



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 3DY4 / pdb_00003dy4
Title : Crystal structure of yeast 20S proteasome in complex with spirolactacystin
Authors : Groll, M.; Balskus, E.; Jacobsen, E.
Deposited on : 2008-07-25
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

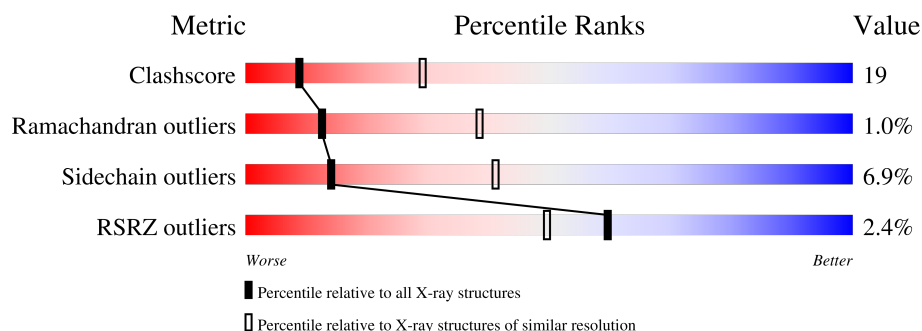
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3% 66% 30% .
1	O	250	4% 64% 33% .
2	B	244	6% 55% 41% .
2	P	244	7% 56% 39% 5%
3	C	241	5% 55% 39% 5%
3	Q	241	8% 57% 37% 5%

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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 50588 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

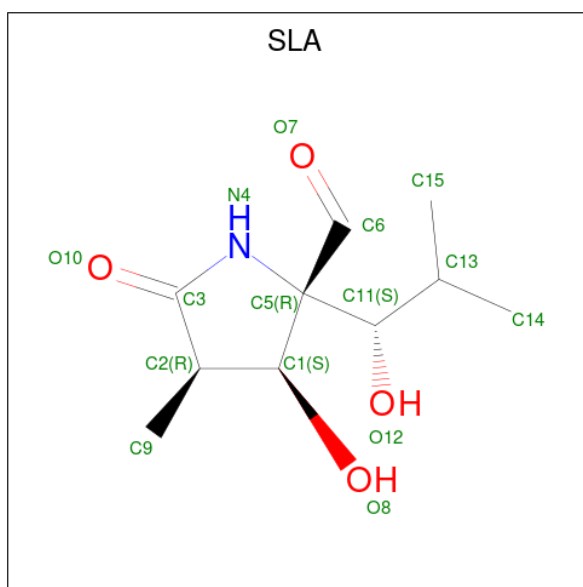
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is Omuralide, open form (CCD ID: SLA) (formula: C₁₀H₁₇NO₄).



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

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	38	Total	O	0	0
			38	38		
16	B	26	Total	O	0	0
			26	26		
16	C	30	Total	O	0	0
			30	30		
16	D	28	Total	O	0	0
			28	28		
16	E	17	Total	O	0	0
			17	17		
16	F	41	Total	O	0	0
			41	41		
16	G	45	Total	O	0	0
			45	45		
16	H	36	Total	O	0	0
			36	36		

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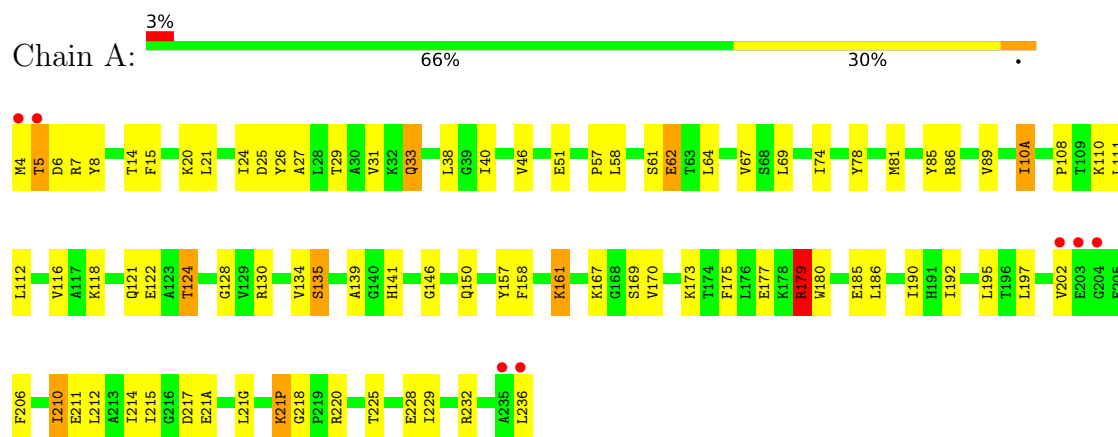
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	I	48	Total 48	O 48	0	0
16	J	33	Total 33	O 33	0	0
16	K	27	Total 27	O 27	0	0
16	L	41	Total 41	O 41	0	0
16	M	54	Total 54	O 54	0	0
16	N	45	Total 45	O 45	0	0
16	O	25	Total 25	O 25	0	0
16	P	19	Total 19	O 19	0	0
16	Q	18	Total 18	O 18	0	0
16	R	21	Total 21	O 21	0	0
16	S	15	Total 15	O 15	0	0
16	T	30	Total 30	O 30	0	0
16	U	50	Total 50	O 50	0	0
16	V	36	Total 36	O 36	0	0
16	W	46	Total 46	O 46	0	0
16	X	36	Total 36	O 36	0	0
16	Y	26	Total 26	O 26	0	0
16	Z	34	Total 34	O 34	0	0
16	1	58	Total 58	O 58	0	0
16	2	57	Total 57	O 57	0	0

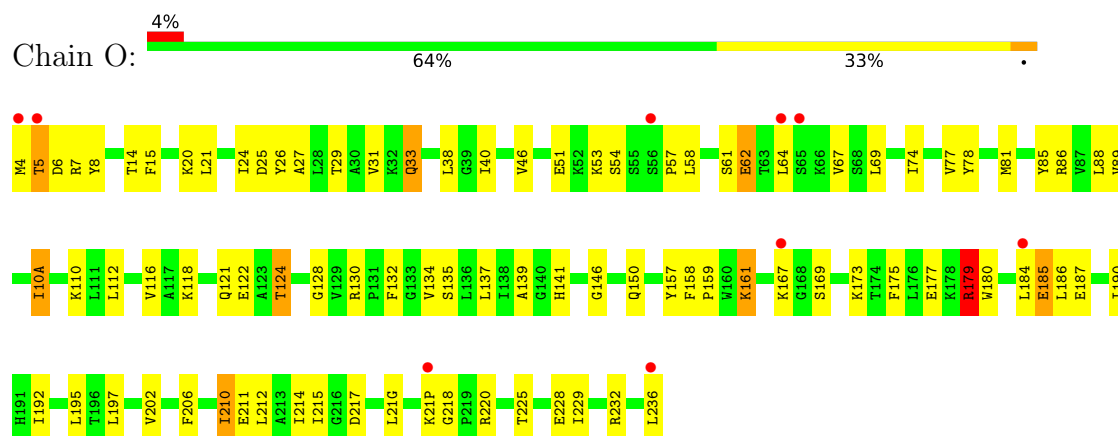
3 Residue-property plots [i](#)

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

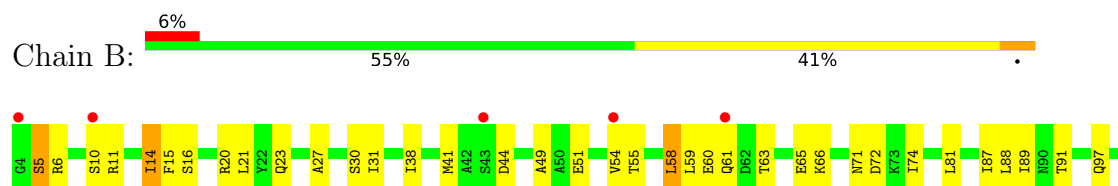
• Molecule 1: Proteasome component Y7

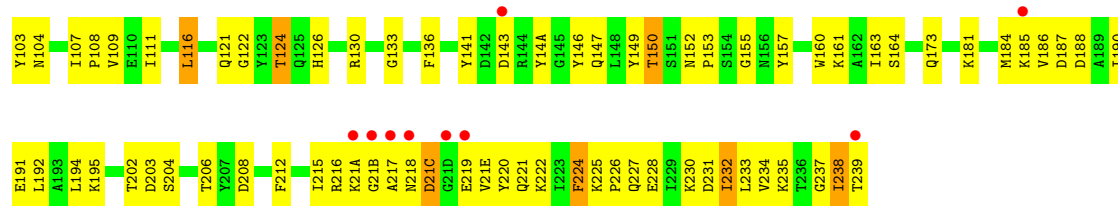


• Molecule 1: Proteasome component Y7

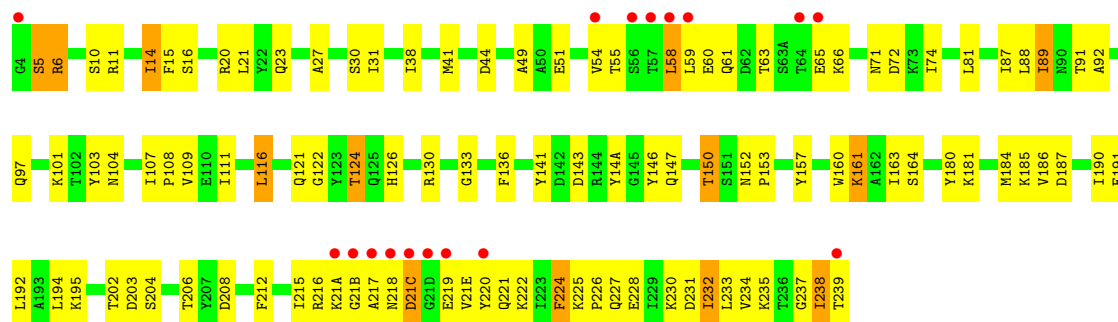


• Molecule 2: Proteasome component Y13

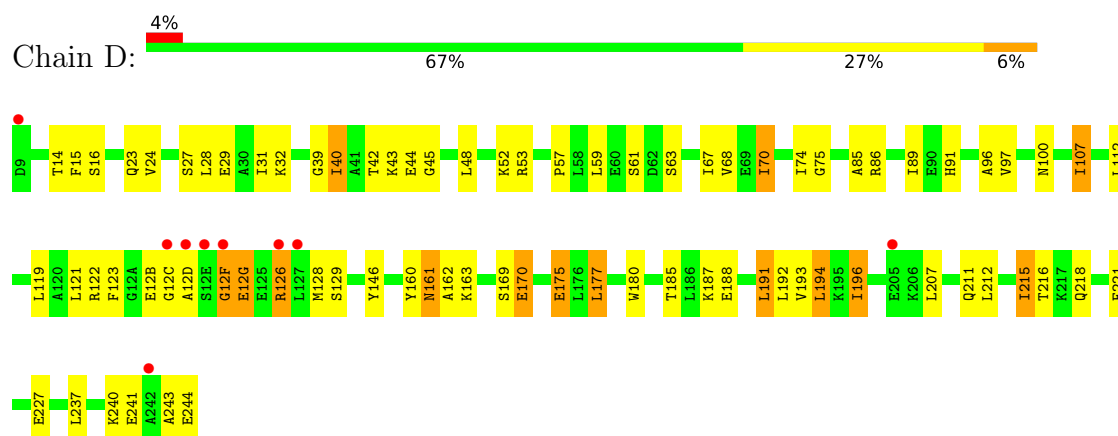




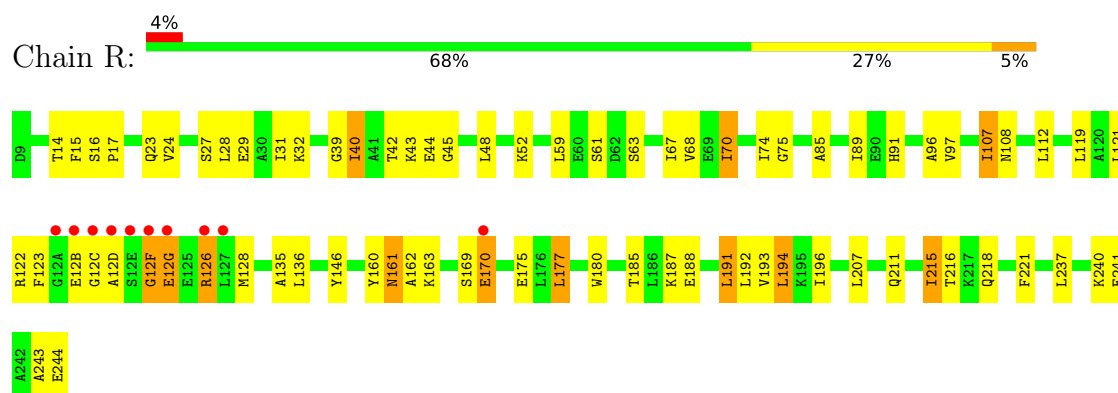
• Molecule 2: Proteasome component Y13



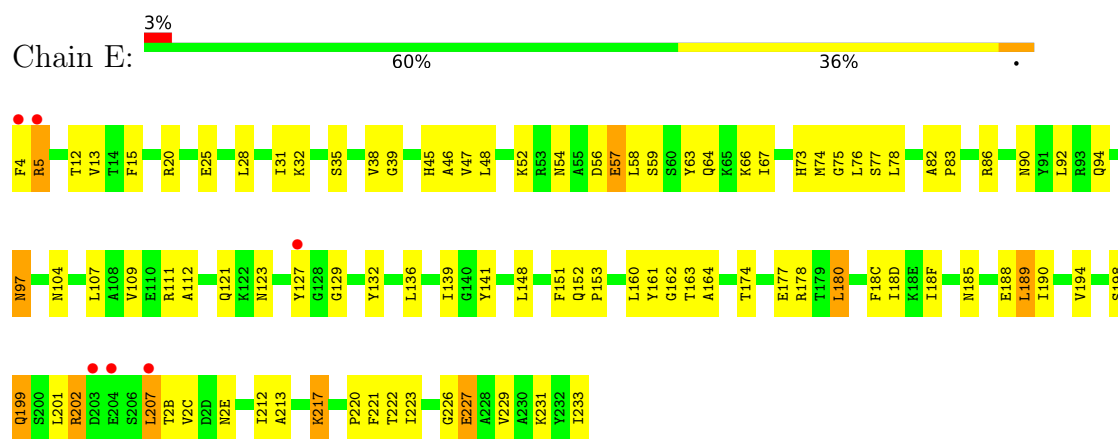
- Molecule 4: Proteasome component PUP2



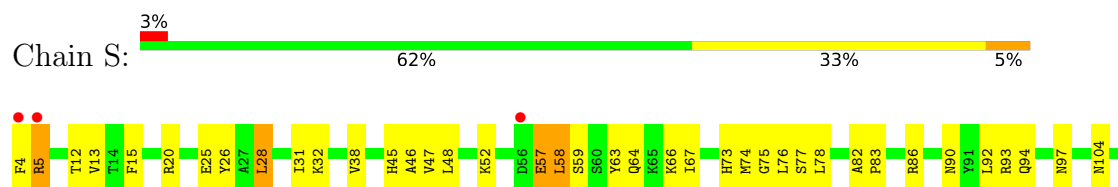
- Molecule 4: Proteasome component PUP2

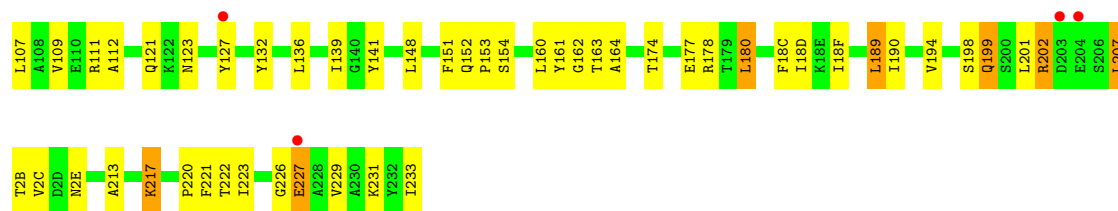


- Molecule 5: Proteasome component PRE5

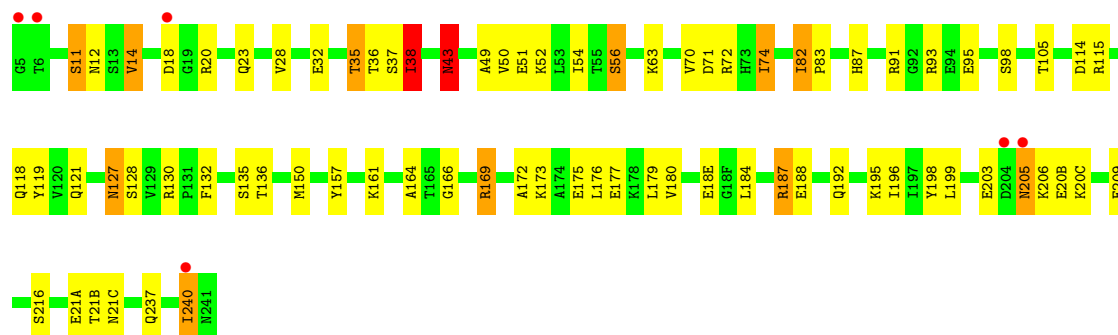


- Molecule 5: Proteasome component PRE5

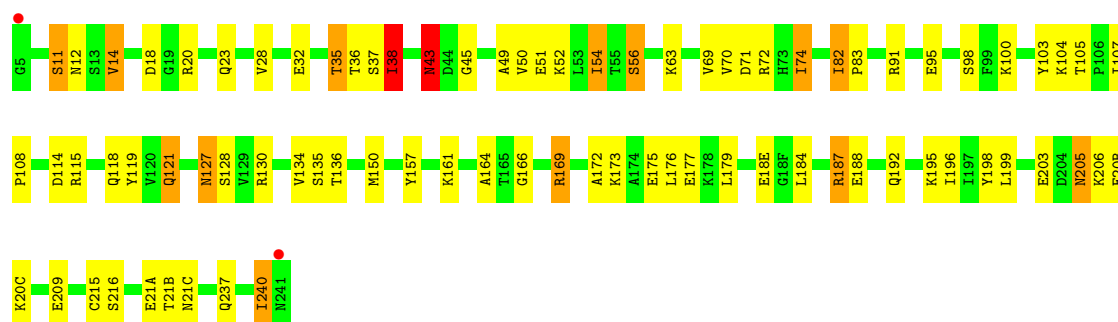




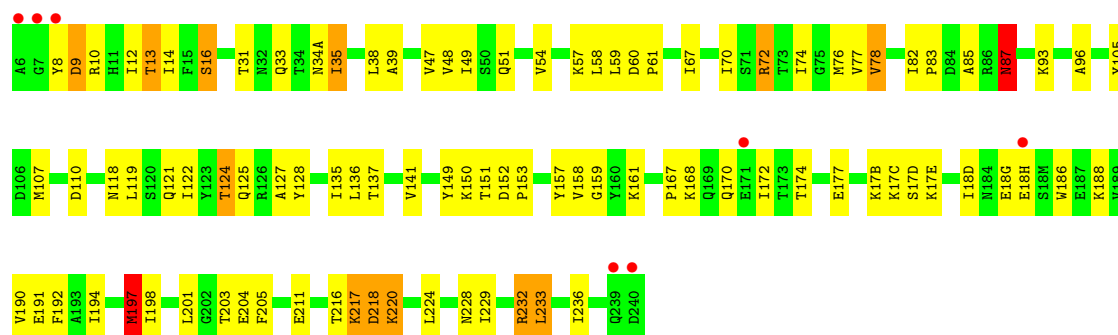
● Molecule 6: Proteasome component C1



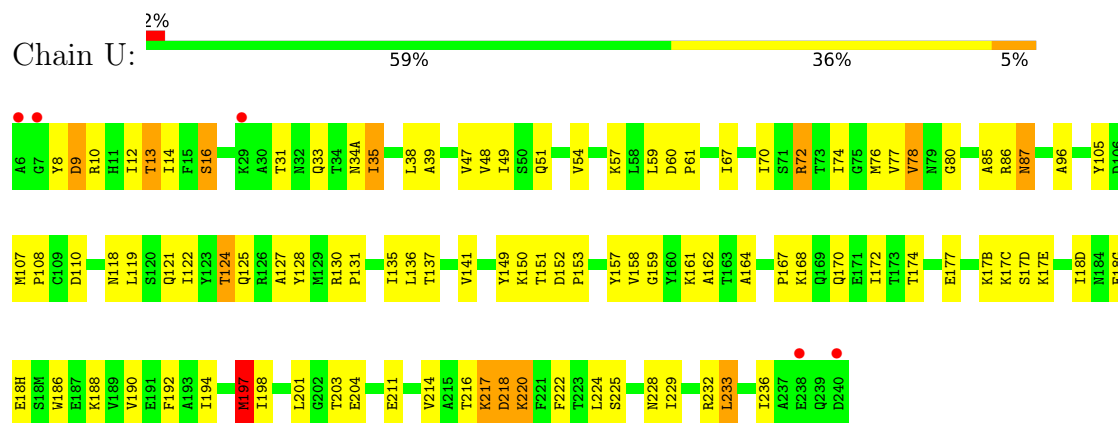
● Molecule 6: Proteasome component C1



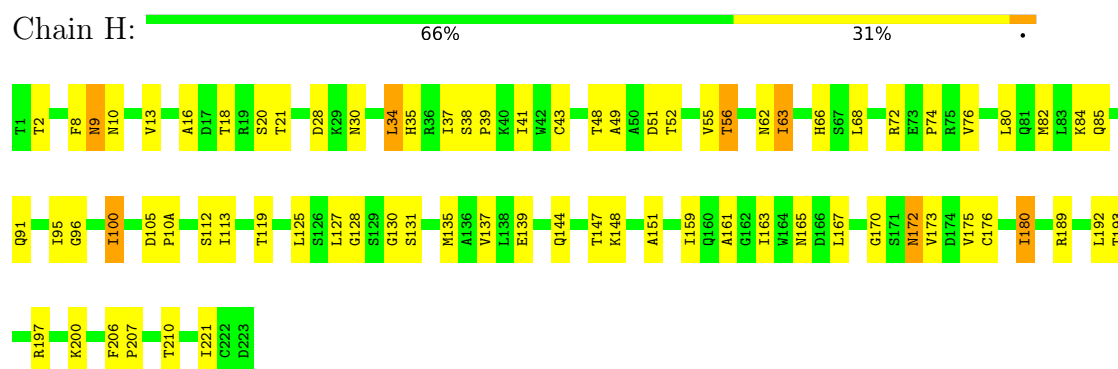
● Molecule 7: Proteasome component C7-alpha



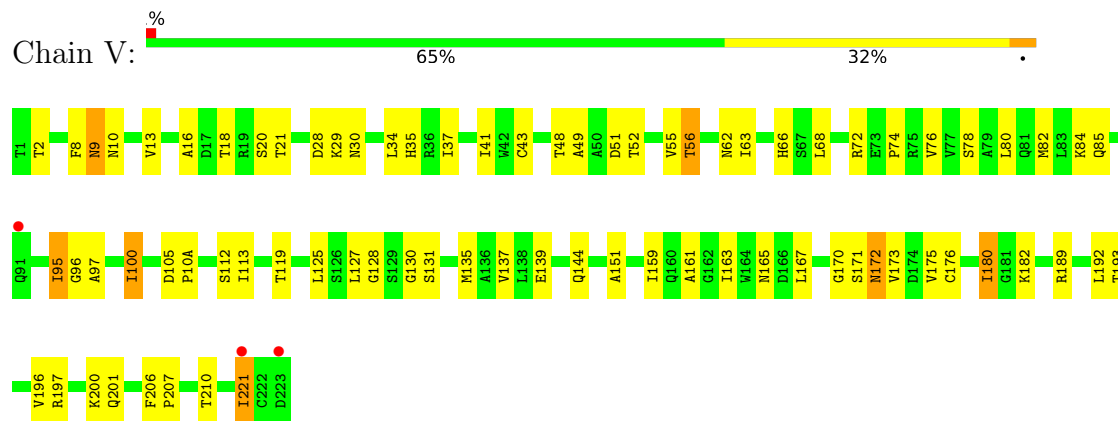
- Molecule 7: Proteasome component C7-alpha



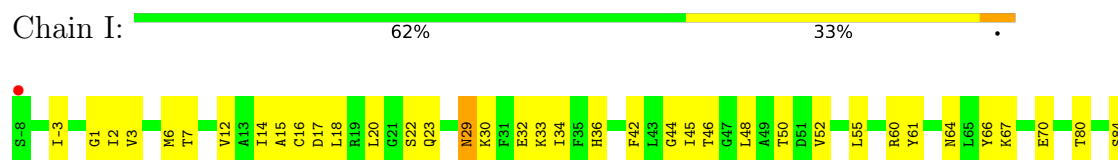
- Molecule 8: Proteasome component PUP1

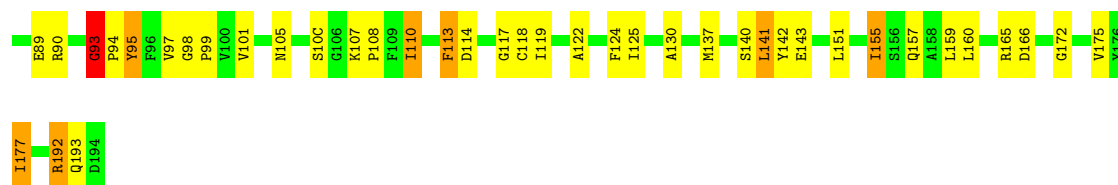


- Molecule 8: Proteasome component PUP1

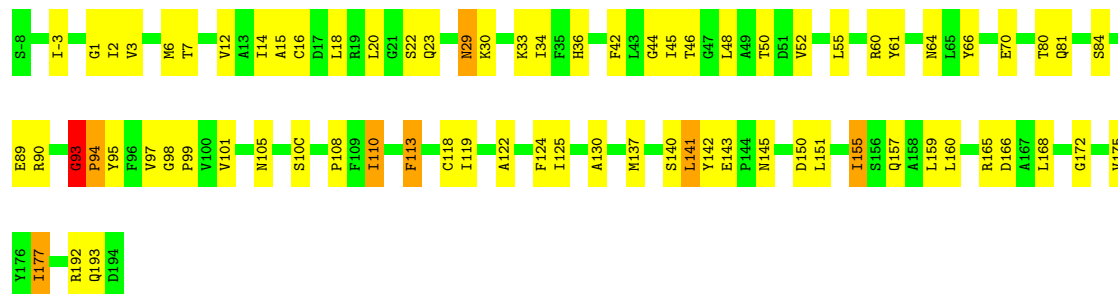


- Molecule 9: Proteasome component PUP3

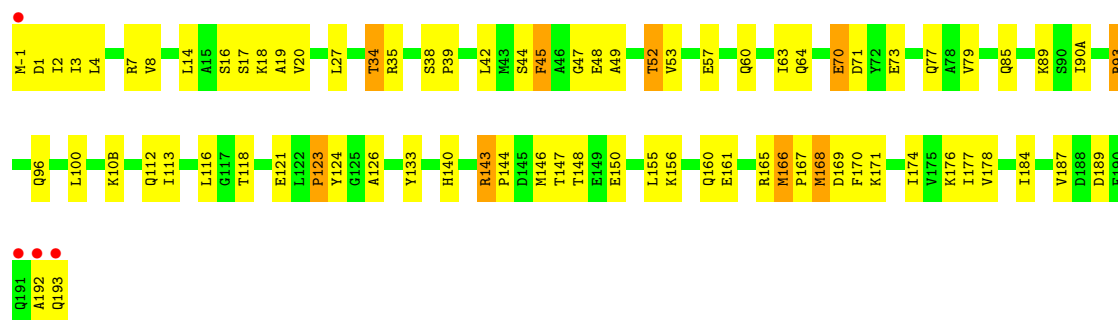




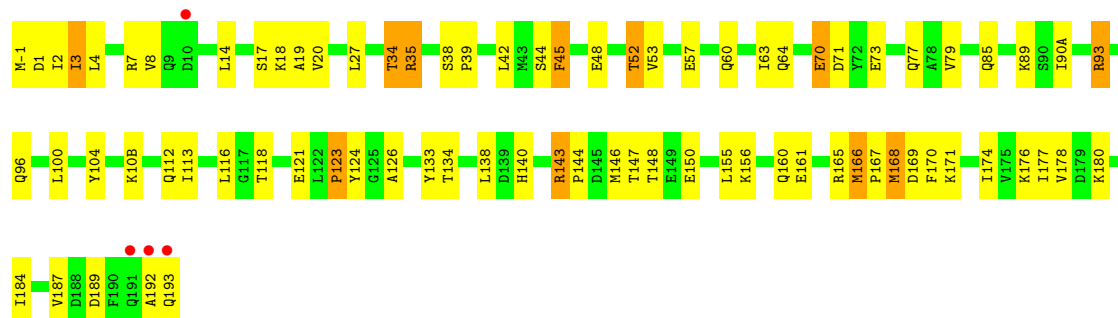
• Molecule 9: Proteasome component PUP3



• Molecule 10: Proteasome component C11

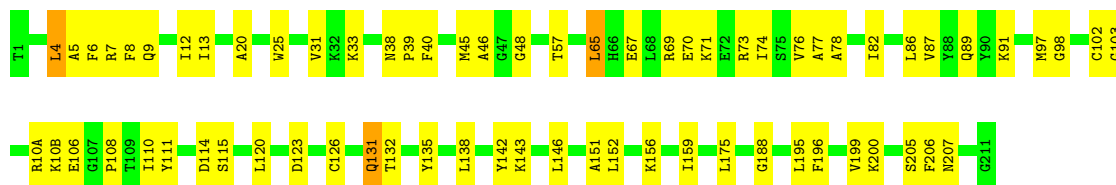


• Molecule 10: Proteasome component C11



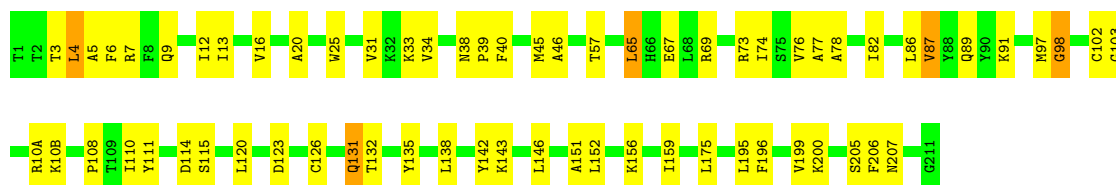
• Molecule 11: Proteasome component PRE2

Chain K:  67% 31% .



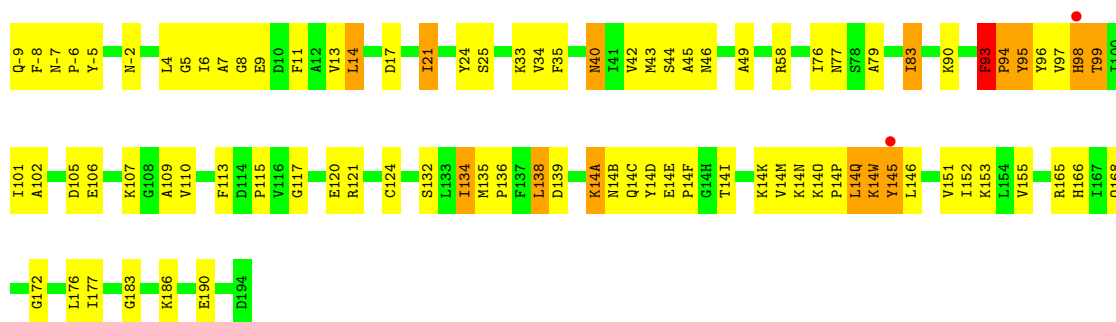
• Molecule 11: Proteasome component PRE2

Chain Y:  69% 29% .



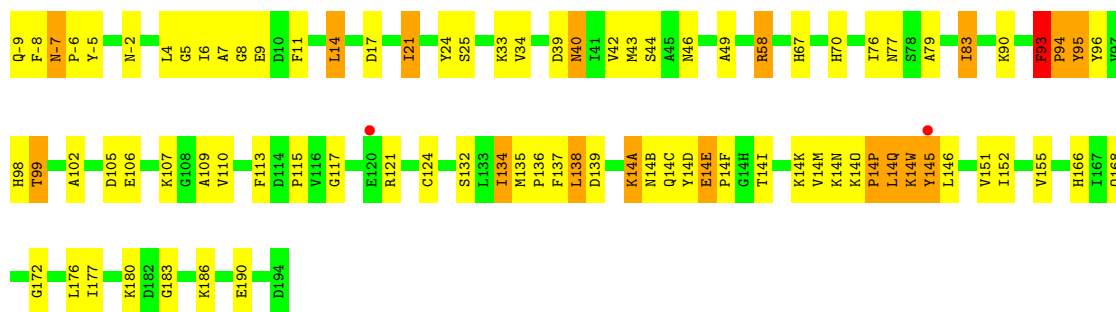
• Molecule 12: Proteasome component C5

Chain L:  % 59% 34% 6% .



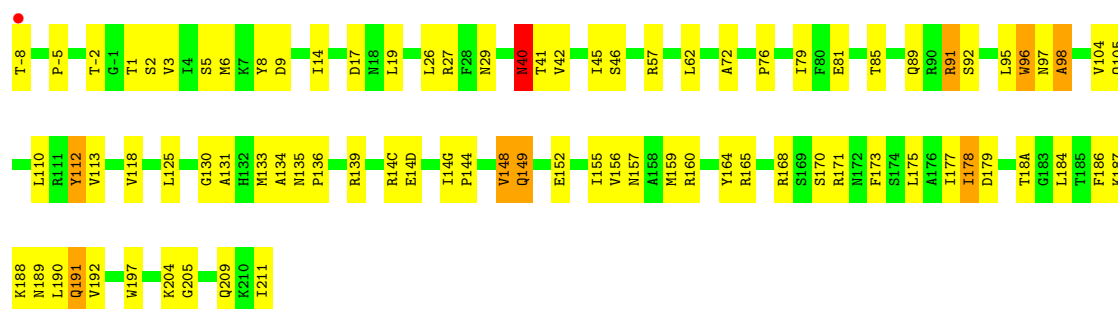
• Molecule 12: Proteasome component C5

Chain Z:  % 61% 31% 8% .

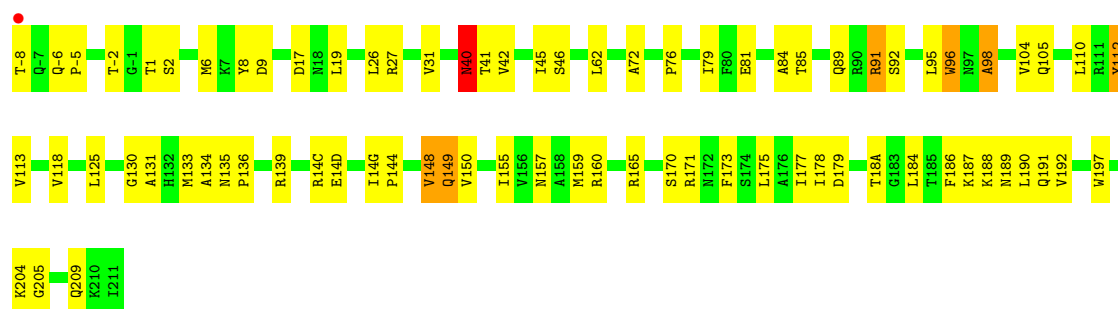


• Molecule 13: Proteasome component PRE4

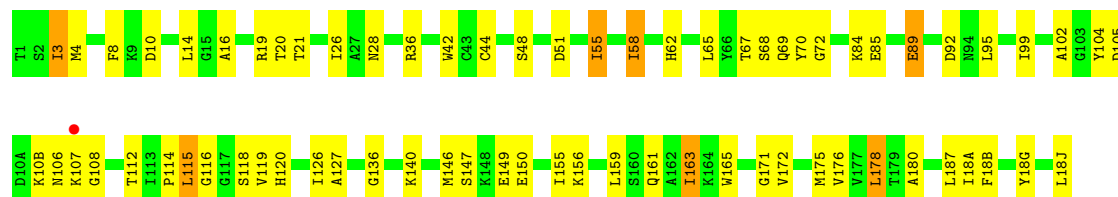
Chain M:  64% 33% .



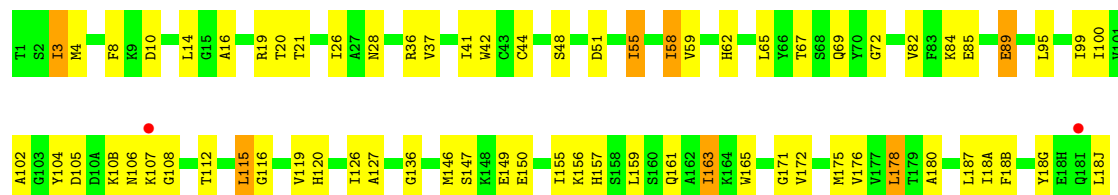
• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.16Å 301.97Å 144.05Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.80) 97.2 (15.00-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.256 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50588	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/1952	0.94	8/2642 (0.3%)
1	O	0.43	0/1952	0.94	8/2642 (0.3%)
2	B	0.45	0/1935	0.95	7/2618 (0.3%)
2	P	0.47	0/1935	0.95	5/2618 (0.2%)
3	C	0.42	0/1920	0.89	4/2598 (0.2%)
3	Q	0.41	0/1920	0.89	4/2598 (0.2%)
4	D	0.44	0/1887	0.91	8/2541 (0.3%)
4	R	0.43	0/1887	0.91	7/2541 (0.3%)
5	E	0.42	0/1823	0.92	4/2463 (0.2%)
5	S	0.42	0/1823	0.92	6/2463 (0.2%)
6	F	0.44	0/1937	0.98	9/2614 (0.3%)
6	T	0.45	0/1937	0.98	11/2614 (0.4%)
7	G	0.49	0/1959	1.00	13/2652 (0.5%)
7	U	0.48	0/1959	1.00	14/2652 (0.5%)
8	H	0.48	0/1716	0.94	4/2326 (0.2%)
8	V	0.45	0/1716	0.94	5/2326 (0.2%)
9	I	0.45	0/1611	1.01	11/2174 (0.5%)
9	W	0.47	0/1611	1.02	11/2174 (0.5%)
10	J	0.46	0/1613	0.99	10/2173 (0.5%)
10	X	0.47	0/1613	1.00	11/2173 (0.5%)
11	K	0.46	0/1681	0.94	4/2274 (0.2%)
11	Y	0.45	0/1681	0.93	4/2274 (0.2%)
12	L	0.46	0/1795	1.02	10/2420 (0.4%)
12	Z	0.45	0/1795	1.03	9/2420 (0.4%)
13	1	0.48	0/1855	0.98	9/2514 (0.4%)
13	M	0.47	0/1855	0.98	10/2514 (0.4%)
14	2	0.49	0/1541	0.94	2/2087 (0.1%)
14	N	0.51	0/1541	0.95	2/2087 (0.1%)
All	All	0.46	0/50450	0.96	210/68192 (0.3%)

There are no bond length outliers.

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	27	ARG	N-CA-C	10.87	122.70	111.07
13	1	27	ARG	N-CA-C	10.72	122.55	111.07
12	Z	93	PHE	CA-C-N	9.22	129.06	120.21
12	Z	93	PHE	C-N-CA	9.22	129.06	120.21
4	D	70	ILE	N-CA-C	-8.94	103.14	111.45
4	R	70	ILE	N-CA-C	-8.63	103.42	111.45
6	T	12	ASN	N-CA-C	8.31	120.42	111.36
6	F	12	ASN	N-CA-C	8.18	120.27	111.36
2	P	238	ILE	N-CA-C	-8.14	105.25	113.47
7	G	16	SER	N-CA-C	-8.12	99.77	110.40
2	B	238	ILE	N-CA-C	-7.95	105.45	113.47
12	L	93	PHE	CA-C-N	7.92	128.98	120.11
12	L	93	PHE	C-N-CA	7.92	128.98	120.11
7	U	16	SER	N-CA-C	-7.58	100.47	110.40
1	O	161	LYS	N-CA-C	-7.47	102.07	112.45
1	A	161	LYS	N-CA-C	-7.46	102.08	112.45
11	Y	57	THR	N-CA-C	-7.42	103.28	111.36
1	A	128	GLY	N-CA-C	7.40	124.28	113.48
3	Q	161	SER	N-CA-C	-7.36	102.95	112.23
6	T	161	LYS	N-CA-C	-7.35	102.23	112.45
11	K	57	THR	N-CA-C	-7.29	103.41	111.36
9	W	143	GLU	CA-C-N	7.28	127.31	119.89
9	W	143	GLU	C-N-CA	7.28	127.31	119.89
3	C	161	SER	N-CA-C	-7.26	103.09	112.23
5	E	57	GLU	N-CA-C	-7.21	103.63	113.30
1	O	128	GLY	N-CA-C	7.21	124.01	113.48
12	L	117	GLY	N-CA-C	7.20	123.44	114.37
6	F	161	LYS	N-CA-C	-7.04	102.66	112.45
13	1	98	ALA	N-CA-C	-7.04	97.43	108.90
10	J	123	PRO	N-CA-C	-6.94	104.10	113.40
4	R	161	ASN	N-CA-C	-6.94	103.81	112.90
9	I	143	GLU	CA-C-N	6.93	126.96	119.89
9	I	143	GLU	C-N-CA	6.93	126.96	119.89
9	I	98	GLY	CA-C-N	6.93	126.91	119.78
9	I	98	GLY	C-N-CA	6.93	126.91	119.78
6	F	63	LYS	N-CA-C	6.89	121.93	112.90
6	F	135	SER	N-CA-C	-6.87	98.53	109.59
7	G	161	LYS	N-CA-C	-6.84	103.28	111.69
7	G	54	VAL	CA-C-N	6.83	126.29	118.85
7	G	54	VAL	C-N-CA	6.83	126.29	118.85
2	B	203	ASP	N-CA-C	-6.81	104.97	113.28
5	S	57	GLU	N-CA-C	-6.81	104.18	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	108	THR	N-CA-C	-6.80	101.37	110.55
6	T	14	VAL	N-CA-C	6.79	118.36	108.58
13	1	95	LEU	N-CA-C	-6.75	96.66	108.20
9	W	60	ARG	N-CA-C	-6.74	103.86	111.14
13	1	9	ASP	N-CA-C	6.71	119.45	111.33
3	C	70	ILE	N-CA-C	-6.70	106.05	111.81
12	L	115	PRO	N-CA-C	-6.70	105.49	113.86
13	M	9	ASP	N-CA-C	6.69	119.42	111.33
13	M	98	ALA	N-CA-C	-6.67	98.03	108.90
9	W	98	GLY	CA-C-N	6.66	126.64	119.78
9	W	98	GLY	C-N-CA	6.66	126.64	119.78
2	P	203	ASP	N-CA-C	-6.65	105.17	113.28
6	T	63	LYS	N-CA-C	6.64	121.60	112.90
6	F	14	VAL	N-CA-C	6.64	118.14	108.58
4	D	161	ASN	N-CA-C	-6.63	104.21	112.90
3	Q	108	THR	N-CA-C	-6.63	101.60	110.55
13	M	-2	THR	N-CA-C	6.56	119.87	109.50
13	M	95	LEU	N-CA-C	-6.49	97.11	108.20
6	T	135	SER	N-CA-C	-6.47	99.18	109.59
9	W	93	GLY	CA-C-N	6.45	126.42	120.03
9	W	93	GLY	C-N-CA	6.45	126.42	120.03
12	Z	115	PRO	N-CA-C	-6.43	105.83	113.86
7	U	161	LYS	N-CA-C	-6.41	103.81	111.69
8	H	180	ILE	N-CA-C	6.38	117.89	110.62
10	X	123	PRO	N-CA-C	-6.38	104.86	113.40
7	U	54	VAL	CA-C-N	6.37	125.79	118.85
7	U	54	VAL	C-N-CA	6.37	125.79	118.85
9	I	142	TYR	N-CA-C	6.33	118.96	110.35
12	Z	117	GLY	N-CA-C	6.32	122.33	114.37
9	I	93	GLY	CA-C-N	6.30	126.27	120.03
9	I	93	GLY	C-N-CA	6.30	126.27	120.03
9	W	142	TYR	N-CA-C	6.29	118.90	110.35
1	A	185	GLU	N-CA-C	-6.25	100.74	110.42
1	O	185	GLU	N-CA-C	-6.16	100.87	110.42
7	G	9	ASP	N-CA-C	-6.14	105.85	113.15
13	1	-2	THR	N-CA-C	6.13	119.19	109.50
7	U	127	ALA	N-CA-C	6.13	118.93	111.82
12	Z	49	ALA	N-CA-C	6.11	118.72	111.33
3	Q	70	ILE	N-CA-C	-6.11	105.87	111.67
2	B	161	LYS	N-CA-C	-6.11	103.96	112.45
2	P	161	LYS	N-CA-C	-6.09	103.99	112.45
9	I	60	ARG	N-CA-C	-6.06	104.60	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	16	SER	N-CA-C	-6.04	103.18	110.13
6	T	38	ILE	N-CA-C	6.04	117.41	108.65
6	F	38	ILE	N-CA-C	5.99	117.33	108.65
13	M	189	ASN	N-CA-C	5.98	120.16	112.86
6	F	71	ASP	CB-CA-C	-5.96	109.72	116.63
12	L	49	ALA	N-CA-C	5.96	118.54	111.33
8	V	180	ILE	N-CA-C	5.95	117.40	110.62
2	B	109	VAL	N-CA-C	5.94	116.59	110.36
8	H	100	ILE	N-CA-C	-5.91	98.62	107.37
6	F	240	ILE	N-CA-C	-5.91	106.98	112.83
13	1	189	ASN	N-CA-C	5.90	120.06	112.86
9	W	95	TYR	N-CA-C	-5.90	100.88	110.20
10	X	165	ARG	N-CA-C	5.89	120.54	113.23
1	O	81	MET	N-CA-C	5.88	117.79	108.67
4	D	218	GLN	N-CA-C	5.86	117.47	111.14
4	D	63	SER	N-CA-C	-5.85	106.00	113.02
10	X	27	LEU	N-CA-C	5.85	117.74	111.36
11	Y	131	GLN	N-CA-C	5.84	118.12	111.11
10	J	166	MET	CA-C-N	5.83	125.53	119.05
10	J	166	MET	C-N-CA	5.83	125.53	119.05
6	T	71	ASP	CB-CA-C	-5.82	109.88	116.63
12	L	21	ILE	N-CA-C	5.82	117.30	108.80
7	U	9	ASP	N-CA-C	-5.82	106.22	113.15
11	K	131	GLN	N-CA-C	5.81	118.08	111.11
12	Z	94	PRO	N-CA-C	5.81	119.35	111.22
4	D	61	SER	N-CA-C	5.80	119.88	112.34
13	M	40	ASN	N-CA-C	-5.80	105.57	114.16
4	R	61	SER	N-CA-C	5.80	119.88	112.34
7	G	13	THR	N-CA-C	5.80	118.61	109.39
12	L	94	PRO	N-CA-C	5.79	119.61	111.33
10	X	45	PHE	N-CA-C	5.74	117.79	109.07
9	I	141	LEU	N-CA-C	5.73	117.53	111.28
8	V	100	ILE	N-CA-C	-5.73	98.89	107.37
2	P	109	VAL	N-CA-C	5.73	116.37	110.36
7	U	13	THR	N-CA-C	5.71	118.47	109.39
10	J	45	PHE	N-CA-C	5.68	117.71	109.07
9	W	141	LEU	N-CA-C	5.68	117.47	111.28
12	Z	21	ILE	N-CA-C	5.67	117.07	108.80
4	R	218	GLN	N-CA-C	5.65	117.25	111.14
4	R	63	SER	N-CA-C	-5.64	106.25	113.02
12	L	95	TYR	N-CA-C	-5.64	99.33	108.41
6	T	240	ILE	N-CA-C	-5.62	107.27	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	166	MET	CA-C-N	5.59	125.25	119.05
10	X	166	MET	C-N-CA	5.59	125.25	119.05
5	E	161	TYR	N-CA-C	-5.58	105.20	112.23
14	2	99	ILE	N-CA-C	5.57	116.61	108.53
14	N	99	ILE	N-CA-C	5.57	116.61	108.53
13	M	45	ILE	N-CA-C	5.57	116.50	108.48
7	U	60	ASP	CA-C-N	5.55	126.78	119.84
7	U	60	ASP	C-N-CA	5.55	126.78	119.84
7	G	60	ASP	CA-C-N	5.53	126.75	119.84
7	G	60	ASP	C-N-CA	5.53	126.75	119.84
12	Z	95	TYR	N-CA-C	-5.52	100.11	108.67
10	X	93	ARG	CA-C-N	5.50	125.26	119.76
10	X	93	ARG	C-N-CA	5.50	125.26	119.76
10	J	143	ARG	CA-C-N	5.49	125.84	119.47
10	J	143	ARG	C-N-CA	5.49	125.84	119.47
14	N	115	LEU	N-CA-C	5.48	117.96	111.33
10	J	165	ARG	N-CA-C	5.45	119.99	113.23
1	A	10(A)	ILE	CB-CA-C	-5.45	105.37	111.80
10	X	143	ARG	CA-C-N	5.44	125.78	119.47
10	X	143	ARG	C-N-CA	5.44	125.78	119.47
9	I	95	TYR	N-CA-C	-5.44	101.61	110.20
14	2	115	LEU	N-CA-C	5.44	117.91	111.33
7	G	127	ALA	N-CA-C	5.42	119.15	112.54
7	U	197	MET	N-CA-C	-5.41	105.46	111.36
13	1	40	ASN	N-CA-C	-5.37	106.21	114.16
10	J	27	LEU	N-CA-C	5.37	118.05	111.82
3	Q	62(A)	ILE	N-CA-C	5.37	117.27	111.58
5	S	161	TYR	N-CA-C	-5.37	105.47	112.23
11	K	102	CYS	N-CA-C	5.34	117.67	109.07
7	G	197	MET	N-CA-C	-5.33	105.55	111.36
1	A	179	ARG	N-CA-C	5.32	119.03	112.54
7	G	218	ASP	N-CA-C	5.30	118.90	111.74
5	E	152	GLN	CA-C-N	5.28	126.44	119.84
5	E	152	GLN	C-N-CA	5.28	126.44	119.84
5	S	152	GLN	CA-C-N	5.28	126.43	119.84
5	S	152	GLN	C-N-CA	5.28	126.43	119.84
1	A	81	MET	N-CA-C	5.27	116.84	108.67
7	U	78	VAL	N-CA-C	5.27	115.49	108.11
1	O	179	ARG	N-CA-C	5.27	119.33	113.01
6	T	43	ASN	N-CA-C	5.26	119.33	113.01
1	A	78	TYR	N-CA-C	5.26	116.27	108.86
9	I	117	GLY	N-CA-C	5.26	120.95	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	29	ASN	N-CA-C	5.26	120.34	113.30
9	W	145	ASN	N-CA-C	5.24	118.42	111.30
11	Y	102	CYS	N-CA-C	5.23	117.49	109.07
2	B	188	ASP	N-CA-C	-5.23	105.66	111.36
6	F	43	ASN	N-CA-C	5.23	119.28	113.01
4	R	16	SER	N-CA-C	-5.22	104.12	110.13
10	J	93	ARG	CA-C-N	5.20	124.96	119.76
10	J	93	ARG	C-N-CA	5.20	124.96	119.76
4	D	16	SER	N-CA-C	-5.18	104.18	110.13
13	M	97	ASN	N-CA-C	5.18	116.85	109.14
8	V	21	THR	N-CA-C	5.18	117.68	109.50
8	V	172	ASN	N-CA-C	5.17	117.40	109.95
8	H	21	THR	N-CA-C	5.17	117.67	109.50
8	H	172	ASN	N-CA-C	5.17	117.40	109.95
12	L	145	TYR	N-CA-C	5.15	118.47	110.17
3	C	62(A)	ILE	N-CA-C	5.15	117.04	111.58
1	O	21(P)	LYS	N-CA-C	5.15	119.65	113.17
1	A	21(P)	LYS	N-CA-C	5.14	119.64	113.17
12	Z	145	TYR	N-CA-C	5.13	118.43	110.17
8	V	182	LYS	N-CA-C	5.13	117.99	109.94
7	U	218	ASP	N-CA-C	5.12	118.64	111.74
13	I	31	VAL	N-CA-C	5.11	115.69	107.73
1	O	10(A)	ILE	CB-CA-C	-5.10	105.78	111.80
7	U	80	GLY	CA-C-N	5.10	125.10	119.90
7	U	80	GLY	C-N-CA	5.10	125.10	119.90
7	G	78	VAL	N-CA-C	5.10	115.25	108.11
4	D	129	SER	N-CA-C	5.09	118.75	112.54
11	Y	98	GLY	N-CA-C	-5.09	101.11	113.18
7	G	87	ASN	N-CA-C	-5.08	105.65	111.14
12	L	35	PHE	N-CA-C	5.08	117.84	109.72
10	X	134	THR	N-CA-C	5.07	119.50	112.45
2	P	16	SER	N-CA-C	-5.06	102.68	110.07
6	T	134	VAL	CB-CA-C	-5.06	104.77	111.80
11	K	188	GLY	N-CA-C	5.04	125.14	113.18
1	O	78	TYR	N-CA-C	5.04	115.97	108.86
4	R	169	SER	N-CA-C	5.04	121.54	110.80
5	S	58	LEU	N-CA-C	-5.04	107.17	113.72
6	T	54	ILE	CB-CA-C	-5.03	107.59	113.22
13	I	45	ILE	N-CA-C	5.02	115.70	108.48
5	S	154	SER	N-CA-C	-5.01	106.43	112.54
4	D	169	SER	N-CA-C	5.01	121.47	110.80
2	B	155	GLY	N-CA-C	-5.00	108.18	115.63

There are no chirality outliers.

There are no planarity outliers.

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	66	0
1	O	1915	0	1926	68	0
2	B	1905	0	1901	107	0
2	P	1905	0	1901	108	0
3	C	1891	0	1900	114	0
3	Q	1891	0	1900	104	0
4	D	1862	0	1836	73	0
4	R	1862	0	1836	68	0
5	E	1795	0	1797	78	0
5	S	1795	0	1797	77	0
6	F	1897	0	1886	69	0
6	T	1897	0	1886	73	0
7	G	1921	0	1910	76	0
7	U	1921	0	1910	79	0
8	H	1685	0	1687	48	0
8	V	1685	0	1687	48	0
9	I	1581	0	1574	61	0
9	W	1581	0	1574	58	0
10	J	1585	0	1590	77	0
10	X	1585	0	1590	78	0
11	K	1644	0	1594	52	0
11	Y	1644	0	1594	53	0
12	L	1757	0	1711	65	0
12	Z	1757	0	1711	70	0
13	1	1824	0	1832	64	0
13	M	1824	0	1832	68	0
14	2	1512	0	1481	63	0
14	N	1512	0	1481	63	0
15	H	15	0	16	1	0
15	K	15	0	16	1	0
15	V	15	0	16	1	0
15	Y	15	0	16	1	0
16	1	58	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	2	57	0	0	2	0
16	A	38	0	0	2	0
16	B	26	0	0	2	0
16	C	30	0	0	5	0
16	D	28	0	0	2	0
16	E	17	0	0	0	0
16	F	41	0	0	2	0
16	G	45	0	0	2	0
16	H	36	0	0	1	0
16	I	48	0	0	3	0
16	J	33	0	0	2	0
16	K	27	0	0	2	0
16	L	41	0	0	2	0
16	M	54	0	0	6	0
16	N	45	0	0	3	0
16	O	25	0	0	2	0
16	P	19	0	0	0	0
16	Q	18	0	0	2	0
16	R	21	0	0	3	0
16	S	15	0	0	3	0
16	T	30	0	0	2	0
16	U	50	0	0	5	0
16	V	36	0	0	2	0
16	W	46	0	0	1	0
16	X	36	0	0	0	0
16	Y	26	0	0	3	0
16	Z	34	0	0	6	0
All	All	50588	0	49314	1840	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 19.

All (1840) 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)
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.32	1.11
5:S:2(B):THR:H	5:S:2(E):ASN:ND2	1.49	1.11
5:E:2(B):THR:H	5:E:2(E):ASN:ND2	1.48	1.09
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.31	1.08
4:R:68:VAL:HG21	4:R:89:ILE:HD13	1.35	1.07
7:U:96:ALA:HA	7:U:107:MET:HE2	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:VAL:HG21	4:D:89:ILE:HD13	1.40	1.02
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.23	1.02
10:J:168:MET:HE3	10:X:168:MET:HE3	1.43	1.01
7:G:96:ALA:HA	7:G:107:MET:HE2	1.41	0.99
1:A:15:PHE:H	2:B:23:GLN:HE22	1.11	0.98
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.27	0.98
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.07	0.98
11:Y:33:LYS:HG2	11:Y:45:MET:HE2	1.45	0.97
1:O:15:PHE:H	2:P:23:GLN:HE22	1.07	0.97
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.65	0.97
2:B:71:ASN:ND2	2:B:72:ASP:H	1.63	0.96
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.03	0.95
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.29	0.95
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.67	0.95
11:K:33:LYS:HG2	11:K:45:MET:HE2	1.48	0.94
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.07	0.93
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.33	0.93
2:P:71:ASN:ND2	2:P:72:ASP:H	1.65	0.93
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.17	0.93
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.34	0.92
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.35	0.92
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.17	0.91
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.35	0.91
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.52	0.91
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.04	0.91
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.87	0.90
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.53	0.89
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.55	0.89
3:C:232:TYR:O	3:C:236:ILE:HG13	1.72	0.89
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.54	0.88
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.88	0.88
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.35	0.88
11:K:142:TYR:O	11:K:143:LYS:HD2	1.72	0.88
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.17	0.88
2:B:202:THR:HG22	2:B:204:SER:H	1.39	0.87
13:M:149:GLN:NE2	13:M:149:GLN:H	1.73	0.87
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.74	0.87
2:P:202:THR:HG22	2:P:204:SER:H	1.37	0.87
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.75	0.85
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.59	0.85
3:C:163:GLN:NE2	3:C:164:THR:H	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:ILE:HD11	6:F:49:ALA:HB3	1.58	0.84
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.77	0.84
2:B:71:ASN:HD22	2:B:72:ASP:H	1.26	0.84
12:L:33:LYS:HD2	12:L:46:ASN:ND2	1.93	0.84
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.75	0.84
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.78	0.84
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.89	0.83
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.60	0.83
6:T:38:ILE:HD11	6:T:49:ALA:HB3	1.59	0.83
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.59	0.83
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.79	0.82
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.77	0.82
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	1.94	0.82
10:J:-1:MET:HG2	10:J:1:ASP:H	1.45	0.82
13:1:149:GLN:NE2	13:1:149:GLN:H	1.78	0.81
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.44	0.81
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.62	0.81
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.79	0.81
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.63	0.81
2:B:15:PHE:H	3:C:23:GLN:HE22	1.26	0.80
3:Q:201:VAL:CG2	3:Q:210:ILE:HD11	2.10	0.80
10:X:-1:MET:HG2	10:X:1:ASP:H	1.44	0.80
6:F:192:GLN:O	6:F:196:ILE:HG12	1.81	0.80
2:P:71:ASN:HD22	2:P:72:ASP:H	1.27	0.80
3:C:185:THR:HB	3:C:188:GLU:HG2	1.63	0.80
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.17	0.80
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.46	0.80
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.63	0.80
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.29	0.80
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.46	0.80
2:B:121:GLN:O	2:B:124:THR:HB	1.82	0.79
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.47	0.79
3:C:201:VAL:CG2	3:C:210:ILE:HD11	2.10	0.79
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.28	0.79
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.81	0.79
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.62	0.79
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.78	0.79
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.95	0.79
3:C:163:GLN:HE21	3:C:164:THR:H	1.30	0.79
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.65	0.79
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	1.96	0.78
5:S:15:PHE:H	6:T:23:GLN:HE22	1.32	0.78
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.66	0.78
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.30	0.78
11:Y:31:VAL:HG11	11:Y:45:MET:HE1	1.64	0.78
4:D:40:ILE:HG13	4:D:193:VAL:HG23	1.66	0.78
7:U:121:GLN:O	7:U:124:THR:HB	1.83	0.78
3:C:33:ARG:HH11	3:C:33:ARG:CB	1.97	0.78
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.81	0.78
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.47	0.78
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.49	0.78
7:U:86:ARG:HD2	16:U:248:HOH:O	1.84	0.78
10:J:156:LYS:O	10:J:160:GLN:HG3	1.84	0.78
6:T:192:GLN:O	6:T:196:ILE:HG12	1.83	0.77
11:K:31:VAL:HG11	11:K:45:MET:HE1	1.67	0.77
3:C:15:PHE:H	4:D:23:GLN:HE22	1.29	0.77
2:P:121:GLN:O	2:P:124:THR:HB	1.85	0.77
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	1.98	0.77
7:G:87:ASN:C	7:G:87:ASN:HD22	1.92	0.77
7:G:198:ILE:HG23	7:G:203:THR:O	1.84	0.77
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.19	0.77
7:U:87:ASN:C	7:U:87:ASN:HD22	1.93	0.77
9:W:7:THR:HG23	9:W:110:ILE:HD13	1.67	0.77
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.00	0.76
10:J:168:MET:HE3	10:X:168:MET:CE	2.15	0.76
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.82	0.76
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.01	0.76
3:Q:197:LEU:O	3:Q:201:VAL:HG23	1.85	0.76
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.50	0.76
10:J:168:MET:CE	10:X:168:MET:HE3	2.14	0.76
11:K:143:LYS:O	11:K:146:LEU:HD13	1.85	0.76
9:I:7:THR:HG23	9:I:110:ILE:HD13	1.67	0.76
3:C:185:THR:HG22	3:C:187:GLU:N	2.01	0.76
3:C:185:THR:HG22	3:C:187:GLU:H	1.49	0.76
10:X:156:LYS:O	10:X:160:GLN:HG3	1.84	0.76
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.86	0.76
5:E:207:LEU:HD23	5:E:207:LEU:H	1.50	0.76
4:R:40:ILE:HG13	4:R:193:VAL:HG23	1.68	0.76
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.67	0.76
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.51	0.76
5:E:2(B):THR:N	5:E:2(E):ASN:ND2	2.31	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.87	0.75
13:1:42:VAL:HG23	13:1:178:ILE:HD11	1.69	0.75
7:U:217:LYS:HA	7:U:217:LYS:HE3	1.67	0.75
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.68	0.75
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.87	0.75
7:G:121:GLN:O	7:G:124:THR:HB	1.86	0.74
1:O:179:ARG:HB3	1:O:179:ARG:HH11	1.52	0.74
5:S:207:LEU:HD23	5:S:207:LEU:H	1.50	0.74
10:J:168:MET:HG2	10:X:168:MET:HE3	1.70	0.74
3:C:41:LYS:HG2	3:C:161:SER:O	1.88	0.74
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.53	0.73
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.36	0.73
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.69	0.73
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.68	0.73
1:O:159:PRO:O	2:P:59:LEU:HD12	1.88	0.73
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.71	0.73
3:C:197:LEU:O	3:C:201:VAL:HG23	1.87	0.73
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.71	0.73
5:S:2(B):THR:N	5:S:2(E):ASN:ND2	2.32	0.73
7:U:198:ILE:HG23	7:U:203:THR:O	1.88	0.72
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.70	0.72
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.71	0.72
4:R:68:VAL:CG2	4:R:89:ILE:HD13	2.18	0.72
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.53	0.72
1:O:121:GLN:O	1:O:124:THR:HB	1.90	0.72
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.55	0.72
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.70	0.71
1:A:7:ARG:HB2	2:B:5:SER:OG	1.90	0.71
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.73	0.71
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.72	0.71
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.71	0.71
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.55	0.71
12:Z:-8:PHE:HB2	13:1:-8:THR:HG23	1.71	0.71
12:Z:109:ALA:HA	16:Z:202:HOH:O	1.91	0.71
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.72	0.71
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.55	0.71
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.14	0.70
10:X:147:THR:HG23	10:X:150:GLU:OE2	1.91	0.70
14:2:155:ILE:HG22	14:2:175:MET:HE2	1.72	0.70
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.73	0.70
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.74	0.70
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.55	0.70
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.73	0.70
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.73	0.70
12:L:-9:GLN:NE2	12:L:-8:PHE:H	1.90	0.70
2:P:71:ASN:ND2	2:P:72:ASP:N	2.40	0.70
6:T:173:LYS:O	6:T:177:GLU:HG3	1.91	0.70
13:1:41:THR:OG1	13:1:76:PRO:HG3	1.91	0.69
2:B:71:ASN:ND2	2:B:72:ASP:N	2.38	0.69
1:A:121:GLN:O	1:A:124:THR:HB	1.92	0.69
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.27	0.69
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.57	0.69
13:M:57:ARG:NE	16:M:243:HOH:O	2.25	0.69
2:B:71:ASN:HD22	2:B:72:ASP:N	1.89	0.69
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.28	0.69
5:E:15:PHE:H	6:F:23:GLN:HE22	1.39	0.69
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.73	0.69
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.74	0.69
10:J:90(A):ILE:HG12	10:J:116:LEU:HA	1.74	0.69
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.38	0.69
6:F:173:LYS:O	6:F:177:GLU:HG3	1.93	0.69
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.58	0.69
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.74	0.69
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.07	0.68
5:S:132:TYR:O	5:S:153:PRO:HB3	1.93	0.68
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.73	0.68
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.06	0.68
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.75	0.68
10:J:147:THR:HG23	10:J:150:GLU:OE2	1.93	0.68
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.76	0.68
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.74	0.68
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	1.76	0.68
2:P:71:ASN:HD22	2:P:72:ASP:N	1.90	0.68
10:X:-1:MET:HG2	10:X:1:ASP:N	2.09	0.68
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.75	0.68
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.07	0.68
14:N:107:LYS:HG2	14:N:108:GLY:H	1.60	0.67
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.76	0.67
14:N:155:ILE:HG22	14:N:175:MET:HE2	1.75	0.67
5:S:207:LEU:H	5:S:207:LEU:CD2	2.06	0.67
5:E:132:TYR:O	5:E:153:PRO:HB3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:GLN:HE21	3:C:164:THR:N	1.92	0.67
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.59	0.67
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.76	0.67
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.24	0.67
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.91	0.67
5:E:207:LEU:H	5:E:207:LEU:CD2	2.07	0.67
2:P:234:VAL:HA	2:P:239:THR:HA	1.77	0.67
14:2:107:LYS:HG2	14:2:108:GLY:H	1.58	0.67
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.10	0.67
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.77	0.67
12:Z:-9:GLN:NE2	12:Z:-8:PHE:H	1.93	0.67
2:P:190:ILE:HG21	2:P:232:ILE:HD11	1.76	0.66
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.76	0.66
4:D:162:ALA:HB3	5:E:58:LEU:HD23	1.77	0.66
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.77	0.66
10:X:90(A):ILE:HG12	10:X:116:LEU:HA	1.76	0.66
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.58	0.66
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.76	0.66
10:J:168:MET:HE3	10:X:168:MET:HG2	1.76	0.66
11:K:7:ARG:HD2	11:K:108:PRO:O	1.96	0.66
14:2:21:THR:HG22	14:2:26:ILE:HA	1.77	0.66
3:C:76:LEU:HD12	3:C:138:ILE:HG12	1.76	0.66
7:G:96:ALA:CA	7:G:107:MET:HE2	2.22	0.66
2:P:185:LYS:HD3	2:P:186:VAL:N	2.10	0.66
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.92	0.66
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.77	0.66
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.76	0.66
2:B:185:LYS:HD3	2:B:186:VAL:N	2.11	0.66
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.77	0.66
3:Q:201:VAL:HG21	3:Q:210:ILE:CD1	2.19	0.66
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.78	0.66
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.78	0.66
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.78	0.66
7:U:96:ALA:HA	7:U:107:MET:CE	2.23	0.66
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.78	0.65
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.86	0.65
10:J:-1:MET:HG2	10:J:1:ASP:N	2.10	0.65
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.11	0.65
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.27	0.65
7:G:96:ALA:HA	7:G:107:MET:CE	2.24	0.65
1:O:161:LYS:HD2	2:P:58:LEU:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.79	0.65
3:Q:70:ILE:HD12	3:Q:112:LEU:HD11	1.79	0.65
6:F:35:THR:HG21	6:F:51:GLU:O	1.97	0.65
8:H:165:ASN:HD22	13:1:139:ARG:NH1	1.91	0.65
6:T:177:GLU:OE2	7:U:57:LYS:HE2	1.96	0.65
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.61	0.65
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.78	0.65
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.22	0.64
11:K:142:TYR:C	11:K:143:LYS:HD2	2.21	0.64
9:W:124:PHE:O	9:W:125:ILE:HD12	1.98	0.64
8:H:128:GLY:O	8:H:131:SER:HB2	1.96	0.64
14:N:21:THR:HG22	14:N:26:ILE:HA	1.80	0.64
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.32	0.64
2:B:190:ILE:HG21	2:B:232:ILE:HD11	1.79	0.64
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.28	0.64
5:S:227:GLU:H	5:S:227:GLU:CD	2.06	0.64
2:B:234:VAL:HA	2:B:239:THR:HA	1.78	0.64
14:N:3:ILE:HD11	14:N:127:ALA:HB3	1.78	0.64
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.78	0.64
1:O:7:ARG:HB2	2:P:5:SER:OG	1.97	0.64
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.79	0.64
1:A:206:PHE:CE1	1:A:210:ILE:HD11	2.33	0.64
3:C:41:LYS:HD3	3:C:161:SER:HA	1.80	0.64
14:N:107:LYS:HG2	14:N:108:GLY:N	2.13	0.64
7:U:59:LEU:O	7:U:61:PRO:HD3	1.97	0.64
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.80	0.64
13:M:40:ASN:HD22	13:M:40:ASN:H	1.46	0.64
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.11	0.64
3:C:35:THR:HB	3:C:51:GLU:HG3	1.79	0.64
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.13	0.64
1:O:15:PHE:H	2:P:23:GLN:NE2	1.89	0.63
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.80	0.63
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.80	0.63
10:J:168:MET:HG2	10:X:168:MET:CE	2.28	0.63
6:T:172:ALA:O	6:T:176:LEU:HD23	1.97	0.63
5:E:227:GLU:H	5:E:227:GLU:CD	2.05	0.63
2:P:228:GLU:O	2:P:232:ILE:HG22	1.99	0.63
8:V:128:GLY:O	8:V:131:SER:HB2	1.99	0.63
14:2:106:ASN:O	14:2:107:LYS:HB3	1.99	0.63
10:J:2:ILE:O	10:J:3:ILE:HD13	1.99	0.63
10:J:147:THR:OG1	10:J:150:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.34	0.63
13:M:159:MET:HE1	16:M:246:HOH:O	1.99	0.63
2:B:41:MET:HE3	16:B:240:HOH:O	1.99	0.63
4:D:68:VAL:CG2	4:D:89:ILE:HD13	2.22	0.63
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.32	0.63
12:Z:6:ILE:HG12	12:Z:124:CYS:HB2	1.79	0.63
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.81	0.63
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.80	0.63
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.10	0.63
13:1:40:ASN:H	13:1:40:ASN:HD22	1.46	0.63
4:D:175:GLU:HG2	4:D:196:ILE:HD13	1.80	0.63
2:B:163:ILE:HG12	2:B:164:SER:N	2.14	0.62
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.81	0.62
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.93	0.62
3:C:201:VAL:HG21	3:C:210:ILE:CD1	2.19	0.62
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.12	0.62
9:W:113:PHE:CD2	9:W:113:PHE:N	2.66	0.62
11:Y:7:ARG:HD2	11:Y:108:PRO:O	1.99	0.62
13:M:139:ARG:NH1	8:V:165:ASN:HD22	1.93	0.62
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.80	0.62
10:J:52:THR:HG22	10:J:53:VAL:N	2.14	0.62
2:P:163:ILE:HG12	2:P:164:SER:N	2.13	0.62
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.81	0.62
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.81	0.62
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.15	0.62
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.33	0.62
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.28	0.62
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.35	0.62
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.11	0.62
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.30	0.62
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.79	0.62
2:B:228:GLU:O	2:B:232:ILE:HG22	2.00	0.62
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.13	0.62
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.81	0.62
2:P:122:GLY:C	2:P:124:THR:H	2.08	0.62
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.13	0.62
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.81	0.62
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.14	0.62
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.81	0.62
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.00	0.62
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.30	0.62
12:L:6:ILE:HG12	12:L:124:CYS:HB2	1.80	0.62
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.97	0.62
2:P:41:MET:HE3	16:Q:247:HOH:O	1.99	0.62
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.87	0.62
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.82	0.62
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.35	0.61
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.48	0.61
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.34	0.61
10:X:143:ARG:O	10:X:146:MET:HG3	2.00	0.61
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.65	0.61
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	2.07	0.61
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.47	0.61
2:P:239:THR:HG22	2:P:239:THR:OXT	1.99	0.61
4:R:207:LEU:HD23	4:R:207:LEU:C	2.26	0.61
8:V:172:ASN:ND2	8:V:193:THR:HA	2.14	0.61
3:C:15:PHE:N	4:D:23:GLN:HE22	1.98	0.61
9:I:16:CYS:SG	9:I:34:ILE:HG12	2.39	0.61
10:X:2:ILE:O	10:X:3:ILE:HD13	2.01	0.61
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.66	0.61
7:G:59:LEU:O	7:G:61:PRO:HD3	2.00	0.61
9:I:113:PHE:CD2	9:I:113:PHE:N	2.66	0.61
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.31	0.61
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.30	0.61
7:U:96:ALA:CA	7:U:107:MET:HE2	2.21	0.61
7:U:218:ASP:O	7:U:220:LYS:HB2	1.99	0.61
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.16	0.61
1:O:206:PHE:CE1	1:O:210:ILE:HD11	2.35	0.61
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.81	0.61
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.81	0.61
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.29	0.61
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.06	0.61
13:1:149:GLN:H	13:1:149:GLN:HE21	1.49	0.61
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.82	0.61
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.82	0.61
11:Y:31:VAL:CG1	11:Y:45:MET:HE1	2.30	0.61
14:2:107:LYS:HG2	14:2:108:GLY:N	2.13	0.61
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.65	0.61
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.31	0.61
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.82	0.60
7:G:77:VAL:HG12	7:G:137:THR:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:35:THR:HG21	6:T:51:GLU:O	2.01	0.60
6:F:38:ILE:CD1	6:F:49:ALA:HB3	2.31	0.60
14:N:106:ASN:O	14:N:107:LYS:HB3	2.00	0.60
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.96	0.60
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.31	0.60
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.82	0.60
12:Z:151:VAL:O	12:Z:155:VAL:HG23	2.01	0.60
9:W:16:CYS:SG	9:W:34:ILE:HG12	2.41	0.60
10:X:52:THR:HG22	10:X:53:VAL:N	2.16	0.60
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.36	0.60
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.82	0.60
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.01	0.60
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.32	0.60
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.84	0.60
2:B:181:LYS:O	2:B:184:MET:HG3	2.02	0.60
7:G:87:ASN:C	7:G:87:ASN:ND2	2.60	0.60
13:1:40:ASN:HD22	13:1:40:ASN:N	2.00	0.60
1:A:20:LYS:HE3	1:A:25:ASP:OD1	2.02	0.60
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.16	0.60
10:J:156:LYS:HE2	10:J:160:GLN:NE2	2.17	0.60
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.31	0.60
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.83	0.60
6:F:177:GLU:OE2	7:G:57:LYS:HE2	2.01	0.60
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.67	0.60
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.16	0.59
11:K:74:ILE:HA	16:K:322:HOH:O	2.02	0.59
14:N:92:ASP:HB2	16:N:199:HOH:O	2.01	0.59
10:X:156:LYS:HE2	10:X:160:GLN:NE2	2.18	0.59
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.32	0.59
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.85	0.59
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.84	0.59
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.48	0.59
13:M:40:ASN:HD22	13:M:40:ASN:N	2.00	0.59
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.30	0.59
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.84	0.59
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.84	0.59
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.65	0.59
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.85	0.59
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.37	0.59
3:C:14:ILE:HB	4:D:23:GLN:NE2	2.18	0.59
6:T:130:ARG:HG2	6:T:130:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:O	1:A:177:GLU:HG3	2.03	0.59
10:J:168:MET:CE	10:X:168:MET:HG2	2.33	0.59
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.84	0.59
9:W:110:ILE:HG13	9:W:125:ILE:HD13	1.83	0.59
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.83	0.59
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.17	0.59
11:K:31:VAL:CG1	11:K:45:MET:HE1	2.33	0.59
14:N:3:ILE:O	14:N:3:ILE:HD13	2.03	0.59
2:P:190:ILE:CG2	2:P:232:ILE:HD11	2.32	0.59
6:T:127:ASN:HD22	6:T:128:SER:N	2.01	0.59
14:2:3:ILE:O	14:2:3:ILE:HD13	2.03	0.59
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.33	0.59
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.67	0.59
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.85	0.59
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.85	0.59
14:2:3:ILE:HD11	14:2:127:ALA:HB3	1.83	0.59
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.83	0.59
9:I:124:PHE:O	9:I:125:ILE:HD12	2.02	0.59
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.67	0.59
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.85	0.58
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.11	0.58
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.67	0.58
13:1:113:VAL:HA	13:1:118:VAL:O	2.03	0.58
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.38	0.58
1:O:20:LYS:HE3	1:O:25:ASP:OD1	2.03	0.58
2:P:181:LYS:O	2:P:184:MET:HG3	2.03	0.58
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.84	0.58
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	2.03	0.58
14:2:161:GLN:NE2	14:2:165:TRP:HE1	1.99	0.58
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.68	0.58
7:G:77:VAL:CG1	7:G:137:THR:HB	2.33	0.58
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.33	0.58
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.85	0.58
6:T:237:GLN:O	6:T:240:ILE:HG22	2.03	0.58
7:U:131:PRO:HB3	16:U:258:HOH:O	2.02	0.58
7:U:228:ASN:HB3	16:U:242:HOH:O	2.04	0.58
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.39	0.58
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.51	0.58
2:B:239:THR:HG22	2:B:239:THR:OXT	2.01	0.58
6:T:38:ILE:CD1	6:T:49:ALA:HB3	2.31	0.58
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:172:ALA:O	6:F:176:LEU:HD23	2.03	0.58
6:F:20(B):GLU:HG3	6:F:20(C):LYS:H	1.68	0.58
1:O:173:LYS:O	1:O:177:GLU:HG3	2.03	0.58
3:Q:195:ARG:HG3	3:Q:236:ILE:CD1	2.33	0.58
10:X:113:ILE:HA	10:X:118:THR:O	2.04	0.58
1:A:69:LEU:HD23	1:A:69:LEU:C	2.29	0.58
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.84	0.58
14:N:156:LYS:HG2	14:N:18(J):LEU:CD1	2.34	0.58
14:2:156:LYS:HG2	14:2:18(J):LEU:CD1	2.33	0.58
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.68	0.58
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.37	0.58
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.85	0.58
12:L:166:HIS:HD2	12:L:168:GLN:H	1.52	0.58
4:R:107:ILE:HG22	16:R:247:HOH:O	2.03	0.58
7:G:218:ASP:O	7:G:220:LYS:HB2	2.03	0.57
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.86	0.57
4:D:207:LEU:C	4:D:207:LEU:HD23	2.29	0.57
4:R:24:VAL:O	4:R:27:SER:HB3	2.04	0.57
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.34	0.57
4:D:24:VAL:O	4:D:27:SER:HB3	2.04	0.57
4:D:215:ILE:C	4:D:215:ILE:HD13	2.29	0.57
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.01	0.57
14:2:172:VAL:HB	14:2:18(A):ILE:HD11	1.86	0.57
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.34	0.57
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.87	0.57
9:I:110:ILE:HG13	9:I:125:ILE:HD13	1.85	0.57
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.87	0.57
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.62	0.57
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.87	0.57
2:B:122:GLY:C	2:B:124:THR:H	2.11	0.57
2:P:143:ASP:OD2	10:X:10(B):LYS:HE2	2.04	0.57
2:P:186:VAL:HG21	2:P:216:ARG:HG2	1.85	0.57
7:U:130:ARG:HB2	16:U:262:HOH:O	2.03	0.57
13:M:149:GLN:H	13:M:149:GLN:HE21	1.46	0.57
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.05	0.57
3:C:195:ARG:HG3	3:C:236:ILE:CD1	2.34	0.57
5:E:111:ARG:HG2	5:E:111:ARG:NH1	2.20	0.57
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.87	0.57
12:L:-9:GLN:CD	12:L:-8:PHE:N	2.63	0.57
12:L:145:TYR:CD1	12:L:146:LEU:N	2.72	0.57
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:207:LEU:HD23	5:S:207:LEU:N	2.20	0.57
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.86	0.57
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.39	0.57
5:E:207:LEU:HD23	5:E:207:LEU:N	2.20	0.57
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.87	0.57
1:O:69:LEU:C	1:O:69:LEU:HD23	2.30	0.57
2:B:11:ARG:O	2:B:14:ILE:HD13	2.05	0.56
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.40	0.56
11:K:86:LEU:HD13	11:K:86:LEU:C	2.30	0.56
7:U:77:VAL:CG1	7:U:137:THR:HB	2.35	0.56
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.34	0.56
6:F:38:ILE:HG22	6:F:164:ALA:HA	1.87	0.56
6:F:130:ARG:HG2	6:F:130:ARG:HH11	1.70	0.56
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.35	0.56
12:L:-9:GLN:CD	12:L:-8:PHE:H	2.13	0.56
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.38	0.56
2:P:88:LEU:HB3	2:P:116:LEU:HD21	1.87	0.56
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.39	0.56
9:W:48:LEU:HG	9:W:50:THR:HG22	1.87	0.56
11:Y:45:MET:HE3	15:Y:301:SLA:H11	1.87	0.56
12:Z:99:THR:HG22	16:Z:199:HOH:O	2.04	0.56
3:C:242:GLU:O	3:C:243:GLN:HB2	2.06	0.56
4:D:85:ALA:O	4:D:89:ILE:HG13	2.06	0.56
5:E:86:ARG:O	5:E:90:ASN:HB2	2.05	0.56
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.70	0.56
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	2.05	0.56
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.06	0.56
3:Q:14:ILE:HB	4:R:23:GLN:NE2	2.20	0.56
7:U:77:VAL:HG12	7:U:137:THR:HB	1.85	0.56
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.87	0.56
12:Z:76:ILE:HG22	16:Z:218:HOH:O	2.03	0.56
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.70	0.56
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.70	0.56
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.74	0.56
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.41	0.56
6:F:127:ASN:HD22	6:F:128:SER:N	2.03	0.56
2:P:227:GLN:OE1	2:P:230:LYS:HD3	2.05	0.56
5:S:46:ALA:HB1	5:S:139:ILE:HB	1.87	0.56
5:S:86:ARG:O	5:S:90:ASN:HB2	2.05	0.56
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.35	0.56
8:H:172:ASN:ND2	8:H:193:THR:HA	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:192:LEU:O	4:R:196:ILE:HG13	2.06	0.56
6:T:20(B):GLU:HG3	6:T:20(C):LYS:H	1.70	0.56
9:W:122:ALA:HB3	9:W:125:ILE:CD1	2.35	0.56
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.69	0.56
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.54	0.56
2:B:227:GLN:OE1	2:B:230:LYS:HD3	2.05	0.56
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.88	0.56
3:C:229:ILE:O	3:C:233:VAL:HG23	2.06	0.56
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.88	0.56
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.71	0.56
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.31	0.56
2:B:20:ARG:NH2	3:C:33:ARG:HH21	2.03	0.56
2:B:143:ASP:OD2	10:J:10(B):LYS:HE2	2.06	0.56
2:B:186:VAL:HG21	2:B:216:ARG:HG2	1.88	0.56
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.87	0.56
10:X:44:SER:OG	10:X:100:LEU:HB2	2.05	0.56
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	2.07	0.56
13:1:41:THR:HG21	13:1:79:ILE:HD12	1.88	0.56
3:C:70:ILE:HD12	3:C:112:LEU:HD11	1.88	0.55
10:J:113:ILE:HA	10:J:118:THR:O	2.06	0.55
13:M:113:VAL:HA	13:M:118:VAL:O	2.06	0.55
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.06	0.55
8:V:200:LYS:HE3	9:W:140:SER:O	2.06	0.55
14:N:172:VAL:HB	14:N:18(A):ILE:HD11	1.88	0.55
1:O:15:PHE:N	2:P:23:GLN:HE22	1.90	0.55
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.89	0.55
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.36	0.55
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.87	0.55
2:P:87:ILE:O	2:P:91:THR:HG23	2.06	0.55
10:X:-1:MET:CG	10:X:1:ASP:H	2.19	0.55
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.06	0.55
3:C:227:GLU:H	3:C:227:GLU:CD	2.15	0.55
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.89	0.55
3:C:46:VAL:O	3:C:215:VAL:HG12	2.07	0.55
6:F:70:VAL:HB	6:F:74:ILE:HB	1.88	0.55
11:K:45:MET:HE3	15:K:301:SLA:H11	1.88	0.55
14:N:67:THR:HA	14:N:72:GLY:O	2.06	0.55
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.04	0.55
4:R:85:ALA:O	4:R:89:ILE:HG13	2.06	0.55
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.07	0.55
1:A:141:HIS:HA	1:A:146:GLY:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:200:LYS:HE3	11:K:206:PHE:O	2.06	0.55
12:L:151:VAL:O	12:L:155:VAL:HG23	2.06	0.55
13:M:41:THR:HG21	13:M:79:ILE:HD12	1.88	0.55
13:M:184:LEU:HD23	13:M:184:LEU:C	2.31	0.55
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.07	0.55
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.21	0.55
7:G:136:LEU:O	7:G:150:LYS:HA	2.07	0.55
12:L:105:ASP:OD2	12:L:107:LYS:HB2	2.07	0.55
3:Q:163:GLN:NE2	3:Q:163:GLN:HA	2.21	0.55
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.88	0.55
8:V:84:LYS:HG3	8:V:85:GLN:N	2.22	0.55
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.37	0.55
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.88	0.55
8:V:18:THR:HB	8:V:30:ASN:HD22	1.72	0.55
3:C:163:GLN:NE2	3:C:163:GLN:HA	2.21	0.55
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.89	0.55
12:L:177:ILE:HD12	12:L:177:ILE:N	2.22	0.55
1:O:14:THR:O	1:O:21:LEU:HD23	2.06	0.55
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.42	0.55
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.41	0.55
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.07	0.54
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.89	0.54
1:O:8:TYR:HD2	7:U:128:TYR:HB3	1.72	0.54
2:P:11:ARG:O	2:P:14:ILE:HD13	2.07	0.54
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.37	0.54
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.72	0.54
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.36	0.54
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.23	0.54
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.22	0.54
1:O:141:HIS:HA	1:O:146:GLY:O	2.07	0.54
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.89	0.54
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.07	0.54
3:Q:242:GLU:O	3:Q:243:GLN:HB2	2.06	0.54
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.89	0.54
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.07	0.54
10:J:133:TYR:HD1	16:Y:319:HOH:O	1.89	0.54
13:M:187:LYS:HB3	13:M:190:LEU:HD11	1.89	0.54
3:Q:85:SER:O	3:Q:89:ILE:HD12	2.06	0.54
5:S:74:MET:HE2	5:S:109:VAL:HA	1.88	0.54
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.90	0.54
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.88	0.54
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.37	0.54
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.90	0.54
9:I:48:LEU:HG	9:I:50:THR:HG22	1.88	0.54
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.42	0.54
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.90	0.54
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.43	0.54
2:P:235:LYS:C	2:P:237:GLY:H	2.16	0.54
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.89	0.54
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.89	0.54
2:B:27:ALA:O	2:B:31:ILE:HG12	2.08	0.54
6:F:237:GLN:O	6:F:240:ILE:HG22	2.08	0.54
11:K:48:GLY:HA2	16:K:318:HOH:O	2.08	0.54
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.07	0.54
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.89	0.54
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.23	0.54
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.23	0.54
8:H:18:THR:HB	8:H:30:ASN:HD22	1.73	0.54
8:H:41:ILE:HG12	8:H:76:VAL:HG22	1.89	0.54
8:H:139:GLU:OE1	13:1:165:ARG:NH1	2.36	0.54
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.38	0.54
6:T:70:VAL:HB	6:T:74:ILE:HB	1.89	0.54
8:V:172:ASN:HD22	8:V:193:THR:HA	1.73	0.54
2:B:87:ILE:O	2:B:91:THR:HG23	2.07	0.54
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.38	0.54
9:I:122:ALA:HB3	9:I:125:ILE:CD1	2.38	0.54
7:U:172:ILE:HD12	7:U:197:MET:CE	2.37	0.54
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.90	0.54
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.72	0.54
13:M:1:THR:HG22	16:M:214:HOH:O	2.07	0.54
5:S:73:HIS:HE1	5:S:107:LEU:O	1.90	0.54
8:V:196:VAL:HG23	16:V:319:HOH:O	2.07	0.54
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.08	0.54
12:L:134:ILE:HG22	12:L:138:LEU:HD22	1.90	0.54
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.42	0.54
12:Z:-5:TYR:CE2	12:Z:96:TYR:HB2	2.43	0.54
2:B:163:ILE:HG12	2:B:164:SER:H	1.72	0.53
2:P:44:ASP:OD2	2:P:186:VAL:HG23	2.08	0.53
2:P:224:PHE:N	2:P:224:PHE:CD2	2.76	0.53
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.08	0.53
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:136:LEU:O	7:U:150:LYS:HA	2.08	0.53
10:X:48:GLU:HB2	10:X:96:GLN:HB2	1.89	0.53
3:C:150:GLN:HG2	3:C:151:THR:N	2.22	0.53
5:E:227:GLU:CD	5:E:227:GLU:N	2.66	0.53
8:H:200:LYS:HE3	9:I:140:SER:O	2.08	0.53
11:K:25:TRP:CH2	12:L:132:SER:HA	2.42	0.53
3:Q:229:ILE:O	3:Q:233:VAL:HG23	2.08	0.53
7:U:87:ASN:C	7:U:87:ASN:ND2	2.60	0.53
10:X:19:ALA:HB2	10:X:171:LYS:HG2	1.90	0.53
12:Z:-9:GLN:CD	12:Z:-8:PHE:N	2.65	0.53
5:E:46:ALA:HB1	5:E:139:ILE:HB	1.90	0.53
5:E:18(C):PHE:O	5:E:18(F):ILE:HG12	2.09	0.53
8:H:2:THR:HG22	8:H:159:ILE:HD13	1.90	0.53
10:J:143:ARG:O	10:J:146:MET:HG3	2.08	0.53
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.38	0.53
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.07	0.53
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.91	0.53
10:J:44:SER:OG	10:J:100:LEU:HB2	2.09	0.53
13:M:125:LEU:HA	16:M:225:HOH:O	2.09	0.53
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.91	0.53
5:E:74:MET:HE2	5:E:109:VAL:HA	1.90	0.53
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.89	0.53
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.91	0.53
13:M:17:ASP:HA	13:M:173:PHE:CB	2.38	0.53
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.90	0.53
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.89	0.53
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.38	0.53
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.44	0.53
4:D:112:LEU:C	4:D:112:LEU:HD13	2.34	0.53
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.07	0.53
2:P:163:ILE:HG12	2:P:164:SER:H	1.73	0.53
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.90	0.53
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.90	0.53
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.44	0.53
2:B:224:PHE:N	2:B:224:PHE:CD2	2.76	0.53
5:E:73:HIS:HE1	5:E:107:LEU:O	1.90	0.53
7:G:172:ILE:HD12	7:G:197:MET:CE	2.39	0.53
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.91	0.53
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.91	0.53
13:1:14(C):ARG:HH11	13:1:14(C):ARG:HG3	1.73	0.53
2:B:235:LYS:C	2:B:237:GLY:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:LYS:O	3:C:58:LEU:HB2	2.09	0.53
4:D:185:THR:HG23	4:D:188:GLU:OE1	2.09	0.53
3:Q:172:VAL:O	3:Q:176:LEU:HG	2.09	0.53
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.24	0.53
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	1.90	0.53
2:B:224:PHE:N	2:B:224:PHE:HD2	2.07	0.53
3:C:190:VAL:O	3:C:194:VAL:HG23	2.08	0.53
3:C:224:LEU:HD12	3:C:224:LEU:N	2.24	0.53
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.09	0.53
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.74	0.53
9:I:16:CYS:HB3	9:I:34:ILE:HD11	1.91	0.53
12:L:5:GLY:O	12:L:124:CYS:HA	2.08	0.53
6:T:127:ASN:HD22	6:T:127:ASN:C	2.17	0.53
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.44	0.53
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.89	0.53
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.38	0.53
12:L:90:LYS:HE3	12:L:93:PHE:O	2.07	0.53
14:N:159:LEU:O	14:N:163:ILE:HD12	2.09	0.53
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.24	0.53
6:T:38:ILE:HG22	6:T:164:ALA:HA	1.91	0.53
2:B:51:GLU:CD	2:B:202:THR:HG23	2.34	0.52
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.90	0.52
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.38	0.52
7:G:233:LEU:O	7:G:236:ILE:HG12	2.09	0.52
9:I:67:LYS:HB3	16:I:216:HOH:O	2.09	0.52
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.89	0.52
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.90	0.52
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.92	0.52
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.73	0.52
2:P:224:PHE:N	2:P:224:PHE:HD2	2.07	0.52
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.39	0.52
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.91	0.52
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.91	0.52
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.39	0.52
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.08	0.52
9:I:29:ASN:ND2	9:I:29:ASN:H	2.07	0.52
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.55	0.52
2:P:150:THR:O	2:P:157:TYR:HA	2.09	0.52
5:S:201:LEU:O	5:S:202:ARG:HB2	2.09	0.52
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.90	0.52
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.90	0.52
4:D:192:LEU:O	4:D:196:ILE:HG13	2.10	0.52
9:I:29:ASN:C	9:I:29:ASN:HD22	2.18	0.52
10:J:52:THR:CG2	10:J:53:VAL:N	2.73	0.52
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.73	0.52
7:U:233:LEU:O	7:U:236:ILE:HG12	2.09	0.52
9:W:29:ASN:ND2	9:W:29:ASN:H	2.08	0.52
13:1:187:LYS:HB3	13:1:190:LEU:HD11	1.91	0.52
1:A:170:VAL:N	16:A:250:HOH:O	2.43	0.52
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.90	0.52
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.91	0.52
10:J:63:ILE:HD12	10:J:79:VAL:HG22	1.91	0.52
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.91	0.52
2:P:186:VAL:HG11	2:P:216:ARG:HD3	1.92	0.52
3:Q:15:PHE:H	4:R:23:GLN:NE2	2.04	0.52
3:Q:150:GLN:HG2	3:Q:151:THR:N	2.24	0.52
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.90	0.52
13:1:17:ASP:HA	13:1:173:PHE:CB	2.39	0.52
2:B:126:HIS:HA	16:C:264:HOH:O	2.10	0.52
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.90	0.52
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.92	0.52
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.66	0.52
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.92	0.52
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.91	0.52
1:A:112:LEU:O	1:A:116:VAL:HG23	2.10	0.52
3:C:227:GLU:OE1	3:C:227:GLU:N	2.30	0.52
2:P:27:ALA:O	2:P:31:ILE:HG12	2.09	0.52
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.09	0.52
1:A:150:GLN:O	1:A:157:TYR:HA	2.10	0.52
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.73	0.52
8:H:34:LEU:HB2	16:H:323:HOH:O	2.10	0.52
2:P:108:PRO:HB2	2:P:111:ILE:HD12	1.92	0.52
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.45	0.52
4:R:112:LEU:HD13	4:R:112:LEU:C	2.35	0.52
5:S:18(C):PHE:O	5:S:18(F):ILE:HG12	2.09	0.52
9:W:124:PHE:C	9:W:125:ILE:HD12	2.34	0.52
2:B:108:PRO:HB2	2:B:111:ILE:HD12	1.92	0.52
4:D:59:LEU:HD13	4:D:59:LEU:C	2.34	0.52
3:Q:121:GLN:NE2	3:Q:121:GLN:C	2.68	0.52
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.91	0.52
7:U:18(H):GLU:CD	7:U:18(H):GLU:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:193:GLN:HG2	10:X:193:GLN:OXT	2.08	0.52
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.45	0.52
12:Z:105:ASP:OD2	12:Z:107:LYS:HB2	2.10	0.52
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.92	0.52
2:B:160:TRP:HA	3:C:59:GLN:HA	1.92	0.51
8:H:52:THR:O	8:H:56:THR:HB	2.10	0.51
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.59	0.51
5:S:227:GLU:CD	5:S:227:GLU:N	2.67	0.51
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.93	0.51
2:B:150:THR:O	2:B:157:TYR:HA	2.10	0.51
2:B:220:TYR:CE1	2:B:222:LYS:HB2	2.45	0.51
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.32	0.51
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.10	0.51
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.11	0.51
2:B:44:ASP:OD2	2:B:186:VAL:HG23	2.10	0.51
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.92	0.51
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.90	0.51
2:P:190:ILE:HG21	2:P:232:ILE:CD1	2.40	0.51
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.93	0.51
4:R:59:LEU:HD13	4:R:59:LEU:C	2.35	0.51
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.10	0.51
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.92	0.51
9:W:29:ASN:C	9:W:29:ASN:HD22	2.18	0.51
9:W:61:TYR:CD1	9:W:61:TYR:C	2.89	0.51
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.41	0.51
12:Z:-9:GLN:CD	12:Z:-8:PHE:H	2.17	0.51
10:J:48:GLU:HB2	10:J:96:GLN:HB2	1.91	0.51
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.39	0.51
4:R:215:ILE:HD13	4:R:215:ILE:C	2.36	0.51
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.41	0.51
13:1:184:LEU:C	13:1:184:LEU:HD23	2.35	0.51
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.74	0.51
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.46	0.51
1:O:150:GLN:O	1:O:157:TYR:HA	2.10	0.51
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.93	0.51
13:1:1:THR:OG1	13:1:2:SER:N	2.43	0.51
6:F:28:VAL:O	6:F:32:GLU:HG3	2.10	0.51
6:F:184:LEU:CD1	6:F:188:GLU:HB3	2.37	0.51
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.93	0.51
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.10	0.51
9:W:122:ALA:HB3	9:W:125:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:GLY:C	2:B:124:THR:N	2.69	0.51
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.46	0.51
9:I:124:PHE:C	9:I:125:ILE:HD12	2.36	0.51
10:J:16:SER:HB2	16:J:202:HOH:O	2.10	0.51
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.41	0.51
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.09	0.51
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.93	0.51
5:S:123:ASN:HD22	5:S:123:ASN:N	2.07	0.51
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.46	0.51
14:2:67:THR:HA	14:2:72:GLY:O	2.11	0.51
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.92	0.51
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.74	0.51
9:W:16:CYS:HB3	9:W:34:ILE:HD11	1.92	0.51
4:D:240:LYS:O	4:D:243:ALA:HB3	2.11	0.51
9:I:105:ASN:HB3	9:I:10(C):SER:OG	2.11	0.51
10:J:148:THR:HG21	10:J:177:ILE:HD13	1.93	0.51
2:P:160:TRP:CD2	2:P:163:ILE:HD12	2.46	0.51
4:R:237:LEU:O	4:R:241:GLU:HG3	2.11	0.51
7:U:168:LYS:O	7:U:172:ILE:HG12	2.11	0.51
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.92	0.51
2:B:6:ARG:HH12	4:D:12(B):GLU:CD	2.18	0.51
2:B:20:ARG:HG2	2:B:20:ARG:HH11	1.76	0.51
11:K:4:LEU:C	11:K:4:LEU:CD2	2.84	0.51
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.51
9:W:101:VAL:O	9:W:110:ILE:HA	2.11	0.51
1:A:7:ARG:NH1	5:E:127:TYR:HD2	2.08	0.50
1:A:27:ALA:O	1:A:31:VAL:HG23	2.11	0.50
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.10	0.50
3:C:121:GLN:NE2	3:C:121:GLN:C	2.69	0.50
4:D:177:LEU:HA	5:E:58:LEU:HD11	1.93	0.50
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.45	0.50
1:O:212:LEU:HD23	1:O:212:LEU:C	2.36	0.50
12:L:79:ALA:O	12:L:83:ILE:HG13	2.11	0.50
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.10	0.50
1:A:29:THR:O	1:A:33:GLN:HG2	2.11	0.50
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.93	0.50
8:H:84:LYS:HG3	8:H:85:GLN:N	2.26	0.50
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.45	0.50
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.47	0.50
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.10	0.50
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	1.94	0.50
3:C:52:ARG:HD2	3:C:208:LYS:O	2.11	0.50
4:D:237:LEU:O	4:D:241:GLU:HG3	2.12	0.50
10:J:168:MET:CG	10:X:168:MET:HE3	2.38	0.50
3:Q:159:SER:HB2	16:Q:257:HOH:O	2.11	0.50
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.92	0.50
3:C:235:GLN:O	3:C:239:GLU:HG2	2.11	0.50
1:O:27:ALA:O	1:O:31:VAL:HG23	2.12	0.50
8:V:2:THR:HG22	8:V:159:ILE:HD13	1.92	0.50
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.46	0.50
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.85	0.50
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.47	0.50
2:B:111:ILE:HD11	10:J:70:GLU:HG2	1.92	0.50
3:C:224:LEU:N	3:C:224:LEU:CD1	2.75	0.50
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.12	0.50
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.76	0.50
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.47	0.50
5:S:199:GLN:N	5:S:199:GLN:HE21	2.09	0.50
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.12	0.50
3:C:173:ARG:O	3:C:177:GLU:HG3	2.12	0.50
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.41	0.50
8:H:175:VAL:HG12	8:H:176:CYS:N	2.25	0.50
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.12	0.50
5:S:177:GLU:OE1	6:T:56:SER:HB2	2.11	0.50
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.92	0.50
12:Z:180:LYS:HG2	16:Z:228:HOH:O	2.10	0.50
3:C:172:VAL:O	3:C:176:LEU:HG	2.11	0.50
3:C:228:GLU:O	3:C:232:TYR:HD1	1.94	0.50
4:D:70:ILE:HG13	4:D:74:ILE:HG22	1.93	0.50
6:F:199:LEU:HD12	6:F:240:ILE:HD12	1.94	0.50
14:N:147:SER:OG	14:N:150:GLU:HG3	2.11	0.50
1:O:10(A):ILE:N	1:O:10(A):ILE:HD12	2.27	0.50
10:X:52:THR:CG2	10:X:53:VAL:N	2.74	0.50
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.94	0.50
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.47	0.50
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.93	0.50
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.93	0.50
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.46	0.50
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.94	0.50
11:K:46:ALA:HB3	11:K:98:GLY:O	2.12	0.50
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:185:THR:HG23	4:R:188:GLU:OE1	2.11	0.50
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.42	0.49
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.46	0.49
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.40	0.49
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.93	0.49
7:G:18(D):ILE:HD12	7:G:18(D):ILE:N	2.27	0.49
8:H:16:ALA:HA	8:H:159:ILE:HD12	1.94	0.49
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.76	0.49
2:P:202:THR:CG2	2:P:204:SER:HB2	2.42	0.49
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.11	0.49
6:T:130:ARG:HG2	6:T:130:ARG:NH1	2.27	0.49
1:A:212:LEU:HD23	1:A:212:LEU:C	2.36	0.49
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.77	0.49
1:O:29:THR:O	1:O:33:GLN:HG2	2.11	0.49
2:P:51:GLU:CD	2:P:202:THR:HG23	2.36	0.49
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.11	0.49
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.75	0.49
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.43	0.49
5:E:233:ILE:HG22	5:E:233:ILE:OXT	2.12	0.49
12:L:-5:TYR:CE2	12:L:96:TYR:HB2	2.47	0.49
14:N:3:ILE:H	14:N:3:ILE:HD12	1.77	0.49
2:P:111:ILE:HD11	10:X:70:GLU:HG2	1.93	0.49
2:P:202:THR:HG21	2:P:204:SER:HB2	1.92	0.49
7:U:70:ILE:HG13	7:U:74:ILE:HG22	1.94	0.49
13:1:125:LEU:HA	16:1:217:HOH:O	2.12	0.49
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.12	0.49
7:G:70:ILE:HG13	7:G:74:ILE:HG22	1.94	0.49
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.47	0.49
4:R:121:LEU:HA	4:R:123:PHE:HE1	1.78	0.49
5:S:220:PRO:O	5:S:222:THR:HG23	2.12	0.49
6:T:157:TYR:CD1	6:T:157:TYR:C	2.90	0.49
8:V:52:THR:O	8:V:56:THR:HB	2.11	0.49
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.42	0.49
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.47	0.49
2:B:20:ARG:CZ	3:C:33:ARG:HH21	2.26	0.49
5:E:123:ASN:N	5:E:123:ASN:HD22	2.10	0.49
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.12	0.49
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.95	0.49
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.94	0.49
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.94	0.49
1:A:14:THR:O	1:A:21:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PRO:HG3	7:G:177:GLU:CD	2.38	0.49
2:B:61:GLN:NE2	2:B:226:PRO:HG3	2.28	0.49
5:E:201:LEU:O	5:E:202:ARG:HB2	2.11	0.49
3:Q:87:ILE:N	3:Q:87:ILE:CD1	2.76	0.49
4:R:240:LYS:O	4:R:243:ALA:HB3	2.13	0.49
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.92	0.49
9:W:105:ASN:HB3	9:W:10(C):SER:OG	2.11	0.49
1:A:10(A):ILE:N	1:A:10(A):ILE:HD12	2.28	0.49
3:C:159:SER:O	4:D:59:LEU:HD22	2.13	0.49
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.93	0.49
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.43	0.49
6:F:38:ILE:HG22	6:F:164:ALA:CA	2.41	0.49
6:F:127:ASN:HD22	6:F:127:ASN:C	2.20	0.49
1:O:112:LEU:O	1:O:116:VAL:HG23	2.12	0.49
7:U:8:TYR:C	7:U:10:ARG:H	2.21	0.49
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.93	0.49
10:J:-1:MET:CG	10:J:1:ASP:H	2.19	0.49
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.47	0.49
3:Q:159:SER:O	4:R:59:LEU:HD22	2.13	0.49
3:Q:241:GLN:O	3:Q:243:GLN:N	2.41	0.49
2:B:51:GLU:OE1	2:B:202:THR:HG23	2.12	0.49
2:B:191:GLU:O	2:B:195:LYS:HG2	2.13	0.49
7:G:151:THR:HG22	7:G:157:TYR:CB	2.42	0.49
12:L:17:ASP:OD2	12:L:33:LYS:NZ	2.45	0.49
12:L:43:MET:HG2	12:L:44:SER:N	2.28	0.49
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.94	0.49
11:K:131:GLN:HG3	11:K:132:THR:N	2.28	0.49
1:O:122:GLU:C	1:O:124:THR:H	2.21	0.49
3:Q:55:THR:HG22	3:Q:56:LEU:CD2	2.41	0.49
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.95	0.49
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.48	0.49
1:A:130:ARG:HG2	7:G:125:GLN:HG3	1.94	0.48
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.48	0.48
9:I:101:VAL:O	9:I:110:ILE:HA	2.14	0.48
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.42	0.48
10:X:166:MET:CE	10:X:168:MET:HB2	2.43	0.48
2:B:235:LYS:C	2:B:237:GLY:N	2.70	0.48
10:J:168:MET:HE3	10:X:168:MET:CG	2.42	0.48
11:K:97:MET:O	11:K:114:ASP:HA	2.13	0.48
12:L:109:ALA:HA	16:L:225:HOH:O	2.13	0.48
13:M:112:TYR:C	13:M:112:TYR:CD2	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.29	0.48
6:T:18:ASP:OD1	6:T:20:ARG:HD3	2.14	0.48
7:U:38:LEU:C	7:U:38:LEU:HD12	2.38	0.48
8:V:49:ALA:HB2	15:V:301:SLA:H16	1.95	0.48
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.48	0.48
12:L:76:ILE:HG23	12:L:77:ASN:N	2.29	0.48
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.42	0.48
7:U:18(D):ILE:HD12	7:U:18(D):ILE:N	2.29	0.48
10:X:4:LEU:HD23	10:X:126:ALA:HB2	1.95	0.48
10:X:148:THR:HG21	10:X:177:ILE:HD13	1.96	0.48
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.13	0.48
2:B:160:TRP:CD2	2:B:163:ILE:HD12	2.48	0.48
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.15	0.48
11:K:207:ASN:HD21	10:X:144:PRO:HG2	1.78	0.48
12:L:42:VAL:HG23	12:L:102:ALA:HB3	1.95	0.48
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.48	0.48
9:W:113:PHE:HA	9:W:118:CYS:O	2.14	0.48
13:1:150:VAL:HG21	16:1:232:HOH:O	2.13	0.48
14:2:105:ASP:OD2	14:2:106:ASN:N	2.44	0.48
3:C:65:SER:HB2	16:C:252:HOH:O	2.14	0.48
3:C:102:THR:OG1	3:C:103:LEU:HD22	2.13	0.48
5:E:226:GLY:O	5:E:229:VAL:HG22	2.14	0.48
7:G:8:TYR:C	7:G:10:ARG:H	2.21	0.48
7:G:9:ASP:OD2	7:G:16:SER:HA	2.13	0.48
10:J:39:PRO:HG2	10:J:73:GLU:CD	2.38	0.48
13:M:1:THR:OG1	13:M:2:SER:N	2.46	0.48
2:P:220:TYR:CE1	2:P:222:LYS:HB2	2.48	0.48
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.28	0.48
2:B:186:VAL:HG11	2:B:216:ARG:HD3	1.95	0.48
5:E:190:ILE:O	5:E:194:VAL:HG23	2.13	0.48
5:E:199:GLN:HE21	5:E:199:GLN:N	2.10	0.48
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.82	0.48
1:O:169:SER:O	1:O:173:LYS:HG3	2.14	0.48
5:S:233:ILE:HG22	5:S:233:ILE:OXT	2.14	0.48
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.44	0.48
10:X:39:PRO:HG2	10:X:73:GLU:CD	2.39	0.48
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.44	0.48
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.49	0.48
13:1:91:ARG:HG3	13:1:92:SER:N	2.28	0.48
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.14	0.48
5:E:220:PRO:O	5:E:222:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.44	0.48
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.49	0.48
2:P:6:ARG:HH12	4:R:12(B):GLU:CD	2.22	0.48
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.96	0.48
2:P:191:GLU:O	2:P:195:LYS:HG2	2.14	0.48
2:P:235:LYS:C	2:P:237:GLY:N	2.70	0.48
7:U:9:ASP:OD2	7:U:16:SER:HA	2.14	0.48
7:U:203:THR:HG22	7:U:204:GLU:O	2.13	0.48
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.13	0.48
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.95	0.48
8:H:172:ASN:HD22	8:H:193:THR:HA	1.79	0.48
8:V:175:VAL:HG12	8:V:176:CYS:N	2.29	0.48
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.49	0.48
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.96	0.48
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.13	0.48
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.77	0.48
1:A:169:SER:O	1:A:173:LYS:HG3	2.14	0.48
4:D:86:ARG:HA	4:D:86:ARG:HD3	1.77	0.48
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.13	0.48
4:R:241:GLU:C	4:R:243:ALA:H	2.21	0.48
6:T:100:LYS:NZ	16:T:267:HOH:O	2.47	0.48
9:W:80:THR:HG22	9:W:119:ILE:HD13	1.96	0.48
10:X:93:ARG:NH2	11:Y:91:LYS:HD3	2.28	0.48
2:B:55:THR:HG22	2:B:59:LEU:HD23	1.96	0.47
2:B:202:THR:HG21	2:B:204:SER:HB2	1.95	0.47
6:F:52:LYS:HB2	6:F:209:GLU:O	2.14	0.47
7:G:18(H):GLU:CD	7:G:18(H):GLU:H	2.21	0.47
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.43	0.47
7:U:47:VAL:HG12	7:U:49:ILE:CD1	2.44	0.47
14:2:58:ILE:HG22	14:2:62:HIS:HD2	1.79	0.47
4:D:241:GLU:C	4:D:243:ALA:H	2.21	0.47
16:F:252:HOH:O	14:N:70:TYR:HE2	1.97	0.47
6:T:28:VAL:O	6:T:32:GLU:HG3	2.14	0.47
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.27	0.47
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.68	0.47
7:G:38:LEU:C	7:G:38:LEU:HD12	2.39	0.47
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.14	0.47
10:J:189:ASP:O	10:J:193:GLN:HB2	2.15	0.47
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.44	0.47
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.80	0.47
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:63:ILE:HD12	10:X:79:VAL:HG22	1.95	0.47
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.95	0.47
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.30	0.47
1:A:186:LEU:O	1:A:190:ILE:HG13	2.14	0.47
3:C:87:ILE:N	3:C:87:ILE:CD1	2.76	0.47
10:J:166:MET:CE	10:J:168:MET:HB2	2.43	0.47
14:N:18(A):ILE:HD13	14:N:18(B):PHE:N	2.29	0.47
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.15	0.47
2:P:21(A):LYS:O	2:P:217:ALA:N	2.47	0.47
16:R:258:HOH:O	12:Z:70:HIS:HE1	1.95	0.47
5:S:67:ILE:HG21	5:S:213:ALA:HB2	1.96	0.47
7:U:35:ILE:HD11	16:U:285:HOH:O	2.14	0.47
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.95	0.47
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.93	0.47
4:D:170:GLU:N	4:D:170:GLU:OE1	2.46	0.47
7:G:93:LYS:HD3	14:N:68:SER:HB3	1.96	0.47
9:I:61:TYR:CD1	9:I:61:TYR:C	2.92	0.47
4:R:70:ILE:HG13	4:R:74:ILE:HG22	1.95	0.47
6:T:136:THR:O	6:T:150:MET:HA	2.14	0.47
14:2:3:ILE:HB	14:2:44:CYS:HB3	1.95	0.47
14:2:116:GLY:HA3	16:2:190:HOH:O	2.14	0.47
4:D:91:HIS:CE1	4:D:119:LEU:HD21	2.49	0.47
4:D:121:LEU:HA	4:D:123:PHE:HE1	1.79	0.47
13:M:168:ARG:HB2	16:M:240:HOH:O	2.14	0.47
1:O:8:TYR:CD2	7:U:128:TYR:HB3	2.49	0.47
1:O:62:GLU:CD	1:O:62:GLU:H	2.22	0.47
3:Q:102:THR:OG1	3:Q:103:LEU:HD22	2.13	0.47
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.29	0.47
14:2:18(A):ILE:HD13	14:2:18(B):PHE:N	2.29	0.47
1:A:8:TYR:CD2	7:G:128:TYR:HB3	2.48	0.47
1:A:62:GLU:CD	1:A:62:GLU:H	2.21	0.47
2:B:11:ARG:HD2	3:C:10:ARG:CZ	2.44	0.47
2:B:190:ILE:HG21	2:B:232:ILE:CD1	2.42	0.47
4:D:122:ARG:HG2	4:D:122:ARG:NH1	2.29	0.47
6:F:130:ARG:HG2	6:F:130:ARG:NH1	2.29	0.47
7:G:168:LYS:O	7:G:172:ILE:HG12	2.14	0.47
7:G:203:THR:HG22	7:G:204:GLU:O	2.15	0.47
10:J:133:TYR:HE1	16:Y:219:HOH:O	1.97	0.47
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.96	0.47
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.29	0.47
2:P:60:GLU:OE1	2:P:60:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.78	0.47
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.96	0.47
5:S:2(C):VAL:HG22	5:S:226:GLY:C	2.40	0.47
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.45	0.47
9:W:89:GLU:HG2	9:W:90:ARG:NH1	2.30	0.47
10:X:45:PHE:CE1	10:X:52:THR:HG23	2.50	0.47
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.15	0.47
3:C:85:SER:O	3:C:89:ILE:HD12	2.14	0.47
9:I:192:ARG:HD3	16:I:242:HOH:O	2.14	0.47
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.96	0.47
13:M:149:GLN:NE2	13:M:149:GLN:N	2.54	0.47
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.97	0.47
2:P:20:ARG:HG2	2:P:20:ARG:HH11	1.78	0.47
2:P:27:ALA:O	2:P:30:SER:HB3	2.15	0.47
2:P:38:ILE:HG12	2:P:164:SER:HB3	1.97	0.47
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.15	0.47
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	2.14	0.47
6:T:52:LYS:HB2	6:T:209:GLU:O	2.14	0.47
8:V:16:ALA:HA	8:V:159:ILE:HD12	1.95	0.47
10:X:189:ASP:O	10:X:193:GLN:HB2	2.14	0.47
12:Z:43:MET:HG2	12:Z:44:SER:N	2.28	0.47
2:B:21(A):LYS:O	2:B:217:ALA:N	2.47	0.47
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.49	0.47
10:J:112:GLN:NE2	10:J:126:ALA:H	2.12	0.47
11:K:205:SER:HB2	10:X:140:HIS:HA	1.96	0.47
2:P:55:THR:HG22	2:P:59:LEU:HD23	1.96	0.47
4:R:170:GLU:OE1	4:R:170:GLU:N	2.48	0.47
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.29	0.47
13:1:157:ASN:HB3	16:1:248:HOH:O	2.13	0.47
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.97	0.47
6:F:157:TYR:CD1	6:F:157:TYR:C	2.92	0.47
12:L:176:LEU:CD1	12:L:186:LYS:HG2	2.45	0.47
1:O:5:THR:O	1:O:7:ARG:HG2	2.15	0.47
5:S:15:PHE:H	6:T:23:GLN:NE2	2.06	0.47
8:V:41:ILE:HG12	8:V:76:VAL:HG22	1.97	0.47
8:V:206:PHE:CE2	9:W:157:GLN:HG3	2.50	0.47
9:W:20:LEU:C	9:W:20:LEU:HD13	2.39	0.47
9:W:177:ILE:HD13	9:W:177:ILE:N	2.30	0.47
10:X:7:ARG:HG2	10:X:7:ARG:NH1	2.29	0.47
2:B:60:GLU:OE1	2:B:60:GLU:HA	2.15	0.46
2:B:202:THR:CG2	2:B:204:SER:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:48:VAL:C	7:G:49:ILE:HD12	2.41	0.46
12:L:135:MET:CE	9:W:165:ARG:NH2	2.78	0.46
2:P:232:ILE:O	2:P:232:ILE:HG13	2.14	0.46
3:Q:33:ARG:HG2	3:Q:33:ARG:O	2.15	0.46
11:Y:97:MET:O	11:Y:114:ASP:HA	2.14	0.46
1:A:5:THR:O	1:A:7:ARG:HG2	2.15	0.46
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.45	0.46
3:C:234:THR:HG22	3:C:238:GLN:HE21	1.80	0.46
5:E:18(D):ILE:HG12	5:E:18(D):ILE:O	2.14	0.46
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.62	0.46
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.97	0.46
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.97	0.46
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.30	0.46
8:V:63:ILE:CG2	8:V:74:PRO:HB3	2.45	0.46
9:W:89:GLU:O	9:W:90:ARG:NH1	2.48	0.46
10:X:90(A):ILE:HD13	10:X:90(A):ILE:HA	1.79	0.46
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.16	0.46
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.97	0.46
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.43	0.46
14:N:26:ILE:HB	13:1:165:ARG:HA	1.98	0.46
11:Y:132:THR:HG22	16:Y:219:HOH:O	2.15	0.46
13:1:171:ARG:O	13:1:192:VAL:HG23	2.16	0.46
3:C:122:ARG:NH2	16:C:267:HOH:O	2.49	0.46
5:E:47:VAL:CG2	5:E:189:LEU:HD13	2.42	0.46
9:I:122:ALA:HB3	9:I:125:ILE:HD11	1.96	0.46
11:K:12:ILE:HG23	11:K:110:ILE:HD11	1.97	0.46
2:P:51:GLU:OE1	2:P:202:THR:HG23	2.16	0.46
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.40	0.46
5:S:90:ASN:ND2	16:S:245:HOH:O	2.47	0.46
6:T:38:ILE:HG22	6:T:164:ALA:CA	2.44	0.46
12:Z:79:ALA:O	12:Z:83:ILE:HG13	2.15	0.46
13:1:133:MET:O	13:1:136:PRO:HD2	2.16	0.46
1:A:110:LYS:HG2	16:A:245:HOH:O	2.14	0.46
3:C:15:PHE:H	4:D:23:GLN:NE2	2.03	0.46
5:E:198:SER:HA	5:E:201:LEU:HG	1.98	0.46
6:F:166:GLY:O	6:F:169:ARG:HB3	2.15	0.46
12:L:9:GLU:O	12:L:107:LYS:HD3	2.16	0.46
14:N:116:GLY:HA3	16:N:195:HOH:O	2.15	0.46
1:O:130:ARG:HG2	7:U:125:GLN:HG3	1.98	0.46
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.97	0.46
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:29:GLU:OE2	4:R:32:LYS:HD2	2.16	0.46
9:W:33:LYS:O	9:W:44:GLY:HA2	2.16	0.46
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.16	0.46
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.15	0.46
7:G:141:VAL:HG21	7:G:216:THR:HA	1.97	0.46
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	1.98	0.46
3:Q:185:THR:CB	3:Q:188:GLU:HG2	2.41	0.46
3:Q:234:THR:HG22	3:Q:238:GLN:HE21	1.80	0.46
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.97	0.46
6:T:172:ALA:C	6:T:176:LEU:HD23	2.41	0.46
7:U:158:VAL:HG22	7:U:159:GLY:N	2.31	0.46
9:W:22:SER:O	9:W:23:GLN:HB2	2.15	0.46
11:Y:12:ILE:HG23	11:Y:110:ILE:HD11	1.98	0.46
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.80	0.46
9:I:20:LEU:HD13	9:I:20:LEU:C	2.41	0.46
10:J:85:GLN:O	10:J:89:LYS:HG3	2.16	0.46
13:M:40:ASN:N	13:M:40:ASN:ND2	2.64	0.46
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.31	0.46
8:V:100:ILE:HD11	8:V:127:LEU:HG	1.98	0.46
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.50	0.46
14:2:3:ILE:HG22	14:2:16:ALA:HB1	1.97	0.46
14:2:19:ARG:HG3	14:2:26:ILE:HG23	1.98	0.46
14:2:147:SER:OG	14:2:150:GLU:HG3	2.16	0.46
2:B:20:ARG:HG2	2:B:20:ARG:NH1	2.28	0.46
2:B:232:ILE:O	2:B:232:ILE:HG13	2.14	0.46
5:E:148:LEU:HD23	5:E:162:GLY:HA2	1.97	0.46
8:H:9:ASN:OD1	8:H:10:ASN:N	2.49	0.46
1:A:217:ASP:O	1:A:220:ARG:HA	2.16	0.46
5:E:2(C):VAL:HG22	5:E:226:GLY:C	2.41	0.46
9:I:33:LYS:O	9:I:44:GLY:HA2	2.16	0.46
10:J:140:HIS:HA	11:Y:205:SER:HB2	1.97	0.46
11:K:13:ILE:HD12	11:K:152:LEU:HD23	1.98	0.46
12:L:-2:ASN:HA	12:L:21:ILE:O	2.15	0.46
5:S:190:ILE:O	5:S:194:VAL:HG23	2.15	0.46
6:T:91:ARG:HG2	6:T:119:TYR:CD2	2.51	0.46
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.46	0.46
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.16	0.46
7:G:158:VAL:HG22	7:G:159:GLY:N	2.31	0.46
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.51	0.46
13:M:171:ARG:O	13:M:192:VAL:HG23	2.16	0.46
4:R:29:GLU:OE2	4:R:29:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.16	0.46
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.16	0.46
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.16	0.45
9:I:22:SER:O	9:I:23:GLN:HB2	2.16	0.45
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.16	0.45
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.51	0.45
7:U:190:VAL:O	7:U:194:ILE:HD12	2.16	0.45
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.97	0.45
12:Z:9:GLU:O	12:Z:107:LYS:HD3	2.15	0.45
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.97	0.45
13:1:148:VAL:HG23	16:1:227:HOH:O	2.16	0.45
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.98	0.45
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.99	0.45
3:C:79:SER:HA	16:C:261:HOH:O	2.15	0.45
4:D:187:LYS:O	4:D:191:LEU:HD22	2.16	0.45
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.97	0.45
2:P:136:PHE:O	2:P:150:THR:HA	2.17	0.45
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.51	0.45
4:R:91:HIS:CE1	4:R:119:LEU:HD21	2.51	0.45
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.98	0.45
10:X:166:MET:HA	10:X:167:PRO:HD3	1.80	0.45
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.17	0.45
1:A:38:LEU:C	1:A:38:LEU:HD12	2.40	0.45
13:M:17:ASP:HA	13:M:173:PHE:HA	1.98	0.45
2:P:121:GLN:HG2	3:Q:83:ALA:HB1	1.97	0.45
2:P:122:GLY:C	2:P:124:THR:N	2.68	0.45
8:V:9:ASN:OD1	8:V:10:ASN:N	2.48	0.45
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.99	0.45
12:Z:17:ASP:OD2	12:Z:33:LYS:NZ	2.45	0.45
14:2:10(B):LYS:O	14:2:10(B):LYS:HD3	2.17	0.45
1:A:4:MET:O	1:A:5:THR:O	2.34	0.45
1:A:122:GLU:C	1:A:124:THR:H	2.23	0.45
4:D:91:HIS:CG	4:D:119:LEU:HD11	2.52	0.45
6:F:199:LEU:HD12	6:F:240:ILE:CD1	2.46	0.45
8:H:48:THR:HB	8:H:51:ASP:HB2	1.97	0.45
9:I:113:PHE:HA	9:I:118:CYS:O	2.16	0.45
10:J:14:LEU:HD12	10:J:42:LEU:HD23	1.98	0.45
11:K:146:LEU:HD23	11:K:151:ALA:HA	1.98	0.45
2:P:194:LEU:HD13	2:P:233:LEU:HD12	1.98	0.45
5:S:226:GLY:O	5:S:229:VAL:HG22	2.16	0.45
7:U:13:THR:HB	7:U:124:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:60:GLN:O	10:X:64:GLN:HG3	2.16	0.45
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.14	0.45
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.32	0.45
7:G:190:VAL:O	7:G:194:ILE:HD12	2.15	0.45
12:L:17:ASP:HA	12:L:172:GLY:O	2.17	0.45
12:L:139:ASP:O	12:L:14(A):LYS:HG2	2.17	0.45
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.98	0.45
3:Q:101:LEU:HD11	10:X:57:GLU:HB3	1.99	0.45
3:Q:112:LEU:O	3:Q:116:VAL:HG23	2.16	0.45
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.99	0.45
6:T:11:SER:HB3	6:T:14:VAL:CG2	2.46	0.45
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.97	0.45
11:Y:40:PHE:CD1	11:Y:73:ARG:NH1	2.85	0.45
12:Z:139:ASP:O	12:Z:14(A):LYS:HG2	2.16	0.45
13:1:149:GLN:NE2	13:1:149:GLN:N	2.58	0.45
1:A:67:VAL:CG2	1:A:211:GLU:HG2	2.47	0.45
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.51	0.45
3:C:186:VAL:O	3:C:190:VAL:HG23	2.17	0.45
9:I:89:GLU:O	9:I:90:ARG:NH1	2.50	0.45
13:M:46:SER:OG	13:M:98:ALA:HB3	2.16	0.45
14:N:105:ASP:OD2	14:N:106:ASN:N	2.45	0.45
6:T:166:GLY:O	6:T:169:ARG:HB3	2.17	0.45
14:2:172:VAL:HB	14:2:18(A):ILE:CD1	2.46	0.45
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.52	0.45
6:F:18:ASP:OD1	6:F:20:ARG:HD3	2.16	0.45
6:F:136:THR:O	6:F:150:MET:HA	2.17	0.45
8:H:49:ALA:HB2	15:H:301:SLA:H16	1.97	0.45
12:L:-9:GLN:NE2	12:L:-8:PHE:N	2.64	0.45
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	1.98	0.45
13:1:133:MET:C	13:1:136:PRO:HD2	2.42	0.45
1:A:7:ARG:NH1	5:E:127:TYR:CD2	2.85	0.45
8:H:135:MET:HE3	13:1:165:ARG:NH2	2.31	0.45
14:N:58:ILE:HG22	14:N:62:HIS:HD2	1.82	0.45
1:O:4:MET:O	1:O:5:THR:O	2.35	0.45
1:O:38:LEU:C	1:O:38:LEU:HD12	2.42	0.45
2:P:61:GLN:NE2	2:P:226:PRO:HG3	2.31	0.45
3:Q:158:SER:CB	4:R:59:LEU:HD21	2.46	0.45
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.51	0.45
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.52	0.45
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.31	0.45
7:U:48:VAL:C	7:U:49:ILE:HD12	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.99	0.45
10:X:112:GLN:NE2	10:X:126:ALA:H	2.14	0.45
12:Z:99:THR:CG2	16:Z:199:HOH:O	2.64	0.45
13:1:175:LEU:HD23	13:1:175:LEU:C	2.42	0.45
14:2:14:LEU:O	14:2:175:MET:HA	2.16	0.45
2:B:38:ILE:HG12	2:B:164:SER:HB3	1.98	0.45
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.47	0.45
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.47	0.45
9:I:137:MET:CE	9:I:141:LEU:HD11	2.47	0.45
11:K:6:PHE:HA	11:K:123:ASP:O	2.16	0.45
13:M:164:TYR:O	14:2:26:ILE:HD12	2.17	0.45
14:N:3:ILE:HG22	14:N:16:ALA:HB1	1.98	0.45
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.81	0.45
12:Z:58:ARG:NH2	16:Z:227:HOH:O	2.50	0.45
3:C:112:LEU:O	3:C:116:VAL:HG23	2.17	0.45
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.17	0.45
6:F:127:ASN:ND2	6:F:127:ASN:H	2.15	0.45
7:G:203:THR:HG22	7:G:204:GLU:N	2.32	0.45
9:I:3:VAL:HG23	9:I:46:THR:HG22	1.98	0.45
11:K:67:GLU:OE1	11:K:74:ILE:HG22	2.17	0.45
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.80	0.45
12:L:14(Q):LEU:O	12:L:14(W):LYS:C	2.59	0.45
1:O:217:ASP:O	1:O:220:ARG:HA	2.17	0.45
5:S:2(C):VAL:O	5:S:226:GLY:HA2	2.17	0.45
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.98	0.45
1:A:197:LEU:HD23	1:A:210:ILE:HD13	1.98	0.44
6:F:127:ASN:HD22	6:F:127:ASN:N	2.15	0.44
2:P:121:GLN:NE2	2:P:121:GLN:C	2.75	0.44
6:T:127:ASN:C	6:T:127:ASN:ND2	2.75	0.44
10:X:77:GLN:C	10:X:77:GLN:NE2	2.74	0.44
14:2:4:MET:CB	14:2:126:ILE:HG22	2.47	0.44
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.17	0.44
1:A:85:TYR:O	1:A:89:VAL:HG23	2.17	0.44
2:B:21(C):ASP:OD2	2:B:219:GLU:HB3	2.16	0.44
5:E:2(C):VAL:O	5:E:226:GLY:HA2	2.18	0.44
7:G:211:GLU:HA	16:G:256:HOH:O	2.18	0.44
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.53	0.44
13:M:91:ARG:HG3	13:M:92:SER:N	2.31	0.44
13:M:165:ARG:HA	14:2:26:ILE:HB	1.98	0.44
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.99	0.44
3:Q:18:ASP:OD2	3:Q:20:HIS:ND1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:52:ARG:NH2	3:Q:211:GLU:HB3	2.31	0.44
5:S:93:ARG:HD2	16:S:245:HOH:O	2.16	0.44
5:S:123:ASN:N	5:S:123:ASN:ND2	2.65	0.44
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.16	0.44
3:C:52:ARG:NH2	3:C:211:GLU:HB3	2.32	0.44
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.99	0.44
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.98	0.44
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.99	0.44
14:N:85:GLU:O	14:N:89:GLU:HB2	2.18	0.44
14:N:18(A):ILE:HD13	14:N:18(B):PHE:H	1.82	0.44
3:Q:33:ARG:CB	3:Q:33:ARG:NH1	2.67	0.44
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.98	0.44
5:S:90:ASN:O	5:S:94:GLN:HG3	2.17	0.44
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.47	0.44
11:Y:76:VAL:HG22	11:Y:103:GLY:HA3	1.98	0.44
13:1:112:TYR:C	13:1:112:TYR:CD2	2.94	0.44
2:B:41:MET:HE1	3:C:60:ASP:OD1	2.17	0.44
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.98	0.44
3:C:55:THR:HG22	3:C:56:LEU:CD2	2.44	0.44
3:C:241:GLN:O	3:C:243:GLN:N	2.41	0.44
4:D:12(F):GLY:HA3	16:D:262:HOH:O	2.17	0.44
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.51	0.44
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.99	0.44
9:I:6:MET:HE1	9:I:155:ILE:HA	2.00	0.44
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.98	0.44
1:O:184:LEU:HB2	16:O:246:HOH:O	2.17	0.44
2:P:21(C):ASP:OD2	2:P:219:GLU:HB3	2.17	0.44
4:R:91:HIS:CG	4:R:119:LEU:HD11	2.52	0.44
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.99	0.44
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.99	0.44
2:B:31:ILE:HD11	2:B:133:GLY:C	2.43	0.44
3:C:55:THR:C	3:C:56:LEU:HD22	2.43	0.44
3:C:107:VAL:HA	16:C:250:HOH:O	2.17	0.44
13:M:130:GLY:O	13:M:134:ALA:HB3	2.17	0.44
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.53	0.44
10:X:178:VAL:HG22	10:X:184:ILE:HG12	2.00	0.44
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.82	0.44
14:2:18(A):ILE:HD13	14:2:18(B):PHE:H	1.83	0.44
3:C:72:SER:O	3:C:221:ILE:HD12	2.17	0.44
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.99	0.44
5:E:66:LYS:O	5:E:77:SER:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:ASN:N	6:F:43:ASN:ND2	2.66	0.44
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.48	0.44
1:O:186:LEU:O	1:O:190:ILE:HG13	2.18	0.44
5:S:198:SER:HA	5:S:201:LEU:HG	1.99	0.44
6:T:187:ARG:HH11	6:T:187:ARG:CG	2.30	0.44
7:U:141:VAL:HG21	7:U:216:THR:HA	2.00	0.44
8:V:78:SER:O	8:V:82:MET:HG3	2.18	0.44
9:W:15:ALA:HB2	9:W:175:VAL:HG22	2.00	0.44
2:B:97:GLN:NE2	16:B:246:HOH:O	2.50	0.44
3:C:18:ASP:OD2	3:C:20:HIS:ND1	2.51	0.44
8:H:62:ASN:HB3	8:H:82:MET:HE1	1.99	0.44
9:I:15:ALA:HB1	9:I:159:LEU:HD22	2.00	0.44
9:I:80:THR:HG22	9:I:119:ILE:HD13	1.98	0.44
9:I:84:SER:HB2	9:I:119:ILE:HD11	2.00	0.44
12:L:93:PHE:N	12:L:94:PRO:HD3	2.33	0.44
13:M:85:THR:O	13:M:89:GLN:HG3	2.18	0.44
10:X:52:THR:HG22	10:X:53:VAL:H	1.83	0.44
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.17	0.44
4:D:29:GLU:OE2	4:D:29:GLU:HA	2.18	0.44
5:E:4:PHE:CG	5:E:5:ARG:N	2.86	0.44
9:I:15:ALA:HB2	9:I:175:VAL:HG22	1.98	0.44
10:J:167:PRO:C	10:X:168:MET:HE2	2.43	0.44
11:K:195:LEU:O	11:K:199:VAL:HG23	2.18	0.44
11:K:200:LYS:HG3	11:K:206:PHE:HB2	2.00	0.44
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.53	0.44
3:Q:215:VAL:HG23	3:Q:221:ILE:HG13	1.99	0.44
5:S:20:ARG:HB3	5:S:25:GLU:OE2	2.17	0.44
9:W:3:VAL:HG23	9:W:46:THR:HG22	1.99	0.44
10:X:85:GLN:O	10:X:89:LYS:HG3	2.17	0.44
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.53	0.44
13:1:177:ILE:HD12	13:1:177:ILE:N	2.33	0.44
4:D:42:THR:C	4:D:44:GLU:H	2.26	0.44
5:E:104:ASN:HB2	13:M:81:GLU:HG2	2.00	0.44
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.18	0.44
11:K:86:LEU:O	11:K:89:GLN:HB2	2.17	0.44
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.53	0.44
1:O:67:VAL:CG2	1:O:211:GLU:HG2	2.48	0.44
7:U:152:ASP:HB2	7:U:153:PRO:HD2	2.00	0.44
14:2:146:MET:HB3	14:2:150:GLU:HB2	2.00	0.44
4:D:170:GLU:N	4:D:170:GLU:CD	2.76	0.43
6:F:172:ALA:C	6:F:176:LEU:HD23	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:LEU:HD23	10:J:126:ALA:HB2	2.00	0.43
13:M:177:ILE:HD12	13:M:177:ILE:N	2.33	0.43
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.53	0.43
14:N:14:LEU:O	14:N:175:MET:HA	2.17	0.43
4:R:187:LYS:O	4:R:191:LEU:HD22	2.18	0.43
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.18	0.43
13:1:131:ALA:HA	13:1:135:ASN:ND2	2.33	0.43
3:C:215:VAL:HG23	3:C:221:ILE:HG13	1.99	0.43
5:E:90:ASN:O	5:E:94:GLN:HG3	2.17	0.43
6:F:180:VAL:HG21	7:G:58:LEU:HD23	2.00	0.43
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.33	0.43
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.33	0.43
10:J:45:PHE:CD1	10:J:52:THR:HG23	2.53	0.43
10:J:144:PRO:HG2	11:Y:207:ASN:HD21	1.83	0.43
10:J:178:VAL:HG22	10:J:184:ILE:HG12	2.00	0.43
13:M:3:VAL:HG23	13:M:46:SER:HB3	2.00	0.43
1:O:197:LEU:HD23	1:O:210:ILE:HD13	1.99	0.43
3:Q:215:VAL:HG23	3:Q:221:ILE:CG1	2.48	0.43
5:S:180:LEU:O	5:S:18(D):ILE:HG22	2.19	0.43
7:U:151:THR:HG22	7:U:157:TYR:CB	2.46	0.43
8:V:221:ILE:HD13	8:V:221:ILE:N	2.33	0.43
11:Y:114:ASP:C	11:Y:114:ASP:OD1	2.61	0.43
8:H:30:ASN:O	8:H:189:ARG:NH2	2.51	0.43
9:I:114:ASP:HB2	16:I:231:HOH:O	2.17	0.43
12:L:13:VAL:HG12	12:L:177:ILE:HG13	2.00	0.43
13:M:211:ILE:HD11	16:2:196:HOH:O	2.18	0.43
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.16	0.43
5:S:4:PHE:CG	5:S:5:ARG:N	2.86	0.43
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.89	0.43
7:U:203:THR:HG22	7:U:204:GLU:N	2.33	0.43
8:V:48:THR:HB	8:V:51:ASP:HB2	1.99	0.43
2:B:15:PHE:N	3:C:23:GLN:HE22	2.05	0.43
3:C:55:THR:O	3:C:56:LEU:HD22	2.17	0.43
10:J:77:GLN:NE2	10:J:77:GLN:C	2.76	0.43
2:P:235:LYS:HD3	2:P:235:LYS:N	2.33	0.43
4:R:68:VAL:HG21	4:R:89:ILE:CD1	2.27	0.43
7:U:186:TRP:O	7:U:190:VAL:HG23	2.18	0.43
7:U:188:LYS:HD3	7:U:188:LYS:HA	1.78	0.43
12:Z:113:PHE:N	12:Z:113:PHE:CD1	2.87	0.43
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.53	0.43
14:2:44:CYS:HB2	14:2:100:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:TYR:HE1	4:D:216:THR:HA	1.83	0.43
5:E:177:GLU:OE1	6:F:56:SER:HB2	2.19	0.43
8:H:84:LYS:HE2	8:H:119:THR:CG2	2.48	0.43
8:H:167:LEU:HD12	12:Z:24:TYR:HA	2.00	0.43
9:I:45:ILE:HB	9:I:52:VAL:HG13	2.00	0.43
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.80	0.43
12:L:113:PHE:N	12:L:113:PHE:CD1	2.86	0.43
14:N:10(B):LYS:O	14:N:10(B):LYS:HD3	2.18	0.43
4:R:42:THR:C	4:R:44:GLU:H	2.26	0.43
6:T:199:LEU:HD12	6:T:240:ILE:CD1	2.49	0.43
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	2.01	0.43
13:1:17:ASP:HA	13:1:173:PHE:HA	1.99	0.43
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.53	0.43
12:L:43:MET:HG3	12:L:101:ILE:HG22	2.01	0.43
13:M:175:LEU:HD23	13:M:175:LEU:C	2.42	0.43
14:N:105:ASP:HB2	16:N:218:HOH:O	2.18	0.43
1:O:186:LEU:HD21	1:O:214:ILE:HD12	2.01	0.43
5:S:66:LYS:O	5:S:77:SER:HA	2.18	0.43
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.18	0.43
4:D:161:ASN:HB3	4:D:180:TRP:CZ2	2.53	0.43
6:F:18(E):GLU:H	6:F:18(E):GLU:CD	2.26	0.43
14:N:172:VAL:HB	14:N:18(A):ILE:CD1	2.48	0.43
2:P:103:TYR:O	2:P:104:ASN:HB2	2.18	0.43
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.18	0.43
12:Z:14(Q):LEU:O	12:Z:14(W):LYS:C	2.60	0.43
5:E:54:ASN:ND2	5:E:56:ASP:O	2.52	0.43
7:G:186:TRP:O	7:G:190:VAL:HG23	2.19	0.43
9:I:15:ALA:CB	9:I:175:VAL:HG22	2.49	0.43
12:L:98:HIS:HD2	16:L:198:HOH:O	2.01	0.43
13:M:165:ARG:NH2	8:V:135:MET:HE3	2.34	0.43
14:N:114:PRO:HD2	14:N:118:SER:O	2.19	0.43
2:P:74:ILE:C	2:P:221:GLN:HE22	2.27	0.43
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.82	0.43
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.83	0.43
3:C:33:ARG:O	3:C:33:ARG:HG2	2.19	0.43
3:C:215:VAL:HG23	3:C:221:ILE:CG1	2.49	0.43
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.99	0.43
4:D:243:ALA:O	4:D:244:GLU:HB2	2.18	0.43
8:H:100:ILE:HD11	8:H:127:LEU:HG	2.01	0.43
10:J:60:GLN:O	10:J:64:GLN:HG3	2.18	0.43
10:J:85:GLN:HG2	10:J:89:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:97:MET:HG2	11:K:115:SER:HB3	2.01	0.43
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.18	0.43
3:Q:72:SER:O	3:Q:221:ILE:HD12	2.19	0.43
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.48	0.43
3:C:158:SER:CB	4:D:59:LEU:HD21	2.49	0.43
4:D:14:THR:HG22	4:D:15:PHE:N	2.33	0.43
4:D:241:GLU:C	4:D:243:ALA:N	2.77	0.43
6:F:11:SER:HB3	6:F:14:VAL:CG2	2.49	0.43
8:H:63:ILE:CG2	8:H:74:PRO:HB3	2.49	0.43
10:J:166:MET:HA	10:J:167:PRO:HD3	1.82	0.43
12:L:24:TYR:HA	8:V:167:LEU:HD12	2.00	0.43
14:N:3:ILE:HD13	14:N:3:ILE:C	2.43	0.43
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.17	0.43
4:R:241:GLU:C	4:R:243:ALA:N	2.77	0.43
7:U:192:PHE:CD1	7:U:192:PHE:C	2.97	0.43
16:V:334:HOH:O	9:W:150:ASP:HA	2.19	0.43
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.54	0.42
7:G:192:PHE:CD1	7:G:192:PHE:C	2.97	0.42
9:I:137:MET:HE3	9:I:141:LEU:CD1	2.49	0.42
14:N:4:MET:CB	14:N:126:ILE:HG22	2.49	0.42
14:N:14:LEU:HD11	14:N:102:ALA:CB	2.49	0.42
14:N:146:MET:HB3	14:N:150:GLU:HB2	1.99	0.42
1:O:77:VAL:CG1	1:O:137:LEU:HB2	2.49	0.42
4:R:17:PRO:HA	5:S:26:TYR:CD1	2.54	0.42
4:R:243:ALA:O	4:R:244:GLU:HB2	2.19	0.42
5:S:174:THR:O	5:S:178:ARG:HB2	2.19	0.42
6:T:199:LEU:HD12	6:T:240:ILE:HD12	2.00	0.42
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.54	0.42
8:V:62:ASN:HB3	8:V:82:MET:HE1	1.99	0.42
12:Z:-5:TYR:CD2	12:Z:96:TYR:HB2	2.54	0.42
3:C:52:ARG:HB2	3:C:209:ASN:HA	2.01	0.42
3:C:215:VAL:O	3:C:215:VAL:HG13	2.19	0.42
3:C:225:SER:O	3:C:226:SER:C	2.62	0.42
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.83	0.42
6:F:91:ARG:HG2	6:F:119:TYR:CD2	2.53	0.42
9:I:89:GLU:HG2	9:I:90:ARG:NH1	2.33	0.42
1:O:58:LEU:HB3	7:U:162:ALA:O	2.19	0.42
2:P:21(E):VAL:HG12	2:P:220:TYR:N	2.34	0.42
2:P:222:LYS:HZ1	2:P:228:GLU:CD	2.27	0.42
6:T:18(E):GLU:CD	6:T:18(E):GLU:H	2.27	0.42
9:W:84:SER:HB2	9:W:119:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.19	0.42
4:R:14:THR:HG22	4:R:15:PHE:N	2.33	0.42
10:X:169:ASP:OD1	10:X:171:LYS:HD3	2.19	0.42
13:1:130:GLY:O	13:1:134:ALA:HB3	2.20	0.42
2:B:136:PHE:O	2:B:150:THR:HA	2.19	0.42
3:C:106:PRO:HG2	3:C:143:PRO:HG2	2.00	0.42
6:F:205:ASN:C	6:F:20(B):GLU:H	2.27	0.42
7:G:170:GLN:HB3	16:G:265:HOH:O	2.18	0.42
8:H:206:PHE:CE2	9:I:157:GLN:HG3	2.55	0.42
9:I:14:ILE:HG23	9:I:14:ILE:O	2.20	0.42
11:K:5:ALA:HA	11:K:13:ILE:O	2.19	0.42
12:L:14:LEU:HD13	12:L:34:VAL:HG13	2.00	0.42
12:L:145:TYR:HD1	12:L:146:LEU:N	2.15	0.42
1:O:33:GLN:CA	1:O:33:GLN:NE2	2.80	0.42
1:O:85:TYR:O	1:O:89:VAL:HG23	2.19	0.42
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.42
2:P:147:GLN:HG2	3:Q:62(A):ILE:HG21	2.01	0.42
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	2.01	0.42
3:Q:215:VAL:O	3:Q:215:VAL:HG13	2.19	0.42
10:X:70:GLU:O	10:X:71:ASP:C	2.63	0.42
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.54	0.42
1:A:108:PRO:HG2	1:A:111:LEU:HG	2.01	0.42
2:B:194:LEU:HD13	2:B:233:LEU:HD12	2.00	0.42
9:I:1:GLY:HA2	9:I:17:ASP:OD1	2.19	0.42
11:K:33:LYS:O	11:K:45:MET:N	2.52	0.42
13:M:133:MET:C	13:M:136:PRO:HD2	2.45	0.42
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.84	0.42
4:R:170:GLU:N	4:R:170:GLU:CD	2.78	0.42
6:T:127:ASN:ND2	6:T:127:ASN:H	2.17	0.42
7:U:31:THR:HG21	7:U:135:ILE:HG13	2.02	0.42
10:X:85:GLN:HG2	10:X:89:LYS:HE3	2.00	0.42
13:1:40:ASN:N	13:1:40:ASN:ND2	2.64	0.42
14:2:159:LEU:O	14:2:163:ILE:HD12	2.20	0.42
4:D:39:GLY:O	4:D:162:ALA:HA	2.20	0.42
4:D:194:LEU:HD22	4:D:212:LEU:HD11	2.02	0.42
9:I:6:MET:HB3	9:I:151:LEU:HD11	2.01	0.42
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.54	0.42
2:P:185:LYS:HD3	2:P:186:VAL:H	1.85	0.42
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.85	0.42
6:T:43:ASN:N	6:T:43:ASN:ND2	2.67	0.42
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:36:ARG:HG3	14:2:42:TRP:NE1	2.34	0.42
1:A:33:GLN:CA	1:A:33:GLN:NE2	2.80	0.42
3:C:36:CYS:H	3:C:51:GLU:HG2	1.85	0.42
3:C:160:TRP:NE1	4:D:59:LEU:HD23	2.35	0.42
5:E:18(C):PHE:CD1	5:E:18(C):PHE:C	2.98	0.42
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.50	0.42
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.54	0.42
11:K:114:ASP:OD1	11:K:114:ASP:C	2.63	0.42
1:O:53:LYS:O	1:O:54:SER:C	2.63	0.42
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.84	0.42
9:W:15:ALA:HB1	9:W:159:LEU:HD22	2.01	0.42
11:Y:67:GLU:OE1	11:Y:74:ILE:HG22	2.19	0.42
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.20	0.42
3:C:197:LEU:HD13	3:C:210:ILE:HD12	2.02	0.42
3:C:234:THR:C	3:C:236:ILE:N	2.77	0.42
5:E:45:HIS:HB2	5:E:189:LEU:HD12	2.02	0.42
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.55	0.42
6:F:205:ASN:O	6:F:20(B):GLU:N	2.53	0.42
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.20	0.42
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	2.02	0.42
4:R:12(D):ALA:HB3	4:R:126:ARG:CG	2.50	0.42
9:W:15:ALA:CB	9:W:175:VAL:HG22	2.49	0.42
12:Z:-6:PRO:HG2	12:Z:-5:TYR:CD1	2.55	0.42
12:Z:134:ILE:O	12:Z:137:PHE:HB3	2.20	0.42
13:1:46:SER:OG	13:1:98:ALA:HB3	2.20	0.42
2:B:186:VAL:HG21	2:B:216:ARG:CG	2.50	0.42
3:C:209:ASN:O	3:C:210:ILE:HD13	2.19	0.42
5:E:180:LEU:O	5:E:18(D):ILE:HG22	2.18	0.42
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.01	0.42
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.85	0.42
8:V:30:ASN:O	8:V:189:ARG:NH2	2.50	0.42
13:1:159:MET:HE3	16:1:240:HOH:O	2.18	0.42
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.80	0.42
9:I:93:GLY:N	9:I:94:PRO:CD	2.83	0.42
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.83	0.42
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.01	0.42
14:N:4:MET:HB3	14:N:126:ILE:HG22	2.02	0.42
1:O:195:LEU:HD23	1:O:236:LEU:HD11	2.02	0.42
2:P:186:VAL:HG11	2:P:216:ARG:CD	2.50	0.42
4:R:96:ALA:HA	4:R:107:ILE:HG21	2.02	0.42
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.84	0.42
2:B:235:LYS:N	2:B:235:LYS:HD3	2.34	0.41
4:D:29:GLU:OE2	4:D:32:LYS:HD2	2.20	0.41
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.38	0.41
7:G:31:THR:HG21	7:G:135:ILE:HG13	2.01	0.41
10:J:168:MET:HE3	10:X:168:MET:SD	2.59	0.41
12:L:45:ALA:HB1	12:L:97:VAL:HG21	2.02	0.41
13:M:40:ASN:HD22	13:M:41:THR:N	2.18	0.41
13:M:131:ALA:HA	13:M:135:ASN:ND2	2.35	0.41
1:O:7:ARG:HD3	5:S:127:TYR:CD2	2.55	0.41
2:P:31:ILE:HD11	2:P:133:GLY:C	2.44	0.41
6:T:127:ASN:HD22	6:T:127:ASN:N	2.16	0.41
7:U:17(C):LYS:HB2	7:U:17(C):LYS:HE3	1.81	0.41
9:W:6:MET:HE1	9:W:155:ILE:HA	2.01	0.41
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.55	0.41
2:B:27:ALA:O	2:B:30:SER:HB3	2.20	0.41
2:B:141:TYR:CD1	2:B:141:TYR:C	2.98	0.41
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.45	0.41
6:F:93:ARG:HD3	16:F:268:HOH:O	2.20	0.41
8:H:72:ARG:HG3	8:H:72:ARG:NH1	2.34	0.41
9:I:18:LEU:CD2	9:I:32:GLU:HG2	2.49	0.41
1:O:88:LEU:HG	1:O:132:PHE:CE2	2.55	0.41
2:P:161:LYS:HB3	2:P:180:TYR:CE2	2.55	0.41
4:R:108:ASN:HB3	16:R:255:HOH:O	2.21	0.41
5:S:45:HIS:HB2	5:S:189:LEU:HD12	2.01	0.41
5:S:93:ARG:NH1	16:S:245:HOH:O	2.53	0.41
6:T:69:VAL:HG23	6:T:74:ILE:O	2.20	0.41
6:T:114:ASP:O	6:T:118:GLN:HG2	2.19	0.41
12:Z:14(E):GLU:OE2	12:Z:14(P):PRO:HD2	2.21	0.41
4:D:100:ASN:HB3	16:D:248:HOH:O	2.19	0.41
5:E:174:THR:O	5:E:178:ARG:HB2	2.21	0.41
6:F:21(B):THR:O	6:F:21(C):ASN:CB	2.68	0.41
8:H:172:ASN:HB3	8:H:192:LEU:O	2.20	0.41
9:I:177:ILE:HD13	9:I:177:ILE:N	2.35	0.41
12:L:107:LYS:HD3	12:L:107:LYS:HA	1.93	0.41
5:S:28:LEU:HA	5:S:31:ILE:HD12	2.02	0.41
5:S:46:ALA:CB	5:S:139:ILE:HB	2.50	0.41
5:S:160:LEU:HD13	5:S:163:THR:HB	2.02	0.41
5:S:18(C):PHE:CD1	5:S:18(C):PHE:C	2.98	0.41
6:T:169:ARG:O	6:T:173:LYS:HG3	2.20	0.41
6:T:205:ASN:C	6:T:20(B):GLU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:14:ILE:O	9:W:14:ILE:HG23	2.20	0.41
9:W:168:LEU:HD22	16:W:205:HOH:O	2.19	0.41
10:X:48:GLU:CB	10:X:96:GLN:HB2	2.49	0.41
10:X:104:TYR:CD1	10:X:180:LYS:HA	2.55	0.41
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.50	0.41
11:Y:97:MET:HG2	11:Y:115:SER:HB3	2.02	0.41
1:A:195:LEU:HD23	1:A:236:LEU:HD11	2.03	0.41
6:F:127:ASN:ND2	6:F:127:ASN:N	2.68	0.41
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.03	0.41
9:I:18:LEU:HD12	9:I:172:GLY:HA3	2.03	0.41
10:J:-1:MET:HE2	10:J:47:GLY:HA2	2.03	0.41
11:K:76:VAL:HG22	11:K:103:GLY:HA3	2.01	0.41
12:L:120:GLU:OE1	12:L:120:GLU:HA	2.20	0.41
3:Q:76:LEU:HD22	3:Q:89:ILE:HG13	2.01	0.41
4:R:194:LEU:HD12	4:R:194:LEU:HA	1.92	0.41
6:T:45:GLY:HA3	6:T:215:CYS:O	2.20	0.41
6:T:103:TYR:O	6:T:104:LYS:HB3	2.20	0.41
9:W:6:MET:HB3	9:W:151:LEU:HD11	2.03	0.41
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.56	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.83	0.41
1:A:26:TYR:O	1:A:29:THR:HB	2.20	0.41
2:B:74:ILE:C	2:B:221:GLN:HE22	2.28	0.41
3:C:185:THR:CB	3:C:188:GLU:HG2	2.43	0.41
5:E:185:ASN:OD1	5:E:188:GLU:HG2	2.21	0.41
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.51	0.41
2:P:233:LEU:HD12	2:P:233:LEU:HA	1.92	0.41
3:Q:209:ASN:O	3:Q:210:ILE:HD13	2.20	0.41
3:Q:225:SER:O	3:Q:226:SER:C	2.61	0.41
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.86	0.41
7:U:107:MET:HA	7:U:108:PRO:HD3	1.90	0.41
7:U:225:SER:H	7:U:228:ASN:HB2	1.85	0.41
8:V:95:ILE:O	8:V:97:ALA:N	2.53	0.41
11:Y:3:THR:HG22	11:Y:16:VAL:HG12	2.02	0.41
14:2:85:GLU:O	14:2:89:GLU:HB2	2.20	0.41
4:D:96:ALA:HA	4:D:107:ILE:HG21	2.02	0.41
4:D:227:GLU:OE2	4:D:227:GLU:N	2.39	0.41
6:F:43:ASN:N	6:F:43:ASN:HD22	2.18	0.41
7:G:39:ALA:CB	7:G:48:VAL:HG12	2.48	0.41
8:H:38:SER:O	8:H:39:PRO:C	2.62	0.41
10:J:90(A):ILE:HD13	10:J:90(A):ILE:HA	1.79	0.41
2:P:89:ILE:O	2:P:92:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:21(B):THR:O	6:T:21(C):ASN:CB	2.68	0.41
7:U:164:ALA:CB	7:U:172:ILE:HB	2.51	0.41
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.33	0.41
14:2:37:VAL:HG22	14:2:41:ILE:O	2.21	0.41
14:2:107:LYS:CG	14:2:108:GLY:H	2.26	0.41
2:B:15:PHE:H	3:C:23:GLN:NE2	2.06	0.41
3:C:46:VAL:HG11	3:C:139:ALA:HB1	2.02	0.41
6:F:127:ASN:C	6:F:127:ASN:ND2	2.78	0.41
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.88	0.41
10:J:70:GLU:O	10:J:71:ASP:C	2.63	0.41
10:J:77:GLN:HB2	16:J:206:HOH:O	2.21	0.41
2:P:215:ILE:O	2:P:215:ILE:HG22	2.20	0.41
12:Z:135:MET:O	12:Z:136:PRO:C	2.63	0.41
6:F:91:ARG:O	6:F:95:GLU:HB2	2.20	0.41
7:G:82:ILE:HG22	7:G:83:PRO:HD3	2.02	0.41
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.01	0.41
10:J:7:ARG:HG2	10:J:7:ARG:NH1	2.34	0.41
11:K:78:ALA:O	11:K:82:ILE:HG12	2.20	0.41
14:N:172:VAL:CB	14:N:18(A):ILE:HD11	2.50	0.41
4:R:161:ASN:HB3	4:R:180:TRP:CZ2	2.55	0.41
9:W:18:LEU:HD12	9:W:172:GLY:HA3	2.02	0.41
14:2:59:VAL:HG22	14:2:82:VAL:HG12	2.03	0.41
1:A:46:VAL:HG11	1:A:139:ALA:HB1	2.03	0.41
1:A:186:LEU:HD21	1:A:214:ILE:HD12	2.01	0.41
1:A:21(A):GLU:OE2	1:A:21(P):LYS:HB2	2.21	0.41
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.36	0.41
2:B:103:TYR:O	2:B:104:ASN:HB2	2.20	0.41
2:B:222:LYS:HZ1	2:B:228:GLU:CD	2.29	0.41
4:D:12(D):ALA:HB3	4:D:126:ARG:CG	2.51	0.41
5:E:160:LEU:HD13	5:E:163:THR:HB	2.03	0.41
6:F:114:ASP:O	6:F:118:GLN:HG2	2.20	0.41
7:G:13:THR:HB	7:G:124:THR:O	2.20	0.41
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.84	0.41
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.56	0.41
13:M:152:GLU:O	13:M:156:VAL:HG23	2.20	0.41
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.61	0.41
1:O:58:LEU:HA	1:O:58:LEU:HD23	1.83	0.41
1:O:175:PHE:O	1:O:179:ARG:HG2	2.21	0.41
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.20	0.41
4:R:135:ALA:O	4:R:136:LEU:HD23	2.20	0.41
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.51	0.41
12:Z:107:LYS:HD3	12:Z:107:LYS:HA	1.94	0.41
12:Z:176:LEU:CD1	12:Z:186:LYS:HG2	2.51	0.41
14:2:104:TYR:CD1	14:2:104:TYR:C	2.98	0.41
14:2:172:VAL:CB	14:2:18(A):ILE:HD11	2.49	0.41
1:A:58:LEU:HD23	1:A:58:LEU:HA	1.86	0.41
5:E:38:VAL:HG12	5:E:39:GLY:N	2.35	0.41
8:H:147:THR:O	8:H:148:LYS:C	2.62	0.41
10:J:93:ARG:NH2	11:K:91:LYS:HD3	2.36	0.41
10:J:169:ASP:OD1	10:J:171:LYS:HD3	2.21	0.41
2:P:63:THR:O	2:P:63:THR:HG22	2.20	0.41
2:P:231:ASP:O	2:P:235:LYS:HG2	2.21	0.41
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	2.01	0.41
3:Q:234:THR:C	3:Q:236:ILE:N	2.77	0.41
4:R:146:TYR:HE1	4:R:216:THR:HA	1.85	0.41
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.64	0.41
12:Z:39:ASP:OD2	12:Z:67:HIS:HE1	2.04	0.41
12:Z:145:TYR:HD1	12:Z:146:LEU:N	2.17	0.41
5:E:20:ARG:HB3	5:E:25:GLU:OE2	2.21	0.40
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.85	0.40
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.56	0.40
10:J:167:PRO:O	10:X:168:MET:HE2	2.21	0.40
11:K:76:VAL:N	11:K:106:GLU:OE2	2.50	0.40
2:P:235:LYS:O	2:P:237:GLY:N	2.54	0.40
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.56	0.40
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.36	0.40
1:A:31:VAL:HG11	1:A:135:SER:HB2	2.04	0.40
1:A:175:PHE:O	1:A:179:ARG:HG2	2.21	0.40
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.19	0.40
10:J:168:MET:HE2	10:X:167:PRO:C	2.46	0.40
12:L:135:MET:O	12:L:136:PRO:C	2.64	0.40
1:O:26:TYR:O	1:O:29:THR:HB	2.20	0.40
1:O:46:VAL:HG11	1:O:139:ALA:HB1	2.02	0.40
1:O:110:LYS:HG2	16:O:243:HOH:O	2.20	0.40
6:T:205:ASN:O	6:T:20(B):GLU:N	2.53	0.40
9:W:177:ILE:N	9:W:177:ILE:CD1	2.85	0.40
14:2:14:LEU:HD11	14:2:102:ALA:CB	2.51	0.40
14:2:51:ASP:O	14:2:55:ILE:HG13	2.21	0.40
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.46	0.40
3:C:36:CYS:N	3:C:51:GLU:HG2	2.36	0.40
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:LYS:O	4:D:53:ARG:HB3	2.21	0.40
10:J:48:GLU:CB	10:J:96:GLN:HB2	2.51	0.40
10:J:167:PRO:HB2	10:X:168:MET:HE1	2.03	0.40
10:J:168:MET:HE1	10:X:167:PRO:HB2	2.03	0.40
13:M:157:ASN:ND2	16:M:265:HOH:O	2.54	0.40
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.47	0.40
4:R:39:GLY:O	4:R:162:ALA:HA	2.20	0.40
9:W:81:GLN:NE2	9:W:81:GLN:HA	2.35	0.40
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	2.04	0.40
12:Z:-9:GLN:NE2	12:Z:-8:PHE:N	2.65	0.40
2:B:63:THR:O	2:B:63:THR:HG22	2.20	0.40
5:E:38:VAL:CG1	5:E:39:GLY:N	2.84	0.40
8:H:175:VAL:CG1	8:H:176:CYS:N	2.84	0.40
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.57	0.40
12:L:153:LYS:HG2	8:V:201:GLN:CG	2.52	0.40
1:O:185:GLU:OE1	1:O:187:GLU:HB2	2.21	0.40
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.37	0.40
13:1:84:ALA:HA	13:1:113:VAL:HG21	2.04	0.40
13:1:85:THR:O	13:1:89:GLN:HG3	2.22	0.40
13:1:133:MET:HE1	13:1:165:ARG:HG3	2.02	0.40
2:B:231:ASP:O	2:B:235:LYS:HG2	2.21	0.40
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.84	0.40
11:K:70:GLU:O	11:K:71:LYS:C	2.65	0.40
6:T:121:GLN:NE2	16:T:248:HOH:O	2.54	0.40
7:U:214:VAL:HB	7:U:222:PHE:CZ	2.56	0.40
9:W:137:MET:CE	9:W:141:LEU:HD11	2.52	0.40
10:X:45:PHE:CD1	10:X:52:THR:HG23	2.57	0.40
10:X:143:ARG:HA	10:X:144:PRO:HD3	1.95	0.40
11:Y:33:LYS:O	11:Y:45:MET:N	2.52	0.40
12:Z:42:VAL:HG12	12:Z:176:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	230 (93%)	15 (6%)	3 (1%)	10	34
1	O	248/250 (99%)	230 (93%)	15 (6%)	3 (1%)	10	34
2	B	242/244 (99%)	220 (91%)	19 (8%)	3 (1%)	10	34
2	P	242/244 (99%)	220 (91%)	18 (7%)	4 (2%)	7	25
3	C	239/241 (99%)	218 (91%)	17 (7%)	4 (2%)	7	25
3	Q	239/241 (99%)	218 (91%)	17 (7%)	4 (2%)	7	25
4	D	240/242 (99%)	219 (91%)	16 (7%)	5 (2%)	5	20
4	R	240/242 (99%)	217 (90%)	18 (8%)	5 (2%)	5	20
5	E	231/233 (99%)	212 (92%)	15 (6%)	4 (2%)	7	25
5	S	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	7	25
6	F	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	16	44
6	T	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	16	44
7	G	241/243 (99%)	228 (95%)	12 (5%)	1 (0%)	30	60
7	U	241/243 (99%)	228 (95%)	12 (5%)	1 (0%)	30	60
8	H	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	9	30
8	V	220/222 (99%)	209 (95%)	8 (4%)	3 (1%)	9	30
9	I	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	24	55
9	W	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	24	55
10	J	196/198 (99%)	188 (96%)	4 (2%)	4 (2%)	6	21
10	X	196/198 (99%)	187 (95%)	6 (3%)	3 (2%)	8	28
11	K	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
11	Y	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
12	L	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	24	55
12	Z	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	24	55
13	1	231/233 (99%)	214 (93%)	15 (6%)	2 (1%)	14	41
13	M	231/233 (99%)	214 (93%)	15 (6%)	2 (1%)	14	41
14	2	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6312/6368 (99%)	5892 (93%)	354 (6%)	66 (1%)	12	38

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
3	C	58	LEU
4	D	12(G)	GLU
6	F	205	ASN
10	J	192	ALA
1	O	5	THR
3	Q	58	LEU
4	R	12(G)	GLU
6	T	205	ASN
10	X	192	ALA
1	A	61	SER
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	203	THR
5	E	202	ARG
6	F	206	LYS
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	203	THR
5	S	202	ARG
6	T	206	LYS
3	C	179	ASN
3	C	183	PRO
4	D	128	MET
5	E	180	LEU
7	G	220	LYS
9	I	93	GLY
1	O	61	SER
3	Q	179	ASN
3	Q	183	PRO
4	R	128	MET
5	S	180	LEU
7	U	220	LYS
9	W	93	GLY
5	E	217	LYS
10	J	49	ALA
13	M	96	TRP
2	P	6	ARG
5	S	217	LYS
8	V	96	GLY
4	D	43	LYS

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Mol	Chain	Res	Type
4	D	12(C)	GLY
5	E	5	ARG
8	H	91	GLN
1	O	167	LYS
4	R	12(C)	GLY
8	V	171	SER
1	A	167	LYS
8	H	9	ASN
10	J	8	VAL
13	M	72	ALA
4	R	43	LYS
5	S	5	ARG
8	V	9	ASN
10	X	8	VAL
13	1	72	ALA
13	1	96	TRP
10	X	187	VAL
12	Z	93	PHE
8	H	96	GLY
10	J	187	VAL
4	D	12(F)	GLY
12	L	93	PHE
4	R	12(F)	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%)	194 (93%)	15 (7%)	13	39
1	O	209/209 (100%)	194 (93%)	15 (7%)	13	39
2	B	203/203 (100%)	189 (93%)	14 (7%)	14	41
2	P	203/203 (100%)	189 (93%)	14 (7%)	14	41
3	C	213/213 (100%)	194 (91%)	19 (9%)	9	29
3	Q	213/213 (100%)	193 (91%)	20 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	198/198 (100%)	185 (93%)	13 (7%)	15	43
4	R	198/198 (100%)	186 (94%)	12 (6%)	17	46
5	E	192/192 (100%)	176 (92%)	16 (8%)	10	32
5	S	192/192 (100%)	176 (92%)	16 (8%)	10	32
6	F	201/201 (100%)	185 (92%)	16 (8%)	11	34
6	T	201/201 (100%)	185 (92%)	16 (8%)	11	34
7	G	207/207 (100%)	195 (94%)	12 (6%)	18	49
7	U	207/207 (100%)	195 (94%)	12 (6%)	18	49
8	H	181/181 (100%)	168 (93%)	13 (7%)	13	39
8	V	181/181 (100%)	169 (93%)	12 (7%)	15	43
9	I	172/172 (100%)	164 (95%)	8 (5%)	23	57
9	W	172/172 (100%)	163 (95%)	9 (5%)	21	53
10	J	175/175 (100%)	168 (96%)	7 (4%)	28	63
10	X	175/175 (100%)	167 (95%)	8 (5%)	24	58
11	K	169/169 (100%)	162 (96%)	7 (4%)	27	62
11	Y	169/169 (100%)	163 (96%)	6 (4%)	31	66
12	L	185/185 (100%)	159 (86%)	26 (14%)	3	12
12	Z	185/185 (100%)	158 (85%)	27 (15%)	3	11
13	1	199/199 (100%)	191 (96%)	8 (4%)	28	63
13	M	199/199 (100%)	190 (96%)	9 (4%)	24	58
14	2	162/162 (100%)	152 (94%)	10 (6%)	16	45
14	N	162/162 (100%)	152 (94%)	10 (6%)	16	45
All	All	5332/5332 (100%)	4962 (93%)	370 (7%)	14	41

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	33	GLN
1	A	40	ILE
1	A	62	GLU
1	A	64	LEU
1	A	74	ILE
1	A	124	THR

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Mol	Chain	Res	Type
1	A	134	VAL
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
1	A	192	ILE
1	A	210	ILE
1	A	215	ILE
1	A	229	ILE
2	B	5	SER
2	B	10	SER
2	B	14	ILE
2	B	58	LEU
2	B	89	ILE
2	B	116	LEU
2	B	124	THR
2	B	14(A)	TYR
2	B	150	THR
2	B	192	LEU
2	B	206	THR
2	B	224	PHE
2	B	232	ILE
2	B	238	ILE
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU
3	C	28	LEU
3	C	33	ARG
3	C	57	LYS
3	C	61	THR
3	C	66	LYS
3	C	70	ILE
3	C	87	ILE
3	C	89	ILE
3	C	135	SER
3	C	14(A)	ARG
3	C	14(B)	ASP
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	224	LEU
3	C	236	ILE
4	D	28	LEU

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Mol	Chain	Res	Type
4	D	31	ILE
4	D	40	ILE
4	D	48	LEU
4	D	107	ILE
4	D	126	ARG
4	D	170	GLU
4	D	175	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	196	ILE
4	D	215	ILE
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	64	GLN
5	E	76	LEU
5	E	78	LEU
5	E	97	ASN
5	E	121	GLN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	223	ILE
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	35	THR
6	F	38	ILE
6	F	43	ASN
6	F	54	ILE
6	F	56	SER
6	F	72	ARG
6	F	74	ILE
6	F	82	ILE
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	169	ARG

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Mol	Chain	Res	Type
6	F	187	ARG
6	F	203	GLU
7	G	33	GLN
7	G	35	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	122	ILE
7	G	124	THR
7	G	197	MET
7	G	217	LYS
7	G	229	ILE
7	G	232	ARG
7	G	233	LEU
8	H	13	VAL
8	H	34	LEU
8	H	37	ILE
8	H	43	CYS
8	H	55	VAL
8	H	56	THR
8	H	63	ILE
8	H	68	LEU
8	H	95	ILE
8	H	144	GLN
8	H	180	ILE
8	H	197	ARG
8	H	221	ILE
9	I	-3	ILE
9	I	29	ASN
9	I	110	ILE
9	I	113	PHE
9	I	155	ILE
9	I	160	LEU
9	I	177	ILE
9	I	192	ARG
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	121	GLU
10	J	155	LEU
10	J	168	MET

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Mol	Chain	Res	Type
11	K	4	LEU
11	K	8	PHE
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	138	LEU
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	83	ILE
12	L	98	HIS
12	L	99	THR
12	L	106	GLU
12	L	134	ILE
12	L	138	LEU
12	L	14(A)	LYS
12	L	14(B)	ASN
12	L	14(C)	GLN
12	L	14(D)	TYR
12	L	14(E)	GLU
12	L	14(F)	PRO
12	L	14(I)	THR
12	L	14(K)	LYS
12	L	14(M)	VAL
12	L	14(N)	LYS
12	L	14(O)	LYS
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS
12	L	152	ILE
12	L	190	GLU
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	148	VAL
13	M	149	GLN
13	M	178	ILE
13	M	191	GLN
13	M	204	LYS

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Mol	Chain	Res	Type
14	N	3	ILE
14	N	55	ILE
14	N	58	ILE
14	N	84	LYS
14	N	89	GLU
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU
14	N	163	ILE
14	N	178	LEU
1	O	24	ILE
1	O	33	GLN
1	O	40	ILE
1	O	62	GLU
1	O	64	LEU
1	O	74	ILE
1	O	124	THR
1	O	134	VAL
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
1	O	192	ILE
1	O	210	ILE
1	O	215	ILE
1	O	229	ILE
2	P	5	SER
2	P	10	SER
2	P	14	ILE
2	P	58	LEU
2	P	89	ILE
2	P	116	LEU
2	P	124	THR
2	P	14(A)	TYR
2	P	150	THR
2	P	192	LEU
2	P	206	THR
2	P	224	PHE
2	P	232	ILE
2	P	238	ILE
3	Q	10	ARG
3	Q	14	ILE
3	Q	25	GLU

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Mol	Chain	Res	Type
3	Q	28	LEU
3	Q	33	ARG
3	Q	57	LYS
3	Q	61	THR
3	Q	66	LYS
3	Q	70	ILE
3	Q	87	ILE
3	Q	89	ILE
3	Q	100	ARG
3	Q	135	SER
3	Q	14(A)	ARG
3	Q	14(B)	ASP
3	Q	163	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	224	LEU
3	Q	236	ILE
4	R	28	LEU
4	R	31	ILE
4	R	40	ILE
4	R	48	LEU
4	R	107	ILE
4	R	126	ARG
4	R	170	GLU
4	R	175	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
5	S	12	THR
5	S	13	VAL
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	64	GLN
5	S	76	LEU
5	S	78	LEU
5	S	97	ASN
5	S	121	GLN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU

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Mol	Chain	Res	Type
5	S	223	ILE
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	35	THR
6	T	38	ILE
6	T	43	ASN
6	T	54	ILE
6	T	56	SER
6	T	72	ARG
6	T	74	ILE
6	T	82	ILE
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	169	ARG
6	T	187	ARG
6	T	203	GLU
7	U	33	GLN
7	U	35	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	122	ILE
7	U	124	THR
7	U	197	MET
7	U	217	LYS
7	U	229	ILE
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	34	LEU
8	V	37	ILE
8	V	43	CYS
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	95	ILE
8	V	144	GLN
8	V	180	ILE
8	V	197	ARG

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Mol	Chain	Res	Type
8	V	221	ILE
9	W	-3	ILE
9	W	29	ASN
9	W	94	PRO
9	W	110	ILE
9	W	113	PHE
9	W	155	ILE
9	W	160	LEU
9	W	177	ILE
9	W	192	ARG
10	X	3	ILE
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	121	GLU
10	X	155	LEU
10	X	168	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
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	83	ILE
12	Z	98	HIS
12	Z	99	THR
12	Z	106	GLU
12	Z	134	ILE
12	Z	138	LEU
12	Z	14(A)	LYS
12	Z	14(B)	ASN
12	Z	14(C)	GLN
12	Z	14(D)	TYR
12	Z	14(E)	GLU
12	Z	14(F)	PRO
12	Z	14(I)	THR

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Mol	Chain	Res	Type
12	Z	14(K)	LYS
12	Z	14(M)	VAL
12	Z	14(N)	LYS
12	Z	14(O)	LYS
12	Z	14(P)	PRO
12	Z	14(Q)	LEU
12	Z	14(W)	LYS
12	Z	152	ILE
12	Z	190	GLU
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	148	VAL
13	1	149	GLN
13	1	191	GLN
13	1	204	LYS
14	2	3	ILE
14	2	55	ILE
14	2	58	ILE
14	2	84	LYS
14	2	89	GLU
14	2	115	LEU
14	2	119	VAL
14	2	149	GLU
14	2	163	ILE
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (237) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	145	ASN
2	B	23	GLN
2	B	33	HIS
2	B	71	ASN
2	B	97	GLN
2	B	104	ASN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN

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Mol	Chain	Res	Type
2	B	173	GLN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	120	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	199	GLN
4	D	20(A)	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	73	HIS
5	E	95	GLN
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	144	ASN

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Mol	Chain	Res	Type
6	F	192	GLN
6	F	241	ASN
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
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	109	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	220	ASN
9	I	29	ASN
9	I	81	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	160	GLN
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	24	ASN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
11	K	208	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	27	ASN

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Mol	Chain	Res	Type
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
12	L	168	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	132	HIS
13	M	135	ASN
13	M	149	GLN
13	M	157	ASN
13	M	191	GLN
14	N	62	HIS
14	N	69	GLN
14	N	106	ASN
14	N	141	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	145	ASN
2	P	23	GLN
2	P	33	HIS
2	P	71	ASN
2	P	97	GLN
2	P	104	ASN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	173	GLN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN

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Mol	Chain	Res	Type
3	Q	120	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	147	GLN
4	R	161	ASN
4	R	199	GLN
4	R	20(A)	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	73	HIS
5	S	95	GLN
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	144	ASN
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN

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Mol	Chain	Res	Type
7	U	170	GLN
7	U	178	ASN
7	U	18(C)	HIS
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	66	HIS
8	V	91	GLN
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	220	ASN
9	W	29	ASN
9	W	81	GLN
9	W	161	ASN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	64	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	160	GLN
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	24	ASN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	27	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	85	HIS

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Mol	Chain	Res	Type
12	Z	1(I)	ASN
12	Z	166	HIS
12	Z	168	GLN
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	191	GLN
14	2	62	HIS
14	2	69	GLN
14	2	106	ASN
14	2	141	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SLA	V	301	8	10,15,15	3.15	2 (20%)	13,23,23	1.50	3 (23%)
15	SLA	H	301	8	10,15,15	2.87	2 (20%)	13,23,23	1.52	3 (23%)
15	SLA	K	301	11	10,15,15	2.72	1 (10%)	13,23,23	1.66	3 (23%)
15	SLA	Y	301	11	10,15,15	2.79	1 (10%)	13,23,23	1.66	3 (23%)

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	SLA	V	301	8	-	0/6/32/32	0/1/1/1
15	SLA	H	301	8	-	0/6/32/32	0/1/1/1
15	SLA	K	301	11	-	0/6/32/32	0/1/1/1
15	SLA	Y	301	11	-	0/6/32/32	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	301	SLA	C13-C11	9.16	1.61	1.53
15	H	301	SLA	C13-C11	8.24	1.60	1.53
15	Y	301	SLA	C13-C11	8.11	1.60	1.53
15	K	301	SLA	C13-C11	7.88	1.60	1.53
15	H	301	SLA	O8-C1	2.32	1.47	1.42
15	V	301	SLA	C9-C2	2.05	1.57	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	SLA	C5-N4-C3	3.64	117.00	114.58
15	K	301	SLA	C5-N4-C3	3.61	116.98	114.58
15	H	301	SLA	O7-C6-C5	-3.07	119.52	124.25
15	V	301	SLA	O7-C6-C5	-3.01	119.60	124.25
15	K	301	SLA	O10-C3-C2	-2.98	123.80	126.17
15	Y	301	SLA	O7-C6-C5	-2.91	119.77	124.25
15	Y	301	SLA	O10-C3-C2	-2.88	123.89	126.17
15	H	301	SLA	C5-N4-C3	2.74	116.40	114.58
15	K	301	SLA	O7-C6-C5	-2.67	120.14	124.25
15	V	301	SLA	O10-C3-C2	-2.53	124.16	126.17
15	V	301	SLA	C5-N4-C3	2.47	116.22	114.58
15	H	301	SLA	O10-C3-C2	-2.35	124.30	126.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	V	301	SLA	1	0
15	H	301	SLA	1	0
15	K	301	SLA	1	0
15	Y	301	SLA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.13	7 (2%)	55	45	32, 46, 77, 100	0
1	O	250/250 (100%)	0.04	9 (3%)	46	37	35, 54, 79, 99	0
2	B	244/244 (100%)	0.12	14 (5%)	29	22	31, 51, 84, 113	0
2	P	244/244 (100%)	0.26	17 (6%)	22	16	34, 53, 88, 114	0
3	C	241/241 (100%)	0.24	13 (5%)	31	24	35, 55, 105, 122	0
3	Q	241/241 (100%)	0.44	20 (8%)	17	12	38, 58, 106, 122	0
4	D	242/242 (100%)	0.16	9 (3%)	45	36	38, 54, 87, 119	0
4	R	242/242 (100%)	0.23	10 (4%)	41	33	41, 56, 89, 119	0
5	E	233/233 (100%)	0.07	6 (2%)	57	47	37, 54, 80, 105	0
5	S	233/233 (100%)	0.06	7 (3%)	52	42	37, 55, 80, 106	0
6	F	244/244 (100%)	-0.07	6 (2%)	58	48	31, 48, 85, 103	0
6	T	244/244 (100%)	-0.19	2 (0%)	82	75	30, 45, 85, 99	0
7	G	243/243 (100%)	-0.18	7 (2%)	53	43	28, 43, 71, 108	0
7	U	243/243 (100%)	-0.15	5 (2%)	63	54	29, 44, 70, 106	0
8	H	222/222 (100%)	-0.36	0	100	100	28, 42, 59, 91	0
8	V	222/222 (100%)	-0.28	3 (1%)	73	64	33, 45, 62, 93	0
9	I	204/204 (100%)	-0.46	1 (0%)	87	82	26, 44, 62, 78	0
9	W	204/204 (100%)	-0.38	0	100	100	32, 43, 64, 77	0
10	J	198/198 (100%)	-0.25	4 (2%)	65	56	32, 46, 62, 118	0
10	X	198/198 (100%)	-0.15	4 (2%)	65	56	32, 46, 64, 120	0
11	K	212/212 (100%)	-0.21	0	100	100	30, 45, 61, 73	0
11	Y	212/212 (100%)	-0.28	0	100	100	30, 46, 63, 74	0
12	L	222/222 (100%)	-0.19	2 (0%)	81	74	28, 46, 69, 89	0
12	Z	222/222 (100%)	-0.25	2 (0%)	81	74	31, 45, 70, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.45	1 (0%)	88 84	29, 40, 54, 62	0
13	M	233/233 (100%)	-0.44	1 (0%)	88 84	27, 42, 56, 63	0
14	2	196/196 (100%)	-0.36	2 (1%)	79 72	23, 39, 58, 78	0
14	N	196/196 (100%)	-0.47	1 (0%)	87 82	29, 38, 58, 76	0
All	All	6368/6368 (100%)	-0.12	153 (2%)	59 49	23, 47, 79, 122	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(D)	ALA	10.1
4	R	12(D)	ALA	8.8
4	D	12(E)	SER	8.6
4	R	12(E)	SER	8.5
3	Q	56	LEU	7.5
4	D	12(C)	GLY	6.8
7	U	240	ASP	6.8
3	C	55	THR	6.1
7	G	6	ALA	5.5
13	1	-8	THR	5.5
6	F	5	GLY	5.5
2	P	54	VAL	5.3
3	C	56	LEU	5.3
4	R	127	LEU	5.0
4	R	12(C)	GLY	4.9
5	S	4	PHE	4.9
4	R	126	ARG	4.5
1	O	5	THR	4.5
10	X	192	ALA	4.5
2	B	21(B)	GLY	4.4
2	B	54	VAL	4.3
2	B	217	ALA	4.3
2	B	21(D)	GLY	4.1
7	G	240	ASP	4.1
10	J	192	ALA	4.1
10	J	193	GLN	4.0
1	A	5	THR	3.9
2	B	4	GLY	3.8
14	2	107	LYS	3.8
10	X	193	GLN	3.8
3	Q	240	LYS	3.8
3	C	54	SER	3.8

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Mol	Chain	Res	Type	RSRZ
7	U	6	ALA	3.7
6	F	6	THR	3.7
2	P	21(A)	LYS	3.7
2	P	217	ALA	3.7
12	L	145	TYR	3.7
3	Q	58	LEU	3.6
2	P	21(C)	ASP	3.6
3	Q	55	THR	3.6
1	A	204	GLY	3.6
2	P	4	GLY	3.5
3	Q	207	ALA	3.5
7	G	239	GLN	3.4
4	D	126	ARG	3.4
2	P	21(D)	GLY	3.4
2	B	143	ASP	3.4
7	G	8	TYR	3.4
5	E	4	PHE	3.3
3	C	206	GLY	3.3
2	P	21(B)	GLY	3.3
5	S	5	ARG	3.3
3	C	240	LYS	3.3
10	J	-1	MET	3.2
3	Q	236	ILE	3.2
1	O	56	SER	3.2
2	P	239	THR	3.2
1	O	21(P)	LYS	3.1
14	N	107	LYS	3.1
3	Q	210	ILE	3.0
9	I	-8	SER	3.0
2	B	239	THR	3.0
3	C	207	ALA	3.0
1	A	203	GLU	3.0
5	E	127	TYR	2.9
10	X	10	ASP	2.9
2	P	218	ASN	2.9
3	Q	57	LYS	2.9
4	R	12(B)	GLU	2.9
1	O	4	MET	2.9
4	D	127	LEU	2.8
10	X	191	GLN	2.8
7	U	7	GLY	2.8
2	P	219	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
6	F	204	ASP	2.8
13	M	-8	THR	2.7
3	Q	54	SER	2.7
3	Q	241	GLN	2.7
5	S	127	TYR	2.7
4	R	12(A)	GLY	2.7
3	C	242	GLU	2.7
4	D	242	ALA	2.6
3	Q	203	THR	2.6
3	Q	44	ASN	2.6
2	B	21(A)	LYS	2.6
3	C	59	GLN	2.6
3	Q	187	GLU	2.6
5	S	203	ASP	2.6
2	P	56	SER	2.6
5	E	203	ASP	2.6
4	R	12(F)	GLY	2.6
6	T	5	GLY	2.6
5	S	204	GLU	2.6
8	V	91	GLN	2.6
3	Q	209	ASN	2.6
4	D	12(F)	GLY	2.5
4	R	12(G)	GLU	2.5
7	G	171	GLU	2.5
12	Z	120	GLU	2.5
2	B	218	ASN	2.5
12	Z	145	TYR	2.5
2	P	65	GLU	2.5
7	G	18(H)	GLU	2.5
1	O	236	LEU	2.5
2	B	61	GLN	2.5
3	Q	243	GLN	2.5
5	E	5	ARG	2.5
2	P	64	THR	2.5
5	E	204	GLU	2.4
3	C	238	GLN	2.4
3	C	52	ARG	2.4
1	A	235	ALA	2.4
2	P	220	TYR	2.4
3	C	241	GLN	2.4
3	Q	238	GLN	2.4
1	A	4	MET	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	208	LYS	2.4
1	O	65	SER	2.4
6	F	240	ILE	2.4
1	A	202	VAL	2.4
2	B	219	GLU	2.4
2	P	57	THR	2.4
4	D	9	ASP	2.3
3	Q	208	LYS	2.3
1	A	236	LEU	2.3
8	V	223	ASP	2.3
6	T	241	ASN	2.3
5	S	227	GLU	2.3
5	S	56	ASP	2.3
2	B	185	LYS	2.3
7	G	7	GLY	2.2
2	B	43	SER	2.2
1	O	64	LEU	2.2
10	J	191	GLN	2.2
3	Q	206	GLY	2.2
3	Q	183	PRO	2.2
6	F	18	ASP	2.1
1	O	184	LEU	2.1
2	P	59	LEU	2.1
4	D	205	GLU	2.1
7	U	29	LYS	2.1
3	C	203	THR	2.1
2	P	58	LEU	2.1
14	2	18(I)	GLN	2.1
2	B	10	SER	2.1
5	E	207	LEU	2.1
8	V	221	ILE	2.1
1	O	167	LYS	2.0
7	U	238	GLU	2.0
12	L	98	HIS	2.0
6	F	205	ASN	2.0
3	Q	242	GLU	2.0
4	R	170	GLU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	SLA	V	301	15/15	0.91	0.12	47,49,53,53	0
15	SLA	Y	301	15/15	0.92	0.09	36,40,43,44	0
15	SLA	H	301	15/15	0.94	0.10	47,49,50,53	0
15	SLA	K	301	15/15	0.95	0.09	41,43,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.