



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:58 AM UTC

PDB ID : 3BDM / pdb_00003bdm
Title : yeast 20S proteasome:glidobactin A-complex
Authors : Groll, M.; Dudler, R.; Kaiser, M.
Deposited on : 2007-11-15
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

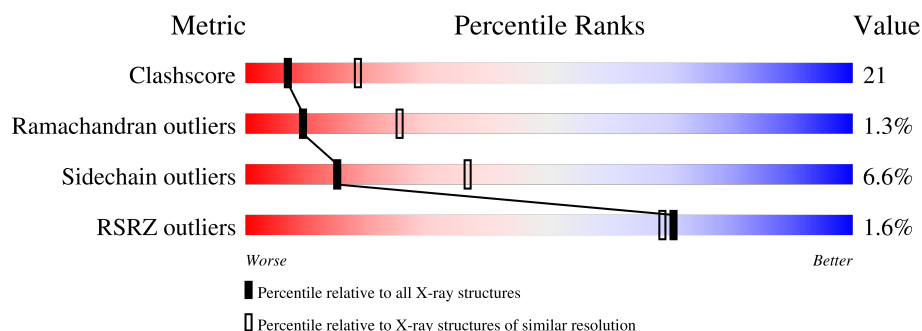
1 Overall quality at a glance

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))
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	2% 63% 33% .
1	O	250	2% 64% 32% .
2	B	258	3% 53% 36% 5% 5%
2	P	258	3% 51% 39% 5% 5%
3	C	254	3% 48% 41% 6% 5%
3	Q	254	4% 48% 41% 6% 5%

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	287	
6	T	287	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	241	
12	Z	241	
13	O	266	
13	M	266	
14	1	196	
14	N	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51022 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
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	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
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	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
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	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
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	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
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

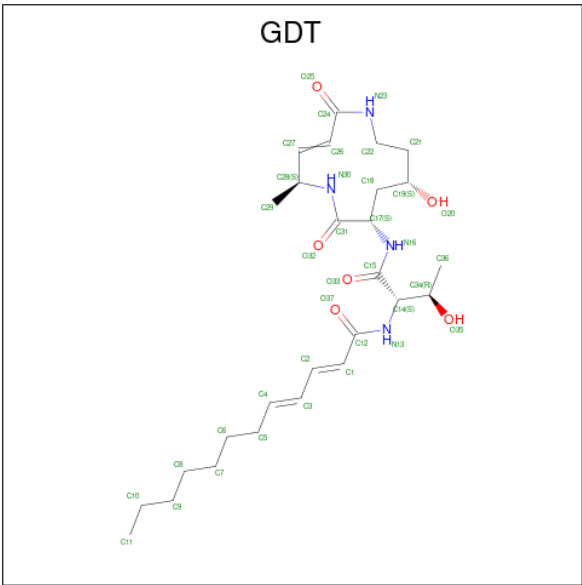
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	1	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is (2E,4E)-N-[(2S,3R)-3-hydroxy-1-[(3Z,5S,8S,10S)-10-hydroxy-5-methyl-2,7-dioxo-1,6-diazacyclododec-3-en-8-yl]amino]-1-oxobutan-2-yl]dodeca-2,4-dienamide (CCD ID: GDT) (formula: C₂₇H₄₄N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			37	27	4	6		
15	K	1	Total	C	N	O	0	0
			37	27	4	6		
15	V	1	Total	C	N	O	0	0
			37	27	4	6		
15	Y	1	Total	C	N	O	0	0
			37	27	4	6		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	57	Total	O	0	0
			57	57		
16	B	38	Total	O	0	0
			38	38		
16	C	42	Total	O	0	0
			42	42		
16	D	40	Total	O	0	0
			40	40		
16	E	24	Total	O	0	0
			24	24		
16	F	46	Total	O	0	0
			46	46		
16	G	61	Total	O	0	0
			61	61		
16	H	48	Total	O	0	0
			48	48		

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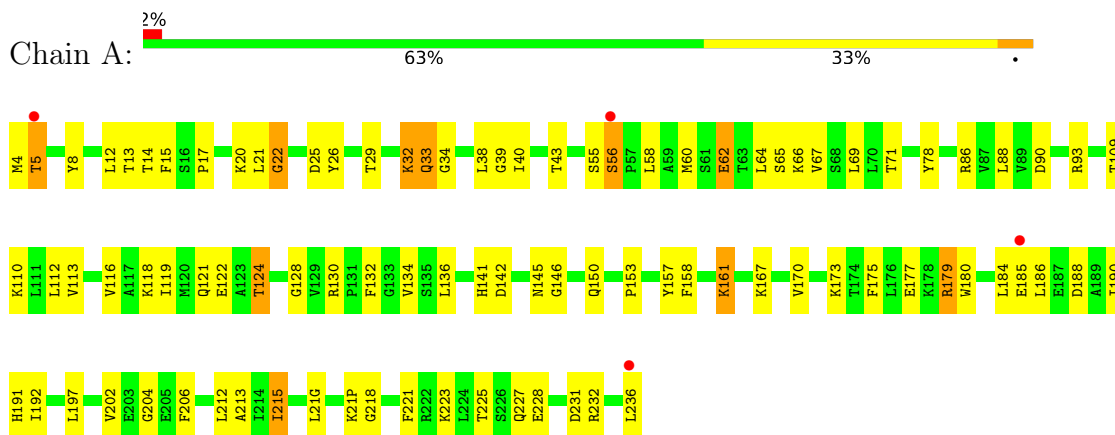
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	I	66	Total 66	O 66	0	0
16	J	52	Total 52	O 52	0	0
16	K	46	Total 46	O 46	0	0
16	L	60	Total 60	O 60	0	0
16	M	69	Total 69	O 69	0	0
16	N	56	Total 56	O 56	0	0
16	O	33	Total 33	O 33	0	0
16	P	32	Total 32	O 32	0	0
16	Q	26	Total 26	O 26	0	0
16	R	34	Total 34	O 34	0	0
16	S	20	Total 20	O 20	0	0
16	T	39	Total 39	O 39	0	0
16	U	58	Total 58	O 58	0	0
16	V	47	Total 47	O 47	0	0
16	W	60	Total 60	O 60	0	0
16	X	42	Total 42	O 42	0	0
16	Y	49	Total 49	O 49	0	0
16	Z	53	Total 53	O 53	0	0
16	0	74	Total 74	O 74	0	0
16	1	64	Total 64	O 64	0	0

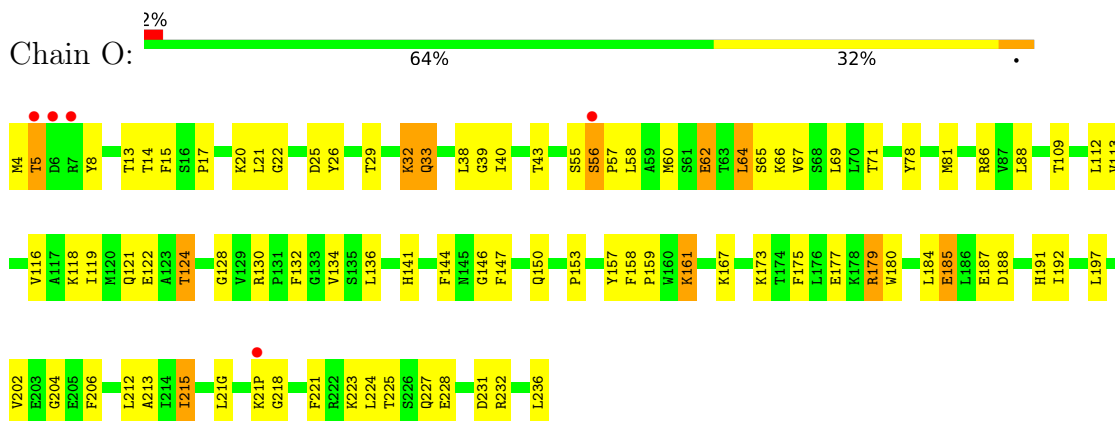
3 Residue-property plots [i](#)

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.

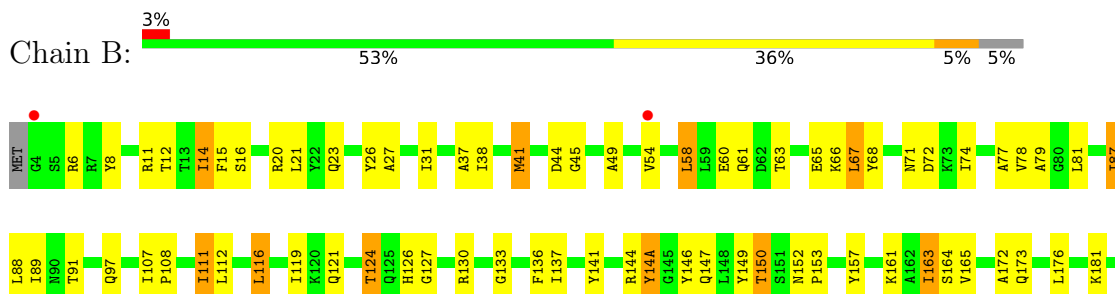
- Molecule 1: Proteasome component Y7

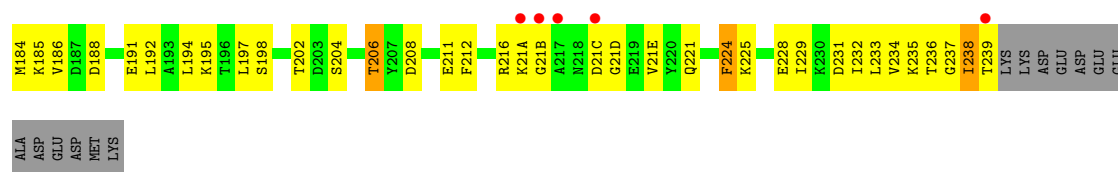


- Molecule 1: Proteasome component Y7

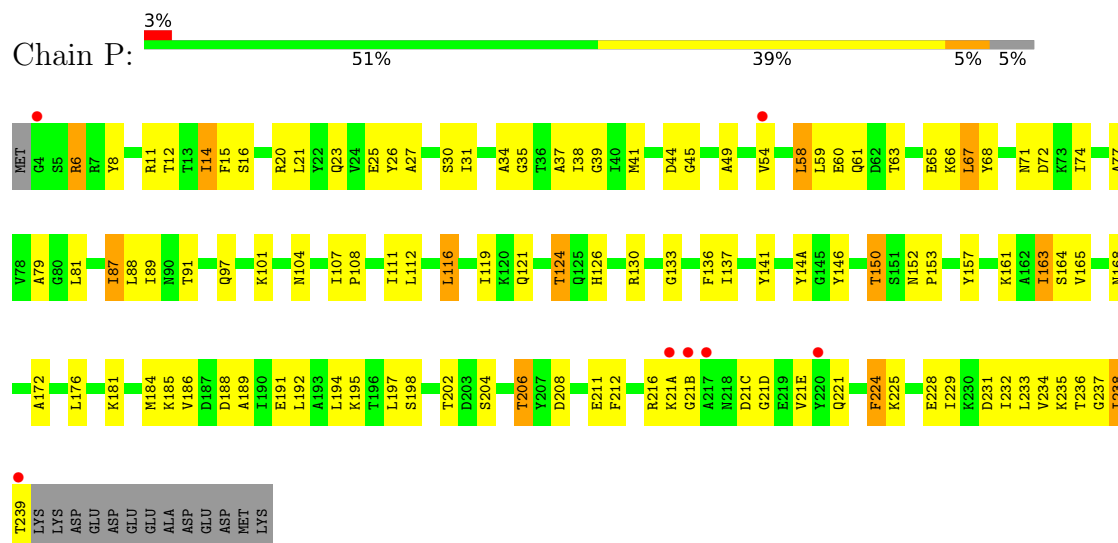


- Molecule 2: Proteasome component Y13

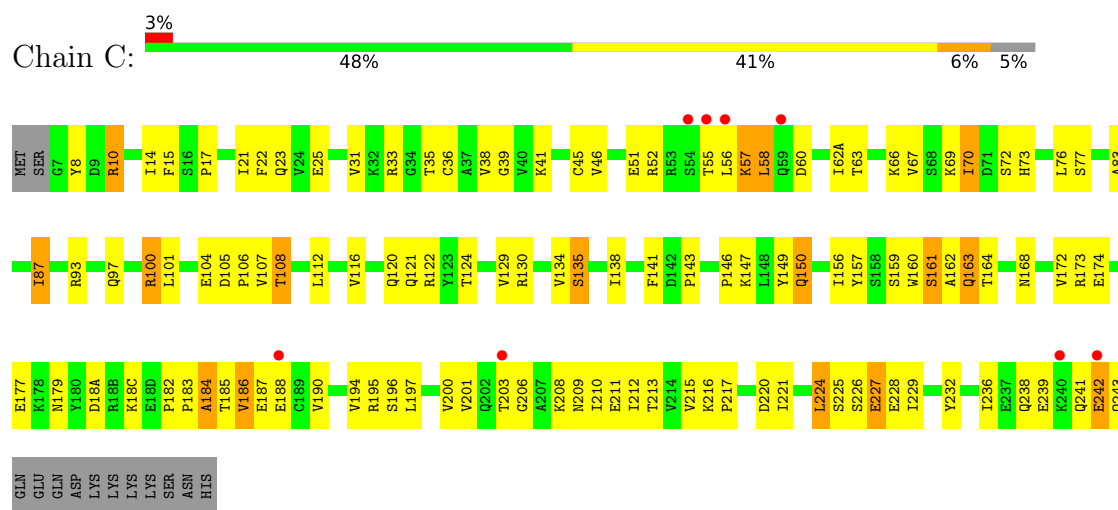




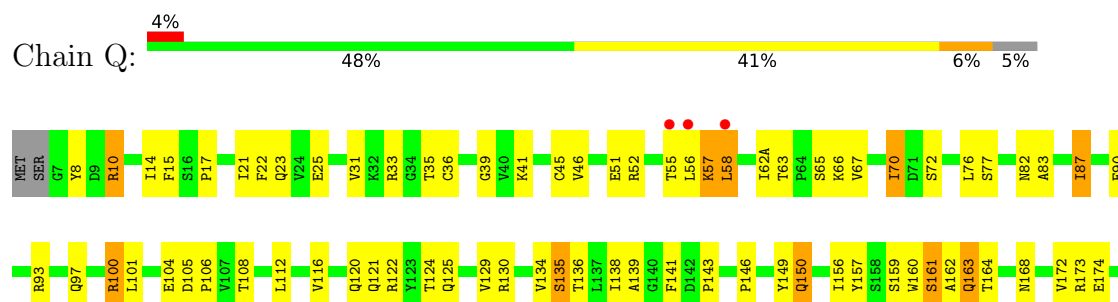
• Molecule 2: Proteasome component Y13

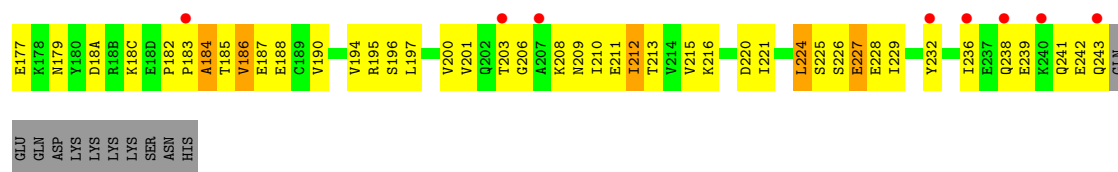


• Molecule 3: Proteasome component PRE6

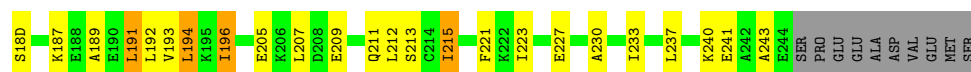
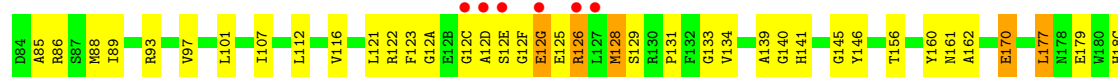


• Molecule 3: Proteasome component PRE6

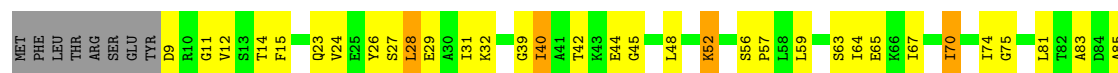




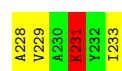
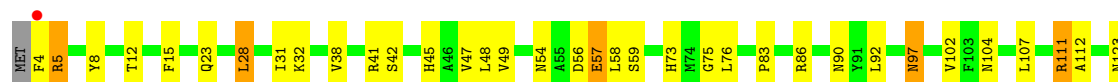
• Molecule 4: Proteasome component PUP2



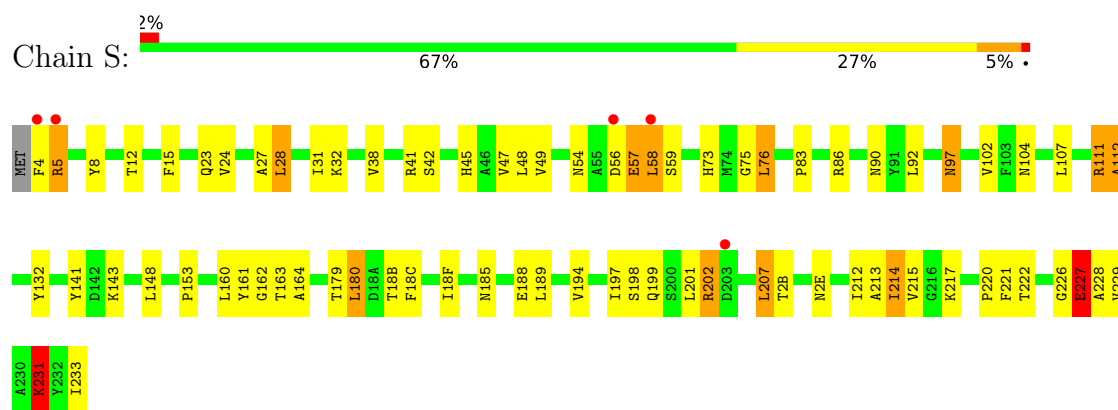
• Molecule 4: Proteasome component PUP2



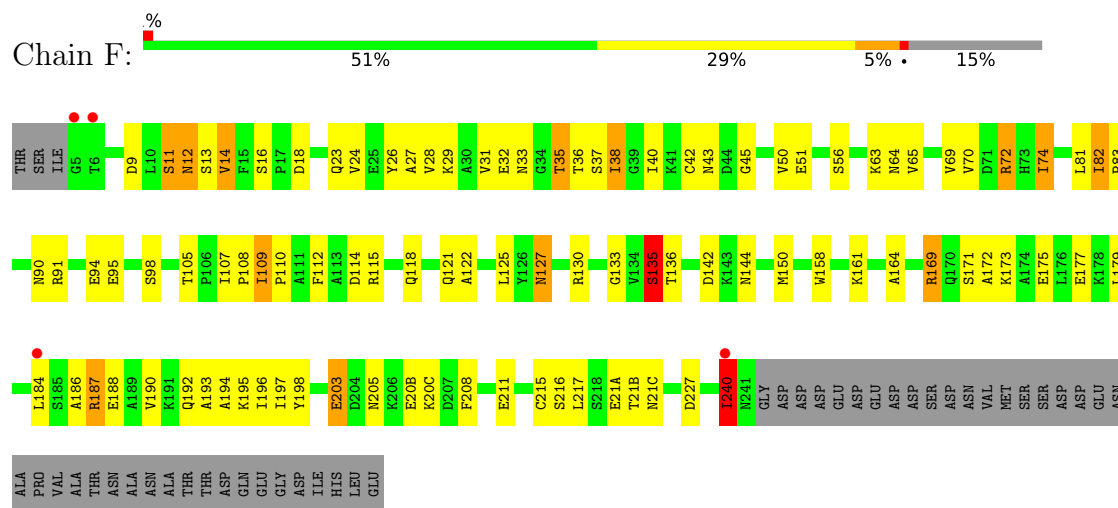
• Molecule 5: Proteasome component PRE5



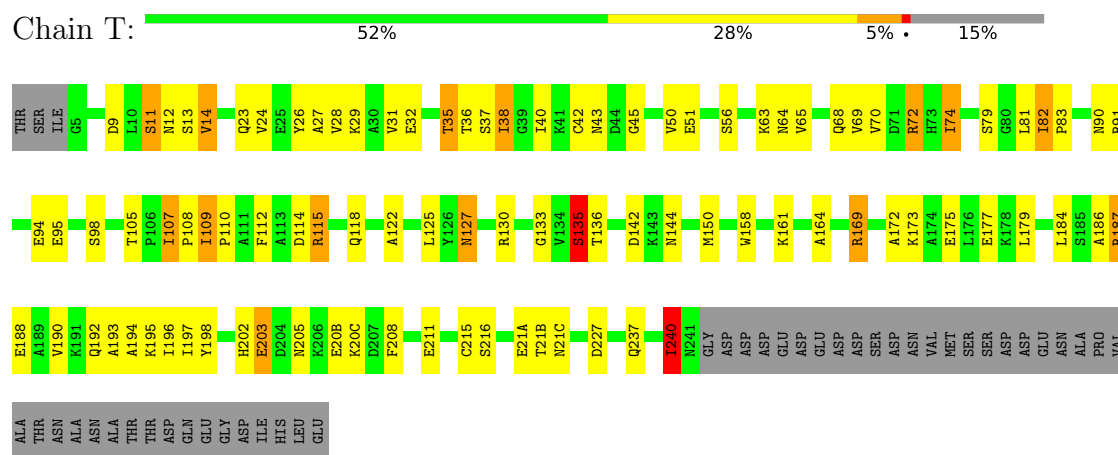
• Molecule 5: Proteasome component PRE5



- Molecule 6: Proteasome component C1

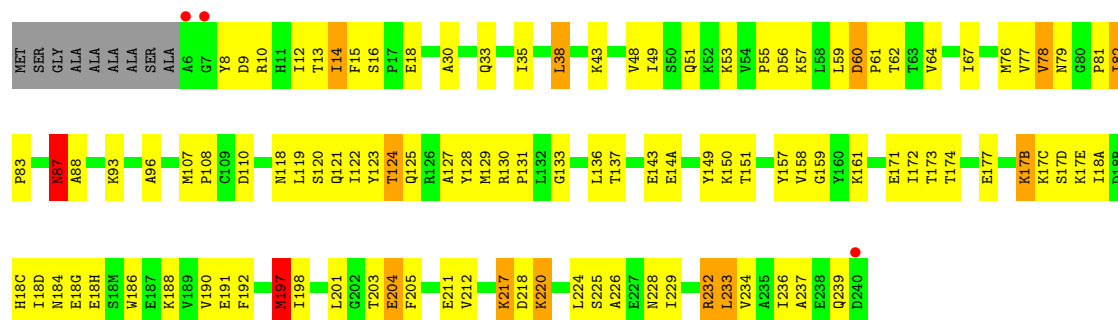


- Molecule 6: Proteasome component C1

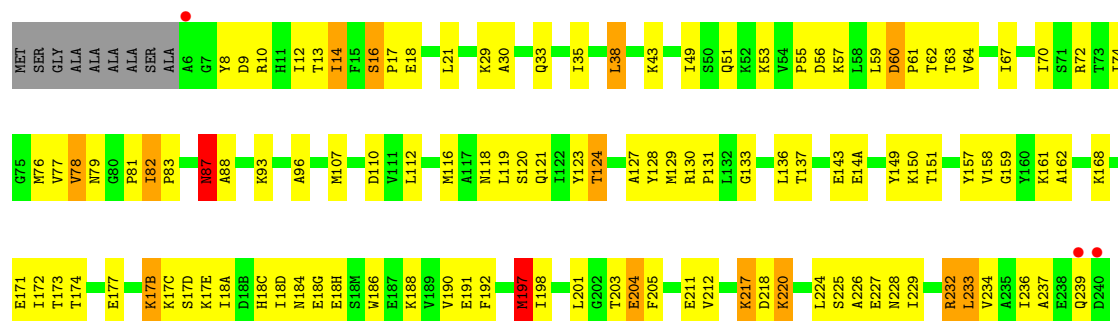


- Molecule 7: Proteasome component C7-alpha

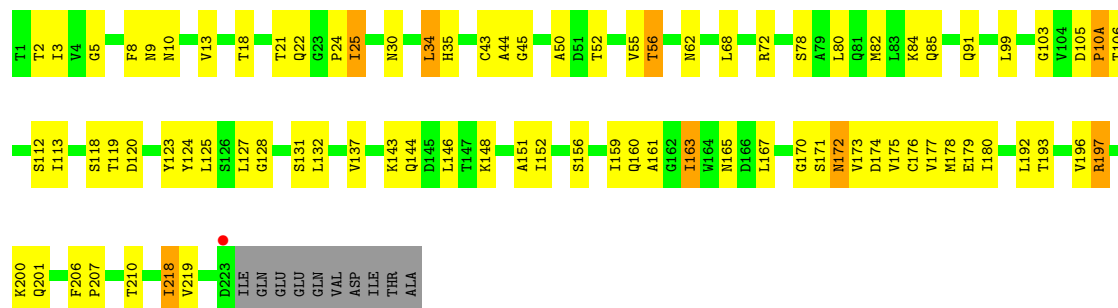




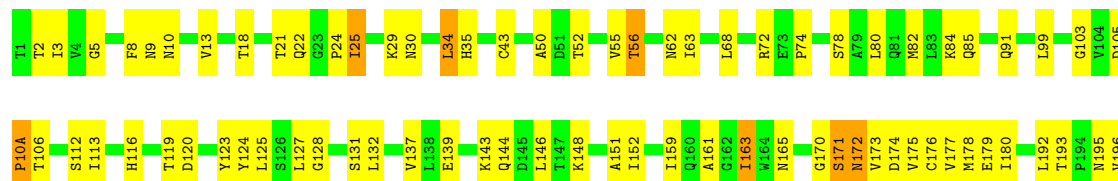
• Molecule 7: Proteasome component C7-alpha

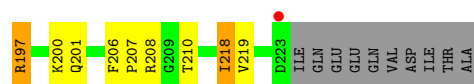


• Molecule 8: Proteasome component PUP1

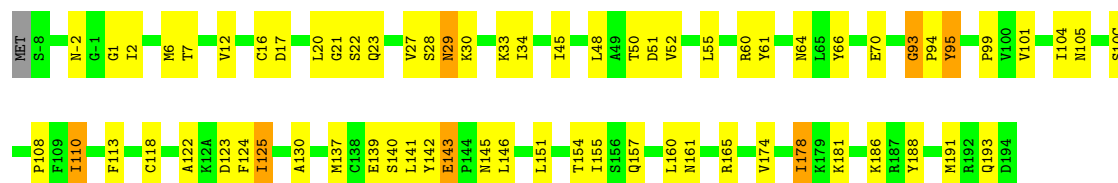


• Molecule 8: Proteasome component PUP1

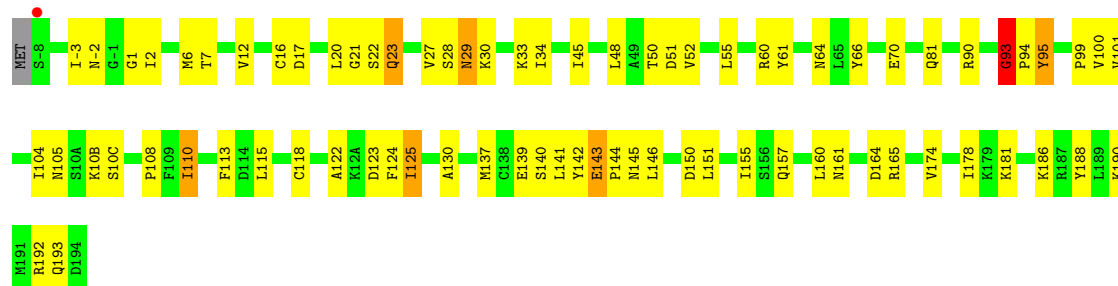




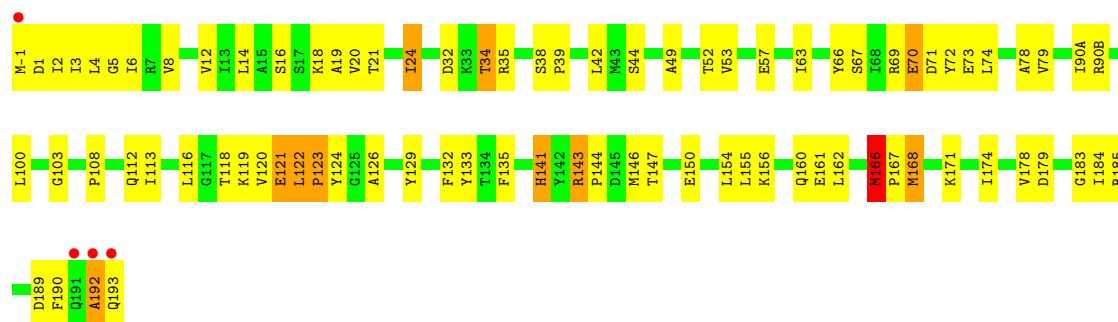
• Molecule 9: Proteasome component PUP3



• Molecule 9: Proteasome component PUP3

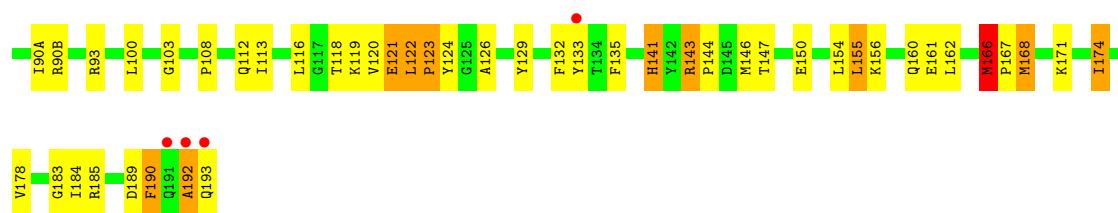


• Molecule 10: Proteasome component C11

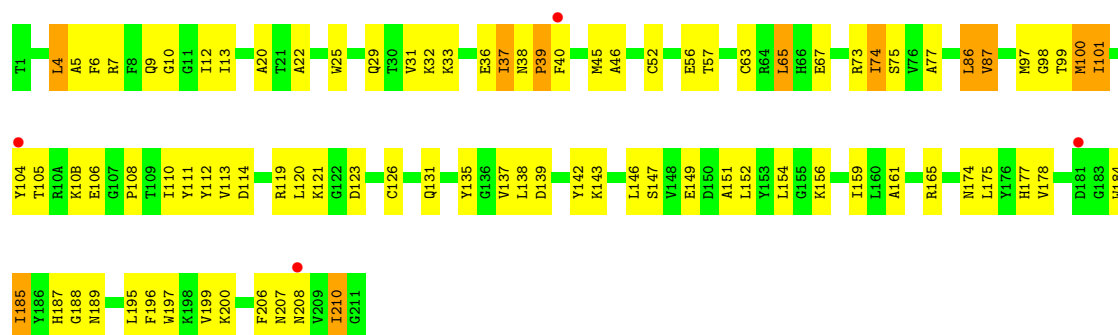


• Molecule 10: Proteasome component C11

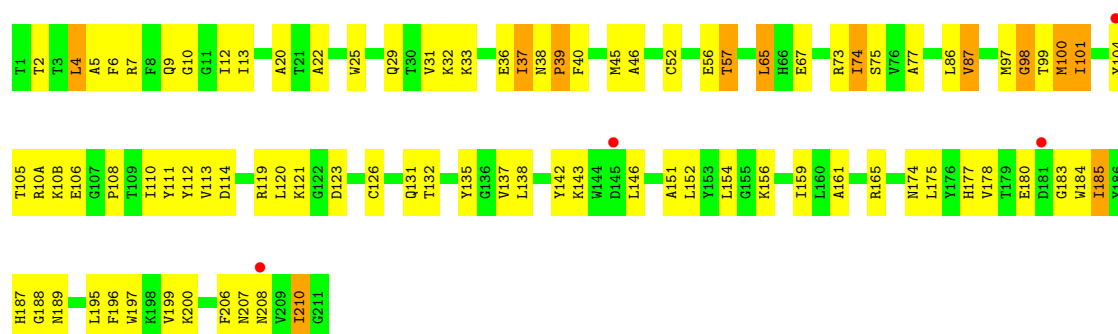




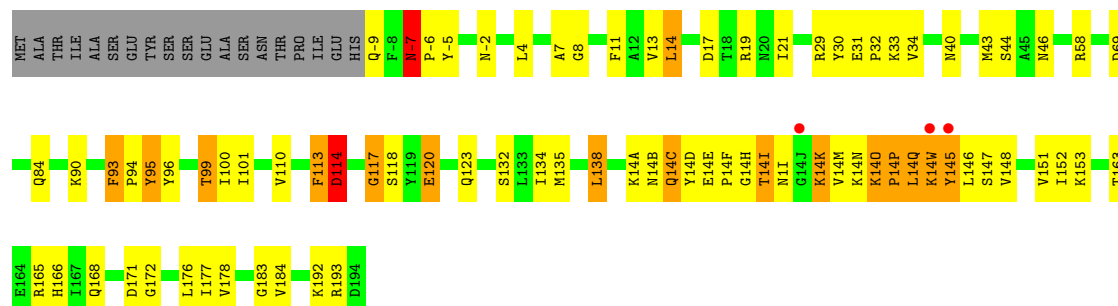
- Molecule 11: Proteasome component PRE2



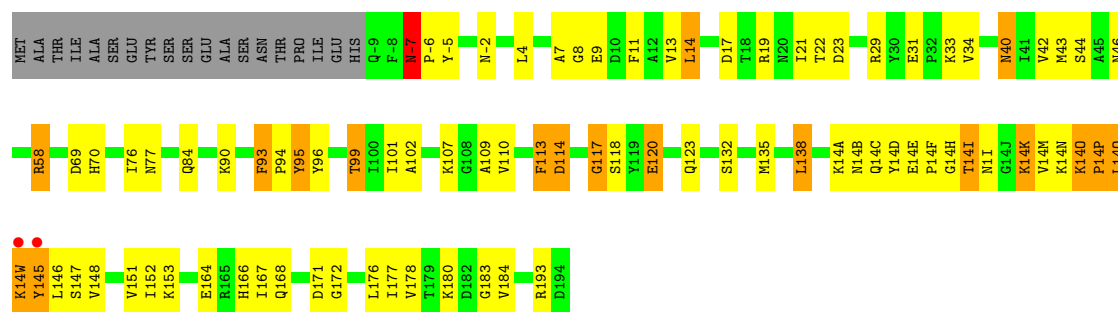
- Molecule 11: Proteasome component PRE2



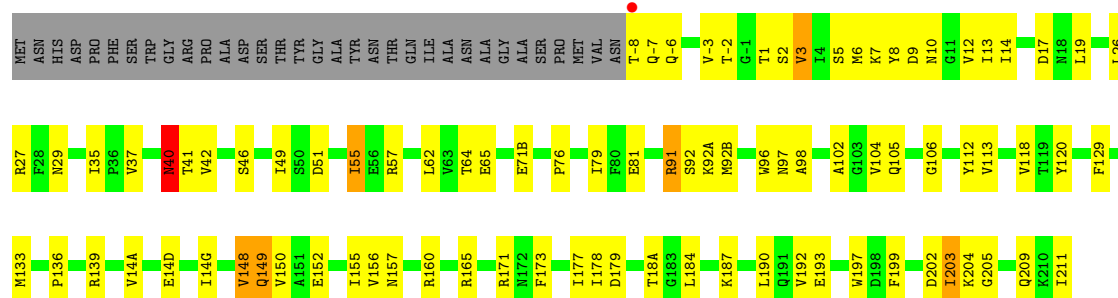
- Molecule 12: Proteasome component C5



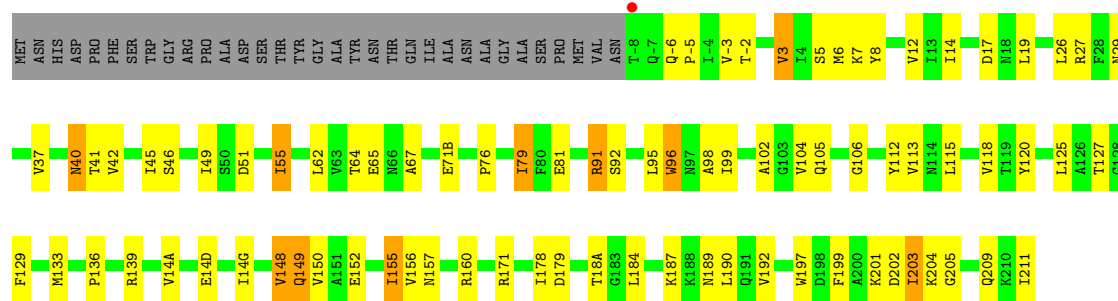
- Molecule 12: Proteasome component C5



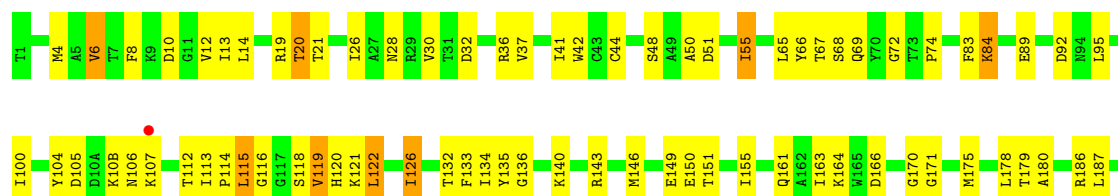
• Molecule 13: Proteasome component PRE4



• Molecule 13: Proteasome component PRE4

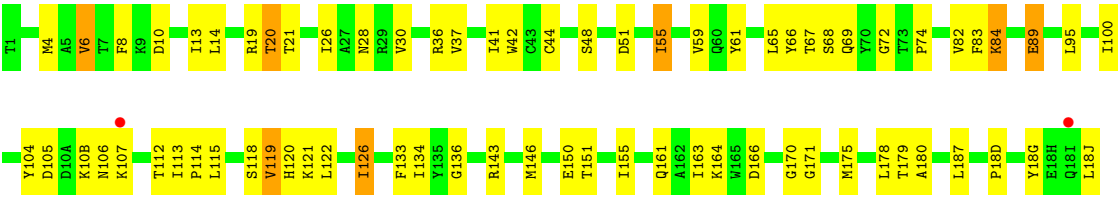


• Molecule 14: Proteasome component PRE3





● 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	132.77Å 302.79Å 143.21Å 90.00° 112.24° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.00-2.70) 97.3 (15.00-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.262 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51022	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/1952	0.95	8/2642 (0.3%)
1	O	0.44	0/1952	0.94	6/2642 (0.2%)
2	B	0.44	0/1934	0.91	2/2618 (0.1%)
2	P	0.45	0/1934	0.92	2/2618 (0.1%)
3	C	0.43	0/1919	0.91	5/2598 (0.2%)
3	Q	0.42	0/1919	0.91	5/2598 (0.2%)
4	D	0.45	0/1886	0.94	6/2541 (0.2%)
4	R	0.44	0/1886	0.93	7/2541 (0.3%)
5	E	0.45	0/1823	0.95	3/2463 (0.1%)
5	S	0.45	0/1823	0.95	5/2463 (0.2%)
6	F	0.46	0/1936	0.98	9/2614 (0.3%)
6	T	0.47	0/1936	0.99	11/2614 (0.4%)
7	G	0.49	0/1959	1.02	15/2652 (0.6%)
7	U	0.48	0/1959	1.02	15/2652 (0.6%)
8	H	0.51	0/1715	0.95	6/2326 (0.3%)
8	V	0.50	0/1715	0.93	3/2326 (0.1%)
9	I	0.47	0/1611	1.00	9/2174 (0.4%)
9	W	0.49	0/1611	1.02	10/2174 (0.5%)
10	J	0.53	1/1613 (0.1%)	1.02	11/2173 (0.5%)
10	X	0.53	1/1613 (0.1%)	1.03	13/2173 (0.6%)
11	K	0.46	0/1681	0.94	5/2274 (0.2%)
11	Y	0.46	0/1681	0.93	6/2274 (0.3%)
12	L	0.47	0/1795	1.02	11/2420 (0.5%)
12	Z	0.46	0/1795	1.02	8/2420 (0.3%)
13	O	0.52	0/1855	1.00	7/2514 (0.3%)
13	M	0.49	0/1855	0.98	8/2514 (0.3%)
14	1	0.52	0/1541	0.95	0/2087
14	N	0.53	0/1541	0.96	4/2087 (0.2%)
All	All	0.47	2/50440 (0.0%)	0.97	200/68192 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	166	MET	SD-CE	6.66	1.96	1.79
10	J	166	MET	SD-CE	5.57	1.93	1.79

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	27	ARG	N-CA-C	10.78	122.60	111.07
13	O	27	ARG	N-CA-C	10.67	122.49	111.07
12	Z	93	PHE	CA-C-N	9.38	131.57	119.84
12	Z	93	PHE	C-N-CA	9.38	131.57	119.84
12	L	93	PHE	CA-C-N	8.93	131.00	119.84
12	L	93	PHE	C-N-CA	8.93	131.00	119.84
6	T	161	LYS	N-CA-C	-8.36	100.83	112.45
4	D	70	ILE	N-CA-C	-8.36	103.67	111.45
3	Q	70	ILE	N-CA-C	-8.36	102.71	110.82
1	A	161	LYS	N-CA-C	-8.31	101.76	112.23
1	O	161	LYS	N-CA-C	-8.26	101.82	112.23
6	T	12	ASN	N-CA-C	8.25	122.61	112.54
6	F	12	ASN	N-CA-C	8.24	122.60	112.54
6	T	107	ILE	N-CA-C	8.16	117.86	108.96
4	R	70	ILE	N-CA-C	-8.13	103.88	111.45
7	G	161	LYS	N-CA-C	-8.12	102.00	112.23
6	F	161	LYS	N-CA-C	-8.10	101.19	112.45
9	W	60	ARG	N-CA-C	-7.98	102.18	111.03
7	U	161	LYS	N-CA-C	-7.96	102.20	112.23
10	J	166	MET	CA-C-N	7.93	127.49	119.24
10	J	166	MET	C-N-CA	7.93	127.49	119.24
9	W	142	TYR	N-CA-C	7.93	120.55	110.24
9	I	142	TYR	N-CA-C	7.76	120.33	110.24
10	X	166	MET	CA-C-N	7.63	127.17	119.24
10	X	166	MET	C-N-CA	7.63	127.17	119.24
3	C	70	ILE	N-CA-C	-7.53	102.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	60	ARG	N-CA-C	-7.53	102.67	111.03
5	E	102	VAL	N-CA-C	7.47	117.55	110.53
1	A	78	TYR	N-CA-C	7.32	117.92	108.34
5	E	57	GLU	N-CA-C	-7.29	103.54	113.30
1	O	78	TYR	N-CA-C	7.22	117.79	108.34
2	B	161	LYS	N-CA-C	-7.14	104.19	113.12
5	S	102	VAL	N-CA-C	7.06	117.17	110.53
5	S	57	GLU	N-CA-C	-7.06	103.84	113.30
4	D	63	SER	N-CA-C	-7.01	104.60	113.02
4	R	63	SER	N-CA-C	-6.87	104.77	113.02
13	M	-2	THR	N-CA-C	6.87	120.71	109.85
13	O	-2	THR	N-CA-C	6.69	120.42	109.85
12	L	117	GLY	N-CA-C	6.64	122.73	114.37
7	G	16	SER	N-CA-C	-6.62	101.73	110.40
12	Z	117	GLY	N-CA-C	6.62	122.71	114.37
12	L	-7	ASN	CA-C-N	6.46	126.59	119.87
12	L	-7	ASN	C-N-CA	6.46	126.59	119.87
7	U	16	SER	N-CA-C	-6.43	101.97	110.40
12	Z	-7	ASN	CA-C-N	6.41	126.53	119.87
12	Z	-7	ASN	C-N-CA	6.41	126.53	119.87
2	P	16	SER	N-CA-C	-6.36	102.82	110.13
10	J	143	ARG	CA-C-N	6.35	126.27	119.28
10	J	143	ARG	C-N-CA	6.35	126.27	119.28
6	T	14	VAL	N-CA-C	6.35	117.27	108.89
4	R	161	ASN	N-CA-C	-6.35	104.59	112.90
7	G	13	THR	N-CA-C	6.30	119.08	109.62
13	O	98	ALA	N-CA-C	-6.29	98.13	108.76
2	P	161	LYS	N-CA-C	-6.23	103.79	112.45
10	X	143	ARG	CA-C-N	6.21	126.11	119.28
10	X	143	ARG	C-N-CA	6.21	126.11	119.28
9	I	95	TYR	N-CA-C	-6.20	99.89	109.76
6	F	240	ILE	N-CA-C	-6.17	103.97	113.16
7	G	127	ALA	N-CA-C	6.16	117.99	111.28
4	D	129	SER	N-CA-C	6.12	118.03	111.36
7	U	127	ALA	N-CA-C	6.10	118.01	111.36
3	Q	161	SER	N-CA-C	-6.06	104.59	112.23
6	T	240	ILE	N-CA-C	-6.05	104.15	113.16
9	W	95	TYR	N-CA-C	-6.04	99.43	109.46
2	B	16	SER	N-CA-C	-6.04	103.19	110.13
11	K	131	GLN	N-CA-C	6.04	117.86	111.28
13	M	98	ALA	N-CA-C	-6.02	98.58	108.76
9	W	-3	ILE	N-CA-C	-5.99	107.05	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	185	GLU	N-CA-C	-5.98	101.67	110.52
7	U	13	THR	N-CA-C	5.95	118.54	109.62
1	A	128	GLY	N-CA-C	5.93	122.14	113.48
1	A	71	THR	N-CA-C	-5.92	101.33	108.14
7	U	60	ASP	CA-C-N	5.92	127.23	119.84
7	U	60	ASP	C-N-CA	5.92	127.23	119.84
13	O	95	LEU	N-CA-C	-5.89	98.12	108.20
3	C	161	SER	N-CA-C	-5.89	104.81	112.23
7	G	9	ASP	N-CA-C	-5.89	106.14	113.15
1	A	185	GLU	N-CA-C	-5.88	101.81	110.52
4	D	128	MET	N-CA-C	-5.84	98.36	110.80
7	G	82	ILE	CA-C-N	-5.81	112.60	119.05
7	G	82	ILE	C-N-CA	-5.81	112.60	119.05
9	I	94	PRO	N-CA-C	5.80	119.34	111.22
1	O	128	GLY	N-CA-C	5.79	121.94	113.48
6	F	82	ILE	CB-CA-C	-5.77	108.22	113.70
1	O	66	LYS	N-CA-C	-5.77	106.08	113.23
4	D	161	ASN	N-CA-C	-5.75	104.99	112.23
10	X	122	LEU	CA-C-N	5.73	125.10	118.85
10	X	122	LEU	C-N-CA	5.73	125.10	118.85
11	Y	188	GLY	N-CA-C	5.73	121.78	112.61
1	A	66	LYS	N-CA-C	-5.73	106.13	113.23
10	X	141	HIS	N-CA-C	5.73	119.35	112.93
10	X	123	PRO	N-CA-C	-5.72	105.73	113.40
10	J	123	PRO	N-CA-C	-5.71	105.75	113.40
4	R	128	MET	N-CA-C	-5.71	98.63	110.80
1	A	34	GLY	N-CA-C	5.70	118.61	112.33
9	W	143	GLU	CA-C-N	5.70	125.65	119.78
9	W	143	GLU	C-N-CA	5.70	125.65	119.78
8	H	45	GLY	N-CA-C	5.68	121.39	111.46
9	W	94	PRO	N-CA-C	5.66	119.15	111.22
12	L	69	ASP	N-CA-C	5.62	117.21	111.14
7	U	9	ASP	N-CA-C	-5.61	106.47	113.15
3	C	186	VAL	N-CA-C	-5.61	104.90	110.62
8	V	132	LEU	N-CA-C	5.60	117.39	111.28
9	I	178	ILE	N-CA-C	5.58	115.98	108.17
8	H	21	THR	N-CA-C	5.58	117.66	109.24
13	M	29	ASN	N-CA-C	5.56	121.95	113.61
11	K	188	GLY	N-CA-C	5.56	121.51	112.61
6	T	82	ILE	CB-CA-C	-5.56	108.42	113.70
11	Y	57	THR	N-CA-C	-5.56	105.30	111.36
10	X	183	GLY	N-CA-C	5.55	117.17	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	132	LEU	N-CA-C	5.55	117.33	111.28
1	O	71	THR	N-CA-C	-5.53	101.78	108.14
7	G	60	ASP	CA-C-N	5.52	126.74	119.84
7	G	60	ASP	C-N-CA	5.52	126.74	119.84
4	D	61	SER	N-CA-C	5.52	119.52	112.34
6	T	135	SER	N-CA-C	-5.52	100.18	109.07
3	C	22	PHE	N-CA-C	5.51	117.28	111.28
6	F	135	SER	N-CA-C	-5.50	99.93	108.90
7	G	78	VAL	N-CA-C	5.50	115.87	108.17
3	Q	22	PHE	N-CA-C	5.50	117.28	111.28
3	Q	186	VAL	N-CA-C	-5.48	105.03	110.62
11	K	29	GLN	N-CA-C	-5.48	105.39	113.61
11	Y	22	ALA	N-CA-C	-5.46	98.31	107.32
6	F	14	VAL	N-CA-C	5.43	116.59	109.21
6	F	208	PHE	N-CA-C	5.42	117.31	109.07
3	C	108	THR	N-CA-C	-5.40	102.52	110.52
6	T	38	ILE	N-CA-C	5.40	116.48	108.65
6	F	38	ILE	N-CA-C	5.39	116.47	108.65
7	U	82	ILE	CA-C-N	-5.39	113.07	119.05
7	U	82	ILE	C-N-CA	-5.39	113.07	119.05
12	L	114	ASP	CA-C-N	-5.38	114.07	119.56
12	L	114	ASP	C-N-CA	-5.38	114.07	119.56
12	Z	113	PHE	N-CA-C	5.38	118.04	109.81
11	Y	131	GLN	N-CA-C	5.37	117.14	111.28
7	U	17(B)	LYS	N-CA-C	-5.36	105.55	111.71
11	K	22	ALA	N-CA-C	-5.35	98.50	107.32
11	Y	29	GLN	N-CA-C	-5.34	105.59	113.61
6	T	208	PHE	N-CA-C	5.33	117.29	109.24
3	Q	108	THR	N-CA-C	-5.33	102.64	110.52
7	U	74	ILE	N-CA-C	5.31	115.61	108.17
5	S	112	ALA	N-CA-C	-5.30	105.40	111.07
10	J	122	LEU	CA-C-N	5.30	124.62	118.85
10	J	122	LEU	C-N-CA	5.30	124.62	118.85
8	V	21	THR	N-CA-C	5.30	117.03	109.14
13	O	189	ASN	N-CA-C	5.29	119.32	112.86
4	R	129	SER	N-CA-C	5.29	117.96	111.82
9	W	145	ASN	N-CA-C	5.27	118.71	111.54
7	G	15	PHE	N-CA-C	5.26	117.92	110.50
10	X	27	LEU	N-CA-C	5.26	117.93	111.82
1	A	12	LEU	N-CA-C	-5.26	106.54	113.17
9	I	145	ASN	N-CA-C	5.25	118.68	111.54
13	M	3	VAL	N-CA-C	-5.25	99.97	107.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	122	LEU	N-CA-C	5.24	116.73	108.55
10	J	183	GLY	N-CA-C	5.24	116.85	111.56
5	E	161	TYR	N-CA-C	-5.23	106.05	112.90
7	U	87	ASN	N-CA-C	-5.22	105.48	111.07
7	G	17(B)	LYS	N-CA-C	-5.21	105.72	111.71
12	L	95	TYR	N-CA-C	-5.21	100.68	108.96
7	G	43	LYS	N-CA-C	-5.20	105.67	112.23
6	T	227	ASP	N-CA-C	5.20	116.64	110.97
10	J	49	ALA	N-CA-C	5.20	119.95	111.37
8	V	172	ASN	N-CA-C	5.20	117.44	109.95
7	U	43	LYS	N-CA-C	-5.19	105.69	112.23
14	N	122	LEU	CA-C-N	5.18	124.68	119.19
14	N	122	LEU	C-N-CA	5.18	124.68	119.19
7	G	197	MET	N-CA-C	-5.18	105.53	111.07
13	O	3	VAL	N-CA-C	-5.18	100.07	107.78
5	S	161	TYR	N-CA-C	-5.17	106.12	112.90
11	K	57	THR	N-CA-C	-5.17	105.72	111.36
12	Z	69	ASP	N-CA-C	5.17	116.72	111.14
14	N	12	VAL	N-CA-C	5.17	115.09	107.75
7	U	197	MET	N-CA-C	-5.17	105.54	111.07
12	L	113	PHE	N-CA-C	5.16	118.00	109.85
9	I	143	GLU	CA-C-N	5.16	125.44	119.92
9	I	143	GLU	C-N-CA	5.16	125.44	119.92
6	T	115	ARG	N-CA-C	-5.15	105.56	111.07
8	H	172	ASN	N-CA-C	5.13	117.34	109.95
7	U	78	VAL	N-CA-C	5.10	115.31	108.17
11	Y	98	GLY	N-CA-C	-5.10	101.10	113.18
8	H	44	ALA	CA-C-N	-5.10	118.19	121.65
8	H	44	ALA	C-N-CA	-5.10	118.19	121.65
14	N	115	LEU	N-CA-C	5.09	117.49	111.33
13	M	40	ASN	N-CA-C	-5.09	106.63	114.16
13	O	29	ASN	N-CA-C	5.08	121.24	113.61
6	F	227	ASP	N-CA-C	5.08	116.51	110.97
12	L	134	ILE	N-CA-C	5.07	116.53	111.00
9	W	93	GLY	N-CA-C	-5.06	102.01	112.34
4	R	152	GLU	CA-C-N	5.06	124.78	119.82
4	R	152	GLU	C-N-CA	5.06	124.78	119.82
9	I	93	GLY	N-CA-C	-5.05	102.03	112.34
10	X	190	PHE	N-CA-C	-5.05	107.07	114.39
10	X	93	ARG	CA-C-N	5.05	124.98	119.78
10	X	93	ARG	C-N-CA	5.05	124.98	119.78
13	M	97	ASN	N-CA-C	5.04	116.47	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	58	LEU	N-CA-C	-5.03	107.20	113.38
12	Z	95	TYR	N-CA-C	-5.02	100.97	108.96
10	J	141	HIS	N-CA-C	5.02	119.05	113.02
7	G	87	ASN	N-CA-C	-5.01	105.51	110.97
9	W	27	VAL	N-CA-C	5.01	115.96	111.90
13	M	35	ILE	N-CA-C	5.01	112.51	107.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	80	0
1	O	1915	0	1926	86	0
2	B	1904	0	1901	110	0
2	P	1904	0	1901	111	0
3	C	1890	0	1900	128	0
3	Q	1890	0	1900	123	0
4	D	1861	0	1836	84	0
4	R	1861	0	1836	83	0
5	E	1795	0	1797	77	0
5	S	1795	0	1797	80	0
6	F	1896	0	1886	84	0
6	T	1896	0	1886	86	0
7	G	1921	0	1910	90	0
7	U	1921	0	1910	101	0
8	H	1684	0	1687	65	0
8	V	1684	0	1687	68	0
9	I	1581	0	1574	62	0
9	W	1581	0	1574	68	0
10	J	1585	0	1590	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1585	0	1590	78	0
11	K	1644	0	1594	80	0
11	Y	1644	0	1594	85	0
12	L	1757	0	1711	61	0
12	Z	1757	0	1711	74	0
13	O	1824	0	1832	65	0
13	M	1824	0	1832	69	0
14	1	1512	0	1481	66	0
14	N	1512	0	1481	68	0
15	H	37	0	43	2	0
15	K	37	0	43	2	0
15	V	37	0	43	3	0
15	Y	37	0	43	4	0
16	O	74	0	0	4	0
16	1	64	0	0	3	0
16	A	57	0	0	5	0
16	B	38	0	0	3	0
16	C	42	0	0	8	0
16	D	40	0	0	4	0
16	E	24	0	0	1	0
16	F	46	0	0	5	0
16	G	61	0	0	5	0
16	H	48	0	0	2	0
16	I	66	0	0	3	0
16	J	52	0	0	4	0
16	K	46	0	0	2	0
16	L	60	0	0	2	0
16	M	69	0	0	4	0
16	N	56	0	0	3	0
16	O	33	0	0	3	0
16	P	32	0	0	4	0
16	Q	26	0	0	3	0
16	R	34	0	0	3	0
16	S	20	0	0	1	0
16	T	39	0	0	6	0
16	U	58	0	0	11	0
16	V	47	0	0	6	0
16	W	60	0	0	4	0
16	X	42	0	0	6	0
16	Y	49	0	0	2	0
16	Z	53	0	0	8	0
All	All	51022	0	49422	2087	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (2087) 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)
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.14	1.10
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.15	1.09
10:J:168:MET:HE3	10:X:168:MET:HE3	1.09	1.09
14:N:136:GLY:HA2	14:1:161:GLN:HE21	1.12	1.07
14:N:161:GLN:HE21	14:1:136:GLY:HA2	1.15	1.06
2:P:71:ASN:ND2	2:P:72:ASP:H	1.56	1.04
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.24	1.01
2:B:71:ASN:ND2	2:B:72:ASP:H	1.58	1.01
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.06	1.00
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.29	0.98
2:P:202:THR:HG22	2:P:204:SER:H	1.29	0.97
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.28	0.96
3:C:52:ARG:HH21	3:C:211:GLU:HB3	1.31	0.95
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.31	0.94
1:O:86:ARG:HE	7:U:118:ASN:HD21	0.97	0.94
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.47	0.94
3:C:76:LEU:HD12	3:C:138:ILE:HG12	1.50	0.94
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.67	0.93
1:O:15:PHE:H	2:P:23:GLN:HE22	1.14	0.92
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.31	0.92
2:B:202:THR:HG22	2:B:204:SER:H	1.32	0.92
7:G:96:ALA:HA	7:G:107:MET:HE2	1.52	0.92
14:N:136:GLY:HA2	14:1:161:GLN:NE2	1.83	0.92
10:J:-1:MET:HG2	10:J:1:ASP:H	1.34	0.91
13:M:149:GLN:NE2	13:M:149:GLN:H	1.69	0.91
10:J:133:TYR:HD1	16:Y:524:HOH:O	1.53	0.90
14:N:161:GLN:NE2	14:1:136:GLY:HA2	1.85	0.90
7:U:96:ALA:HA	7:U:107:MET:HE2	1.51	0.90
1:A:15:PHE:H	2:B:23:GLN:HE22	1.18	0.90
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.54	0.90
10:X:-1:MET:HG2	10:X:1:ASP:H	1.34	0.90
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.17	0.89
11:K:12:ILE:HB	11:K:178:VAL:HB	1.55	0.89
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.54	0.88
10:J:156:LYS:O	10:J:160:GLN:HG3	1.74	0.88
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.89	0.88
7:G:77:VAL:HG12	7:G:137:THR:HB	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:GLN:HE21	3:C:164:THR:H	1.15	0.88
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.73	0.87
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.56	0.87
3:C:163:GLN:NE2	3:C:164:THR:H	1.72	0.87
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	1.89	0.87
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	1.88	0.87
13:O:149:GLN:NE2	13:O:149:GLN:H	1.73	0.87
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.40	0.86
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.88	0.86
10:X:156:LYS:O	10:X:160:GLN:HG3	1.74	0.86
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.19	0.86
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.88	0.86
14:1:84:LYS:HG3	14:1:119:VAL:HG22	1.56	0.86
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.58	0.85
7:U:77:VAL:HG12	7:U:137:THR:HB	1.58	0.85
2:B:163:ILE:HD13	2:B:164:SER:H	1.39	0.85
11:K:143:LYS:O	11:K:146:LEU:HD13	1.76	0.85
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.20	0.85
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.57	0.85
10:J:168:MET:CE	10:X:168:MET:HE3	2.02	0.85
3:Q:52:ARG:NH2	3:Q:211:GLU:HB3	1.91	0.85
5:S:214:ILE:HD12	5:S:215:VAL:N	1.92	0.85
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.58	0.85
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.21	0.85
3:C:52:ARG:NH2	3:C:211:GLU:HB3	1.92	0.84
10:J:168:MET:HE3	10:X:168:MET:CE	2.02	0.84
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.21	0.84
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.75	0.84
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.42	0.83
2:B:15:PHE:H	3:C:23:GLN:HE22	1.26	0.83
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.43	0.83
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.61	0.83
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.92	0.82
13:M:149:GLN:H	13:M:149:GLN:HE21	1.27	0.82
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.43	0.82
3:C:185:THR:HG22	3:C:187:GLU:H	1.44	0.82
6:F:192:GLN:O	6:F:196:ILE:HG12	1.80	0.82
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.95	0.82
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	1.94	0.81
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.44	0.81
14:N:126:ILE:HD13	14:N:126:ILE:H	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:69:VAL:HG12	16:T:306:HOH:O	1.78	0.81
2:B:185:LYS:HD3	2:B:186:VAL:N	1.97	0.80
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.81	0.80
13:O:149:GLN:H	13:O:149:GLN:HE21	1.30	0.80
6:T:192:GLN:O	6:T:196:ILE:HG12	1.82	0.80
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.79	0.80
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.63	0.80
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	1.97	0.80
13:O:157:ASN:HD22	13:O:160:ARG:HH11	1.29	0.79
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.31	0.79
7:U:217:LYS:HA	7:U:217:LYS:HE3	1.62	0.79
7:U:87:ASN:C	7:U:87:ASN:HD22	1.90	0.79
2:P:185:LYS:HD3	2:P:186:VAL:N	1.97	0.79
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.45	0.79
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.65	0.78
11:Y:210:ILE:HB	16:Y:539:HOH:O	1.83	0.78
7:G:87:ASN:C	7:G:87:ASN:HD22	1.91	0.78
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.96	0.78
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.66	0.78
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.48	0.78
14:1:126:ILE:HD13	14:1:126:ILE:H	1.49	0.78
5:E:214:ILE:HD12	5:E:215:VAL:N	1.99	0.77
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.47	0.77
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.83	0.77
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.66	0.77
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.66	0.77
3:C:33:ARG:NH1	3:C:33:ARG:HB2	1.98	0.77
2:P:163:ILE:CD1	2:P:164:SER:H	1.98	0.77
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.67	0.77
13:O:76:PRO:HD2	13:O:105:GLN:OE1	1.85	0.77
11:K:142:TYR:O	11:K:143:LYS:HD2	1.85	0.77
2:P:71:ASN:ND2	2:P:72:ASP:N	2.33	0.77
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.32	0.76
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.67	0.76
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.67	0.76
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.67	0.76
12:L:123:GLN:HG3	12:L:145:TYR:OH	1.86	0.76
2:B:71:ASN:ND2	2:B:72:ASP:N	2.34	0.75
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.69	0.75
3:C:163:GLN:HE21	3:C:164:THR:N	1.84	0.75
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	1.86	0.75
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.67	0.75
2:B:163:ILE:CD1	2:B:164:SER:H	1.99	0.75
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.69	0.75
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.87	0.75
1:O:179:ARG:HB3	1:O:179:ARG:HH11	1.50	0.75
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.50	0.74
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.87	0.74
6:F:35:THR:HG21	6:F:51:GLU:O	1.87	0.74
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.50	0.74
14:N:51:ASP:O	14:N:55:ILE:HD12	1.86	0.74
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.01	0.74
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.88	0.74
11:K:184:TRP:C	11:K:185:ILE:HD13	2.11	0.73
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.88	0.73
14:1:51:ASP:O	14:1:55:ILE:HD12	1.86	0.73
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.34	0.73
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.68	0.73
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.01	0.73
11:Y:184:TRP:C	11:Y:185:ILE:HD13	2.14	0.73
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.88	0.73
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.69	0.73
14:1:146:MET:HE2	14:1:150:GLU:HB3	1.70	0.73
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.52	0.73
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.01	0.73
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.03	0.73
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.69	0.73
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.89	0.73
3:C:33:ARG:HH11	3:C:33:ARG:CB	2.02	0.72
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.71	0.72
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.54	0.72
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.71	0.72
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.38	0.72
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.87	0.72
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.05	0.71
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.36	0.71
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.72	0.71
3:C:35:THR:HB	3:C:51:GLU:HG3	1.72	0.71
6:T:35:THR:HG21	6:T:51:GLU:O	1.91	0.71
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.72	0.71
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.03	0.71
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.71	0.71
7:G:96:ALA:HA	7:G:107:MET:CE	2.20	0.71
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.25	0.71
6:F:122:ALA:HA	6:F:125:LEU:HD12	1.71	0.71
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.74	0.70
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.73	0.70
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.55	0.70
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.73	0.70
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.72	0.70
7:U:96:ALA:HA	7:U:107:MET:CE	2.20	0.70
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.74	0.70
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.07	0.70
14:1:36:ARG:HG3	14:1:42:TRP:CE2	2.26	0.70
13:O:37:VAL:HG11	13:O:79:ILE:HD13	1.74	0.70
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.22	0.70
4:D:162:ALA:HB3	5:E:58:LEU:HD23	1.73	0.70
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.73	0.69
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.72	0.69
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.72	0.69
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.36	0.69
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.74	0.69
14:N:161:GLN:HE21	14:1:136:GLY:CA	1.99	0.69
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.75	0.69
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.75	0.69
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.74	0.69
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.73	0.69
6:T:68:GLN:HA	16:T:312:HOH:O	1.91	0.69
10:J:133:TYR:HE1	16:X:222:HOH:O	1.75	0.69
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.90	0.69
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.74	0.68
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.04	0.68
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.27	0.68
13:O:6:MET:HG2	13:O:155:ILE:HD11	1.74	0.68
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.76	0.68
3:C:15:PHE:H	4:D:23:GLN:HE22	1.39	0.68
3:C:232:TYR:O	3:C:236:ILE:HG13	1.94	0.68
2:B:27:ALA:O	2:B:31:ILE:HG12	1.94	0.68
13:M:37:VAL:HG11	13:M:79:ILE:HD13	1.75	0.68
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.76	0.68
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:142:TYR:C	11:K:143:LYS:HD2	2.19	0.68
13:M:211:ILE:HG12	16:M:243:HOH:O	1.93	0.68
1:O:121:GLN:O	1:O:124:THR:HB	1.94	0.67
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.24	0.67
6:T:122:ALA:HA	6:T:125:LEU:HD12	1.75	0.67
14:1:36:ARG:HG3	14:1:42:TRP:CZ2	2.29	0.67
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.76	0.67
4:R:140:GLY:HA2	4:R:215:ILE:HG12	1.74	0.67
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.75	0.67
12:L:1(I):ASN:O	12:L:14(K):LYS:HG2	1.94	0.67
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.76	0.67
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.10	0.67
3:Q:211:GLU:C	3:Q:212:ILE:HD13	2.19	0.67
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.76	0.67
11:K:104:TYR:CE2	11:K:108:PRO:HG3	2.30	0.67
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.76	0.67
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.77	0.67
13:M:40:ASN:HD22	13:M:40:ASN:H	1.43	0.67
2:P:87:ILE:O	2:P:91:THR:HG23	1.95	0.67
7:U:218:ASP:O	7:U:220:LYS:HB2	1.95	0.67
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.77	0.66
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.77	0.66
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.77	0.66
14:1:112:THR:HG22	14:1:120:HIS:HB2	1.77	0.66
1:A:121:GLN:O	1:A:124:THR:HB	1.94	0.66
2:B:87:ILE:O	2:B:91:THR:HG23	1.95	0.66
9:I:6:MET:HE1	9:I:155:ILE:HA	1.78	0.66
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.93	0.66
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.08	0.66
3:Q:101:LEU:HD11	10:X:57:GLU:HB3	1.77	0.66
3:C:41:LYS:HG2	3:C:161:SER:O	1.94	0.66
3:C:177:GLU:OE2	4:D:57:PRO:HD2	1.95	0.66
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.44	0.66
7:G:77:VAL:CG1	7:G:137:THR:HB	2.25	0.66
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.61	0.66
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.78	0.66
12:Z:-6:PRO:O	13:O:91:ARG:NH1	2.29	0.66
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.10	0.66
7:G:198:ILE:HG23	7:G:203:THR:O	1.95	0.66
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.76	0.66
13:M:57:ARG:NE	16:M:245:HOH:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:177:GLU:HG2	2:P:58:LEU:HD22	1.78	0.66
11:Y:104:TYR:CE2	11:Y:108:PRO:HG3	2.31	0.66
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.78	0.66
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.78	0.66
10:X:63:ILE:HD11	10:X:79:VAL:HG13	1.77	0.66
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.94	0.66
10:J:63:ILE:HD11	10:J:79:VAL:HG13	1.77	0.66
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.09	0.66
2:P:163:ILE:HD13	2:P:164:SER:H	1.61	0.66
2:P:163:ILE:HD12	2:P:164:SER:N	2.11	0.66
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.78	0.66
3:C:211:GLU:C	3:C:212:ILE:HD13	2.21	0.65
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.77	0.65
1:A:188:ASP:O	1:A:192:ILE:HG12	1.96	0.65
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.77	0.65
7:U:130:ARG:HB2	16:U:293:HOH:O	1.96	0.65
16:X:222:HOH:O	11:Y:132:THR:HG22	1.95	0.65
16:B:254:HOH:O	3:C:62(A):ILE:HD11	1.95	0.65
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.78	0.65
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.32	0.65
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.78	0.65
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.94	0.65
7:U:77:VAL:CG1	7:U:137:THR:HB	2.26	0.65
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.26	0.65
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.77	0.65
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.32	0.65
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.78	0.65
1:A:67:VAL:HB	1:A:223:LYS:NZ	2.12	0.65
2:B:108:PRO:HB2	2:B:111:ILE:HD12	1.79	0.65
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.78	0.65
1:O:86:ARG:NE	7:U:118:ASN:HD21	1.82	0.65
2:P:234:VAL:HA	2:P:239:THR:HA	1.79	0.65
6:T:79:SER:HA	16:T:316:HOH:O	1.96	0.65
13:O:40:ASN:H	13:O:40:ASN:HD22	1.41	0.65
1:A:170:VAL:HB	16:A:253:HOH:O	1.96	0.65
2:P:27:ALA:O	2:P:31:ILE:HG12	1.97	0.65
5:S:73:HIS:HE1	5:S:107:LEU:O	1.79	0.65
12:Z:1(I):ASN:O	12:Z:14(K):LYS:HG2	1.97	0.65
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.77	0.65
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.32	0.65
4:R:24:VAL:O	4:R:28:LEU:HD22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:121:GLN:O	7:U:124:THR:HB	1.96	0.65
5:E:73:HIS:HE1	5:E:107:LEU:O	1.80	0.65
7:U:59:LEU:O	7:U:61:PRO:HD3	1.96	0.65
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.77	0.64
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.79	0.64
14:N:105:ASP:OD2	14:N:106:ASN:N	2.30	0.64
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.21	0.64
7:G:218:ASP:O	7:G:220:LYS:HB2	1.96	0.64
11:K:73:ARG:NH2	11:K:104:TYR:O	2.30	0.64
1:O:188:ASP:O	1:O:192:ILE:HG12	1.97	0.64
1:O:67:VAL:HB	1:O:223:LYS:HZ1	1.62	0.64
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.33	0.64
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.28	0.64
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.80	0.64
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.63	0.64
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.80	0.64
2:P:163:ILE:CD1	2:P:164:SER:N	2.61	0.64
8:V:18:THR:HB	8:V:30:ASN:HD22	1.63	0.64
10:X:44:SER:OG	10:X:100:LEU:HB2	1.98	0.64
12:Z:109:ALA:HA	16:Z:207:HOH:O	1.98	0.64
5:E:231:LYS:H	5:E:231:LYS:HD2	1.63	0.64
16:L:201:HOH:O	9:W:192:ARG:HG3	1.96	0.64
10:X:52:THR:HG23	10:X:53:VAL:N	2.13	0.64
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.28	0.64
1:A:86:ARG:NE	7:G:118:ASN:HD21	1.89	0.63
7:G:177:GLU:O	7:G:17(B):LYS:HG3	1.99	0.63
14:N:136:GLY:CA	14:1:161:GLN:HE21	1.99	0.63
5:S:231:LYS:H	5:S:231:LYS:HD2	1.63	0.63
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.80	0.63
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.78	0.63
6:F:33:ASN:HB2	16:F:326:HOH:O	1.98	0.63
10:J:52:THR:HG23	10:J:53:VAL:N	2.13	0.63
6:T:173:LYS:O	6:T:177:GLU:HG3	1.98	0.63
9:W:101:VAL:O	9:W:110:ILE:HA	1.98	0.63
2:P:163:ILE:HD12	2:P:164:SER:H	1.64	0.63
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.33	0.63
7:G:121:GLN:O	7:G:124:THR:HB	1.97	0.63
2:P:71:ASN:HD22	2:P:72:ASP:H	1.42	0.63
6:T:127:ASN:HD22	6:T:127:ASN:N	1.96	0.63
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.79	0.63
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:VAL:HA	2:B:239:THR:HA	1.80	0.63
5:S:198:SER:HA	5:S:201:LEU:HG	1.81	0.63
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.81	0.63
5:E:198:SER:HA	5:E:201:LEU:HG	1.80	0.63
11:K:208:ASN:HD21	9:W:29:ASN:HD21	1.45	0.63
2:P:202:THR:HG22	2:P:204:SER:N	2.09	0.63
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.81	0.63
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.81	0.62
1:O:69:LEU:C	1:O:69:LEU:HD23	2.24	0.62
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.80	0.62
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.99	0.62
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.62	0.62
8:V:128:GLY:O	8:V:131:SER:HB2	1.98	0.62
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.81	0.62
6:F:127:ASN:N	6:F:127:ASN:HD22	1.97	0.62
10:J:141:HIS:HB2	10:J:154:LEU:HD11	1.82	0.62
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.80	0.62
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.64	0.62
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.79	0.62
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.80	0.62
5:E:132:TYR:O	5:E:153:PRO:HB3	1.99	0.62
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.81	0.62
13:O:157:ASN:ND2	13:O:160:ARG:HH11	1.96	0.62
2:B:163:ILE:CD1	2:B:164:SER:N	2.62	0.62
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.82	0.62
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.80	0.62
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.82	0.62
7:U:16:SER:HA	16:U:316:HOH:O	2.00	0.62
7:U:87:ASN:C	7:U:87:ASN:ND2	2.56	0.62
11:Y:12:ILE:HG13	11:Y:108:PRO:HB3	1.81	0.62
11:Y:74:ILE:HG13	11:Y:75:SER:N	2.13	0.62
2:B:112:LEU:HD23	2:B:112:LEU:C	2.25	0.62
7:G:93:LYS:HD3	14:N:68:SER:HB3	1.82	0.62
11:K:12:ILE:HG13	11:K:108:PRO:HB3	1.82	0.62
5:S:15:PHE:H	6:T:23:GLN:HE22	1.46	0.62
8:H:18:THR:HB	8:H:30:ASN:HD22	1.65	0.62
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.15	0.62
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.35	0.62
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.64	0.61
8:V:34:LEU:HD22	8:V:174:ASP:HB3	1.81	0.61
4:D:24:VAL:O	4:D:28:LEU:HD22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:173:LYS:O	6:F:177:GLU:HG3	2.00	0.61
7:G:172:ILE:HD11	7:G:201:LEU:CD2	2.30	0.61
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.82	0.61
1:O:67:VAL:HB	1:O:223:LYS:NZ	2.15	0.61
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.35	0.61
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	1.82	0.61
10:J:63:ILE:CD1	10:J:79:VAL:HG13	2.31	0.61
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.34	0.61
3:Q:14:ILE:HB	4:R:23:GLN:NE2	2.15	0.61
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.65	0.61
2:P:112:LEU:HD23	2:P:112:LEU:C	2.24	0.61
10:X:141:HIS:HB2	10:X:154:LEU:HD11	1.81	0.61
14:1:175:MET:HB2	14:1:187:LEU:HB2	1.82	0.61
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.36	0.61
1:O:197:LEU:O	1:O:202:VAL:HG23	2.01	0.61
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.01	0.61
1:A:197:LEU:O	1:A:202:VAL:HG23	2.01	0.61
8:H:5:GLY:O	8:H:124:TYR:HA	2.01	0.61
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.00	0.61
10:X:-1:MET:CG	10:X:1:ASP:H	2.12	0.61
14:1:44:CYS:HB2	14:1:100:ILE:HB	1.83	0.61
14:1:105:ASP:OD2	14:1:106:ASN:N	2.32	0.61
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.63	0.61
12:L:166:HIS:HD2	12:L:168:GLN:H	1.46	0.61
10:X:63:ILE:CD1	10:X:79:VAL:HG13	2.29	0.61
3:C:14:ILE:HB	4:D:23:GLN:NE2	2.16	0.61
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.66	0.61
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.83	0.61
9:I:104:ILE:HD12	9:I:178:ILE:HG22	1.83	0.61
12:L:178:VAL:HG22	12:L:184:VAL:HG22	1.82	0.61
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.82	0.61
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.64	0.61
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.31	0.60
5:E:227:GLU:N	5:E:227:GLU:CD	2.59	0.60
11:K:74:ILE:HG13	11:K:75:SER:N	2.15	0.60
12:Z:-7:ASN:C	12:Z:-7:ASN:HD22	2.09	0.60
1:A:69:LEU:HD23	1:A:69:LEU:C	2.25	0.60
10:J:133:TYR:CE1	16:X:222:HOH:O	2.50	0.60
5:S:220:PRO:O	5:S:222:THR:HG23	2.00	0.60
12:Z:21:ILE:C	12:Z:21:ILE:HD12	2.26	0.60
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.97	0.60
7:U:198:ILE:HG23	7:U:203:THR:O	2.01	0.60
8:V:196:VAL:HG23	16:V:520:HOH:O	2.00	0.60
2:B:202:THR:HG22	2:B:204:SER:N	2.11	0.60
3:C:182:PRO:O	3:C:184:ALA:N	2.35	0.60
13:M:40:ASN:HD22	13:M:40:ASN:N	1.98	0.60
9:W:6:MET:HE1	9:W:155:ILE:HA	1.82	0.60
10:X:190:PHE:C	10:X:192:ALA:H	2.10	0.60
11:K:99:THR:HG22	11:K:113:VAL:O	2.01	0.60
10:X:42:LEU:HB2	10:X:184:ILE:HD13	1.82	0.60
7:G:59:LEU:O	7:G:61:PRO:HD3	2.02	0.60
1:O:60:MET:HB3	1:O:62:GLU:OE1	2.02	0.60
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.83	0.60
14:1:48:SER:HB3	14:1:51:ASP:HB2	1.84	0.60
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.84	0.60
14:1:84:LYS:HG3	14:1:119:VAL:CG2	2.30	0.60
8:H:34:LEU:HD22	8:H:174:ASP:HB3	1.82	0.60
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.83	0.60
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.65	0.60
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.84	0.60
2:P:71:ASN:HD22	2:P:72:ASP:N	1.96	0.60
2:P:79:ALA:HA	16:P:281:HOH:O	2.02	0.60
6:F:63:LYS:O	6:F:65:VAL:N	2.34	0.60
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.02	0.60
11:K:208:ASN:ND2	9:W:29:ASN:HD21	1.99	0.59
14:N:21:THR:HG22	14:N:26:ILE:HA	1.84	0.59
5:S:227:GLU:CD	5:S:227:GLU:N	2.60	0.59
7:U:17:PRO:HD3	16:U:316:HOH:O	2.01	0.59
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.31	0.59
9:W:104:ILE:HD12	9:W:178:ILE:HG22	1.83	0.59
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.03	0.59
2:B:181:LYS:O	2:B:184:MET:HG3	2.03	0.59
5:E:220:PRO:O	5:E:222:THR:HG23	2.02	0.59
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.85	0.59
10:J:44:SER:OG	10:J:100:LEU:HB2	2.02	0.59
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.38	0.59
2:P:108:PRO:HB2	2:P:111:ILE:HD12	1.85	0.59
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.84	0.59
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.14	0.59
7:U:225:SER:O	7:U:229:ILE:HD12	2.03	0.59
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:212:LEU:HD23	1:O:212:LEU:C	2.28	0.59
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.86	0.59
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	2.01	0.59
3:C:107:VAL:HA	16:C:260:HOH:O	2.02	0.59
5:E:226:GLY:O	5:E:229:VAL:HG22	2.02	0.59
5:S:132:TYR:O	5:S:153:PRO:HB3	2.02	0.59
6:T:63:LYS:O	6:T:65:VAL:N	2.34	0.59
6:T:109:ILE:N	6:T:109:ILE:CD1	2.65	0.59
6:T:109:ILE:HD13	6:T:142:ASP:HB3	1.82	0.59
7:U:53:LYS:O	7:U:55:PRO:HD3	2.02	0.59
14:1:21:THR:HG22	14:1:26:ILE:HA	1.83	0.59
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.38	0.59
9:I:101:VAL:O	9:I:110:ILE:HA	2.02	0.59
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.83	0.59
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.66	0.59
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.85	0.59
4:R:86:ARG:HB2	16:R:1021:HOH:O	2.02	0.59
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.32	0.59
8:V:208:ARG:HG3	16:V:537:HOH:O	2.00	0.59
9:W:29:ASN:ND2	9:W:29:ASN:H	2.01	0.59
6:F:109:ILE:N	6:F:109:ILE:CD1	2.65	0.59
7:G:122:ILE:HA	16:G:273:HOH:O	2.02	0.59
3:Q:224:LEU:CD1	3:Q:224:LEU:H	2.15	0.59
7:U:172:ILE:HD11	7:U:201:LEU:CD2	2.32	0.59
8:V:5:GLY:O	8:V:124:TYR:HA	2.03	0.59
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.35	0.59
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.03	0.59
3:C:185:THR:HB	3:C:188:GLU:HG2	1.84	0.59
6:F:109:ILE:HD13	6:F:109:ILE:H	1.68	0.59
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.33	0.59
2:P:137:ILE:HD11	2:P:165:VAL:HG22	1.85	0.59
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.85	0.58
9:I:29:ASN:ND2	9:I:29:ASN:H	2.01	0.58
2:P:181:LYS:O	2:P:184:MET:HG3	2.03	0.58
4:R:177:LEU:HD13	5:S:58:LEU:HD11	1.84	0.58
7:U:8:TYR:C	7:U:10:ARG:H	2.11	0.58
8:V:84:LYS:HG3	8:V:85:GLN:N	2.18	0.58
6:F:90:ASN:O	6:F:94:GLU:HG3	2.03	0.58
10:J:135:PHE:HB3	11:Y:165:ARG:HE	1.67	0.58
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.03	0.58
13:O:179:ASP:HB3	13:O:18(A):THR:OG1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.68	0.58
3:C:185:THR:HG22	3:C:187:GLU:N	2.14	0.58
7:G:8:TYR:C	7:G:10:ARG:H	2.10	0.58
13:M:197:TRP:CH2	14:1:171:GLY:HA2	2.38	0.58
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.03	0.58
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.86	0.58
5:S:226:GLY:O	5:S:229:VAL:HG22	2.04	0.58
2:B:163:ILE:HD13	2:B:164:SER:N	2.13	0.58
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.66	0.58
13:M:184:LEU:HD23	13:M:184:LEU:C	2.28	0.58
1:A:60:MET:HB3	1:A:62:GLU:OE1	2.02	0.58
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.85	0.58
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.86	0.58
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.86	0.58
2:B:141:TYR:CD1	2:B:141:TYR:C	2.82	0.58
5:E:207:LEU:HD23	5:E:207:LEU:H	1.68	0.58
3:Q:182:PRO:O	3:Q:184:ALA:N	2.37	0.58
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.86	0.58
14:1:133:PHE:HE2	14:1:166:ASP:HB2	1.67	0.58
3:C:227:GLU:H	3:C:227:GLU:CD	2.11	0.58
8:H:128:GLY:O	8:H:131:SER:HB2	2.04	0.58
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.10	0.58
1:O:62:GLU:CD	1:O:62:GLU:H	2.12	0.58
7:U:72:ARG:HG2	16:U:321:HOH:O	2.03	0.58
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.39	0.58
2:B:71:ASN:HD22	2:B:72:ASP:N	1.99	0.58
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.66	0.58
12:L:135:MET:CE	9:W:165:ARG:NH2	2.66	0.58
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.04	0.58
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.86	0.58
4:D:192:LEU:O	4:D:196:ILE:HG13	2.04	0.58
10:J:190:PHE:C	10:J:192:ALA:H	2.10	0.58
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.69	0.58
11:Y:111:TYR:CE1	11:Y:121:LYS:HB2	2.39	0.58
3:C:224:LEU:CD1	3:C:224:LEU:H	2.17	0.57
5:E:15:PHE:H	6:F:23:GLN:HE22	1.50	0.57
7:G:151:THR:HG22	7:G:157:TYR:CB	2.34	0.57
8:H:24:PRO:HG2	8:H:25:ILE:HD13	1.86	0.57
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.86	0.57
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.86	0.57
5:S:49:VAL:HG13	5:S:212:ILE:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.19	0.57
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.85	0.57
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.85	0.57
6:F:69:VAL:HG12	16:F:289:HOH:O	2.04	0.57
12:L:14(H):GLY:C	12:L:1(I):ASN:H	2.12	0.57
14:N:133:PHE:HE2	14:N:166:ASP:HB2	1.69	0.57
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.39	0.57
8:V:106:THR:HG21	16:V:511:HOH:O	2.03	0.57
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.34	0.57
10:J:-1:MET:CG	10:J:1:ASP:H	2.12	0.57
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.70	0.57
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.18	0.57
1:A:212:LEU:HD23	1:A:212:LEU:C	2.29	0.57
3:C:36:CYS:H	3:C:51:GLU:HG2	1.69	0.57
3:C:190:VAL:O	3:C:194:VAL:HG23	2.05	0.57
7:G:53:LYS:O	7:G:55:PRO:HD3	2.04	0.57
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.34	0.57
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.34	0.57
1:A:62:GLU:CD	1:A:62:GLU:H	2.12	0.57
11:K:13:ILE:HD12	11:K:152:LEU:HD23	1.85	0.57
11:K:25:TRP:CH2	12:L:132:SER:HA	2.39	0.57
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.69	0.57
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.04	0.57
10:X:52:THR:CG2	10:X:53:VAL:N	2.67	0.57
10:X:156:LYS:HE2	10:X:160:GLN:NE2	2.19	0.57
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.35	0.57
7:G:87:ASN:C	7:G:87:ASN:ND2	2.59	0.57
11:K:184:TRP:O	11:K:185:ILE:HD13	2.04	0.57
12:L:21:ILE:C	12:L:21:ILE:HD12	2.30	0.57
13:M:91:ARG:HG3	13:M:92:SER:N	2.18	0.57
1:O:159:PRO:O	2:P:59:LEU:HD12	2.04	0.57
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.85	0.57
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.85	0.57
11:K:7:ARG:HD2	11:K:108:PRO:O	2.04	0.57
6:T:109:ILE:N	6:T:109:ILE:HD12	2.18	0.57
6:T:136:THR:O	6:T:150:MET:HA	2.05	0.57
10:X:44:SER:HG	10:X:100:LEU:HB2	1.70	0.57
13:O:152:GLU:O	13:O:156:VAL:HG23	2.04	0.57
10:J:-1:MET:HG2	10:J:1:ASP:N	2.14	0.57
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.12	0.57
10:X:90(A):ILE:HG12	10:X:116:LEU:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.87	0.57
13:0:12:VAL:HG21	13:0:102:ALA:HB1	1.87	0.57
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.87	0.57
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.05	0.57
6:F:63:LYS:O	6:F:65:VAL:HG23	2.05	0.57
6:F:91:ARG:O	6:F:95:GLU:HB2	2.05	0.57
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.02	0.56
2:B:121:GLN:O	2:B:124:THR:HB	2.05	0.56
6:F:136:THR:O	6:F:150:MET:HA	2.05	0.56
14:N:30:VAL:HG11	13:0:199:PHE:CE2	2.40	0.56
6:T:91:ARG:O	6:T:95:GLU:HB2	2.05	0.56
3:C:228:GLU:O	3:C:232:TYR:HD1	1.89	0.56
11:K:165:ARG:HE	10:X:135:PHE:HB3	1.70	0.56
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.20	0.56
6:T:90:ASN:O	6:T:94:GLU:HG3	2.05	0.56
8:V:200:LYS:HE3	9:W:140:SER:O	2.05	0.56
2:B:71:ASN:HD22	2:B:72:ASP:H	1.45	0.56
5:E:45:HIS:HB3	5:E:214:ILE:HD11	1.88	0.56
10:J:52:THR:CG2	10:J:53:VAL:N	2.68	0.56
10:J:74:LEU:HD23	16:J:205:HOH:O	2.05	0.56
5:S:207:LEU:HD23	5:S:207:LEU:H	1.69	0.56
6:T:63:LYS:O	6:T:65:VAL:HG23	2.05	0.56
9:I:154:THR:HG23	16:I:224:HOH:O	2.04	0.56
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.87	0.56
8:V:25:ILE:HD13	8:V:25:ILE:N	2.21	0.56
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.86	0.56
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.41	0.56
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.40	0.56
12:Z:14(H):GLY:C	12:Z:1(I):ASN:H	2.13	0.56
2:P:141:TYR:CD1	2:P:141:TYR:C	2.83	0.56
7:U:228:ASN:HB3	16:U:295:HOH:O	2.04	0.56
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.06	0.56
13:0:51:ASP:O	13:0:55:ILE:HD12	2.05	0.56
14:1:61:TYR:HA	16:1:214:HOH:O	2.05	0.56
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.71	0.56
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.38	0.56
4:R:85:ALA:O	4:R:89:ILE:HG12	2.05	0.56
5:S:45:HIS:HB3	5:S:214:ILE:HD11	1.88	0.56
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.05	0.56
11:Y:9:GLN:CD	11:Y:10:GLY:N	2.64	0.56
4:D:112:LEU:C	4:D:112:LEU:HD13	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:LYS:HG3	8:H:85:GLN:N	2.20	0.56
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.87	0.56
7:U:172:ILE:HD12	7:U:197:MET:CE	2.36	0.56
7:U:18(A):ILE:CD1	7:U:18(C):HIS:O	2.53	0.56
13:O:19:LEU:HD21	13:O:26:LEU:HD22	1.87	0.56
3:C:55:THR:O	3:C:56:LEU:HD22	2.05	0.56
8:H:105:ASP:O	8:H:106:THR:N	2.38	0.56
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.53	0.56
3:Q:224:LEU:H	3:Q:224:LEU:HD12	1.70	0.56
4:D:177:LEU:HD13	5:E:58:LEU:CD1	2.36	0.56
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.41	0.56
13:M:13:ILE:HB	13:M:155:ILE:HD12	1.88	0.56
2:P:38:ILE:HG13	2:P:164:SER:HB3	1.88	0.56
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.41	0.56
14:1:8:PHE:CE1	14:1:10:ASP:HB2	2.41	0.56
14:1:19:ARG:HG3	14:1:26:ILE:HG23	1.88	0.56
5:E:207:LEU:H	5:E:207:LEU:CD2	2.19	0.55
11:K:45:MET:HG3	11:K:52:CYS:HB2	1.88	0.55
8:V:148:LYS:O	8:V:152:ILE:HG13	2.05	0.55
13:O:157:ASN:HD22	13:O:160:ARG:NH1	2.03	0.55
7:G:172:ILE:HD12	7:G:197:MET:CE	2.37	0.55
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.06	0.55
10:X:113:ILE:HA	10:X:118:THR:O	2.06	0.55
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.06	0.55
13:O:14(D):GLU:O	13:O:14(G):ILE:HG13	2.05	0.55
2:B:38:ILE:HG13	2:B:164:SER:HB3	1.88	0.55
3:C:173:ARG:O	3:C:177:GLU:HG3	2.07	0.55
3:C:224:LEU:HD12	3:C:224:LEU:N	2.22	0.55
4:D:227:GLU:OE2	4:D:227:GLU:N	2.34	0.55
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.71	0.55
9:I:6:MET:CE	9:I:155:ILE:HA	2.36	0.55
10:J:156:LYS:HE2	10:J:160:GLN:NE2	2.21	0.55
11:K:4:LEU:HD11	11:K:159:ILE:HG12	1.89	0.55
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.42	0.55
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.33	0.55
13:O:41:THR:OG1	13:O:76:PRO:HG3	2.06	0.55
2:B:194:LEU:HD12	2:B:236:THR:HG21	1.88	0.55
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.35	0.55
8:H:165:ASN:ND2	13:O:139:ARG:HH11	2.04	0.55
13:M:152:GLU:O	13:M:156:VAL:HG23	2.06	0.55
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:VAL:O	3:C:190:VAL:HG23	2.07	0.55
7:G:18(A):ILE:CD1	7:G:18(C):HIS:O	2.53	0.55
8:H:196:VAL:HG23	16:H:521:HOH:O	2.06	0.55
11:K:32:LYS:N	11:K:32:LYS:HD2	2.22	0.55
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.42	0.55
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.06	0.55
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.87	0.55
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.07	0.55
4:R:205:GLU:HA	4:R:205:GLU:OE2	2.06	0.55
11:Y:4:LEU:HD11	11:Y:159:ILE:HG12	1.89	0.55
11:Y:45:MET:HG3	11:Y:52:CYS:HB2	1.89	0.55
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.07	0.55
2:B:224:PHE:N	2:B:224:PHE:CD2	2.75	0.55
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.36	0.55
5:S:207:LEU:H	5:S:207:LEU:CD2	2.20	0.55
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.88	0.55
3:C:227:GLU:OE1	3:C:227:GLU:N	2.37	0.55
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.37	0.55
14:1:133:PHE:CE2	14:1:166:ASP:HB2	2.41	0.55
2:B:15:PHE:N	3:C:23:GLN:HE22	2.02	0.55
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.42	0.55
3:C:121:GLN:NE2	3:C:121:GLN:C	2.65	0.55
3:C:122:ARG:NH2	16:C:280:HOH:O	2.39	0.55
4:D:85:ALA:O	4:D:89:ILE:HG12	2.07	0.55
10:J:190:PHE:HA	10:J:193:GLN:HB2	1.89	0.55
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.42	0.55
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.89	0.55
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.89	0.55
13:0:178:ILE:CD1	13:0:184:LEU:HG	2.36	0.55
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.21	0.55
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.02	0.55
13:M:199:PHE:CE2	14:1:30:VAL:HG11	2.41	0.55
8:H:200:LYS:HE3	9:I:140:SER:O	2.06	0.54
10:J:113:ILE:HA	10:J:118:THR:O	2.07	0.54
11:K:9:GLN:CD	11:K:10:GLY:N	2.65	0.54
11:K:207:ASN:HD21	10:X:144:PRO:HG2	1.73	0.54
12:L:163:THR:HG21	16:L:247:HOH:O	2.06	0.54
3:Q:57:LYS:HG2	3:Q:208:LYS:NZ	2.23	0.54
3:Q:87:ILE:HD13	3:Q:87:ILE:N	2.21	0.54
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.71	0.54
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:PHE:N	2:B:224:PHE:HD2	2.04	0.54
8:H:148:LYS:O	8:H:152:ILE:HG13	2.07	0.54
8:H:218:ILE:N	8:H:218:ILE:HD13	2.23	0.54
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.88	0.54
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.07	0.54
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.06	0.54
6:T:127:ASN:HD22	6:T:127:ASN:H	1.53	0.54
10:J:2:ILE:O	10:J:3:ILE:HD13	2.07	0.54
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.23	0.54
13:M:51:ASP:O	13:M:55:ILE:HD12	2.07	0.54
14:N:6:VAL:HG23	14:N:155:ILE:HD11	1.89	0.54
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.07	0.54
2:P:121:GLN:O	2:P:124:THR:HB	2.06	0.54
2:P:185:LYS:HD3	2:P:186:VAL:H	1.72	0.54
7:U:151:THR:HG22	7:U:157:TYR:CB	2.37	0.54
14:1:18(G):TYR:HA	14:1:18(J):LEU:HG	1.88	0.54
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.38	0.54
3:C:57:LYS:HG2	3:C:208:LYS:NZ	2.23	0.54
3:C:224:LEU:H	3:C:224:LEU:HD12	1.72	0.54
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.36	0.54
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.38	0.54
11:K:33:LYS:HE2	15:K:500:GDT:H29	1.88	0.54
11:K:67:GLU:CD	11:K:73:ARG:HA	2.33	0.54
11:K:200:LYS:HE3	11:K:206:PHE:O	2.07	0.54
3:Q:65:SER:HB2	16:Q:257:HOH:O	2.07	0.54
5:S:143:LYS:HD2	13:O:71(B):GLU:O	2.07	0.54
13:O:184:LEU:HD23	13:O:184:LEU:C	2.32	0.54
5:E:194:VAL:O	5:E:197:ILE:HG22	2.07	0.54
11:K:63:CYS:HB2	16:K:540:HOH:O	2.07	0.54
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.42	0.54
1:O:191:HIS:HE1	1:O:236:LEU:HA	1.72	0.54
2:P:6:ARG:HD2	4:R:9:ASP:N	2.22	0.54
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.22	0.54
14:N:171:GLY:HA2	13:O:197:TRP:CH2	2.42	0.54
1:O:86:ARG:NE	7:U:118:ASN:ND2	2.46	0.54
11:Y:33:LYS:HE2	15:Y:500:GDT:H29	1.88	0.54
4:D:40:ILE:HG13	4:D:193:VAL:HG23	1.89	0.54
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.36	0.54
4:R:42:THR:C	4:R:44:GLU:H	2.16	0.54
4:R:88:MET:HE2	4:R:116:VAL:CG1	2.38	0.54
4:R:112:LEU:HD13	4:R:112:LEU:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:32:LYS:N	11:Y:32:LYS:HD2	2.22	0.54
2:B:15:PHE:H	3:C:23:GLN:NE2	2.02	0.54
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.71	0.54
14:N:143:ARG:NH2	14:N:146:MET:HE3	2.23	0.54
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.89	0.54
1:A:17:PRO:HA	2:B:26:TYR:CD1	2.43	0.54
8:H:159:ILE:O	8:H:163:ILE:HD12	2.08	0.54
14:N:146:MET:CE	14:N:150:GLU:HB3	2.37	0.54
13:O:113:VAL:HA	13:O:118:VAL:O	2.08	0.54
1:A:191:HIS:HE1	1:A:236:LEU:HA	1.72	0.54
4:D:88:MET:HE2	4:D:116:VAL:CG1	2.38	0.54
7:G:192:PHE:C	7:G:192:PHE:CD1	2.85	0.54
8:H:165:ASN:HD22	13:O:139:ARG:HH11	1.56	0.54
12:L:177:ILE:HD12	12:L:177:ILE:N	2.22	0.54
3:Q:122:ARG:NH2	16:Q:261:HOH:O	2.40	0.54
4:R:177:LEU:HD13	5:S:58:LEU:CD1	2.36	0.54
7:U:79:ASN:HA	16:U:302:HOH:O	2.07	0.54
10:X:52:THR:CG2	10:X:53:VAL:H	2.21	0.54
11:Y:184:TRP:O	11:Y:185:ILE:HD13	2.08	0.54
13:O:40:ASN:HD22	13:O:40:ASN:N	1.97	0.54
6:F:121:GLN:NE2	16:F:300:HOH:O	2.41	0.53
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.89	0.53
8:V:172:ASN:ND2	8:V:193:THR:HA	2.23	0.53
7:G:225:SER:O	7:G:229:ILE:HD12	2.08	0.53
8:H:34:LEU:HB2	16:H:522:HOH:O	2.07	0.53
8:H:143:LYS:HG2	8:H:146:LEU:HD21	1.90	0.53
10:J:135:PHE:HB3	11:Y:165:ARG:NE	2.23	0.53
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.39	0.53
2:P:224:PHE:HD2	2:P:224:PHE:N	2.06	0.53
7:U:87:ASN:HD22	7:U:88:ALA:N	2.07	0.53
7:U:172:ILE:HD12	7:U:197:MET:HE2	1.91	0.53
10:X:39:PRO:HG2	10:X:73:GLU:CD	2.34	0.53
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.23	0.53
8:V:22:GLN:HG2	15:V:500:GDT:H36B	1.90	0.53
5:E:49:VAL:HG13	5:E:212:ILE:CD1	2.39	0.53
8:H:25:ILE:HD13	8:H:25:ILE:N	2.23	0.53
9:I:29:ASN:HD21	11:Y:208:ASN:HD21	1.55	0.53
13:M:149:GLN:NE2	13:M:149:GLN:N	2.49	0.53
14:N:133:PHE:CE2	14:N:166:ASP:HB2	2.43	0.53
1:O:150:GLN:O	1:O:157:TYR:HA	2.08	0.53
7:U:131:PRO:HB3	16:U:312:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.90	0.53
9:W:6:MET:CE	9:W:155:ILE:HA	2.38	0.53
4:D:29:GLU:OE2	4:D:32:LYS:HD2	2.08	0.53
13:O:8:TYR:CE2	13:O:148:VAL:HG22	2.43	0.53
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.56	0.53
7:G:30:ALA:O	7:G:33:GLN:HB2	2.08	0.53
7:G:172:ILE:HD12	7:G:197:MET:HE2	1.91	0.53
12:L:93:PHE:N	12:L:94:PRO:HD3	2.22	0.53
4:R:192:LEU:O	4:R:196:ILE:HG13	2.09	0.53
7:U:192:PHE:C	7:U:192:PHE:CD1	2.86	0.53
9:W:48:LEU:HG	9:W:50:THR:HG22	1.91	0.53
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.38	0.53
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.90	0.53
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.44	0.53
4:D:81:LEU:O	4:D:134:VAL:HB	2.09	0.53
10:J:162:LEU:O	10:J:166:MET:HB2	2.08	0.53
11:K:37:ILE:O	11:K:38:ASN:HB3	2.09	0.53
8:V:18:THR:CB	8:V:30:ASN:HD22	2.22	0.53
11:Y:38:ASN:O	11:Y:40:PHE:N	2.41	0.53
15:Y:500:GDT:H8	12:Z:96:TYR:CE2	2.44	0.53
13:O:149:GLN:NE2	13:O:149:GLN:N	2.52	0.53
2:B:74:ILE:C	2:B:221:GLN:HE22	2.17	0.53
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.90	0.53
5:E:227:GLU:CD	5:E:227:GLU:H	2.17	0.53
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.90	0.53
7:U:158:VAL:HG22	7:U:159:GLY:N	2.22	0.53
8:V:74:PRO:HA	16:V:516:HOH:O	2.09	0.53
11:Y:67:GLU:CD	11:Y:73:ARG:HA	2.33	0.53
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	1.99	0.53
14:1:146:MET:HE2	14:1:150:GLU:CB	2.39	0.53
9:I:104:ILE:HG21	9:I:181:LYS:HG2	1.91	0.53
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.44	0.53
3:Q:15:PHE:N	4:R:23:GLN:HE22	2.06	0.53
4:R:29:GLU:OE2	4:R:32:LYS:HD2	2.09	0.53
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.89	0.53
13:O:91:ARG:HG3	13:O:92:SER:N	2.24	0.53
13:O:205:GLY:HA3	13:O:209:GLN:HB3	1.91	0.53
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.91	0.53
9:I:48:LEU:HG	9:I:50:THR:HG22	1.90	0.53
10:J:90(A):ILE:HG12	10:J:116:LEU:HA	1.91	0.53
10:J:189:ASP:O	10:J:193:GLN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.67	0.53
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.09	0.53
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.90	0.53
11:Y:40:PHE:HB3	11:Y:73:ARG:HH21	1.73	0.53
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.43	0.52
2:B:137:ILE:HD11	2:B:165:VAL:HG22	1.90	0.52
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.91	0.52
2:P:224:PHE:N	2:P:224:PHE:CD2	2.77	0.52
5:S:214:ILE:HD12	5:S:215:VAL:H	1.70	0.52
6:T:109:ILE:CD1	6:T:109:ILE:H	2.21	0.52
7:U:30:ALA:O	7:U:33:GLN:HB2	2.09	0.52
7:U:38:LEU:HD23	7:U:197:MET:HE3	1.90	0.52
8:V:143:LYS:HG2	8:V:146:LEU:HD21	1.90	0.52
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.33	0.52
14:1:114:PRO:HD2	14:1:118:SER:O	2.09	0.52
14:1:146:MET:CE	14:1:150:GLU:HB3	2.37	0.52
1:A:227:GLN:NE2	1:A:231:ASP:OD1	2.42	0.52
7:G:136:LEU:O	7:G:150:LYS:HA	2.09	0.52
8:H:172:ASN:ND2	8:H:193:THR:HA	2.24	0.52
5:S:194:VAL:O	5:S:197:ILE:HG22	2.08	0.52
8:V:105:ASP:O	8:V:106:THR:N	2.43	0.52
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.43	0.52
2:B:71:ASN:CG	2:B:72:ASP:H	2.17	0.52
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.90	0.52
5:E:214:ILE:CD1	5:E:215:VAL:N	2.71	0.52
6:F:186:ALA:O	6:F:190:VAL:HG23	2.10	0.52
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.90	0.52
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.91	0.52
10:X:190:PHE:HA	10:X:193:GLN:HB2	1.89	0.52
13:O:7:LYS:HG3	13:O:14(G):ILE:HD13	1.91	0.52
1:A:150:GLN:O	1:A:157:TYR:HA	2.09	0.52
7:G:158:VAL:HG22	7:G:159:GLY:N	2.24	0.52
3:Q:121:GLN:NE2	3:Q:121:GLN:C	2.68	0.52
6:T:70:VAL:HB	6:T:74:ILE:HB	1.90	0.52
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.45	0.52
8:V:78:SER:O	8:V:82:MET:HG3	2.09	0.52
4:D:22:PHE:HB2	16:D:280:HOH:O	2.09	0.52
4:D:24:VAL:O	4:D:27:SER:HB3	2.10	0.52
13:M:14(D):GLU:O	13:M:14(G):ILE:HG13	2.08	0.52
3:Q:112:LEU:O	3:Q:116:VAL:HG23	2.09	0.52
8:V:218:ILE:HD13	8:V:218:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.91	0.52
13:M:113:VAL:HA	13:M:118:VAL:O	2.08	0.52
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.91	0.52
7:U:18(A):ILE:HD12	7:U:18(C):HIS:O	2.10	0.52
13:O:171:ARG:O	13:O:192:VAL:HG23	2.10	0.52
3:C:15:PHE:N	4:D:23:GLN:HE22	2.08	0.52
5:E:54:ASN:ND2	5:E:56:ASP:O	2.43	0.52
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.92	0.52
10:J:42:LEU:HB2	10:J:184:ILE:HD13	1.90	0.52
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.45	0.52
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.91	0.52
14:1:163:ILE:HG23	14:1:170:GLY:HA2	1.92	0.52
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.44	0.52
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	2.07	0.52
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.45	0.52
14:N:67:THR:HA	14:N:72:GLY:O	2.10	0.52
4:R:175:GLU:HG2	4:R:196:ILE:HD13	1.91	0.52
9:W:29:ASN:HB2	16:W:218:HOH:O	2.10	0.52
10:X:103:GLY:HA2	10:X:178:VAL:HG11	1.92	0.52
14:N:106:ASN:O	14:N:107:LYS:HB3	2.09	0.52
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.40	0.52
2:B:185:LYS:HD3	2:B:186:VAL:H	1.72	0.52
16:P:258:HOH:O	3:Q:62(A):ILE:HD11	2.10	0.52
7:U:93:LYS:HD3	14:1:68:SER:HB3	1.91	0.52
10:X:189:ASP:O	10:X:193:GLN:HB2	2.10	0.52
12:Z:180:LYS:HG2	16:Z:247:HOH:O	2.10	0.52
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.74	0.51
4:D:121:LEU:HA	4:D:123:PHE:HE1	1.74	0.51
9:I:124:PHE:O	9:I:125:ILE:HD13	2.10	0.51
11:K:38:ASN:O	11:K:40:PHE:N	2.43	0.51
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.91	0.51
6:T:72:ARG:HD2	13:O:64:THR:OG1	2.10	0.51
11:Y:101:ILE:HD13	11:Y:101:ILE:N	2.25	0.51
13:O:105:GLN:HG3	16:O:260:HOH:O	2.09	0.51
3:C:39:GLY:O	3:C:162:ALA:HA	2.11	0.51
11:K:86:LEU:HD13	11:K:86:LEU:C	2.35	0.51
2:P:206:THR:HB	2:P:208:ASP:OD1	2.11	0.51
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.46	0.51
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.93	0.51
6:F:70:VAL:HB	6:F:74:ILE:HB	1.92	0.51
6:F:109:ILE:HD13	6:F:142:ASP:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.25	0.51
15:K:500:GDT:H8	12:L:96:TYR:CE2	2.45	0.51
13:M:7:LYS:HG3	13:M:14(G):ILE:HD13	1.92	0.51
13:M:40:ASN:N	13:M:40:ASN:ND2	2.58	0.51
13:M:157:ASN:HD22	13:M:160:ARG:NH1	2.05	0.51
3:Q:212:ILE:HG22	3:Q:213:THR:N	2.26	0.51
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.91	0.51
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.93	0.51
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.45	0.51
3:C:160:TRP:NE1	4:D:59:LEU:HD23	2.25	0.51
3:C:197:LEU:O	3:C:201:VAL:HG23	2.11	0.51
13:M:203:ILE:HG22	13:M:203:ILE:O	2.09	0.51
3:C:212:ILE:HG22	3:C:213:THR:N	2.25	0.51
7:G:87:ASN:HD22	7:G:88:ALA:N	2.08	0.51
10:J:24:ILE:HD11	10:X:129:TYR:HB3	1.92	0.51
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.45	0.51
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.75	0.51
14:1:106:ASN:O	14:1:107:LYS:HB3	2.10	0.51
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.92	0.51
2:P:194:LEU:HD12	2:P:236:THR:HG21	1.92	0.51
5:S:41:ARG:NH1	5:S:42:SER:O	2.43	0.51
11:Y:37:ILE:O	11:Y:38:ASN:HB3	2.09	0.51
1:A:202:VAL:HG21	1:A:206:PHE:CD1	2.45	0.51
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.93	0.51
4:D:12(E):SER:HB2	5:E:123:ASN:OD1	2.11	0.51
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.93	0.51
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.93	0.51
6:T:45:GLY:HA3	6:T:215:CYS:O	2.11	0.51
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.46	0.51
6:F:127:ASN:HD22	6:F:127:ASN:H	1.56	0.51
7:G:18(D):ILE:O	7:G:18(G):GLU:N	2.44	0.51
13:M:-3:VAL:HG12	13:M:49:ILE:HG13	1.92	0.51
13:M:205:GLY:HA2	16:1:193:HOH:O	2.11	0.51
10:X:121:GLU:O	10:X:122:LEU:HD23	2.10	0.51
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.92	0.51
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.91	0.51
9:I:30:LYS:NZ	11:Y:210:ILE:HD13	2.26	0.51
1:O:227:GLN:NE2	1:O:231:ASP:OD1	2.43	0.51
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.93	0.51
4:R:121:LEU:HA	4:R:123:PHE:HE1	1.73	0.51
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:0:-3:VAL:HG12	13:0:49:ILE:HG13	1.91	0.51
9:I:1:GLY:HA2	9:I:17:ASP:OD1	2.11	0.51
9:I:101:VAL:HG23	9:I:113:PHE:HE2	1.76	0.51
13:M:3:VAL:HG23	13:M:46:SER:HB3	1.93	0.51
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.40	0.51
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.10	0.51
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	1.93	0.51
12:Z:70:HIS:HE1	16:Z:226:HOH:O	1.94	0.51
14:1:10(B):LYS:O	14:1:10(B):LYS:HD3	2.11	0.51
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.92	0.50
2:B:136:PHE:O	2:B:150:THR:HA	2.10	0.50
10:J:69:ARG:HD2	16:J:216:HOH:O	2.10	0.50
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.37	0.50
13:M:178:ILE:CD1	13:M:184:LEU:HG	2.40	0.50
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.50
14:N:13:ILE:HD12	14:N:151:THR:HG22	1.92	0.50
10:X:2:ILE:O	10:X:3:ILE:HD13	2.11	0.50
10:X:16:SER:HB2	16:X:229:HOH:O	2.11	0.50
11:Y:31:VAL:HA	12:Z:120:GLU:OE2	2.11	0.50
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.68	0.50
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.41	0.50
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.06	0.50
6:T:237:GLN:O	6:T:240:ILE:HG22	2.11	0.50
9:W:45:ILE:HG22	9:W:52:VAL:HG22	1.93	0.50
3:C:112:LEU:O	3:C:116:VAL:HG23	2.11	0.50
4:D:42:THR:C	4:D:44:GLU:H	2.19	0.50
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.92	0.50
5:E:143:LYS:HD2	13:M:71(B):GLU:O	2.11	0.50
8:H:18:THR:CB	8:H:30:ASN:HD22	2.24	0.50
10:J:103:GLY:HA2	10:J:178:VAL:HG11	1.93	0.50
7:U:81:PRO:HD2	7:U:133:GLY:O	2.11	0.50
2:B:127:GLY:N	16:B:275:HOH:O	2.44	0.50
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.93	0.50
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.93	0.50
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.12	0.50
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.37	0.50
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.77	0.50
2:P:74:ILE:C	2:P:221:GLN:HE22	2.19	0.50
3:Q:120:GLN:O	3:Q:124:THR:HG23	2.12	0.50
5:S:226:GLY:O	5:S:228:ALA:N	2.44	0.50
13:0:104:VAL:HG13	13:0:106:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.94	0.50
8:H:10:ASN:HD22	8:H:179:GLU:CG	2.24	0.50
10:J:39:PRO:HG2	10:J:73:GLU:CD	2.36	0.50
10:J:179:ASP:HB2	16:J:217:HOH:O	2.10	0.50
11:K:101:ILE:HD13	11:K:101:ILE:N	2.27	0.50
7:U:225:SER:O	7:U:226:ALA:C	2.55	0.50
10:X:74:LEU:HD22	10:X:78:ALA:CB	2.42	0.50
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.27	0.50
14:1:10:ASP:O	14:1:179:THR:HG22	2.12	0.50
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.25	0.50
10:J:129:TYR:HB3	10:X:24:ILE:HD11	1.92	0.50
11:K:6:PHE:HA	11:K:123:ASP:O	2.12	0.50
11:K:32:LYS:HB2	16:K:542:HOH:O	2.11	0.50
2:B:206:THR:HB	2:B:208:ASP:OD1	2.11	0.50
3:C:87:ILE:HD13	3:C:87:ILE:N	2.26	0.50
4:D:177:LEU:HA	5:E:58:LEU:HD11	1.93	0.50
7:G:228:ASN:HB3	16:G:255:HOH:O	2.12	0.50
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.47	0.50
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.93	0.50
2:P:71:ASN:CG	2:P:72:ASP:H	2.16	0.50
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.77	0.50
9:W:104:ILE:HG21	9:W:181:LYS:HG2	1.93	0.50
10:X:39:PRO:HG2	10:X:73:GLU:OE2	2.12	0.50
10:J:52:THR:CG2	10:J:53:VAL:H	2.24	0.50
11:K:67:GLU:HG2	11:K:73:ARG:HA	1.94	0.50
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.12	0.50
5:S:227:GLU:CD	5:S:227:GLU:H	2.19	0.50
12:Z:123:GLN:HG3	12:Z:145:TYR:HH	1.74	0.50
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.94	0.49
7:G:38:LEU:HD23	7:G:197:MET:CE	2.42	0.49
8:H:22:GLN:HG2	15:H:500:GDT:H36B	1.94	0.49
14:N:114:PRO:HD2	14:N:118:SER:O	2.12	0.49
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.12	0.49
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.94	0.49
5:S:86:ARG:O	5:S:90:ASN:HB2	2.11	0.49
6:T:186:ALA:O	6:T:190:VAL:HG23	2.12	0.49
7:U:49:ILE:HD12	7:U:212:VAL:HG22	1.93	0.49
10:X:19:ALA:HB2	10:X:171:LYS:HG2	1.92	0.49
2:B:31:ILE:HD11	2:B:133:GLY:C	2.37	0.49
3:C:69:LYS:HG3	16:C:277:HOH:O	2.12	0.49
4:D:29:GLU:OE2	4:D:29:GLU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.47	0.49
10:J:112:GLN:NE2	10:J:126:ALA:H	2.10	0.49
1:O:39:GLY:C	1:O:40:ILE:HG13	2.37	0.49
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.12	0.49
2:P:136:PHE:O	2:P:150:THR:HA	2.12	0.49
2:P:168:ASN:HA	16:P:275:HOH:O	2.12	0.49
3:Q:201:VAL:HG21	3:Q:210:ILE:CD1	2.41	0.49
4:R:59:LEU:HD13	4:R:59:LEU:C	2.37	0.49
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.74	0.49
10:X:162:LEU:O	10:X:166:MET:HB2	2.11	0.49
12:Z:147:SER:O	12:Z:151:VAL:HG23	2.12	0.49
14:1:6:VAL:HG23	14:1:155:ILE:HD11	1.93	0.49
1:A:109:THR:O	1:A:113:VAL:HG23	2.12	0.49
2:B:235:LYS:C	2:B:237:GLY:H	2.20	0.49
11:K:46:ALA:HB3	11:K:98:GLY:O	2.12	0.49
3:Q:39:GLY:O	3:Q:162:ALA:HA	2.11	0.49
3:Q:62(A):ILE:HG13	3:Q:63:THR:N	2.28	0.49
7:U:136:LEU:O	7:U:150:LYS:HA	2.12	0.49
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.94	0.49
9:W:186:LYS:HE2	9:W:188:TYR:CE1	2.47	0.49
5:E:226:GLY:O	5:E:228:ALA:N	2.44	0.49
6:F:45:GLY:HA3	6:F:215:CYS:O	2.12	0.49
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.93	0.49
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.41	0.49
8:V:10:ASN:HD22	8:V:179:GLU:CG	2.26	0.49
8:V:52:THR:O	8:V:56:THR:HB	2.13	0.49
12:Z:11:PHE:CZ	12:Z:148:VAL:HA	2.47	0.49
1:A:86:ARG:NE	7:G:118:ASN:ND2	2.56	0.49
7:G:225:SER:O	7:G:226:ALA:C	2.55	0.49
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.93	0.49
11:K:146:LEU:HD23	11:K:151:ALA:HA	1.93	0.49
11:K:165:ARG:NE	10:X:135:PHE:HB3	2.27	0.49
2:P:97:GLN:OE1	9:W:64:ASN:HB3	2.13	0.49
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.94	0.49
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.48	0.49
4:R:194:LEU:HD12	4:R:207:LEU:HD11	1.94	0.49
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.12	0.49
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.13	0.49
13:O:-6:GLN:HG3	13:O:-6:GLN:O	2.13	0.49
13:O:40:ASN:N	13:O:40:ASN:ND2	2.58	0.49
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.26	0.49
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.93	0.49
4:D:14:THR:HG23	5:E:23:GLN:NE2	2.28	0.49
4:D:194:LEU:HD12	4:D:207:LEU:HD11	1.95	0.49
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.27	0.49
2:P:12:THR:HB	2:P:23:GLN:HG3	1.93	0.49
2:P:225:LYS:HB2	2:P:228:GLU:HG3	1.95	0.49
4:R:81:LEU:O	4:R:134:VAL:HB	2.13	0.49
10:X:4:LEU:HD23	10:X:126:ALA:HB2	1.94	0.49
14:1:104:TYR:OH	14:1:180:ALA:HB2	2.12	0.49
2:B:235:LYS:HD3	2:B:235:LYS:N	2.28	0.49
7:G:81:PRO:HD2	7:G:133:GLY:O	2.13	0.49
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.95	0.49
11:K:126:CYS:HB2	11:K:135:TYR:CZ	2.48	0.49
14:N:146:MET:HE2	14:N:150:GLU:CB	2.38	0.49
3:Q:125:GLN:NE2	16:Q:270:HOH:O	2.46	0.49
7:U:18(D):ILE:O	7:U:18(G):GLU:N	2.45	0.49
10:X:100:LEU:CD2	10:X:112:GLN:HG3	2.42	0.49
2:B:126:HIS:CB	3:C:129:VAL:HG12	2.35	0.49
3:C:120:GLN:O	3:C:124:THR:HG23	2.13	0.49
4:D:56:SER:OG	4:D:57:PRO:HD2	2.12	0.49
4:D:101:LEU:N	16:D:257:HOH:O	2.45	0.49
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.48	0.49
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.95	0.49
8:H:159:ILE:HG22	8:H:163:ILE:CD1	2.43	0.49
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.48	0.49
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.12	0.49
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.93	0.49
8:H:52:THR:O	8:H:56:THR:HB	2.12	0.49
6:T:20(B):GLU:CD	6:T:20(C):LYS:HE3	2.38	0.49
4:D:240:LYS:O	4:D:243:ALA:HB3	2.13	0.49
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.11	0.49
9:I:165:ARG:HG2	16:Z:218:HOH:O	2.13	0.49
12:L:11:PHE:CZ	12:L:148:VAL:HA	2.48	0.49
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.11	0.49
4:R:40:ILE:HG13	4:R:193:VAL:HG23	1.93	0.49
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.39	0.49
6:T:127:ASN:H	6:T:127:ASN:ND2	2.11	0.49
8:V:24:PRO:HG2	8:V:25:ILE:HD13	1.94	0.49
3:C:225:SER:O	3:C:229:ILE:HG13	2.12	0.48
6:F:109:ILE:CD1	6:F:109:ILE:H	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:79:ASN:HA	16:G:284:HOH:O	2.13	0.48
12:L:145:TYR:CD1	12:L:146:LEU:N	2.81	0.48
2:P:72:ASP:O	2:P:221:GLN:HG3	2.12	0.48
4:R:29:GLU:OE2	4:R:29:GLU:HA	2.12	0.48
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.43	0.48
5:S:49:VAL:HG13	5:S:212:ILE:HD11	1.95	0.48
9:W:104:ILE:CD1	9:W:178:ILE:HG22	2.43	0.48
10:X:-1:MET:HG2	10:X:1:ASP:N	2.15	0.48
12:Z:123:GLN:CG	12:Z:145:TYR:OH	2.61	0.48
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.94	0.48
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.43	0.48
13:M:171:ARG:O	13:M:192:VAL:HG23	2.13	0.48
14:N:10:ASP:O	14:N:179:THR:HG22	2.13	0.48
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.28	0.48
4:R:240:LYS:O	4:R:243:ALA:HB3	2.13	0.48
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.48	0.48
13:O:42:VAL:HG23	13:O:178:ILE:HD11	1.94	0.48
7:G:233:LEU:O	7:G:236:ILE:HG12	2.13	0.48
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.38	0.48
5:S:48:LEU:HB2	5:S:213:ALA:HB3	1.95	0.48
5:S:207:LEU:HD23	5:S:207:LEU:N	2.29	0.48
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.82	0.48
5:E:207:LEU:HD23	5:E:207:LEU:N	2.28	0.48
1:O:122:GLU:C	1:O:124:THR:H	2.21	0.48
4:R:24:VAL:O	4:R:27:SER:HB3	2.13	0.48
5:S:54:ASN:ND2	5:S:56:ASP:O	2.45	0.48
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.95	0.48
11:Y:67:GLU:HG2	11:Y:73:ARG:HA	1.96	0.48
13:O:42:VAL:CG2	13:O:178:ILE:HD11	2.44	0.48
2:B:21(A):LYS:HE2	2:B:21(D):GLY:O	2.14	0.48
3:C:45:CYS:HA	3:C:141:PHE:HZ	1.79	0.48
7:G:8:TYR:C	7:G:10:ARG:N	2.72	0.48
14:N:83:PHE:HB3	14:N:113:ILE:HD13	1.95	0.48
1:O:14:THR:O	1:O:21:LEU:HD23	2.12	0.48
3:Q:225:SER:O	3:Q:229:ILE:HG13	2.12	0.48
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.48	0.48
7:U:226:ALA:HB3	16:U:344:HOH:O	2.14	0.48
9:W:100:VAL:HG13	9:W:125:ILE:HG21	1.95	0.48
14:1:67:THR:HA	14:1:72:GLY:O	2.13	0.48
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.37	0.48
2:B:12:THR:HB	2:B:23:GLN:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:GLN:C	3:C:243:GLN:H	2.22	0.48
10:J:100:LEU:CD2	10:J:112:GLN:HG3	2.43	0.48
1:O:22:GLY:O	1:O:25:ASP:HB2	2.14	0.48
5:S:104:ASN:HB2	13:O:81:GLU:HG2	1.96	0.48
6:T:240:ILE:HD12	6:T:240:ILE:O	2.14	0.48
9:W:1:GLY:HA2	9:W:17:ASP:OD1	2.13	0.48
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.96	0.48
14:1:121:LYS:O	14:1:122:LEU:HD23	2.13	0.48
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.95	0.48
11:Y:112:TYR:O	11:Y:119:ARG:HA	2.13	0.48
14:1:143:ARG:NH2	14:1:146:MET:HE3	2.28	0.48
2:B:225:LYS:HB2	2:B:228:GLU:HG3	1.95	0.48
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.13	0.48
4:D:59:LEU:HD13	4:D:59:LEU:C	2.38	0.48
9:I:104:ILE:CD1	9:I:178:ILE:HG22	2.43	0.48
10:J:121:GLU:O	10:J:122:LEU:HD23	2.13	0.48
8:V:197:ARG:NH2	9:W:139:GLU:O	2.47	0.48
9:W:137:MET:HE2	9:W:161:ASN:HB2	1.96	0.48
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.14	0.48
1:A:14:THR:O	1:A:21:LEU:HD23	2.13	0.48
1:A:67:VAL:HB	1:A:223:LYS:HZ2	1.78	0.48
3:Q:70:ILE:HG21	3:Q:112:LEU:HD21	1.96	0.48
1:A:90:ASP:OD1	16:A:245:HOH:O	2.20	0.48
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.49	0.48
3:C:70:ILE:HG21	3:C:112:LEU:HD21	1.95	0.48
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.95	0.48
5:E:4:PHE:CG	5:E:5:ARG:N	2.81	0.48
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.14	0.48
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.14	0.48
10:J:67:SER:O	10:J:71:ASP:N	2.46	0.48
11:K:67:GLU:OE1	11:K:73:ARG:HA	2.14	0.48
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.62	0.48
2:P:11:ARG:O	2:P:14:ILE:HD13	2.14	0.48
2:P:235:LYS:C	2:P:237:GLY:H	2.21	0.48
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.94	0.48
5:S:49:VAL:HG22	5:S:212:ILE:HD12	1.96	0.48
7:U:233:LEU:O	7:U:236:ILE:HG12	2.13	0.48
9:W:22:SER:O	9:W:23:GLN:HB2	2.14	0.48
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.79	0.48
13:O:203:ILE:O	13:O:203:ILE:HG22	2.13	0.48
10:J:190:PHE:C	10:J:192:ALA:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:195:LEU:O	11:K:199:VAL:HG23	2.14	0.47
1:O:202:VAL:HG21	1:O:206:PHE:CD1	2.48	0.47
10:X:129:TYR:O	10:X:132:PHE:HB2	2.14	0.47
14:1:66:TYR:CD2	14:1:74:PRO:HB3	2.49	0.47
5:E:41:ARG:NH1	5:E:42:SER:O	2.47	0.47
11:K:112:TYR:O	11:K:119:ARG:HA	2.14	0.47
12:L:84:GLN:HG3	12:L:117:GLY:O	2.13	0.47
12:L:123:GLN:HG3	12:L:145:TYR:HH	1.77	0.47
1:O:109:THR:O	1:O:113:VAL:HG23	2.13	0.47
2:P:31:ILE:HD11	2:P:133:GLY:C	2.40	0.47
4:R:237:LEU:C	4:R:237:LEU:HD13	2.39	0.47
7:U:38:LEU:HD23	7:U:197:MET:CE	2.44	0.47
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.97	0.47
12:Z:84:GLN:HG3	12:Z:117:GLY:O	2.14	0.47
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.49	0.47
7:G:55:PRO:HG2	7:G:56:ASP:H	1.78	0.47
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.95	0.47
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.96	0.47
8:H:78:SER:O	8:H:82:MET:HG3	2.15	0.47
10:J:74:LEU:HD22	10:J:78:ALA:CB	2.44	0.47
2:P:235:LYS:HD3	2:P:235:LYS:N	2.28	0.47
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.44	0.47
7:U:18(H):GLU:CD	7:U:18(H):GLU:N	2.73	0.47
9:W:7:THR:CG2	9:W:110:ILE:HG13	2.45	0.47
13:0:14(A):VAL:O	13:0:14(A):VAL:HG23	2.14	0.47
1:A:215:ILE:HD11	1:A:221:PHE:HD1	1.79	0.47
2:B:38:ILE:HD13	2:B:197:LEU:HG	1.96	0.47
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.43	0.47
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.77	0.47
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.29	0.47
7:U:120:SER:HA	7:U:123:TYR:CD2	2.50	0.47
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.14	0.47
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.95	0.47
12:Z:31:GLU:OE1	13:0:120:TYR:HA	2.15	0.47
3:Q:15:PHE:H	4:R:23:GLN:NE2	2.10	0.47
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.96	0.47
6:T:114:ASP:O	6:T:118:GLN:HG2	2.14	0.47
7:U:38:LEU:CD2	7:U:197:MET:HE3	2.45	0.47
13:0:37:VAL:HG11	13:0:79:ILE:CD1	2.43	0.47
5:E:86:ARG:O	5:E:90:ASN:HB2	2.15	0.47
7:G:217:LYS:HA	7:G:217:LYS:CE	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:7:THR:CG2	9:I:110:ILE:HG13	2.45	0.47
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.49	0.47
2:P:150:THR:O	2:P:157:TYR:HA	2.15	0.47
2:P:228:GLU:O	2:P:232:ILE:HG22	2.14	0.47
5:S:226:GLY:O	5:S:227:GLU:C	2.57	0.47
8:V:18:THR:HB	8:V:30:ASN:HA	1.97	0.47
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.96	0.47
11:Y:67:GLU:OE1	11:Y:73:ARG:HA	2.14	0.47
14:1:65:LEU:HG	14:1:69:GLN:NE2	2.29	0.47
1:A:39:GLY:C	1:A:40:ILE:HG13	2.39	0.47
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.13	0.47
3:C:46:VAL:HG22	3:C:146:PRO:HB2	1.96	0.47
3:C:62(A):ILE:HG13	3:C:63:THR:N	2.30	0.47
5:E:179:THR:HG22	5:E:18(B):THR:HB	1.96	0.47
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.14	0.47
7:G:60:ASP:OD2	7:G:62:THR:OG1	2.32	0.47
8:H:172:ASN:HD22	8:H:193:THR:HA	1.80	0.47
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.78	0.47
14:N:10(B):LYS:O	14:N:10(B):LYS:HD3	2.14	0.47
1:O:175:PHE:O	1:O:179:ARG:HG2	2.14	0.47
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.27	0.47
3:Q:241:GLN:C	3:Q:243:GLN:H	2.22	0.47
4:R:227:GLU:OE2	4:R:227:GLU:N	2.36	0.47
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.30	0.47
8:V:172:ASN:HD22	8:V:193:THR:HA	1.79	0.47
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.48	0.47
12:Z:19:ARG:NE	12:Z:171:ASP:OD2	2.38	0.47
12:Z:94:PRO:HA	16:Z:198:HOH:O	2.13	0.47
3:C:14:ILE:HB	4:D:23:GLN:HE22	1.80	0.47
4:D:112:LEU:HD13	4:D:112:LEU:O	2.14	0.47
5:E:28:LEU:HD12	5:E:153:PRO:HD2	1.96	0.47
5:E:220:PRO:O	5:E:221:PHE:C	2.58	0.47
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.50	0.47
8:H:103:GLY:HA2	8:H:178:MET:SD	2.54	0.47
3:Q:156:ILE:HD13	4:R:83:ALA:HB2	1.96	0.47
4:R:65:GLU:HA	16:R:750:HOH:O	2.13	0.47
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.14	0.47
5:S:220:PRO:O	5:S:221:PHE:C	2.56	0.47
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.50	0.47
6:F:127:ASN:H	6:F:127:ASN:ND2	2.12	0.47
13:M:-7:GLN:HB3	16:M:228:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:65:LEU:HG	14:N:69:GLN:NE2	2.30	0.47
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.50	0.47
6:T:68:GLN:HG2	16:T:312:HOH:O	2.14	0.47
8:V:2:THR:HG22	8:V:159:ILE:HD13	1.97	0.47
9:W:29:ASN:ND2	9:W:29:ASN:N	2.63	0.47
13:O:3:VAL:HG23	13:O:46:SER:HB3	1.97	0.47
2:B:176:LEU:HD23	2:B:192:LEU:HD22	1.96	0.47
2:B:176:LEU:HD23	2:B:192:LEU:CD2	2.45	0.47
9:I:110:ILE:O	9:I:110:ILE:HD12	2.15	0.47
11:K:210:ILE:O	11:K:210:ILE:HG22	2.14	0.47
3:Q:8:TYR:CZ	3:Q:10:ARG:HB2	2.50	0.47
4:R:189:ALA:O	4:R:193:VAL:HG23	2.16	0.47
5:S:4:PHE:CG	5:S:5:ARG:N	2.82	0.47
7:U:186:TRP:O	7:U:190:VAL:HG23	2.15	0.47
9:W:29:ASN:H	9:W:29:ASN:HD22	1.62	0.47
14:1:65:LEU:HG	14:1:69:GLN:HE21	1.80	0.47
14:1:112:THR:CG2	14:1:120:HIS:HB2	2.43	0.47
1:A:22:GLY:O	1:A:25:ASP:HB2	2.15	0.46
6:F:169:ARG:HE	6:F:169:ARG:HB3	1.46	0.46
7:G:35:ILE:HD11	7:G:53:LYS:HG3	1.98	0.46
10:J:144:PRO:HG2	11:Y:207:ASN:HD21	1.80	0.46
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.50	0.46
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.97	0.46
4:R:86:ARG:HA	4:R:86:ARG:HD3	1.80	0.46
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.79	0.46
10:X:112:GLN:NE2	10:X:126:ALA:H	2.13	0.46
2:B:60:GLU:OE1	2:B:60:GLU:HA	2.16	0.46
3:C:236:ILE:HA	3:C:239:GLU:HG2	1.97	0.46
13:M:104:VAL:HG13	13:M:106:GLY:O	2.14	0.46
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.44	0.46
2:B:45:GLY:HA2	2:B:146:TYR:CE1	2.51	0.46
8:H:62:ASN:CB	8:H:82:MET:HE1	2.46	0.46
2:P:60:GLU:OE1	2:P:60:GLU:HA	2.14	0.46
3:Q:62(A):ILE:O	3:Q:63:THR:C	2.58	0.46
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.97	0.46
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.44	0.46
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.96	0.46
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.97	0.46
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.15	0.46
3:C:55:THR:C	3:C:56:LEU:HD22	2.41	0.46
3:C:69:LYS:N	16:C:277:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:211:GLU:O	3:C:212:ILE:HD13	2.16	0.46
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.79	0.46
5:E:188:GLU:OE1	5:E:188:GLU:HA	2.13	0.46
6:F:184:LEU:CD1	6:F:188:GLU:HB3	2.45	0.46
7:G:203:THR:HG22	7:G:204:GLU:N	2.31	0.46
9:I:51:ASP:OD1	10:J:90(B):ARG:NH2	2.48	0.46
9:I:105:ASN:HB3	9:I:10(C):SER:OG	2.15	0.46
2:P:231:ASP:O	2:P:235:LYS:HG2	2.16	0.46
3:Q:14:ILE:HB	4:R:23:GLN:HE22	1.78	0.46
6:T:127:ASN:N	6:T:127:ASN:ND2	2.63	0.46
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.50	0.46
1:A:186:LEU:O	1:A:190:ILE:HG13	2.16	0.46
7:G:38:LEU:CD2	7:G:197:MET:HE3	2.45	0.46
16:T:320:HOH:O	13:O:67:ALA:HB3	2.15	0.46
9:W:12:VAL:HG12	9:W:108:PRO:HB3	1.97	0.46
9:W:93:GLY:C	16:W:215:HOH:O	2.59	0.46
1:A:32:LYS:HA	1:A:32:LYS:CE	2.45	0.46
5:E:48:LEU:HB2	5:E:213:ALA:HB3	1.97	0.46
12:L:43:MET:CG	12:L:44:SER:N	2.79	0.46
12:L:166:HIS:CD2	12:L:168:GLN:H	2.32	0.46
2:P:38:ILE:HD13	2:P:197:LEU:HG	1.98	0.46
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.97	0.46
9:W:61:TYR:CD1	9:W:61:TYR:C	2.94	0.46
9:W:101:VAL:HG23	9:W:113:PHE:HE2	1.81	0.46
9:W:110:ILE:CD1	9:W:122:ALA:O	2.63	0.46
10:X:2:ILE:O	10:X:16:SER:HA	2.16	0.46
3:C:57:LYS:O	3:C:58:LEU:HB2	2.15	0.46
3:C:100:ARG:O	3:C:104:GLU:N	2.49	0.46
4:D:237:LEU:C	4:D:237:LEU:HD13	2.41	0.46
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.96	0.46
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.31	0.46
8:H:218:ILE:HG22	8:H:219:VAL:N	2.31	0.46
9:I:29:ASN:H	9:I:29:ASN:HD22	1.63	0.46
10:J:129:TYR:O	10:J:132:PHE:HB2	2.15	0.46
12:L:147:SER:O	12:L:151:VAL:HG23	2.14	0.46
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.16	0.46
14:N:14:LEU:O	14:N:175:MET:HA	2.15	0.46
14:N:116:GLY:HA3	16:N:194:HOH:O	2.16	0.46
1:O:215:ILE:HD11	1:O:221:PHE:HD1	1.81	0.46
2:P:176:LEU:HD23	2:P:192:LEU:HD22	1.98	0.46
2:P:185:LYS:O	2:P:188:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.81	0.46
6:T:169:ARG:O	6:T:173:LYS:HG3	2.15	0.46
8:V:62:ASN:CB	8:V:82:MET:HE1	2.45	0.46
8:V:103:GLY:HA2	8:V:178:MET:SD	2.56	0.46
10:X:67:SER:O	10:X:71:ASP:N	2.49	0.46
12:Z:43:MET:CG	12:Z:44:SER:N	2.78	0.46
13:O:133:MET:O	13:O:136:PRO:HD2	2.16	0.46
14:1:13:ILE:HD12	14:1:151:THR:HG22	1.97	0.46
14:1:83:PHE:HB3	14:1:113:ILE:HD13	1.98	0.46
1:A:32:LYS:HE2	1:A:32:LYS:CA	2.45	0.46
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.46	0.46
1:A:112:LEU:O	1:A:116:VAL:HG23	2.15	0.46
11:K:137:VAL:HG21	11:K:161:ALA:HB2	1.98	0.46
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.81	0.46
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.46	0.46
2:P:21(A):LYS:HE2	2:P:21(D):GLY:O	2.15	0.46
10:X:185:ARG:HG2	10:X:185:ARG:HH11	1.81	0.46
14:1:14:LEU:O	14:1:175:MET:HA	2.15	0.46
1:A:38:LEU:C	1:A:38:LEU:HD12	2.41	0.46
2:B:228:GLU:O	2:B:232:ILE:HG22	2.15	0.46
2:B:229:ILE:O	2:B:233:LEU:HB2	2.16	0.46
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.81	0.46
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.81	0.46
8:H:18:THR:HB	8:H:30:ASN:HA	1.98	0.46
10:J:39:PRO:HG2	10:J:73:GLU:OE2	2.16	0.46
13:M:177:ILE:C	13:M:178:ILE:HD13	2.41	0.46
1:O:144:PHE:CE2	9:W:10(B):LYS:HD2	2.51	0.46
3:Q:160:TRP:NE1	4:R:59:LEU:HD23	2.31	0.46
14:1:89:GLU:OE1	14:1:89:GLU:HA	2.14	0.46
1:A:175:PHE:O	1:A:179:ARG:HG2	2.16	0.46
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.45	0.46
1:O:112:LEU:O	1:O:116:VAL:HG23	2.15	0.46
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.15	0.46
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.46	0.46
6:T:179:LEU:CD2	6:T:192:GLN:HG2	2.42	0.46
7:U:55:PRO:HG2	7:U:56:ASP:H	1.80	0.46
13:O:45:ILE:HG12	13:O:99:ILE:HG12	1.99	0.46
14:1:67:THR:O	14:1:68:SER:C	2.58	0.46
3:C:8:TYR:CZ	3:C:10:ARG:HB2	2.51	0.45
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.96	0.45
9:I:191:MET:HE2	16:I:203:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	2.00	0.45
14:N:161:GLN:O	14:N:164:LYS:HB3	2.16	0.45
16:P:258:HOH:O	3:Q:62(A):ILE:CD1	2.63	0.45
6:F:42:CYS:HB2	6:F:184:LEU:O	2.16	0.45
6:F:130:ARG:HG2	6:F:130:ARG:HH11	1.81	0.45
3:Q:212:ILE:HD13	3:Q:212:ILE:N	2.30	0.45
3:C:100:ARG:NH2	16:C:278:HOH:O	2.49	0.45
14:N:67:THR:O	14:N:68:SER:C	2.60	0.45
3:Q:236:ILE:HA	3:Q:239:GLU:HG2	1.97	0.45
4:R:56:SER:OG	4:R:57:PRO:HD2	2.16	0.45
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.81	0.45
5:S:47:VAL:HG12	5:S:48:LEU:N	2.32	0.45
5:S:179:THR:HG22	5:S:18(B):THR:HB	1.97	0.45
9:W:123:ASP:OD1	9:W:124:PHE:N	2.45	0.45
2:B:63:THR:O	2:B:63:THR:HG22	2.16	0.45
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.97	0.45
2:B:185:LYS:O	2:B:188:ASP:HB2	2.17	0.45
5:E:185:ASN:C	5:E:185:ASN:HD22	2.25	0.45
8:H:218:ILE:N	8:H:218:ILE:CD1	2.79	0.45
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.15	0.45
5:S:214:ILE:HD12	5:S:214:ILE:C	2.41	0.45
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.98	0.45
7:U:227:GLU:HG2	16:U:344:HOH:O	2.16	0.45
9:W:105:ASN:HB3	9:W:10(C):SER:OG	2.16	0.45
3:C:62(A):ILE:O	3:C:63:THR:C	2.59	0.45
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.51	0.45
4:D:213:SER:CB	4:D:223:ILE:HA	2.46	0.45
6:F:115:ARG:HG2	16:F:293:HOH:O	2.16	0.45
1:O:67:VAL:HG11	1:O:213:ALA:HB3	1.99	0.45
4:R:209:GLU:HG3	4:R:230:ALA:HB2	1.98	0.45
5:S:188:GLU:OE1	5:S:188:GLU:HA	2.16	0.45
7:U:218:ASP:O	7:U:220:LYS:CB	2.64	0.45
11:Y:126:CYS:HB2	11:Y:135:TYR:CZ	2.50	0.45
12:Z:114:ASP:HB2	12:Z:118:SER:N	2.31	0.45
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.29	0.45
1:A:13:THR:O	2:B:130:ARG:HD3	2.17	0.45
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.98	0.45
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.47	0.45
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.51	0.45
3:C:156:ILE:HD13	4:D:83:ALA:HB2	1.99	0.45
3:C:238:GLN:O	3:C:242:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:PHE:HB2	5:E:23:GLN:OE1	2.17	0.45
13:M:17:ASP:OD2	13:M:17:ASP:C	2.59	0.45
2:P:66:LYS:O	2:P:77:ALA:HA	2.17	0.45
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.52	0.45
9:W:190:LYS:HA	16:W:233:HOH:O	2.16	0.45
6:F:171:SER:N	16:F:308:HOH:O	2.34	0.45
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.80	0.45
10:J:166:MET:HE2	10:J:166:MET:HB3	1.83	0.45
12:L:17:ASP:HA	12:L:172:GLY:O	2.16	0.45
12:L:14(O):LYS:CG	12:L:14(P):PRO:HD2	2.47	0.45
13:M:37:VAL:HG11	13:M:79:ILE:CD1	2.45	0.45
13:M:149:GLN:HE21	13:M:149:GLN:N	2.04	0.45
14:N:126:ILE:HD13	14:N:126:ILE:N	2.22	0.45
1:O:32:LYS:HE2	1:O:32:LYS:CA	2.45	0.45
1:O:184:LEU:HB2	16:O:248:HOH:O	2.15	0.45
5:S:86:ARG:HH11	5:S:86:ARG:CG	2.29	0.45
11:Y:210:ILE:O	11:Y:210:ILE:HG22	2.16	0.45
14:1:155:ILE:HG22	14:1:175:MET:HE2	1.99	0.45
5:E:49:VAL:HG13	5:E:212:ILE:HD11	1.98	0.45
8:H:9:ASN:OD1	8:H:10:ASN:N	2.49	0.45
9:I:123:ASP:OD1	9:I:124:PHE:N	2.47	0.45
1:O:26:TYR:O	1:O:29:THR:HB	2.16	0.45
1:O:134:VAL:O	1:O:153:PRO:HG3	2.17	0.45
3:Q:97:GLN:NE2	3:Q:97:GLN:HA	2.32	0.45
7:U:203:THR:HG22	7:U:204:GLU:N	2.31	0.45
10:X:4:LEU:HD23	10:X:126:ALA:CB	2.46	0.45
2:B:11:ARG:O	2:B:14:ILE:HD13	2.17	0.45
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.52	0.45
4:D:122:ARG:HG2	4:D:122:ARG:NH1	2.30	0.45
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.17	0.45
4:D:170:GLU:N	4:D:170:GLU:OE1	2.50	0.45
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.47	0.45
14:N:92:ASP:HB2	16:N:198:HOH:O	2.17	0.45
1:O:55:SER:O	1:O:56:SER:HB2	2.17	0.45
3:Q:100:ARG:O	3:Q:104:GLU:N	2.47	0.45
3:Q:159:SER:O	4:R:59:LEU:HD22	2.17	0.45
5:S:97:ASN:HD22	5:S:97:ASN:HA	1.62	0.45
6:T:28:VAL:O	6:T:32:GLU:HG3	2.17	0.45
7:U:8:TYR:C	7:U:10:ARG:N	2.73	0.45
10:X:166:MET:HA	10:X:167:PRO:HD3	1.73	0.45
11:Y:152:LEU:HD11	11:Y:187:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:0:17:ASP:OD2	13:0:17:ASP:C	2.60	0.45
14:1:59:VAL:HG22	14:1:82:VAL:HG12	1.98	0.45
2:B:21(A):LYS:HE3	2:B:21(E):VAL:HG23	1.99	0.45
6:F:169:ARG:O	6:F:173:LYS:HG3	2.17	0.45
7:G:123:TYR:CE1	7:G:129:MET:HE3	2.52	0.45
11:K:152:LEU:HD11	11:K:187:HIS:CD2	2.52	0.45
14:N:126:ILE:H	14:N:126:ILE:CD1	2.24	0.45
2:P:176:LEU:HD23	2:P:192:LEU:CD2	2.46	0.45
2:P:229:ILE:O	2:P:233:LEU:HB2	2.16	0.45
9:W:113:PHE:HA	9:W:118:CYS:O	2.17	0.45
13:0:190:LEU:N	13:0:190:LEU:CD1	2.80	0.45
1:A:93:ARG:NH1	16:A:245:HOH:O	2.34	0.44
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.98	0.44
3:C:67:VAL:HG22	3:C:77:SER:HB3	1.99	0.44
3:C:150:GLN:O	3:C:157:TYR:HA	2.17	0.44
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.52	0.44
12:L:-2:ASN:HA	12:L:21:ILE:O	2.16	0.44
1:O:32:LYS:HA	1:O:32:LYS:CE	2.46	0.44
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.42	0.44
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.44
2:B:231:ASP:O	2:B:235:LYS:HG2	2.17	0.44
4:D:23:GLN:HA	4:D:23:GLN:OE1	2.16	0.44
5:E:49:VAL:HG22	5:E:212:ILE:HD12	1.99	0.44
6:F:13:SER:HB2	7:G:130:ARG:HD3	1.98	0.44
6:F:81:LEU:HD12	6:F:133:GLY:HA3	1.99	0.44
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.51	0.44
8:H:123:TYR:OH	13:0:202:ASP:HB2	2.17	0.44
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.27	0.44
14:N:186:ARG:O	14:N:187:LEU:HD23	2.18	0.44
1:O:147:PHE:HZ	16:O:261:HOH:O	2.00	0.44
2:P:224:PHE:HD2	2:P:224:PHE:H	1.65	0.44
5:S:160:LEU:HD13	5:S:163:THR:HB	1.99	0.44
10:X:5:GLY:O	10:X:124:TYR:HA	2.16	0.44
10:X:143:ARG:O	10:X:146:MET:HG3	2.17	0.44
12:Z:31:GLU:HA	16:Z:208:HOH:O	2.18	0.44
1:A:122:GLU:C	1:A:124:THR:H	2.23	0.44
2:B:41:MET:HE1	3:C:60:ASP:OD1	2.16	0.44
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.69	0.44
5:E:160:LEU:HD13	5:E:163:THR:HB	1.98	0.44
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.48	0.44
2:P:45:GLY:HA2	2:P:146:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:68:TYR:CG	2:P:89:ILE:HD13	2.52	0.44
5:S:15:PHE:H	6:T:23:GLN:NE2	2.13	0.44
5:S:214:ILE:CD1	5:S:215:VAL:N	2.74	0.44
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.99	0.44
8:V:116:HIS:HB2	16:V:545:HOH:O	2.16	0.44
1:A:55:SER:O	1:A:56:SER:HB2	2.17	0.44
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.48	0.44
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.52	0.44
5:E:226:GLY:O	5:E:227:GLU:C	2.59	0.44
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.98	0.44
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.30	0.44
1:O:21(P):LYS:HB2	16:O:253:HOH:O	2.17	0.44
3:Q:31:VAL:HG11	3:Q:135:SER:HB2	2.00	0.44
3:Q:163:GLN:NE2	3:Q:173:ARG:HE	2.01	0.44
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.47	0.44
7:U:234:VAL:O	7:U:237:ALA:HB3	2.18	0.44
8:V:218:ILE:HG22	8:V:219:VAL:N	2.33	0.44
10:X:190:PHE:C	10:X:192:ALA:N	2.72	0.44
14:1:4:MET:HB3	14:1:126:ILE:HG22	1.99	0.44
1:A:136:LEU:O	1:A:150:GLN:HA	2.18	0.44
2:B:78:VAL:HG12	2:B:79:ALA:N	2.33	0.44
2:B:150:THR:O	2:B:157:TYR:HA	2.17	0.44
3:C:93:ARG:NH1	10:J:69:ARG:HA	2.32	0.44
10:J:4:LEU:HD23	10:J:126:ALA:HB2	1.98	0.44
12:L:19:ARG:HG2	12:L:21:ILE:HG23	1.99	0.44
12:L:14(Q):LEU:O	12:L:14(W):LYS:C	2.59	0.44
12:L:165:ARG:CZ	8:V:29:LYS:HE2	2.48	0.44
2:P:27:ALA:O	2:P:30:SER:HB3	2.17	0.44
2:P:63:THR:O	2:P:63:THR:HG22	2.17	0.44
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.66	0.44
2:P:235:LYS:C	2:P:237:GLY:N	2.75	0.44
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.17	0.44
3:Q:87:ILE:N	3:Q:87:ILE:CD1	2.80	0.44
4:R:107:ILE:HG22	16:R:338:HOH:O	2.18	0.44
5:S:201:LEU:O	5:S:202:ARG:HB2	2.16	0.44
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.17	0.44
14:1:13:ILE:HD12	14:1:151:THR:CG2	2.47	0.44
1:A:67:VAL:HG11	1:A:213:ALA:HB3	1.99	0.44
1:A:141:HIS:HA	1:A:146:GLY:O	2.17	0.44
3:C:206:GLY:CA	3:C:209:ASN:HD22	2.30	0.44
5:E:8:TYR:OH	6:F:9:ASP:OD2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:179:LEU:CD2	6:F:192:GLN:HG2	2.44	0.44
7:G:234:VAL:O	7:G:237:ALA:HB3	2.17	0.44
8:H:152:ILE:HD11	8:H:177:VAL:HG21	2.00	0.44
8:H:197:ARG:NH2	9:I:139:GLU:O	2.51	0.44
11:K:135:TYR:O	11:K:139:ASP:HB2	2.18	0.44
14:N:37:VAL:CG2	14:N:41:ILE:HG22	2.48	0.44
1:O:81:MET:HE1	7:U:21:LEU:HD11	1.98	0.44
1:O:221:PHE:CD2	1:O:221:PHE:C	2.95	0.44
3:Q:41:LYS:HD3	3:Q:160:TRP:O	2.18	0.44
2:B:66:LYS:O	2:B:77:ALA:HA	2.18	0.44
4:D:189:ALA:O	4:D:193:VAL:HG23	2.17	0.44
5:E:47:VAL:HG12	5:E:48:LEU:N	2.31	0.44
6:F:50:VAL:HG12	6:F:211:GLU:HB3	1.98	0.44
6:F:114:ASP:O	6:F:118:GLN:HG2	2.18	0.44
11:K:31:VAL:HA	12:L:120:GLU:OE2	2.18	0.44
14:N:121:LYS:O	14:N:122:LEU:HD23	2.18	0.44
2:P:141:TYR:CG	2:P:21(E):VAL:HG21	2.53	0.44
3:Q:57:LYS:HG2	3:Q:208:LYS:HZ1	1.81	0.44
1:A:130:ARG:HG2	7:G:125:GLN:HG3	2.00	0.44
1:A:21(P):LYS:N	16:A:286:HOH:O	2.43	0.44
2:B:238:ILE:O	2:B:239:THR:O	2.36	0.44
3:C:57:LYS:HG2	3:C:208:LYS:HZ1	1.83	0.44
5:E:201:LEU:O	5:E:202:ARG:HB2	2.17	0.44
7:G:120:SER:HA	7:G:123:TYR:CD2	2.53	0.44
10:J:185:ARG:HG2	10:J:185:ARG:HH11	1.82	0.44
11:K:97:MET:O	11:K:114:ASP:HA	2.17	0.44
2:P:37:ALA:O	2:P:164:SER:HA	2.18	0.44
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.48	0.44
6:T:50:VAL:HG12	6:T:211:GLU:HB3	1.99	0.44
7:U:197:MET:HG2	7:U:205:PHE:CE1	2.53	0.44
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.47	0.44
15:V:500:GDT:H3	9:W:115:LEU:HD21	2.00	0.44
15:Y:500:GDT:H8	12:Z:96:TYR:CZ	2.53	0.44
13:O:190:LEU:N	13:O:190:LEU:HD12	2.32	0.44
7:G:49:ILE:CD1	7:G:212:VAL:HG22	2.47	0.44
9:I:110:ILE:C	9:I:110:ILE:CD1	2.91	0.44
9:I:186:LYS:HE2	9:I:188:TYR:CE1	2.52	0.44
11:K:177:HIS:O	11:K:184:TRP:HA	2.17	0.44
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.50	0.44
1:O:141:HIS:HA	1:O:146:GLY:O	2.18	0.44
2:P:112:LEU:HD23	2:P:112:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ALA:O	2:B:164:SER:HA	2.17	0.43
4:D:86:ARG:HA	4:D:86:ARG:HD3	1.81	0.43
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.47	0.43
6:F:28:VAL:O	6:F:32:GLU:HG3	2.17	0.43
8:H:201:GLN:HG3	12:Z:153:LYS:HG2	2.00	0.43
9:I:16:CYS:SG	9:I:34:ILE:HG12	2.58	0.43
9:I:61:TYR:CD1	9:I:61:TYR:C	2.95	0.43
10:J:100:LEU:HD21	10:J:112:GLN:HG3	2.00	0.43
11:K:5:ALA:HA	11:K:13:ILE:O	2.18	0.43
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.99	0.43
8:V:22:GLN:CG	15:V:500:GDT:H36B	2.48	0.43
13:O:150:VAL:HG21	16:O:231:HOH:O	2.17	0.43
4:D:93:ARG:HD2	16:D:258:HOH:O	2.17	0.43
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.48	0.43
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.99	0.43
9:I:137:MET:HE2	9:I:161:ASN:HB2	2.00	0.43
12:L:192:LYS:HE3	8:V:195:ASN:HB3	2.00	0.43
14:N:18(D):PRO:HA	14:N:18(G):TYR:CE2	2.53	0.43
1:O:58:LEU:HB3	7:U:162:ALA:O	2.19	0.43
3:Q:224:LEU:CD1	3:Q:224:LEU:N	2.78	0.43
3:Q:241:GLN:O	3:Q:243:GLN:N	2.46	0.43
5:S:76:LEU:O	5:S:76:LEU:HD23	2.19	0.43
7:U:49:ILE:CD1	7:U:212:VAL:HG22	2.48	0.43
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.17	0.43
11:Y:65:LEU:HD12	11:Y:65:LEU:HA	1.87	0.43
11:Y:174:ASN:HD22	11:Y:174:ASN:HA	1.65	0.43
12:Z:58:ARG:NH2	16:Z:244:HOH:O	2.47	0.43
2:B:224:PHE:HD2	2:B:224:PHE:H	1.64	0.43
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.53	0.43
13:M:-6:GLN:HG3	13:M:-6:GLN:O	2.17	0.43
14:N:116:GLY:CA	16:N:194:HOH:O	2.65	0.43
3:Q:238:GLN:O	3:Q:242:GLU:HG3	2.17	0.43
4:R:14:THR:HG22	4:R:15:PHE:N	2.34	0.43
6:T:13:SER:HB2	7:U:130:ARG:HD3	1.99	0.43
6:T:130:ARG:HG2	6:T:130:ARG:HH11	1.82	0.43
6:T:169:ARG:HE	6:T:169:ARG:HB3	1.47	0.43
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.78	0.43
8:V:206:PHE:CZ	9:W:157:GLN:HG3	2.54	0.43
2:B:68:TYR:CG	2:B:89:ILE:HD13	2.53	0.43
2:B:72:ASP:O	2:B:221:GLN:HG3	2.18	0.43
2:B:112:LEU:HD23	2:B:112:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LYS:HE2	16:C:263:HOH:O	2.18	0.43
7:G:130:ARG:HG3	7:G:131:PRO:O	2.18	0.43
13:M:92(A):LYS:O	13:M:92(B):MET:HB2	2.18	0.43
1:O:15:PHE:H	2:P:23:GLN:NE2	1.97	0.43
2:P:44:ASP:OD1	2:P:185:LYS:HE3	2.19	0.43
3:Q:67:VAL:HG22	3:Q:77:SER:HB3	2.00	0.43
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.47	0.43
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.18	0.43
4:R:187:LYS:O	4:R:191:LEU:HD22	2.19	0.43
10:X:100:LEU:HD21	10:X:112:GLN:HG3	2.00	0.43
2:B:172:ALA:O	2:B:176:LEU:HG	2.17	0.43
7:G:18(H):GLU:CD	7:G:18(H):GLU:N	2.77	0.43
10:J:14:LEU:HD12	10:J:42:LEU:HD23	2.00	0.43
13:M:211:ILE:HD11	14:1:36:ARG:CD	2.49	0.43
1:O:62:GLU:C	1:O:64:LEU:H	2.27	0.43
3:Q:104:GLU:O	3:Q:105:ASP:HB2	2.17	0.43
3:Q:215:VAL:HG23	3:Q:221:ILE:HG13	2.01	0.43
6:T:11:SER:HB3	6:T:14:VAL:HG23	2.00	0.43
6:T:81:LEU:HD12	6:T:133:GLY:HA3	2.01	0.43
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.84	0.43
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.32	0.43
7:U:151:THR:HB	16:U:303:HOH:O	2.18	0.43
8:V:62:ASN:HB3	8:V:82:MET:HE1	2.01	0.43
8:V:72:ARG:HH11	8:V:72:ARG:CG	2.31	0.43
10:X:143:ARG:HG2	10:X:143:ARG:HH11	1.83	0.43
11:Y:100:MET:HE2	11:Y:100:MET:HB2	1.83	0.43
12:Z:107:LYS:HA	12:Z:107:LYS:HD3	1.93	0.43
12:Z:14(Q):LEU:O	12:Z:14(W):LYS:C	2.60	0.43
2:B:38:ILE:HG13	2:B:164:SER:CB	2.48	0.43
2:B:163:ILE:HD12	2:B:164:SER:N	2.33	0.43
3:C:97:GLN:NE2	3:C:97:GLN:HA	2.33	0.43
6:F:203:GLU:OE1	6:F:203:GLU:HA	2.19	0.43
8:H:43:CYS:SG	8:H:99:LEU:HB3	2.59	0.43
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.00	0.43
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.44	0.43
9:I:20:LEU:HD13	9:I:20:LEU:C	2.44	0.43
9:I:110:ILE:O	9:I:110:ILE:CD1	2.66	0.43
2:P:38:ILE:HG13	2:P:164:SER:CB	2.49	0.43
6:T:24:VAL:O	6:T:27:ALA:HB3	2.18	0.43
11:Y:36:GLU:OE2	11:Y:184:TRP:CH2	2.72	0.43
11:Y:177:HIS:O	11:Y:184:TRP:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:0:125:LEU:HA	16:0:217:HOH:O	2.17	0.43
4:D:14:THR:HG22	4:D:15:PHE:N	2.33	0.43
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	2.00	0.43
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.53	0.43
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	2.01	0.43
8:H:2:THR:HG22	8:H:159:ILE:HD13	2.01	0.43
1:O:215:ILE:O	1:O:215:ILE:HG22	2.17	0.43
2:P:88:LEU:HB3	2:P:116:LEU:HD21	2.01	0.43
2:P:21(A):LYS:HE3	2:P:21(E):VAL:HG23	2.00	0.43
9:W:55:LEU:HD21	9:W:95:TYR:CD1	2.54	0.43
12:Z:19:ARG:HG2	12:Z:21:ILE:HG23	2.01	0.43
12:Z:14(H):GLY:C	12:Z:1(I):ASN:N	2.77	0.43
13:0:5:SER:HB3	13:0:14:ILE:HG13	2.01	0.43
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.77	0.43
3:C:18(A):ASP:OD2	3:C:18(C):LYS:HG2	2.19	0.43
3:C:206:GLY:HA3	3:C:209:ASN:HD22	1.83	0.43
5:E:162:GLY:O	5:E:163:THR:HB	2.19	0.43
10:J:5:GLY:O	10:J:124:TYR:HA	2.19	0.43
10:J:70:GLU:O	10:J:71:ASP:C	2.61	0.43
1:O:13:THR:O	2:P:130:ARG:HD3	2.19	0.43
11:Y:105:THR:OG1	11:Y:106:GLU:HG3	2.19	0.43
11:Y:184:TRP:O	11:Y:184:TRP:CE3	2.72	0.43
4:D:141:HIS:HA	4:D:145:GLY:O	2.19	0.43
6:F:177:GLU:OE2	7:G:57:LYS:HE2	2.19	0.43
8:H:175:VAL:HG12	8:H:176:CYS:N	2.33	0.43
10:J:4:LEU:HD23	10:J:126:ALA:CB	2.49	0.43
10:J:24:ILE:O	10:X:133:TYR:OH	2.32	0.43
1:O:191:HIS:CE1	1:O:236:LEU:HA	2.53	0.43
2:P:14:ILE:HB	3:Q:23:GLN:NE2	2.33	0.43
4:R:213:SER:CB	4:R:223:ILE:HA	2.48	0.43
7:U:171:GLU:OE1	7:U:171:GLU:N	2.51	0.43
12:Z:43:MET:CB	12:Z:101:ILE:HG22	2.46	0.43
1:A:110:LYS:HG2	16:A:246:HOH:O	2.18	0.43
3:C:220:ASP:HA	16:C:290:HOH:O	2.19	0.43
4:D:40:ILE:HG13	4:D:193:VAL:HG22	2.00	0.43
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.48	0.43
11:K:197:TRP:CE3	11:K:197:TRP:HA	2.54	0.43
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.54	0.43
1:O:43:THR:HG23	1:O:184:LEU:O	2.18	0.43
4:R:23:GLN:OE1	4:R:23:GLN:HA	2.18	0.43
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:207:LEU:HD21	4:R:233:ILE:HG12	2.01	0.43
6:T:203:GLU:HA	6:T:203:GLU:OE1	2.19	0.43
7:U:35:ILE:HD11	7:U:53:LYS:HG3	2.00	0.43
7:U:123:TYR:CE1	7:U:129:MET:HE3	2.53	0.43
9:W:-2:ASN:HA	9:W:21:GLY:O	2.19	0.43
9:W:7:THR:HG23	9:W:110:ILE:HG13	2.01	0.43
11:Y:97:MET:O	11:Y:114:ASP:HA	2.19	0.43
14:1:146:MET:HE1	16:1:230:HOH:O	2.18	0.43
3:C:159:SER:O	4:D:59:LEU:HD22	2.18	0.42
3:C:195:ARG:HG3	3:C:236:ILE:HD13	2.01	0.42
3:C:215:VAL:HG23	3:C:221:ILE:HG13	2.01	0.42
7:G:186:TRP:O	7:G:190:VAL:HG23	2.19	0.42
9:I:27:VAL:HG13	16:J:232:HOH:O	2.19	0.42
11:K:105:THR:OG1	11:K:106:GLU:HG3	2.19	0.42
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.53	0.42
13:M:150:VAL:HG21	16:M:266:HOH:O	2.18	0.42
6:T:177:GLU:OE2	7:U:57:LYS:HE2	2.19	0.42
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.48	0.42
7:U:168:LYS:O	7:U:172:ILE:HG12	2.19	0.42
13:0:187:LYS:HB3	13:0:190:LEU:HD11	2.01	0.42
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.64	0.42
6:F:122:ALA:HA	6:F:125:LEU:CD1	2.43	0.42
7:G:171:GLU:N	7:G:171:GLU:OE1	2.52	0.42
8:H:10:ASN:ND2	8:H:179:GLU:HG2	2.34	0.42
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.53	0.42
11:K:156:LYS:HB2	11:K:175:LEU:HD11	2.01	0.42
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.00	0.42
13:M:187:LYS:HB3	13:M:190:LEU:HD11	2.00	0.42
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.77	0.42
4:R:191:LEU:HD12	4:R:237:LEU:HB2	1.99	0.42
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	2.01	0.42
1:A:202:VAL:HG21	1:A:206:PHE:CE1	2.54	0.42
2:B:44:ASP:OD1	2:B:185:LYS:HE3	2.20	0.42
3:C:41:LYS:HD3	3:C:160:TRP:O	2.18	0.42
4:D:209:GLU:HG3	4:D:230:ALA:HB2	2.01	0.42
7:G:188:LYS:HD3	7:G:188:LYS:HA	1.89	0.42
7:G:211:GLU:HA	16:G:260:HOH:O	2.18	0.42
8:H:112:SER:OG	8:H:120:ASP:HB2	2.19	0.42
9:I:-2:ASN:HA	9:I:21:GLY:O	2.19	0.42
9:I:137:MET:HE3	9:I:141:LEU:CD1	2.49	0.42
2:P:172:ALA:O	2:P:176:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:206:GLY:CA	3:Q:209:ASN:HD22	2.32	0.42
8:V:159:ILE:O	8:V:163:ILE:HD12	2.19	0.42
2:B:235:LYS:C	2:B:237:GLY:N	2.73	0.42
3:C:73:HIS:CE1	3:C:106:PRO:HB2	2.54	0.42
3:C:108:THR:N	16:C:260:HOH:O	2.50	0.42
5:E:214:ILE:HD12	5:E:214:ILE:C	2.44	0.42
2:P:202:THR:CG2	2:P:204:SER:HB2	2.49	0.42
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.49	0.42
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.33	0.42
12:Z:14(H):GLY:O	12:Z:1(I):ASN:N	2.53	0.42
1:A:173:LYS:O	1:A:177:GLU:HG3	2.20	0.42
1:A:221:PHE:CD2	1:A:221:PHE:C	2.97	0.42
2:B:144:ARG:HG3	10:J:72:TYR:CZ	2.55	0.42
4:D:97:VAL:HG21	11:K:65:LEU:CD1	2.44	0.42
11:K:36:GLU:OE2	11:K:184:TRP:CH2	2.73	0.42
12:L:43:MET:CB	12:L:101:ILE:HG22	2.48	0.42
14:N:30:VAL:HG11	13:O:199:PHE:HE2	1.84	0.42
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	2.02	0.42
5:S:185:ASN:C	5:S:185:ASN:HD22	2.27	0.42
6:T:115:ARG:HG2	16:T:315:HOH:O	2.19	0.42
8:V:218:ILE:N	8:V:218:ILE:CD1	2.83	0.42
12:Z:14(O):LYS:CG	12:Z:14(P):PRO:HD2	2.49	0.42
13:O:157:ASN:HB3	16:O:250:HOH:O	2.19	0.42
3:C:36:CYS:H	3:C:51:GLU:CG	2.33	0.42
16:E:238:HOH:O	6:F:12:ASN:HB2	2.19	0.42
12:L:113:PHE:CD1	12:L:113:PHE:N	2.87	0.42
13:M:9:ASP:C	13:M:10:ASN:HD22	2.28	0.42
1:O:15:PHE:N	2:P:23:GLN:HE22	1.98	0.42
3:Q:36:CYS:H	3:Q:51:GLU:CG	2.33	0.42
4:R:40:ILE:HG13	4:R:193:VAL:HG22	2.00	0.42
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.49	0.42
5:S:107:LEU:HA	16:S:253:HOH:O	2.19	0.42
8:V:9:ASN:OD1	8:V:10:ASN:N	2.52	0.42
8:V:10:ASN:ND2	8:V:179:GLU:HG2	2.35	0.42
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.46	0.42
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	2.02	0.42
2:B:186:VAL:HG21	2:B:216:ARG:CD	2.46	0.42
6:F:11:SER:HB3	6:F:14:VAL:HG23	2.00	0.42
10:J:166:MET:HA	10:J:167:PRO:HD3	1.73	0.42
12:L:30:TYR:CZ	12:L:32:PRO:HG3	2.55	0.42
12:L:114:ASP:HB2	12:L:118:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:14(H):GLY:O	12:L:1(I):ASN:N	2.53	0.42
13:M:190:LEU:N	13:M:190:LEU:CD1	2.83	0.42
1:O:136:LEU:O	1:O:150:GLN:HA	2.18	0.42
1:O:173:LYS:O	1:O:177:GLU:HG3	2.20	0.42
7:U:63:THR:HG21	16:U:325:HOH:O	2.19	0.42
7:U:70:ILE:HG21	7:U:112:LEU:HD21	2.01	0.42
9:W:20:LEU:C	9:W:20:LEU:HD13	2.44	0.42
10:X:113:ILE:CG1	10:X:119:LYS:HG3	2.49	0.42
11:Y:137:VAL:HG21	11:Y:161:ALA:HB2	2.02	0.42
11:Y:197:TRP:HA	11:Y:197:TRP:CE3	2.54	0.42
14:1:146:MET:HB3	14:1:150:GLU:HB2	2.02	0.42
1:A:58:LEU:HD12	7:G:173:THR:HG23	2.01	0.42
1:A:88:LEU:HG	1:A:132:PHE:CE2	2.55	0.42
1:A:191:HIS:CE1	1:A:236:LEU:HA	2.53	0.42
5:E:179:THR:O	5:E:180:LEU:C	2.61	0.42
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.83	0.42
8:H:62:ASN:HB3	8:H:82:MET:HE1	2.01	0.42
8:H:167:LEU:HD22	12:Z:167:ILE:O	2.20	0.42
9:I:12:VAL:HG12	9:I:108:PRO:HB3	2.02	0.42
9:I:22:SER:O	9:I:23:GLN:HB2	2.20	0.42
9:I:113:PHE:HA	9:I:118:CYS:O	2.19	0.42
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	2.01	0.42
13:M:202:ASP:HB2	8:V:123:TYR:OH	2.19	0.42
1:O:38:LEU:C	1:O:38:LEU:HD12	2.45	0.42
8:V:175:VAL:HG12	8:V:176:CYS:N	2.34	0.42
9:W:124:PHE:O	9:W:125:ILE:HD13	2.19	0.42
2:B:6:ARG:HD2	4:D:9:ASP:N	2.34	0.42
2:B:202:THR:CG2	2:B:204:SER:HB2	2.50	0.42
13:M:42:VAL:HG23	13:M:178:ILE:HD11	2.01	0.42
1:O:8:TYR:HD2	7:U:128:TYR:HB3	1.84	0.42
1:O:57:PRO:HG2	7:U:177:GLU:HG2	2.01	0.42
2:P:137:ILE:CD1	2:P:165:VAL:HG22	2.48	0.42
2:P:238:ILE:O	2:P:239:THR:O	2.38	0.42
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.35	0.42
7:U:18:GLU:CD	7:U:18:GLU:N	2.78	0.42
9:W:16:CYS:SG	9:W:34:ILE:HG12	2.59	0.42
13:O:133:MET:C	13:O:136:PRO:HD2	2.45	0.42
16:G:249:HOH:O	8:H:82:MET:HA	2.20	0.42
10:J:133:TYR:OH	10:X:24:ILE:HG13	2.20	0.42
14:N:4:MET:HB3	14:N:126:ILE:HG22	2.02	0.42
6:T:42:CYS:HB2	6:T:184:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:194:ALA:O	6:T:198:TYR:HD1	2.02	0.42
7:U:217:LYS:HA	7:U:217:LYS:CE	2.41	0.42
11:Y:2:THR:HG22	11:Y:159:ILE:HD13	2.02	0.42
11:Y:75:SER:HA	11:Y:105:THR:HG21	2.02	0.42
15:Y:500:GDT:H36A	12:Z:114:ASP:OD2	2.20	0.42
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.32	0.42
12:Z:11:PHE:CE1	12:Z:148:VAL:HA	2.55	0.42
14:1:161:GLN:O	14:1:164:LYS:HB3	2.20	0.42
14:1:18(D):PRO:HA	14:1:18(G):TYR:CE2	2.55	0.42
1:A:134:VAL:O	1:A:153:PRO:HG3	2.20	0.41
1:A:179:ARG:HH11	1:A:179:ARG:CB	2.28	0.41
1:A:215:ILE:O	1:A:215:ILE:HG22	2.19	0.41
3:C:38:VAL:HG22	3:C:39:GLY:N	2.35	0.41
4:D:156:THR:HG22	5:E:83:PRO:HD3	2.02	0.41
10:J:2:ILE:O	10:J:16:SER:HA	2.20	0.41
1:O:29:THR:O	1:O:33:GLN:HG2	2.19	0.41
1:O:88:LEU:HG	1:O:132:PHE:CE2	2.54	0.41
3:Q:206:GLY:HA3	3:Q:209:ASN:HD22	1.85	0.41
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.20	0.41
7:U:60:ASP:OD2	7:U:62:THR:OG1	2.36	0.41
9:W:164:ASP:HA	16:W:213:HOH:O	2.20	0.41
11:Y:87:VAL:HG21	11:Y:97:MET:HE2	2.02	0.41
11:Y:138:LEU:HD12	11:Y:154:LEU:HG	2.01	0.41
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.35	0.41
5:E:15:PHE:H	6:F:23:GLN:NE2	2.17	0.41
7:G:48:VAL:O	7:G:48:VAL:HG23	2.20	0.41
7:G:110:ASP:OD2	7:G:110:ASP:N	2.53	0.41
10:J:35:ARG:HD3	10:J:35:ARG:HA	1.78	0.41
10:J:143:ARG:HG2	10:J:143:ARG:HH11	1.85	0.41
12:L:153:LYS:HG2	8:V:201:GLN:HG3	2.01	0.41
13:M:1:THR:OG1	13:M:2:SER:N	2.52	0.41
13:M:17:ASP:HA	13:M:173:PHE:HA	2.02	0.41
6:T:202:HIS:O	6:T:202:HIS:CG	2.73	0.41
6:T:21(B):THR:O	6:T:21(C):ASN:CB	2.67	0.41
8:V:112:SER:OG	8:V:120:ASP:HB2	2.20	0.41
9:W:81:GLN:HA	9:W:81:GLN:NE2	2.34	0.41
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.45	0.41
11:Y:10(B):LYS:N	11:Y:10(B):LYS:CD	2.68	0.41
12:Z:113:PHE:N	12:Z:113:PHE:CD1	2.87	0.41
13:0:201:LYS:HG3	13:0:202:ASP:OD2	2.20	0.41
3:C:212:ILE:HD13	3:C:212:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:42:THR:C	4:D:44:GLU:N	2.78	0.41
4:D:191:LEU:HD12	4:D:237:LEU:HB2	2.02	0.41
11:K:52:CYS:O	11:K:56:GLU:HB2	2.21	0.41
11:K:138:LEU:HD12	11:K:154:LEU:HG	2.01	0.41
3:Q:18(A):ASP:OD2	3:Q:18(C):LYS:HG2	2.20	0.41
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.55	0.41
4:R:170:GLU:OE1	4:R:170:GLU:N	2.53	0.41
6:T:95:GLU:CD	6:T:115:ARG:HD2	2.46	0.41
9:W:124:PHE:C	9:W:125:ILE:HD13	2.45	0.41
10:X:46:ALA:HA	16:X:223:HOH:O	2.19	0.41
14:1:126:ILE:HD13	14:1:126:ILE:N	2.24	0.41
14:1:126:ILE:H	14:1:126:ILE:CD1	2.26	0.41
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.20	0.41
3:C:104:GLU:O	3:C:105:ASP:HB2	2.19	0.41
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.20	0.41
8:H:105:ASP:C	8:H:106:THR:H	2.27	0.41
8:H:105:ASP:C	8:H:106:THR:N	2.79	0.41
10:J:-1:MET:CG	10:J:1:ASP:N	2.81	0.41
12:L:11:PHE:CE1	12:L:148:VAL:HA	2.55	0.41
3:Q:72:SER:O	3:Q:221:ILE:HD12	2.20	0.41
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	2.02	0.41
4:R:141:HIS:HA	4:R:145:GLY:O	2.21	0.41
5:S:28:LEU:HD12	5:S:153:PRO:HD2	2.02	0.41
5:S:162:GLY:O	5:S:163:THR:HB	2.19	0.41
5:S:2(B):THR:C	5:S:233:ILE:HD13	2.46	0.41
6:T:31:VAL:HG11	6:T:135:SER:HB2	2.02	0.41
11:Y:180:GLU:C	11:Y:183:GLY:H	2.27	0.41
13:0:-5:PRO:HD3	13:0:96:TRP:CE2	2.56	0.41
14:1:55:ILE:HD11	14:1:95:LEU:HD22	2.01	0.41
2:B:107:ILE:HG23	2:B:107:ILE:O	2.20	0.41
3:C:134:VAL:HG12	3:C:135:SER:N	2.35	0.41
4:D:39:GLY:O	4:D:162:ALA:HA	2.20	0.41
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.85	0.41
5:E:86:ARG:HH11	5:E:86:ARG:CG	2.33	0.41
6:F:172:ALA:O	6:F:173:LYS:C	2.64	0.41
6:F:240:ILE:HD12	6:F:240:ILE:O	2.19	0.41
8:H:22:GLN:CG	15:H:500:GDT:H36B	2.50	0.41
8:H:25:ILE:N	8:H:25:ILE:CD1	2.84	0.41
11:K:174:ASN:HD22	11:K:174:ASN:HA	1.65	0.41
11:K:210:ILE:HD13	9:W:30:LYS:NZ	2.35	0.41
12:L:31:GLU:OE1	13:M:120:TYR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:150:GLN:HE21	3:Q:150:GLN:HB3	1.68	0.41
4:R:179:GLU:O	4:R:18(C):HIS:HD2	2.04	0.41
9:W:51:ASP:OD1	10:X:90(B):ARG:NH2	2.53	0.41
11:Y:114:ASP:OD1	11:Y:114:ASP:C	2.63	0.41
12:Z:43:MET:HG2	12:Z:44:SER:N	2.34	0.41
14:1:20:THR:OG1	14:1:28:ASN:HB3	2.21	0.41
1:A:43:THR:HG23	1:A:184:LEU:O	2.19	0.41
2:B:97:GLN:OE1	9:I:64:ASN:HB3	2.20	0.41
2:B:141:TYR:CG	2:B:21(E):VAL:HG21	2.54	0.41
2:B:191:GLU:O	2:B:195:LYS:HG2	2.20	0.41
4:D:123:PHE:CE2	4:D:131:PRO:HG3	2.56	0.41
4:D:237:LEU:O	4:D:241:GLU:HG3	2.20	0.41
6:F:24:VAL:O	6:F:27:ALA:HB3	2.19	0.41
6:F:31:VAL:HG11	6:F:135:SER:HB2	2.03	0.41
7:G:191:GLU:CG	7:G:232:ARG:HG3	2.50	0.41
9:I:-2:ASN:HB3	16:I:200:HOH:O	2.20	0.41
9:I:124:PHE:C	9:I:125:ILE:HD13	2.45	0.41
12:L:4:LEU:HD13	12:L:138:LEU:HD21	2.01	0.41
2:P:21:LEU:O	2:P:25:GLU:HG2	2.20	0.41
3:Q:93:ARG:NH1	10:X:69:ARG:HA	2.36	0.41
4:R:12:VAL:HG13	4:R:12(B):GLU:OE1	2.20	0.41
4:R:237:LEU:O	4:R:241:GLU:HG3	2.20	0.41
6:T:109:ILE:HD13	6:T:109:ILE:H	1.84	0.41
8:V:29:LYS:NZ	9:W:139:GLU:OE2	2.54	0.41
1:A:29:THR:O	1:A:33:GLN:HG2	2.20	0.41
3:C:163:GLN:NE2	3:C:163:GLN:HA	2.34	0.41
6:F:16:SER:OG	6:F:18:ASP:OD2	2.37	0.41
8:H:206:PHE:CZ	9:I:157:GLN:HG3	2.56	0.41
10:J:167:PRO:O	10:X:168:MET:HE2	2.21	0.41
13:M:177:ILE:O	13:M:178:ILE:HD13	2.20	0.41
1:O:161:LYS:HG3	2:P:58:LEU:O	2.20	0.41
1:O:212:LEU:HD22	1:O:224:LEU:HD12	2.02	0.41
5:S:86:ARG:HG3	5:S:86:ARG:NH1	2.32	0.41
12:Z:22:THR:O	12:Z:23:ASP:HB2	2.20	0.41
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.51	0.41
13:O:-3:VAL:HG12	13:O:49:ILE:CG1	2.50	0.41
1:A:4:MET:O	1:A:5:THR:O	2.39	0.41
2:B:97:GLN:HA	2:B:97:GLN:NE2	2.35	0.41
4:D:207:LEU:HD21	4:D:233:ILE:HG12	2.02	0.41
6:F:26:TYR:O	6:F:29:LYS:HB2	2.21	0.41
6:F:194:ALA:O	6:F:198:TYR:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:110:ILE:CD1	9:I:122:ALA:O	2.69	0.41
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.33	0.41
11:K:87:VAL:HG21	11:K:97:MET:HE2	2.03	0.41
14:N:136:GLY:O	14:N:140:LYS:HG2	2.21	0.41
2:P:34:ALA:O	2:P:35:GLY:C	2.64	0.41
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.51	0.41
5:S:24:VAL:O	5:S:27:ALA:HB3	2.21	0.41
7:U:130:ARG:HG3	7:U:131:PRO:O	2.21	0.41
7:U:191:GLU:CG	7:U:232:ARG:HG3	2.51	0.41
8:V:43:CYS:SG	8:V:99:LEU:HB3	2.60	0.41
10:X:18:LYS:HD3	10:X:174:ILE:HG12	2.03	0.41
11:Y:52:CYS:O	11:Y:56:GLU:HB2	2.20	0.41
14:1:143:ARG:O	14:1:146:MET:HG3	2.21	0.41
1:A:26:TYR:O	1:A:29:THR:HB	2.21	0.41
2:B:144:ARG:CZ	2:B:14(A):TYR:CE2	3.04	0.41
3:C:31:VAL:HG11	3:C:135:SER:HB2	2.02	0.41
3:C:163:GLN:NE2	3:C:164:THR:N	2.52	0.41
4:D:179:GLU:O	4:D:18(C):HIS:HD2	2.03	0.41
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.51	0.41
5:E:2(B):THR:C	5:E:233:ILE:HD13	2.46	0.41
6:F:38:ILE:HG12	6:F:197:ILE:HD11	2.03	0.41
7:G:18:GLU:N	7:G:18:GLU:CD	2.79	0.41
7:G:107:MET:HA	7:G:108:PRO:HD3	1.92	0.41
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.02	0.41
7:G:218:ASP:O	7:G:220:LYS:CB	2.66	0.41
8:H:72:ARG:HG3	8:H:72:ARG:NH1	2.34	0.41
10:J:90(A):ILE:HD12	10:J:90(A):ILE:HA	1.87	0.41
11:K:100:MET:HA	11:K:111:TYR:O	2.21	0.41
11:K:100:MET:HE2	11:K:100:MET:HB2	1.80	0.41
13:M:112:TYR:CD2	13:M:112:TYR:C	2.99	0.41
14:N:36:ARG:CD	13:O:211:ILE:HD11	2.51	0.41
14:N:132:THR:HA	14:N:135:TYR:CD2	2.55	0.41
14:N:146:MET:HB3	14:N:150:GLU:HB2	2.03	0.41
2:P:44:ASP:OD2	2:P:44:ASP:N	2.52	0.41
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	2.02	0.41
3:Q:150:GLN:O	3:Q:157:TYR:HA	2.21	0.41
4:R:112:LEU:HD13	4:R:112:LEU:O	2.21	0.41
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.88	0.41
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.21	0.41
8:V:170:GLY:O	8:V:171:SER:HB2	2.21	0.41
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:100:MET:HA	11:Y:111:TYR:O	2.21	0.41
12:Z:76:ILE:HG22	16:Z:229:HOH:O	2.21	0.41
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.35	0.41
14:1:10(B):LYS:HD3	14:1:10(B):LYS:C	2.46	0.41
1:A:13:THR:HG22	1:A:21:LEU:HD22	2.02	0.41
2:B:44:ASP:OD2	2:B:44:ASP:N	2.53	0.41
16:B:254:HOH:O	3:C:62(A):ILE:CD1	2.63	0.41
3:C:72:SER:O	3:C:221:ILE:HD12	2.20	0.41
3:C:106:PRO:HG2	3:C:143:PRO:HG3	2.02	0.41
10:J:143:ARG:HB2	10:J:146:MET:HG3	2.03	0.41
11:K:4:LEU:HD22	11:K:4:LEU:C	2.46	0.41
14:N:55:ILE:HD11	14:N:95:LEU:HD22	2.03	0.41
14:N:143:ARG:O	14:N:146:MET:HG3	2.21	0.41
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.36	0.41
4:R:70:ILE:HB	4:R:74:ILE:HG22	2.03	0.41
5:S:179:THR:O	5:S:180:LEU:C	2.64	0.41
7:U:112:LEU:O	7:U:116:MET:HG2	2.20	0.41
6:F:217:LEU:HD12	6:F:217:LEU:HA	1.90	0.40
6:F:21(B):THR:O	6:F:21(C):ASN:CB	2.69	0.40
7:G:18:GLU:CD	7:G:18:GLU:H	2.29	0.40
10:J:112:GLN:NE2	10:J:126:ALA:N	2.69	0.40
13:M:193:GLU:HA	13:M:193:GLU:OE2	2.21	0.40
1:O:4:MET:O	1:O:5:THR:O	2.39	0.40
2:P:38:ILE:HG22	2:P:39:GLY:N	2.36	0.40
2:P:112:LEU:C	2:P:112:LEU:CD2	2.94	0.40
2:P:191:GLU:O	2:P:195:LYS:HG2	2.20	0.40
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.52	0.40
3:Q:136:THR:O	3:Q:150:GLN:HA	2.21	0.40
5:S:8:TYR:OH	6:T:9:ASP:OD2	2.32	0.40
6:T:109:ILE:HB	6:T:110:PRO:HD3	2.02	0.40
8:V:152:ILE:HD11	8:V:177:VAL:HG21	2.02	0.40
16:V:540:HOH:O	9:W:150:ASP:HA	2.21	0.40
13:O:112:TYR:HE1	13:O:127:THR:HG22	1.86	0.40
3:C:201:VAL:HG21	3:C:210:ILE:CD1	2.46	0.40
4:D:46:VAL:HG11	4:D:139:ALA:HB1	2.03	0.40
5:E:226:GLY:C	5:E:228:ALA:N	2.79	0.40
8:H:156:SER:O	8:H:160:GLN:HG3	2.22	0.40
9:I:51:ASP:CG	10:J:90(B):ARG:HH21	2.29	0.40
11:K:147:SER:C	11:K:149:GLU:N	2.78	0.40
13:M:133:MET:C	13:M:136:PRO:HD2	2.47	0.40
1:O:179:ARG:HH11	1:O:179:ARG:CB	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.56	0.40
3:Q:90:GLU:HA	3:Q:90:GLU:OE2	2.21	0.40
4:R:39:GLY:O	4:R:162:ALA:HA	2.21	0.40
5:S:179:THR:HG22	5:S:179:THR:O	2.21	0.40
6:T:26:TYR:O	6:T:29:LYS:HB2	2.22	0.40
11:Y:184:TRP:C	11:Y:184:TRP:CE3	2.99	0.40
14:1:55:ILE:HD11	14:1:95:LEU:CD2	2.50	0.40
2:B:137:ILE:CD1	2:B:165:VAL:HG22	2.52	0.40
4:D:187:LYS:O	4:D:191:LEU:HD22	2.21	0.40
10:J:66:TYR:CE2	10:J:74:LEU:HG	2.56	0.40
10:J:143:ARG:O	10:J:146:MET:HG3	2.21	0.40
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.87	0.40
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.21	0.40
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.22	0.40
4:R:18(C):HIS:O	4:R:18(E):SER:N	2.54	0.40
6:T:82:ILE:O	6:T:83:PRO:C	2.63	0.40
7:U:18(H):GLU:CD	7:U:18(H):GLU:H	2.29	0.40
9:W:110:ILE:CD1	9:W:110:ILE:O	2.70	0.40
9:W:143:GLU:HA	9:W:144:PRO:HD3	1.88	0.40
14:1:37:VAL:CG2	14:1:41:ILE:HG22	2.51	0.40
3:C:46:VAL:O	3:C:215:VAL:HG12	2.21	0.40
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.57	0.40
8:H:118:SER:HB3	14:N:50:ALA:N	2.37	0.40
11:K:4:LEU:CD1	11:K:159:ILE:HG12	2.51	0.40
14:N:32:ASP:OD1	14:N:186:ARG:NH2	2.54	0.40
1:O:17:PRO:HA	2:P:26:TYR:CE1	2.57	0.40
1:O:185:GLU:OE1	1:O:187:GLU:HB2	2.22	0.40
2:P:20:ARG:HG2	2:P:20:ARG:NH1	2.37	0.40
2:P:184:MET:HE2	2:P:189:ALA:N	2.37	0.40
10:X:135:PHE:HZ	16:X:213:HOH:O	2.04	0.40
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.57	0.40
4:D:82:THR:N	16:D:256:HOH:O	2.55	0.40
11:K:67:GLU:CG	11:K:73:ARG:HA	2.52	0.40
3:Q:82:ASN:O	3:Q:83:ALA:C	2.64	0.40
3:Q:163:GLN:NE2	3:Q:163:GLN:HA	2.36	0.40
4:R:197:LEU:O	4:R:201:MET:HG3	2.21	0.40
6:T:172:ALA:O	6:T:173:LYS:C	2.65	0.40
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.04	0.40
10:X:155:LEU:HD23	10:X:155:LEU:HA	1.85	0.40
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.87	0.40
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.21	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%)	15 (6%)	5 (2%)	6	16
1	O	248/250 (99%)	228 (92%)	16 (6%)	4 (2%)	7	20
2	B	242/258 (94%)	220 (91%)	19 (8%)	3 (1%)	10	27
2	P	242/258 (94%)	219 (90%)	19 (8%)	4 (2%)	7	19
3	C	239/254 (94%)	215 (90%)	18 (8%)	6 (2%)	4	11
3	Q	239/254 (94%)	217 (91%)	17 (7%)	5 (2%)	5	15
4	D	240/260 (92%)	215 (90%)	20 (8%)	5 (2%)	5	15
4	R	240/260 (92%)	216 (90%)	18 (8%)	6 (2%)	4	11
5	E	231/234 (99%)	210 (91%)	15 (6%)	6 (3%)	4	11
5	S	231/234 (99%)	210 (91%)	16 (7%)	5 (2%)	5	14
6	F	242/287 (84%)	228 (94%)	12 (5%)	2 (1%)	16	37
6	T	242/287 (84%)	226 (93%)	14 (6%)	2 (1%)	16	37
7	G	241/252 (96%)	225 (93%)	13 (5%)	3 (1%)	10	27
7	U	241/252 (96%)	225 (93%)	13 (5%)	3 (1%)	10	27
8	H	220/232 (95%)	203 (92%)	13 (6%)	4 (2%)	6	18
8	V	220/232 (95%)	204 (93%)	12 (6%)	4 (2%)	6	18
9	I	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	24	48
9	W	202/205 (98%)	190 (94%)	10 (5%)	2 (1%)	12	32
10	J	196/198 (99%)	184 (94%)	10 (5%)	2 (1%)	12	32
10	X	196/198 (99%)	184 (94%)	10 (5%)	2 (1%)	12	32
11	K	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	24	48
11	Y	210/212 (99%)	193 (92%)	16 (8%)	1 (0%)	24	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	220/241 (91%)	208 (94%)	11 (5%)	1 (0%)	24	48
12	Z	220/241 (91%)	208 (94%)	11 (5%)	1 (0%)	24	48
13	O	231/266 (87%)	212 (92%)	18 (8%)	1 (0%)	30	54
13	M	231/266 (87%)	213 (92%)	17 (7%)	1 (0%)	30	54
14	1	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6690 (94%)	5840 (92%)	392 (6%)	80 (1%)	9	25

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	56	SER
3	C	58	LEU
4	D	12(G)	GLU
6	F	64	ASN
7	G	220	LYS
10	J	192	ALA
1	O	5	THR
1	O	56	SER
3	Q	58	LEU
4	R	12(G)	GLU
5	S	202	ARG
6	T	64	ASN
7	U	220	LYS
10	X	192	ALA
1	A	167	LYS
2	B	54	VAL
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
4	D	18(D)	SER
5	E	5	ARG
5	E	180	LEU
5	E	202	ARG
5	E	227	GLU
5	E	231	LYS
7	G	184	ASN
11	K	39	PRO
12	L	14(I)	THR

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Mol	Chain	Res	Type
1	O	167	LYS
2	P	54	VAL
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	18(D)	SER
5	S	5	ARG
5	S	227	GLU
5	S	231	LYS
7	U	184	ASN
11	Y	39	PRO
12	Z	14(I)	THR
3	C	184	ALA
4	D	128	MET
7	G	239	GLN
8	H	10(A)	PRO
13	M	96	TRP
1	O	204	GLY
3	Q	184	ALA
4	R	128	MET
5	S	180	LEU
7	U	239	GLN
8	V	10(A)	PRO
1	A	204	GLY
4	D	12(C)	GLY
6	F	205	ASN
9	I	93	GLY
4	R	12(C)	GLY
6	T	205	ASN
8	V	91	GLN
9	W	93	GLY
3	C	179	ASN
5	E	18(A)	ASP
8	H	91	GLN
3	Q	179	ASN
8	V	171	SER
9	W	23	GLN
13	0	96	TRP
3	C	242	GLU
8	H	171	SER
2	P	6	ARG
4	R	11	GLY

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Mol	Chain	Res	Type
4	R	12(E)	SER
8	H	180	ILE
10	J	8	VAL
10	X	8	VAL
2	B	21(B)	GLY
2	P	21(B)	GLY
8	V	180	ILE
1	A	22	GLY
4	D	11	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	199 (95%)	10 (5%)	23	50
1	O	209/209 (100%)	199 (95%)	10 (5%)	23	50
2	B	203/216 (94%)	186 (92%)	17 (8%)	10	26
2	P	203/216 (94%)	186 (92%)	17 (8%)	10	26
3	C	213/226 (94%)	201 (94%)	12 (6%)	19	44
3	Q	213/226 (94%)	200 (94%)	13 (6%)	17	40
4	D	198/215 (92%)	184 (93%)	14 (7%)	13	33
4	R	198/215 (92%)	184 (93%)	14 (7%)	13	33
5	E	192/193 (100%)	179 (93%)	13 (7%)	14	35
5	S	192/193 (100%)	179 (93%)	13 (7%)	14	35
6	F	201/238 (84%)	185 (92%)	16 (8%)	11	28
6	T	201/238 (84%)	185 (92%)	16 (8%)	11	28
7	G	207/210 (99%)	195 (94%)	12 (6%)	18	42
7	U	207/210 (99%)	195 (94%)	12 (6%)	18	42
8	H	181/190 (95%)	171 (94%)	10 (6%)	19	45
8	V	181/190 (95%)	170 (94%)	11 (6%)	17	40
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	167 (97%)	5 (3%)	37	67
10	J	175/175 (100%)	166 (95%)	9 (5%)	21	48
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	185/201 (92%)	162 (88%)	23 (12%)	4	11
12	Z	185/201 (92%)	162 (88%)	23 (12%)	4	11
13	O	199/224 (89%)	186 (94%)	13 (6%)	15	37
13	M	199/224 (89%)	189 (95%)	10 (5%)	22	48
14	I	162/162 (100%)	152 (94%)	10 (6%)	16	39
14	N	162/162 (100%)	151 (93%)	11 (7%)	14	35
All	All	5332/5602 (95%)	4981 (93%)	351 (7%)	15	36

All (351) 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	65	SER
1	A	119	ILE
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
1	A	215	ILE
2	B	8	TYR
2	B	14	ILE
2	B	41	MET
2	B	58	LEU
2	B	67	LEU
2	B	87	ILE
2	B	111	ILE
2	B	116	LEU
2	B	119	ILE
2	B	124	THR
2	B	14(A)	TYR
2	B	150	THR

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Mol	Chain	Res	Type
2	B	163	ILE
2	B	198	SER
2	B	206	THR
2	B	224	PHE
2	B	238	ILE
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	66	LYS
3	C	87	ILE
3	C	100	ARG
3	C	135	SER
3	C	150	GLN
3	C	163	GLN
3	C	174	GLU
3	C	224	LEU
3	C	227	GLU
4	D	28	LEU
4	D	31	ILE
4	D	40	ILE
4	D	48	LEU
4	D	52	LYS
4	D	64	ILE
4	D	107	ILE
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	196	ILE
4	D	215	ILE
5	E	12	THR
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	111	ARG
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	214	ILE

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Mol	Chain	Res	Type
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	35	THR
6	F	43	ASN
6	F	56	SER
6	F	72	ARG
6	F	74	ILE
6	F	98	SER
6	F	105	THR
6	F	109	ILE
6	F	127	ASN
6	F	135	SER
6	F	144	ASN
6	F	169	ARG
6	F	187	ARG
6	F	203	GLU
6	F	240	ILE
7	G	14	ILE
7	G	38	LEU
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	14(A)	GLU
7	G	174	THR
7	G	197	MET
7	G	204	GLU
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	13	VAL
8	H	25	ILE
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	144	GLN
8	H	163	ILE
8	H	197	ARG
8	H	218	ILE
9	I	29	ASN
9	I	110	ILE

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Mol	Chain	Res	Type
9	I	125	ILE
9	I	160	LEU
10	J	6	ILE
10	J	21	THR
10	J	24	ILE
10	J	34	THR
10	J	70	GLU
10	J	121	GLU
10	J	155	LEU
10	J	166	MET
10	J	168	MET
11	K	4	LEU
11	K	37	ILE
11	K	39	PRO
11	K	65	LEU
11	K	74	ILE
11	K	86	LEU
11	K	87	VAL
11	K	100	MET
11	K	101	ILE
11	K	110	ILE
11	K	185	ILE
11	K	210	ILE
12	L	-7	ASN
12	L	14	LEU
12	L	58	ARG
12	L	99	THR
12	L	100	ILE
12	L	114	ASP
12	L	120	GLU
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

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Mol	Chain	Res	Type
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS
12	L	152	ILE
13	M	40	ASN
13	M	55	ILE
13	M	62	LEU
13	M	65	GLU
13	M	91	ARG
13	M	129	PHE
13	M	148	VAL
13	M	149	GLN
13	M	203	ILE
13	M	204	LYS
14	N	6	VAL
14	N	20	THR
14	N	55	ILE
14	N	84	LYS
14	N	89	GLU
14	N	115	LEU
14	N	119	VAL
14	N	126	ILE
14	N	134	ILE
14	N	149	GLU
14	N	178	LEU
1	O	32	LYS
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	65	SER
1	O	119	ILE
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
1	O	215	ILE
2	P	8	TYR
2	P	14	ILE
2	P	41	MET
2	P	58	LEU
2	P	67	LEU
2	P	87	ILE
2	P	104	ASN

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Mol	Chain	Res	Type
2	P	116	LEU
2	P	119	ILE
2	P	124	THR
2	P	14(A)	TYR
2	P	150	THR
2	P	163	ILE
2	P	198	SER
2	P	206	THR
2	P	224	PHE
2	P	238	ILE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	66	LYS
3	Q	87	ILE
3	Q	100	ARG
3	Q	135	SER
3	Q	150	GLN
3	Q	163	GLN
3	Q	174	GLU
3	Q	212	ILE
3	Q	224	LEU
3	Q	227	GLU
4	R	28	LEU
4	R	31	ILE
4	R	40	ILE
4	R	48	LEU
4	R	52	LYS
4	R	64	ILE
4	R	107	ILE
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	196	ILE
4	R	215	ILE
5	S	12	THR
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU

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Mol	Chain	Res	Type
5	S	97	ASN
5	S	111	ARG
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	214	ILE
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	35	THR
6	T	43	ASN
6	T	56	SER
6	T	72	ARG
6	T	74	ILE
6	T	98	SER
6	T	105	THR
6	T	109	ILE
6	T	127	ASN
6	T	135	SER
6	T	144	ASN
6	T	169	ARG
6	T	187	ARG
6	T	203	GLU
6	T	240	ILE
7	U	14	ILE
7	U	38	LEU
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	14(A)	GLU
7	U	174	THR
7	U	197	MET
7	U	204	GLU
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	25	ILE
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	63	ILE

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Mol	Chain	Res	Type
8	V	68	LEU
8	V	144	GLN
8	V	163	ILE
8	V	197	ARG
8	V	218	ILE
9	W	29	ASN
9	W	90	ARG
9	W	110	ILE
9	W	125	ILE
9	W	160	LEU
10	X	6	ILE
10	X	24	ILE
10	X	34	THR
10	X	52	THR
10	X	70	GLU
10	X	121	GLU
10	X	155	LEU
10	X	166	MET
10	X	168	MET
10	X	174	ILE
11	Y	4	LEU
11	Y	37	ILE
11	Y	39	PRO
11	Y	65	LEU
11	Y	74	ILE
11	Y	87	VAL
11	Y	100	MET
11	Y	101	ILE
11	Y	110	ILE
11	Y	185	ILE
11	Y	210	ILE
12	Z	-7	ASN
12	Z	14	LEU
12	Z	40	ASN
12	Z	58	ARG
12	Z	99	THR
12	Z	114	ASP
12	Z	120	GLU
12	Z	138	LEU
12	Z	14(A)	LYS
12	Z	14(B)	ASN
12	Z	14(C)	GLN

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Mol	Chain	Res	Type
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
12	Z	14(W)	LYS
12	Z	152	ILE
13	0	40	ASN
13	0	55	ILE
13	0	62	LEU
13	0	65	GLU
13	0	79	ILE
13	0	91	ARG
13	0	115	LEU
13	0	129	PHE
13	0	148	VAL
13	0	149	GLN
13	0	155	ILE
13	0	203	ILE
13	0	204	LYS
14	1	6	VAL
14	1	20	THR
14	1	55	ILE
14	1	84	LYS
14	1	89	GLU
14	1	115	LEU
14	1	119	VAL
14	1	126	ILE
14	1	134	ILE
14	1	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (235) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	145	ASN

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Mol	Chain	Res	Type
1	A	191	HIS
2	B	23	GLN
2	B	71	ASN
2	B	90	ASN
2	B	95	HIS
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	97	GLN
3	C	120	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	230	ASN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	20(A)	ASN
4	D	211	GLN
4	D	226	ASN
5	E	7	ASN
5	E	73	HIS
5	E	95	GLN
5	E	97	ASN
5	E	104	ASN
5	E	114	HIS
5	E	121	GLN
5	E	125	GLN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN

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Mol	Chain	Res	Type
6	F	192	GLN
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	18(C)	HIS
7	G	184	ASN
7	G	228	ASN
8	H	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	220	ASN
9	I	29	ASN
9	I	64	ASN
9	I	81	GLN
9	I	193	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	64	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	160	GLN
10	J	186	GLN
10	J	193	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	189	ASN
11	K	207	ASN
11	K	208	ASN

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Mol	Chain	Res	Type
12	L	-9	GLN
12	L	-7	ASN
12	L	-2	ASN
12	L	20	ASN
12	L	27	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	140	ASN
12	L	141	GLN
12	L	14(B)	ASN
12	L	1(I)	ASN
12	L	166	HIS
12	L	168	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	69	GLN
14	N	94	ASN
14	N	106	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	145	ASN
1	O	191	HIS
2	P	23	GLN
2	P	33	HIS
2	P	71	ASN
2	P	90	ASN
2	P	95	HIS
2	P	121	GLN
2	P	125	GLN

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Mol	Chain	Res	Type
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	230	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	20(A)	ASN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN
5	S	73	HIS
5	S	95	GLN
5	S	97	ASN
5	S	104	ASN
5	S	114	HIS
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
7	U	11	HIS
7	U	32	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN

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Mol	Chain	Res	Type
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	18(C)	HIS
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	91	GLN
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	220	ASN
9	W	29	ASN
9	W	64	ASN
9	W	81	GLN
9	W	193	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	64	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	160	GLN
10	X	186	GLN
10	X	193	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	-2	ASN
12	Z	20	ASN
12	Z	27	ASN

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Mol	Chain	Res	Type
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	84	GLN
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
12	Z	168	GLN
13	0	10	ASN
13	0	40	ASN
13	0	89	GLN
13	0	93	ASN
13	0	132	HIS
13	0	149	GLN
13	0	157	ASN
13	0	189	ASN
13	0	191	GLN
14	1	69	GLN
14	1	106	ASN
14	1	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	GDT	K	500	11	36,37,37	2.19	3 (8%)	42,46,46	1.81	8 (19%)
15	GDT	V	500	8	36,37,37	2.35	3 (8%)	42,46,46	1.72	8 (19%)
15	GDT	Y	500	11	36,37,37	1.98	2 (5%)	42,46,46	1.89	8 (19%)
15	GDT	H	500	8	36,37,37	2.26	4 (11%)	42,46,46	1.73	8 (19%)

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	GDT	K	500	11	-	9/50/50/50	0/0/1/1
15	GDT	V	500	8	-	12/50/50/50	0/0/1/1
15	GDT	Y	500	11	-	9/50/50/50	0/0/1/1
15	GDT	H	500	8	-	11/50/50/50	0/0/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	500	GDT	C26-C27	12.00	1.59	1.32
15	H	500	GDT	C26-C27	11.74	1.58	1.32
15	K	500	GDT	C26-C27	11.36	1.57	1.32
15	Y	500	GDT	C26-C27	10.00	1.54	1.32
15	V	500	GDT	C14-N13	3.18	1.52	1.45
15	H	500	GDT	C14-N13	2.80	1.51	1.45
15	V	500	GDT	C31-N30	2.59	1.39	1.34
15	K	500	GDT	C22-N23	-2.42	1.40	1.46
15	H	500	GDT	C31-N30	2.34	1.39	1.34
15	K	500	GDT	C14-N13	2.09	1.50	1.45
15	H	500	GDT	C12-N13	2.07	1.38	1.34
15	Y	500	GDT	C14-N13	2.00	1.50	1.45

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	500	GDT	C27-C26-C24	-6.38	107.68	122.67
15	Y	500	GDT	C26-C24-N23	6.04	128.30	115.07
15	K	500	GDT	C27-C26-C24	-5.80	109.04	122.67
15	K	500	GDT	C26-C24-N23	5.75	127.67	115.07
15	V	500	GDT	C26-C24-N23	4.95	125.91	115.07
15	H	500	GDT	C27-C26-C24	-4.87	111.21	122.67
15	H	500	GDT	C26-C24-N23	4.67	125.30	115.07
15	V	500	GDT	C27-C26-C24	-4.62	111.81	122.67
15	H	500	GDT	C1-C12-N13	4.11	121.64	114.61
15	V	500	GDT	C1-C12-N13	4.07	121.58	114.61
15	Y	500	GDT	O25-C24-C26	-3.79	114.21	122.95
15	K	500	GDT	O25-C24-C26	-3.68	114.47	122.95
15	H	500	GDT	C22-N23-C24	3.41	127.37	122.46
15	K	500	GDT	C1-C12-N13	3.32	120.30	114.61
15	V	500	GDT	O25-C24-C26	-3.30	115.34	122.95
15	Y	500	GDT	C1-C12-N13	3.30	120.25	114.61
15	V	500	GDT	C22-N23-C24	3.23	127.11	122.46
15	Y	500	GDT	O25-C24-N23	-3.06	117.49	122.29
15	H	500	GDT	O25-C24-C26	-2.89	116.29	122.95
15	K	500	GDT	O25-C24-N23	-2.84	117.83	122.29
15	K	500	GDT	C22-N23-C24	2.78	126.46	122.46
15	Y	500	GDT	C22-N23-C24	2.72	126.37	122.46
15	H	500	GDT	O37-C12-C1	-2.69	116.75	122.95
15	Y	500	GDT	C28-N30-C31	-2.57	119.34	122.93
15	H	500	GDT	C3-C2-C1	-2.57	118.58	124.65
15	H	500	GDT	O25-C24-N23	-2.47	118.41	122.29
15	K	500	GDT	C28-N30-C31	-2.42	119.56	122.93
15	V	500	GDT	C3-C2-C1	-2.41	118.94	124.65
15	V	500	GDT	O37-C12-C1	-2.34	117.56	122.95
15	Y	500	GDT	O37-C12-C1	-2.33	117.59	122.95
15	V	500	GDT	O25-C24-N23	-2.26	118.75	122.29
15	K	500	GDT	O37-C12-C1	-2.22	117.83	122.95

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	500	GDT	N16-C17-C18-C19
15	H	500	GDT	C26-C27-C28-N30
15	H	500	GDT	C24-C26-C27-C28
15	H	500	GDT	C26-C24-N23-C22
15	H	500	GDT	O25-C24-N23-C22
15	H	500	GDT	O20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
15	K	500	GDT	C26-C27-C28-N30
15	K	500	GDT	C24-C26-C27-C28
15	K	500	GDT	C26-C24-N23-C22
15	K	500	GDT	O25-C24-N23-C22
15	V	500	GDT	N16-C17-C18-C19
15	V	500	GDT	C26-C27-C28-N30
15	V	500	GDT	C24-C26-C27-C28
15	V	500	GDT	C26-C24-N23-C22
15	V	500	GDT	O25-C24-N23-C22
15	Y	500	GDT	C26-C27-C28-N30
15	Y	500	GDT	C24-C26-C27-C28
15	Y	500	GDT	C26-C24-N23-C22
15	Y	500	GDT	O25-C24-N23-C22
15	H	500	GDT	C26-C27-C28-C29
15	K	500	GDT	C26-C27-C28-C29
15	V	500	GDT	C26-C27-C28-C29
15	Y	500	GDT	C26-C27-C28-C29
15	K	500	GDT	N23-C24-C26-C27
15	H	500	GDT	C4-C5-C6-C7
15	V	500	GDT	C4-C5-C6-C7
15	K	500	GDT	O25-C24-C26-C27
15	Y	500	GDT	O25-C24-C26-C27
15	Y	500	GDT	N23-C24-C26-C27
15	V	500	GDT	C31-C17-C18-C19
15	V	500	GDT	O20-C19-C21-C22
15	H	500	GDT	C31-C17-C18-C19
15	Y	500	GDT	C17-C18-C19-O20
15	H	500	GDT	C18-C19-C21-C22
15	V	500	GDT	C3-C4-C5-C6
15	V	500	GDT	C18-C19-C21-C22
15	H	500	GDT	C3-C4-C5-C6
15	K	500	GDT	C31-C17-C18-C19
15	K	500	GDT	O20-C19-C21-C22
15	Y	500	GDT	O20-C19-C21-C22
15	V	500	GDT	O25-C24-C26-C27

There are no ring outliers.

4 monomers are involved in 11 short contacts:

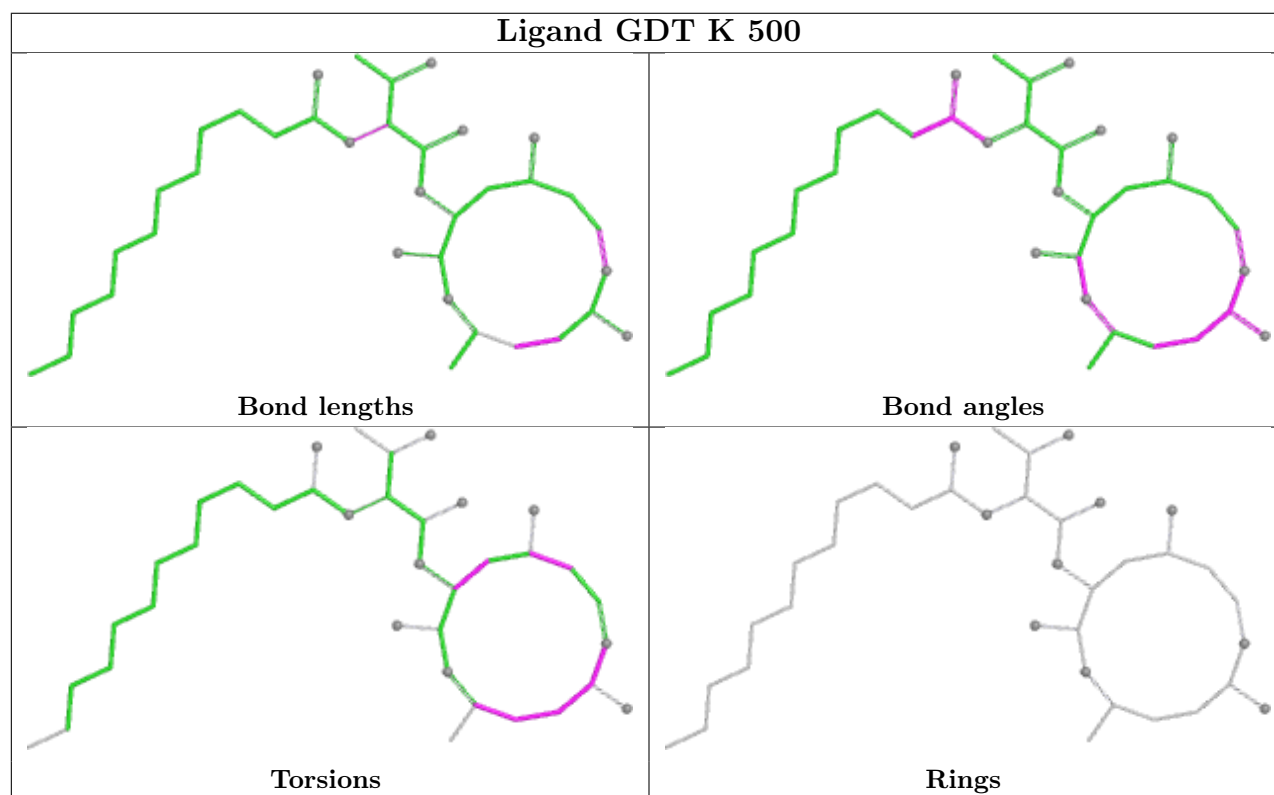
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	500	GDT	2	0
15	V	500	GDT	3	0

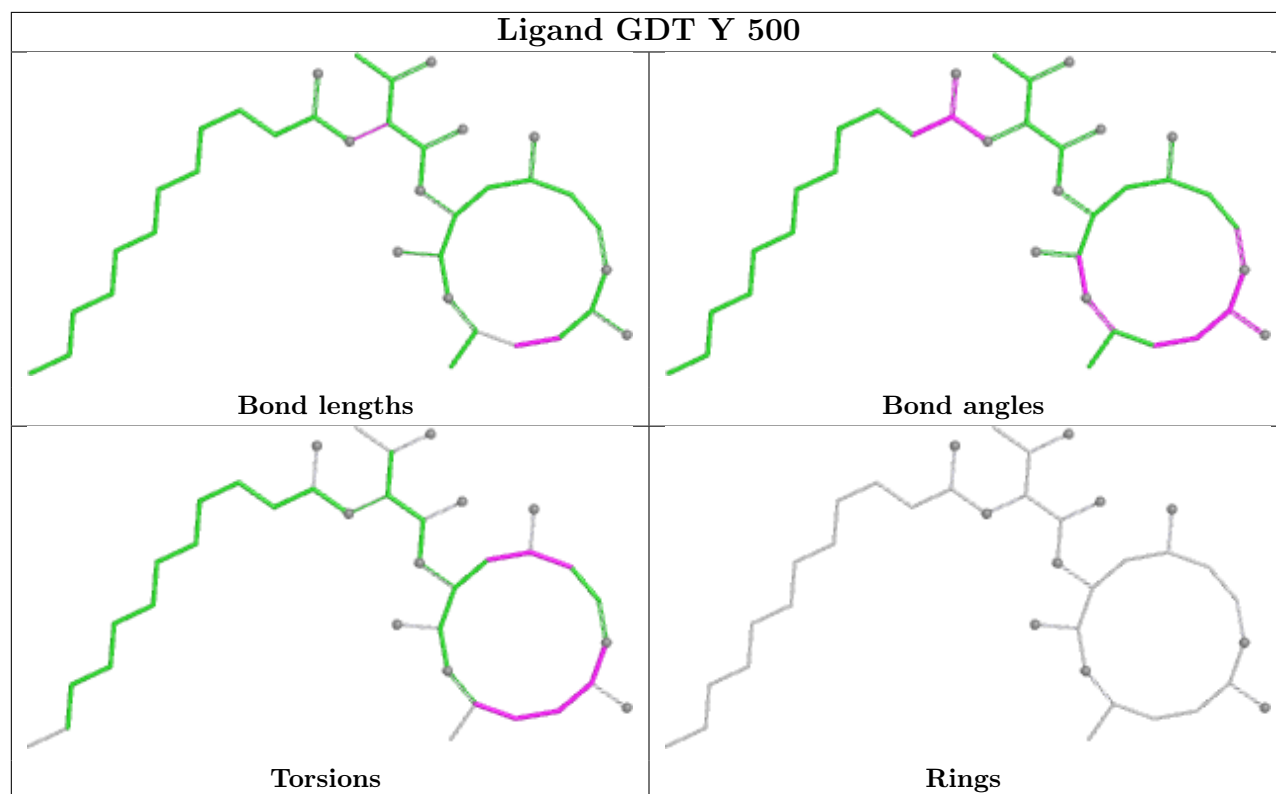
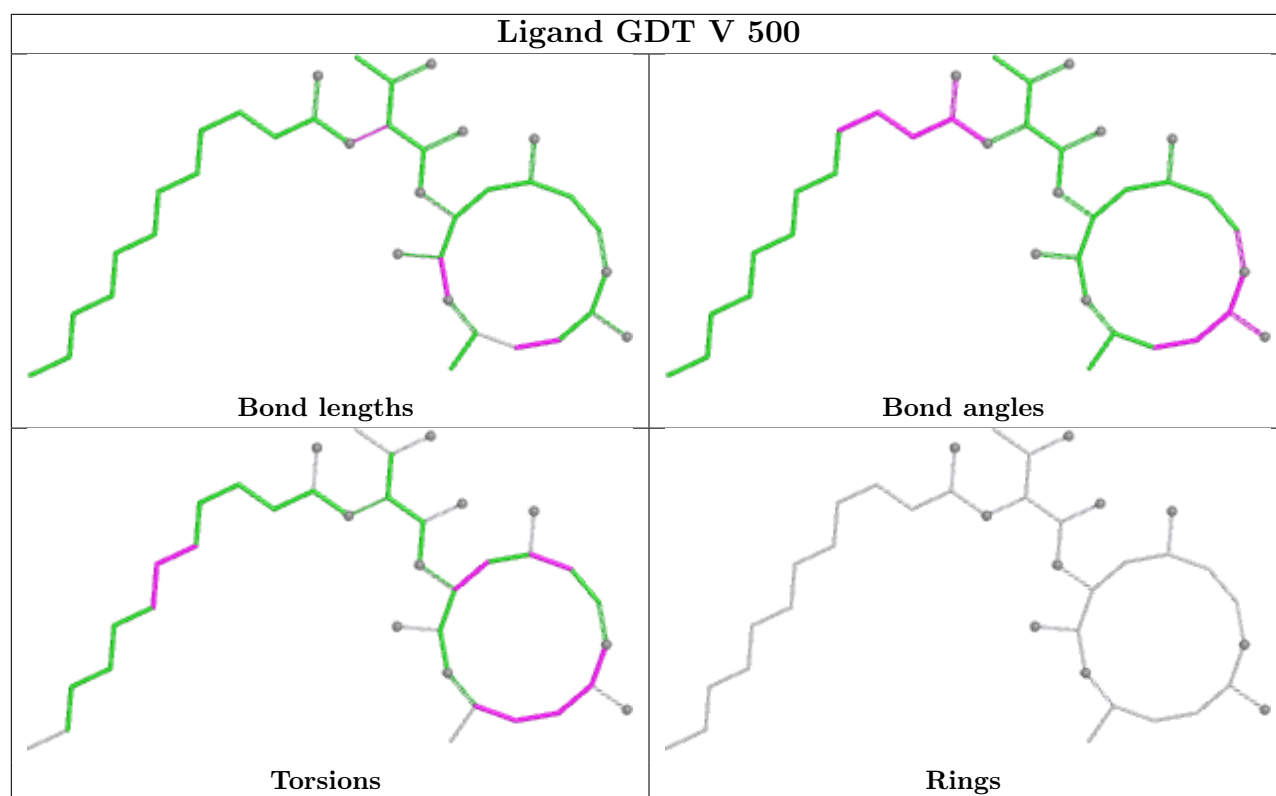
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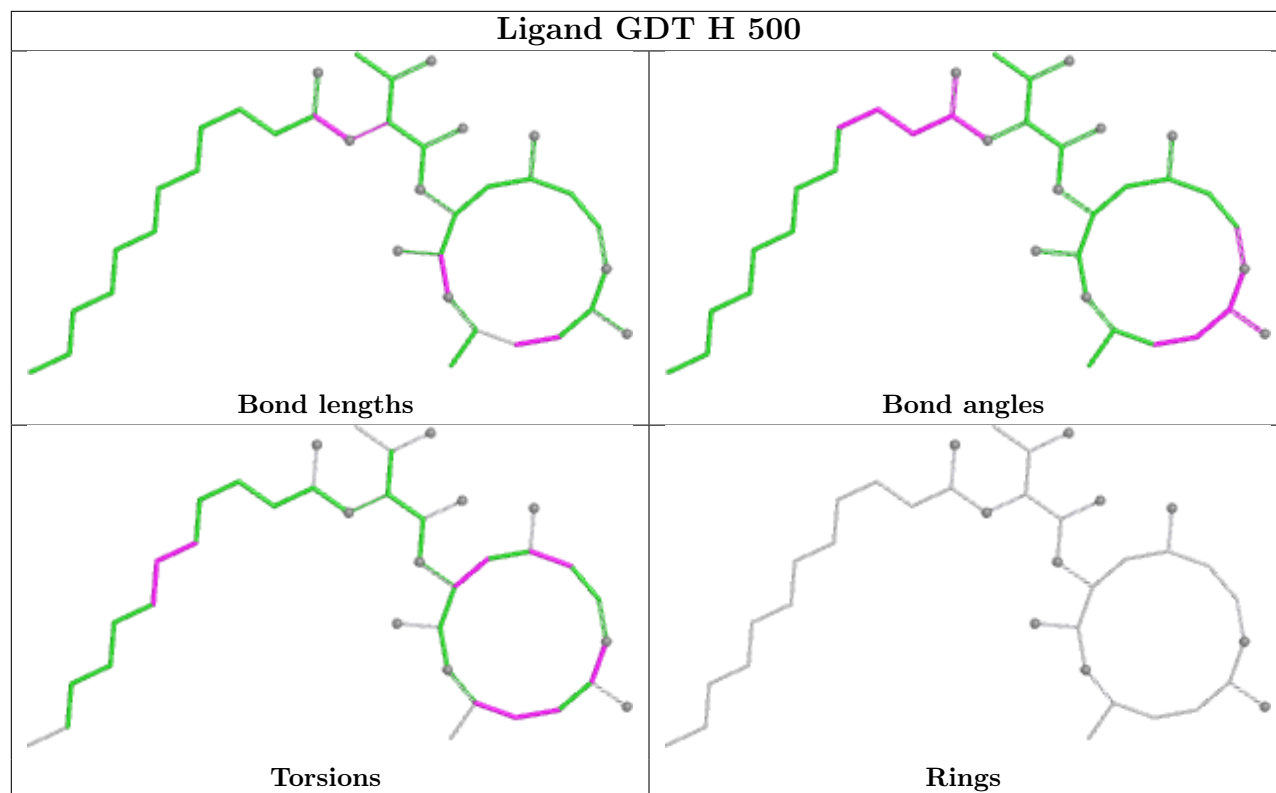
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Y	500	GDT	4	0
15	H	500	GDT	2	0

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%)	-0.17	4 (1%) 70 68	34, 52, 82, 108	0
1	O	250/250 (100%)	-0.08	5 (2%) 65 62	37, 60, 85, 105	0
2	B	244/258 (94%)	0.02	7 (2%) 53 50	34, 58, 92, 117	0
2	P	244/258 (94%)	0.08	7 (2%) 53 50	38, 58, 92, 117	0
3	C	241/254 (94%)	0.15	8 (3%) 49 45	35, 62, 106, 123	0
3	Q	241/254 (94%)	0.27	11 (4%) 37 34	41, 66, 110, 124	0
4	D	242/260 (93%)	0.04	7 (2%) 53 50	39, 58, 90, 123	0
4	R	242/260 (93%)	0.09	7 (2%) 53 50	42, 62, 94, 125	0
5	E	233/234 (99%)	-0.13	2 (0%) 81 80	37, 58, 84, 108	0
5	S	233/234 (99%)	-0.06	5 (2%) 63 61	32, 58, 88, 107	0
6	F	244/287 (85%)	-0.17	4 (1%) 70 68	32, 53, 88, 102	0
6	T	244/287 (85%)	-0.15	0 100 100	29, 52, 87, 105	0
7	G	243/252 (96%)	-0.29	3 (1%) 76 75	29, 48, 78, 113	0
7	U	243/252 (96%)	-0.20	3 (1%) 76 75	33, 52, 78, 112	0
8	H	222/232 (95%)	-0.39	1 (0%) 87 86	27, 43, 64, 106	0
8	V	222/232 (95%)	-0.40	1 (0%) 87 86	28, 46, 64, 109	0
9	I	204/205 (99%)	-0.45	0 100 100	31, 50, 66, 79	0
9	W	204/205 (99%)	-0.47	1 (0%) 87 86	31, 48, 66, 78	0
10	J	198/198 (100%)	-0.28	4 (2%) 65 62	33, 49, 70, 119	0
10	X	198/198 (100%)	-0.24	6 (3%) 52 49	36, 49, 69, 124	0
11	K	212/212 (100%)	-0.17	4 (1%) 66 63	30, 51, 78, 85	0
11	Y	212/212 (100%)	-0.15	4 (1%) 66 63	33, 54, 76, 85	0
12	L	222/241 (92%)	-0.28	3 (1%) 73 72	32, 50, 74, 90	0
12	Z	222/241 (92%)	-0.29	2 (0%) 81 80	37, 50, 74, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	0	233/266 (87%)	-0.41	1 (0%) 88 87	29, 44, 61, 69	0
13	M	233/266 (87%)	-0.48	1 (0%) 88 87	27, 45, 60, 69	0
14	1	196/196 (100%)	-0.39	2 (1%) 79 78	32, 42, 62, 84	0
14	N	196/196 (100%)	-0.41	1 (0%) 87 86	28, 41, 63, 83	0
All	All	6368/6690 (95%)	-0.18	104 (1%) 70 68	27, 52, 85, 125	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	12(E)	SER	8.1
3	Q	56	LEU	6.8
4	R	12(D)	ALA	6.6
4	D	12(D)	ALA	6.2
4	D	12(E)	SER	5.8
10	X	192	ALA	5.4
2	P	217	ALA	5.2
4	R	12(C)	GLY	5.1
4	D	12(C)	GLY	4.8
4	D	127	LEU	4.6
7	G	6	ALA	4.5
12	L	145	TYR	4.5
2	B	21(A)	LYS	4.4
1	A	5	THR	4.2
2	B	217	ALA	4.2
2	P	21(B)	GLY	4.1
3	C	56	LEU	3.8
10	J	192	ALA	3.8
2	B	54	VAL	3.8
7	U	240	ASP	3.8
4	R	127	LEU	3.6
2	P	239	THR	3.6
3	Q	236	ILE	3.5
2	B	21(B)	GLY	3.5
3	C	55	THR	3.4
10	X	-1	MET	3.4
10	X	133	TYR	3.4
12	Z	145	TYR	3.3
5	E	4	PHE	3.2
6	F	5	GLY	3.1
3	Q	240	LYS	3.1
10	X	193	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	P	4	GLY	3.0
5	S	4	PHE	3.0
5	E	203	ASP	3.0
10	J	-1	MET	2.9
3	Q	243	GLN	2.9
4	R	126	ARG	2.9
3	Q	58	LEU	2.9
13	O	-8	THR	2.8
11	Y	104	TYR	2.8
4	D	126	ARG	2.8
3	Q	55	THR	2.8
11	K	40	PHE	2.7
10	J	191	GLN	2.7
1	O	56	SER	2.7
3	C	54	SER	2.7
4	R	12(F)	GLY	2.7
3	C	59	GLN	2.6
3	C	242	GLU	2.6
10	X	10	ASP	2.6
7	G	240	ASP	2.6
1	O	5	THR	2.5
2	B	239	THR	2.5
11	Y	181	ASP	2.5
1	A	185	GLU	2.5
8	V	223	ASP	2.5
2	P	21(A)	LYS	2.4
4	D	10	ARG	2.4
14	1	18(I)	GLN	2.4
7	U	6	ALA	2.4
1	O	21(P)	LYS	2.4
10	X	191	GLN	2.4
1	A	56	SER	2.4
3	Q	207	ALA	2.4
11	Y	145	ASP	2.3
2	B	4	GLY	2.3
2	P	54	VAL	2.3
11	K	208	ASN	2.3
10	J	193	GLN	2.3
13	M	-8	THR	2.2
2	B	21(C)	ASP	2.2
3	C	240	LYS	2.2
14	1	107	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	188	GLU	2.2
11	Y	208	ASN	2.2
7	U	239	GLN	2.2
5	S	5	ARG	2.2
3	Q	232	TYR	2.2
7	G	7	GLY	2.2
11	K	181	ASP	2.2
2	P	220	TYR	2.2
12	Z	14(W)	LYS	2.2
5	S	203	ASP	2.2
9	W	-8	SER	2.2
1	O	7	ARG	2.1
3	C	203	THR	2.1
3	Q	238	GLN	2.1
14	N	107	LYS	2.1
6	F	184	LEU	2.1
4	R	244	GLU	2.1
1	A	236	LEU	2.1
11	K	104	TYR	2.1
12	L	14(J)	GLY	2.1
6	F	6	THR	2.1
8	H	223	ASP	2.1
12	L	14(W)	LYS	2.1
1	O	6	ASP	2.0
4	D	12(G)	GLU	2.0
3	Q	203	THR	2.0
3	Q	183	PRO	2.0
5	S	56	ASP	2.0
5	S	58	LEU	2.0
6	F	240	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

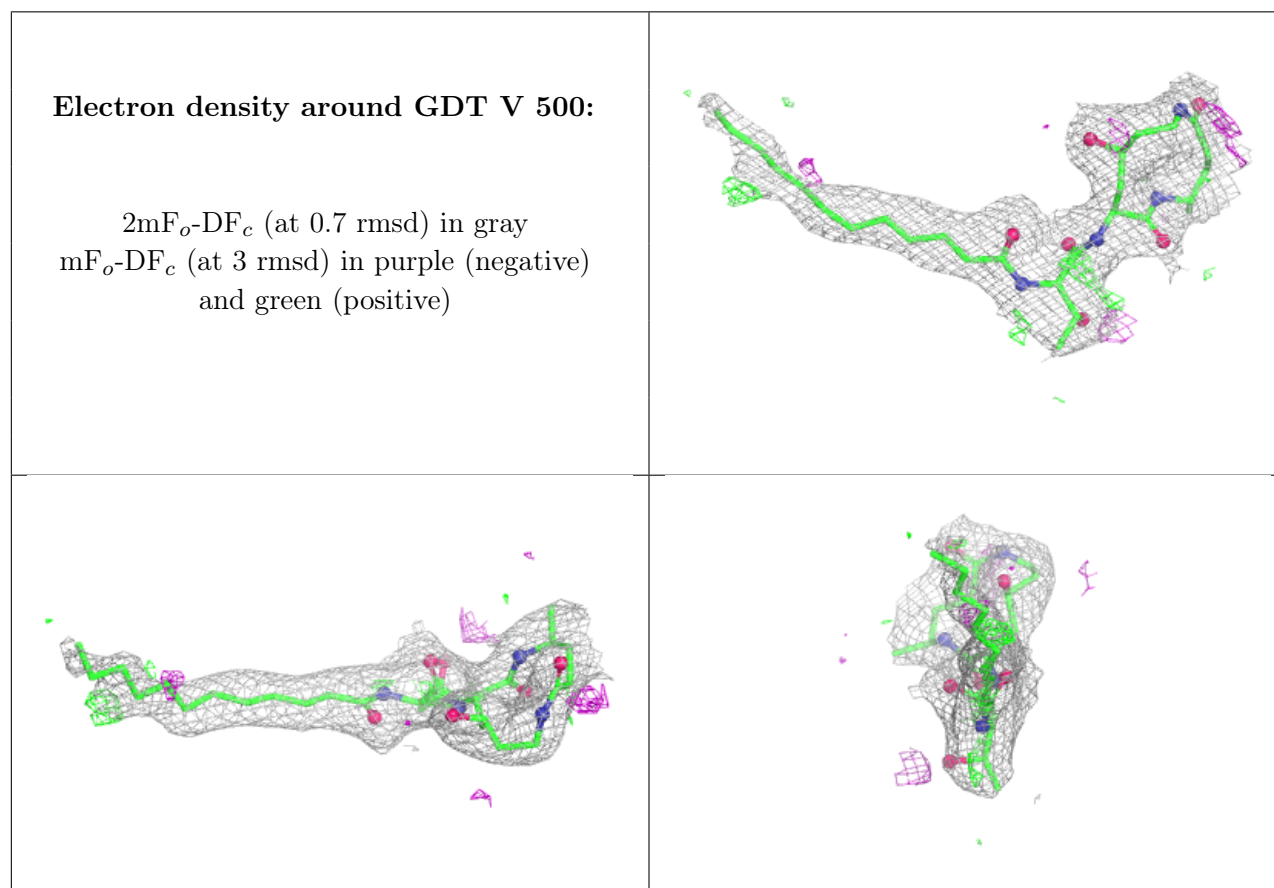
There are no oligosaccharides in this entry.

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.

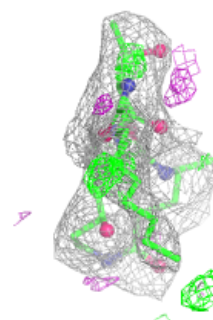
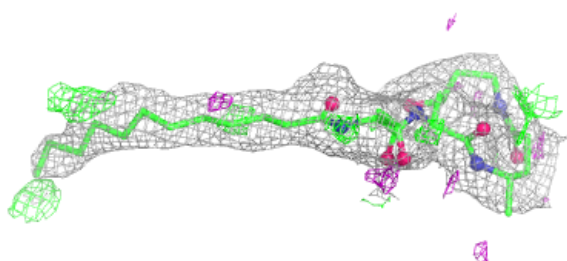
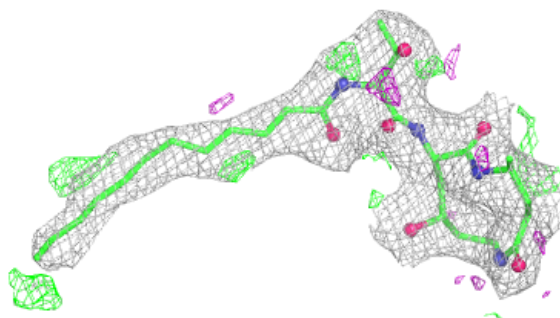
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	GDT	V	500	37/37	0.91	0.12	35,40,62,63	0
15	GDT	H	500	37/37	0.92	0.09	31,35,53,53	0
15	GDT	K	500	37/37	0.93	0.08	31,41,46,47	0
15	GDT	Y	500	37/37	0.93	0.08	39,44,55,56	0

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.

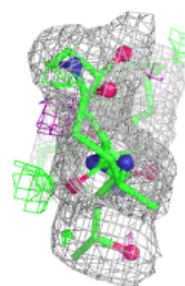
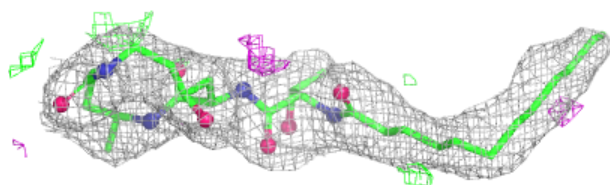
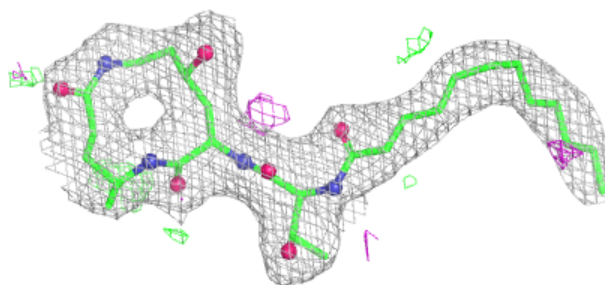


Electron density around GDT H 500:

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

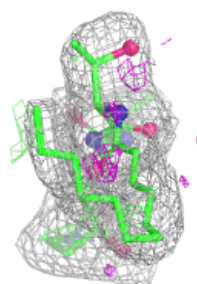
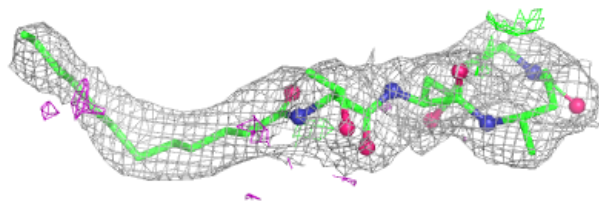
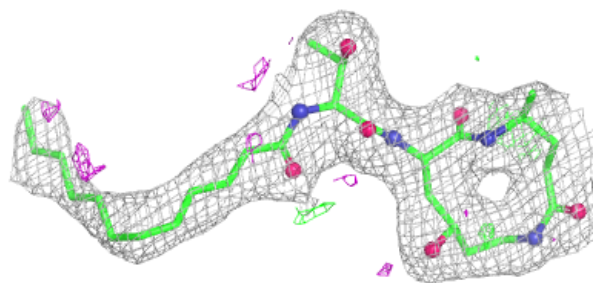
**Electron density around GDT K 500:**

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



Electron density around GDT Y 500:

$2mF_o-DF_c$ (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.