



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:07 PM UTC

PDB ID : 3OKJ / pdb_00003okj
Title : Alpha-keto-aldehyde binding mechanism reveals a novel lead structure motif for proteasome inhibition
Authors : Groll, M.; Poynor, M.; Gallastegui, P.; Stein, M.; Schmidt, B.; Kloetzel, P.M.; Huber, R.
Deposited on : 2010-08-25
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:

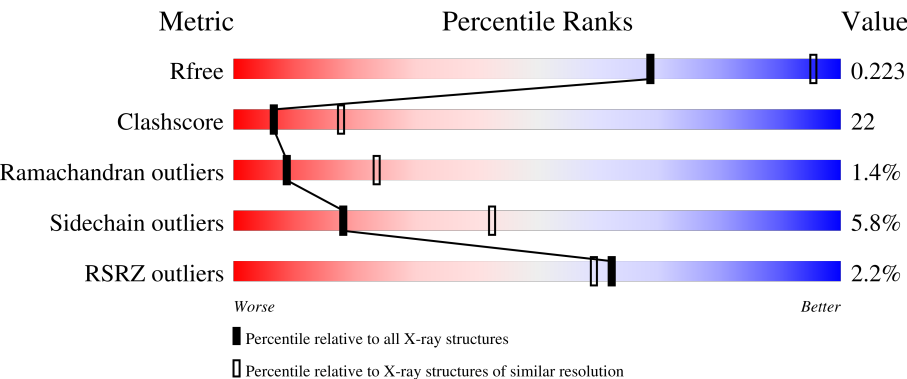
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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	% 68%29%.
1	O	250	% 66%30%.
2	B	244	4% 57%38%5%
2	P	244	4% 56%39%5%

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Mol	Chain	Length	Quality of chain
3	C	241	
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	1	233	
13	M	233	
14	2	196	
14	N	196	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	EP9	K	300	X	X	-	-
15	EP9	Y	300	X	X	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50851 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1731	1101	295	331	4			

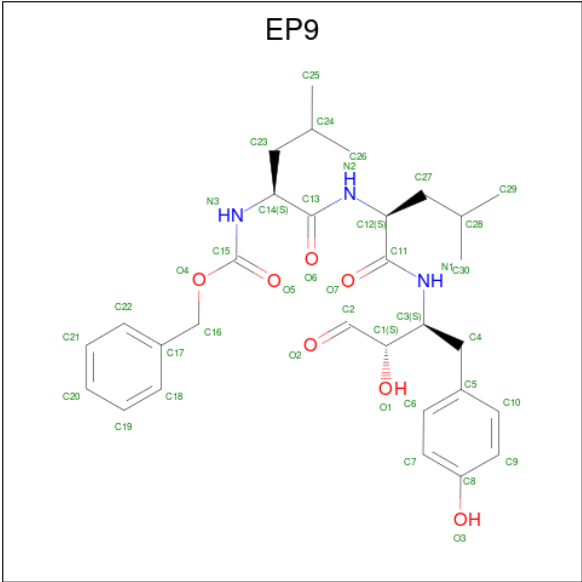
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1807	1143	308	349	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1487	941	245	294	7			

- Molecule 15 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S,3S)-3-hydroxy-1-(4-hydroxyphenyl)-4-oxobutan-2-yl]-L-leucinamide (CCD ID: EP9) (formula: C₃₀H₄₁N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			39	30	3	6		
15	Y	1	Total	C	N	O	0	0
			39	30	3	6		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	52	Total	O	0	0
			52	52		
16	B	38	Total	O	0	0
			38	38		
16	C	39	Total	O	0	0
			39	39		
16	D	42	Total	O	0	0
			42	42		
16	E	20	Total	O	0	0
			20	20		
16	F	47	Total	O	0	0
			47	47		
16	G	60	Total	O	0	0
			60	60		
16	H	49	Total	O	0	0
			49	49		
16	I	62	Total	O	0	0
			62	62		
16	J	49	Total	O	0	0
			49	49		

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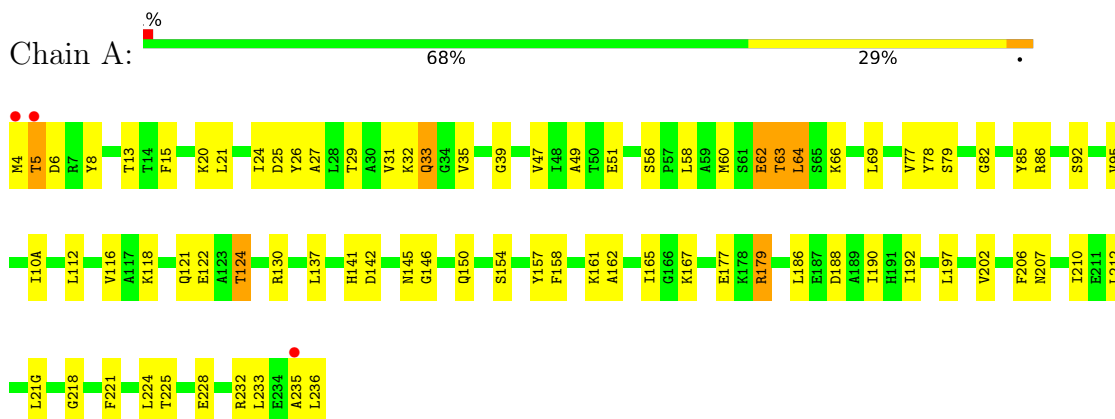
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	K	44	Total 44	O 44	0	0
16	L	57	Total 57	O 57	0	0
16	M	68	Total 68	O 68	0	0
16	N	58	Total 58	O 58	0	0
16	O	34	Total 34	O 34	0	0
16	P	28	Total 28	O 28	0	0
16	Q	28	Total 28	O 28	0	0
16	R	32	Total 32	O 32	0	0
16	S	18	Total 18	O 18	0	0
16	T	40	Total 40	O 40	0	0
16	U	61	Total 61	O 61	0	0
16	V	44	Total 44	O 44	0	0
16	W	58	Total 58	O 58	0	0
16	X	41	Total 41	O 41	0	0
16	Y	47	Total 47	O 47	0	0
16	Z	47	Total 47	O 47	0	0
16	1	74	Total 74	O 74	0	0
16	2	56	Total 56	O 56	0	0

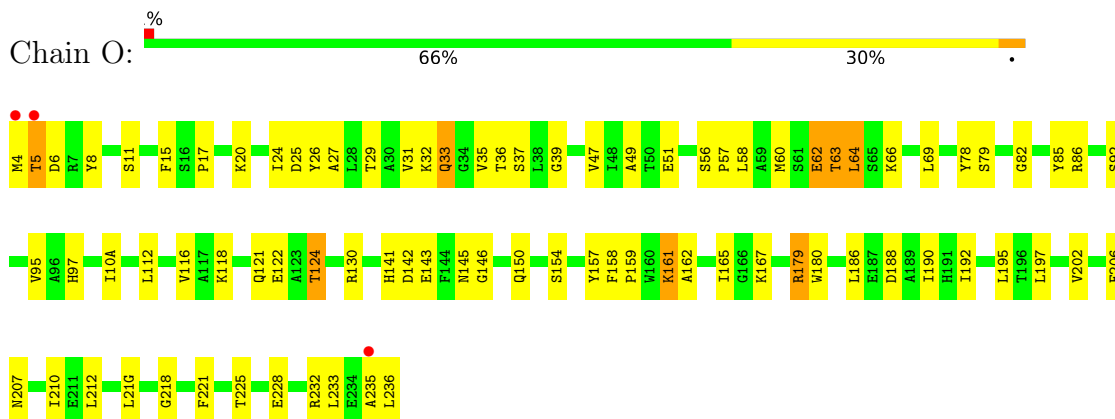
3 Residue-property plots [i](#)

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

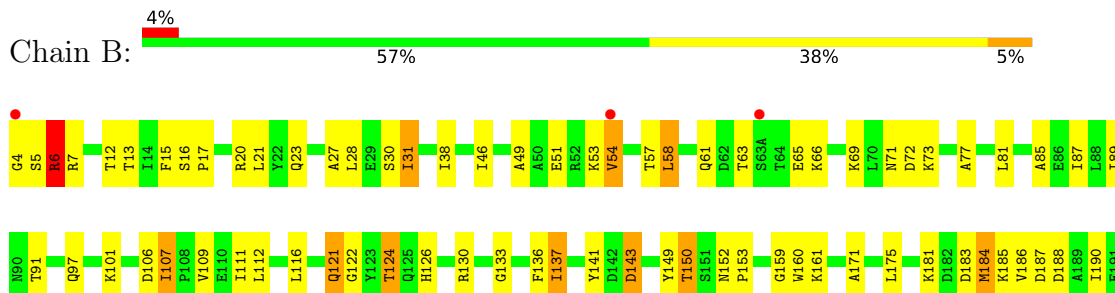
- Molecule 1: Proteasome component Y7



- Molecule 1: Proteasome component Y7

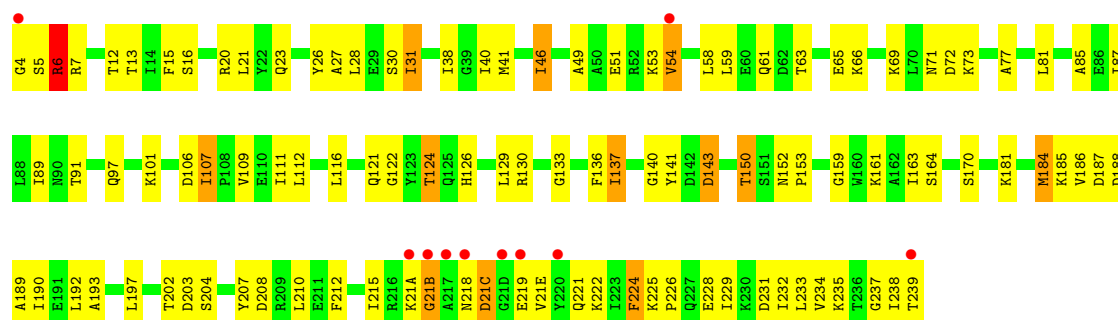


- Molecule 2: Proteasome component Y13

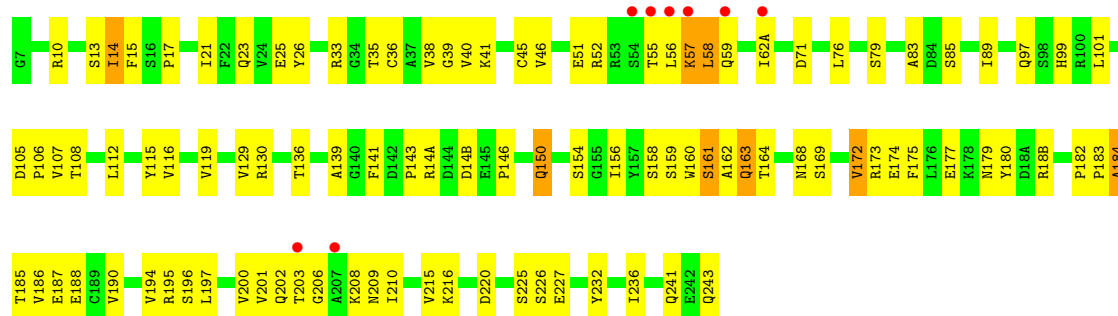




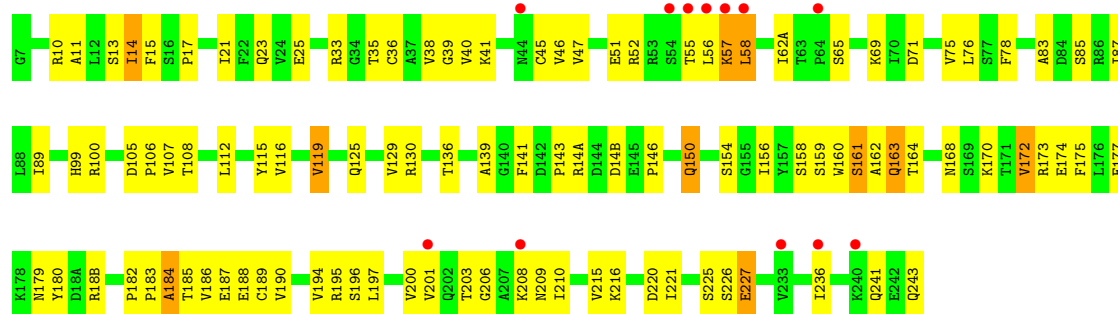
• Molecule 2: Proteasome component Y13



• Molecule 3: Proteasome component PRE6

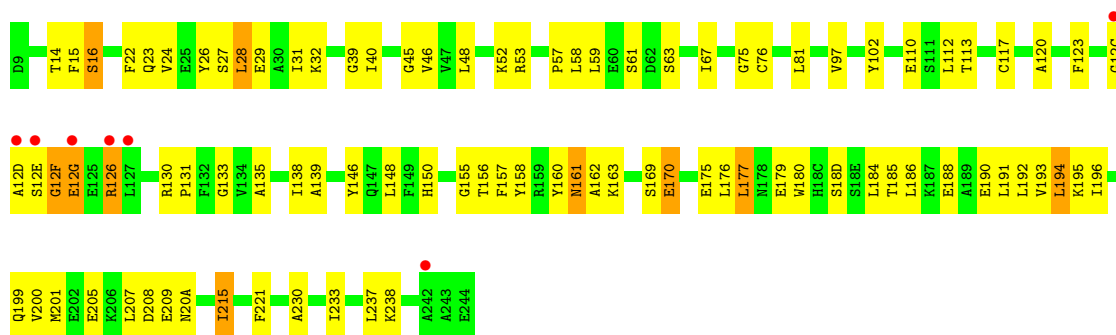


• Molecule 3: Proteasome component PRE6



• Molecule 4: Proteasome component PUP2

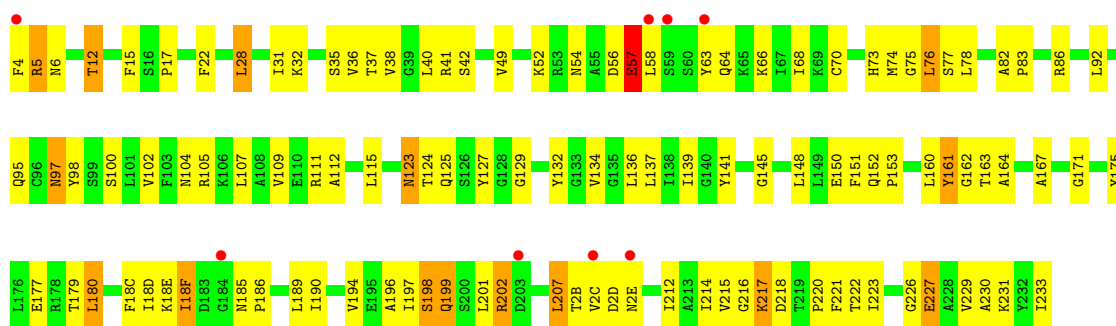




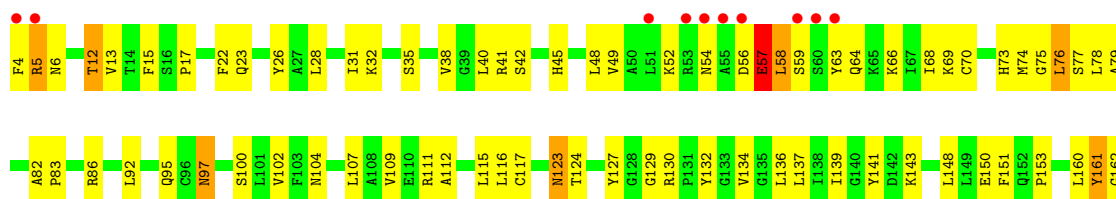
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5

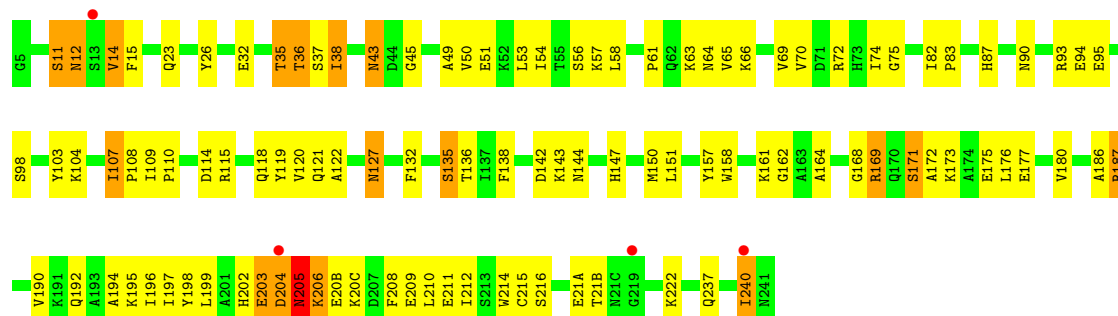


• Molecule 5: Proteasome component PRE5

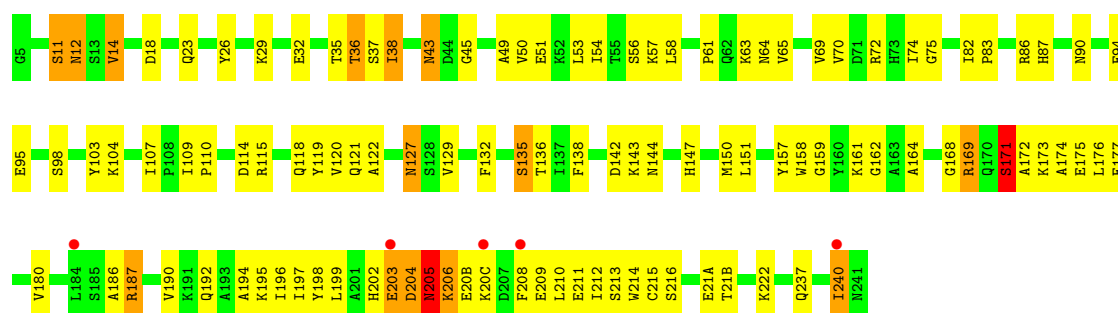




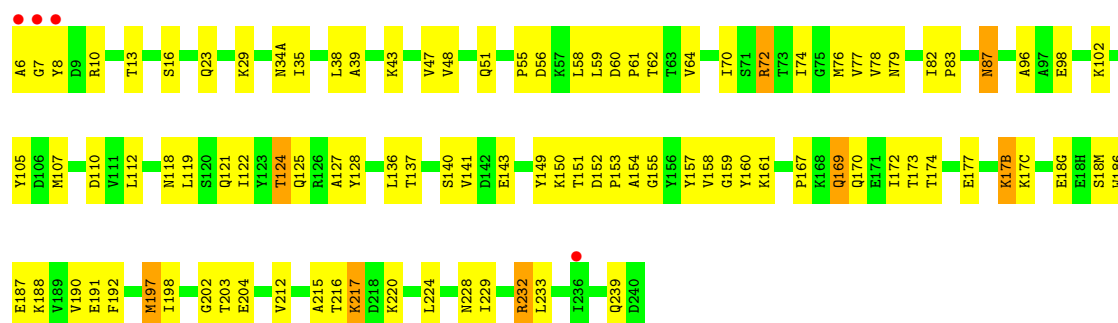
• Molecule 6: Proteasome component C1



• Molecule 6: Proteasome component C1

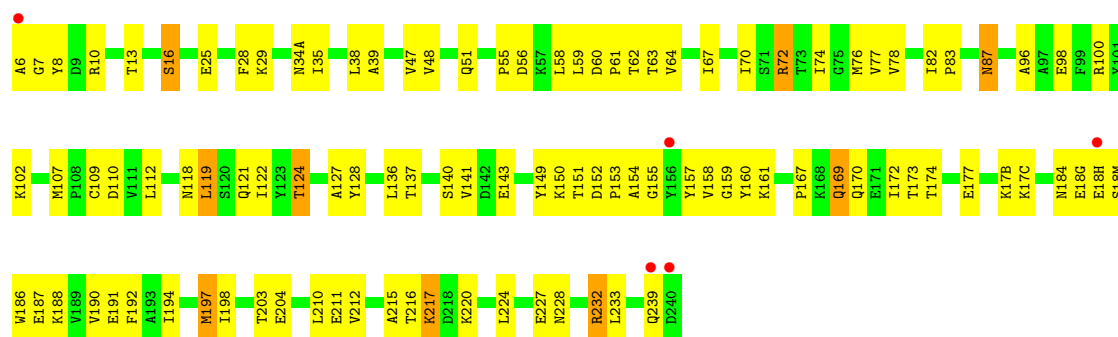


• Molecule 7: Proteasome component C7-alpha



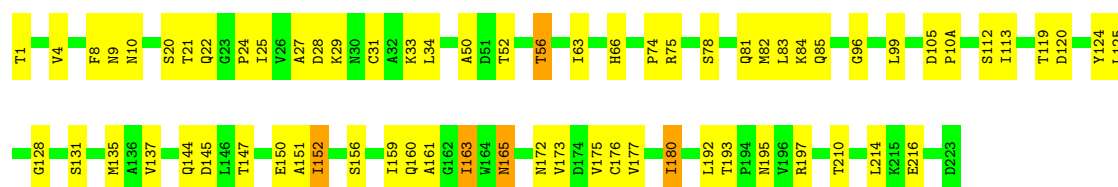
• Molecule 7: Proteasome component C7-alpha





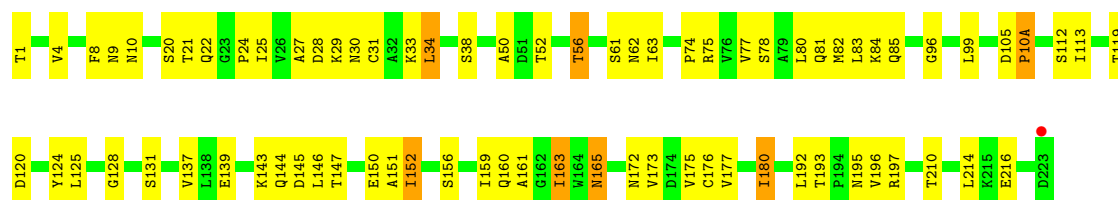
• Molecule 8: Proteasome component PUP1

Chain H: 69% 28% .



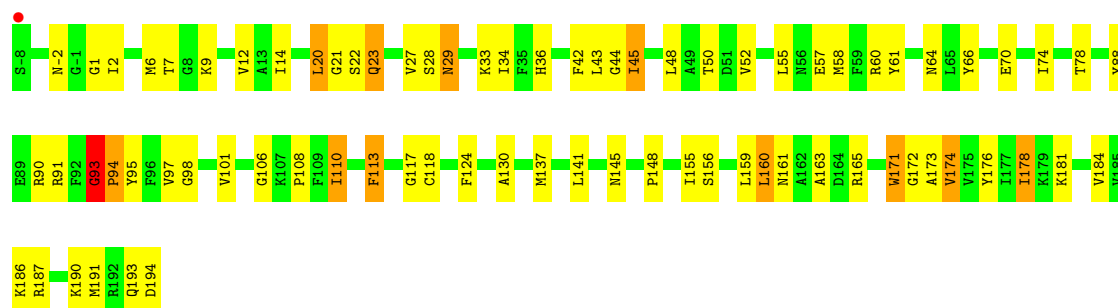
• Molecule 8: Proteasome component PUP1

Chain V: 66% 31% .



• Molecule 9: Proteasome component PUP3

Chain I: 62% 32% 5%

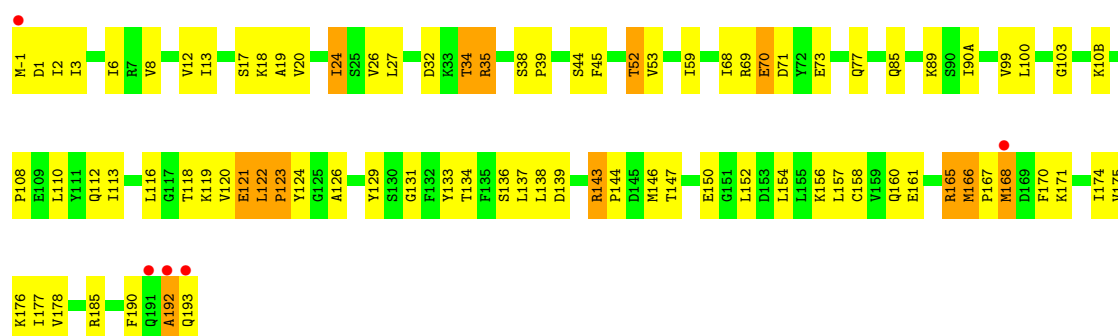


• Molecule 9: Proteasome component PUP3

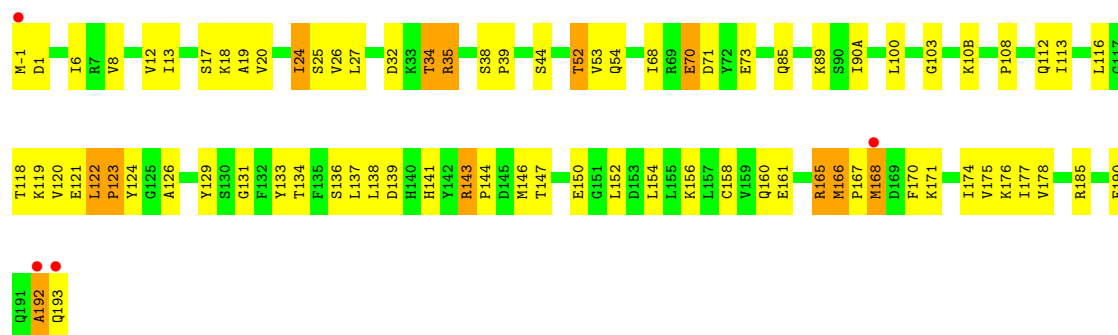
Chain W: 63% 32% 5%



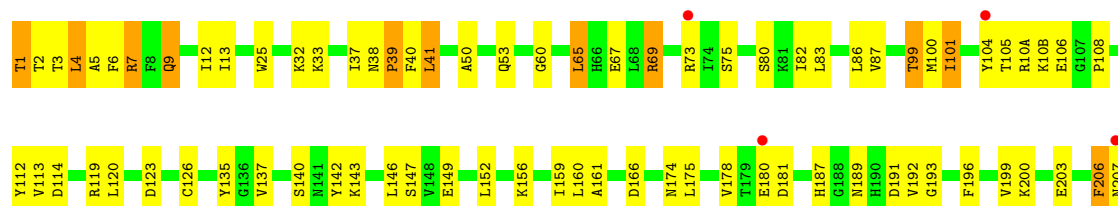
• Molecule 10: Proteasome component C11



• Molecule 10: Proteasome component C11

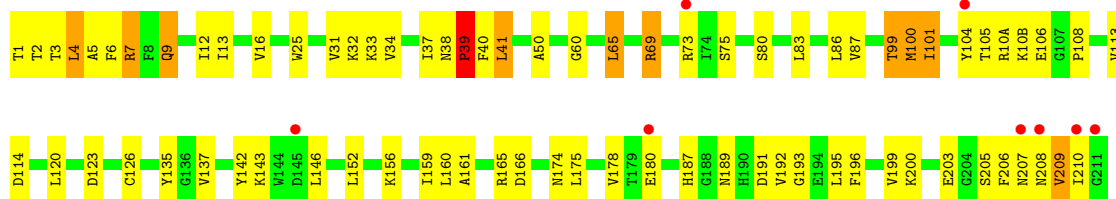


• Molecule 11: Proteasome component PRE2

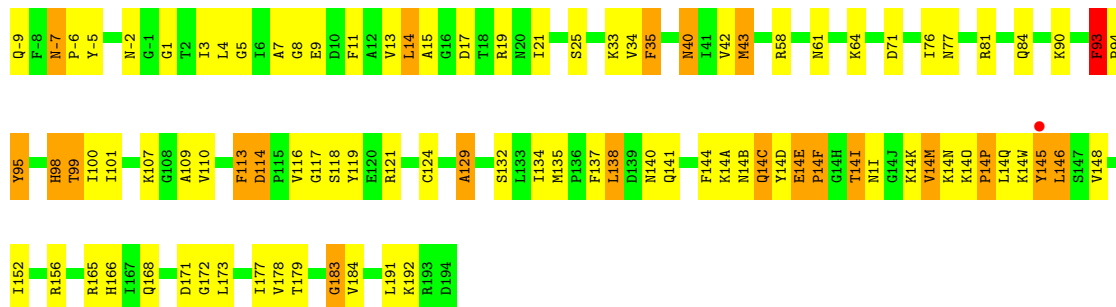




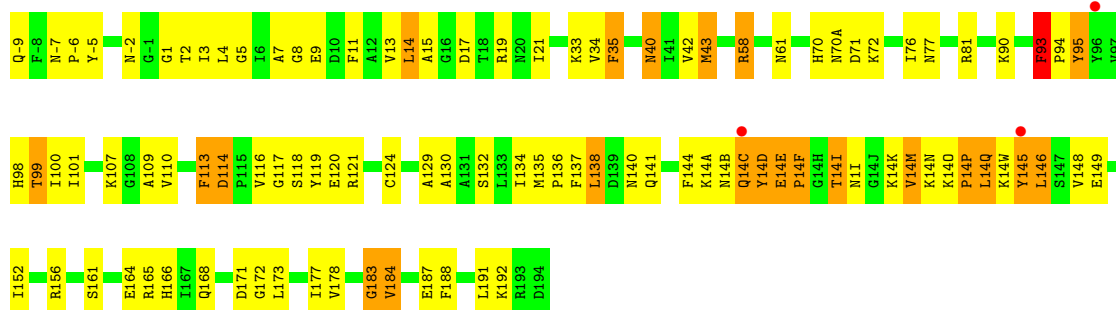
• Molecule 11: Proteasome component PRE2



• Molecule 12: Proteasome component C5

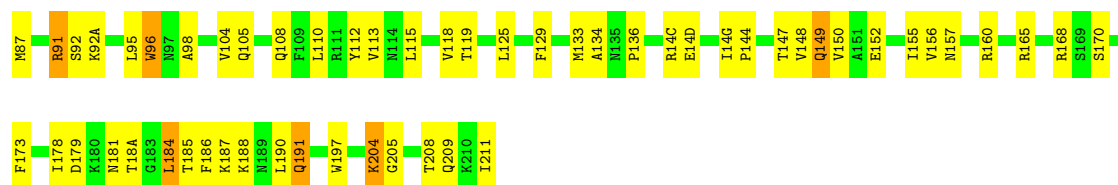


• Molecule 12: Proteasome component C5

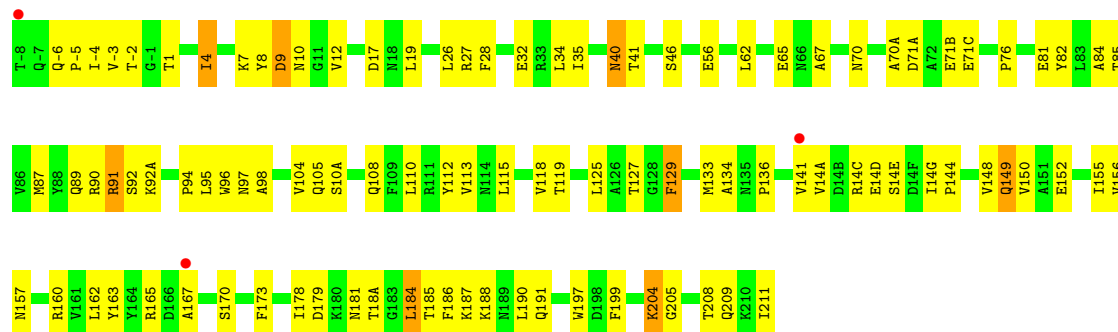


• Molecule 13: Proteasome component PRE4

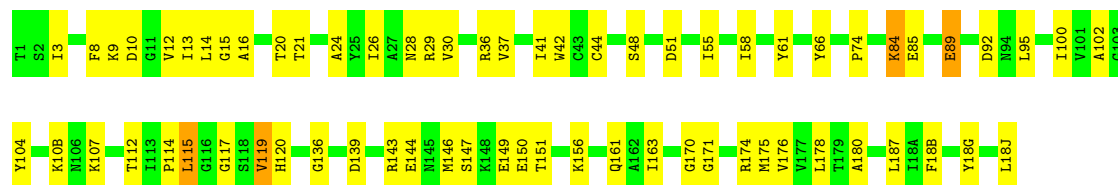




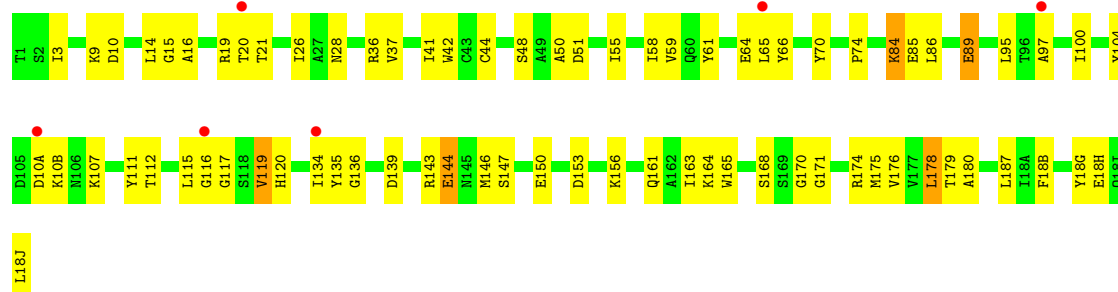
• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.59Å 299.83Å 143.60Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (15.00-2.70) 99.1 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.259 0.220 , 0.223	Depositor DCC
R_{free} test set	14272 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.890	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 77.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50851	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EP9

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	0.44	0/1952	0.93	5/2642 (0.2%)
1	O	0.42	0/1952	0.93	6/2642 (0.2%)
2	B	0.44	0/1935	0.92	8/2618 (0.3%)
2	P	0.44	0/1935	0.92	7/2618 (0.3%)
3	C	0.43	0/1920	0.94	3/2598 (0.1%)
3	Q	0.42	0/1920	0.94	3/2598 (0.1%)
4	D	0.44	0/1887	0.92	5/2541 (0.2%)
4	R	0.43	0/1887	0.92	4/2541 (0.2%)
5	E	0.41	0/1823	0.92	3/2463 (0.1%)
5	S	0.42	0/1823	0.93	5/2463 (0.2%)
6	F	0.44	0/1937	0.95	9/2614 (0.3%)
6	T	0.44	0/1937	0.96	9/2614 (0.3%)
7	G	0.46	0/1959	0.97	10/2652 (0.4%)
7	U	0.44	0/1959	0.96	9/2652 (0.3%)
8	H	0.46	0/1716	0.94	2/2326 (0.1%)
8	V	0.46	0/1716	0.94	2/2326 (0.1%)
9	I	0.45	0/1611	1.00	11/2174 (0.5%)
9	W	0.47	0/1611	1.01	11/2174 (0.5%)
10	J	0.51	0/1613	1.00	10/2173 (0.5%)
10	X	0.50	0/1613	0.99	10/2173 (0.5%)
11	K	0.51	0/1681	0.96	3/2274 (0.1%)
11	Y	0.50	0/1681	0.96	1/2274 (0.0%)
12	L	0.46	0/1795	1.03	13/2420 (0.5%)
12	Z	0.43	0/1747	1.03	13/2328 (0.6%)
13	1	0.46	0/1816	0.91	4/2430 (0.2%)
13	M	0.48	0/1855	0.96	6/2514 (0.2%)
14	2	0.46	0/1495	0.95	1/1996 (0.1%)
14	N	0.48	0/1541	0.94	1/2087 (0.0%)
All	All	0.45	0/50317	0.95	174/67925 (0.3%)

There are no bond length outliers.

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	27	ARG	N-CA-C	9.13	121.00	111.14
6	T	12	ASN	N-CA-C	9.12	120.83	111.07
6	F	12	ASN	N-CA-C	9.11	120.81	111.07
13	M	27	ARG	N-CA-C	9.08	120.95	111.14
1	A	161	LYS	N-CA-C	-8.42	101.87	112.90
7	G	161	LYS	N-CA-C	-8.21	102.70	112.89
1	O	161	LYS	N-CA-C	-8.08	102.32	112.90
3	C	161	SER	N-CA-C	-7.93	102.62	111.82
7	U	161	LYS	N-CA-C	-7.91	103.08	112.89
3	Q	161	SER	N-CA-C	-7.81	102.39	112.23
7	G	127	ALA	N-CA-C	7.81	119.48	110.97
6	T	161	LYS	N-CA-C	-7.66	101.81	112.45
6	F	135	SER	N-CA-C	-7.60	97.01	109.40
6	T	135	SER	N-CA-C	-7.56	97.07	109.40
7	U	127	ALA	N-CA-C	7.53	119.17	110.97
4	R	161	ASN	N-CA-C	-7.38	103.23	112.90
12	L	117	GLY	N-CA-C	7.30	124.41	114.92
6	F	161	LYS	N-CA-C	-7.17	102.48	112.45
4	D	161	ASN	N-CA-C	-7.13	103.55	112.90
12	Z	145	TYR	N-CA-C	7.01	121.26	109.76
12	Z	117	GLY	N-CA-C	7.00	124.02	114.92
9	I	60	ARG	N-CA-C	-6.96	103.62	111.07
12	L	145	TYR	N-CA-C	6.92	121.10	109.76
2	B	137	ILE	N-CA-C	-6.91	97.66	107.75
9	W	60	ARG	N-CA-C	-6.85	103.74	111.07
2	P	137	ILE	N-CA-C	-6.84	97.76	107.75
11	Y	206	PHE	N-CA-C	-6.84	102.88	111.90
4	R	169	SER	N-CA-C	6.83	118.42	110.97
7	U	128	TYR	N-CA-C	6.82	120.70	112.38
11	K	206	PHE	N-CA-C	-6.82	102.90	111.90
7	G	128	TYR	N-CA-C	6.79	120.66	112.38
12	Z	134	ILE	N-CA-C	6.64	118.23	111.00
4	D	169	SER	N-CA-C	6.58	118.15	110.97
8	V	21	THR	N-CA-C	6.58	119.42	109.23
7	G	16	SER	N-CA-C	-6.54	101.60	110.36
9	W	23	GLN	CB-CA-C	-6.53	109.06	116.63
10	J	123	PRO	N-CA-C	-6.51	104.68	113.40
13	M	-2	THR	N-CA-C	6.51	119.61	109.52
7	U	16	SER	N-CA-C	-6.48	101.68	110.36
9	I	117	GLY	N-CA-C	6.45	124.36	115.27
8	H	21	THR	N-CA-C	6.45	119.22	109.23
12	Z	95	TYR	N-CA-C	-6.45	98.71	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	78	TYR	N-CA-C	6.44	116.77	108.34
10	J	27	LEU	N-CA-C	6.41	119.08	111.71
12	L	134	ILE	N-CA-C	6.40	117.98	111.00
10	X	27	LEU	N-CA-C	6.39	119.06	111.71
10	X	123	PRO	N-CA-C	-6.36	104.88	113.40
10	X	165	ARG	N-CA-C	6.36	121.16	113.41
1	A	78	TYR	N-CA-C	6.34	116.65	108.34
10	J	165	ARG	N-CA-C	6.33	121.14	113.41
12	Z	183	GLY	N-CA-C	6.33	117.95	111.56
10	J	166	MET	CA-C-N	6.27	126.18	119.28
10	J	166	MET	C-N-CA	6.27	126.18	119.28
1	O	143	GLU	N-CA-C	6.27	118.92	111.33
12	L	183	GLY	N-CA-C	6.24	117.86	111.56
12	L	95	TYR	N-CA-C	-6.23	99.06	108.96
10	J	143	ARG	CA-C-N	6.23	126.13	119.28
10	J	143	ARG	C-N-CA	6.23	126.13	119.28
6	T	14	VAL	N-CA-C	6.19	117.56	109.58
9	W	117	GLY	N-CA-C	6.19	124.00	115.27
7	U	17(B)	LYS	N-CA-C	-6.18	104.54	111.28
5	E	161	TYR	N-CA-C	-6.12	104.88	112.90
12	L	93	PHE	CA-C-N	6.12	126.47	119.92
12	L	93	PHE	C-N-CA	6.12	126.47	119.92
9	I	23	GLN	CB-CA-C	-6.12	109.54	116.63
6	F	14	VAL	N-CA-C	6.10	117.45	109.58
10	X	143	ARG	CA-C-N	6.08	125.97	119.28
10	X	143	ARG	C-N-CA	6.08	125.97	119.28
2	B	161	LYS	N-CA-C	-6.08	104.94	112.90
9	W	95	TYR	N-CA-C	-6.04	99.80	109.96
12	Z	93	PHE	CA-C-N	6.04	126.38	119.92
12	Z	93	PHE	C-N-CA	6.04	126.38	119.92
4	R	63	SER	N-CA-C	-5.98	105.74	113.16
13	1	-2	THR	N-CA-C	5.95	118.74	109.52
10	X	166	MET	CA-C-N	5.95	125.82	119.28
10	X	166	MET	C-N-CA	5.95	125.82	119.28
4	D	63	SER	N-CA-C	-5.94	105.79	113.16
9	I	178	ILE	N-CA-C	5.93	116.42	108.11
2	P	16	SER	N-CA-C	-5.91	102.45	110.36
12	L	146	LEU	N-CA-C	5.89	118.36	110.35
7	G	17(B)	LYS	N-CA-C	-5.89	104.86	111.28
12	Z	114	ASP	N-CA-C	-5.88	102.18	110.29
10	X	134	THR	N-CA-C	5.85	119.60	112.23
2	B	109	VAL	N-CA-C	5.82	116.47	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	178	ILE	N-CA-C	5.81	116.25	108.11
10	J	134	THR	N-CA-C	5.80	119.54	112.23
5	S	161	TYR	N-CA-C	-5.80	105.30	112.90
6	F	240	ILE	N-CA-C	-5.78	105.20	113.07
12	Z	146	LEU	N-CA-C	5.78	118.22	110.35
2	B	16	SER	N-CA-C	-5.78	102.62	110.36
8	V	165	ASN	N-CA-C	5.77	120.04	112.89
2	B	203	ASP	N-CA-C	-5.76	105.83	112.92
5	S	57	GLU	N-CA-C	-5.75	106.12	113.02
2	P	203	ASP	N-CA-C	-5.71	106.21	112.72
1	A	10(A)	ILE	CB-CA-C	-5.66	105.87	111.30
6	T	240	ILE	N-CA-C	-5.63	105.41	113.07
7	U	74	ILE	N-CA-C	5.63	116.06	108.17
7	G	13	THR	N-CA-C	5.62	118.33	109.39
9	I	95	TYR	N-CA-C	-5.58	100.58	109.96
2	P	109	VAL	N-CA-C	5.58	116.21	110.36
8	H	165	ASN	N-CA-C	5.56	119.78	112.89
14	N	117	GLY	N-CA-C	-5.55	107.36	115.63
6	T	107	ILE	CA-C-N	5.54	125.47	119.76
6	T	107	ILE	C-N-CA	5.54	125.47	119.76
14	2	117	GLY	N-CA-C	-5.52	107.41	115.63
6	F	171	SER	N-CA-C	-5.51	105.17	111.07
12	L	98	HIS	N-CA-C	-5.51	100.26	109.24
9	I	94	PRO	N-CA-C	5.50	119.20	111.33
13	M	92(A)	LYS	N-CA-C	-5.50	105.88	112.59
12	Z	113	PHE	N-CA-C	5.47	118.50	109.85
13	M	98	ALA	N-CA-C	-5.47	99.52	108.76
1	A	66	LYS	N-CA-C	-5.47	106.66	113.38
5	E	57	GLU	N-CA-C	-5.47	106.46	113.02
12	L	114	ASP	N-CA-C	-5.46	102.27	110.24
1	O	10(A)	ILE	CB-CA-C	-5.46	106.06	111.30
1	O	235	ALA	N-CA-C	-5.45	106.50	112.72
6	T	171	SER	N-CA-C	-5.45	105.24	111.07
12	Z	98	HIS	N-CA-C	-5.44	100.37	109.24
9	W	94	PRO	N-CA-C	5.43	119.09	111.33
9	W	143	GLU	CA-C-N	5.42	126.18	120.11
9	W	143	GLU	C-N-CA	5.42	126.18	120.11
2	B	107	ILE	N-CA-C	5.41	114.25	108.95
7	G	74	ILE	N-CA-C	5.40	115.73	108.17
10	J	122	LEU	CA-C-N	5.39	124.73	118.85
10	J	122	LEU	C-N-CA	5.39	124.73	118.85
12	L	35	PHE	N-CA-C	5.39	118.02	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	38	ILE	N-CA-C	5.34	115.05	108.53
5	E	223	ILE	N-CA-C	5.34	115.58	108.11
12	L	129	ALA	N-CA-C	5.33	117.51	111.11
7	G	220	LYS	N-CA-C	5.33	116.51	108.46
3	Q	108	THR	N-CA-C	-5.31	102.66	110.52
7	G	155	GLY	N-CA-C	-5.30	107.90	115.64
12	Z	35	PHE	N-CA-C	5.30	118.19	109.72
5	S	223	ILE	N-CA-C	5.29	115.52	108.11
13	1	92(A)	LYS	N-CA-C	-5.29	106.06	112.88
2	P	107	ILE	N-CA-C	5.29	114.13	108.95
13	M	9	ASP	N-CA-C	5.28	117.04	111.28
9	I	98	GLY	CA-C-N	5.28	125.18	119.85
9	I	98	GLY	C-N-CA	5.28	125.18	119.85
7	U	13	THR	N-CA-C	5.28	117.78	109.39
6	F	38	ILE	N-CA-C	5.27	114.96	108.53
10	X	122	LEU	CA-C-N	5.27	124.59	118.85
10	X	122	LEU	C-N-CA	5.27	124.59	118.85
2	B	210	LEU	N-CA-C	5.25	117.17	109.24
5	S	102	VAL	N-CA-C	5.22	115.89	110.82
1	O	66	LYS	N-CA-C	-5.22	106.96	113.38
12	L	113	PHE	N-CA-C	5.21	118.08	109.85
9	W	93	GLY	CA-C-N	5.19	125.92	120.11
9	W	93	GLY	C-N-CA	5.19	125.92	120.11
9	W	27	VAL	N-CA-C	5.18	115.71	111.62
5	S	58	LEU	N-CA-C	-5.18	106.99	113.72
13	M	95	LEU	N-CA-C	-5.17	98.13	107.75
3	C	108	THR	N-CA-C	-5.17	102.86	110.52
2	B	57	THR	N-CA-C	-5.16	105.73	111.36
6	F	107	ILE	CA-C-N	5.14	125.06	119.76
6	F	107	ILE	C-N-CA	5.14	125.06	119.76
9	I	27	VAL	N-CA-C	5.11	115.66	111.62
2	P	161	LYS	N-CA-C	-5.10	105.37	112.45
9	I	93	GLY	CA-C-N	5.09	125.82	120.11
9	I	93	GLY	C-N-CA	5.09	125.82	120.11
2	P	210	LEU	N-CA-C	5.08	116.92	109.24
1	A	235	ALA	N-CA-C	-5.08	106.94	112.72
4	D	16	SER	N-CA-C	-5.07	102.78	110.39
4	R	180	TRP	N-CA-C	5.07	117.82	109.76
7	U	155	GLY	N-CA-C	-5.06	108.25	115.64
7	U	220	LYS	N-CA-C	5.06	116.10	108.46
3	Q	119	VAL	N-CA-C	-5.04	105.58	110.42
7	G	43	LYS	N-CA-C	-5.02	105.90	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	169	SER	N-CA-C	-5.02	105.94	111.71
11	K	181	ASP	N-CA-C	-5.02	107.00	112.72
11	K	1	THR	CB-CA-C	-5.02	98.06	109.10
13	1	9	ASP	N-CA-C	5.01	116.75	111.28
12	Z	184	VAL	N-CA-C	5.01	115.06	107.80
4	D	179	GLU	N-CA-C	5.01	118.16	111.75

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	60	0
1	O	1915	0	1926	62	0
2	B	1905	0	1901	101	0
2	P	1905	0	1901	101	0
3	C	1891	0	1900	99	0
3	Q	1891	0	1900	101	0
4	D	1862	0	1836	67	0
4	R	1862	0	1836	88	0
5	E	1795	0	1797	110	0
5	S	1795	0	1797	127	0
6	F	1897	0	1886	85	0
6	T	1897	0	1886	85	0
7	G	1921	0	1910	83	0
7	U	1921	0	1910	89	0
8	H	1685	0	1688	47	0
8	V	1685	0	1688	55	0
9	I	1581	0	1574	65	0
9	W	1581	0	1574	61	0
10	J	1585	0	1590	101	0
10	X	1585	0	1590	95	0
11	K	1644	0	1592	102	0
11	Y	1644	0	1592	95	0
12	L	1757	0	1711	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1731	0	1642	102	0
13	1	1807	0	1785	109	0
13	M	1824	0	1832	74	0
14	2	1487	0	1411	75	0
14	N	1512	0	1481	54	0
15	K	39	0	39	1	0
15	Y	39	0	39	2	0
16	1	74	0	0	6	0
16	2	56	0	0	5	0
16	A	52	0	0	0	0
16	B	38	0	0	3	0
16	C	39	0	0	3	0
16	D	42	0	0	0	0
16	E	20	0	0	4	0
16	F	47	0	0	6	0
16	G	60	0	0	4	0
16	H	49	0	0	1	0
16	I	62	0	0	3	0
16	J	49	0	0	11	0
16	K	44	0	0	6	0
16	L	57	0	0	3	0
16	M	68	0	0	5	0
16	N	58	0	0	3	0
16	O	34	0	0	0	0
16	P	28	0	0	3	0
16	Q	28	0	0	5	0
16	R	32	0	0	7	0
16	S	18	0	0	4	0
16	T	40	0	0	2	0
16	U	61	0	0	4	0
16	V	44	0	0	4	0
16	W	58	0	0	3	0
16	X	41	0	0	3	0
16	Y	47	0	0	4	0
16	Z	47	0	0	1	0
All	All	50851	0	49140	2127	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 22.

All (2127) 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)
10:J:168:MET:HE3	10:X:168:MET:HE3	1.27	1.11
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.31	1.08
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.32	1.08
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.10	1.08
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.08	1.06
14:2:135:TYR:CD1	14:2:135:TYR:CZ	2.41	1.03
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.23	1.02
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.22	1.02
7:G:96:ALA:HA	7:G:107:MET:HE2	1.41	1.02
12:Z:14(D):TYR:CE1	12:Z:14(D):TYR:CE2	2.40	1.01
14:2:111:TYR:CE1	14:2:111:TYR:CG	2.42	0.99
11:K:208:ASN:HB3	16:K:776:HOH:O	1.61	0.99
7:U:96:ALA:HA	7:U:107:MET:HE2	1.44	0.98
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.28	0.97
2:P:202:THR:HG22	2:P:204:SER:H	1.28	0.95
14:2:70:TYR:CE1	14:2:70:TYR:CE2	2.41	0.95
2:B:202:THR:HG22	2:B:204:SER:H	1.28	0.95
5:S:207:LEU:HD23	5:S:207:LEU:H	1.31	0.95
10:J:-1:MET:HG2	10:J:1:ASP:H	1.31	0.95
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.49	0.95
12:Z:2:THR:C	12:Z:3:ILE:CA	2.40	0.94
10:J:24:ILE:HD11	10:X:129:TYR:HB3	1.50	0.94
10:X:-1:MET:HG2	10:X:1:ASP:H	1.33	0.94
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.31	0.93
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.31	0.93
2:P:71:ASN:ND2	2:P:72:ASP:H	1.67	0.93
14:2:50:ALA:C	14:2:51:ASP:CA	2.42	0.93
2:B:71:ASN:ND2	2:B:72:ASP:H	1.66	0.93
5:E:207:LEU:HD23	5:E:207:LEU:H	1.33	0.93
14:2:85:GLU:C	14:2:86:LEU:CA	2.42	0.93
14:2:64:GLU:C	14:2:65:LEU:CA	2.42	0.92
12:Z:3:ILE:HD11	12:Z:100:ILE:HD13	1.50	0.91
12:Z:-6:PRO:C	12:Z:-5:TYR:CA	2.43	0.91
12:Z:187:GLU:C	12:Z:188:PHE:CA	2.43	0.91
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.36	0.91
3:C:185:THR:HB	3:C:188:GLU:HG2	1.51	0.91
13:1:157:ASN:HD22	13:1:160:ARG:HH11	0.91	0.91
3:C:185:THR:HG22	3:C:187:GLU:H	1.35	0.91
12:L:3:ILE:HD11	12:L:100:ILE:HD13	1.52	0.91
12:Z:14(Q):LEU:C	12:Z:14(W):LYS:CA	2.44	0.90
13:1:98:ALA:N	13:1:98:ALA:C	2.28	0.90
11:K:207:ASN:HD21	10:X:144:PRO:CG	1.84	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PHE:H	3:C:23:GLN:HE22	1.18	0.90
13:1:14(D):GLU:C	13:1:14(E):SER:CA	2.44	0.90
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.53	0.90
10:J:144:PRO:CG	11:Y:207:ASN:HD21	1.85	0.89
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.54	0.89
13:1:94:PRO:C	13:1:95:LEU:CA	2.46	0.89
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.55	0.89
14:2:134:ILE:CG2	14:2:134:ILE:CG1	2.50	0.89
13:1:14(C):ARG:HH11	13:1:14(C):ARG:HG3	1.37	0.89
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.19	0.89
13:M:157:ASN:HD22	13:M:160:ARG:HH11	0.92	0.89
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.38	0.88
14:2:134:ILE:CG2	14:2:134:ILE:CA	2.52	0.88
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.38	0.88
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.55	0.88
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.38	0.88
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	1.89	0.88
10:J:129:TYR:HB3	10:X:24:ILE:HD11	1.55	0.87
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.73	0.87
13:1:208:THR:CB	13:1:208:THR:C	2.48	0.87
9:W:137:MET:HE2	9:W:161:ASN:HB2	1.56	0.87
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.39	0.87
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.88	0.87
13:1:87:MET:CB	13:1:87:MET:C	2.48	0.87
14:2:97:ALA:C	14:2:97:ALA:CB	2.48	0.87
14:2:18(H):GLU:CG	14:2:18(H):GLU:CA	2.53	0.87
14:2:134:ILE:CG1	14:2:134:ILE:CA	2.53	0.86
13:1:167:ALA:CB	13:1:167:ALA:C	2.49	0.86
13:M:40:ASN:HD22	13:M:40:ASN:H	1.23	0.86
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.40	0.85
13:1:40:ASN:H	13:1:40:ASN:HD22	1.23	0.85
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.56	0.85
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.56	0.85
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.73	0.85
14:2:164:LYS:CA	14:2:165:TRP:N	2.40	0.85
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.75	0.85
9:I:137:MET:HE2	9:I:161:ASN:HB2	1.58	0.85
12:Z:140:ASN:C	12:Z:140:ASN:CB	2.49	0.85
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.57	0.85
13:1:71(C):GLU:C	13:1:71(C):GLU:CB	2.49	0.85
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:ND2	12:Z:-7:ASN:CB	2.40	0.84
6:T:54:ILE:HD11	6:T:209:GLU:HB2	1.59	0.84
12:Z:168:GLN:NE2	12:Z:168:GLN:CG	2.41	0.84
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.41	0.84
10:J:168:MET:HE3	10:X:168:MET:CE	2.07	0.84
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.91	0.84
14:2:10(A):ASP:CA	14:2:10(B):LYS:N	2.41	0.84
6:F:54:ILE:HD11	6:F:209:GLU:HB2	1.60	0.84
1:O:179:ARG:HB3	1:O:179:ARG:HH11	1.41	0.83
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.25	0.83
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.92	0.83
10:J:168:MET:CE	10:X:168:MET:HE3	2.07	0.83
13:1:89:GLN:CA	13:1:90:ARG:N	2.41	0.83
13:1:98:ALA:C	13:1:98:ALA:CB	2.50	0.83
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.75	0.83
12:L:3:ILE:CD1	12:L:100:ILE:HD13	2.07	0.83
14:2:97:ALA:CB	14:2:97:ALA:N	2.41	0.83
11:K:1:THR:HA	11:K:33:LYS:NZ	1.94	0.82
12:Z:3:ILE:CD1	12:Z:100:ILE:HD13	2.08	0.82
13:1:141:VAL:CA	13:1:14(A):VAL:N	2.42	0.82
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.60	0.82
12:Z:77:ASN:ND2	12:Z:77:ASN:CB	2.43	0.82
13:1:167:ALA:CB	13:1:167:ALA:N	2.42	0.82
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.27	0.82
14:2:10:ASP:CG	14:2:10:ASP:CA	2.53	0.82
1:O:15:PHE:H	2:P:23:GLN:HE22	1.26	0.82
12:Z:14(B):ASN:CA	12:Z:14(B):ASN:CG	2.53	0.81
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.45	0.81
12:Z:140:ASN:CB	12:Z:140:ASN:N	2.42	0.81
9:W:29:ASN:HD22	9:W:29:ASN:H	1.28	0.81
13:1:162:LEU:CA	13:1:163:TYR:N	2.43	0.81
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.44	0.81
12:Z:9:GLU:CB	12:Z:9:GLU:CD	2.54	0.81
13:1:105:GLN:CA	13:1:10(A):SER:N	2.44	0.81
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.81	0.81
12:Z:148:VAL:CA	12:Z:149:GLU:N	2.44	0.81
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.80	0.81
12:L:166:HIS:HD2	12:L:168:GLN:H	1.29	0.80
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.62	0.80
9:I:29:ASN:H	9:I:29:ASN:HD22	1.30	0.80
11:K:99:THR:HG22	11:K:113:VAL:HB	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:129:ALA:CA	12:Z:130:ALA:N	2.45	0.80
13:1:98:ALA:N	13:1:98:ALA:CB	2.44	0.80
3:C:186:VAL:O	3:C:190:VAL:HG23	1.82	0.80
13:1:96:TRP:CA	13:1:97:ASN:N	2.44	0.80
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.29	0.80
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.63	0.80
3:C:15:PHE:H	4:D:23:GLN:HE22	1.26	0.79
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.82	0.79
14:N:9:LYS:O	14:N:107:LYS:HD3	1.83	0.79
13:1:71(C):GLU:CB	13:1:71(C):GLU:N	2.45	0.79
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.94	0.79
10:J:156:LYS:HE2	10:J:160:GLN:NE2	1.98	0.79
14:2:65:LEU:CA	14:2:65:LEU:CG	2.61	0.79
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.46	0.79
2:P:85:ALA:O	2:P:89:ILE:HG12	1.84	0.79
9:W:29:ASN:HD22	9:W:29:ASN:N	1.80	0.79
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.65	0.78
2:B:51:GLU:OE2	2:B:202:THR:HG23	1.83	0.78
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.65	0.78
13:1:87:MET:CB	13:1:87:MET:N	2.46	0.78
14:2:9:LYS:O	14:2:107:LYS:HD3	1.83	0.78
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.66	0.78
4:R:72:ARG:HG3	16:R:1302:HOH:O	1.83	0.78
1:A:15:PHE:H	2:B:23:GLN:HE22	1.32	0.77
13:1:208:THR:CB	13:1:208:THR:N	2.46	0.77
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.64	0.77
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.49	0.77
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.31	0.77
10:X:156:LYS:HE2	10:X:160:GLN:NE2	1.99	0.77
12:Z:14(D):TYR:CE1	12:Z:14(D):TYR:OH	2.38	0.77
9:I:29:ASN:HD22	9:I:29:ASN:N	1.82	0.77
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.19	0.76
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.68	0.76
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.65	0.76
2:P:51:GLU:OE2	2:P:202:THR:HG23	1.86	0.76
6:T:186:ALA:O	6:T:190:VAL:HG23	1.86	0.76
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.50	0.76
11:K:208:ASN:HD21	9:W:29:ASN:CG	1.92	0.76
2:P:87:ILE:O	2:P:91:THR:HG23	1.86	0.76
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.66	0.76
10:X:156:LYS:O	10:X:160:GLN:HG3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:19:ARG:NE	14:2:19:ARG:CG	2.49	0.76
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.67	0.76
2:B:85:ALA:O	2:B:89:ILE:HG12	1.86	0.75
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.67	0.75
10:X:6:ILE:HD11	10:X:154:LEU:HD23	1.67	0.75
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.17	0.75
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.68	0.75
5:S:201:LEU:O	5:S:202:ARG:HB2	1.85	0.75
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.49	0.75
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.21	0.75
2:P:124:THR:CG2	3:Q:130:ARG:HH21	1.99	0.75
14:2:70:TYR:CE2	14:2:70:TYR:OH	2.40	0.75
5:E:18(C):PHE:O	5:E:18(F):ILE:HG12	1.86	0.75
5:E:201:LEU:O	5:E:202:ARG:HB2	1.87	0.75
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.69	0.75
9:I:90:ARG:HD2	16:I:1159:HOH:O	1.87	0.75
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.02	0.75
13:M:149:GLN:NE2	13:M:149:GLN:H	1.86	0.74
10:J:133:TYR:OH	16:J:876:HOH:O	2.05	0.74
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.17	0.74
7:U:59:LEU:O	7:U:61:PRO:HD3	1.87	0.74
12:Z:14(D):TYR:CE2	12:Z:14(D):TYR:OH	2.40	0.74
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.50	0.74
5:S:227:GLU:H	5:S:227:GLU:CD	1.96	0.74
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.69	0.74
9:I:29:ASN:CG	11:Y:208:ASN:HD21	1.96	0.73
1:A:58:LEU:HD12	7:G:173:THR:HG23	1.71	0.73
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.69	0.73
3:Q:159:SER:HB2	16:Q:1140:HOH:O	1.87	0.73
2:P:202:THR:HG22	2:P:204:SER:N	2.03	0.73
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.70	0.73
14:2:70:TYR:CE1	14:2:70:TYR:OH	2.41	0.73
10:J:156:LYS:O	10:J:160:GLN:HG3	1.87	0.73
7:G:59:LEU:O	7:G:61:PRO:HD3	1.89	0.73
5:S:207:LEU:H	5:S:207:LEU:CD2	2.01	0.73
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.68	0.73
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.23	0.73
5:S:18(C):PHE:O	5:S:18(F):ILE:HG12	1.89	0.73
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.02	0.73
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.69	0.73
14:2:97:ALA:C	14:2:97:ALA:N	2.47	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:GLU:O	2:B:232:ILE:HG22	1.89	0.73
7:U:121:GLN:O	7:U:124:THR:HB	1.88	0.73
12:Z:-7:ASN:CB	12:Z:-7:ASN:OD1	2.37	0.73
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.69	0.73
9:I:194:ASP:O	16:I:230:HOH:O	2.07	0.73
2:P:228:GLU:O	2:P:232:ILE:HG22	1.89	0.73
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.70	0.73
9:I:29:ASN:N	9:I:29:ASN:ND2	2.36	0.72
10:J:6:ILE:HD11	10:J:154:LEU:HD23	1.71	0.72
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.69	0.72
12:Z:140:ASN:C	12:Z:140:ASN:N	2.47	0.72
13:1:149:GLN:NE2	13:1:149:GLN:H	1.86	0.72
7:G:121:GLN:O	7:G:124:THR:HB	1.89	0.72
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.71	0.72
6:F:186:ALA:O	6:F:190:VAL:HG23	1.89	0.72
5:E:207:LEU:H	5:E:207:LEU:CD2	2.03	0.72
13:1:162:LEU:O	13:1:163:TYR:N	2.23	0.72
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.72	0.72
13:1:87:MET:C	13:1:87:MET:N	2.48	0.72
5:E:227:GLU:H	5:E:227:GLU:CD	1.97	0.72
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.72	0.72
12:Z:-7:ASN:ND2	12:Z:-7:ASN:OD1	2.23	0.72
2:P:159:GLY:HA3	3:Q:62(A):ILE:CD1	2.20	0.71
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.03	0.71
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.53	0.71
9:W:29:ASN:N	9:W:29:ASN:ND2	2.34	0.71
12:Z:120:GLU:CG	12:Z:120:GLU:OE1	2.38	0.71
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.04	0.71
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.91	0.71
2:B:202:THR:HG22	2:B:204:SER:N	2.03	0.71
9:W:194:ASP:O	16:W:228:HOH:O	2.06	0.71
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.71	0.71
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.73	0.71
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.26	0.70
11:K:207:ASN:ND2	10:X:144:PRO:HG3	2.04	0.70
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	1.88	0.70
6:T:70:VAL:HB	6:T:74:ILE:HB	1.73	0.70
7:G:96:ALA:CA	7:G:107:MET:HE2	2.19	0.70
12:Z:168:GLN:NE2	12:Z:168:GLN:OE1	2.24	0.70
12:Z:148:VAL:O	12:Z:149:GLU:N	2.25	0.70
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.06	0.70
7:U:198:ILE:HG23	7:U:203:THR:O	1.91	0.70
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.72	0.70
9:W:156:SER:O	9:W:160:LEU:HB2	1.91	0.70
12:Z:168:GLN:CG	12:Z:168:GLN:OE1	2.40	0.70
13:1:162:LEU:CA	13:1:162:LEU:O	2.39	0.70
13:1:167:ALA:C	13:1:167:ALA:N	2.49	0.70
2:B:87:ILE:O	2:B:91:THR:HG23	1.90	0.70
7:U:96:ALA:CA	7:U:107:MET:HE2	2.20	0.70
13:1:89:GLN:CA	13:1:89:GLN:O	2.40	0.70
13:1:141:VAL:O	13:1:14(A):VAL:N	2.24	0.70
1:O:121:GLN:O	1:O:124:THR:HB	1.92	0.70
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.07	0.70
12:Z:77:ASN:CB	12:Z:77:ASN:OD1	2.40	0.70
13:1:89:GLN:O	13:1:90:ARG:N	2.25	0.70
13:1:141:VAL:CA	13:1:141:VAL:O	2.40	0.70
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.40	0.70
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.27	0.70
9:I:6:MET:CE	9:I:155:ILE:HA	2.22	0.69
1:A:121:GLN:O	1:A:124:THR:HB	1.92	0.69
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.38	0.69
13:M:150:VAL:HG21	16:M:1069:HOH:O	1.93	0.69
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.74	0.69
12:Z:77:ASN:ND2	12:Z:77:ASN:OD1	2.25	0.69
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.74	0.69
12:Z:129:ALA:O	12:Z:130:ALA:N	2.25	0.69
13:1:105:GLN:O	13:1:10(A):SER:N	2.25	0.69
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.75	0.69
12:Z:148:VAL:CA	12:Z:148:VAL:O	2.40	0.69
12:Z:120:GLU:CG	12:Z:120:GLU:OE2	2.41	0.69
6:F:70:VAL:HB	6:F:74:ILE:HB	1.73	0.69
13:1:105:GLN:CA	13:1:105:GLN:O	2.40	0.69
14:2:164:LYS:O	14:2:165:TRP:N	2.25	0.69
9:I:156:SER:O	9:I:160:LEU:HB2	1.92	0.69
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.74	0.69
14:2:164:LYS:CA	14:2:164:LYS:O	2.40	0.69
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.22	0.69
5:S:190:ILE:HG23	5:S:212:ILE:HD13	1.74	0.69
2:B:159:GLY:HA3	3:C:62(A):ILE:CD1	2.23	0.68
7:G:198:ILE:HG23	7:G:203:THR:O	1.92	0.68
10:J:52:THR:HG22	10:J:53:VAL:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.08	0.68
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.57	0.68
9:W:6:MET:CE	9:W:155:ILE:HA	2.22	0.68
9:W:43:LEU:HD21	9:W:45:ILE:HD11	1.75	0.68
11:Y:1:THR:HA	11:Y:33:LYS:NZ	2.08	0.68
2:B:71:ASN:ND2	2:B:72:ASP:N	2.41	0.68
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.73	0.68
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.29	0.68
12:Z:129:ALA:CA	12:Z:129:ALA:O	2.41	0.68
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.75	0.68
14:2:168:SER:CA	14:2:168:SER:OG	2.41	0.68
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.75	0.68
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.24	0.68
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.08	0.68
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.38	0.68
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.03	0.68
2:P:71:ASN:ND2	2:P:72:ASP:N	2.42	0.68
13:1:96:TRP:O	13:1:97:ASN:N	2.26	0.68
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	1.93	0.68
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.76	0.68
14:2:10(A):ASP:CA	14:2:10(A):ASP:O	2.41	0.68
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	2.09	0.68
5:E:97:ASN:HD21	12:L:61:ASN:ND2	1.92	0.67
5:S:52:LYS:HB3	5:S:63:TYR:O	1.93	0.67
8:H:159:ILE:O	8:H:163:ILE:HD12	1.95	0.67
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	1.93	0.67
11:Y:210:ILE:HB	16:Y:1150:HOH:O	1.94	0.67
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.58	0.67
14:2:10(A):ASP:O	14:2:10(B):LYS:N	2.26	0.67
10:J:85:GLN:HB3	16:J:201:HOH:O	1.93	0.67
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.76	0.67
5:S:73:HIS:HE1	5:S:107:LEU:O	1.77	0.67
5:S:132:TYR:O	5:S:153:PRO:HB3	1.95	0.67
10:X:52:THR:HG22	10:X:53:VAL:N	2.08	0.67
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.75	0.67
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.57	0.67
1:O:62:GLU:C	1:O:64:LEU:H	2.03	0.67
8:V:78:SER:O	8:V:82:MET:HG3	1.93	0.67
13:1:96:TRP:CA	13:1:96:TRP:O	2.42	0.67
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.08	0.67
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:69:VAL:HG12	16:F:319:HOH:O	1.93	0.67
6:T:35:THR:HG21	6:T:51:GLU:O	1.95	0.66
1:A:62:GLU:C	1:A:64:LEU:H	2.03	0.66
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.95	0.66
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.96	0.66
5:E:73:HIS:HE1	5:E:107:LEU:O	1.78	0.66
9:I:43:LEU:HD21	9:I:45:ILE:HD11	1.76	0.66
13:M:211:ILE:HD11	14:2:36:ARG:HD3	1.75	0.66
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.30	0.66
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.60	0.66
3:C:71:ASP:HA	10:J:68:ILE:HD13	1.77	0.66
7:U:77:VAL:HG12	7:U:137:THR:HB	1.78	0.66
5:S:143:LYS:HE3	16:1:722:HOH:O	1.94	0.66
8:V:196:VAL:HG23	16:V:652:HOH:O	1.94	0.66
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.10	0.66
5:E:190:ILE:HG23	5:E:212:ILE:HD13	1.77	0.66
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.76	0.66
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.77	0.66
13:1:41:THR:OG1	13:1:76:PRO:HG3	1.96	0.66
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	1.96	0.66
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.26	0.66
13:1:67:ALA:HB3	16:1:1339:HOH:O	1.95	0.66
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.78	0.66
6:F:35:THR:HG21	6:F:51:GLU:O	1.95	0.66
11:K:1:THR:HA	11:K:33:LYS:HZ3	1.59	0.66
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.26	0.66
13:1:71(C):GLU:C	13:1:71(C):GLU:N	2.54	0.66
13:1:208:THR:C	13:1:208:THR:N	2.53	0.66
7:G:172:ILE:HD13	7:G:197:MET:HE1	1.78	0.66
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.77	0.66
16:J:876:HOH:O	10:X:25:SER:OG	2.13	0.66
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.36	0.66
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.09	0.65
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.77	0.65
7:G:77:VAL:HG12	7:G:137:THR:HB	1.78	0.65
4:D:207:LEU:C	4:D:207:LEU:HD23	2.22	0.65
9:W:43:LEU:CD2	9:W:45:ILE:HD11	2.27	0.65
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.32	0.65
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.77	0.65
10:J:32:ASP:OD2	10:J:34:THR:HG22	1.96	0.65
11:K:53:GLN:HE22	12:L:119:TYR:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.96	0.65
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.78	0.65
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.32	0.65
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.78	0.65
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.96	0.65
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.08	0.64
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.33	0.64
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.26	0.64
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.61	0.64
2:B:121:GLN:O	2:B:124:THR:HB	1.97	0.64
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.78	0.64
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.77	0.64
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.92	0.64
7:U:227:GLU:HG2	16:U:1255:HOH:O	1.96	0.64
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.12	0.64
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.26	0.64
5:E:12:THR:HG21	5:E:124:THR:HA	1.80	0.64
5:E:54:ASN:ND2	5:E:56:ASP:O	2.29	0.64
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.36	0.64
11:K:142:TYR:O	11:K:143:LYS:HD2	1.96	0.64
4:R:207:LEU:HD23	4:R:207:LEU:C	2.22	0.64
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.27	0.64
9:I:43:LEU:CD2	9:I:45:ILE:HD11	2.28	0.64
11:K:143:LYS:O	11:K:146:LEU:HD13	1.97	0.64
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.31	0.64
5:S:107:LEU:HD12	16:S:1319:HOH:O	1.98	0.64
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.13	0.64
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.28	0.64
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.45	0.64
2:P:101:LYS:NZ	10:X:85:GLN:HE22	1.96	0.64
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.27	0.64
6:T:237:GLN:O	6:T:240:ILE:HG22	1.97	0.64
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.80	0.64
5:E:132:TYR:O	5:E:153:PRO:HB3	1.98	0.64
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.33	0.64
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.46	0.64
12:Z:173:LEU:HB2	12:Z:191:LEU:HD11	1.79	0.64
3:C:185:THR:HG22	3:C:187:GLU:N	2.09	0.63
10:J:69:ARG:HD2	16:J:514:HOH:O	1.99	0.63
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.79	0.63
13:M:41:THR:OG1	13:M:76:PRO:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.79	0.63
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.95	0.63
8:V:84:LYS:HG3	8:V:85:GLN:N	2.14	0.63
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.79	0.63
8:V:81:GLN:O	8:V:85:GLN:HG3	1.97	0.63
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.11	0.63
9:I:6:MET:HE1	9:I:155:ILE:HA	1.80	0.63
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.81	0.63
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.13	0.63
2:B:181:LYS:O	2:B:184:MET:HG3	1.98	0.63
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.34	0.63
5:E:52:LYS:HB3	5:E:63:TYR:O	1.98	0.63
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.64	0.63
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.60	0.63
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.81	0.63
14:2:89:GLU:OE1	14:2:89:GLU:HA	1.96	0.63
14:N:36:ARG:HD3	13:1:211:ILE:HD11	1.81	0.63
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.10	0.63
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.99	0.63
5:E:97:ASN:ND2	12:L:61:ASN:HD21	1.97	0.63
12:L:114:ASP:CB	12:L:118:SER:HB3	2.29	0.63
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	1.98	0.63
2:P:185:LYS:HE2	2:P:187:ASP:OD1	1.99	0.63
4:R:185:THR:OG1	4:R:188:GLU:HG3	1.99	0.63
9:W:6:MET:HE1	9:W:155:ILE:HA	1.80	0.63
2:B:185:LYS:HE2	2:B:187:ASP:OD1	1.99	0.62
3:C:195:ARG:HD3	16:C:1019:HOH:O	1.99	0.62
5:E:95:GLN:HG3	5:E:115:LEU:HD13	1.81	0.62
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.29	0.62
12:Z:114:ASP:CB	12:Z:118:SER:HB3	2.28	0.62
6:F:36:THR:HG22	6:F:51:GLU:OE2	2.00	0.62
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.81	0.62
8:V:159:ILE:O	8:V:163:ILE:HD12	1.99	0.62
13:1:152:GLU:O	13:1:156:VAL:HG23	1.99	0.62
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.80	0.62
1:O:60:MET:HE3	1:O:63:THR:HG21	1.80	0.62
1:A:186:LEU:O	1:A:190:ILE:HG13	1.99	0.62
6:F:51:GLU:OE1	6:F:53:LEU:HD21	1.99	0.62
8:H:84:LYS:HG3	8:H:85:GLN:N	2.13	0.62
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.45	0.62
8:H:29:LYS:HE2	12:Z:165:ARG:NH2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:173:LEU:HB2	12:L:191:LEU:HD11	1.82	0.62
2:P:121:GLN:O	2:P:124:THR:HB	1.98	0.62
4:D:185:THR:OG1	4:D:188:GLU:HG3	1.99	0.62
13:M:152:GLU:O	13:M:156:VAL:HG23	1.99	0.62
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.62	0.62
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.81	0.62
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.28	0.62
9:I:160:LEU:HD11	9:I:191:MET:HB3	1.80	0.62
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.12	0.62
5:S:95:GLN:HG3	5:S:115:LEU:HD13	1.81	0.62
7:G:72:ARG:HB3	16:G:1063:HOH:O	1.99	0.62
13:M:40:ASN:H	13:M:40:ASN:ND2	1.97	0.62
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.82	0.62
13:1:14(C):ARG:HH11	13:1:14(C):ARG:CG	2.11	0.62
10:J:26:VAL:HG23	10:X:165:ARG:O	1.98	0.62
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.82	0.62
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.33	0.62
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.82	0.62
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.80	0.61
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.35	0.61
2:P:185:LYS:HD3	2:P:186:VAL:N	2.15	0.61
6:T:36:THR:HG22	6:T:51:GLU:OE2	2.00	0.61
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.80	0.61
2:B:185:LYS:HD3	2:B:186:VAL:N	2.15	0.61
3:C:41:LYS:HG2	3:C:161:SER:O	2.00	0.61
4:D:207:LEU:CD2	4:D:233:ILE:HD12	2.31	0.61
8:H:78:SER:O	8:H:82:MET:HG3	2.00	0.61
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.15	0.61
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.82	0.61
7:U:172:ILE:HD13	7:U:197:MET:HE1	1.80	0.61
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.98	0.61
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.81	0.61
5:S:54:ASN:ND2	5:S:56:ASP:O	2.33	0.61
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.82	0.61
8:H:81:GLN:O	8:H:85:GLN:HG3	2.01	0.61
14:N:89:GLU:OE1	14:N:89:GLU:HA	2.00	0.61
9:W:160:LEU:HD11	9:W:191:MET:HB3	1.81	0.61
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.36	0.61
7:G:87:ASN:C	7:G:87:ASN:HD22	2.09	0.61
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.36	0.61
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:186:LEU:O	1:O:190:ILE:HG13	2.00	0.61
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.00	0.61
5:S:139:ILE:HG22	5:S:148:LEU:HD13	1.82	0.61
11:Y:180:GLU:HB3	16:Y:812:HOH:O	1.99	0.61
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.01	0.61
12:L:98:HIS:HD2	16:L:200:HOH:O	1.82	0.61
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.15	0.61
7:U:87:ASN:C	7:U:87:ASN:HD22	2.09	0.61
6:F:237:GLN:O	6:F:240:ILE:HG22	2.01	0.60
11:K:208:ASN:ND2	11:K:209:VAL:N	2.48	0.60
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.31	0.60
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.13	0.60
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.83	0.60
4:R:53:ARG:O	4:R:53:ARG:HG2	2.01	0.60
5:S:12:THR:HG21	5:S:124:THR:HA	1.82	0.60
5:S:207:LEU:HD23	5:S:207:LEU:N	2.11	0.60
3:C:13:SER:O	4:D:130:ARG:HD3	2.01	0.60
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.83	0.60
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.31	0.60
4:R:207:LEU:CD2	4:R:233:ILE:HD12	2.30	0.60
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.65	0.60
15:Y:300:EP9:H36	15:Y:300:EP9:O1	2.01	0.60
9:I:9:LYS:HD3	9:I:145:ASN:HD22	1.66	0.60
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.00	0.60
13:M:14(C):ARG:HH11	13:M:14(C):ARG:CG	2.12	0.60
3:Q:14:ILE:H	3:Q:14:ILE:HD13	1.67	0.60
4:R:186:LEU:O	4:R:190:GLU:HG3	2.01	0.60
5:E:227:GLU:CD	5:E:227:GLU:N	2.60	0.60
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.09	0.60
1:A:60:MET:HE3	1:A:63:THR:HG21	1.83	0.60
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.36	0.60
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.02	0.60
15:K:300:EP9:O1	15:K:300:EP9:H36	2.01	0.60
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.82	0.60
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.50	0.60
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.84	0.60
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.37	0.60
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.16	0.60
4:R:175:GLU:HB3	4:R:196:ILE:HD13	1.84	0.60
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.01	0.60
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:9:LYS:HD3	9:W:145:ASN:HD22	1.66	0.60
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.32	0.60
5:E:28:LEU:HA	5:E:31:ILE:HD13	1.83	0.60
2:P:181:LYS:O	2:P:184:MET:HG3	2.02	0.60
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.32	0.60
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.50	0.59
12:L:90:LYS:HE3	12:L:93:PHE:O	2.02	0.59
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.15	0.59
7:U:217:LYS:HA	7:U:217:LYS:HE3	1.85	0.59
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.01	0.59
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.84	0.59
13:1:40:ASN:H	13:1:40:ASN:ND2	1.98	0.59
13:1:40:ASN:HD22	13:1:40:ASN:N	1.90	0.59
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.84	0.59
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.38	0.59
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.85	0.59
3:C:57:LYS:O	3:C:58:LEU:HB2	2.02	0.59
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.84	0.59
12:L:177:ILE:HD12	12:L:177:ILE:N	2.17	0.59
10:J:-1:MET:HG2	10:J:1:ASP:N	2.11	0.59
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.03	0.59
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.84	0.59
2:P:101:LYS:HZ2	10:X:85:GLN:HE22	1.51	0.59
3:C:175:PHE:O	3:C:179:ASN:HB2	2.03	0.59
5:E:35:SER:HB3	5:E:66:LYS:HZ3	1.67	0.59
10:J:100:LEU:CD2	10:J:112:GLN:HG3	2.33	0.59
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.84	0.59
8:V:52:THR:O	8:V:56:THR:HB	2.03	0.59
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	1.84	0.59
2:P:239:THR:HG22	2:P:239:THR:OXT	2.03	0.59
3:C:185:THR:HG22	3:C:186:VAL:N	2.17	0.58
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	2.03	0.58
4:D:112:LEU:C	4:D:112:LEU:HD13	2.27	0.58
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.68	0.58
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.67	0.58
7:G:118:ASN:O	7:G:122:ILE:HD12	2.03	0.58
11:K:208:ASN:ND2	9:W:29:ASN:CG	2.60	0.58
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.38	0.58
11:Y:10(A):ARG:HB3	11:Y:10(B):LYS:HE3	1.85	0.58
5:S:227:GLU:CD	5:S:227:GLU:N	2.60	0.58
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:100:LEU:CD2	10:X:112:GLN:HG3	2.33	0.58
12:Z:120:GLU:OE1	12:Z:120:GLU:OE2	2.20	0.58
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.10	0.58
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.16	0.58
8:H:52:THR:O	8:H:56:THR:HB	2.04	0.58
3:Q:69:LYS:HB2	16:Q:814:HOH:O	2.02	0.58
7:U:186:TRP:O	7:U:190:VAL:HG23	2.02	0.58
8:V:1:THR:OG1	16:V:263:HOH:O	2.14	0.58
3:C:14:ILE:HD13	3:C:14:ILE:H	1.68	0.58
10:J:144:PRO:HD3	11:Y:207:ASN:ND2	2.18	0.58
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	1.85	0.58
5:S:35:SER:HB3	5:S:66:LYS:NZ	2.19	0.58
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.02	0.58
1:A:69:LEU:HD23	1:A:69:LEU:C	2.28	0.58
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.18	0.58
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.30	0.58
10:J:165:ARG:O	10:X:26:VAL:HG23	2.03	0.58
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.38	0.58
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.68	0.58
11:Y:200:LYS:HE2	16:Y:772:HOH:O	2.04	0.58
2:B:112:LEU:HD23	2:B:112:LEU:C	2.29	0.58
5:E:207:LEU:HD23	5:E:207:LEU:N	2.13	0.58
11:K:10(A):ARG:HB3	11:K:10(B):LYS:HE3	1.85	0.58
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.86	0.58
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.86	0.58
7:U:197:MET:HA	7:U:197:MET:HE3	1.86	0.58
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.19	0.58
1:O:24:ILE:HD12	1:O:154:SER:HA	1.86	0.58
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.86	0.58
4:R:112:LEU:HD13	4:R:112:LEU:C	2.29	0.58
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.33	0.58
11:Y:1:THR:HA	11:Y:33:LYS:HZ3	1.69	0.57
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.19	0.57
10:J:168:MET:HG2	10:X:168:MET:CE	2.35	0.57
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.84	0.57
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.86	0.57
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.85	0.57
10:J:52:THR:CG2	10:J:53:VAL:N	2.67	0.57
5:S:134:VAL:O	5:S:153:PRO:HG3	2.04	0.57
12:Z:19:ARG:NE	12:Z:171:ASP:OD2	2.34	0.57
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.86	0.57
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.19	0.57
11:K:1:THR:HG22	11:K:2:THR:N	2.18	0.57
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.35	0.57
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.34	0.57
9:W:178:ILE:HG23	9:W:184:VAL:HG22	1.85	0.57
2:B:239:THR:HG22	2:B:239:THR:OXT	2.05	0.57
10:J:168:MET:CE	10:X:168:MET:HG2	2.33	0.57
6:T:203:GLU:O	6:T:206:LYS:HD2	2.04	0.57
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.85	0.57
5:E:198:SER:HA	5:E:201:LEU:HG	1.86	0.57
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.04	0.57
10:X:44:SER:OG	10:X:100:LEU:HB2	2.04	0.57
3:C:197:LEU:O	3:C:201:VAL:HG23	2.05	0.57
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.19	0.57
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.87	0.57
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.04	0.57
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.35	0.57
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.34	0.57
7:U:232:ARG:HA	7:U:232:ARG:NE	2.20	0.57
8:V:128:GLY:O	8:V:131:SER:HB2	2.05	0.57
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.86	0.57
4:D:53:ARG:O	4:D:53:ARG:HG2	2.04	0.57
3:Q:41:LYS:HG2	3:Q:161:SER:O	2.04	0.57
8:V:156:SER:O	8:V:160:GLN:HG3	2.04	0.57
13:1:150:VAL:HG21	16:1:323:HOH:O	2.04	0.57
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.86	0.57
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.53	0.57
7:G:136:LEU:O	7:G:150:LYS:HA	2.05	0.57
8:H:165:ASN:OD1	13:1:136:PRO:HA	2.04	0.57
5:S:123:ASN:HD22	5:S:123:ASN:N	2.03	0.57
10:X:52:THR:HG22	10:X:53:VAL:H	1.70	0.57
10:X:190:PHE:C	10:X:192:ALA:H	2.12	0.57
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.39	0.56
14:N:85:GLU:O	14:N:89:GLU:HB2	2.05	0.56
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.86	0.56
5:S:198:SER:HA	5:S:201:LEU:HG	1.87	0.56
8:V:34:LEU:HB2	16:V:578:HOH:O	2.05	0.56
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.35	0.56
6:F:136:THR:HB	16:F:1005:HOH:O	2.05	0.56
7:G:186:TRP:O	7:G:190:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:133:TYR:CE1	16:J:876:HOH:O	2.53	0.56
11:K:180:GLU:CB	16:K:924:HOH:O	2.53	0.56
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.39	0.56
16:R:886:HOH:O	12:Z:70:HIS:HE1	1.87	0.56
11:Y:208:ASN:ND2	11:Y:209:VAL:N	2.53	0.56
1:A:24:ILE:HD12	1:A:154:SER:HA	1.87	0.56
4:D:175:GLU:HB3	4:D:196:ILE:HD13	1.87	0.56
5:E:123:ASN:N	5:E:123:ASN:HD22	2.02	0.56
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.40	0.56
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.05	0.56
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.40	0.56
5:S:28:LEU:HA	5:S:31:ILE:HD13	1.86	0.56
10:X:52:THR:CG2	10:X:53:VAL:N	2.68	0.56
12:Z:-7:ASN:ND2	12:Z:-7:ASN:CA	2.68	0.56
14:2:21:THR:HG22	14:2:26:ILE:HA	1.87	0.56
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.14	0.56
11:K:10(A):ARG:H	11:K:10(B):LYS:HZ2	1.54	0.56
1:O:69:LEU:C	1:O:69:LEU:HD23	2.31	0.56
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.88	0.56
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.87	0.56
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.88	0.56
7:G:158:VAL:HG22	7:G:159:GLY:N	2.21	0.56
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.06	0.56
12:Z:35:PHE:O	12:Z:42:VAL:HA	2.05	0.56
5:E:134:VAL:O	5:E:153:PRO:HG3	2.04	0.56
5:E:2(C):VAL:HA	5:E:233:ILE:HD11	1.88	0.56
7:G:197:MET:HA	7:G:197:MET:HE3	1.86	0.56
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.71	0.56
6:T:172:ALA:C	6:T:176:LEU:HD23	2.30	0.56
2:B:159:GLY:HA3	3:C:62(A):ILE:HD12	1.88	0.56
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.20	0.56
10:J:143:ARG:O	10:J:146:MET:HG3	2.05	0.56
14:N:14:LEU:O	14:N:175:MET:HA	2.05	0.56
4:R:24:VAL:O	4:R:27:SER:HB3	2.05	0.56
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.87	0.56
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.71	0.56
8:H:156:SER:O	8:H:160:GLN:HG3	2.06	0.56
3:Q:65:SER:HB2	16:Q:303:HOH:O	2.06	0.56
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.20	0.56
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.41	0.56
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.88	0.55
9:I:29:ASN:CG	11:Y:208:ASN:ND2	2.64	0.55
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.21	0.55
14:2:14:LEU:O	14:2:175:MET:HA	2.06	0.55
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.06	0.55
7:G:232:ARG:NE	7:G:232:ARG:HA	2.21	0.55
11:K:1:THR:CG2	11:K:3:THR:HG23	2.36	0.55
11:K:7:ARG:HH11	11:K:108:PRO:HB2	1.71	0.55
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.42	0.55
2:P:224:PHE:N	2:P:224:PHE:CD2	2.75	0.55
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.89	0.55
2:B:15:PHE:H	3:C:23:GLN:NE2	1.98	0.55
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.88	0.55
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.88	0.55
10:J:24:ILE:CD1	10:X:129:TYR:HB3	2.32	0.55
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	2.06	0.55
1:O:62:GLU:CD	1:O:62:GLU:H	2.13	0.55
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.31	0.55
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.41	0.55
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.04	0.55
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.87	0.55
4:D:24:VAL:O	4:D:27:SER:HB3	2.06	0.55
6:T:159:GLY:HA3	7:U:63:THR:HG21	1.88	0.55
6:F:172:ALA:C	6:F:176:LEU:HD23	2.31	0.55
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.88	0.55
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.87	0.55
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.88	0.55
7:U:118:ASN:O	7:U:122:ILE:HD12	2.05	0.55
11:Y:4:LEU:CD1	11:Y:159:ILE:HG12	2.37	0.55
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.89	0.55
10:X:112:GLN:NE2	10:X:126:ALA:H	2.04	0.55
3:C:35:THR:HB	3:C:51:GLU:HG3	1.88	0.55
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.89	0.55
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.21	0.55
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.07	0.55
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.88	0.55
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.35	0.55
4:R:196:ILE:O	4:R:200:VAL:HG22	2.07	0.55
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.86	0.55
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.07	0.55
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:12:ASN:HB2	16:F:574:HOH:O	2.07	0.55
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.42	0.55
10:J:44:SER:OG	10:J:100:LEU:HB2	2.07	0.55
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.72	0.55
12:L:172:GLY:C	12:L:191:LEU:HD12	2.32	0.55
2:P:112:LEU:HD23	2:P:112:LEU:C	2.32	0.55
7:U:136:LEU:O	7:U:150:LYS:HA	2.06	0.55
11:Y:7:ARG:HH11	11:Y:108:PRO:HB2	1.71	0.55
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.32	0.55
4:D:186:LEU:O	4:D:190:GLU:HG3	2.07	0.55
5:E:74:MET:HE2	5:E:109:VAL:HG22	1.89	0.55
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.88	0.55
10:J:133:TYR:CZ	16:J:876:HOH:O	2.60	0.55
13:M:40:ASN:HD22	13:M:40:ASN:N	1.90	0.55
2:B:202:THR:CG2	2:B:204:SER:HB2	2.36	0.54
16:I:230:HOH:O	11:Y:166:ASP:O	2.18	0.54
10:J:52:THR:HG22	10:J:53:VAL:H	1.68	0.54
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.37	0.54
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.89	0.54
9:W:14:ILE:HG23	9:W:34:ILE:HD13	1.89	0.54
11:Y:32:LYS:N	11:Y:32:LYS:HD2	2.22	0.54
1:A:62:GLU:CD	1:A:62:GLU:H	2.16	0.54
4:D:207:LEU:HD23	4:D:208:ASP:N	2.23	0.54
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.88	0.54
14:N:21:THR:HG22	14:N:26:ILE:HA	1.89	0.54
14:N:10(B):LYS:C	14:N:10(B):LYS:HD3	2.32	0.54
3:Q:112:LEU:O	3:Q:116:VAL:HG23	2.08	0.54
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.66	0.54
12:L:35:PHE:O	12:L:42:VAL:HA	2.08	0.54
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.90	0.54
2:P:186:VAL:O	2:P:190:ILE:HG13	2.08	0.54
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.89	0.54
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.08	0.54
13:1:35:ILE:HG12	13:1:56:GLU:HG2	1.90	0.54
12:L:129:ALA:HB1	12:L:166:HIS:CE1	2.42	0.54
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.90	0.54
13:M:211:ILE:HD11	14:2:36:ARG:CD	2.36	0.54
2:P:202:THR:CG2	2:P:204:SER:HB2	2.37	0.54
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.89	0.54
4:D:40:ILE:HG13	4:D:193:VAL:HG23	1.89	0.54
10:J:190:PHE:C	10:J:192:ALA:H	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:99:THR:CG2	11:K:113:VAL:HB	2.36	0.54
1:O:197:LEU:O	1:O:202:VAL:HG23	2.08	0.54
14:2:85:GLU:O	14:2:89:GLU:HB2	2.06	0.54
8:H:144:GLN:O	8:H:145:ASP:HB2	2.08	0.54
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.08	0.54
7:U:158:VAL:HG22	7:U:159:GLY:N	2.23	0.54
1:A:79:SER:HB2	1:A:165:ILE:HD12	1.90	0.54
11:K:4:LEU:CD1	11:K:159:ILE:HG12	2.37	0.54
14:N:136:GLY:CA	14:2:161:GLN:HE21	2.10	0.54
4:R:113:THR:HG23	4:R:138:ILE:HD12	1.90	0.54
5:S:2(C):VAL:HA	5:S:233:ILE:HD11	1.89	0.54
1:A:188:ASP:O	1:A:192:ILE:HG13	2.08	0.54
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.90	0.54
7:U:38:LEU:C	7:U:38:LEU:HD12	2.33	0.54
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.07	0.54
2:B:224:PHE:N	2:B:224:PHE:CD2	2.75	0.54
4:D:196:ILE:O	4:D:200:VAL:HG22	2.08	0.54
11:K:86:LEU:HD13	11:K:86:LEU:C	2.33	0.54
11:K:137:VAL:HG21	11:K:161:ALA:HB2	1.90	0.54
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.20	0.54
14:N:92:ASP:HB2	16:N:197:HOH:O	2.07	0.54
5:S:35:SER:HB3	5:S:66:LYS:HZ3	1.73	0.54
6:T:194:ALA:O	6:T:198:TYR:HD1	1.91	0.54
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.90	0.54
1:A:197:LEU:O	1:A:202:VAL:HG23	2.08	0.53
2:B:186:VAL:O	2:B:190:ILE:HG13	2.07	0.53
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.09	0.53
6:F:203:GLU:O	6:F:206:LYS:HD2	2.08	0.53
9:I:58:MET:O	9:I:61:TYR:HB3	2.07	0.53
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.08	0.53
3:Q:13:SER:O	4:R:130:ARG:HD3	2.08	0.53
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	1.91	0.53
1:O:27:ALA:O	1:O:31:VAL:HG23	2.08	0.53
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.38	0.53
12:Z:172:GLY:C	12:Z:191:LEU:HD12	2.33	0.53
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.09	0.53
5:E:220:PRO:O	5:E:221:PHE:C	2.52	0.53
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.89	0.53
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.90	0.53
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.71	0.53
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.90	0.53
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.73	0.53
9:W:48:LEU:HG	9:W:50:THR:HG22	1.91	0.53
9:W:58:MET:O	9:W:61:TYR:HB3	2.08	0.53
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.76	0.53
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.08	0.53
3:C:182:PRO:O	3:C:184:ALA:N	2.42	0.53
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.43	0.53
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.09	0.53
8:H:28:ASP:OD1	8:H:31:CYS:HB3	2.08	0.53
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.07	0.53
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.08	0.53
14:2:174:ARG:HD2	16:2:307:HOH:O	2.08	0.53
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.72	0.53
7:G:212:VAL:HB	7:G:224:LEU:HD12	1.91	0.53
8:V:10:ASN:C	8:V:180:ILE:HD12	2.33	0.53
10:X:113:ILE:HA	10:X:118:THR:O	2.08	0.53
3:C:97:GLN:NE2	16:C:6:HOH:O	2.41	0.53
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.24	0.53
7:U:109:CYS:HB3	16:U:1330:HOH:O	2.09	0.53
8:V:112:SER:OG	8:V:120:ASP:HB2	2.08	0.53
9:W:33:LYS:O	9:W:44:GLY:HA2	2.08	0.53
4:D:113:THR:HG23	4:D:138:ILE:HD12	1.90	0.53
5:E:58:LEU:HD12	5:E:58:LEU:N	2.24	0.53
9:I:33:LYS:O	9:I:44:GLY:HA2	2.09	0.53
12:L:145:TYR:CD1	12:L:146:LEU:N	2.76	0.53
13:M:147:THR:HG23	16:M:1069:HOH:O	2.08	0.53
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.08	0.53
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.24	0.53
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.91	0.53
5:S:69:LYS:HD3	16:S:1020:HOH:O	2.08	0.53
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.39	0.53
6:T:147:HIS:HD2	16:T:242:HOH:O	1.91	0.53
13:1:19:LEU:HD12	13:1:28:PHE:O	2.08	0.53
2:B:71:ASN:HD22	2:B:72:ASP:H	1.52	0.53
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.89	0.53
6:F:45:GLY:HA3	6:F:215:CYS:O	2.08	0.53
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.74	0.53
10:J:-1:MET:N	16:J:1335:HOH:O	2.42	0.53
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.90	0.53
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:35:ILE:HG12	13:M:56:GLU:HG2	1.91	0.53
3:Q:182:PRO:O	3:Q:184:ALA:N	2.42	0.53
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.38	0.53
5:E:152:GLN:HG3	16:E:919:HOH:O	2.07	0.52
13:M:14(C):ARG:HG3	13:M:14(C):ARG:NH1	2.18	0.52
14:2:51:ASP:O	14:2:55:ILE:HG13	2.08	0.52
3:C:173:ARG:O	3:C:177:GLU:HG3	2.09	0.52
12:L:17:ASP:HA	12:L:172:GLY:O	2.09	0.52
10:X:13:ILE:HD13	10:X:152:LEU:HD23	1.91	0.52
2:B:211:GLU:HA	16:B:526:HOH:O	2.09	0.52
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.35	0.52
7:G:87:ASN:C	7:G:87:ASN:ND2	2.67	0.52
9:I:113:PHE:CD2	9:I:113:PHE:N	2.77	0.52
10:J:113:ILE:HA	10:J:118:THR:O	2.10	0.52
11:K:200:LYS:HE2	16:K:1088:HOH:O	2.08	0.52
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.92	0.52
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.92	0.52
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.90	0.52
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.91	0.52
12:L:21:ILE:C	12:L:21:ILE:HD12	2.35	0.52
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.45	0.52
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.91	0.52
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.08	0.52
6:T:45:GLY:HA3	6:T:215:CYS:O	2.10	0.52
10:X:136:SER:HA	10:X:139:ASP:HB2	1.91	0.52
11:Y:10(A):ARG:H	11:Y:10(B):LYS:HZ2	1.57	0.52
7:G:98:GLU:HG2	7:G:102:LYS:HD3	1.92	0.52
8:H:128:GLY:O	8:H:131:SER:HB2	2.09	0.52
9:I:113:PHE:HA	9:I:118:CYS:O	2.10	0.52
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.24	0.52
11:Y:105:THR:OG1	11:Y:106:GLU:HG3	2.10	0.52
13:1:187:LYS:HB3	13:1:190:LEU:HD11	1.92	0.52
14:2:143:ARG:O	14:2:146:MET:HG3	2.10	0.52
5:E:17:PRO:HA	6:F:26:TYR:CD2	2.44	0.52
8:H:210:THR:HG21	12:Z:14(C):GLN:HG2	1.91	0.52
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.09	0.52
6:T:136:THR:O	6:T:150:MET:HA	2.10	0.52
1:A:206:PHE:CE1	1:A:210:ILE:HD11	2.45	0.52
11:K:32:LYS:N	11:K:32:LYS:HD2	2.24	0.52
11:K:73:ARG:NH2	11:K:105:THR:HA	2.25	0.52
11:K:207:ASN:ND2	10:X:144:PRO:HD3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.91	0.52
5:E:167:ALA:HB3	16:E:1131:HOH:O	2.10	0.52
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.68	0.52
13:M:136:PRO:HA	8:V:165:ASN:OD1	2.10	0.52
1:O:79:SER:HB2	1:O:165:ILE:HD12	1.90	0.52
8:V:28:ASP:OD1	8:V:31:CYS:HB3	2.09	0.52
9:W:113:PHE:HA	9:W:118:CYS:O	2.09	0.52
11:Y:73:ARG:NH2	11:Y:105:THR:HA	2.24	0.52
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.75	0.52
2:B:238:ILE:O	2:B:239:THR:O	2.27	0.52
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.91	0.52
9:I:7:THR:HG23	9:I:110:ILE:HG12	1.92	0.52
10:J:100:LEU:HD21	10:J:112:GLN:HG3	1.91	0.52
1:O:62:GLU:O	1:O:64:LEU:N	2.43	0.52
1:O:122:GLU:C	1:O:124:THR:H	2.18	0.52
2:P:136:PHE:O	2:P:150:THR:HA	2.10	0.52
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.10	0.52
4:R:207:LEU:HD23	4:R:208:ASP:N	2.24	0.52
8:V:84:LYS:HD2	16:2:268:HOH:O	2.09	0.52
8:V:144:GLN:O	8:V:145:ASP:HB2	2.10	0.52
9:W:7:THR:HG23	9:W:110:ILE:HG12	1.92	0.52
2:B:224:PHE:N	2:B:224:PHE:HD2	2.08	0.52
7:G:140:SER:HA	7:G:215:ALA:HB1	1.92	0.52
11:K:53:GLN:HE21	12:L:84:GLN:HE22	1.57	0.52
13:M:17:ASP:HA	13:M:173:PHE:CB	2.40	0.52
3:Q:85:SER:O	3:Q:89:ILE:HD13	2.09	0.52
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.92	0.52
6:T:36:THR:CG2	6:T:51:GLU:OE2	2.58	0.52
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.92	0.52
7:U:192:PHE:C	7:U:192:PHE:CD1	2.88	0.52
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.92	0.52
8:V:152:ILE:HD11	8:V:177:VAL:HG21	1.91	0.52
11:Y:1:THR:CG2	11:Y:3:THR:HG23	2.40	0.52
4:D:39:GLY:O	4:D:162:ALA:HA	2.10	0.51
8:H:112:SER:OG	8:H:120:ASP:HB2	2.09	0.51
11:K:143:LYS:HB2	11:K:146:LEU:HD12	1.92	0.51
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.34	0.51
4:R:40:ILE:HG13	4:R:193:VAL:HG23	1.90	0.51
7:U:98:GLU:HG2	7:U:102:LYS:HD3	1.91	0.51
7:U:140:SER:HA	7:U:215:ALA:HB1	1.91	0.51
10:X:-1:MET:HG2	10:X:1:ASP:N	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.91	0.51
5:E:175:TYR:HB2	5:E:199:GLN:HG2	1.93	0.51
7:G:77:VAL:CG1	7:G:137:THR:HB	2.39	0.51
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.45	0.51
11:K:12:ILE:HB	11:K:178:VAL:HB	1.92	0.51
7:U:77:VAL:CG1	7:U:137:THR:HB	2.39	0.51
7:U:87:ASN:C	7:U:87:ASN:ND2	2.66	0.51
11:Y:75:SER:HA	11:Y:105:THR:HG21	1.91	0.51
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.10	0.51
13:M:187:LYS:HB3	13:M:190:LEU:HD11	1.91	0.51
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.10	0.51
8:V:175:VAL:HG12	8:V:176:CYS:N	2.25	0.51
10:X:103:GLY:HA2	10:X:178:VAL:HG11	1.92	0.51
11:Y:137:VAL:HG21	11:Y:161:ALA:HB2	1.91	0.51
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.93	0.51
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.92	0.51
11:K:75:SER:HA	11:K:105:THR:HG21	1.91	0.51
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.09	0.51
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.92	0.51
2:P:224:PHE:N	2:P:224:PHE:HD2	2.08	0.51
5:S:18(C):PHE:CA	5:S:18(F):ILE:HG12	2.40	0.51
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.91	0.51
3:C:158:SER:CB	4:D:59:LEU:HD21	2.40	0.51
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.93	0.51
10:J:136:SER:HA	10:J:139:ASP:HB2	1.91	0.51
11:K:105:THR:OG1	11:K:106:GLU:HG3	2.11	0.51
2:P:13:THR:O	3:Q:130:ARG:HD3	2.10	0.51
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.46	0.51
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.43	0.51
7:U:82:ILE:N	7:U:83:PRO:HD2	2.26	0.51
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.10	0.51
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.73	0.51
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.93	0.51
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.93	0.51
1:O:188:ASP:O	1:O:192:ILE:HG13	2.10	0.51
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.93	0.51
10:X:143:ARG:O	10:X:146:MET:HG3	2.11	0.51
12:Z:21:ILE:C	12:Z:21:ILE:HD12	2.35	0.51
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.11	0.51
9:I:6:MET:HE3	9:I:155:ILE:CG1	2.38	0.51
2:P:101:LYS:HZ3	10:X:85:GLN:NE2	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.11	0.51
1:A:27:ALA:O	1:A:31:VAL:HG23	2.10	0.51
1:A:62:GLU:O	1:A:64:LEU:N	2.43	0.51
1:A:122:GLU:C	1:A:124:THR:H	2.19	0.51
2:B:136:PHE:O	2:B:150:THR:HA	2.10	0.51
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.92	0.51
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.92	0.51
7:G:18(G):GLU:CG	7:G:188:LYS:HB2	2.39	0.51
8:H:152:ILE:HD11	8:H:177:VAL:HG21	1.93	0.51
9:I:48:LEU:HG	9:I:50:THR:HG22	1.92	0.51
14:N:161:GLN:HE21	14:2:136:GLY:CA	2.08	0.51
11:Y:180:GLU:CB	16:Y:812:HOH:O	2.58	0.51
3:C:112:LEU:O	3:C:116:VAL:HG23	2.10	0.51
2:P:143:ASP:OD2	10:X:10(B):LYS:HE2	2.11	0.51
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.33	0.51
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	2.09	0.51
6:F:136:THR:O	6:F:150:MET:HA	2.11	0.50
7:G:38:LEU:C	7:G:38:LEU:HD12	2.36	0.50
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.40	0.50
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.76	0.50
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.93	0.50
5:S:58:LEU:N	5:S:58:LEU:HD12	2.26	0.50
10:X:39:PRO:HG2	10:X:73:GLU:CD	2.35	0.50
13:1:4:ILE:CD1	13:1:155:ILE:HG23	2.41	0.50
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.93	0.50
5:E:68:ILE:HB	5:E:76:LEU:HD21	1.92	0.50
6:F:203:GLU:C	6:F:205:ASN:H	2.19	0.50
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.93	0.50
4:R:17:PRO:HA	5:S:26:TYR:CG	2.45	0.50
5:S:175:TYR:HB2	5:S:199:GLN:HG2	1.93	0.50
2:B:27:ALA:O	2:B:31:ILE:HG12	2.11	0.50
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.92	0.50
9:I:20:LEU:HD13	9:I:20:LEU:C	2.36	0.50
10:J:112:GLN:NE2	10:J:126:ALA:H	2.08	0.50
1:O:4:MET:CG	1:O:5:THR:H	2.25	0.50
9:W:20:LEU:C	9:W:20:LEU:HD13	2.36	0.50
9:W:113:PHE:CD2	9:W:113:PHE:N	2.79	0.50
6:F:36:THR:CG2	6:F:51:GLU:OE2	2.59	0.50
6:F:56:SER:OG	6:F:57:LYS:N	2.43	0.50
7:G:82:ILE:N	7:G:83:PRO:HD2	2.25	0.50
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:220:PRO:O	5:S:221:PHE:C	2.54	0.50
10:X:100:LEU:HD21	10:X:112:GLN:HG3	1.92	0.50
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.53	0.50
7:G:192:PHE:C	7:G:192:PHE:CD1	2.89	0.50
10:J:131:GLY:HA3	16:J:594:HOH:O	2.11	0.50
4:R:192:LEU:O	4:R:196:ILE:HG13	2.12	0.50
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.40	0.50
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.77	0.50
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.94	0.50
5:S:68:ILE:HB	5:S:76:LEU:HD21	1.92	0.50
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.92	0.50
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.93	0.50
16:E:1080:HOH:O	12:L:64:LYS:HE3	2.10	0.50
6:F:192:GLN:NE2	6:F:195:LYS:HE2	2.27	0.50
14:N:143:ARG:O	14:N:146:MET:HG3	2.11	0.50
1:O:159:PRO:O	2:P:59:LEU:HD12	2.12	0.50
4:R:207:LEU:HD21	4:R:233:ILE:HD12	1.94	0.50
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.27	0.50
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.92	0.50
12:Z:58:ARG:NH2	16:Z:1275:HOH:O	2.45	0.50
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.46	0.50
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.75	0.50
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.94	0.50
10:J:24:ILE:O	10:J:24:ILE:HG12	2.11	0.50
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.47	0.50
11:K:104:TYR:CE1	11:K:180:GLU:OE2	2.65	0.50
13:M:66:ASN:HB3	16:M:226:HOH:O	2.11	0.50
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.54	0.50
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.94	0.50
6:T:192:GLN:NE2	6:T:195:LYS:HE2	2.26	0.50
7:U:107:MET:CE	7:U:112:LEU:HD13	2.39	0.50
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.93	0.50
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.93	0.50
11:Y:208:ASN:CG	11:Y:209:VAL:N	2.67	0.50
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.94	0.50
6:F:63:LYS:O	6:F:65:VAL:HG23	2.12	0.49
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.95	0.49
11:K:114:ASP:C	11:K:114:ASP:OD1	2.55	0.49
13:M:19:LEU:HD12	13:M:28:PHE:O	2.11	0.49
14:N:51:ASP:O	14:N:55:ILE:HG13	2.12	0.49
1:O:62:GLU:C	1:O:64:LEU:N	2.69	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:12(D):ALA:HA	5:S:129:GLY:HA2	1.93	0.49
7:U:212:VAL:HB	7:U:224:LEU:HD12	1.93	0.49
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.12	0.49
3:C:227:GLU:OE1	3:C:227:GLU:N	2.43	0.49
4:R:29:GLU:HA	4:R:29:GLU:OE2	2.11	0.49
13:1:112:TYR:O	13:1:119:THR:HA	2.12	0.49
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.41	0.49
3:C:168:ASN:O	3:C:172:VAL:HG12	2.12	0.49
5:E:226:GLY:O	5:E:229:VAL:HG22	2.12	0.49
8:H:82:MET:HA	16:H:228:HOH:O	2.12	0.49
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.48	0.49
1:O:31:VAL:HG13	1:O:79:SER:O	2.13	0.49
5:S:57:GLU:C	5:S:58:LEU:HD12	2.38	0.49
10:X:19:ALA:HB2	10:X:171:LYS:HG2	1.93	0.49
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.12	0.49
4:D:207:LEU:HD21	4:D:233:ILE:HD12	1.95	0.49
8:H:10:ASN:C	8:H:180:ILE:HD12	2.37	0.49
10:J:52:THR:HG22	10:J:53:VAL:HG23	1.95	0.49
4:R:176:LEU:CD2	4:R:196:ILE:HD12	2.43	0.49
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.42	0.49
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.27	0.49
10:X:190:PHE:C	10:X:192:ALA:N	2.69	0.49
13:1:17:ASP:HA	13:1:173:PHE:CB	2.42	0.49
2:B:71:ASN:HD22	2:B:72:ASP:N	2.07	0.49
4:D:29:GLU:OE2	4:D:29:GLU:HA	2.12	0.49
7:G:158:VAL:HG13	7:G:160:TYR:CE1	2.48	0.49
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.93	0.49
4:R:198:LYS:HA	16:R:425:HOH:O	2.11	0.49
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.94	0.49
13:1:14(C):ARG:CG	13:1:14(C):ARG:NH1	2.74	0.49
3:C:185:THR:CG2	3:C:186:VAL:N	2.75	0.49
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.94	0.49
10:J:190:PHE:C	10:J:192:ALA:N	2.71	0.49
3:Q:136:THR:O	3:Q:150:GLN:HA	2.11	0.49
6:T:63:LYS:O	6:T:65:VAL:HG23	2.13	0.49
9:W:101:VAL:O	9:W:110:ILE:HA	2.13	0.49
6:F:43:ASN:N	6:F:43:ASN:HD22	2.10	0.49
7:G:118:ASN:O	7:G:122:ILE:CD1	2.61	0.49
8:H:124:TYR:O	8:H:125:LEU:HD23	2.12	0.49
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.76	0.49
11:K:10(B):LYS:N	11:K:10(B):LYS:CD	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.93	0.49
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.95	0.49
14:N:175:MET:HE3	14:N:18(B):PHE:CE2	2.47	0.49
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.95	0.49
10:X:13:ILE:HD13	10:X:152:LEU:CD2	2.42	0.49
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.42	0.49
3:Q:85:SER:O	3:Q:89:ILE:CD1	2.60	0.49
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.21	0.49
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.77	0.49
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.95	0.49
2:B:15:PHE:N	3:C:23:GLN:HE22	1.98	0.49
5:E:57:GLU:C	5:E:58:LEU:HD12	2.37	0.49
11:K:10(A):ARG:H	11:K:10(B):LYS:NZ	2.10	0.49
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.94	0.49
2:P:170:SER:HB3	16:P:943:HOH:O	2.12	0.49
5:S:74:MET:HE2	5:S:109:VAL:HG22	1.95	0.49
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.48	0.49
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.47	0.48
12:L:178:VAL:HG22	12:L:184:VAL:HG22	1.95	0.48
14:N:147:SER:OG	14:N:150:GLU:HG3	2.13	0.48
2:P:238:ILE:O	2:P:239:THR:O	2.31	0.48
4:R:17:PRO:HG3	5:S:26:TYR:CE2	2.48	0.48
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.95	0.48
12:Z:152:ILE:O	12:Z:156:ARG:HG3	2.12	0.48
3:C:227:GLU:H	3:C:227:GLU:CD	2.22	0.48
4:D:14:THR:HG22	4:D:15:PHE:N	2.29	0.48
5:E:100:SER:O	5:E:104:ASN:N	2.45	0.48
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.94	0.48
8:H:175:VAL:HG12	8:H:176:CYS:N	2.27	0.48
12:L:14(I):THR:O	12:L:1(I):ASN:HB3	2.13	0.48
13:M:4:ILE:CD1	13:M:155:ILE:HG23	2.43	0.48
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.95	0.48
2:P:27:ALA:O	2:P:31:ILE:HG12	2.12	0.48
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.42	0.48
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.38	0.48
13:1:113:VAL:HA	13:1:118:VAL:O	2.13	0.48
16:B:565:HOH:O	3:C:33:ARG:HD2	2.12	0.48
4:D:176:LEU:CD2	4:D:196:ILE:HD12	2.43	0.48
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.78	0.48
7:U:18(G):GLU:CG	7:U:188:LYS:HB2	2.40	0.48
3:C:136:THR:O	3:C:150:GLN:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.49	0.48
4:R:100:ASN:HB3	16:R:371:HOH:O	2.12	0.48
6:T:203:GLU:C	6:T:205:ASN:H	2.20	0.48
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.95	0.48
10:X:10(B):LYS:HB2	10:X:10(B):LYS:NZ	2.28	0.48
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.48	0.48
13:1:14(C):ARG:HG3	13:1:14(C):ARG:NH1	2.16	0.48
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.24	0.48
12:L:140:ASN:O	12:L:144:PHE:HA	2.13	0.48
6:T:54:ILE:HG12	6:T:208:PHE:HA	1.96	0.48
11:Y:80:SER:HA	11:Y:101:ILE:HD12	1.96	0.48
14:2:66:TYR:CE2	14:2:74:PRO:HB3	2.49	0.48
1:A:4:MET:CG	1:A:5:THR:H	2.26	0.48
11:K:142:TYR:C	11:K:143:LYS:HD2	2.38	0.48
14:N:36:ARG:CD	13:1:211:ILE:HD11	2.42	0.48
2:P:6:ARG:HD2	4:R:9:ASP:N	2.29	0.48
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.12	0.48
3:Q:115:TYR:O	3:Q:119:VAL:HG23	2.13	0.48
6:T:43:ASN:HD22	6:T:43:ASN:N	2.10	0.48
11:Y:83:LEU:HD23	11:Y:99:THR:HG21	1.95	0.48
12:Z:14(Q):LEU:C	12:Z:14(W):LYS:C	2.81	0.48
3:C:36:CYS:H	3:C:51:GLU:HG2	1.79	0.48
5:E:161:TYR:OH	6:F:61:PRO:HD2	2.13	0.48
10:J:13:ILE:HD13	10:J:152:LEU:HD23	1.94	0.48
11:K:208:ASN:CG	11:K:209:VAL:N	2.66	0.48
12:L:135:MET:CE	9:W:165:ARG:NH2	2.77	0.48
2:P:71:ASN:HD22	2:P:72:ASP:N	2.08	0.48
4:R:39:GLY:O	4:R:162:ALA:HA	2.14	0.48
4:R:121:LEU:N	16:R:853:HOH:O	2.43	0.48
10:X:6:ILE:CD1	10:X:154:LEU:HD23	2.41	0.48
11:Y:104:TYR:CE1	11:Y:180:GLU:OE2	2.67	0.48
5:E:4:PHE:CG	5:E:5:ARG:N	2.82	0.48
6:T:56:SER:OG	6:T:57:LYS:N	2.45	0.48
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.48	0.48
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.29	0.48
12:Z:14(I):THR:O	12:Z:1(I):ASN:HB3	2.13	0.48
2:B:202:THR:HG21	2:B:204:SER:HB2	1.96	0.48
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.44	0.48
6:F:194:ALA:O	6:F:198:TYR:HD1	1.95	0.48
7:G:170:GLN:HB3	16:G:725:HOH:O	2.13	0.48
10:J:39:PRO:HG2	10:J:73:GLU:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:144:PRO:HD3	11:Y:207:ASN:CG	2.38	0.48
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.95	0.48
2:P:71:ASN:HD22	2:P:72:ASP:H	1.52	0.48
3:Q:76:LEU:C	3:Q:76:LEU:HD23	2.38	0.48
3:Q:18(B):ARG:HH21	4:R:58:LEU:C	2.21	0.48
11:Y:114:ASP:C	11:Y:114:ASP:OD1	2.56	0.48
13:1:157:ASN:HB3	16:1:558:HOH:O	2.14	0.48
1:A:112:LEU:O	1:A:116:VAL:HG23	2.14	0.48
3:C:79:SER:HA	16:C:625:HOH:O	2.14	0.48
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.49	0.48
10:J:144:PRO:CD	11:Y:207:ASN:ND2	2.76	0.48
11:K:1:THR:HA	11:K:33:LYS:HZ2	1.76	0.48
11:K:207:ASN:CG	10:X:144:PRO:HD3	2.39	0.48
1:O:206:PHE:CE1	1:O:210:ILE:HD11	2.49	0.48
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.14	0.48
4:R:14:THR:HG22	4:R:15:PHE:N	2.29	0.48
11:Y:73:ARG:HH22	11:Y:105:THR:HA	1.78	0.48
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.13	0.48
13:1:9:ASP:OD1	13:1:10:ASN:N	2.47	0.48
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.95	0.47
8:H:172:ASN:HD22	8:H:193:THR:HA	1.78	0.47
13:M:112:TYR:O	13:M:119:THR:HA	2.13	0.47
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.46	0.47
3:Q:185:THR:CG2	3:Q:186:VAL:N	2.77	0.47
5:S:78:LEU:O	5:S:78:LEU:HD12	2.14	0.47
5:S:194:VAL:O	5:S:197:ILE:HG22	2.14	0.47
1:A:29:THR:O	1:A:33:GLN:HG2	2.14	0.47
6:F:63:LYS:O	6:F:65:VAL:N	2.47	0.47
11:K:73:ARG:HH22	11:K:105:THR:HA	1.79	0.47
11:K:180:GLU:HB3	16:K:924:HOH:O	2.13	0.47
12:L:3:ILE:HD12	12:L:3:ILE:O	2.14	0.47
13:M:9:ASP:OD1	13:M:10:ASN:N	2.48	0.47
1:O:112:LEU:O	1:O:116:VAL:HG23	2.14	0.47
5:S:226:GLY:O	5:S:229:VAL:HG22	2.14	0.47
7:U:118:ASN:O	7:U:122:ILE:CD1	2.62	0.47
2:B:234:VAL:HA	2:B:239:THR:HA	1.96	0.47
5:E:18(C):PHE:C	5:E:18(F):ILE:HG12	2.39	0.47
7:G:70:ILE:HG21	7:G:112:LEU:HD21	1.96	0.47
9:I:101:VAL:O	9:I:110:ILE:HA	2.14	0.47
13:M:113:VAL:HA	13:M:118:VAL:O	2.13	0.47
4:R:120:ALA:CB	4:R:155:GLY:HA2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:77:SER:OG	5:S:137:LEU:HB2	2.14	0.47
10:X:90(A):ILE:HG12	10:X:116:LEU:HA	1.97	0.47
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.63	0.47
3:C:76:LEU:HD23	3:C:76:LEU:C	2.39	0.47
3:C:101:LEU:HD13	16:J:715:HOH:O	2.14	0.47
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.97	0.47
7:G:8:TYR:C	7:G:10:ARG:H	2.22	0.47
11:K:104:TYR:CD1	11:K:180:GLU:OE2	2.67	0.47
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.39	0.47
6:T:35:THR:CG2	6:T:36:THR:N	2.77	0.47
5:E:52:LYS:CB	5:E:63:TYR:HB3	2.44	0.47
10:J:10(B):LYS:NZ	10:J:10(B):LYS:HB2	2.29	0.47
2:P:141:TYR:CD1	2:P:141:TYR:C	2.92	0.47
6:T:192:GLN:O	6:T:196:ILE:HG13	2.15	0.47
7:U:158:VAL:HG13	7:U:160:TYR:CE1	2.49	0.47
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.50	0.47
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.95	0.47
5:E:52:LYS:O	5:E:63:TYR:HD2	1.98	0.47
7:G:107:MET:CE	7:G:112:LEU:HD13	2.41	0.47
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.97	0.47
11:K:6:PHE:HA	11:K:123:ASP:O	2.15	0.47
2:P:231:ASP:O	2:P:235:LYS:HG2	2.15	0.47
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.43	0.47
10:X:24:ILE:O	10:X:24:ILE:HG12	2.13	0.47
12:Z:14(E):GLU:OE2	12:Z:14(P):PRO:HD2	2.14	0.47
2:B:141:TYR:CD1	2:B:141:TYR:C	2.93	0.47
3:C:190:VAL:O	3:C:194:VAL:HG23	2.14	0.47
5:E:18(C):PHE:CA	5:E:18(F):ILE:HG12	2.41	0.47
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.30	0.47
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.97	0.47
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.50	0.47
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.95	0.47
10:J:185:ARG:HG2	10:J:185:ARG:HH11	1.80	0.47
12:L:1:GLY:HA3	12:L:33:LYS:NZ	2.29	0.47
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.96	0.47
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.97	0.47
1:O:142:ASP:OD1	1:O:145:ASN:HB2	2.15	0.47
2:P:77:ALA:HB3	2:P:137:ILE:HB	1.97	0.47
2:P:107:ILE:HG22	16:P:410:HOH:O	2.15	0.47
2:P:234:VAL:HA	2:P:239:THR:HA	1.96	0.47
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:216:GLY:O	5:S:218:ASP:N	2.47	0.47
6:T:63:LYS:O	6:T:65:VAL:N	2.48	0.47
6:T:69:VAL:HG12	16:T:811:HOH:O	2.15	0.47
7:U:70:ILE:HG21	7:U:112:LEU:HD21	1.96	0.47
12:Z:1:GLY:HA3	12:Z:33:LYS:NZ	2.29	0.47
12:Z:15:ALA:HB1	12:Z:173:LEU:HD11	1.96	0.47
12:Z:14(E):GLU:HB2	12:Z:14(I):THR:HG21	1.96	0.47
13:1:160:ARG:NE	16:1:905:HOH:O	2.37	0.47
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.49	0.47
13:M:14(C):ARG:CG	13:M:14(C):ARG:NH1	2.74	0.47
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.97	0.47
6:F:21(B):THR:HG22	6:F:222:LYS:HD3	1.97	0.47
9:I:172:GLY:O	9:I:173:ALA:HB2	2.14	0.47
4:R:208:ASP:C	4:R:20(A):ASN:H	2.23	0.47
6:T:49:ALA:HA	6:T:211:GLU:O	2.14	0.47
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.96	0.47
11:Y:50:ALA:CB	12:Z:116:VAL:HG23	2.45	0.47
13:1:8:TYR:O	13:1:108:GLN:NE2	2.48	0.47
3:C:40:VAL:HG12	3:C:162:ALA:CB	2.45	0.47
6:F:54:ILE:HG12	6:F:208:PHE:HA	1.97	0.47
9:I:-2:ASN:HA	9:I:21:GLY:O	2.16	0.47
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.30	0.47
5:S:4:PHE:CG	5:S:5:ARG:N	2.82	0.47
2:B:101:LYS:HG3	9:I:57:GLU:HB3	1.97	0.46
3:C:45:CYS:HA	3:C:141:PHE:HZ	1.80	0.46
6:F:36:THR:HB	6:F:168:GLY:H	1.80	0.46
11:K:82:ILE:HG13	16:K:1154:HOH:O	2.14	0.46
13:M:69(C):LEU:HB2	13:M:71(C):GLU:HB2	1.97	0.46
13:M:168:ARG:HB2	16:M:503:HOH:O	2.15	0.46
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.51	0.46
3:Q:40:VAL:HG12	3:Q:162:ALA:CB	2.45	0.46
5:S:18(C):PHE:C	5:S:18(F):ILE:HG12	2.39	0.46
11:Y:4:LEU:HD11	11:Y:159:ILE:HG12	1.97	0.46
11:Y:10(A):ARG:H	11:Y:10(B):LYS:NZ	2.12	0.46
3:C:85:SER:O	3:C:89:ILE:HD13	2.15	0.46
9:I:14:ILE:HG23	9:I:34:ILE:HD13	1.97	0.46
10:J:103:GLY:HA2	10:J:178:VAL:HG11	1.97	0.46
11:K:199:VAL:O	11:K:203:GLU:HB3	2.14	0.46
12:L:5:GLY:O	12:L:124:CYS:HA	2.15	0.46
12:L:14(E):GLU:HB2	12:L:14(I):THR:HG21	1.97	0.46
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:160:LEU:HD13	5:S:163:THR:HB	1.97	0.46
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.16	0.46
8:V:124:TYR:O	8:V:125:LEU:HD23	2.15	0.46
11:Y:199:VAL:O	11:Y:203:GLU:HB3	2.16	0.46
5:E:216:GLY:O	5:E:218:ASP:N	2.49	0.46
7:G:187:GLU:O	7:G:191:GLU:HG3	2.16	0.46
11:K:191:ASP:OD2	11:K:193:GLY:N	2.48	0.46
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.97	0.46
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.50	0.46
4:R:97:VAL:HG11	11:Y:65:LEU:HD22	1.97	0.46
11:Y:104:TYR:CD1	11:Y:180:GLU:OE2	2.69	0.46
13:1:87:MET:HE3	13:1:115:LEU:HA	1.97	0.46
14:2:44:CYS:HB2	14:2:100:ILE:HB	1.96	0.46
3:C:163:GLN:HG3	3:C:164:THR:N	2.30	0.46
5:E:111:ARG:HG2	5:E:111:ARG:NH1	2.29	0.46
4:R:161:ASN:N	5:S:58:LEU:O	2.43	0.46
5:S:52:LYS:O	5:S:63:TYR:HD2	1.97	0.46
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.97	0.46
10:X:193:GLN:HG2	10:X:193:GLN:OXT	2.15	0.46
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.96	0.46
12:Z:76:ILE:CG2	12:Z:77:ASN:N	2.78	0.46
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.97	0.46
1:A:150:GLN:O	1:A:157:TYR:HA	2.16	0.46
11:K:166:ASP:O	16:W:228:HOH:O	2.21	0.46
1:O:82:GLY:O	1:O:85:TYR:HB3	2.15	0.46
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.50	0.46
10:X:156:LYS:HE2	10:X:160:GLN:HE22	1.78	0.46
13:1:17:ASP:C	13:1:17:ASP:OD2	2.57	0.46
4:D:29:GLU:OE2	4:D:32:LYS:HD2	2.15	0.46
5:E:160:LEU:HD13	5:E:163:THR:HB	1.96	0.46
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.16	0.46
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.96	0.46
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.15	0.46
10:X:185:ARG:HG2	10:X:185:ARG:HH11	1.80	0.46
11:Y:104:TYR:CE2	11:Y:108:PRO:HG3	2.51	0.46
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.15	0.46
13:1:204:LYS:N	13:1:204:LYS:HD3	2.31	0.46
14:2:147:SER:OG	14:2:150:GLU:HG3	2.15	0.46
5:E:194:VAL:O	5:E:197:ILE:HG22	2.15	0.46
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.98	0.46
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.75	0.46
6:F:49:ALA:HA	6:F:211:GLU:O	2.15	0.46
13:M:149:GLN:H	13:M:149:GLN:HE21	1.62	0.46
2:P:27:ALA:O	2:P:30:SER:HB3	2.15	0.46
3:Q:71:ASP:OD1	3:Q:100:ARG:NH1	2.46	0.46
4:R:156:THR:HG22	5:S:82:ALA:HB3	1.96	0.46
7:U:8:TYR:C	7:U:10:ARG:H	2.24	0.46
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.97	0.46
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.46	0.46
2:B:231:ASP:O	2:B:235:LYS:HG2	2.16	0.46
11:K:1:THR:CA	11:K:33:LYS:HZ3	2.28	0.46
14:N:139:ASP:HB3	14:2:161:GLN:HE22	1.81	0.46
1:O:29:THR:O	1:O:33:GLN:HG2	2.15	0.46
4:R:16:SER:HA	4:R:22:PHE:CZ	2.51	0.46
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.16	0.46
6:T:90:ASN:O	6:T:94:GLU:HG3	2.16	0.46
9:W:-2:ASN:HA	9:W:21:GLY:O	2.15	0.46
10:X:85:GLN:O	10:X:89:LYS:HG3	2.16	0.46
11:Y:10(B):LYS:N	11:Y:10(B):LYS:CD	2.62	0.46
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.30	0.46
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.16	0.46
10:J:129:TYR:HB3	10:X:24:ILE:CD1	2.38	0.46
12:L:15:ALA:HB1	12:L:173:LEU:HD11	1.97	0.46
7:U:172:ILE:CD1	7:U:197:MET:HE1	2.46	0.46
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.98	0.46
9:W:6:MET:HE3	9:W:155:ILE:CG1	2.40	0.46
9:W:150:ASP:HA	16:W:1181:HOH:O	2.15	0.46
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.51	0.46
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.50	0.46
3:C:115:TYR:O	3:C:119:VAL:HG23	2.16	0.45
4:D:16:SER:HA	4:D:22:PHE:CZ	2.51	0.45
4:D:102:TYR:O	12:L:81:ARG:HG3	2.16	0.45
7:G:34(A):ASN:ND2	7:G:167:PRO:HG2	2.31	0.45
7:G:79:ASN:HA	16:G:926:HOH:O	2.16	0.45
11:K:4:LEU:HD11	11:K:159:ILE:HG12	1.98	0.45
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.98	0.45
5:S:4:PHE:O	5:S:6:ASN:N	2.49	0.45
5:S:41:ARG:NH1	5:S:42:SER:O	2.49	0.45
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.98	0.45
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.31	0.45
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:VAL:HG22	3:C:39:GLY:N	2.31	0.45
6:F:162:GLY:O	7:G:58:LEU:HB3	2.15	0.45
12:L:3:ILE:HD12	12:L:3:ILE:C	2.41	0.45
12:L:93:PHE:N	12:L:94:PRO:HD3	2.30	0.45
13:M:204:LYS:HD3	13:M:204:LYS:N	2.31	0.45
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.46	0.45
7:U:228:ASN:HB3	16:U:242:HOH:O	2.16	0.45
7:U:232:ARG:HA	7:U:232:ARG:HE	1.80	0.45
1:A:82:GLY:O	1:A:85:TYR:HB3	2.16	0.45
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.51	0.45
6:F:35:THR:CG2	6:F:36:THR:N	2.78	0.45
7:G:18(M):SER:HB2	7:G:187:GLU:OE2	2.17	0.45
10:J:13:ILE:HD13	10:J:152:LEU:CD2	2.46	0.45
11:K:104:TYR:CE2	11:K:108:PRO:HG3	2.50	0.45
14:N:29:ARG:HG2	16:N:860:HOH:O	2.15	0.45
1:O:141:HIS:HA	1:O:146:GLY:O	2.17	0.45
4:R:29:GLU:OE2	4:R:32:LYS:HD2	2.16	0.45
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.17	0.45
7:U:6:ALA:C	7:U:8:TYR:H	2.24	0.45
7:U:60:ASP:OD2	7:U:62:THR:OG1	2.35	0.45
12:Z:3:ILE:C	12:Z:3:ILE:HD12	2.41	0.45
2:B:5:SER:C	2:B:7:ARG:N	2.74	0.45
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.17	0.45
11:K:207:ASN:ND2	10:X:144:PRO:CD	2.80	0.45
4:R:156:THR:CG2	5:S:83:PRO:HD3	2.43	0.45
8:V:75:ARG:HA	8:V:105:ASP:OD1	2.15	0.45
13:1:184:LEU:C	13:1:184:LEU:HD23	2.41	0.45
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.98	0.45
2:B:143:ASP:OD2	10:J:10(B):LYS:HE2	2.16	0.45
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.31	0.45
2:P:5:SER:C	2:P:7:ARG:N	2.73	0.45
2:P:234:VAL:HG22	2:P:239:THR:HA	1.98	0.45
2:P:235:LYS:HD3	2:P:235:LYS:N	2.31	0.45
3:Q:11:ALA:CB	4:R:12:VAL:HG11	2.47	0.45
5:S:162:GLY:O	6:T:58:LEU:HD13	2.17	0.45
6:T:36:THR:HB	6:T:168:GLY:H	1.81	0.45
6:T:172:ALA:O	6:T:176:LEU:HD23	2.17	0.45
6:T:21(B):THR:HG22	6:T:222:LYS:HD3	1.97	0.45
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.80	0.45
8:V:172:ASN:HD22	8:V:193:THR:HA	1.81	0.45
11:Y:205:SER:C	11:Y:207:ASN:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:3:ILE:HD13	12:Z:100:ILE:HD13	1.96	0.45
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.46	0.45
3:C:154:SER:OG	3:C:156:ILE:HG12	2.17	0.45
7:G:60:ASP:OD2	7:G:62:THR:OG1	2.33	0.45
7:G:152:ASP:OD1	7:G:154:ALA:HB3	2.17	0.45
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.99	0.45
9:I:93:GLY:N	9:I:94:PRO:CD	2.80	0.45
11:K:4:LEU:C	11:K:4:LEU:CD2	2.89	0.45
13:M:87:MET:HE3	13:M:115:LEU:HA	1.98	0.45
13:M:91:ARG:HG3	13:M:92:SER:N	2.30	0.45
13:M:184:LEU:HD23	13:M:184:LEU:C	2.42	0.45
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.52	0.45
6:T:205:ASN:O	6:T:20(B):GLU:N	2.50	0.45
7:U:152:ASP:OD1	7:U:154:ALA:HB3	2.16	0.45
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.99	0.45
4:D:120:ALA:CB	4:D:155:GLY:HA2	2.46	0.45
6:F:127:ASN:N	6:F:127:ASN:HD22	2.13	0.45
6:F:192:GLN:O	6:F:196:ILE:HG13	2.16	0.45
11:K:83:LEU:HD23	11:K:99:THR:HG21	1.97	0.45
1:O:92:SER:O	1:O:95:VAL:HG12	2.17	0.45
1:O:150:GLN:O	1:O:157:TYR:HA	2.16	0.45
3:Q:125:GLN:NE2	16:Q:872:HOH:O	2.50	0.45
6:T:176:LEU:O	6:T:180:VAL:HG23	2.16	0.45
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.98	0.45
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.90	0.45
11:Y:174:ASN:HD21	11:Y:189:ASN:HB2	1.82	0.45
5:E:4:PHE:O	5:E:6:ASN:N	2.50	0.45
5:E:52:LYS:HB2	5:E:63:TYR:HB3	1.98	0.45
6:F:93:ARG:HD2	16:F:842:HOH:O	2.16	0.45
10:J:6:ILE:CD1	10:J:154:LEU:HD23	2.45	0.45
10:J:166:MET:HA	10:J:167:PRO:HD3	1.79	0.45
11:K:1:THR:CG2	11:K:2:THR:N	2.80	0.45
12:L:14(E):GLU:OE2	12:L:14(P):PRO:HD2	2.16	0.45
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.47	0.45
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.97	0.45
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.99	0.45
5:S:179:THR:HG22	5:S:179:THR:O	2.17	0.45
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.99	0.45
9:W:172:GLY:O	9:W:173:ALA:HB2	2.17	0.45
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.16	0.45
13:1:-4:ILE:HG22	13:1:-3:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ALA:HB3	2:B:137:ILE:HB	1.99	0.45
3:C:150:GLN:HE21	3:C:150:GLN:HB3	1.64	0.45
4:D:208:ASP:C	4:D:20(A):ASN:H	2.25	0.45
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.98	0.45
12:L:76:ILE:CG2	12:L:77:ASN:N	2.80	0.45
13:M:8:TYR:O	13:M:108:GLN:NE2	2.49	0.45
4:R:17:PRO:HA	5:S:26:TYR:CD2	2.52	0.45
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.50	0.45
6:T:142:ASP:O	6:T:144:ASN:N	2.50	0.45
9:W:155:ILE:CG2	9:W:156:SER:N	2.79	0.45
10:X:52:THR:HG22	10:X:53:VAL:HG23	1.98	0.45
10:X:138:LEU:HD21	10:X:158:CYS:SG	2.56	0.45
11:Y:191:ASP:OD2	11:Y:193:GLY:N	2.50	0.45
5:E:78:LEU:HD12	5:E:78:LEU:O	2.17	0.45
10:J:24:ILE:O	10:X:133:TYR:OH	2.34	0.45
11:K:143:LYS:HB2	11:K:146:LEU:HD11	1.96	0.45
13:M:40:ASN:ND2	13:M:40:ASN:N	2.56	0.45
2:P:184:MET:HE3	2:P:188:ASP:HB3	1.99	0.45
4:R:32:LYS:HG3	16:R:962:HOH:O	2.17	0.45
5:S:15:PHE:H	6:T:23:GLN:HE22	1.63	0.45
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.49	0.45
6:T:173:LYS:O	6:T:177:GLU:HG3	2.17	0.45
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.31	0.45
14:2:10(A):ASP:N	14:2:10(B):LYS:N	2.65	0.45
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.52	0.44
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.52	0.44
4:D:123:PHE:CZ	4:D:131:PRO:HG3	2.52	0.44
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.52	0.44
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.74	0.44
10:J:-1:MET:CG	10:J:1:ASP:H	2.14	0.44
12:L:9:GLU:O	12:L:107:LYS:HA	2.16	0.44
13:M:208:THR:HG22	8:V:77:VAL:HB	1.99	0.44
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.65	0.44
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.64	0.44
2:P:202:THR:HG21	2:P:204:SER:HB2	1.97	0.44
8:V:4:VAL:HG22	8:V:159:ILE:CD1	2.43	0.44
11:Y:143:LYS:HB2	11:Y:146:LEU:HD12	1.94	0.44
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.47	0.44
14:2:15:GLY:HA2	14:2:174:ARG:O	2.18	0.44
14:2:116:GLY:HA3	16:2:191:HOH:O	2.16	0.44
2:B:97:GLN:NE2	16:B:246:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:MET:HE3	2:B:188:ASP:HB3	1.99	0.44
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.75	0.44
3:C:46:VAL:HG22	3:C:146:PRO:HB2	1.98	0.44
6:F:119:TYR:O	6:F:122:ALA:HB3	2.17	0.44
13:M:133:MET:HE1	13:M:165:ARG:HG3	1.99	0.44
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.45	0.44
2:P:63:THR:O	2:P:63:THR:HG22	2.18	0.44
2:P:122:GLY:C	2:P:124:THR:H	2.25	0.44
3:Q:170:LYS:HB2	16:Q:833:HOH:O	2.16	0.44
5:S:78:LEU:HD12	5:S:78:LEU:C	2.42	0.44
9:W:6:MET:HE3	9:W:155:ILE:HA	1.97	0.44
9:W:93:GLY:N	9:W:94:PRO:CD	2.78	0.44
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.33	0.44
5:E:77:SER:OG	5:E:137:LEU:HB2	2.16	0.44
6:F:75:GLY:O	6:F:138:PHE:HA	2.17	0.44
6:F:210:LEU:HD21	6:F:212:ILE:HD11	2.00	0.44
7:G:232:ARG:HA	7:G:232:ARG:HE	1.82	0.44
11:K:174:ASN:HD21	11:K:189:ASN:HB2	1.81	0.44
13:M:148:VAL:HG23	16:M:502:HOH:O	2.16	0.44
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.99	0.44
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	2.00	0.44
10:X:166:MET:HE3	10:X:166:MET:HB3	1.72	0.44
1:A:207:ASN:HA	1:A:233:LEU:CD1	2.48	0.44
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.47	0.44
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.17	0.44
4:D:230:ALA:O	4:D:233:ILE:HB	2.18	0.44
7:G:48:VAL:HG23	7:G:48:VAL:O	2.17	0.44
7:G:172:ILE:CD1	7:G:197:MET:HE1	2.45	0.44
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	1.98	0.44
14:N:37:VAL:HG22	14:N:41:ILE:O	2.18	0.44
14:N:161:GLN:HE22	14:2:139:ASP:HB3	1.81	0.44
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.33	0.44
5:S:74:MET:HE2	5:S:109:VAL:HA	1.99	0.44
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.47	0.44
1:A:212:LEU:HD22	1:A:224:LEU:HD12	2.00	0.44
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.99	0.44
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.18	0.44
7:G:6:ALA:C	7:G:8:TYR:H	2.25	0.44
9:I:88:TYR:CE1	9:I:91:ARG:HD3	2.52	0.44
13:M:32:GLU:OE1	13:M:34:LEU:HB2	2.17	0.44
14:N:66:TYR:CE2	14:N:74:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:221:PHE:CD2	1:O:221:PHE:C	2.95	0.44
7:U:29:LYS:HD2	7:U:29:LYS:HA	1.72	0.44
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.17	0.44
9:W:6:MET:HG2	9:W:124:PHE:HB3	1.98	0.44
10:X:131:GLY:HA3	16:X:322:HOH:O	2.18	0.44
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	2.00	0.44
3:C:55:THR:C	3:C:56:LEU:HD22	2.43	0.44
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.99	0.44
7:G:151:THR:HG22	7:G:157:TYR:CB	2.48	0.44
9:I:6:MET:HE3	9:I:155:ILE:HA	1.97	0.44
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.48	0.44
10:J:85:GLN:O	10:J:89:LYS:HG3	2.17	0.44
10:J:144:PRO:CD	11:Y:207:ASN:HD21	2.28	0.44
12:L:3:ILE:HD13	12:L:100:ILE:HD13	1.94	0.44
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.33	0.44
2:P:101:LYS:HG3	9:W:57:GLU:HB3	2.00	0.44
4:R:46:VAL:HG11	4:R:139:ALA:HB1	2.00	0.44
5:S:161:TYR:OH	6:T:61:PRO:HD2	2.17	0.44
12:Z:114:ASP:HB3	12:Z:118:SER:H	1.82	0.44
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.32	0.44
6:F:90:ASN:O	6:F:94:GLU:HG3	2.18	0.44
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.99	0.44
9:I:155:ILE:CG2	9:I:156:SER:N	2.80	0.44
11:K:10(A):ARG:HB3	11:K:10(B):LYS:CE	2.47	0.44
7:U:39:ALA:HA	7:U:47:VAL:O	2.18	0.44
10:X:68:ILE:HG13	16:X:290:HOH:O	2.18	0.44
2:B:234:VAL:HG22	2:B:239:THR:HA	1.99	0.44
4:D:192:LEU:O	4:D:196:ILE:HG13	2.17	0.44
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.82	0.44
6:F:214:TRP:CH2	6:F:21(A):GLU:HB3	2.52	0.44
2:P:124:THR:HG22	3:Q:130:ARG:NH2	2.15	0.44
5:S:40:LEU:N	5:S:40:LEU:HD23	2.32	0.44
5:S:117:CYS:SG	6:T:86:ARG:HD3	2.58	0.44
5:S:214:ILE:HG12	5:S:215:VAL:N	2.32	0.44
6:T:127:ASN:HD22	6:T:127:ASN:N	2.14	0.44
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.75	0.44
9:W:1:GLY:HA3	9:W:33:LYS:HE2	2.00	0.44
10:X:175:VAL:HG21	10:X:190:PHE:CD2	2.53	0.44
2:B:63:THR:O	2:B:63:THR:HG22	2.17	0.44
2:B:183:ASP:O	2:B:184:MET:O	2.36	0.44
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:ASN:N	6:F:43:ASN:ND2	2.65	0.44
6:F:103:TYR:O	6:F:104:LYS:HB3	2.18	0.44
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.33	0.44
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.83	0.44
12:L:76:ILE:HG23	12:L:77:ASN:N	2.32	0.44
13:M:184:LEU:HD23	13:M:185:THR:N	2.32	0.44
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.52	0.44
6:T:43:ASN:N	6:T:43:ASN:ND2	2.65	0.44
6:T:103:TYR:O	6:T:104:LYS:HB3	2.17	0.44
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.81	0.44
12:Z:3:ILE:HD12	12:Z:3:ILE:O	2.17	0.44
13:1:149:GLN:H	13:1:149:GLN:HE21	1.62	0.44
2:B:122:GLY:C	2:B:124:THR:H	2.26	0.43
2:B:149:TYR:CE1	3:C:62(A):ILE:HD13	2.53	0.43
3:C:57:LYS:HD2	3:C:58:LEU:N	2.33	0.43
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.53	0.43
7:G:203:THR:HG22	7:G:204:GLU:O	2.18	0.43
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.47	0.43
9:I:55:LEU:HD23	9:I:55:LEU:HA	1.86	0.43
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.99	0.43
4:R:123:PHE:CZ	4:R:131:PRO:HG3	2.53	0.43
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.53	0.43
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.52	0.43
13:1:190:LEU:N	13:1:190:LEU:HD12	2.33	0.43
1:A:221:PHE:C	1:A:221:PHE:CD2	2.95	0.43
5:E:179:THR:HG22	5:E:179:THR:O	2.18	0.43
12:L:152:ILE:O	12:L:156:ARG:HG3	2.18	0.43
13:M:179:ASP:C	13:M:181:ASN:H	2.26	0.43
5:S:49:VAL:HG13	5:S:212:ILE:HG12	2.00	0.43
5:S:214:ILE:O	5:S:221:PHE:HA	2.18	0.43
11:Y:160:LEU:CD1	11:Y:192:VAL:HG13	2.48	0.43
4:D:201:MET:HE2	4:D:201:MET:HB3	1.90	0.43
5:E:40:LEU:N	5:E:40:LEU:HD23	2.33	0.43
9:I:28:SER:CB	10:J:120:VAL:HG21	2.48	0.43
12:L:5:GLY:HA2	12:L:13:VAL:O	2.18	0.43
1:O:39:GLY:HA2	1:O:47:VAL:O	2.18	0.43
16:S:656:HOH:O	6:T:12:ASN:HB2	2.18	0.43
7:U:48:VAL:O	7:U:48:VAL:HG23	2.17	0.43
8:V:214:LEU:HD11	9:W:190:LYS:HA	1.99	0.43
11:Y:65:LEU:O	11:Y:69:ARG:HB2	2.19	0.43
12:Z:5:GLY:HA2	12:Z:13:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:8:GLY:HA3	12:Z:11:PHE:CZ	2.53	0.43
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.53	0.43
13:1:133:MET:HE1	13:1:165:ARG:HG3	2.01	0.43
14:2:144:GLU:HG2	16:2:1115:HOH:O	2.17	0.43
1:A:39:GLY:HA2	1:A:47:VAL:O	2.18	0.43
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.48	0.43
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.54	0.43
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.53	0.43
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.19	0.43
3:Q:225:SER:O	3:Q:226:SER:C	2.62	0.43
5:S:162:GLY:O	5:S:163:THR:HB	2.17	0.43
13:1:179:ASP:C	13:1:181:ASN:H	2.27	0.43
2:B:121:GLN:NE2	2:B:121:GLN:C	2.77	0.43
3:C:85:SER:O	3:C:89:ILE:CD1	2.66	0.43
5:E:18(F):ILE:HB	5:E:189:LEU:HG	2.01	0.43
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.99	0.43
6:F:205:ASN:O	6:F:20(B):GLU:N	2.51	0.43
8:H:159:ILE:HG22	8:H:163:ILE:CD1	2.49	0.43
11:K:65:LEU:O	11:K:69:ARG:HB2	2.19	0.43
11:K:75:SER:HB2	11:K:106:GLU:OE2	2.18	0.43
3:Q:163:GLN:CA	3:Q:163:GLN:NE2	2.80	0.43
7:U:34(A):ASN:ND2	7:U:167:PRO:HG2	2.32	0.43
7:U:141:VAL:HG21	7:U:216:THR:HA	2.00	0.43
11:Y:40:PHE:CD2	11:Y:40:PHE:N	2.86	0.43
13:1:91:ARG:HG3	13:1:92:SER:N	2.33	0.43
2:B:13:THR:O	3:C:130:ARG:HD3	2.19	0.43
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.18	0.43
6:F:157:TYR:CD1	6:F:157:TYR:C	2.96	0.43
11:K:80:SER:HA	11:K:101:ILE:HD12	2.01	0.43
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.53	0.43
2:P:235:LYS:C	2:P:237:GLY:H	2.27	0.43
4:R:123:PHE:CE1	4:R:131:PRO:HG3	2.53	0.43
7:U:18(M):SER:HB2	7:U:187:GLU:OE2	2.17	0.43
9:W:14:ILE:HG22	9:W:176:TYR:HB2	2.00	0.43
10:X:17:SER:HB2	10:X:170:PHE:HB2	2.00	0.43
10:X:154:LEU:HD12	10:X:154:LEU:HA	1.85	0.43
13:1:186:PHE:HE1	13:1:188:LYS:HG3	1.84	0.43
2:B:207:TYR:CG	2:B:208:ASP:N	2.87	0.43
4:D:158:TYR:HB3	4:D:160:TYR:CE1	2.54	0.43
5:E:78:LEU:HD12	5:E:78:LEU:C	2.44	0.43
6:F:203:GLU:OE1	6:F:203:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:137:MET:SD	12:Z:136:PRO:HB2	2.59	0.43
12:L:114:ASP:HB3	12:L:118:SER:H	1.84	0.43
14:N:58:ILE:O	14:N:61:TYR:HB3	2.19	0.43
3:Q:173:ARG:HB2	3:Q:173:ARG:NH1	2.34	0.43
5:S:100:SER:O	5:S:104:ASN:N	2.46	0.43
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.01	0.43
13:1:82:TYR:O	13:1:85:THR:HB	2.18	0.43
2:B:81:LEU:HD23	2:B:133:GLY:HA3	2.00	0.43
7:G:198:ILE:O	7:G:202:GLY:N	2.52	0.43
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.39	0.43
3:Q:99:HIS:CG	3:Q:107:VAL:HG12	2.54	0.43
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.19	0.43
5:S:171:GLY:HA3	5:S:199:GLN:O	2.19	0.43
7:U:169:GLN:NE2	7:U:170:GLN:N	2.67	0.43
8:V:30:ASN:C	8:V:30:ASN:HD22	2.27	0.43
11:Y:1:THR:HG22	11:Y:2:THR:N	2.33	0.43
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.19	0.43
3:C:225:SER:O	3:C:226:SER:C	2.62	0.43
5:E:177:GLU:HA	6:F:58:LEU:HD21	2.00	0.43
8:H:1:THR:HG23	8:H:33:LYS:HD3	2.00	0.43
9:I:6:MET:HG2	9:I:124:PHE:HB3	2.00	0.43
11:K:25:TRP:CH2	12:L:132:SER:HA	2.53	0.43
11:K:160:LEU:CD1	11:K:192:VAL:HG13	2.49	0.43
14:N:115:LEU:HD12	14:N:115:LEU:HA	1.85	0.43
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	2.01	0.43
5:S:18(F):ILE:HB	5:S:189:LEU:HG	2.00	0.43
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.53	0.43
8:V:22:GLN:HG3	8:V:27:ALA:HB2	2.01	0.43
1:A:13:THR:HG22	1:A:21:LEU:HD22	2.00	0.43
1:A:49:ALA:HB2	1:A:212:LEU:HG	2.00	0.43
2:B:235:LYS:HD3	2:B:235:LYS:N	2.34	0.43
2:B:238:ILE:C	2:B:239:THR:O	2.62	0.43
3:C:159:SER:O	4:D:59:LEU:HD22	2.19	0.43
4:D:150:HIS:O	4:D:157:PHE:HA	2.18	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.48	0.43
11:K:208:ASN:ND2	11:K:209:VAL:H	2.15	0.43
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	2.01	0.43
2:P:5:SER:O	2:P:7:ARG:N	2.52	0.43
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	2.01	0.43
3:Q:154:SER:OG	3:Q:156:ILE:HG12	2.18	0.43
3:Q:18(B):ARG:HH22	4:R:59:LEU:C	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:158:TYR:HB3	4:R:160:TYR:CE1	2.54	0.43
4:R:230:ALA:O	4:R:233:ILE:HB	2.18	0.43
6:T:109:ILE:HB	6:T:110:PRO:HD3	2.00	0.43
7:U:203:THR:HG22	7:U:204:GLU:O	2.18	0.43
10:X:166:MET:HA	10:X:167:PRO:HD3	1.79	0.43
1:A:39:GLY:O	1:A:162:ALA:HA	2.19	0.42
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.54	0.42
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.59	0.42
4:D:123:PHE:CE1	4:D:131:PRO:HG3	2.54	0.42
5:E:5:ARG:HG3	5:E:22:PHE:CD1	2.54	0.42
6:F:186:ALA:HB3	16:F:698:HOH:O	2.17	0.42
7:G:55:PRO:HG2	7:G:56:ASP:H	1.84	0.42
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.00	0.42
8:H:75:ARG:HA	8:H:105:ASP:OD1	2.19	0.42
10:J:17:SER:HB2	10:J:170:PHE:HB2	2.01	0.42
11:K:41:LEU:HD23	11:K:41:LEU:HA	1.91	0.42
11:K:50:ALA:CB	12:L:116:VAL:HG23	2.48	0.42
2:P:184:MET:HE1	2:P:189:ALA:HA	2.00	0.42
5:S:79:ALA:HA	16:S:257:HOH:O	2.19	0.42
6:T:109:ILE:HG21	6:T:147:HIS:HB2	2.00	0.42
7:U:151:THR:HG22	7:U:157:TYR:CB	2.49	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.49	0.42
14:2:37:VAL:HG22	14:2:41:ILE:O	2.18	0.42
3:C:241:GLN:C	3:C:243:GLN:H	2.27	0.42
5:E:214:ILE:O	5:E:221:PHE:HA	2.18	0.42
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.37	0.42
12:L:25:SER:HB3	16:L:444:HOH:O	2.19	0.42
2:P:41:MET:HG3	2:P:46:ILE:HD13	2.02	0.42
3:Q:159:SER:O	4:R:59:LEU:HD22	2.19	0.42
4:R:117:CYS:HB3	4:R:155:GLY:O	2.19	0.42
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.55	0.42
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	2.01	0.42
11:Y:75:SER:HB2	11:Y:106:GLU:OE2	2.19	0.42
13:1:7:LYS:HB3	13:1:12:VAL:HG12	2.01	0.42
13:1:184:LEU:HD23	13:1:185:THR:N	2.34	0.42
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.50	0.42
3:C:46:VAL:O	3:C:215:VAL:HG12	2.20	0.42
5:E:125:GLN:HB3	16:E:1296:HOH:O	2.19	0.42
5:E:216:GLY:O	5:E:217:LYS:C	2.62	0.42
11:K:137:VAL:HG21	11:K:161:ALA:CB	2.49	0.42
13:M:115:LEU:HD23	13:M:115:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:28:LEU:HA	2:P:31:ILE:HG13	2.00	0.42
2:P:53:LYS:O	2:P:54:VAL:O	2.38	0.42
2:P:73:LYS:HE2	2:P:106:ASP:OD2	2.19	0.42
2:P:163:ILE:HG13	2:P:164:SER:N	2.34	0.42
3:Q:241:GLN:C	3:Q:243:GLN:H	2.28	0.42
6:T:214:TRP:CH2	6:T:21(A):GLU:HB3	2.54	0.42
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.49	0.42
7:U:191:GLU:CG	7:U:232:ARG:HG3	2.49	0.42
10:X:185:ARG:HG2	10:X:185:ARG:NH1	2.35	0.42
11:Y:4:LEU:HD13	11:Y:159:ILE:CD1	2.50	0.42
11:Y:9:GLN:NE2	11:Y:146:LEU:O	2.52	0.42
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.54	0.42
11:Y:38:ASN:C	11:Y:38:ASN:OD1	2.61	0.42
14:2:179:THR:HB	16:2:917:HOH:O	2.19	0.42
1:A:62:GLU:C	1:A:64:LEU:N	2.69	0.42
1:A:92:SER:O	1:A:95:VAL:HG12	2.19	0.42
2:B:28:LEU:HA	2:B:31:ILE:HG13	2.01	0.42
4:D:194:LEU:HD12	4:D:194:LEU:HA	1.86	0.42
7:G:228:ASN:HB3	16:G:255:HOH:O	2.18	0.42
8:H:83:LEU:HD13	8:H:113:ILE:HD12	2.02	0.42
10:J:68:ILE:HG13	16:J:810:HOH:O	2.18	0.42
11:K:40:PHE:CD2	11:K:40:PHE:N	2.87	0.42
13:M:-4:ILE:HG22	13:M:-3:VAL:HG23	2.01	0.42
13:M:7:LYS:HB3	13:M:12:VAL:HG12	2.01	0.42
13:M:17:ASP:OD2	13:M:17:ASP:C	2.63	0.42
2:P:6:ARG:HH11	2:P:6:ARG:HG3	1.83	0.42
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.19	0.42
2:P:121:GLN:NE2	2:P:121:GLN:C	2.78	0.42
4:R:238:LYS:HE2	4:R:238:LYS:HB3	1.81	0.42
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.54	0.42
6:T:127:ASN:HD22	6:T:127:ASN:C	2.27	0.42
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.34	0.42
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.49	0.42
12:Z:14(E):GLU:O	12:Z:14(F):PRO:C	2.62	0.42
1:A:35:VAL:HG11	1:A:51:GLU:HB3	2.01	0.42
2:B:27:ALA:O	2:B:30:SER:HB3	2.19	0.42
7:G:39:ALA:HA	7:G:47:VAL:O	2.19	0.42
9:I:1:GLY:HA3	9:I:33:LYS:HE2	2.00	0.42
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.54	0.42
11:K:140:SER:OG	10:X:141:HIS:HE1	2.02	0.42
12:L:179:THR:HG21	16:L:1161:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:171:SER:O	6:T:174:ALA:HB3	2.20	0.42
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.00	0.42
13:1:4:ILE:HG21	13:1:134:ALA:CB	2.49	0.42
14:2:58:ILE:O	14:2:61:TYR:HB3	2.18	0.42
2:B:101:LYS:NZ	10:J:85:GLN:HE22	2.16	0.42
2:B:238:ILE:O	2:B:238:ILE:HG22	2.19	0.42
5:E:98:TYR:CE1	5:E:102:VAL:HG21	2.55	0.42
5:E:171:GLY:HA3	5:E:199:GLN:O	2.19	0.42
5:E:179:THR:O	5:E:180:LEU:C	2.63	0.42
10:J:113:ILE:CG1	10:J:119:LYS:HG3	2.47	0.42
10:J:133:TYR:HE1	16:J:876:HOH:O	1.99	0.42
11:K:180:GLU:HB2	16:K:924:HOH:O	2.17	0.42
2:P:222:LYS:HZ1	2:P:228:GLU:CD	2.27	0.42
4:R:160:TYR:HA	5:S:59:SER:HA	2.01	0.42
6:T:202:HIS:O	6:T:202:HIS:CG	2.73	0.42
11:Y:143:LYS:HB2	11:Y:146:LEU:HD11	1.96	0.42
14:2:55:ILE:O	14:2:59:VAL:HG23	2.20	0.42
1:A:77:VAL:HG12	1:A:137:LEU:HB2	2.00	0.42
2:B:53:LYS:O	2:B:54:VAL:O	2.38	0.42
5:E:185:ASN:HA	5:E:186:PRO:HD2	1.94	0.42
6:F:11:SER:HB3	6:F:14:VAL:CG2	2.50	0.42
9:I:22:SER:O	9:I:23:GLN:HB2	2.20	0.42
9:I:74:ILE:HD11	9:I:78:THR:HG22	2.01	0.42
12:L:13:VAL:HG12	12:L:177:ILE:HG13	2.00	0.42
13:M:-4:ILE:HG22	13:M:-3:VAL:N	2.35	0.42
13:M:1:THR:OG1	13:M:2:SER:N	2.53	0.42
13:M:4:ILE:HG21	13:M:134:ALA:CB	2.49	0.42
13:M:147:THR:OG1	13:M:150:VAL:HG23	2.19	0.42
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.49	0.42
1:O:39:GLY:O	1:O:162:ALA:HA	2.19	0.42
2:P:81:LEU:HD23	2:P:133:GLY:HA3	2.00	0.42
2:P:229:ILE:O	2:P:233:LEU:HB2	2.19	0.42
3:Q:47:VAL:HG23	3:Q:189:CYS:SG	2.59	0.42
4:R:150:HIS:O	4:R:157:PHE:HA	2.19	0.42
5:S:116:LEU:HD23	5:S:116:LEU:HA	1.90	0.42
5:S:160:LEU:HD12	5:S:163:THR:HG21	2.01	0.42
7:U:96:ALA:HA	7:U:107:MET:CE	2.32	0.42
7:U:119:LEU:HD12	7:U:119:LEU:HA	1.85	0.42
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.50	0.42
9:W:7:THR:CG2	9:W:110:ILE:HG12	2.50	0.42
13:1:115:LEU:N	13:1:115:LEU:HD23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:HA	1:A:146:GLY:O	2.20	0.42
2:B:12:THR:HB	2:B:23:GLN:HG3	2.02	0.42
2:B:229:ILE:O	2:B:233:LEU:HB2	2.20	0.42
3:C:173:ARG:NH1	3:C:173:ARG:HB2	2.35	0.42
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.15	0.42
16:P:462:HOH:O	3:Q:87:ILE:HD11	2.20	0.42
7:U:25:GLU:O	7:U:28:PHE:HB2	2.20	0.42
7:U:186:TRP:CZ3	7:U:224:LEU:HD21	2.54	0.42
7:U:187:GLU:O	7:U:191:GLU:HG3	2.19	0.42
11:Y:104:TYR:CZ	11:Y:180:GLU:HB2	2.55	0.42
13:1:1:THR:O	13:1:46:SER:HB2	2.20	0.42
3:C:46:VAL:HG11	3:C:139:ALA:HB1	2.01	0.42
4:D:46:VAL:HG11	4:D:139:ALA:HB1	2.01	0.42
4:D:170:GLU:N	4:D:170:GLU:OE1	2.53	0.42
4:D:207:LEU:C	4:D:207:LEU:CD2	2.92	0.42
8:H:214:LEU:HD11	9:I:190:LYS:HA	2.02	0.42
10:J:2:ILE:O	10:J:3:ILE:HD13	2.19	0.42
10:J:77:GLN:NE2	10:J:77:GLN:C	2.78	0.42
10:J:168:MET:HE3	10:X:168:MET:HG2	2.01	0.42
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.54	0.42
2:P:5:SER:C	2:P:7:ARG:H	2.28	0.42
2:P:12:THR:HB	2:P:23:GLN:HG3	2.02	0.42
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.19	0.42
5:S:5:ARG:HG3	5:S:22:PHE:CD1	2.54	0.42
7:U:67:ILE:HD12	7:U:211:GLU:HG2	2.01	0.42
11:Y:7:ARG:HG3	11:Y:12:ILE:HG12	2.02	0.42
11:Y:100:MET:HE2	11:Y:100:MET:HB2	1.81	0.42
12:Z:90:LYS:HB3	12:Z:93:PHE:O	2.19	0.42
13:1:-4:ILE:HG22	13:1:-3:VAL:N	2.34	0.42
3:C:52:ARG:HD2	3:C:208:LYS:O	2.19	0.42
3:C:163:GLN:NE2	3:C:164:THR:H	2.17	0.42
6:F:142:ASP:O	6:F:144:ASN:N	2.53	0.42
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.76	0.42
10:J:168:MET:CE	10:X:168:MET:CE	2.85	0.42
14:N:15:GLY:HA2	14:N:174:ARG:O	2.20	0.42
3:Q:163:GLN:NE2	3:Q:164:THR:H	2.17	0.42
4:R:102:TYR:O	12:Z:81:ARG:HG3	2.19	0.42
4:R:170:GLU:OE1	4:R:170:GLU:N	2.53	0.42
6:T:157:TYR:CD1	6:T:157:TYR:C	2.97	0.42
11:Y:31:VAL:HG11	15:Y:300:EP9:C9	2.50	0.42
5:E:38:VAL:HG22	5:E:164:ALA:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:MET:HE2	5:E:109:VAL:HA	2.02	0.41
5:E:137:LEU:CD2	5:E:150:GLU:HG3	2.50	0.41
6:F:173:LYS:O	6:F:177:GLU:HG3	2.20	0.41
11:K:208:ASN:HD21	9:W:29:ASN:ND2	2.17	0.41
11:K:208:ASN:O	11:K:209:VAL:C	2.63	0.41
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.84	0.41
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.85	0.41
4:R:195:LYS:HE2	4:R:199:GLN:OE1	2.20	0.41
4:R:205:GLU:OE2	4:R:205:GLU:HA	2.20	0.41
5:S:137:LEU:CD2	5:S:150:GLU:HG3	2.50	0.41
8:V:128:GLY:O	8:V:131:SER:CB	2.68	0.41
1:A:130:ARG:HG2	7:G:125:GLN:HG3	2.03	0.41
4:D:215:ILE:C	4:D:215:ILE:HD13	2.45	0.41
5:E:49:VAL:HG13	5:E:212:ILE:HG12	2.00	0.41
6:F:127:ASN:HD22	6:F:127:ASN:C	2.28	0.41
6:F:127:ASN:ND2	6:F:127:ASN:H	2.19	0.41
7:G:141:VAL:HG21	7:G:216:THR:HA	2.01	0.41
8:H:192:LEU:HD23	8:H:192:LEU:HA	1.91	0.41
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.54	0.41
4:R:207:LEU:C	4:R:207:LEU:CD2	2.92	0.41
14:2:150:GLU:O	14:2:153:ASP:HB2	2.20	0.41
14:2:18(G):TYR:CD1	14:2:18(G):TYR:C	2.98	0.41
1:A:31:VAL:HG13	1:A:79:SER:O	2.20	0.41
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.55	0.41
4:D:97:VAL:HG11	11:K:65:LEU:HD22	2.02	0.41
5:E:141:TYR:CE1	5:E:145:GLY:HA2	2.56	0.41
10:J:20:VAL:HG11	11:K:120:LEU:HD11	2.01	0.41
10:J:138:LEU:HD21	10:J:158:CYS:SG	2.60	0.41
12:L:-2:ASN:HA	12:L:21:ILE:O	2.20	0.41
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.34	0.41
5:S:4:PHE:O	5:S:5:ARG:C	2.63	0.41
6:T:29:LYS:HD3	6:T:29:LYS:HA	1.92	0.41
6:T:204:ASP:OD1	6:T:204:ASP:N	2.52	0.41
8:V:143:LYS:HG2	8:V:146:LEU:HD21	2.01	0.41
1:A:26:TYR:CD1	1:A:26:TYR:N	2.85	0.41
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.19	0.41
4:D:117:CYS:HB3	4:D:155:GLY:O	2.21	0.41
4:D:195:LYS:HE2	4:D:199:GLN:OE1	2.20	0.41
6:F:204:ASP:OD1	6:F:204:ASP:N	2.54	0.41
8:H:135:MET:HE3	13:1:165:ARG:NH2	2.36	0.41
9:I:7:THR:CG2	9:I:110:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:14(E):GLU:O	12:L:14(F):PRO:C	2.64	0.41
13:M:26:LEU:HD12	14:2:164:LYS:O	2.21	0.41
14:N:114:PRO:HG2	16:N:194:HOH:O	2.21	0.41
1:O:26:TYR:N	1:O:26:TYR:CD1	2.86	0.41
4:R:148:LEU:HB3	4:R:160:TYR:O	2.20	0.41
5:S:76:LEU:O	5:S:76:LEU:HD23	2.19	0.41
7:U:18(H):GLU:CD	7:U:18(H):GLU:N	2.79	0.41
7:U:194:ILE:HG23	7:U:210:LEU:HD11	2.02	0.41
9:W:61:TYR:CD1	9:W:61:TYR:C	2.98	0.41
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.02	0.41
11:Y:10(A):ARG:HB3	11:Y:10(B):LYS:CE	2.48	0.41
12:Z:161:SER:O	12:Z:164:GLU:HB2	2.20	0.41
3:C:18(B):ARG:HH21	4:D:58:LEU:C	2.28	0.41
10:J:185:ARG:HG2	10:J:185:ARG:NH1	2.35	0.41
11:K:38:ASN:OD1	11:K:38:ASN:C	2.63	0.41
2:P:225:LYS:O	2:P:226:PRO:C	2.63	0.41
5:S:38:VAL:HG22	5:S:164:ALA:CB	2.50	0.41
5:S:229:VAL:O	5:S:230:ALA:C	2.62	0.41
6:T:75:GLY:O	6:T:138:PHE:HA	2.20	0.41
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.86	0.41
11:Y:152:LEU:HD11	11:Y:187:HIS:CE1	2.55	0.41
13:I:32:GLU:OE1	13:I:34:LEU:HB2	2.19	0.41
2:B:222:LYS:HZ1	2:B:228:GLU:CD	2.28	0.41
4:D:148:LEU:HB3	4:D:160:TYR:O	2.20	0.41
5:E:41:ARG:NH1	5:E:42:SER:O	2.54	0.41
8:H:24:PRO:HG2	8:H:25:ILE:CD1	2.49	0.41
9:I:14:ILE:HG22	9:I:176:TYR:HB2	2.02	0.41
10:J:175:VAL:HG21	10:J:190:PHE:CD2	2.55	0.41
11:K:4:LEU:HD13	11:K:159:ILE:CD1	2.50	0.41
4:R:177:LEU:HD13	5:S:58:LEU:HD11	2.02	0.41
5:S:45:HIS:HB2	5:S:189:LEU:HD12	2.02	0.41
10:X:113:ILE:CG1	10:X:119:LYS:HG3	2.45	0.41
11:Y:137:VAL:HG21	11:Y:161:ALA:CB	2.50	0.41
2:B:6:ARG:HG3	2:B:6:ARG:HH11	1.84	0.41
5:E:139:ILE:HG22	5:E:148:LEU:CD1	2.50	0.41
5:E:229:VAL:O	5:E:230:ALA:C	2.64	0.41
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.50	0.41
8:H:172:ASN:ND2	8:H:193:THR:HA	2.36	0.41
10:J:70:GLU:O	10:J:71:ASP:C	2.63	0.41
10:J:168:MET:HE2	10:X:167:PRO:C	2.45	0.41
11:K:104:TYR:CZ	11:K:180:GLU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:147:SER:C	11:K:149:GLU:N	2.77	0.41
1:O:35:VAL:HG11	1:O:51:GLU:HB3	2.01	0.41
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.21	0.41
1:O:207:ASN:HA	1:O:233:LEU:CD1	2.49	0.41
2:P:235:LYS:C	2:P:237:GLY:N	2.78	0.41
3:Q:11:ALA:HB3	4:R:12:VAL:HG11	2.01	0.41
4:R:121:LEU:HD13	5:S:130:ARG:NH2	2.33	0.41
5:S:13:VAL:CG2	6:T:129:VAL:C	2.93	0.41
5:S:216:GLY:O	5:S:217:LYS:C	2.63	0.41
6:T:127:ASN:C	6:T:127:ASN:ND2	2.79	0.41
6:T:162:GLY:O	7:U:58:LEU:HB3	2.21	0.41
7:U:118:ASN:HD22	7:U:118:ASN:HA	1.67	0.41
8:V:38:SER:HA	16:V:1269:HOH:O	2.20	0.41
10:X:70:GLU:O	10:X:71:ASP:C	2.64	0.41
10:X:85:GLN:HG2	10:X:89:LYS:HE3	2.02	0.41
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.21	0.41
13:1:40:ASN:ND2	13:1:40:ASN:N	2.57	0.41
2:B:5:SER:O	2:B:7:ARG:N	2.54	0.41
7:G:186:TRP:CZ3	7:G:224:LEU:HD21	2.54	0.41
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.55	0.41
14:N:26:ILE:HB	13:1:165:ARG:HA	2.03	0.41
1:O:11:SER:OG	2:P:129:LEU:HA	2.21	0.41
2:P:71:ASN:CG	2:P:72:ASP:H	2.27	0.41
2:P:73:LYS:O	2:P:140:GLY:HA2	2.21	0.41
3:Q:78:PHE:CD1	3:Q:78:PHE:C	2.99	0.41
3:Q:158:SER:CB	4:R:59:LEU:HD21	2.50	0.41
6:T:87:HIS:HD2	6:T:132:PHE:CE2	2.37	0.41
8:V:24:PRO:HG2	8:V:25:ILE:CD1	2.51	0.41
9:W:22:SER:O	9:W:23:GLN:HB2	2.21	0.41
12:Z:70(A):ASN:O	12:Z:72:LYS:N	2.54	0.41
13:1:205:GLY:HA3	16:1:367:HOH:O	2.20	0.41
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.69	0.41
1:A:233:LEU:O	1:A:236:LEU:HB2	2.20	0.41
2:B:73:LYS:HE2	2:B:106:ASP:OD2	2.20	0.41
2:B:126:HIS:HB3	3:C:129:VAL:HG12	2.02	0.41
2:B:225:LYS:O	2:B:226:PRO:C	2.61	0.41
2:B:235:LYS:C	2:B:237:GLY:N	2.79	0.41
3:C:14:ILE:HD13	3:C:14:ILE:N	2.36	0.41
4:D:24:VAL:O	4:D:28:LEU:HD13	2.21	0.41
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.86	0.41
4:D:238:LYS:HE2	4:D:238:LYS:HB3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:LEU:HD23	5:E:76:LEU:O	2.21	0.41
5:E:18(C):PHE:CD1	5:E:18(D):ILE:N	2.89	0.41
5:E:214:ILE:HG12	5:E:215:VAL:N	2.35	0.41
6:F:65:VAL:HG12	6:F:66:LYS:N	2.35	0.41
6:F:114:ASP:O	6:F:118:GLN:HG2	2.21	0.41
6:F:214:TRP:CD1	6:F:214:TRP:N	2.89	0.41
9:I:171:TRP:HH2	11:Y:165:ARG:NH1	2.19	0.41
10:J:34:THR:CG2	10:J:176:LYS:NZ	2.83	0.41
10:J:110:LEU:O	10:J:121:GLU:HG2	2.21	0.41
10:J:157:LEU:HD12	10:J:157:LEU:HA	1.93	0.41
13:M:82:TYR:O	13:M:85:THR:HB	2.20	0.41
1:O:97:HIS:HD2	8:V:61:SER:OG	2.04	0.41
2:P:207:TYR:CG	2:P:208:ASP:N	2.89	0.41
2:P:238:ILE:O	2:P:238:ILE:HG22	2.20	0.41
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.84	0.41
5:S:48:LEU:HG	5:S:139:ILE:HD13	2.02	0.41
5:S:139:ILE:HG22	5:S:148:LEU:CD1	2.49	0.41
6:T:119:TYR:O	6:T:122:ALA:HB3	2.21	0.41
7:U:100:ARG:HH11	7:U:100:ARG:HG3	1.85	0.41
8:V:1:THR:HG23	8:V:33:LYS:HD3	2.03	0.41
8:V:83:LEU:HD13	8:V:113:ILE:HD12	2.03	0.41
9:W:110:ILE:CD1	9:W:125:ILE:HG12	2.51	0.41
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.56	0.41
13:1:-6:GLN:O	13:1:-4:ILE:HD12	2.21	0.41
13:1:19:LEU:HD21	13:1:26:LEU:HD22	2.03	0.41
1:A:236:LEU:C	1:A:236:LEU:HD13	2.46	0.41
2:B:235:LYS:C	2:B:237:GLY:H	2.29	0.41
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	2.13	0.41
6:F:15:PHE:HB2	7:G:23:GLN:OE1	2.20	0.41
6:F:93:ARG:CD	16:F:842:HOH:O	2.69	0.41
6:F:202:HIS:O	6:F:202:HIS:CG	2.74	0.41
9:I:171:TRP:HH2	11:Y:165:ARG:HH11	1.68	0.41
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.75	0.41
12:L:90:LYS:HB3	12:L:93:PHE:O	2.21	0.41
12:L:148:VAL:O	12:L:152:ILE:HG13	2.21	0.41
13:M:-5:PRO:C	13:M:-4:ILE:HD12	2.46	0.41
1:O:195:LEU:HD23	1:O:236:LEU:HD21	2.03	0.41
2:P:40:ILE:HD12	2:P:193:ALA:HB2	2.03	0.41
4:R:194:LEU:HD22	4:R:212:LEU:HD11	2.03	0.41
6:T:11:SER:HB3	6:T:14:VAL:CG2	2.51	0.41
6:T:114:ASP:O	6:T:118:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:158:VAL:CG2	7:U:159:GLY:N	2.84	0.41
9:W:88:TYR:CE1	9:W:91:ARG:HD3	2.56	0.41
6:F:176:LEU:O	6:F:180:VAL:HG23	2.20	0.40
7:G:158:VAL:CG2	7:G:159:GLY:N	2.83	0.40
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.21	0.40
9:I:160:LEU:HD12	9:I:160:LEU:HA	1.95	0.40
10:J:45:PHE:HB3	10:J:99:VAL:HG12	2.02	0.40
10:J:90(A):ILE:HG12	10:J:116:LEU:HD23	2.03	0.40
11:K:200:LYS:HE3	11:K:206:PHE:O	2.20	0.40
14:N:12:VAL:HG22	14:N:13:ILE:N	2.36	0.40
14:N:24:ALA:HB3	13:1:129:PHE:HE2	1.86	0.40
14:N:30:VAL:HG11	13:1:199:PHE:CE2	2.56	0.40
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	2.02	0.40
7:U:55:PRO:HG2	7:U:56:ASP:H	1.85	0.40
12:Z:70:HIS:O	12:Z:70(A):ASN:C	2.65	0.40
13:1:-5:PRO:C	13:1:-4:ILE:HD12	2.46	0.40
2:B:5:SER:C	2:B:7:ARG:H	2.29	0.40
2:B:20:ARG:HG2	2:B:20:ARG:HH11	1.85	0.40
2:B:160:TRP:CZ3	3:C:59:GLN:HG2	2.57	0.40
4:D:156:THR:HG22	5:E:83:PRO:HD3	2.03	0.40
6:F:172:ALA:O	6:F:176:LEU:HD23	2.19	0.40
7:G:169:GLN:HE21	7:G:169:GLN:HB3	1.66	0.40
7:G:191:GLU:CG	7:G:232:ARG:HG3	2.51	0.40
8:H:160:GLN:O	8:H:161:ALA:C	2.64	0.40
11:K:112:TYR:O	11:K:119:ARG:HA	2.22	0.40
4:R:160:TYR:HA	5:S:58:LEU:O	2.20	0.40
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.56	0.40
4:R:207:LEU:HD21	4:R:233:ILE:CD1	2.51	0.40
10:X:-1:MET:CG	10:X:1:ASP:H	2.15	0.40
10:X:143:ARG:HA	10:X:144:PRO:HD3	1.90	0.40
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.21	0.40
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.50	0.40
2:B:171:ALA:O	2:B:175:LEU:HG	2.21	0.40
4:D:12(D):ALA:HB3	4:D:126:ARG:HG3	2.04	0.40
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.57	0.40
6:F:195:LYS:O	6:F:199:LEU:HD13	2.22	0.40
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.56	0.40
10:J:59:ILE:HD13	10:J:59:ILE:HA	1.96	0.40
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.46	0.40
14:N:18(G):TYR:C	14:N:18(G):TYR:CD1	2.99	0.40
4:R:65:GLU:HA	16:R:750:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:18:ASP:OD2	6:T:18:ASP:N	2.51	0.40
10:X:34:THR:CG2	10:X:176:LYS:NZ	2.84	0.40
4:D:207:LEU:HD21	4:D:233:ILE:CD1	2.51	0.40
5:E:36:VAL:HG22	5:E:37:THR:N	2.35	0.40
5:E:105:ARG:HB2	13:M:78:TYR:CE1	2.56	0.40
7:G:229:ILE:O	7:G:232:ARG:N	2.55	0.40
10:J:85:GLN:HG2	10:J:89:LYS:HE3	2.03	0.40
10:J:156:LYS:HE2	10:J:160:GLN:HE22	1.77	0.40
11:K:5:ALA:HA	11:K:13:ILE:O	2.21	0.40
11:K:53:GLN:HE21	12:L:84:GLN:NE2	2.19	0.40
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.34	0.40
14:N:13:ILE:HD12	14:N:151:THR:HG22	2.02	0.40
1:O:36:THR:HG22	1:O:37:SER:N	2.36	0.40
1:O:233:LEU:O	1:O:236:LEU:HB2	2.20	0.40
5:S:17:PRO:HA	6:T:26:TYR:CD2	2.57	0.40
7:U:16:SER:HA	16:U:584:HOH:O	2.21	0.40
8:V:62:ASN:HB3	8:V:82:MET:HE1	2.03	0.40
8:V:112:SER:HG	8:V:120:ASP:HB2	1.85	0.40
12:Z:148:VAL:O	12:Z:152:ILE:HG13	2.21	0.40
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.85	0.40
13:1:162:LEU:O	13:1:163:TYR:CA	2.69	0.40
1:A:232:ARG:NH1	1:A:232:ARG:CG	2.84	0.40
3:C:232:TYR:O	3:C:236:ILE:HG13	2.20	0.40
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.36	0.40
9:I:2:ILE:HD11	9:I:163:ALA:HB2	2.03	0.40
11:K:9:GLN:NE2	11:K:146:LEU:O	2.55	0.40
11:K:67:GLU:HG2	11:K:73:ARG:HA	2.04	0.40
11:K:152:LEU:HD11	11:K:187:HIS:CE1	2.57	0.40
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.52	0.40
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.57	0.40
1:O:236:LEU:HD13	1:O:236:LEU:C	2.46	0.40
6:T:212:ILE:HG22	6:T:213:SER:N	2.37	0.40
9:W:2:ILE:HD11	9:W:163:ALA:HB2	2.04	0.40
10:X:54:GLN:NE2	16:X:874:HOH:O	2.52	0.40
13:1:70:ASN:ND2	13:1:70(A):ALA:HA	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	228 (92%)	16 (6%)	4 (2%)	7	20
1	O	248/250 (99%)	228 (92%)	16 (6%)	4 (2%)	7	20
2	B	242/244 (99%)	217 (90%)	19 (8%)	6 (2%)	4	11
2	P	242/244 (99%)	219 (90%)	17 (7%)	6 (2%)	4	11
3	C	239/241 (99%)	219 (92%)	15 (6%)	5 (2%)	5	15
3	Q	239/241 (99%)	220 (92%)	15 (6%)	4 (2%)	7	19
4	D	240/242 (99%)	220 (92%)	13 (5%)	7 (3%)	3	9
4	R	240/242 (99%)	219 (91%)	14 (6%)	7 (3%)	3	9
5	E	231/233 (99%)	203 (88%)	21 (9%)	7 (3%)	3	8
5	S	231/233 (99%)	201 (87%)	23 (10%)	7 (3%)	3	8
6	F	242/244 (99%)	222 (92%)	16 (7%)	4 (2%)	7	19
6	T	242/244 (99%)	222 (92%)	16 (7%)	4 (2%)	7	19
7	G	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	16	37
7	U	241/243 (99%)	228 (95%)	10 (4%)	3 (1%)	10	27
8	H	220/222 (99%)	206 (94%)	12 (6%)	2 (1%)	14	35
8	V	220/222 (99%)	206 (94%)	11 (5%)	3 (1%)	9	23
9	I	202/204 (99%)	191 (95%)	10 (5%)	1 (0%)	24	48
9	W	202/204 (99%)	190 (94%)	11 (5%)	1 (0%)	24	48
10	J	196/198 (99%)	183 (93%)	11 (6%)	2 (1%)	12	32
10	X	196/198 (99%)	184 (94%)	10 (5%)	2 (1%)	12	32
11	K	210/212 (99%)	196 (93%)	13 (6%)	1 (0%)	24	48
11	Y	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	12	32
12	L	220/222 (99%)	205 (93%)	13 (6%)	2 (1%)	14	35
12	Z	207/222 (93%)	195 (94%)	10 (5%)	2 (1%)	12	32
13	1	212/233 (91%)	197 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	213 (92%)	17 (7%)	1 (0%)	30	54
14	2	183/196 (93%)	171 (93%)	12 (7%)	0	100	100
14	N	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
All	All	6269/6368 (98%)	5788 (92%)	392 (6%)	89 (1%)	9	23

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
2	B	184	MET
2	B	21(C)	ASP
3	C	58	LEU
4	D	12(G)	GLU
5	E	5	ARG
5	E	202	ARG
5	E	217	LYS
10	J	192	ALA
2	P	184	MET
2	P	21(C)	ASP
3	Q	58	LEU
4	R	61	SER
4	R	12(G)	GLU
5	S	5	ARG
5	S	202	ARG
5	S	217	LYS
10	X	192	ALA
12	Z	71	ASP
1	A	63	THR
1	A	167	LYS
2	B	21(B)	GLY
3	C	183	PRO
3	C	203	THR
4	D	61	SER
4	D	18(D)	SER
4	D	209	GLU
6	F	64	ASN
6	F	143	LYS
6	F	206	LYS
8	H	9	ASN
11	K	209	VAL
12	L	71	ASP

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Mol	Chain	Res	Type
13	M	96	TRP
1	O	63	THR
1	O	167	LYS
2	P	54	VAL
2	P	21(B)	GLY
3	Q	183	PRO
3	Q	203	THR
4	R	18(D)	SER
4	R	209	GLU
6	T	64	ASN
6	T	143	LYS
6	T	206	LYS
8	V	9	ASN
11	Y	209	VAL
1	A	5	THR
4	D	12(C)	GLY
4	D	12(F)	GLY
5	E	64	GLN
7	G	239	GLN
9	I	93	GLY
10	J	8	VAL
1	O	5	THR
2	P	6	ARG
4	R	12(C)	GLY
4	R	12(F)	GLY
5	S	64	GLN
7	U	239	GLN
8	V	96	GLY
9	W	93	GLY
2	B	6	ARG
2	B	143	ASP
4	D	12(E)	SER
5	E	231	LYS
6	F	205	ASN
8	H	96	GLY
4	R	12(E)	SER
5	S	180	LEU
6	T	205	ASN
10	X	8	VAL
5	E	180	LEU
7	G	7	GLY
2	P	143	ASP

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Mol	Chain	Res	Type
3	Q	184	ALA
5	S	231	LYS
3	C	184	ALA
3	C	202	GLN
5	E	18(F)	ILE
5	S	18(F)	ILE
7	U	7	GLY
7	U	184	ASN
12	Z	93	PHE
12	L	93	PHE
1	O	56	SER
1	A	56	SER
8	V	10(A)	PRO
11	Y	39	PRO

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%)	192 (95%)	11 (5%)	20	45
2	P	203/203 (100%)	194 (96%)	9 (4%)	25	53
3	C	213/213 (100%)	203 (95%)	10 (5%)	23	51
3	Q	213/213 (100%)	202 (95%)	11 (5%)	21	47
4	D	198/198 (100%)	185 (93%)	13 (7%)	15	36
4	R	198/198 (100%)	185 (93%)	13 (7%)	15	36
5	E	192/192 (100%)	180 (94%)	12 (6%)	16	39
5	S	192/192 (100%)	181 (94%)	11 (6%)	18	43
6	F	201/201 (100%)	186 (92%)	15 (8%)	12	31
6	T	201/201 (100%)	187 (93%)	14 (7%)	14	34
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%)	174 (96%)	7 (4%)	28	57
8	V	181/181 (100%)	174 (96%)	7 (4%)	28	57
9	I	172/172 (100%)	162 (94%)	10 (6%)	18	42
9	W	172/172 (100%)	162 (94%)	10 (6%)	18	42
10	J	175/175 (100%)	165 (94%)	10 (6%)	18	43
10	X	175/175 (100%)	165 (94%)	10 (6%)	18	43
11	K	169/169 (100%)	157 (93%)	12 (7%)	13	33
11	Y	169/169 (100%)	158 (94%)	11 (6%)	15	37
12	L	185/185 (100%)	163 (88%)	22 (12%)	5	13
12	Z	171/185 (92%)	152 (89%)	19 (11%)	6	15
13	1	193/199 (97%)	181 (94%)	12 (6%)	16	39
13	M	199/199 (100%)	186 (94%)	13 (6%)	15	37
14	2	152/162 (94%)	146 (96%)	6 (4%)	28	57
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	59
All	All	5302/5332 (99%)	4996 (94%)	306 (6%)	18	42

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
2	B	6	ARG
2	B	31	ILE
2	B	46	ILE
2	B	58	LEU
2	B	116	LEU
2	B	121	GLN
2	B	124	THR
2	B	150	THR
2	B	192	LEU
2	B	216	ARG

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Mol	Chain	Res	Type
2	B	224	PHE
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU
3	C	57	LYS
3	C	14(A)	ARG
3	C	14(B)	ASP
3	C	150	GLN
3	C	163	GLN
3	C	172	VAL
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	184	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	123	ASN
5	E	198	SER
5	E	199	GLN
5	E	207	LEU
5	E	222	THR
5	E	227	GLU
6	F	11	SER
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	72	ARG
6	F	98	SER

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Mol	Chain	Res	Type
6	F	121	GLN
6	F	127	ASN
6	F	135	SER
6	F	169	ARG
6	F	171	SER
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
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	34	LEU
8	H	56	THR
8	H	99	LEU
8	H	152	ILE
8	H	163	ILE
8	H	180	ILE
8	H	197	ARG
9	I	20	LEU
9	I	29	ASN
9	I	45	ILE
9	I	110	ILE
9	I	113	PHE
9	I	148	PRO
9	I	159	LEU
9	I	160	LEU
9	I	171	TRP
9	I	174	VAL
10	J	24	ILE
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	121	GLU
10	J	122	LEU

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Mol	Chain	Res	Type
10	J	137	LEU
10	J	168	MET
10	J	177	ILE
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	39	PRO
11	K	41	LEU
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	99	THR
11	K	100	MET
11	K	101	ILE
11	K	210	ILE
12	L	-9	GLN
12	L	-7	ASN
12	L	14	LEU
12	L	40	ASN
12	L	43	MET
12	L	58	ARG
12	L	99	THR
12	L	138	LEU
12	L	14(A)	LYS
12	L	14(B)	ASN
12	L	14(C)	GLN
12	L	14(D)	TYR
12	L	14(E)	GLU
12	L	14(F)	PRO
12	L	14(I)	THR
12	L	14(K)	LYS
12	L	14(M)	VAL
12	L	14(N)	LYS
12	L	14(O)	LYS
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS
13	M	4	ILE
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU
13	M	71(A)	ASP

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Mol	Chain	Res	Type
13	M	71(B)	GLU
13	M	71(C)	GLU
13	M	91	ARG
13	M	129	PHE
13	M	149	GLN
13	M	184	LEU
13	M	191	GLN
13	M	204	LYS
14	N	84	LYS
14	N	89	GLU
14	N	115	LEU
14	N	119	VAL
14	N	144	GLU
14	N	149	GLU
1	O	32	LYS
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
2	P	6	ARG
2	P	31	ILE
2	P	46	ILE
2	P	58	LEU
2	P	116	LEU
2	P	124	THR
2	P	150	THR
2	P	192	LEU
2	P	224	PHE
3	Q	10	ARG
3	Q	14	ILE
3	Q	25	GLU
3	Q	57	LYS
3	Q	14(A)	ARG
3	Q	14(B)	ASP
3	Q	150	GLN
3	Q	163	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	227	GLU
4	R	28	LEU

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Mol	Chain	Res	Type
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	177	LEU
4	R	184	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	12	THR
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	123	ASN
5	S	198	SER
5	S	207	LEU
5	S	222	THR
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	36	THR
6	T	43	ASN
6	T	72	ARG
6	T	98	SER
6	T	121	GLN
6	T	127	ASN
6	T	135	SER
6	T	169	ARG
6	T	171	SER
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	169	GLN

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Mol	Chain	Res	Type
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	34	LEU
8	V	56	THR
8	V	99	LEU
8	V	152	ILE
8	V	163	ILE
8	V	180	ILE
8	V	197	ARG
9	W	20	LEU
9	W	29	ASN
9	W	45	ILE
9	W	110	ILE
9	W	113	PHE
9	W	148	PRO
9	W	159	LEU
9	W	160	LEU
9	W	171	TRP
9	W	174	VAL
10	X	24	ILE
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	121	GLU
10	X	122	LEU
10	X	137	LEU
10	X	168	MET
10	X	177	ILE
11	Y	4	LEU
11	Y	7	ARG
11	Y	9	GLN
11	Y	39	PRO
11	Y	41	LEU
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	99	THR
11	Y	100	MET
11	Y	101	ILE

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Mol	Chain	Res	Type
12	Z	-9	GLN
12	Z	14	LEU
12	Z	40	ASN
12	Z	43	MET
12	Z	58	ARG
12	Z	99	THR
12	Z	138	LEU
12	Z	14(A)	LYS
12	Z	14(C)	GLN
12	Z	14(D)	TYR
12	Z	14(E)	GLU
12	Z	14(F)	PRO
12	Z	14(I)	THR
12	Z	14(K)	LYS
12	Z	14(M)	VAL
12	Z	14(N)	LYS
12	Z	14(O)	LYS
12	Z	14(P)	PRO
12	Z	14(Q)	LEU
13	1	4	ILE
13	1	40	ASN
13	1	62	LEU
13	1	65	GLU
13	1	71(A)	ASP
13	1	71(B)	GLU
13	1	91	ARG
13	1	129	PHE
13	1	149	GLN
13	1	184	LEU
13	1	191	GLN
13	1	204	LYS
14	2	84	LYS
14	2	89	GLU
14	2	115	LEU
14	2	119	VAL
14	2	144	GLU
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (226) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN

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Mol	Chain	Res	Type
1	A	97	HIS
1	A	145	ASN
2	B	23	GLN
2	B	71	ASN
2	B	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	211	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	95	GLN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	152	GLN
5	E	170	GLN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	87	HIS

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Mol	Chain	Res	Type
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
6	F	221	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
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	208	ASN
7	G	228	ASN
8	H	10	ASN
8	H	30	ASN
8	H	35	HIS
8	H	66	HIS
8	H	144	GLN
8	H	172	ASN
8	H	190	ASN
8	H	201	GLN
9	I	29	ASN
9	I	56	ASN
9	I	64	ASN
9	I	81	GLN
9	I	145	ASN
9	I	193	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	160	GLN
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	53	GLN
11	K	85	ASN
11	K	141	ASN
11	K	174	ASN
11	K	187	HIS
11	K	207	ASN
11	K	208	ASN
12	L	-7	ASN
12	L	27	ASN
12	L	40	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	14(B)	ASN
12	L	1(I)	ASN
12	L	166	HIS
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	54	HIS
13	M	89	GLN
13	M	93	ASN
13	M	132	HIS
13	M	149	GLN
13	M	157	ASN
13	M	189	ASN
13	M	191	GLN
14	N	38	HIS
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	145	ASN
2	P	23	GLN
2	P	71	ASN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN

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Mol	Chain	Res	Type
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
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	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	95	GLN
5	S	104	ASN
5	S	114	HIS
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	152	GLN
5	S	156	ASN
5	S	170	GLN
5	S	185	ASN
5	S	199	GLN
6	T	23	GLN
6	T	43	ASN
6	T	62	GLN
6	T	87	HIS
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
7	U	32	ASN
7	U	34(A)	ASN
7	U	87	ASN

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Mol	Chain	Res	Type
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	35	HIS
8	V	66	HIS
8	V	144	GLN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	56	ASN
9	W	64	ASN
9	W	81	GLN
9	W	145	ASN
9	W	193	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
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	141	ASN
11	Y	174	ASN
11	Y	187	HIS
11	Y	207	ASN
11	Y	208	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	70(A)	ASN

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Mol	Chain	Res	Type
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	40	ASN
13	1	54	HIS
13	1	93	ASN
13	1	132	HIS
13	1	149	GLN
13	1	157	ASN
13	1	189	ASN
13	1	191	GLN
14	2	141	ASN
14	2	145	ASN
14	2	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	EP9	K	300	11	39,40,41	3.84	26 (66%)	51,53,54	2.36	13 (25%)
15	EP9	Y	300	11	39,40,41	4.03	24 (61%)	51,53,54	2.09	11 (21%)

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	EP9	K	300	11	1/1/9/13	18/41/41/43	0/2/2/2
15	EP9	Y	300	11	1/1/9/13	21/41/41/43	0/2/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	300	EP9	O5-C15	10.89	1.41	1.21
15	K	300	EP9	C19-C18	9.54	1.55	1.38
15	K	300	EP9	O5-C15	8.53	1.37	1.21
15	Y	300	EP9	C19-C18	8.26	1.53	1.38
15	Y	300	EP9	O4-C15	7.73	1.50	1.35
15	Y	300	EP9	C7-C6	6.67	1.49	1.38
15	K	300	EP9	O4-C15	6.63	1.48	1.35
15	K	300	EP9	C7-C8	5.83	1.49	1.39
15	Y	300	EP9	C21-C22	5.49	1.48	1.38
15	K	300	EP9	C21-C22	5.32	1.48	1.38
15	Y	300	EP9	C16-C17	5.29	1.63	1.50
15	K	300	EP9	C7-C6	5.15	1.47	1.38
15	K	300	EP9	C20-C19	4.79	1.48	1.38
15	K	300	EP9	C21-C20	4.73	1.48	1.38
15	Y	300	EP9	C22-C17	4.71	1.48	1.38
15	Y	300	EP9	O7-C11	4.70	1.32	1.23
15	K	300	EP9	O6-C13	4.69	1.32	1.23
15	K	300	EP9	C18-C17	4.51	1.47	1.38
15	Y	300	EP9	C20-C19	4.48	1.48	1.38
15	K	300	EP9	C10-C5	4.36	1.47	1.38
15	Y	300	EP9	C3-N1	4.34	1.53	1.46
15	Y	300	EP9	O3-C8	4.33	1.46	1.37
15	Y	300	EP9	O6-C13	4.24	1.31	1.23
15	K	300	EP9	C3-N1	4.24	1.53	1.46
15	Y	300	EP9	C15-N3	4.17	1.45	1.34
15	Y	300	EP9	C21-C20	4.12	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	300	EP9	C22-C17	4.08	1.47	1.38
15	Y	300	EP9	C4-C5	4.08	1.61	1.51
15	K	300	EP9	C16-C17	3.89	1.59	1.50
15	Y	300	EP9	C4-C3	3.83	1.61	1.53
15	K	300	EP9	O3-C8	3.78	1.45	1.37
15	Y	300	EP9	O1-C1	3.59	1.52	1.43
15	K	300	EP9	C4-C3	3.54	1.60	1.53
15	Y	300	EP9	C6-C5	3.53	1.45	1.38
15	K	300	EP9	O7-C11	3.46	1.30	1.23
15	K	300	EP9	O4-C16	3.36	1.52	1.45
15	Y	300	EP9	C7-C8	3.23	1.45	1.39
15	K	300	EP9	C6-C5	3.20	1.45	1.38
15	Y	300	EP9	C10-C5	3.15	1.45	1.38
15	K	300	EP9	C4-C5	3.12	1.58	1.51
15	K	300	EP9	C14-C13	3.06	1.60	1.52
15	Y	300	EP9	C30-C28	2.69	1.65	1.51
15	Y	300	EP9	C18-C17	2.61	1.44	1.38
15	Y	300	EP9	C27-C12	2.59	1.61	1.53
15	K	300	EP9	C9-C8	2.53	1.43	1.39
15	Y	300	EP9	C12-C11	2.48	1.59	1.52
15	K	300	EP9	C27-C12	2.26	1.60	1.53
15	K	300	EP9	C10-C9	2.21	1.42	1.38
15	K	300	EP9	C30-C28	2.19	1.63	1.51
15	K	300	EP9	C27-C28	2.03	1.61	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	300	EP9	O4-C15-N3	8.98	129.65	110.45
15	Y	300	EP9	O4-C15-N3	7.47	126.43	110.45
15	K	300	EP9	O4-C15-O5	-6.34	112.09	124.26
15	Y	300	EP9	O4-C15-O5	-5.82	113.11	124.26
15	K	300	EP9	O5-C15-N3	-5.65	115.61	124.86
15	Y	300	EP9	O5-C15-N3	-5.30	116.17	124.86
15	K	300	EP9	C27-C12-N2	-5.20	98.84	110.58
15	K	300	EP9	C4-C3-N1	-4.95	103.05	110.08
15	Y	300	EP9	C27-C12-N2	-4.48	100.46	110.58
15	Y	300	EP9	C16-O4-C15	3.31	123.39	115.93
15	Y	300	EP9	C14-N3-C15	-3.25	112.84	120.93
15	Y	300	EP9	C11-C12-N2	-3.14	102.62	111.11
15	K	300	EP9	C14-N3-C15	-3.03	113.40	120.93
15	K	300	EP9	C11-C12-N2	-2.83	103.45	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	300	EP9	O6-C13-C14	-2.69	114.84	120.48
15	Y	300	EP9	C4-C3-N1	-2.67	106.30	110.08
15	K	300	EP9	O6-C13-C14	-2.43	115.40	120.48
15	K	300	EP9	C24-C23-C14	-2.42	108.90	115.40
15	Y	300	EP9	C24-C23-C14	-2.37	109.04	115.40
15	K	300	EP9	O6-C13-N2	-2.34	118.77	122.96
15	K	300	EP9	C16-C17-C18	2.17	125.65	120.64
15	K	300	EP9	O7-C11-C12	-2.16	115.94	120.48
15	Y	300	EP9	C13-C14-N3	-2.05	105.57	111.11
15	K	300	EP9	C12-C11-N1	2.02	120.94	116.63

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	K	300	EP9	C1
15	Y	300	EP9	C1

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	K	300	EP9	C1-C3-N1-C11
15	K	300	EP9	C4-C3-N1-C11
15	Y	300	EP9	O1-C1-C3-C4
15	Y	300	EP9	C1-C3-N1-C11
15	Y	300	EP9	C4-C3-N1-C11
15	Y	300	EP9	O5-C15-O4-C16
15	Y	300	EP9	O5-C15-N3-C14
15	K	300	EP9	O5-C15-O4-C16
15	K	300	EP9	C11-C12-C27-C28
15	Y	300	EP9	C11-C12-C27-C28
15	K	300	EP9	C3-C4-C5-C10
15	K	300	EP9	C12-C11-N1-C3
15	K	300	EP9	C14-C23-C24-C25
15	K	300	EP9	C14-C23-C24-C26
15	Y	300	EP9	C14-C23-C24-C26
15	Y	300	EP9	C3-C4-C5-C6
15	Y	300	EP9	C3-C4-C5-C10
15	K	300	EP9	O1-C1-C3-N1
15	Y	300	EP9	O1-C1-C3-N1
15	Y	300	EP9	C14-C23-C24-C25
15	K	300	EP9	C3-C4-C5-C6
15	K	300	EP9	O5-C15-N3-C14

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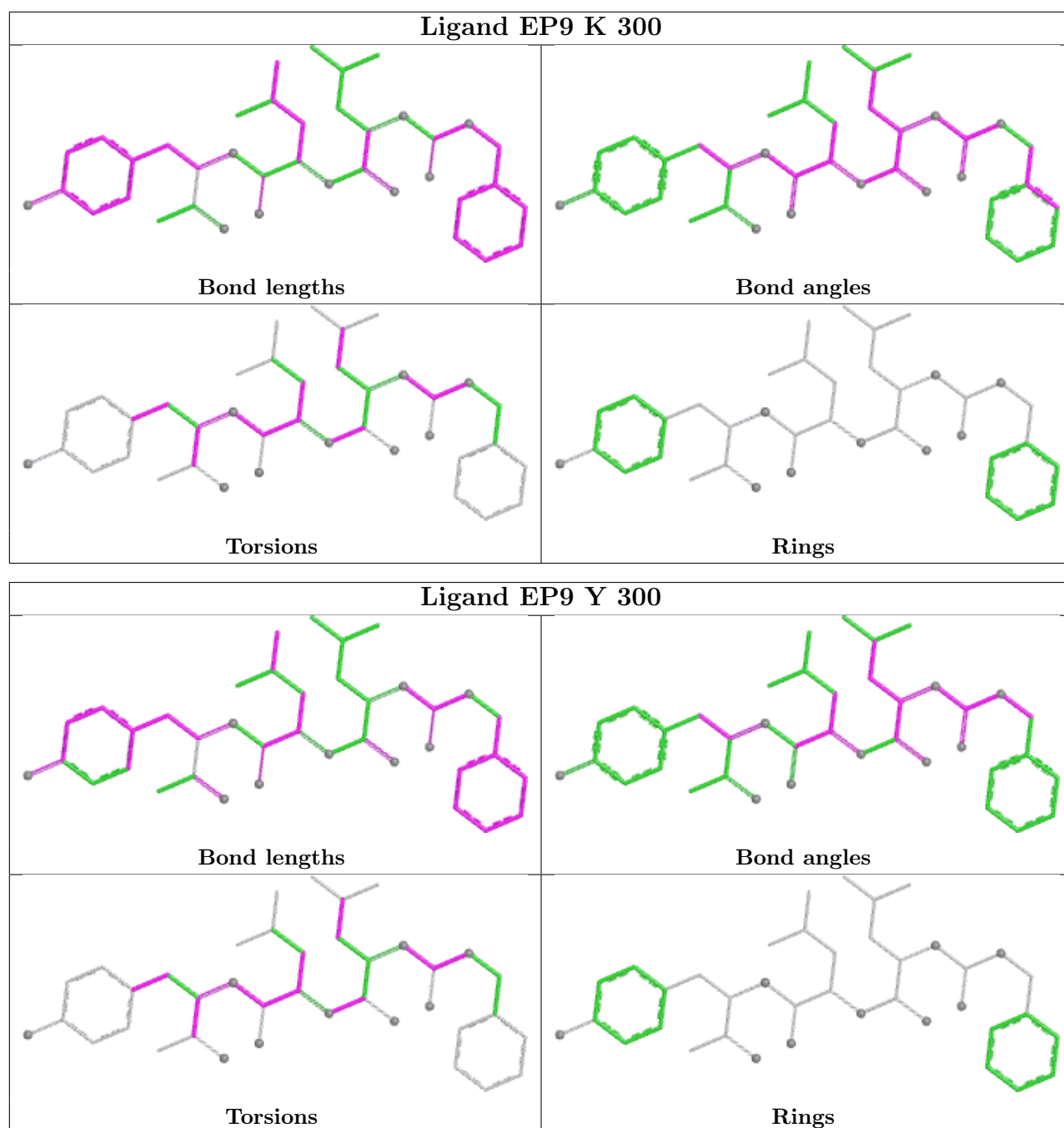
Mol	Chain	Res	Type	Atoms
15	K	300	EP9	C2-C1-C3-N1
15	Y	300	EP9	C2-C1-C3-N1
15	K	300	EP9	N2-C12-C27-C28
15	K	300	EP9	O6-C13-N2-C12
15	Y	300	EP9	C12-C11-N1-C3
15	Y	300	EP9	O6-C13-N2-C12
15	Y	300	EP9	O7-C11-C12-N2
15	Y	300	EP9	N3-C15-O4-C16
15	K	300	EP9	O7-C11-C12-N2
15	Y	300	EP9	N2-C12-C27-C28
15	K	300	EP9	O1-C1-C3-C4
15	K	300	EP9	O4-C15-N3-C14
15	Y	300	EP9	O4-C15-N3-C14
15	Y	300	EP9	C2-C1-C3-C4
15	K	300	EP9	O7-C11-C12-C27
15	Y	300	EP9	O7-C11-C12-C27
15	Y	300	EP9	N1-C11-C12-N2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	300	EP9	1	0
15	Y	300	EP9	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	-0.12	3 (1%) 76 75	49, 69, 99, 124	0
1	O	250/250 (100%)	-0.07	3 (1%) 76 75	50, 70, 100, 123	0
2	B	244/244 (100%)	0.12	9 (3%) 45 41	51, 70, 107, 130	0
2	P	244/244 (100%)	0.14	10 (4%) 41 37	51, 71, 108, 130	0
3	C	241/241 (100%)	0.21	8 (3%) 49 45	53, 76, 125, 143	0
3	Q	241/241 (100%)	0.32	12 (4%) 34 30	56, 78, 126, 143	0
4	D	242/242 (100%)	0.18	7 (2%) 53 50	51, 76, 109, 140	0
4	R	242/242 (100%)	0.21	7 (2%) 53 50	52, 77, 109, 140	0
5	E	233/233 (100%)	0.34	8 (3%) 48 44	56, 82, 110, 126	0
5	S	233/233 (100%)	0.64	16 (6%) 23 20	57, 84, 110, 125	0
6	F	244/244 (100%)	0.13	4 (1%) 70 68	51, 73, 109, 120	0
6	T	244/244 (100%)	0.25	5 (2%) 65 62	52, 73, 110, 120	0
7	G	243/243 (100%)	-0.03	4 (1%) 70 68	48, 68, 97, 129	0
7	U	243/243 (100%)	-0.03	5 (2%) 63 61	50, 69, 97, 128	0
8	H	222/222 (100%)	-0.16	0 100 100	49, 64, 83, 125	0
8	V	222/222 (100%)	-0.17	1 (0%) 87 86	51, 65, 84, 125	0
9	I	204/204 (100%)	-0.28	1 (0%) 87 86	44, 62, 81, 98	0
9	W	204/204 (100%)	-0.29	1 (0%) 87 86	46, 62, 82, 98	0
10	J	198/198 (100%)	-0.21	5 (2%) 58 55	46, 60, 81, 137	0
10	X	198/198 (100%)	-0.27	4 (2%) 65 62	46, 60, 80, 137	0
11	K	212/212 (100%)	-0.16	7 (3%) 49 45	42, 60, 83, 105	0
11	Y	212/212 (100%)	-0.11	8 (3%) 44 40	43, 61, 84, 107	0
12	L	222/222 (100%)	-0.18	1 (0%) 87 86	46, 64, 89, 111	0
12	Z	222/222 (100%)	0.04	3 (1%) 73 72	49, 69, 94, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	0.03	3 (1%) 75 73	49, 69, 86, 90	0
13	M	233/233 (100%)	-0.20	2 (0%) 81 80	46, 64, 82, 87	0
14	2	196/196 (100%)	0.06	6 (3%) 51 48	51, 65, 85, 99	0
14	N	196/196 (100%)	-0.26	0 100 100	48, 61, 82, 95	0
All	All	6368/6368 (100%)	0.01	143 (2%) 62 59	42, 68, 104, 143	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(D)	ALA	7.9
4	D	12(C)	GLY	7.0
3	Q	56	LEU	6.5
4	R	12(D)	ALA	6.4
11	K	104	TYR	5.8
11	Y	104	TYR	5.6
10	J	192	ALA	5.3
3	C	56	LEU	5.0
4	D	12(E)	SER	4.9
2	P	217	ALA	4.9
4	D	126	ARG	4.9
4	R	12(C)	GLY	4.8
2	B	217	ALA	4.8
7	U	240	ASP	4.8
2	B	21(B)	GLY	4.8
5	S	4	PHE	4.7
3	C	55	THR	4.7
4	R	12(E)	SER	4.7
11	Y	208	ASN	4.6
10	X	192	ALA	4.0
12	Z	145	TYR	4.0
3	Q	58	LEU	3.9
3	C	54	SER	3.9
5	S	2(E)	ASN	3.8
4	R	127	LEU	3.8
5	S	55	ALA	3.7
4	R	126	ARG	3.7
5	E	4	PHE	3.7
10	X	193	GLN	3.6
2	B	239	THR	3.6
10	J	193	GLN	3.5
12	L	145	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
7	U	6	ALA	3.4
10	X	-1	MET	3.4
10	J	168	MET	3.4
13	1	167	ALA	3.4
11	K	208	ASN	3.4
11	K	207	ASN	3.3
11	Y	73	ARG	3.3
4	D	127	LEU	3.2
5	S	210	LEU	3.1
3	Q	55	THR	3.1
10	J	-1	MET	3.1
7	G	6	ALA	3.1
14	2	65	LEU	3.1
13	1	-8	THR	3.1
5	S	59	SER	3.1
1	A	235	ALA	3.1
5	S	60	SER	3.1
2	P	21(B)	GLY	3.0
1	O	4	MET	2.9
5	E	63	TYR	2.9
7	G	7	GLY	2.9
5	S	5	ARG	2.9
5	S	230	ALA	2.9
5	S	18(C)	PHE	2.9
1	A	4	MET	2.8
5	S	63	TYR	2.8
1	O	235	ALA	2.8
2	P	54	VAL	2.8
2	P	220	TYR	2.8
5	E	203	ASP	2.7
13	M	-8	THR	2.7
11	K	210	ILE	2.7
2	P	21(D)	GLY	2.7
11	K	73	ARG	2.7
14	2	97	ALA	2.7
3	Q	236	ILE	2.7
10	X	168	MET	2.6
11	Y	207	ASN	2.6
11	Y	210	ILE	2.6
11	Y	211	GLY	2.6
4	D	242	ALA	2.6
5	E	2(C)	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
14	2	20	THR	2.5
6	F	204	ASP	2.5
6	F	240	ILE	2.5
3	C	207	ALA	2.5
5	E	58	LEU	2.5
7	U	18(H)	GLU	2.5
11	K	211	GLY	2.5
2	B	54	VAL	2.5
2	P	218	ASN	2.5
14	2	134	ILE	2.5
2	B	21(D)	GLY	2.5
7	U	156	TYR	2.5
5	S	53	ARG	2.4
6	F	219	GLY	2.4
3	Q	233	VAL	2.4
2	B	218	ASN	2.4
1	O	5	THR	2.4
5	S	56	ASP	2.4
3	Q	240	LYS	2.4
5	S	54	ASN	2.3
3	Q	57	LYS	2.3
5	S	51	LEU	2.3
8	V	223	ASP	2.3
9	W	-8	SER	2.3
11	Y	145	ASP	2.3
2	P	4	GLY	2.3
7	U	239	GLN	2.3
5	S	18(F)	ILE	2.3
4	R	158	TYR	2.3
7	G	236	ILE	2.2
2	P	239	THR	2.2
11	K	180	GLU	2.2
7	G	8	TYR	2.2
3	C	59	GLN	2.2
12	Z	14(C)	GLN	2.2
2	B	4	GLY	2.2
1	A	5	THR	2.2
3	Q	64	PRO	2.2
4	R	12(F)	GLY	2.2
5	E	59	SER	2.2
11	Y	180	GLU	2.2
14	2	10(A)	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	Q	201	VAL	2.2
13	1	141	VAL	2.2
4	D	12(G)	GLU	2.2
10	J	191	GLN	2.2
2	B	63(A)	SER	2.2
3	Q	54	SER	2.2
3	Q	208	LYS	2.1
5	E	184	GLY	2.1
14	2	116	GLY	2.1
3	C	62(A)	ILE	2.1
3	C	203	THR	2.1
6	T	208	PHE	2.1
2	P	21(A)	LYS	2.1
2	B	238	ILE	2.1
6	T	240	ILE	2.1
6	T	203	GLU	2.1
5	S	180	LEU	2.1
13	M	61	ASP	2.0
2	P	219	GLU	2.0
3	Q	44	ASN	2.0
12	Z	96	TYR	2.0
3	C	57	LYS	2.0
6	T	20(C)	LYS	2.0
6	F	13	SER	2.0
9	I	-8	SER	2.0
6	T	184	LEU	2.0
5	E	2(E)	ASN	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,

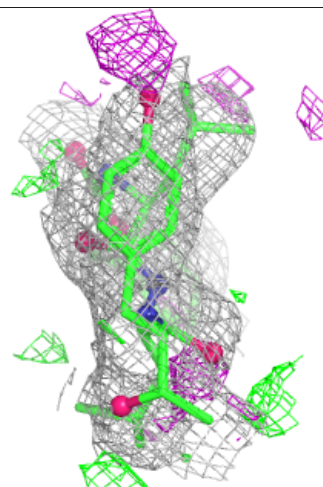
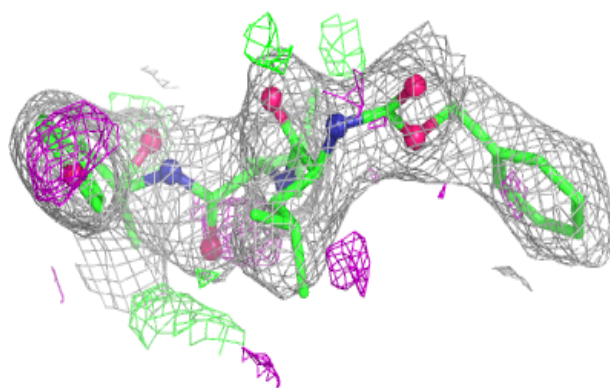
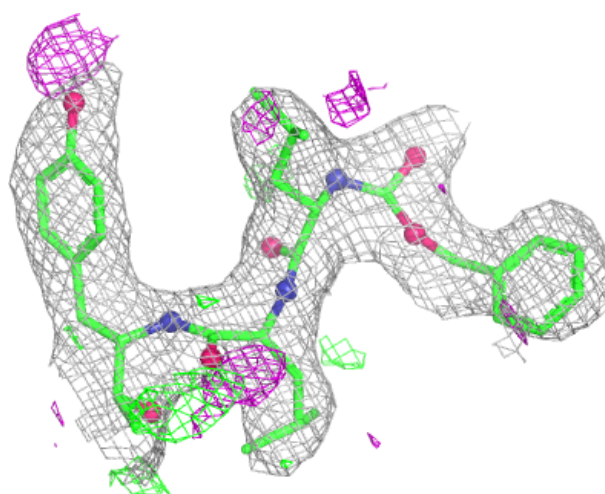
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	EP9	Y	300	39/40	0.91	0.10	43,50,69,70	0
15	EP9	K	300	39/40	0.92	0.10	40,47,69,71	0

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

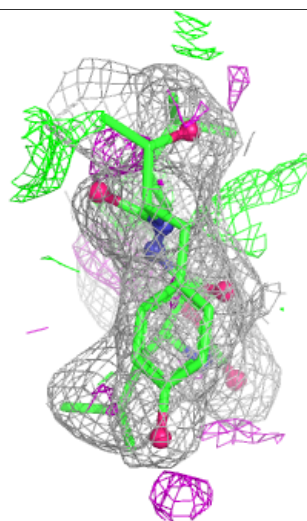
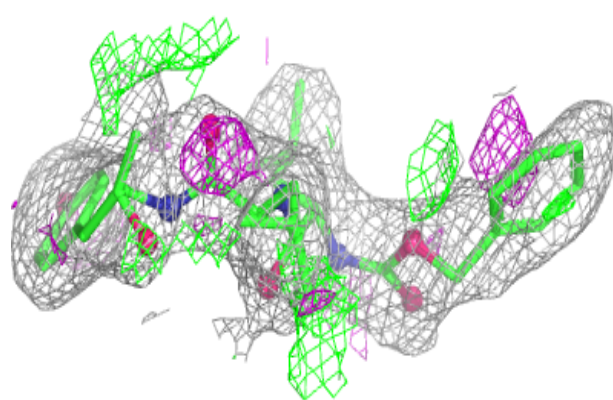
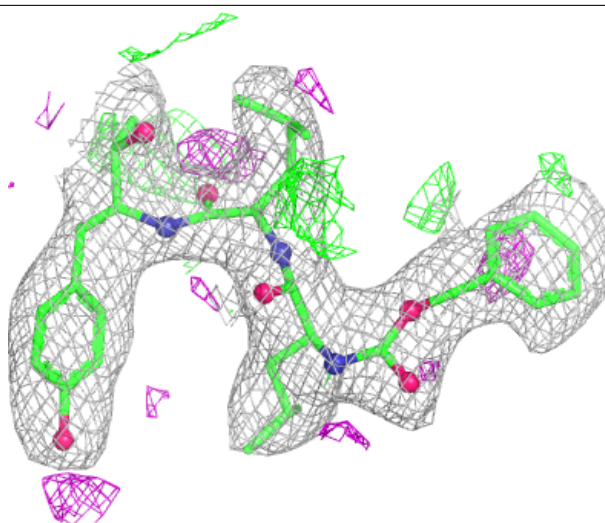
Electron density around EP9 Y 300:

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



Electron density around EP9 K 300:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.