O	1:O:113:VAL:HG23	2.17	0.44
5:S:18(C):PHE:CD1	5:S:18(D):ILE:N	2.85	0.44
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.27	0.44
8:V:9:ASN:OD1	8:V:10:ASN:N	2.51	0.44
10:X:37:LEU:HD13	10:X:63:ILE:HD11	1.98	0.44
1:A:67:VAL:HG11	1:A:213:ALA:HB3	1.99	0.44
2:B:63:THR:O	2:B:63:THR:HG22	2.18	0.44
7:G:131:PRO:HB3	17:G:243:HOH:O	2.16	0.44
8:H:34:LEU:HA	8:H:43:CYS:O	2.18	0.44
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.52	0.44
13:M:35:ILE:N	13:M:35:ILE:HD12	2.33	0.44
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.14	0.44
2:P:63:THR:O	2:P:63:THR:HG22	2.17	0.44
3:Q:99:HIS:CG	3:Q:107:VAL:HG12	2.52	0.44
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.98	0.44
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.18	0.44
8:V:3:ILE:CD1	8:V:46:ALA:HB2	2.48	0.44
8:V:36:ARG:HG3	8:V:38:SER:O	2.17	0.44
8:V:63:ILE:CG2	8:V:74:PRO:HB3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.00	0.44
12:Z:113:PHE:N	12:Z:113:PHE:CD1	2.86	0.44
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.52	0.44
6:F:24:VAL:O	6:F:27:ALA:HB3	2.17	0.44
11:K:119:ARG:HG2	17:K:1232:HOH:O	2.18	0.44
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.59	0.44
7:U:13:THR:HB	7:U:124:THR:O	2.18	0.44
12:Z:11:PHE:CE1	12:Z:148:VAL:HA	2.52	0.44
12:Z:185:ARG:HB3	12:Z:185:ARG:NH1	2.32	0.44
13:1:35:ILE:HD11	13:1:56:GLU:HG3	1.98	0.44
13:1:45:ILE:HG12	13:1:99:ILE:HG12	1.98	0.44
2:B:107:ILE:CD1	2:B:112:LEU:N	2.78	0.44
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.52	0.44
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.52	0.44
4:D:196:ILE:HD12	4:D:196:ILE:H	1.83	0.44
5:E:31:ILE:HD12	5:E:31:ILE:H	1.82	0.44
8:H:15:ALA:HB1	8:H:159:ILE:HD13	1.97	0.44
10:J:35:ARG:HD3	10:J:35:ARG:HA	1.76	0.44
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.53	0.44
14:N:132:THR:HA	14:N:135:TYR:CD2	2.52	0.44
2:P:171:ALA:O	2:P:175:LEU:HG	2.18	0.44
2:P:232:ILE:O	2:P:232:ILE:HG12	2.18	0.44
3:Q:19:GLY:O	4:R:30:ALA:HB2	2.17	0.44
4:R:42:THR:C	4:R:44:GLU:H	2.21	0.44
5:S:43:ASN:HB2	5:S:183:ASP:OD1	2.17	0.44
5:S:116:LEU:HD23	5:S:116:LEU:HA	1.86	0.44
8:V:34:LEU:HA	8:V:43:CYS:O	2.17	0.44
13:1:147:THR:HB	13:1:149:GLN:HE22	1.83	0.44
14:2:37:VAL:HG22	14:2:41:ILE:HG22	1.99	0.44
14:2:147:SER:OG	14:2:150:GLU:HG3	2.17	0.44
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.32	0.44
13:M:184:LEU:HD23	13:M:184:LEU:C	2.37	0.44
1:O:29:THR:O	1:O:33:GLN:HG2	2.17	0.44
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.16	0.44
6:T:18:ASP:OD1	6:T:20:ARG:HD3	2.17	0.44
6:T:172:ALA:C	6:T:176:LEU:HD23	2.38	0.44
10:X:70:GLU:O	10:X:71:ASP:C	2.56	0.44
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.17	0.44
14:2:107:LYS:HG2	14:2:108:GLY:N	2.33	0.44
5:E:160:LEU:HD13	5:E:163:THR:HB	1.99	0.44
9:I:35:PHE:CD1	9:I:45:ILE:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:160:ARG:HB2	13:M:192:VAL:HG13	2.00	0.44
1:O:47:VAL:CG2	1:O:212:LEU:HD21	2.48	0.44
1:O:190:ILE:HD11	1:O:214:ILE:HG22	1.99	0.44
5:S:220:PRO:O	5:S:221:PHE:C	2.55	0.44
7:U:35:ILE:HD11	7:U:53:LYS:CG	2.46	0.44
9:W:155:ILE:HD13	9:W:155:ILE:C	2.38	0.44
10:X:19:ALA:HB2	10:X:171:LYS:HG2	1.98	0.44
11:Y:126:CYS:HB2	11:Y:135:TYR:CZ	2.53	0.44
11:Y:172:SER:CA	11:Y:192:VAL:HG23	2.46	0.44
7:G:198:ILE:O	7:G:202:GLY:N	2.50	0.44
13:M:74:LEU:HB3	13:M:79:ILE:HD11	2.00	0.44
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.52	0.44
1:O:24:ILE:HD13	1:O:131:PRO:HG2	1.99	0.44
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.31	0.44
2:P:21:LEU:O	2:P:25:GLU:HG2	2.17	0.44
10:X:93:ARG:CZ	11:Y:91:LYS:HD3	2.48	0.44
13:1:184:LEU:C	13:1:184:LEU:HD23	2.38	0.44
14:2:6:VAL:O	14:2:12:VAL:HG23	2.17	0.44
1:A:150:GLN:O	1:A:157:TYR:HA	2.17	0.43
4:D:18:GLU:OE2	4:D:18:GLU:N	2.50	0.43
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.52	0.43
8:H:1:THR:CG2	8:H:2:THR:N	2.80	0.43
1:O:17:PRO:HG3	2:P:26:TYR:CZ	2.53	0.43
3:Q:123:TYR:CD1	3:Q:132:PHE:HE1	2.36	0.43
4:R:70:ILE:HB	4:R:74:ILE:HG22	2.00	0.43
10:X:152:LEU:HD21	10:X:177:ILE:HD11	2.00	0.43
11:Y:12:ILE:HG23	11:Y:110:ILE:HD11	2.00	0.43
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.53	0.43
2:B:5:SER:O	2:B:7:ARG:N	2.50	0.43
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.33	0.43
5:E:4:PHE:O	5:E:6:ASN:N	2.51	0.43
10:J:70:GLU:O	10:J:71:ASP:C	2.56	0.43
12:L:21:ILE:HD11	12:L:168:GLN:NE2	2.33	0.43
13:M:13:ILE:HB	13:M:155:ILE:CD1	2.48	0.43
1:O:62:GLU:O	1:O:64:LEU:N	2.47	0.43
2:P:39:GLY:O	2:P:162:ALA:HA	2.18	0.43
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.14	0.43
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.51	0.43
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.33	0.43
6:T:49:ALA:HA	6:T:211:GLU:O	2.18	0.43
9:W:61:TYR:CD1	9:W:61:TYR:C	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HG22	1:A:21:LEU:HD22	2.01	0.43
3:C:70:ILE:HD11	3:C:76:LEU:HD13	1.99	0.43
5:E:95:GLN:HG3	5:E:115:LEU:HD13	2.00	0.43
5:E:230:ALA:C	5:E:232:TYR:H	2.21	0.43
10:J:17:SER:HB2	10:J:170:PHE:HB2	2.00	0.43
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.47	0.43
12:L:113:PHE:N	12:L:113:PHE:CD1	2.86	0.43
13:M:112:TYR:O	13:M:119:THR:HA	2.18	0.43
8:V:18:THR:HB	8:V:30:ASN:HA	2.00	0.43
14:2:126:ILE:N	14:2:126:ILE:CD1	2.81	0.43
2:B:231:ASP:O	2:B:235:LYS:HG2	2.19	0.43
4:D:24:VAL:O	4:D:28:LEU:HD13	2.18	0.43
6:F:39:GLY:HA3	6:F:137:ILE:HG21	2.00	0.43
7:G:70:ILE:HA	7:G:93:LYS:HG2	2.01	0.43
10:J:34:THR:CG2	10:J:176:LYS:HZ2	2.31	0.43
12:L:8:GLY:O	12:L:108:GLY:HA3	2.17	0.43
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.33	0.43
1:O:177:GLU:HG2	2:P:58:LEU:HD22	2.01	0.43
5:S:134:VAL:O	5:S:153:PRO:HG3	2.19	0.43
5:S:216:GLY:O	5:S:217:LYS:C	2.57	0.43
8:V:192:LEU:HA	8:V:192:LEU:HD23	1.77	0.43
10:X:166:MET:HA	10:X:167:PRO:HD3	1.72	0.43
14:2:38:HIS:HB3	14:2:41:ILE:HB	2.01	0.43
2:B:10:SER:HB2	17:B:248:HOH:O	2.18	0.43
2:B:17:PRO:HA	3:C:26:TYR:CZ	2.54	0.43
2:B:39:GLY:O	2:B:162:ALA:HA	2.19	0.43
4:D:215:ILE:HD13	4:D:215:ILE:O	2.18	0.43
5:E:18(C):PHE:CD1	5:E:18(D):ILE:N	2.86	0.43
6:F:157:TYR:CD1	6:F:157:TYR:C	2.91	0.43
11:K:13:ILE:HD12	11:K:152:LEU:HD23	2.01	0.43
11:K:14:VAL:HB	11:K:176:TYR:HB2	2.00	0.43
11:K:19:ARG:HG2	11:K:21:THR:HG23	2.01	0.43
12:L:52:GLY:O	12:L:56:VAL:HG23	2.18	0.43
13:M:190:LEU:HD12	13:M:190:LEU:N	2.33	0.43
1:O:67:VAL:HG11	1:O:213:ALA:HB3	1.99	0.43
2:P:97:GLN:HG2	17:P:297:HOH:O	2.19	0.43
2:P:120:LYS:HZ1	2:P:136:PHE:HD1	1.67	0.43
2:P:150:THR:O	2:P:157:TYR:HA	2.18	0.43
2:P:21(A):LYS:HG3	2:P:219:GLU:O	2.18	0.43
2:P:234:VAL:HA	2:P:239:THR:HA	2.00	0.43
8:V:49:ALA:HB1	9:W:118:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HD21	1:A:214:ILE:HD12	2.01	0.43
2:B:194:LEU:O	2:B:198:SER:HB2	2.19	0.43
5:E:207:LEU:O	5:E:233:ILE:HD12	2.18	0.43
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.49	0.43
7:G:139:VAL:HA	7:G:147:SER:O	2.18	0.43
2:P:150:THR:HG22	2:P:160:TRP:HE1	1.84	0.43
5:S:4:PHE:O	5:S:6:ASN:N	2.52	0.43
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.18	0.43
8:V:1:THR:CG2	8:V:2:THR:N	2.82	0.43
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.19	0.43
2:B:235:LYS:HD3	2:B:235:LYS:N	2.34	0.43
3:C:123:TYR:CD1	3:C:132:PHE:HE1	2.37	0.43
5:E:116:LEU:HD23	5:E:116:LEU:HA	1.88	0.43
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.81	0.43
7:G:47:VAL:CG1	7:G:49:ILE:HD11	2.48	0.43
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.48	0.43
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.33	0.43
4:R:192:LEU:O	4:R:196:ILE:HD13	2.19	0.43
4:R:196:ILE:HD12	4:R:196:ILE:N	2.34	0.43
5:S:67:ILE:HD11	5:S:77:SER:HB3	1.98	0.43
6:T:21:ASN:C	6:T:21:ASN:OD1	2.57	0.43
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	2.00	0.43
11:Y:74:ILE:HG13	11:Y:75:SER:N	2.33	0.43
1:A:175:PHE:O	1:A:179:ARG:HG2	2.19	0.43
2:B:150:THR:O	2:B:157:TYR:HA	2.19	0.43
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.54	0.43
5:E:146:ALA:N	17:E:1070:HOH:O	2.51	0.43
7:G:220:LYS:HG2	7:G:221:PHE:N	2.34	0.43
8:H:63:ILE:CG2	8:H:74:PRO:HB3	2.49	0.43
10:J:93:ARG:CZ	11:K:91:LYS:HD3	2.49	0.43
11:K:207:ASN:ND2	10:X:144:PRO:HD3	2.34	0.43
12:L:3:ILE:CD1	12:L:3:ILE:N	2.80	0.43
12:L:185:ARG:NH1	17:L:1161:HOH:O	2.38	0.43
13:M:17:ASP:HA	13:M:173:PHE:HB3	2.01	0.43
13:M:150:VAL:HG21	17:M:1069:HOH:O	2.18	0.43
1:O:184:LEU:HB2	17:O:486:HOH:O	2.19	0.43
5:S:83:PRO:O	5:S:86:ARG:HB3	2.18	0.43
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.54	0.43
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.34	0.43
7:U:67:ILE:HD12	7:U:211:GLU:CG	2.44	0.43
8:V:100:ILE:CD1	8:V:112:SER:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.18	0.43
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.53	0.43
14:2:8:PHE:HE1	14:2:10:ASP:HB2	1.84	0.43
1:A:188:ASP:O	1:A:192:ILE:HG12	2.18	0.43
2:B:222:LYS:NZ	2:B:228:GLU:OE2	2.47	0.43
2:B:228:GLU:O	2:B:232:ILE:HG22	2.19	0.43
3:C:55:THR:C	3:C:56:LEU:HD22	2.40	0.43
3:C:212:ILE:HD12	3:C:212:ILE:N	2.33	0.43
3:C:215:VAL:O	3:C:215:VAL:HG13	2.19	0.43
6:F:91:ARG:O	6:F:95:GLU:HB2	2.19	0.43
10:J:18:LYS:CD	10:J:174:ILE:HG13	2.45	0.43
12:L:148:VAL:O	12:L:152:ILE:HG13	2.19	0.43
1:O:92:SER:O	1:O:95:VAL:HG12	2.18	0.43
3:Q:156:ILE:HD12	3:Q:156:ILE:N	2.33	0.43
7:U:74:ILE:HD12	7:U:109:CYS:HA	2.00	0.43
9:W:174:VAL:HG21	9:W:186:LYS:HE3	2.01	0.43
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.33	0.43
2:B:224:PHE:HD2	2:B:224:PHE:H	1.66	0.43
3:C:160:TRP:NE1	4:D:59:LEU:HD23	2.34	0.43
6:F:130:ARG:HG2	6:F:130:ARG:HH11	1.84	0.43
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.49	0.43
9:I:6:MET:HE3	9:I:155:ILE:HA	2.01	0.43
11:K:9:GLN:CD	11:K:10:GLY:N	2.71	0.43
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.87	0.43
11:K:131:GLN:HG3	11:K:132:THR:N	2.34	0.43
11:K:174:ASN:ND2	11:K:189:ASN:HB2	2.34	0.43
14:N:14:LEU:N	14:N:14:LEU:HD12	2.33	0.43
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.17	0.43
6:T:91:ARG:O	6:T:95:GLU:HB2	2.19	0.43
6:T:172:ALA:O	6:T:173:LYS:C	2.57	0.43
11:Y:19:ARG:HG2	11:Y:21:THR:HG23	2.01	0.43
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	2.01	0.43
2:B:234:VAL:HA	2:B:239:THR:HA	2.00	0.42
3:C:227:GLU:OE1	3:C:227:GLU:N	2.49	0.42
6:F:14:VAL:HG12	6:F:15:PHE:N	2.33	0.42
6:F:137:ILE:HD11	6:F:163:ALA:CB	2.47	0.42
8:H:101:VAL:HG12	8:H:113:ILE:CD1	2.48	0.42
9:I:3:VAL:HG22	9:I:16:CYS:HB3	2.01	0.42
11:K:5:ALA:HA	11:K:13:ILE:O	2.19	0.42
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.33	0.42
12:L:160:THR:O	12:L:164:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:147:THR:HB	13:M:149:GLN:HE22	1.84	0.42
2:P:113:VAL:HG22	2:P:138:TYR:CG	2.54	0.42
4:R:23:GLN:HB3	4:R:131:PRO:HG2	2.01	0.42
6:T:103:TYR:O	6:T:104:LYS:HB3	2.19	0.42
8:V:156:SER:HA	8:V:159:ILE:HD12	2.00	0.42
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	2.00	0.42
3:C:190:VAL:HG13	3:C:212:ILE:HG21	2.01	0.42
3:C:225:SER:O	3:C:226:SER:C	2.58	0.42
6:F:52:LYS:HB2	6:F:209:GLU:O	2.19	0.42
8:H:56:THR:HG22	8:H:57:GLN:N	2.33	0.42
10:J:190:PHE:C	10:J:192:ALA:H	2.22	0.42
11:K:10(A):ARG:HD3	11:K:180:GLU:OE1	2.20	0.42
13:M:125:LEU:HA	17:M:224:HOH:O	2.19	0.42
4:R:79:SER:O	4:R:134:VAL:HG23	2.18	0.42
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.34	0.42
12:Z:4:LEU:O	12:Z:14:LEU:HD23	2.18	0.42
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.32	0.42
2:B:122:GLY:C	2:B:124:THR:N	2.73	0.42
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.54	0.42
4:D:70:ILE:HB	4:D:74:ILE:HG22	2.00	0.42
4:D:197:LEU:O	4:D:201:MET:HG3	2.19	0.42
5:E:83:PRO:O	5:E:86:ARG:HB3	2.19	0.42
6:F:66:LYS:HE3	6:F:82:ILE:HD12	2.01	0.42
6:F:172:ALA:O	6:F:173:LYS:C	2.57	0.42
7:G:229:ILE:O	7:G:232:ARG:HB2	2.19	0.42
10:J:152:LEU:HD21	10:J:177:ILE:HD11	2.02	0.42
12:L:42:VAL:HG23	12:L:102:ALA:HB3	2.01	0.42
14:N:85:GLU:HA	14:N:85:GLU:OE2	2.20	0.42
2:P:121:GLN:NE2	2:P:121:GLN:C	2.73	0.42
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.79	0.42
7:U:82:ILE:N	7:U:83:PRO:HD2	2.34	0.42
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.49	0.42
10:X:136:SER:HA	17:X:559:HOH:O	2.20	0.42
12:Z:82:ASN:C	12:Z:82:ASN:HD22	2.20	0.42
12:Z:93:PHE:N	12:Z:94:PRO:CD	2.81	0.42
1:A:13:THR:CG2	1:A:24:ILE:HD11	2.43	0.42
4:D:70:ILE:HD11	4:D:89:ILE:HG23	2.01	0.42
4:D:230:ALA:HA	4:D:233:ILE:HD12	2.00	0.42
7:G:35:ILE:HD11	7:G:53:LYS:CG	2.47	0.42
7:G:87:ASN:HD22	7:G:88:ALA:N	2.17	0.42
8:H:112:SER:OG	8:H:120:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:93:GLY:N	9:I:94:PRO:HD3	2.34	0.42
9:I:174:VAL:HG21	9:I:186:LYS:HE3	2.01	0.42
10:J:168:MET:HE1	10:X:167:PRO:C	2.39	0.42
2:P:194:LEU:HD13	2:P:233:LEU:HD12	2.01	0.42
5:S:91:TYR:CD1	5:S:119:LYS:HD2	2.54	0.42
5:S:160:LEU:HD13	5:S:163:THR:HB	2.00	0.42
6:T:39:GLY:HA3	6:T:137:ILE:HG21	2.02	0.42
6:T:130:ARG:HG2	6:T:130:ARG:HH11	1.84	0.42
6:T:210:LEU:HD12	6:T:211:GLU:H	1.85	0.42
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.19	0.42
1:A:207:ASN:HA	1:A:233:LEU:CD1	2.49	0.42
3:C:197:LEU:O	3:C:201:VAL:HG23	2.19	0.42
5:E:114:HIS:HB3	6:F:86:ARG:NH2	2.34	0.42
6:F:187:ARG:HG3	6:F:187:ARG:NH1	2.34	0.42
7:G:168:LYS:HD3	17:G:1365:HOH:O	2.19	0.42
7:G:206:SER:O	7:G:233:LEU:HD21	2.19	0.42
11:K:104:TYR:CE1	11:K:180:GLU:HB2	2.54	0.42
12:L:59:PHE:CD1	12:L:83:ILE:CD1	2.98	0.42
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.54	0.42
1:O:160:TRP:CE3	1:O:163:THR:HB	2.55	0.42
3:Q:47:VAL:CG1	3:Q:212:ILE:HG23	2.50	0.42
4:R:215:ILE:HD13	4:R:215:ILE:O	2.20	0.42
5:S:18(C):PHE:C	5:S:18(E):LYS:N	2.73	0.42
6:T:157:TYR:CD1	6:T:157:TYR:C	2.93	0.42
7:U:8:TYR:C	7:U:10:ARG:N	2.72	0.42
7:U:18(D):ILE:HG22	7:U:18(G):GLU:HB2	2.01	0.42
8:V:37:ILE:CD1	8:V:43:CYS:HB2	2.49	0.42
11:Y:104:TYR:CE1	11:Y:180:GLU:HB2	2.55	0.42
3:C:97:GLN:HG3	10:J:65:LEU:HB2	2.00	0.42
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.59	0.42
4:D:147:GLN:HG2	4:D:159:ARG:CZ	2.49	0.42
13:M:100:ILE:HD13	13:M:112:TYR:CB	2.47	0.42
5:S:18(C):PHE:C	5:S:18(E):LYS:H	2.23	0.42
5:S:226:GLY:O	5:S:227:GLU:C	2.58	0.42
6:T:202:HIS:O	6:T:202:HIS:CG	2.73	0.42
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.50	0.42
2:B:20:ARG:HG2	2:B:20:ARG:HH11	1.85	0.42
2:B:107:ILE:HD13	2:B:108:PRO:C	2.36	0.42
2:B:232:ILE:HG12	2:B:232:ILE:O	2.19	0.42
4:D:42:THR:C	4:D:44:GLU:H	2.22	0.42
5:E:150:GLU:O	5:E:157:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:54:ILE:HG12	6:F:208:PHE:HA	2.02	0.42
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.55	0.42
2:P:39:GLY:C	2:P:148:LEU:HD21	2.40	0.42
2:P:215:ILE:HD12	2:P:215:ILE:N	2.34	0.42
6:T:151:LEU:HD13	6:T:157:TYR:HB3	2.02	0.42
7:U:118:ASN:O	7:U:122:ILE:HD13	2.19	0.42
7:U:188:LYS:HD3	7:U:188:LYS:HA	1.88	0.42
8:V:3:ILE:O	8:V:3:ILE:HG12	2.19	0.42
11:Y:10(A):ARG:HD3	11:Y:180:GLU:OE1	2.20	0.42
12:Z:160:THR:O	12:Z:164:GLU:HG2	2.20	0.42
14:2:48:SER:HB3	14:2:51:ASP:HB2	2.02	0.42
14:2:18(A):ILE:HD13	14:2:18(B):PHE:H	1.75	0.42
1:A:29:THR:O	1:A:33:GLN:HG2	2.19	0.42
3:C:224:LEU:HD12	3:C:224:LEU:N	2.35	0.42
5:E:194:VAL:CG1	5:E:207:LEU:HD11	2.50	0.42
9:I:61:TYR:CD1	9:I:61:TYR:C	2.93	0.42
11:K:76:VAL:HG12	11:K:111:TYR:HD2	1.85	0.42
4:R:96:ALA:HA	4:R:107:ILE:HG21	2.01	0.42
4:R:147:GLN:HG2	4:R:159:ARG:CZ	2.50	0.42
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.35	0.42
5:S:230:ALA:C	5:S:232:TYR:H	2.23	0.42
8:V:56:THR:HG22	8:V:57:GLN:N	2.34	0.42
10:X:59:ILE:HD12	10:X:59:ILE:N	2.35	0.42
11:Y:40:PHE:CD1	11:Y:73:ARG:NH1	2.88	0.42
12:Z:76:ILE:CG2	12:Z:77:ASN:N	2.83	0.42
12:Z:167:ILE:C	12:Z:167:ILE:HD12	2.39	0.42
2:B:17:PRO:HA	3:C:26:TYR:CE2	2.55	0.42
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.50	0.42
7:G:179:HIS:ND1	7:G:179:HIS:C	2.73	0.42
7:G:187:GLU:O	7:G:191:GLU:HG3	2.20	0.42
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.00	0.42
2:P:194:LEU:O	2:P:198:SER:HB2	2.19	0.42
2:P:235:LYS:HD3	2:P:235:LYS:N	2.34	0.42
5:S:194:VAL:CG1	5:S:207:LEU:HD11	2.50	0.42
6:T:14:VAL:HG12	6:T:15:PHE:N	2.35	0.42
6:T:43:ASN:N	6:T:43:ASN:ND2	2.67	0.42
7:U:179:HIS:ND1	7:U:179:HIS:C	2.73	0.42
11:Y:76:VAL:HG22	11:Y:103:GLY:HA3	2.01	0.42
12:Z:79:ALA:O	12:Z:82:ASN:HB3	2.20	0.42
12:Z:145:TYR:HD1	12:Z:146:LEU:N	2.17	0.42
14:2:98:GLY:C	14:2:99:ILE:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:139:GLU:OE1	13:1:165:ARG:NH1	2.53	0.42
10:J:3:ILE:HG23	17:J:195:HOH:O	2.20	0.42
10:J:65:LEU:HD21	10:J:69:ARG:HH22	1.84	0.42
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.20	0.42
12:L:194:ASP:HB2	8:V:163:ILE:HG23	2.02	0.42
13:M:8:TYR:HB2	13:M:146:THR:O	2.20	0.42
14:N:107:LYS:HG2	14:N:108:GLY:H	1.84	0.42
1:O:38:LEU:C	1:O:38:LEU:HD12	2.40	0.42
1:O:136:LEU:O	1:O:150:GLN:HA	2.20	0.42
2:P:101:LYS:HG3	9:W:57:GLU:HB3	2.02	0.42
2:P:184:MET:HE3	2:P:188:ASP:CB	2.48	0.42
6:T:35:THR:CG2	6:T:36:THR:N	2.81	0.42
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.85	0.42
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.50	0.42
7:U:206:SER:O	7:U:233:LEU:HD21	2.20	0.42
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.84	0.42
9:W:126:VAL:HG11	9:W:134:LEU:HB3	2.02	0.42
10:X:85:GLN:O	10:X:89:LYS:HG3	2.20	0.42
11:Y:157:ARG:O	11:Y:160:LEU:HB3	2.20	0.42
13:1:157:ASN:O	13:1:161:VAL:HG23	2.20	0.42
14:2:14:LEU:HD12	14:2:14:LEU:N	2.34	0.42
1:A:92:SER:O	1:A:95:VAL:HG12	2.20	0.41
4:D:79:SER:O	4:D:134:VAL:HG23	2.20	0.41
5:E:216:GLY:O	5:E:217:LYS:C	2.58	0.41
6:F:35:THR:CG2	6:F:36:THR:N	2.83	0.41
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.55	0.41
7:G:18(D):ILE:HG22	7:G:18(G):GLU:HB2	2.02	0.41
9:I:58:MET:O	9:I:61:TYR:HB3	2.20	0.41
11:K:2:THR:OG1	11:K:130:GLY:HA3	2.20	0.41
17:L:199:HOH:O	9:W:192:ARG:HG3	2.19	0.41
14:N:8:PHE:HE1	14:N:10:ASP:HB2	1.84	0.41
1:O:175:PHE:O	1:O:179:ARG:HG2	2.19	0.41
1:O:179:ARG:HH11	1:O:179:ARG:CB	2.23	0.41
1:O:207:ASN:HA	1:O:233:LEU:CD1	2.50	0.41
3:Q:97:GLN:HE21	3:Q:97:GLN:CA	2.33	0.41
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.80	0.41
8:V:221:ILE:HD12	8:V:221:ILE:N	2.35	0.41
11:Y:7:ARG:CG	11:Y:12:ILE:HD13	2.45	0.41
13:1:190:LEU:N	13:1:190:LEU:CD1	2.82	0.41
1:A:40:ILE:HD12	1:A:193:ALA:HB2	2.02	0.41
2:B:138:TYR:HB2	2:B:149:TYR:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:LYS:O	2:B:234:VAL:HG23	2.21	0.41
4:D:180:TRP:HA	4:D:184:LEU:HD11	2.03	0.41
5:E:67:ILE:HD13	5:E:213:ALA:HB2	2.02	0.41
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	2.02	0.41
5:E:198:SER:HA	5:E:201:LEU:CD1	2.50	0.41
6:F:81:LEU:HA	17:F:313:HOH:O	2.20	0.41
8:H:18:THR:HB	8:H:30:ASN:HA	2.01	0.41
9:I:-2:ASN:HA	9:I:21:GLY:O	2.19	0.41
10:J:190:PHE:HA	10:J:193:GLN:HB2	2.03	0.41
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.20	0.41
12:L:164:GLU:OE1	12:L:192:LYS:HD3	2.20	0.41
13:M:82:TYR:O	13:M:85:THR:HB	2.19	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.41
11:Y:76:VAL:CG2	11:Y:103:GLY:HA3	2.50	0.41
11:Y:124:ILE:CG2	11:Y:138:LEU:HD23	2.51	0.41
13:1:160:ARG:HB2	13:1:192:VAL:HG13	2.02	0.41
14:2:97:ALA:HB1	14:2:99:ILE:CD1	2.49	0.41
1:A:7:ARG:HH11	5:E:127:TYR:HD2	1.68	0.41
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.56	0.41
7:G:158:VAL:HG22	7:G:159:GLY:H	1.85	0.41
8:H:14:ILE:O	8:H:14:ILE:HG13	2.20	0.41
8:H:170:GLY:O	8:H:171:SER:HB2	2.20	0.41
11:K:124:ILE:CG2	11:K:138:LEU:HD23	2.50	0.41
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.02	0.41
14:N:107:LYS:HG2	14:N:108:GLY:N	2.35	0.41
1:O:4:MET:O	1:O:5:THR:O	2.39	0.41
1:O:57:PRO:HG2	7:U:177:GLU:HG2	2.01	0.41
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.41
5:S:121:GLN:OE1	5:S:125:GLN:NE2	2.53	0.41
5:S:198:SER:HA	5:S:201:LEU:CD1	2.50	0.41
6:T:109:ILE:HG22	6:T:149:TYR:HE2	1.85	0.41
10:X:18:LYS:CD	10:X:174:ILE:HG13	2.45	0.41
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.20	0.41
12:Z:129:ALA:HB1	12:Z:166:HIS:NE2	2.35	0.41
1:A:86:ARG:NE	7:G:118:ASN:HD21	2.18	0.41
1:A:166:GLY:O	1:A:167:LYS:C	2.58	0.41
3:C:14:ILE:HB	4:D:23:GLN:NE2	2.35	0.41
3:C:224:LEU:N	3:C:224:LEU:CD1	2.84	0.41
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.35	0.41
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.77	0.41
7:G:18(D):ILE:O	7:G:18(G):GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.82	0.41
1:O:159:PRO:O	2:P:59:LEU:HD12	2.21	0.41
2:P:233:LEU:HD12	2:P:233:LEU:HA	1.91	0.41
4:R:52:LYS:HE3	4:R:211:GLN:HB2	2.01	0.41
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.50	0.41
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	2.03	0.41
13:1:14(C):ARG:HH11	13:1:14(C):ARG:CG	2.25	0.41
14:2:44:CYS:HB2	14:2:100:ILE:HB	2.01	0.41
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.81	0.41
7:G:217:LYS:HA	7:G:217:LYS:CE	2.43	0.41
7:G:224:LEU:HB3	7:G:228:ASN:HB2	2.03	0.41
9:I:55:LEU:HD12	9:I:97:VAL:HG21	2.01	0.41
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.21	0.41
11:K:45:MET:SD	16:K:2(I):H10:C15	3.08	0.41
11:K:104:TYR:HA	11:K:107:GLY:O	2.20	0.41
12:L:4:LEU:O	12:L:14:LEU:HD23	2.21	0.41
1:O:35:VAL:CG1	1:O:51:GLU:HB3	2.50	0.41
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.21	0.41
5:S:4:PHE:O	5:S:5:ARG:C	2.59	0.41
6:T:151:LEU:CD1	6:T:157:TYR:HB3	2.51	0.41
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.48	0.41
7:U:220:LYS:HG2	7:U:221:PHE:N	2.34	0.41
9:W:81:GLN:HG2	17:W:949:HOH:O	2.20	0.41
16:Y:2(I):H10:H22A	12:Z:125:ARG:HH21	1.86	0.41
12:Z:6:ILE:HG12	12:Z:124:CYS:HB2	2.02	0.41
13:1:17:ASP:C	13:1:17:ASP:OD2	2.59	0.41
13:1:184:LEU:HD23	13:1:185:THR:N	2.34	0.41
14:2:4:MET:CB	14:2:126:ILE:HG22	2.51	0.41
14:2:105:ASP:HB3	14:2:106:ASN:HB2	2.02	0.41
2:B:186:VAL:O	2:B:190:ILE:HG13	2.20	0.41
3:C:97:GLN:HE21	3:C:97:GLN:CA	2.32	0.41
3:C:150:GLN:HE21	3:C:150:GLN:HB3	1.65	0.41
4:D:52:LYS:HE3	4:D:211:GLN:HB2	2.02	0.41
5:E:226:GLY:O	5:E:227:GLU:C	2.58	0.41
7:G:188:LYS:HA	7:G:188:LYS:HD3	1.89	0.41
8:H:149:GLU:OE2	8:H:149:GLU:N	2.54	0.41
9:I:80:THR:HG23	9:I:113:PHE:CZ	2.56	0.41
10:J:3:ILE:HG22	10:J:100:LEU:HD12	2.01	0.41
11:K:167:ALA:HB1	9:W:167:ALA:O	2.21	0.41
14:N:105:ASP:HB3	14:N:106:ASN:HB2	2.02	0.41
3:Q:102:THR:OG1	3:Q:103:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.36	0.41
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.21	0.41
8:V:67:SER:HB2	8:V:74:PRO:HG3	2.01	0.41
8:V:149:GLU:OE2	8:V:149:GLU:N	2.53	0.41
10:X:105:ASP:O	10:X:106:ASN:N	2.53	0.41
11:Y:40:PHE:CD1	11:Y:73:ARG:CZ	3.04	0.41
1:A:31:VAL:HG13	1:A:79:SER:O	2.21	0.41
2:B:144:ARG:NH1	10:J:72:TYR:HB2	2.36	0.41
4:D:192:LEU:O	4:D:196:ILE:HD13	2.20	0.41
5:E:136:LEU:HB2	5:E:151:PHE:HB3	2.02	0.41
6:F:61:PRO:O	6:F:62:GLN:HB2	2.20	0.41
6:F:90:ASN:HD22	6:F:90:ASN:HA	1.64	0.41
6:F:184:LEU:CD1	6:F:188:GLU:HB3	2.47	0.41
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.02	0.41
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.36	0.41
13:M:36:PRO:HA	13:M:42:VAL:HA	2.03	0.41
13:M:137:LEU:HD11	13:M:161:VAL:HG21	2.03	0.41
1:O:58:LEU:HB3	7:U:162:ALA:O	2.21	0.41
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.36	0.41
4:R:180:TRP:HA	4:R:184:LEU:HD11	2.02	0.41
5:S:76:LEU:HA	5:S:137:LEU:O	2.21	0.41
6:T:179:LEU:HD21	6:T:192:GLN:HG2	2.02	0.41
8:V:78:SER:O	8:V:82:MET:HG3	2.21	0.41
9:W:55:LEU:HD12	9:W:97:VAL:HG21	2.01	0.41
9:W:93:GLY:N	9:W:94:PRO:HD3	2.35	0.41
12:Z:14(D):TYR:CG	12:Z:14(J):GLY:HA2	2.56	0.41
13:1:4:ILE:HD12	13:1:155:ILE:HD12	2.03	0.41
2:B:113:VAL:HG22	2:B:138:TYR:CG	2.56	0.41
6:F:107:ILE:O	6:F:107:ILE:HG23	2.20	0.41
6:F:179:LEU:HD21	6:F:192:GLN:HG2	2.02	0.41
7:G:46:THR:HG21	7:G:139:VAL:HB	2.02	0.41
10:J:119:LYS:HE2	17:J:408:HOH:O	2.21	0.41
12:L:6:ILE:HG12	12:L:124:CYS:CB	2.50	0.41
2:P:20:ARG:HG2	2:P:20:ARG:HH11	1.85	0.41
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	2.03	0.41
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.55	0.41
7:U:229:ILE:O	7:U:232:ARG:HB2	2.21	0.41
11:Y:74:ILE:HD11	11:Y:78:ALA:HB1	2.02	0.41
13:1:125:LEU:HA	17:1:217:HOH:O	2.19	0.41
13:1:137:LEU:HD11	13:1:161:VAL:HG21	2.02	0.41
13:1:14(C):ARG:NH1	13:1:14(C):ARG:CG	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:C	1:A:74:ILE:HG13	2.41	0.41
1:A:79:SER:HB2	1:A:165:ILE:HD12	2.02	0.41
1:A:124:THR:CG2	1:A:124:THR:O	2.69	0.41
1:A:160:TRP:CE3	1:A:163:THR:HB	2.56	0.41
2:B:107:ILE:HD11	2:B:111:ILE:HB	2.03	0.41
2:B:194:LEU:HD13	2:B:233:LEU:HD12	2.03	0.41
5:E:2(C):VAL:O	5:E:226:GLY:HA2	2.21	0.41
6:F:13:SER:HB2	7:G:130:ARG:HD3	2.03	0.41
6:F:103:TYR:O	6:F:104:LYS:HB3	2.21	0.41
7:G:203:THR:HG22	7:G:204:GLU:N	2.35	0.41
8:H:208:ARG:NH1	9:I:149:GLU:HB2	2.35	0.41
8:H:221:ILE:HD12	8:H:221:ILE:N	2.35	0.41
10:J:63:ILE:HD13	10:J:63:ILE:N	2.36	0.41
11:K:50:ALA:CB	12:L:116:VAL:HG23	2.48	0.41
11:K:83:LEU:CD2	11:K:101:ILE:HD11	2.51	0.41
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.50	0.41
12:L:145:TYR:HD1	12:L:146:LEU:N	2.18	0.41
13:M:45:ILE:HG12	13:M:99:ILE:HG12	2.03	0.41
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.20	0.41
14:N:37:VAL:HG22	14:N:41:ILE:HG22	2.01	0.41
1:O:205:GLU:HA	1:O:205:GLU:OE2	2.21	0.41
1:O:21(L):ILE:HD11	8:V:186:TYR:CD2	2.56	0.41
4:R:12:VAL:HG23	4:R:12(A):GLY:HA2	2.02	0.41
4:R:160:TYR:HB3	4:R:162:ALA:O	2.21	0.41
5:S:4:PHE:CG	5:S:5:ARG:N	2.88	0.41
7:U:40:VAL:HB	7:U:18(D):ILE:HD13	2.03	0.41
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.02	0.41
10:X:7:ARG:HH11	10:X:7:ARG:HG2	1.86	0.41
10:X:66:TYR:CE2	10:X:74:LEU:HG	2.56	0.41
10:X:85:GLN:HG2	10:X:89:LYS:HE3	2.03	0.41
10:X:190:PHE:HA	10:X:193:GLN:HB2	2.03	0.41
11:Y:9:GLN:CD	11:Y:10:GLY:N	2.74	0.41
13:1:209:GLN:N	17:1:367:HOH:O	2.54	0.41
14:2:32:ASP:HA	17:2:307:HOH:O	2.21	0.41
14:2:134:ILE:C	14:2:134:ILE:HD12	2.41	0.41
1:A:136:LEU:O	1:A:150:GLN:HA	2.21	0.41
2:B:21(A):LYS:HG3	2:B:219:GLU:O	2.20	0.41
4:D:101:LEU:CD1	11:K:57:THR:HG22	2.51	0.41
4:D:196:ILE:HD12	4:D:196:ILE:N	2.35	0.41
5:E:136:LEU:HD12	5:E:151:PHE:CD2	2.56	0.41
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:ASN:N	6:F:43:ASN:ND2	2.69	0.41
6:F:49:ALA:HB1	6:F:212:ILE:CD1	2.51	0.41
7:G:49:ILE:CD1	7:G:49:ILE:N	2.80	0.41
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.02	0.41
8:H:156:SER:HA	8:H:159:ILE:HD12	2.01	0.41
10:J:-1:MET:CG	10:J:1:ASP:H	2.31	0.41
11:K:40:PHE:CD1	11:K:73:ARG:CZ	3.04	0.41
12:L:43:MET:HG2	12:L:44:SER:N	2.36	0.41
13:M:62:LEU:HD13	13:M:79:ILE:HD13	2.02	0.41
14:N:38:HIS:HB3	14:N:41:ILE:HB	2.02	0.41
14:N:143:ARG:O	14:N:146:MET:HG3	2.21	0.41
2:P:39:GLY:O	2:P:148:LEU:HD21	2.21	0.41
2:P:230:LYS:O	2:P:234:VAL:HG23	2.21	0.41
7:U:79:ASN:HA	17:U:252:HOH:O	2.20	0.41
8:V:62:ASN:HB3	8:V:82:MET:HE1	2.03	0.41
9:W:46:THR:HA	17:W:608:HOH:O	2.21	0.41
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.80	0.41
12:Z:-5:TYR:CD2	12:Z:96:TYR:HB2	2.55	0.41
12:Z:52:GLY:O	12:Z:56:VAL:HG23	2.21	0.41
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.20	0.41
14:2:51:ASP:O	14:2:55:ILE:HG13	2.22	0.41
8:H:18:THR:OG1	8:H:171:SER:HB2	2.21	0.40
9:I:126:VAL:HG11	9:I:134:LEU:HB3	2.03	0.40
10:J:133:TYR:OH	10:X:24:ILE:CG1	2.68	0.40
11:K:90:TYR:O	11:K:91:LYS:C	2.59	0.40
12:L:54:ALA:O	12:L:58:ARG:HB2	2.21	0.40
2:P:215:ILE:O	2:P:215:ILE:HG22	2.21	0.40
5:S:31:ILE:HD13	5:S:152:GLN:OE1	2.21	0.40
9:W:20:LEU:HA	17:W:240:HOH:O	2.21	0.40
10:X:190:PHE:C	10:X:192:ALA:H	2.22	0.40
11:Y:31:VAL:HG11	16:Y:2(I):H10:C15	2.51	0.40
11:Y:31:VAL:CG1	16:Y:2(I):H10:C15	2.99	0.40
12:Z:70(A):ASN:O	12:Z:72:LYS:N	2.54	0.40
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.18	0.40
1:A:24:ILE:HD12	1:A:24:ILE:N	2.36	0.40
3:C:19:GLY:O	4:D:30:ALA:HB2	2.21	0.40
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.49	0.40
5:E:27:ALA:O	5:E:31:ILE:HD12	2.21	0.40
6:F:21:ASN:C	6:F:21:ASN:OD1	2.59	0.40
6:F:35:THR:HG21	6:F:51:GLU:O	2.21	0.40
6:F:83:PRO:HB2	17:F:1240:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:172:ALA:C	6:F:176:LEU:HD23	2.42	0.40
7:G:13:THR:HB	7:G:124:THR:O	2.21	0.40
8:H:62:ASN:HB3	8:H:82:MET:HE1	2.04	0.40
9:I:16:CYS:SG	9:I:34:ILE:HG12	2.60	0.40
14:N:116:GLY:HA3	17:N:194:HOH:O	2.21	0.40
3:Q:156:ILE:CD1	3:Q:156:ILE:H	2.34	0.40
4:R:40:ILE:HG12	4:R:193:VAL:CG2	2.51	0.40
5:S:39:GLY:O	5:S:162:GLY:HA2	2.21	0.40
5:S:198:SER:HA	5:S:201:LEU:CG	2.46	0.40
7:U:35:ILE:HD13	7:U:53:LYS:HE3	2.03	0.40
7:U:198:ILE:O	7:U:202:GLY:N	2.51	0.40
9:W:58:MET:O	9:W:61:TYR:HB3	2.21	0.40
11:Y:109:THR:HA	17:Y:595:HOH:O	2.21	0.40
12:Z:95:TYR:O	12:Z:97:VAL:N	2.53	0.40
1:A:4:MET:O	1:A:5:THR:O	2.39	0.40
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.87	0.40
1:A:205:GLU:HA	1:A:205:GLU:OE2	2.21	0.40
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.03	0.40
3:C:79:SER:HA	17:C:625:HOH:O	2.22	0.40
3:C:210:ILE:HG22	3:C:212:ILE:CD1	2.52	0.40
4:D:12(G):GLU:HG2	4:D:125:GLU:N	2.34	0.40
8:H:192:LEU:HD23	8:H:192:LEU:HA	1.79	0.40
11:K:17:ASP:CG	11:K:33:LYS:HZ2	2.25	0.40
11:K:76:VAL:HG22	11:K:103:GLY:HA3	2.03	0.40
12:L:133:LEU:N	12:L:133:LEU:HD12	2.36	0.40
12:L:176:LEU:HG	12:L:186:LYS:HG3	2.03	0.40
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.50	0.40
6:T:126:TYR:HE1	7:U:129:MET:SD	2.45	0.40
9:W:84:SER:OG	9:W:119:ILE:HD11	2.21	0.40
10:X:123:PRO:HB3	10:X:142:TYR:CE2	2.57	0.40
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.58	0.40
12:Z:32:PRO:CD	17:Z:1177:HOH:O	2.65	0.40
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	2.03	0.40
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.56	0.40
1:A:21(I):TYR:HE2	1:A:21(L):ILE:HD12	1.87	0.40
2:B:39:GLY:C	2:B:148:LEU:HD21	2.42	0.40
3:C:125:GLN:HB2	4:D:130:ARG:HG2	2.03	0.40
4:D:161:ASN:HB3	4:D:180:TRP:CZ2	2.56	0.40
6:F:151:LEU:HD13	6:F:157:TYR:HB3	2.03	0.40
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.86	0.40
9:I:55:LEU:HD23	9:I:55:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:93:GLY:H	9:I:94:PRO:HD3	1.87	0.40
10:J:123:PRO:HB3	10:J:142:TYR:CE2	2.55	0.40
10:J:133:TYR:CZ	10:J:166:MET:HG3	2.57	0.40
12:L:104:LEU:HA	12:L:107:LYS:O	2.22	0.40
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.20	0.40
2:P:122:GLY:C	2:P:124:THR:N	2.74	0.40
4:R:115:SER:O	4:R:118:ASP:HB2	2.22	0.40
7:U:203:THR:HG22	7:U:204:GLU:N	2.36	0.40
11:Y:45:MET:SD	16:Y:2(I):H10:C15	3.09	0.40
11:Y:174:ASN:HD22	11:Y:174:ASN:HA	1.69	0.40
13:1:8:TYR:HB2	13:1:146:THR:O	2.21	0.40
14:2:133:PHE:HE2	14:2:166:ASP:HB2	1.86	0.40
3:C:241:GLN:O	3:C:243:GLN:N	2.50	0.40
5:E:4:PHE:O	5:E:5:ARG:C	2.58	0.40
7:G:12:ILE:HD13	7:G:12:ILE:H	1.85	0.40
13:M:1:THR:OG1	13:M:2:SER:N	2.55	0.40
1:O:45:GLY:HA2	1:O:147:PHE:CE2	2.57	0.40
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	2.03	0.40
5:S:66:LYS:O	5:S:77:SER:HA	2.20	0.40
6:T:43:ASN:ND2	6:T:43:ASN:H	2.20	0.40
6:T:114:ASP:O	6:T:118:GLN:HG2	2.21	0.40
6:T:195:LYS:NZ	6:T:196:ILE:CD1	2.85	0.40
7:U:99:PHE:CD1	7:U:99:PHE:C	2.95	0.40
8:V:100:ILE:HG12	8:V:127:LEU:HD12	2.03	0.40
9:W:-2:ASN:HA	9:W:21:GLY:O	2.22	0.40
10:X:121:GLU:O	10:X:122:LEU:HD23	2.21	0.40
11:Y:50:ALA:CB	12:Z:116:VAL:HG23	2.51	0.40
11:Y:76:VAL:HG12	11:Y:111:TYR:HD2	1.86	0.40
12:Z:40:ASN:ND2	17:Z:799:HOH:O	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	248/250 (99%)	226 (91%)	15 (6%)	7 (3%)	5	17
1	O	248/250 (99%)	226 (91%)	14 (6%)	8 (3%)	4	13
2	B	242/244 (99%)	217 (90%)	18 (7%)	7 (3%)	4	15
2	P	242/244 (99%)	217 (90%)	19 (8%)	6 (2%)	5	19
3	C	239/241 (99%)	219 (92%)	15 (6%)	5 (2%)	7	23
3	Q	239/241 (99%)	217 (91%)	17 (7%)	5 (2%)	7	23
4	D	240/242 (99%)	217 (90%)	18 (8%)	5 (2%)	7	23
4	R	240/242 (99%)	216 (90%)	19 (8%)	5 (2%)	7	23
5	E	231/233 (99%)	201 (87%)	24 (10%)	6 (3%)	5	18
5	S	231/233 (99%)	203 (88%)	22 (10%)	6 (3%)	5	18
6	F	242/244 (99%)	224 (93%)	17 (7%)	1 (0%)	34	66
6	T	242/244 (99%)	223 (92%)	18 (7%)	1 (0%)	34	66
7	G	241/243 (99%)	223 (92%)	15 (6%)	3 (1%)	13	39
7	U	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	13	39
8	H	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	11	34
8	V	220/222 (99%)	205 (93%)	12 (6%)	3 (1%)	11	34
9	I	202/204 (99%)	189 (94%)	10 (5%)	3 (2%)	10	33
9	W	202/204 (99%)	189 (94%)	11 (5%)	2 (1%)	15	44
10	J	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	10	33
10	X	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	10	33
11	K	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
11	Y	210/212 (99%)	200 (95%)	9 (4%)	1 (0%)	29	61
12	L	220/222 (99%)	201 (91%)	18 (8%)	1 (0%)	29	61
12	Z	220/222 (99%)	201 (91%)	18 (8%)	1 (0%)	29	61
13	1	231/233 (99%)	208 (90%)	21 (9%)	2 (1%)	17	46
13	M	231/233 (99%)	210 (91%)	19 (8%)	2 (1%)	17	46
14	2	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
14	N	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
All	All	6312/6368 (99%)	5789 (92%)	431 (7%)	92 (2%)	10	33

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	167	LYS
2	B	54	VAL
3	C	58	LEU
3	C	203	THR
4	D	12(G)	GLU
5	E	5	ARG
5	E	202	ARG
6	F	143	LYS
12	L	71	ASP
1	O	5	THR
1	O	167	LYS
2	P	54	VAL
3	Q	58	LEU
3	Q	203	THR
4	R	12(G)	GLU
5	S	5	ARG
5	S	202	ARG
6	T	143	LYS
12	Z	71	ASP
1	A	53	LYS
2	B	6	ARG
2	B	21(B)	GLY
2	B	21(C)	ASP
5	E	180	LEU
5	E	217	LYS
5	E	231	LYS
7	G	239	GLN
8	H	9	ASN
8	H	96	GLY
10	J	49	ALA
10	J	192	ALA
1	O	53	LYS
2	P	6	ARG
2	P	21(B)	GLY
2	P	21(C)	ASP
5	S	180	LEU
5	S	217	LYS
8	V	9	ASN
8	V	96	GLY
10	X	49	ALA
10	X	192	ALA
13	1	96	TRP

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Mol	Chain	Res	Type
1	A	63	THR
2	B	20(A)	SER
4	D	12(F)	GLY
5	E	18(A)	ASP
13	M	96	TRP
1	O	63	THR
2	P	20(A)	SER
4	R	120	ALA
4	R	12(F)	GLY
5	S	18(A)	ASP
5	S	231	LYS
7	U	184	ASN
7	U	239	GLN
1	A	100	TYR
3	C	183	PRO
3	C	202	GLN
4	D	120	ALA
4	D	12(C)	GLY
7	G	184	ASN
3	Q	183	PRO
3	Q	202	GLN
4	R	12(C)	GLY
7	U	55	PRO
8	V	171	SER
4	D	18(D)	SER
7	G	55	PRO
8	H	171	SER
9	I	23	GLN
9	I	93	GLY
9	I	106	GLY
13	M	1	THR
1	O	100	TYR
3	Q	53	ARG
9	W	93	GLY
9	W	106	GLY
13	1	1	THR
1	A	208	GLY
2	B	64	THR
3	C	53	ARG
1	O	56	SER
1	O	208	GLY
4	R	18(D)	SER

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Mol	Chain	Res	Type
1	A	56	SER
10	J	8	VAL
10	X	8	VAL
1	O	22	GLY
2	P	186	VAL
2	B	186	VAL
11	Y	39	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	209/209 (100%)	204 (98%)	5 (2%)	49	81
1	O	209/209 (100%)	204 (98%)	5 (2%)	49	81
2	B	203/203 (100%)	188 (93%)	15 (7%)	13	37
2	P	203/203 (100%)	188 (93%)	15 (7%)	13	37
3	C	213/213 (100%)	204 (96%)	9 (4%)	30	63
3	Q	213/213 (100%)	203 (95%)	10 (5%)	26	59
4	D	198/198 (100%)	186 (94%)	12 (6%)	18	48
4	R	198/198 (100%)	186 (94%)	12 (6%)	18	48
5	E	192/192 (100%)	172 (90%)	20 (10%)	7	21
5	S	192/192 (100%)	174 (91%)	18 (9%)	8	26
6	F	201/201 (100%)	188 (94%)	13 (6%)	17	44
6	T	201/201 (100%)	188 (94%)	13 (6%)	17	44
7	G	207/207 (100%)	197 (95%)	10 (5%)	25	58
7	U	207/207 (100%)	197 (95%)	10 (5%)	25	58
8	H	181/181 (100%)	173 (96%)	8 (4%)	28	61
8	V	181/181 (100%)	170 (94%)	11 (6%)	18	48
9	I	172/172 (100%)	165 (96%)	7 (4%)	30	64
9	W	172/172 (100%)	166 (96%)	6 (4%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	175/175 (100%)	169 (97%)	6 (3%)	37	71
10	X	175/175 (100%)	169 (97%)	6 (3%)	37	71
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	75
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	75
12	L	185/185 (100%)	172 (93%)	13 (7%)	15	40
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17	44
13	1	199/199 (100%)	191 (96%)	8 (4%)	31	65
13	M	199/199 (100%)	191 (96%)	8 (4%)	31	65
14	2	162/162 (100%)	154 (95%)	8 (5%)	25	57
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
All	All	5332/5332 (100%)	5057 (95%)	275 (5%)	23	55

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
2	B	58	LEU
2	B	62	ASP
2	B	67	LEU
2	B	71	ASN
2	B	107	ILE
2	B	116	LEU
2	B	121	GLN
2	B	156	ASN
2	B	158	THR
2	B	192	LEU
2	B	198	SER
2	B	212	PHE
2	B	218	ASN
2	B	224	PHE
2	B	232	ILE
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU

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Mol	Chain	Res	Type
3	C	57	LYS
3	C	121	GLN
3	C	150	GLN
3	C	163	GLN
3	C	174	GLU
3	C	208	LYS
4	D	28	LEU
4	D	48	LEU
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	170	GLU
4	D	175	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
5	E	11	ASP
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	117	CYS
5	E	121	GLN
5	E	178	ARG
5	E	18(D)	ILE
5	E	185	ASN
5	E	199	GLN
5	E	207	LEU
5	E	2(C)	VAL
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	35	THR
6	F	43	ASN
6	F	98	SER

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Mol	Chain	Res	Type
6	F	121	GLN
6	F	127	ASN
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	21(C)	ASN
7	G	12	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	157	TYR
7	G	169	GLN
7	G	197	MET
7	G	232	ARG
7	G	233	LEU
8	H	31	CYS
8	H	34	LEU
8	H	41	ILE
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	144	GLN
8	H	197	ARG
9	I	20	LEU
9	I	29	ASN
9	I	45	ILE
9	I	90	ARG
9	I	113	PHE
9	I	116	ILE
9	I	160	LEU
10	J	35	ARG
10	J	52	THR
10	J	63	ILE
10	J	77	GLN
10	J	90	SER
10	J	168	MET
11	K	4	LEU
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	65	LEU
11	K	87	VAL
11	K	104	TYR
12	L	-7	ASN
12	L	3	ILE
12	L	14	LEU
12	L	21	ILE
12	L	40	ASN
12	L	46	ASN
12	L	58	ARG
12	L	70(A)	ASN
12	L	82	ASN
12	L	99	THR
12	L	112	SER
12	L	120	GLU
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	204	LYS
14	N	13	ILE
14	N	84	LYS
14	N	89	GLU
14	N	10(B)	LYS
14	N	149	GLU
1	O	33	GLN
1	O	64	LEU
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
2	P	58	LEU
2	P	62	ASP
2	P	67	LEU
2	P	71	ASN
2	P	116	LEU
2	P	121	GLN
2	P	156	ASN
2	P	158	THR

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Mol	Chain	Res	Type
2	P	187	ASP
2	P	192	LEU
2	P	198	SER
2	P	212	PHE
2	P	218	ASN
2	P	224	PHE
2	P	232	ILE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	121	GLN
3	Q	150	GLN
3	Q	156	ILE
3	Q	163	GLN
3	Q	165	ILE
3	Q	174	GLU
3	Q	208	LYS
4	R	28	LEU
4	R	48	LEU
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	170	GLU
4	R	175	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	11	ASP
5	S	12	THR
5	S	13	VAL
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	117	CYS
5	S	121	GLN
5	S	178	ARG
5	S	185	ASN

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Mol	Chain	Res	Type
5	S	199	GLN
5	S	207	LEU
5	S	2(C)	VAL
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	35	THR
6	T	43	ASN
6	T	98	SER
6	T	121	GLN
6	T	127	ASN
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
7	U	14	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	157	TYR
7	U	169	GLN
7	U	197	MET
7	U	232	ARG
7	U	233	LEU
8	V	3	ILE
8	V	30	ASN
8	V	31	CYS
8	V	34	LEU
8	V	41	ILE
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	197	ARG
9	W	20	LEU
9	W	29	ASN
9	W	90	ARG

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Mol	Chain	Res	Type
9	W	113	PHE
9	W	155	ILE
9	W	160	LEU
10	X	35	ARG
10	X	52	THR
10	X	77	GLN
10	X	90	SER
10	X	90(A)	ILE
10	X	168	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	87	VAL
11	Y	104	TYR
12	Z	-7	ASN
12	Z	14	LEU
12	Z	21	ILE
12	Z	40	ASN
12	Z	46	ASN
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	99	THR
12	Z	112	SER
12	Z	120	GLU
12	Z	145	TYR
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
14	2	3	ILE
14	2	13	ILE
14	2	84	LYS
14	2	89	GLU
14	2	10(B)	LYS
14	2	126	ILE
14	2	149	GLU
14	2	18(A)	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (203) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	156	ASN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	87	HIS

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Mol	Chain	Res	Type
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
8	H	22	GLN
8	H	66	HIS
8	H	114	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
9	I	29	ASN
9	I	64	ASN
9	I	81	GLN
9	I	145	ASN
10	J	36	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN

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Mol	Chain	Res	Type
12	L	70(A)	ASN
12	L	82	ASN
12	L	123	GLN
12	L	14(C)	GLN
12	L	1(I)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	10	ASN
13	M	18	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	191	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	145	ASN
2	P	23	GLN
2	P	71	ASN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	161	ASN

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Mol	Chain	Res	Type
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	87	HIS
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
9	W	29	ASN
9	W	81	GLN
9	W	145	ASN
10	X	36	GLN
10	X	54	GLN
10	X	77	GLN

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Mol	Chain	Res	Type
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	85	HIS
12	Z	123	GLN
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	18	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	191	GLN
14	2	38	HIS
14	2	145	ASN
14	2	157	HIS
14	2	161	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	MES	Y	1(L)	-	12,12,12	2.74	6 (50%)	14,16,16	3.16	5 (35%)
15	MES	K	1(L)	-	12,12,12	2.75	8 (66%)	14,16,16	3.19	6 (42%)
16	H10	K	2(I)	-	27,29,29	3.41	18 (66%)	36,43,43	1.05	3 (8%)
16	H10	Y	2(I)	-	27,29,29	3.32	18 (66%)	36,43,43	1.01	2 (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	MES	Y	1(L)	-	-	3/6/14/14	0/1/1/1
15	MES	K	1(L)	-	-	5/6/14/14	0/1/1/1
16	H10	K	2(I)	-	-	2/14/45/45	0/5/4/4
16	H10	Y	2(I)	-	-	2/14/45/45	0/5/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	2(I)	H10	O13-N9	-11.07	1.25	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	2(I)	H10	O13-N9	-10.31	1.26	1.40
16	Y	2(I)	H10	C26-C1	5.58	1.62	1.52
15	Y	1(L)	MES	C8-S	5.23	1.84	1.77
16	K	2(I)	H10	C26-C1	5.22	1.61	1.52
15	K	1(L)	MES	C8-S	4.98	1.84	1.77
16	K	2(I)	H10	C25-C1	4.96	1.61	1.52
16	Y	2(I)	H10	C25-C1	4.95	1.61	1.52
16	K	2(I)	H10	C17-C3	4.45	1.47	1.38
16	K	2(I)	H10	C18-C1	4.36	1.60	1.52
15	Y	1(L)	MES	C7-C8	-4.34	1.40	1.52
16	Y	2(I)	H10	C18-C1	4.05	1.59	1.52
16	Y	2(I)	H10	C17-C3	4.03	1.46	1.38
15	K	1(L)	MES	C7-C8	-3.80	1.42	1.52
15	Y	1(L)	MES	O1-C6	-3.78	1.27	1.42
16	Y	2(I)	H10	C20-C19	3.44	1.61	1.52
15	K	1(L)	MES	O1-C6	-3.43	1.28	1.42
16	K	2(I)	H10	C24-C19	3.12	1.60	1.52
16	Y	2(I)	H10	C24-C19	3.05	1.60	1.52
16	K	2(I)	H10	C24-C23	3.00	1.60	1.52
16	Y	2(I)	H10	C22-C23	2.99	1.60	1.52
16	K	2(I)	H10	C20-C19	2.95	1.60	1.52
16	Y	2(I)	H10	C24-C23	2.95	1.60	1.52
16	K	2(I)	H10	C6-C7	-2.88	1.16	1.19
16	K	2(I)	H10	C22-C21	2.87	1.60	1.52
16	Y	2(I)	H10	C18-C19	2.80	1.61	1.54
15	K	1(L)	MES	O2S-S	-2.79	1.36	1.45
15	K	1(L)	MES	C3-N4	2.75	1.54	1.46
16	K	2(I)	H10	C22-C23	2.73	1.59	1.52
16	K	2(I)	H10	C18-C19	2.73	1.61	1.54
16	Y	2(I)	H10	C6-C7	-2.72	1.16	1.19
16	Y	2(I)	H10	C22-C21	2.71	1.59	1.52
16	K	2(I)	H10	C4-C3	2.69	1.43	1.38
16	Y	2(I)	H10	C4-C3	2.65	1.43	1.38
15	K	1(L)	MES	O1-C2	2.62	1.53	1.42
15	K	1(L)	MES	O1S-S	2.61	1.52	1.45
15	Y	1(L)	MES	C3-N4	2.61	1.54	1.46
16	Y	2(I)	H10	C20-C21	2.46	1.59	1.52
16	K	2(I)	H10	C4-C5	2.43	1.43	1.39
15	Y	1(L)	MES	O1-C2	2.38	1.52	1.42
16	K	2(I)	H10	C16-C17	2.33	1.43	1.38
16	Y	2(I)	H10	C16-C15	2.31	1.43	1.38
15	K	1(L)	MES	C5-C6	2.23	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	1(L)	MES	C5-C6	2.20	1.59	1.50
16	K	2(I)	H10	C20-C21	2.13	1.58	1.52
16	Y	2(I)	H10	C15-C5	2.12	1.43	1.39
16	Y	2(I)	H10	C4-C5	2.10	1.43	1.39
16	Y	2(I)	H10	C16-C17	2.07	1.43	1.38
16	K	2(I)	H10	C16-C15	2.05	1.43	1.38
16	K	2(I)	H10	C15-C5	2.04	1.43	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Y	1(L)	MES	O1S-S-C8	-9.48	95.50	106.92
15	K	1(L)	MES	O1S-S-C8	-9.44	95.55	106.92
15	Y	1(L)	MES	O2S-S-C8	4.18	111.95	106.92
15	Y	1(L)	MES	O3S-S-O2S	3.87	120.72	111.27
15	K	1(L)	MES	O3S-S-O2S	3.84	120.65	111.27
15	K	1(L)	MES	O1-C2-C3	-2.73	105.79	111.80
15	K	1(L)	MES	C7-N4-C3	2.70	118.13	111.23
16	K	2(I)	H10	C14-C8-N9	2.62	114.41	110.24
16	Y	2(I)	H10	C14-C8-N9	2.60	114.38	110.24
16	K	2(I)	H10	C26-C1-C18	-2.60	106.39	109.89
16	Y	2(I)	H10	O11-C10-N12	-2.30	118.34	122.77
16	K	2(I)	H10	O11-C10-N12	-2.27	118.40	122.77
15	K	1(L)	MES	O3S-S-C8	2.25	109.41	105.77
15	K	1(L)	MES	C6-C5-N4	2.22	113.47	110.10
15	Y	1(L)	MES	O1-C2-C3	-2.07	107.24	111.80
15	Y	1(L)	MES	C7-N4-C3	2.02	116.39	111.23

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	K	1(L)	MES	C7-C8-S-O1S
15	K	1(L)	MES	C7-C8-S-O3S
15	Y	1(L)	MES	C7-C8-S-O1S
15	Y	1(L)	MES	C7-C8-S-O2S
15	Y	1(L)	MES	C7-C8-S-O3S
16	K	2(I)	H10	C5-C6-C7-C8
16	Y	2(I)	H10	C5-C6-C7-C8
15	K	1(L)	MES	C8-C7-N4-C3
15	K	1(L)	MES	C8-C7-N4-C5
15	K	1(L)	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
16	K	2(I)	H10	C14-C8-N9-O13
16	Y	2(I)	H10	C14-C8-N9-O13

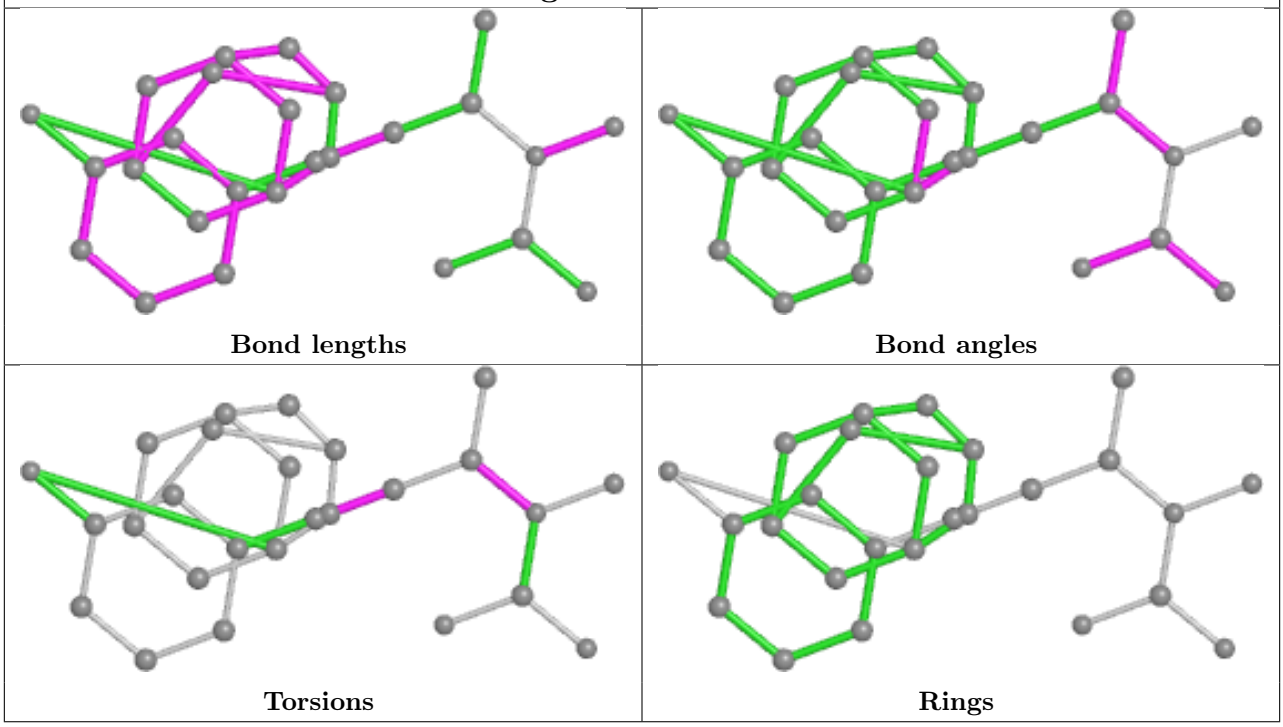
There are no ring outliers.

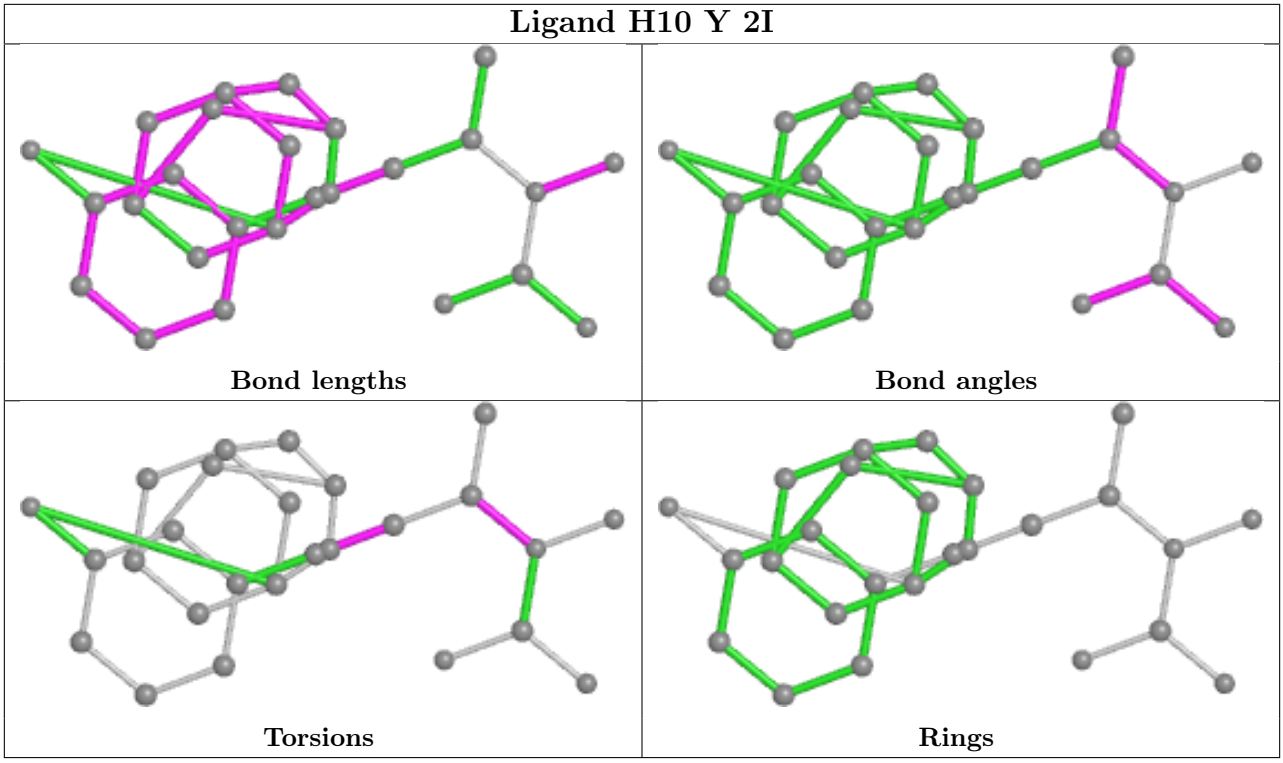
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	2(I)	H10	4	0
16	Y	2(I)	H10	7	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 then 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.

Ligand H10 K 2I





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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.35	1 (0%)	92	91	47, 64, 92, 112	0
1	O	250/250 (100%)	-0.28	4 (1%)	72	66	48, 65, 94, 112	0
2	B	244/244 (100%)	-0.19	5 (2%)	65	56	47, 67, 103, 129	0
2	P	244/244 (100%)	-0.06	6 (2%)	57	47	46, 67, 103, 129	0
3	C	241/241 (100%)	-0.06	6 (2%)	57	47	50, 69, 118, 136	0
3	Q	241/241 (100%)	0.06	16 (6%)	18	11	51, 70, 118, 136	0
4	D	242/242 (100%)	-0.12	6 (2%)	57	47	49, 70, 102, 133	0
4	R	242/242 (100%)	-0.13	8 (3%)	46	36	48, 70, 103, 133	0
5	E	233/233 (100%)	-0.21	2 (0%)	84	80	52, 74, 98, 121	0
5	S	233/233 (100%)	0.02	10 (4%)	35	25	52, 75, 99, 121	0
6	F	244/244 (100%)	-0.24	2 (0%)	86	81	48, 65, 100, 112	0
6	T	244/244 (100%)	-0.24	1 (0%)	92	91	48, 65, 101, 113	0
7	G	243/243 (100%)	-0.37	4 (1%)	72	66	45, 61, 88, 120	0
7	U	243/243 (100%)	-0.32	2 (0%)	86	81	46, 62, 87, 119	0
8	H	222/222 (100%)	-0.39	1 (0%)	91	88	46, 59, 78, 110	0
8	V	222/222 (100%)	-0.41	2 (0%)	84	80	48, 61, 78, 109	0
9	I	204/204 (100%)	-0.36	1 (0%)	91	88	42, 58, 81, 95	0
9	W	204/204 (100%)	-0.21	1 (0%)	91	88	44, 58, 80, 96	0
10	J	198/198 (100%)	-0.46	2 (1%)	82	77	44, 58, 75, 128	0
10	X	198/198 (100%)	-0.43	3 (1%)	73	68	46, 58, 74, 128	0
11	K	212/212 (100%)	-0.43	0	100	100	42, 57, 73, 84	0
11	Y	212/212 (100%)	-0.45	0	100	100	44, 58, 73, 84	0
12	L	222/222 (100%)	-0.37	1 (0%)	91	88	42, 59, 81, 100	0
12	Z	222/222 (100%)	-0.37	2 (0%)	84	80	42, 60, 81, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/233 (100%)	-0.53	1 (0%) 92 91	45, 57, 71, 80	0
13	M	233/233 (100%)	-0.47	1 (0%) 92 91	44, 58, 72, 79	0
14	2	196/196 (100%)	-0.48	0 100 100	44, 54, 75, 87	0
14	N	196/196 (100%)	-0.56	0 100 100	42, 53, 74, 88	0
All	All	6368/6368 (100%)	-0.29	88 (1%) 75 70	42, 62, 95, 136	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(D)	ALA	8.6
4	D	12(E)	SER	7.9
4	D	12(F)	GLY	7.6
4	D	12(C)	GLY	7.3
4	R	12(F)	GLY	6.5
7	U	240	ASP	5.7
4	R	12(D)	ALA	5.5
7	U	6	ALA	5.4
2	P	218	ASN	5.2
3	C	56	LEU	5.1
3	C	55	THR	5.1
4	R	126	ARG	4.6
2	B	218	ASN	4.5
7	G	6	ALA	4.2
5	S	5	ARG	4.1
4	R	12(E)	SER	4.0
3	Q	56	LEU	4.0
1	A	4	MET	4.0
3	Q	55	THR	3.9
5	S	233	ILE	3.9
8	V	223	ASP	3.8
2	B	217	ALA	3.8
5	E	4	PHE	3.8
4	D	126	ARG	3.5
6	F	240	ILE	3.4
4	D	12(G)	GLU	3.3
2	P	217	ALA	3.3
10	J	193	GLN	3.3
3	Q	54	SER	3.2
13	M	-8	THR	3.2
10	X	193	GLN	3.2
3	Q	242	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
3	Q	238	GLN	3.1
3	Q	236	ILE	3.1
12	Z	145	TYR	3.1
1	O	236	LEU	3.0
5	E	5	ARG	3.0
5	S	197	ILE	2.9
5	S	206	SER	2.8
12	L	145	TYR	2.8
4	R	12(B)	GLU	2.8
4	R	12(C)	GLY	2.8
5	S	231	LYS	2.8
5	S	232	TYR	2.8
2	B	232	ILE	2.8
2	P	219	GLU	2.7
6	F	204	ASP	2.6
7	G	240	ASP	2.6
1	O	4	MET	2.6
8	H	222	CYS	2.6
4	R	12(G)	GLU	2.6
7	G	237	ALA	2.5
10	J	191	GLN	2.5
5	S	4	PHE	2.5
10	X	191	GLN	2.5
2	P	21(C)	ASP	2.5
3	Q	203	THR	2.5
3	Q	202	GLN	2.5
2	B	21(B)	GLY	2.4
1	O	5	THR	2.4
3	Q	241	GLN	2.4
1	O	235	ALA	2.4
3	Q	239	GLU	2.4
13	1	-8	THR	2.4
12	Z	14(W)	LYS	2.3
3	C	239	GLU	2.3
7	G	239	GLN	2.3
3	Q	200	VAL	2.3
9	W	-8	SER	2.3
3	C	212	ILE	2.3
3	C	202	GLN	2.3
3	Q	179	ASN	2.2
9	I	-8	SER	2.2
8	V	222	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	Q	233	VAL	2.2
2	P	239	THR	2.2
2	P	21(B)	GLY	2.2
3	Q	189	CYS	2.2
5	S	178	ARG	2.1
4	R	127	LEU	2.1
2	B	54	VAL	2.1
3	Q	234	THR	2.1
10	X	192	ALA	2.1
3	C	240	LYS	2.1
5	S	223	ILE	2.0
5	S	195	GLU	2.0
3	Q	237	GLU	2.0
6	T	240	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

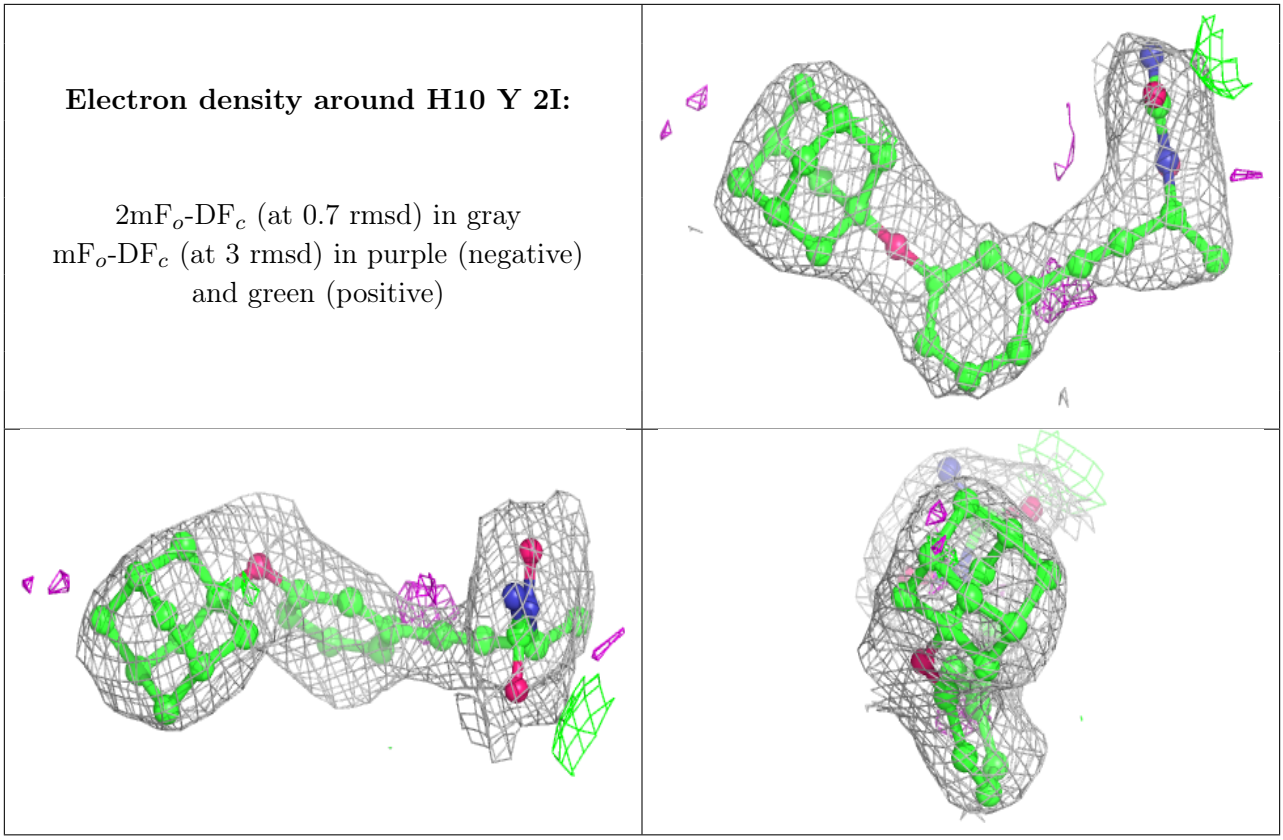
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	H10	Y	2(I)	26/26	0.94	0.18	46,51,60,62	0
16	H10	K	2(I)	26/26	0.96	0.20	46,50,57,58	0
15	MES	Y	1(L)	12/12	0.96	0.18	63,70,75,76	0
15	MES	K	1(L)	12/12	0.97	0.16	62,70,76,77	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

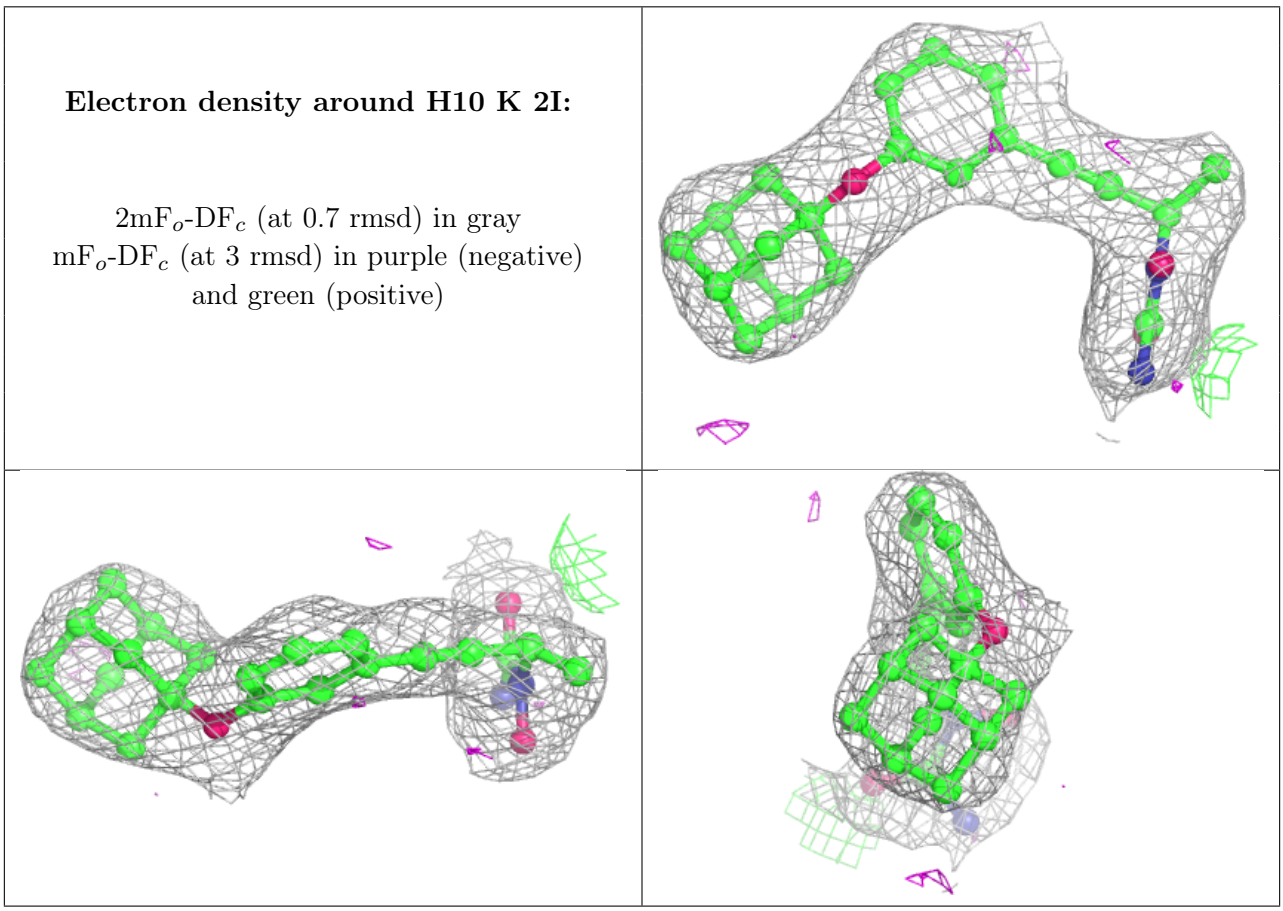
Electron density around H10 Y 2I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around H10 K 2I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.