Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 10:09 AM EST

PDB ID	:	3DY3
Title	:	Crystal structure of yeast 20S proteasome in complex with the epimer form of spirolactacystin
Authors	:	Groll, M.; Balskus, E.; Jacobsen, E.
Deposited on	:	2008-07-25
Resolution	:	2.81 Å(reported)

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

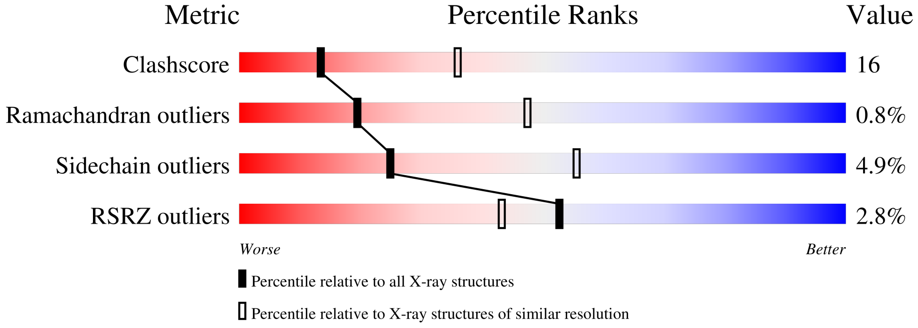
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

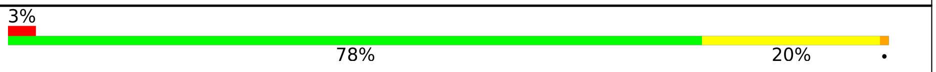
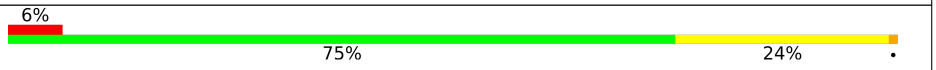
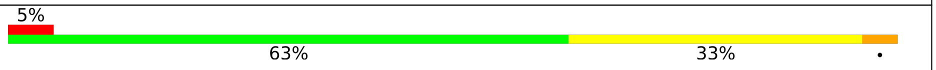
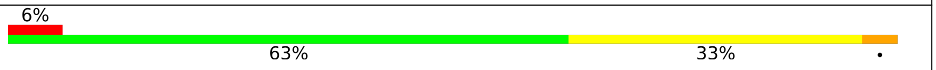
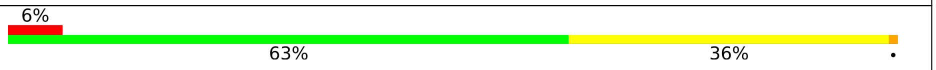
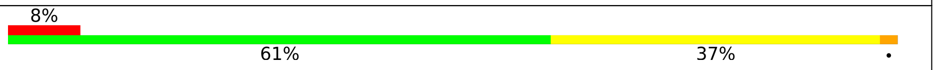
The reported resolution of this entry is 2.81 Å.

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))
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	250	
1	O	250	
2	B	244	
2	P	244	
3	C	241	
3	Q	241	

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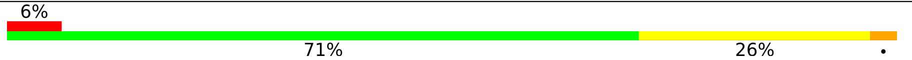
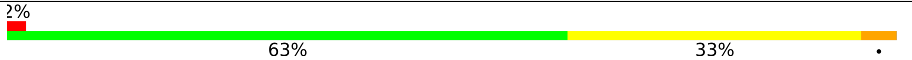
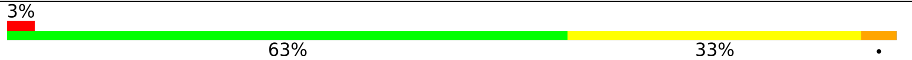
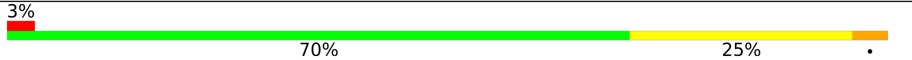
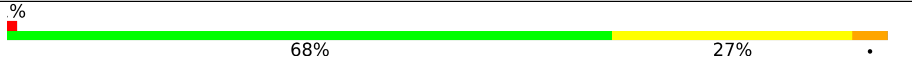
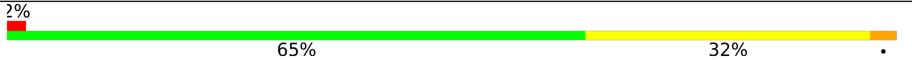
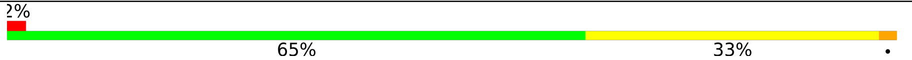
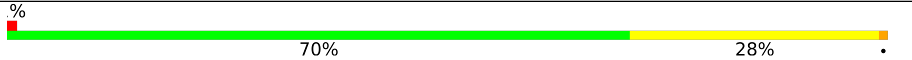
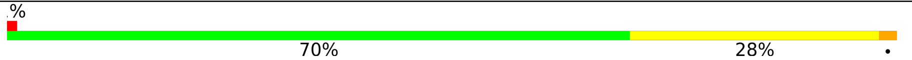
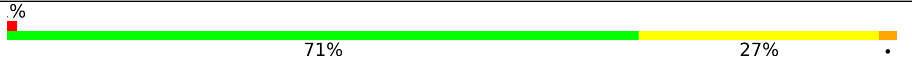
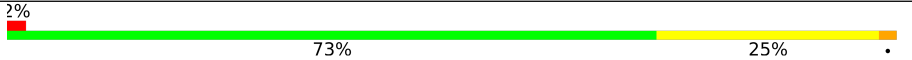
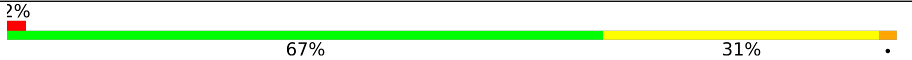
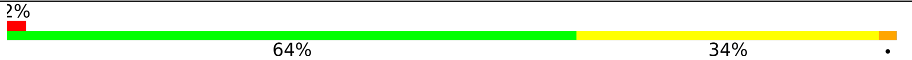
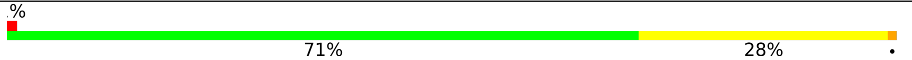
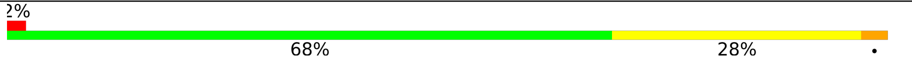
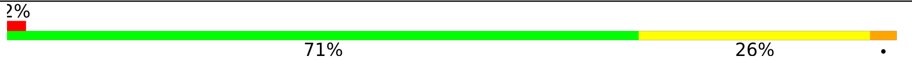
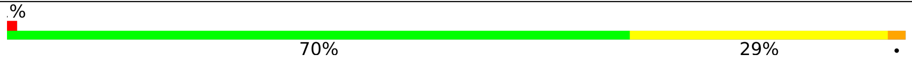
Mol	Chain	Length	Quality of chain
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50584 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 1915 1219 315 377 4	0	0	0
1	O	250	Total C N O S 1915 1219 315 377 4	0	0	0

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

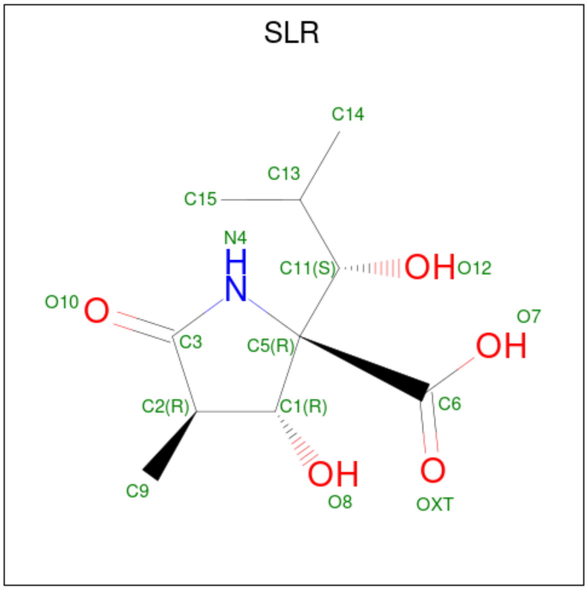
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is (3R,4R)-3-hydroxy-2-[(1S)-1-hydroxy-2-methylpropyl]-4-methyl-5-oxo-D-proline (three-letter code: SLR) (formula: $C_{10}H_{17}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total C N O 15 10 1 4	0	0
15	Y	1	Total C N O 15 10 1 4	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	35	Total O 35 35	0	0
16	B	27	Total O 27 27	0	0
16	C	32	Total O 32 32	0	0
16	D	23	Total O 23 23	0	0
16	E	15	Total O 15 15	0	0
16	F	35	Total O 35 35	0	0
16	G	51	Total O 51 51	0	0
16	H	41	Total O 41 41	0	0
16	I	51	Total O 51 51	0	0
16	J	38	Total O 38 38	0	0

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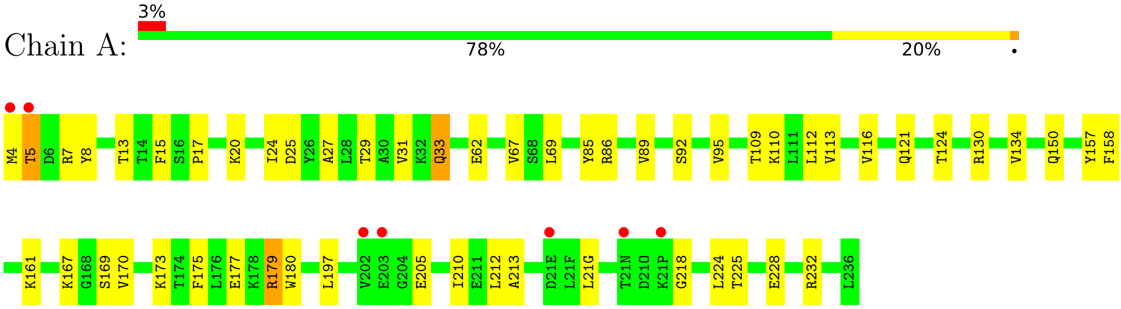
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	33	Total O 33 33	0	0
16	L	43	Total O 43 43	0	0
16	M	56	Total O 56 56	0	0
16	N	49	Total O 49 49	0	0
16	O	28	Total O 28 28	0	0
16	P	18	Total O 18 18	0	0
16	Q	19	Total O 19 19	0	0
16	R	19	Total O 19 19	0	0
16	S	16	Total O 16 16	0	0
16	T	30	Total O 30 30	0	0
16	U	48	Total O 48 48	0	0
16	V	36	Total O 36 36	0	0
16	W	40	Total O 40 40	0	0
16	X	36	Total O 36 36	0	0
16	Y	36	Total O 36 36	0	0
16	Z	36	Total O 36 36	0	0
16	1	64	Total O 64 64	0	0
16	2	51	Total O 51 51	0	0

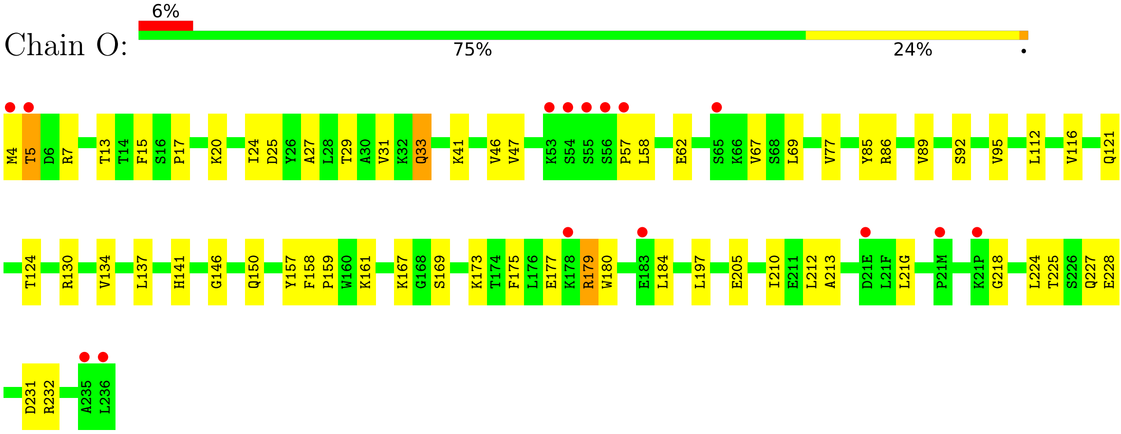
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

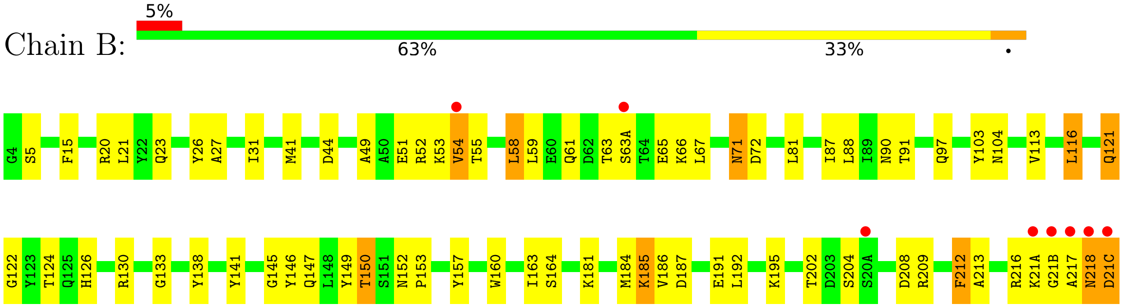
- Molecule 1: Proteasome component Y7

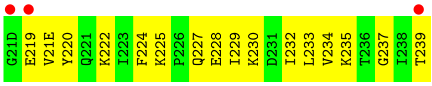


- Molecule 1: Proteasome component Y7

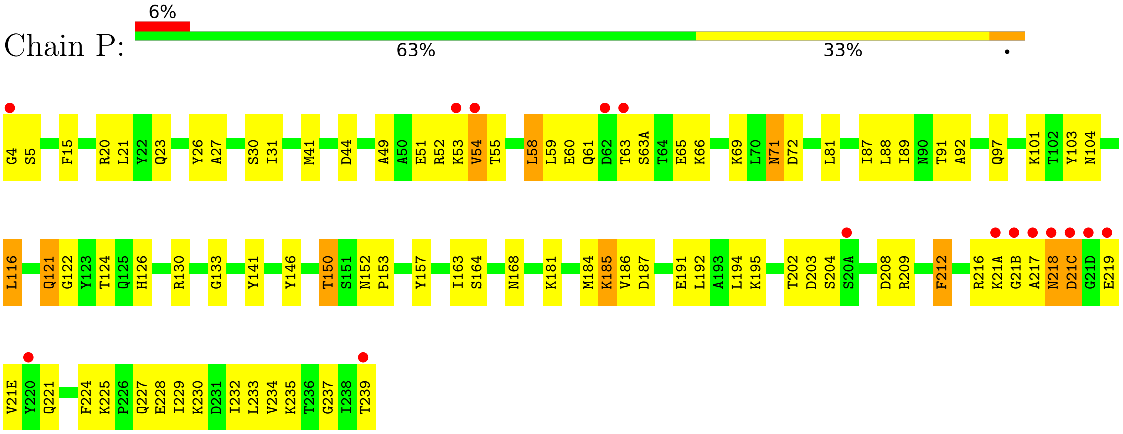


- Molecule 2: Proteasome component Y13

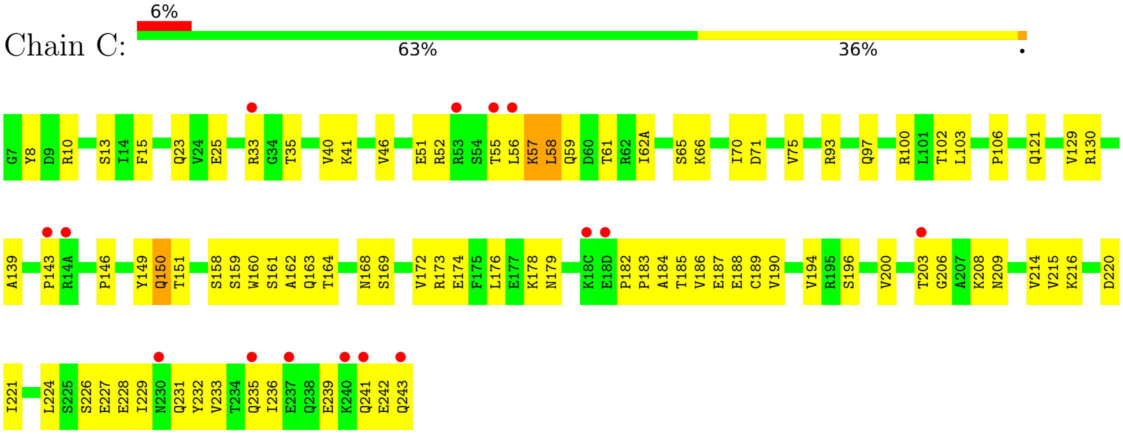




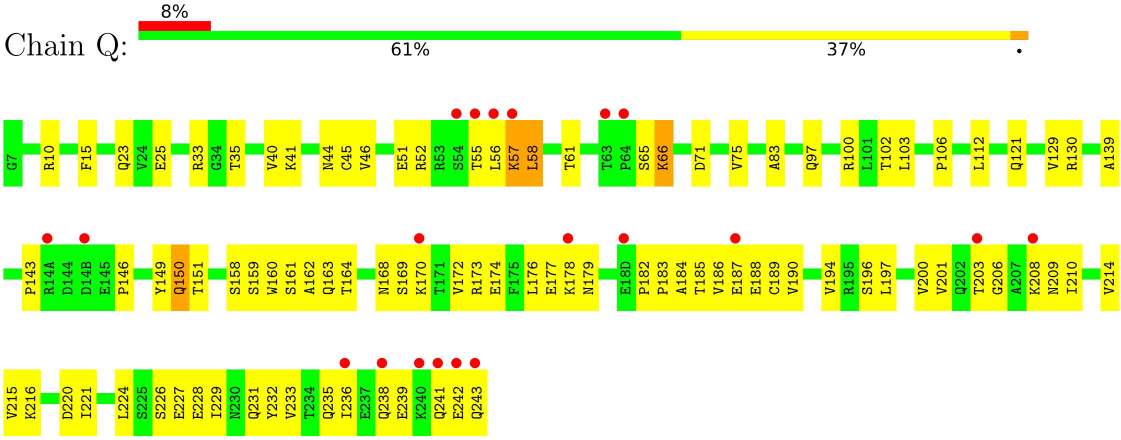
- Molecule 2: Proteasome component Y13



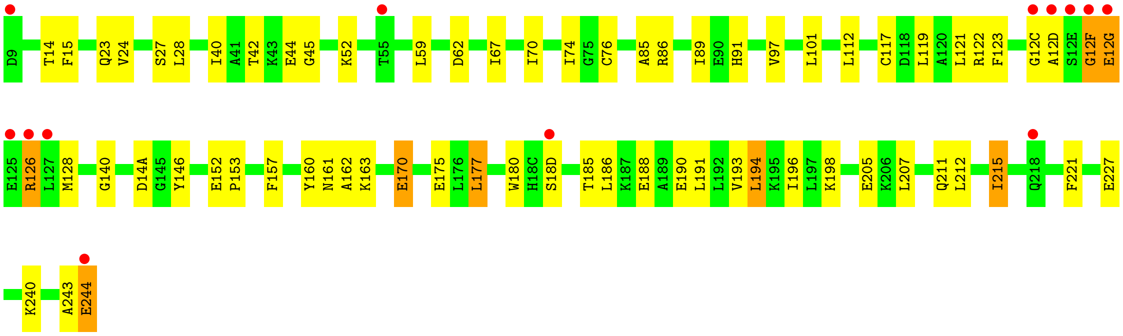
- Molecule 3: Proteasome component PRE6



- Molecule 3: Proteasome component PRE6

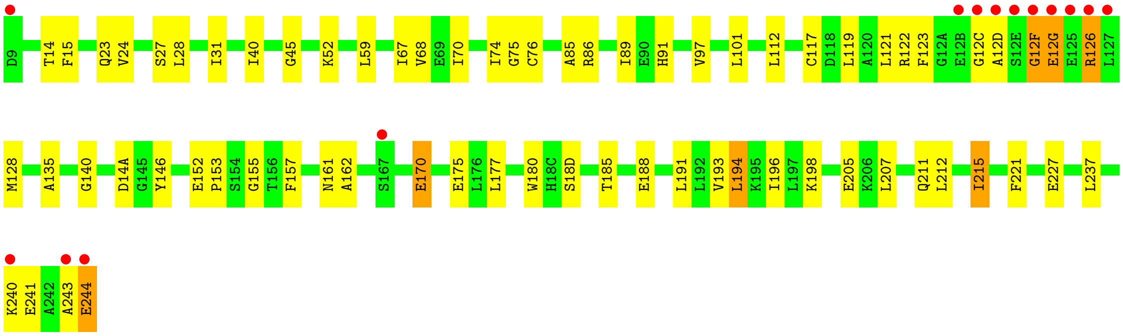


- Molecule 4: Proteasome component PUP2



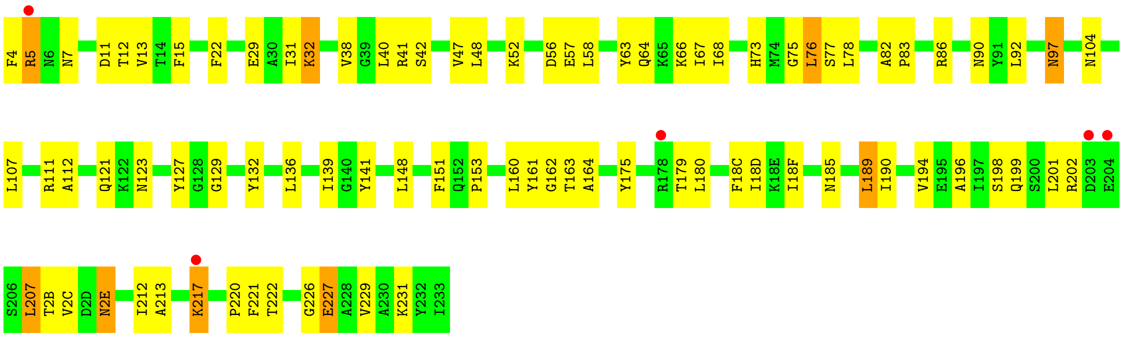
- Molecule 4: Proteasome component PUP2

Chain R:



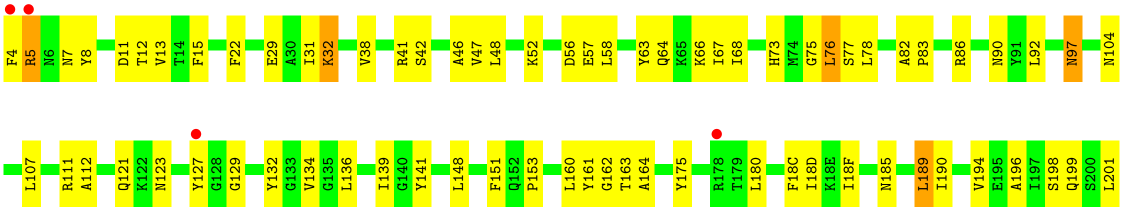
- Molecule 5: Proteasome component PRE5

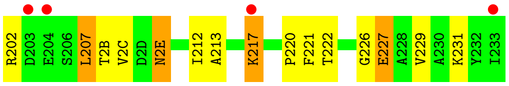
Chain E:



- Molecule 5: Proteasome component PRE5

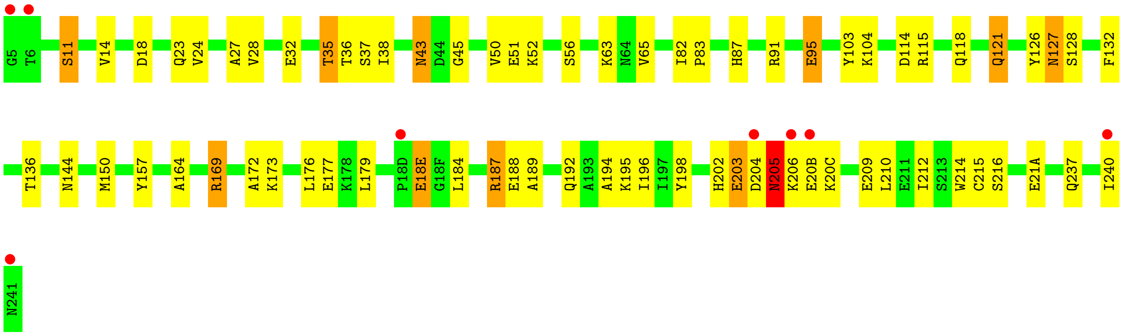
Chain S:





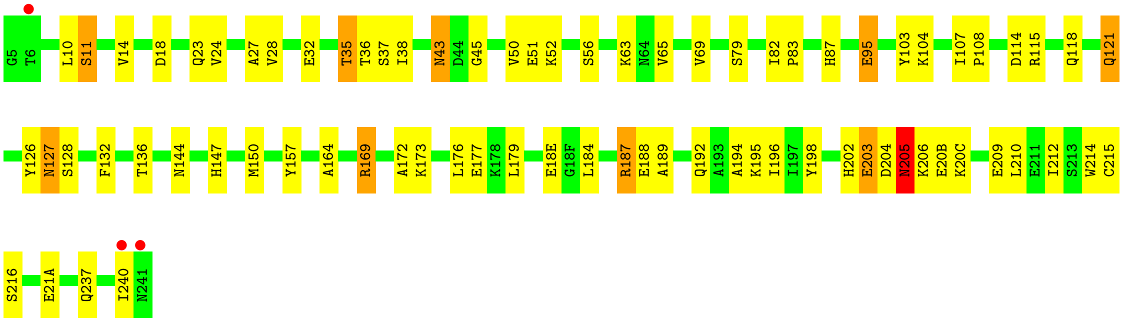
- Molecule 6: Proteasome component C1

Chain F:



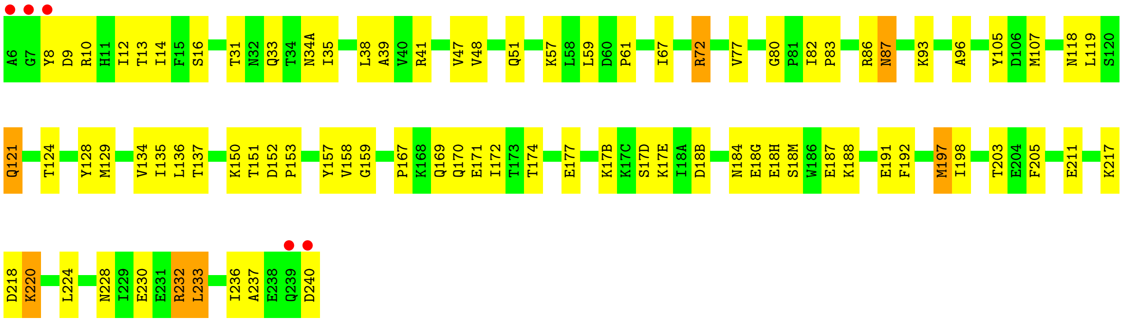
- Molecule 6: Proteasome component C1

Chain T:



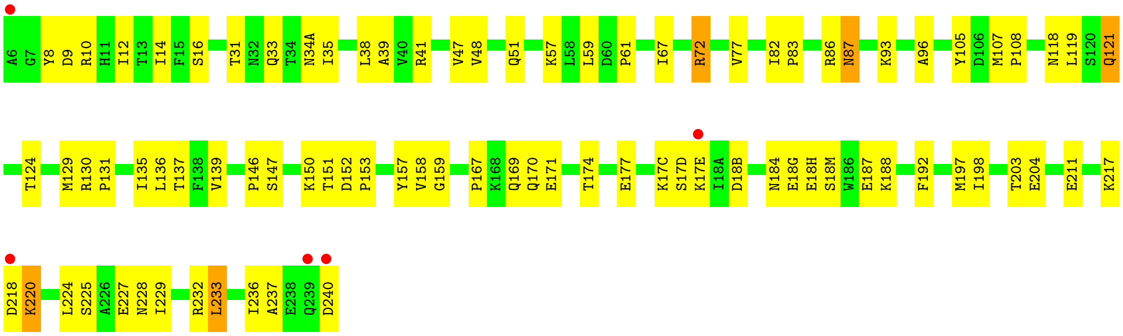
- Molecule 7: Proteasome component C7-alpha

Chain G:

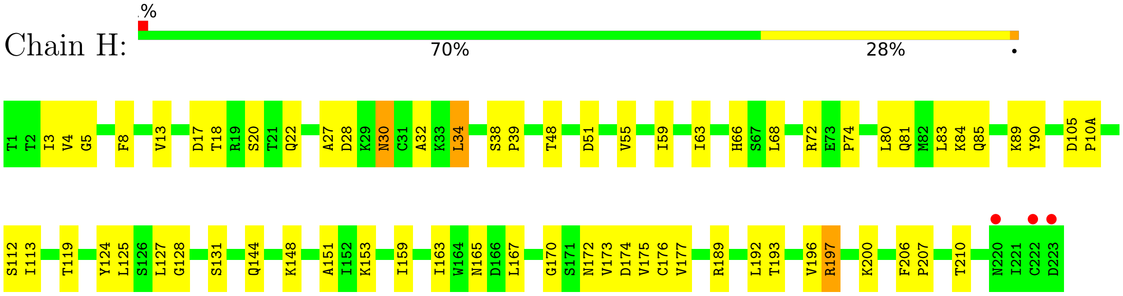


- Molecule 7: Proteasome component C7-alpha

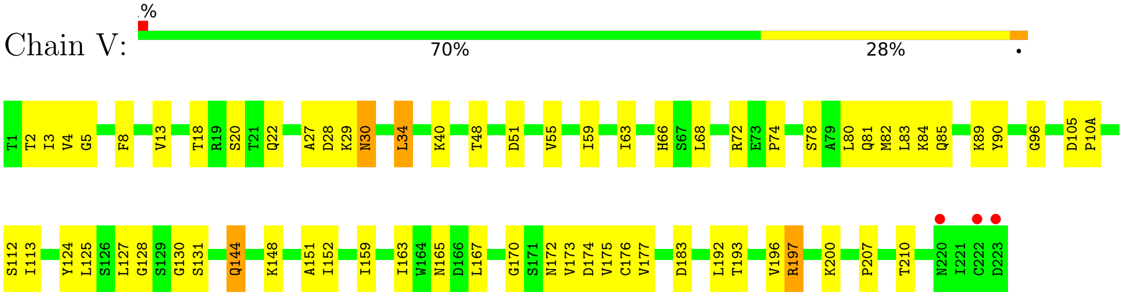
Chain U:



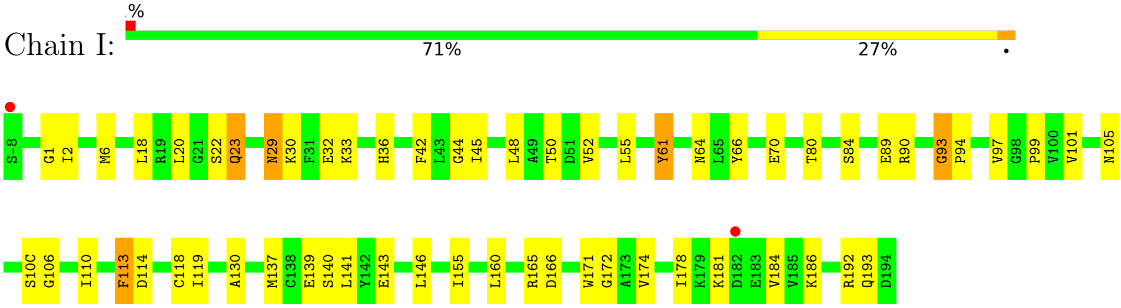
- Molecule 8: Proteasome component PUP1



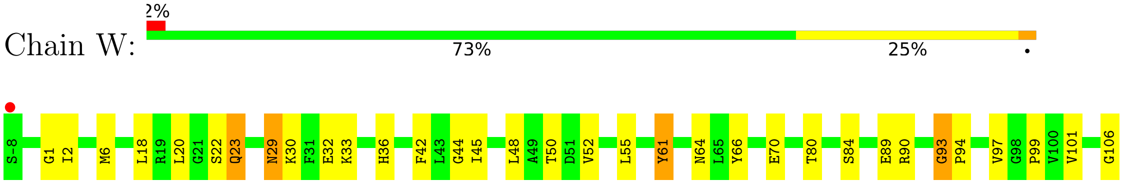
- Molecule 8: Proteasome component PUP1

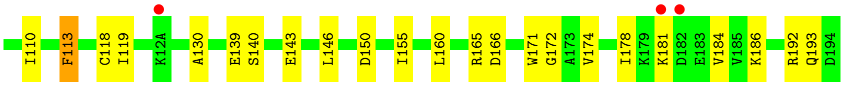


- Molecule 9: Proteasome component PUP3

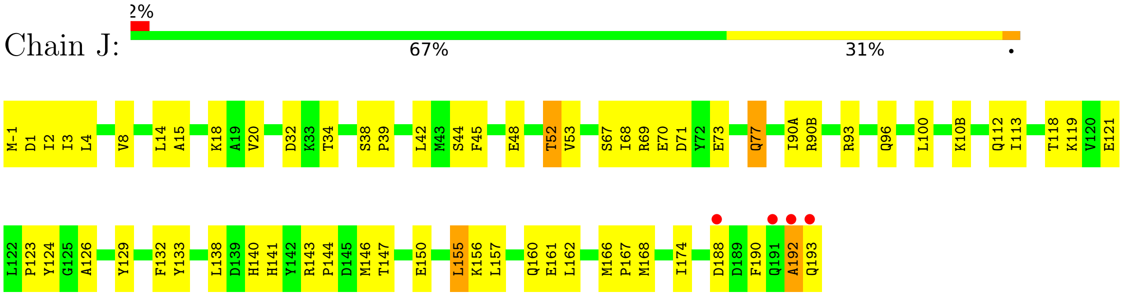


- Molecule 9: Proteasome component PUP3

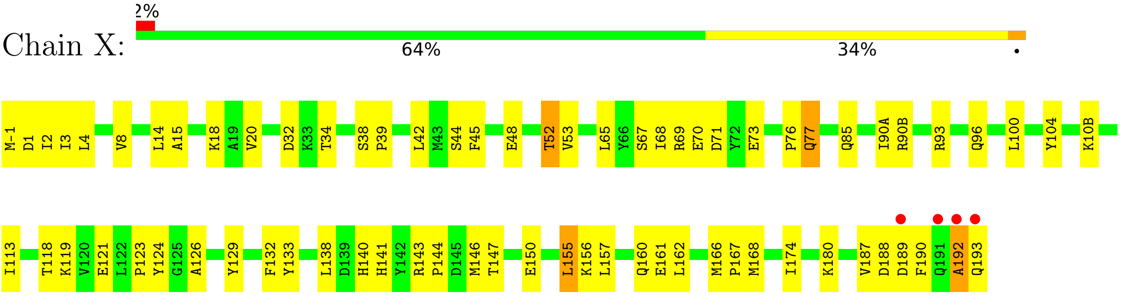




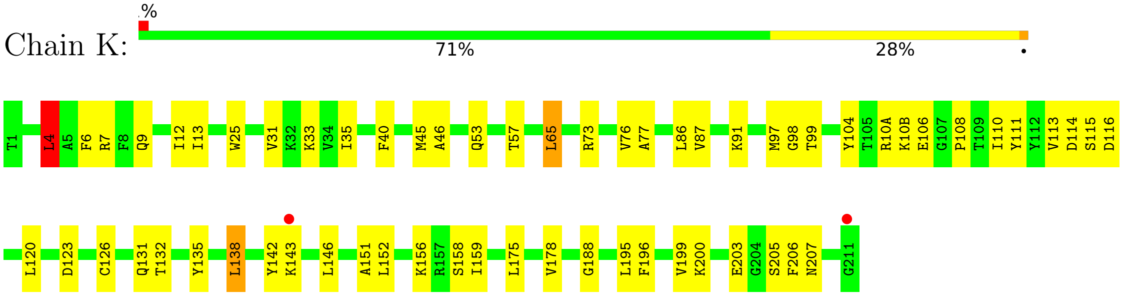
- Molecule 10: Proteasome component C11



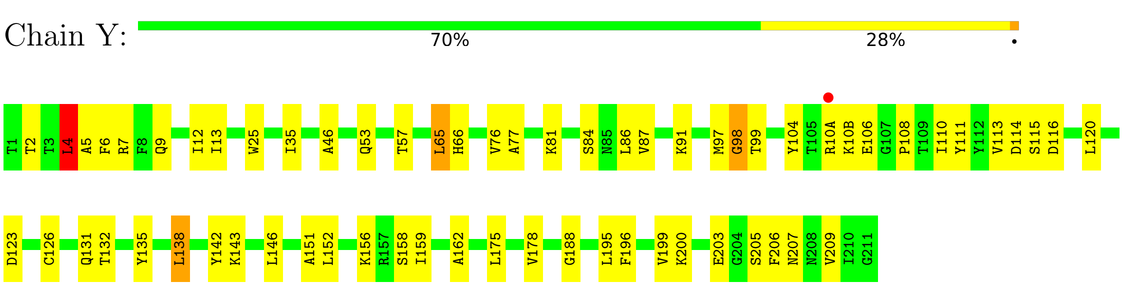
- Molecule 10: Proteasome component C11



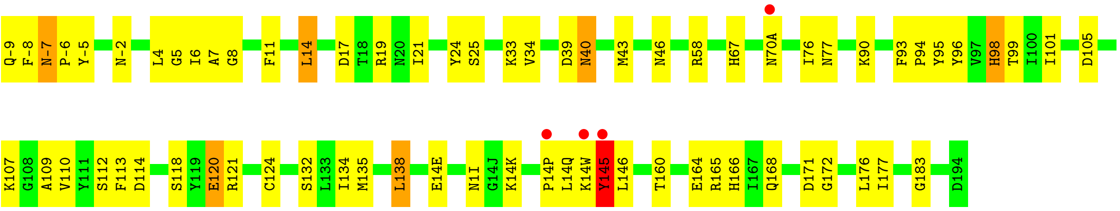
- Molecule 11: Proteasome component PRE2



- Molecule 11: Proteasome component PRE2

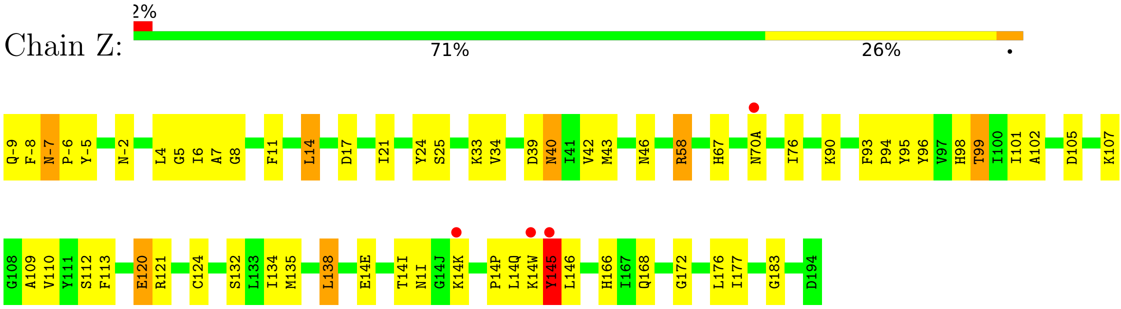


- Molecule 12: Proteasome component C5



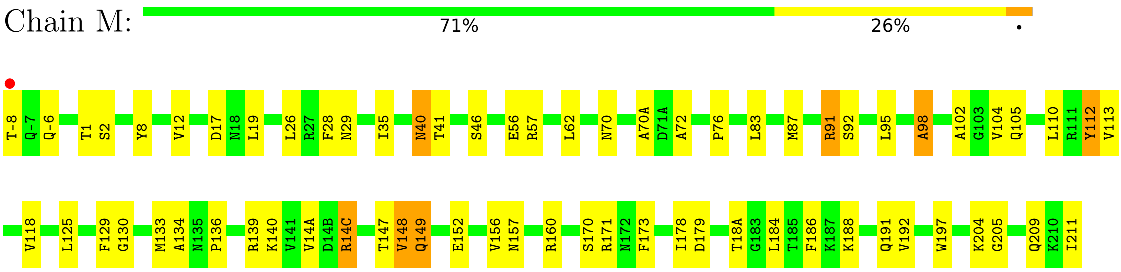
- Molecule 12: Proteasome component C5

Chain Z:



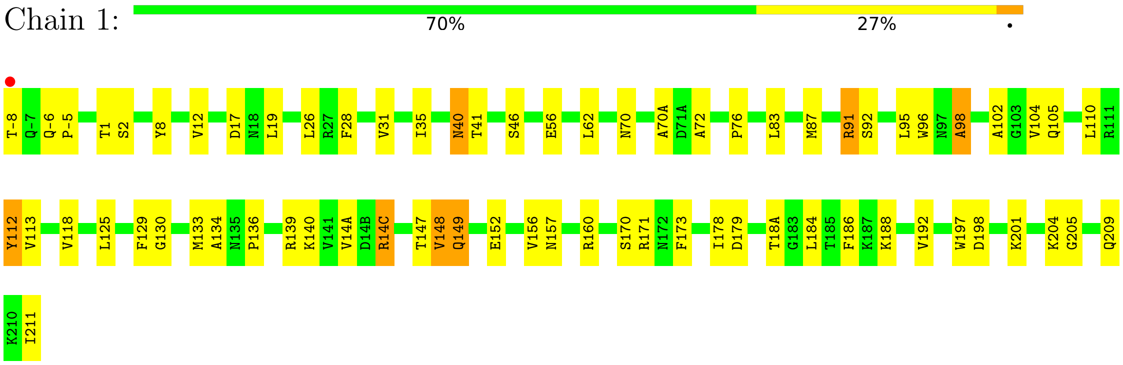
- Molecule 13: Proteasome component PRE4

Chain M:



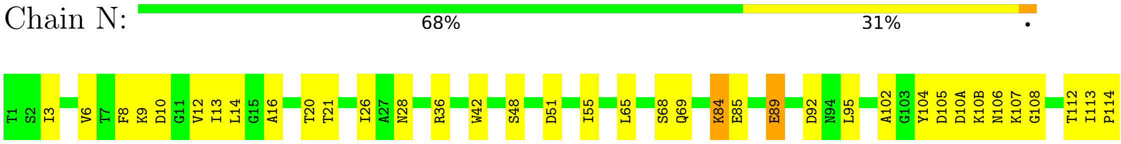
- Molecule 13: Proteasome component PRE4

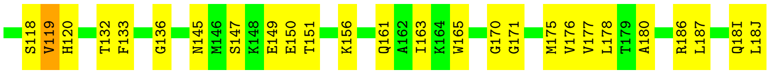
Chain 1:



- Molecule 14: Proteasome component PRE3

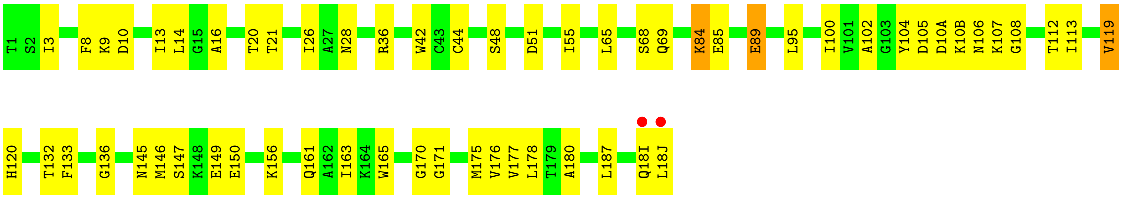
Chain N:





- Molecule 14: Proteasome component PRE3

Chain 2:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.15Å 301.86Å 144.08Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	15.00 – 2.81 20.02 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.81) 98.7 (20.02-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.245 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	50584	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.38	0/1952	0.63	0/2642
1	O	0.37	0/1952	0.63	0/2642
2	B	0.38	0/1935	0.63	0/2618
2	P	0.38	0/1935	0.64	0/2618
3	C	0.35	0/1920	0.61	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.36	0/1887	0.63	0/2541
4	R	0.35	0/1887	0.62	0/2541
5	E	0.35	0/1823	0.61	0/2463
5	S	0.35	0/1823	0.61	0/2463
6	F	0.38	0/1937	0.62	0/2614
6	T	0.38	0/1937	0.63	0/2614
7	G	0.40	0/1959	0.63	0/2652
7	U	0.39	0/1959	0.63	0/2652
8	H	0.40	0/1716	0.66	0/2326
8	V	0.37	0/1716	0.65	0/2326
9	I	0.39	0/1611	0.64	0/2174
9	W	0.40	0/1611	0.65	0/2174
10	J	0.37	0/1613	0.64	0/2173
10	X	0.38	0/1613	0.64	0/2173
11	K	0.40	0/1681	0.67	2/2274 (0.1%)
11	Y	0.38	0/1681	0.66	3/2274 (0.1%)
12	L	0.40	0/1795	0.65	0/2420
12	Z	0.39	0/1795	0.65	0/2420
13	1	0.41	0/1855	0.67	2/2514 (0.1%)
13	M	0.39	0/1855	0.66	2/2514 (0.1%)
14	2	0.40	0/1541	0.65	0/2087
14	N	0.41	0/1541	0.65	0/2087
All	All	0.38	0/50450	0.64	9/68192 (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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.58	128.13	115.30
11	K	4	LEU	CA-CB-CG	5.35	127.61	115.30
13	1	95	LEU	N-CA-C	-5.16	97.07	111.00
11	Y	188	GLY	N-CA-C	5.12	125.91	113.10
11	Y	98	GLY	N-CA-C	-5.09	100.37	113.10
11	K	188	GLY	N-CA-C	5.04	125.71	113.10
13	M	98	ALA	N-CA-C	-5.04	97.40	111.00
13	1	98	ALA	N-CA-C	-5.02	97.45	111.00
13	M	95	LEU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	53	0
1	O	1915	0	1926	65	0
2	B	1905	0	1901	87	0
2	P	1905	0	1901	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1891	0	1900	92	0
3	Q	1891	0	1900	90	0
4	D	1862	0	1836	53	0
4	R	1862	0	1836	50	0
5	E	1795	0	1797	67	0
5	S	1795	0	1797	70	0
6	F	1897	0	1886	62	0
6	T	1897	0	1886	68	0
7	G	1921	0	1910	62	0
7	U	1921	0	1910	69	0
8	H	1685	0	1688	47	0
8	V	1685	0	1688	45	0
9	I	1581	0	1574	51	0
9	W	1581	0	1574	50	0
10	J	1585	0	1590	67	0
10	X	1585	0	1590	66	0
11	K	1644	0	1594	53	0
11	Y	1644	0	1594	52	0
12	L	1757	0	1711	62	0
12	Z	1757	0	1711	63	0
13	1	1824	0	1832	57	0
13	M	1824	0	1832	61	0
14	2	1512	0	1481	50	0
14	N	1512	0	1481	52	0
15	K	15	0	16	0	0
15	Y	15	0	16	0	0
16	1	64	0	0	1	0
16	2	51	0	0	1	0
16	A	35	0	0	2	0
16	B	27	0	0	3	0
16	C	32	0	0	5	0
16	D	23	0	0	1	0
16	E	15	0	0	0	0
16	F	35	0	0	1	0
16	G	51	0	0	2	0
16	H	41	0	0	4	0
16	I	51	0	0	1	0
16	J	38	0	0	1	0
16	K	33	0	0	0	0
16	L	43	0	0	2	0
16	M	56	0	0	4	0
16	N	49	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	O	28	0	0	2	0
16	P	18	0	0	2	0
16	Q	19	0	0	4	0
16	R	19	0	0	0	0
16	S	16	0	0	0	0
16	T	30	0	0	5	0
16	U	48	0	0	6	0
16	V	36	0	0	1	0
16	W	40	0	0	1	0
16	X	36	0	0	3	0
16	Y	36	0	0	2	0
16	Z	36	0	0	7	0
All	All	50584	0	49284	1590	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 16.

All (1590) 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)
7:U:96:ALA:HA	7:U:107:MET:HE2	1.27	1.16
7:G:96:ALA:HA	7:G:107:MET:HE2	1.27	1.14
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.22	1.02
2:B:71:ASN:ND2	2:B:72:ASP:H	1.60	0.99
2:B:202:THR:HG22	2:B:204:SER:H	1.27	0.99
2:P:202:THR:HG22	2:P:204:SER:H	1.26	0.99
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.27	0.99
2:P:71:ASN:ND2	2:P:72:ASP:H	1.60	0.99
1:O:15:PHE:H	2:P:23:GLN:HE22	1.07	0.98
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	0.96	0.96
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.47	0.95
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.30	0.95
3:C:15:PHE:H	4:D:23:GLN:HE22	1.07	0.95
3:C:163:GLN:HE21	3:C:164:THR:H	0.95	0.95
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.46	0.94
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	0.95	0.94
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.01	0.94
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.30	0.94
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.16	0.94
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.68	0.93
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:THR:HB	3:C:188:GLU:HG2	1.49	0.93
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.48	0.92
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.32	0.92
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.85	0.91
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.05	0.91
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.86	0.90
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.70	0.89
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.93	0.89
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.36	0.89
5:E:2(B):THR:H	5:E:2(E):ASN:ND2	1.69	0.89
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.15	0.88
5:S:2(B):THR:H	5:S:2(E):ASN:ND2	1.71	0.88
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.53	0.88
3:C:163:GLN:NE2	3:C:164:THR:H	1.71	0.88
5:E:207:LEU:HD23	5:E:207:LEU:H	1.39	0.88
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.40	0.87
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.39	0.86
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.74	0.86
5:S:207:LEU:HD23	5:S:207:LEU:H	1.41	0.86
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.40	0.85
1:A:15:PHE:H	2:B:23:GLN:HE22	1.24	0.84
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.59	0.84
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.42	0.84
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.26	0.84
2:B:15:PHE:H	3:C:23:GLN:HE22	1.24	0.84
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.76	0.84
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.77	0.83
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.43	0.82
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.61	0.82
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.79	0.82
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.93	0.82
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.80	0.82
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.43	0.81
13:M:40:ASN:H	13:M:40:ASN:HD22	1.29	0.81
13:1:35:ILE:HG12	13:1:56:GLU:HG3	1.62	0.81
3:C:163:GLN:HE21	3:C:164:THR:N	1.78	0.81
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.63	0.81
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.93	0.80
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.95	0.80
7:G:87:ASN:C	7:G:87:ASN:HD22	1.84	0.80
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.47	0.80
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.79	0.80
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.48	0.79
2:P:71:ASN:HD22	2:P:72:ASP:H	1.27	0.79
13:1:40:ASN:H	13:1:40:ASN:HD22	1.28	0.79
2:B:71:ASN:HD22	2:B:72:ASP:H	1.29	0.78
7:U:87:ASN:C	7:U:87:ASN:HD22	1.87	0.78
6:F:35:THR:HG21	6:F:51:GLU:O	1.83	0.78
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.82	0.78
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.98	0.77
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.77	0.77
2:P:124:THR:CG2	3:Q:130:ARG:HH21	1.98	0.77
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.48	0.77
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.67	0.77
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.48	0.76
2:P:71:ASN:ND2	2:P:72:ASP:N	2.34	0.76
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.49	0.76
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.32	0.76
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.21	0.75
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.21	0.75
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.48	0.75
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.69	0.75
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.85	0.75
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.66	0.75
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.32	0.75
13:M:149:GLN:NE2	13:M:149:GLN:H	1.85	0.75
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.52	0.74
2:B:121:GLN:O	2:B:124:THR:HB	1.87	0.74
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.86	0.74
6:T:35:THR:HG21	6:T:51:GLU:O	1.87	0.74
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.52	0.74
7:U:121:GLN:O	7:U:124:THR:HB	1.87	0.74
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.52	0.74
2:B:71:ASN:ND2	2:B:72:ASP:N	2.34	0.74
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.70	0.73
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.70	0.73
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	2.02	0.73
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.71	0.73
11:K:143:LYS:O	11:K:146:LEU:HD13	1.89	0.73
13:M:57:ARG:NE	16:M:240:HOH:O	2.22	0.73
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.54	0.73
7:U:96:ALA:CA	7:U:107:MET:HE2	2.15	0.73
2:P:121:GLN:O	2:P:124:THR:HB	1.89	0.73
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.69	0.72
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.89	0.72
13:1:149:GLN:H	13:1:149:GLN:NE2	1.87	0.72
5:S:15:PHE:H	6:T:23:GLN:HE22	1.38	0.72
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.02	0.72
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.70	0.72
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.89	0.72
2:P:227:GLN:OE1	2:P:230:LYS:HD3	1.89	0.72
7:G:121:GLN:O	7:G:124:THR:HB	1.89	0.72
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.90	0.72
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.03	0.72
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.20	0.72
12:Z:109:ALA:HA	16:Z:204:HOH:O	1.90	0.72
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.89	0.72
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.88	0.71
7:G:198:ILE:HG23	7:G:203:THR:O	1.90	0.71
3:C:15:PHE:N	4:D:23:GLN:HE22	1.86	0.71
7:U:96:ALA:HA	7:U:107:MET:CE	2.15	0.71
3:C:41:LYS:HG2	3:C:161:SER:O	1.90	0.71
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.02	0.71
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.03	0.71
4:R:185:THR:OG1	4:R:188:GLU:HG3	1.91	0.71
1:A:179:ARG:HH11	1:A:179:ARG:HB3	1.54	0.71
2:B:227:GLN:OE1	2:B:230:LYS:HD3	1.90	0.71
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.54	0.71
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.53	0.71
3:C:185:THR:HG22	3:C:187:GLU:H	1.55	0.71
7:G:96:ALA:CA	7:G:107:MET:HE2	2.15	0.71
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.71	0.71
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.73	0.71
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.73	0.71
12:L:-9:GLN:NE2	12:L:-8:PHE:H	1.89	0.71
6:T:173:LYS:O	6:T:177:GLU:HG3	1.91	0.71
12:Z:-9:GLN:NE2	12:Z:-8:PHE:H	1.88	0.71
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.73	0.70
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.06	0.70
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.07	0.70
10:X:156:LYS:O	10:X:160:GLN:HG3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.06	0.70
6:F:173:LYS:O	6:F:177:GLU:HG3	1.92	0.70
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.92	0.70
11:K:142:TYR:O	11:K:143:LYS:HD2	1.91	0.70
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.74	0.70
5:E:207:LEU:H	5:E:207:LEU:CD2	2.05	0.70
3:C:15:PHE:H	4:D:23:GLN:NE2	1.86	0.70
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.74	0.70
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.89	0.70
5:S:207:LEU:H	5:S:207:LEU:CD2	2.05	0.70
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.74	0.69
12:Z:76:ILE:HG22	16:Z:221:HOH:O	1.92	0.69
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.04	0.69
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.72	0.69
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.92	0.69
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.07	0.69
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.74	0.69
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.74	0.69
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.07	0.69
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.75	0.69
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.75	0.69
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.92	0.69
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.22	0.69
10:J:156:LYS:O	10:J:160:GLN:HG3	1.93	0.69
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.74	0.69
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.75	0.69
12:Z:-8:PHE:HB2	13:1:-8:THR:HG23	1.75	0.69
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.74	0.68
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.06	0.68
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.41	0.68
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.75	0.68
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.27	0.68
4:D:185:THR:OG1	4:D:188:GLU:HG3	1.92	0.68
10:J:32:ASP:OD2	10:J:34:THR:HG22	1.93	0.68
14:N:186:ARG:HD3	16:N:228:HOH:O	1.93	0.68
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.24	0.68
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.75	0.68
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.76	0.68
4:D:162:ALA:HB3	5:E:58:LEU:HD23	1.76	0.67
3:C:41:LYS:HD3	3:C:161:SER:HA	1.75	0.67
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.76	0.67
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.77	0.67
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.29	0.67
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.76	0.67
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.77	0.67
8:V:172:ASN:HD22	8:V:193:THR:HA	1.60	0.67
8:V:81:GLN:O	8:V:85:GLN:HG3	1.94	0.67
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.77	0.66
13:1:40:ASN:HD22	13:1:40:ASN:N	1.92	0.66
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.78	0.66
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.76	0.66
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.78	0.66
7:U:198:ILE:HG23	7:U:203:THR:O	1.95	0.66
5:E:132:TYR:O	5:E:153:PRO:HB3	1.96	0.66
1:O:159:PRO:O	2:P:59:LEU:HD12	1.96	0.66
2:P:185:LYS:HD3	2:P:186:VAL:N	2.10	0.66
2:B:181:LYS:O	2:B:184:MET:HG3	1.95	0.66
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.59	0.66
10:J:147:THR:OG1	10:J:150:GLU:HG3	1.96	0.66
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.78	0.66
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.78	0.66
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.76	0.65
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.77	0.65
1:O:121:GLN:O	1:O:124:THR:HB	1.97	0.65
2:P:71:ASN:HD22	2:P:72:ASP:N	1.93	0.65
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.78	0.65
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.77	0.65
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	1.97	0.65
10:J:168:MET:HG2	10:X:168:MET:CE	2.26	0.65
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.11	0.65
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.76	0.65
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.79	0.65
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.61	0.65
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.32	0.65
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.79	0.65
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.31	0.65
2:B:185:LYS:HD3	2:B:186:VAL:N	2.11	0.64
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.79	0.64
9:I:6:MET:HE1	9:I:155:ILE:HA	1.78	0.64
2:P:181:LYS:O	2:P:184:MET:HG3	1.96	0.64
5:S:198:SER:HA	5:S:201:LEU:HG	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.78	0.64
10:J:168:MET:CE	10:X:168:MET:HG2	2.28	0.64
10:J:52:THR:HG22	10:J:53:VAL:N	2.11	0.64
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.09	0.64
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	2.01	0.64
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.60	0.64
10:X:147:THR:HG23	10:X:150:GLU:OE2	1.97	0.64
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.80	0.64
8:H:81:GLN:O	8:H:85:GLN:HG3	1.97	0.64
8:H:172:ASN:HD22	8:H:193:THR:HA	1.61	0.64
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	1.97	0.64
3:C:35:THR:HB	3:C:51:GLU:HG3	1.78	0.64
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.79	0.64
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.81	0.63
7:U:59:LEU:O	7:U:61:PRO:HD3	1.98	0.63
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.33	0.63
3:C:71:ASP:HA	10:J:68:ILE:HD11	1.81	0.63
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.80	0.63
4:R:85:ALA:O	4:R:89:ILE:HG12	1.98	0.63
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.28	0.63
2:B:71:ASN:HD22	2:B:72:ASP:N	1.95	0.63
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.81	0.63
10:X:147:THR:OG1	10:X:150:GLU:HG3	1.98	0.63
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.79	0.63
8:H:18:THR:HB	8:H:30:ASN:HD22	1.64	0.63
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.34	0.63
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.80	0.63
3:C:185:THR:HG22	3:C:187:GLU:N	2.12	0.63
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.14	0.63
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.81	0.63
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.79	0.63
13:M:40:ASN:HD22	13:M:40:ASN:N	1.92	0.63
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.93	0.62
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.80	0.62
3:Q:65:SER:HB2	16:Q:247:HOH:O	1.98	0.62
4:R:97:VAL:HG21	11:Y:65:LEU:CD1	2.28	0.62
3:C:46:VAL:O	3:C:215:VAL:HG12	1.99	0.62
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.81	0.62
11:Y:114:ASP:OD1	11:Y:116:ASP:HB2	2.00	0.62
1:A:121:GLN:O	1:A:124:THR:HB	1.98	0.62
7:G:233:LEU:O	7:G:236:ILE:HG13	2.00	0.62

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
5:E:198:SER:HA	5:E:201:LEU:HG	1.80	0.62
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	1.81	0.62
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.48	0.62
10:X:52:THR:HG22	10:X:53:VAL:N	2.14	0.62
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.29	0.62
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.00	0.62
11:K:7:ARG:HD2	11:K:108:PRO:O	2.00	0.62
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.80	0.62
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.14	0.62
12:L:90:LYS:HE3	12:L:93:PHE:O	2.00	0.62
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.14	0.62
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.30	0.61
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.80	0.61
3:Q:46:VAL:O	3:Q:215:VAL:HG12	1.99	0.61
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.99	0.61
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.80	0.61
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.30	0.61
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.81	0.61
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.82	0.61
5:S:132:TYR:O	5:S:153:PRO:HB3	1.99	0.61
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.82	0.61
3:C:227:GLU:OE1	3:C:227:GLU:N	2.29	0.61
8:V:18:THR:HB	8:V:30:ASN:HD22	1.66	0.61
8:V:196:VAL:HG23	16:V:242:HOH:O	2.00	0.61
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.00	0.61
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.83	0.61
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.01	0.61
8:H:128:GLY:O	8:H:131:SER:HB2	2.00	0.61
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.01	0.61
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.64	0.60
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.01	0.60
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.83	0.60
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.83	0.60
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.84	0.60
9:W:150:ASP:HA	16:W:230:HOH:O	2.00	0.60
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.66	0.60
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.50	0.60
4:D:122:ARG:HH11	4:D:122:ARG:HG2	1.65	0.60
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.83	0.60
14:N:92:ASP:HB2	16:N:199:HOH:O	2.01	0.60
8:V:128:GLY:O	8:V:131:SER:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:195:LEU:O	11:K:199:VAL:HG23	2.01	0.60
3:Q:170:LYS:HB2	16:Q:255:HOH:O	2.01	0.60
7:U:233:LEU:O	7:U:236:ILE:HG13	2.02	0.60
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.83	0.60
2:P:163:ILE:HG13	2:P:164:SER:N	2.16	0.60
8:V:172:ASN:ND2	8:V:193:THR:HA	2.17	0.60
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.02	0.60
7:G:87:ASN:C	7:G:87:ASN:ND2	2.55	0.60
2:P:234:VAL:HA	2:P:239:THR:HA	1.84	0.60
5:E:15:PHE:H	6:F:23:GLN:HE22	1.49	0.60
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.84	0.60
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.02	0.60
10:X:48:GLU:HB2	10:X:96:GLN:HB2	1.83	0.60
4:D:97:VAL:HG21	11:K:65:LEU:CD1	2.27	0.59
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.84	0.59
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.67	0.59
6:T:127:ASN:HD22	6:T:128:SER:N	2.00	0.59
10:J:45:PHE:CD1	10:J:52:THR:HG23	2.36	0.59
11:K:114:ASP:OD1	11:K:116:ASP:HB2	2.02	0.59
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.84	0.59
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.82	0.59
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.83	0.59
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.32	0.59
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.02	0.59
2:P:88:LEU:HB3	2:P:116:LEU:HD21	1.82	0.59
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.84	0.59
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.85	0.59
3:C:186:VAL:O	3:C:190:VAL:HG23	2.02	0.59
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.18	0.59
1:O:15:PHE:N	2:P:23:GLN:HE22	1.91	0.59
3:Q:15:PHE:H	4:R:23:GLN:NE2	1.94	0.59
1:A:173:LYS:O	1:A:177:GLU:HG3	2.03	0.59
4:D:85:ALA:O	4:D:89:ILE:HG12	2.03	0.59
8:H:172:ASN:ND2	8:H:193:THR:HA	2.18	0.59
11:K:138:LEU:HD13	11:K:158:SER:OG	2.03	0.59
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.83	0.59
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.85	0.59
10:X:10(B):LYS:HB2	10:X:10(B):LYS:NZ	2.18	0.59
12:Z:21:ILE:C	12:Z:21:ILE:HD12	2.23	0.59
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.83	0.59
6:F:127:ASN:HD22	6:F:128:SER:N	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:21:ILE:C	12:L:21:ILE:HD12	2.23	0.58
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.67	0.58
10:X:44:SER:OG	10:X:100:LEU:HB2	2.02	0.58
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.68	0.58
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.68	0.58
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.03	0.58
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.19	0.58
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.50	0.58
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.85	0.58
3:C:232:TYR:O	3:C:236:ILE:HG13	2.03	0.58
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.85	0.58
7:G:59:LEU:O	7:G:61:PRO:HD3	2.03	0.58
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.69	0.58
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.83	0.58
1:A:7:ARG:HB2	2:B:5:SER:OG	2.03	0.58
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.38	0.58
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.03	0.58
4:R:207:LEU:C	4:R:207:LEU:HD23	2.24	0.58
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.86	0.58
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.84	0.58
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.36	0.58
5:E:180:LEU:O	5:E:18(D):ILE:HG22	2.03	0.58
5:E:190:ILE:O	5:E:194:VAL:HG23	2.04	0.58
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.39	0.58
1:O:173:LYS:O	1:O:177:GLU:HG3	2.04	0.58
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.04	0.58
7:U:218:ASP:O	7:U:220:LYS:HB2	2.04	0.58
7:G:217:LYS:HE3	7:G:217:LYS:HA	1.84	0.58
10:J:3:ILE:HG22	10:J:100:LEU:CD1	2.34	0.58
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.85	0.57
10:J:48:GLU:HB2	10:J:96:GLN:HB2	1.85	0.57
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.86	0.57
3:Q:159:SER:HB2	16:Q:260:HOH:O	2.03	0.57
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.85	0.57
5:E:86:ARG:O	5:E:90:ASN:HB2	2.04	0.57
1:O:161:LYS:HD2	2:P:58:LEU:HA	1.84	0.57
7:U:236:ILE:HD12	7:U:237:ALA:N	2.19	0.57
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.86	0.57
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.69	0.57
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.04	0.57
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.86	0.57
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.84	0.57
5:S:86:ARG:O	5:S:90:ASN:HB2	2.04	0.57
6:T:147:HIS:HD2	16:T:242:HOH:O	1.86	0.57
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.09	0.57
5:S:207:LEU:HD23	5:S:207:LEU:N	2.18	0.57
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.33	0.57
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.86	0.57
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.87	0.57
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.51	0.57
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.86	0.57
2:B:234:VAL:HA	2:B:239:THR:HA	1.85	0.57
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.87	0.57
5:S:180:LEU:O	5:S:18(D):ILE:HG22	2.04	0.57
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.40	0.57
5:E:207:LEU:HD23	5:E:207:LEU:N	2.16	0.57
7:G:96:ALA:HA	7:G:107:MET:CE	2.17	0.57
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.87	0.57
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.87	0.57
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.87	0.57
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.35	0.57
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.53	0.57
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.53	0.57
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.39	0.57
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.86	0.57
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.35	0.57
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.86	0.57
3:C:190:VAL:O	3:C:194:VAL:HG23	2.05	0.56
6:T:121:GLN:NE2	16:T:248:HOH:O	2.38	0.56
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.86	0.56
12:L:98:HIS:HD2	16:L:198:HOH:O	1.88	0.56
2:P:202:THR:HG21	2:P:204:SER:HB2	1.87	0.56
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.87	0.56
4:D:227:GLU:OE2	4:D:227:GLU:N	2.33	0.56
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.87	0.56
4:D:91:HIS:CG	4:D:119:LEU:HD11	2.40	0.56
4:D:207:LEU:HD23	4:D:207:LEU:C	2.26	0.56
5:E:123:ASN:N	5:E:123:ASN:HD22	2.03	0.56
7:U:87:ASN:C	7:U:87:ASN:ND2	2.57	0.56
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.40	0.56
3:C:102:THR:OG1	3:C:103:LEU:HD22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.87	0.56
10:J:44:SER:OG	10:J:100:LEU:HB2	2.05	0.56
14:N:147:SER:OG	14:N:150:GLU:HG3	2.06	0.56
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.07	0.56
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.87	0.56
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.87	0.56
10:X:3:ILE:HG22	10:X:100:LEU:CD1	2.36	0.56
3:C:227:GLU:H	3:C:227:GLU:CD	2.10	0.56
7:G:218:ASP:O	7:G:220:LYS:HB2	2.06	0.56
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.88	0.56
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.35	0.55
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.86	0.55
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.88	0.55
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.05	0.55
7:U:131:PRO:HB3	16:U:259:HOH:O	2.06	0.55
8:V:84:LYS:HG3	8:V:85:GLN:N	2.21	0.55
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.88	0.55
5:S:73:HIS:HE1	5:S:107:LEU:O	1.89	0.55
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.88	0.55
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.53	0.55
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.88	0.55
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.36	0.55
3:C:224:LEU:HD12	3:C:224:LEU:N	2.21	0.55
7:G:77:VAL:CG1	7:G:137:THR:HB	2.36	0.55
5:S:190:ILE:O	5:S:194:VAL:HG23	2.06	0.55
12:Z:-5:TYR:CE2	12:Z:96:TYR:HB2	2.41	0.55
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.89	0.55
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.37	0.55
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.06	0.55
10:X:45:PHE:CD1	10:X:52:THR:HG23	2.41	0.55
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.88	0.55
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.21	0.55
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.71	0.55
10:J:14:LEU:HD12	10:J:42:LEU:HD23	1.89	0.55
10:J:15:ALA:HB2	10:J:155:LEU:HD11	1.89	0.55
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.41	0.55
1:A:150:GLN:O	1:A:157:TYR:HA	2.07	0.55
2:B:163:ILE:HG13	2:B:164:SER:N	2.22	0.55
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.72	0.55
2:P:239:THR:OXT	2:P:239:THR:HG22	2.07	0.55
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.07	0.55

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.89	0.55
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.42	0.55
14:N:156:LYS:HG2	14:N:18(J):LEU:CD1	2.37	0.55
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.70	0.55
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.89	0.55
5:E:226:GLY:O	5:E:229:VAL:HG22	2.06	0.55
3:Q:102:THR:OG1	3:Q:103:LEU:HD22	2.06	0.55
4:R:91:HIS:CG	4:R:119:LEU:HD11	2.42	0.55
8:H:172:ASN:HB3	8:H:192:LEU:O	2.07	0.54
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.40	0.54
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.89	0.54
14:2:156:LYS:HG2	14:2:18(J):LEU:CD1	2.37	0.54
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.42	0.54
11:K:25:TRP:CH2	12:L:132:SER:HA	2.42	0.54
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.22	0.54
7:U:77:VAL:CG1	7:U:137:THR:HB	2.38	0.54
2:B:202:THR:HG21	2:B:204:SER:HB2	1.90	0.54
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.22	0.54
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.38	0.54
3:C:229:ILE:O	3:C:233:VAL:HG23	2.08	0.54
12:L:177:ILE:N	12:L:177:ILE:HD12	2.22	0.54
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.42	0.54
7:G:171:GLU:N	7:G:171:GLU:OE1	2.38	0.54
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.07	0.54
9:I:29:ASN:HD22	9:I:29:ASN:C	2.11	0.54
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.90	0.54
7:U:228:ASN:HB3	16:U:242:HOH:O	2.06	0.54
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.90	0.54
1:O:150:GLN:O	1:O:157:TYR:HA	2.07	0.54
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.89	0.54
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.07	0.54
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.43	0.54
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.37	0.53
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.11	0.53
6:T:79:SER:HA	16:T:268:HOH:O	2.06	0.53
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.90	0.53
10:X:15:ALA:HB2	10:X:155:LEU:HD11	1.90	0.53
6:F:28:VAL:O	6:F:32:GLU:HG3	2.07	0.53
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.90	0.53
8:V:172:ASN:HB3	8:V:192:LEU:O	2.08	0.53
5:E:73:HIS:HE1	5:E:107:LEU:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.89	0.53
2:P:103:TYR:O	2:P:104:ASN:HB2	2.08	0.53
4:D:175:GLU:HG2	4:D:196:ILE:HG12	1.90	0.53
11:K:200:LYS:HE3	11:K:206:PHE:O	2.08	0.53
12:L:109:ALA:HA	16:L:225:HOH:O	2.07	0.53
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.43	0.53
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.90	0.53
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.90	0.53
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.08	0.53
5:E:227:GLU:CD	5:E:227:GLU:H	2.12	0.53
1:O:7:ARG:HB2	2:P:5:SER:OG	2.08	0.53
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.08	0.53
13:1:12:VAL:HG21	13:1:102:ALA:HB1	1.89	0.53
11:K:46:ALA:HB3	11:K:98:GLY:O	2.09	0.53
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.08	0.53
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.44	0.53
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.57	0.53
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.90	0.53
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.55	0.53
14:2:65:LEU:HG	14:2:69:GLN:NE2	2.24	0.53
3:C:13:SER:HA	16:C:251:HOH:O	2.08	0.53
7:G:236:ILE:HD12	7:G:237:ALA:N	2.23	0.53
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.90	0.53
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.39	0.53
12:L:166:HIS:HD2	12:L:168:GLN:H	1.56	0.53
3:Q:71:ASP:HA	10:X:68:ILE:HD11	1.89	0.53
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.90	0.53
7:G:86:ARG:HD2	16:G:254:HOH:O	2.09	0.53
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.90	0.53
4:R:175:GLU:HG2	4:R:196:ILE:HG12	1.90	0.53
5:S:123:ASN:HD22	5:S:123:ASN:N	2.04	0.53
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.91	0.53
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.92	0.53
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.38	0.53
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.73	0.53
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.29	0.53
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.91	0.53
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.13	0.53
2:P:122:GLY:C	2:P:124:THR:H	2.13	0.53
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.57	0.53
3:Q:172:VAL:O	3:Q:176:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:177:GLU:OE2	7:U:57:LYS:HE2	2.09	0.53
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.91	0.53
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.08	0.52
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.39	0.52
14:N:20:THR:HG1	14:N:28:ASN:HB3	1.74	0.52
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.39	0.52
13:1:149:GLN:H	13:1:149:GLN:HE21	1.57	0.52
8:H:59:ILE:HG12	8:H:83:LEU:HG	1.92	0.52
2:B:239:THR:HG22	2:B:239:THR:OXT	2.09	0.52
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.73	0.52
5:S:226:GLY:O	5:S:229:VAL:HG22	2.09	0.52
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.40	0.52
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.30	0.52
2:P:168:ASN:HA	16:P:252:HOH:O	2.07	0.52
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.45	0.52
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.09	0.52
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.92	0.52
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.09	0.52
10:J:3:ILE:HG22	10:J:100:LEU:HD12	1.92	0.52
10:J:168:MET:HG2	10:X:168:MET:HE2	1.91	0.52
12:L:39:ASP:OD2	12:L:67:HIS:HE1	1.92	0.52
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.44	0.52
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.74	0.52
7:U:171:GLU:N	7:U:171:GLU:OE1	2.37	0.52
10:X:76:PRO:HD2	16:X:206:HOH:O	2.10	0.52
14:2:14:LEU:O	14:2:175:MET:HA	2.10	0.52
3:C:75:VAL:HG13	3:C:221:ILE:HD13	1.91	0.52
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.22	0.52
14:2:147:SER:OG	14:2:150:GLU:HG3	2.10	0.52
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.25	0.52
2:B:41:MET:HE3	16:B:240:HOH:O	2.10	0.52
3:Q:229:ILE:O	3:Q:233:VAL:HG23	2.10	0.52
5:S:86:ARG:HG3	5:S:86:ARG:HH11	1.75	0.52
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.10	0.52
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.90	0.52
12:Z:39:ASP:OD2	12:Z:67:HIS:HE1	1.92	0.52
2:B:55:THR:HG22	2:B:59:LEU:HD23	1.91	0.52
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.92	0.52
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.10	0.52
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.92	0.52
9:I:114:ASP:HB2	16:I:236:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:184:LEU:HD23	13:M:184:LEU:C	2.30	0.52
2:P:228:GLU:O	2:P:232:ILE:HG22	2.10	0.52
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	1.92	0.52
3:Q:185:THR:CB	3:Q:188:GLU:HG2	2.32	0.52
9:W:89:GLU:O	9:W:90:ARG:NH1	2.42	0.52
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.76	0.51
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.91	0.51
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.10	0.51
12:L:-5:TYR:CE2	12:L:96:TYR:HB2	2.45	0.51
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.10	0.51
2:P:202:THR:HG22	2:P:204:SER:N	2.10	0.51
6:T:20(B):GLU:CD	6:T:20(C):LYS:HE3	2.31	0.51
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.44	0.51
13:1:104:VAL:CG2	13:1:178:ILE:HG22	2.38	0.51
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.93	0.51
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.39	0.51
10:X:143:ARG:O	10:X:146:MET:HG3	2.10	0.51
8:H:84:LYS:HG3	8:H:85:GLN:N	2.25	0.51
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.37	0.51
1:O:69:LEU:C	1:O:69:LEU:HD23	2.31	0.51
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.45	0.51
11:Y:12:ILE:HG23	11:Y:110:ILE:HD11	1.92	0.51
13:1:14(A):VAL:HG23	13:1:14(A):VAL:O	2.11	0.51
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.26	0.51
13:M:211:ILE:HD11	14:2:36:ARG:CD	2.40	0.51
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.41	0.51
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.31	0.51
6:T:103:TYR:O	6:T:104:LYS:HB3	2.09	0.51
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.26	0.51
11:Y:35:ILE:CD1	11:Y:53:GLN:HA	2.40	0.51
11:Y:35:ILE:HD13	11:Y:53:GLN:HA	1.92	0.51
2:P:21(C):ASP:OD2	2:P:219:GLU:HB3	2.11	0.51
13:1:91:ARG:HG3	13:1:92:SER:N	2.25	0.51
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.45	0.51
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.92	0.51
14:N:65:LEU:HG	14:N:69:GLN:NE2	2.26	0.51
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.26	0.51
14:2:20:THR:HG1	14:2:28:ASN:HB3	1.76	0.51
11:K:6:PHE:HA	11:K:123:ASP:O	2.10	0.51
10:X:93:ARG:NH2	11:Y:91:LYS:HD3	2.26	0.51
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:TRP:HA	3:C:59:GLN:HA	1.93	0.51
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.41	0.51
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.93	0.51
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.41	0.51
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.26	0.51
2:P:55:THR:HG22	2:P:59:LEU:HD23	1.93	0.51
5:S:227:GLU:CD	5:S:227:GLU:H	2.13	0.51
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.94	0.50
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.93	0.50
6:T:172:ALA:O	6:T:176:LEU:HD23	2.11	0.50
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.40	0.50
9:W:55:LEU:HD11	9:W:97:VAL:HG21	1.93	0.50
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.92	0.50
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.41	0.50
4:R:24:VAL:O	4:R:27:SER:HB3	2.11	0.50
12:Z:99:THR:HG22	16:Z:201:HOH:O	2.11	0.50
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.40	0.50
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.24	0.50
12:L:-2:ASN:HA	12:L:21:ILE:O	2.11	0.50
12:L:17:ASP:HA	12:L:172:GLY:O	2.11	0.50
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.46	0.50
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.41	0.50
9:W:29:ASN:HD22	9:W:29:ASN:C	2.13	0.50
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.29	0.50
1:A:69:LEU:C	1:A:69:LEU:HD23	2.31	0.50
5:S:4:PHE:CG	5:S:5:ARG:N	2.79	0.50
7:U:8:TYR:C	7:U:10:ARG:H	2.15	0.50
7:U:9:ASP:OD2	7:U:16:SER:HA	2.12	0.50
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.12	0.50
13:1:113:VAL:HA	13:1:118:VAL:O	2.12	0.50
1:A:212:LEU:HD22	1:A:224:LEU:HD12	1.94	0.50
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.92	0.50
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.41	0.50
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.42	0.50
7:G:93:LYS:HD3	14:N:68:SER:HB3	1.94	0.50
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.12	0.50
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.92	0.50
9:W:101:VAL:O	9:W:110:ILE:HA	2.12	0.50
12:Z:14(E):GLU:OE2	12:Z:14(P):PRO:HD2	2.11	0.50
2:B:21(C):ASP:OD2	2:B:219:GLU:HB3	2.10	0.50
3:C:224:LEU:N	3:C:224:LEU:CD1	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:192:GLN:O	6:F:196:ILE:HG13	2.12	0.50
9:I:55:LEU:HD11	9:I:97:VAL:HG21	1.93	0.50
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.93	0.50
5:S:161:TYR:CD1	5:S:18(D):ILE:HD13	2.47	0.50
12:Z:90:LYS:HE2	16:Z:196:HOH:O	2.12	0.50
2:B:103:TYR:O	2:B:104:ASN:HB2	2.11	0.50
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.94	0.50
5:S:220:PRO:O	5:S:222:THR:HG23	2.12	0.50
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.47	0.50
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.12	0.50
1:A:170:VAL:HB	16:A:250:HOH:O	2.12	0.50
2:B:228:GLU:O	2:B:232:ILE:HG22	2.11	0.50
4:D:170:GLU:OE1	4:D:170:GLU:N	2.44	0.50
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.92	0.50
12:L:1(I):ASN:O	12:L:14(K):LYS:HG2	2.11	0.50
13:M:14(C):ARG:HH11	13:M:14(C):ARG:CG	2.22	0.50
9:W:48:LEU:HG	9:W:50:THR:HG22	1.94	0.50
10:X:4:LEU:HD23	10:X:126:ALA:HB2	1.93	0.50
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.46	0.50
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.22	0.49
5:E:4:PHE:CG	5:E:5:ARG:N	2.78	0.49
5:E:66:LYS:O	5:E:77:SER:HA	2.12	0.49
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.94	0.49
10:J:133:TYR:HE1	16:X:220:HOH:O	1.94	0.49
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.47	0.49
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.12	0.49
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.12	0.49
2:B:191:GLU:O	2:B:195:LYS:HG2	2.12	0.49
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.12	0.49
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.94	0.49
5:S:67:ILE:HG21	5:S:213:ALA:HB2	1.93	0.49
6:T:35:THR:CG2	6:T:36:THR:N	2.75	0.49
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.95	0.49
12:L:135:MET:CE	9:W:165:ARG:NH2	2.76	0.49
6:T:28:VAL:O	6:T:32:GLU:HG3	2.12	0.49
3:C:97:GLN:HA	3:C:97:GLN:NE2	2.26	0.49
4:D:70:ILE:HB	4:D:74:ILE:HG22	1.94	0.49
8:V:59:ILE:HG12	8:V:83:LEU:HG	1.93	0.49
13:1:184:LEU:C	13:1:184:LEU:HD23	2.33	0.49
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.95	0.49
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:3:ILE:HG22	10:X:100:LEU:HD12	1.95	0.49
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.41	0.49
6:F:179:LEU:CD2	6:F:192:GLN:HG2	2.42	0.49
6:T:192:GLN:O	6:T:196:ILE:HG13	2.12	0.49
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.42	0.49
7:G:136:LEU:O	7:G:150:LYS:HA	2.12	0.49
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.95	0.49
1:O:175:PHE:O	1:O:179:ARG:HG2	2.12	0.49
10:X:90(B):ARG:NH1	16:X:205:HOH:O	2.43	0.49
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.11	0.49
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.48	0.49
10:J:133:TYR:HD1	16:Y:322:HOH:O	1.96	0.49
13:M:152:GLU:O	13:M:156:VAL:HG23	2.12	0.49
14:N:36:ARG:CD	13:1:211:ILE:HD11	2.43	0.49
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.94	0.49
3:Q:97:GLN:HA	3:Q:97:GLN:NE2	2.28	0.49
6:T:237:GLN:O	6:T:240:ILE:HG22	2.12	0.49
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.95	0.49
10:X:190:PHE:HA	10:X:193:GLN:HB2	1.95	0.49
11:Y:199:VAL:O	11:Y:203:GLU:HB3	2.13	0.49
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.43	0.49
2:B:27:ALA:O	2:B:31:ILE:HG13	2.13	0.49
3:C:172:VAL:O	3:C:176:LEU:HG	2.13	0.49
6:F:103:TYR:O	6:F:104:LYS:HB3	2.13	0.49
6:F:126:TYR:HE1	7:G:129:MET:SD	2.36	0.49
6:F:184:LEU:CD1	6:F:188:GLU:HB3	2.42	0.49
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.28	0.49
10:J:190:PHE:HA	10:J:193:GLN:HB2	1.94	0.49
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.25	0.49
13:M:19:LEU:HD12	13:M:28:PHE:O	2.13	0.49
13:M:40:ASN:N	13:M:40:ASN:ND2	2.60	0.49
14:N:106:ASN:O	14:N:107:LYS:HB3	2.13	0.49
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.94	0.49
4:D:205:GLU:OE2	4:D:205:GLU:HA	2.13	0.49
13:M:17:ASP:HA	13:M:173:PHE:CB	2.42	0.49
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.48	0.49
4:R:170:GLU:N	4:R:170:GLU:OE1	2.46	0.49
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.66	0.49
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.94	0.48
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.47	0.48
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:14(E):GLU:OE2	12:L:14(P):PRO:HD2	2.13	0.48
13:M:35:ILE:HD12	13:M:35:ILE:N	2.28	0.48
14:N:14:LEU:O	14:N:175:MET:HA	2.12	0.48
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.28	0.48
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.93	0.48
13:1:40:ASN:N	13:1:40:ASN:ND2	2.60	0.48
4:D:24:VAL:O	4:D:27:SER:HB3	2.12	0.48
9:I:93:GLY:H	9:I:94:PRO:HD3	1.78	0.48
9:I:93:GLY:N	9:I:94:PRO:CD	2.76	0.48
9:I:101:VAL:O	9:I:110:ILE:HA	2.13	0.48
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.41	0.48
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.95	0.48
11:K:35:ILE:CD1	11:K:53:GLN:HA	2.43	0.48
2:P:186:VAL:HG21	2:P:216:ARG:HG2	1.95	0.48
2:B:122:GLY:C	2:B:124:THR:H	2.15	0.48
11:K:35:ILE:HD13	11:K:53:GLN:HA	1.95	0.48
13:M:46:SER:OG	13:M:98:ALA:HB3	2.14	0.48
1:O:159:PRO:HB2	2:P:60:GLU:HB3	1.95	0.48
7:U:72:ARG:HG2	16:U:267:HOH:O	2.13	0.48
7:U:152:ASP:HB2	7:U:153:PRO:HD2	1.95	0.48
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.95	0.48
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.96	0.48
12:Z:1(I):ASN:O	12:Z:14(K):LYS:HG2	2.14	0.48
1:A:4:MET:HG2	6:F:126:TYR:CE2	2.49	0.48
1:A:29:THR:O	1:A:33:GLN:HG2	2.13	0.48
2:B:21(A):LYS:O	2:B:217:ALA:N	2.46	0.48
3:C:159:SER:O	4:D:59:LEU:HD22	2.14	0.48
7:G:9:ASP:OD2	7:G:16:SER:HA	2.13	0.48
9:I:48:LEU:HG	9:I:50:THR:HG22	1.95	0.48
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.48	0.48
13:1:35:ILE:N	13:1:35:ILE:HD12	2.27	0.48
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.95	0.48
3:C:100:ARG:HH12	3:C:106:PRO:HB3	1.74	0.48
10:J:168:MET:HE3	10:X:168:MET:HG2	1.94	0.48
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.48	0.48
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.95	0.48
4:R:227:GLU:OE2	4:R:227:GLU:N	2.35	0.48
7:U:158:VAL:HG22	7:U:159:GLY:N	2.29	0.48
9:W:6:MET:HE3	9:W:155:ILE:HA	1.96	0.48
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	2.13	0.48
13:1:19:LEU:HD12	13:1:28:PHE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:176:LEU:HD22	6:F:196:ILE:HD13	1.95	0.48
7:G:72:ARG:HB2	7:G:72:ARG:NH1	2.28	0.48
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.79	0.48
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.41	0.48
8:V:72:ARG:HG3	8:V:72:ARG:HH11	1.79	0.48
10:X:113:ILE:HA	10:X:118:THR:O	2.13	0.48
4:D:112:LEU:C	4:D:112:LEU:HD13	2.33	0.48
9:I:22:SER:O	9:I:23:GLN:HB2	2.14	0.48
11:K:12:ILE:HG23	11:K:110:ILE:HD11	1.95	0.48
11:K:199:VAL:O	11:K:203:GLU:HB3	2.14	0.48
2:P:21(A):LYS:O	2:P:217:ALA:N	2.47	0.48
4:R:205:GLU:HA	4:R:205:GLU:OE2	2.13	0.48
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.96	0.48
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.95	0.48
3:C:150:GLN:HG2	3:C:151:THR:N	2.28	0.48
7:G:77:VAL:HG12	7:G:137:THR:HB	1.95	0.48
9:I:89:GLU:O	9:I:90:ARG:NH1	2.47	0.48
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.12	0.48
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.78	0.48
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.95	0.48
13:1:1:THR:OG1	13:1:2:SER:N	2.44	0.48
14:2:106:ASN:O	14:2:107:LYS:HB3	2.14	0.48
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.29	0.48
2:B:185:LYS:HD3	2:B:187:ASP:H	1.79	0.48
5:E:86:ARG:HG3	5:E:86:ARG:HH11	1.78	0.48
13:M:186:PHE:HE1	13:M:188:LYS:HG3	1.79	0.48
14:N:113:ILE:HG12	14:N:119:VAL:HG13	1.94	0.48
1:O:169:SER:O	1:O:173:LYS:HG3	2.14	0.48
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.96	0.48
6:T:176:LEU:HD22	6:T:196:ILE:HD13	1.96	0.48
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.29	0.48
9:W:22:SER:O	9:W:23:GLN:HB2	2.14	0.48
3:C:242:GLU:O	3:C:243:GLN:HB2	2.14	0.47
5:E:161:TYR:CD1	5:E:18(D):ILE:HD13	2.49	0.47
4:R:70:ILE:HB	4:R:74:ILE:HG22	1.96	0.47
7:U:136:LEU:O	7:U:150:LYS:HA	2.13	0.47
9:W:6:MET:CE	9:W:155:ILE:HA	2.44	0.47
13:1:14(C):ARG:HH11	13:1:14(C):ARG:CG	2.21	0.47
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.44	0.47
1:A:13:THR:O	2:B:130:ARG:HD3	2.14	0.47
9:I:6:MET:CE	9:I:155:ILE:HA	2.43	0.47

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
12:L:166:HIS:CD2	12:L:168:GLN:H	2.32	0.47
14:N:13:ILE:HG12	14:N:177:VAL:HG13	1.96	0.47
1:O:15:PHE:H	2:P:23:GLN:NE2	1.92	0.47
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.29	0.47
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.97	0.47
14:2:3:ILE:HG22	14:2:16:ALA:HB2	1.96	0.47
1:A:110:LYS:HG2	16:A:245:HOH:O	2.13	0.47
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.43	0.47
4:D:122:ARG:HG2	4:D:122:ARG:NH1	2.27	0.47
6:F:20(B):GLU:HG3	6:F:20(C):LYS:H	1.78	0.47
9:I:18:LEU:CD2	9:I:32:GLU:HG2	2.44	0.47
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.44	0.47
9:W:80:THR:HG22	9:W:119:ILE:HD13	1.96	0.47
11:Y:66:HIS:HA	16:Y:333:HOH:O	2.14	0.47
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.82	0.47
13:1:83:LEU:O	13:1:87:MET:HG2	2.14	0.47
14:2:113:ILE:HG12	14:2:119:VAL:HG13	1.95	0.47
12:L:134:ILE:HG22	12:L:138:LEU:HD22	1.96	0.47
1:O:24:ILE:HD11	1:O:124:THR:HG23	1.95	0.47
2:P:224:PHE:N	2:P:224:PHE:CD2	2.83	0.47
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.76	0.47
5:S:7:ASN:O	6:T:10:LEU:HD22	2.14	0.47
6:T:136:THR:O	6:T:150:MET:HA	2.14	0.47
1:A:85:TYR:O	1:A:89:VAL:HG23	2.14	0.47
1:A:169:SER:O	1:A:173:LYS:HG3	2.14	0.47
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.50	0.47
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.97	0.47
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.26	0.47
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	2.14	0.47
2:P:44:ASP:OD2	2:P:186:VAL:HG23	2.14	0.47
2:P:229:ILE:O	2:P:233:LEU:HB2	2.15	0.47
5:S:66:LYS:O	5:S:77:SER:HA	2.13	0.47
16:T:244:HOH:O	7:U:86:ARG:HD2	2.14	0.47
12:Z:-9:GLN:NE2	12:Z:-8:PHE:N	2.59	0.47
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.49	0.47
1:A:5:THR:O	1:A:7:ARG:HG2	2.14	0.47
1:A:24:ILE:HD11	1:A:124:THR:HG23	1.96	0.47
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.96	0.47
11:K:142:TYR:C	11:K:143:LYS:HD2	2.35	0.47
12:L:145:TYR:CD1	12:L:146:LEU:N	2.82	0.47
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:160:LEU:HD13	5:S:163:THR:HB	1.97	0.47
5:S:18(C):PHE:HA	5:S:18(F):ILE:CD1	2.44	0.47
9:W:61:TYR:CD1	9:W:61:TYR:C	2.88	0.47
10:X:52:THR:CG2	10:X:53:VAL:N	2.78	0.47
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.30	0.47
5:E:111:ARG:HG2	5:E:111:ARG:NH1	2.25	0.47
7:G:8:TYR:C	7:G:10:ARG:H	2.16	0.47
7:G:158:VAL:HG22	7:G:159:GLY:N	2.30	0.47
8:H:3:ILE:CD1	8:H:127:LEU:HB2	2.43	0.47
10:J:140:HIS:HA	11:Y:205:SER:HB2	1.95	0.47
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.49	0.47
13:M:91:ARG:HG3	13:M:92:SER:N	2.29	0.47
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.49	0.47
14:N:105:ASP:OD2	14:N:106:ASN:N	2.38	0.47
14:N:120:HIS:HA	16:N:234:HOH:O	2.14	0.47
1:O:27:ALA:O	1:O:31:VAL:HG23	2.13	0.47
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.97	0.47
2:P:191:GLU:O	2:P:195:LYS:HG2	2.12	0.47
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.29	0.47
5:S:123:ASN:N	5:S:123:ASN:ND2	2.63	0.47
8:V:175:VAL:HG12	8:V:176:CYS:N	2.29	0.47
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.50	0.47
9:W:93:GLY:H	9:W:94:PRO:HD3	1.78	0.47
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.80	0.47
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.50	0.47
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	1.97	0.47
13:1:186:PHE:HE1	13:1:188:LYS:HG3	1.79	0.47
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.44	0.47
8:H:5:GLY:O	8:H:124:TYR:HA	2.15	0.47
10:J:168:MET:HG2	10:X:168:MET:HE3	1.96	0.47
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.95	0.47
14:N:9:LYS:HA	14:N:145:ASN:HD22	1.80	0.47
9:W:93:GLY:N	9:W:94:PRO:CD	2.77	0.47
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.97	0.47
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.14	0.47
13:1:104:VAL:HG23	13:1:178:ILE:CG2	2.43	0.47
3:C:163:GLN:HG3	3:C:164:THR:N	2.29	0.47
6:F:136:THR:O	6:F:150:MET:HA	2.15	0.47
8:H:175:VAL:HG12	8:H:176:CYS:N	2.29	0.47
3:Q:242:GLU:O	3:Q:243:GLN:HB2	2.13	0.47
14:2:9:LYS:HA	14:2:145:ASN:HD22	1.80	0.47

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
14:2:107:LYS:HG2	14:2:108:GLY:H	1.79	0.47
1:A:175:PHE:O	1:A:179:ARG:HG2	2.15	0.47
10:J:143:ARG:O	10:J:146:MET:HG3	2.15	0.47
14:N:85:GLU:O	14:N:89:GLU:HB2	2.15	0.47
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.96	0.47
6:T:179:LEU:CD2	6:T:192:GLN:HG2	2.40	0.47
6:T:20(B):GLU:HG3	6:T:20(C):LYS:H	1.79	0.47
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.80	0.46
10:J:52:THR:CG2	10:J:53:VAL:N	2.76	0.46
2:P:20:ARG:HG2	2:P:20:ARG:HH11	1.80	0.46
2:P:185:LYS:HD3	2:P:187:ASP:H	1.79	0.46
11:Y:200:LYS:NZ	11:Y:209:VAL:O	2.39	0.46
1:A:92:SER:O	1:A:95:VAL:HG12	2.14	0.46
12:L:5:GLY:O	12:L:124:CYS:HA	2.15	0.46
14:N:107:LYS:HG2	14:N:108:GLY:H	1.80	0.46
1:O:29:THR:O	1:O:33:GLN:HG2	2.14	0.46
3:Q:182:PRO:O	3:Q:184:ALA:N	2.49	0.46
6:T:127:ASN:HD22	6:T:127:ASN:C	2.19	0.46
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.96	0.46
13:1:17:ASP:HA	13:1:173:PHE:CB	2.45	0.46
4:D:240:LYS:O	4:D:243:ALA:HB3	2.15	0.46
7:G:38:LEU:C	7:G:38:LEU:HD12	2.35	0.46
10:J:113:ILE:HA	10:J:118:THR:O	2.16	0.46
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.16	0.46
1:A:4:MET:O	1:A:5:THR:O	2.33	0.46
1:A:112:LEU:O	1:A:116:VAL:HG23	2.16	0.46
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.98	0.46
6:F:20(B):GLU:OE1	6:F:20(C):LYS:HE3	2.15	0.46
9:I:80:THR:HG22	9:I:119:ILE:HD13	1.97	0.46
1:O:24:ILE:HD11	1:O:124:THR:CG2	2.46	0.46
2:P:224:PHE:N	2:P:224:PHE:HD2	2.14	0.46
11:Y:87:VAL:HG11	11:Y:115:SER:HA	1.96	0.46
12:Z:39:ASP:OD2	12:Z:67:HIS:CE1	2.68	0.46
13:1:8:TYR:CZ	13:1:148:VAL:HG13	2.51	0.46
2:B:224:PHE:N	2:B:224:PHE:CD2	2.83	0.46
4:D:91:HIS:CE1	4:D:119:LEU:HD21	2.51	0.46
5:E:18(C):PHE:HA	5:E:18(F):ILE:CD1	2.46	0.46
5:E:220:PRO:O	5:E:222:THR:HG23	2.14	0.46
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.79	0.46
13:M:17:ASP:HA	13:M:173:PHE:HA	1.98	0.46
13:M:35:ILE:CG1	13:M:56:GLU:HG3	2.41	0.46

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.98	0.46
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.35	0.46
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.45	0.46
8:H:196:VAL:HG23	16:H:244:HOH:O	2.14	0.46
13:M:83:LEU:O	13:M:87:MET:HG2	2.15	0.46
13:M:113:VAL:HA	13:M:118:VAL:O	2.15	0.46
3:C:8:TYR:HB3	16:C:269:HOH:O	2.15	0.46
3:C:103:LEU:HD13	16:C:270:HOH:O	2.15	0.46
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.98	0.46
2:B:224:PHE:N	2:B:224:PHE:HD2	2.14	0.46
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.97	0.46
6:F:121:GLN:NE2	16:F:257:HOH:O	2.49	0.46
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.98	0.46
10:J:168:MET:HE2	10:X:168:MET:HG2	1.97	0.46
11:K:31:VAL:CG1	11:K:45:MET:HE1	2.46	0.46
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.31	0.46
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.98	0.46
14:2:85:GLU:O	14:2:89:GLU:HB2	2.16	0.46
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.36	0.46
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.16	0.46
1:O:5:THR:O	1:O:7:ARG:HG2	2.15	0.46
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.46	0.46
8:V:5:GLY:O	8:V:124:TYR:HA	2.16	0.46
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.98	0.46
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.51	0.46
6:F:172:ALA:O	6:F:176:LEU:HD23	2.16	0.46
8:H:48:THR:HB	8:H:51:ASP:HB2	1.98	0.46
11:K:10(A):ARG:HH11	11:K:10(A):ARG:HG2	1.81	0.46
14:N:3:ILE:HG22	14:N:16:ALA:HB2	1.97	0.46
5:S:227:GLU:CD	5:S:227:GLU:N	2.69	0.46
3:C:169:SER:HA	3:C:172:VAL:CG1	2.47	0.45
6:F:194:ALA:O	6:F:198:TYR:HD1	1.98	0.45
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.37	0.45
2:P:27:ALA:O	2:P:31:ILE:HG13	2.17	0.45
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.98	0.45
2:P:97:GLN:NE2	16:P:244:HOH:O	2.46	0.45
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.75	0.45
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.36	0.45
13:1:152:GLU:O	13:1:156:VAL:HG23	2.16	0.45
2:B:229:ILE:O	2:B:233:LEU:HB2	2.15	0.45
4:D:86:ARG:HA	4:D:86:ARG:HD3	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.98	0.45
6:F:43:ASN:N	6:F:43:ASN:HD22	2.14	0.45
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.98	0.45
8:H:72:ARG:HG3	8:H:72:ARG:HH11	1.80	0.45
10:J:93:ARG:NH2	11:K:91:LYS:HD3	2.31	0.45
11:K:13:ILE:HD12	11:K:152:LEU:HD23	1.98	0.45
12:L:105:ASP:OD2	12:L:107:LYS:HB2	2.16	0.45
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.45	0.45
6:T:184:LEU:HD21	6:T:189:ALA:HA	1.97	0.45
6:T:194:ALA:O	6:T:198:TYR:HD1	1.99	0.45
7:U:227:GLU:HG2	16:U:283:HOH:O	2.16	0.45
13:1:31:VAL:HA	16:1:267:HOH:O	2.15	0.45
11:K:131:GLN:HG3	11:K:132:THR:N	2.31	0.45
12:L:-9:GLN:NE2	12:L:-8:PHE:N	2.61	0.45
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.99	0.45
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.97	0.45
6:T:43:ASN:N	6:T:43:ASN:HD22	2.14	0.45
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.98	0.45
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.32	0.45
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.98	0.45
3:C:57:LYS:O	3:C:58:LEU:HB2	2.16	0.45
3:C:182:PRO:O	3:C:184:ALA:N	2.49	0.45
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.81	0.45
13:M:112:TYR:C	13:M:112:TYR:CD2	2.89	0.45
13:M:149:GLN:H	13:M:149:GLN:HE21	1.57	0.45
1:O:4:MET:O	1:O:5:THR:O	2.34	0.45
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.51	0.45
2:P:194:LEU:HD13	2:P:233:LEU:HD12	1.98	0.45
6:T:20(B):GLU:OE1	6:T:20(C):LYS:HE3	2.16	0.45
8:V:34:LEU:HD22	8:V:174:ASP:HB3	1.98	0.45
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.37	0.45
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.31	0.45
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.46	0.45
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.31	0.45
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.50	0.45
2:B:20:ARG:HG2	2:B:20:ARG:HH11	1.80	0.45
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.98	0.45
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.97	0.45
4:R:112:LEU:HD13	4:R:112:LEU:C	2.37	0.45
6:T:69:VAL:HG12	16:T:262:HOH:O	2.15	0.45
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:N	2:B:23:GLN:HE22	2.04	0.45
2:B:63:THR:HG22	2:B:63:THR:O	2.17	0.45
2:B:186:VAL:HG21	2:B:216:ARG:HG2	1.97	0.45
5:E:5:ARG:HG3	5:E:22:PHE:CE2	2.51	0.45
11:K:31:VAL:HG11	11:K:45:MET:CE	2.47	0.45
11:K:76:VAL:N	11:K:106:GLU:OE2	2.46	0.45
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.17	0.45
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.14	0.45
12:Z:43:MET:CB	12:Z:101:ILE:HG22	2.47	0.45
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.98	0.45
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.99	0.45
3:C:235:GLN:O	3:C:239:GLU:HG2	2.16	0.45
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.63	0.45
5:E:227:GLU:CD	5:E:227:GLU:N	2.70	0.45
6:F:237:GLN:O	6:F:240:ILE:HG22	2.16	0.45
11:K:146:LEU:HD23	11:K:151:ALA:HA	1.99	0.45
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.31	0.45
2:P:4:GLY:HA3	5:S:127:TYR:CZ	2.52	0.45
2:P:150:THR:O	2:P:157:TYR:HA	2.16	0.45
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.98	0.45
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.16	0.45
4:R:12(D):ALA:HA	5:S:129:GLY:HA2	1.98	0.45
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.51	0.45
6:T:126:TYR:HE1	7:U:129:MET:SD	2.39	0.45
7:U:130:ARG:HB2	16:U:263:HOH:O	2.17	0.45
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.97	0.45
5:E:160:LEU:HD13	5:E:163:THR:HB	1.99	0.45
10:J:52:THR:HG22	10:J:53:VAL:HG23	1.99	0.45
11:K:97:MET:O	11:K:114:ASP:HA	2.17	0.45
10:X:166:MET:HA	10:X:167:PRO:HD3	1.80	0.45
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.81	0.45
13:1:70:ASN:ND2	13:1:70(A):ALA:HA	2.32	0.45
7:G:152:ASP:HB2	7:G:153:PRO:HD2	1.97	0.45
8:H:89:LYS:HE3	8:H:90:TYR:CE2	2.52	0.45
11:K:65:LEU:HD12	11:K:65:LEU:HA	1.84	0.45
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.70	0.45
12:L:93:PHE:N	12:L:94:PRO:HD3	2.32	0.45
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.47	0.45
5:S:48:LEU:HB2	5:S:213:ALA:HB3	1.98	0.45
7:U:39:ALA:HA	7:U:47:VAL:O	2.17	0.45
1:A:17:PRO:HA	2:B:26:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ILE:O	2:B:91:THR:HG23	2.17	0.45
2:B:209:ARG:CZ	2:B:209:ARG:HB3	2.46	0.45
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.17	0.45
4:D:59:LEU:HD13	4:D:59:LEU:C	2.37	0.45
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.98	0.45
1:O:67:VAL:HG11	1:O:213:ALA:HB2	1.99	0.45
1:O:85:TYR:O	1:O:89:VAL:HG23	2.17	0.45
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.98	0.45
2:B:44:ASP:OD2	2:B:186:VAL:HG23	2.17	0.44
4:D:62:ASP:OD2	4:D:62:ASP:N	2.45	0.44
5:E:123:ASN:N	5:E:123:ASN:ND2	2.63	0.44
5:E:2(B):THR:N	5:E:2(E):ASN:ND2	2.50	0.44
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.52	0.44
1:O:184:LEU:HB2	16:O:247:HOH:O	2.17	0.44
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.99	0.44
3:Q:159:SER:O	4:R:59:LEU:HD22	2.17	0.44
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.17	0.44
9:W:93:GLY:H	9:W:94:PRO:CD	2.29	0.44
9:W:178:ILE:HG23	9:W:184:VAL:HG22	1.99	0.44
10:X:140:HIS:CD2	10:X:141:HIS:NE2	2.85	0.44
1:A:24:ILE:HD11	1:A:124:THR:CG2	2.47	0.44
4:D:243:ALA:O	4:D:244:GLU:HB2	2.17	0.44
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.33	0.44
4:R:240:LYS:O	4:R:243:ALA:HB3	2.17	0.44
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.86	0.44
8:V:3:ILE:CD1	8:V:127:LEU:HB2	2.44	0.44
12:Z:-9:GLN:HE21	12:Z:-8:PHE:H	1.62	0.44
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.71	0.44
6:F:184:LEU:HD21	6:F:189:ALA:HA	1.99	0.44
9:I:93:GLY:H	9:I:94:PRO:CD	2.29	0.44
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.99	0.44
10:J:38:SER:HA	16:J:207:HOH:O	2.16	0.44
10:J:77:GLN:NE2	10:J:77:GLN:C	2.71	0.44
13:M:29:ASN:N	16:M:245:HOH:O	2.50	0.44
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.45	0.44
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.68	0.44
7:U:188:LYS:HD3	7:U:188:LYS:HA	1.84	0.44
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.52	0.44
4:D:198:LYS:HB2	4:D:207:LEU:HD13	1.99	0.44
4:D:211:GLN:HA	16:D:258:HOH:O	2.17	0.44
7:G:18(M):SER:HB2	7:G:187:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:4:MET:SD	1:O:5:THR:N	2.84	0.44
1:O:92:SER:O	1:O:95:VAL:HG12	2.17	0.44
4:R:91:HIS:CE1	4:R:119:LEU:HD21	2.51	0.44
4:R:140:GLY:HA2	4:R:215:ILE:HG12	1.99	0.44
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.17	0.44
9:W:18:LEU:CD2	9:W:32:GLU:HG2	2.47	0.44
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.52	0.44
10:X:193:GLN:OXT	10:X:193:GLN:HG2	2.17	0.44
1:A:27:ALA:O	1:A:31:VAL:HG23	2.16	0.44
3:C:55:THR:C	3:C:56:LEU:HD22	2.38	0.44
3:C:185:THR:CB	3:C:188:GLU:HG2	2.34	0.44
11:K:207:ASN:HD21	10:X:144:PRO:HG2	1.83	0.44
12:L:39:ASP:OD2	12:L:67:HIS:CE1	2.69	0.44
14:N:107:LYS:HG2	14:N:108:GLY:N	2.33	0.44
3:Q:35:THR:OG1	3:Q:66:LYS:NZ	2.49	0.44
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.18	0.44
6:T:63:LYS:O	6:T:65:VAL:N	2.50	0.44
9:W:113:PHE:CD2	9:W:113:PHE:N	2.85	0.44
14:2:107:LYS:HG2	14:2:108:GLY:N	2.33	0.44
1:A:62:GLU:CD	1:A:62:GLU:H	2.21	0.44
2:B:150:THR:O	2:B:157:TYR:HA	2.17	0.44
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.53	0.44
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.16	0.44
6:F:11:SER:HB3	6:F:14:VAL:CG2	2.47	0.44
6:F:35:THR:CG2	6:F:36:THR:N	2.79	0.44
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.47	0.44
9:I:80:THR:HG23	9:I:113:PHE:CZ	2.53	0.44
2:P:21:LEU:HD13	2:P:124:THR:HG23	2.00	0.44
2:P:87:ILE:O	2:P:91:THR:HG23	2.17	0.44
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.47	0.44
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.47	0.44
10:X:52:THR:HG22	10:X:53:VAL:HG23	1.99	0.44
11:Y:97:MET:O	11:Y:114:ASP:HA	2.17	0.44
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.83	0.44
11:K:87:VAL:CG1	11:K:115:SER:HA	2.48	0.44
13:M:70:ASN:ND2	13:M:70(A):ALA:HA	2.32	0.44
2:P:63:THR:HG22	2:P:63:THR:O	2.17	0.44
3:Q:33:ARG:O	3:Q:33:ARG:HG2	2.17	0.44
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.52	0.44
7:U:77:VAL:HG12	7:U:137:THR:HB	1.99	0.44
1:A:197:LEU:HD23	1:A:210:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.52	0.44
9:I:61:TYR:CD1	9:I:61:TYR:C	2.92	0.44
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.81	0.44
11:K:87:VAL:HG11	11:K:115:SER:HA	2.00	0.44
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.47	0.44
1:O:17:PRO:HA	2:P:26:TYR:CE1	2.53	0.44
6:T:11:SER:HB3	6:T:14:VAL:CG2	2.47	0.44
8:V:40:LYS:HE2	8:V:183:ASP:HA	2.00	0.44
9:W:6:MET:HE3	9:W:155:ILE:CG1	2.38	0.44
14:2:105:ASP:OD2	14:2:106:ASN:N	2.37	0.44
2:B:145:GLY:O	2:B:147:GLN:HG3	2.18	0.44
3:C:52:ARG:HB2	3:C:209:ASN:HA	2.00	0.44
3:Q:100:ARG:HH12	3:Q:106:PRO:HB3	1.75	0.44
7:U:139:VAL:HA	7:U:147:SER:O	2.18	0.44
1:A:109:THR:O	1:A:113:VAL:HG23	2.18	0.43
2:B:126:HIS:HA	16:B:260:HOH:O	2.18	0.43
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.18	0.43
8:H:200:LYS:HE3	9:I:140:SER:O	2.18	0.43
13:M:171:ARG:HG3	13:M:192:VAL:HB	1.98	0.43
5:S:97:ASN:HD22	5:S:97:ASN:HA	1.61	0.43
8:V:3:ILE:CG1	8:V:127:LEU:HB2	2.47	0.43
9:W:174:VAL:HG21	9:W:186:LYS:CE	2.48	0.43
10:X:190:PHE:C	10:X:192:ALA:H	2.22	0.43
1:A:4:MET:SD	1:A:5:THR:N	2.83	0.43
7:G:39:ALA:HA	7:G:47:VAL:O	2.18	0.43
10:J:90(A):ILE:HD12	10:J:90(A):ILE:HA	1.77	0.43
10:J:190:PHE:C	10:J:192:ALA:H	2.21	0.43
12:L:-9:GLN:HE21	12:L:-8:PHE:H	1.66	0.43
13:M:8:TYR:CZ	13:M:148:VAL:HG13	2.52	0.43
2:P:41:MET:HE3	16:Q:246:HOH:O	2.18	0.43
3:Q:150:GLN:HG2	3:Q:151:THR:N	2.32	0.43
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.48	0.43
8:V:200:LYS:HE3	9:W:140:SER:O	2.18	0.43
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.54	0.43
12:Z:120:GLU:OE1	12:Z:120:GLU:HA	2.18	0.43
13:1:112:TYR:C	13:1:112:TYR:CD2	2.90	0.43
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.98	0.43
4:D:101:LEU:CD1	11:K:57:THR:HG22	2.49	0.43
5:E:48:LEU:HB2	5:E:213:ALA:HB3	2.00	0.43
7:G:192:PHE:CD1	7:G:192:PHE:C	2.92	0.43
8:H:3:ILE:CG1	8:H:127:LEU:HB2	2.48	0.43

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.81	0.43
4:R:198:LYS:HB2	4:R:207:LEU:HD13	2.00	0.43
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.99	0.43
12:Z:-5:TYR:CD2	12:Z:96:TYR:HB2	2.53	0.43
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.17	0.43
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.53	0.43
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.99	0.43
11:K:86:LEU:C	11:K:86:LEU:HD13	2.39	0.43
12:L:90:LYS:HE2	16:M:254:HOH:O	2.19	0.43
1:O:57:PRO:HG2	7:U:177:GLU:HG2	2.01	0.43
1:O:112:LEU:O	1:O:116:VAL:HG23	2.18	0.43
1:O:197:LEU:HD23	1:O:210:ILE:HD12	1.99	0.43
2:P:202:THR:CG2	2:P:204:SER:HB2	2.48	0.43
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	2.00	0.43
4:R:59:LEU:C	4:R:59:LEU:HD13	2.39	0.43
6:T:45:GLY:HA3	6:T:215:CYS:O	2.18	0.43
13:1:46:SER:OG	13:1:98:ALA:HB3	2.18	0.43
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.18	0.43
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.42	0.43
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.33	0.43
13:M:-6:GLN:HG3	13:M:-6:GLN:O	2.17	0.43
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.00	0.43
2:P:122:GLY:C	2:P:124:THR:N	2.71	0.43
4:R:68:VAL:HG21	4:R:89:ILE:HD12	2.01	0.43
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.49	0.43
6:T:169:ARG:O	6:T:173:LYS:HG3	2.19	0.43
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.34	0.43
6:T:202:HIS:O	6:T:202:HIS:CG	2.71	0.43
6:T:203:GLU:C	6:T:205:ASN:H	2.22	0.43
7:U:18(M):SER:HB2	7:U:187:GLU:OE2	2.17	0.43
8:V:48:THR:HB	8:V:51:ASP:HB2	2.00	0.43
3:C:33:ARG:O	3:C:33:ARG:HG2	2.18	0.43
3:C:228:GLU:O	3:C:232:TYR:HD1	2.01	0.43
6:F:114:ASP:O	6:F:118:GLN:HG2	2.19	0.43
9:I:33:LYS:O	9:I:44:GLY:HA2	2.18	0.43
12:L:24:TYR:HA	8:V:167:LEU:HD12	2.01	0.43
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.99	0.43
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.53	0.43
7:U:31:THR:HG21	7:U:135:ILE:HG13	2.01	0.43
12:Z:58:ARG:NH2	16:Z:229:HOH:O	2.51	0.43
6:F:127:ASN:HD22	6:F:127:ASN:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:SER:O	8:H:39:PRO:C	2.57	0.43
9:I:137:MET:HE3	9:I:141:LEU:HD11	2.00	0.43
1:O:62:GLU:CD	1:O:62:GLU:H	2.22	0.43
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.49	0.43
7:U:192:PHE:CD1	7:U:192:PHE:C	2.91	0.43
3:C:70:ILE:O	10:J:68:ILE:HD13	2.19	0.43
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.53	0.43
5:E:29:GLU:HA	5:E:32:LYS:HE3	2.00	0.43
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.54	0.43
1:O:7:ARG:HD3	5:S:127:TYR:HD2	1.84	0.43
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.17	0.43
4:R:243:ALA:O	4:R:244:GLU:HB2	2.19	0.43
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.00	0.43
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.49	0.43
11:Y:76:VAL:N	11:Y:106:GLU:OE2	2.49	0.43
12:Z:6:ILE:HG12	12:Z:124:CYS:HB2	2.01	0.43
12:Z:99:THR:CG2	16:Z:201:HOH:O	2.65	0.43
3:C:241:GLN:C	3:C:243:GLN:H	2.23	0.43
5:E:52:LYS:HB3	5:E:63:TYR:HB3	2.01	0.43
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.49	0.43
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.19	0.43
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.54	0.43
10:J:18:LYS:HD3	10:J:174:ILE:HG13	2.00	0.43
10:J:124:TYR:CD2	10:J:138:LEU:HD13	2.54	0.43
2:P:27:ALA:O	2:P:30:SER:HB3	2.19	0.43
2:P:209:ARG:HB3	2:P:209:ARG:CZ	2.48	0.43
3:Q:241:GLN:C	3:Q:243:GLN:H	2.22	0.43
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	2.00	0.43
7:U:17(C):LYS:HB2	7:U:17(C):LYS:HE3	1.81	0.43
10:X:39:PRO:HG2	10:X:73:GLU:OE2	2.19	0.43
10:X:10(B):LYS:HB2	10:X:10(B):LYS:HZ2	1.84	0.43
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	2.00	0.43
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.48	0.43
14:2:163:ILE:HG23	14:2:170:GLY:HA2	2.00	0.43
2:B:122:GLY:C	2:B:124:THR:N	2.73	0.43
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.23	0.43
3:C:57:LYS:C	3:C:57:LYS:HD2	2.39	0.43
7:G:188:LYS:HA	7:G:188:LYS:HD3	1.84	0.43
9:I:29:ASN:ND2	9:I:29:ASN:H	2.16	0.43
11:K:205:SER:HB2	10:X:140:HIS:HA	2.00	0.43
12:L:6:ILE:HG12	12:L:124:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:114:PRO:HD2	14:N:118:SER:O	2.19	0.43
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.18	0.43
7:U:38:LEU:C	7:U:38:LEU:HD12	2.39	0.43
13:1:17:ASP:HA	13:1:173:PHE:HA	2.01	0.43
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.83	0.42
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ3	1.82	0.42
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.87	0.42
2:P:44:ASP:OD2	2:P:44:ASP:N	2.50	0.42
6:T:24:VAL:O	6:T:27:ALA:HB3	2.19	0.42
8:V:18:THR:HB	8:V:30:ASN:HA	2.01	0.42
9:W:29:ASN:ND2	9:W:29:ASN:H	2.17	0.42
11:Y:65:LEU:HD12	11:Y:65:LEU:HA	1.84	0.42
14:2:55:ILE:HD11	14:2:95:LEU:HD13	2.00	0.42
5:E:4:PHE:CD2	5:E:5:ARG:N	2.86	0.42
6:F:43:ASN:N	6:F:43:ASN:ND2	2.67	0.42
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.17	0.42
12:L:14(Q):LEU:O	12:L:14(W):LYS:C	2.58	0.42
4:R:194:LEU:HD12	4:R:194:LEU:HA	1.89	0.42
5:S:8:TYR:CE1	6:T:10:LEU:HD23	2.55	0.42
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.49	0.42
7:U:146:PRO:HD2	16:U:287:HOH:O	2.18	0.42
9:W:18:LEU:HD12	9:W:172:GLY:HA3	2.01	0.42
9:W:143:GLU:HG3	9:W:146:LEU:HD21	2.00	0.42
10:X:157:LEU:HD12	10:X:157:LEU:HA	1.91	0.42
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.18	0.42
6:F:127:ASN:HD22	6:F:127:ASN:C	2.19	0.42
9:I:113:PHE:N	9:I:113:PHE:CD2	2.86	0.42
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.54	0.42
10:J:39:PRO:HG2	10:J:73:GLU:OE2	2.18	0.42
13:M:110:LEU:HG	13:M:125:LEU:HD12	2.00	0.42
13:M:147:THR:HB	13:M:149:GLN:NE2	2.34	0.42
13:M:211:ILE:HD11	14:2:36:ARG:HD3	2.01	0.42
14:N:6:VAL:O	14:N:12:VAL:HG23	2.19	0.42
14:N:132:THR:O	14:2:133:PHE:HA	2.19	0.42
1:O:77:VAL:CG1	1:O:137:LEU:HB2	2.49	0.42
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.16	0.42
2:P:186:VAL:HG11	2:P:216:ARG:CD	2.49	0.42
5:S:29:GLU:HA	5:S:32:LYS:HE3	2.01	0.42
5:S:41:ARG:NH1	5:S:42:SER:O	2.52	0.42
8:V:148:LYS:HE3	8:V:177:VAL:HG11	2.02	0.42
9:W:20:LEU:HD13	9:W:20:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:THR:HG22	2:B:204:SER:N	2.11	0.42
8:H:18:THR:HB	8:H:30:ASN:HA	2.01	0.42
8:H:148:LYS:HE3	8:H:177:VAL:HG11	2.01	0.42
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.48	0.42
1:O:58:LEU:HA	1:O:58:LEU:HD23	1.81	0.42
9:W:80:THR:HG23	9:W:113:PHE:CZ	2.55	0.42
10:X:129:TYR:O	10:X:132:PHE:HB2	2.19	0.42
3:C:46:VAL:HG22	3:C:146:PRO:HB2	2.01	0.42
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.59	0.42
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.49	0.42
6:F:91:ARG:O	6:F:95:GLU:HB2	2.20	0.42
9:I:113:PHE:HA	9:I:118:CYS:O	2.19	0.42
11:K:33:LYS:HG2	11:K:45:MET:CE	2.49	0.42
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.09	0.42
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.49	0.42
1:O:77:VAL:HG12	1:O:137:LEU:HB2	2.00	0.42
6:T:43:ASN:N	6:T:43:ASN:ND2	2.66	0.42
6:T:52:LYS:HB2	6:T:209:GLU:O	2.19	0.42
8:V:89:LYS:HE3	8:V:90:TYR:CE2	2.55	0.42
13:1:130:GLY:O	13:1:134:ALA:HB3	2.20	0.42
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.48	0.42
4:D:14:THR:HG22	4:D:15:PHE:N	2.35	0.42
7:G:12:ILE:HG13	7:G:14:ILE:HG23	2.01	0.42
8:H:113:ILE:HG12	8:H:119:THR:HG22	2.00	0.42
11:K:99:THR:HG22	11:K:113:VAL:O	2.20	0.42
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.19	0.42
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.60	0.42
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.20	0.42
10:X:77:GLN:NE2	10:X:77:GLN:C	2.73	0.42
14:2:146:MET:HE3	14:2:150:GLU:HB3	2.02	0.42
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.84	0.42
3:C:71:ASP:HA	10:J:68:ILE:HD13	2.00	0.42
6:F:63:LYS:O	6:F:65:VAL:N	2.52	0.42
6:F:169:ARG:O	6:F:173:LYS:HG3	2.20	0.42
10:J:129:TYR:O	10:J:132:PHE:HB2	2.19	0.42
14:N:36:ARG:HD2	13:1:211:ILE:HD11	2.02	0.42
1:O:41:LYS:NZ	2:P:60:GLU:OE2	2.44	0.42
5:S:52:LYS:HB3	5:S:63:TYR:HB3	2.01	0.42
6:T:87:HIS:HD2	6:T:132:PHE:CE2	2.37	0.42
7:U:41:ARG:NH2	7:U:18(B):ASP:OD2	2.52	0.42
9:W:113:PHE:HA	9:W:118:CYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:171:ARG:HG3	13:1:192:VAL:HB	2.00	0.42
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.19	0.42
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.50	0.42
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.54	0.42
6:F:52:LYS:HB2	6:F:209:GLU:O	2.20	0.42
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.38	0.42
6:F:177:GLU:OE2	7:G:57:LYS:HE2	2.19	0.42
8:H:167:LEU:HD12	12:Z:24:TYR:HA	2.01	0.42
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.47	0.42
12:L:14:LEU:HD13	12:L:34:VAL:HG13	2.01	0.42
2:P:235:LYS:N	2:P:235:LYS:HD3	2.35	0.42
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.83	0.42
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.55	0.42
10:X:-1:MET:HG2	10:X:1:ASP:N	2.34	0.42
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	2.01	0.42
13:1:110:LEU:HG	13:1:125:LEU:HD12	2.01	0.42
13:1:198:ASP:OD1	13:1:201:LYS:NZ	2.49	0.42
5:E:7:ASN:HD22	5:E:7:ASN:HA	1.72	0.42
5:E:179:THR:HG22	5:E:179:THR:O	2.20	0.42
6:F:35:THR:CG2	6:F:51:GLU:O	2.62	0.42
7:G:172:ILE:HD13	7:G:197:MET:CE	2.50	0.42
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.01	0.42
12:L:120:GLU:HA	12:L:120:GLU:OE1	2.19	0.42
13:M:211:ILE:HD11	14:2:36:ARG:HD2	2.02	0.42
2:P:233:LEU:HD12	2:P:233:LEU:HA	1.92	0.42
4:R:14:THR:HG22	4:R:15:PHE:N	2.34	0.42
5:S:5:ARG:HG3	5:S:22:PHE:CE2	2.55	0.42
5:S:2(B):THR:N	5:S:2(E):ASN:ND2	2.51	0.42
6:T:157:TYR:CD1	6:T:157:TYR:C	2.93	0.42
13:1:133:MET:C	13:1:136:PRO:HD2	2.40	0.42
3:C:93:ARG:NH1	10:J:69:ARG:HA	2.35	0.42
1:O:205:GLU:OE2	1:O:205:GLU:HA	2.20	0.42
3:Q:214:VAL:HG23	3:Q:224:LEU:HD11	2.02	0.42
4:R:31:ILE:HD13	4:R:135:ALA:HB2	2.02	0.42
5:S:134:VAL:O	5:S:153:PRO:HG3	2.20	0.42
7:U:236:ILE:HD12	7:U:236:ILE:C	2.40	0.42
8:V:78:SER:O	8:V:82:MET:HG3	2.20	0.42
11:Y:2:THR:HG21	11:Y:162:ALA:CB	2.50	0.42
2:B:202:THR:CG2	2:B:204:SER:HB2	2.50	0.41
6:F:203:GLU:C	6:F:205:ASN:H	2.23	0.41
7:G:72:ARG:HG2	16:G:246:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:206:PHE:N	16:H:258:HOH:O	2.45	0.41
10:J:4:LEU:HD23	10:J:126:ALA:HB2	2.01	0.41
11:K:31:VAL:HG12	11:K:45:MET:HE1	2.02	0.41
12:L:113:PHE:CD1	12:L:113:PHE:N	2.87	0.41
13:M:130:GLY:O	13:M:134:ALA:HB3	2.20	0.41
1:O:33:GLN:CA	1:O:33:GLN:NE2	2.82	0.41
1:O:141:HIS:HA	1:O:146:GLY:O	2.20	0.41
2:P:235:LYS:C	2:P:237:GLY:H	2.23	0.41
3:Q:224:LEU:CD1	3:Q:224:LEU:H	2.33	0.41
1:A:33:GLN:CA	1:A:33:GLN:NE2	2.81	0.41
2:B:235:LYS:C	2:B:237:GLY:H	2.23	0.41
3:C:97:GLN:NE2	16:C:244:HOH:O	2.51	0.41
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.50	0.41
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.55	0.41
12:L:43:MET:CB	12:L:101:ILE:HG22	2.48	0.41
1:O:218:GLY:N	16:O:258:HOH:O	2.28	0.41
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.20	0.41
2:P:89:ILE:O	2:P:92:ALA:HB3	2.21	0.41
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.55	0.41
7:U:93:LYS:HD3	14:2:68:SER:HB3	2.01	0.41
7:U:107:MET:HA	7:U:108:PRO:HD3	1.91	0.41
8:V:144:GLN:HE21	8:V:144:GLN:HB2	1.64	0.41
12:Z:4:LEU:HD12	12:Z:5:GLY:N	2.35	0.41
13:1:133:MET:O	13:1:136:PRO:HD2	2.21	0.41
2:B:15:PHE:N	3:C:23:GLN:HE22	2.03	0.41
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.15	0.41
3:C:224:LEU:CD1	3:C:224:LEU:H	2.32	0.41
4:D:177:LEU:HD22	5:E:58:LEU:HD13	2.01	0.41
8:H:153:LYS:HD2	16:H:247:HOH:O	2.19	0.41
9:I:29:ASN:HD21	9:I:30:LYS:NZ	2.19	0.41
12:L:4:LEU:HD12	12:L:5:GLY:N	2.35	0.41
2:P:186:VAL:HG11	2:P:216:ARG:HD3	2.02	0.41
4:R:152:GLU:HB3	4:R:153:PRO:CD	2.50	0.41
6:T:114:ASP:O	6:T:118:GLN:HG2	2.19	0.41
6:T:127:ASN:HD22	6:T:127:ASN:N	2.17	0.41
9:W:84:SER:HB2	9:W:119:ILE:HD11	2.03	0.41
10:X:67:SER:O	10:X:71:ASP:N	2.54	0.41
14:2:156:LYS:HE3	16:2:229:HOH:O	2.19	0.41
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.55	0.41
6:F:45:GLY:HA3	6:F:215:CYS:O	2.20	0.41
7:G:13:THR:HB	7:G:124:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:12:ILE:HB	11:K:178:VAL:HB	2.03	0.41
11:K:207:ASN:ND2	10:X:144:PRO:HD3	2.36	0.41
13:M:1:THR:HG22	16:M:214:HOH:O	2.20	0.41
13:M:133:MET:C	13:M:136:PRO:HD2	2.41	0.41
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.88	0.41
14:2:44:CYS:HB2	14:2:100:ILE:HB	2.02	0.41
7:G:41:ARG:NH2	7:G:18(B):ASP:OD2	2.53	0.41
7:G:230:GLU:OE2	7:G:230:GLU:HA	2.19	0.41
9:I:18:LEU:HD12	9:I:172:GLY:HA3	2.02	0.41
10:J:67:SER:O	10:J:71:ASP:N	2.53	0.41
14:N:133:PHE:HA	14:2:132:THR:O	2.20	0.41
1:O:227:GLN:NE2	1:O:231:ASP:OD1	2.54	0.41
3:C:40:VAL:HG23	3:C:189:CYS:SG	2.61	0.41
9:I:174:VAL:HG21	9:I:186:LYS:CE	2.50	0.41
10:J:90(B):ARG:HG2	10:J:90(B):ARG:HH11	1.86	0.41
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.51	0.41
1:O:86:ARG:NE	7:U:118:ASN:ND2	2.58	0.41
5:S:15:PHE:H	6:T:23:GLN:NE2	2.12	0.41
7:U:35:ILE:HG23	7:U:51:GLN:HB2	2.03	0.41
3:C:65:SER:HB2	16:C:253:HOH:O	2.20	0.41
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.86	0.41
10:X:187:VAL:O	10:X:189:ASP:N	2.53	0.41
12:Z:-6:PRO:HG2	12:Z:-5:TYR:CD1	2.56	0.41
2:B:220:TYR:CE1	2:B:222:LYS:HB2	2.56	0.41
2:B:235:LYS:N	2:B:235:LYS:HD3	2.34	0.41
4:D:42:THR:C	4:D:44:GLU:H	2.24	0.41
6:F:24:VAL:O	6:F:27:ALA:HB3	2.20	0.41
9:I:29:ASN:HD21	9:I:30:LYS:HZ3	1.67	0.41
10:J:39:PRO:HG2	10:J:73:GLU:CD	2.41	0.41
12:L:114:ASP:HB2	12:L:118:SER:HB3	2.03	0.41
14:N:21:THR:HG22	14:N:26:ILE:HA	2.03	0.41
2:P:202:THR:HG22	2:P:203:ASP:N	2.36	0.41
4:R:237:LEU:O	4:R:241:GLU:HG3	2.21	0.41
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.36	0.41
3:C:214:VAL:HG23	3:C:224:LEU:HD11	2.03	0.41
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.86	0.41
6:F:18(E):GLU:CD	6:F:18(E):GLU:H	2.24	0.41
6:F:202:HIS:O	6:F:202:HIS:CG	2.73	0.41
8:H:34:LEU:HD22	8:H:174:ASP:HB3	2.01	0.41
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.09	0.41
10:J:93:ARG:HG2	10:J:93:ARG:HH11	1.86	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
10:J:157:LEU:HD12	10:J:157:LEU:HA	1.88	0.41
12:L:76:ILE:HG23	12:L:77:ASN:N	2.36	0.41
12:L:160:THR:O	12:L:164:GLU:HG2	2.20	0.41
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.20	0.41
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.21	0.41
5:S:7:ASN:HD22	5:S:7:ASN:HA	1.73	0.41
8:V:148:LYS:O	8:V:152:ILE:HG13	2.20	0.41
4:D:152:GLU:HB3	4:D:153:PRO:CD	2.51	0.41
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.36	0.41
7:G:35:ILE:HG23	7:G:51:GLN:HB2	2.02	0.41
9:I:20:LEU:C	9:I:20:LEU:HD13	2.42	0.41
9:I:84:SER:HB2	9:I:119:ILE:HD11	2.03	0.41
10:J:166:MET:HA	10:J:167:PRO:HD3	1.82	0.41
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.56	0.41
1:O:57:PRO:HG3	7:U:177:GLU:OE1	2.21	0.41
2:P:52:ARG:NH2	2:P:63(A):SER:HB3	2.36	0.41
3:Q:40:VAL:HG23	3:Q:189:CYS:SG	2.61	0.41
3:Q:57:LYS:HD2	3:Q:57:LYS:C	2.41	0.41
4:R:117:CYS:HB3	4:R:155:GLY:O	2.21	0.41
6:T:35:THR:HG23	6:T:36:THR:N	2.36	0.41
6:T:127:ASN:C	6:T:127:ASN:ND2	2.75	0.41
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.86	0.41
9:W:33:LYS:O	9:W:44:GLY:HA2	2.21	0.41
10:X:104:TYR:CD1	10:X:180:LYS:HA	2.56	0.41
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.51	0.41
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.56	0.41
14:2:21:THR:HG22	14:2:26:ILE:HA	2.03	0.41
3:C:227:GLU:O	3:C:231:GLN:HG3	2.21	0.40
4:D:186:LEU:O	4:D:190:GLU:HG3	2.22	0.40
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.57	0.40
10:J:-1:MET:HG2	10:J:1:ASP:N	2.35	0.40
10:J:112:GLN:HE22	10:J:126:ALA:H	1.69	0.40
10:J:140:HIS:CD2	10:J:141:HIS:NE2	2.89	0.40
10:J:144:PRO:HG2	11:Y:207:ASN:HD21	1.86	0.40
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.22	0.40
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.19	0.40
3:Q:112:LEU:O	3:Q:112:LEU:HD13	2.21	0.40
3:Q:227:GLU:O	3:Q:231:GLN:HG3	2.21	0.40
10:X:133:TYR:CZ	10:X:166:MET:HG3	2.55	0.40
11:Y:81:LYS:HA	11:Y:84:SER:HB3	2.02	0.40
12:Z:105:ASP:OD2	12:Z:107:LYS:HB2	2.20	0.40

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
13:1:147:THR:HB	13:1:149:GLN:NE2	2.36	0.40
1:A:7:ARG:NH1	5:E:127:TYR:CD2	2.90	0.40
2:B:44:ASP:OD2	2:B:44:ASP:N	2.52	0.40
2:B:113:VAL:HG22	2:B:138:TYR:CD2	2.57	0.40
2:B:233:LEU:HD12	2:B:233:LEU:HA	1.92	0.40
5:E:41:ARG:NH1	5:E:42:SER:O	2.54	0.40
7:G:31:THR:HG21	7:G:135:ILE:HG13	2.02	0.40
7:G:18(H):GLU:CD	7:G:18(H):GLU:H	2.23	0.40
8:H:34:LEU:HB2	16:H:245:HOH:O	2.21	0.40
9:I:105:ASN:HB3	9:I:10(C):SER:OG	2.22	0.40
3:Q:44:ASN:O	3:Q:45:CYS:HB3	2.21	0.40
3:Q:201:VAL:HG21	3:Q:210:ILE:HG12	2.03	0.40
7:U:225:SER:O	7:U:229:ILE:HG13	2.22	0.40
9:W:29:ASN:HD21	9:W:30:LYS:NZ	2.19	0.40
1:A:67:VAL:HG11	1:A:213:ALA:HB2	2.02	0.40
2:B:90:ASN:HB2	16:B:262:HOH:O	2.20	0.40
2:B:186:VAL:HG11	2:B:216:ARG:CD	2.51	0.40
8:H:30:ASN:O	8:H:189:ARG:NH2	2.53	0.40
8:H:32:ALA:HB2	8:H:189:ARG:NH1	2.36	0.40
9:I:93:GLY:N	9:I:94:PRO:HD3	2.36	0.40
13:M:1:THR:OG1	13:M:2:SER:N	2.45	0.40
13:M:12:VAL:CG2	13:M:102:ALA:HB1	2.51	0.40
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.65	0.40
1:O:13:THR:O	2:P:130:ARG:HD3	2.22	0.40
7:U:18(H):GLU:H	7:U:18(H):GLU:CD	2.24	0.40
7:U:203:THR:HG22	7:U:204:GLU:O	2.21	0.40
10:X:65:LEU:HD21	10:X:69:ARG:NH2	2.36	0.40
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.22	0.40
11:Y:12:ILE:HB	11:Y:178:VAL:HB	2.02	0.40
12:Z:90:LYS:CE	16:Z:196:HOH:O	2.70	0.40
1:A:205:GLU:HA	1:A:205:GLU:OE2	2.21	0.40
7:G:80:GLY:HA3	7:G:134:VAL:HG12	2.03	0.40
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.52	0.40
10:X:143:ARG:HA	10:X:144:PRO:HD3	1.95	0.40
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.90	0.40
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.22	0.40
12:Z:14(Q):LEU:O	12:Z:14(W):LYS:C	2.59	0.40
2:B:67:LEU:HD23	2:B:213:ALA:HB2	2.03	0.40
3:C:46:VAL:HG11	3:C:139:ALA:HB1	2.03	0.40
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.57	0.40
5:E:40:LEU:HD23	5:E:40:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:157:TYR:CD1	6:F:157:TYR:C	2.94	0.40
8:H:17:ASP:HA	8:H:172:ASN:O	2.22	0.40
10:J:133:TYR:CZ	10:J:166:MET:HG3	2.56	0.40
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.56	0.40
13:M:14(C):ARG:CG	13:M:14(C):ARG:NH1	2.84	0.40
1:O:46:VAL:HG12	1:O:47:VAL:N	2.36	0.40
1:O:67:VAL:HG11	1:O:213:ALA:HB3	2.03	0.40
3:Q:238:GLN:O	3:Q:242:GLU:HG3	2.21	0.40
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.84	0.40
5:S:46:ALA:HB1	5:S:139:ILE:HB	2.04	0.40
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	231 (93%)	15 (6%)	2 (1%)	19	47
1	O	248/250 (99%)	231 (93%)	15 (6%)	2 (1%)	19	47
2	B	242/244 (99%)	221 (91%)	18 (7%)	3 (1%)	13	37
2	P	242/244 (99%)	220 (91%)	19 (8%)	3 (1%)	13	37
3	C	239/241 (99%)	216 (90%)	19 (8%)	4 (2%)	9	27
3	Q	239/241 (99%)	216 (90%)	19 (8%)	4 (2%)	9	27
4	D	240/242 (99%)	219 (91%)	16 (7%)	5 (2%)	7	22
4	R	240/242 (99%)	219 (91%)	16 (7%)	5 (2%)	7	22
5	E	231/233 (99%)	211 (91%)	17 (7%)	3 (1%)	12	34
5	S	231/233 (99%)	211 (91%)	17 (7%)	3 (1%)	12	34
6	F	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	19	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	19	47
7	G	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	34	64
7	U	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	34	64
8	H	220/222 (99%)	205 (93%)	15 (7%)	0	100	100
8	V	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	29	59
9	I	202/204 (99%)	193 (96%)	7 (4%)	2 (1%)	15	42
9	W	202/204 (99%)	192 (95%)	8 (4%)	2 (1%)	15	42
10	J	196/198 (99%)	185 (94%)	8 (4%)	3 (2%)	10	31
10	X	196/198 (99%)	183 (93%)	10 (5%)	3 (2%)	10	31
11	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
11	Y	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
12	L	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
12	Z	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
13	1	231/233 (99%)	217 (94%)	13 (6%)	1 (0%)	34	64
13	M	231/233 (99%)	215 (93%)	15 (6%)	1 (0%)	34	64
14	2	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
14	N	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
All	All	6312/6368 (99%)	5895 (93%)	364 (6%)	53 (1%)	19	47

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
3	C	58	LEU
4	D	12(G)	GLU
10	J	192	ALA
1	O	5	THR
3	Q	58	LEU
4	R	12(G)	GLU
10	X	192	ALA
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
4	D	128	MET

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Mol	Chain	Res	Type
5	E	202	ARG
6	F	205	ASN
6	F	206	LYS
9	I	93	GLY
10	J	188	ASP
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	128	MET
5	S	202	ARG
6	T	205	ASN
6	T	206	LYS
9	W	93	GLY
10	X	188	ASP
3	C	179	ASN
4	D	12(C)	GLY
4	D	18(D)	SER
5	E	5	ARG
5	E	217	LYS
7	G	220	LYS
3	Q	179	ASN
4	R	12(C)	GLY
4	R	18(D)	SER
5	S	217	LYS
7	U	220	LYS
5	S	5	ARG
4	D	12(F)	GLY
9	I	23	GLN
4	R	12(F)	GLY
9	W	23	GLN
1	A	167	LYS
13	M	72	ALA
1	O	167	LYS
10	X	8	VAL
13	1	72	ALA
10	J	8	VAL
8	V	96	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	205 (98%)	4 (2%)	57	84
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	84
2	B	203/203 (100%)	194 (96%)	9 (4%)	28	60
2	P	203/203 (100%)	194 (96%)	9 (4%)	28	60
3	C	213/213 (100%)	203 (95%)	10 (5%)	26	57
3	Q	213/213 (100%)	203 (95%)	10 (5%)	26	57
4	D	198/198 (100%)	188 (95%)	10 (5%)	24	54
4	R	198/198 (100%)	188 (95%)	10 (5%)	24	54
5	E	192/192 (100%)	172 (90%)	20 (10%)	7	20
5	S	192/192 (100%)	172 (90%)	20 (10%)	7	20
6	F	201/201 (100%)	185 (92%)	16 (8%)	12	32
6	T	201/201 (100%)	185 (92%)	16 (8%)	12	32
7	G	207/207 (100%)	196 (95%)	11 (5%)	22	52
7	U	207/207 (100%)	196 (95%)	11 (5%)	22	52
8	H	181/181 (100%)	174 (96%)	7 (4%)	32	64
8	V	181/181 (100%)	174 (96%)	7 (4%)	32	64
9	I	172/172 (100%)	166 (96%)	6 (4%)	36	68
9	W	172/172 (100%)	166 (96%)	6 (4%)	36	68
10	J	175/175 (100%)	170 (97%)	5 (3%)	42	74
10	X	175/175 (100%)	170 (97%)	5 (3%)	42	74
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	73
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	73
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	43
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17	43
13	1	199/199 (100%)	189 (95%)	10 (5%)	24	55
13	M	199/199 (100%)	189 (95%)	10 (5%)	24	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2	162/162 (100%)	156 (96%)	6 (4%)	34	66
14	N	162/162 (100%)	156 (96%)	6 (4%)	34	66
All	All	5332/5332 (100%)	5070 (95%)	262 (5%)	25	55

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	134	VAL
1	A	158	PHE
1	A	179	ARG
2	B	58	LEU
2	B	71	ASN
2	B	116	LEU
2	B	121	GLN
2	B	150	THR
2	B	185	LYS
2	B	192	LEU
2	B	212	PHE
2	B	218	ASN
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	61	THR
3	C	66	LYS
3	C	121	GLN
3	C	150	GLN
3	C	174	GLU
3	C	178	LYS
3	C	208	LYS
4	D	28	LEU
4	D	76	CYS
4	D	126	ARG
4	D	14(A)	ASP
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	244	GLU
5	E	11	ASP

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Mol	Chain	Res	Type
5	E	12	THR
5	E	13	VAL
5	E	32	LYS
5	E	56	ASP
5	E	57	GLU
5	E	64	GLN
5	E	76	LEU
5	E	78	LEU
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	2(C)	VAL
5	E	2(E)	ASN
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	18	ASP
6	F	35	THR
6	F	43	ASN
6	F	56	SER
6	F	95	GLU
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	169	ARG
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
7	G	33	GLN
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	169	GLN
7	G	184	ASN

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Mol	Chain	Res	Type
7	G	197	MET
7	G	232	ARG
7	G	233	LEU
7	G	240	ASP
8	H	13	VAL
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	61	TYR
9	I	113	PHE
9	I	160	LEU
9	I	171	TRP
9	I	192	ARG
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	121	GLU
10	J	155	LEU
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	104	TYR
11	K	138	LEU
12	L	-7	ASN
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	70(A)	ASN
12	L	98	HIS
12	L	99	THR
12	L	112	SER
12	L	120	GLU
12	L	138	LEU
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG

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Mol	Chain	Res	Type
13	M	112	TYR
13	M	129	PHE
13	M	140	LYS
13	M	14(C)	ARG
13	M	148	VAL
13	M	149	GLN
13	M	204	LYS
14	N	84	LYS
14	N	89	GLU
14	N	10(A)	ASP
14	N	119	VAL
14	N	149	GLU
14	N	18(I)	GLN
1	O	33	GLN
1	O	134	VAL
1	O	158	PHE
1	O	179	ARG
2	P	58	LEU
2	P	71	ASN
2	P	116	LEU
2	P	121	GLN
2	P	150	THR
2	P	185	LYS
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	61	THR
3	Q	66	LYS
3	Q	121	GLN
3	Q	150	GLN
3	Q	174	GLU
3	Q	178	LYS
3	Q	208	LYS
4	R	28	LEU
4	R	76	CYS
4	R	126	ARG
4	R	14(A)	ASP
4	R	170	GLU
4	R	177	LEU

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Mol	Chain	Res	Type
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	244	GLU
5	S	11	ASP
5	S	12	THR
5	S	13	VAL
5	S	32	LYS
5	S	56	ASP
5	S	57	GLU
5	S	64	GLN
5	S	76	LEU
5	S	78	LEU
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	2(C)	VAL
5	S	2(E)	ASN
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	18	ASP
6	T	35	THR
6	T	43	ASN
6	T	56	SER
6	T	95	GLU
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	169	ARG
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
7	U	33	GLN
7	U	72	ARG

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Mol	Chain	Res	Type
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	232	ARG
7	U	233	LEU
7	U	240	ASP
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	144	GLN
8	V	197	ARG
9	W	29	ASN
9	W	61	TYR
9	W	113	PHE
9	W	160	LEU
9	W	171	TRP
9	W	192	ARG
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
10	X	155	LEU
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	104	TYR
11	Y	138	LEU
12	Z	-7	ASN
12	Z	14	LEU
12	Z	25	SER
12	Z	40	ASN
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	112	SER
12	Z	120	GLU

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Mol	Chain	Res	Type
12	Z	138	LEU
12	Z	145	TYR
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	140	LYS
13	1	14(C)	ARG
13	1	148	VAL
13	1	149	GLN
13	1	204	LYS
14	2	84	LYS
14	2	89	GLU
14	2	10(A)	ASP
14	2	119	VAL
14	2	149	GLU
14	2	18(I)	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (199) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	227	GLN
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	238	GLN

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Mol	Chain	Res	Type
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	161	ASN
4	D	211	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	156	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	87	HIS
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	11	HIS
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	18(C)	HIS
7	G	184	ASN
8	H	30	ASN
8	H	66	HIS
8	H	114	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN

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Mol	Chain	Res	Type
8	H	190	ASN
9	I	29	ASN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	186	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	85	HIS
12	L	98	HIS
12	L	1(I)	ASN
12	L	166	HIS
13	M	-7	GLN
13	M	10	ASN
13	M	18	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	191	GLN
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	227	GLN
2	P	23	GLN
2	P	71	ASN

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Mol	Chain	Res	Type
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	161	ASN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	87	HIS
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN

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Mol	Chain	Res	Type
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	18(C)	HIS
7	U	184	ASN
8	V	30	ASN
8	V	66	HIS
8	V	91	GLN
8	V	114	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	85	HIS
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	18	ASN

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Mol	Chain	Res	Type
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	191	GLN
14	2	69	GLN
14	2	141	ASN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	SLR	Y	301	11	11,15,16	2.86	2 (18%)	11,23,25	2.16	4 (36%)
15	SLR	K	301	11	11,15,16	2.84	2 (18%)	11,23,25	2.14	4 (36%)

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	SLR	Y	301	11	-	3/12/32/35	0/1/1/1
15	SLR	K	301	11	-	3/12/32/35	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	301	SLR	C13-C11	7.19	1.59	1.53
15	K	301	SLR	C13-C11	6.93	1.59	1.53
15	Y	301	SLR	O7-C6	-5.44	1.24	1.42
15	K	301	SLR	O7-C6	-5.39	1.24	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	K	301	SLR	O7-C6-C5	3.86	121.41	111.37
15	Y	301	SLR	C9-C2-C1	-3.82	112.51	116.54
15	Y	301	SLR	O7-C6-C5	3.65	120.87	111.37
15	K	301	SLR	C9-C2-C1	-3.53	112.82	116.54
15	Y	301	SLR	O12-C11-C13	-2.79	103.92	109.90
15	K	301	SLR	O12-C11-C13	-2.75	104.00	109.90
15	K	301	SLR	O10-C3-C2	-2.54	124.16	126.17
15	Y	301	SLR	O10-C3-C2	-2.52	124.17	126.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	K	301	SLR	C1-C5-C6-O7
15	K	301	SLR	N4-C5-C6-O7
15	K	301	SLR	C11-C5-C6-O7
15	Y	301	SLR	C1-C5-C6-O7
15	Y	301	SLR	N4-C5-C6-O7
15	Y	301	SLR	C11-C5-C6-O7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.28	7 (2%)	53	43	27, 43, 74, 104	0
1	O	250/250 (100%)	-0.11	15 (6%)	21	14	31, 52, 78, 101	0
2	B	244/244 (100%)	-0.10	11 (4%)	33	23	29, 49, 82, 111	0
2	P	244/244 (100%)	-0.00	15 (6%)	21	13	29, 51, 87, 113	0
3	C	241/241 (100%)	0.06	15 (6%)	20	13	31, 54, 102, 119	0
3	Q	241/241 (100%)	0.25	20 (8%)	11	6	37, 57, 105, 120	0
4	D	242/242 (100%)	-0.01	13 (5%)	25	17	35, 51, 84, 116	0
4	R	242/242 (100%)	0.07	14 (5%)	23	15	36, 55, 89, 116	0
5	E	233/233 (100%)	-0.22	5 (2%)	63	54	34, 51, 77, 103	0
5	S	233/233 (100%)	-0.23	8 (3%)	45	35	33, 51, 79, 105	0
6	F	244/244 (100%)	-0.28	8 (3%)	46	36	30, 44, 86, 106	0
6	T	244/244 (100%)	-0.39	3 (1%)	79	73	26, 43, 82, 103	0
7	G	243/243 (100%)	-0.34	5 (2%)	63	54	23, 39, 68, 112	0
7	U	243/243 (100%)	-0.29	5 (2%)	63	54	27, 42, 69, 113	0
8	H	222/222 (100%)	-0.47	3 (1%)	75	69	25, 40, 58, 89	0
8	V	222/222 (100%)	-0.42	3 (1%)	75	69	33, 43, 60, 96	0
9	I	204/204 (100%)	-0.55	2 (0%)	82	77	28, 41, 59, 77	0
9	W	204/204 (100%)	-0.55	4 (1%)	65	56	30, 42, 61, 78	0
10	J	198/198 (100%)	-0.33	4 (2%)	65	56	30, 44, 61, 118	0
10	X	198/198 (100%)	-0.29	4 (2%)	65	56	28, 45, 62, 120	0
11	K	212/212 (100%)	-0.40	2 (0%)	84	80	28, 43, 61, 69	0
11	Y	212/212 (100%)	-0.47	1 (0%)	91	88	27, 44, 63, 72	0
12	L	222/222 (100%)	-0.38	4 (1%)	68	61	26, 43, 65, 86	0
12	Z	222/222 (100%)	-0.41	4 (1%)	68	61	28, 42, 68, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/233 (100%)	-0.54	1 (0%) 92 91	24, 38, 53, 60	0
13	M	233/233 (100%)	-0.52	1 (0%) 92 91	25, 39, 54, 61	0
14	2	196/196 (100%)	-0.53	2 (1%) 82 77	23, 37, 56, 77	0
14	N	196/196 (100%)	-0.54	0 100 100	26, 36, 57, 74	0
All	All	6368/6368 (100%)	-0.28	179 (2%) 53 43	23, 45, 78, 120	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	U	240	ASP	11.4
4	R	12(D)	ALA	10.5
4	D	12(E)	SER	10.1
4	R	12(E)	SER	9.9
3	C	55	THR	9.1
4	D	12(D)	ALA	8.7
10	X	192	ALA	8.5
3	Q	55	THR	8.1
7	G	240	ASP	7.4
6	F	5	GLY	6.8
2	P	217	ALA	6.6
4	D	12(F)	GLY	6.6
4	R	12(C)	GLY	6.5
4	D	12(C)	GLY	6.4
2	P	218	ASN	6.4
7	G	6	ALA	6.4
10	J	192	ALA	6.2
10	X	191	GLN	6.2
10	X	193	GLN	6.1
2	B	217	ALA	5.9
4	R	12(F)	GLY	5.9
2	P	21(C)	ASP	5.8
7	U	6	ALA	5.7
2	B	218	ASN	5.6
13	1	-8	THR	5.3
10	J	191	GLN	5.2
4	R	127	LEU	5.2
8	V	223	ASP	5.0
3	Q	56	LEU	5.0
1	O	5	THR	5.0
1	A	4	MET	5.0
2	P	54	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
3	Q	203	THR	4.9
1	O	4	MET	4.8
1	A	5	THR	4.8
2	B	54	VAL	4.7
3	C	56	LEU	4.7
4	R	126	ARG	4.5
2	P	219	GLU	4.3
3	Q	242	GLU	4.3
3	Q	63	THR	4.2
4	D	12(G)	GLU	4.2
5	S	203	ASP	4.1
5	E	203	ASP	4.1
2	B	21(B)	GLY	4.1
3	Q	243	GLN	4.0
12	L	145	TYR	4.0
4	R	9	ASP	4.0
8	H	222	CYS	3.9
4	D	126	ARG	3.9
9	I	-8	SER	3.9
5	S	4	PHE	3.9
12	Z	14(W)	LYS	3.9
3	C	241	GLN	3.8
13	M	-8	THR	3.7
14	2	18(I)	GLN	3.6
4	D	244	GLU	3.6
2	P	21(B)	GLY	3.6
1	O	56	SER	3.6
7	G	8	TYR	3.5
3	C	203	THR	3.5
8	H	223	ASP	3.5
10	J	193	GLN	3.5
12	L	14(P)	PRO	3.4
6	F	206	LYS	3.4
6	F	241	ASN	3.4
12	L	14(W)	LYS	3.4
3	C	14(A)	ARG	3.3
4	R	12(G)	GLU	3.3
9	W	-8	SER	3.3
2	B	219	GLU	3.3
1	O	55	SER	3.3
10	J	188	ASP	3.3
1	O	235	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	239	THR	3.2
7	U	239	GLN	3.2
12	Z	145	TYR	3.2
5	S	5	ARG	3.2
3	C	33	ARG	3.2
3	C	240	LYS	3.2
6	F	6	THR	3.2
7	G	239	GLN	3.1
5	E	204	GLU	3.1
6	F	20(B)	GLU	3.1
1	A	203	GLU	3.1
5	S	233	ILE	3.1
2	P	21(A)	LYS	3.1
4	R	125	GLU	3.1
4	R	244	GLU	3.1
2	P	62	ASP	3.1
9	W	12(A)	LYS	3.0
6	T	241	ASN	3.0
3	Q	18(D)	GLU	3.0
7	U	17(E)	LYS	3.0
3	Q	240	LYS	3.0
1	O	21(P)	LYS	3.0
3	Q	54	SER	3.0
1	O	53	LYS	2.9
4	D	125	GLU	2.9
10	X	189	ASP	2.9
3	Q	236	ILE	2.8
2	P	4	GLY	2.8
3	Q	208	LYS	2.8
3	Q	241	GLN	2.8
11	Y	10(A)	ARG	2.8
3	Q	238	GLN	2.8
2	B	21(C)	ASP	2.8
3	C	243	GLN	2.8
8	V	220	ASN	2.8
3	Q	187	GLU	2.7
6	F	240	ILE	2.7
4	R	243	ALA	2.7
2	B	21(A)	LYS	2.7
8	V	222	CYS	2.7
9	W	181	LYS	2.7
3	Q	14(A)	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	127	LEU	2.7
6	F	204	ASP	2.7
6	T	240	ILE	2.7
3	Q	178	LYS	2.7
4	D	9	ASP	2.6
5	S	204	GLU	2.6
7	G	7	GLY	2.6
4	R	12(B)	GLU	2.5
5	E	5	ARG	2.5
3	C	230	ASN	2.5
3	Q	170	LYS	2.5
2	P	239	THR	2.5
5	S	178	ARG	2.5
2	P	63	THR	2.5
2	P	220	TYR	2.5
1	O	57	PRO	2.4
3	C	237	GLU	2.4
8	H	220	ASN	2.4
4	D	55	THR	2.4
7	U	218	ASP	2.4
3	C	53	ARG	2.4
1	O	178	LYS	2.3
3	C	18(C)	LYS	2.3
1	O	54	SER	2.3
14	2	18(J)	LEU	2.3
2	P	21(D)	GLY	2.3
1	A	21(P)	LYS	2.3
5	E	217	LYS	2.3
2	P	20(A)	SER	2.3
5	S	127	TYR	2.3
11	K	211	GLY	2.3
4	D	218	GLN	2.2
1	A	21(N)	THR	2.2
4	R	167	SER	2.2
6	F	18(D)	PRO	2.2
11	K	143	LYS	2.2
4	D	18(D)	SER	2.2
1	O	183	GLU	2.2
2	B	20(A)	SER	2.2
3	C	143	PRO	2.2
5	E	178	ARG	2.2
1	A	21(E)	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	236	LEU	2.1
9	I	182	ASP	2.1
9	W	182	ASP	2.1
2	P	53	LYS	2.1
2	B	21(D)	GLY	2.1
1	O	21(E)	ASP	2.1
3	Q	57	LYS	2.1
12	Z	14(K)	LYS	2.1
1	O	21(M)	PRO	2.1
6	T	6	THR	2.1
12	Z	70(A)	ASN	2.1
1	A	202	VAL	2.1
3	Q	64	PRO	2.1
5	S	217	LYS	2.1
2	B	63(A)	SER	2.0
3	Q	14(B)	ASP	2.0
3	C	18(D)	GLU	2.0
3	C	235	GLN	2.0
1	O	65	SER	2.0
4	R	240	LYS	2.0
12	L	70(A)	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SLR	Y	301	15/16	0.94	0.19	46,48,49,51	0
15	SLR	K	301	15/16	0.95	0.19	42,42,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.