



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:33 PM UTC

PDB ID : 4LQI / pdb_00004lqi
Title : Yeast 20S Proteasome in complex with Vibralactone
Authors : List, A.; Zeiler, E.; Gallastegui, N.; Rusch, M.; Hedberg, C.; Sieber, S.A.; Groll, M.
Deposited on : 2013-07-18
Resolution : 2.70 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

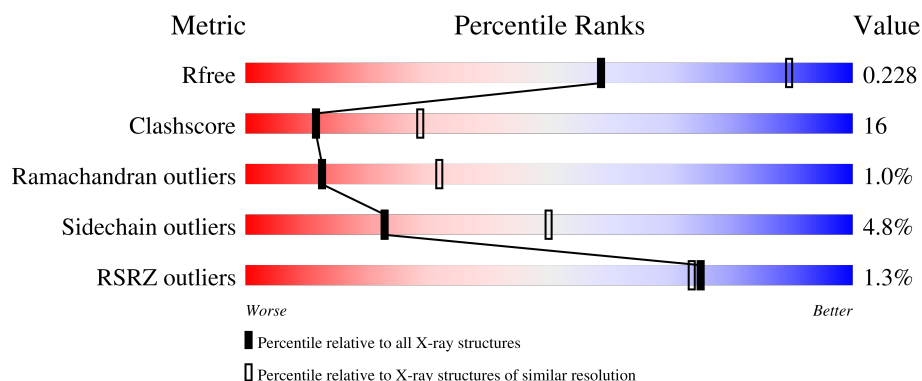
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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% 74% 24%
1	O	250	72% 27%
2	B	244	3% 62% 32% 6%
2	P	244	4% 64% 32% 5%
3	C	241	3% 59% 38%

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Mol	Chain	Length	Quality of chain
3	Q	241	
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	M	233	
13	a	233	
14	N	196	
14	b	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50942 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 subunit alpha type-2.

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 subunit alpha type-3.

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 subunit alpha type-4.

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 subunit alpha type-5.

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 subunit alpha type-6.

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 subunit alpha type-7.

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 subunit alpha type-1.

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 subunit beta type-2.

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 subunit beta type-3.

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 subunit beta type-4.

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 subunit beta type-5.

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 subunit beta type-6.

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			

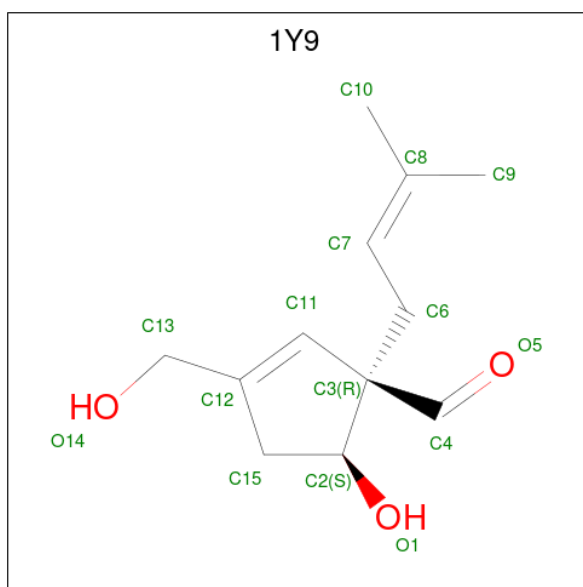
- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is vibrallactone, bound form (CCD ID: 1Y9) (formula: C₁₂H₁₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	K	1	Total	C	O	0	0
			15	12	3		
15	N	1	Total	C	O	0	0
			15	12	3		
15	Y	1	Total	C	O	0	0
			15	12	3		
15	b	1	Total	C	O	0	0
			15	12	3		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	56	Total	O	0	0
			56	56		
16	B	36	Total	O	0	0
			36	36		
16	C	42	Total	O	0	0
			42	42		
16	D	38	Total	O	0	0
			38	38		
16	E	23	Total	O	0	0
			23	23		
16	F	49	Total	O	0	0
			49	49		
16	G	61	Total	O	0	0
			61	61		
16	H	49	Total	O	0	0
			49	49		

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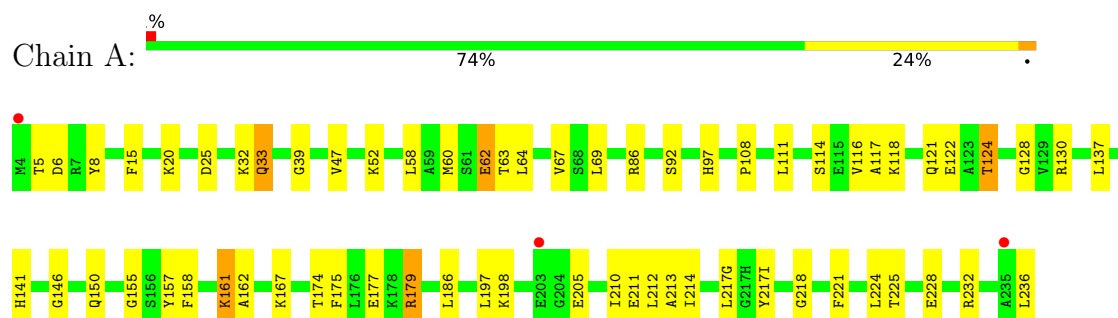
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	I	70	Total 70	O 70	0	0
16	J	53	Total 53	O 53	0	0
16	K	46	Total 46	O 46	0	0
16	L	56	Total 56	O 56	0	0
16	M	73	Total 73	O 73	0	0
16	N	57	Total 57	O 57	0	0
16	O	31	Total 31	O 31	0	0
16	P	28	Total 28	O 28	0	0
16	Q	28	Total 28	O 28	0	0
16	R	31	Total 31	O 31	0	0
16	S	20	Total 20	O 20	0	0
16	T	38	Total 38	O 38	0	0
16	U	62	Total 62	O 62	0	0
16	V	46	Total 46	O 46	0	0
16	W	61	Total 61	O 61	0	0
16	X	52	Total 52	O 52	0	0
16	Y	46	Total 46	O 46	0	0
16	Z	52	Total 52	O 52	0	0
16	a	75	Total 75	O 75	0	0
16	b	55	Total 55	O 55	0	0

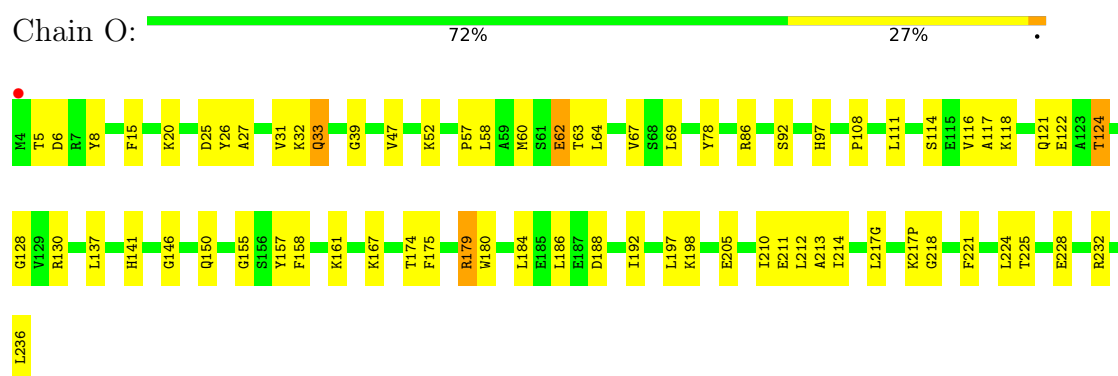
3 Residue-property plots

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

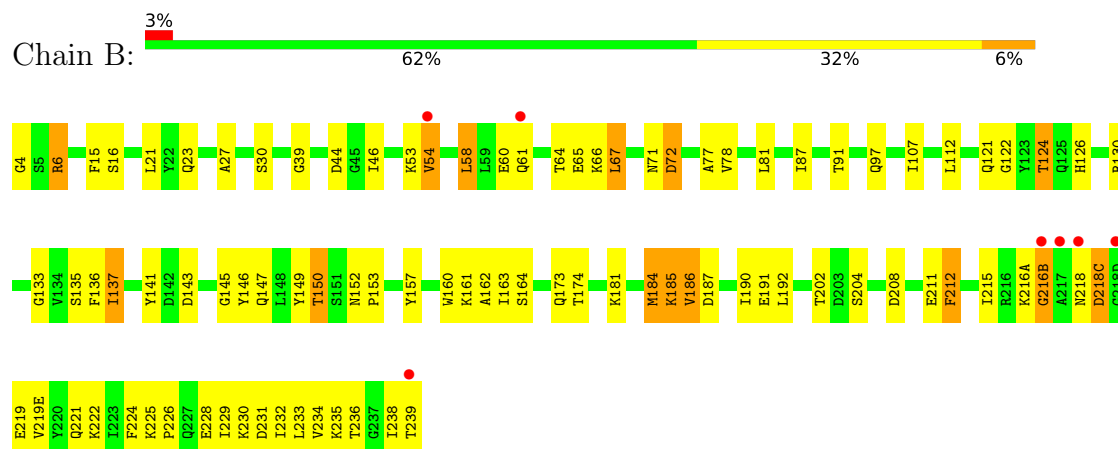
• Molecule 1: Proteasome subunit alpha type-2



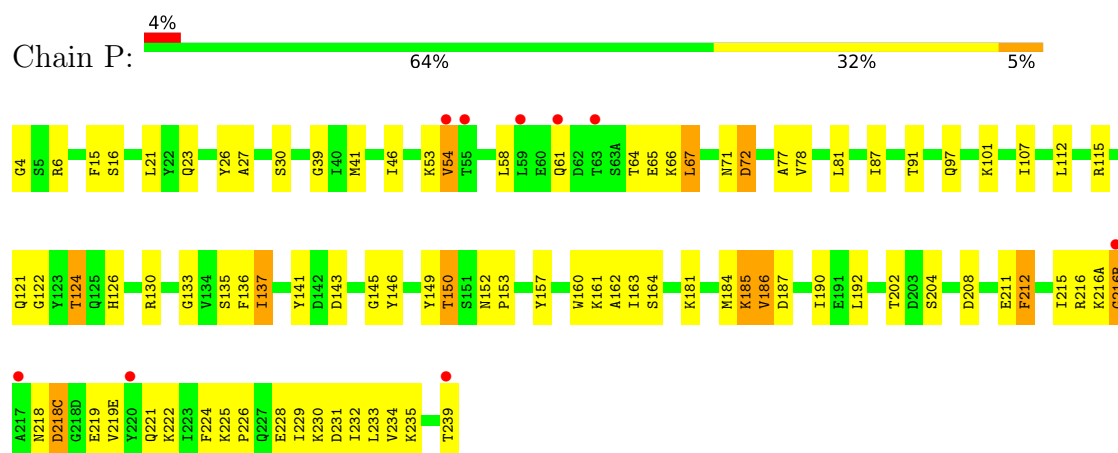
• Molecule 1: Proteasome subunit alpha type-2



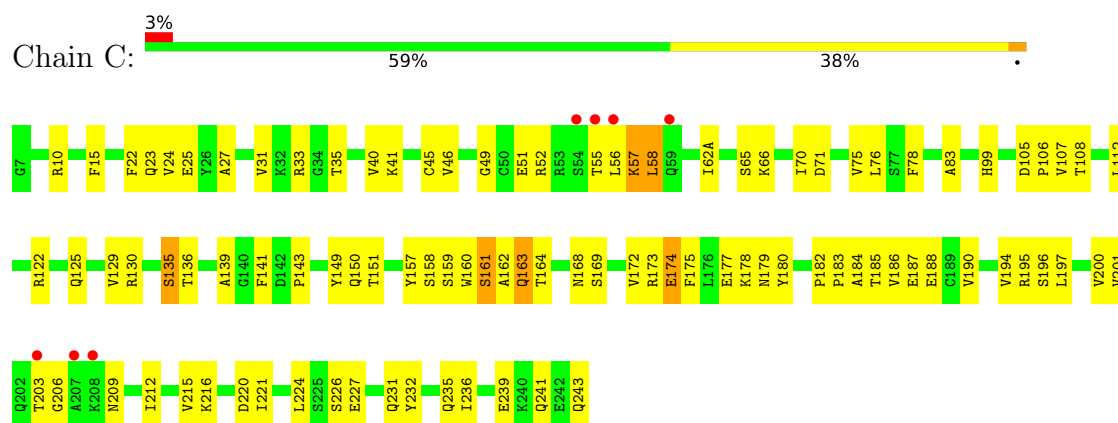
• Molecule 2: Proteasome subunit alpha type-3



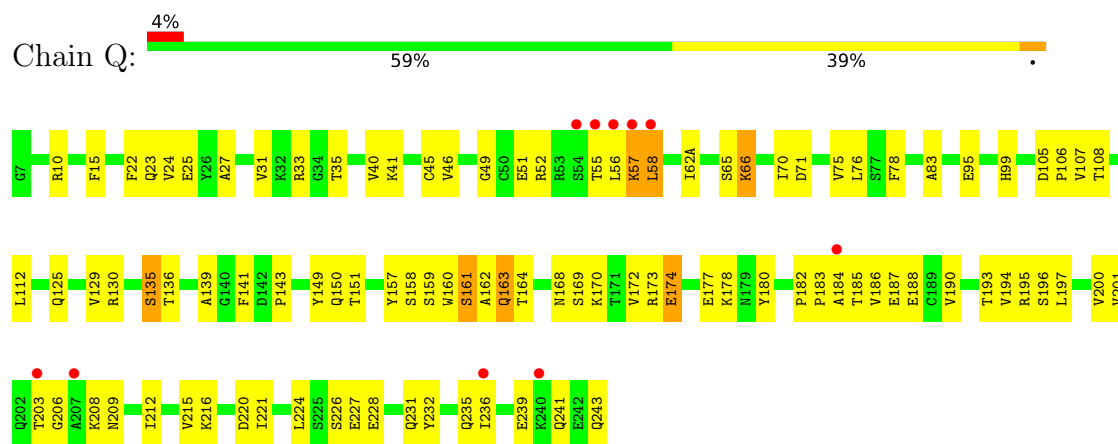
- Molecule 2: Proteasome subunit alpha type-3



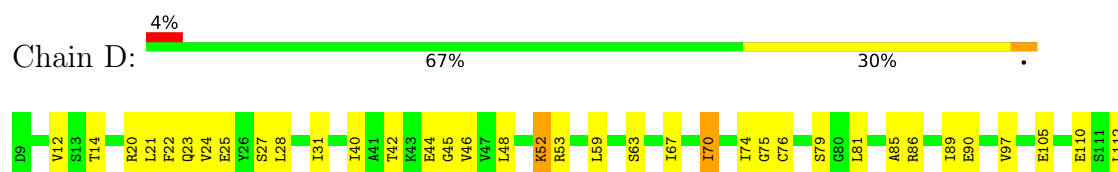
- Molecule 3: Proteasome subunit alpha type-4



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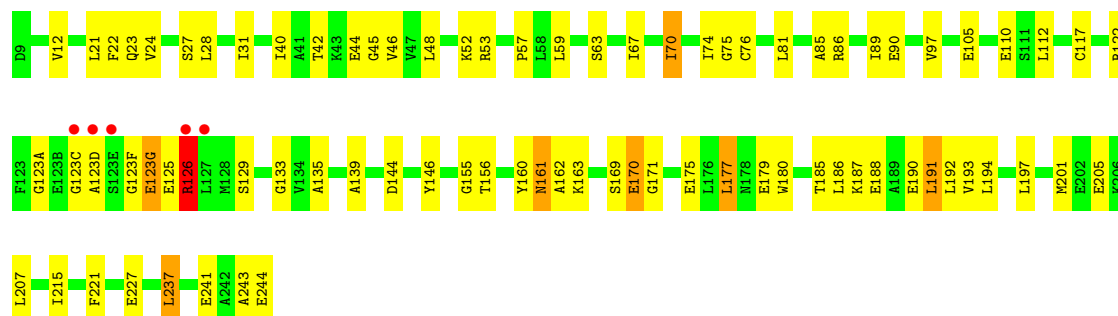


- Molecule 4: Proteasome subunit alpha type-5

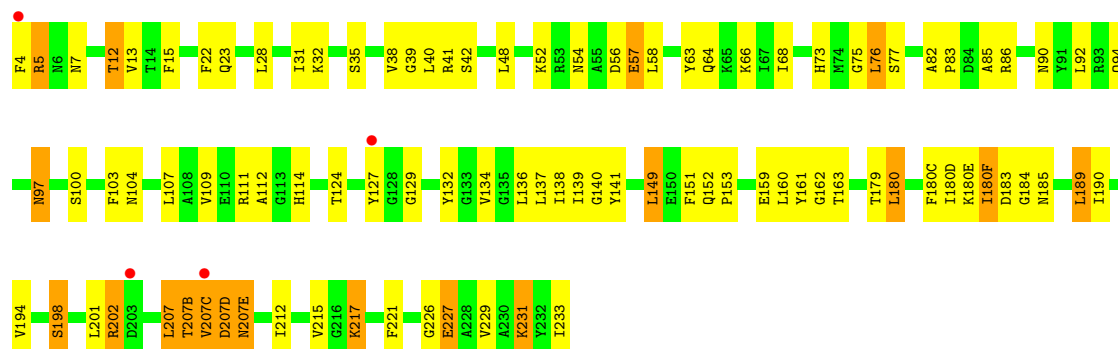




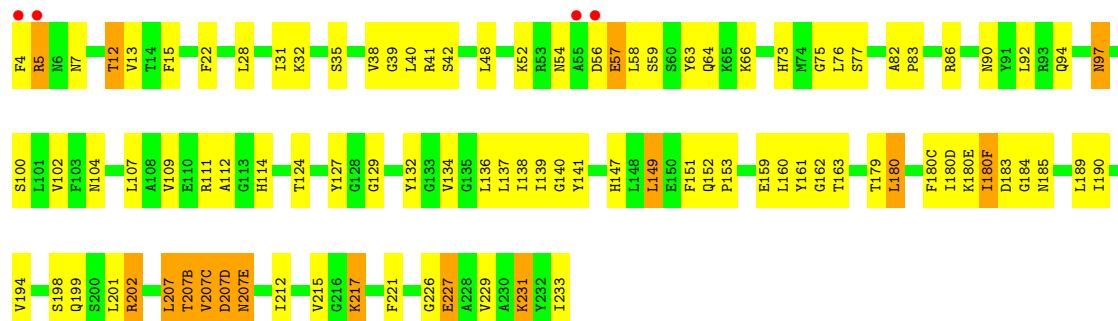
• Molecule 4: Proteasome subunit alpha type-5



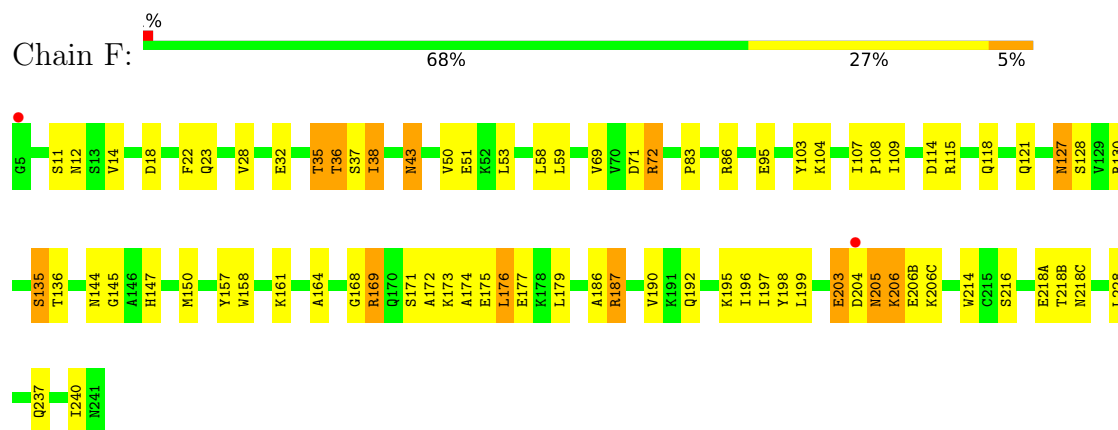
• Molecule 5: Proteasome subunit alpha type-6



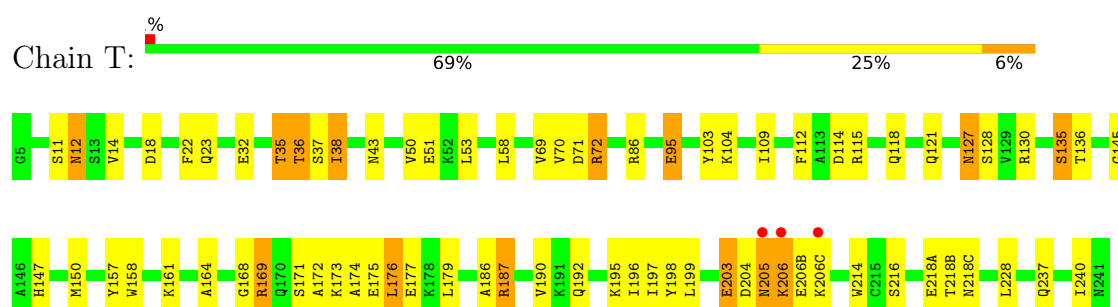
• Molecule 5: Proteasome subunit alpha type-6



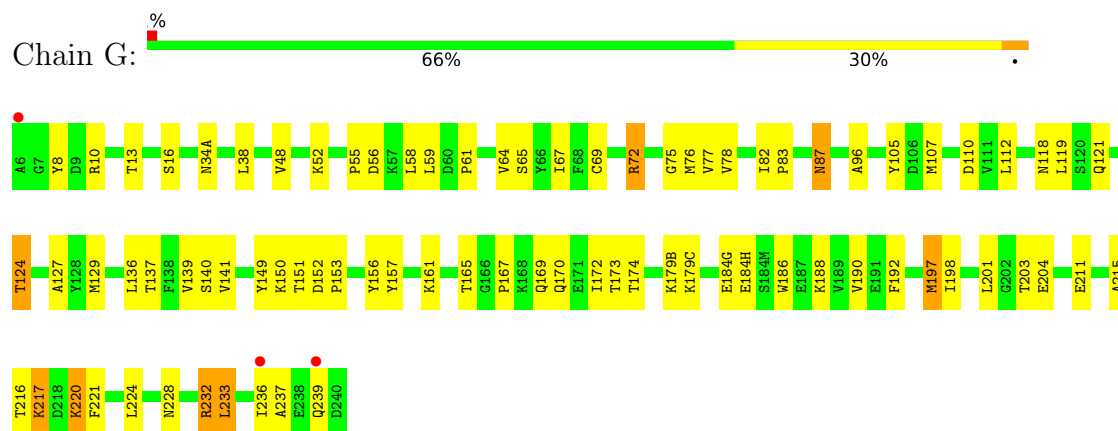
- Molecule 6: Proteasome subunit alpha type-7



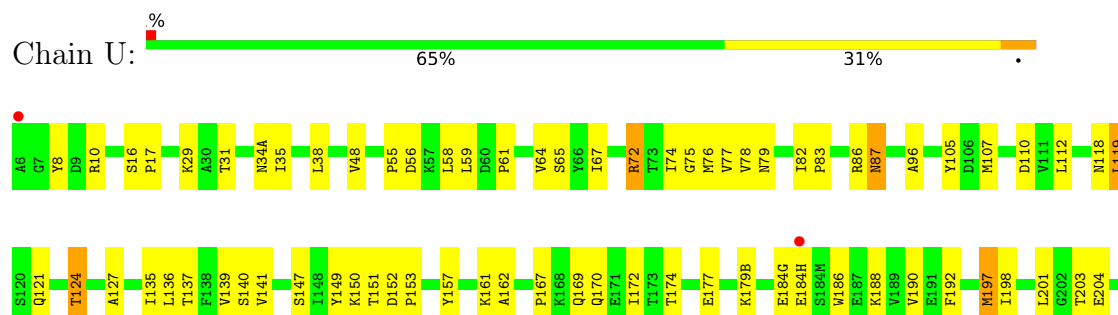
- Molecule 6: Proteasome subunit alpha type-7

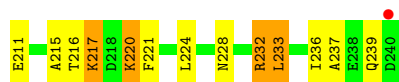


- Molecule 7: Proteasome subunit alpha type-1

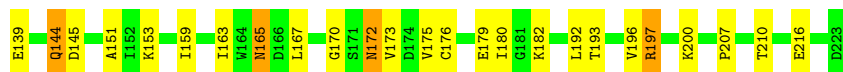


- Molecule 7: Proteasome subunit alpha type-1

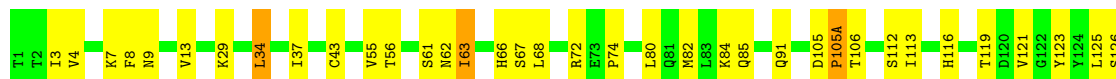




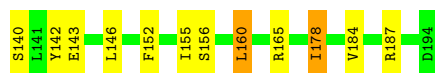
• Molecule 8: Proteasome subunit beta type-2



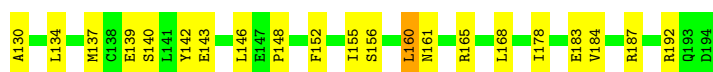
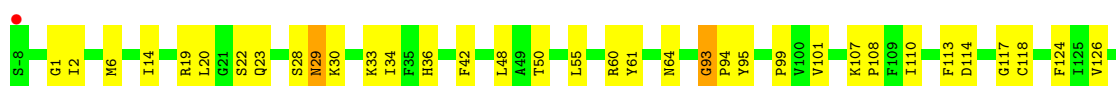
• Molecule 8: Proteasome subunit beta type-2



• Molecule 9: Proteasome subunit beta type-3

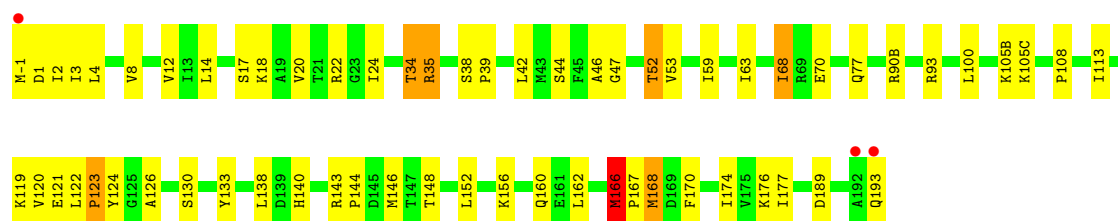


• Molecule 9: Proteasome subunit beta type-3

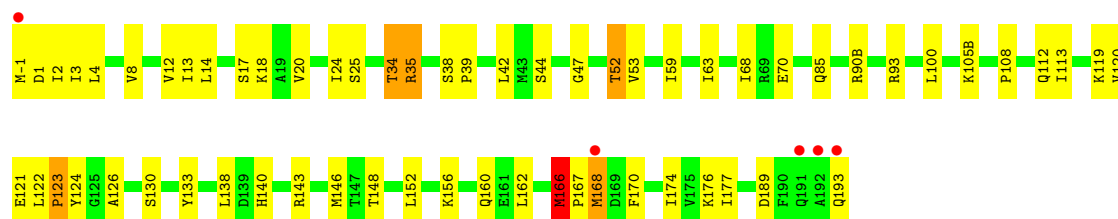


• Molecule 10: Proteasome subunit beta type-4

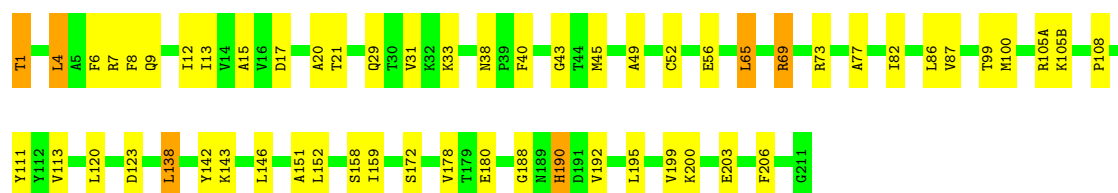




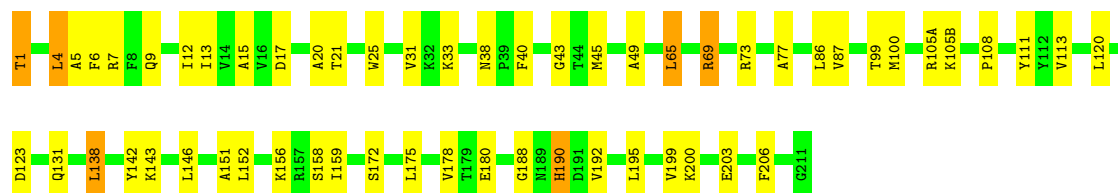
• Molecule 10: Proteasome subunit beta type-4



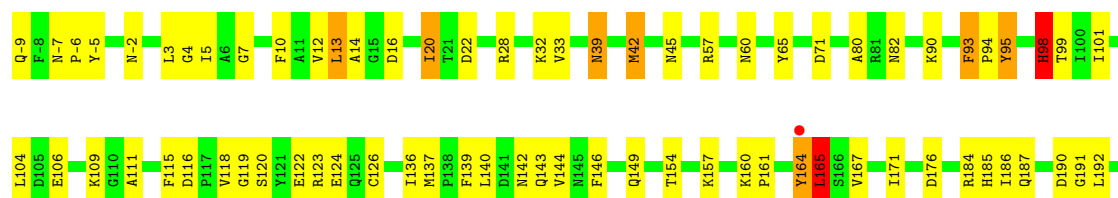
• Molecule 11: Proteasome subunit beta type-5



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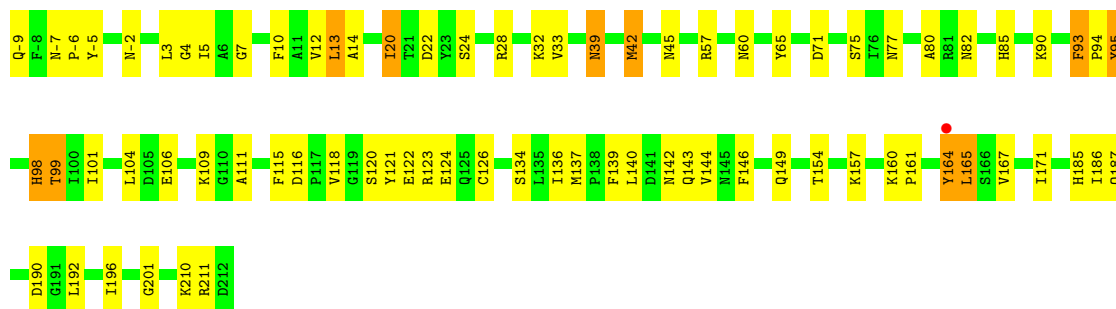
• Molecule 12: Proteasome subunit beta type-6





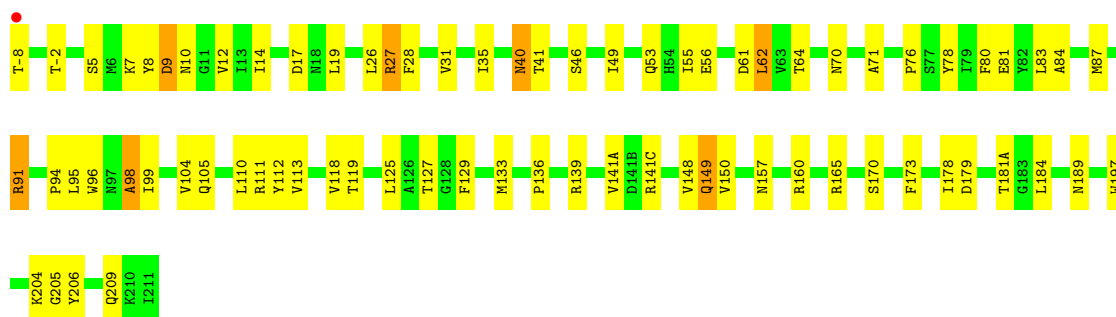
• Molecule 12: Proteasome subunit beta type-6

Chain Z: 65% 31% 5%



• Molecule 13: Proteasome subunit beta type-7

Chain M: 68% 29% 3%



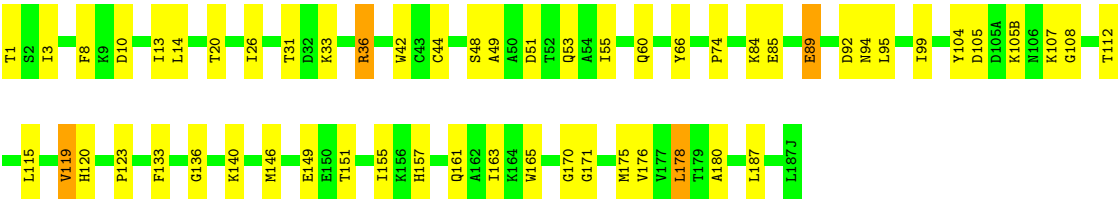
• Molecule 13: Proteasome subunit beta type-7

Chain a: 67% 30% 3%

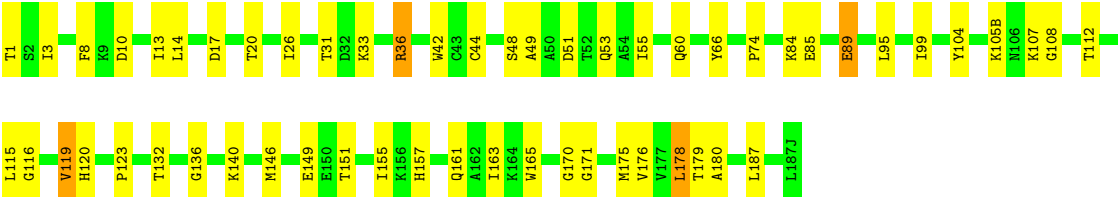


• Molecule 14: Proteasome subunit beta type-1

Chain N: 71% 27% 2%



● Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.86Å 299.40Å 144.99Å 90.00° 113.07° 90.00°	Depositor
Resolution (Å)	14.99 – 2.70 14.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (14.99-2.70) 98.9 (14.99-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.202 , 0.227 0.202 , 0.228	Depositor DCC
R_{free} test set	14347 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50942	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1Y9

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	0.43	0/1952	0.94	3/2642 (0.1%)
1	O	0.43	0/1952	0.93	4/2642 (0.2%)
2	B	0.44	0/1935	0.90	6/2618 (0.2%)
2	P	0.44	0/1935	0.90	6/2618 (0.2%)
3	C	0.42	0/1920	0.92	4/2598 (0.2%)
3	Q	0.41	0/1920	0.92	4/2598 (0.2%)
4	D	0.42	0/1887	0.91	6/2541 (0.2%)
4	R	0.42	0/1887	0.91	6/2541 (0.2%)
5	E	0.41	0/1823	0.91	5/2463 (0.2%)
5	S	0.40	0/1823	0.92	7/2463 (0.3%)
6	F	0.43	0/1937	0.96	9/2614 (0.3%)
6	T	0.42	0/1937	0.97	8/2614 (0.3%)
7	G	0.45	0/1959	0.95	6/2652 (0.2%)
7	U	0.45	0/1959	0.96	6/2652 (0.2%)
8	H	0.45	0/1716	0.93	5/2326 (0.2%)
8	V	0.44	0/1716	0.95	3/2326 (0.1%)
9	I	0.44	0/1611	0.99	7/2174 (0.3%)
9	W	0.44	0/1611	0.99	6/2174 (0.3%)
10	J	0.47	0/1613	0.97	6/2173 (0.3%)
10	X	0.47	0/1613	0.97	6/2173 (0.3%)
11	K	0.46	0/1681	0.91	2/2274 (0.1%)
11	Y	0.45	0/1681	0.92	1/2274 (0.0%)
12	L	0.43	0/1795	1.02	12/2420 (0.5%)
12	Z	0.44	0/1795	1.02	11/2420 (0.5%)
13	M	0.46	0/1855	0.93	8/2514 (0.3%)
13	a	0.45	0/1855	0.95	10/2514 (0.4%)
14	N	0.47	0/1541	0.92	2/2087 (0.1%)
14	b	0.46	0/1541	0.92	4/2087 (0.2%)
All	All	0.44	0/50450	0.94	163/68192 (0.2%)

There are no bond length outliers.

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	12	ASN	N-CA-C	8.82	120.89	111.28
6	F	12	ASN	N-CA-C	8.70	120.76	111.28
6	F	161	LYS	N-CA-C	-8.33	100.87	112.45
13	a	2	SER	N-CA-C	8.27	121.93	110.35
6	T	161	LYS	N-CA-C	-8.23	101.01	112.45
12	L	95	TYR	N-CA-C	-8.14	96.80	109.25
7	G	161	LYS	N-CA-C	-8.09	101.74	111.69
12	Z	95	TYR	N-CA-C	-8.08	96.89	109.25
2	B	161	LYS	N-CA-C	-7.90	103.77	113.41
12	Z	93	PHE	CA-C-N	7.83	127.88	119.89
12	Z	93	PHE	C-N-CA	7.83	127.88	119.89
7	U	161	LYS	N-CA-C	-7.79	102.11	111.69
1	A	161	LYS	N-CA-C	-7.64	101.83	112.45
6	F	135	SER	N-CA-C	-7.63	96.96	109.40
2	P	161	LYS	N-CA-C	-7.62	104.12	113.41
12	L	93	PHE	CA-C-N	7.61	127.66	119.89
12	L	93	PHE	C-N-CA	7.61	127.66	119.89
1	O	161	LYS	N-CA-C	-7.60	101.88	112.45
6	T	135	SER	N-CA-C	-7.34	96.94	108.90
2	P	16	SER	N-CA-C	-7.32	101.71	110.13
14	N	99	ILE	N-CA-C	7.32	118.35	108.11
4	R	169	SER	N-CA-C	7.29	119.91	111.02
8	H	37	ILE	N-CA-C	-7.26	104.70	111.45
4	R	161	ASN	N-CA-C	-7.22	103.44	112.90
4	D	169	SER	N-CA-C	7.21	119.82	111.02
11	K	188	GLY	N-CA-C	7.08	123.93	112.61
4	D	161	ASN	N-CA-C	-7.05	103.67	112.90
10	X	166	MET	CA-C-N	7.03	127.01	119.28
10	X	166	MET	C-N-CA	7.03	127.01	119.28
7	U	16	SER	N-CA-C	-7.00	101.23	110.40
7	G	16	SER	N-CA-C	-6.99	101.25	110.40
8	V	37	ILE	N-CA-C	-6.96	104.97	111.45
11	Y	188	GLY	N-CA-C	6.93	123.71	112.61
2	B	16	SER	N-CA-C	-6.93	102.16	110.13
10	J	166	MET	CA-C-N	6.86	126.82	119.28
10	J	166	MET	C-N-CA	6.86	126.82	119.28
9	W	95	TYR	N-CA-C	-6.86	99.36	110.20
13	a	27	ARG	N-CA-C	6.85	120.08	111.24
13	M	27	ARG	N-CA-C	6.74	119.94	111.24
5	S	57	GLU	N-CA-C	-6.74	104.80	113.16
3	C	161	SER	N-CA-C	-6.73	104.02	111.36
3	Q	161	SER	N-CA-C	-6.71	104.05	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	161	TYR	N-CA-C	-6.61	104.25	112.90
13	a	98	ALA	N-CA-C	-6.58	97.55	108.34
8	V	180	ILE	N-CA-C	6.54	120.20	111.17
5	E	161	TYR	N-CA-C	-6.53	104.35	112.90
8	H	180	ILE	N-CA-C	6.51	120.15	111.17
7	U	220	LYS	N-CA-C	6.49	118.26	108.46
14	b	99	ILE	N-CA-C	6.48	117.82	108.48
13	M	98	ALA	N-CA-C	-6.48	97.71	108.34
4	R	70	ILE	N-CA-C	-6.46	106.26	111.81
7	G	127	ALA	N-CA-C	6.45	120.41	112.54
5	E	57	GLU	N-CA-C	-6.39	105.24	113.16
3	C	22	PHE	N-CA-C	6.33	117.85	111.07
7	G	179(B)	LYS	N-CA-C	-6.31	104.40	111.28
10	J	123	PRO	N-CA-C	-6.31	104.95	113.40
4	D	70	ILE	N-CA-C	-6.26	106.42	111.81
13	a	-2	THR	N-CA-C	6.26	119.74	109.72
12	Z	165	LEU	N-CA-C	6.23	119.28	110.50
2	P	72	ASP	N-CA-C	-6.22	105.73	113.38
12	Z	118	VAL	N-CA-C	6.21	118.23	111.77
7	G	220	LYS	N-CA-C	6.21	117.83	108.46
12	L	165	LEU	N-CA-C	6.21	119.25	110.50
9	I	95	TYR	N-CA-C	-6.20	100.41	110.20
12	L	118	VAL	N-CA-C	6.18	118.20	111.77
6	F	14	VAL	N-CA-C	6.18	117.04	108.89
9	W	117	GLY	N-CA-C	6.17	122.94	114.92
6	T	145	GLY	N-CA-C	6.17	120.58	111.76
7	U	179(B)	LYS	N-CA-C	-6.15	104.57	111.28
9	I	117	GLY	N-CA-C	6.13	122.89	114.92
10	X	123	PRO	N-CA-C	-6.06	105.28	113.40
7	U	127	ALA	N-CA-C	6.04	119.91	112.54
13	a	9	ASP	N-CA-C	6.04	118.64	111.33
13	M	9	ASP	N-CA-C	6.04	118.63	111.33
13	M	-2	THR	N-CA-C	6.03	119.37	109.72
1	O	137	LEU	N-CA-C	-6.03	98.45	108.34
6	F	145	GLY	N-CA-C	6.02	120.37	111.76
1	O	128	GLY	N-CA-C	6.00	123.55	114.61
10	J	122	LEU	N-CA-C	5.97	117.87	108.55
5	S	22	PHE	N-CA-C	5.96	117.78	111.28
5	E	22	PHE	N-CA-C	5.95	117.76	111.28
1	A	128	GLY	N-CA-C	5.92	123.43	114.61
10	J	93	ARG	CA-C-N	5.91	125.84	119.76
10	J	93	ARG	C-N-CA	5.91	125.84	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	107	ILE	N-CA-C	5.89	114.72	108.95
3	Q	108	THR	N-CA-C	-5.87	101.83	110.52
12	L	164	TYR	N-CA-C	5.86	119.80	109.96
12	L	20	ILE	N-CA-C	5.85	117.34	108.80
3	Q	70	ILE	N-CA-C	-5.83	105.40	111.58
6	T	14	VAL	N-CA-C	5.82	116.57	108.89
10	X	122	LEU	N-CA-C	5.80	117.60	108.55
12	Z	164	TYR	N-CA-C	5.78	119.68	109.96
2	B	72	ASP	N-CA-C	-5.78	106.28	113.38
13	a	95	LEU	N-CA-C	-5.77	97.02	107.75
12	L	136	ILE	N-CA-C	5.75	116.40	110.82
12	Z	136	ILE	N-CA-C	5.74	116.39	110.82
10	X	93	ARG	CA-C-N	5.74	125.67	119.76
10	X	93	ARG	C-N-CA	5.74	125.67	119.76
6	F	38	ILE	N-CA-C	5.72	115.51	108.53
5	S	152	GLN	CA-C-N	5.67	126.93	119.84
5	S	152	GLN	C-N-CA	5.67	126.93	119.84
3	C	70	ILE	N-CA-C	-5.64	105.60	111.58
3	C	108	THR	N-CA-C	-5.61	102.22	110.52
2	P	137	ILE	N-CA-C	-5.59	99.59	107.75
6	T	38	ILE	N-CA-C	5.57	115.33	108.53
5	E	152	GLN	CA-C-N	5.57	126.80	119.84
5	E	152	GLN	C-N-CA	5.57	126.80	119.84
13	M	189	ASN	N-CA-C	5.56	119.10	111.54
2	B	137	ILE	N-CA-C	-5.54	99.66	107.75
1	A	137	LEU	N-CA-C	-5.54	99.26	108.34
12	Z	20	ILE	N-CA-C	5.53	116.88	108.80
8	H	100	ILE	N-CA-C	-5.53	99.68	107.75
3	Q	22	PHE	N-CA-C	5.51	117.72	111.11
2	P	78	VAL	N-CA-C	5.49	116.89	108.71
9	I	93	GLY	N-CA-C	-5.46	101.21	112.34
9	W	93	GLY	N-CA-C	-5.46	101.21	112.34
4	R	129	SER	N-CA-C	5.45	119.03	112.38
6	T	71	ASP	CB-CA-C	-5.45	110.31	116.63
14	N	123	PRO	N-CA-C	-5.44	106.44	113.57
6	F	71	ASP	CB-CA-C	-5.41	110.36	116.63
4	R	63	SER	N-CA-C	-5.39	106.68	113.20
13	a	189	ASN	N-CA-C	5.37	118.84	111.54
13	M	31	VAL	N-CA-C	5.37	116.10	107.73
4	R	144	ASP	N-CA-C	5.36	118.04	111.82
8	H	172	ASN	N-CA-C	5.35	117.65	109.95
9	W	60	ARG	N-CA-C	-5.33	105.38	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	107	ILE	N-CA-C	5.32	114.17	108.95
13	M	95	LEU	N-CA-C	-5.32	97.85	107.75
6	T	22	PHE	N-CA-C	5.32	117.77	111.33
6	F	144	ASN	N-CA-C	5.31	117.25	108.49
2	B	78	VAL	N-CA-C	5.30	116.61	108.71
4	D	144	ASP	N-CA-C	5.30	117.97	111.82
9	I	60	ARG	N-CA-C	-5.29	105.43	111.14
8	H	165	ASN	N-CA-C	5.27	119.72	113.28
12	Z	22	ASP	CB-CA-C	-5.27	110.06	117.23
6	F	22	PHE	N-CA-C	5.23	117.66	111.33
7	U	74	ILE	N-CA-C	5.22	115.83	108.36
5	S	102	VAL	N-CA-C	5.22	115.88	110.82
4	D	63	SER	N-CA-C	-5.20	106.71	113.16
13	a	198	ASP	N-CA-C	5.20	116.95	111.28
13	M	94	PRO	N-CA-C	5.20	119.21	111.41
1	O	78	TYR	N-CA-C	5.19	115.90	108.74
7	G	13	THR	N-CA-C	5.17	117.61	109.39
13	a	31	VAL	N-CA-C	5.15	115.76	107.73
11	K	29	GLN	N-CA-C	-5.15	105.89	113.61
5	S	199	GLN	N-CA-C	-5.14	106.79	113.16
14	b	17	ASP	N-CA-C	-5.13	102.41	110.36
8	V	172	ASN	N-CA-C	5.12	117.31	109.95
14	b	116	GLY	N-CA-C	5.12	119.94	113.24
4	D	129	SER	N-CA-C	5.11	118.62	112.38
12	Z	124	GLU	N-CA-C	5.11	116.95	109.24
12	L	22	ASP	CB-CA-C	-5.10	110.29	117.23
12	Z	98	HIS	N-CA-C	-5.10	98.96	107.99
9	I	114	ASP	N-CA-C	-5.09	102.93	110.46
13	a	94	PRO	N-CA-C	5.08	119.03	111.41
9	I	142	TYR	N-CA-C	5.07	118.48	109.96
12	L	119	GLY	N-CA-C	5.07	121.74	114.64
9	W	142	TYR	N-CA-C	5.06	118.46	109.96
12	L	124	GLU	N-CA-C	5.06	116.88	109.24
9	W	114	ASP	N-CA-C	-5.05	103.27	110.59
12	L	98	HIS	N-CA-C	-5.04	99.06	107.99
9	I	178	ILE	N-CA-C	5.03	115.22	108.17
14	b	123	PRO	N-CA-C	-5.02	106.68	113.40

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	57	0
1	O	1915	0	1926	61	0
2	B	1905	0	1901	81	0
2	P	1905	0	1901	79	0
3	C	1891	0	1900	96	0
3	Q	1891	0	1900	101	0
4	D	1862	0	1836	54	0
4	R	1862	0	1836	55	0
5	E	1795	0	1797	90	0
5	S	1795	0	1797	87	0
6	F	1897	0	1886	62	0
6	T	1897	0	1886	62	0
7	G	1921	0	1910	74	0
7	U	1921	0	1910	80	0
8	H	1685	0	1688	46	0
8	V	1685	0	1688	44	0
9	I	1581	0	1574	39	0
9	W	1581	0	1574	43	0
10	J	1585	0	1590	68	0
10	X	1585	0	1590	71	0
11	K	1644	0	1594	51	0
11	Y	1644	0	1594	52	0
12	L	1757	0	1711	56	0
12	Z	1757	0	1711	61	0
13	M	1824	0	1832	58	0
13	a	1824	0	1832	59	0
14	N	1512	0	1480	47	0
14	b	1512	0	1480	45	0
15	K	15	0	17	3	0
15	N	15	0	17	3	0
15	Y	15	0	17	3	0
15	b	15	0	17	3	0
16	A	56	0	0	0	0
16	B	36	0	0	1	0
16	C	42	0	0	2	0
16	D	38	0	0	2	0
16	E	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	F	49	0	0	2	0
16	G	61	0	0	4	0
16	H	49	0	0	4	0
16	I	70	0	0	3	0
16	J	53	0	0	3	0
16	K	46	0	0	2	0
16	L	56	0	0	1	0
16	M	73	0	0	1	0
16	N	57	0	0	4	0
16	O	31	0	0	2	0
16	P	28	0	0	2	0
16	Q	28	0	0	4	0
16	R	31	0	0	1	0
16	S	20	0	0	0	0
16	T	38	0	0	3	0
16	U	62	0	0	2	0
16	V	46	0	0	3	0
16	W	61	0	0	2	0
16	X	52	0	0	3	0
16	Y	46	0	0	1	0
16	Z	52	0	0	3	0
16	a	75	0	0	0	0
16	b	55	0	0	2	0
All	All	50942	0	49318	1587	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1587) 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)
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.14	1.13
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.13	1.09
2:P:202:THR:HG22	2:P:204:SER:H	1.13	1.09
2:B:202:THR:HG22	2:B:204:SER:H	1.14	1.07
10:J:168:MET:HE3	10:X:168:MET:HE3	1.37	1.03
7:G:96:ALA:HA	7:G:107:MET:HE2	1.42	1.01
11:K:105(B):LYS:H	11:K:105(B):LYS:HD2	1.26	1.00
7:U:96:ALA:HA	7:U:107:MET:HE2	1.44	0.99
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.47	0.97
11:Y:105(B):LYS:H	11:Y:105(B):LYS:HD2	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.10	0.96
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.32	0.94
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.46	0.94
5:S:207:LEU:HD23	5:S:207:LEU:H	1.32	0.93
2:B:15:PHE:H	3:C:23:GLN:HE22	1.04	0.93
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.34	0.92
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.32	0.92
5:E:207:LEU:HD23	5:E:207:LEU:H	1.33	0.91
1:O:15:PHE:H	2:P:23:GLN:HE22	1.17	0.91
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.53	0.91
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.32	0.90
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.20	0.89
13:a:157:ASN:HD22	13:a:160:ARG:HH11	1.12	0.89
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.54	0.89
3:C:15:PHE:H	4:D:23:GLN:HE22	1.21	0.88
7:G:217:LYS:HE3	7:G:217:LYS:HA	1.54	0.87
5:E:12:THR:HG21	5:E:124:THR:HA	1.56	0.87
2:B:71:ASN:ND2	2:B:72:ASP:H	1.71	0.87
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.40	0.86
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.39	0.86
3:C:185:THR:HB	3:C:188:GLU:HG2	1.57	0.86
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.89	0.86
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.58	0.85
5:S:12:THR:HG21	5:S:124:THR:HA	1.57	0.85
5:E:207:LEU:HA	5:E:207(E):ASN:ND2	1.91	0.85
1:A:15:PHE:H	2:B:23:GLN:HE22	1.21	0.85
15:N:201:1Y9:H12	16:N:321:HOH:O	1.76	0.85
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.42	0.85
1:A:179:ARG:HH11	1:A:179:ARG:HB3	1.42	0.85
3:C:185:THR:HG22	3:C:187:GLU:H	1.42	0.84
2:P:71:ASN:ND2	2:P:72:ASP:H	1.74	0.84
5:S:207:LEU:HA	5:S:207(E):ASN:ND2	1.90	0.84
8:H:172:ASN:HD22	8:H:193:THR:HA	1.42	0.84
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.58	0.83
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.43	0.83
14:N:161:GLN:NE2	14:b:136:GLY:HA2	1.92	0.83
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.76	0.83
8:V:172:ASN:HD22	8:V:193:THR:HA	1.41	0.83
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.27	0.82
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.61	0.82
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:136:GLY:HA2	14:b:161:GLN:NE2	1.94	0.82
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.60	0.82
13:a:157:ASN:HD22	13:a:160:ARG:NH1	1.78	0.81
7:G:184(G):GLU:HG2	7:G:188:LYS:HB2	1.62	0.81
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.61	0.80
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.93	0.80
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.64	0.80
13:M:40:ASN:H	13:M:40:ASN:HD22	1.27	0.80
5:S:207:LEU:HA	5:S:207(E):ASN:HD22	1.45	0.80
13:a:141(C):ARG:HG3	13:a:141(C):ARG:HH11	1.46	0.79
10:J:156:LYS:O	10:J:160:GLN:HG3	1.83	0.79
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.80	0.79
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.46	0.79
13:a:40:ASN:HD22	13:a:40:ASN:H	1.26	0.79
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.31	0.79
9:W:192:ARG:HG3	16:W:207:HOH:O	1.82	0.78
8:H:165:ASN:HD22	13:a:139:ARG:HH11	1.28	0.78
3:C:163:GLN:NE2	3:C:164:THR:H	1.82	0.78
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.65	0.78
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.47	0.78
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.82	0.78
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.32	0.78
12:L:42:MET:HB2	12:L:101:ILE:HG22	1.66	0.78
4:R:243:ALA:O	4:R:244:GLU:HB2	1.85	0.77
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.66	0.77
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.66	0.77
1:A:124:THR:CG2	2:B:130:ARG:HH21	1.98	0.77
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.98	0.77
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.65	0.77
10:X:156:LYS:O	10:X:160:GLN:HG3	1.83	0.77
13:a:157:ASN:ND2	13:a:160:ARG:HH11	1.83	0.76
2:P:202:THR:HG22	2:P:204:SER:N	1.97	0.76
4:D:243:ALA:O	4:D:244:GLU:HB2	1.85	0.75
3:Q:65:SER:HB2	16:Q:303:HOH:O	1.85	0.75
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.67	0.75
2:B:15:PHE:N	3:C:23:GLN:HE22	1.84	0.75
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.16	0.75
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.35	0.75
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.69	0.74
14:b:1:THR:HG23	14:b:33:LYS:NZ	2.01	0.74
7:G:172:ILE:HD13	7:G:197:MET:HE1	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:219:GLU:HG2	2:P:219(E):VAL:H	1.52	0.74
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.69	0.74
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.36	0.74
2:B:219:GLU:HG2	2:B:219(E):VAL:H	1.51	0.74
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.17	0.74
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.53	0.73
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.00	0.73
3:C:163:GLN:HE21	3:C:164:THR:H	1.36	0.73
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.18	0.73
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.54	0.73
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.69	0.73
12:Z:42:MET:HB2	12:Z:101:ILE:HG22	1.70	0.73
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.85	0.73
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.71	0.73
11:Y:45:MET:HE3	15:Y:301:1Y9:H9	1.71	0.73
12:Z:185:HIS:HD2	12:Z:187:GLN:H	1.35	0.73
4:D:123(D):ALA:HA	5:E:129:GLY:HA2	1.71	0.72
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.19	0.72
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.19	0.72
14:N:107:LYS:HG2	14:N:108:GLY:H	1.53	0.72
2:B:219:GLU:HG2	2:B:219(E):VAL:N	2.05	0.72
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.72	0.72
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.71	0.72
10:J:168:MET:CE	10:X:168:MET:HE3	2.18	0.72
5:E:207:LEU:H	5:E:207:LEU:CD2	2.03	0.71
2:P:219:GLU:HG2	2:P:219(E):VAL:N	2.06	0.71
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.72	0.71
14:N:1:THR:HG23	14:N:33:LYS:NZ	2.05	0.71
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.72	0.71
5:S:207:LEU:H	5:S:207:LEU:CD2	2.03	0.71
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.21	0.71
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.26	0.71
12:L:185:HIS:HD2	12:L:187:GLN:H	1.39	0.70
13:a:104:VAL:HG23	13:a:178:ILE:HG22	1.73	0.70
14:N:1:THR:HG23	14:N:33:LYS:HZ3	1.54	0.70
10:J:168:MET:HE3	10:X:168:MET:CE	2.17	0.70
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.06	0.70
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.27	0.70
14:N:49:ALA:HB2	15:N:201:1Y9:H13	1.72	0.70
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.05	0.70
5:S:180(C):PHE:HA	5:S:180(F):ILE:HG13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:THR:HG22	2:B:204:SER:N	1.98	0.69
5:E:180(C):PHE:HA	5:E:180(F):ILE:HG13	1.73	0.69
6:T:127:ASN:C	6:T:127:ASN:HD22	1.99	0.69
8:V:196:VAL:HG23	16:V:320:HOH:O	1.90	0.69
13:a:8:TYR:CE2	13:a:148:VAL:HG22	2.27	0.69
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.22	0.69
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.26	0.69
3:C:71:ASP:HA	10:J:68:ILE:HD13	1.74	0.69
12:L:12:VAL:HG12	12:L:196:ILE:HG13	1.73	0.69
6:T:203:GLU:O	6:T:206:LYS:HD2	1.92	0.69
7:U:59:LEU:O	7:U:61:PRO:HD3	1.93	0.69
14:b:55:ILE:HD11	14:b:95:LEU:HD13	1.74	0.69
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.40	0.69
11:K:45:MET:HE3	15:K:301:1Y9:H9	1.74	0.69
7:U:172:ILE:HD13	7:U:197:MET:HE1	1.72	0.69
14:b:49:ALA:HB2	15:b:201:1Y9:H13	1.73	0.69
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.40	0.69
7:G:59:LEU:O	7:G:61:PRO:HD3	1.93	0.69
5:S:132:TYR:O	5:S:153:PRO:HB3	1.92	0.69
6:F:203:GLU:O	6:F:206:LYS:HD2	1.93	0.68
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.93	0.68
5:E:132:TYR:O	5:E:153:PRO:HB3	1.94	0.68
5:S:207(B):THR:H	5:S:207(E):ASN:HD22	1.41	0.68
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.29	0.68
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.24	0.68
14:b:107:LYS:HG2	14:b:108:GLY:H	1.57	0.68
11:Y:105(B):LYS:H	11:Y:105(B):LYS:CD	2.06	0.68
2:B:121:GLN:O	2:B:124:THR:HB	1.95	0.68
1:O:121:GLN:O	1:O:124:THR:HB	1.94	0.68
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.29	0.68
12:Z:12:VAL:HG12	12:Z:196:ILE:HG13	1.75	0.68
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.76	0.67
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.76	0.67
13:a:19:LEU:HB2	13:a:170:SER:HB2	1.75	0.67
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.30	0.67
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.94	0.67
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.76	0.67
12:L:116:ASP:HB2	12:L:120:SER:HB3	1.77	0.67
5:E:207:LEU:HD23	5:E:207:LEU:N	2.08	0.67
6:F:127:ASN:C	6:F:127:ASN:HD22	2.00	0.67
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:13:LEU:HD13	12:Z:33:VAL:HG13	1.76	0.67
12:Z:116:ASP:HB2	12:Z:120:SER:HB3	1.76	0.67
3:C:41:LYS:HG2	3:C:161:SER:O	1.94	0.67
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.30	0.67
11:Y:49:ALA:HB2	15:Y:301:1Y9:H13	1.76	0.67
5:S:207:LEU:HD23	5:S:207:LEU:N	2.08	0.67
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.77	0.67
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.60	0.66
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.78	0.66
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.95	0.66
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.75	0.66
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.31	0.66
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.92	0.66
12:L:13:LEU:HD13	12:L:33:VAL:HG13	1.77	0.66
7:G:121:GLN:O	7:G:124:THR:HB	1.95	0.66
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.77	0.66
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.77	0.66
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.25	0.66
11:K:49:ALA:HB2	15:K:301:1Y9:H13	1.78	0.66
3:C:241:GLN:C	3:C:243:GLN:H	2.03	0.66
13:M:40:ASN:HD22	13:M:40:ASN:N	1.90	0.66
5:S:104:ASN:HB2	13:a:81:GLU:HG2	1.77	0.66
1:A:121:GLN:O	1:A:124:THR:HB	1.95	0.66
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.43	0.66
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.07	0.66
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.78	0.65
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.78	0.65
3:Q:241:GLN:C	3:Q:243:GLN:H	2.04	0.65
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.26	0.65
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.12	0.65
5:S:15:PHE:H	6:T:23:GLN:HE22	1.45	0.65
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.77	0.65
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.61	0.65
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.78	0.65
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.79	0.65
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.79	0.65
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.32	0.65
14:b:105(B):LYS:HD3	14:b:105(B):LYS:C	2.22	0.64
7:U:121:GLN:O	7:U:124:THR:HB	1.97	0.64
12:Z:99:THR:HG23	16:Z:307:HOH:O	1.97	0.64
14:b:112:THR:HG22	14:b:120:HIS:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.63	0.64
5:E:15:PHE:H	6:F:23:GLN:HE22	1.46	0.64
6:T:35:THR:HG21	6:T:51:GLU:O	1.97	0.64
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.78	0.64
2:B:71:ASN:ND2	2:B:72:ASP:N	2.44	0.64
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.33	0.64
8:V:34:LEU:HB2	16:V:318:HOH:O	1.98	0.64
15:b:201:1Y9:H12	16:b:323:HOH:O	1.97	0.64
2:B:15:PHE:H	3:C:23:GLN:NE2	1.88	0.63
3:C:105:ASP:OD2	3:C:106:PRO:HD2	1.98	0.63
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.78	0.63
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.79	0.63
6:F:35:THR:HG21	6:F:51:GLU:O	1.98	0.63
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.81	0.63
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.62	0.63
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.81	0.63
5:S:160:LEU:HD13	5:S:163:THR:HB	1.80	0.63
10:J:-1:MET:HG2	10:J:1:ASP:H	1.63	0.63
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.99	0.63
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.80	0.63
13:a:110:LEU:HG	13:a:125:LEU:HD12	1.80	0.63
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.63	0.63
7:G:233:LEU:O	7:G:236:ILE:HG13	1.99	0.63
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.12	0.63
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.64	0.63
16:R:316:HOH:O	12:Z:85:HIS:HD2	1.82	0.62
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.81	0.62
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.79	0.62
5:E:160:LEU:HD13	5:E:163:THR:HB	1.80	0.62
7:G:77:VAL:HG12	7:G:137:THR:HB	1.81	0.62
10:J:166:MET:CE	10:J:168:MET:HB2	2.30	0.62
2:P:121:GLN:O	2:P:124:THR:HB	1.98	0.62
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.82	0.62
4:R:207:LEU:C	4:R:207:LEU:HD23	2.25	0.62
5:S:86:ARG:HG3	5:S:86:ARG:HH11	1.65	0.62
2:B:181:LYS:O	2:B:184:MET:HG3	2.00	0.62
14:N:107:LYS:HG2	14:N:108:GLY:N	2.14	0.62
2:P:71:ASN:ND2	2:P:72:ASP:N	2.46	0.62
1:A:20:LYS:HE3	1:A:25:ASP:OD1	2.00	0.62
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.12	0.62
11:K:172:SER:HA	11:K:192:VAL:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:105(B):LYS:HD3	14:N:105(B):LYS:C	2.24	0.62
13:a:35:ILE:HG12	13:a:56:GLU:HG3	1.82	0.62
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.64	0.62
8:H:172:ASN:ND2	8:H:193:THR:HG22	2.15	0.62
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.15	0.61
12:L:20:ILE:C	12:L:20:ILE:HD12	2.24	0.61
11:K:105(B):LYS:H	11:K:105(B):LYS:CD	2.05	0.61
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.00	0.61
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.97	0.61
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.82	0.61
12:Z:20:ILE:HD12	12:Z:20:ILE:C	2.26	0.61
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.83	0.61
13:a:40:ASN:HD22	13:a:40:ASN:N	1.90	0.61
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.83	0.61
7:G:198:ILE:HG23	7:G:203:THR:O	2.01	0.61
1:O:20:LYS:HE3	1:O:25:ASP:OD1	2.00	0.61
11:Y:172:SER:HA	11:Y:192:VAL:HG23	1.82	0.61
10:J:168:MET:HG2	10:X:168:MET:CE	2.31	0.61
11:K:138:LEU:HD13	11:K:158:SER:OG	2.01	0.61
3:Q:159:SER:HB2	16:Q:322:HOH:O	2.00	0.61
3:Q:170:LYS:HB2	16:Q:315:HOH:O	1.99	0.61
5:S:198:SER:HA	5:S:201:LEU:HG	1.82	0.61
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.83	0.61
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.83	0.61
10:X:166:MET:CE	10:X:168:MET:HB2	2.31	0.61
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.83	0.60
5:E:198:SER:HA	5:E:201:LEU:HG	1.82	0.60
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.00	0.60
4:D:162:ALA:HB3	5:E:58:LEU:HD23	1.83	0.60
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.82	0.60
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.83	0.60
3:C:65:SER:HB2	16:C:311:HOH:O	2.01	0.60
4:D:205:GLU:OE2	4:D:205:GLU:HA	2.01	0.60
7:U:198:ILE:HG23	7:U:203:THR:O	2.01	0.60
10:X:-1:MET:HG2	10:X:1:ASP:H	1.65	0.60
6:F:69:VAL:HG12	16:F:308:HOH:O	2.00	0.60
9:I:165:ARG:NH2	12:Z:137:MET:HE3	2.16	0.60
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.83	0.60
5:E:86:ARG:HG3	5:E:86:ARG:HH11	1.65	0.60
5:S:227:GLU:CD	5:S:227:GLU:H	2.09	0.60
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:GLN:HE21	3:C:164:THR:N	1.99	0.60
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.83	0.60
7:U:233:LEU:O	7:U:236:ILE:HG13	2.01	0.60
10:J:4:LEU:HD23	10:J:126:ALA:HB2	1.83	0.60
10:J:168:MET:CE	10:X:168:MET:HG2	2.31	0.60
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.82	0.60
11:Y:105(B):LYS:HD2	11:Y:105(B):LYS:N	2.06	0.60
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.84	0.60
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.83	0.60
1:A:97:HIS:HD2	8:H:61:SER:OG	1.84	0.59
12:L:93:PHE:N	12:L:94:PRO:HD3	2.17	0.59
10:X:4:LEU:HD23	10:X:126:ALA:HB2	1.84	0.59
14:b:20:THR:HG23	14:b:31:THR:OG1	2.02	0.59
10:J:-1:MET:HG2	10:J:1:ASP:N	2.17	0.59
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.84	0.59
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.83	0.59
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.85	0.59
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.83	0.59
14:N:85:GLU:O	14:N:89:GLU:HB2	2.03	0.59
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.84	0.59
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.02	0.59
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.84	0.59
4:D:207:LEU:HD23	4:D:207:LEU:C	2.28	0.59
12:L:149:GLN:HG2	8:V:210:THR:CG2	2.32	0.59
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.85	0.59
14:N:20:THR:HG23	14:N:31:THR:OG1	2.02	0.59
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.85	0.59
5:S:180(D):ILE:HG23	5:S:180(E):LYS:HG3	1.85	0.59
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.85	0.59
12:Z:-6:PRO:O	13:a:91:ARG:NH1	2.34	0.59
14:b:84:LYS:HG3	14:b:119:VAL:HG22	1.83	0.59
2:B:224:PHE:H	2:B:224:PHE:HD2	1.51	0.59
5:E:227:GLU:CD	5:E:227:GLU:H	2.09	0.59
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.67	0.59
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.18	0.58
1:A:69:LEU:C	1:A:69:LEU:HD23	2.28	0.58
7:G:69:CYS:HB3	16:G:341:HOH:O	2.02	0.58
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.84	0.58
11:K:105(B):LYS:HD2	11:K:105(B):LYS:N	2.07	0.58
7:U:77:VAL:HG12	7:U:137:THR:HB	1.83	0.58
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.39	0.58
4:D:24:VAL:O	4:D:27:SER:HB3	2.03	0.58
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.38	0.58
4:D:123(D):ALA:HB3	4:D:126:ARG:HD3	1.85	0.58
5:E:180(D):ILE:HG23	5:E:180(E):LYS:HG3	1.86	0.58
3:C:232:TYR:O	3:C:236:ILE:HG13	2.03	0.58
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.38	0.58
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.86	0.58
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.86	0.58
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.86	0.58
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.86	0.58
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.85	0.58
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.85	0.58
7:G:184(G):GLU:CG	7:G:188:LYS:HB2	2.33	0.58
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.85	0.58
13:a:84:ALA:HA	13:a:113:VAL:HG21	1.86	0.58
14:b:107:LYS:HG2	14:b:108:GLY:N	2.18	0.58
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.34	0.57
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.04	0.57
10:X:143:ARG:O	10:X:146:MET:HG3	2.03	0.57
2:B:228:GLU:O	2:B:232:ILE:HG22	2.04	0.57
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.87	0.57
10:J:143:ARG:O	10:J:146:MET:HG3	2.04	0.57
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.52	0.57
4:R:205:GLU:HA	4:R:205:GLU:OE2	2.04	0.57
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.86	0.57
13:a:141(A):VAL:O	13:a:141(A):VAL:HG23	2.04	0.57
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.86	0.57
13:a:141(C):ARG:HH11	13:a:141(C):ARG:CG	2.15	0.57
7:G:77:VAL:CG1	7:G:137:THR:HB	2.35	0.57
2:P:181:LYS:O	2:P:184:MET:HG3	2.04	0.57
10:X:-1:MET:HG2	10:X:1:ASP:N	2.18	0.57
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.87	0.57
2:B:230:LYS:O	2:B:234:VAL:HG23	2.04	0.57
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.34	0.57
14:b:1:THR:HG23	14:b:33:LYS:HZ2	1.69	0.57
12:L:98:HIS:HD2	16:L:305:HOH:O	1.86	0.57
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.34	0.57
9:W:6:MET:CE	9:W:155:ILE:HA	2.35	0.57
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.87	0.57
12:L:137:MET:HE3	9:W:165:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:107:LYS:CG	14:N:108:GLY:H	2.18	0.57
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.53	0.57
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.85	0.57
6:T:127:ASN:HD22	6:T:128:SER:N	2.02	0.57
12:Z:82:ASN:C	12:Z:82:ASN:HD22	2.12	0.57
4:R:123(D):ALA:HB3	4:R:126:ARG:HD3	1.86	0.57
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.40	0.57
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.35	0.56
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.05	0.56
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.86	0.56
12:L:-2:ASN:HA	12:L:20:ILE:O	2.05	0.56
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.05	0.56
12:Z:-2:ASN:HA	12:Z:20:ILE:O	2.04	0.56
16:B:319:HOH:O	3:C:33:ARG:HD2	2.05	0.56
7:U:136:LEU:O	7:U:150:LYS:HA	2.05	0.56
9:W:29:ASN:ND2	9:W:29:ASN:H	2.03	0.56
12:Z:116:ASP:CB	12:Z:120:SER:HB3	2.36	0.56
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.86	0.56
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.70	0.56
2:P:224:PHE:H	2:P:224:PHE:HD2	1.52	0.56
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.87	0.56
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.86	0.56
6:T:127:ASN:C	6:T:127:ASN:ND2	2.63	0.56
14:b:105(B):LYS:HD3	14:b:105(B):LYS:O	2.05	0.56
14:b:161:GLN:NE2	14:b:165:TRP:HE1	2.03	0.56
3:C:169:SER:HA	3:C:172:VAL:CG1	2.36	0.56
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.21	0.56
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.87	0.56
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.40	0.56
2:P:228:GLU:O	2:P:232:ILE:HG22	2.04	0.56
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.20	0.56
10:J:189:ASP:O	10:J:193:GLN:HB2	2.04	0.56
11:K:82:ILE:HG13	16:K:439:HOH:O	2.05	0.56
12:L:111:ALA:HB2	12:L:123:ARG:NH2	2.20	0.56
3:Q:31:VAL:HG11	3:Q:135:SER:HB2	1.88	0.56
7:U:197:MET:HE3	7:U:197:MET:HA	1.87	0.56
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.30	0.56
3:C:185:THR:HG22	3:C:187:GLU:N	2.18	0.56
6:F:127:ASN:C	6:F:127:ASN:ND2	2.63	0.56
6:F:127:ASN:HD22	6:F:128:SER:N	2.04	0.56
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:85:GLU:O	14:b:89:GLU:HB2	2.04	0.56
1:O:197:LEU:HD23	1:O:210:ILE:HD12	1.87	0.56
5:S:97:ASN:HD21	12:Z:60:ASN:ND2	2.03	0.56
5:S:227:GLU:CD	5:S:227:GLU:N	2.63	0.56
7:U:172:ILE:CD1	7:U:197:MET:HE1	2.36	0.56
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	1.87	0.56
4:D:112:LEU:C	4:D:112:LEU:HD13	2.31	0.56
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.88	0.56
10:J:14:LEU:HD12	10:J:42:LEU:HD23	1.88	0.56
13:M:141(C):ARG:HH11	13:M:141(C):ARG:CG	2.17	0.56
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.04	0.56
5:S:134:VAL:O	5:S:153:PRO:HG3	2.06	0.56
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.87	0.56
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.21	0.56
9:W:6:MET:HG2	9:W:124:PHE:HB3	1.88	0.56
10:X:189:ASP:O	10:X:193:GLN:HB2	2.06	0.56
1:A:150:GLN:O	1:A:157:TYR:HA	2.06	0.56
7:G:136:LEU:O	7:G:150:LYS:HA	2.05	0.56
7:G:172:ILE:CD1	7:G:197:MET:HE1	2.34	0.56
1:A:197:LEU:HD23	1:A:210:ILE:HD12	1.87	0.56
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.88	0.56
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.71	0.56
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.88	0.56
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.36	0.56
8:H:210:THR:CG2	12:Z:149:GLN:HG2	2.36	0.56
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.87	0.56
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.88	0.56
1:A:32:LYS:HA	1:A:32:LYS:HE2	1.89	0.55
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.41	0.55
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.21	0.55
11:K:99:THR:HG22	11:K:113:VAL:O	2.05	0.55
4:R:112:LEU:HD13	4:R:112:LEU:C	2.31	0.55
5:S:41:ARG:NH1	5:S:42:SER:O	2.39	0.55
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.71	0.55
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.41	0.55
2:B:218:ASN:O	2:B:218(C):ASP:HB2	2.06	0.55
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.71	0.55
12:L:3:LEU:HD11	12:L:140:LEU:HD21	1.89	0.55
13:M:141(A):VAL:HG23	13:M:141(A):VAL:O	2.06	0.55
2:P:141:TYR:CD1	2:P:219(E):VAL:HG21	2.41	0.55
7:G:197:MET:HE3	7:G:197:MET:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:197:TRP:CH2	14:b:171:GLY:HA2	2.41	0.55
1:O:69:LEU:C	1:O:69:LEU:HD23	2.31	0.55
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.40	0.55
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.89	0.55
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.87	0.55
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.22	0.55
5:E:227:GLU:CD	5:E:227:GLU:N	2.64	0.55
11:K:1:THR:HG23	11:K:33:LYS:NZ	2.20	0.55
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.55	0.55
7:U:86:ARG:HD2	16:U:309:HOH:O	2.07	0.55
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.41	0.55
14:b:1:THR:HG23	14:b:33:LYS:HZ3	1.70	0.55
9:I:6:MET:HG2	9:I:124:PHE:HB3	1.89	0.55
12:L:116:ASP:CB	12:L:120:SER:HB3	2.36	0.55
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.87	0.55
12:Z:111:ALA:HB2	12:Z:123:ARG:NH2	2.22	0.55
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.88	0.55
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.37	0.55
10:X:105(B):LYS:HB2	10:X:105(B):LYS:NZ	2.22	0.55
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.89	0.55
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.19	0.55
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	1.87	0.55
12:Z:28:ARG:NH1	12:Z:190:ASP:OD1	2.36	0.55
9:I:6:MET:CE	9:I:155:ILE:HA	2.36	0.55
2:P:230:LYS:O	2:P:234:VAL:HG23	2.06	0.55
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.37	0.55
7:U:77:VAL:CG1	7:U:137:THR:HB	2.37	0.55
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.89	0.54
14:N:105:ASP:HB2	16:N:334:HOH:O	2.08	0.54
1:O:150:GLN:O	1:O:157:TYR:HA	2.07	0.54
3:Q:163:GLN:NE2	3:Q:163:GLN:HA	2.22	0.54
4:R:24:VAL:O	4:R:27:SER:HB3	2.08	0.54
11:Y:1:THR:HG23	11:Y:33:LYS:NZ	2.22	0.54
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.07	0.54
3:C:57:LYS:O	3:C:58:LEU:HB2	2.07	0.54
12:L:82:ASN:C	12:L:82:ASN:HD22	2.15	0.54
4:R:123(D):ALA:HA	5:S:129:GLY:HA2	1.89	0.54
7:U:96:ALA:CA	7:U:107:MET:HE2	2.28	0.54
12:Z:3:LEU:HD11	12:Z:140:LEU:HD21	1.89	0.54
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.05	0.54
5:S:109:VAL:HG12	5:S:149:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:69:VAL:HG12	16:T:324:HOH:O	2.07	0.54
13:a:19:LEU:HD21	13:a:26:LEU:HD22	1.89	0.54
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.21	0.54
3:C:197:LEU:O	3:C:201:VAL:HG23	2.07	0.54
7:G:96:ALA:CA	7:G:107:MET:HE2	2.27	0.54
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.89	0.54
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.88	0.54
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.36	0.54
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.37	0.54
5:E:109:VAL:HG12	5:E:149:LEU:HD22	1.90	0.54
11:K:86:LEU:C	11:K:86:LEU:HD13	2.32	0.54
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.89	0.54
2:P:71:ASN:HD22	2:P:72:ASP:N	2.05	0.54
2:P:218:ASN:O	2:P:218(C):ASP:HB2	2.06	0.54
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.71	0.54
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.42	0.54
14:N:14:LEU:O	14:N:175:MET:HA	2.08	0.54
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.73	0.54
9:W:156:SER:O	9:W:160:LEU:HB2	2.08	0.54
1:A:186:LEU:HD21	1:A:214:ILE:HD12	1.90	0.54
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.88	0.54
8:V:175:VAL:HG12	8:V:176:CYS:N	2.23	0.54
14:b:14:LEU:O	14:b:175:MET:HA	2.08	0.54
3:C:31:VAL:HG11	3:C:135:SER:HB2	1.89	0.54
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.89	0.54
10:J:124:TYR:CD2	10:J:138:LEU:HD13	2.42	0.54
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.08	0.54
13:M:149:GLN:NE2	13:M:149:GLN:H	2.06	0.54
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.18	0.54
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.73	0.54
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.90	0.54
3:C:57:LYS:HD2	3:C:58:LEU:N	2.24	0.53
7:U:96:ALA:HA	7:U:107:MET:CE	2.30	0.53
7:U:236:ILE:HD12	7:U:236:ILE:C	2.33	0.53
2:B:71:ASN:HD22	2:B:72:ASP:N	2.03	0.53
13:a:104:VAL:CG2	13:a:178:ILE:HG22	2.38	0.53
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.91	0.53
14:N:105(B):LYS:HD3	14:N:105(B):LYS:O	2.09	0.53
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	1.89	0.53
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.89	0.53
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.23	0.53
13:a:149:GLN:H	13:a:149:GLN:NE2	2.06	0.53
14:b:175:MET:HB2	14:b:187:LEU:HB2	1.89	0.53
3:C:169:SER:HA	3:C:172:VAL:HG12	1.90	0.53
5:E:41:ARG:NH1	5:E:42:SER:O	2.42	0.53
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.39	0.53
3:Q:169:SER:HA	3:Q:172:VAL:HG12	1.89	0.53
7:U:55:PRO:HG2	7:U:56:ASP:H	1.73	0.53
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.73	0.53
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.39	0.53
4:D:187:LYS:O	4:D:191:LEU:HD22	2.09	0.53
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.39	0.53
12:Z:32:LYS:HD2	12:Z:45:ASN:HD22	1.73	0.53
2:P:239:THR:OXT	2:P:239:THR:HG22	2.09	0.53
6:T:206(B):GLU:HG3	6:T:206(C):LYS:H	1.72	0.53
6:F:206(B):GLU:HG3	6:F:206(C):LYS:H	1.72	0.53
8:H:175:VAL:HG12	8:H:176:CYS:N	2.22	0.53
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.23	0.53
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.07	0.53
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.74	0.53
5:S:162:GLY:O	6:T:58:LEU:HD13	2.08	0.53
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.90	0.53
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.21	0.53
3:C:45:CYS:HA	3:C:141:PHE:HZ	1.74	0.53
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.74	0.53
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.21	0.53
10:J:105(B):LYS:HB2	10:J:105(B):LYS:NZ	2.23	0.53
13:M:46:SER:OG	13:M:98:ALA:HB3	2.09	0.53
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.39	0.53
13:a:76:PRO:HD2	13:a:105:GLN:OE1	2.09	0.53
9:I:29:ASN:ND2	9:I:29:ASN:H	2.07	0.52
14:N:171:GLY:HA2	13:a:197:TRP:CH2	2.44	0.52
14:b:161:GLN:HE22	14:b:165:TRP:HE1	1.57	0.52
2:B:216(A):LYS:O	2:B:216(B):GLY:C	2.52	0.52
5:E:134:VAL:O	5:E:153:PRO:HG3	2.08	0.52
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.39	0.52
12:L:7:GLY:HA3	12:L:10:PHE:CE2	2.44	0.52
12:L:32:LYS:HD2	12:L:45:ASN:HD22	1.74	0.52
2:P:216(A):LYS:O	2:P:216(B):GLY:C	2.52	0.52
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.40	0.52
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.39	0.52
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.90	0.52
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.73	0.52
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.09	0.52
3:C:75:VAL:HG13	3:C:221:ILE:HD13	1.91	0.52
3:C:186:VAL:O	3:C:190:VAL:HG23	2.10	0.52
1:O:60:MET:HE3	1:O:63:THR:HG21	1.92	0.52
2:P:87:ILE:O	2:P:91:THR:HG23	2.09	0.52
12:Z:7:GLY:HA3	12:Z:10:PHE:CE2	2.44	0.52
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.45	0.52
11:K:190:HIS:HA	16:K:444:HOH:O	2.10	0.52
7:U:107:MET:HE3	7:U:112:LEU:HB2	1.91	0.52
13:a:46:SER:OG	13:a:98:ALA:HB3	2.08	0.52
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.56	0.52
3:C:163:GLN:NE2	3:C:163:GLN:HA	2.23	0.52
9:I:156:SER:O	9:I:160:LEU:HB2	2.10	0.52
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.10	0.52
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.10	0.52
7:U:184(G):GLU:CG	7:U:188:LYS:HB2	2.34	0.52
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.06	0.52
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.93	0.52
1:O:175:PHE:O	1:O:179:ARG:HG2	2.09	0.52
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.92	0.52
5:S:54:ASN:ND2	5:S:56:ASP:O	2.43	0.52
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.91	0.52
12:Z:82:ASN:C	12:Z:82:ASN:ND2	2.67	0.52
3:C:46:VAL:O	3:C:215:VAL:HG12	2.10	0.52
13:M:17:ASP:HA	13:M:173:PHE:CB	2.40	0.52
13:M:40:ASN:N	13:M:40:ASN:ND2	2.57	0.52
1:O:97:HIS:HD2	8:V:61:SER:OG	1.93	0.52
7:U:141:VAL:HG21	7:U:216:THR:HA	1.92	0.52
7:U:151:THR:HG22	7:U:157:TYR:CB	2.40	0.52
14:b:107:LYS:CG	14:b:108:GLY:H	2.21	0.52
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.72	0.52
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.92	0.52
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.92	0.52
5:S:66:LYS:O	5:S:77:SER:HA	2.09	0.52
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.45	0.52
6:F:186:ALA:O	6:F:190:VAL:HG23	2.10	0.51
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.45	0.51
11:Y:190:HIS:N	11:Y:190:HIS:CD2	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:190:HIS:N	11:K:190:HIS:CD2	2.78	0.51
14:N:155:ILE:HG22	14:N:175:MET:HE2	1.92	0.51
4:R:243:ALA:O	4:R:244:GLU:CB	2.57	0.51
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.36	0.51
2:B:112:LEU:HD23	2:B:112:LEU:C	2.35	0.51
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.40	0.51
6:F:237:GLN:O	6:F:240:ILE:HG22	2.10	0.51
7:G:107:MET:HE3	7:G:112:LEU:HB2	1.93	0.51
12:L:164:TYR:CD1	12:L:165:LEU:N	2.78	0.51
2:P:121:GLN:NE2	2:P:121:GLN:C	2.69	0.51
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.46	0.51
13:a:17:ASP:HA	13:a:173:PHE:CB	2.40	0.51
13:a:41:THR:OG1	13:a:76:PRO:HG3	2.11	0.51
7:G:55:PRO:HG2	7:G:56:ASP:H	1.74	0.51
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.51
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.46	0.51
1:O:186:LEU:HD21	1:O:214:ILE:HD12	1.92	0.51
4:R:187:LYS:O	4:R:191:LEU:HD22	2.10	0.51
6:T:237:GLN:O	6:T:240:ILE:HG22	2.09	0.51
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.45	0.51
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.92	0.51
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.93	0.51
14:b:155:ILE:HG22	14:b:175:MET:HE2	1.93	0.51
5:E:97:ASN:HD21	12:L:60:ASN:ND2	2.09	0.51
11:K:142:TYR:O	11:K:143:LYS:HD2	2.11	0.51
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.10	0.51
10:J:52:THR:CG2	10:J:53:VAL:N	2.73	0.51
3:Q:182:PRO:O	3:Q:184:ALA:N	2.44	0.51
4:R:85:ALA:O	4:R:89:ILE:HG12	2.10	0.51
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.41	0.51
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.32	0.51
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.92	0.51
12:Z:164:TYR:CD1	12:Z:165:LEU:N	2.79	0.51
13:a:83:LEU:O	13:a:87:MET:HG2	2.11	0.51
5:E:162:GLY:O	6:F:58:LEU:HD13	2.11	0.51
7:G:217:LYS:HE3	7:G:217:LYS:CA	2.36	0.51
9:I:50:THR:HG22	16:I:207:HOH:O	2.11	0.51
3:C:46:VAL:HG11	3:C:139:ALA:HB1	1.92	0.51
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.40	0.51
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.92	0.51
12:L:149:GLN:HG2	8:V:210:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.46	0.51
6:T:147:HIS:HD2	16:T:302:HOH:O	1.94	0.51
10:X:52:THR:HG23	10:X:53:VAL:N	2.26	0.51
2:B:239:THR:HG22	2:B:239:THR:OXT	2.11	0.51
5:E:54:ASN:ND2	5:E:56:ASP:O	2.43	0.51
11:K:12:ILE:HB	11:K:178:VAL:HB	1.92	0.51
14:N:89:GLU:OE1	14:N:89:GLU:HA	2.09	0.51
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.93	0.51
13:a:205:GLY:HA3	13:a:209:GLN:HB3	1.92	0.51
1:A:212:LEU:HD22	1:A:224:LEU:HD12	1.93	0.50
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.26	0.50
5:E:201:LEU:O	5:E:202:ARG:HB2	2.11	0.50
7:G:141:VAL:HG21	7:G:216:THR:HA	1.93	0.50
7:G:151:THR:HG22	7:G:157:TYR:CB	2.41	0.50
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.93	0.50
8:H:139:GLU:OE2	8:H:139:GLU:HA	2.11	0.50
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.26	0.50
1:A:197:LEU:CD2	1:A:210:ILE:HD12	2.41	0.50
10:J:105(B):LYS:HB2	10:J:105(B):LYS:HZ2	1.76	0.50
13:M:83:LEU:O	13:M:87:MET:HG2	2.11	0.50
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.94	0.50
3:C:235:GLN:O	3:C:239:GLU:HG2	2.11	0.50
10:J:44:SER:OG	10:J:100:LEU:HB2	2.11	0.50
4:R:186:LEU:O	4:R:190:GLU:HG3	2.12	0.50
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.93	0.50
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.93	0.50
7:U:65:SER:HA	7:U:211:GLU:OE2	2.11	0.50
12:Z:-9:GLN:HG2	13:a:-8:THR:HG21	1.93	0.50
14:b:89:GLU:HA	14:b:89:GLU:OE1	2.11	0.50
10:J:52:THR:HG23	10:J:53:VAL:N	2.25	0.50
3:C:241:GLN:C	3:C:243:GLN:N	2.69	0.50
5:E:66:LYS:O	5:E:77:SER:HA	2.11	0.50
11:K:4:LEU:HD22	11:K:4:LEU:C	2.37	0.50
11:K:195:LEU:O	11:K:199:VAL:HG23	2.11	0.50
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.10	0.50
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.12	0.50
3:Q:241:GLN:C	3:Q:243:GLN:N	2.69	0.50
8:V:62:ASN:HB3	8:V:82:MET:HE1	1.94	0.50
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.11	0.50
10:X:52:THR:CG2	10:X:53:VAL:N	2.75	0.50
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.94	0.50
1:O:62:GLU:H	1:O:62:GLU:CD	2.19	0.50
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.15	0.50
1:O:141:HIS:HA	1:O:146:GLY:O	2.12	0.50
8:V:72:ARG:HG3	8:V:72:ARG:HH11	1.77	0.50
9:W:29:ASN:H	9:W:29:ASN:HD22	1.60	0.50
11:Y:1:THR:HG23	11:Y:33:LYS:HZ3	1.77	0.50
1:A:175:PHE:O	1:A:179:ARG:HG2	2.10	0.50
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.93	0.50
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.77	0.50
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.93	0.50
5:S:149:LEU:HD12	5:S:159:GLU:HA	1.94	0.50
2:B:121:GLN:NE2	2:B:121:GLN:C	2.70	0.50
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.93	0.50
11:Y:143:LYS:O	11:Y:146:LEU:HD13	2.12	0.50
7:G:184(G):GLU:HG2	7:G:188:LYS:HB3	1.94	0.49
5:S:77:SER:OG	5:S:137:LEU:HB2	2.12	0.49
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.94	0.49
1:A:62:GLU:CD	1:A:62:GLU:H	2.19	0.49
6:F:157:TYR:C	6:F:157:TYR:CD1	2.90	0.49
8:H:165:ASN:HD22	13:a:139:ARG:NH1	2.05	0.49
12:L:82:ASN:C	12:L:82:ASN:ND2	2.70	0.49
5:S:73:HIS:HE1	5:S:107:LEU:O	1.94	0.49
5:S:97:ASN:HD21	12:Z:60:ASN:HD21	1.59	0.49
3:C:182:PRO:O	3:C:184:ALA:N	2.45	0.49
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.48	0.49
4:D:227:GLU:OE2	4:D:227:GLU:N	2.42	0.49
1:O:197:LEU:CD2	1:O:210:ILE:HD12	2.42	0.49
6:T:157:TYR:CD1	6:T:157:TYR:C	2.90	0.49
8:V:172:ASN:HB3	8:V:192:LEU:O	2.12	0.49
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.12	0.49
3:C:35:THR:HB	3:C:51:GLU:HG3	1.94	0.49
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.13	0.49
8:H:165:ASN:ND2	13:a:139:ARG:HH11	2.04	0.49
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.94	0.49
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.95	0.49
2:B:122:GLY:C	2:B:124:THR:H	2.19	0.49
3:C:41:LYS:HD3	3:C:161:SER:HA	1.95	0.49
5:E:77:SER:OG	5:E:137:LEU:HB2	2.13	0.49
8:H:172:ASN:HB3	8:H:192:LEU:O	2.13	0.49
5:S:180(C):PHE:HA	5:S:180(F):ILE:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.61	0.49
3:Q:125:GLN:NE2	16:Q:318:HOH:O	2.45	0.49
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.47	0.49
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.60	0.49
9:W:113:PHE:HA	9:W:118:CYS:O	2.13	0.49
4:D:85:ALA:O	4:D:89:ILE:HG12	2.13	0.49
5:E:149:LEU:HD12	5:E:159:GLU:HA	1.94	0.49
7:G:236:ILE:C	7:G:236:ILE:HD12	2.37	0.49
13:M:112:TYR:CE1	13:M:127:THR:HG22	2.48	0.49
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.95	0.49
6:T:186:ALA:O	6:T:190:VAL:HG23	2.13	0.49
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.94	0.48
3:C:227:GLU:N	3:C:227:GLU:OE1	2.46	0.48
5:E:73:HIS:HE1	5:E:107:LEU:O	1.96	0.48
12:L:28:ARG:NH1	12:L:190:ASP:OD1	2.38	0.48
12:L:39:ASN:HD21	12:L:201:GLY:HA2	1.78	0.48
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.13	0.48
5:S:201:LEU:O	5:S:202:ARG:HB2	2.12	0.48
4:D:243:ALA:O	4:D:244:GLU:CB	2.58	0.48
7:G:65:SER:HA	7:G:211:GLU:OE2	2.13	0.48
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.39	0.48
2:P:112:LEU:C	2:P:112:LEU:HD23	2.38	0.48
3:Q:49:GLY:HA2	3:Q:212:ILE:HD13	1.95	0.48
7:U:236:ILE:HD12	7:U:237:ALA:N	2.27	0.48
13:a:184:LEU:HD23	13:a:184:LEU:C	2.38	0.48
7:G:192:PHE:CD1	7:G:192:PHE:C	2.90	0.48
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.07	0.48
2:P:122:GLY:C	2:P:124:THR:H	2.21	0.48
2:P:163:ILE:HG13	2:P:164:SER:N	2.29	0.48
6:T:36:THR:HB	6:T:168:GLY:H	1.79	0.48
11:Y:33:LYS:HA	11:Y:45:MET:HE2	1.93	0.48
1:A:141:HIS:HA	1:A:146:GLY:O	2.14	0.48
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.14	0.48
4:R:170:GLU:N	4:R:170:GLU:OE1	2.46	0.48
7:U:87:ASN:C	7:U:87:ASN:HD22	2.21	0.48
7:U:192:PHE:CD1	7:U:192:PHE:C	2.90	0.48
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.94	0.48
10:X:44:SER:OG	10:X:100:LEU:HB2	2.12	0.48
1:A:60:MET:HE3	1:A:63:THR:HG21	1.94	0.48
2:B:87:ILE:O	2:B:91:THR:HG23	2.14	0.48
4:D:53:ARG:O	4:D:53:ARG:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:38:LEU:C	7:G:38:LEU:HD12	2.39	0.48
10:J:133:TYR:HD1	16:Y:422:HOH:O	1.94	0.48
4:R:227:GLU:OE2	4:R:227:GLU:N	2.43	0.48
6:T:176:LEU:HB3	7:U:58:LEU:CD2	2.43	0.48
5:E:111:ARG:HG2	5:E:111:ARG:NH1	2.29	0.48
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.77	0.48
8:H:105:ASP:HB2	8:H:105(A):PRO:CD	2.43	0.48
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.60	0.48
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.22	0.48
6:T:35:THR:CG2	6:T:36:THR:N	2.76	0.48
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.44	0.48
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.22	0.48
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.94	0.48
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.29	0.48
5:S:207(C):VAL:CG1	5:S:207(D):ASP:N	2.76	0.48
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.28	0.48
7:U:186:TRP:O	7:U:190:VAL:HG23	2.13	0.48
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.29	0.48
3:C:227:GLU:H	3:C:227:GLU:CD	2.22	0.48
4:D:117:CYS:HB3	4:D:155:GLY:O	2.14	0.48
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.43	0.48
1:O:205:GLU:OE2	1:O:205:GLU:HA	2.13	0.48
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.49	0.48
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.28	0.48
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.96	0.48
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.48	0.48
7:G:220:LYS:HG2	7:G:221:PHE:N	2.28	0.48
11:K:142:TYR:C	11:K:143:LYS:HD2	2.39	0.48
4:R:40:ILE:CD1	4:R:193:VAL:HG23	2.42	0.48
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.28	0.48
9:W:6:MET:HE1	9:W:155:ILE:HA	1.96	0.48
9:W:178:ILE:HG23	9:W:184:VAL:HG22	1.94	0.48
5:E:207(C):VAL:CG1	5:E:207(D):ASP:N	2.77	0.48
7:G:236:ILE:HD12	7:G:237:ALA:N	2.29	0.48
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.95	0.48
7:U:203:THR:HG22	7:U:204:GLU:N	2.29	0.48
9:W:126:VAL:HG11	9:W:134:LEU:HB3	1.96	0.48
13:a:5:SER:HB3	13:a:14:ILE:HG13	1.96	0.48
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.95	0.47
4:D:170:GLU:OE1	4:D:170:GLU:N	2.46	0.47
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:70:ASN:ND2	13:M:71:ALA:HA	2.29	0.47
13:M:184:LEU:HD23	13:M:184:LEU:C	2.38	0.47
1:O:217(P):LYS:HE3	16:O:315:HOH:O	2.13	0.47
3:Q:76:LEU:C	3:Q:76:LEU:HD23	2.38	0.47
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.96	0.47
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.42	0.47
7:G:48:VAL:HG23	7:G:48:VAL:O	2.14	0.47
9:I:152:PHE:CE1	9:I:187:ARG:HD2	2.49	0.47
12:L:-9:GLN:HG2	13:M:-8:THR:HG21	1.96	0.47
1:O:86:ARG:NE	7:U:118:ASN:HD21	2.07	0.47
7:U:8:TYR:C	7:U:10:ARG:H	2.22	0.47
7:U:107:MET:CE	7:U:112:LEU:HD13	2.44	0.47
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.29	0.47
1:A:205:GLU:HA	1:A:205:GLU:OE2	2.13	0.47
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.14	0.47
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.94	0.47
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.79	0.47
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.95	0.47
13:a:40:ASN:N	13:a:40:ASN:ND2	2.57	0.47
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.49	0.47
6:F:114:ASP:O	6:F:118:GLN:HG2	2.13	0.47
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.39	0.47
4:R:53:ARG:O	4:R:53:ARG:HG2	2.15	0.47
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.49	0.47
6:F:136:THR:O	6:F:150:MET:HA	2.15	0.47
8:H:210:THR:HG21	12:Z:149:GLN:HG2	1.96	0.47
14:N:49:ALA:CB	15:N:201:1Y9:H13	2.43	0.47
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.77	0.47
5:S:73:HIS:CD2	5:S:73:HIS:H	2.33	0.47
5:S:207(B):THR:N	5:S:207(E):ASN:HD22	2.11	0.47
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.30	0.47
1:O:179:ARG:HH11	1:O:179:ARG:CB	2.23	0.47
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.96	0.47
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.47	0.47
4:R:123(G):GLU:HG2	4:R:125:GLU:H	1.80	0.47
4:R:237:LEU:HD22	4:R:241:GLU:HG3	1.96	0.47
5:S:207(C):VAL:HG22	5:S:226:GLY:C	2.40	0.47
1:A:67:VAL:HG11	1:A:213:ALA:HB3	1.95	0.47
8:H:72:ARG:HG3	8:H:72:ARG:HH11	1.78	0.47
11:K:33:LYS:HA	11:K:45:MET:HE2	1.96	0.47
5:S:35:SER:HB3	5:S:66:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:87:ASN:C	7:U:87:ASN:ND2	2.73	0.47
7:U:220:LYS:HG2	7:U:221:PHE:N	2.29	0.47
12:Z:185:HIS:CD2	12:Z:187:GLN:H	2.24	0.47
14:b:112:THR:CG2	14:b:120:HIS:HB2	2.44	0.47
1:A:92:SER:OG	1:A:116:VAL:HG22	2.15	0.47
5:E:73:HIS:H	5:E:73:HIS:CD2	2.32	0.47
7:G:186:TRP:O	7:G:190:VAL:HG23	2.15	0.47
1:O:124:THR:HG22	2:P:130:ARG:NH2	2.15	0.47
2:P:235:LYS:N	2:P:235:LYS:HD3	2.29	0.47
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.47	0.47
7:U:232:ARG:NE	7:U:232:ARG:HA	2.30	0.47
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.45	0.47
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.49	0.47
3:C:49:GLY:HA2	3:C:212:ILE:HD13	1.96	0.47
7:G:203:THR:HG22	7:G:204:GLU:N	2.29	0.47
10:J:46:ALA:HA	16:J:221:HOH:O	2.14	0.47
14:N:8:PHE:HB2	14:N:146:MET:O	2.15	0.47
4:R:117:CYS:HB3	4:R:155:GLY:O	2.14	0.47
5:S:12:THR:CG2	5:S:124:THR:HA	2.38	0.47
7:U:75:GLY:HA3	7:U:221:PHE:CE2	2.50	0.47
9:W:6:MET:HE3	9:W:155:ILE:HA	1.96	0.47
9:W:143:GLU:CG	9:W:146:LEU:HD21	2.44	0.47
11:Y:49:ALA:HB2	15:Y:301:1Y9:C10	2.45	0.47
13:a:112:TYR:HE1	13:a:127:THR:HG22	1.80	0.47
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.15	0.47
5:E:64:GLN:NE2	5:E:82:ALA:HB2	2.30	0.47
7:G:96:ALA:HA	7:G:107:MET:CE	2.29	0.47
10:J:166:MET:HA	10:J:167:PRO:HD3	1.76	0.47
11:K:13:ILE:HD12	11:K:152:LEU:HD23	1.96	0.47
3:Q:227:GLU:CD	3:Q:227:GLU:H	2.22	0.47
6:T:203:GLU:HG3	6:T:206:LYS:NZ	2.30	0.47
9:W:152:PHE:CE1	9:W:187:ARG:HD2	2.50	0.47
10:X:18:LYS:HD3	10:X:174:ILE:CG1	2.45	0.47
2:B:71:ASN:CG	2:B:72:ASP:H	2.23	0.46
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.45	0.46
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.49	0.46
6:T:114:ASP:O	6:T:118:GLN:HG2	2.15	0.46
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.97	0.46
13:a:40:ASN:H	13:a:40:ASN:ND2	2.06	0.46
2:B:141:TYR:CD1	2:B:141:TYR:C	2.94	0.46
2:B:141:TYR:CE2	2:B:145:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.79	0.46
9:I:113:PHE:HA	9:I:118:CYS:O	2.15	0.46
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.79	0.46
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.58	0.46
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.96	0.46
6:F:36:THR:HB	6:F:168:GLY:H	1.79	0.46
6:F:203:GLU:HG3	6:F:206:LYS:NZ	2.30	0.46
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.97	0.46
8:H:167:LEU:HD22	12:Z:186:ILE:O	2.15	0.46
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.81	0.46
11:K:38:ASN:C	11:K:38:ASN:OD1	2.57	0.46
12:L:186:ILE:O	8:V:167:LEU:HD22	2.15	0.46
13:M:104:VAL:HG23	13:M:178:ILE:CG2	2.42	0.46
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.16	0.46
14:b:3:ILE:HB	14:b:44:CYS:HB3	1.97	0.46
2:B:146:TYR:OH	2:B:216(A):LYS:HB2	2.14	0.46
7:G:72:ARG:HB2	7:G:72:ARG:NH1	2.30	0.46
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.79	0.46
10:J:168:MET:HE2	10:X:167:PRO:C	2.40	0.46
11:K:105(A):ARG:HG2	11:K:105(A):ARG:HH11	1.79	0.46
11:K:172:SER:CA	11:K:192:VAL:HG23	2.45	0.46
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.96	0.46
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.29	0.46
5:S:190:ILE:O	5:S:194:VAL:HG23	2.16	0.46
9:W:61:TYR:CD1	9:W:61:TYR:C	2.94	0.46
13:a:49:ILE:O	13:a:53:GLN:HG3	2.16	0.46
2:B:136:PHE:O	2:B:150:THR:HA	2.16	0.46
3:C:122:ARG:NH2	16:C:327:HOH:O	2.47	0.46
4:D:12:VAL:HG23	4:D:123(A):GLY:HA2	1.98	0.46
4:D:70:ILE:HD12	4:D:74:ILE:HG22	1.96	0.46
4:D:123(D):ALA:HA	5:E:129:GLY:CA	2.42	0.46
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.46	0.46
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.30	0.46
5:E:207(C):VAL:HG22	5:E:226:GLY:C	2.40	0.46
11:K:143:LYS:O	11:K:146:LEU:HD13	2.16	0.46
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.08	0.46
1:O:67:VAL:HG11	1:O:213:ALA:HB3	1.96	0.46
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.46	0.46
12:Z:80:ALA:HA	12:Z:115:PHE:HZ	1.80	0.46
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.50	0.46
3:C:76:LEU:HD23	3:C:76:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:205:GLU:OE2	4:D:205:GLU:CA	2.64	0.46
7:G:87:ASN:C	7:G:87:ASN:HD22	2.23	0.46
4:R:70:ILE:HD12	4:R:74:ILE:HG22	1.96	0.46
7:U:82:ILE:N	7:U:83:PRO:HD2	2.31	0.46
7:U:217:LYS:HE3	7:U:217:LYS:CA	2.36	0.46
10:X:3:ILE:HG22	10:X:100:LEU:CD1	2.45	0.46
13:a:112:TYR:CE1	13:a:127:THR:HG22	2.51	0.46
2:B:163:ILE:HG13	2:B:164:SER:N	2.30	0.46
10:J:3:ILE:HG22	10:J:100:LEU:CD1	2.45	0.46
11:K:1:THR:HG23	11:K:33:LYS:HZ3	1.81	0.46
11:K:13:ILE:HG13	11:K:151:ALA:HB1	1.98	0.46
2:P:115:ARG:HG2	16:P:304:HOH:O	2.15	0.46
6:T:192:GLN:O	6:T:196:ILE:HG13	2.15	0.46
11:Y:172:SER:CA	11:Y:192:VAL:HG23	2.45	0.46
1:A:97:HIS:CD2	8:H:61:SER:OG	2.66	0.46
6:F:218(B):THR:O	6:F:218(C):ASN:HB2	2.16	0.46
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.97	0.46
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.51	0.46
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.97	0.46
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.46	0.46
13:a:141(C):ARG:CG	13:a:141(C):ARG:NH1	2.78	0.46
14:b:13:ILE:HD12	14:b:151:THR:CG2	2.45	0.46
5:E:97:ASN:HD21	12:L:60:ASN:HD21	1.63	0.46
9:I:29:ASN:H	9:I:29:ASN:HD22	1.64	0.46
1:O:217(P):LYS:HB2	16:O:315:HOH:O	2.16	0.46
10:X:148:THR:HG21	10:X:177:ILE:HD13	1.98	0.46
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.40	0.46
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.96	0.46
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.99	0.46
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.51	0.46
2:P:136:PHE:O	2:P:150:THR:HA	2.16	0.46
7:U:38:LEU:C	7:U:38:LEU:HD12	2.41	0.46
2:B:186:VAL:O	2:B:190:ILE:HG13	2.16	0.45
4:D:90:GLU:OE2	11:K:69:ARG:NH1	2.49	0.45
5:E:40:LEU:N	5:E:40:LEU:HD23	2.31	0.45
6:F:192:GLN:O	6:F:196:ILE:HG13	2.16	0.45
7:G:82:ILE:N	7:G:83:PRO:HD2	2.31	0.45
8:H:7:LYS:HG3	8:H:123:TYR:HA	1.98	0.45
8:H:196:VAL:HG23	16:H:324:HOH:O	2.15	0.45
11:K:200:LYS:HE3	11:K:206:PHE:O	2.17	0.45
7:U:203:THR:HG22	7:U:204:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:104:VAL:HG23	13:a:178:ILE:CG2	2.42	0.45
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.32	0.45
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.98	0.45
9:I:6:MET:HE1	9:I:155:ILE:HA	1.97	0.45
9:I:143:GLU:CG	9:I:146:LEU:HD21	2.46	0.45
10:J:148:THR:HG21	10:J:177:ILE:HD13	1.98	0.45
12:L:154:THR:O	12:L:157:LYS:HB2	2.16	0.45
12:Z:210:LYS:HG3	16:Z:334:HOH:O	2.15	0.45
1:A:212:LEU:HD22	1:A:224:LEU:CD1	2.46	0.45
13:M:9:ASP:OD1	13:M:10:ASN:N	2.49	0.45
14:N:26:ILE:HB	13:a:165:ARG:HA	1.98	0.45
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.46	0.45
2:P:185:LYS:HD3	2:P:186:VAL:N	2.32	0.45
2:P:231:ASP:O	2:P:235:LYS:HG2	2.17	0.45
2:B:185:LYS:HD3	2:B:186:VAL:N	2.31	0.45
3:C:150:GLN:HG2	3:C:151:THR:N	2.32	0.45
5:E:190:ILE:O	5:E:194:VAL:HG23	2.16	0.45
9:I:55:LEU:HD23	9:I:55:LEU:HA	1.80	0.45
10:J:24:ILE:HG12	10:X:133:TYR:OH	2.16	0.45
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.49	0.45
6:T:173:LYS:O	6:T:177:GLU:HG3	2.17	0.45
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.81	0.45
6:F:35:THR:CG2	6:F:36:THR:N	2.78	0.45
9:I:90:ARG:HD2	16:I:266:HOH:O	2.17	0.45
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.83	0.45
11:K:6:PHE:HA	11:K:123:ASP:O	2.17	0.45
12:L:140:LEU:O	12:L:144:VAL:HB	2.16	0.45
2:P:146:TYR:OH	2:P:216(A):LYS:HB2	2.16	0.45
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.95	0.45
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.99	0.45
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.52	0.45
9:W:101:VAL:O	9:W:110:ILE:HA	2.17	0.45
10:X:3:ILE:N	16:X:247:HOH:O	2.44	0.45
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	1.99	0.45
2:B:235:LYS:HD3	2:B:235:LYS:N	2.31	0.45
3:C:174:GLU:O	3:C:178:LYS:HD2	2.17	0.45
4:R:86:ARG:HA	4:R:86:ARG:HD3	1.82	0.45
10:X:105(B):LYS:HB2	10:X:105(B):LYS:HZ2	1.80	0.45
13:a:9:ASP:OD1	13:a:10:ASN:N	2.49	0.45
6:F:173:LYS:O	6:F:177:GLU:HG3	2.17	0.45
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:232:ARG:HA	7:G:232:ARG:NE	2.32	0.45
9:I:101:VAL:O	9:I:110:ILE:HA	2.16	0.45
14:N:36:ARG:HH21	14:N:60:GLN:HE21	1.65	0.45
3:Q:136:THR:O	3:Q:150:GLN:HA	2.16	0.45
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.52	0.45
5:S:226:GLY:O	5:S:229:VAL:HG22	2.17	0.45
12:Z:39:ASN:ND2	16:Z:326:HOH:O	2.49	0.45
12:Z:154:THR:O	12:Z:157:LYS:HB2	2.17	0.45
13:a:70:ASN:ND2	13:a:70(D):ALA:HA	2.32	0.45
14:b:104:TYR:OH	14:b:180:ALA:HB2	2.17	0.45
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.65	0.45
4:D:123(G):GLU:HG2	4:D:125:GLU:H	1.82	0.45
7:G:87:ASN:C	7:G:87:ASN:ND2	2.75	0.45
10:J:35:ARG:NH2	16:J:239:HOH:O	2.50	0.45
10:J:105(C):LYS:NZ	16:J:248:HOH:O	2.49	0.45
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.52	0.45
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.99	0.45
7:U:48:VAL:CG1	7:U:139:VAL:HG11	2.47	0.45
13:a:113:VAL:HA	13:a:118:VAL:O	2.17	0.45
5:E:100:SER:O	5:E:104:ASN:HA	2.17	0.45
10:J:166:MET:HE2	10:J:168:MET:HB2	1.98	0.45
13:M:7:LYS:HB3	13:M:12:VAL:HG12	1.98	0.45
14:N:140:LYS:NZ	14:b:157:HIS:HD2	2.15	0.45
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.17	0.45
14:b:49:ALA:CB	15:b:201:1Y9:H13	2.43	0.45
14:b:66:TYR:CD2	14:b:74:PRO:HB3	2.51	0.45
1:A:179:ARG:HH11	1:A:179:ARG:CB	2.22	0.45
2:B:218(C):ASP:OD2	2:B:219:GLU:HB3	2.16	0.45
5:E:226:GLY:O	5:E:229:VAL:HG22	2.17	0.45
7:G:8:TYR:C	7:G:10:ARG:H	2.23	0.45
2:P:39:GLY:O	2:P:162:ALA:HA	2.17	0.45
5:S:179:THR:O	5:S:179:THR:HG22	2.16	0.45
6:T:187:ARG:NH1	6:T:228:LEU:HD13	2.32	0.45
9:W:48:LEU:HG	9:W:50:THR:HG22	1.99	0.45
13:a:7:LYS:HB3	13:a:12:VAL:HG12	1.99	0.45
14:b:48:SER:HB3	14:b:51:ASP:HB2	1.99	0.45
4:D:42:THR:C	4:D:44:GLU:H	2.25	0.44
4:D:186:LEU:O	4:D:190:GLU:HG3	2.16	0.44
10:J:18:LYS:HD3	10:J:174:ILE:CG1	2.47	0.44
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.52	0.44
2:P:141:TYR:CD1	2:P:141:TYR:C	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:224:PHE:N	2:P:224:PHE:CD2	2.85	0.44
3:Q:33:ARG:O	3:Q:33:ARG:HG2	2.16	0.44
5:S:207(C):VAL:HA	5:S:233:ILE:HD11	1.99	0.44
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.98	0.44
7:U:184(H):GLU:CD	7:U:184(H):GLU:H	2.24	0.44
7:U:197:MET:HE2	7:U:201:LEU:HG	1.99	0.44
10:X:25:SER:HB2	11:Y:131:GLN:NE2	2.32	0.44
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.52	0.44
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.99	0.44
5:E:38:VAL:HG12	5:E:39:GLY:N	2.32	0.44
6:F:176:LEU:HB3	7:G:58:LEU:HD21	1.99	0.44
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.52	0.44
1:O:58:LEU:HB3	7:U:162:ALA:O	2.17	0.44
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.99	0.44
8:V:7:LYS:HG3	8:V:123:TYR:HA	1.99	0.44
12:Z:139:PHE:CE1	12:Z:143:GLN:HG3	2.52	0.44
2:B:143:ASP:OD2	10:J:105(B):LYS:HE2	2.18	0.44
5:E:179:THR:HG22	5:E:179:THR:O	2.17	0.44
5:E:180(C):PHE:HA	5:E:180(F):ILE:CG1	2.44	0.44
5:E:207(B):THR:N	5:E:207(E):ASN:HD22	2.10	0.44
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.17	0.44
6:F:216:SER:HB3	6:F:218(A):GLU:HB2	2.00	0.44
8:H:144:GLN:O	8:H:145:ASP:HB2	2.17	0.44
8:H:200:LYS:HE3	9:I:140:SER:O	2.17	0.44
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.99	0.44
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.47	0.44
6:T:216:SER:HB3	6:T:218(A):GLU:HB2	1.99	0.44
7:U:48:VAL:HG23	7:U:48:VAL:O	2.16	0.44
3:C:163:GLN:NE2	3:C:163:GLN:CA	2.79	0.44
9:I:6:MET:HE3	9:I:155:ILE:HA	1.97	0.44
9:I:61:TYR:CD1	9:I:61:TYR:C	2.96	0.44
1:O:221:PHE:C	1:O:221:PHE:CD2	2.95	0.44
5:S:140:GLY:HA2	5:S:215:VAL:HG11	1.98	0.44
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.32	0.44
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.48	0.44
12:Z:5:ILE:HG12	12:Z:126:CYS:HB2	1.99	0.44
12:Z:167:VAL:O	12:Z:171:ILE:HG13	2.18	0.44
14:b:8:PHE:HB2	14:b:146:MET:O	2.17	0.44
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.52	0.44
8:H:165:ASN:ND2	13:a:139:ARG:HD2	2.32	0.44
12:L:185:HIS:CD2	12:L:187:GLN:H	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:194:LEU:HD12	4:R:194:LEU:HA	1.83	0.44
5:S:86:ARG:HG3	5:S:86:ARG:NH1	2.32	0.44
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.34	0.44
8:V:105:ASP:O	8:V:106:THR:N	2.51	0.44
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.52	0.44
13:a:19:LEU:HD12	13:a:20:GLY:H	1.83	0.44
8:H:62:ASN:HB3	8:H:82:MET:HE1	1.98	0.44
10:J:133:TYR:OH	10:X:24:ILE:HG12	2.17	0.44
12:L:80:ALA:HA	12:L:115:PHE:HZ	1.82	0.44
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.33	0.44
5:S:207(C):VAL:HG13	5:S:207(D):ASP:N	2.31	0.44
11:Y:105(A):ARG:HH11	11:Y:105(A):ARG:HG2	1.81	0.44
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.15	0.44
4:D:86:ARG:HA	4:D:86:ARG:HD3	1.83	0.44
7:G:48:VAL:CG1	7:G:139:VAL:HG11	2.47	0.44
9:I:126:VAL:HG11	9:I:134:LEU:HB3	1.99	0.44
10:J:167:PRO:C	10:X:168:MET:HE2	2.43	0.44
10:J:168:MET:HG2	10:X:168:MET:HE3	2.00	0.44
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.26	0.44
12:L:93:PHE:N	12:L:94:PRO:CD	2.81	0.44
5:S:40:LEU:N	5:S:40:LEU:HD23	2.32	0.44
5:S:180(F):ILE:HG22	5:S:180(F):ILE:O	2.18	0.44
8:V:67:SER:HB2	8:V:74:PRO:HG3	2.00	0.44
2:B:150:THR:O	2:B:157:TYR:HA	2.17	0.44
5:E:86:ARG:HG3	5:E:86:ARG:NH1	2.33	0.44
5:E:207(C):VAL:HG13	5:E:207(D):ASP:N	2.31	0.44
7:G:184(H):GLU:H	7:G:184(H):GLU:CD	2.26	0.44
10:J:168:MET:HE3	10:X:168:MET:HG2	1.98	0.44
12:L:139:PHE:CE1	12:L:143:GLN:HG3	2.52	0.44
3:Q:112:LEU:O	3:Q:112:LEU:HD13	2.18	0.44
4:R:185:THR:HG23	4:R:188:GLU:OE1	2.17	0.44
5:S:180(C):PHE:HA	5:S:180(F):ILE:CD1	2.48	0.44
6:T:187:ARG:HH12	6:T:228:LEU:HD13	1.83	0.44
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.98	0.44
12:Z:39:ASN:HD21	12:Z:201:GLY:HA2	1.82	0.44
12:Z:140:LEU:O	12:Z:144:VAL:HB	2.18	0.44
1:A:221:PHE:C	1:A:221:PHE:CD2	2.96	0.44
5:E:12:THR:CG2	5:E:124:THR:HA	2.38	0.44
12:L:14:ALA:HB1	12:L:192:LEU:HD11	2.00	0.44
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.53	0.44
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:143:ASP:OD2	10:X:105(B):LYS:HE2	2.18	0.44
7:U:184(H):GLU:CD	7:U:184(H):GLU:N	2.76	0.44
12:Z:14:ALA:HB1	12:Z:192:LEU:HD11	1.99	0.44
14:b:36:ARG:HH21	14:b:60:GLN:HE21	1.66	0.44
3:C:136:THR:O	3:C:150:GLN:HA	2.17	0.43
10:J:2:ILE:HB	10:J:17:SER:HB3	1.99	0.43
2:P:41:MET:HE2	16:P:305:HOH:O	2.18	0.43
2:P:101:LYS:NZ	10:X:85:GLN:HE22	2.09	0.43
2:P:218(C):ASP:OD2	2:P:219:GLU:HB3	2.18	0.43
2:P:225:LYS:O	2:P:226:PRO:C	2.60	0.43
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.99	0.43
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.48	0.43
4:D:14:THR:HG23	5:E:23:GLN:NE2	2.33	0.43
7:G:140:SER:HA	7:G:215:ALA:HB1	1.98	0.43
13:M:165:ARG:HA	14:b:26:ILE:HB	1.99	0.43
6:T:204:ASP:OD1	6:T:204:ASP:N	2.51	0.43
7:U:140:SER:HA	7:U:215:ALA:HB1	1.99	0.43
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.53	0.43
9:W:55:LEU:HD23	9:W:55:LEU:HA	1.82	0.43
13:a:80:PHE:CD1	13:a:80:PHE:C	2.95	0.43
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.48	0.43
3:C:33:ARG:O	3:C:33:ARG:HG2	2.16	0.43
4:D:122:ARG:HH11	4:D:122:ARG:HG2	1.83	0.43
5:E:207(C):VAL:HA	5:E:233:ILE:HD11	2.00	0.43
7:G:110:ASP:HB3	7:G:149:TYR:CE2	2.53	0.43
7:G:179(C):LYS:HE3	7:G:179(C):LYS:HB2	1.72	0.43
7:G:184(G):GLU:CG	7:G:188:LYS:CB	2.94	0.43
13:M:80:PHE:CD1	13:M:80:PHE:C	2.96	0.43
1:O:236:LEU:HD13	1:O:236:LEU:C	2.43	0.43
2:P:71:ASN:CG	2:P:72:ASP:H	2.23	0.43
2:P:150:THR:O	2:P:157:TYR:HA	2.18	0.43
3:Q:24:VAL:O	3:Q:27:ALA:HB3	2.18	0.43
3:Q:40:VAL:HG22	3:Q:193:THR:OG1	2.18	0.43
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.53	0.43
6:T:171:SER:O	6:T:174:ALA:HB3	2.19	0.43
2:B:46:ILE:HD11	2:B:146:TYR:HB3	2.00	0.43
2:B:222:LYS:NZ	2:B:228:GLU:OE2	2.50	0.43
2:B:225:LYS:O	2:B:226:PRO:C	2.60	0.43
3:C:227:GLU:O	3:C:231:GLN:HG3	2.18	0.43
5:E:138:ILE:HD12	5:E:138:ILE:N	2.33	0.43
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:186:VAL:O	2:P:190:ILE:HG13	2.18	0.43
6:T:38:ILE:HG12	6:T:197:ILE:HD11	2.00	0.43
6:T:136:THR:O	6:T:150:MET:HA	2.17	0.43
6:T:218(B):THR:O	6:T:218(C):ASN:HB2	2.17	0.43
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.85	0.43
9:W:20:LEU:HD13	9:W:20:LEU:C	2.43	0.43
4:D:185:THR:HG23	4:D:188:GLU:OE1	2.18	0.43
11:K:105(A):ARG:HD3	11:K:180:GLU:OE1	2.18	0.43
12:L:160:LYS:HG3	12:L:161:PRO:HD2	2.00	0.43
13:M:113:VAL:HA	13:M:118:VAL:O	2.19	0.43
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.53	0.43
7:U:119:LEU:HD12	7:U:119:LEU:HA	1.88	0.43
12:Z:-9:GLN:HE21	13:a:-8:THR:HG21	1.82	0.43
6:F:103:TYR:O	6:F:104:LYS:HB3	2.19	0.43
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.54	0.43
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.54	0.43
10:J:126:ALA:HB1	10:J:130:SER:HB2	2.01	0.43
12:L:5:ILE:HG12	12:L:126:CYS:HB2	2.01	0.43
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.19	0.43
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.19	0.43
1:O:212:LEU:HD22	1:O:224:LEU:CD1	2.48	0.43
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.19	0.43
3:Q:215:VAL:HG13	3:Q:215:VAL:O	2.19	0.43
6:T:72:ARG:HD2	13:a:64:THR:OG1	2.19	0.43
10:X:90(B):ARG:HG2	10:X:90(B):ARG:HH11	1.84	0.43
11:Y:13:ILE:HG13	11:Y:151:ALA:HB1	2.00	0.43
1:A:217(G):LEU:HG	1:A:217(I):TYR:CE1	2.54	0.43
2:B:122:GLY:C	2:B:124:THR:N	2.77	0.43
3:C:224:LEU:HD12	3:C:224:LEU:N	2.34	0.43
4:D:105:GLU:OE1	12:L:65:TYR:OH	2.29	0.43
11:K:105(A):ARG:HG2	11:K:105(A):ARG:NH1	2.34	0.43
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.00	0.43
1:O:39:GLY:HA2	1:O:47:VAL:O	2.18	0.43
3:Q:31:VAL:CG1	3:Q:135:SER:HB2	2.48	0.43
4:R:12:VAL:HG23	4:R:123(A):GLY:HA2	2.00	0.43
4:R:81:LEU:HD12	4:R:133:GLY:HA3	2.01	0.43
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.54	0.43
13:a:112:TYR:O	13:a:119:THR:HA	2.18	0.43
13:a:133:MET:HE1	13:a:165:ARG:HG3	2.01	0.43
14:b:179:THR:HB	16:b:341:HOH:O	2.18	0.43
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:SER:CB	10:J:120:VAL:HG21	2.48	0.43
14:N:13:ILE:HD12	14:N:151:THR:HG22	2.00	0.43
2:P:77:ALA:HB3	2:P:137:ILE:HB	1.99	0.43
6:T:12:ASN:HB2	16:T:301:HOH:O	2.17	0.43
12:Z:116:ASP:HB3	12:Z:120:SER:H	1.83	0.43
1:A:39:GLY:HA2	1:A:47:VAL:O	2.19	0.43
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.19	0.43
5:E:180(C):PHE:HA	5:E:180(F):ILE:CD1	2.49	0.43
5:E:180(C):PHE:CD1	5:E:180(C):PHE:C	2.97	0.43
8:H:105:ASP:O	8:H:106:THR:N	2.51	0.43
11:K:40:PHE:CD1	11:K:73:ARG:CZ	3.02	0.43
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.53	0.43
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.77	0.43
5:E:179:THR:O	5:E:180:LEU:C	2.61	0.43
11:K:43:GLY:HA2	11:K:100:MET:O	2.19	0.43
12:L:167:VAL:O	12:L:171:ILE:HG13	2.18	0.43
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.00	0.43
13:M:179:ASP:HB3	13:M:181(A):THR:OG1	2.19	0.43
1:O:92:SER:OG	1:O:116:VAL:HG22	2.18	0.43
4:R:105:GLU:OE1	12:Z:65:TYR:OH	2.30	0.43
9:W:14:ILE:HG23	9:W:34:ILE:HD13	2.00	0.43
10:X:166:MET:HE2	10:X:168:MET:HB2	1.99	0.43
11:Y:40:PHE:CD1	11:Y:73:ARG:CZ	3.02	0.43
8:H:3:ILE:O	8:H:126:SER:HA	2.19	0.42
13:M:133:MET:HE1	13:M:165:ARG:HG3	2.01	0.42
2:P:27:ALA:O	2:P:30:SER:HB3	2.18	0.42
7:U:79:ASN:HA	16:U:312:HOH:O	2.19	0.42
7:U:110:ASP:HB3	7:U:149:TYR:CE2	2.54	0.42
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.01	0.42
10:X:126:ALA:HB1	10:X:130:SER:HB2	2.00	0.42
13:a:19:LEU:HD12	13:a:28:PHE:O	2.19	0.42
2:B:224:PHE:N	2:B:224:PHE:CD2	2.85	0.42
6:F:187:ARG:NH1	6:F:228:LEU:HD13	2.33	0.42
7:G:184(H):GLU:CD	7:G:184(H):GLU:N	2.77	0.42
10:J:52:THR:CG2	10:J:53:VAL:H	2.32	0.42
1:O:33:GLN:CA	1:O:33:GLN:NE2	2.82	0.42
3:Q:227:GLU:O	3:Q:231:GLN:HG3	2.19	0.42
4:R:42:THR:C	4:R:44:GLU:H	2.27	0.42
5:S:38:VAL:HG12	5:S:39:GLY:N	2.33	0.42
5:S:179:THR:O	5:S:180:LEU:C	2.62	0.42
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.84	0.42
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.25	0.42
13:a:17:ASP:OD2	13:a:17:ASP:C	2.62	0.42
14:b:13:ILE:HD12	14:b:151:THR:HG22	2.00	0.42
14:b:163:ILE:HG23	14:b:170:GLY:HA2	2.01	0.42
3:C:186:VAL:HG21	3:C:216:LYS:HE2	2.00	0.42
5:E:140:GLY:HA2	5:E:215:VAL:HG11	2.01	0.42
5:E:160:LEU:CD2	6:F:59:LEU:HD12	2.49	0.42
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.19	0.42
7:G:129:MET:HE3	16:G:330:HOH:O	2.19	0.42
8:H:34:LEU:HB2	16:H:325:HOH:O	2.19	0.42
10:J:77:GLN:NE2	10:J:77:GLN:C	2.78	0.42
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.54	0.42
5:S:100:SER:O	5:S:104:ASN:HA	2.19	0.42
5:S:180(C):PHE:CD1	5:S:180(C):PHE:C	2.97	0.42
8:V:144:GLN:O	8:V:145:ASP:HB2	2.19	0.42
11:Y:105(A):ARG:HD3	11:Y:180:GLU:OE1	2.20	0.42
2:B:77:ALA:HB3	2:B:137:ILE:HB	2.00	0.42
13:M:27:ARG:HD3	13:M:28:PHE:CZ	2.55	0.42
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.82	0.42
11:Y:25:TRP:CH2	12:Z:134:SER:HA	2.54	0.42
3:C:173:ARG:O	3:C:177:GLU:HG3	2.19	0.42
6:F:187:ARG:HH11	6:F:187:ARG:CG	2.32	0.42
11:K:49:ALA:HB2	15:K:301:1Y9:C10	2.46	0.42
12:L:20:ILE:C	12:L:20:ILE:CD1	2.93	0.42
13:M:150:VAL:HG21	16:M:360:HOH:O	2.20	0.42
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.54	0.42
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.18	0.42
3:Q:174:GLU:O	3:Q:178:LYS:HD2	2.18	0.42
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.85	0.42
6:T:103:TYR:O	6:T:104:LYS:HB3	2.18	0.42
12:Z:10:PHE:CE1	12:Z:167:VAL:HA	2.54	0.42
14:b:8:PHE:CE1	14:b:10:ASP:HB2	2.54	0.42
5:E:90:ASN:O	5:E:94:GLN:HG3	2.19	0.42
6:F:38:ILE:HG12	6:F:197:ILE:HD11	2.01	0.42
6:F:187:ARG:HH12	6:F:228:LEU:HD13	1.85	0.42
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.35	0.42
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.19	0.42
8:H:153:LYS:HD2	16:H:328:HOH:O	2.19	0.42
8:H:196:VAL:HA	16:H:344:HOH:O	2.19	0.42
12:L:4:GLY:O	12:L:126:CYS:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:49:ILE:O	13:M:53:GLN:HG3	2.19	0.42
13:M:112:TYR:O	13:M:119:THR:HA	2.20	0.42
1:O:108:PRO:CG	1:O:111:LEU:HD12	2.50	0.42
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	2.01	0.42
3:Q:241:GLN:O	3:Q:243:GLN:N	2.48	0.42
10:X:2:ILE:HB	10:X:17:SER:HB3	2.01	0.42
12:Z:4:GLY:O	12:Z:126:CYS:HA	2.20	0.42
1:A:52:LYS:HG3	1:A:211:GLU:HB2	2.01	0.42
6:F:172:ALA:O	6:F:176:LEU:HD23	2.19	0.42
6:F:172:ALA:O	6:F:176:LEU:CD2	2.68	0.42
8:H:84:LYS:HG3	8:H:85:GLN:N	2.34	0.42
10:J:140:HIS:CE1	11:Y:203:GLU:OE2	2.73	0.42
11:K:17:ASP:OD2	11:K:33:LYS:NZ	2.49	0.42
12:L:16:ASP:HA	12:L:191:GLY:O	2.19	0.42
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.19	0.42
1:O:198:LYS:HE3	1:O:236:LEU:HD11	2.02	0.42
8:V:200:LYS:HE3	9:W:140:SER:O	2.19	0.42
9:W:29:ASN:HD22	9:W:29:ASN:C	2.26	0.42
13:a:37:VAL:HG11	13:a:79:ILE:CD1	2.49	0.42
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.19	0.42
1:A:86:ARG:NE	7:G:118:ASN:HD21	2.11	0.42
1:A:111:LEU:O	1:A:114:SER:HB3	2.20	0.42
3:C:112:LEU:HD13	3:C:112:LEU:O	2.19	0.42
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.54	0.42
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.35	0.42
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.19	0.42
3:Q:99:HIS:CG	3:Q:107:VAL:HG12	2.55	0.42
4:R:160:TYR:HA	5:S:58:LEU:O	2.20	0.42
5:S:97:ASN:ND2	12:Z:60:ASN:HD21	2.16	0.42
9:W:137:MET:HE2	9:W:161:ASN:HB2	2.01	0.42
10:X:13:ILE:HD13	10:X:152:LEU:HD23	2.01	0.42
1:A:236:LEU:HD13	1:A:236:LEU:C	2.45	0.42
4:D:81:LEU:HD12	4:D:133:GLY:HA3	2.02	0.42
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.01	0.42
10:J:-1:MET:CG	10:J:1:ASP:H	2.31	0.42
12:L:104:LEU:HA	12:L:109:LYS:O	2.19	0.42
13:M:133:MET:C	13:M:136:PRO:HD2	2.45	0.42
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.02	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.42
3:Q:125:GLN:O	3:Q:125:GLN:HG3	2.20	0.42
4:R:179:GLU:HB3	4:R:192:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:183:ASP:O	5:S:185:ASN:N	2.53	0.42
10:X:38:SER:HA	16:X:224:HOH:O	2.18	0.42
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.42
1:A:33:GLN:CA	1:A:33:GLN:NE2	2.83	0.42
2:B:39:GLY:O	2:B:162:ALA:HA	2.20	0.42
2:B:121:GLN:HG3	3:C:83:ALA:HB1	2.01	0.42
3:C:24:VAL:O	3:C:27:ALA:HB3	2.19	0.42
3:C:190:VAL:O	3:C:194:VAL:HG23	2.20	0.42
4:D:79:SER:HA	16:D:305:HOH:O	2.18	0.42
5:E:85:ALA:HB2	5:E:134:VAL:HG21	2.02	0.42
8:H:5:GLY:O	8:H:124:TYR:HA	2.20	0.42
11:K:52:CYS:O	11:K:56:GLU:HB2	2.20	0.42
3:Q:150:GLN:HG2	3:Q:151:THR:N	2.34	0.42
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.85	0.42
5:S:90:ASN:O	5:S:94:GLN:HG3	2.20	0.42
11:Y:105(A):ARG:HG2	11:Y:105(A):ARG:NH1	2.35	0.42
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.20	0.42
9:I:48:LEU:HG	9:I:50:THR:HG22	2.01	0.41
10:J:-1:MET:HE2	10:J:47:GLY:HA2	2.02	0.41
2:P:186:VAL:HG21	2:P:216:ARG:HD3	2.01	0.41
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.35	0.41
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.20	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.83	0.41
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.55	0.41
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.55	0.41
4:D:147:GLN:HA	16:D:324:HOH:O	2.19	0.41
5:E:160:LEU:HD23	6:F:59:LEU:HA	2.02	0.41
7:G:107:MET:CE	7:G:112:LEU:HD13	2.49	0.41
9:I:20:LEU:C	9:I:20:LEU:HD13	2.45	0.41
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.51	0.41
10:J:90(B):ARG:HG2	10:J:90(B):ARG:HH11	1.85	0.41
1:O:111:LEU:O	1:O:114:SER:HB3	2.21	0.41
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.47	0.41
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.85	0.41
4:R:156:THR:HG22	5:S:82:ALA:HB3	2.02	0.41
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.32	0.41
8:V:116:HIS:HB2	16:V:344:HOH:O	2.20	0.41
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.94	0.41
3:C:31:VAL:CG1	3:C:135:SER:HB2	2.49	0.41
3:C:125:GLN:O	3:C:125:GLN:HG3	2.21	0.41
7:G:197:MET:HE2	7:G:201:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:203:THR:HG22	7:G:204:GLU:O	2.21	0.41
8:H:179:GLU:CD	8:H:182:LYS:HE2	2.46	0.41
9:I:114:ASP:HB2	16:I:252:HOH:O	2.19	0.41
12:L:176:ASP:OD1	8:V:204:TYR:OH	2.36	0.41
13:M:55:ILE:HD13	13:M:99:ILE:HD11	2.03	0.41
1:O:27:ALA:O	1:O:31:VAL:HG23	2.19	0.41
1:O:180:TRP:HA	1:O:184:LEU:HD11	2.02	0.41
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.67	0.41
8:V:3:ILE:O	8:V:126:SER:HA	2.21	0.41
10:X:20:VAL:HA	16:X:232:HOH:O	2.19	0.41
12:Z:115:PHE:CD2	12:Z:121:TYR:HB3	2.55	0.41
2:B:229:ILE:O	2:B:233:LEU:HB2	2.21	0.41
2:B:231:ASP:O	2:B:235:LYS:HG2	2.20	0.41
4:D:20:ARG:HD3	4:D:25:GLU:OE2	2.19	0.41
5:E:207(B):THR:H	5:E:207(E):ASN:HB3	1.86	0.41
9:I:22:SER:O	9:I:23:GLN:HB2	2.20	0.41
10:J:143:ARG:HA	10:J:144:PRO:HD3	1.95	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.01	0.41
14:N:92:ASP:HB2	16:N:309:HOH:O	2.20	0.41
5:S:139:ILE:HA	5:S:147:HIS:O	2.20	0.41
5:S:207(B):THR:H	5:S:207(E):ASN:HB3	1.84	0.41
9:W:22:SER:O	9:W:23:GLN:HB2	2.21	0.41
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.56	0.41
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.01	0.41
1:A:39:GLY:O	1:A:162:ALA:HA	2.21	0.41
2:B:191:GLU:HG3	2:B:236:THR:HG22	2.02	0.41
5:E:103:PHE:CE2	13:M:62:LEU:HD21	2.56	0.41
6:F:204:ASP:OD1	6:F:204:ASP:N	2.53	0.41
6:F:214:TRP:CH2	6:F:218(A):GLU:HB3	2.55	0.41
7:G:165:THR:HG23	16:G:335:HOH:O	2.21	0.41
14:N:133:PHE:HA	14:b:132:THR:O	2.20	0.41
2:P:46:ILE:HD11	2:P:146:TYR:HB3	2.01	0.41
5:S:138:ILE:N	5:S:138:ILE:HD12	2.35	0.41
8:V:148:LYS:O	8:V:152:ILE:HG13	2.21	0.41
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	2.02	0.41
12:Z:75:SER:HB2	12:Z:77:ASN:OD1	2.20	0.41
13:a:80:PHE:CE1	13:a:111:ARG:HD3	2.55	0.41
1:A:58:LEU:HD12	7:G:173:THR:HG23	2.03	0.41
2:B:238:ILE:HG22	2:B:238:ILE:O	2.20	0.41
4:D:21:LEU:O	4:D:22:PHE:C	2.64	0.41
5:E:103:PHE:O	13:M:78:TYR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:5:ILE:HG12	12:L:126:CYS:CB	2.50	0.41
1:O:86:ARG:NE	7:U:118:ASN:ND2	2.62	0.41
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	2.02	0.41
3:Q:78:PHE:CD1	3:Q:78:PHE:C	2.99	0.41
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.21	0.41
9:W:183:GLU:HA	16:W:243:HOH:O	2.21	0.41
10:X:25:SER:HB2	11:Y:131:GLN:HE22	1.86	0.41
11:Y:17:ASP:OD2	11:Y:33:LYS:NZ	2.49	0.41
12:Z:5:ILE:HG12	12:Z:126:CYS:CB	2.50	0.41
1:A:108:PRO:CG	1:A:111:LEU:HD12	2.51	0.41
2:B:27:ALA:O	2:B:30:SER:HB3	2.21	0.41
3:C:175:PHE:O	3:C:179:ASN:HB2	2.21	0.41
4:D:179:GLU:HB3	4:D:192:LEU:HD21	2.01	0.41
5:E:114:HIS:HB3	6:F:86:ARG:NH2	2.36	0.41
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.33	0.41
13:M:19:LEU:HD12	13:M:28:PHE:O	2.20	0.41
2:P:229:ILE:O	2:P:233:LEU:HB2	2.20	0.41
3:Q:95:GLU:OE2	3:Q:95:GLU:HA	2.21	0.41
4:R:197:LEU:O	4:R:201:MET:HG3	2.20	0.41
6:T:172:ALA:O	6:T:176:LEU:HD23	2.21	0.41
8:V:128:GLY:O	8:V:131:SER:HB2	2.20	0.41
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.50	0.41
11:Y:43:GLY:HA2	11:Y:100:MET:O	2.20	0.41
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.12	0.41
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.88	0.41
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.84	0.41
8:H:67:SER:HB2	8:H:74:PRO:HG3	2.02	0.41
12:L:196:ILE:N	12:L:196:ILE:HD12	2.36	0.41
14:N:53:GLN:HG2	13:a:206:TYR:CZ	2.55	0.41
14:N:94:ASN:ND2	16:N:346:HOH:O	2.30	0.41
1:O:117:ALA:HB1	1:O:155:GLY:O	2.20	0.41
1:O:122:GLU:C	1:O:124:THR:H	2.28	0.41
1:O:188:ASP:O	1:O:192:ILE:HG13	2.21	0.41
2:P:53:LYS:O	2:P:54:VAL:O	2.39	0.41
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.48	0.41
10:X:59:ILE:O	10:X:63:ILE:HG12	2.21	0.41
12:Z:104:LEU:HA	12:Z:109:LYS:O	2.20	0.41
12:Z:160:LYS:HG3	12:Z:161:PRO:HD2	2.03	0.41
12:Z:196:ILE:N	12:Z:196:ILE:HD12	2.36	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.87	0.41
1:A:161:LYS:HE3	2:B:60:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:ARG:HG3	3:C:236:ILE:HD13	2.03	0.41
4:D:52:LYS:HB2	4:D:209(B):ASN:C	2.46	0.41
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.85	0.41
4:D:238:LYS:HE2	4:D:238:LYS:HB3	1.89	0.41
7:G:151:THR:HG22	7:G:157:TYR:HB3	2.01	0.41
7:G:151:THR:HA	7:G:156:TYR:O	2.21	0.41
9:I:29:ASN:HD22	9:I:29:ASN:C	2.29	0.41
10:J:59:ILE:O	10:J:63:ILE:HG12	2.20	0.41
14:N:157:HIS:HD2	14:b:140:LYS:NZ	2.19	0.41
2:P:149:TYR:CZ	3:Q:62(A):ILE:HD12	2.56	0.41
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.21	0.41
3:Q:159:SER:O	4:R:59:LEU:HD22	2.21	0.41
4:R:112:LEU:HD13	4:R:112:LEU:O	2.20	0.41
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.56	0.41
6:T:214:TRP:CH2	6:T:218(A):GLU:HB3	2.55	0.41
7:U:35:ILE:HD13	7:U:35:ILE:HA	1.92	0.41
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.99	0.41
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.84	0.41
6:F:28:VAL:O	6:F:32:GLU:HG3	2.21	0.41
12:L:142:ASN:O	12:L:146:PHE:HA	2.20	0.41
12:L:184:ARG:NH2	8:V:29:LYS:HE2	2.36	0.41
2:P:160:TRP:CD2	2:P:163:ILE:HD13	2.55	0.41
2:P:185:LYS:O	2:P:186:VAL:C	2.63	0.41
3:Q:150:GLN:O	3:Q:157:TYR:HA	2.21	0.41
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	2.03	0.41
7:U:151:THR:HG22	7:U:157:TYR:HB3	2.03	0.41
8:V:84:LYS:HG3	8:V:85:GLN:N	2.36	0.41
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.20	0.41
12:Z:28:ARG:NH1	12:Z:211:ARG:HB3	2.36	0.41
3:C:150:GLN:O	3:C:157:TYR:HA	2.22	0.40
5:E:180(F):ILE:O	5:E:180(F):ILE:HG22	2.20	0.40
6:F:83:PRO:HB2	16:F:343:HOH:O	2.20	0.40
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.52	0.40
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.36	0.40
12:L:28:ARG:NH1	12:L:211:ARG:HB3	2.36	0.40
13:M:141(C):ARG:CG	13:M:141(C):ARG:NH1	2.79	0.40
14:N:107:LYS:CG	14:N:108:GLY:N	2.81	0.40
3:Q:35:THR:OG1	3:Q:66:LYS:NZ	2.54	0.40
5:S:31:ILE:HD11	5:S:153:PRO:HG2	2.03	0.40
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.36	0.40
6:T:36:THR:CG2	6:T:51:GLU:OE2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:31:THR:HG21	7:U:135:ILE:HG13	2.03	0.40
7:U:139:VAL:HA	7:U:147:SER:O	2.21	0.40
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.03	0.40
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.21	0.40
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	2.03	0.40
12:Z:142:ASN:O	12:Z:146:PHE:HA	2.20	0.40
13:a:133:MET:C	13:a:136:PRO:HD2	2.46	0.40
2:B:44:ASP:OD2	2:B:44:ASP:N	2.54	0.40
3:C:215:VAL:HG13	3:C:215:VAL:O	2.20	0.40
11:K:8:PHE:CE2	11:K:13:ILE:HG12	2.56	0.40
11:K:203:GLU:OE2	10:X:140:HIS:CE1	2.74	0.40
13:M:206:TYR:CZ	14:b:53:GLN:HG2	2.55	0.40
1:O:32:LYS:HA	1:O:32:LYS:CE	2.51	0.40
4:R:170:GLU:HG2	4:R:171:GLY:N	2.36	0.40
6:T:35:THR:CG2	6:T:51:GLU:O	2.67	0.40
13:a:179:ASP:HB3	13:a:181(A):THR:OG1	2.21	0.40
3:C:78:PHE:CD1	3:C:78:PHE:C	2.99	0.40
5:E:180(E):LYS:O	5:E:183:ASP:N	2.52	0.40
6:F:43:ASN:N	6:F:43:ASN:ND2	2.70	0.40
6:F:171:SER:O	6:F:174:ALA:HB3	2.21	0.40
8:H:126:SER:O	8:H:127:LEU:HD23	2.21	0.40
13:M:139:ARG:HD2	8:V:165:ASN:ND2	2.35	0.40
1:O:52:LYS:HG3	1:O:211:GLU:HB2	2.02	0.40
2:P:15:PHE:N	3:Q:23:GLN:HE22	2.05	0.40
5:S:207(B):THR:OG1	5:S:207(E):ASN:HB3	2.22	0.40
6:T:172:ALA:O	6:T:176:LEU:CD2	2.70	0.40
10:X:-1:MET:HE2	10:X:47:GLY:HA2	2.03	0.40
10:X:52:THR:CG2	10:X:53:VAL:H	2.34	0.40
10:X:100:LEU:HD21	10:X:112:GLN:HG3	2.04	0.40
12:Z:20:ILE:C	12:Z:20:ILE:CD1	2.94	0.40
13:a:37:VAL:HG11	13:a:79:ILE:HD13	2.04	0.40
1:A:117:ALA:HB1	1:A:155:GLY:O	2.21	0.40
1:A:122:GLU:C	1:A:124:THR:H	2.29	0.40
2:B:53:LYS:O	2:B:54:VAL:O	2.40	0.40
2:B:185:LYS:O	2:B:186:VAL:C	2.65	0.40
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.86	0.40
4:D:112:LEU:HD13	4:D:112:LEU:O	2.22	0.40
5:E:4:PHE:CG	5:E:5:ARG:N	2.89	0.40
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.51	0.40
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.03	0.40
10:J:22:ARG:HD3	10:J:22:ARG:HA	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:21:LEU:O	4:R:22:PHE:C	2.64	0.40
5:S:4:PHE:CG	5:S:5:ARG:N	2.88	0.40
10:X:193:GLN:HG2	10:X:193:GLN:OXT	2.22	0.40
5:E:40:LEU:HG	5:E:189:LEU:HD22	2.03	0.40
5:E:86:ARG:O	5:E:90:ASN:HB2	2.22	0.40
5:E:183:ASP:O	5:E:185:ASN:N	2.54	0.40
6:F:36:THR:CG2	6:F:51:GLU:OE2	2.69	0.40
7:G:52:LYS:HA	16:G:320:HOH:O	2.22	0.40
10:J:168:MET:HE2	10:X:167:PRO:O	2.20	0.40
12:L:90:LYS:HE3	12:L:93:PHE:O	2.22	0.40
2:P:26:TYR:CD1	2:P:26:TYR:N	2.87	0.40
3:Q:228:GLU:O	3:Q:232:TYR:HD1	2.05	0.40
5:S:180(E):LYS:O	5:S:183:ASP:N	2.52	0.40
5:S:194:VAL:CG1	5:S:207:LEU:HD11	2.52	0.40
6:T:35:THR:HG23	6:T:51:GLU:HB3	2.03	0.40
6:T:203:GLU:HA	6:T:203:GLU:OE1	2.21	0.40
9:W:19:ARG:HD3	9:W:168:LEU:O	2.21	0.40
9:W:29:ASN:ND2	9:W:29:ASN:N	2.65	0.40
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.22	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%)	235 (95%)	11 (4%)	2 (1%)	16	37
1	O	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	16	37
2	B	242/244 (99%)	219 (90%)	16 (7%)	7 (3%)	3	9
2	P	242/244 (99%)	219 (90%)	17 (7%)	6 (2%)	4	11
3	C	239/241 (99%)	226 (95%)	10 (4%)	3 (1%)	9	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	239/241 (99%)	225 (94%)	11 (5%)	3 (1%)	9	25
4	D	240/242 (99%)	223 (93%)	13 (5%)	4 (2%)	7	19
4	R	240/242 (99%)	221 (92%)	15 (6%)	4 (2%)	7	19
5	E	231/233 (99%)	208 (90%)	16 (7%)	7 (3%)	3	8
5	S	231/233 (99%)	208 (90%)	16 (7%)	7 (3%)	3	8
6	F	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	16	37
6	T	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	16	37
7	G	241/243 (99%)	227 (94%)	13 (5%)	1 (0%)	30	54
7	U	241/243 (99%)	227 (94%)	13 (5%)	1 (0%)	30	54
8	H	220/222 (99%)	209 (95%)	9 (4%)	2 (1%)	14	35
8	V	220/222 (99%)	209 (95%)	8 (4%)	3 (1%)	9	23
9	I	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	196/198 (99%)	186 (95%)	9 (5%)	1 (0%)	24	48
10	X	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	24	48
11	K	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	24	48
12	Z	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	24	48
13	M	231/233 (99%)	219 (95%)	11 (5%)	1 (0%)	30	54
13	a	231/233 (99%)	219 (95%)	11 (5%)	1 (0%)	30	54
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6312/6368 (99%)	5946 (94%)	304 (5%)	62 (1%)	12	32

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
2	B	218(C)	ASP
3	C	58	LEU
3	C	203	THR
4	D	123(G)	GLU
12	L	71	ASP

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Mol	Chain	Res	Type
2	P	54	VAL
2	P	218(C)	ASP
3	Q	58	LEU
3	Q	203	THR
4	R	123(G)	GLU
12	Z	71	ASP
1	A	5	THR
1	A	167	LYS
2	B	6	ARG
2	B	216(B)	GLY
3	C	183	PRO
5	E	5	ARG
5	E	180	LEU
5	E	202	ARG
6	F	205	ASN
1	O	5	THR
1	O	167	LYS
2	P	6	ARG
2	P	216(B)	GLY
3	Q	183	PRO
5	S	5	ARG
5	S	180	LEU
5	S	202	ARG
6	T	205	ASN
4	D	123(C)	GLY
6	F	206	LYS
8	H	91	GLN
4	R	123(C)	GLY
6	T	206	LYS
8	V	91	GLN
13	a	96	TRP
2	B	184	MET
5	E	217	LYS
13	M	96	TRP
5	S	217	LYS
2	B	64	THR
5	E	231	LYS
7	G	239	GLN
5	S	231	LYS
7	U	239	GLN
4	D	123(F)	GLY
4	D	126	ARG

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Mol	Chain	Res	Type
10	J	8	VAL
2	P	64	THR
4	R	123(F)	GLY
4	R	126	ARG
8	V	9	ASN
10	X	8	VAL
2	B	186	VAL
2	P	186	VAL
5	S	184	GLY
8	V	105(A)	PRO
8	H	105(A)	PRO
5	E	180(F)	ILE
5	E	184	GLY
5	S	180(F)	ILE

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%)	202 (97%)	7 (3%)	33	63
1	O	209/209 (100%)	202 (97%)	7 (3%)	33	63
2	B	203/203 (100%)	194 (96%)	9 (4%)	25	53
2	P	203/203 (100%)	195 (96%)	8 (4%)	28	57
3	C	213/213 (100%)	206 (97%)	7 (3%)	33	63
3	Q	213/213 (100%)	206 (97%)	7 (3%)	33	63
4	D	198/198 (100%)	187 (94%)	11 (6%)	19	44
4	R	198/198 (100%)	186 (94%)	12 (6%)	17	40
5	E	192/192 (100%)	174 (91%)	18 (9%)	8	21
5	S	192/192 (100%)	175 (91%)	17 (9%)	9	23
6	F	201/201 (100%)	186 (92%)	15 (8%)	12	31
6	T	201/201 (100%)	185 (92%)	16 (8%)	11	28
7	G	207/207 (100%)	198 (96%)	9 (4%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	207/207 (100%)	198 (96%)	9 (4%)	26	54
8	H	181/181 (100%)	171 (94%)	10 (6%)	19	45
8	V	181/181 (100%)	171 (94%)	10 (6%)	19	45
9	I	172/172 (100%)	170 (99%)	2 (1%)	63	84
9	W	172/172 (100%)	169 (98%)	3 (2%)	53	79
10	J	175/175 (100%)	167 (95%)	8 (5%)	24	51
10	X	175/175 (100%)	168 (96%)	7 (4%)	28	56
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	46
11	Y	169/169 (100%)	160 (95%)	9 (5%)	20	46
12	L	185/185 (100%)	176 (95%)	9 (5%)	22	49
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	49
13	M	199/199 (100%)	192 (96%)	7 (4%)	32	61
13	a	199/199 (100%)	191 (96%)	8 (4%)	28	56
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	59
14	b	162/162 (100%)	156 (96%)	6 (4%)	30	59
All	All	5332/5332 (100%)	5077 (95%)	255 (5%)	23	50

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	124	THR
1	A	158	PHE
1	A	174	THR
1	A	179	ARG
2	B	58	LEU
2	B	67	LEU
2	B	124	THR
2	B	135	SER
2	B	150	THR
2	B	174	THR
2	B	185	LYS
2	B	192	LEU
2	B	212	PHE
3	C	10	ARG

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Mol	Chain	Res	Type
3	C	25	GLU
3	C	57	LYS
3	C	66	LYS
3	C	135	SER
3	C	163	GLN
3	C	174	GLU
4	D	28	LEU
4	D	48	LEU
4	D	52	LYS
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	215	ILE
4	D	237	LEU
5	E	7	ASN
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	149	LEU
5	E	189	LEU
5	E	198	SER
5	E	207	LEU
5	E	207(B)	THR
5	E	207(C)	VAL
5	E	207(D)	ASP
5	E	207(E)	ASN
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	18	ASP
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	72	ARG
6	F	121	GLN

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Mol	Chain	Res	Type
6	F	127	ASN
6	F	130	ARG
6	F	135	SER
6	F	169	ARG
6	F	176	LEU
6	F	187	ARG
6	F	203	GLU
6	F	205	ASN
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	169	GLN
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	13	VAL
8	H	34	LEU
8	H	43	CYS
8	H	55	VAL
8	H	56	THR
8	H	63	ILE
8	H	68	LEU
8	H	121	VAL
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	160	LEU
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	121	GLU
10	J	166	MET
10	J	168	MET
11	K	1	THR
11	K	4	LEU
11	K	9	GLN
11	K	21	THR
11	K	65	LEU

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Mol	Chain	Res	Type
11	K	69	ARG
11	K	87	VAL
11	K	138	LEU
11	K	190	HIS
12	L	13	LEU
12	L	39	ASN
12	L	42	MET
12	L	57	ARG
12	L	98	HIS
12	L	99	THR
12	L	106	GLU
12	L	122	GLU
12	L	165	LEU
13	M	40	ASN
13	M	61	ASP
13	M	62	LEU
13	M	91	ARG
13	M	129	PHE
13	M	149	GLN
13	M	204	LYS
14	N	36	ARG
14	N	89	GLU
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU
14	N	178	LEU
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	124	THR
1	O	158	PHE
1	O	174	THR
1	O	179	ARG
2	P	58	LEU
2	P	67	LEU
2	P	124	THR
2	P	135	SER
2	P	150	THR
2	P	185	LYS
2	P	192	LEU
2	P	212	PHE
3	Q	10	ARG

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Mol	Chain	Res	Type
3	Q	25	GLU
3	Q	57	LYS
3	Q	66	LYS
3	Q	135	SER
3	Q	163	GLN
3	Q	174	GLU
4	R	28	LEU
4	R	48	LEU
4	R	52	LYS
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	170	GLU
4	R	175	GLU
4	R	177	LEU
4	R	191	LEU
4	R	215	ILE
4	R	237	LEU
5	S	7	ASN
5	S	12	THR
5	S	13	VAL
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	149	LEU
5	S	189	LEU
5	S	207	LEU
5	S	207(B)	THR
5	S	207(C)	VAL
5	S	207(D)	ASP
5	S	207(E)	ASN
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	18	ASP
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	72	ARG
6	T	95	GLU

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Mol	Chain	Res	Type
6	T	121	GLN
6	T	127	ASN
6	T	130	ARG
6	T	135	SER
6	T	169	ARG
6	T	176	LEU
6	T	187	ARG
6	T	203	GLU
6	T	205	ASN
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	169	GLN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	34	LEU
8	V	43	CYS
8	V	55	VAL
8	V	56	THR
8	V	63	ILE
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	197	ARG
9	W	29	ASN
9	W	148	PRO
9	W	160	LEU
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	121	GLU
10	X	166	MET
10	X	168	MET
11	Y	1	THR
11	Y	4	LEU
11	Y	9	GLN
11	Y	21	THR

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Mol	Chain	Res	Type
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	138	LEU
11	Y	190	HIS
12	Z	13	LEU
12	Z	24	SER
12	Z	39	ASN
12	Z	42	MET
12	Z	57	ARG
12	Z	98	HIS
12	Z	99	THR
12	Z	106	GLU
12	Z	122	GLU
13	a	40	ASN
13	a	61	ASP
13	a	62	LEU
13	a	91	ARG
13	a	129	PHE
13	a	148	VAL
13	a	149	GLN
13	a	204	LYS
14	b	36	ARG
14	b	89	GLU
14	b	115	LEU
14	b	119	VAL
14	b	149	GLU
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (238) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	173	GLN
2	B	177	GLN

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Mol	Chain	Res	Type
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	243	GLN
4	D	23	GLN
4	D	99	HIS
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	178	ASN
4	D	211	GLN
4	D	226	ASN
5	E	7	ASN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	125	GLN
5	E	152	GLN
5	E	185	ASN
5	E	199	GLN
5	E	207(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
6	F	205	ASN
6	F	241	ASN
7	G	11	HIS
7	G	32	ASN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN

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Mol	Chain	Res	Type
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	85	GLN
8	H	86	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	56	ASN
9	I	81	GLN
9	I	145	ASN
9	I	157	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	64	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	160	GLN
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	39	ASN
12	L	45	ASN
12	L	60	ASN
12	L	70	ASN
12	L	82	ASN

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Mol	Chain	Res	Type
12	L	98	HIS
12	L	142	ASN
12	L	143	GLN
12	L	148	ASN
12	L	155	ASN
12	L	185	HIS
12	L	187	GLN
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	132	HIS
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	189	ASN
13	M	191	GLN
14	N	38	HIS
14	N	60	GLN
14	N	69	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
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
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN

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Mol	Chain	Res	Type
3	Q	243	GLN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	209(A)	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	152	GLN
5	S	185	ASN
5	S	199	GLN
5	S	207(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
6	T	205	ASN
6	T	241	ASN
7	U	11	HIS
7	U	32	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	66	HIS

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Mol	Chain	Res	Type
8	V	85	GLN
8	V	86	HIS
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	56	ASN
9	W	81	GLN
9	W	145	ASN
9	W	157	GLN
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	141	HIS
10	X	160	GLN
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	39	ASN
12	Z	45	ASN
12	Z	60	ASN
12	Z	70	ASN
12	Z	84	GLN
12	Z	98	HIS
12	Z	142	ASN
12	Z	143	GLN
12	Z	148	ASN
12	Z	155	ASN
12	Z	185	HIS

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Mol	Chain	Res	Type
12	Z	187	GLN
13	a	-7	GLN
13	a	10	ASN
13	a	40	ASN
13	a	89	GLN
13	a	93	ASN
13	a	132	HIS
13	a	149	GLN
13	a	157	ASN
13	a	172	ASN
13	a	189	ASN
13	a	191	GLN
14	b	38	HIS
14	b	60	GLN
14	b	69	GLN
14	b	145	ASN
14	b	157	HIS
14	b	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	1Y9	K	301	11	13,15,15	2.36	2 (15%)	9,21,21	1.52	2 (22%)
15	1Y9	b	201	14	13,15,15	2.24	1 (7%)	9,21,21	1.75	2 (22%)
15	1Y9	N	201	14	13,15,15	2.24	1 (7%)	9,21,21	1.80	2 (22%)
15	1Y9	Y	301	11	13,15,15	2.35	2 (15%)	9,21,21	1.49	2 (22%)

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	1Y9	K	301	11	-	5/10/26/26	0/1/1/1
15	1Y9	b	201	14	-	5/10/26/26	0/1/1/1
15	1Y9	N	201	14	-	5/10/26/26	0/1/1/1
15	1Y9	Y	301	11	-	4/10/26/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	301	1Y9	O5-C4	7.68	1.44	1.20
15	N	201	1Y9	O5-C4	7.45	1.44	1.20
15	b	201	1Y9	O5-C4	7.35	1.43	1.20
15	Y	301	1Y9	O5-C4	7.31	1.43	1.20
15	Y	301	1Y9	C15-C2	3.12	1.55	1.52
15	K	301	1Y9	C15-C2	2.42	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	201	1Y9	C3-C6-C7	4.10	120.66	113.69
15	b	201	1Y9	C3-C6-C7	3.69	119.95	113.69
15	K	301	1Y9	C3-C6-C7	3.35	119.38	113.69
15	Y	301	1Y9	C3-C6-C7	3.11	118.98	113.69
15	Y	301	1Y9	O5-C4-C3	-2.42	119.10	125.56
15	K	301	1Y9	O5-C4-C3	-2.40	119.14	125.56
15	N	201	1Y9	O5-C4-C3	-2.36	119.26	125.56
15	b	201	1Y9	O5-C4-C3	-2.30	119.40	125.56

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	K	301	1Y9	C2-C3-C4-O5
15	K	301	1Y9	C6-C3-C4-O5
15	N	201	1Y9	C2-C3-C4-O5
15	N	201	1Y9	C6-C3-C4-O5
15	Y	301	1Y9	C2-C3-C4-O5
15	Y	301	1Y9	C6-C3-C4-O5
15	b	201	1Y9	C2-C3-C4-O5
15	b	201	1Y9	C6-C3-C4-O5
15	N	201	1Y9	C3-C6-C7-C8
15	K	301	1Y9	C3-C6-C7-C8
15	Y	301	1Y9	C3-C6-C7-C8
15	b	201	1Y9	C3-C6-C7-C8
15	K	301	1Y9	C11-C3-C4-O5
15	N	201	1Y9	C11-C3-C4-O5
15	Y	301	1Y9	C11-C3-C4-O5
15	b	201	1Y9	C11-C3-C4-O5
15	K	301	1Y9	C11-C12-C13-O14
15	N	201	1Y9	C11-C12-C13-O14
15	b	201	1Y9	C11-C12-C13-O14

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	301	1Y9	3	0
15	b	201	1Y9	3	0
15	N	201	1Y9	3	0
15	Y	301	1Y9	3	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%)	-0.30	3 (1%) 76 75	44, 58, 89, 114	0
1	O	250/250 (100%)	-0.32	1 (0%) 88 87	44, 59, 91, 114	0
2	B	244/244 (100%)	-0.07	7 (2%) 53 50	42, 62, 102, 124	0
2	P	244/244 (100%)	0.01	9 (3%) 45 41	42, 63, 103, 124	0
3	C	241/241 (100%)	0.01	7 (2%) 53 50	45, 67, 117, 132	0
3	Q	241/241 (100%)	0.05	10 (4%) 41 37	47, 69, 118, 133	0
4	D	242/242 (100%)	0.02	9 (3%) 45 41	45, 66, 98, 133	0
4	R	242/242 (100%)	-0.00	5 (2%) 63 61	46, 67, 97, 133	0
5	E	233/233 (100%)	-0.01	4 (1%) 69 67	49, 69, 95, 121	0
5	S	233/233 (100%)	0.06	4 (1%) 69 67	49, 70, 95, 120	0
6	F	244/244 (100%)	-0.14	2 (0%) 82 81	45, 62, 99, 114	0
6	T	244/244 (100%)	-0.05	3 (1%) 76 75	46, 63, 99, 115	0
7	G	243/243 (100%)	-0.33	3 (1%) 76 75	40, 57, 87, 123	0
7	U	243/243 (100%)	-0.33	3 (1%) 76 75	39, 57, 86, 124	0
8	H	222/222 (100%)	-0.40	0 100 100	41, 55, 77, 108	0
8	V	222/222 (100%)	-0.44	1 (0%) 87 86	42, 56, 78, 110	0
9	I	204/204 (100%)	-0.59	0 100 100	39, 53, 71, 84	0
9	W	204/204 (100%)	-0.52	1 (0%) 87 86	40, 53, 72, 85	0
10	J	198/198 (100%)	-0.37	3 (1%) 72 70	42, 55, 74, 133	0
10	X	198/198 (100%)	-0.36	5 (2%) 58 55	43, 56, 73, 133	0
11	K	212/212 (100%)	-0.50	0 100 100	39, 54, 73, 83	0
11	Y	212/212 (100%)	-0.47	0 100 100	40, 54, 74, 84	0
12	L	222/222 (100%)	-0.41	1 (0%) 87 86	38, 55, 78, 97	0
12	Z	222/222 (100%)	-0.44	1 (0%) 87 86	39, 55, 76, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.46	1 (0%)	88	87	39, 56, 71, 79	0
13	a	233/233 (100%)	-0.50	1 (0%)	88	87	39, 55, 71, 79	0
14	N	196/196 (100%)	-0.55	0	100	100	39, 51, 72, 85	0
14	b	196/196 (100%)	-0.53	0	100	100	40, 51, 72, 85	0
All	All	6368/6368 (100%)	-0.27	84 (1%)	75	73	38, 58, 91, 133	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	123(D)	ALA	9.3
4	D	123(E)	SER	6.4
4	R	123(D)	ALA	6.3
7	U	240	ASP	6.1
4	D	123(C)	GLY	5.9
3	Q	56	LEU	5.9
4	R	123(E)	SER	5.1
3	C	55	THR	5.1
3	C	56	LEU	5.0
7	G	6	ALA	4.8
7	U	6	ALA	4.7
2	B	217	ALA	4.7
2	B	216(B)	GLY	4.7
4	D	126	ARG	4.6
5	S	4	PHE	4.6
2	P	217	ALA	4.3
4	R	123(C)	GLY	4.2
10	J	193	GLN	4.1
10	X	193	GLN	4.0
5	E	4	PHE	4.0
4	D	123(F)	GLY	4.0
6	F	204	ASP	4.0
4	R	126	ARG	3.9
3	Q	58	LEU	3.9
10	X	192	ALA	3.7
2	B	218(D)	GLY	3.5
2	P	216(B)	GLY	3.5
10	J	192	ALA	3.4
3	C	54	SER	3.4
2	P	220	TYR	3.4
12	Z	164	TYR	3.1
12	L	164	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
6	F	5	GLY	3.0
4	R	127	LEU	2.8
2	B	239	THR	2.8
13	a	-8	THR	2.8
1	A	235	ALA	2.8
8	V	223	ASP	2.7
7	G	239	GLN	2.7
3	Q	240	LYS	2.7
3	Q	55	THR	2.7
13	M	-8	THR	2.7
5	S	5	ARG	2.7
2	P	54	VAL	2.6
3	C	207	ALA	2.6
6	T	206	LYS	2.6
3	Q	184	ALA	2.6
5	S	56	ASP	2.5
4	D	243	ALA	2.5
3	Q	57	LYS	2.5
3	C	203	THR	2.4
10	X	191	GLN	2.4
2	P	59	LEU	2.4
10	X	-1	MET	2.4
1	A	203	GLU	2.4
6	T	206(C)	LYS	2.3
2	B	61	GLN	2.3
2	P	61	GLN	2.3
10	J	-1	MET	2.3
4	D	242	ALA	2.3
1	O	4	MET	2.3
5	E	203	ASP	2.2
7	G	236	ILE	2.2
1	A	4	MET	2.2
2	P	55	THR	2.2
3	C	208	LYS	2.2
2	P	63	THR	2.2
4	D	127	LEU	2.2
2	P	239	THR	2.2
5	E	127	TYR	2.2
3	Q	236	ILE	2.2
4	D	123(G)	GLU	2.1
3	Q	207	ALA	2.1
3	Q	203	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	59	GLN	2.1
5	S	55	ALA	2.1
7	U	184(H)	GLU	2.1
10	X	168	MET	2.1
3	Q	54	SER	2.0
2	B	218	ASN	2.0
6	T	205	ASN	2.0
5	E	207(C)	VAL	2.0
9	W	-8	SER	2.0
2	B	54	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
15	1Y9	Y	301	15/15	0.85	0.16	67,75,78,80	0
15	1Y9	b	201	15/15	0.86	0.17	65,73,76,80	0
15	1Y9	N	201	15/15	0.90	0.15	65,71,74,75	0
15	1Y9	K	301	15/15	0.91	0.13	68,74,78,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.