Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:48 PM GMT

PDB ID	:	4FZG
Title	:	20S yeast proteasome in complex with glidobactin
Authors	:	Stein, M.; Beck, P.; Kaiser, M.; Dudler, R.; Becker, C.F.W.; Groll, M.
Deposited on	:	2012-07-06
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

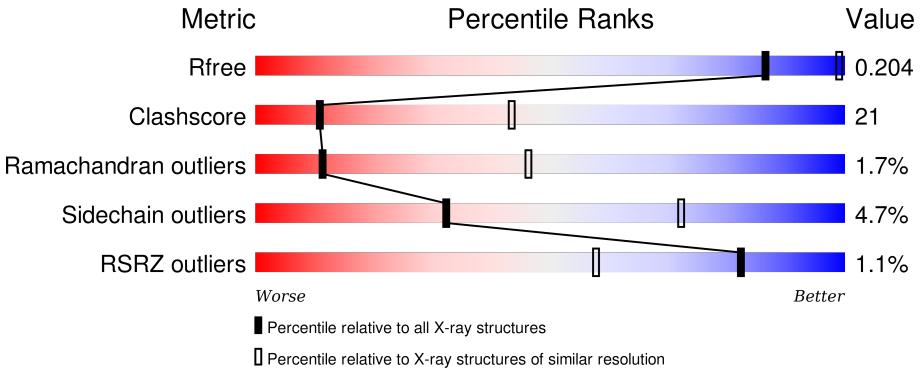
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	65% 33%
1	O	250	64% 34%
2	B	244	54% 41% 5%
2	P	244	3% 54% 41% 5%
3	C	241	57% 40%

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Mol	Chain	Length	Quality of chain
3	Q	241	3% 56% 41%
4	D	242	2% 63% 35%
4	R	242	2% 62% 36%
5	E	233	2% 52% 41% 7%
5	S	233	2% 51% 42% 6%
6	F	244	% 59% 36% 5%
6	T	244	2% 58% 38%
7	G	243	% 63% 33%
7	U	243	% 60% 35% 5%
8	H	222	68% 28%
8	V	222	66% 31%
9	I	204	64% 33%
9	W	204	65% 32%
10	J	198	2% 63% 36%
10	X	198	2% 60% 39%
11	K	212	62% 36%
11	Y	212	64% 34%
12	L	222	58% 39%
12	Z	222	59% 36%
13	M	233	62% 35%
13	a	233	94% 6%
14	N	196	68% 29%
14	b	196	95% 5%
15	c	4	100%
15	d	4	100%

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Mol	Chain	Length	Quality of chain
15	e	4	100%
15	f	4	100%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50986 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
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is a protein called Glidobactin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	0	0	0
			37	27	4	6			
15	d	4	Total	C	N	O	0	0	0
			37	27	4	6			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	e	4	Total C N O 37 27 4 6	0	0	0
15	f	4	Total C N O 37 27 4 6	0	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	56	Total O 56 56	0	0
16	B	35	Total O 35 35	0	0
16	C	41	Total O 41 41	0	0
16	D	39	Total O 39 39	0	0
16	E	25	Total O 25 25	0	0
16	F	45	Total O 45 45	0	0
16	G	59	Total O 59 59	0	0
16	H	52	Total O 52 52	0	0
16	I	61	Total O 61 61	0	0
16	J	55	Total O 55 55	0	0
16	K	41	Total O 41 41	0	0
16	L	57	Total O 57 57	0	0
16	M	63	Total O 63 63	0	0
16	N	61	Total O 61 61	0	0
16	O	34	Total O 34 34	0	0
16	P	27	Total O 27 27	0	0
16	Q	29	Total O 29 29	0	0

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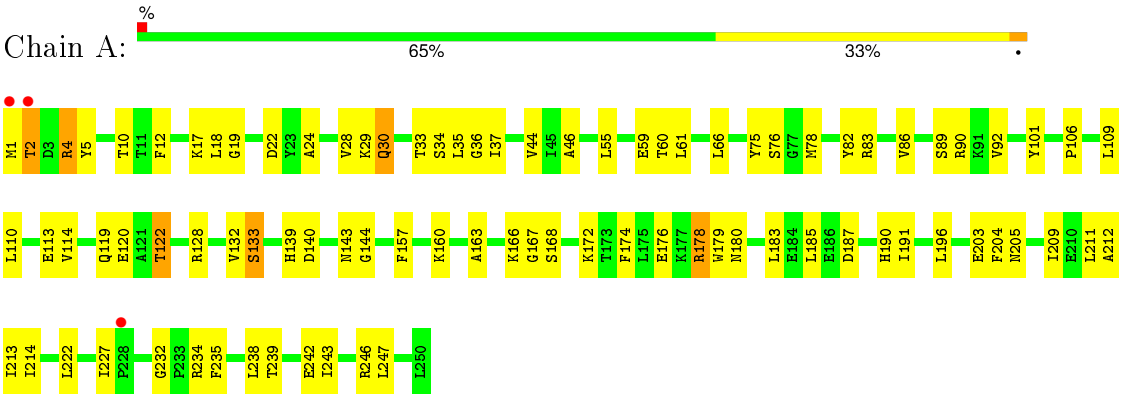
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	R	31	Total O 31 31	0	0
16	S	21	Total O 21 21	0	0
16	T	36	Total O 36 36	0	0
16	U	63	Total O 63 63	0	0
16	V	46	Total O 46 46	0	0
16	W	47	Total O 47 47	0	0
16	X	47	Total O 47 47	0	0
16	Y	44	Total O 44 44	0	0
16	Z	49	Total O 49 49	0	0
16	a	72	Total O 72 72	0	0
16	b	54	Total O 54 54	0	0

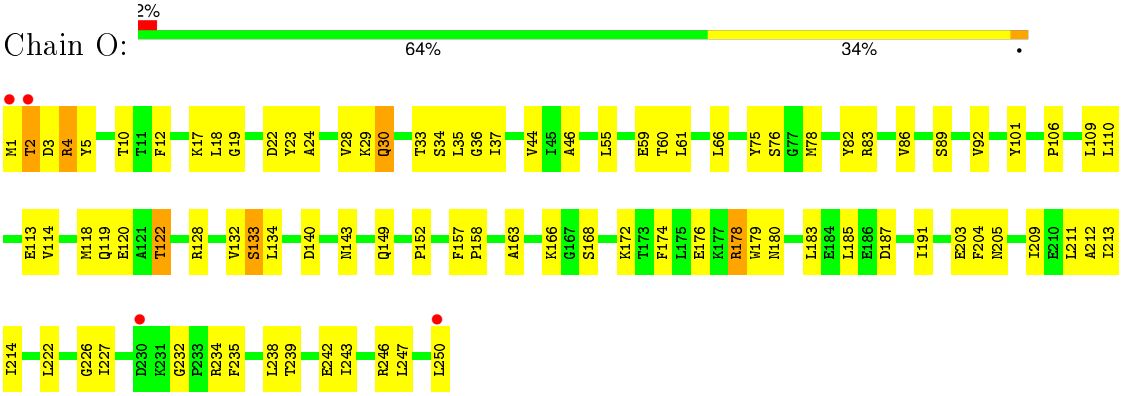
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

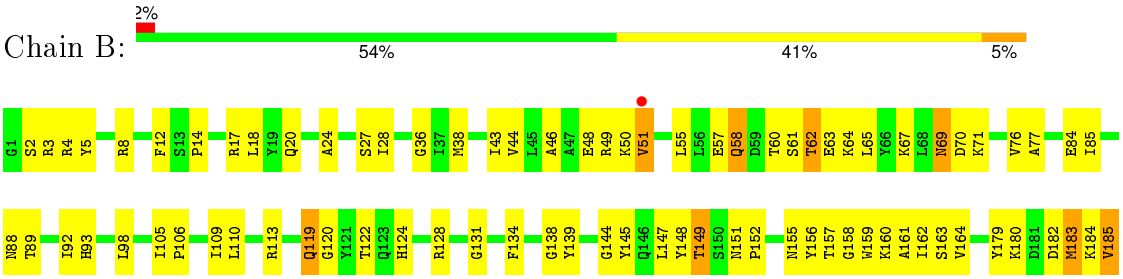
- Molecule 1: Proteasome component Y7

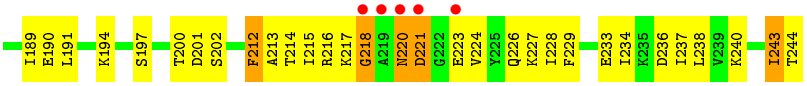


- Molecule 1: Proteasome component Y7

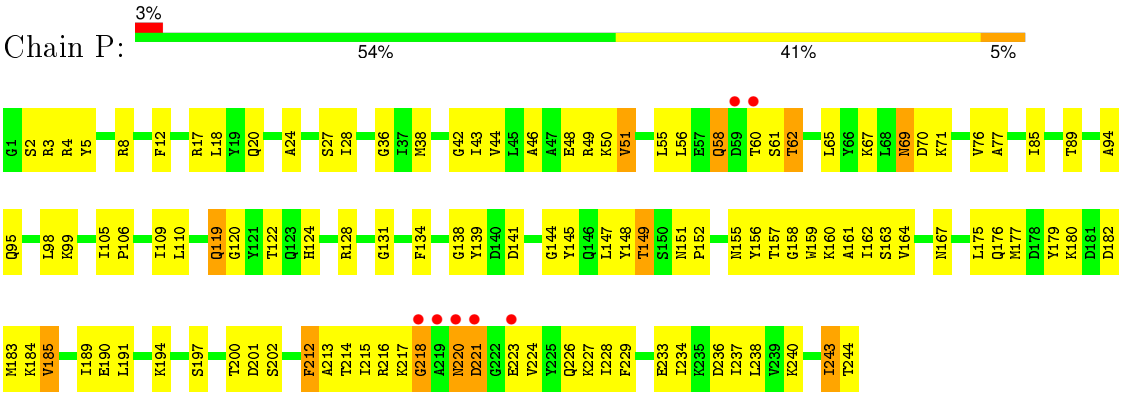


- Molecule 2: Proteasome component Y13

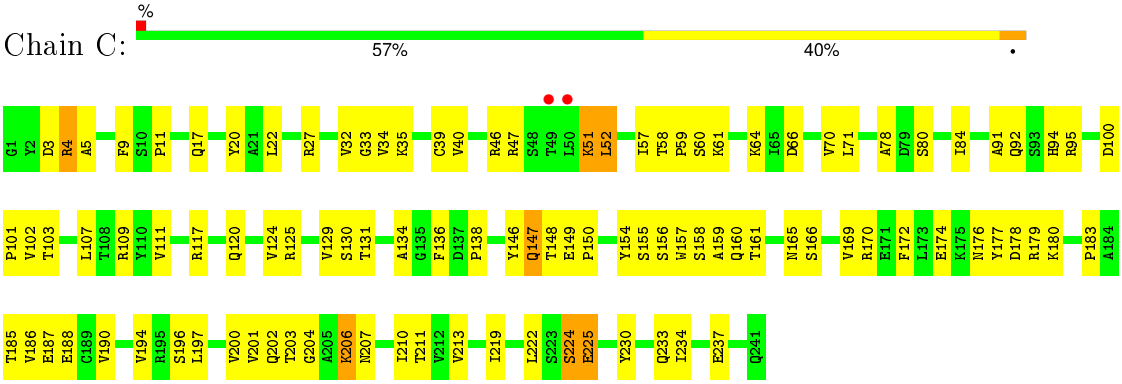




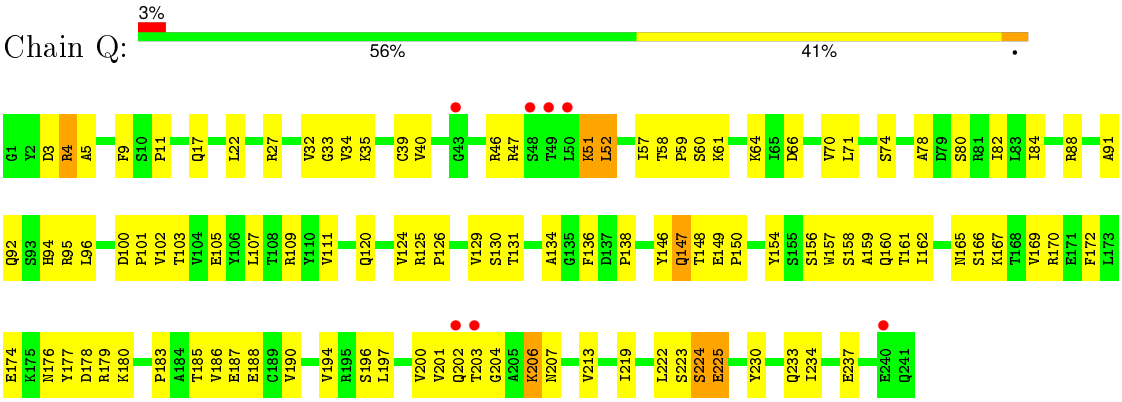
• Molecule 2: Proteasome component Y13



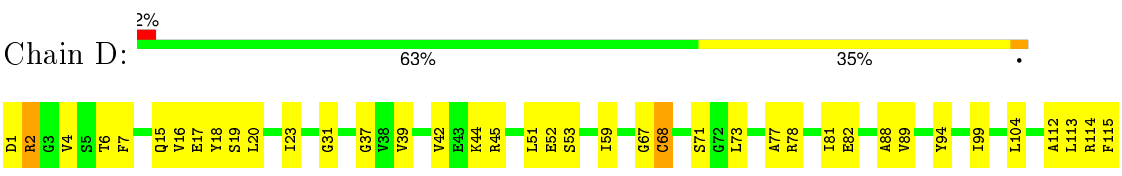
• Molecule 3: Proteasome component PRE6

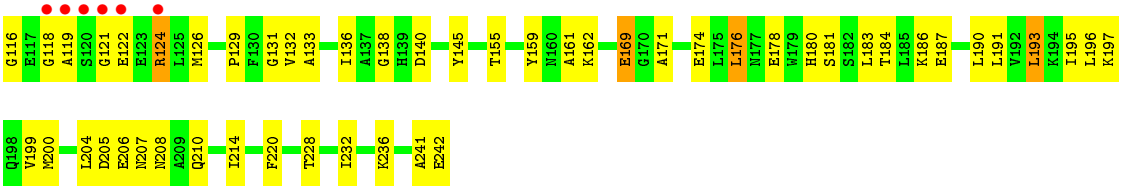


• Molecule 3: Proteasome component PRE6



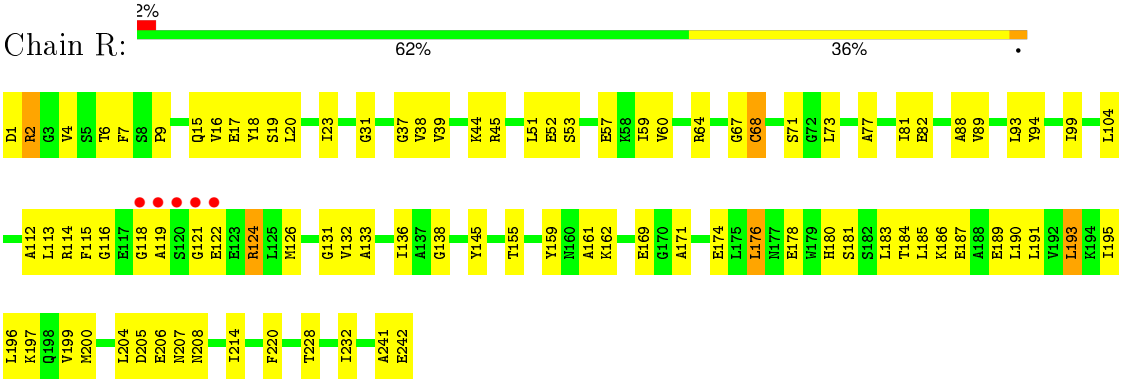
• Molecule 4: Proteasome component PUP2





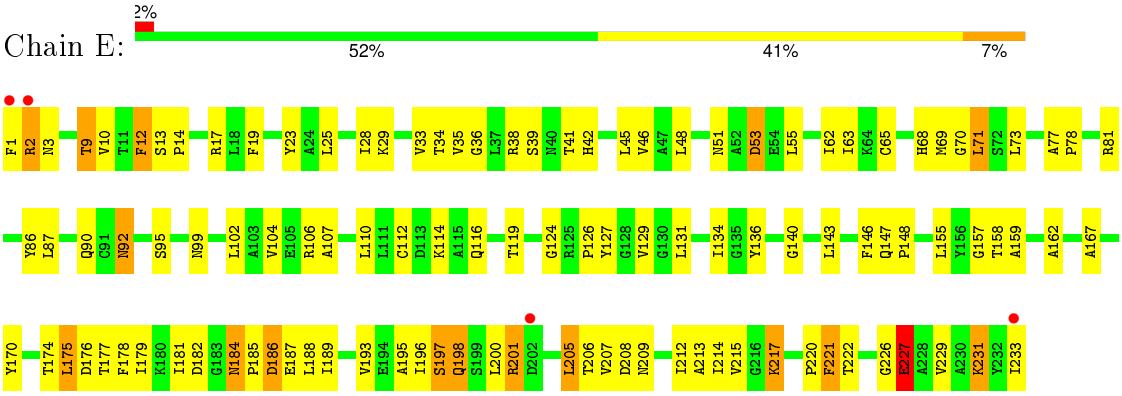
• Molecule 4: Proteasome component PUP2

Chain R:



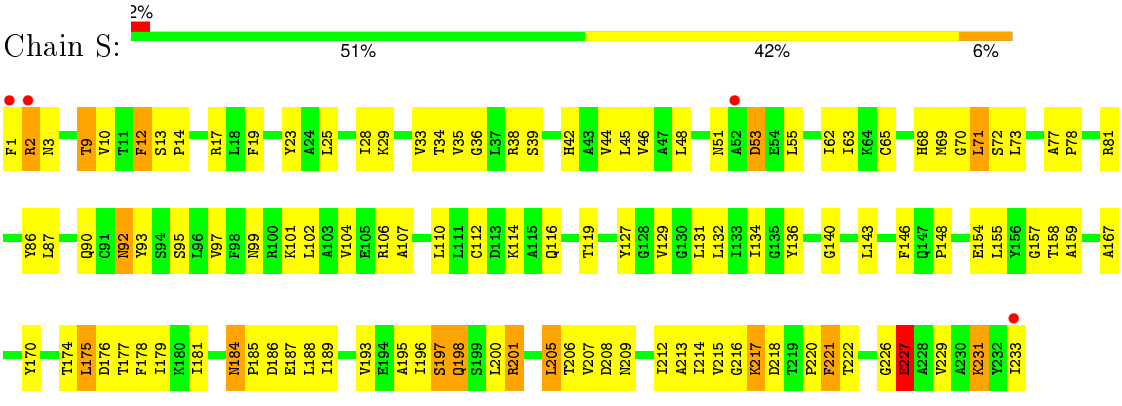
• Molecule 5: Proteasome component PRE5

Chain E:



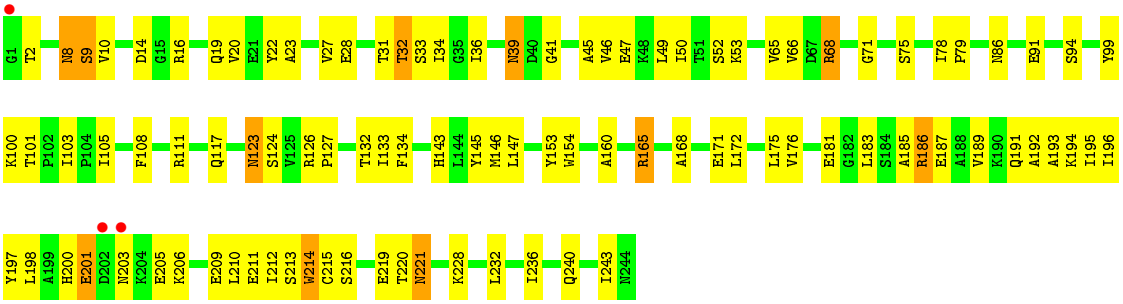
• Molecule 5: Proteasome component PRE5

Chain S:



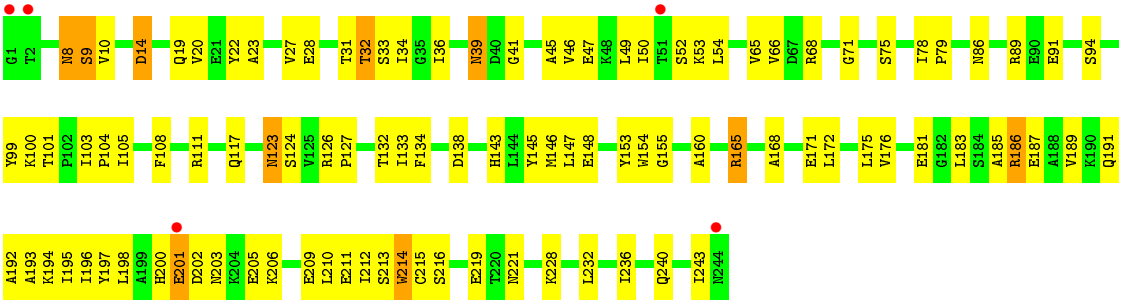
• Molecule 6: Proteasome component C1

Chain F:



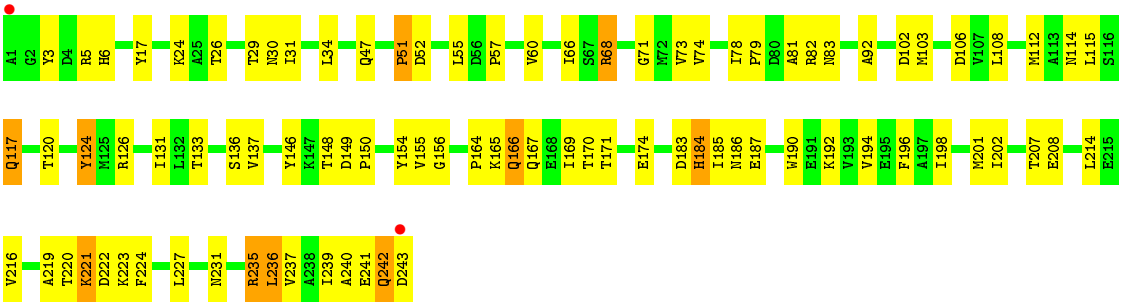
• Molecule 6: Proteasome component C1

Chain T:



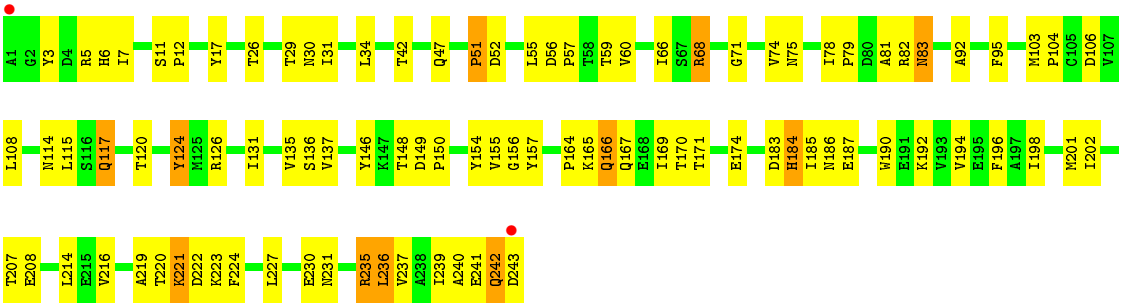
• Molecule 7: Proteasome component C7-alpha

Chain G:



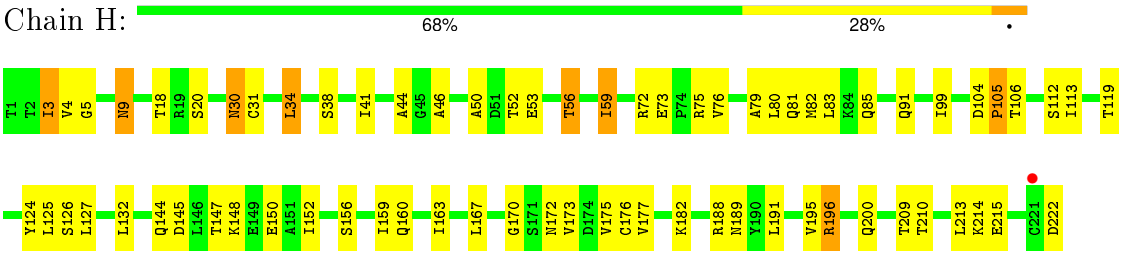
• Molecule 7: Proteasome component C7-alpha

Chain U:



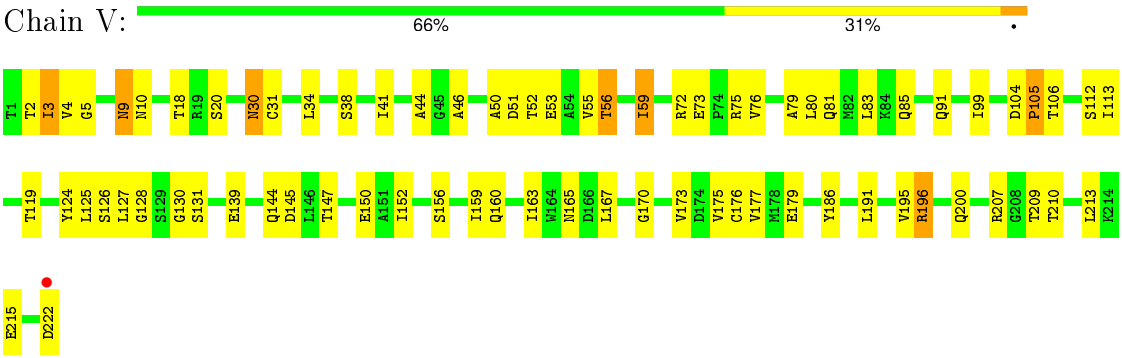
• Molecule 8: Proteasome component PUP1

Chain H:



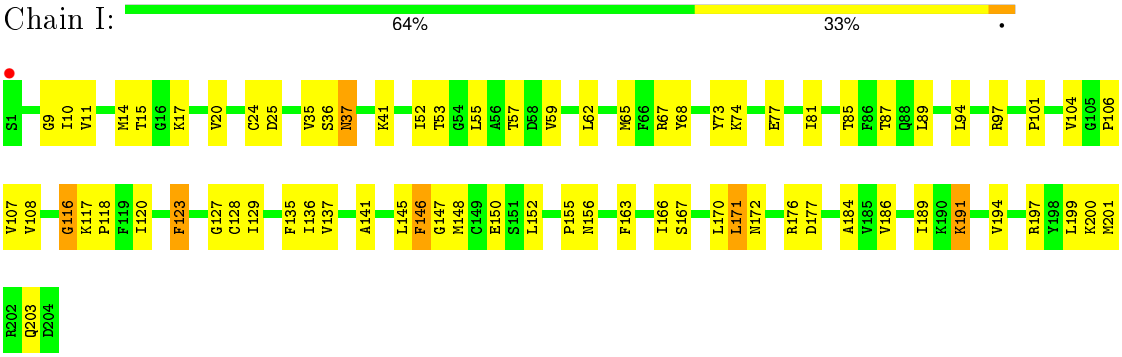
• Molecule 8: Proteasome component PUP1

Chain V:



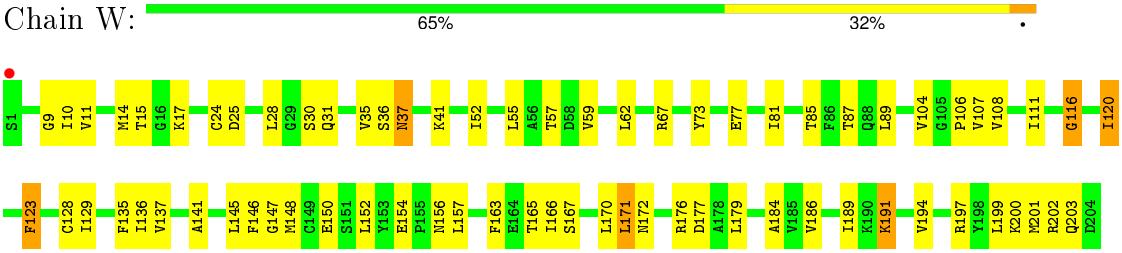
• Molecule 9: Proteasome component PUP3

Chain I:



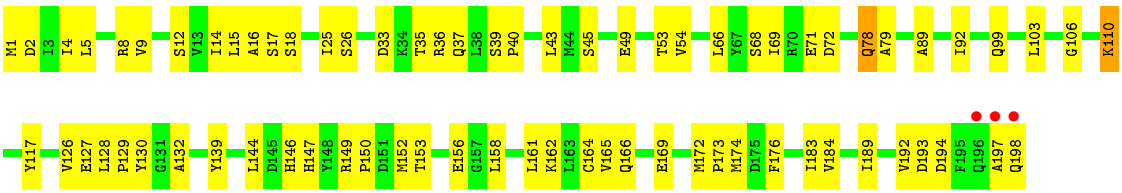
• Molecule 9: Proteasome component PUP3

Chain W:

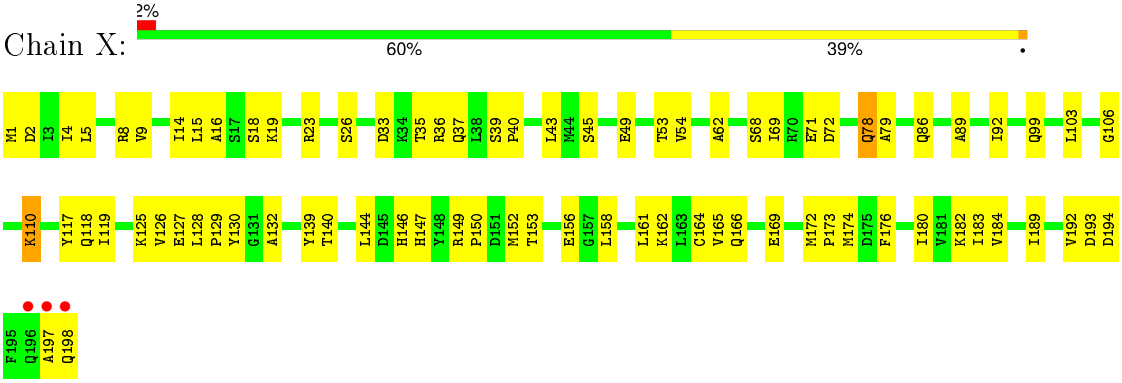


• Molecule 10: Proteasome component C11

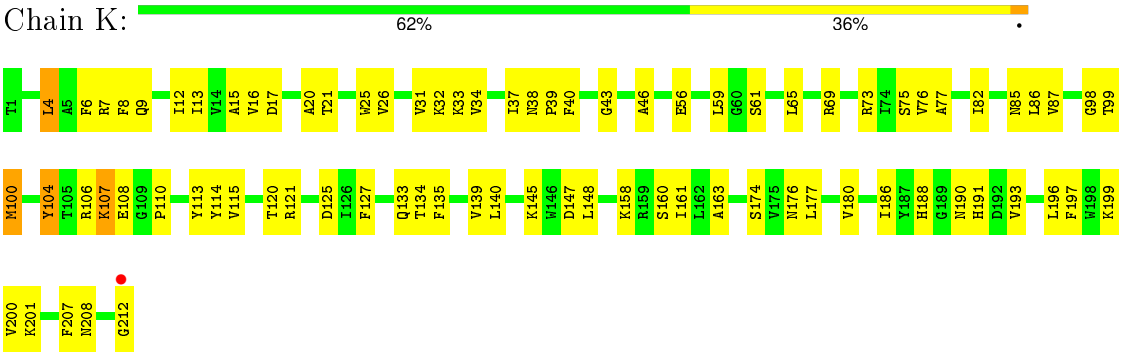
Chain J:



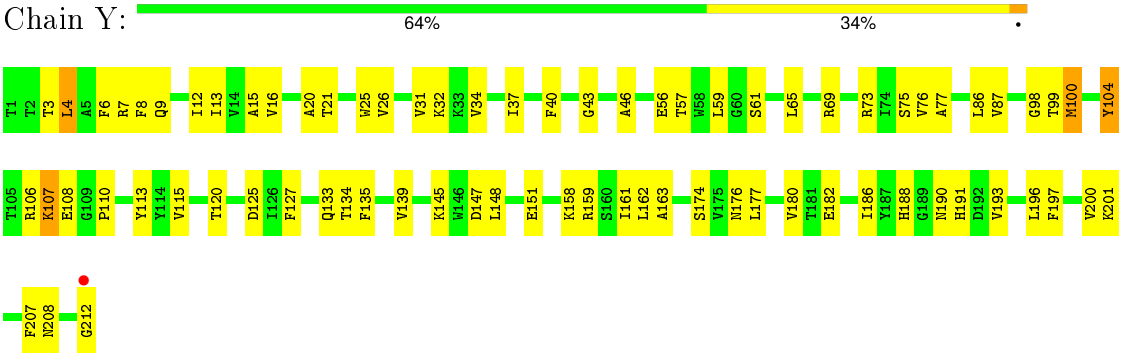
• Molecule 10: Proteasome component C11



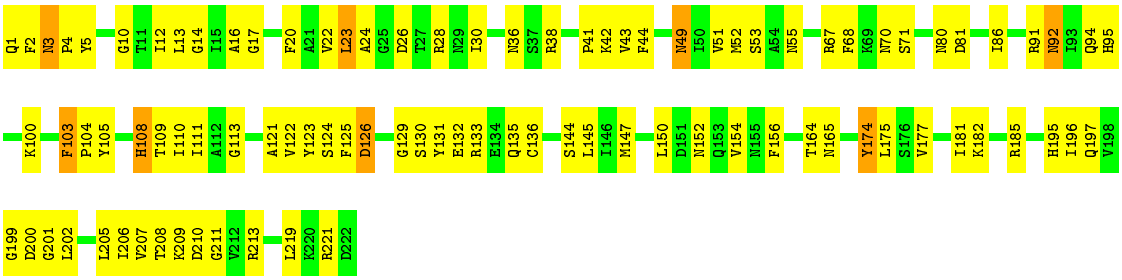
• Molecule 11: Proteasome component PRE2



• Molecule 11: Proteasome component PRE2

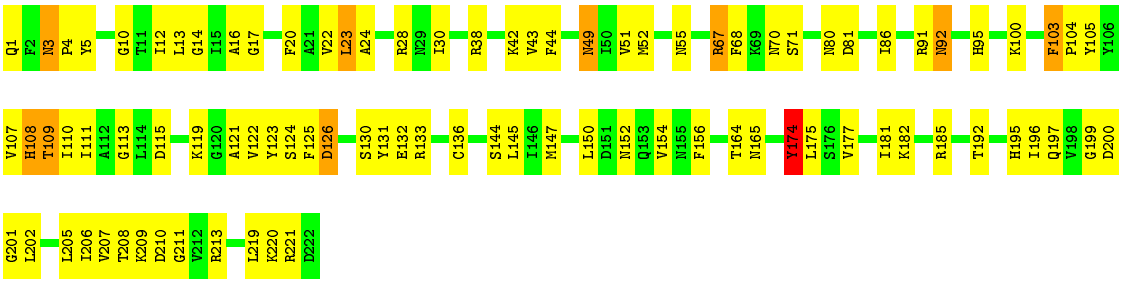


• Molecule 12: Proteasome component C5



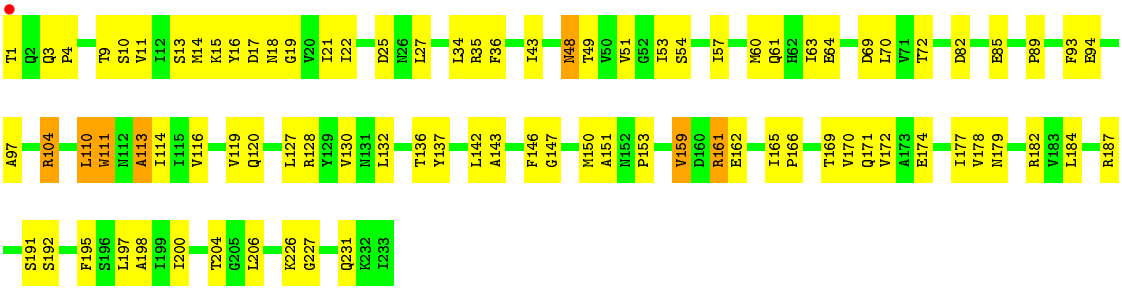
• Molecule 12: Proteasome component C5

Chain Z:



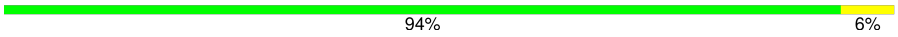
• Molecule 13: Proteasome component PRE4

Chain M:



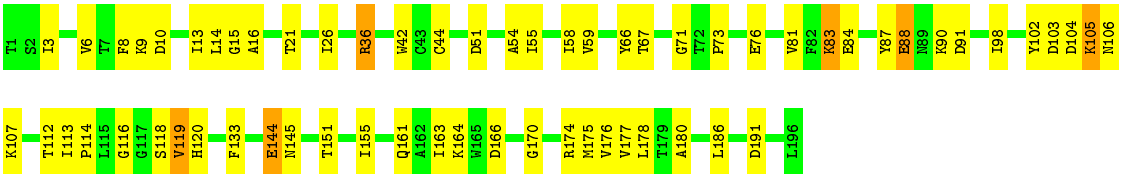
• Molecule 13: Proteasome component PRE4

Chain a:



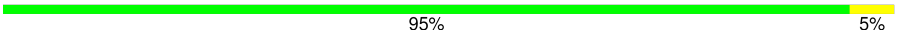
• Molecule 14: Proteasome component PRE3

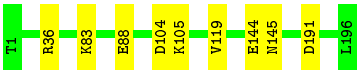
Chain N:



• Molecule 14: Proteasome component PRE3

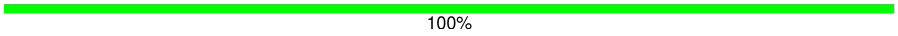
Chain b:





• Molecule 15: Glidobactin

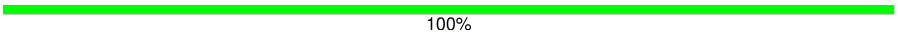
Chain c:



There are no outlier residues recorded for this chain.

• Molecule 15: Glidobactin

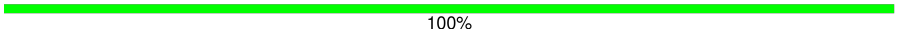
Chain d:



There are no outlier residues recorded for this chain.

• Molecule 15: Glidobactin

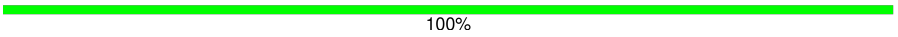
Chain e:



There are no outlier residues recorded for this chain.

• Molecule 15: Glidobactin

Chain f:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.77Å 300.35Å 144.49Å 90.00° 112.67° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 24.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-3.00) 99.6 (24.92-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 2.99Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.197 , 0.226 0.204 , 0.204	Depositor DCC
R_{free} test set	10412 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 209581 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50986	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0W6, LYO, MH9

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	0.39	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.38	0/1935	0.63	0/2618
2	P	0.39	0/1935	0.64	0/2618
3	C	0.35	0/1920	0.61	0/2598
3	Q	0.36	0/1920	0.62	0/2598
4	D	0.36	0/1887	0.63	0/2541
4	R	0.38	0/1887	0.64	0/2541
5	E	0.36	0/1823	0.59	0/2463
5	S	0.37	0/1823	0.59	0/2463
6	F	0.39	0/1937	0.61	0/2614
6	T	0.39	0/1937	0.61	0/2614
7	G	0.39	0/1959	0.62	0/2652
7	U	0.38	0/1959	0.62	0/2652
8	H	0.39	0/1716	0.66	0/2326
8	V	0.38	0/1716	0.66	0/2326
9	I	0.40	0/1611	0.65	0/2174
9	W	0.42	0/1611	0.65	0/2174
10	J	0.42	0/1613	0.64	0/2173
10	X	0.42	0/1613	0.64	0/2173
11	K	0.41	0/1681	0.65	0/2274
11	Y	0.42	0/1681	0.65	0/2274
12	L	0.41	0/1795	0.66	0/2420
12	Z	0.41	0/1795	0.66	0/2420
13	M	0.40	0/1855	0.67	2/2514 (0.1%)
13	a	0.40	0/1855	0.67	2/2514 (0.1%)
14	N	0.41	0/1541	0.64	0/2087
14	b	0.40	0/1541	0.64	0/2087
15	c	1.04	0/6	0.80	0/7
15	d	1.14	0/6	1.13	0/7
15	e	1.08	0/6	0.74	0/7
15	f	0.86	0/6	1.12	0/7

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.39	0/50474	0.64	4/68220 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	110	LEU	N-CA-C	-5.98	94.85	111.00
13	M	110	LEU	N-CA-C	-5.75	95.47	111.00
13	a	113	ALA	N-CA-C	-5.25	96.83	111.00
13	M	113	ALA	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	174	TYR	Sidechain
12	Z	174	TYR	Sidechain

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	1929	80	0
1	O	1915	0	1929	78	0
2	B	1905	0	1904	106	0
2	P	1905	0	1904	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1891	0	1903	93	0
3	Q	1891	0	1903	94	0
4	D	1862	0	1839	69	0
4	R	1862	0	1839	72	0
5	E	1795	0	1800	121	0
5	S	1795	0	1800	134	0
6	F	1897	0	1889	77	0
6	T	1897	0	1889	83	0
7	G	1921	0	1913	79	0
7	U	1921	0	1913	89	0
8	H	1685	0	1687	56	0
8	V	1685	0	1687	59	0
9	I	1581	0	1574	71	0
9	W	1581	0	1574	73	0
10	J	1585	0	1590	71	0
10	X	1585	0	1590	79	0
11	K	1644	0	1594	73	0
11	Y	1644	0	1594	70	0
12	L	1757	0	1711	82	0
12	Z	1757	0	1711	82	0
13	M	1824	0	1832	75	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	47	0
14	b	1512	0	1481	0	0
15	c	37	0	42	0	0
15	d	37	0	42	0	0
15	e	37	0	42	0	0
15	f	37	0	42	0	0
16	A	56	0	0	2	0
16	B	35	0	0	1	0
16	C	41	0	0	4	0
16	D	39	0	0	3	0
16	E	25	0	0	3	0
16	F	45	0	0	4	0
16	G	59	0	0	6	0
16	H	52	0	0	5	0
16	I	61	0	0	4	0
16	J	55	0	0	3	0
16	K	41	0	0	4	0
16	L	57	0	0	3	0
16	M	63	0	0	7	0
16	N	61	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	O	34	0	0	0	0
16	P	27	0	0	6	0
16	Q	29	0	0	8	0
16	R	31	0	0	4	0
16	S	21	0	0	3	0
16	T	36	0	0	7	0
16	U	63	0	0	6	0
16	V	46	0	0	3	0
16	W	47	0	0	8	0
16	X	47	0	0	4	0
16	Y	44	0	0	4	0
16	Z	49	0	0	6	0
16	a	72	0	0	0	0
16	b	54	0	0	0	0
All	All	50986	0	49460	1934	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 21.

All (1934) 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)
1:A:176:GLU:HG2	2:B:55:LEU:HD21	1.30	1.10
2:B:43:ILE:HD11	2:B:145:TYR:HB3	1.36	1.06
2:P:43:ILE:HD11	2:P:145:TYR:HB3	1.37	1.04
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.25	1.01
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.25	1.01
1:A:176:GLU:HG2	2:B:55:LEU:CD2	1.91	0.99
11:K:107:LYS:H	11:K:107:LYS:HD2	1.24	0.98
1:O:12:PHE:H	2:P:20:GLN:HE22	1.11	0.97
2:B:223:GLU:HG2	2:B:224:VAL:H	1.27	0.97
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.25	0.97
2:P:200:THR:HG22	2:P:202:SER:H	1.27	0.97
2:P:223:GLU:HG2	2:P:224:VAL:H	1.29	0.97
10:X:162:LYS:O	10:X:166:GLN:HG3	1.68	0.94
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.48	0.94
2:B:200:THR:HG22	2:B:202:SER:H	1.29	0.93
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.49	0.92
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.50	0.92
3:Q:160:GLN:NE2	3:Q:161:THR:H	1.67	0.92
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.33	0.91
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.51	0.91
10:J:162:LYS:O	10:J:166:GLN:HG3	1.68	0.91
2:B:69:ASN:ND2	2:B:70:ASP:H	1.69	0.90
3:C:160:GLN:NE2	3:C:161:THR:H	1.67	0.90
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.53	0.90
3:Q:60:SER:HB2	16:Q:303:HOH:O	1.72	0.89
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.52	0.89
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.55	0.88
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.37	0.88
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.36	0.88
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.39	0.87
3:C:160:GLN:HE21	3:C:161:THR:N	1.72	0.87
2:P:69:ASN:ND2	2:P:70:ASP:H	1.72	0.87
1:A:12:PHE:H	2:B:20:GLN:HE22	1.18	0.86
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.18	0.86
3:Q:160:GLN:HE21	3:Q:161:THR:N	1.71	0.86
1:A:46:ALA:HB2	1:A:211:LEU:HG	1.56	0.85
1:O:46:ALA:HB2	1:O:211:LEU:HG	1.55	0.85
2:B:12:PHE:H	3:C:17:GLN:HE22	1.20	0.85
11:K:135:PHE:HA	16:X:212:HOH:O	1.74	0.85
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.58	0.85
1:O:128:ARG:HH21	7:U:120:THR:CG2	1.89	0.85
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.41	0.84
3:Q:160:GLN:HE21	3:Q:161:THR:H	0.85	0.84
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.60	0.84
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.41	0.83
3:C:185:THR:HG22	3:C:187:GLU:H	1.42	0.83
5:E:205:LEU:H	5:E:205:LEU:HD23	1.44	0.82
9:W:202:ARG:HG3	16:W:307:HOH:O	1.78	0.82
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.22	0.82
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.61	0.81
10:J:1:MET:HG2	10:J:2:ASP:H	1.45	0.81
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.61	0.81
1:A:30:GLN:HA	1:A:30:GLN:HE21	1.45	0.81
5:S:205:LEU:HD23	5:S:205:LEU:H	1.44	0.81
5:S:12:PHE:HB2	6:T:19:GLN:HE22	1.46	0.81
6:T:65:VAL:HG12	16:T:322:HOH:O	1.80	0.80
3:C:160:GLN:HE21	3:C:161:THR:H	0.86	0.80
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.79	0.80
1:A:128:ARG:HH21	7:G:120:THR:CG2	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:52:MET:HB2	12:L:111:ILE:HG22	1.65	0.79
5:E:200:LEU:HD11	5:E:205:LEU:HD22	1.65	0.79
1:O:30:GLN:HE21	1:O:30:GLN:HA	1.46	0.79
9:I:14:MET:HE3	9:I:166:ILE:HA	1.63	0.79
4:R:155:THR:HG22	5:S:77:ALA:HB3	1.66	0.78
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.65	0.78
4:D:241:ALA:O	4:D:242:GLU:HB2	1.83	0.78
11:K:107:LYS:H	11:K:107:LYS:CD	1.95	0.78
4:R:241:ALA:O	4:R:242:GLU:HB2	1.82	0.78
5:E:69:MET:HE2	5:E:104:VAL:HG22	1.66	0.78
9:W:35:VAL:HG13	16:X:227:HOH:O	1.82	0.78
5:S:200:LEU:HD11	5:S:205:LEU:HD22	1.65	0.78
10:X:1:MET:HG2	10:X:2:ASP:H	1.47	0.77
8:H:81:GLN:O	8:H:85:GLN:HG3	1.84	0.77
5:S:197:SER:HA	5:S:200:LEU:HG	1.65	0.77
5:S:189:ILE:HG23	5:S:212:ILE:HD13	1.66	0.77
3:Q:80:SER:O	3:Q:84:ILE:HG12	1.84	0.77
13:M:130:VAL:HG23	13:M:136:THR:HG22	1.67	0.77
9:W:14:MET:HE3	9:W:166:ILE:HA	1.66	0.77
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.67	0.77
7:G:68:ARG:HB3	16:G:352:HOH:O	1.85	0.77
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.14	0.76
3:C:66:ASP:HA	10:J:69:ILE:HD13	1.67	0.76
6:F:65:VAL:HG12	16:F:308:HOH:O	1.85	0.76
5:E:197:SER:HA	5:E:200:LEU:HG	1.66	0.76
8:V:81:GLN:O	8:V:85:GLN:HG3	1.86	0.76
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.66	0.76
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.83	0.76
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.67	0.76
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.67	0.76
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.68	0.76
2:B:223:GLU:HG2	2:B:224:VAL:N	2.00	0.76
7:U:55:LEU:O	7:U:57:PRO:HD3	1.85	0.76
3:C:80:SER:O	3:C:84:ILE:HG12	1.85	0.76
11:Y:107:LYS:CD	11:Y:107:LYS:H	1.95	0.75
12:Z:52:MET:HB2	12:Z:111:ILE:HG22	1.66	0.75
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.67	0.75
2:B:122:THR:CG2	3:C:125:ARG:HH21	1.99	0.75
5:E:189:ILE:HG23	5:E:212:ILE:HD13	1.68	0.75
12:L:17:GLY:HA3	12:L:20:PHE:CE2	2.22	0.75
12:Z:17:GLY:HA3	12:Z:20:PHE:CE2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:213:VAL:HG23	3:Q:219:ILE:HG12	1.68	0.75
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.69	0.74
7:G:55:LEU:O	7:G:57:PRO:HD3	1.87	0.74
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.68	0.74
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.33	0.74
6:T:31:THR:HG21	6:T:47:GLU:O	1.88	0.74
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.67	0.74
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.68	0.74
6:F:34:ILE:HG22	6:F:160:ALA:CB	2.16	0.74
3:C:9:PHE:H	4:D:15:GLN:HE22	1.33	0.74
2:P:223:GLU:HG2	2:P:224:VAL:N	2.02	0.74
7:G:103:MET:HE3	7:G:108:LEU:HD13	1.70	0.73
7:U:221:LYS:HE3	7:U:221:LYS:HA	1.70	0.73
1:O:178:ARG:HB3	1:O:178:ARG:HH11	1.52	0.73
7:G:103:MET:HE3	7:G:108:LEU:HB2	1.71	0.72
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.36	0.72
3:Q:156:SER:HB2	16:Q:323:HOH:O	1.89	0.72
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.69	0.72
3:C:35:LYS:HG2	3:C:158:SER:O	1.88	0.72
5:E:81:ARG:HG3	5:E:81:ARG:HH11	1.54	0.72
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.02	0.72
6:T:31:THR:HG22	6:T:32:THR:N	2.04	0.72
1:A:204:PHE:CE1	1:A:209:ILE:HD11	2.23	0.72
5:S:81:ARG:HG3	5:S:81:ARG:HH11	1.53	0.72
11:K:208:ASN:HD21	10:X:150:PRO:HG3	1.54	0.72
14:N:51:ASP:O	14:N:55:ILE:HG12	1.90	0.72
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.87	0.72
6:F:31:THR:HG21	6:F:47:GLU:O	1.90	0.72
8:H:3:ILE:CD1	8:H:127:LEU:HB2	2.20	0.72
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.72	0.72
7:U:11:SER:HA	16:U:326:HOH:O	1.90	0.72
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.71	0.72
5:E:12:PHE:HB2	6:F:19:GLN:NE2	2.05	0.71
1:O:119:GLN:O	1:O:122:THR:HB	1.91	0.71
7:G:221:LYS:HE3	7:G:221:LYS:HA	1.71	0.71
10:X:33:ASP:OD2	10:X:35:THR:HG22	1.89	0.71
3:C:64:LYS:HE3	3:C:219:ILE:HD12	1.71	0.71
1:A:178:ARG:HH11	1:A:178:ARG:HB3	1.54	0.71
2:B:119:GLN:O	2:B:122:THR:HB	1.90	0.71
2:P:119:GLN:O	2:P:122:THR:HB	1.90	0.71
3:C:213:VAL:HG23	3:C:219:ILE:HG12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:30:ASN:HD22	7:G:164:PRO:HG2	1.56	0.71
10:J:139:TYR:HD1	16:Y:319:HOH:O	1.74	0.71
8:V:3:ILE:CD1	8:V:127:LEU:HB2	2.19	0.71
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.02	0.71
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.73	0.71
6:F:196:ILE:HG21	6:F:210:LEU:HD13	1.72	0.71
12:L:22:VAL:HG12	12:L:206:ILE:HG13	1.73	0.71
4:D:159:TYR:CE2	4:D:162:LYS:HD3	2.26	0.71
8:V:52:THR:O	8:V:56:THR:HB	1.91	0.71
8:V:53:GLU:O	8:V:56:THR:HG22	1.91	0.70
4:D:186:LYS:O	4:D:190:LEU:HD23	1.91	0.70
5:S:205:LEU:HA	5:S:209:ASN:ND2	2.06	0.70
1:O:204:PHE:CE1	1:O:209:ILE:HD11	2.27	0.70
4:R:186:LYS:O	4:R:190:LEU:HD23	1.91	0.70
10:J:33:ASP:OD2	10:J:35:THR:HG22	1.90	0.70
11:K:107:LYS:N	11:K:107:LYS:HD2	2.05	0.70
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.72	0.70
6:T:196:ILE:HG21	6:T:210:LEU:HD13	1.72	0.70
2:P:122:THR:CG2	3:Q:125:ARG:HH21	2.02	0.70
1:A:119:GLN:O	1:A:122:THR:HB	1.90	0.70
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.26	0.70
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.91	0.70
7:U:30:ASN:HD22	7:U:164:PRO:HG2	1.56	0.70
13:M:48:ASN:H	13:M:48:ASN:HD22	1.38	0.70
12:Z:22:VAL:HG12	12:Z:206:ILE:HG13	1.73	0.70
7:U:117:GLN:O	7:U:120:THR:HB	1.92	0.69
13:M:51:VAL:HG22	13:M:116:VAL:HG22	1.74	0.69
3:Q:64:LYS:HE3	3:Q:219:ILE:HD12	1.73	0.69
8:H:52:THR:O	8:H:56:THR:HB	1.92	0.69
3:C:204:GLY:HA3	3:C:207:ASN:HB2	1.75	0.69
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.25	0.69
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.74	0.69
10:X:14:ILE:HD13	10:X:158:LEU:HD23	1.74	0.69
11:K:208:ASN:HD21	10:X:150:PRO:CG	2.06	0.69
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.27	0.69
3:Q:35:LYS:HG2	3:Q:158:SER:O	1.92	0.69
14:N:105:LYS:HD3	14:N:105:LYS:O	1.93	0.69
7:G:117:GLN:O	7:G:120:THR:HB	1.91	0.69
3:C:51:LYS:O	3:C:52:LEU:HB2	1.93	0.69
9:W:17:LYS:HD3	9:W:156:ASN:HD22	1.57	0.69
13:M:174:GLU:O	13:M:178:VAL:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:202:LEU:HB2	12:Z:219:LEU:HD11	1.75	0.68
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.90	0.68
13:M:172:VAL:HG21	16:M:350:HOH:O	1.94	0.68
6:F:31:THR:HG22	6:F:32:THR:N	2.07	0.68
12:Z:126:ASP:HB2	12:Z:130:SER:H	1.57	0.68
9:I:17:LYS:HD3	9:I:156:ASN:HD22	1.58	0.68
5:E:205:LEU:HA	5:E:209:ASN:ND2	2.08	0.68
5:S:77:ALA:HB3	5:S:78:PRO:HD3	1.75	0.68
12:L:126:ASP:HB2	12:L:130:SER:H	1.57	0.68
6:T:78:ILE:HB	6:T:79:PRO:HD3	1.76	0.68
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.76	0.68
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	1.75	0.68
1:O:176:GLU:HG2	2:P:55:LEU:HD21	1.76	0.67
10:J:149:ARG:O	10:J:152:MET:HG3	1.95	0.67
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.75	0.67
5:S:127:TYR:O	5:S:148:PRO:HB3	1.94	0.67
5:S:206:THR:H	5:S:209:ASN:HD22	1.41	0.67
12:L:202:LEU:HB2	12:L:219:LEU:HD11	1.75	0.67
5:E:207:VAL:HG13	5:E:208:ASP:N	2.09	0.67
2:B:43:ILE:CD1	2:B:145:TYR:HB3	2.22	0.67
14:N:21:THR:HG22	14:N:26:ILE:HA	1.77	0.67
5:E:167:ALA:HB2	5:E:195:ALA:O	1.95	0.67
4:R:180:HIS:O	4:R:183:LEU:HD12	1.95	0.67
5:S:136:TYR:CE2	5:S:217:LYS:HA	2.29	0.66
1:A:172:LYS:O	1:A:176:GLU:HG3	1.95	0.66
1:O:178:ARG:HB3	1:O:178:ARG:NH1	2.10	0.66
5:S:12:PHE:HB2	6:T:19:GLN:NE2	2.10	0.66
5:E:77:ALA:HB3	5:E:78:PRO:HD3	1.76	0.66
4:D:180:HIS:O	4:D:183:LEU:HD12	1.95	0.66
5:S:207:VAL:HG13	5:S:208:ASP:N	2.10	0.66
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.11	0.66
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.31	0.66
10:J:14:ILE:HD13	10:J:158:LEU:HD23	1.78	0.66
9:W:148:MET:HE3	9:W:152:LEU:HD11	1.78	0.66
5:E:136:TYR:CE2	5:E:217:LYS:HA	2.31	0.66
6:F:147:LEU:HB3	16:F:333:HOH:O	1.96	0.66
3:Q:51:LYS:HD2	3:Q:52:LEU:N	2.11	0.66
5:S:167:ALA:HB2	5:S:195:ALA:O	1.96	0.66
6:F:78:ILE:HB	6:F:79:PRO:HD3	1.77	0.65
6:T:143:HIS:HD2	16:T:301:HOH:O	1.78	0.65
1:O:176:GLU:HG2	2:P:55:LEU:CD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:VAL:HA	5:E:233:ILE:HD11	1.79	0.65
3:C:60:SER:HB2	16:C:309:HOH:O	1.96	0.65
12:L:28:ARG:NE	12:L:200:ASP:OD2	2.30	0.65
12:L:195:HIS:HD2	12:L:197:GLN:H	1.44	0.65
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.77	0.65
2:P:85:ILE:O	2:P:89:THR:HG23	1.96	0.65
1:A:178:ARG:HB3	1:A:178:ARG:NH1	2.11	0.65
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.30	0.65
6:F:191:GLN:O	6:F:195:ILE:HG12	1.97	0.65
2:P:48:GLU:OE2	2:P:200:THR:HG23	1.96	0.65
10:X:149:ARG:O	10:X:152:MET:HG3	1.97	0.65
3:Q:66:ASP:HA	10:X:69:ILE:HD13	1.78	0.65
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.25	0.65
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.10	0.65
2:P:119:GLN:HG3	3:Q:78:ALA:HB1	1.79	0.65
10:J:150:PRO:HG3	11:Y:208:ASN:HD21	1.60	0.65
5:E:193:VAL:O	5:E:196:ILE:HG22	1.97	0.65
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.79	0.65
7:U:202:ILE:HG23	7:U:207:THR:O	1.96	0.65
12:L:38:ARG:NH1	12:L:221:ARG:HB3	2.12	0.65
12:Z:181:ILE:O	12:Z:185:ARG:HG3	1.96	0.65
13:M:153:PRO:HA	8:V:165:ASN:OD1	1.97	0.65
12:Z:38:ARG:NH1	12:Z:221:ARG:HB3	2.11	0.65
5:S:9:THR:HG21	5:S:119:THR:HA	1.78	0.65
3:C:27:ARG:HD2	16:C:319:HOH:O	1.96	0.65
2:B:48:GLU:OE2	2:B:200:THR:HG23	1.97	0.64
5:S:207:VAL:HA	5:S:233:ILE:HD11	1.79	0.64
9:I:14:MET:HE3	9:I:166:ILE:CA	2.26	0.64
3:C:51:LYS:HD2	3:C:52:LEU:N	2.12	0.64
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.79	0.64
5:E:9:THR:HG21	5:E:119:THR:HA	1.79	0.64
13:M:89:PRO:HD2	13:M:120:GLN:OE1	1.97	0.64
10:X:127:GLU:O	10:X:128:LEU:HD23	1.97	0.64
2:B:69:ASN:ND2	2:B:70:ASP:N	2.44	0.64
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.45	0.64
12:Z:28:ARG:NE	12:Z:200:ASP:OD2	2.30	0.64
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.79	0.64
9:I:148:MET:HE3	9:I:152:LEU:HD11	1.80	0.64
5:S:193:VAL:O	5:S:196:ILE:HG22	1.98	0.64
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.61	0.64
7:G:148:THR:HG22	7:G:154:TYR:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.45	0.64
2:P:217:LYS:HG3	2:P:223:GLU:O	1.97	0.64
10:J:53:THR:HG23	10:J:54:VAL:N	2.13	0.64
8:H:3:ILE:HG12	8:H:99:ILE:HD12	1.78	0.64
6:T:147:LEU:HD13	6:T:153:TYR:HB3	1.79	0.64
4:R:94:TYR:O	12:Z:91:ARG:HG3	1.98	0.64
2:B:217:LYS:HG3	2:B:223:GLU:O	1.98	0.64
3:C:27:ARG:HB2	3:C:27:ARG:NH1	2.12	0.64
10:J:127:GLU:O	10:J:128:LEU:HD23	1.97	0.64
2:P:158:GLY:HA3	3:Q:57:ILE:CD1	2.28	0.64
5:S:90:GLN:HG3	5:S:110:LEU:HD13	1.78	0.64
7:U:103:MET:HE3	7:U:108:LEU:HB2	1.80	0.64
9:W:120:ILE:HD12	9:W:136:ILE:HD13	1.79	0.64
12:Z:13:LEU:HD11	12:Z:150:LEU:CD2	2.28	0.64
13:M:49:THR:OG1	13:M:89:PRO:HG3	1.98	0.64
11:Y:145:LYS:O	11:Y:148:LEU:HD13	1.98	0.64
7:G:202:ILE:HG23	7:G:207:THR:O	1.97	0.64
1:A:246:ARG:HG3	1:A:246:ARG:HH11	1.63	0.64
13:M:161:ARG:CG	13:M:161:ARG:HH11	2.10	0.63
12:Z:13:LEU:HD12	12:Z:14:GLY:H	1.63	0.63
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.28	0.63
8:H:53:GLU:O	8:H:56:THR:HG22	1.98	0.63
6:F:36:ILE:HD12	6:F:192:ALA:HB2	1.80	0.63
5:S:69:MET:HE2	5:S:104:VAL:HA	1.79	0.63
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.33	0.63
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.44	0.63
3:Q:27:ARG:HB2	3:Q:27:ARG:NH1	2.13	0.63
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.64	0.63
1:O:246:ARG:HH11	1:O:246:ARG:HG3	1.61	0.63
5:E:206:THR:H	5:E:209:ASN:HD22	1.44	0.63
10:J:150:PRO:CG	11:Y:208:ASN:HD21	2.10	0.63
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.79	0.63
5:E:90:GLN:HG3	5:E:110:LEU:HD13	1.80	0.63
13:M:114:ILE:HB	13:M:130:VAL:HG12	1.80	0.63
2:B:220:ASN:O	2:B:221:ASP:HB2	1.99	0.63
7:U:148:THR:HG22	7:U:154:TYR:HB2	1.81	0.63
4:R:9:PRO:HA	5:S:23:TYR:CD2	2.34	0.63
4:D:155:THR:HG22	5:E:77:ALA:HB3	1.80	0.63
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.34	0.63
6:T:31:THR:CG2	6:T:32:THR:N	2.62	0.63
11:K:21:THR:HG22	11:K:26:VAL:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:30:GLN:CA	1:O:30:GLN:HE21	2.12	0.63
5:S:69:MET:HE2	5:S:104:VAL:HG22	1.79	0.63
9:I:120:ILE:HD12	9:I:136:ILE:HD13	1.79	0.63
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.99	0.63
6:T:185:ALA:O	6:T:189:VAL:HG23	1.99	0.63
11:Y:21:THR:HG22	11:Y:26:VAL:HA	1.81	0.63
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.34	0.62
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.80	0.62
3:C:101:PRO:HG2	3:C:138:PRO:CG	2.29	0.62
6:T:191:GLN:O	6:T:195:ILE:HG12	1.99	0.62
8:V:195:VAL:HG23	16:V:316:HOH:O	1.99	0.62
1:O:28:VAL:HG13	1:O:76:SER:O	1.99	0.62
5:E:127:TYR:O	5:E:148:PRO:HB3	1.99	0.62
2:B:158:GLY:HA3	3:C:57:ILE:CD1	2.29	0.62
1:O:172:LYS:O	1:O:176:GLU:HG3	1.99	0.62
5:E:207:VAL:HG13	5:E:208:ASP:H	1.64	0.62
6:F:147:LEU:HD13	6:F:153:TYR:HB3	1.81	0.62
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.79	0.62
4:R:193:LEU:HD21	4:R:232:ILE:HD12	1.82	0.62
10:X:53:THR:HG23	10:X:54:VAL:N	2.14	0.62
4:D:94:TYR:O	12:L:91:ARG:HG3	1.99	0.62
13:M:119:VAL:HG23	13:M:200:ILE:HG22	1.79	0.62
12:L:181:ILE:O	12:L:185:ARG:HG3	2.00	0.62
11:Y:7:ARG:HG2	11:Y:110:PRO:HB2	1.80	0.62
2:P:69:ASN:ND2	2:P:70:ASP:N	2.46	0.62
11:K:208:ASN:ND2	10:X:150:PRO:HD3	2.14	0.62
8:H:132:LEU:HB2	16:H:315:HOH:O	1.99	0.62
2:B:85:ILE:O	2:B:89:THR:HG23	2.00	0.62
3:C:190:VAL:O	3:C:194:VAL:HG23	2.00	0.62
11:K:7:ARG:HG2	11:K:110:PRO:HB2	1.82	0.62
12:L:13:LEU:HD11	12:L:150:LEU:CD2	2.29	0.62
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.63	0.62
12:L:13:LEU:HD12	12:L:14:GLY:H	1.63	0.61
3:Q:91:ALA:O	3:Q:95:ARG:HG3	2.00	0.61
9:W:9:GLY:HA2	9:W:25:ASP:OD1	2.00	0.61
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.82	0.61
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.35	0.61
12:Z:3:ASN:ND2	12:Z:5:TYR:H	1.97	0.61
10:J:45:SER:OG	10:J:103:LEU:HB2	2.00	0.61
13:M:179:ASN:ND2	13:M:182:ARG:HH11	1.98	0.61
10:X:45:SER:OG	10:X:103:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:51:PRO:HG2	7:G:52:ASP:H	1.65	0.61
6:F:31:THR:CG2	6:F:32:THR:N	2.63	0.61
14:N:6:VAL:CG2	14:N:155:ILE:HD11	2.31	0.61
7:U:198:ILE:HG23	7:U:214:LEU:HD11	1.83	0.61
3:C:91:ALA:O	3:C:95:ARG:HG3	2.00	0.61
2:B:89:THR:HG22	16:B:335:HOH:O	2.00	0.61
5:E:45:LEU:HG	5:E:134:ILE:HD13	1.81	0.61
4:D:197:LYS:HG3	16:D:310:HOH:O	2.00	0.61
2:B:180:LYS:O	2:B:183:MET:HG3	2.01	0.61
7:G:155:VAL:HG22	7:G:156:GLY:N	2.16	0.61
2:P:220:ASN:O	2:P:221:ASP:HB2	1.99	0.61
5:S:207:VAL:HG13	5:S:208:ASP:H	1.65	0.61
6:T:186:ARG:HH11	6:T:186:ARG:HG3	1.66	0.61
8:V:3:ILE:HG12	8:V:99:ILE:HD12	1.83	0.61
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.83	0.61
10:J:150:PRO:HD3	11:Y:208:ASN:ND2	2.16	0.61
5:E:162:ALA:HB3	16:E:321:HOH:O	2.00	0.60
1:A:128:ARG:NH2	7:G:120:THR:HG22	2.08	0.60
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.83	0.60
4:D:193:LEU:HD21	4:D:232:ILE:HD12	1.83	0.60
12:Z:103:PHE:N	12:Z:104:PRO:HD3	2.16	0.60
1:A:160:LYS:HE3	2:B:57:GLU:OE1	2.00	0.60
11:Y:107:LYS:N	11:Y:107:LYS:HD2	2.05	0.60
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.83	0.60
3:C:101:PRO:HG2	3:C:138:PRO:HG3	1.82	0.60
14:N:8:PHE:HE2	14:N:13:ILE:HG13	1.67	0.60
12:L:3:ASN:ND2	12:L:5:TYR:H	1.98	0.60
7:U:5:ARG:HD3	7:U:17:TYR:CD2	2.36	0.60
3:Q:101:PRO:HG2	3:Q:138:PRO:CG	2.31	0.60
4:R:45:ARG:HG2	4:R:45:ARG:O	2.00	0.60
2:B:18:LEU:HD13	2:B:122:THR:HG23	1.82	0.60
2:P:18:LEU:HD13	2:P:122:THR:HG23	1.82	0.60
3:Q:167:LYS:HB2	16:Q:316:HOH:O	2.01	0.60
6:F:185:ALA:O	6:F:189:VAL:HG23	2.01	0.60
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.66	0.60
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.82	0.60
9:W:14:MET:HE3	9:W:166:ILE:CA	2.31	0.60
5:S:45:LEU:HG	5:S:134:ILE:HD13	1.83	0.60
2:B:233:GLU:O	2:B:237:ILE:HG22	2.02	0.60
4:R:60:VAL:HA	16:R:324:HOH:O	2.02	0.60
7:G:194:VAL:O	7:G:198:ILE:HG13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:119:ALA:HB3	4:R:124:ARG:HD3	1.83	0.60
5:E:14:PRO:HA	6:F:22:TYR:CD2	2.36	0.60
12:L:206:ILE:HD12	12:L:206:ILE:N	2.17	0.60
1:A:17:LYS:HE3	1:A:22:ASP:OD1	2.01	0.60
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.82	0.60
6:T:8:ASN:HB3	6:T:123:ASN:HA	1.84	0.59
1:A:66:LEU:C	1:A:66:LEU:HD23	2.22	0.59
11:K:106:ARG:HG2	11:K:106:ARG:HH11	1.67	0.59
11:Y:106:ARG:HH11	11:Y:106:ARG:HG2	1.67	0.59
2:P:180:LYS:O	2:P:183:MET:HG3	2.02	0.59
14:N:14:LEU:O	14:N:175:MET:HA	2.01	0.59
1:O:128:ARG:NH2	7:U:120:THR:HG22	2.06	0.59
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.84	0.59
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.00	0.59
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.84	0.59
11:K:61:SER:O	11:K:65:LEU:HD23	2.01	0.59
6:T:36:ILE:HD12	6:T:192:ALA:HB2	1.84	0.59
5:S:73:LEU:HD12	5:S:73:LEU:O	2.03	0.59
9:W:171:LEU:CD2	9:W:199:LEU:HD13	2.33	0.59
10:J:53:THR:HG23	10:J:54:VAL:HG23	1.83	0.59
7:U:51:PRO:HG2	7:U:52:ASP:H	1.68	0.59
1:O:66:LEU:C	1:O:66:LEU:HD23	2.23	0.59
6:F:186:ARG:HG3	6:F:186:ARG:HH11	1.66	0.59
7:G:185:ILE:N	7:G:185:ILE:HD12	2.18	0.59
5:S:200:LEU:O	5:S:201:ARG:HB2	2.03	0.59
13:M:150:MET:C	13:M:153:PRO:HD2	2.23	0.59
3:Q:101:PRO:HG2	3:Q:138:PRO:HG3	1.84	0.59
7:G:198:ILE:HG23	7:G:214:LEU:HD11	1.85	0.59
7:U:239:ILE:C	7:U:239:ILE:HD12	2.23	0.59
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.68	0.59
6:F:8:ASN:HB3	6:F:123:ASN:HA	1.85	0.59
5:E:35:VAL:HG22	5:E:159:ALA:HB2	1.85	0.59
5:S:181:ILE:HG21	5:S:187:GLU:HB2	1.85	0.59
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.68	0.59
5:S:95:SER:O	5:S:99:ASN:HA	2.03	0.58
4:R:1:ASP:O	4:R:2:ARG:HB2	2.03	0.58
6:T:183:LEU:HD11	6:T:187:GLU:HB3	1.85	0.58
11:Y:61:SER:O	11:Y:65:LEU:HD23	2.03	0.58
11:K:145:LYS:O	11:K:148:LEU:HD13	2.03	0.58
12:Z:14:GLY:O	12:Z:136:CYS:HA	2.03	0.58
5:E:95:SER:O	5:E:99:ASN:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:26:SER:HB2	11:Y:133:GLN:HE22	1.69	0.58
3:Q:92:GLN:HG2	16:Q:302:HOH:O	2.02	0.58
9:W:137:VAL:HG11	9:W:145:LEU:HB3	1.85	0.58
5:E:73:LEU:HD12	5:E:73:LEU:O	2.03	0.58
12:Z:206:ILE:HD12	12:Z:206:ILE:N	2.17	0.58
6:T:8:ASN:O	6:T:10:VAL:N	2.33	0.58
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.85	0.58
4:R:197:LYS:HA	16:R:304:HOH:O	2.03	0.58
1:O:29:LYS:HE2	1:O:29:LYS:HA	1.85	0.58
1:O:17:LYS:HE3	1:O:22:ASP:OD1	2.04	0.58
5:E:51:ASN:ND2	5:E:53:ASP:O	2.36	0.58
7:U:155:VAL:HG22	7:U:156:GLY:N	2.18	0.58
2:P:95:GLN:HG2	16:P:306:HOH:O	2.02	0.58
1:O:211:LEU:HD22	1:O:238:LEU:CD1	2.30	0.58
6:T:105:ILE:HG21	6:T:143:HIS:HB2	1.86	0.58
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.85	0.58
10:J:129:PRO:HB2	10:J:130:TYR:CD1	2.39	0.58
8:V:156:SER:O	8:V:160:GLN:HG3	2.03	0.58
7:U:185:ILE:N	7:U:185:ILE:HD12	2.19	0.58
11:Y:145:LYS:HB2	11:Y:148:LEU:CD1	2.34	0.58
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.86	0.58
4:D:119:ALA:HB3	4:D:124:ARG:HD3	1.84	0.58
2:P:233:GLU:O	2:P:237:ILE:HG22	2.03	0.58
4:D:45:ARG:O	4:D:45:ARG:HG2	2.02	0.58
12:L:103:PHE:N	12:L:104:PRO:HD3	2.17	0.58
6:T:132:THR:O	6:T:146:MET:HA	2.04	0.58
1:A:29:LYS:HA	1:A:29:LYS:HE2	1.85	0.58
6:F:132:THR:O	6:F:146:MET:HA	2.04	0.58
12:L:52:MET:CB	12:L:111:ILE:HG22	2.33	0.58
5:E:55:LEU:HD12	5:E:55:LEU:N	2.19	0.58
5:S:42:HIS:HD2	5:S:214:ILE:HD11	1.69	0.58
8:H:156:SER:O	8:H:160:GLN:HG3	2.04	0.58
7:U:31:ILE:HG23	7:U:47:GLN:HB2	1.86	0.58
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.85	0.57
12:L:14:GLY:O	12:L:136:CYS:HA	2.04	0.57
4:R:89:VAL:HG21	11:Y:65:LEU:HD22	1.86	0.57
6:F:183:LEU:HD11	6:F:187:GLU:HB3	1.84	0.57
3:Q:230:TYR:O	3:Q:234:ILE:HG13	2.04	0.57
9:I:170:LEU:HD21	9:I:184:ALA:HB1	1.86	0.57
2:P:200:THR:HG22	2:P:202:SER:N	2.09	0.57
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:83:LYS:HG3	14:N:119:VAL:HG22	1.85	0.57
12:Z:109:THR:HG23	16:Z:309:HOH:O	2.03	0.57
7:U:68:ARG:HB2	7:U:68:ARG:HH11	1.69	0.57
2:P:43:ILE:CD1	2:P:145:TYR:HB3	2.23	0.57
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.04	0.57
5:E:42:HIS:HD2	5:E:214:ILE:HD11	1.69	0.57
11:K:75:SER:HB2	11:K:108:GLU:OE2	2.04	0.57
1:A:28:VAL:HG13	1:A:76:SER:O	2.04	0.57
5:E:200:LEU:O	5:E:201:ARG:HB2	2.03	0.57
5:S:35:VAL:HG22	5:S:159:ALA:HB2	1.86	0.57
5:E:134:ILE:HG22	5:E:143:LEU:HD13	1.87	0.57
11:K:197:PHE:CE1	9:W:203:GLN:HG3	2.39	0.57
1:O:180:ASN:H	1:O:183:LEU:HD12	1.69	0.57
10:X:53:THR:HG23	10:X:54:VAL:HG23	1.86	0.57
12:Z:3:ASN:HD22	12:Z:3:ASN:C	2.06	0.57
12:Z:100:LYS:HE3	12:Z:103:PHE:O	2.04	0.57
13:M:21:ILE:HG23	13:M:197:LEU:HD21	1.85	0.57
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.03	0.57
6:F:175:LEU:HD11	6:F:191:GLN:HG3	1.86	0.57
12:Z:3:ASN:HD22	12:Z:4:PRO:CD	2.18	0.57
6:F:8:ASN:O	6:F:10:VAL:N	2.33	0.57
1:A:37:ILE:N	1:A:37:ILE:HD12	2.19	0.57
1:A:180:ASN:H	1:A:183:LEU:HD12	1.70	0.57
9:W:31:GLN:HB3	16:W:334:HOH:O	2.04	0.57
6:T:75:SER:HA	16:T:330:HOH:O	2.05	0.57
9:I:14:MET:HE3	9:I:166:ILE:HG13	1.87	0.57
3:C:66:ASP:OD1	3:C:95:ARG:NH1	2.36	0.57
4:D:176:LEU:HD13	5:E:55:LEU:HD11	1.87	0.57
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.70	0.57
7:U:68:ARG:HB2	7:U:68:ARG:NH1	2.19	0.57
9:W:170:LEU:HD21	9:W:184:ALA:HB1	1.87	0.57
7:G:239:ILE:HD12	7:G:239:ILE:C	2.25	0.57
9:W:55:LEU:HG	9:W:57:THR:HG22	1.86	0.57
6:F:32:THR:HG23	6:F:47:GLU:OE2	2.05	0.57
9:I:55:LEU:HG	9:I:57:THR:HG22	1.87	0.57
9:W:165:THR:HG23	16:W:318:HOH:O	2.05	0.57
7:U:216:VAL:HB	7:U:227:LEU:HD12	1.87	0.57
8:H:34:LEU:HB2	16:H:326:HOH:O	2.03	0.57
9:I:14:MET:CE	9:I:166:ILE:HA	2.32	0.56
6:T:32:THR:HG23	6:T:47:GLU:OE2	2.05	0.56
1:A:211:LEU:HD23	1:A:212:ALA:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:68:ARG:HB2	7:G:68:ARG:HH11	1.70	0.56
13:M:179:ASN:HB3	16:M:318:HOH:O	2.04	0.56
14:N:59:VAL:HG22	14:N:81:VAL:HG12	1.88	0.56
1:O:78:MET:H	1:O:132:VAL:HG12	1.70	0.56
7:G:5:ARG:HD3	7:G:17:TYR:CD2	2.40	0.56
2:B:119:GLN:HG3	3:C:78:ALA:HB1	1.87	0.56
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.35	0.56
1:O:211:LEU:HD23	1:O:212:ALA:N	2.21	0.56
1:A:110:LEU:O	1:A:114:VAL:HG23	2.06	0.56
5:E:181:ILE:HG21	5:E:187:GLU:HB2	1.86	0.56
12:L:3:ASN:HD22	12:L:3:ASN:C	2.08	0.56
13:M:18:ASN:HB2	16:M:359:HOH:O	2.05	0.56
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.35	0.56
1:O:37:ILE:HD12	1:O:37:ILE:N	2.20	0.56
3:Q:107:LEU:O	3:Q:111:VAL:HG23	2.04	0.56
1:A:176:GLU:CG	2:B:55:LEU:HD21	2.21	0.56
7:U:194:VAL:O	7:U:198:ILE:HG13	2.04	0.56
4:D:89:VAL:HG21	11:K:65:LEU:HD22	1.87	0.56
4:R:82:GLU:OE2	11:Y:69:ARG:NH1	2.38	0.56
8:H:73:GLU:OE1	8:H:73:GLU:HA	2.03	0.56
2:P:38:MET:HG3	2:P:43:ILE:CD1	2.36	0.56
10:J:174:MET:CE	10:X:174:MET:HG2	2.36	0.56
1:O:110:LEU:O	1:O:114:VAL:HG23	2.05	0.56
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.41	0.56
9:W:14:MET:CE	9:W:166:ILE:HA	2.35	0.56
7:G:68:ARG:HB2	7:G:68:ARG:NH1	2.20	0.56
2:P:106:PRO:HD2	2:P:109:ILE:HD12	1.87	0.56
1:A:113:GLU:HA	1:A:113:GLU:OE1	2.06	0.56
5:S:134:ILE:HG22	5:S:143:LEU:HD13	1.86	0.56
6:T:175:LEU:HD11	6:T:191:GLN:HG3	1.87	0.56
13:M:197:LEU:HD23	13:M:198:ALA:N	2.21	0.56
12:L:68:PHE:O	12:L:71:SER:HB3	2.06	0.56
9:I:9:GLY:HA2	9:I:25:ASP:OD1	2.05	0.56
5:E:231:LYS:HD2	5:E:231:LYS:H	1.70	0.56
1:A:35:LEU:HB3	1:A:163:ALA:HB2	1.88	0.56
9:I:171:LEU:CD2	9:I:199:LEU:HD13	2.35	0.56
5:S:184:ASN:OD1	5:S:187:GLU:HG2	2.06	0.56
13:M:179:ASN:ND2	13:M:182:ARG:NH1	2.54	0.56
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.88	0.56
11:K:145:LYS:HB2	11:K:148:LEU:CD1	2.35	0.56
7:G:3:TYR:C	7:G:5:ARG:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:183:ASP:O	7:U:184:HIS:HB3	2.06	0.56
4:D:1:ASP:O	4:D:2:ARG:HB2	2.05	0.56
5:S:181:ILE:CG2	5:S:187:GLU:HB2	2.35	0.56
1:A:90:ARG:NH1	16:A:309:HOH:O	2.35	0.56
3:C:230:TYR:O	3:C:234:ILE:HG13	2.04	0.56
5:S:51:ASN:ND2	5:S:53:ASP:O	2.39	0.56
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.04	0.55
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.88	0.55
5:E:205:LEU:H	5:E:205:LEU:CD2	2.17	0.55
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.88	0.55
3:C:107:LEU:O	3:C:111:VAL:HG23	2.06	0.55
7:G:216:VAL:HB	7:G:227:LEU:HD12	1.87	0.55
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.41	0.55
2:B:49:ARG:NH2	2:B:58:GLN:HE21	2.04	0.55
9:W:37:ASN:ND2	9:W:37:ASN:H	2.04	0.55
14:N:84:GLU:HA	14:N:84:GLU:OE2	2.06	0.55
7:U:103:MET:HE3	7:U:108:LEU:CD1	2.34	0.55
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.87	0.55
6:F:105:ILE:HG21	6:F:143:HIS:HB2	1.87	0.55
6:F:205:GLU:HG3	6:F:206:LYS:HG3	1.88	0.55
4:D:104:LEU:C	4:D:104:LEU:HD13	2.27	0.55
3:C:185:THR:HB	3:C:188:GLU:HG2	1.87	0.55
5:E:69:MET:HE2	5:E:104:VAL:HA	1.88	0.55
14:N:13:ILE:HD12	14:N:151:THR:HG22	1.89	0.55
6:T:205:GLU:HG3	6:T:206:LYS:HG3	1.89	0.55
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.89	0.55
5:S:65:CYS:SG	5:S:87:LEU:HD23	2.47	0.55
9:W:17:LYS:HD3	9:W:156:ASN:HB3	1.89	0.55
2:P:49:ARG:NH2	2:P:58:GLN:HE21	2.04	0.55
2:P:99:LYS:HZ2	10:X:86:GLN:HE22	1.54	0.55
10:J:174:MET:HG2	10:X:174:MET:CE	2.37	0.55
5:S:55:LEU:N	5:S:55:LEU:HD12	2.21	0.55
2:P:99:LYS:NZ	10:X:86:GLN:NE2	2.54	0.55
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.41	0.55
1:O:158:PRO:O	2:P:56:LEU:HD12	2.07	0.55
7:G:183:ASP:O	7:G:184:HIS:HB3	2.07	0.55
12:Z:68:PHE:O	12:Z:71:SER:HB3	2.07	0.55
7:U:169:ILE:HD12	7:U:201:MET:CE	2.36	0.55
9:I:203:GLN:HG3	11:Y:197:PHE:CE1	2.42	0.55
13:M:25:ASP:HA	13:M:195:PHE:CB	2.36	0.55
10:J:26:SER:HB2	11:K:133:GLN:HE22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.71	0.55
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.88	0.55
9:I:97:ARG:HD2	16:I:357:HOH:O	2.06	0.55
1:O:239:THR:OG1	1:O:242:GLU:HG3	2.07	0.55
5:S:189:ILE:HD12	5:S:189:ILE:N	2.22	0.55
5:S:35:VAL:HG12	5:S:36:GLY:N	2.22	0.55
5:E:184:ASN:OD1	5:E:187:GLU:HG2	2.05	0.55
10:J:53:THR:CG2	10:J:54:VAL:N	2.70	0.55
2:B:159:TRP:CE3	2:B:162:ILE:HD13	2.41	0.55
2:P:228:ILE:HD12	2:P:228:ILE:N	2.22	0.55
5:S:1:PHE:O	5:S:3:ASN:N	2.40	0.55
10:X:146:HIS:HD2	10:X:147:HIS:CE1	2.25	0.55
2:P:244:THR:OXT	2:P:244:THR:HG22	2.07	0.55
10:X:149:ARG:HH11	10:X:149:ARG:HG2	1.72	0.54
5:E:181:ILE:CG2	5:E:187:GLU:HB2	2.36	0.54
12:L:3:ASN:HD22	12:L:4:PRO:N	2.05	0.54
7:U:230:GLU:HG2	16:U:357:HOH:O	2.07	0.54
6:T:193:ALA:O	6:T:197:TYR:HD1	1.89	0.54
8:V:73:GLU:OE1	8:V:73:GLU:HA	2.05	0.54
1:A:211:LEU:HD22	1:A:238:LEU:CD1	2.29	0.54
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.42	0.54
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.89	0.54
12:L:121:ALA:HB2	12:L:133:ARG:NH2	2.22	0.54
7:G:235:ARG:HA	7:G:235:ARG:HE	1.72	0.54
1:A:83:ARG:HE	7:G:114:ASN:ND2	2.05	0.54
2:P:190:GLU:O	2:P:194:LYS:HG2	2.07	0.54
1:A:78:MET:H	1:A:132:VAL:HG12	1.73	0.54
2:P:162:ILE:HG13	2:P:163:SER:N	2.23	0.54
9:W:141:ALA:HB2	9:W:177:ASP:HB2	1.89	0.54
5:S:12:PHE:H	6:T:19:GLN:HE22	1.54	0.54
12:Z:52:MET:CB	12:Z:111:ILE:HG22	2.34	0.54
5:S:185:PRO:HG2	5:S:186:ASP:H	1.72	0.54
6:T:147:LEU:CD1	6:T:153:TYR:HB3	2.37	0.54
12:Z:121:ALA:HB2	12:Z:133:ARG:NH2	2.22	0.54
6:F:66:VAL:HG11	6:F:108:PHE:CE1	2.42	0.54
11:Y:75:SER:HB2	11:Y:108:GLU:OE2	2.07	0.54
7:G:169:ILE:HD12	7:G:201:MET:CE	2.37	0.54
9:I:37:ASN:ND2	9:I:37:ASN:H	2.05	0.54
5:E:99:ASN:HB2	13:M:94:GLU:HG2	1.88	0.54
1:O:89:SER:O	1:O:92:VAL:HG12	2.08	0.54
2:B:24:ALA:O	2:B:28:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:TYR:CD1	5:E:114:LYS:HD2	2.42	0.54
4:R:104:LEU:C	4:R:104:LEU:HD13	2.28	0.54
1:O:12:PHE:N	2:P:20:GLN:HE22	1.94	0.54
2:P:119:GLN:NE2	16:P:310:HOH:O	2.41	0.54
9:W:14:MET:HE3	9:W:166:ILE:HG13	1.88	0.54
10:X:139:TYR:CE2	10:X:172:MET:HG3	2.43	0.54
2:P:180:LYS:HE2	2:P:182:ASP:OD1	2.08	0.54
9:W:137:VAL:CG1	9:W:145:LEU:HB3	2.37	0.54
1:O:239:THR:O	1:O:243:ILE:HG12	2.08	0.54
9:I:137:VAL:HG11	9:I:145:LEU:HB3	1.88	0.54
9:I:141:ALA:HB2	9:I:177:ASP:HB2	1.88	0.54
1:A:4:ARG:HB2	2:B:2:SER:OG	2.08	0.54
5:S:205:LEU:CD2	5:S:205:LEU:H	2.17	0.54
7:G:103:MET:HB3	16:G:306:HOH:O	2.07	0.54
2:P:159:TRP:CE3	2:P:162:ILE:HD13	2.42	0.54
7:U:78:ILE:N	7:U:79:PRO:HD2	2.23	0.54
12:L:108:HIS:HE1	12:L:124:SER:HB2	1.73	0.54
5:E:13:SER:HB3	5:E:17:ARG:H	1.73	0.54
7:G:112:MET:HE3	16:G:331:HOH:O	2.07	0.54
2:B:69:ASN:HD22	2:B:70:ASP:H	1.52	0.54
12:L:3:ASN:HD22	12:L:4:PRO:CD	2.20	0.54
13:M:21:ILE:CG2	13:M:197:LEU:HD21	2.38	0.54
10:X:130:TYR:CD2	10:X:144:LEU:HD13	2.43	0.54
2:B:190:GLU:O	2:B:194:LYS:HG2	2.08	0.54
14:N:9:LYS:O	14:N:107:LYS:HD3	2.07	0.54
9:W:171:LEU:HD21	9:W:199:LEU:HD13	1.89	0.54
7:G:103:MET:HE3	7:G:108:LEU:CB	2.38	0.54
2:B:106:PRO:HD2	2:B:109:ILE:HD12	1.89	0.54
12:Z:3:ASN:HD22	12:Z:4:PRO:N	2.05	0.54
7:U:190:TRP:O	7:U:194:VAL:HG23	2.08	0.54
7:G:190:TRP:O	7:G:194:VAL:HG23	2.08	0.54
11:Y:151:GLU:HB2	16:Y:332:HOH:O	2.07	0.54
2:B:244:THR:OXT	2:B:244:THR:HG22	2.08	0.54
8:H:3:ILE:HB	8:H:44:ALA:HB1	1.90	0.53
5:S:35:VAL:HG22	5:S:159:ALA:CB	2.38	0.53
5:E:35:VAL:HG22	5:E:159:ALA:CB	2.37	0.53
13:M:48:ASN:HD22	13:M:48:ASN:N	2.01	0.53
5:S:214:ILE:HG12	5:S:215:VAL:N	2.23	0.53
7:U:137:VAL:HG21	7:U:220:THR:HA	1.90	0.53
11:Y:176:ASN:HD22	11:Y:190:ASN:HA	1.73	0.53
7:G:235:ARG:NE	7:G:235:ARG:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:52:SER:OG	6:F:53:LYS:N	2.41	0.53
5:S:231:LYS:H	5:S:231:LYS:HD2	1.73	0.53
6:T:66:VAL:HG11	6:T:108:PHE:CE1	2.43	0.53
1:O:113:GLU:HA	1:O:113:GLU:OE1	2.08	0.53
9:I:17:LYS:HD3	9:I:156:ASN:HB3	1.91	0.53
10:J:149:ARG:HH11	10:J:149:ARG:HG2	1.73	0.53
9:I:137:VAL:CG1	9:I:145:LEU:HB3	2.39	0.53
11:K:38:ASN:HB3	16:K:335:HOH:O	2.09	0.53
4:D:184:THR:HG23	4:D:187:GLU:OE1	2.09	0.53
5:E:189:ILE:HD12	5:E:189:ILE:N	2.23	0.53
5:E:35:VAL:HG12	5:E:36:GLY:N	2.22	0.53
5:E:185:PRO:HG2	5:E:186:ASP:H	1.73	0.53
5:E:1:PHE:O	5:E:3:ASN:N	2.42	0.53
7:U:235:ARG:HE	7:U:235:ARG:HA	1.73	0.53
4:R:9:PRO:HG3	5:S:23:TYR:CE2	2.43	0.53
2:B:180:LYS:HE2	2:B:182:ASP:OD1	2.09	0.53
7:U:3:TYR:C	7:U:5:ARG:H	2.11	0.53
10:J:146:HIS:HD2	10:J:147:HIS:CE1	2.26	0.53
4:D:82:GLU:OE2	11:K:69:ARG:NH1	2.42	0.53
12:L:100:LYS:HE3	12:L:103:PHE:O	2.08	0.53
8:H:59:ILE:HG12	8:H:83:LEU:HD23	1.91	0.53
7:G:31:ILE:HG23	7:G:47:GLN:HB2	1.90	0.53
2:B:105:ILE:HD11	2:B:109:ILE:CG2	2.38	0.53
5:S:226:GLY:O	5:S:229:VAL:HG22	2.09	0.53
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.91	0.53
10:J:153:THR:OG1	10:J:156:GLU:HG3	2.08	0.53
2:B:84:GLU:HA	2:B:84:GLU:OE2	4.13	0.53
2:B:38:MET:HG3	2:B:43:ILE:CD1	2.39	0.53
9:W:148:MET:CE	9:W:172:ASN:HB2	2.39	0.53
2:P:99:LYS:NZ	10:X:86:GLN:HE22	2.07	0.53
7:U:235:ARG:NE	7:U:235:ARG:HA	2.23	0.53
11:K:176:ASN:HD22	11:K:190:ASN:HA	1.73	0.53
1:O:4:ARG:HB2	2:P:2:SER:OG	2.09	0.53
3:Q:40:VAL:HG11	3:Q:134:ALA:HB1	1.89	0.53
2:P:24:ALA:O	2:P:28:ILE:HG12	2.08	0.53
6:F:39:ASN:HD22	6:F:39:ASN:N	2.07	0.53
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.89	0.53
2:P:69:ASN:HD22	2:P:70:ASP:H	1.53	0.53
9:I:14:MET:CE	9:I:166:ILE:HG13	2.39	0.53
10:J:130:TYR:CD2	10:J:144:LEU:HD13	2.43	0.53
1:A:140:ASP:OD1	1:A:143:ASN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:59:ILE:HG12	8:V:83:LEU:HD23	1.90	0.53
3:Q:165:ASN:O	3:Q:169:VAL:HG12	2.09	0.53
10:X:53:THR:CG2	10:X:54:VAL:N	2.72	0.53
9:I:116:GLY:HA2	9:I:191:LYS:HD3	1.90	0.53
3:C:117:ARG:NH2	16:C:326:HOH:O	2.41	0.53
9:I:74:LYS:HD3	16:I:325:HOH:O	2.08	0.53
6:F:193:ALA:O	6:F:197:TYR:HD1	1.92	0.53
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.08	0.53
1:A:89:SER:O	1:A:92:VAL:HG12	2.08	0.52
9:W:17:LYS:CD	9:W:156:ASN:HD22	2.22	0.52
12:Z:123:TYR:CE1	12:Z:133:ARG:HB2	2.44	0.52
1:A:239:THR:OG1	1:A:242:GLU:HG3	2.09	0.52
14:N:67:THR:HA	14:N:71:GLY:O	2.09	0.52
1:O:140:ASP:OD1	1:O:143:ASN:HB2	2.09	0.52
5:E:63:ILE:HB	5:E:71:LEU:CD2	2.39	0.52
3:Q:233:GLN:O	3:Q:237:GLU:HG2	2.09	0.52
3:C:170:ARG:O	3:C:174:GLU:HG3	2.10	0.52
1:O:44:VAL:HG23	1:O:211:LEU:HD21	1.92	0.52
5:E:226:GLY:O	5:E:229:VAL:HG22	2.10	0.52
4:D:89:VAL:HG11	11:K:65:LEU:CD2	2.40	0.52
1:A:239:THR:O	1:A:243:ILE:HG12	2.09	0.52
2:B:228:ILE:N	2:B:228:ILE:HD12	2.24	0.52
1:O:35:LEU:HB3	1:O:163:ALA:HB2	1.90	0.52
4:D:16:VAL:O	4:D:19:SER:HB3	2.09	0.52
5:E:214:ILE:HG12	5:E:215:VAL:N	2.24	0.52
12:L:123:TYR:CE1	12:L:133:ARG:HB2	2.44	0.52
7:G:137:VAL:HG21	7:G:220:THR:HA	1.91	0.52
1:A:5:TYR:HD2	7:G:124:TYR:HB3	1.74	0.52
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.89	0.52
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.90	0.52
7:U:165:LYS:O	7:U:169:ILE:HG12	2.10	0.52
10:X:129:PRO:HB2	10:X:130:TYR:CD1	2.44	0.52
16:J:205:HOH:O	11:Y:135:PHE:HA	2.09	0.52
1:O:28:VAL:HG11	1:O:133:SER:HB2	1.92	0.52
10:J:5:LEU:HD23	10:J:132:ALA:HB2	1.91	0.52
5:E:147:GLN:HG3	16:E:314:HOH:O	2.08	0.52
9:W:28:LEU:HA	16:W:315:HOH:O	2.09	0.52
2:P:200:THR:HG22	2:P:201:ASP:N	2.23	0.52
3:Q:170:ARG:O	3:Q:174:GLU:HG3	2.10	0.52
9:I:171:LEU:HD21	9:I:199:LEU:HD13	1.91	0.52
2:B:162:ILE:HG13	2:B:163:SER:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:ILE:N	7:G:79:PRO:HD2	2.24	0.52
9:W:81:ILE:HD11	9:W:85:THR:HG22	1.91	0.52
9:W:14:MET:CE	9:W:166:ILE:HG13	2.40	0.52
10:X:153:THR:OG1	10:X:156:GLU:HG3	2.10	0.52
5:E:81:ARG:HG3	5:E:81:ARG:NH1	2.21	0.52
14:N:105:LYS:HD3	14:N:105:LYS:C	2.29	0.52
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.43	0.52
1:A:10:THR:HG22	1:A:18:LEU:HD22	1.92	0.52
1:A:101:TYR:CE1	9:I:89:LEU:HD13	2.45	0.52
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.92	0.52
5:S:63:ILE:HB	5:S:71:LEU:CD2	2.40	0.52
13:M:54:SER:OG	13:M:113:ALA:HB3	2.10	0.52
5:E:197:SER:HA	5:E:200:LEU:CG	2.40	0.52
9:I:166:ILE:CG2	9:I:167:SER:N	2.72	0.52
5:S:178:PHE:CD1	5:S:179:ILE:N	2.78	0.52
1:O:82:TYR:O	1:O:86:VAL:HG23	2.10	0.52
3:C:40:VAL:HG11	3:C:134:ALA:HB1	1.92	0.52
3:C:233:GLN:O	3:C:237:GLU:HG2	2.10	0.52
4:R:57:GLU:HA	16:R:312:HOH:O	2.09	0.52
1:A:30:GLN:CA	1:A:30:GLN:HE21	2.12	0.52
5:S:81:ARG:HG3	5:S:81:ARG:NH1	2.20	0.52
10:J:174:MET:HE3	10:X:174:MET:HE3	1.92	0.52
5:E:178:PHE:CD1	5:E:179:ILE:N	2.78	0.52
3:Q:66:ASP:OD1	3:Q:95:ARG:NH1	2.38	0.52
12:Z:195:HIS:CD2	12:Z:197:GLN:H	2.27	0.52
2:P:105:ILE:HD11	2:P:109:ILE:CG2	2.40	0.52
1:O:106:PRO:HD2	1:O:109:LEU:HD12	1.92	0.52
5:E:38:ARG:NH1	5:E:39:SER:O	2.43	0.52
10:X:36:ARG:O	10:X:43:LEU:HD12	2.10	0.52
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.40	0.52
8:V:3:ILE:HB	8:V:44:ALA:HB1	1.92	0.51
6:T:45:ALA:HA	6:T:211:GLU:O	2.10	0.51
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.91	0.51
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.92	0.51
8:H:144:GLN:O	8:H:145:ASP:HB2	2.10	0.51
13:M:53:ILE:HG21	13:M:60:MET:HG3	1.92	0.51
3:C:32:VAL:HG22	3:C:33:GLY:N	2.24	0.51
10:J:8:ARG:HH11	10:J:8:ARG:HG2	1.76	0.51
2:B:119:GLN:CG	3:C:78:ALA:HB1	2.40	0.51
10:J:139:TYR:CE2	10:J:172:MET:HG3	2.45	0.51
1:A:179:TRP:HA	1:A:183:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:184:THR:HG23	4:R:187:GLU:OE1	2.10	0.51
9:W:135:PHE:O	9:W:136:ILE:HD12	2.10	0.51
3:C:27:ARG:CB	3:C:27:ARG:HH11	2.23	0.51
9:W:163:PHE:CE1	9:W:197:ARG:HD2	2.45	0.51
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.92	0.51
13:M:227:GLY:HA3	13:M:231:GLN:HB3	1.92	0.51
2:B:200:THR:HG22	2:B:201:ASP:N	2.26	0.51
4:R:159:TYR:HA	5:S:55:LEU:O	2.10	0.51
13:M:150:MET:O	13:M:153:PRO:HD2	2.11	0.51
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.92	0.51
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.91	0.51
9:W:116:GLY:HA2	9:W:191:LYS:HD3	1.91	0.51
6:T:52:SER:OG	6:T:53:LYS:N	2.42	0.51
5:S:227:GLU:CD	5:S:227:GLU:H	2.14	0.51
5:S:106:ARG:HH11	5:S:106:ARG:HG2	1.76	0.51
9:I:17:LYS:CD	9:I:156:ASN:HD22	2.24	0.51
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.93	0.51
10:J:15:LEU:HD12	10:J:43:LEU:HD23	1.91	0.51
5:S:14:PRO:HA	6:T:22:TYR:CD2	2.45	0.51
1:A:183:LEU:HD21	1:A:191:ILE:HD11	1.92	0.51
9:W:148:MET:HE2	9:W:172:ASN:HB2	1.92	0.51
1:A:227:ILE:HD12	1:A:227:ILE:N	2.26	0.51
5:S:86:TYR:CD1	5:S:114:LYS:HD2	2.46	0.51
5:S:38:ARG:NH1	5:S:39:SER:O	2.43	0.51
8:H:18:THR:HB	8:H:30:ASN:HD22	1.76	0.51
3:Q:96:LEU:HD13	16:X:237:HOH:O	2.10	0.51
6:T:39:ASN:HD22	6:T:39:ASN:N	2.07	0.51
3:C:165:ASN:O	3:C:169:VAL:HG12	2.11	0.51
11:Y:106:ARG:NH1	11:Y:106:ARG:HG2	2.26	0.51
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.46	0.51
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.40	0.51
1:A:82:TYR:O	1:A:86:VAL:HG23	2.11	0.51
3:Q:160:GLN:HG3	3:Q:161:THR:N	2.25	0.51
9:I:135:PHE:O	9:I:136:ILE:HD12	2.10	0.51
4:R:176:LEU:HD13	5:S:55:LEU:HD11	1.92	0.51
11:K:73:ARG:NH2	11:K:104:TYR:O	2.44	0.51
14:N:8:PHE:HE1	14:N:10:ASP:HB2	1.76	0.51
1:O:179:TRP:HA	1:O:183:LEU:HD11	1.92	0.51
1:O:183:LEU:HD21	1:O:191:ILE:HD11	1.93	0.51
9:I:73:TYR:CZ	9:I:77:GLU:HG3	2.46	0.51
12:Z:44:PHE:O	12:Z:51:VAL:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:4:PRO:HD3	13:M:111:TRP:CE2	2.46	0.51
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.91	0.51
10:X:14:ILE:HD13	10:X:158:LEU:CD2	2.39	0.51
3:C:27:ARG:NH1	3:C:27:ARG:CB	2.74	0.51
9:I:148:MET:CE	9:I:172:ASN:HB2	2.40	0.51
11:K:196:LEU:O	11:K:196:LEU:HD12	2.11	0.51
11:K:12:ILE:HB	11:K:180:VAL:HB	1.93	0.51
4:D:114:ARG:HG2	4:D:114:ARG:HH11	1.76	0.51
12:L:126:ASP:HB2	12:L:130:SER:N	2.26	0.50
2:B:148:TYR:CE1	3:C:57:ILE:HD13	2.46	0.50
7:G:167:GLN:NE2	7:G:171:THR:HG23	2.25	0.50
3:Q:32:VAL:HG22	3:Q:33:GLY:N	2.26	0.50
3:C:5:ALA:HB3	4:D:4:VAL:HG11	1.92	0.50
11:Y:8:PHE:CE2	11:Y:13:ILE:HG12	2.47	0.50
3:C:94:HIS:CD2	3:C:102:VAL:HG12	2.46	0.50
5:E:65:CYS:SG	5:E:87:LEU:HD23	2.51	0.50
10:X:5:LEU:HD23	10:X:132:ALA:HB2	1.93	0.50
9:W:73:TYR:CZ	9:W:77:GLU:HG3	2.46	0.50
6:F:45:ALA:HA	6:F:211:GLU:O	2.10	0.50
9:I:35:VAL:HG13	16:J:242:HOH:O	2.11	0.50
12:L:213:ARG:NH1	12:L:213:ARG:HB3	2.25	0.50
12:L:195:HIS:CD2	12:L:197:GLN:H	2.27	0.50
3:Q:27:ARG:CB	3:Q:27:ARG:HH11	2.24	0.50
4:R:89:VAL:HG11	11:Y:65:LEU:CD2	2.41	0.50
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.94	0.50
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.93	0.50
3:C:131:THR:O	3:C:147:GLN:HA	2.11	0.50
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.46	0.50
11:K:16:VAL:HG21	11:K:34:VAL:HG23	1.93	0.50
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.93	0.50
13:M:57:ILE:O	13:M:61:GLN:HG3	2.11	0.50
9:W:179:LEU:HD22	16:W:311:HOH:O	2.10	0.50
3:C:160:GLN:HG3	3:C:161:THR:N	2.26	0.50
12:L:13:LEU:HD12	12:L:14:GLY:N	2.25	0.50
3:Q:100:ASP:OD2	3:Q:101:PRO:HD2	2.11	0.50
11:Y:176:ASN:ND2	11:Y:190:ASN:HA	2.26	0.50
11:K:8:PHE:CE2	11:K:13:ILE:HG12	2.46	0.50
13:M:43:ILE:HD12	13:M:64:GLU:HG3	1.94	0.50
6:T:9:SER:HB2	7:U:126:ARG:HD3	1.93	0.50
3:Q:27:ARG:CB	3:Q:27:ARG:NH1	2.74	0.50
3:C:100:ASP:OD2	3:C:101:PRO:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:15:LEU:HD12	10:X:43:LEU:HD23	1.93	0.50
14:N:144:GLU:O	14:N:145:ASN:HB2	2.12	0.50
3:Q:126:PRO:HB3	16:Q:307:HOH:O	2.10	0.50
4:R:114:ARG:HH11	4:R:114:ARG:HG2	1.76	0.50
1:O:59:GLU:C	1:O:61:LEU:H	2.14	0.50
14:N:66:TYR:CD2	14:N:73:PRO:HB3	2.47	0.50
3:C:197:LEU:O	3:C:201:VAL:HG23	2.12	0.50
9:W:107:VAL:HG13	9:W:136:ILE:HG21	1.94	0.50
6:F:196:ILE:HG21	6:F:210:LEU:CD1	2.42	0.50
4:D:31:GLY:O	4:D:161:ALA:HA	2.11	0.50
5:E:214:ILE:O	5:E:221:PHE:HA	2.11	0.50
5:S:63:ILE:HB	5:S:71:LEU:HD21	1.94	0.50
11:K:25:TRP:CH2	12:L:144:SER:HA	2.47	0.50
13:M:165:ILE:N	13:M:166:PRO:HD2	2.27	0.50
8:V:18:THR:HB	8:V:30:ASN:HD22	1.77	0.50
2:P:69:ASN:HD22	2:P:70:ASP:N	2.09	0.50
4:R:31:GLY:HA2	4:R:39:VAL:O	2.11	0.50
7:U:207:THR:HG22	7:U:208:GLU:N	2.27	0.50
7:U:167:GLN:NE2	7:U:171:THR:HG23	2.27	0.50
13:M:162:GLU:O	13:M:165:ILE:HG12	2.12	0.50
6:T:41:GLY:HA3	6:T:215:CYS:O	2.12	0.50
9:W:189:ILE:N	9:W:189:ILE:HD12	2.27	0.50
7:U:136:SER:HA	7:U:219:ALA:HB1	1.94	0.50
12:L:113:GLY:HA2	12:L:207:VAL:HG11	1.94	0.50
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.93	0.50
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.59	0.50
4:R:241:ALA:O	4:R:242:GLU:CB	2.56	0.50
4:D:31:GLY:HA2	4:D:39:VAL:O	2.11	0.50
1:O:246:ARG:NH1	1:O:246:ARG:HG3	2.27	0.50
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.12	0.50
5:E:63:ILE:HB	5:E:71:LEU:HD21	1.94	0.50
9:I:189:ILE:HD12	9:I:189:ILE:N	2.27	0.50
14:N:116:GLY:HA3	16:N:209:HOH:O	2.12	0.50
1:A:174:PHE:O	1:A:178:ARG:HG2	2.12	0.49
6:F:147:LEU:CD1	6:F:153:TYR:HB3	2.42	0.49
11:K:176:ASN:ND2	11:K:190:ASN:HA	2.26	0.49
12:Z:152:ASN:O	12:Z:156:PHE:HA	2.12	0.49
10:J:161:LEU:O	10:J:164:CYS:N	2.45	0.49
10:J:18:SER:HB2	10:J:176:PHE:HB2	1.94	0.49
5:E:227:GLU:CD	5:E:227:GLU:H	2.14	0.49
5:E:12:PHE:H	6:F:19:GLN:HE22	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:99:LYS:HZ3	10:X:86:GLN:NE2	2.11	0.49
9:W:189:ILE:HA	9:W:194:VAL:HG22	1.95	0.49
6:F:154:TRP:CZ3	7:G:60:VAL:HA	2.47	0.49
10:J:194:ASP:O	10:J:198:GLN:HB2	2.12	0.49
12:Z:220:LYS:HG3	16:Z:331:HOH:O	2.10	0.49
6:F:41:GLY:HA3	6:F:215:CYS:O	2.11	0.49
5:S:101:LYS:HA	16:S:313:HOH:O	2.11	0.49
2:B:69:ASN:HD22	2:B:70:ASP:N	2.07	0.49
10:J:36:ARG:O	10:J:43:LEU:HD12	2.12	0.49
11:K:199:LYS:HB2	16:K:336:HOH:O	2.12	0.49
7:U:74:VAL:HG11	7:U:81:ALA:CB	2.42	0.49
6:T:20:VAL:O	6:T:23:ALA:HB3	2.13	0.49
8:V:144:GLN:O	8:V:145:ASP:HB2	2.12	0.49
11:K:85:ASN:ND2	16:K:320:HOH:O	2.44	0.49
7:G:74:VAL:HG11	7:G:81:ALA:CB	2.43	0.49
5:S:189:ILE:HD12	5:S:189:ILE:H	1.76	0.49
5:S:189:ILE:CG2	5:S:212:ILE:HD13	2.41	0.49
7:U:231:ASN:HB3	16:U:302:HOH:O	2.12	0.49
9:I:123:PHE:CD2	9:I:123:PHE:N	2.80	0.49
5:S:13:SER:HB3	5:S:17:ARG:H	1.77	0.49
1:A:106:PRO:HD2	1:A:109:LEU:HD12	1.94	0.49
6:F:198:LEU:HD12	6:F:198:LEU:H	1.78	0.49
8:V:4:VAL:HG12	8:V:126:SER:CB	2.42	0.49
1:O:36:GLY:HA2	1:O:44:VAL:O	2.12	0.49
5:E:69:MET:CE	5:E:104:VAL:HA	2.41	0.49
5:S:73:LEU:HD12	5:S:73:LEU:C	2.33	0.49
6:F:20:VAL:O	6:F:23:ALA:HB3	2.13	0.49
3:C:148:THR:HG22	3:C:154:TYR:HB3	1.94	0.49
4:D:68:CYS:HB2	4:D:136:ILE:HA	1.94	0.49
12:L:208:THR:C	12:L:210:ASP:H	2.15	0.49
10:X:8:ARG:HH11	10:X:8:ARG:HG2	1.78	0.49
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.58	0.49
1:A:36:GLY:HA2	1:A:44:VAL:O	2.12	0.49
2:P:162:ILE:HG13	2:P:163:SER:H	1.78	0.49
12:L:92:ASN:C	12:L:92:ASN:HD22	2.16	0.49
9:I:163:PHE:CE1	9:I:197:ARG:HD2	2.47	0.49
1:O:5:TYR:HD2	7:U:124:TYR:HB3	1.77	0.49
7:G:136:SER:HA	7:G:219:ALA:HB1	1.94	0.49
10:J:78:GLN:C	10:J:78:GLN:NE2	2.65	0.49
2:P:98:LEU:HG	9:W:67:ARG:HH21	1.78	0.49
4:R:204:LEU:HD23	4:R:205:ASP:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:78:GLN:C	10:X:78:GLN:NE2	2.66	0.49
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.33	0.49
5:S:214:ILE:O	5:S:221:PHE:HA	2.13	0.49
3:C:51:LYS:O	3:C:52:LEU:CB	2.61	0.49
5:E:179:ILE:HG12	5:E:179:ILE:O	2.12	0.49
16:P:305:HOH:O	3:Q:57:ILE:HD11	2.12	0.49
2:P:94:ALA:HB3	16:P:306:HOH:O	2.11	0.49
8:V:104:ASP:O	8:V:106:THR:N	2.45	0.49
14:N:133:PHE:HE2	14:N:166:ASP:HB2	1.77	0.49
3:Q:103:THR:HG23	16:Q:314:HOH:O	2.12	0.49
11:Y:196:LEU:O	11:Y:196:LEU:HD12	2.12	0.49
11:Y:56:GLU:O	11:Y:59:LEU:HB3	2.13	0.49
3:Q:131:THR:O	3:Q:147:GLN:HA	2.12	0.49
3:Q:148:THR:HG22	3:Q:154:TYR:HB3	1.94	0.49
11:Y:32:LYS:N	11:Y:32:LYS:HD2	2.27	0.49
6:T:198:LEU:H	6:T:198:LEU:HD12	1.77	0.49
5:E:189:ILE:H	5:E:189:ILE:HD12	1.78	0.49
1:O:23:TYR:CE1	7:U:12:PRO:HA	2.48	0.49
3:C:186:VAL:O	3:C:190:VAL:HG23	2.13	0.49
12:L:4:PRO:O	13:M:104:ARG:NH1	2.38	0.49
7:G:170:THR:O	7:G:174:GLU:HB2	2.13	0.49
1:A:59:GLU:C	1:A:61:LEU:H	2.16	0.49
6:F:232:LEU:O	6:F:236:ILE:HD13	2.12	0.49
14:N:103:ASP:HB3	14:N:106:ASN:HB2	1.93	0.49
6:T:31:THR:CG2	6:T:32:THR:H	2.24	0.49
12:Z:126:ASP:CB	12:Z:130:SER:H	2.25	0.49
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.95	0.49
6:T:240:GLN:O	6:T:243:ILE:HG22	2.12	0.49
2:B:55:LEU:HD22	2:B:55:LEU:N	2.28	0.49
2:B:200:THR:HG22	2:B:202:SER:N	2.12	0.49
9:W:166:ILE:CG2	9:W:167:SER:N	2.76	0.49
5:E:207:VAL:CG1	5:E:208:ASP:N	2.76	0.49
11:K:106:ARG:HG2	11:K:106:ARG:NH1	2.28	0.49
6:T:172:LEU:O	6:T:176:VAL:HG23	2.12	0.49
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.93	0.48
4:D:113:LEU:HD23	4:D:115:PHE:HE1	1.77	0.48
9:W:87:THR:HG22	9:W:129:ILE:HD13	1.93	0.48
1:O:33:THR:HG22	1:O:34:SER:N	2.27	0.48
10:J:17:SER:HB2	16:J:215:HOH:O	2.13	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG21	1.94	0.48
1:O:227:ILE:N	1:O:227:ILE:HD12	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:75:ASN:HA	16:U:308:HOH:O	2.13	0.48
5:S:197:SER:HA	5:S:200:LEU:CG	2.39	0.48
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.94	0.48
10:X:53:THR:CG2	10:X:54:VAL:H	2.27	0.48
3:Q:96:LEU:HD22	10:X:62:ALA:HB2	1.94	0.48
4:R:68:CYS:HB2	4:R:136:ILE:HA	1.95	0.48
3:Q:166:SER:HA	3:Q:169:VAL:CG1	2.43	0.48
7:U:103:MET:HE3	7:U:108:LEU:CB	2.43	0.48
5:S:200:LEU:HD11	5:S:205:LEU:CD2	2.40	0.48
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.26	0.48
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.49	0.48
11:Y:133:GLN:HG3	11:Y:134:THR:N	2.27	0.48
2:P:105:ILE:HG12	2:P:110:LEU:HB2	1.95	0.48
2:P:44:VAL:HG22	2:P:214:THR:HG22	1.95	0.48
1:O:10:THR:HG22	1:O:18:LEU:HD22	1.95	0.48
14:N:114:PRO:HD2	14:N:118:SER:O	2.14	0.48
8:H:167:LEU:HD22	12:Z:196:ILE:O	2.13	0.48
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.96	0.48
3:Q:120:GLN:O	3:Q:120:GLN:HG3	2.13	0.48
6:F:2:THR:HG23	12:Z:126:ASP:OD2	100.68	0.48
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.42	0.48
9:I:81:ILE:HD11	9:I:85:THR:HG22	1.94	0.48
4:D:44:LYS:HB2	4:D:208:ASN:C	2.34	0.48
12:L:44:PHE:O	12:L:51:VAL:HA	2.13	0.48
6:T:28:GLU:HB3	6:T:165:ARG:NH2	2.28	0.48
8:V:20:SER:HB2	8:V:31:CYS:SG	2.54	0.48
6:T:14:ASP:OD2	6:T:14:ASP:N	2.44	0.48
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.95	0.48
10:J:4:ILE:O	10:J:132:ALA:HA	2.14	0.48
14:N:14:LEU:N	14:N:14:LEU:HD12	2.29	0.48
2:P:159:TRP:CD2	2:P:162:ILE:HD13	2.49	0.48
12:L:152:ASN:O	12:L:156:PHE:HA	2.12	0.48
3:C:58:THR:HG23	3:C:59:PRO:HD2	1.95	0.48
3:Q:34:VAL:HG12	3:Q:159:ALA:HB1	1.95	0.48
12:Z:208:THR:C	12:Z:210:ASP:H	2.16	0.48
8:H:148:LYS:HD3	16:H:344:HOH:O	2.12	0.48
9:W:123:PHE:CD2	9:W:123:PHE:N	2.81	0.48
12:Z:42:LYS:HD2	12:Z:55:ASN:ND2	2.28	0.48
3:Q:5:ALA:HB3	4:R:4:VAL:HG11	1.94	0.48
2:P:36:GLY:O	2:P:161:ALA:HA	2.14	0.48
1:O:174:PHE:O	1:O:178:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:179:ILE:O	5:S:179:ILE:HG12	2.13	0.48
5:S:181:ILE:HG21	5:S:187:GLU:CB	2.44	0.48
12:L:201:GLY:C	12:L:219:LEU:HD12	2.33	0.48
8:H:104:ASP:O	8:H:106:THR:N	2.46	0.48
10:X:161:LEU:O	10:X:164:CYS:N	2.46	0.48
2:B:44:VAL:HG22	2:B:214:THR:HG22	1.96	0.48
10:X:194:ASP:O	10:X:198:GLN:HB2	2.13	0.48
5:S:174:THR:HG22	5:S:177:THR:HB	1.96	0.48
4:R:113:LEU:HD23	4:R:115:PHE:HE1	1.78	0.48
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.49	0.48
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.43	0.48
3:Q:51:LYS:O	3:Q:52:LEU:CB	2.60	0.48
2:B:159:TRP:CD2	2:B:162:ILE:HD13	2.49	0.48
10:X:4:ILE:O	10:X:132:ALA:HA	2.14	0.48
7:U:237:VAL:O	7:U:240:ALA:HB3	2.14	0.48
11:Y:99:THR:HG22	11:Y:115:VAL:O	2.13	0.48
8:V:4:VAL:HG12	8:V:126:SER:HB3	1.95	0.48
4:R:31:GLY:O	4:R:161:ALA:HA	2.13	0.48
10:J:53:THR:CG2	10:J:54:VAL:H	2.26	0.48
5:E:73:LEU:HD12	5:E:73:LEU:C	2.33	0.48
12:L:196:ILE:O	8:V:167:LEU:HD22	2.14	0.48
8:H:72:ARG:NH1	8:H:72:ARG:HG3	2.27	0.48
6:F:41:GLY:CA	6:F:215:CYS:O	2.62	0.48
6:T:168:ALA:O	6:T:172:LEU:HD23	2.14	0.48
14:N:91:ASP:HB2	16:N:212:HOH:O	2.13	0.48
3:C:34:VAL:HG12	3:C:159:ALA:HB1	1.96	0.48
16:F:305:HOH:O	7:G:82:ARG:HD2	2.14	0.48
6:F:27:VAL:HG13	6:F:75:SER:O	2.14	0.48
7:G:102:ASP:HA	16:G:315:HOH:O	2.14	0.48
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.95	0.48
1:A:120:GLU:C	1:A:122:THR:H	2.18	0.47
7:G:207:THR:HG22	7:G:208:GLU:N	2.29	0.47
5:S:69:MET:CE	5:S:104:VAL:HA	2.43	0.47
1:A:28:VAL:HG11	1:A:133:SER:HB2	1.95	0.47
2:B:49:ARG:HH21	2:B:58:GLN:HE21	1.62	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.47
3:Q:179:ARG:HH22	4:R:52:GLU:HA	1.79	0.47
11:K:99:THR:HG22	11:K:115:VAL:O	2.14	0.47
10:X:110:LYS:HB2	10:X:110:LYS:NZ	2.29	0.47
2:P:139:TYR:HA	2:P:144:GLY:O	2.14	0.47
12:Z:126:ASP:HB2	12:Z:130:SER:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:169:THR:HA	16:M:323:HOH:O	2.14	0.47
7:U:236:LEU:O	7:U:239:ILE:HG13	2.14	0.47
5:E:227:GLU:CD	5:E:227:GLU:N	2.67	0.47
5:S:68:HIS:HE1	5:S:102:LEU:O	1.97	0.47
5:E:106:ARG:HH11	5:E:106:ARG:HG2	1.79	0.47
4:D:37:GLY:HA2	4:D:145:TYR:CD1	2.50	0.47
13:M:15:LYS:HG3	13:M:165:ILE:HD12	1.96	0.47
6:T:198:LEU:HD12	6:T:198:LEU:N	2.30	0.47
7:U:170:THR:O	7:U:174:GLU:HB2	2.14	0.47
11:K:32:LYS:N	11:K:32:LYS:HD2	2.29	0.47
12:Z:92:ASN:C	12:Z:92:ASN:HD22	2.16	0.47
8:H:4:VAL:HG12	8:H:126:SER:CB	2.43	0.47
7:G:103:MET:CE	7:G:108:LEU:HD13	2.41	0.47
6:F:191:GLN:NE2	6:F:194:LYS:CE	2.77	0.47
13:M:119:VAL:HG23	13:M:200:ILE:CG2	2.45	0.47
14:N:13:ILE:HG12	14:N:177:VAL:HG13	1.97	0.47
12:L:86:ILE:HG23	12:L:123:TYR:HE2	1.79	0.47
11:K:4:LEU:HD22	11:K:4:LEU:O	2.14	0.47
2:B:76:VAL:HG22	2:B:134:PHE:CE2	2.49	0.47
6:T:212:ILE:HG22	6:T:213:SER:N	2.28	0.47
4:D:204:LEU:HD23	4:D:204:LEU:C	2.34	0.47
4:D:204:LEU:HD23	4:D:205:ASP:N	2.29	0.47
4:D:140:ASP:HA	16:D:337:HOH:O	2.14	0.47
6:F:31:THR:CG2	6:F:32:THR:H	2.27	0.47
10:J:14:ILE:HD13	10:J:158:LEU:CD2	2.44	0.47
7:G:165:LYS:O	7:G:169:ILE:HG12	2.15	0.47
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.44	0.47
11:K:196:LEU:HD12	11:K:200:VAL:HG23	1.96	0.47
12:Z:192:THR:HG21	16:Z:331:HOH:O	2.13	0.47
4:R:204:LEU:HD23	4:R:204:LEU:C	2.34	0.47
3:Q:74:SER:OG	3:Q:162:ILE:HG13	2.15	0.47
6:F:103:ILE:HG22	16:F:327:HOH:O	2.13	0.47
3:Q:94:HIS:CD2	3:Q:102:VAL:HG12	2.48	0.47
6:F:212:ILE:HG22	6:F:213:SER:N	2.29	0.47
13:M:63:ILE:HD11	13:M:110:LEU:HD13	1.95	0.47
12:Z:213:ARG:NH1	12:Z:213:ARG:HB3	2.28	0.47
9:I:107:VAL:HG13	9:I:136:ILE:HG21	1.96	0.47
12:Z:3:ASN:ND2	12:Z:3:ASN:C	2.67	0.47
4:R:113:LEU:HB2	16:R:318:HOH:O	2.14	0.47
4:D:67:GLY:HA3	4:D:220:PHE:CD2	2.49	0.47
10:J:89:ALA:O	10:J:92:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:SER:HB2	8:H:31:CYS:SG	2.55	0.47
3:C:71:LEU:HD22	3:C:84:ILE:CD1	2.45	0.47
5:E:42:HIS:CD2	5:E:214:ILE:HD11	2.48	0.47
5:E:181:ILE:HG21	5:E:187:GLU:CB	2.45	0.47
5:S:207:VAL:CG1	5:S:208:ASP:N	2.78	0.47
1:A:33:THR:HG22	1:A:34:SER:N	2.29	0.47
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.44	0.47
5:S:102:LEU:HA	16:S:321:HOH:O	2.15	0.47
4:R:16:VAL:O	4:R:19:SER:HB3	2.14	0.47
11:Y:139:VAL:HG21	11:Y:163:ALA:HB2	1.96	0.47
5:E:174:THR:HG22	5:E:177:THR:HB	1.95	0.47
13:M:147:GLY:O	13:M:151:ALA:HB3	2.14	0.47
6:T:89:ARG:HD2	16:T:307:HOH:O	2.14	0.47
8:V:99:ILE:HG13	8:V:127:LEU:HD12	1.97	0.47
2:B:36:GLY:O	2:B:161:ALA:HA	2.14	0.47
3:C:66:ASP:HA	10:J:69:ILE:CD1	2.41	0.47
13:M:16:TYR:CZ	13:M:170:VAL:HG22	2.50	0.47
2:P:49:ARG:HH21	2:P:58:GLN:HE21	1.63	0.47
5:S:2:ARG:HG3	5:S:19:PHE:CE1	2.50	0.47
5:S:154:GLU:HG3	16:S:306:HOH:O	2.14	0.47
12:Z:95:HIS:HE1	16:Z:303:HOH:O	1.98	0.47
7:G:26:THR:HG21	7:G:131:ILE:HG13	1.96	0.47
6:F:50:ILE:HD11	6:F:209:GLU:HB2	1.96	0.47
3:Q:71:LEU:HD22	3:Q:84:ILE:CD1	2.44	0.47
5:S:42:HIS:CD2	5:S:214:ILE:HD11	2.48	0.47
5:S:178:PHE:HA	5:S:181:ILE:CG1	2.44	0.47
2:B:50:LYS:O	2:B:51:VAL:O	2.33	0.47
7:U:103:MET:CE	7:U:108:LEU:HD13	2.37	0.47
7:G:103:MET:HE3	7:G:108:LEU:CD1	2.43	0.47
5:E:68:HIS:HE1	5:E:102:LEU:O	1.98	0.47
13:M:35:ARG:HD3	13:M:36:PHE:CZ	2.50	0.47
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.97	0.47
14:N:102:TYR:OH	14:N:180:ALA:HB2	2.15	0.47
11:K:86:LEU:C	11:K:86:LEU:HD13	2.36	0.47
1:A:176:GLU:HG2	2:B:55:LEU:HD23	1.90	0.46
8:H:4:VAL:HG12	8:H:126:SER:HB3	1.97	0.46
9:W:14:MET:HG2	9:W:135:PHE:HB3	1.96	0.46
2:B:189:ILE:HG23	2:B:212:PHE:CE2	2.50	0.46
12:Z:113:GLY:HA2	12:Z:207:VAL:HG11	1.96	0.46
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.49	0.46
13:M:184:LEU:HD13	16:M:314:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD21	1:A:213:ILE:HD12	1.97	0.46
9:I:176:ARG:NH2	12:Z:147:MET:CE	2.79	0.46
2:B:139:TYR:HA	2:B:144:GLY:O	2.15	0.46
9:W:15:THR:HG23	9:W:120:ILE:HG12	1.96	0.46
9:W:15:THR:CG2	9:W:120:ILE:HG12	2.45	0.46
4:D:241:ALA:O	4:D:242:GLU:CB	2.57	0.46
5:S:193:VAL:HG22	5:S:212:ILE:HD11	1.97	0.46
12:Z:17:GLY:HA3	12:Z:20:PHE:CZ	2.49	0.46
7:G:92:ALA:HA	7:G:103:MET:CE	2.45	0.46
14:N:44:CYS:HB2	14:N:98:ILE:HB	1.97	0.46
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.95	0.46
5:E:205:LEU:N	5:E:205:LEU:HD23	2.22	0.46
2:P:148:TYR:CE1	3:Q:57:ILE:HD13	2.50	0.46
6:T:41:GLY:CA	6:T:215:CYS:O	2.63	0.46
2:B:98:LEU:HG	9:I:67:ARG:HH21	1.80	0.46
8:V:38:SER:OG	8:V:41:ILE:HG13	2.15	0.46
14:N:15:GLY:HA2	14:N:174:ARG:O	2.14	0.46
12:Z:67:ARG:NH2	16:Z:347:HOH:O	2.39	0.46
6:T:126:ARG:HG2	6:T:126:ARG:HH11	1.80	0.46
12:Z:108:HIS:HE1	12:Z:124:SER:HB2	1.80	0.46
5:S:205:LEU:HD23	5:S:205:LEU:N	2.21	0.46
5:S:143:LEU:CD2	5:S:157:GLY:HA2	2.45	0.46
5:E:143:LEU:CD2	5:E:157:GLY:HA2	2.45	0.46
5:S:25:LEU:O	5:S:28:ILE:HB	2.15	0.46
1:O:24:ALA:O	1:O:28:VAL:HG23	2.16	0.46
12:L:3:ASN:ND2	12:L:3:ASN:C	2.69	0.46
5:E:14:PRO:HA	6:F:22:TYR:CE2	2.50	0.46
6:T:123:ASN:HD22	6:T:124:SER:N	2.13	0.46
7:U:227:LEU:HB3	7:U:231:ASN:HB2	1.97	0.46
5:S:227:GLU:N	5:S:227:GLU:CD	2.68	0.46
10:J:78:GLN:HE21	10:J:79:ALA:N	2.14	0.46
10:X:78:GLN:HE21	10:X:79:ALA:N	2.14	0.46
9:I:101:PRO:HA	16:I:310:HOH:O	2.15	0.46
8:H:213:LEU:HD22	11:Y:212:GLY:HA2	1.98	0.46
7:U:196:PHE:C	7:U:196:PHE:CD1	2.89	0.46
3:C:166:SER:HA	3:C:169:VAL:CG1	2.45	0.46
12:Z:150:LEU:O	12:Z:154:VAL:HB	2.16	0.46
5:S:129:VAL:O	5:S:148:PRO:HG3	2.15	0.46
6:F:123:ASN:HD22	6:F:123:ASN:N	2.12	0.46
9:I:87:THR:HG22	9:I:129:ILE:HD13	1.97	0.46
2:P:189:ILE:HG23	2:P:212:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:145:LEU:O	9:W:147:GLY:HA3	2.15	0.46
6:T:50:ILE:HD11	6:T:209:GLU:HB2	1.98	0.46
7:G:71:GLY:HA3	7:G:224:PHE:CE2	2.51	0.46
3:C:120:GLN:O	3:C:120:GLN:HG3	2.15	0.46
3:C:222:LEU:N	3:C:222:LEU:HD12	2.31	0.46
14:N:113:ILE:HG12	14:N:119:VAL:HG13	1.96	0.46
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	1.97	0.46
11:Y:196:LEU:HD12	11:Y:200:VAL:HG23	1.96	0.46
14:N:3:ILE:HD12	14:N:44:CYS:HB3	1.96	0.46
6:F:240:GLN:O	6:F:243:ILE:HG22	2.15	0.46
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.14	0.46
4:R:93:LEU:CD1	11:Y:57:THR:HG22	2.45	0.46
2:B:217:LYS:O	2:B:218:GLY:C	2.53	0.46
2:B:43:ILE:HD11	2:B:145:TYR:CB	2.26	0.46
9:I:167:SER:O	9:I:171:LEU:HD23	2.16	0.46
13:M:130:VAL:HG23	13:M:136:THR:CG2	2.42	0.46
13:M:48:ASN:ND2	13:M:48:ASN:N	2.64	0.46
12:Z:201:GLY:C	12:Z:219:LEU:HD12	2.36	0.46
5:E:207:VAL:HG22	5:E:226:GLY:HA2	1.98	0.46
5:S:207:VAL:HG22	5:S:226:GLY:HA2	1.97	0.46
13:M:94:GLU:OE2	13:M:94:GLU:HA	2.16	0.46
2:B:61:SER:O	2:B:62:THR:OG1	2.30	0.46
7:U:7:ILE:HA	16:U:335:HOH:O	2.14	0.46
7:U:26:THR:HG21	7:U:131:ILE:HG13	1.97	0.46
8:V:173:VAL:HB	8:V:191:LEU:HB2	1.98	0.46
8:V:152:ILE:HD11	8:V:177:VAL:HG21	1.97	0.46
7:U:34:LEU:C	7:U:34:LEU:HD12	2.36	0.46
4:R:37:GLY:HA2	4:R:145:TYR:CD1	2.50	0.46
12:Z:86:ILE:HG23	12:Z:123:TYR:HE2	1.81	0.46
11:K:4:LEU:CD1	11:K:161:ILE:HD11	2.46	0.46
9:W:73:TYR:CE1	9:W:77:GLU:HG3	2.51	0.46
9:I:106:PRO:HB2	9:I:123:PHE:CD2	2.50	0.46
12:L:51:VAL:HG12	12:L:205:LEU:HD23	1.98	0.46
6:F:99:TYR:O	6:F:100:LYS:HB3	2.16	0.46
1:A:205:ASN:HA	1:A:247:LEU:CD1	2.46	0.46
2:P:236:ASP:O	2:P:240:LYS:HG2	2.16	0.46
8:H:200:GLN:HG2	12:Z:182:LYS:HA	1.98	0.46
2:P:167:ASN:HA	16:P:319:HOH:O	2.16	0.46
3:Q:161:THR:HG23	3:Q:166:SER:HB2	1.98	0.46
2:B:77:ALA:HB2	2:B:164:VAL:HG23	1.97	0.46
9:W:201:MET:HB2	16:W:307:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:177:VAL:O	12:L:181:ILE:HG13	2.16	0.46
2:B:162:ILE:HG13	2:B:163:SER:H	1.80	0.46
11:K:4:LEU:C	11:K:4:LEU:HD22	2.37	0.46
3:Q:58:THR:HG23	3:Q:59:PRO:HD2	1.97	0.46
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.98	0.46
4:R:67:GLY:HA3	4:R:220:PHE:CD2	2.50	0.46
14:N:88:GLU:OE1	14:N:88:GLU:HA	2.15	0.46
6:T:191:GLN:NE2	6:T:194:LYS:CE	2.79	0.46
2:B:158:GLY:HA3	3:C:57:ILE:HD12	1.97	0.46
11:K:4:LEU:HD13	11:K:161:ILE:HD11	1.97	0.46
12:Z:208:THR:O	12:Z:210:ASP:N	2.49	0.46
6:F:172:LEU:O	6:F:176:VAL:HG23	2.16	0.46
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.46
6:F:126:ARG:HH11	6:F:126:ARG:HG2	1.81	0.46
5:E:200:LEU:HD11	5:E:205:LEU:CD2	2.41	0.45
11:K:208:ASN:ND2	10:X:150:PRO:CG	2.75	0.45
4:D:161:ALA:HB3	5:E:55:LEU:HD23	1.99	0.45
7:U:166:GLN:NE2	7:U:167:GLN:N	2.64	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.45
12:Z:51:VAL:HG12	12:Z:205:LEU:HD23	1.98	0.45
6:F:198:LEU:N	6:F:198:LEU:HD12	2.31	0.45
4:R:44:LYS:HB2	4:R:208:ASN:C	2.37	0.45
12:L:42:LYS:HD2	12:L:55:ASN:ND2	2.30	0.45
8:H:196:ARG:NH2	9:I:150:GLU:O	2.50	0.45
8:V:179:GLU:N	16:V:326:HOH:O	2.48	0.45
12:L:17:GLY:HA3	12:L:20:PHE:CZ	2.51	0.45
1:A:29:LYS:NZ	1:A:168:SER:OG	2.47	0.45
8:H:38:SER:OG	8:H:41:ILE:HG13	2.16	0.45
13:M:11:VAL:O	13:M:143:ALA:HA	2.17	0.45
2:P:77:ALA:HB2	2:P:164:VAL:HG23	1.97	0.45
12:L:125:PHE:CD1	12:L:125:PHE:N	2.83	0.45
13:M:85:GLU:OE2	13:M:85:GLU:HA	2.16	0.45
5:E:25:LEU:O	5:E:28:ILE:HB	2.15	0.45
10:X:53:THR:HG23	10:X:54:VAL:H	1.82	0.45
6:F:8:ASN:ND2	6:F:127:PRO:HD3	2.31	0.45
5:E:2:ARG:HG3	5:E:19:PHE:CE1	2.50	0.45
9:I:73:TYR:CE1	9:I:77:GLU:HG3	2.51	0.45
9:I:189:ILE:HA	9:I:194:VAL:HG22	1.98	0.45
6:T:71:GLY:O	6:T:134:PHE:HA	2.16	0.45
1:A:44:VAL:HG23	1:A:211:LEU:HD21	1.97	0.45
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:ILE:HG12	2:B:110:LEU:HB2	1.98	0.45
2:P:55:LEU:N	2:P:55:LEU:HD22	2.31	0.45
6:T:8:ASN:ND2	6:T:127:PRO:HD3	2.31	0.45
11:K:196:LEU:O	11:K:200:VAL:HG23	2.17	0.45
8:H:213:LEU:HG	9:I:200:LYS:HB2	1.98	0.45
2:P:50:LYS:O	2:P:51:VAL:O	2.33	0.45
2:B:236:ASP:O	2:B:240:LYS:HG2	2.15	0.45
4:D:71:SER:O	4:D:132:VAL:HG23	2.17	0.45
3:Q:129:VAL:HG12	3:Q:130:SER:N	2.32	0.45
8:H:195:VAL:HA	16:H:346:HOH:O	2.17	0.45
4:R:71:SER:O	4:R:132:VAL:HG23	2.15	0.45
10:X:89:ALA:O	10:X:92:ILE:HG22	2.16	0.45
6:F:133:ILE:HA	6:F:145:TYR:O	2.16	0.45
6:F:201:GLU:HA	6:F:201:GLU:OE1	2.17	0.45
2:B:43:ILE:CG2	2:B:147:LEU:HD13	2.46	0.45
9:I:14:MET:HG2	9:I:135:PHE:HB3	1.98	0.45
1:A:246:ARG:HG3	1:A:246:ARG:NH1	2.28	0.45
8:H:79:ALA:O	8:H:83:LEU:HG	2.16	0.45
6:T:232:LEU:O	6:T:236:ILE:HD13	2.16	0.45
3:Q:46:ARG:HD2	3:Q:206:LYS:O	2.17	0.45
2:P:76:VAL:HG22	2:P:134:PHE:CE2	2.51	0.45
4:R:6:THR:HG22	4:R:7:PHE:N	2.31	0.45
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.99	0.45
7:G:34:LEU:C	7:G:34:LEU:HD12	2.37	0.45
12:Z:125:PHE:CD1	12:Z:125:PHE:N	2.84	0.45
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.51	0.45
12:L:150:LEU:O	12:L:154:VAL:HB	2.15	0.45
12:L:126:ASP:CB	12:L:130:SER:H	2.26	0.45
6:T:123:ASN:N	6:T:123:ASN:HD22	2.14	0.45
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.52	0.45
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.51	0.45
11:Y:4:LEU:CD1	11:Y:161:ILE:HD11	2.46	0.45
9:W:106:PRO:HB2	9:W:123:PHE:CD2	2.51	0.45
12:L:12:ILE:HG13	12:L:110:ILE:HD12	1.99	0.45
6:T:148:GLU:HG2	16:T:326:HOH:O	2.16	0.45
2:P:185:VAL:HG21	2:P:216:ARG:HG3	1.99	0.45
8:H:152:ILE:HD11	8:H:177:VAL:HG21	1.99	0.45
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.17	0.45
6:F:71:GLY:O	6:F:134:PHE:HA	2.15	0.45
1:O:120:GLU:C	1:O:122:THR:H	2.19	0.45
3:Q:146:TYR:CE1	3:Q:156:SER:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:159:TYR:HA	5:E:55:LEU:O	2.17	0.45
6:T:196:ILE:HG21	6:T:210:LEU:CD1	2.43	0.45
14:N:155:ILE:HG22	14:N:175:MET:HE2	1.99	0.45
9:I:170:LEU:CD2	9:I:184:ALA:HB1	2.47	0.45
6:T:99:TYR:O	6:T:100:LYS:HB3	2.15	0.45
6:T:133:ILE:HA	6:T:145:TYR:O	2.17	0.45
10:X:106:GLY:HA2	10:X:184:VAL:HG11	1.98	0.45
11:Y:191:HIS:N	11:Y:191:HIS:CD2	2.85	0.45
8:V:3:ILE:HD12	8:V:46:ALA:HB2	1.99	0.45
9:I:15:THR:CG2	9:I:120:ILE:HG12	2.47	0.45
5:S:207:VAL:CG1	5:S:208:ASP:H	2.29	0.45
7:G:185:ILE:N	7:G:185:ILE:CD1	2.79	0.45
2:P:67:LYS:CE	2:P:228:ILE:HD11	2.47	0.45
2:P:149:THR:O	2:P:156:TYR:HA	2.17	0.45
12:L:135:GLN:NE2	12:L:174:TYR:OH	2.50	0.45
16:T:303:HOH:O	7:U:82:ARG:HD2	2.17	0.45
8:H:173:VAL:HB	8:H:191:LEU:HB2	1.99	0.45
3:C:172:PHE:O	3:C:176:ASN:HB2	2.16	0.45
3:Q:222:LEU:N	3:Q:222:LEU:HD12	2.32	0.45
8:H:3:ILE:HD12	8:H:46:ALA:HB2	1.98	0.45
3:C:3:ASP:O	3:C:4:ARG:C	2.55	0.45
5:S:36:GLY:O	5:S:157:GLY:HA2	2.17	0.45
6:T:47:GLU:OE1	6:T:49:LEU:HD21	2.17	0.45
1:A:204:PHE:CD1	1:A:209:ILE:HD11	2.52	0.45
4:R:180:HIS:H	4:R:183:LEU:CD1	2.30	0.45
11:K:174:SER:HA	11:K:193:VAL:HG23	1.99	0.45
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.99	0.45
11:K:46:ALA:HB3	11:K:98:GLY:O	2.17	0.45
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.17	0.45
2:P:17:ARG:HH11	2:P:17:ARG:HG2	1.81	0.45
5:E:207:VAL:CG1	5:E:208:ASP:H	2.28	0.45
4:R:180:HIS:H	4:R:183:LEU:HD11	1.82	0.45
5:E:136:TYR:CE1	5:E:140:GLY:HA2	2.52	0.45
10:X:103:LEU:HA	10:X:103:LEU:HD23	1.74	0.45
1:O:180:ASN:H	1:O:183:LEU:CD1	2.30	0.45
13:M:21:ILE:HB	13:M:177:ILE:HD12	1.98	0.45
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.46	0.45
11:K:186:ILE:O	11:K:188:HIS:HD2	2.00	0.45
2:P:71:LYS:O	2:P:138:GLY:HA2	2.17	0.45
9:W:111:ILE:N	16:W:306:HOH:O	2.31	0.45
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:165:VAL:O	10:J:169:GLU:HG3	2.17	0.45
12:L:95:HIS:HE1	16:L:304:HOH:O	2.00	0.45
5:E:129:VAL:O	5:E:148:PRO:HG3	2.17	0.44
4:D:178:GLU:HB3	4:D:191:LEU:HD21	2.00	0.44
4:D:17:GLU:O	4:D:20:LEU:HB2	2.18	0.44
7:U:241:GLU:O	7:U:242:GLN:HB2	2.17	0.44
11:K:139:VAL:HG21	11:K:163:ALA:HB2	2.00	0.44
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.52	0.44
5:S:155:LEU:HD12	5:S:158:THR:HG21	1.99	0.44
3:Q:51:LYS:HD2	3:Q:52:LEU:H	1.82	0.44
8:V:72:ARG:NH1	8:V:72:ARG:HG3	2.30	0.44
13:M:19:GLY:HA3	13:M:200:ILE:O	2.17	0.44
14:N:6:VAL:HG21	14:N:155:ILE:HD11	1.99	0.44
3:Q:107:LEU:HD13	3:Q:107:LEU:O	2.17	0.44
11:K:133:GLN:HG3	11:K:134:THR:N	2.32	0.44
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.99	0.44
11:K:201:LYS:HE3	11:K:207:PHE:O	2.17	0.44
1:A:1:MET:CG	1:A:2:THR:H	2.30	0.44
7:U:92:ALA:HA	7:U:103:MET:CE	2.46	0.44
13:M:161:ARG:CG	13:M:161:ARG:NH1	2.74	0.44
9:W:108:VAL:O	9:W:120:ILE:HA	2.18	0.44
9:W:167:SER:O	9:W:171:LEU:HD23	2.17	0.44
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.48	0.44
11:Y:196:LEU:O	11:Y:200:VAL:HG23	2.17	0.44
2:P:141:ASP:OD2	10:X:110:LYS:HE2	2.17	0.44
12:L:174:TYR:CD1	12:L:175:LEU:N	2.86	0.44
7:G:237:VAL:O	7:G:240:ALA:HB3	2.16	0.44
4:R:196:LEU:O	4:R:200:MET:HG3	2.16	0.44
13:M:191:SER:HB2	16:M:322:HOH:O	2.17	0.44
2:P:229:PHE:CD2	2:P:229:PHE:N	2.85	0.44
5:S:136:TYR:CE1	5:S:140:GLY:HA2	2.52	0.44
10:X:117:TYR:CE1	10:X:127:GLU:HG3	2.52	0.44
7:U:185:ILE:CD1	7:U:185:ILE:N	2.80	0.44
7:G:236:LEU:O	7:G:239:ILE:HG13	2.18	0.44
5:E:175:LEU:O	5:E:177:THR:N	2.51	0.44
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.82	0.44
4:D:6:THR:HG22	4:D:7:PHE:N	2.31	0.44
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.51	0.44
2:P:60:THR:O	2:P:60:THR:HG22	2.18	0.44
2:P:217:LYS:O	2:P:218:GLY:C	2.54	0.44
6:F:47:GLU:OE1	6:F:49:LEU:HD21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:174:MET:CE	10:X:174:MET:HE3	2.47	0.44
2:B:105:ILE:HD11	2:B:109:ILE:HG22	1.99	0.44
10:J:150:PRO:CG	11:Y:208:ASN:ND2	2.81	0.44
2:P:158:GLY:HA3	3:Q:57:ILE:HD11	2.00	0.44
6:T:123:ASN:HD22	6:T:123:ASN:C	2.21	0.44
1:A:24:ALA:O	1:A:28:VAL:HG23	2.17	0.44
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.98	0.44
2:B:67:LYS:CE	2:B:228:ILE:HD11	2.48	0.44
3:C:129:VAL:HG12	3:C:130:SER:N	2.32	0.44
11:K:56:GLU:O	11:K:59:LEU:HB3	2.17	0.44
9:I:11:VAL:HG22	9:I:24:CYS:HB3	1.99	0.44
10:J:117:TYR:CE1	10:J:127:GLU:HG3	2.52	0.44
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.47	0.44
10:X:5:LEU:HB2	10:X:16:ALA:HB3	2.00	0.44
12:L:213:ARG:CB	12:L:213:ARG:HH11	2.30	0.44
4:D:171:ALA:O	4:D:174:GLU:HB3	2.17	0.44
6:F:28:GLU:HB3	6:F:165:ARG:NH2	2.33	0.44
7:U:71:GLY:HA3	7:U:224:PHE:CE2	2.52	0.44
3:Q:3:ASP:O	3:Q:4:ARG:C	2.54	0.44
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	1.98	0.44
9:W:157:LEU:HG	16:W:327:HOH:O	2.17	0.44
2:P:243:ILE:O	2:P:243:ILE:HG22	2.17	0.44
12:Z:154:VAL:O	12:Z:154:VAL:HG12	2.18	0.44
5:S:157:GLY:O	5:S:158:THR:HB	2.17	0.44
10:J:172:MET:HA	10:J:173:PRO:HD3	1.70	0.44
12:L:24:ALA:HB1	12:L:202:LEU:HD11	2.00	0.44
6:F:123:ASN:HD22	6:F:124:SER:N	2.16	0.44
13:M:14:MET:HE3	13:M:159:VAL:CG2	2.47	0.44
12:L:208:THR:O	12:L:210:ASP:N	2.51	0.44
8:H:41:ILE:HD13	8:H:76:VAL:HA	1.98	0.44
12:L:182:LYS:HA	8:V:200:GLN:HG2	1.99	0.44
2:B:237:ILE:O	2:B:237:ILE:HG13	2.18	0.44
11:K:4:LEU:HA	11:K:127:PHE:O	2.18	0.44
8:V:9:ASN:HD21	8:V:147:THR:HA	1.82	0.44
14:N:87:TYR:O	14:N:90:LYS:HG2	2.18	0.44
1:O:1:MET:CG	1:O:2:THR:H	2.30	0.44
2:B:60:THR:O	2:B:60:THR:HG22	2.18	0.44
9:I:15:THR:HG23	9:I:120:ILE:HG12	2.00	0.44
7:G:155:VAL:CG2	7:G:156:GLY:N	2.80	0.44
6:T:123:ASN:ND2	6:T:123:ASN:C	2.72	0.44
2:P:105:ILE:HD11	2:P:109:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:41:PRO:HA	16:L:344:HOH:O	2.16	0.44
1:O:185:LEU:HD21	1:O:213:ILE:HD12	1.99	0.44
4:R:73:LEU:N	4:R:131:GLY:O	2.47	0.44
13:M:165:ILE:HB	13:M:166:PRO:CD	2.49	0.43
9:I:53:THR:HA	16:I:305:HOH:O	2.18	0.43
2:B:234:ILE:O	2:B:238:LEU:HB2	2.18	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.43
7:G:196:PHE:CD1	7:G:196:PHE:C	2.91	0.43
5:E:48:LEU:HD12	5:E:209:ASN:OD1	2.18	0.43
5:S:48:LEU:HD12	5:S:209:ASN:OD1	2.17	0.43
9:I:108:VAL:O	9:I:120:ILE:HA	2.18	0.43
5:E:193:VAL:HG22	5:E:212:ILE:HD11	2.00	0.43
4:R:89:VAL:HG21	11:Y:65:LEU:CD2	2.48	0.43
7:G:3:TYR:C	7:G:5:ARG:N	2.70	0.43
9:W:37:ASN:C	9:W:37:ASN:HD22	2.21	0.43
2:B:28:ILE:HD11	2:B:131:GLY:C	2.38	0.43
2:B:149:THR:O	2:B:156:TYR:HA	2.18	0.43
8:V:51:ASP:O	8:V:55:VAL:HG12	2.18	0.43
1:O:118:MET:HE2	1:O:152:PRO:HA	2.00	0.43
10:J:68:SER:O	10:J:72:ASP:N	2.51	0.43
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.18	0.43
14:N:161:GLN:O	14:N:164:LYS:HB3	2.18	0.43
5:S:205:LEU:HA	5:S:209:ASN:HD22	1.81	0.43
5:S:170:TYR:HB2	5:S:198:GLN:HG2	2.00	0.43
8:H:5:GLY:O	8:H:124:TYR:HA	2.18	0.43
5:S:1:PHE:CG	5:S:2:ARG:N	2.86	0.43
13:M:53:ILE:CD1	13:M:60:MET:HG3	2.47	0.43
9:I:104:VAL:HG23	9:I:106:PRO:HD3	2.00	0.43
7:G:241:GLU:O	7:G:242:GLN:HB2	2.18	0.43
7:U:222:ASP:O	7:U:223:LYS:HB2	2.18	0.43
11:Y:43:GLY:HA2	11:Y:100:MET:O	2.19	0.43
14:N:54:ALA:O	14:N:58:ILE:HG12	2.18	0.43
1:O:203:GLU:OE2	1:O:203:GLU:HA	2.19	0.43
5:S:70:GLY:HA3	5:S:221:PHE:CZ	2.52	0.43
4:D:89:VAL:HG21	11:K:65:LEU:CD2	2.48	0.43
2:P:237:ILE:O	2:P:237:ILE:HG13	2.18	0.43
2:P:194:LYS:O	2:P:197:SER:HB3	2.18	0.43
2:P:28:ILE:HD11	2:P:131:GLY:C	2.38	0.43
2:B:71:LYS:O	2:B:138:GLY:HA2	2.18	0.43
7:U:149:ASP:HB2	7:U:150:PRO:HD2	2.00	0.43
3:Q:172:PHE:O	3:Q:176:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:12:ILE:HG13	12:Z:110:ILE:HD12	2.00	0.43
1:A:214:ILE:HD11	1:A:235:PHE:HD1	1.84	0.43
11:Y:186:ILE:O	11:Y:188:HIS:HD2	2.00	0.43
10:X:68:SER:O	10:X:72:ASP:N	2.52	0.43
10:J:37:GLN:HG3	10:J:189:ILE:HG13	2.01	0.43
6:T:201:GLU:HA	6:T:201:GLU:OE1	2.19	0.43
12:Z:30:ILE:HD11	12:Z:197:GLN:NE2	2.34	0.43
3:Q:11:PRO:HA	4:R:18:TYR:CE1	2.53	0.43
2:P:2:SER:O	2:P:4:ARG:N	2.52	0.43
6:F:168:ALA:O	6:F:172:LEU:HD23	2.17	0.43
9:W:11:VAL:HG22	9:W:24:CYS:HB3	2.00	0.43
13:M:13:SER:HB3	13:M:22:ILE:HG13	2.00	0.43
1:O:226:GLY:HA3	8:V:186:TYR:HB3	2.00	0.43
8:V:213:LEU:HG	9:W:200:LYS:HB2	1.99	0.43
2:B:120:GLY:C	2:B:122:THR:H	2.21	0.43
2:B:122:THR:HG22	3:C:125:ARG:NH2	2.18	0.43
3:C:161:THR:HG23	3:C:166:SER:HB2	2.00	0.43
8:V:210:THR:CG2	9:W:199:LEU:HD22	2.49	0.43
12:L:30:ILE:HD11	12:L:197:GLN:NE2	2.33	0.43
11:K:76:VAL:N	11:K:108:GLU:OE2	2.51	0.43
13:M:53:ILE:HD12	13:M:60:MET:HG3	2.00	0.43
12:L:208:THR:C	12:L:210:ASP:N	2.72	0.43
4:D:115:PHE:CZ	4:D:129:PRO:HG3	2.54	0.43
8:H:9:ASN:HD21	8:H:147:THR:HA	1.82	0.43
10:J:106:GLY:HA2	10:J:184:VAL:HG11	1.99	0.43
3:C:46:ARG:HD2	3:C:206:LYS:O	2.18	0.43
8:V:207:ARG:HG3	16:V:335:HOH:O	2.19	0.43
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.19	0.43
13:M:3:GLN:HG3	13:M:3:GLN:O	2.18	0.43
10:J:172:MET:HG2	10:J:173:PRO:HD2	2.01	0.43
10:X:172:MET:HG2	10:X:173:PRO:HD2	2.01	0.43
5:E:70:GLY:HA3	5:E:221:PHE:CZ	2.54	0.43
4:D:180:HIS:H	4:D:183:LEU:HD11	1.83	0.43
9:I:37:ASN:HD22	9:I:37:ASN:C	2.22	0.43
2:B:194:LYS:O	2:B:197:SER:HB3	2.18	0.43
2:B:185:VAL:HG21	2:B:216:ARG:HG3	2.00	0.43
4:R:77:ALA:O	4:R:81:ILE:HG12	2.18	0.43
8:H:210:THR:CG2	9:I:199:LEU:HD22	2.48	0.43
5:E:157:GLY:O	5:E:158:THR:HB	2.19	0.43
11:K:208:ASN:ND2	10:X:150:PRO:CD	2.80	0.43
10:J:174:MET:HE1	10:X:173:PRO:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:220:PRO:O	5:S:221:PHE:C	2.57	0.43
14:N:8:PHE:CE2	14:N:13:ILE:HG13	2.51	0.43
7:U:155:VAL:CG2	7:U:156:GLY:N	2.82	0.43
4:D:4:VAL:HG23	4:D:116:GLY:HA2	2.01	0.43
14:N:133:PHE:CE2	14:N:166:ASP:HB2	2.53	0.43
5:S:175:LEU:O	5:S:177:THR:N	2.51	0.43
11:K:212:GLY:HA2	8:V:213:LEU:HD22	2.01	0.43
11:K:6:PHE:HA	11:K:125:ASP:O	2.18	0.43
8:V:5:GLY:O	8:V:124:TYR:HA	2.19	0.43
13:M:93:PHE:CE1	13:M:128:ARG:HD3	2.54	0.43
2:P:42:GLY:HA2	2:P:145:TYR:CE1	2.53	0.43
2:P:120:GLY:C	2:P:122:THR:H	2.22	0.43
10:X:149:ARG:NH1	10:X:149:ARG:HG2	2.34	0.43
12:L:199:GLY:O	12:L:200:ASP:HB2	2.19	0.43
12:Z:199:GLY:O	12:Z:200:ASP:HB2	2.18	0.43
7:U:68:ARG:CB	7:U:68:ARG:HH11	2.32	0.43
8:V:79:ALA:O	8:V:83:LEU:HG	2.19	0.43
3:C:109:ARG:HD3	3:C:154:TYR:OH	2.19	0.43
3:Q:147:GLN:HB3	3:Q:147:GLN:HE21	1.49	0.43
1:O:205:ASN:HA	1:O:247:LEU:CD1	2.49	0.43
8:V:4:VAL:HG22	8:V:159:ILE:CD1	2.42	0.43
10:X:149:ARG:HA	10:X:150:PRO:HD3	1.89	0.43
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.83	0.43
11:Y:76:VAL:N	11:Y:108:GLU:OE2	2.52	0.43
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.48	0.43
10:J:198:GLN:OXT	10:J:198:GLN:HG2	2.18	0.43
7:U:74:VAL:HG11	7:U:81:ALA:HB2	2.01	0.43
12:Z:10:GLY:HA3	12:Z:42:LYS:NZ	2.34	0.43
12:L:147:MET:CE	9:W:176:ARG:NH2	2.81	0.43
7:U:103:MET:CE	7:U:108:LEU:HB2	2.46	0.42
5:S:181:ILE:O	5:S:181:ILE:HG22	2.19	0.42
2:B:148:TYR:OH	3:C:57:ILE:HB	2.19	0.42
13:M:17:ASP:OD1	13:M:18:ASN:N	2.52	0.42
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.39	0.42
2:B:213:ALA:HA	2:B:227:LYS:O	2.19	0.42
4:R:23:ILE:HD13	4:R:133:ALA:HB2	2.01	0.42
4:D:77:ALA:O	4:D:81:ILE:HG12	2.19	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.00	0.42
2:B:229:PHE:CD2	2:B:229:PHE:N	2.86	0.42
11:K:191:HIS:N	11:K:191:HIS:CD2	2.86	0.42
2:B:243:ILE:O	2:B:243:ILE:HG22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	0.42
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.52	0.42
1:O:29:LYS:NZ	1:O:168:SER:OG	2.51	0.42
12:Z:109:THR:CG2	16:Z:309:HOH:O	2.62	0.42
1:O:183:LEU:HD23	1:O:187:ASP:HB3	2.00	0.42
6:T:214:TRP:CH2	6:T:219:GLU:HB3	2.54	0.42
13:M:25:ASP:HA	13:M:195:PHE:HA	2.00	0.42
1:O:214:ILE:HD11	1:O:235:PHE:HD1	1.84	0.42
9:I:186:VAL:HG21	9:I:199:LEU:HD11	2.01	0.42
4:R:155:THR:CG2	5:S:78:PRO:HD3	2.49	0.42
5:E:220:PRO:O	5:E:221:PHE:C	2.57	0.42
5:E:178:PHE:HA	5:E:181:ILE:CG1	2.46	0.42
6:T:171:GLU:HB3	6:T:195:ILE:CD1	2.49	0.42
5:E:1:PHE:CG	5:E:2:ARG:N	2.87	0.42
12:Z:92:ASN:C	12:Z:92:ASN:ND2	2.73	0.42
11:K:43:GLY:HA2	11:K:100:MET:O	2.19	0.42
9:I:94:LEU:HD12	9:I:127:GLY:HA2	2.01	0.42
12:Z:174:TYR:CD1	12:Z:175:LEU:N	2.86	0.42
3:Q:223:SER:O	3:Q:224:SER:C	2.57	0.42
1:O:234:ARG:HH11	1:O:234:ARG:HG2	1.84	0.42
8:H:172:ASN:ND2	8:H:172:ASN:N	2.66	0.42
1:A:203:GLU:OE2	1:A:203:GLU:HA	2.18	0.42
10:X:35:THR:HG21	10:X:182:LYS:NZ	2.35	0.42
3:Q:158:SER:HB3	3:Q:177:TYR:CE1	2.55	0.42
5:E:170:TYR:CE2	5:E:195:ALA:HB2	2.54	0.42
7:U:106:ASP:N	7:U:106:ASP:OD2	2.52	0.42
7:G:74:VAL:HG11	7:G:81:ALA:HB2	2.02	0.42
8:H:215:GLU:HG3	9:I:197:ARG:HG2	2.01	0.42
4:R:4:VAL:HG23	4:R:116:GLY:HA2	2.01	0.42
11:Y:115:VAL:HA	11:Y:120:THR:O	2.19	0.42
9:I:147:GLY:HA3	12:Z:145:LEU:O	2.19	0.42
6:F:9:SER:HB2	7:G:126:ARG:HD3	2.01	0.42
10:J:49:GLU:HB2	10:J:99:GLN:HB2	2.01	0.42
3:Q:39:CYS:HA	3:Q:136:PHE:HZ	1.84	0.42
13:M:9:THR:OG1	13:M:10:SER:N	2.52	0.42
12:Z:105:TYR:O	12:Z:107:VAL:N	2.51	0.42
1:A:128:ARG:HH11	1:A:128:ARG:HG3	1.84	0.42
7:U:12:PRO:HD3	16:U:326:HOH:O	2.18	0.42
1:A:180:ASN:H	1:A:183:LEU:CD1	2.31	0.42
12:Z:177:VAL:O	12:Z:181:ILE:HG13	2.20	0.42
7:U:3:TYR:C	7:U:5:ARG:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.55	0.42
2:B:4:ARG:HD2	2:B:5:TYR:CZ	2.55	0.42
7:G:29:THR:O	7:G:31:ILE:HG13	2.20	0.42
6:F:214:TRP:N	6:F:214:TRP:CD1	2.88	0.42
8:H:75:ARG:HG3	16:H:318:HOH:O	2.19	0.42
4:D:196:LEU:O	4:D:200:MET:HG3	2.19	0.42
2:P:234:ILE:O	2:P:238:LEU:HB2	2.19	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.42
10:J:110:LYS:HB2	10:J:110:LYS:NZ	2.33	0.42
1:A:30:GLN:CA	1:A:30:GLN:NE2	2.81	0.42
5:E:36:GLY:O	5:E:157:GLY:HA2	2.19	0.42
1:A:204:PHE:CZ	1:A:209:ILE:HD11	2.55	0.42
10:J:174:MET:HE1	10:X:173:PRO:CB	2.50	0.42
5:E:170:TYR:HB2	5:E:198:GLN:HG2	2.00	0.42
4:D:180:HIS:H	4:D:183:LEU:CD1	2.32	0.42
6:F:171:GLU:HB3	6:F:195:ILE:CD1	2.50	0.42
4:R:9:PRO:HG3	5:S:23:TYR:HE2	1.82	0.42
10:J:5:LEU:HB2	10:J:16:ALA:HB3	2.02	0.42
7:U:29:THR:O	7:U:31:ILE:HG13	2.20	0.42
5:S:39:SER:HB3	5:S:188:LEU:HD11	2.02	0.42
6:T:39:ASN:N	6:T:39:ASN:ND2	2.68	0.42
4:R:6:THR:CG2	4:R:7:PHE:N	2.83	0.42
10:X:184:VAL:HG22	10:X:189:ILE:HD12	2.01	0.42
9:I:117:LYS:HA	9:I:118:PRO:HD3	1.88	0.42
5:E:41:THR:HG23	5:E:182:ASP:HB3	2.01	0.42
1:O:134:LEU:O	1:O:149:GLN:HA	2.20	0.42
11:Y:174:SER:HA	11:Y:193:VAL:HG23	2.01	0.42
11:Y:201:LYS:HE3	11:Y:207:PHE:O	2.20	0.42
10:X:49:GLU:HB2	10:X:99:GLN:HB2	2.01	0.42
6:T:103:ILE:HA	6:T:104:PRO:HD3	1.84	0.42
1:O:44:VAL:CG2	1:O:211:LEU:HD21	2.50	0.42
7:G:66:ILE:HG21	7:G:108:LEU:HD21	2.01	0.42
9:W:145:LEU:HA	9:W:145:LEU:HD23	1.88	0.42
3:C:107:LEU:HD13	3:C:107:LEU:O	2.19	0.42
8:V:215:GLU:HG3	9:W:197:ARG:HG2	2.00	0.42
11:Y:4:LEU:O	11:Y:4:LEU:HD22	2.19	0.42
10:X:198:GLN:OXT	10:X:198:GLN:HG2	2.20	0.42
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.85	0.42
4:D:195:ILE:O	4:D:199:VAL:HG22	2.20	0.42
4:D:23:ILE:HD13	4:D:133:ALA:HB2	2.02	0.42
4:R:178:GLU:HB3	4:R:191:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:TYR:CE1	3:C:156:SER:HB3	2.54	0.42
7:U:6:HIS:CD2	7:U:6:HIS:N	2.88	0.42
2:B:17:ARG:HH11	2:B:17:ARG:HG2	1.84	0.42
5:S:35:VAL:HG23	5:S:196:ILE:CD1	2.49	0.42
5:S:36:GLY:O	5:S:158:THR:N	2.48	0.42
10:X:172:MET:HA	10:X:173:PRO:HD3	1.70	0.42
12:Z:28:ARG:HB2	12:Z:200:ASP:HB2	2.01	0.42
2:P:228:ILE:HD12	2:P:228:ILE:H	1.83	0.42
2:P:4:ARG:HD2	2:P:5:TYR:CZ	2.55	0.42
14:N:76:GLU:HB2	16:N:211:HOH:O	2.19	0.42
10:X:165:VAL:O	10:X:169:GLU:HG3	2.20	0.42
9:I:65:MET:O	9:I:68:TYR:HB3	2.20	0.42
4:R:171:ALA:O	4:R:174:GLU:HB3	2.20	0.42
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.01	0.42
2:P:61:SER:O	2:P:62:THR:OG1	2.29	0.42
5:E:131:LEU:HB2	5:E:146:PHE:HB3	2.01	0.42
8:V:175:VAL:HG12	8:V:176:CYS:N	2.35	0.42
5:S:157:GLY:O	6:T:54:LEU:HD13	2.20	0.42
5:S:189:ILE:O	5:S:193:VAL:HG23	2.20	0.42
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.44	0.42
5:E:155:LEU:HD12	5:E:158:THR:HG21	2.02	0.42
3:Q:213:VAL:O	3:Q:213:VAL:HG13	2.20	0.42
5:S:170:TYR:CE2	5:S:195:ALA:HB2	2.54	0.42
10:J:150:PRO:CD	11:Y:208:ASN:ND2	2.83	0.42
4:R:9:PRO:HA	5:S:23:TYR:CE2	2.54	0.42
7:U:135:VAL:O	7:U:136:SER:HB3	2.19	0.42
4:R:195:ILE:O	4:R:199:VAL:HG22	2.20	0.42
11:K:82:ILE:HG13	16:K:334:HOH:O	2.20	0.42
7:U:66:ILE:HG21	7:U:108:LEU:HD21	2.02	0.42
5:S:35:VAL:HG13	5:S:159:ALA:HB2	2.02	0.42
8:H:124:TYR:O	8:H:125:LEU:HD23	2.20	0.42
9:W:170:LEU:CD2	9:W:184:ALA:HB1	2.48	0.42
5:E:39:SER:HB3	5:E:188:LEU:HD11	2.01	0.42
8:H:214:LYS:CG	8:H:215:GLU:N	2.83	0.42
3:C:225:GLU:N	3:C:225:GLU:OE1	2.52	0.42
5:S:33:VAL:HG22	5:S:34:THR:N	2.34	0.42
1:O:101:TYR:CE1	9:W:89:LEU:HD13	2.55	0.42
2:P:43:ILE:CG2	2:P:147:LEU:HD13	2.50	0.41
9:I:171:LEU:HD11	9:I:201:MET:HB3	2.02	0.41
4:R:159:TYR:CD2	4:R:162:LYS:HB2	2.55	0.41
2:B:110:LEU:HD23	2:B:110:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:7:ARG:HD2	11:Y:110:PRO:O	2.20	0.41
1:O:187:ASP:O	1:O:191:ILE:HG13	2.20	0.41
9:W:189:ILE:HG13	9:W:194:VAL:HG22	2.01	0.41
1:O:55:LEU:HD12	7:U:170:THR:HG23	2.02	0.41
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.35	0.41
5:E:23:TYR:CD1	5:E:23:TYR:N	2.88	0.41
5:E:46:VAL:HG13	5:E:212:ILE:HG12	2.03	0.41
13:M:48:ASN:ND2	13:M:48:ASN:H	2.09	0.41
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	2.00	0.41
1:A:187:ASP:O	1:A:191:ILE:HG13	2.20	0.41
5:E:178:PHE:O	5:E:181:ILE:HG13	2.20	0.41
5:S:167:ALA:CB	5:S:195:ALA:O	2.67	0.41
12:L:28:ARG:HB2	12:L:200:ASP:HB2	2.02	0.41
5:S:1:PHE:O	5:S:2:ARG:C	2.59	0.41
12:Z:51:VAL:CG1	12:Z:205:LEU:HD23	2.50	0.41
11:Y:4:LEU:HA	11:Y:127:PHE:O	2.20	0.41
9:I:189:ILE:HG13	9:I:194:VAL:HG22	2.01	0.41
10:X:192:VAL:C	10:X:194:ASP:H	2.23	0.41
4:D:42:VAL:HG22	4:D:59:ILE:HD11	2.03	0.41
8:V:41:ILE:HD13	8:V:76:VAL:HA	2.00	0.41
6:F:168:ALA:C	6:F:172:LEU:HD23	2.41	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.41
2:P:17:ARG:NH1	2:P:17:ARG:HG2	2.35	0.41
10:J:12:SER:HB2	10:J:184:VAL:O	2.20	0.41
10:X:23:ARG:HD3	10:X:23:ARG:HA	1.86	0.41
3:C:179:ARG:HH22	4:D:52:GLU:HA	1.85	0.41
4:R:185:LEU:O	4:R:189:GLU:HG3	2.20	0.41
2:B:160:LYS:HB3	2:B:179:TYR:CZ	2.56	0.41
11:Y:3:THR:HG21	16:Y:333:HOH:O	2.20	0.41
8:V:196:ARG:NH2	9:W:150:GLU:O	2.53	0.41
9:W:62:LEU:HA	9:W:62:LEU:HD23	1.87	0.41
7:G:222:ASP:O	7:G:223:LYS:HB2	2.18	0.41
1:A:187:ASP:O	1:A:190:HIS:HB3	2.20	0.41
10:J:149:ARG:NH1	10:J:149:ARG:HG2	2.35	0.41
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.51	0.41
11:K:115:VAL:HA	11:K:120:THR:O	2.20	0.41
11:K:37:ILE:HD13	11:K:59:LEU:HD23	2.01	0.41
5:S:131:LEU:HD12	5:S:146:PHE:CD2	2.56	0.41
10:X:119:ILE:HG12	10:X:125:LYS:HG3	2.02	0.41
8:H:188:ARG:O	8:H:189:ASN:HB2	2.20	0.41
2:P:160:LYS:HB3	2:P:179:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:95:PHE:CD1	7:U:95:PHE:C	2.94	0.41
4:R:64:ARG:O	4:R:64:ARG:HG2	2.20	0.41
8:V:3:ILE:O	8:V:126:SER:HA	2.20	0.41
3:C:160:GLN:CG	3:C:161:THR:N	2.83	0.41
1:A:122:THR:O	1:A:122:THR:CG2	2.68	0.41
3:C:70:VAL:HG13	3:C:219:ILE:HD13	2.03	0.41
5:E:167:ALA:CB	5:E:195:ALA:O	2.67	0.41
3:C:157:TRP:CZ2	4:D:51:LEU:HD23	2.55	0.41
7:G:166:GLN:NE2	7:G:167:GLN:N	2.68	0.41
6:F:214:TRP:CH2	6:F:219:GLU:HB3	2.55	0.41
7:U:42:THR:HG21	7:U:135:VAL:HB	2.02	0.41
11:Y:4:LEU:HD11	11:Y:161:ILE:HG12	2.02	0.41
3:Q:109:ARG:HD3	3:Q:154:TYR:OH	2.20	0.41
6:T:168:ALA:C	6:T:172:LEU:HD23	2.41	0.41
6:T:148:GLU:HB3	16:T:336:HOH:O	2.19	0.41
3:Q:178:ASP:OD1	3:Q:180:LYS:HB2	2.21	0.41
3:Q:88:ARG:NH1	16:Q:304:HOH:O	2.40	0.41
9:W:171:LEU:HD11	9:W:201:MET:HB3	2.02	0.41
7:G:68:ARG:CB	7:G:68:ARG:HH11	2.32	0.41
5:E:189:ILE:CG2	5:E:212:ILE:HD13	2.44	0.41
10:J:174:MET:CE	10:X:174:MET:CE	2.99	0.41
6:T:191:GLN:O	6:T:194:LYS:HB3	2.20	0.41
3:C:11:PRO:HA	4:D:18:TYR:CE1	2.54	0.41
2:B:24:ALA:O	2:B:27:SER:HB3	2.21	0.41
6:F:39:ASN:N	6:F:39:ASN:ND2	2.68	0.41
10:J:192:VAL:C	10:J:194:ASP:H	2.24	0.41
4:R:205:ASP:O	4:R:207:ASN:N	2.54	0.41
12:Z:208:THR:C	12:Z:210:ASP:N	2.73	0.41
5:E:174:THR:HG22	5:E:174:THR:O	2.20	0.41
6:T:126:ARG:NH1	6:T:126:ARG:HG2	2.35	0.41
4:R:73:LEU:HD12	4:R:131:GLY:HA3	2.03	0.41
3:C:178:ASP:OD1	3:C:180:LYS:HB2	2.21	0.41
6:F:200:HIS:O	6:F:200:HIS:CG	2.74	0.41
3:Q:70:VAL:HG13	3:Q:219:ILE:HD13	2.02	0.41
1:A:183:LEU:HD23	1:A:187:ASP:HB3	2.01	0.41
10:J:158:LEU:HD21	10:J:183:ILE:HD11	2.03	0.41
5:S:23:TYR:CD1	5:S:23:TYR:N	2.88	0.41
4:D:228:THR:HG22	4:D:232:ILE:HD13	2.02	0.41
10:J:8:ARG:HG2	10:J:8:ARG:NH1	2.34	0.41
4:D:205:ASP:O	4:D:207:ASN:N	2.54	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:LEU:HD12	4:D:131:GLY:HA3	2.03	0.41
11:Y:77:ALA:HA	11:Y:113:TYR:CE2	2.55	0.41
7:G:24:LYS:HD2	7:G:24:LYS:HA	1.80	0.41
4:D:236:LYS:HE2	4:D:236:LYS:HB3	1.91	0.41
7:U:103:MET:HA	7:U:104:PRO:HD3	1.94	0.41
12:L:154:VAL:O	12:L:154:VAL:HG12	2.20	0.41
2:B:46:ALA:HB2	2:B:212:PHE:CE1	2.55	0.41
13:M:159:VAL:HG11	13:M:165:ILE:HD13	2.03	0.41
5:S:174:THR:O	5:S:174:THR:HG22	2.21	0.41
10:X:37:GLN:HG3	10:X:189:ILE:HG13	2.03	0.41
10:J:184:VAL:HG22	10:J:189:ILE:HD12	2.03	0.41
16:G:308:HOH:O	8:H:82:MET:HA	2.19	0.41
12:Z:115:ASP:OD2	12:Z:119:LYS:HB2	2.20	0.41
11:Y:159:ARG:O	11:Y:162:LEU:HB3	2.21	0.41
2:P:65:LEU:HD23	2:P:213:ALA:HB2	2.02	0.41
5:S:72:SER:OG	5:S:132:LEU:HB2	2.21	0.41
5:E:35:VAL:HG13	5:E:159:ALA:HB2	2.03	0.41
10:J:172:MET:CE	10:J:174:MET:HB2	2.51	0.41
2:B:134:PHE:O	2:B:149:THR:HA	2.21	0.41
8:V:104:ASP:C	8:V:106:THR:H	2.24	0.41
1:A:139:HIS:HA	1:A:144:GLY:O	2.21	0.41
2:B:63:GLU:HG3	2:B:64:LYS:HG3	2.02	0.41
6:F:86:ASN:HD22	6:F:86:ASN:HA	1.65	0.41
9:W:186:VAL:HG21	9:W:199:LEU:HD11	2.03	0.41
5:E:189:ILE:O	5:E:193:VAL:HG23	2.20	0.41
5:E:35:VAL:HG23	5:E:196:ILE:CD1	2.51	0.41
3:C:158:SER:HB3	3:C:177:TYR:CE1	2.56	0.41
3:C:213:VAL:O	3:C:213:VAL:HG13	2.20	0.41
10:J:25:ILE:O	10:X:139:TYR:OH	2.39	0.41
3:C:51:LYS:HD2	3:C:52:LEU:H	1.82	0.41
5:E:181:ILE:HG22	5:E:181:ILE:O	2.21	0.41
13:M:170:VAL:HG23	16:M:323:HOH:O	2.21	0.41
4:D:193:LEU:HA	4:D:193:LEU:HD12	1.82	0.41
11:Y:106:ARG:HD3	11:Y:182:GLU:OE1	2.21	0.41
6:F:123:ASN:C	6:F:123:ASN:HD22	2.24	0.41
10:X:26:SER:HB2	11:Y:133:GLN:NE2	2.34	0.41
12:L:92:ASN:ND2	12:L:92:ASN:C	2.73	0.41
11:Y:37:ILE:HD13	11:Y:59:LEU:HD23	2.02	0.41
9:W:104:VAL:HG23	9:W:106:PRO:HD3	2.02	0.41
12:Z:213:ARG:HH11	12:Z:213:ARG:CB	2.33	0.41
4:R:38:VAL:HB	4:R:214:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:THR:CG2	4:D:7:PHE:N	2.83	0.41
2:B:65:LEU:HD23	2:B:213:ALA:HB2	2.03	0.41
5:S:93:TYR:CE1	5:S:97:VAL:HG21	2.56	0.41
7:G:6:HIS:CD2	7:G:6:HIS:N	2.87	0.41
2:P:176:GLN:O	2:P:176:GLN:HG2	2.21	0.41
7:G:73:VAL:CG1	7:G:133:THR:HB	2.51	0.41
3:C:92:GLN:HG3	10:J:66:LEU:HB2	2.03	0.41
8:V:128:GLY:O	8:V:131:SER:HB2	2.20	0.41
8:H:175:VAL:HG12	8:H:176:CYS:N	2.36	0.41
5:E:126:PRO:HA	16:E:303:HOH:O	2.20	0.41
2:P:175:LEU:C	2:P:177:MET:H	2.24	0.41
6:T:91:GLU:HG2	6:T:111:ARG:CB	2.35	0.41
2:B:93:HIS:CE1	2:B:113:ARG:HD3	2.56	0.41
8:H:3:ILE:O	8:H:126:SER:HA	2.20	0.41
5:S:12:PHE:N	6:T:19:GLN:HE22	2.18	0.41
12:L:195:HIS:CD2	12:L:197:GLN:HB2	2.56	0.41
7:G:167:GLN:HB3	16:G:339:HOH:O	2.21	0.41
10:X:103:LEU:HD21	10:X:118:GLN:HG3	2.02	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.41
6:T:27:VAL:HG13	6:T:75:SER:O	2.21	0.41
2:B:2:SER:O	2:B:4:ARG:N	2.54	0.41
1:O:3:ASP:OD2	1:O:5:TYR:HB2	2.21	0.41
10:X:140:THR:HG22	10:X:164:CYS:HB3	2.03	0.41
12:L:10:GLY:N	16:L:330:HOH:O	2.54	0.41
3:C:103:THR:N	16:C:306:HOH:O	2.48	0.41
4:R:17:GLU:O	4:R:20:LEU:HB2	2.21	0.41
12:L:36:ASN:HB3	13:M:137:TYR:CZ	2.56	0.41
6:T:138:ASP:OD2	6:T:138:ASP:C	2.60	0.41
3:Q:160:GLN:CG	3:Q:161:THR:N	2.83	0.40
12:L:52:MET:HG2	12:L:53:SER:N	2.36	0.40
3:C:155:SER:HB2	4:D:51:LEU:HD21	2.03	0.40
4:R:228:THR:HG22	4:R:232:ILE:HD13	2.03	0.40
10:J:103:LEU:HD23	10:J:103:LEU:HA	1.77	0.40
2:P:95:GLN:NE2	16:P:307:HOH:O	2.53	0.40
9:W:30:SER:O	9:W:31:GLN:HB2	2.22	0.40
2:P:24:ALA:O	2:P:27:SER:HB3	2.21	0.40
2:P:46:ALA:HB2	2:P:212:PHE:CE1	2.56	0.40
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.21	0.40
12:L:10:GLY:HA3	12:L:42:LYS:NZ	2.36	0.40
8:V:10:ASN:HD22	8:V:179:GLU:HG2	1.86	0.40
11:Y:201:LYS:HG2	16:Y:326:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:213:ALA:HA	2:P:227:LYS:O	2.20	0.40
5:E:33:VAL:HG22	5:E:34:THR:N	2.36	0.40
3:C:210:ILE:CG2	3:C:211:THR:N	2.84	0.40
3:Q:105:GLU:HB3	16:Q:305:HOH:O	2.21	0.40
11:K:77:ALA:HA	11:K:113:TYR:CE2	2.56	0.40
12:L:2:PHE:CB	13:M:1:THR:HG23	2.51	0.40
6:T:200:HIS:O	6:T:200:HIS:CG	2.74	0.40
6:T:86:ASN:HD22	6:T:86:ASN:HA	1.67	0.40
7:U:83:ASN:C	7:U:83:ASN:ND2	2.74	0.40
4:D:78:ARG:HD3	4:D:78:ARG:HA	1.92	0.40
8:H:3:ILE:HD13	8:H:127:LEU:O	2.21	0.40
7:G:103:MET:CE	7:G:108:LEU:HB2	2.47	0.40
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.55	0.40
5:S:184:ASN:HA	5:S:185:PRO:HD2	1.96	0.40
10:J:4:ILE:HG22	10:J:103:LEU:CD1	2.51	0.40
11:K:65:LEU:O	11:K:69:ARG:HB2	2.22	0.40
2:P:110:LEU:C	2:P:110:LEU:HD23	2.41	0.40
9:I:145:LEU:HA	9:I:145:LEU:HD23	1.88	0.40
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.02	0.40
2:B:228:ILE:H	2:B:228:ILE:HD12	1.84	0.40
5:E:188:LEU:HA	5:E:188:LEU:HD23	1.90	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
10:X:110:LYS:HB2	10:X:110:LYS:HZ3	1.87	0.40
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.40
1:A:167:GLY:HA2	16:A:317:HOH:O	2.22	0.40
11:K:140:LEU:HD13	11:K:160:SER:OG	2.21	0.40
11:K:114:TYR:O	11:K:121:ARG:HA	2.21	0.40
5:S:216:GLY:O	5:S:218:ASP:N	2.54	0.40
7:U:56:ASP:C	7:U:56:ASP:OD2	2.60	0.40
1:A:196:LEU:HA	1:A:196:LEU:HD12	1.88	0.40
8:V:3:ILE:HD13	8:V:127:LEU:O	2.21	0.40
5:S:178:PHE:O	5:S:181:ILE:HG13	2.21	0.40
6:F:191:GLN:NE2	6:F:194:LYS:HE2	2.37	0.40
11:K:20:ALA:CB	11:K:31:VAL:HG21	2.49	0.40
10:J:53:THR:HG23	10:J:54:VAL:H	1.83	0.40
5:S:23:TYR:HD1	5:S:23:TYR:N	2.19	0.40
7:G:149:ASP:HB2	7:G:150:PRO:HD2	2.02	0.40
8:V:75:ARG:HA	8:V:104:ASP:OD1	2.21	0.40
9:I:146:PHE:O	9:I:150:GLU:HB2	2.21	0.40
2:P:134:PHE:O	2:P:149:THR:HA	2.21	0.40
9:W:154:GLU:CG	9:W:157:LEU:HD21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:23:ARG:NE	16:X:222:HOH:O	2.42	0.40
3:C:39:CYS:HA	3:C:136:PHE:HZ	1.87	0.40
1:O:250:LEU:C	1:O:250:LEU:HD13	2.42	0.40
4:D:169:GLU:OE1	4:D:169:GLU:N	2.55	0.40
5:S:44:VAL:HG12	5:S:45:LEU:N	2.36	0.40
5:S:46:VAL:HG13	5:S:212:ILE:HG12	2.02	0.40
1:O:204:PHE:CD1	1:O:209:ILE:HD11	2.55	0.40
11:K:7:ARG:HD2	11:K:110:PRO:O	2.22	0.40
12:Z:103:PHE:N	12:Z:104:PRO:CD	2.82	0.40
7:U:155:VAL:HG13	7:U:157:TYR:CE1	2.57	0.40
9:I:20:VAL:CG2	9:I:189:ILE:HB	2.52	0.40
14:N:114:PRO:HA	16:N:220:HOH:O	2.21	0.40
2:B:88:ASN:O	2:B:92:ILE:HG12	2.22	0.40
10:X:19:LYS:HG2	10:X:180:ILE:HG13	2.04	0.40
6:F:14:ASP:OD1	6:F:16:ARG:HD3	2.21	0.40
4:D:210:GLN:HA	16:D:318:HOH:O	2.21	0.40
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.87	0.40
3:Q:225:GLU:N	3:Q:225:GLU:OE1	2.54	0.40
5:S:205:LEU:HA	5:S:209:ASN:HD21	1.83	0.40
10:X:158:LEU:HD21	10:X:183:ILE:HD11	2.02	0.40
13:M:27:LEU:HD11	13:M:34:LEU:HB3	2.04	0.40
5:S:106:ARG:NH1	5:S:106:ARG:HG2	2.35	0.40
5:E:131:LEU:HD12	5:E:146:PHE:CD2	2.56	0.40
3:C:224:SER:HB2	3:C:225:GLU:OE1	2.22	0.40
5:S:131:LEU:HB2	5:S:146:PHE:HB3	2.02	0.40
11:K:17:ASP:CG	11:K:33:LYS:HZ2	2.25	0.40
12:L:94:GLN:HG3	12:L:129:GLY:O	2.21	0.40
6:F:220:THR:O	6:F:221:ASN:CB	2.69	0.40
3:Q:82:ILE:N	3:Q:82:ILE:CD1	2.85	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%)	18 (7%)	4 (2%)	12	48
1	O	248/250 (99%)	224 (90%)	20 (8%)	4 (2%)	12	48
2	B	242/244 (99%)	213 (88%)	21 (9%)	8 (3%)	5	26
2	P	242/244 (99%)	212 (88%)	23 (10%)	7 (3%)	6	29
3	C	239/241 (99%)	214 (90%)	20 (8%)	5 (2%)	9	40
3	Q	239/241 (99%)	215 (90%)	19 (8%)	5 (2%)	9	40
4	D	240/242 (99%)	212 (88%)	19 (8%)	9 (4%)	4	22
4	R	240/242 (99%)	212 (88%)	19 (8%)	9 (4%)	4	22
5	E	231/233 (99%)	202 (87%)	21 (9%)	8 (4%)	4	24
5	S	231/233 (99%)	202 (87%)	22 (10%)	7 (3%)	5	29
6	F	242/244 (99%)	224 (93%)	16 (7%)	2 (1%)	24	66
6	T	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	24	66
7	G	241/243 (99%)	219 (91%)	19 (8%)	3 (1%)	16	56
7	U	241/243 (99%)	218 (90%)	20 (8%)	3 (1%)	16	56
8	H	220/222 (99%)	197 (90%)	20 (9%)	3 (1%)	14	51
8	V	220/222 (99%)	195 (89%)	22 (10%)	3 (1%)	14	51
9	I	202/204 (99%)	185 (92%)	14 (7%)	3 (2%)	13	50
9	W	202/204 (99%)	185 (92%)	15 (7%)	2 (1%)	19	61
10	J	196/198 (99%)	183 (93%)	10 (5%)	3 (2%)	13	50
10	X	196/198 (99%)	182 (93%)	11 (6%)	3 (2%)	13	50
11	K	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
11	Y	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
12	L	220/222 (99%)	199 (90%)	16 (7%)	5 (2%)	8	36
12	Z	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	11	45
13	M	231/233 (99%)	206 (89%)	24 (10%)	1 (0%)	39	80
13	a	231/233 (99%)	206 (89%)	24 (10%)	1 (0%)	39	80
14	N	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	34	76
14	b	194/196 (99%)	183 (94%)	9 (5%)	2 (1%)	19	61
15	c	1/4 (25%)	1 (100%)	0	0	100	100
15	d	1/4 (25%)	1 (100%)	0	0	100	100
15	e	1/4 (25%)	1 (100%)	0	0	100	100
15	f	1/4 (25%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6316/6384 (99%)	5724 (91%)	485 (8%)	107 (2%)	11 46

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	62	THR
2	B	221	ASP
3	C	52	LEU
4	D	122	GLU
5	E	2	ARG
5	E	201	ARG
5	E	217	LYS
6	F	8	ASN
6	F	9	SER
7	G	242	GLN
12	L	81	ASP
2	P	51	VAL
2	P	62	THR
2	P	221	ASP
3	Q	52	LEU
4	R	122	GLU
5	S	2	ARG
5	S	201	ARG
5	S	217	LYS
6	T	8	ASN
6	T	9	SER
7	U	242	GLN
12	Z	81	ASP
2	B	3	ARG
2	B	218	GLY
3	C	203	THR
4	D	53	SER
4	D	126	MET
4	D	181	SER
4	D	206	GLU
5	E	175	LEU
5	E	176	ASP
9	I	191	LYS
10	J	193	ASP
10	J	197	ALA
12	L	164	THR

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Mol	Chain	Res	Type
2	P	3	ARG
2	P	218	GLY
3	Q	203	THR
4	R	53	SER
4	R	126	MET
4	R	181	SER
4	R	206	GLU
5	S	175	LEU
5	S	176	ASP
8	V	9	ASN
8	V	91	GLN
9	W	191	LYS
10	X	193	ASP
10	X	197	ALA
12	Z	164	THR
14	b	191	ASP
1	A	60	THR
3	C	202	GLN
3	C	224	SER
4	D	2	ARG
5	E	227	GLU
8	H	9	ASN
8	H	91	GLN
8	H	105	PRO
12	L	103	PHE
14	N	191	ASP
1	O	2	THR
1	O	60	THR
3	Q	202	GLN
4	R	2	ARG
8	V	105	PRO
12	Z	209	LYS
1	A	2	THR
2	B	183	MET
5	E	221	PHE
10	J	9	VAL
12	L	209	LYS
3	Q	224	SER
5	S	221	PHE
10	X	9	VAL
12	Z	103	PHE
13	a	111	TRP

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Mol	Chain	Res	Type
1	A	166	LYS
2	B	243	ILE
4	D	112	ALA
4	D	118	GLY
7	G	51	PRO
7	G	184	HIS
9	I	116	GLY
12	L	26	ASP
13	M	111	TRP
1	O	19	GLY
1	O	166	LYS
2	P	243	ILE
4	R	112	ALA
4	R	118	GLY
5	S	227	GLU
7	U	51	PRO
7	U	184	HIS
9	W	116	GLY
1	A	19	GLY
4	D	121	GLY
5	E	186	ASP
4	R	121	GLY
14	b	145	ASN
3	C	183	PRO
3	Q	183	PRO
9	I	155	PRO
2	B	185	VAL
2	P	185	VAL

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%)	203 (97%)	6 (3%)	50 84
1	O	209/209 (100%)	203 (97%)	6 (3%)	50 84
2	B	203/203 (100%)	193 (95%)	10 (5%)	31 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	203/203 (100%)	193 (95%)	10 (5%)	31	71
3	C	213/213 (100%)	205 (96%)	8 (4%)	40	78
3	Q	213/213 (100%)	205 (96%)	8 (4%)	40	78
4	D	198/198 (100%)	193 (98%)	5 (2%)	55	86
4	R	198/198 (100%)	193 (98%)	5 (2%)	55	86
5	E	192/192 (100%)	176 (92%)	16 (8%)	14	46
5	S	192/192 (100%)	176 (92%)	16 (8%)	14	46
6	F	201/201 (100%)	186 (92%)	15 (8%)	17	51
6	T	201/201 (100%)	184 (92%)	17 (8%)	13	45
7	G	207/207 (100%)	196 (95%)	11 (5%)	28	67
7	U	207/207 (100%)	196 (95%)	11 (5%)	28	67
8	H	181/181 (100%)	172 (95%)	9 (5%)	30	70
8	V	181/181 (100%)	173 (96%)	8 (4%)	35	74
9	I	172/172 (100%)	168 (98%)	4 (2%)	58	87
9	W	172/172 (100%)	167 (97%)	5 (3%)	50	84
10	J	175/175 (100%)	172 (98%)	3 (2%)	68	91
10	X	175/175 (100%)	172 (98%)	3 (2%)	68	91
11	K	169/169 (100%)	162 (96%)	7 (4%)	37	76
11	Y	169/169 (100%)	162 (96%)	7 (4%)	37	76
12	L	185/185 (100%)	173 (94%)	12 (6%)	21	58
12	Z	185/185 (100%)	172 (93%)	13 (7%)	19	55
13	M	199/199 (100%)	186 (94%)	13 (6%)	21	58
13	a	199/199 (100%)	188 (94%)	11 (6%)	27	65
14	N	162/162 (100%)	155 (96%)	7 (4%)	35	75
14	b	162/162 (100%)	155 (96%)	7 (4%)	35	75
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
All	All	5336/5336 (100%)	5083 (95%)	253 (5%)	32	72

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

Mol	Chain	Res	Type
1	A	4	ARG
1	A	30	GLN
1	A	122	THR
1	A	133	SER
1	A	157	PHE
1	A	178	ARG
2	B	58	GLN
2	B	69	ASN
2	B	119	GLN
2	B	149	THR
2	B	155	ASN
2	B	157	THR
2	B	184	LYS
2	B	191	LEU
2	B	212	PHE
2	B	220	ASN
3	C	4	ARG
3	C	22	LEU
3	C	47	ARG
3	C	51	LYS
3	C	61	LYS
3	C	147	GLN
3	C	206	LYS
3	C	225	GLU
4	D	68	CYS
4	D	124	ARG
4	D	169	GLU
4	D	176	LEU
4	D	193	LEU
5	E	9	THR
5	E	10	VAL
5	E	12	PHE
5	E	29	LYS
5	E	53	ASP
5	E	71	LEU
5	E	92	ASN
5	E	112	CYS
5	E	116	GLN
5	E	184	ASN
5	E	197	SER
5	E	198	GLN
5	E	205	LEU
5	E	222	THR

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Mol	Chain	Res	Type
5	E	227	GLU
5	E	231	LYS
6	F	32	THR
6	F	39	ASN
6	F	68	ARG
6	F	94	SER
6	F	101	THR
6	F	117	GLN
6	F	123	ASN
6	F	165	ARG
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	203	ASN
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	124	TYR
7	G	166	GLN
7	G	186	ASN
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
7	G	243	ASP
8	H	3	ILE
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	59	ILE
8	H	182	LYS
8	H	196	ARG
8	H	209	THR
8	H	222	ASP
9	I	37	ASN
9	I	123	PHE
9	I	146	PHE
9	I	171	LEU
10	J	71	GLU

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Mol	Chain	Res	Type
10	J	78	GLN
10	J	110	LYS
11	K	4	LEU
11	K	9	GLN
11	K	87	VAL
11	K	100	MET
11	K	104	TYR
11	K	107	LYS
11	K	147	ASP
12	L	1	GLN
12	L	3	ASN
12	L	23	LEU
12	L	49	ASN
12	L	67	ARG
12	L	80	ASN
12	L	92	ASN
12	L	108	HIS
12	L	109	THR
12	L	126	ASP
12	L	132	GLU
12	L	165	ASN
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	82	ASP
13	M	104	ARG
13	M	132	LEU
13	M	146	PHE
13	M	159	VAL
13	M	161	ARG
13	M	171	GLN
13	M	204	THR
13	M	206	LEU
13	M	226	LYS
14	N	36	ARG
14	N	83	LYS
14	N	88	GLU
14	N	104	ASP
14	N	105	LYS
14	N	119	VAL
14	N	144	GLU
1	O	4	ARG

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Mol	Chain	Res	Type
1	O	30	GLN
1	O	122	THR
1	O	133	SER
1	O	157	PHE
1	O	178	ARG
2	P	58	GLN
2	P	69	ASN
2	P	119	GLN
2	P	149	THR
2	P	155	ASN
2	P	157	THR
2	P	184	LYS
2	P	191	LEU
2	P	212	PHE
2	P	220	ASN
3	Q	4	ARG
3	Q	22	LEU
3	Q	47	ARG
3	Q	51	LYS
3	Q	61	LYS
3	Q	147	GLN
3	Q	206	LYS
3	Q	225	GLU
4	R	68	CYS
4	R	124	ARG
4	R	169	GLU
4	R	176	LEU
4	R	193	LEU
5	S	9	THR
5	S	10	VAL
5	S	12	PHE
5	S	29	LYS
5	S	53	ASP
5	S	71	LEU
5	S	92	ASN
5	S	112	CYS
5	S	116	GLN
5	S	184	ASN
5	S	197	SER
5	S	198	GLN
5	S	205	LEU
5	S	222	THR

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Mol	Chain	Res	Type
5	S	227	GLU
5	S	231	LYS
6	T	14	ASP
6	T	32	THR
6	T	39	ASN
6	T	68	ARG
6	T	94	SER
6	T	101	THR
6	T	117	GLN
6	T	123	ASN
6	T	165	ARG
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	202	ASP
6	T	203	ASN
6	T	214	TRP
6	T	221	ASN
6	T	228	LYS
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	124	TYR
7	U	166	GLN
7	U	186	ASN
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
7	U	243	ASP
8	V	3	ILE
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	59	ILE
8	V	196	ARG
8	V	209	THR
8	V	222	ASP
9	W	37	ASN
9	W	120	ILE
9	W	123	PHE
9	W	146	PHE

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Mol	Chain	Res	Type
9	W	171	LEU
10	X	71	GLU
10	X	78	GLN
10	X	110	LYS
11	Y	4	LEU
11	Y	9	GLN
11	Y	87	VAL
11	Y	100	MET
11	Y	104	TYR
11	Y	107	LYS
11	Y	147	ASP
12	Z	1	GLN
12	Z	3	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	67	ARG
12	Z	80	ASN
12	Z	92	ASN
12	Z	108	HIS
12	Z	109	THR
12	Z	126	ASP
12	Z	132	GLU
12	Z	165	ASN
12	Z	174	TYR
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	82	ASP
13	a	104	ARG
13	a	146	PHE
13	a	159	VAL
13	a	161	ARG
13	a	171	GLN
13	a	206	LEU
13	a	226	LYS
14	b	36	ARG
14	b	83	LYS
14	b	88	GLU
14	b	104	ASP
14	b	105	LYS
14	b	119	VAL
14	b	144	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (200) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	69	ASN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
3	C	17	GLN
3	C	92	GLN
3	C	147	GLN
3	C	160	GLN
3	C	207	ASN
3	C	241	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	4	ASN
5	E	30	GLN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
5	E	198	GLN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	224	HIS

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Mol	Chain	Res	Type
7	G	6	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
7	G	231	ASN
8	H	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	172	ASN
9	I	37	ASN
9	I	71	ASN
9	I	88	GLN
9	I	156	ASN
10	J	55	GLN
10	J	78	GLN
10	J	86	GLN
10	J	146	HIS
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	188	HIS
11	K	191	HIS
11	K	208	ASN
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	92	ASN
12	L	135	GLN
12	L	152	ASN
12	L	153	GLN

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Mol	Chain	Res	Type
12	L	158	ASN
12	L	165	ASN
12	L	195	HIS
12	L	197	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	60	GLN
14	N	69	GLN
14	N	157	HIS
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	69	ASN
2	P	93	HIS
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	92	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	207	ASN
3	Q	241	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	4	ASN
5	S	30	GLN

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Mol	Chain	Res	Type
5	S	59	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
5	S	198	GLN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	6	HIS
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	172	ASN
9	W	37	ASN
9	W	71	ASN
9	W	88	GLN
9	W	156	ASN
10	X	55	GLN
10	X	78	GLN
10	X	86	GLN
10	X	146	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN

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Mol	Chain	Res	Type
11	Y	133	GLN
11	Y	176	ASN
11	Y	188	HIS
11	Y	191	HIS
11	Y	208	ASN
11	Y	209	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	92	ASN
12	Z	135	GLN
12	Z	152	ASN
12	Z	153	GLN
12	Z	158	ASN
12	Z	165	ASN
12	Z	195	HIS
12	Z	197	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	60	GLN
14	b	69	GLN
14	b	145	ASN
14	b	157	HIS
14	b	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

8 non-standard protein/DNA/RNA residues 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	LYO	c	3	15	8,9,10	0.90	0	7,10,12	1.01	1 (14%)
15	0W6	c	4	8,15	6,6,7	1.58	1 (16%)	4,6,8	0.75	0
15	LYO	d	3	15	8,9,10	0.79	0	7,10,12	1.09	1 (14%)
15	0W6	d	4	11,15	6,6,7	1.21	0	4,6,8	0.50	0
15	LYO	e	3	15	8,9,10	0.85	0	7,10,12	0.97	1 (14%)
15	0W6	e	4	8,15	6,6,7	1.14	0	4,6,8	0.85	0
15	LYO	f	3	15	8,9,10	0.92	0	7,10,12	1.03	1 (14%)
15	0W6	f	4	11,15	6,6,7	1.27	1 (16%)	4,6,8	0.42	0

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	LYO	c	3	15	-	0/7/9/11	0/0/0/0
15	0W6	c	4	8,15	-	0/3/4/5	0/0/0/0
15	LYO	d	3	15	-	0/7/9/11	0/0/0/0
15	0W6	d	4	11,15	-	0/3/4/5	0/0/0/0
15	LYO	e	3	15	-	0/7/9/11	0/0/0/0
15	0W6	e	4	8,15	-	0/3/4/5	0/0/0/0
15	LYO	f	3	15	-	0/7/9/11	0/0/0/0
15	0W6	f	4	11,15	-	0/3/4/5	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	4	0W6	C17-C15	2.09	1.55	1.53
15	c	4	0W6	C17-C15	3.30	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	d	3	LYO	O-C-CA	-2.51	118.94	125.49
15	f	3	LYO	O-C-CA	-2.38	119.30	125.49
15	e	3	LYO	O-C-CA	-2.32	119.43	125.49
15	c	3	LYO	O-C-CA	-2.31	119.46	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.42	3 (1%)	81	55	61, 83, 116, 141	0
1	O	250/250 (100%)	-0.53	4 (1%)	74	47	61, 83, 117, 141	0
2	B	244/244 (100%)	-0.34	6 (2%)	61	30	61, 83, 131, 151	0
2	P	244/244 (100%)	-0.36	7 (2%)	55	26	61, 83, 131, 151	0
3	C	241/241 (100%)	-0.36	2 (0%)	87	67	63, 89, 135, 162	0
3	Q	241/241 (100%)	-0.31	7 (2%)	55	26	65, 91, 136, 162	0
4	D	242/242 (100%)	-0.28	6 (2%)	61	30	61, 90, 125, 155	0
4	R	242/242 (100%)	-0.27	5 (2%)	67	36	63, 91, 126, 155	0
5	E	233/233 (100%)	-0.32	4 (1%)	73	45	67, 95, 125, 145	0
5	S	233/233 (100%)	-0.29	4 (1%)	73	45	68, 95, 125, 145	0
6	F	244/244 (100%)	-0.35	3 (1%)	81	55	64, 87, 124, 141	0
6	T	244/244 (100%)	-0.27	5 (2%)	68	39	65, 87, 125, 140	0
7	G	243/243 (100%)	-0.47	2 (0%)	87	67	62, 84, 116, 152	0
7	U	243/243 (100%)	-0.45	2 (0%)	87	67	63, 83, 115, 153	0
8	H	222/222 (100%)	-0.66	1 (0%)	91	76	59, 75, 98, 140	0
8	V	222/222 (100%)	-0.66	1 (0%)	91	76	61, 74, 98, 142	0
9	I	204/204 (100%)	-0.70	1 (0%)	91	76	57, 75, 99, 117	0
9	W	204/204 (100%)	-0.68	1 (0%)	91	76	58, 75, 99, 116	0
10	J	198/198 (100%)	-0.57	3 (1%)	76	49	56, 76, 99, 161	0
10	X	198/198 (100%)	-0.59	3 (1%)	76	49	57, 77, 98, 162	0
11	K	212/212 (100%)	-0.62	1 (0%)	91	76	55, 75, 99, 115	0
11	Y	212/212 (100%)	-0.62	1 (0%)	91	76	56, 75, 101, 117	0
12	L	222/222 (100%)	-0.64	0	100	100	59, 77, 105, 129	0
12	Z	222/222 (100%)	-0.62	0	100	100	59, 77, 104, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	-0.62	1 (0%) 93 80	59, 77, 99, 111	0
13	a	233/233 (100%)	-0.61	0 100 100	58, 77, 99, 110	0
14	N	196/196 (100%)	-0.65	0 100 100	58, 74, 100, 115	0
14	b	196/196 (100%)	-0.60	0 100 100	58, 74, 101, 114	0
15	c	1/4 (25%)	-0.78	0 100 100	75, 75, 75, 75	0
15	d	1/4 (25%)	-0.63	0 100 100	63, 63, 63, 63	0
15	e	1/4 (25%)	-0.56	0 100 100	75, 75, 75, 75	0
15	f	1/4 (25%)	-1.05	0 100 100	66, 66, 66, 66	0
All	All	6372/6384 (99%)	-0.49	73 (1%) 82 58	55, 81, 120, 162	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	118	GLY	6.4
7	U	243	ASP	6.2
4	R	121	GLY	6.2
4	D	121	GLY	5.7
4	D	120	SER	5.7
2	B	220	ASN	5.6
4	R	118	GLY	5.5
4	D	119	ALA	5.3
2	P	220	ASN	5.2
10	X	198	GLN	5.2
3	C	50	LEU	4.8
3	C	49	THR	4.8
2	B	219	ALA	4.8
2	P	219	ALA	4.7
4	R	119	ALA	4.4
10	J	197	ALA	4.2
10	X	197	ALA	4.2
10	J	198	GLN	4.1
5	E	1	PHE	3.8
4	R	120	SER	3.8
3	Q	50	LEU	3.8
3	Q	48	SER	3.8
7	G	1	ALA	3.6
8	V	222	ASP	3.4
6	F	202	ASP	3.3
5	E	2	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	3.2
1	O	1	MET	3.2
10	J	196	GLN	3.2
3	Q	49	THR	3.2
6	T	1	GLY	3.1
1	A	1	MET	3.1
5	S	1	PHE	2.9
5	E	233	ILE	2.9
7	G	243	ASP	2.9
6	F	203	ASN	2.8
11	Y	212	GLY	2.8
10	X	196	GLN	2.8
11	K	212	GLY	2.7
2	P	218	GLY	2.7
5	E	202	ASP	2.6
5	S	233	ILE	2.6
7	U	1	ALA	2.6
6	F	1	GLY	2.6
6	T	51	THR	2.6
4	D	124	ARG	2.5
2	B	51	VAL	2.4
2	P	221	ASP	2.4
1	A	2	THR	2.4
2	B	218	GLY	2.4
2	P	60	THR	2.4
6	T	2	THR	2.3
13	M	1	THR	2.3
9	I	1	SER	2.3
4	D	122	GLU	2.2
3	Q	203	THR	2.2
5	S	52	ALA	2.2
2	P	223	GLU	2.2
1	O	250	LEU	2.2
1	O	2	THR	2.2
2	B	223	GLU	2.2
6	T	201	GLU	2.2
1	O	230	ASP	2.2
4	R	122	GLU	2.1
2	P	59	ASP	2.1
9	W	1	SER	2.1
3	Q	202	GLN	2.1
6	T	244	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
8	H	221	CYS	2.0
5	S	2	ARG	2.0
3	Q	240	GLU	2.0
1	A	228	PRO	2.0
3	Q	43	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
15	LYO	d	3	10/11	0.96	0.13	-	64,68,71,71	0
15	0W6	f	4	7/8	0.97	0.12	-	67,68,72,73	0
15	0W6	d	4	7/8	0.96	0.13	-	67,67,72,72	0
15	0W6	e	4	7/8	0.95	0.15	-	71,73,77,77	0
15	0W6	c	4	7/8	0.95	0.14	-	70,72,76,77	0
15	LYO	c	3	10/11	0.96	0.12	-	72,74,78,78	0
15	LYO	e	3	10/11	0.93	0.18	-	73,75,78,79	0
15	LYO	f	3	10/11	0.97	0.13	-	64,67,71,72	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.