



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:20 AM UTC

PDB ID : 3GPT / pdb_00003gpt
Title : Crystal structure of the yeast 20S proteasome in complex with Salinosporamide derivatives: slow substrate ligand
Authors : Groll, M.; Macherla, V.R.; Manam, R.R.; Arthur, K.A.M.; Potts, C.B.
Deposited on : 2009-03-23
Resolution : 2.41 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

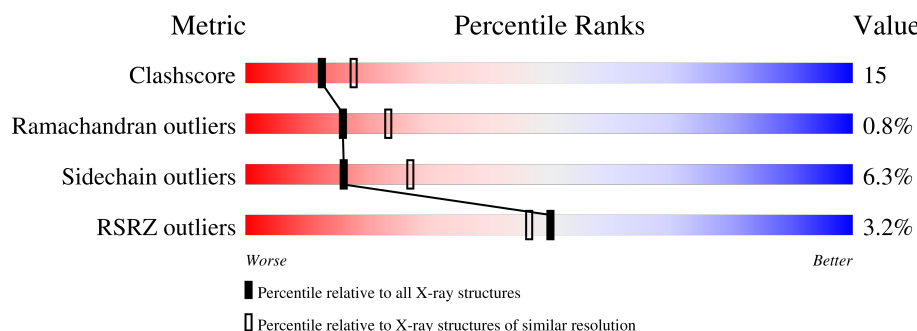
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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% 75% 22% .
1	O	250	3% 75% 22% .
2	B	244	6% 59% 35% 6%
2	P	244	5% 61% 34% 5%
3	C	241	7% 60% 36% .
3	Q	241	9% 59% 37% .

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

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	7			

- Molecule 12 is a protein called Proteasome component C5.

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

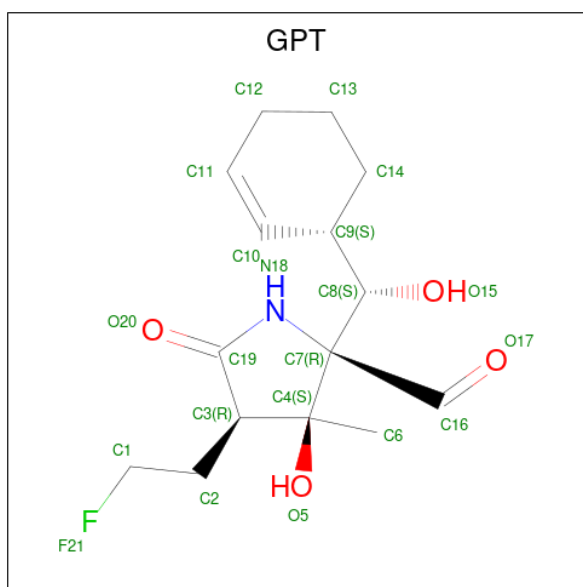
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is (2R,3S,4R)-2-[(S)-(1S)-cyclohex-2-en-1-yl(hydroxy)methyl]-4-(2-fluoroethyl)-3-hydroxy-3-methyl-5-oxopyrrolidine-2-carbaldehyde (CCD ID: GPT) (formula: C₁₅H₂₂FNO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	F	N	O	
			21	15	1	1	4	0
15	K	1	Total	C	F	N	O	
			21	15	1	1	4	0
15	N	1	Total	C	F	N	O	
			21	15	1	1	4	0
15	V	1	Total	C	F	N	O	
			21	15	1	1	4	0
15	Y	1	Total	C	F	N	O	
			21	15	1	1	4	0
15	2	1	Total	C	F	N	O	
			21	15	1	1	4	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	58	Total	O		
			58	58	0	0
16	B	38	Total	O		
			38	38	0	0
16	C	44	Total	O		
			44	44	0	0
16	D	39	Total	O		
			39	39	0	0
16	E	23	Total	O		
			23	23	0	0
16	F	47	Total	O		
			47	47	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	58	Total O 58 58	0	0
16	H	54	Total O 54 54	0	0
16	I	69	Total O 69 69	0	0
16	J	51	Total O 51 51	0	0
16	K	49	Total O 49 49	0	0
16	L	58	Total O 58 58	0	0
16	M	73	Total O 73 73	0	0
16	N	56	Total O 56 56	0	0
16	O	34	Total O 34 34	0	0
16	P	29	Total O 29 29	0	0
16	Q	27	Total O 27 27	0	0
16	R	31	Total O 31 31	0	0
16	S	19	Total O 19 19	0	0
16	T	39	Total O 39 39	0	0
16	U	62	Total O 62 62	0	0
16	V	49	Total O 49 49	0	0
16	W	62	Total O 62 62	0	0
16	X	45	Total O 45 45	0	0
16	Y	48	Total O 48 48	0	0
16	Z	53	Total O 53 53	0	0
16	1	75	Total O 75 75	0	0

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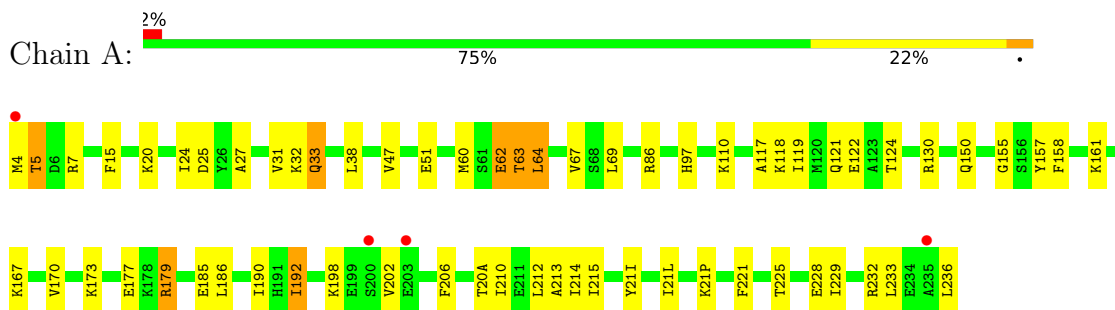
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	56	Total	O	0	0
			56	56		

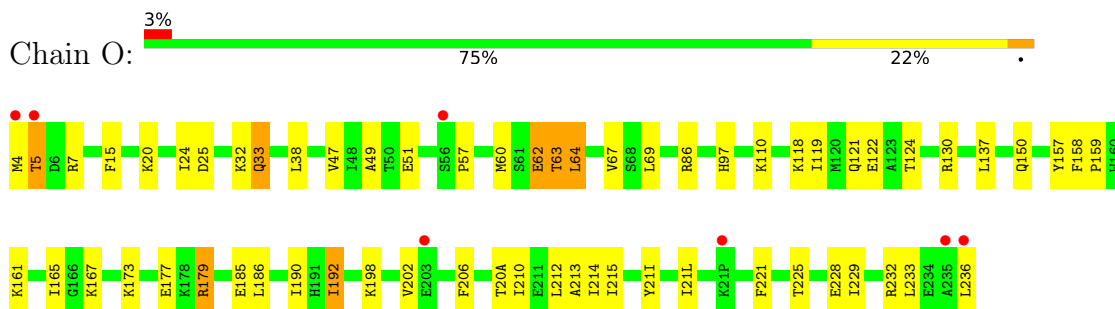
3 Residue-property plots [i](#)

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.

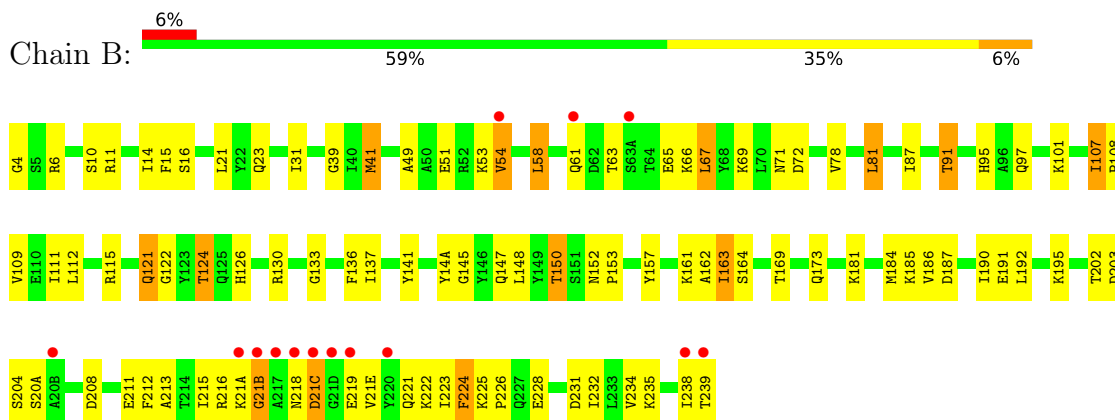
- Molecule 1: Proteasome component Y7



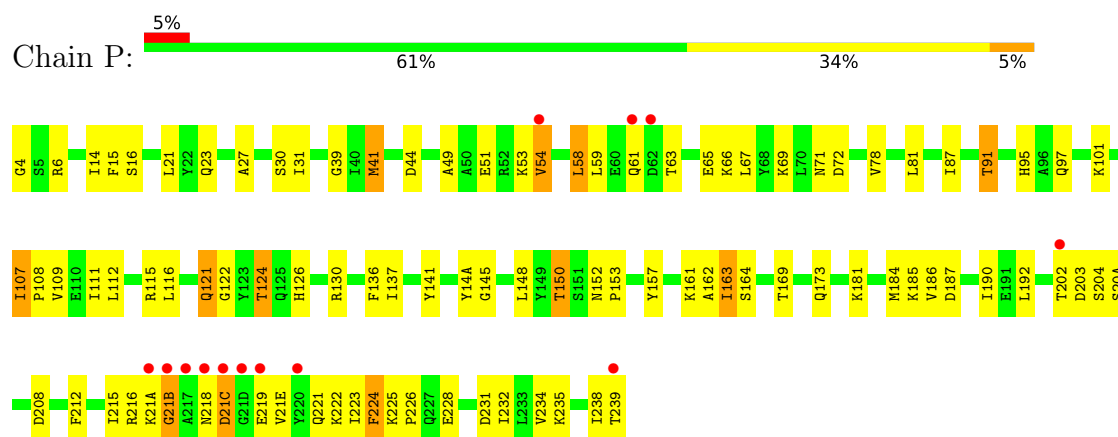
- Molecule 1: Proteasome component Y7



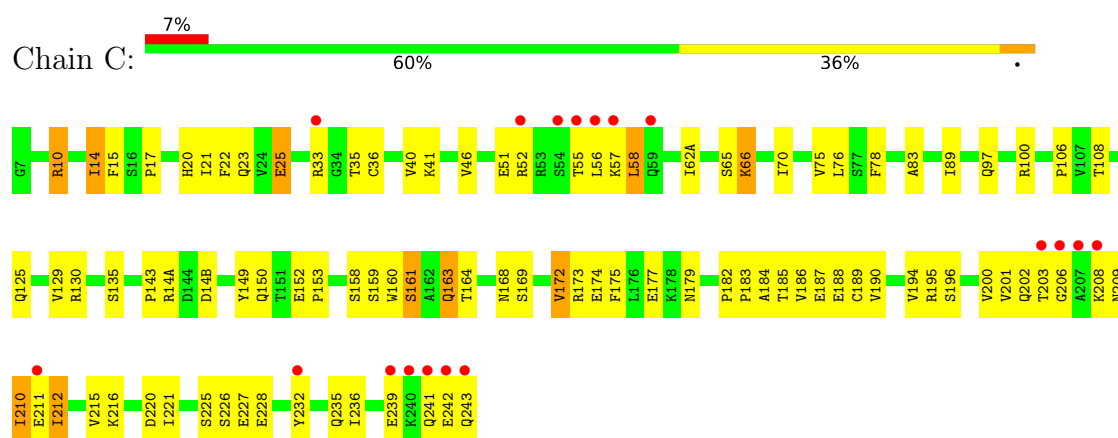
- Molecule 2: Proteasome component Y13



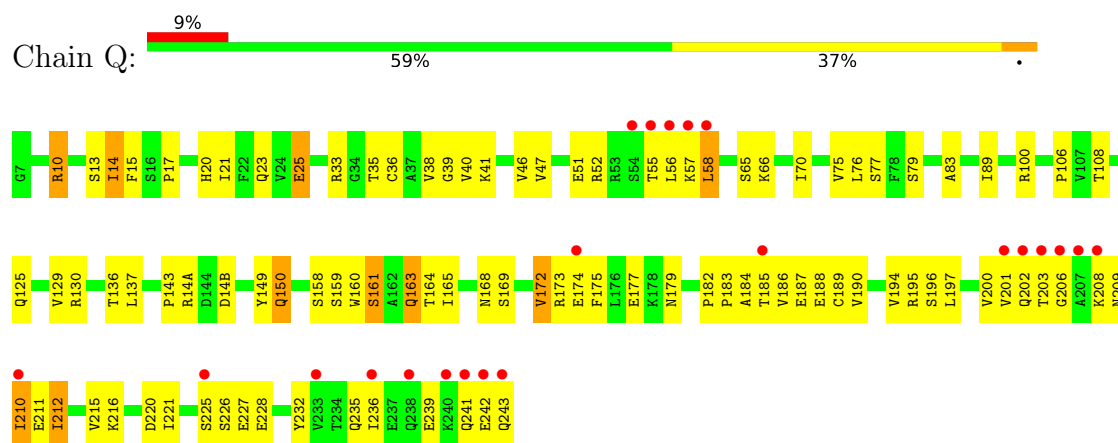
- Molecule 2: Proteasome component Y13



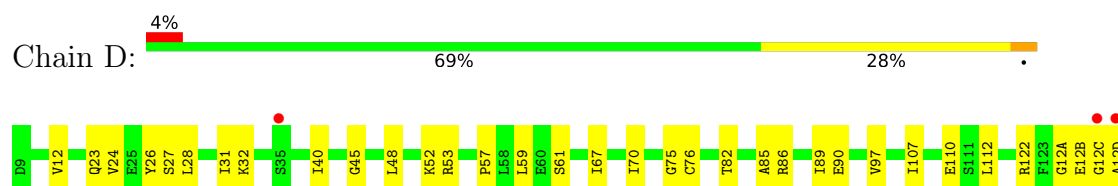
• Molecule 3: Proteasome component PRE6

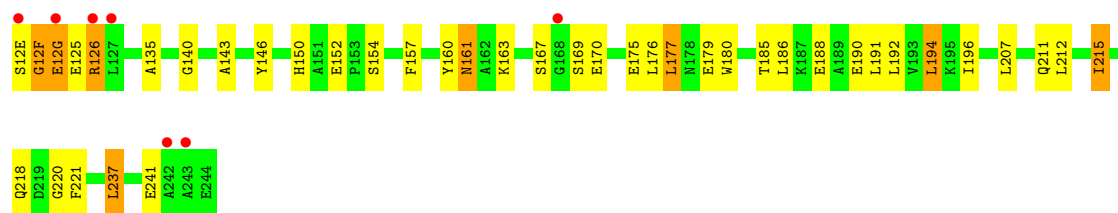


• Molecule 3: Proteasome component PRE6

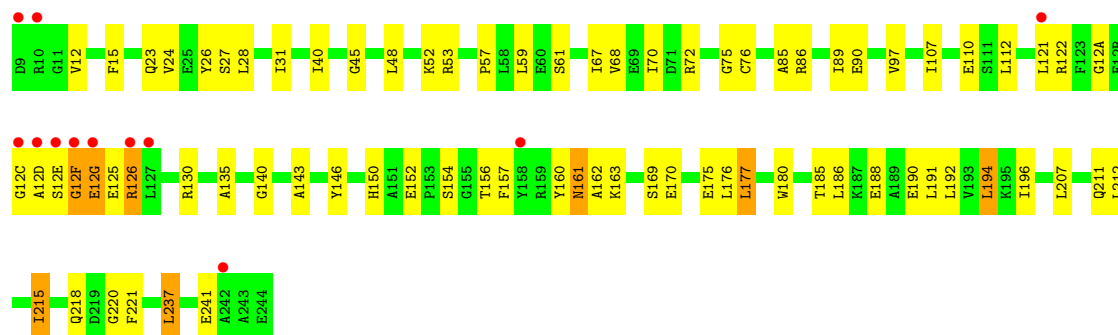


• Molecule 4: Proteasome component PUP2

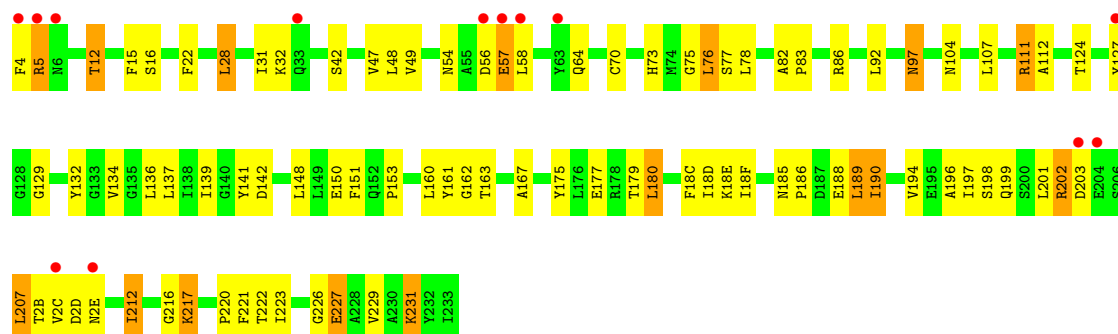




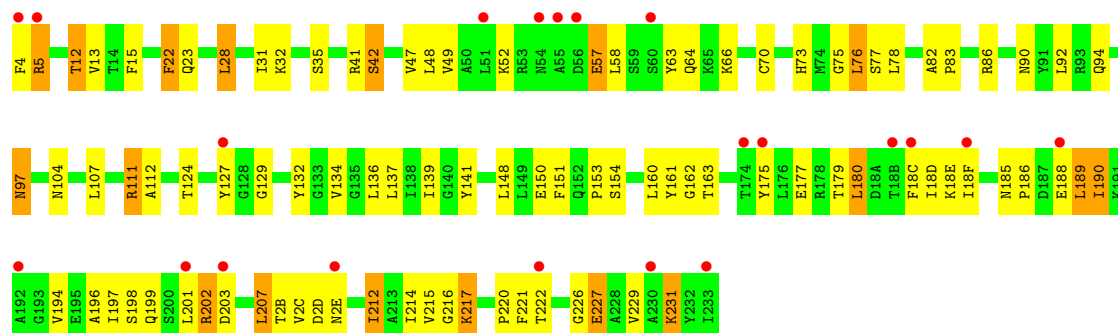
• Molecule 4: Proteasome component PUP2



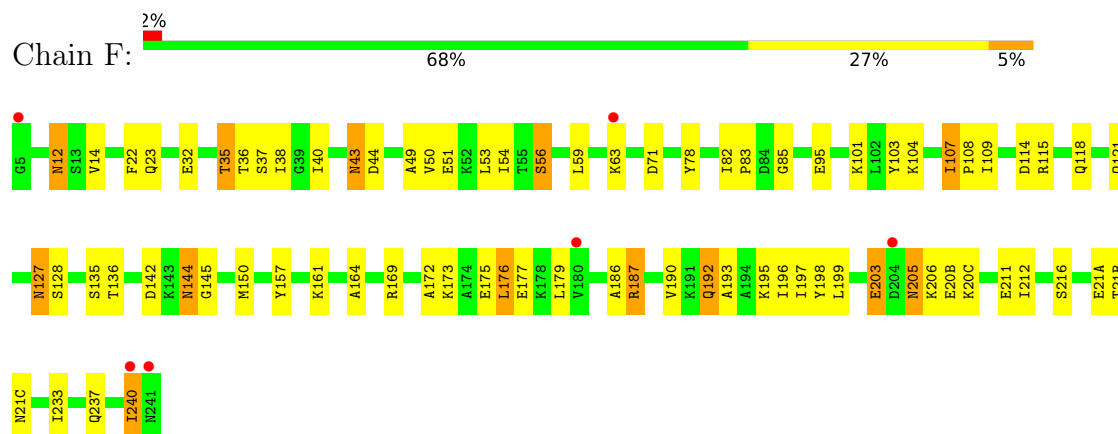
• Molecule 5: Proteasome component PRE5



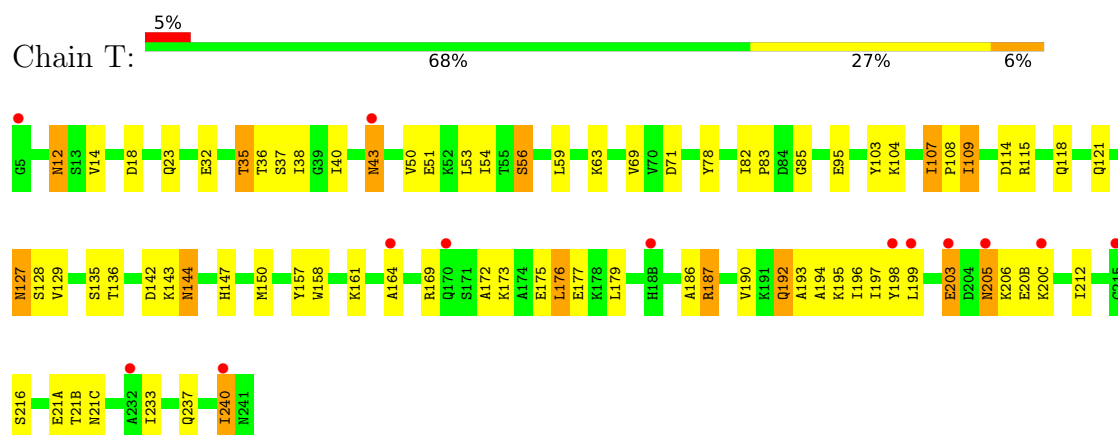
• Molecule 5: Proteasome component PRE5



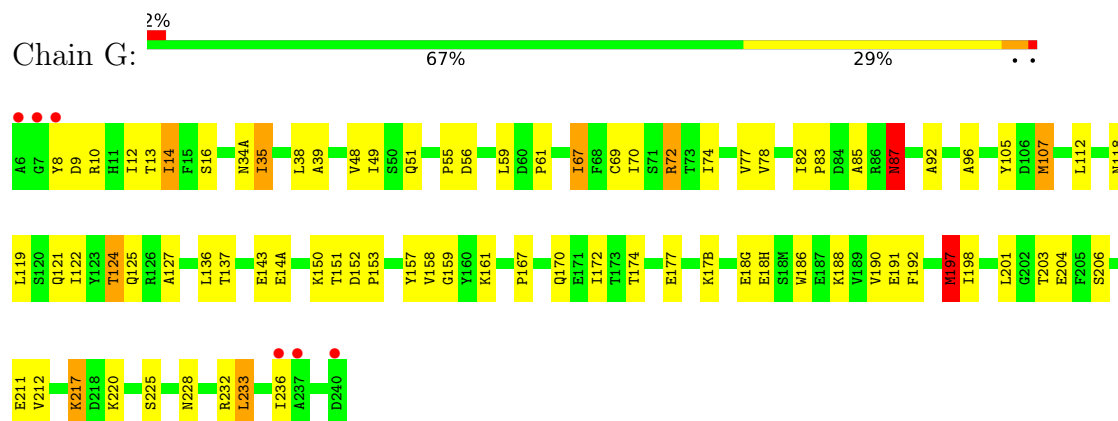
- Molecule 6: Proteasome component C1



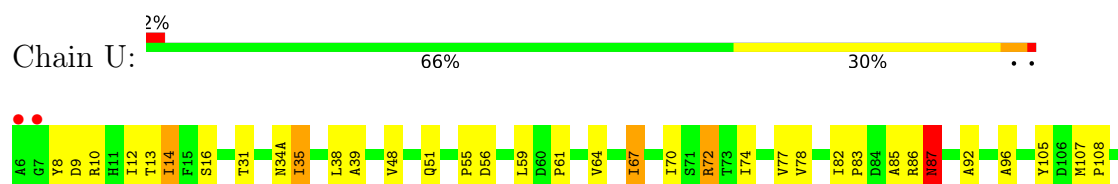
- Molecule 6: Proteasome component C1

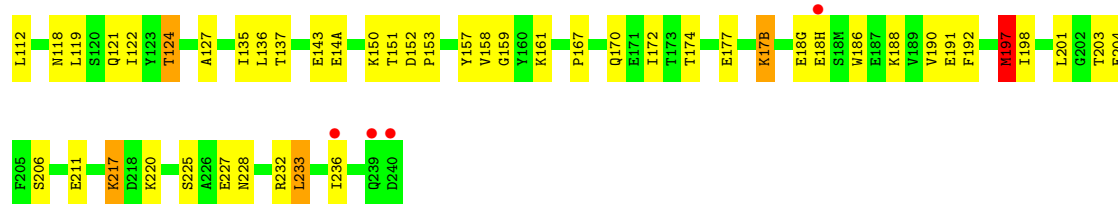


- Molecule 7: Proteasome component C7-alpha

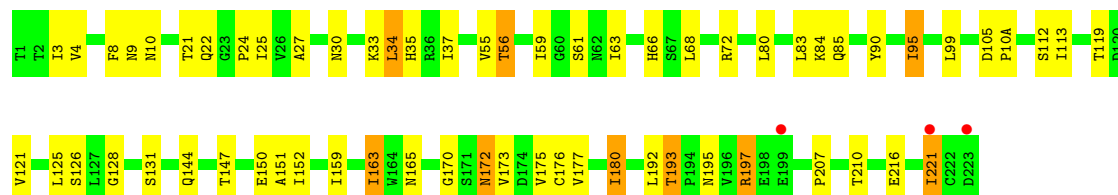
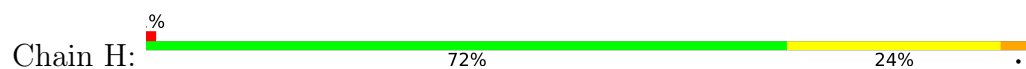


- Molecule 7: Proteasome component C7-alpha

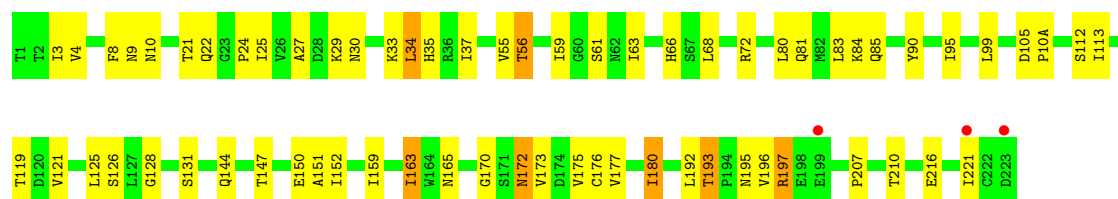




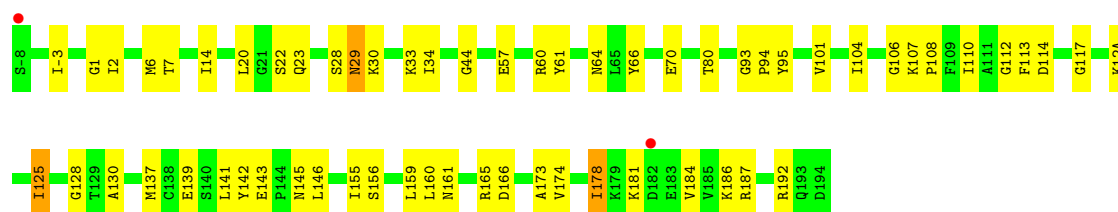
• Molecule 8: Proteasome component PUP1



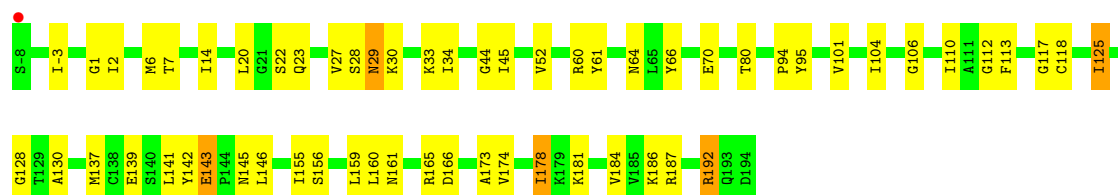
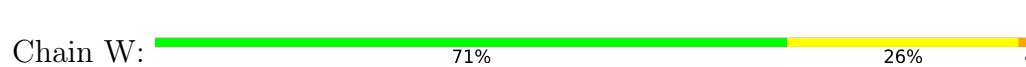
• Molecule 8: Proteasome component PUP1



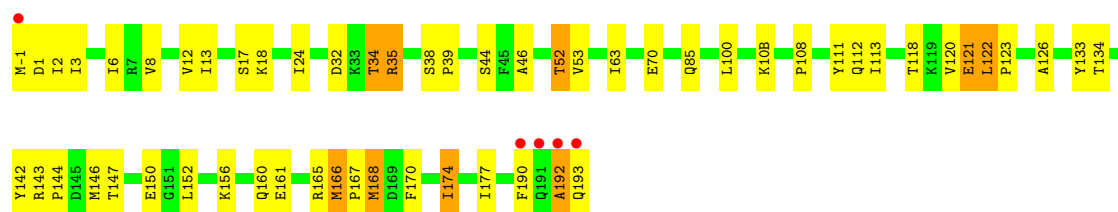
• Molecule 9: Proteasome component PUP3



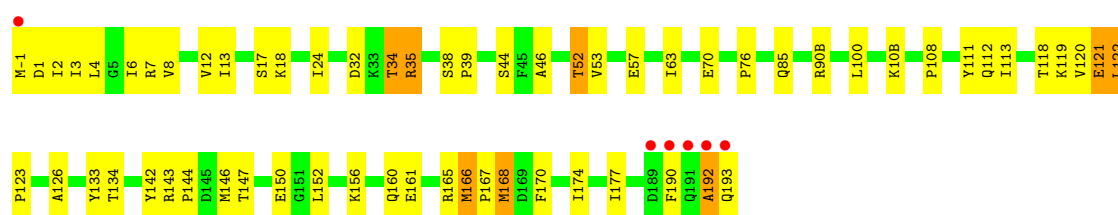
• Molecule 9: Proteasome component PUP3



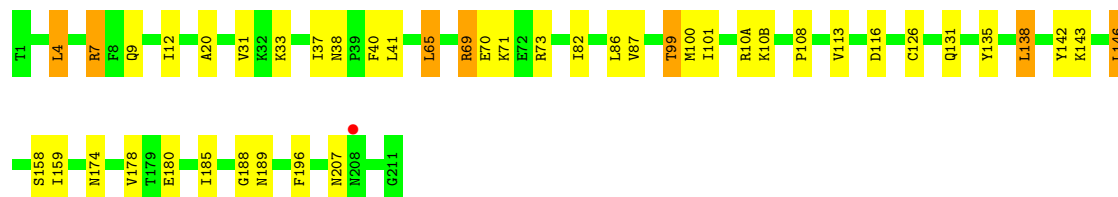
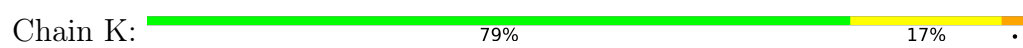
- Molecule 10: Proteasome component C11



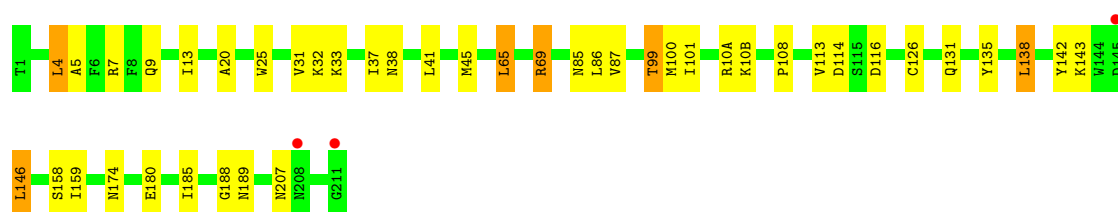
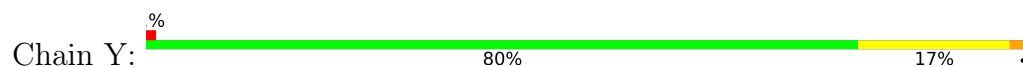
- Molecule 10: Proteasome component C11



- Molecule 11: Proteasome component PRE2



- Molecule 11: Proteasome component PRE2

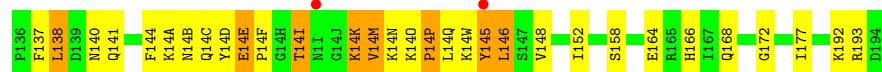


- Molecule 12: Proteasome component C5

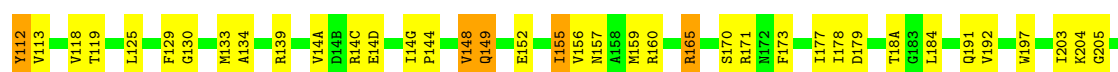




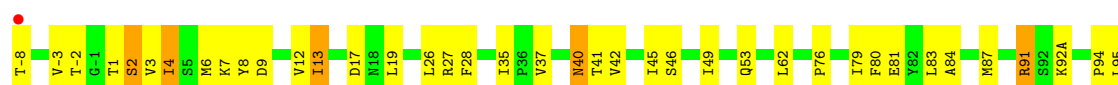
• Molecule 12: Proteasome component C5



• Molecule 13: Proteasome component PRE4



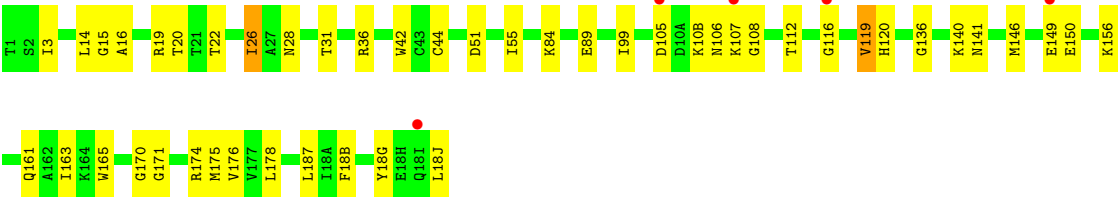
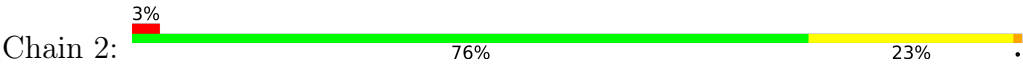
• Molecule 13: Proteasome component PRE4



• 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	134.00Å 301.26Å 143.81Å 90.00° 112.56° 90.00°	Depositor
Resolution (Å)	15.00 – 2.41 15.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.3 (15.00-2.41) 99.2 (15.00-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.245 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.912	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51018	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: GPT

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	0.42	0/1952	0.92	3/2642 (0.1%)
1	O	0.40	0/1952	0.92	3/2642 (0.1%)
2	B	0.40	0/1935	0.91	8/2618 (0.3%)
2	P	0.42	0/1935	0.92	8/2618 (0.3%)
3	C	0.42	0/1920	0.91	4/2598 (0.2%)
3	Q	0.40	0/1920	0.91	3/2598 (0.1%)
4	D	0.41	0/1887	0.89	7/2541 (0.3%)
4	R	0.39	0/1887	0.88	6/2541 (0.2%)
5	E	0.39	0/1823	0.89	4/2463 (0.2%)
5	S	0.40	0/1823	0.90	5/2463 (0.2%)
6	F	0.41	0/1937	0.98	11/2614 (0.4%)
6	T	0.43	0/1937	0.98	9/2614 (0.3%)
7	G	0.47	1/1959 (0.1%)	0.97	9/2652 (0.3%)
7	U	0.45	0/1959	0.97	10/2652 (0.4%)
8	H	0.44	0/1716	0.94	7/2326 (0.3%)
8	V	0.43	0/1716	0.95	7/2326 (0.3%)
9	I	0.44	0/1611	1.02	12/2174 (0.6%)
9	W	0.46	0/1611	1.02	11/2174 (0.5%)
10	J	0.44	0/1613	0.97	8/2173 (0.4%)
10	X	0.45	0/1613	0.98	7/2173 (0.3%)
11	K	0.45	0/1680	0.91	5/2274 (0.2%)
11	Y	0.44	0/1680	0.92	4/2274 (0.2%)
12	L	0.41	0/1795	1.01	12/2420 (0.5%)
12	Z	0.41	0/1795	1.01	9/2420 (0.4%)
13	1	0.47	0/1855	0.95	11/2514 (0.4%)
13	M	0.45	0/1855	0.94	10/2514 (0.4%)
14	2	0.44	0/1541	0.94	3/2087 (0.1%)
14	N	0.45	0/1541	0.94	3/2087 (0.1%)
All	All	0.43	1/50448 (0.0%)	0.94	199/68192 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	107	MET	SD-CE	-5.15	1.66	1.79

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	27	ARG	N-CA-C	11.61	123.49	111.07
13	1	27	ARG	N-CA-C	11.54	123.42	111.07
6	T	12	ASN	N-CA-C	10.46	122.26	111.07
6	F	12	ASN	N-CA-C	10.29	122.08	111.07
1	A	161	LYS	N-CA-C	-9.08	101.01	112.90
12	Z	95	TYR	N-CA-C	-8.78	95.81	109.25
1	O	161	LYS	N-CA-C	-8.73	101.46	112.90
12	L	95	TYR	N-CA-C	-8.73	95.90	109.25
6	F	107	ILE	N-CA-C	8.71	118.46	108.96
6	T	107	ILE	N-CA-C	8.71	118.46	108.96
7	U	161	LYS	N-CA-C	-8.51	101.22	111.69
7	G	161	LYS	N-CA-C	-8.49	101.25	111.69
2	B	161	LYS	N-CA-C	-8.20	103.41	113.41
2	P	161	LYS	N-CA-C	-8.08	103.55	113.41
6	F	63	LYS	N-CA-C	8.00	121.16	111.40
6	T	63	LYS	N-CA-C	7.96	121.11	111.40
11	Y	188	GLY	N-CA-C	7.76	124.30	112.81
7	G	16	SER	N-CA-C	-7.73	101.03	110.31
4	R	161	ASN	N-CA-C	-7.68	102.84	112.90
3	Q	161	SER	N-CA-C	-7.55	103.13	111.36
11	K	188	GLY	N-CA-C	7.51	124.63	112.61
7	U	16	SER	N-CA-C	-7.48	101.33	110.31
2	P	16	SER	N-CA-C	-7.46	101.55	110.13
12	Z	93	PHE	CA-C-N	7.43	127.47	119.89
12	Z	93	PHE	C-N-CA	7.43	127.47	119.89
3	C	161	SER	N-CA-C	-7.41	103.28	111.36
4	D	161	ASN	N-CA-C	-7.37	103.25	112.90
4	D	169	SER	N-CA-C	7.30	118.89	111.07
3	Q	108	THR	N-CA-C	-7.24	100.77	110.55
4	R	169	SER	N-CA-C	7.19	118.77	111.07
12	L	93	PHE	CA-C-N	7.15	127.18	119.89
12	L	93	PHE	C-N-CA	7.15	127.18	119.89
3	C	108	THR	N-CA-C	-7.02	101.08	110.55
7	G	13	THR	N-CA-C	6.90	120.36	109.39
6	T	135	SER	N-CA-C	-6.76	98.71	109.59
7	U	13	THR	N-CA-C	6.69	120.03	109.39
6	T	161	LYS	N-CA-C	-6.64	103.21	112.45
13	1	95	LEU	N-CA-C	-6.62	96.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	135	SER	N-CA-C	-6.60	98.97	109.59
8	H	37	ILE	N-CA-C	-6.55	105.35	111.45
2	B	137	ILE	N-CA-C	-6.54	98.20	107.75
4	D	70	ILE	N-CA-C	-6.46	105.53	111.67
14	N	99	ILE	N-CA-C	6.44	117.13	108.11
14	2	99	ILE	N-CA-C	6.43	117.11	108.11
9	W	60	ARG	N-CA-C	-6.43	104.20	111.14
8	V	37	ILE	N-CA-C	-6.42	105.48	111.45
2	B	16	SER	N-CA-C	-6.42	102.75	110.13
4	R	70	ILE	N-CA-C	-6.39	105.60	111.67
1	O	215	ILE	N-CA-C	-6.38	97.14	107.28
13	M	9	ASP	N-CA-C	6.34	118.19	111.28
13	M	95	LEU	N-CA-C	-6.33	97.38	108.20
6	F	161	LYS	N-CA-C	-6.33	103.66	112.45
13	1	45	ILE	N-CA-C	6.31	116.94	108.11
13	M	45	ILE	N-CA-C	6.29	116.91	108.11
13	1	9	ASP	N-CA-C	6.26	118.10	111.28
9	I	94	PRO	N-CA-C	6.23	120.76	111.41
10	X	166	MET	CA-C-N	6.19	125.75	119.19
10	X	166	MET	C-N-CA	6.19	125.75	119.19
6	T	14	VAL	N-CA-C	6.18	117.48	108.58
7	U	220	LYS	N-CA-C	6.18	117.79	108.46
1	A	215	ILE	N-CA-C	-6.16	97.49	107.28
7	G	197	MET	N-CA-C	-6.14	104.50	111.07
2	P	137	ILE	N-CA-C	-6.12	98.81	107.75
12	Z	134	ILE	N-CA-C	6.12	117.15	111.45
5	S	57	GLU	N-CA-C	-6.12	105.57	113.16
10	J	123	PRO	N-CA-C	-6.10	105.57	113.57
9	W	94	PRO	N-CA-C	6.09	120.55	111.41
7	G	220	LYS	N-CA-C	6.08	117.64	108.46
13	1	98	ALA	N-CA-C	-6.07	98.51	108.76
7	U	197	MET	N-CA-C	-6.01	104.64	111.07
10	X	123	PRO	N-CA-C	-6.01	105.70	113.57
12	L	129	ALA	N-CA-C	5.98	118.32	111.02
5	E	161	TYR	N-CA-C	-5.98	105.07	112.90
8	H	172	ASN	N-CA-C	5.97	118.55	109.95
13	M	98	ALA	N-CA-C	-5.97	98.67	108.76
7	G	127	ALA	N-CA-C	5.96	117.78	111.28
6	F	144	ASN	N-CA-C	5.92	117.65	109.54
13	M	-2	THR	N-CA-C	5.90	118.82	109.50
6	T	144	ASN	N-CA-C	5.90	117.62	109.54
8	H	99	LEU	N-CA-C	5.88	118.80	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	94	PRO	N-CA-C	5.88	120.22	111.41
5	E	57	GLU	N-CA-C	-5.86	105.90	113.16
7	U	127	ALA	N-CA-C	5.81	117.61	111.28
10	J	166	MET	CA-C-N	5.79	125.65	119.28
10	J	166	MET	C-N-CA	5.79	125.65	119.28
12	L	146	LEU	N-CA-C	5.79	118.18	110.53
12	L	134	ILE	N-CA-C	5.79	117.72	111.58
5	E	42	SER	N-CA-C	-5.78	101.14	109.29
8	V	99	LEU	N-CA-C	5.78	118.63	109.50
5	S	161	TYR	N-CA-C	-5.77	105.34	112.90
2	P	72	ASP	N-CA-C	-5.76	106.25	113.28
9	I	95	TYR	N-CA-C	-5.75	101.11	110.20
9	I	60	ARG	N-CA-C	-5.74	104.94	111.14
5	S	42	SER	N-CA-C	-5.71	101.24	109.29
9	W	142	TYR	N-CA-C	5.71	118.55	110.50
12	Z	49	ALA	N-CA-C	5.70	118.23	111.33
9	I	145	ASN	N-CA-C	5.69	119.27	111.54
12	Z	146	LEU	N-CA-C	5.68	118.03	110.53
6	F	14	VAL	N-CA-C	5.67	116.74	108.58
13	M	94	PRO	N-CA-C	5.67	119.91	111.41
9	I	142	TYR	N-CA-C	5.67	118.49	110.50
11	Y	99	THR	N-CA-C	5.65	117.78	109.24
8	V	172	ASN	N-CA-C	5.62	118.40	110.14
12	L	21	ILE	N-CA-C	5.61	116.99	108.80
11	K	99	THR	N-CA-C	5.59	117.68	109.24
9	I	128	GLY	N-CA-C	5.58	118.54	111.85
9	W	95	TYR	N-CA-C	-5.56	100.92	109.76
7	U	74	ILE	N-CA-C	5.55	115.94	108.17
2	B	72	ASP	N-CA-C	-5.55	106.51	113.28
12	L	94	PRO	N-CA-C	5.55	119.93	111.11
9	W	145	ASN	N-CA-C	5.55	119.08	111.54
6	T	71	ASP	CB-CA-C	-5.54	110.21	116.63
2	P	203	ASP	N-CA-C	-5.51	106.22	113.17
9	W	128	GLY	N-CA-C	5.49	118.44	111.85
1	A	185	GLU	N-CA-C	-5.48	102.41	110.52
8	V	193	THR	CA-C-N	5.46	126.40	120.83
8	V	193	THR	C-N-CA	5.46	126.40	120.83
12	Z	21	ILE	N-CA-C	5.46	116.77	108.80
11	Y	131	GLN	N-CA-C	5.44	117.64	111.11
4	D	143	ALA	N-CA-C	5.44	118.71	111.75
12	Z	94	PRO	N-CA-C	5.42	119.73	111.11
11	K	131	GLN	N-CA-C	5.42	117.61	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	185	GLU	N-CA-C	-5.41	102.52	110.52
12	L	117	GLY	N-CA-C	5.39	122.87	115.27
2	B	203	ASP	N-CA-C	-5.37	106.40	113.17
2	P	109	VAL	N-CA-C	5.37	116.00	110.36
10	J	142	TYR	N-CA-C	5.37	118.01	109.96
13	M	165	ARG	N-CA-C	5.35	119.96	113.38
2	B	109	VAL	N-CA-C	5.34	115.97	110.36
13	1	35	ILE	N-CA-C	5.34	113.31	107.60
13	1	-2	THR	N-CA-C	5.34	117.94	109.50
6	F	71	ASP	CB-CA-C	-5.33	110.44	116.63
12	L	49	ALA	N-CA-C	5.32	117.77	111.33
3	Q	70	ILE	N-CA-C	-5.32	105.94	111.58
9	W	117	GLY	N-CA-C	5.32	122.12	115.21
14	2	141	ASN	N-CA-C	5.31	119.76	113.28
4	R	143	ALA	N-CA-C	5.31	118.55	111.75
7	G	74	ILE	N-CA-C	5.31	115.60	108.17
9	I	178	ILE	N-CA-C	5.31	115.54	108.11
11	K	116	ASP	N-CA-C	-5.30	106.76	113.18
9	W	143	GLU	CA-C-N	5.28	125.57	119.92
9	W	143	GLU	C-N-CA	5.28	125.57	119.92
10	X	142	TYR	N-CA-C	5.27	117.87	109.96
3	C	22	PHE	N-CA-C	5.27	117.03	111.28
2	B	78	VAL	N-CA-C	5.27	116.56	108.71
12	L	116	VAL	N-CA-C	5.26	117.24	111.77
4	D	61	SER	N-CA-C	5.26	118.48	111.75
9	I	114	ASP	N-CA-C	-5.25	102.97	110.59
13	1	92(A)	LYS	N-CA-C	-5.25	106.47	112.92
10	X	134	THR	N-CA-C	5.24	119.95	113.50
4	R	61	SER	N-CA-C	5.23	118.45	111.75
10	J	134	THR	N-CA-C	5.23	119.94	113.50
6	F	145	GLY	N-CA-C	5.23	119.24	111.76
13	1	165	ARG	N-CA-C	5.23	119.81	113.38
10	X	165	ARG	N-CA-C	5.21	119.69	113.23
10	J	165	ARG	N-CA-C	5.21	119.69	113.23
7	U	17(B)	LYS	N-CA-C	-5.21	105.78	111.82
4	R	218	GLN	N-CA-C	5.19	116.75	111.14
9	W	23	GLN	CB-CA-C	-5.19	110.17	117.23
12	L	145	TYR	N-CA-C	5.18	118.67	109.96
7	G	206	SER	N-CA-C	-5.18	102.36	110.17
4	D	218	GLN	N-CA-C	5.17	116.72	111.14
8	H	180	ILE	N-CA-C	5.17	120.10	109.34
9	I	117	GLY	N-CA-C	5.17	121.93	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	141	ASN	N-CA-C	5.17	119.58	113.28
2	P	78	VAL	N-CA-C	5.16	116.40	108.71
13	1	2	SER	N-CA-C	5.16	121.78	110.80
9	I	93	GLY	CA-C-N	5.15	125.13	120.03
9	I	93	GLY	C-N-CA	5.15	125.13	120.03
6	T	240	ILE	N-CA-C	-5.15	106.88	112.80
13	M	35	ILE	N-CA-C	5.14	113.11	107.60
3	C	70	ILE	N-CA-C	-5.14	106.13	111.58
8	H	21	THR	N-CA-C	5.14	117.62	109.50
6	F	240	ILE	N-CA-C	-5.14	106.89	112.80
4	D	82	THR	N-CA-C	5.13	117.61	111.71
10	J	122	LEU	N-CA-C	5.13	116.55	108.55
14	2	22	THR	N-CA-C	-5.12	96.77	107.37
2	P	107	ILE	N-CA-C	5.11	113.96	108.95
6	F	22	PHE	N-CA-C	5.11	117.51	111.33
9	I	23	GLN	CB-CA-C	-5.11	110.28	117.23
7	G	87	ASN	N-CA-C	-5.10	105.80	111.36
11	K	82	ILE	N-CA-C	-5.09	105.74	110.53
12	Z	145	TYR	N-CA-C	5.09	118.52	109.96
2	B	107	ILE	N-CA-C	5.09	113.94	108.95
8	H	193	THR	CA-C-N	5.08	126.01	120.83
8	H	193	THR	C-N-CA	5.08	126.01	120.83
10	X	122	LEU	N-CA-C	5.07	116.45	108.55
13	M	2	SER	N-CA-C	5.04	121.54	110.80
7	U	87	ASN	N-CA-C	-5.04	105.86	111.36
11	Y	116	ASP	N-CA-C	-5.04	107.08	113.18
5	S	22	PHE	N-CA-C	5.04	116.77	111.28
14	N	22	THR	N-CA-C	-5.04	96.94	107.37
10	J	174	ILE	N-CA-C	-5.03	101.23	108.53
8	V	21	THR	N-CA-C	5.02	117.43	109.50
9	W	178	ILE	N-CA-C	5.02	115.13	108.11
8	V	180	ILE	N-CA-C	5.01	119.77	109.34
5	S	154	SER	N-CA-C	-5.01	106.42	112.54
7	U	206	SER	N-CA-C	-5.01	102.61	110.17
5	E	16	SER	N-CA-C	-5.00	104.38	110.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	56	0
1	O	1915	0	1926	53	0
2	B	1905	0	1901	86	0
2	P	1905	0	1901	81	0
3	C	1891	0	1900	94	0
3	Q	1891	0	1900	95	0
4	D	1862	0	1836	51	0
4	R	1862	0	1836	56	0
5	E	1795	0	1797	85	0
5	S	1795	0	1797	90	0
6	F	1897	0	1886	66	0
6	T	1897	0	1886	68	0
7	G	1921	0	1910	78	0
7	U	1921	0	1910	84	0
8	H	1685	0	1687	45	0
8	V	1685	0	1687	46	0
9	I	1581	0	1574	40	0
9	W	1581	0	1574	41	0
10	J	1585	0	1590	57	0
10	X	1585	0	1590	62	0
11	K	1643	0	1594	33	0
11	Y	1643	0	1594	33	0
12	L	1757	0	1711	47	0
12	Z	1757	0	1711	49	0
13	1	1824	0	1832	66	0
13	M	1824	0	1832	55	0
14	2	1512	0	1480	39	0
14	N	1512	0	1480	42	0
15	2	21	0	21	2	0
15	H	21	0	21	1	0
15	K	21	0	21	2	0
15	N	21	0	21	2	0
15	V	21	0	21	1	0
15	Y	21	0	21	2	0
16	1	75	0	0	2	0
16	2	56	0	0	1	0
16	A	58	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	38	0	0	2	0
16	C	44	0	0	2	0
16	D	39	0	0	0	0
16	E	23	0	0	2	0
16	F	47	0	0	0	0
16	G	58	0	0	2	0
16	H	54	0	0	1	0
16	I	69	0	0	1	0
16	J	51	0	0	1	0
16	K	49	0	0	1	0
16	L	58	0	0	3	0
16	M	73	0	0	1	0
16	N	56	0	0	2	0
16	O	34	0	0	1	0
16	P	29	0	0	1	0
16	Q	27	0	0	2	0
16	R	31	0	0	2	0
16	S	19	0	0	0	0
16	T	39	0	0	2	0
16	U	62	0	0	3	0
16	V	49	0	0	2	0
16	W	62	0	0	0	0
16	X	45	0	0	6	0
16	Y	48	0	0	2	0
16	Z	53	0	0	4	0
All	All	51018	0	49374	1519	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 15.

All (1519) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:96:ALA:HA	7:U:107:MET:HE2	1.30	1.13
7:G:96:ALA:HA	7:G:107:MET:HE2	1.32	1.11
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.14	1.11
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	1.14	1.07
10:J:168:MET:HE3	10:X:168:MET:HE3	1.34	1.06
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.13	1.06
7:U:9:ASP:HA	7:U:14:ILE:HD11	1.34	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:9:ASP:HA	7:G:14:ILE:HD11	1.34	1.04
2:P:202:THR:HG22	2:P:204:SER:H	1.25	0.99
2:B:202:THR:HG22	2:B:204:SER:H	1.27	0.98
2:B:15:PHE:H	3:C:23:GLN:HE22	1.02	0.97
1:O:15:PHE:H	2:P:23:GLN:HE22	1.15	0.93
2:B:108:PRO:HB2	2:B:111:ILE:HD13	1.51	0.93
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.34	0.92
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.52	0.92
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.49	0.92
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.13	0.91
3:C:15:PHE:H	4:D:23:GLN:HE22	1.17	0.91
13:M:157:ASN:HD22	13:M:160:ARG:HH11	0.97	0.91
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.86	0.91
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.87	0.90
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.20	0.89
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.19	0.89
5:E:207:LEU:HD23	5:E:207:LEU:H	1.38	0.88
13:1:157:ASN:HD22	13:1:160:ARG:HH11	0.96	0.88
5:S:207:LEU:HD23	5:S:207:LEU:H	1.36	0.88
5:S:15:PHE:H	6:T:23:GLN:HE22	1.22	0.87
2:P:108:PRO:HB2	2:P:111:ILE:HD13	1.54	0.86
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.40	0.86
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.88	0.86
1:A:15:PHE:H	2:B:23:GLN:HE22	1.20	0.86
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.24	0.86
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.74	0.86
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.39	0.85
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.77	0.85
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.74	0.85
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.75	0.85
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.39	0.84
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.75	0.84
6:F:109:ILE:HD12	6:F:109:ILE:H	1.42	0.84
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.43	0.84
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.23	0.83
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.60	0.83
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.78	0.83
6:T:109:ILE:HD12	6:T:109:ILE:H	1.44	0.83
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.26	0.83
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.42	0.83
5:E:15:PHE:H	6:F:23:GLN:HE22	1.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:107:LYS:HG2	14:N:108:GLY:H	1.43	0.82
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.44	0.82
14:2:107:LYS:HG2	14:2:108:GLY:H	1.44	0.82
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.27	0.82
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.77	0.82
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.62	0.82
6:T:35:THR:HG21	6:T:51:GLU:O	1.80	0.81
11:K:99:THR:HG22	11:K:113:VAL:O	1.79	0.81
3:C:185:THR:HG22	3:C:187:GLU:H	1.44	0.81
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.63	0.81
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.27	0.81
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.61	0.81
3:C:163:GLN:HE21	3:C:164:THR:H	1.24	0.81
6:F:35:THR:HG21	6:F:51:GLU:O	1.80	0.81
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.62	0.81
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.63	0.80
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.94	0.80
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.62	0.80
13:1:42:VAL:HG23	13:1:178:ILE:HD11	1.64	0.79
3:C:185:THR:HB	3:C:188:GLU:HG2	1.63	0.79
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.62	0.79
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.64	0.79
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.63	0.79
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.65	0.78
3:C:163:GLN:NE2	3:C:164:THR:H	1.81	0.78
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.81	0.78
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.64	0.78
16:B:565:HOH:O	3:C:33:ARG:HD2	1.83	0.78
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.29	0.78
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.66	0.77
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.65	0.77
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.14	0.77
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.65	0.77
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.66	0.76
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.85	0.76
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.66	0.76
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.66	0.76
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.68	0.76
4:D:192:LEU:O	4:D:196:ILE:HG12	1.86	0.76
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.32	0.76
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.16	0.75
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.33	0.75
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.67	0.75
3:C:232:TYR:O	3:C:236:ILE:HG13	1.86	0.75
9:W:6:MET:HE3	9:W:155:ILE:HD12	1.67	0.75
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.52	0.74
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.67	0.74
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.69	0.74
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.03	0.74
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.69	0.74
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.70	0.74
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.87	0.74
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.69	0.74
4:R:192:LEU:O	4:R:196:ILE:HG12	1.86	0.74
12:Z:134:ILE:HD13	12:Z:158:SER:HB3	1.69	0.74
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.01	0.73
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.53	0.73
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.88	0.73
3:Q:65:SER:HB2	16:Q:303:HOH:O	1.89	0.73
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.88	0.73
3:C:41:LYS:HG2	3:C:161:SER:O	1.88	0.73
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.19	0.73
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	1.92	0.73
7:G:217:LYS:HE3	7:G:217:LYS:HA	1.70	0.72
10:J:168:MET:HE3	10:X:168:MET:CE	2.17	0.72
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.89	0.72
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.70	0.72
12:L:134:ILE:HD13	12:L:158:SER:HB3	1.72	0.72
5:S:207:LEU:H	5:S:207:LEU:CD2	2.01	0.72
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.54	0.72
5:E:207:LEU:H	5:E:207:LEU:CD2	2.03	0.72
12:L:166:HIS:HD2	12:L:168:GLN:H	1.37	0.72
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.54	0.72
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.87	0.72
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.20	0.72
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.71	0.72
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.72	0.72
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.53	0.72
10:J:168:MET:CE	10:X:168:MET:HE3	2.18	0.72
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.36	0.72
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:96:ALA:HA	7:G:107:MET:CE	2.16	0.71
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.72	0.71
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.72	0.71
6:T:192:GLN:O	6:T:196:ILE:HG12	1.90	0.71
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.73	0.71
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.03	0.71
11:K:142:TYR:O	11:K:143:LYS:HD2	1.89	0.71
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.03	0.71
5:E:12:THR:HG21	5:E:124:THR:HA	1.72	0.71
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.73	0.71
9:I:6:MET:HE3	9:I:155:ILE:HD12	1.72	0.71
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.05	0.71
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	1.99	0.71
1:A:179:ARG:HH11	1:A:179:ARG:HB3	1.56	0.70
7:U:59:LEU:O	7:U:61:PRO:HD3	1.89	0.70
2:P:41:MET:HE3	16:P:254:HOH:O	1.90	0.70
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.91	0.70
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.88	0.70
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.57	0.70
1:O:60:MET:HE3	1:O:63:THR:HG21	1.71	0.70
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.71	0.70
5:S:12:THR:HG21	5:S:124:THR:HA	1.71	0.70
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.07	0.70
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.74	0.70
6:F:192:GLN:O	6:F:196:ILE:HG12	1.91	0.70
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.99	0.70
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.73	0.70
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.56	0.70
7:U:96:ALA:HA	7:U:107:MET:CE	2.16	0.69
6:F:109:ILE:HD12	6:F:109:ILE:N	2.06	0.69
6:T:109:ILE:HD12	6:T:109:ILE:N	2.07	0.69
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.06	0.69
13:1:40:ASN:H	13:1:40:ASN:HD22	1.39	0.69
3:C:163:GLN:HE21	3:C:164:THR:N	1.91	0.69
10:J:3:ILE:HD13	10:J:46:ALA:HB2	1.75	0.69
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.07	0.69
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.27	0.69
7:G:59:LEU:O	7:G:61:PRO:HD3	1.93	0.69
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.75	0.68
8:H:35:HIS:CB	8:H:56:THR:HG21	2.23	0.68
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.08	0.68
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.58	0.68
7:U:227:GLU:HG2	16:U:1255:HOH:O	1.93	0.68
1:A:60:MET:HE3	1:A:63:THR:HG21	1.76	0.68
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.76	0.68
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.29	0.68
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.42	0.68
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.06	0.68
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.22	0.68
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.91	0.68
13:M:40:ASN:H	13:M:40:ASN:HD22	1.40	0.68
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.09	0.68
7:U:86:ARG:HD2	16:U:248:HOH:O	1.91	0.68
8:V:35:HIS:CB	8:V:56:THR:HG21	2.24	0.68
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.74	0.68
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.90	0.67
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.57	0.67
6:T:237:GLN:O	6:T:240:ILE:HG22	1.95	0.67
2:B:163:ILE:HD13	2:B:164:SER:N	2.09	0.67
3:Q:57:LYS:O	3:Q:58:LEU:HB2	1.94	0.67
5:S:207:LEU:HD23	5:S:207:LEU:N	2.09	0.67
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.75	0.67
3:C:57:LYS:O	3:C:58:LEU:HB2	1.94	0.67
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.75	0.67
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.60	0.67
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.77	0.67
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.77	0.67
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.76	0.67
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.77	0.67
12:Z:148:VAL:O	12:Z:152:ILE:HG12	1.95	0.67
14:2:20:THR:HG23	14:2:31:THR:OG1	1.95	0.67
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.77	0.66
5:E:207:LEU:HD23	5:E:207:LEU:N	2.10	0.66
7:U:121:GLN:O	7:U:124:THR:HB	1.95	0.66
10:J:-1:MET:HG2	10:J:1:ASP:H	1.60	0.66
5:S:227:GLU:CD	5:S:227:GLU:H	2.03	0.66
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.76	0.66
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.94	0.66
6:T:186:ALA:O	6:T:190:VAL:HG23	1.96	0.66
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.43	0.66
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:3:ILE:HD13	10:X:46:ALA:HB2	1.76	0.66
3:C:46:VAL:O	3:C:215:VAL:HG12	1.95	0.66
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.78	0.66
14:N:20:THR:HG23	14:N:31:THR:OG1	1.96	0.66
5:S:49:VAL:HG22	5:S:212:ILE:HD13	1.77	0.66
1:A:121:GLN:O	1:A:124:THR:HB	1.96	0.65
6:F:237:GLN:O	6:F:240:ILE:HG22	1.97	0.65
7:G:233:LEU:O	7:G:236:ILE:HG13	1.96	0.65
1:O:121:GLN:O	1:O:124:THR:HB	1.95	0.65
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.08	0.65
7:G:121:GLN:O	7:G:124:THR:HB	1.97	0.65
8:H:33:LYS:HG2	15:H:224:GPT:H12	1.78	0.65
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.76	0.65
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.97	0.65
7:U:233:LEU:O	7:U:236:ILE:HG13	1.96	0.65
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.77	0.65
3:Q:46:VAL:O	3:Q:215:VAL:HG12	1.96	0.65
12:L:148:VAL:O	12:L:152:ILE:HG12	1.96	0.65
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.78	0.65
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.10	0.65
3:Q:241:GLN:C	3:Q:243:GLN:H	2.05	0.65
7:U:77:VAL:HG12	7:U:137:THR:HB	1.79	0.65
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.79	0.65
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.62	0.65
13:M:165:ARG:C	14:2:26:ILE:HG13	2.22	0.65
2:P:112:LEU:C	2:P:112:LEU:HD23	2.21	0.65
4:R:175:GLU:HG2	4:R:196:ILE:HD12	1.79	0.65
5:E:227:GLU:CD	5:E:227:GLU:H	2.03	0.64
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.78	0.64
2:P:163:ILE:HD13	2:P:164:SER:N	2.11	0.64
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.78	0.64
5:E:226:GLY:O	5:E:229:VAL:HG22	1.96	0.64
14:N:26:ILE:HG13	13:1:165:ARG:C	2.21	0.64
14:N:107:LYS:HG2	14:N:108:GLY:N	2.13	0.64
2:B:112:LEU:HD23	2:B:112:LEU:C	2.22	0.64
3:C:186:VAL:O	3:C:190:VAL:HG23	1.98	0.64
7:U:8:TYR:C	7:U:10:ARG:H	2.05	0.64
8:V:33:LYS:HG2	15:V:224:GPT:H12	1.78	0.64
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.10	0.64
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.78	0.64
5:S:28:LEU:HA	5:S:31:ILE:HD12	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:33:LYS:HG2	15:Y:224:GPT:H12	1.79	0.64
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.30	0.64
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.97	0.64
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.79	0.64
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.45	0.64
7:G:77:VAL:HG12	7:G:137:THR:HB	1.79	0.64
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.32	0.64
10:X:-1:MET:HG2	10:X:1:ASP:H	1.63	0.64
3:C:241:GLN:C	3:C:243:GLN:H	2.05	0.64
6:F:186:ALA:O	6:F:190:VAL:HG23	1.97	0.64
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.28	0.64
10:J:2:ILE:C	10:J:3:ILE:HD12	2.23	0.64
5:S:226:GLY:O	5:S:229:VAL:HG22	1.98	0.64
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.44	0.63
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.33	0.63
13:1:-3:VAL:HG12	13:1:49:ILE:HG13	1.80	0.63
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.63	0.63
5:E:28:LEU:HA	5:E:31:ILE:HD12	1.79	0.63
13:M:-3:VAL:HG12	13:M:49:ILE:HG13	1.81	0.63
7:G:8:TYR:C	7:G:10:ARG:H	2.04	0.63
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.79	0.63
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.81	0.63
5:S:220:PRO:O	5:S:222:THR:HG23	1.98	0.63
2:B:121:GLN:O	2:B:124:THR:HB	1.99	0.63
4:D:175:GLU:HG2	4:D:196:ILE:HD12	1.79	0.63
2:P:185:LYS:HD3	2:P:186:VAL:N	2.14	0.63
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.81	0.63
2:B:181:LYS:O	2:B:184:MET:HG3	1.99	0.63
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.79	0.63
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.80	0.63
5:E:220:PRO:O	5:E:222:THR:HG23	1.99	0.63
9:I:112:GLY:N	9:I:125:ILE:HD12	2.14	0.63
7:U:198:ILE:HG23	7:U:203:THR:O	1.99	0.62
10:X:2:ILE:C	10:X:3:ILE:HD12	2.24	0.62
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.80	0.62
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.99	0.62
2:B:15:PHE:H	3:C:23:GLN:NE2	1.86	0.62
3:C:65:SER:HB2	16:C:274:HOH:O	1.99	0.62
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.46	0.62
14:2:107:LYS:HG2	14:2:108:GLY:N	2.13	0.62
7:G:14:ILE:HD13	7:G:14:ILE:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.81	0.62
1:O:4:MET:SD	1:O:5:THR:N	2.67	0.62
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.81	0.62
10:J:10(B):LYS:HZ2	10:J:10(B):LYS:HB2	1.65	0.62
10:J:156:LYS:O	10:J:160:GLN:HG3	2.00	0.62
11:K:33:LYS:HG2	15:K:224:GPT:H12	1.82	0.62
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.82	0.62
1:O:86:ARG:HH21	7:U:118:ASN:ND2	1.98	0.62
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.81	0.62
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.15	0.62
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.28	0.62
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	1.97	0.62
10:X:156:LYS:O	10:X:160:GLN:HG3	2.00	0.62
2:B:185:LYS:HD3	2:B:186:VAL:N	2.15	0.61
8:H:159:ILE:HG22	8:H:163:ILE:CD1	2.29	0.61
13:1:133:MET:HE1	13:1:165:ARG:HG3	1.82	0.61
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.64	0.61
5:S:18(D):ILE:HG12	5:S:18(D):ILE:O	2.01	0.61
1:A:4:MET:SD	1:A:5:THR:N	2.65	0.61
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.64	0.61
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.82	0.61
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.15	0.61
8:V:172:ASN:HD22	8:V:193:THR:HA	1.66	0.61
1:A:86:ARG:HH21	7:G:118:ASN:ND2	1.97	0.61
1:O:69:LEU:C	1:O:69:LEU:HD23	2.26	0.61
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.81	0.61
2:P:181:LYS:O	2:P:184:MET:HG3	2.00	0.61
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.47	0.61
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.15	0.61
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.31	0.61
5:E:86:ARG:HG3	5:E:86:ARG:HH11	1.65	0.61
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.66	0.61
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.81	0.61
13:1:37:VAL:HG11	13:1:79:ILE:HD13	1.82	0.61
3:C:35:THR:HB	3:C:51:GLU:HG3	1.82	0.61
5:S:132:TYR:O	5:S:153:PRO:HB3	2.01	0.61
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.31	0.61
5:E:18(D):ILE:HG12	5:E:18(D):ILE:O	2.01	0.61
5:S:86:ARG:HG3	5:S:86:ARG:HH11	1.65	0.61
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.83	0.60
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.30	0.60
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.31	0.60
13:1:152:GLU:O	13:1:156:VAL:HG23	2.01	0.60
1:A:69:LEU:C	1:A:69:LEU:HD23	2.26	0.60
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.81	0.60
1:A:97:HIS:HD2	8:H:61:SER:OG	1.85	0.60
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.83	0.60
5:E:49:VAL:HG22	5:E:212:ILE:HD13	1.83	0.60
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.84	0.60
7:U:14:ILE:HD13	7:U:14:ILE:H	1.67	0.60
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.32	0.60
2:P:121:GLN:O	2:P:124:THR:HB	1.99	0.60
13:M:133:MET:HE1	13:M:165:ARG:HG3	1.84	0.60
7:G:198:ILE:HG23	7:G:203:THR:O	2.00	0.59
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.83	0.59
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.84	0.59
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.84	0.59
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.37	0.59
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.33	0.59
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.99	0.59
2:P:231:ASP:O	2:P:235:LYS:HG2	2.03	0.59
5:S:73:HIS:HE1	5:S:107:LEU:O	1.85	0.59
7:G:72:ARG:HB2	7:G:72:ARG:NH1	2.18	0.59
10:J:133:TYR:HD1	16:Y:593:HOH:O	1.85	0.59
13:M:37:VAL:HG11	13:M:79:ILE:CD1	2.33	0.59
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.03	0.59
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.01	0.59
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.01	0.59
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.84	0.59
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.68	0.59
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.66	0.59
5:E:73:HIS:HE1	5:E:107:LEU:O	1.86	0.59
13:M:37:VAL:HG11	13:M:79:ILE:HD13	1.83	0.59
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.84	0.59
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.01	0.59
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.02	0.59
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.03	0.59
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.85	0.59
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.33	0.59
4:R:121:LEU:HB2	16:R:853:HOH:O	2.02	0.59
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.33	0.59
2:B:224:PHE:H	2:B:224:PHE:HD2	1.51	0.58
3:C:173:ARG:O	3:C:177:GLU:HG3	2.03	0.58
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.85	0.58
6:T:173:LYS:O	6:T:177:GLU:HG3	2.03	0.58
10:X:10(B):LYS:HB2	10:X:10(B):LYS:NZ	2.18	0.58
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.17	0.58
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.33	0.58
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.98	0.58
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.86	0.58
6:T:69:VAL:HG12	16:T:811:HOH:O	2.03	0.58
10:X:2:ILE:O	10:X:3:ILE:HD12	2.02	0.58
8:H:159:ILE:HG22	8:H:163:ILE:HD12	1.85	0.58
11:K:31:VAL:HG11	15:K:224:GPT:H11	1.86	0.58
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.32	0.58
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.33	0.58
2:B:231:ASP:O	2:B:235:LYS:HG2	2.03	0.58
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.02	0.58
8:V:159:ILE:HG22	8:V:163:ILE:HD12	1.84	0.58
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.01	0.58
8:H:172:ASN:HD22	8:H:193:THR:HA	1.68	0.58
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.84	0.58
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.86	0.58
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.34	0.58
5:E:132:TYR:O	5:E:153:PRO:HB3	2.03	0.58
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.18	0.58
2:P:224:PHE:H	2:P:224:PHE:HD2	1.49	0.58
5:S:227:GLU:CD	5:S:227:GLU:N	2.61	0.58
6:F:127:ASN:C	6:F:127:ASN:HD22	2.12	0.58
5:E:167:ALA:HB3	16:E:1131:HOH:O	2.03	0.57
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.18	0.57
6:F:109:ILE:H	6:F:109:ILE:CD1	2.16	0.57
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.05	0.57
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.01	0.57
13:1:37:VAL:HG11	13:1:79:ILE:CD1	2.33	0.57
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.86	0.57
10:J:2:ILE:O	10:J:3:ILE:HD12	2.03	0.57
13:M:152:GLU:O	13:M:156:VAL:HG23	2.04	0.57
5:E:227:GLU:CD	5:E:227:GLU:N	2.61	0.57
10:J:52:THR:CG2	10:J:53:VAL:N	2.68	0.57
3:Q:211:GLU:C	3:Q:212:ILE:HD13	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.04	0.57
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.85	0.57
14:N:51:ASP:O	14:N:55:ILE:HG12	2.04	0.57
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.04	0.57
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.86	0.57
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.86	0.57
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.87	0.57
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.69	0.57
11:K:86:LEU:C	11:K:86:LEU:HD13	2.29	0.57
6:T:109:ILE:H	6:T:109:ILE:CD1	2.17	0.57
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.35	0.56
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.68	0.56
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.86	0.56
2:B:202:THR:HG22	2:B:204:SER:N	2.10	0.56
6:F:173:LYS:O	6:F:177:GLU:HG3	2.04	0.56
9:I:7:THR:HG23	9:I:110:ILE:HD13	1.87	0.56
1:O:177:GLU:HG2	2:P:58:LEU:HD22	1.86	0.56
14:2:51:ASP:O	14:2:55:ILE:HG12	2.06	0.56
8:H:34:LEU:HB2	16:H:540:HOH:O	2.04	0.56
9:I:137:MET:HE2	9:I:161:ASN:HB2	1.86	0.56
11:K:138:LEU:HD13	11:K:158:SER:OG	2.05	0.56
8:V:172:ASN:ND2	8:V:193:THR:HA	2.20	0.56
9:W:27:VAL:HG13	16:X:622:HOH:O	2.04	0.56
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.87	0.56
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.05	0.56
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.40	0.56
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.87	0.56
3:C:20:HIS:HB3	3:C:25:GLU:OE1	2.06	0.56
7:G:228:ASN:HB3	16:G:255:HOH:O	2.06	0.56
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.88	0.56
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.05	0.56
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.88	0.56
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.87	0.56
4:R:112:LEU:HD13	4:R:112:LEU:C	2.31	0.56
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.31	0.56
7:U:96:ALA:CA	7:U:107:MET:HE2	2.19	0.56
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.06	0.56
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.35	0.56
13:1:40:ASN:HD22	13:1:40:ASN:N	1.99	0.56
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.87	0.55
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:HB	16:A:402:HOH:O	2.05	0.55
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.41	0.55
7:G:96:ALA:CA	7:G:107:MET:HE2	2.21	0.55
9:I:6:MET:CE	9:I:155:ILE:HA	2.36	0.55
11:Y:31:VAL:HG11	15:Y:224:GPT:H11	1.89	0.55
12:Z:-7:ASN:C	12:Z:-7:ASN:HD22	2.15	0.55
10:J:3:ILE:CD1	10:J:46:ALA:HB2	2.35	0.55
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.42	0.55
9:W:7:THR:HG23	9:W:110:ILE:HD13	1.88	0.55
9:W:137:MET:HE2	9:W:161:ASN:HB2	1.88	0.55
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.06	0.55
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.89	0.55
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.88	0.55
10:X:3:ILE:CD1	10:X:46:ALA:HB2	2.37	0.55
3:C:14:ILE:H	3:C:14:ILE:HD12	1.72	0.55
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.88	0.55
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.42	0.55
4:D:112:LEU:C	4:D:112:LEU:HD13	2.31	0.55
7:G:87:ASN:C	7:G:87:ASN:HD22	2.15	0.55
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.87	0.55
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.37	0.55
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.42	0.55
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.69	0.55
3:C:185:THR:HG22	3:C:187:GLU:N	2.18	0.55
13:M:149:GLN:NE2	13:M:149:GLN:H	2.05	0.55
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.42	0.55
4:R:85:ALA:O	4:R:89:ILE:HG12	2.06	0.55
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.72	0.55
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.89	0.55
3:Q:20:HIS:HB3	3:Q:25:GLU:OE1	2.07	0.55
10:X:52:THR:CG2	10:X:53:VAL:N	2.69	0.55
5:E:198:SER:HA	5:E:201:LEU:HG	1.88	0.55
1:O:62:GLU:H	1:O:62:GLU:CD	2.15	0.55
1:O:97:HIS:HD2	8:V:61:SER:OG	1.89	0.55
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.42	0.55
5:S:198:SER:HA	5:S:201:LEU:HG	1.88	0.55
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.70	0.54
4:D:237:LEU:O	4:D:241:GLU:HG3	2.08	0.54
1:A:21(P):LYS:N	16:A:1147:HOH:O	2.37	0.54
4:D:186:LEU:O	4:D:190:GLU:HG3	2.07	0.54
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.07	0.54
8:H:172:ASN:ND2	8:H:193:THR:HA	2.22	0.54
1:A:62:GLU:CD	1:A:62:GLU:H	2.14	0.54
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.89	0.54
5:S:190:ILE:HG23	5:S:212:ILE:HD12	1.89	0.54
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.72	0.54
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.33	0.54
1:O:62:GLU:C	1:O:64:LEU:H	2.16	0.54
2:P:202:THR:HG22	2:P:204:SER:N	2.08	0.54
7:U:228:ASN:HB3	16:U:242:HOH:O	2.07	0.54
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.43	0.54
4:R:207:LEU:C	4:R:207:LEU:HD23	2.32	0.54
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.89	0.54
6:T:127:ASN:C	6:T:127:ASN:HD22	2.14	0.54
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.89	0.54
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.38	0.54
7:U:192:PHE:CD1	7:U:192:PHE:C	2.86	0.54
8:V:90:TYR:CG	8:V:95:ILE:HD12	2.42	0.54
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.88	0.54
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.42	0.54
3:C:211:GLU:C	3:C:212:ILE:HD13	2.33	0.54
7:G:77:VAL:CG1	7:G:137:THR:HB	2.37	0.54
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.38	0.54
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.42	0.54
13:1:149:GLN:H	13:1:149:GLN:NE2	2.06	0.54
3:C:41:LYS:HD3	3:C:161:SER:HA	1.90	0.54
1:O:198:LYS:HE3	1:O:236:LEU:HD11	1.90	0.54
6:T:203:GLU:O	6:T:206:LYS:HD2	2.08	0.54
11:K:7:ARG:HD2	11:K:108:PRO:O	2.08	0.54
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.73	0.54
2:P:239:THR:OXT	2:P:239:THR:HG22	2.06	0.54
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.33	0.54
2:B:41:MET:HE3	16:B:240:HOH:O	2.08	0.53
4:D:85:ALA:O	4:D:89:ILE:HG12	2.08	0.53
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.90	0.53
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.72	0.53
4:R:186:LEU:O	4:R:190:GLU:HG3	2.08	0.53
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.89	0.53
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.90	0.53
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.07	0.53
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:6:MET:CE	9:W:155:ILE:HA	2.38	0.53
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.90	0.53
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.88	0.53
5:E:78:LEU:HD12	5:E:78:LEU:C	2.33	0.53
7:G:8:TYR:C	7:G:10:ARG:N	2.66	0.53
1:O:20(A):THR:C	1:O:210:ILE:HD12	2.34	0.53
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.43	0.53
7:U:197:MET:HE3	7:U:197:MET:HA	1.89	0.53
4:D:207:LEU:HD23	4:D:207:LEU:C	2.33	0.53
8:H:90:TYR:CG	8:H:95:ILE:HD12	2.43	0.53
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.33	0.53
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.43	0.53
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.38	0.53
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.89	0.53
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.89	0.53
7:G:197:MET:HE3	7:G:197:MET:HA	1.90	0.53
1:A:20(A):THR:C	1:A:210:ILE:HD12	2.34	0.53
2:B:239:THR:HG22	2:B:239:THR:OXT	2.07	0.53
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.09	0.53
7:G:192:PHE:CD1	7:G:192:PHE:C	2.86	0.53
2:P:87:ILE:O	2:P:91:THR:HG23	2.09	0.53
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.95	0.53
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.91	0.53
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.21	0.53
4:R:237:LEU:O	4:R:241:GLU:HG3	2.09	0.53
5:S:15:PHE:H	6:T:23:GLN:NE2	2.01	0.53
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.90	0.53
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.43	0.53
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.91	0.53
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.44	0.52
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.91	0.52
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.09	0.52
1:O:150:GLN:O	1:O:157:TYR:HA	2.09	0.52
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.74	0.52
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.39	0.52
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.91	0.52
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.18	0.52
7:U:77:VAL:CG1	7:U:137:THR:HB	2.39	0.52
6:T:172:ALA:O	6:T:176:LEU:HD22	2.08	0.52
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.09	0.52
2:B:169:THR:O	2:B:173:GLN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.39	0.52
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.90	0.52
7:G:9:ASP:HA	7:G:14:ILE:CD1	2.24	0.52
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.15	0.52
2:P:224:PHE:N	2:P:224:PHE:CD2	2.78	0.52
4:R:59:LEU:C	4:R:59:LEU:HD13	2.35	0.52
5:S:201:LEU:O	5:S:202:ARG:HB2	2.09	0.52
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.21	0.52
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.10	0.52
5:E:201:LEU:O	5:E:202:ARG:HB2	2.10	0.52
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.91	0.52
2:B:224:PHE:N	2:B:224:PHE:CD2	2.78	0.52
6:F:136:THR:O	6:F:150:MET:HA	2.10	0.52
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.39	0.52
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.92	0.52
1:O:159:PRO:O	2:P:59:LEU:HD12	2.10	0.52
10:X:10(B):LYS:HB2	10:X:10(B):LYS:HZ2	1.74	0.52
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.10	0.52
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.90	0.52
13:M:40:ASN:HD22	13:M:40:ASN:N	2.00	0.52
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.10	0.52
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.92	0.52
2:P:224:PHE:HD2	2:P:224:PHE:N	2.08	0.52
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.50	0.52
5:S:78:LEU:C	5:S:78:LEU:HD12	2.35	0.52
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.09	0.52
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.45	0.51
3:C:55:THR:C	3:C:56:LEU:HD22	2.35	0.51
3:C:227:GLU:OE1	3:C:227:GLU:N	2.42	0.51
10:J:24:ILE:HG12	10:J:24:ILE:O	2.09	0.51
14:N:175:MET:HE3	14:N:18(B):PHE:CE2	2.46	0.51
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.91	0.51
6:T:136:THR:O	6:T:150:MET:HA	2.10	0.51
7:U:87:ASN:C	7:U:87:ASN:HD22	2.18	0.51
1:A:150:GLN:O	1:A:157:TYR:HA	2.09	0.51
8:H:165:ASN:HD22	13:1:139:ARG:NH1	2.04	0.51
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.91	0.51
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.91	0.51
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.10	0.51
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.45	0.51
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:34:ILE:HB	16:I:955:HOH:O	2.09	0.51
3:C:15:PHE:CD1	3:C:21:ILE:HD11	2.46	0.51
4:D:24:VAL:O	4:D:27:SER:HB3	2.11	0.51
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.15	0.51
2:P:169:THR:O	2:P:173:GLN:HB2	2.10	0.51
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.41	0.51
5:S:134:VAL:O	5:S:153:PRO:HG3	2.10	0.51
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.92	0.51
2:B:87:ILE:O	2:B:91:THR:HG23	2.11	0.51
2:B:215:ILE:HG13	2:B:221:GLN:HG2	1.93	0.51
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.46	0.51
12:L:129:ALA:HB1	12:L:166:HIS:CE1	2.46	0.51
14:N:20:THR:HG22	15:N:224:GPT:H10	1.92	0.51
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.46	0.51
5:S:160:LEU:HD13	5:S:163:THR:HB	1.92	0.51
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.93	0.51
9:W:29:ASN:C	9:W:29:ASN:HD22	2.18	0.51
2:B:222:LYS:NZ	2:B:228:GLU:OE2	2.43	0.51
4:D:40:ILE:HD11	4:D:176:LEU:HD22	1.93	0.51
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.46	0.51
5:E:190:ILE:HG23	5:E:212:ILE:HD12	1.92	0.51
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.76	0.51
6:F:203:GLU:O	6:F:206:LYS:HD2	2.10	0.51
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.91	0.51
10:J:-1:MET:HG2	10:J:1:ASP:N	2.24	0.51
13:M:7:LYS:HB3	13:M:12:VAL:HG12	1.93	0.51
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.76	0.51
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.74	0.51
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.92	0.51
5:E:15:PHE:H	6:F:23:GLN:NE2	2.04	0.51
8:V:4:VAL:HG12	8:V:126:SER:HB3	1.93	0.51
10:X:113:ILE:HA	10:X:118:THR:O	2.10	0.51
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.45	0.51
4:R:72:ARG:HG3	16:R:1302:HOH:O	2.11	0.51
2:B:224:PHE:HD2	2:B:224:PHE:N	2.08	0.51
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.92	0.51
9:I:29:ASN:C	9:I:29:ASN:HD22	2.19	0.51
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.41	0.51
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.26	0.51
7:U:8:TYR:C	7:U:10:ARG:N	2.67	0.51
12:L:109:ALA:HA	16:L:975:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.93	0.51
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	2.11	0.51
1:A:62:GLU:C	1:A:64:LEU:H	2.18	0.50
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.93	0.50
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.44	0.50
10:X:133:TYR:CZ	10:X:166:MET:HG3	2.46	0.50
4:D:177:LEU:CD2	5:E:58:LEU:HD13	2.41	0.50
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.24	0.50
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.11	0.50
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.46	0.50
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.42	0.50
8:H:4:VAL:HG12	8:H:126:SER:HB3	1.94	0.50
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.41	0.50
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.76	0.50
7:U:9:ASP:HA	7:U:14:ILE:CD1	2.24	0.50
8:V:152:ILE:HD11	8:V:177:VAL:HG21	1.93	0.50
6:F:172:ALA:O	6:F:176:LEU:HD22	2.12	0.50
8:H:128:GLY:O	8:H:131:SER:HB2	2.11	0.50
10:J:167:PRO:O	10:X:168:MET:HE2	2.12	0.50
8:V:196:VAL:HG23	16:V:652:HOH:O	2.11	0.50
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.93	0.50
14:2:20:THR:HG22	15:2:224:GPT:H10	1.94	0.50
1:A:173:LYS:O	1:A:177:GLU:HG3	2.11	0.50
13:M:13:ILE:HB	13:M:155:ILE:HD13	1.92	0.50
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.11	0.50
2:P:63:THR:HG22	2:P:63:THR:O	2.12	0.50
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.93	0.50
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.11	0.50
6:F:53:LEU:HD11	6:F:205:ASN:OD1	2.12	0.50
10:J:24:ILE:HG12	10:X:133:TYR:OH	2.12	0.50
8:H:221:ILE:HD11	9:I:184:VAL:HG21	1.92	0.50
10:J:143:ARG:O	10:J:146:MET:HG3	2.11	0.50
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.93	0.50
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.93	0.50
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.75	0.50
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.94	0.50
5:E:134:VAL:O	5:E:153:PRO:HG3	2.12	0.50
1:O:173:LYS:O	1:O:177:GLU:HG3	2.12	0.50
2:P:215:ILE:HG13	2:P:221:GLN:HG2	1.93	0.50
3:Q:57:LYS:NZ	16:Q:434:HOH:O	2.44	0.50
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.93	0.50
10:X:-1:MET:HG2	10:X:1:ASP:N	2.27	0.50
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.52	0.50
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.12	0.50
16:L:200:HOH:O	9:W:192:ARG:HG3	2.10	0.50
3:Q:15:PHE:CD1	3:Q:21:ILE:HD11	2.46	0.50
10:X:24:ILE:HG12	10:X:24:ILE:O	2.11	0.50
13:1:4:ILE:HD13	13:1:4:ILE:H	1.77	0.50
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.47	0.49
4:D:59:LEU:HD13	4:D:59:LEU:C	2.36	0.49
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.47	0.49
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.37	0.49
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.27	0.49
1:A:38:LEU:HD12	1:A:38:LEU:C	2.37	0.49
2:B:11:ARG:HD2	3:C:10:ARG:NH1	2.27	0.49
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.47	0.49
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.46	0.49
4:D:122:ARG:HH11	4:D:122:ARG:HG2	1.76	0.49
7:G:49:ILE:HD12	7:G:212:VAL:HG22	1.93	0.49
10:J:112:GLN:NE2	10:J:126:ALA:H	2.09	0.49
12:L:145:TYR:CD1	12:L:146:LEU:N	2.80	0.49
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.36	0.49
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.47	0.49
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.59	0.49
7:U:70:ILE:HD12	7:U:92:ALA:HB3	1.94	0.49
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.80	0.49
2:B:63:THR:HG22	2:B:63:THR:O	2.12	0.49
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.70	0.49
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.27	0.49
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.93	0.49
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.95	0.49
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.12	0.49
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.47	0.49
14:2:116:GLY:HA3	16:2:191:HOH:O	2.12	0.49
3:C:15:PHE:N	4:D:23:GLN:HE22	1.98	0.49
4:D:170:GLU:OE1	4:D:170:GLU:N	2.45	0.49
5:E:4:PHE:CG	5:E:5:ARG:N	2.79	0.49
11:K:10(A):ARG:HH11	11:K:10(A):ARG:HG2	1.76	0.49
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.25	0.49
6:T:203:GLU:C	6:T:205:ASN:H	2.20	0.49
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.43	0.49
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.75	0.49
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.25	0.49
10:X:143:ARG:O	10:X:146:MET:HG3	2.11	0.49
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.95	0.49
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	2.12	0.49
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.42	0.49
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.95	0.49
10:J:168:MET:HE2	10:X:167:PRO:O	2.13	0.49
14:N:26:ILE:HB	13:1:165:ARG:HA	1.94	0.49
13:1:7:LYS:HB3	13:1:12:VAL:HG12	1.95	0.49
2:B:15:PHE:N	3:C:23:GLN:HE22	1.87	0.49
7:G:70:ILE:HD12	7:G:92:ALA:HB3	1.94	0.49
7:G:87:ASN:C	7:G:87:ASN:ND2	2.71	0.49
10:J:113:ILE:HA	10:J:118:THR:O	2.12	0.49
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.11	0.49
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.94	0.49
8:V:84:LYS:HG3	8:V:85:GLN:N	2.27	0.49
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.95	0.49
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.94	0.49
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.60	0.49
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	1.94	0.49
4:R:24:VAL:O	4:R:27:SER:HB3	2.12	0.49
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.95	0.49
8:V:128:GLY:O	8:V:131:SER:HB2	2.12	0.49
9:W:20:LEU:HD13	9:W:20:LEU:C	2.38	0.49
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.28	0.49
3:C:52:ARG:HD2	3:C:208:LYS:O	2.13	0.49
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.26	0.49
2:P:150:THR:O	2:P:157:TYR:HA	2.12	0.49
3:Q:14:ILE:CD1	3:Q:14:ILE:C	2.85	0.49
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.13	0.49
9:W:112:GLY:N	9:W:125:ILE:HD12	2.28	0.49
10:X:112:GLN:NE2	10:X:126:ALA:H	2.11	0.49
13:1:184:LEU:C	13:1:184:LEU:HD23	2.38	0.49
3:C:57:LYS:HD2	3:C:58:LEU:N	2.28	0.49
3:C:182:PRO:O	3:C:184:ALA:N	2.46	0.49
6:F:203:GLU:C	6:F:205:ASN:H	2.19	0.49
10:J:133:TYR:OH	10:X:24:ILE:HG12	2.13	0.49
12:L:98:HIS:HD2	16:L:199:HOH:O	1.96	0.49
13:M:165:ARG:HA	14:2:26:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.94	0.49
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.59	0.49
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.25	0.49
13:1:40:ASN:N	13:1:40:ASN:ND2	2.61	0.49
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.13	0.48
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.78	0.48
3:Q:40:VAL:HG23	3:Q:189:CYS:SG	2.52	0.48
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.13	0.48
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.94	0.48
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.94	0.48
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.67	0.48
6:T:109:ILE:CD1	6:T:142:ASP:HB3	2.43	0.48
9:W:178:ILE:HG23	9:W:184:VAL:HG22	1.94	0.48
13:1:40:ASN:H	13:1:40:ASN:ND2	2.10	0.48
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.48	0.48
5:E:160:LEU:HD13	5:E:163:THR:HB	1.94	0.48
10:J:133:TYR:CZ	10:J:166:MET:HG3	2.48	0.48
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.26	0.48
3:Q:182:PRO:O	3:Q:184:ALA:N	2.47	0.48
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.48	0.48
7:U:107:MET:CE	7:U:112:LEU:HD13	2.42	0.48
8:H:152:ILE:HD11	8:H:177:VAL:HG21	1.95	0.48
4:R:40:ILE:HD11	4:R:176:LEU:HD22	1.93	0.48
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.12	0.48
2:B:163:ILE:HD13	2:B:164:SER:H	1.79	0.48
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.94	0.48
13:M:184:LEU:HD23	13:M:184:LEU:C	2.39	0.48
7:G:107:MET:CE	7:G:112:LEU:HD13	2.44	0.48
8:H:84:LYS:HG3	8:H:85:GLN:N	2.27	0.48
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.78	0.48
3:C:190:VAL:O	3:C:194:VAL:HG23	2.14	0.48
6:F:101:LYS:NZ	14:N:85:GLU:OE1	2.46	0.48
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.28	0.48
12:L:166:HIS:CD2	12:L:168:GLN:H	2.24	0.48
11:Y:4:LEU:HD11	11:Y:159:ILE:HG12	1.96	0.48
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.25	0.48
3:C:14:ILE:CD1	3:C:14:ILE:C	2.87	0.48
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.95	0.48
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.96	0.48
1:O:38:LEU:HD12	1:O:38:LEU:C	2.39	0.48
4:R:175:GLU:CG	4:R:196:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:82:ILE:HG22	7:U:83:PRO:HD3	1.95	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.96	0.48
13:M:139:ARG:NH1	8:V:165:ASN:HD22	2.05	0.48
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.49	0.48
5:S:4:PHE:CG	5:S:5:ARG:N	2.80	0.48
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.61	0.48
3:C:40:VAL:HG23	3:C:189:CYS:SG	2.54	0.48
4:D:175:GLU:CG	4:D:196:ILE:HD12	2.44	0.48
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.49	0.48
9:I:20:LEU:C	9:I:20:LEU:HD13	2.39	0.48
10:J:6:ILE:CG2	10:J:13:ILE:HB	2.44	0.48
10:J:133:TYR:HE1	16:X:876:HOH:O	1.97	0.48
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.79	0.48
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.94	0.48
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.39	0.48
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.48	0.47
2:B:150:THR:O	2:B:157:TYR:HA	2.14	0.47
13:M:4:ILE:HD13	13:M:4:ILE:H	1.79	0.47
7:U:203:THR:HG22	7:U:204:GLU:N	2.29	0.47
10:X:6:ILE:CG2	10:X:13:ILE:HB	2.44	0.47
10:X:119:LYS:HE2	16:X:705:HOH:O	2.14	0.47
5:E:177:GLU:OE1	6:F:56:SER:HB2	2.13	0.47
11:K:142:TYR:C	11:K:143:LYS:HD2	2.39	0.47
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.62	0.47
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.14	0.47
8:V:128:GLY:O	8:V:131:SER:CB	2.62	0.47
10:X:120:VAL:HG13	10:X:122:LEU:HG	1.96	0.47
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.14	0.47
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.95	0.47
6:F:109:ILE:CD1	6:F:142:ASP:HB3	2.44	0.47
7:G:186:TRP:O	7:G:190:VAL:HG23	2.13	0.47
9:I:33:LYS:O	9:I:44:GLY:HA2	2.14	0.47
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.49	0.47
13:1:13:ILE:HB	13:1:155:ILE:HD13	1.96	0.47
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.96	0.47
3:C:241:GLN:C	3:C:243:GLN:N	2.71	0.47
8:H:197:ARG:NH2	9:I:139:GLU:O	2.47	0.47
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.96	0.47
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.96	0.47
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.14	0.47
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:186:PRO:O	5:S:190:ILE:HD12	2.15	0.47
7:G:12:ILE:HG13	7:G:14:ILE:HD12	1.97	0.47
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.96	0.47
5:S:179:THR:O	5:S:179:THR:HG22	2.14	0.47
9:W:61:TYR:CD1	9:W:61:TYR:C	2.92	0.47
10:X:44:SER:OG	10:X:100:LEU:HB2	2.14	0.47
1:A:24:ILE:HD11	1:A:124:THR:OG1	2.14	0.47
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.15	0.47
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.97	0.47
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.96	0.47
1:A:233:LEU:O	1:A:236:LEU:HB2	2.15	0.47
8:H:128:GLY:O	8:H:131:SER:CB	2.63	0.47
10:J:52:THR:HG23	10:J:53:VAL:N	2.30	0.47
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.27	0.47
1:O:24:ILE:HD11	1:O:124:THR:OG1	2.15	0.47
3:Q:241:GLN:C	3:Q:243:GLN:N	2.71	0.47
4:R:53:ARG:O	4:R:53:ARG:HG2	2.14	0.47
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.61	0.47
5:E:179:THR:HG22	5:E:179:THR:O	2.15	0.47
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.50	0.47
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.96	0.47
13:1:112:TYR:C	13:1:112:TYR:CD2	2.92	0.47
6:F:127:ASN:HD22	6:F:128:SER:N	2.13	0.47
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.15	0.47
7:G:82:ILE:HG22	7:G:83:PRO:HD3	1.96	0.47
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.97	0.47
10:J:120:VAL:HG13	10:J:122:LEU:HG	1.97	0.47
13:M:17:ASP:HA	13:M:173:PHE:CB	2.45	0.47
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.50	0.47
5:S:77:SER:OG	5:S:137:LEU:HB2	2.15	0.47
6:T:127:ASN:HD22	6:T:128:SER:N	2.13	0.47
8:V:80:LEU:HD12	8:V:113:ILE:CD1	2.40	0.47
9:W:14:ILE:HG12	9:W:34:ILE:HD12	1.97	0.47
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.95	0.47
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.42	0.47
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.80	0.47
13:M:112:TYR:C	13:M:112:TYR:CD2	2.93	0.47
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.11	0.47
4:R:170:GLU:N	4:R:170:GLU:OE1	2.46	0.47
6:T:147:HIS:HD2	16:T:242:HOH:O	1.98	0.47
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.97	0.47
2:B:228:GLU:O	2:B:232:ILE:HG22	2.15	0.46
3:C:163:GLN:NE2	3:C:163:GLN:HA	2.30	0.46
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.77	0.46
10:J:166:MET:HA	10:J:167:PRO:HD3	1.77	0.46
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.30	0.46
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.80	0.46
7:U:186:TRP:O	7:U:190:VAL:HG23	2.15	0.46
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.97	0.46
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.97	0.46
10:J:168:MET:HG2	10:X:168:MET:CE	2.46	0.46
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	2.15	0.46
1:O:233:LEU:O	1:O:236:LEU:HB2	2.15	0.46
2:P:101:LYS:HZ2	10:X:85:GLN:HE21	1.61	0.46
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.29	0.46
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.48	0.46
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.40	0.46
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.45	0.46
8:V:9:ASN:OD1	8:V:10:ASN:N	2.48	0.46
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.25	0.46
4:D:140:GLY:HA2	4:D:215:ILE:HD12	1.97	0.46
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.98	0.46
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.16	0.46
8:V:221:ILE:HD11	9:W:184:VAL:HG21	1.97	0.46
6:F:103:TYR:O	6:F:104:LYS:HB3	2.16	0.46
7:G:203:THR:HG22	7:G:204:GLU:N	2.31	0.46
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.51	0.46
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.30	0.46
8:V:175:VAL:HG12	8:V:176:CYS:N	2.31	0.46
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.97	0.46
7:G:151:THR:HG22	7:G:157:TYR:CB	2.46	0.46
7:G:228:ASN:N	7:G:228:ASN:HD22	2.14	0.46
12:L:140:ASN:O	12:L:144:PHE:HA	2.15	0.46
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.49	0.46
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.59	0.46
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.16	0.46
3:C:20:HIS:C	3:C:21:ILE:HD13	2.41	0.46
6:F:127:ASN:C	6:F:127:ASN:ND2	2.73	0.46
11:K:37:ILE:HB	11:K:41:LEU:HB2	1.97	0.46
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.16	0.46
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.98	0.46
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.31	0.46
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.97	0.46
7:U:87:ASN:C	7:U:87:ASN:ND2	2.72	0.46
2:B:6:ARG:NH1	4:D:12(B):GLU:OE2	2.49	0.46
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.79	0.46
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.16	0.46
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.79	0.46
11:K:4:LEU:HD11	11:K:159:ILE:HG12	1.97	0.46
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.80	0.46
13:M:171:ARG:HG3	13:M:192:VAL:HB	1.97	0.46
14:N:161:GLN:HE21	14:2:136:GLY:CA	2.04	0.46
1:O:60:MET:HE3	1:O:63:THR:CG2	2.45	0.46
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.80	0.46
2:B:101:LYS:HZ2	10:J:85:GLN:NE2	2.14	0.46
4:D:86:ARG:HA	4:D:86:ARG:HD3	1.86	0.46
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.96	0.46
7:G:158:VAL:HG22	7:G:159:GLY:N	2.31	0.46
2:P:122:GLY:C	2:P:124:THR:H	2.23	0.46
3:Q:163:GLN:NE2	3:Q:163:GLN:HA	2.30	0.46
4:R:86:ARG:HA	4:R:86:ARG:HD3	1.84	0.46
6:T:157:TYR:CD1	6:T:157:TYR:C	2.93	0.46
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.59	0.46
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.15	0.46
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.16	0.46
10:J:168:MET:CE	10:X:168:MET:HG2	2.45	0.46
6:T:175:GLU:HB3	6:T:196:ILE:CD1	2.45	0.46
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	1.97	0.46
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.15	0.46
11:Y:85:ASN:ND2	16:Y:215:HOH:O	2.49	0.46
2:B:141:TYR:CE2	2:B:145:GLY:HA2	2.51	0.46
3:C:36:CYS:N	3:C:51:GLU:HG2	2.31	0.46
8:H:9:ASN:OD1	8:H:10:ASN:N	2.49	0.46
1:O:110:LYS:HG2	16:O:376:HOH:O	2.15	0.46
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.98	0.46
8:V:4:VAL:HG12	8:V:126:SER:CB	2.46	0.46
2:B:234:VAL:HA	2:B:239:THR:HA	1.98	0.45
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.98	0.45
5:E:76:LEU:HD23	5:E:76:LEU:C	2.41	0.45
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.98	0.45
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.15	0.45
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.98	0.45
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.81	0.45
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.99	0.45
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.25	0.45
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.98	0.45
5:S:76:LEU:C	5:S:76:LEU:HD23	2.41	0.45
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.17	0.45
3:C:175:PHE:O	3:C:179:ASN:HB2	2.17	0.45
5:E:231:LYS:H	5:E:231:LYS:HD2	1.81	0.45
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.46	0.45
14:N:14:LEU:O	14:N:175:MET:HA	2.17	0.45
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.51	0.45
8:V:197:ARG:NH2	9:W:139:GLU:O	2.50	0.45
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.15	0.45
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.17	0.45
1:A:97:HIS:CD2	8:H:61:SER:OG	2.68	0.45
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.58	0.45
12:L:93:PHE:N	12:L:94:PRO:HD3	2.30	0.45
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.98	0.45
2:P:186:VAL:O	2:P:190:ILE:HG13	2.17	0.45
2:P:228:GLU:O	2:P:232:ILE:HG22	2.15	0.45
4:R:140:GLY:HA2	4:R:215:ILE:HD12	1.99	0.45
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.99	0.45
9:W:33:LYS:O	9:W:44:GLY:HA2	2.15	0.45
1:A:210:ILE:HD12	1:A:210:ILE:N	2.32	0.45
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.97	0.45
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.26	0.45
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.98	0.45
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.81	0.45
14:N:18(E):ASP:OD2	16:N:232:HOH:O	2.21	0.45
2:P:163:ILE:HD13	2:P:164:SER:H	1.81	0.45
5:S:49:VAL:HG12	5:S:197:ILE:HD13	1.97	0.45
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.32	0.45
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.47	0.45
7:U:203:THR:HG22	7:U:204:GLU:O	2.17	0.45
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.52	0.45
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.98	0.45
1:A:110:LYS:HG2	16:A:285:HOH:O	2.16	0.45
2:B:39:GLY:O	2:B:162:ALA:HA	2.16	0.45
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.52	0.45
6:F:35:THR:CG2	6:F:51:GLU:O	2.59	0.45
3:Q:241:GLN:O	3:Q:243:GLN:N	2.47	0.45
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.32	0.45
8:V:3:ILE:O	8:V:126:SER:HA	2.17	0.45
9:W:101:VAL:O	9:W:110:ILE:HA	2.16	0.45
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.97	0.45
10:X:90(B):ARG:NH1	16:X:266:HOH:O	2.42	0.45
13:1:17:ASP:HA	13:1:173:PHE:CB	2.46	0.45
8:H:3:ILE:O	8:H:126:SER:HA	2.17	0.45
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.45
5:S:13:VAL:CG2	6:T:129:VAL:C	2.90	0.45
6:T:35:THR:CG2	6:T:36:THR:N	2.80	0.45
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.82	0.45
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.99	0.45
11:Y:37:ILE:HB	11:Y:41:LEU:HB2	1.99	0.45
12:Z:129:ALA:HB1	12:Z:166:HIS:NE2	2.31	0.45
5:E:160:LEU:HD23	6:F:59:LEU:HA	1.98	0.45
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.52	0.45
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.82	0.45
1:O:186:LEU:O	1:O:190:ILE:HG13	2.17	0.45
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.47	0.45
6:F:114:ASP:O	6:F:118:GLN:HG2	2.17	0.45
8:H:4:VAL:HG12	8:H:126:SER:CB	2.47	0.45
9:I:101:VAL:O	9:I:110:ILE:HA	2.17	0.45
7:U:78:VAL:HG11	7:U:85:ALA:HB2	1.99	0.45
3:C:225:SER:OG	3:C:228:GLU:HG3	2.17	0.45
7:G:136:LEU:O	7:G:150:LYS:HA	2.17	0.45
7:G:217:LYS:HA	7:G:217:LYS:CE	2.45	0.45
11:K:38:ASN:C	11:K:38:ASN:OD1	2.59	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.98	0.45
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.85	0.45
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.99	0.45
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.98	0.45
1:A:221:PHE:C	1:A:221:PHE:CD2	2.95	0.44
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.97	0.44
6:F:175:GLU:HB3	6:F:196:ILE:CD1	2.45	0.44
12:L:5:GLY:O	12:L:124:CYS:HA	2.16	0.44
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.99	0.44
1:O:210:ILE:HD12	1:O:210:ILE:N	2.32	0.44
2:P:121:GLN:NE2	2:P:121:GLN:C	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.52	0.44
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.17	0.44
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.98	0.44
7:U:158:VAL:HG22	7:U:159:GLY:N	2.32	0.44
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.99	0.44
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.18	0.44
13:1:4:ILE:CD1	13:1:159:MET:SD	3.05	0.44
13:1:130:GLY:O	13:1:134:ALA:HB3	2.17	0.44
13:1:157:ASN:HB3	16:1:558:HOH:O	2.16	0.44
14:2:3:ILE:HB	14:2:44:CYS:HB3	2.00	0.44
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.17	0.44
5:E:54:ASN:ND2	5:E:56:ASP:O	2.51	0.44
9:I:61:TYR:CD1	9:I:61:TYR:C	2.95	0.44
13:M:40:ASN:N	13:M:40:ASN:ND2	2.61	0.44
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.47	0.44
2:P:234:VAL:HA	2:P:239:THR:HA	1.98	0.44
5:S:52:LYS:O	5:S:63:TYR:HD2	2.00	0.44
7:U:151:THR:HG22	7:U:157:TYR:CB	2.48	0.44
9:W:29:ASN:ND2	9:W:29:ASN:H	2.15	0.44
5:E:186:PRO:O	5:E:190:ILE:HD12	2.17	0.44
6:F:157:TYR:C	6:F:157:TYR:CD1	2.95	0.44
7:G:38:LEU:C	7:G:38:LEU:HD12	2.43	0.44
12:L:82:ASN:C	12:L:82:ASN:HD22	2.25	0.44
2:P:39:GLY:O	2:P:162:ALA:HA	2.16	0.44
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.99	0.44
12:Z:99:THR:CG2	16:Z:231:HOH:O	2.64	0.44
14:2:14:LEU:O	14:2:175:MET:HA	2.17	0.44
1:O:221:PHE:CD2	1:O:221:PHE:C	2.95	0.44
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.52	0.44
5:S:194:VAL:O	5:S:197:ILE:HG22	2.17	0.44
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.80	0.44
3:C:58:LEU:HD12	3:C:58:LEU:HA	1.84	0.44
3:C:241:GLN:O	3:C:243:GLN:N	2.47	0.44
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.82	0.44
4:R:194:LEU:HD12	4:R:194:LEU:HA	1.88	0.44
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.53	0.44
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.18	0.44
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.53	0.44
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.81	0.44
9:I:6:MET:HE1	9:I:155:ILE:HA	1.99	0.44
13:M:40:ASN:H	13:M:40:ASN:ND2	2.10	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.18	0.44
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.48	0.44
5:S:177:GLU:OE1	6:T:56:SER:HB2	2.17	0.44
7:U:197:MET:HE2	7:U:201:LEU:HG	2.00	0.44
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.83	0.44
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	2.00	0.44
5:E:142:ASP:HB2	16:M:885:HOH:O	2.17	0.44
12:L:17:ASP:HA	12:L:172:GLY:O	2.18	0.44
1:O:47:VAL:HG23	1:O:212:LEU:HD21	1.99	0.44
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.83	0.44
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.53	0.44
6:T:103:TYR:O	6:T:104:LYS:HB3	2.16	0.44
6:T:114:ASP:O	6:T:118:GLN:HG2	2.17	0.44
14:2:106:ASN:O	14:2:107:LYS:HB3	2.18	0.44
3:C:235:GLN:O	3:C:239:GLU:HG2	2.17	0.44
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.83	0.44
16:E:574:HOH:O	6:F:12:ASN:HB2	2.17	0.44
6:F:43:ASN:N	6:F:43:ASN:HD22	2.16	0.44
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	1.99	0.44
9:I:6:MET:HE3	9:I:155:ILE:HA	2.00	0.44
9:I:29:ASN:ND2	9:I:29:ASN:H	2.15	0.44
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.99	0.44
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.99	0.44
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.48	0.44
10:X:52:THR:HG23	10:X:53:VAL:N	2.32	0.44
1:A:186:LEU:O	1:A:190:ILE:HG13	2.17	0.44
4:D:179:GLU:HG3	4:D:192:LEU:HD11	2.00	0.44
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.47	0.44
12:L:192:LYS:HE3	8:V:195:ASN:HB3	2.00	0.44
14:N:106:ASN:O	14:N:107:LYS:HB3	2.18	0.44
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.81	0.44
4:R:68:VAL:HG21	4:R:89:ILE:HD12	2.00	0.44
6:T:35:THR:CG2	6:T:51:GLU:O	2.59	0.44
10:X:76:PRO:HD2	16:X:275:HOH:O	2.17	0.44
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.66	0.44
13:1:14(C):ARG:HH11	13:1:14(C):ARG:CG	2.30	0.44
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.32	0.43
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.00	0.43
7:G:172:ILE:HD11	7:G:201:LEU:CD2	2.48	0.43
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.47	0.43
12:L:177:ILE:N	12:L:177:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.48	0.43
1:O:137:LEU:HG	1:O:165:ILE:HD13	2.00	0.43
2:P:141:TYR:CD1	2:P:141:TYR:C	2.96	0.43
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.18	0.43
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.53	0.43
5:S:231:LYS:H	5:S:231:LYS:HD2	1.83	0.43
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.48	0.43
13:1:113:VAL:HA	13:1:118:VAL:O	2.18	0.43
14:2:19:ARG:NE	14:2:26:ILE:HD13	2.32	0.43
6:F:50:VAL:HG22	6:F:51:GLU:N	2.33	0.43
7:G:203:THR:HG22	7:G:204:GLU:O	2.18	0.43
10:J:18:LYS:HD3	10:J:174:ILE:HG13	2.00	0.43
1:O:5:THR:O	1:O:7:ARG:HG3	2.18	0.43
1:O:21(I):TYR:HE2	1:O:21(L):ILE:HD12	1.83	0.43
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.18	0.43
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.82	0.43
10:X:35:ARG:NH1	10:X:57:GLU:OE2	2.51	0.43
13:1:14(A):VAL:HG23	13:1:14(A):VAL:O	2.18	0.43
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.99	0.43
10:J:44:SER:OG	10:J:100:LEU:HB2	2.17	0.43
3:Q:79:SER:OG	3:Q:165:ILE:HG13	2.18	0.43
5:S:76:LEU:HD23	5:S:76:LEU:O	2.18	0.43
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.47	0.43
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	2.01	0.43
13:1:4:ILE:HD12	13:1:159:MET:SD	2.59	0.43
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.53	0.43
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.49	0.43
5:E:148:LEU:HD23	5:E:162:GLY:HA2	2.00	0.43
9:I:159:LEU:HD21	9:I:173:ALA:HB1	2.00	0.43
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.48	0.43
10:J:52:THR:HG22	10:J:53:VAL:H	1.84	0.43
1:O:212:LEU:HD23	1:O:213:ALA:N	2.33	0.43
3:Q:169:SER:HA	3:Q:172:VAL:HG13	2.01	0.43
7:U:38:LEU:C	7:U:38:LEU:HD12	2.44	0.43
13:1:19:LEU:HD12	13:1:28:PHE:O	2.18	0.43
2:B:122:GLY:C	2:B:124:THR:H	2.26	0.43
4:D:90:GLU:OE2	11:K:69:ARG:NH1	2.52	0.43
5:E:194:VAL:O	5:E:197:ILE:HG22	2.19	0.43
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.48	0.43
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.83	0.43
3:Q:225:SER:OG	3:Q:228:GLU:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:6:MET:HE3	9:W:155:ILE:HA	2.00	0.43
9:W:113:PHE:HA	9:W:118:CYS:O	2.19	0.43
13:1:171:ARG:HG3	13:1:192:VAL:HB	2.00	0.43
1:A:5:THR:O	1:A:7:ARG:HG3	2.18	0.43
2:B:11:ARG:HD2	3:C:10:ARG:CZ	2.48	0.43
2:B:112:LEU:HD23	2:B:112:LEU:O	2.19	0.43
3:C:97:GLN:NE2	16:C:6:HOH:O	2.46	0.43
7:G:225:SER:OG	7:G:228:ASN:ND2	2.51	0.43
2:P:225:LYS:O	2:P:226:PRO:C	2.61	0.43
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.43
3:C:227:GLU:H	3:C:227:GLU:CD	2.27	0.43
12:L:13:VAL:HG12	12:L:177:ILE:HG13	2.00	0.43
3:Q:47:VAL:HG23	3:Q:189:CYS:SG	2.59	0.43
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.27	0.43
4:R:12(D):ALA:HA	5:S:129:GLY:HA2	2.01	0.43
5:S:160:LEU:CD2	6:T:59:LEU:HD12	2.49	0.43
7:U:136:LEU:O	7:U:150:LYS:HA	2.17	0.43
12:Z:82:ASN:C	12:Z:82:ASN:HD22	2.25	0.43
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.48	0.43
2:B:232:ILE:O	2:B:232:ILE:HG13	2.19	0.43
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.46	0.43
13:M:13:ILE:HD13	13:M:177:ILE:HG12	2.00	0.43
2:P:112:LEU:HD23	2:P:112:LEU:O	2.18	0.43
7:U:172:ILE:HD11	7:U:201:LEU:CD2	2.48	0.43
7:U:217:LYS:HA	7:U:217:LYS:CE	2.44	0.43
2:B:39:GLY:C	2:B:148:LEU:HD21	2.43	0.43
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.83	0.43
5:E:77:SER:OG	5:E:137:LEU:HB2	2.17	0.43
1:O:15:PHE:N	2:P:23:GLN:HE22	1.98	0.43
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.45	0.43
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.54	0.43
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.83	0.43
1:A:212:LEU:HD23	1:A:213:ALA:N	2.33	0.43
3:C:21:ILE:HD13	3:C:21:ILE:N	2.34	0.43
3:C:36:CYS:H	3:C:51:GLU:HG2	1.84	0.43
7:G:18(G):GLU:CG	7:G:188:LYS:HB2	2.44	0.43
9:I:14:ILE:HG12	9:I:34:ILE:HD12	2.00	0.43
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.19	0.43
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.18	0.43
9:W:155:ILE:HG23	9:W:156:SER:N	2.34	0.43
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:52:THR:HG22	10:X:53:VAL:H	1.84	0.43
1:A:21(I):TYR:HE2	1:A:21(L):ILE:HD12	1.83	0.42
7:G:67:ILE:HD13	7:G:211:GLU:HG2	2.00	0.42
12:L:99:THR:HG23	12:L:113:PHE:HB2	2.01	0.42
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.54	0.42
8:V:59:ILE:HG12	8:V:83:LEU:HD23	2.00	0.42
10:X:18:LYS:HD3	10:X:174:ILE:HG13	2.00	0.42
12:Z:99:THR:HG22	16:Z:231:HOH:O	2.18	0.42
13:1:13:ILE:HD13	13:1:177:ILE:HG12	2.01	0.42
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.21	0.42
2:B:101:LYS:HG3	9:I:57:GLU:HB3	2.00	0.42
4:D:53:ARG:O	4:D:53:ARG:HG2	2.18	0.42
11:K:100:MET:C	11:K:101:ILE:HD13	2.43	0.42
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.34	0.42
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.76	0.42
13:M:113:VAL:HA	13:M:118:VAL:O	2.19	0.42
2:P:232:ILE:O	2:P:232:ILE:HG13	2.19	0.42
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.18	0.42
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.49	0.42
5:S:104:ASN:HB2	13:1:81:GLU:HG2	2.01	0.42
6:T:43:ASN:N	6:T:43:ASN:HD22	2.16	0.42
6:T:50:VAL:HG22	6:T:51:GLU:N	2.34	0.42
10:X:166:MET:CE	10:X:168:MET:HB2	2.49	0.42
12:L:113:PHE:N	12:L:113:PHE:CD1	2.86	0.42
14:N:107:LYS:CG	14:N:108:GLY:H	2.16	0.42
3:Q:14:ILE:HD12	3:Q:14:ILE:H	1.85	0.42
6:T:127:ASN:C	6:T:127:ASN:ND2	2.74	0.42
8:V:81:GLN:O	8:V:85:GLN:HG3	2.19	0.42
9:W:159:LEU:HD21	9:W:173:ALA:HB1	2.01	0.42
5:E:49:VAL:HG12	5:E:197:ILE:HD13	2.01	0.42
5:E:64:GLN:NE2	5:E:82:ALA:HB2	2.35	0.42
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.20	0.42
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.19	0.42
10:J:166:MET:CE	10:J:168:MET:HB2	2.49	0.42
14:N:116:GLY:HA3	16:N:195:HOH:O	2.18	0.42
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.66	0.42
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.19	0.42
5:S:137:LEU:CD2	5:S:150:GLU:HG3	2.48	0.42
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.84	0.42
6:T:194:ALA:O	6:T:198:TYR:HD1	2.03	0.42
7:U:67:ILE:HD13	7:U:211:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.02	0.42
13:1:112:TYR:O	13:1:119:THR:HA	2.19	0.42
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.17	0.42
3:C:75:VAL:HG13	3:C:221:ILE:HD13	2.02	0.42
8:H:59:ILE:HG12	8:H:83:LEU:HD23	2.02	0.42
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.19	0.42
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.35	0.42
14:N:159:LEU:O	14:N:163:ILE:HG13	2.19	0.42
3:Q:13:SER:O	4:R:130:ARG:HD3	2.19	0.42
5:S:35:SER:HB3	5:S:66:LYS:NZ	2.35	0.42
10:X:113:ILE:HG12	10:X:119:LYS:HG3	2.01	0.42
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.19	0.42
2:B:141:TYR:CD1	2:B:141:TYR:C	2.98	0.42
3:C:66:LYS:HE2	3:C:78:PHE:CZ	2.54	0.42
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.35	0.42
7:G:172:ILE:HD12	7:G:197:MET:CE	2.49	0.42
8:H:72:ARG:HG3	8:H:72:ARG:HH11	1.83	0.42
9:I:155:ILE:HG23	9:I:156:SER:N	2.35	0.42
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.55	0.42
2:P:136:PHE:O	2:P:150:THR:HA	2.20	0.42
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.19	0.42
4:R:150:HIS:O	4:R:157:PHE:HA	2.19	0.42
5:S:41:ARG:NH1	5:S:42:SER:O	2.51	0.42
6:T:78:TYR:CE1	6:T:85:GLY:HA3	2.54	0.42
7:U:228:ASN:N	7:U:228:ASN:HD22	2.16	0.42
2:B:225:LYS:O	2:B:226:PRO:C	2.59	0.42
5:E:137:LEU:CD2	5:E:150:GLU:HG3	2.50	0.42
6:F:53:LEU:HD13	6:F:20(C):LYS:HD2	2.02	0.42
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.33	0.42
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.83	0.42
9:I:12(A):LYS:HE3	9:I:12(A):LYS:HB2	1.88	0.42
13:M:112:TYR:O	13:M:119:THR:HA	2.20	0.42
13:M:130:GLY:O	13:M:134:ALA:HB3	2.19	0.42
14:N:105:ASP:HB3	14:N:106:ASN:HB2	2.01	0.42
1:O:49:ALA:HB2	1:O:212:LEU:HG	2.00	0.42
2:P:44:ASP:OD2	2:P:44:ASP:N	2.52	0.42
12:Z:40:ASN:ND2	16:Z:799:HOH:O	2.49	0.42
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.55	0.42
13:1:1:THR:OG1	13:1:2:SER:N	2.52	0.42
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.33	0.42
14:2:105:ASP:HB3	14:2:106:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.54	0.42
4:D:150:HIS:O	4:D:157:PHE:HA	2.19	0.42
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.32	0.42
2:P:27:ALA:O	2:P:30:SER:HB3	2.20	0.42
2:P:39:GLY:C	2:P:148:LEU:HD21	2.44	0.42
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.19	0.42
3:C:201:VAL:HG21	3:C:210:ILE:HD11	2.01	0.42
5:E:76:LEU:HD23	5:E:76:LEU:O	2.20	0.42
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.35	0.42
8:H:163:ILE:HG23	8:H:170:GLY:HA2	2.01	0.42
11:K:196:PHE:HB3	16:K:214:HOH:O	2.18	0.42
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.02	0.42
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	2.02	0.42
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.20	0.42
3:Q:35:THR:HB	3:Q:51:GLU:CG	2.49	0.42
7:U:121:GLN:NE2	7:U:122:ILE:HD13	2.35	0.42
8:V:34:LEU:HB2	16:V:578:HOH:O	2.19	0.42
10:X:52:THR:CG2	10:X:53:VAL:H	2.33	0.42
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.76	0.42
13:1:49:ILE:O	13:1:53:GLN:HG3	2.20	0.42
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.55	0.42
5:E:179:THR:O	5:E:180:LEU:C	2.63	0.42
7:G:121:GLN:NE2	7:G:122:ILE:HD13	2.35	0.42
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	2.02	0.42
14:N:20:THR:HG22	15:N:224:GPT:C10	2.49	0.42
1:O:179:ARG:HB3	1:O:192:ILE:HD13	2.02	0.42
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.54	0.42
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.35	0.42
11:Y:114:ASP:OD1	11:Y:114:ASP:C	2.63	0.42
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.56	0.41
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.55	0.41
5:E:18(C):PHE:CA	5:E:18(F):ILE:HG13	2.43	0.41
6:F:43:ASN:HD22	6:F:44:ASP:N	2.18	0.41
13:M:19:LEU:HD12	13:M:28:PHE:O	2.21	0.41
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.55	0.41
2:P:122:GLY:C	2:P:124:THR:N	2.77	0.41
7:U:31:THR:HG21	7:U:135:ILE:HG13	2.02	0.41
7:U:18(H):GLU:N	7:U:18(H):GLU:CD	2.78	0.41
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	2.02	0.41
11:Y:32:LYS:O	11:Y:45:MET:CE	2.68	0.41
13:1:3:VAL:O	13:1:126:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB1	1:A:155:GLY:O	2.20	0.41
2:B:191:GLU:O	2:B:195:LYS:HG2	2.20	0.41
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.03	0.41
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.54	0.41
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.50	0.41
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.35	0.41
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.35	0.41
5:S:160:LEU:HD23	6:T:59:LEU:HA	2.01	0.41
7:U:152:ASP:HB2	7:U:153:PRO:HD2	2.01	0.41
7:U:18(H):GLU:CD	7:U:18(H):GLU:H	2.28	0.41
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.34	0.41
16:A:245:HOH:O	2:B:10:SER:HB2	2.20	0.41
3:C:125:GLN:HG3	3:C:125:GLN:O	2.20	0.41
4:D:32:LYS:O	4:D:167:SER:HA	2.21	0.41
5:E:185:ASN:OD1	5:E:188:GLU:HG2	2.21	0.41
6:F:35:THR:CG2	6:F:36:THR:N	2.81	0.41
10:J:167:PRO:C	10:X:168:MET:HE2	2.45	0.41
11:K:12:ILE:HB	11:K:178:VAL:HB	2.03	0.41
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.18	0.41
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	2.01	0.41
6:T:18:ASP:OD2	6:T:18:ASP:N	2.40	0.41
7:U:172:ILE:HD12	7:U:197:MET:CE	2.49	0.41
9:W:6:MET:HE1	9:W:155:ILE:HA	2.02	0.41
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.20	0.41
10:J:35:ARG:NH2	16:J:875:HOH:O	2.52	0.41
10:J:190:PHE:C	10:J:192:ALA:H	2.28	0.41
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.55	0.41
4:R:177:LEU:HA	5:S:58:LEU:HD11	2.02	0.41
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.34	0.41
7:U:12:ILE:HG13	7:U:14:ILE:HD12	2.01	0.41
8:V:72:ARG:HG3	8:V:72:ARG:HH11	1.86	0.41
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.21	0.41
1:A:179:ARG:HB3	1:A:192:ILE:HD13	2.02	0.41
8:H:159:ILE:O	8:H:163:ILE:HD12	2.21	0.41
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.34	0.41
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.35	0.41
7:U:18(G):GLU:CG	7:U:188:LYS:HB2	2.46	0.41
2:B:136:PHE:O	2:B:150:THR:HA	2.21	0.41
2:B:186:VAL:O	2:B:190:ILE:HG13	2.21	0.41
7:G:18(H):GLU:CD	7:G:18(H):GLU:N	2.79	0.41
3:Q:76:LEU:C	3:Q:76:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:97:ASN:CG	12:Z:61:ASN:HD21	2.28	0.41
5:S:216:GLY:O	5:S:217:LYS:C	2.64	0.41
7:U:225:SER:OG	7:U:228:ASN:ND2	2.54	0.41
9:W:45:ILE:HB	9:W:52:VAL:HG13	2.02	0.41
12:Z:58:ARG:NH2	16:Z:1275:HOH:O	2.52	0.41
2:B:122:GLY:C	2:B:124:THR:N	2.79	0.41
2:B:213:ALA:HA	2:B:222:LYS:O	2.20	0.41
3:C:76:LEU:HD23	3:C:76:LEU:C	2.45	0.41
4:R:152:GLU:C	4:R:154:SER:H	2.28	0.41
4:R:175:GLU:OE1	4:R:175:GLU:HA	2.20	0.41
5:S:5:ARG:HG3	5:S:22:PHE:CE1	2.56	0.41
5:S:18(C):PHE:CA	5:S:18(F):ILE:HG13	2.42	0.41
6:T:53:LEU:HD13	6:T:20(C):LYS:HD2	2.02	0.41
10:X:190:PHE:C	10:X:192:ALA:H	2.27	0.41
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.33	0.41
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.88	0.41
13:1:83:LEU:O	13:1:87:MET:HG2	2.20	0.41
14:2:15:GLY:HA2	14:2:174:ARG:O	2.21	0.41
1:A:60:MET:HE3	1:A:63:THR:CG2	2.49	0.41
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.36	0.41
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.16	0.41
2:B:121:GLN:NE2	2:B:121:GLN:C	2.79	0.41
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.56	0.41
4:D:177:LEU:HD13	5:E:58:LEU:HD11	2.03	0.41
5:E:216:GLY:O	5:E:217:LYS:C	2.64	0.41
7:G:69:CYS:HB3	16:G:840:HOH:O	2.19	0.41
10:J:167:PRO:HB2	10:X:168:MET:HE1	2.03	0.41
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.19	0.41
13:1:191:GLN:HE21	13:1:191:GLN:HB3	1.60	0.41
14:2:20:THR:HG22	15:2:224:GPT:C10	2.51	0.41
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	2.02	0.41
1:A:47:VAL:HG23	1:A:212:LEU:HD21	2.02	0.41
1:A:67:VAL:HG11	1:A:213:ALA:HB3	2.02	0.41
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.83	0.41
6:F:49:ALA:HA	6:F:211:GLU:O	2.21	0.41
10:J:52:THR:CG2	10:J:53:VAL:H	2.33	0.41
10:J:168:MET:HE2	10:X:167:PRO:C	2.46	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.03	0.41
2:P:112:LEU:C	2:P:112:LEU:CD2	2.93	0.41
3:Q:136:THR:O	3:Q:150:GLN:HA	2.21	0.41
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:4:PHE:O	5:S:5:ARG:C	2.63	0.41
5:S:90:ASN:O	5:S:94:GLN:HG3	2.20	0.41
5:S:136:LEU:HB2	5:S:151:PHE:HB3	2.02	0.41
5:S:185:ASN:OD1	5:S:188:GLU:HG2	2.21	0.41
7:U:14:ILE:HD13	7:U:14:ILE:N	2.35	0.41
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.21	0.41
11:Y:10(A):ARG:HD3	11:Y:180:GLU:OE1	2.21	0.41
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.56	0.41
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.36	0.41
12:Z:33:LYS:HB3	12:Z:33:LYS:HE2	1.87	0.41
13:1:46:SER:OG	13:1:98:ALA:HB3	2.21	0.41
5:E:4:PHE:O	5:E:5:ARG:C	2.64	0.41
7:G:78:VAL:HG11	7:G:85:ALA:HB2	2.03	0.41
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.50	0.41
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.56	0.41
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.21	0.41
2:B:101:LYS:HZ2	10:J:85:GLN:HE21	1.68	0.40
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.37	0.40
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.82	0.40
11:K:70:GLU:O	11:K:71:LYS:C	2.64	0.40
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.40
9:W:130:ALA:HB2	9:W:166:ASP:CB	2.51	0.40
13:1:146:THR:HA	16:1:323:HOH:O	2.22	0.40
1:A:27:ALA:O	1:A:31:VAL:HG23	2.21	0.40
1:A:130:ARG:HG2	7:G:125:GLN:HG3	2.03	0.40
2:B:67:LEU:HD22	2:B:211:GLU:HB3	2.03	0.40
4:D:215:ILE:HA	4:D:220:GLY:O	2.20	0.40
5:E:97:ASN:CG	12:L:61:ASN:HD21	2.29	0.40
5:E:104:ASN:HB2	13:M:81:GLU:HG2	2.03	0.40
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.35	0.40
7:G:55:PRO:HG2	7:G:56:ASP:H	1.86	0.40
3:Q:212:ILE:HD13	3:Q:212:ILE:N	2.37	0.40
4:R:215:ILE:HA	4:R:220:GLY:O	2.22	0.40
10:X:4:LEU:HD23	10:X:126:ALA:HB2	2.02	0.40
10:X:7:ARG:NE	16:X:194:HOH:O	2.40	0.40
2:B:53:LYS:HG2	2:B:54:VAL:HG23	2.03	0.40
6:F:12:ASN:OD1	6:F:12:ASN:O	2.39	0.40
7:G:197:MET:HE2	7:G:201:LEU:HG	2.02	0.40
12:L:114:ASP:CB	12:L:118:SER:HB3	2.46	0.40
14:N:147:SER:OG	14:N:150:GLU:HG3	2.22	0.40
3:Q:77:SER:OG	3:Q:137:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.52	0.40
7:U:72:ARG:HH11	7:U:72:ARG:CB	2.34	0.40
7:U:107:MET:HA	7:U:108:PRO:HD3	1.90	0.40
9:W:80:THR:HG23	9:W:113:PHE:CZ	2.56	0.40
3:C:169:SER:HA	3:C:172:VAL:HG13	2.02	0.40
4:D:152:GLU:C	4:D:154:SER:H	2.29	0.40
8:H:22:GLN:CG	8:H:27:ALA:HB2	2.44	0.40
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	2.02	0.40
13:M:4:ILE:CD1	13:M:159:MET:SD	3.09	0.40
14:N:48:SER:O	14:N:52:THR:HG23	2.21	0.40
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.19	0.40
1:O:124:THR:HG22	2:P:130:ARG:NH2	2.20	0.40
2:P:53:LYS:HG2	2:P:54:VAL:HG23	2.03	0.40
6:T:12:ASN:OD1	6:T:12:ASN:O	2.39	0.40
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.34	0.40
14:2:107:LYS:CG	14:2:108:GLY:H	2.17	0.40
2:B:81:LEU:HD23	2:B:133:GLY:HA3	2.04	0.40
3:C:57:LYS:HD2	3:C:57:LYS:C	2.47	0.40
3:C:169:SER:HA	3:C:172:VAL:CG1	2.52	0.40
5:E:18(C):PHE:CD1	5:E:18(C):PHE:C	3.00	0.40
7:G:18(H):GLU:CD	7:G:18(H):GLU:H	2.29	0.40
9:I:80:THR:HG23	9:I:113:PHE:CZ	2.57	0.40
11:K:10(A):ARG:HD3	11:K:180:GLU:OE1	2.22	0.40
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.57	0.40
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.37	0.40
14:N:19:ARG:NE	14:N:26:ILE:HD13	2.36	0.40
5:S:214:ILE:HG12	5:S:215:VAL:N	2.36	0.40
7:U:39:ALA:CB	7:U:48:VAL:HG12	2.51	0.40
7:U:55:PRO:HG2	7:U:56:ASP:H	1.87	0.40
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.56	0.40
11:Y:100:MET:C	11:Y:101:ILE:HD13	2.47	0.40
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.56	0.40
12:Z:14(E):GLU:OE2	12:Z:14(P):PRO:HD2	2.22	0.40
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.57	0.40
13:1:133:MET:C	13:1:136:PRO:HD2	2.47	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%)	234 (94%)	11 (4%)	3 (1%)	10	15
1	O	248/250 (99%)	235 (95%)	10 (4%)	3 (1%)	10	15
2	B	242/244 (99%)	219 (90%)	19 (8%)	4 (2%)	7	9
2	P	242/244 (99%)	219 (90%)	19 (8%)	4 (2%)	7	9
3	C	239/241 (99%)	226 (95%)	8 (3%)	5 (2%)	5	6
3	Q	239/241 (99%)	225 (94%)	9 (4%)	5 (2%)	5	6
4	D	240/242 (99%)	232 (97%)	4 (2%)	4 (2%)	7	9
4	R	240/242 (99%)	232 (97%)	4 (2%)	4 (2%)	7	9
5	E	231/233 (99%)	209 (90%)	16 (7%)	6 (3%)	4	4
5	S	231/233 (99%)	209 (90%)	16 (7%)	6 (3%)	4	4
6	F	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	30	42
6	T	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	16	23
7	G	241/243 (99%)	230 (95%)	11 (5%)	0	100	100
7	U	241/243 (99%)	231 (96%)	10 (4%)	0	100	100
8	H	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
8	V	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
9	I	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
9	W	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
10	J	196/198 (99%)	189 (96%)	5 (3%)	2 (1%)	12	18
10	X	196/198 (99%)	190 (97%)	4 (2%)	2 (1%)	12	18
11	K	210/212 (99%)	208 (99%)	2 (1%)	0	100	100
11	Y	210/212 (99%)	208 (99%)	2 (1%)	0	100	100
12	L	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
12	Z	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
13	1	231/233 (99%)	219 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	218 (94%)	13 (6%)	0	100	100
14	2	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6312/6368 (99%)	5999 (95%)	262 (4%)	51 (1%)	16	23

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	LEU
3	C	203	THR
4	D	12(G)	GLU
3	Q	58	LEU
4	R	12(G)	GLU
5	S	217	LYS
1	A	5	THR
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
5	E	202	ARG
5	E	217	LYS
10	J	192	ALA
1	O	5	THR
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	203	THR
5	S	202	ARG
10	X	192	ALA
1	A	167	LYS
2	B	20(A)	SER
3	C	183	PRO
4	D	12(F)	GLY
5	E	5	ARG
5	E	180	LEU
1	O	63	THR
1	O	167	LYS
2	P	20(A)	SER
3	Q	183	PRO
4	R	12(F)	GLY
5	S	5	ARG
5	S	180	LEU

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Mol	Chain	Res	Type
1	A	63	THR
3	C	242	GLU
3	Q	242	GLU
6	T	143	LYS
4	D	12(E)	SER
5	E	203	ASP
5	E	231	LYS
4	R	12(E)	SER
5	S	203	ASP
6	T	205	ASN
3	C	202	GLN
6	F	205	ASN
3	Q	202	GLN
5	S	231	LYS
4	D	12(C)	GLY
4	R	12(C)	GLY
10	X	8	VAL
10	J	8	VAL

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	38
1	O	209/209 (100%)	199 (95%)	10 (5%)	23	38
2	B	203/203 (100%)	186 (92%)	17 (8%)	10	16
2	P	203/203 (100%)	185 (91%)	18 (9%)	9	14
3	C	213/213 (100%)	199 (93%)	14 (7%)	15	25
3	Q	213/213 (100%)	200 (94%)	13 (6%)	17	28
4	D	198/198 (100%)	186 (94%)	12 (6%)	17	28
4	R	198/198 (100%)	186 (94%)	12 (6%)	17	28
5	E	192/192 (100%)	178 (93%)	14 (7%)	13	21
5	S	192/192 (100%)	179 (93%)	13 (7%)	14	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	201/201 (100%)	187 (93%)	14 (7%)	14	22
6	T	201/201 (100%)	186 (92%)	15 (8%)	12	20
7	G	207/207 (100%)	195 (94%)	12 (6%)	18	30
7	U	207/207 (100%)	195 (94%)	12 (6%)	18	30
8	H	181/181 (100%)	168 (93%)	13 (7%)	13	21
8	V	181/181 (100%)	170 (94%)	11 (6%)	17	28
9	I	172/172 (100%)	165 (96%)	7 (4%)	27	44
9	W	172/172 (100%)	165 (96%)	7 (4%)	27	44
10	J	175/175 (100%)	167 (95%)	8 (5%)	24	39
10	X	175/175 (100%)	167 (95%)	8 (5%)	24	39
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	34
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	39
12	L	185/185 (100%)	164 (89%)	21 (11%)	5	8
12	Z	185/185 (100%)	163 (88%)	22 (12%)	5	7
13	1	199/199 (100%)	186 (94%)	13 (6%)	15	25
13	M	199/199 (100%)	185 (93%)	14 (7%)	14	22
14	2	162/162 (100%)	158 (98%)	4 (2%)	42	62
14	N	162/162 (100%)	158 (98%)	4 (2%)	42	62
All	All	5332/5332 (100%)	4997 (94%)	335 (6%)	16	27

All (335) 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	119	ILE
1	A	158	PHE
1	A	179	ARG
1	A	192	ILE
1	A	214	ILE
1	A	229	ILE
2	B	14	ILE
2	B	31	ILE
2	B	41	MET

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Mol	Chain	Res	Type
2	B	58	LEU
2	B	67	LEU
2	B	71	ASN
2	B	81	LEU
2	B	91	THR
2	B	121	GLN
2	B	124	THR
2	B	14(A)	TYR
2	B	150	THR
2	B	163	ILE
2	B	192	LEU
2	B	223	ILE
2	B	224	PHE
2	B	238	ILE
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU
3	C	66	LYS
3	C	89	ILE
3	C	135	SER
3	C	14(A)	ARG
3	C	14(B)	ASP
3	C	150	GLN
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	210	ILE
3	C	212	ILE
4	D	28	LEU
4	D	48	LEU
4	D	52	LYS
4	D	76	CYS
4	D	107	ILE
4	D	110	GLU
4	D	126	ARG
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	28	LEU

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Mol	Chain	Res	Type
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	190	ILE
5	E	199	GLN
5	E	207	LEU
5	E	212	ILE
5	E	223	ILE
5	E	227	GLU
6	F	35	THR
6	F	43	ASN
6	F	54	ILE
6	F	56	SER
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	176	LEU
6	F	187	ARG
6	F	192	GLN
6	F	197	ILE
6	F	203	GLU
6	F	212	ILE
6	F	233	ILE
7	G	14	ILE
7	G	35	ILE
7	G	67	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	14(A)	GLU
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR

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Mol	Chain	Res	Type
8	H	63	ILE
8	H	68	LEU
8	H	95	ILE
8	H	121	VAL
8	H	144	GLN
8	H	163	ILE
8	H	180	ILE
8	H	197	ARG
8	H	221	ILE
9	I	-3	ILE
9	I	22	SER
9	I	29	ASN
9	I	104	ILE
9	I	125	ILE
9	I	160	LEU
9	I	192	ARG
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	63	ILE
10	J	70	GLU
10	J	121	GLU
10	J	168	MET
10	J	177	ILE
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	138	LEU
11	K	146	LEU
11	K	185	ILE
12	L	14	LEU
12	L	21	ILE
12	L	40	ASN
12	L	58	ARG
12	L	98	HIS
12	L	99	THR
12	L	134	ILE
12	L	14(A)	LYS
12	L	14(B)	ASN

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Mol	Chain	Res	Type
12	L	14(C)	GLN
12	L	14(D)	TYR
12	L	14(E)	GLU
12	L	14(F)	PRO
12	L	14(I)	THR
12	L	14(K)	LYS
12	L	14(M)	VAL
12	L	14(N)	LYS
12	L	14(O)	LYS
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS
13	M	4	ILE
13	M	13	ILE
13	M	40	ASN
13	M	62	LEU
13	M	79	ILE
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	148	VAL
13	M	149	GLN
13	M	155	ILE
13	M	191	GLN
13	M	203	ILE
13	M	204	LYS
14	N	26	ILE
14	N	89	GLU
14	N	119	VAL
14	N	149	GLU
1	O	32	LYS
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	119	ILE
1	O	158	PHE
1	O	179	ARG
1	O	192	ILE
1	O	214	ILE
1	O	229	ILE
2	P	14	ILE
2	P	31	ILE

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Mol	Chain	Res	Type
2	P	41	MET
2	P	58	LEU
2	P	67	LEU
2	P	71	ASN
2	P	81	LEU
2	P	91	THR
2	P	116	LEU
2	P	121	GLN
2	P	124	THR
2	P	14(A)	TYR
2	P	150	THR
2	P	163	ILE
2	P	192	LEU
2	P	223	ILE
2	P	224	PHE
2	P	238	ILE
3	Q	10	ARG
3	Q	14	ILE
3	Q	25	GLU
3	Q	66	LYS
3	Q	89	ILE
3	Q	14(A)	ARG
3	Q	14(B)	ASP
3	Q	150	GLN
3	Q	163	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	210	ILE
3	Q	212	ILE
4	R	28	LEU
4	R	48	LEU
4	R	52	LYS
4	R	76	CYS
4	R	107	ILE
4	R	110	GLU
4	R	126	ARG
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	12	THR

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Mol	Chain	Res	Type
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	111	ARG
5	S	189	LEU
5	S	190	ILE
5	S	199	GLN
5	S	207	LEU
5	S	212	ILE
5	S	227	GLU
6	T	35	THR
6	T	43	ASN
6	T	54	ILE
6	T	56	SER
6	T	109	ILE
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	176	LEU
6	T	187	ARG
6	T	192	GLN
6	T	197	ILE
6	T	203	GLU
6	T	212	ILE
6	T	233	ILE
7	U	14	ILE
7	U	35	ILE
7	U	67	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	14(A)	GLU
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL

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Mol	Chain	Res	Type
8	V	56	THR
8	V	63	ILE
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	163	ILE
8	V	180	ILE
8	V	197	ARG
9	W	-3	ILE
9	W	22	SER
9	W	29	ASN
9	W	104	ILE
9	W	125	ILE
9	W	160	LEU
9	W	192	ARG
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	63	ILE
10	X	70	GLU
10	X	121	GLU
10	X	168	MET
10	X	177	ILE
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	138	LEU
11	Y	146	LEU
11	Y	185	ILE
12	Z	14	LEU
12	Z	21	ILE
12	Z	40	ASN
12	Z	58	ARG
12	Z	98	HIS
12	Z	99	THR
12	Z	134	ILE
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
13	1	4	ILE
13	1	13	ILE
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	148	VAL
13	1	149	GLN
13	1	155	ILE
13	1	191	GLN
13	1	203	ILE
13	1	204	LYS
14	2	26	ILE
14	2	89	GLU
14	2	119	VAL
14	2	149	GLU

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

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	150	GLN
2	B	23	GLN
2	B	71	ASN
2	B	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	147	GLN

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Mol	Chain	Res	Type
2	B	156	ASN
2	B	173	GLN
2	B	177	GLN
2	B	218	ASN
2	B	227	GLN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	168	ASN
3	C	179	ASN
3	C	209	ASN
3	C	243	GLN
4	D	23	GLN
4	D	99	HIS
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	94	GLN
5	E	95	GLN
5	E	104	ASN
5	E	121	GLN
5	E	125	GLN
5	E	156	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN

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Mol	Chain	Res	Type
6	F	237	GLN
6	F	241	ASN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	201	GLN
9	I	29	ASN
9	I	36	HIS
9	I	56	ASN
10	J	9	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	85	GLN
10	J	112	GLN
10	J	141	HIS
10	J	160	GLN
10	J	186	GLN
11	K	9	GLN
11	K	24	ASN
11	K	85	ASN
11	K	131	GLN
11	K	141	ASN
11	K	174	ASN
11	K	189	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	27	ASN

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Mol	Chain	Res	Type
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	70	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	98	HIS
12	L	1(I)	ASN
12	L	166	HIS
13	M	-7	GLN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	189	ASN
13	M	191	GLN
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	150	GLN
2	P	23	GLN
2	P	71	ASN
2	P	95	HIS
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	147	GLN
2	P	156	ASN
2	P	173	GLN
2	P	177	GLN
2	P	218	ASN
2	P	227	GLN
3	Q	23	GLN
3	Q	82	ASN
3	Q	120	GLN
3	Q	121	GLN

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Mol	Chain	Res	Type
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	168	ASN
3	Q	179	ASN
3	Q	209	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	94	GLN
5	S	95	GLN
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
6	T	237	GLN
6	T	241	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN

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Mol	Chain	Res	Type
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	66	HIS
8	V	114	HIS
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	201	GLN
9	W	29	ASN
9	W	56	ASN
9	W	81	GLN
10	X	9	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	85	GLN
10	X	112	GLN
10	X	141	HIS
10	X	160	GLN
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	141	ASN
11	Y	174	ASN
11	Y	189	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	27	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	82	ASN

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Mol	Chain	Res	Type
12	Z	84	GLN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	189	ASN
13	1	191	GLN
14	2	69	GLN
14	2	141	ASN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA [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](#)

6 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	GPT	V	224	8	17,22,22	1.64	4 (23%)	22,33,33	1.60	3 (13%)
15	GPT	2	224	14	17,22,22	1.73	3 (17%)	22,33,33	1.68	3 (13%)
15	GPT	K	224	11	17,22,22	1.70	4 (23%)	22,33,33	1.59	4 (18%)
15	GPT	N	224	14	17,22,22	2.15	4 (23%)	22,33,33	1.71	3 (13%)
15	GPT	Y	224	11	17,22,22	2.01	4 (23%)	22,33,33	1.61	7 (31%)
15	GPT	H	224	8	17,22,22	2.19	5 (29%)	22,33,33	1.69	3 (13%)

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	GPT	V	224	8	-	1/7/48/48	0/2/2/2
15	GPT	2	224	14	-	0/7/48/48	0/2/2/2
15	GPT	K	224	11	-	0/7/48/48	0/2/2/2
15	GPT	N	224	14	-	0/7/48/48	0/2/2/2
15	GPT	Y	224	11	-	1/7/48/48	0/2/2/2
15	GPT	H	224	8	-	1/7/48/48	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	224	GPT	C6-C4	4.84	1.58	1.52
15	N	224	GPT	C6-C4	4.80	1.58	1.52
15	H	224	GPT	C6-C4	4.76	1.58	1.52
15	H	224	GPT	C14-C9	4.44	1.62	1.54
15	N	224	GPT	C14-C9	4.22	1.62	1.54
15	N	224	GPT	C9-C8	3.97	1.60	1.54
15	H	224	GPT	C9-C8	3.96	1.60	1.54
15	Y	224	GPT	C14-C9	3.84	1.61	1.54
15	K	224	GPT	C6-C4	3.57	1.56	1.52
15	2	224	GPT	C9-C8	3.53	1.60	1.54
15	Y	224	GPT	C9-C8	3.25	1.59	1.54
15	2	224	GPT	C14-C9	3.17	1.60	1.54
15	2	224	GPT	C6-C4	3.13	1.56	1.52
15	V	224	GPT	C9-C8	2.94	1.59	1.54
15	V	224	GPT	C6-C4	2.86	1.56	1.52
15	K	224	GPT	C14-C9	2.83	1.59	1.54
15	V	224	GPT	C14-C9	2.75	1.59	1.54
15	K	224	GPT	C9-C10	2.70	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	224	GPT	C9-C10	2.65	1.54	1.50
15	K	224	GPT	C9-C8	2.39	1.58	1.54
15	N	224	GPT	C2-C3	2.21	1.59	1.54
15	Y	224	GPT	C9-C10	2.16	1.54	1.50
15	H	224	GPT	C9-C10	2.16	1.54	1.50
15	H	224	GPT	C2-C3	2.14	1.59	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	224	GPT	C4-C3-C19	-4.72	100.23	104.23
15	N	224	GPT	C4-C3-C19	-4.62	100.32	104.23
15	H	224	GPT	C4-C3-C19	-4.33	100.56	104.23
15	V	224	GPT	C7-C8-C9	4.02	119.13	114.09
15	V	224	GPT	C4-C3-C19	-3.96	100.88	104.23
15	K	224	GPT	C4-C3-C19	-3.50	101.26	104.23
15	2	224	GPT	C7-C8-C9	3.46	118.44	114.09
15	Y	224	GPT	C4-C3-C19	-3.41	101.34	104.23
15	H	224	GPT	C7-C8-C9	3.39	118.34	114.09
15	K	224	GPT	C7-C8-C9	3.31	118.24	114.09
15	N	224	GPT	C7-C8-C9	3.18	118.08	114.09
15	H	224	GPT	C1-C2-C3	2.99	118.04	112.37
15	Y	224	GPT	C7-C8-C9	2.78	117.57	114.09
15	V	224	GPT	C1-C2-C3	2.56	117.23	112.37
15	K	224	GPT	C7-N18-C19	2.54	118.03	115.42
15	Y	224	GPT	C7-N18-C19	2.44	117.93	115.42
15	N	224	GPT	O15-C8-C9	-2.22	104.98	109.98
15	Y	224	GPT	C2-C3-C4	2.11	118.45	115.45
15	Y	224	GPT	C1-C2-C3	2.10	116.37	112.37
15	Y	224	GPT	C7-C4-C3	2.10	107.44	104.13
15	K	224	GPT	C2-C3-C4	2.08	118.42	115.45
15	2	224	GPT	C7-N18-C19	2.02	117.50	115.42
15	Y	224	GPT	O15-C8-C9	-2.01	105.44	109.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

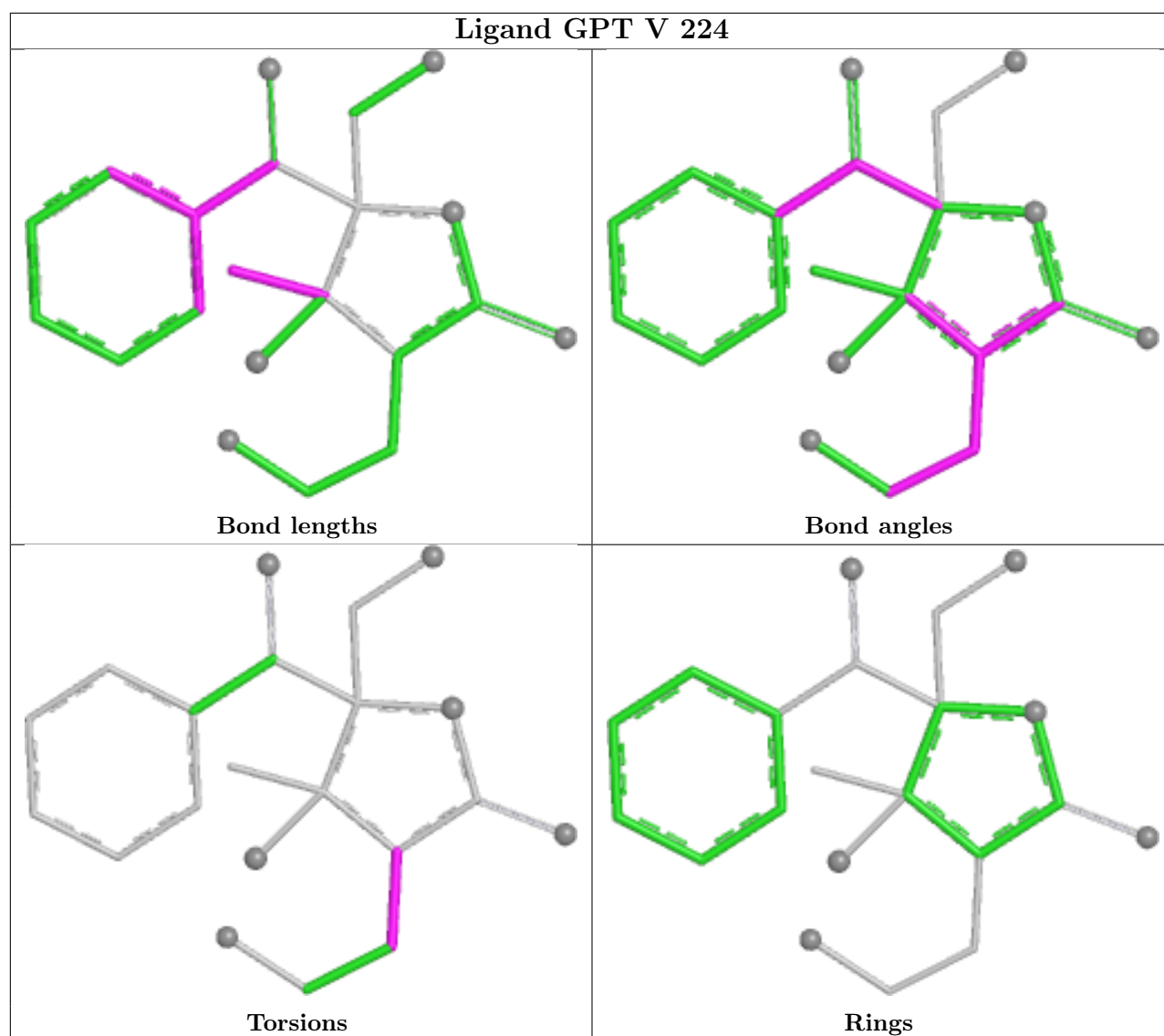
Mol	Chain	Res	Type	Atoms
15	H	224	GPT	C1-C2-C3-C19
15	V	224	GPT	C1-C2-C3-C19
15	Y	224	GPT	C1-C2-C3-C19

There are no ring outliers.

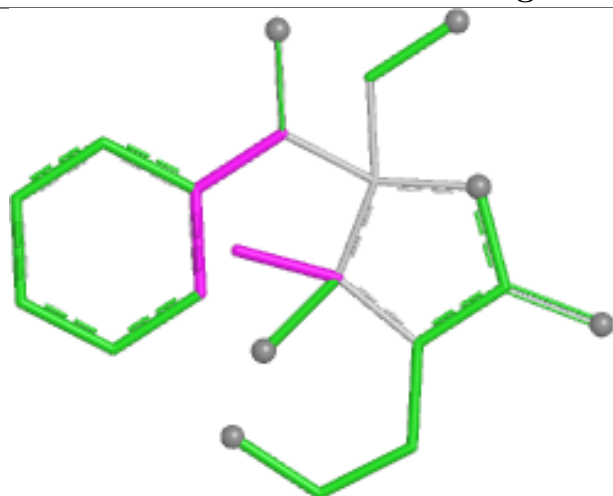
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	V	224	GPT	1	0
15	2	224	GPT	2	0
15	K	224	GPT	2	0
15	N	224	GPT	2	0
15	Y	224	GPT	2	0
15	H	224	GPT	1	0

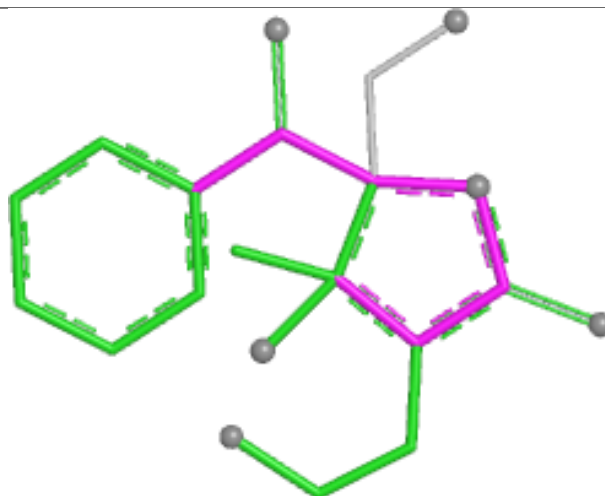
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



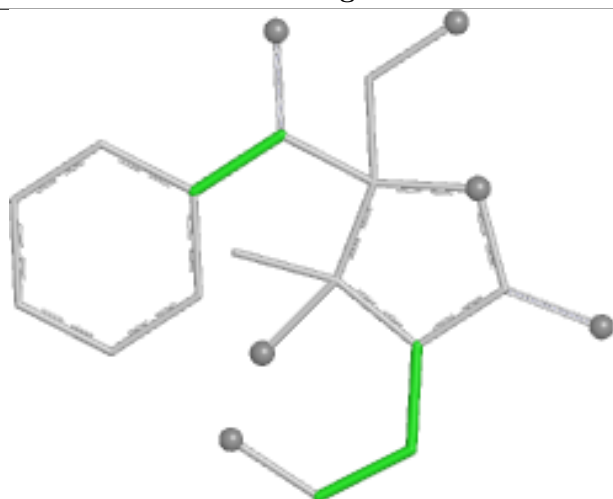
Ligand GPT 2 224



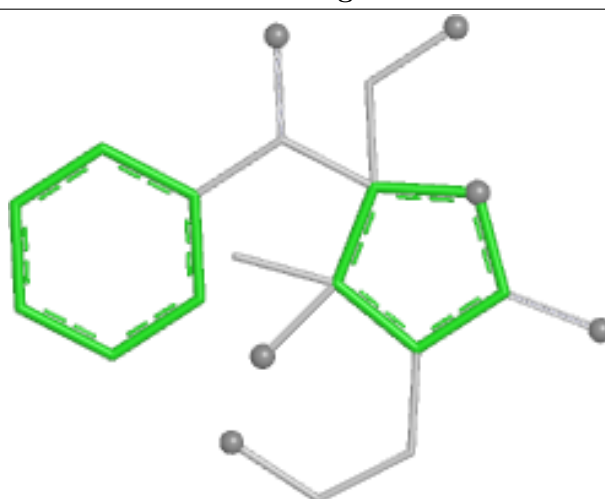
Bond lengths



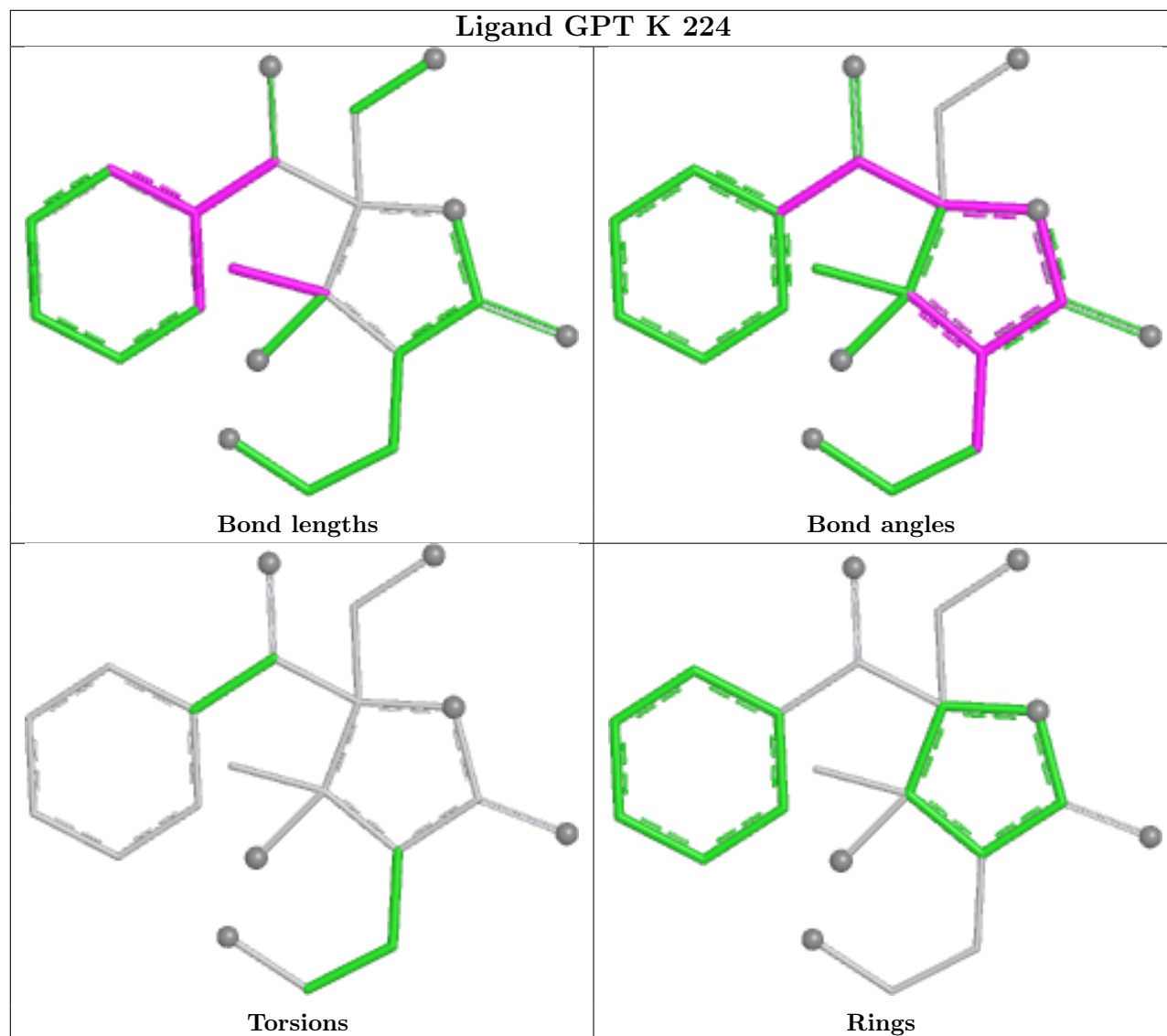
Bond angles

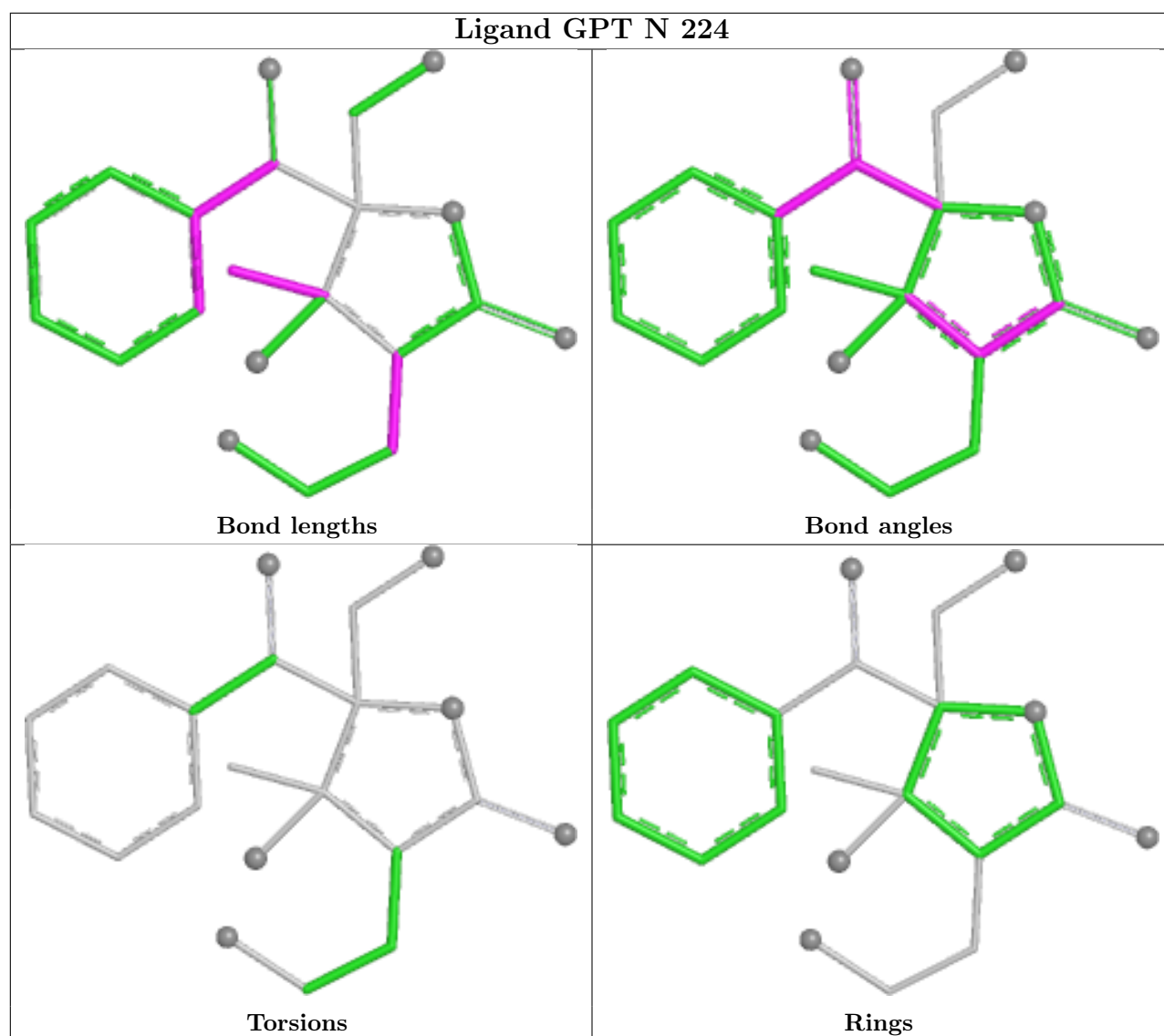


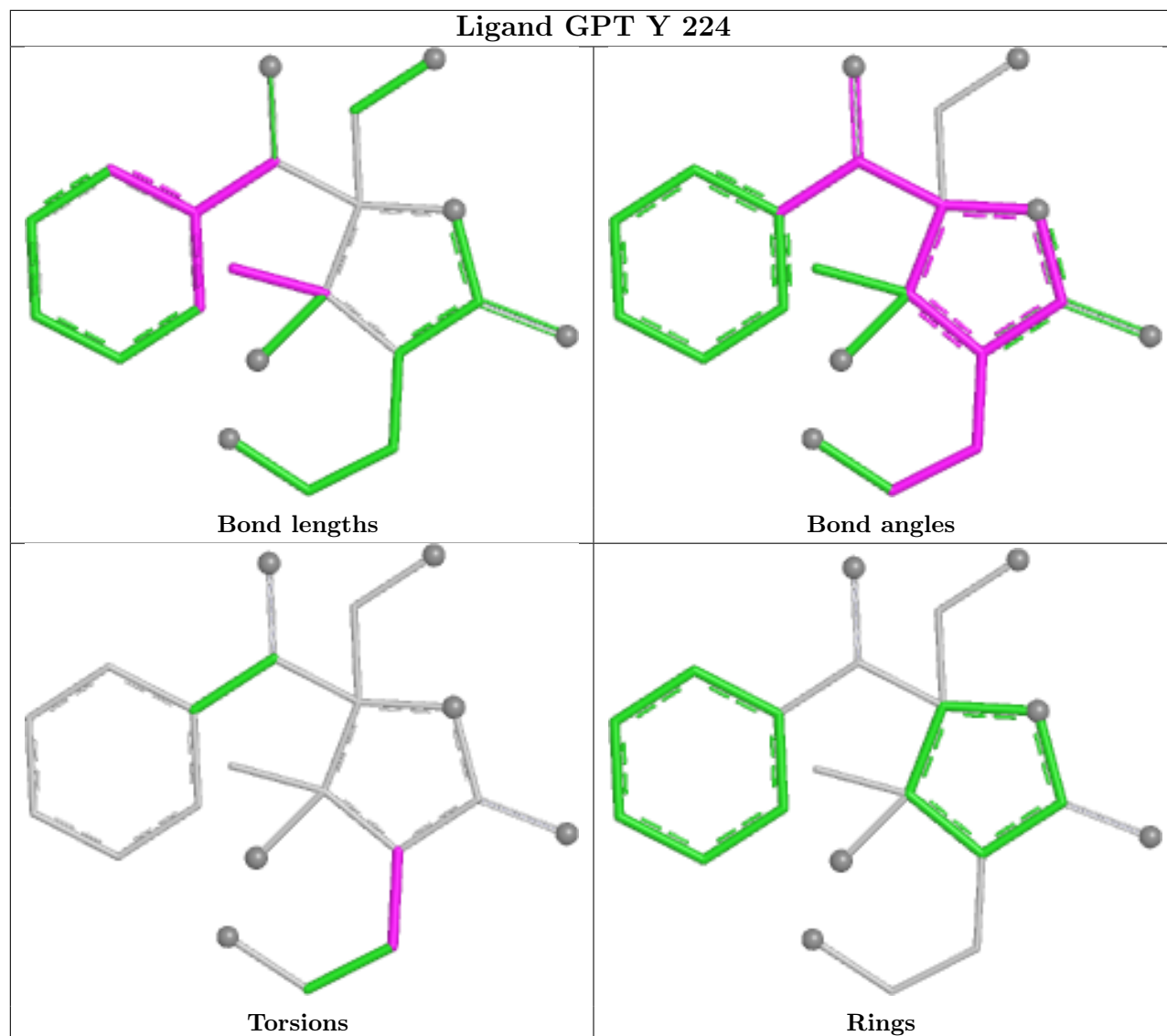
Torsions

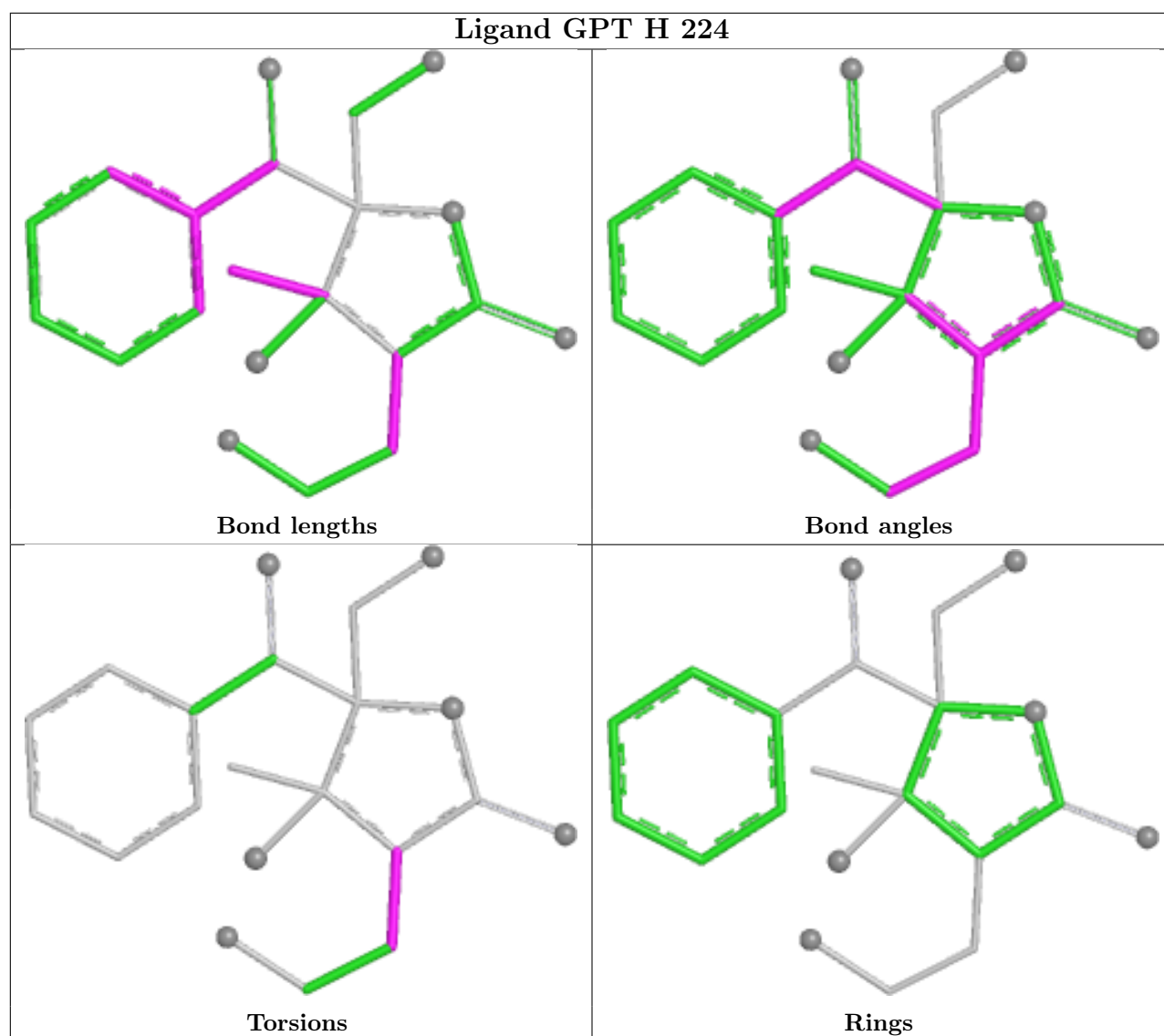


Rings









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%)	-0.11	4 (1%) 70 67	32, 43, 73, 101	0
1	O	250/250 (100%)	0.02	7 (2%) 55 51	34, 48, 76, 101	0
2	B	244/244 (100%)	0.20	14 (5%) 29 25	32, 49, 85, 113	0
2	P	244/244 (100%)	0.26	13 (5%) 32 28	30, 49, 86, 113	0
3	C	241/241 (100%)	0.24	18 (7%) 20 17	30, 50, 104, 117	0
3	Q	241/241 (100%)	0.47	22 (9%) 15 12	36, 56, 106, 117	0
4	D	242/242 (100%)	0.24	10 (4%) 41 37	33, 52, 85, 116	0
4	R	242/242 (100%)	0.33	12 (4%) 34 30	36, 56, 86, 117	0
5	E	233/233 (100%)	0.32	13 (5%) 30 26	39, 55, 83, 106	0
5	S	233/233 (100%)	0.75	21 (9%) 15 12	39, 59, 84, 104	0
6	F	244/244 (100%)	0.15	6 (2%) 58 55	34, 50, 85, 102	0
6	T	244/244 (100%)	0.42	13 (5%) 32 28	32, 52, 87, 103	0
7	G	243/243 (100%)	-0.06	6 (2%) 58 55	31, 44, 72, 108	0
7	U	243/243 (100%)	0.08	6 (2%) 58 55	31, 47, 73, 108	0
8	H	222/222 (100%)	-0.23	3 (1%) 73 70	26, 40, 61, 91	0
8	V	222/222 (100%)	-0.22	3 (1%) 73 70	26, 43, 61, 92	0
9	I	204/204 (100%)	-0.41	2 (0%) 79 77	27, 40, 56, 73	0
9	W	204/204 (100%)	-0.43	1 (0%) 87 86	29, 39, 58, 75	0
10	J	198/198 (100%)	-0.20	5 (2%) 58 55	28, 42, 59, 113	0
10	X	198/198 (100%)	-0.19	6 (3%) 52 49	29, 42, 60, 115	0
11	K	212/212 (100%)	-0.35	1 (0%) 87 86	24, 38, 57, 64	0
11	Y	212/212 (100%)	-0.21	3 (1%) 73 70	28, 43, 60, 69	0
12	L	222/222 (100%)	-0.26	3 (1%) 73 70	26, 41, 63, 82	0
12	Z	222/222 (100%)	-0.20	2 (0%) 81 79	31, 43, 65, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.23	1 (0%) 88 87	28, 42, 57, 64	0
13	M	233/233 (100%)	-0.19	2 (0%) 81 79	29, 43, 58, 65	0
14	2	196/196 (100%)	-0.25	5 (2%) 57 54	27, 40, 60, 75	0
14	N	196/196 (100%)	-0.32	0 100 100	29, 39, 59, 74	0
All	All	6368/6368 (100%)	0.00	202 (3%) 50 47	24, 46, 78, 117	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(D)	ALA	7.3
10	J	192	ALA	7.2
4	D	12(C)	GLY	7.2
7	U	240	ASP	7.0
2	P	217	ALA	6.9
4	R	12(D)	ALA	6.3
2	B	217	ALA	6.2
2	B	21(B)	GLY	6.1
3	C	55	THR	5.8
4	D	12(E)	SER	5.8
5	S	4	PHE	5.7
3	C	56	LEU	5.6
4	D	126	ARG	5.5
4	R	12(C)	GLY	5.5
4	R	12(E)	SER	4.9
2	P	21(B)	GLY	4.8
4	D	127	LEU	4.8
3	Q	56	LEU	4.8
5	E	4	PHE	4.6
2	B	239	THR	4.6
3	C	54	SER	4.5
7	G	6	ALA	4.4
4	R	12(F)	GLY	4.4
4	R	127	LEU	4.3
10	X	192	ALA	4.3
10	X	193	GLN	4.3
12	Z	145	TYR	4.2
4	D	242	ALA	4.2
4	R	126	ARG	4.2
3	Q	58	LEU	4.0
7	G	236	ILE	3.8
2	P	54	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
10	J	191	GLN	3.8
5	S	2(E)	ASN	3.7
7	U	6	ALA	3.7
5	S	5	ARG	3.7
13	1	-8	THR	3.6
10	X	-1	MET	3.6
2	B	218	ASN	3.5
8	H	223	ASP	3.5
6	F	204	ASP	3.4
10	J	193	GLN	3.4
12	L	145	TYR	3.4
2	P	219	GLU	3.4
10	X	191	GLN	3.4
5	S	203	ASP	3.4
6	F	5	GLY	3.3
4	D	243	ALA	3.3
2	P	218	ASN	3.3
5	S	55	ALA	3.3
3	Q	240	LYS	3.3
5	E	203	ASP	3.2
2	B	21(D)	GLY	3.2
2	P	239	THR	3.2
3	C	203	THR	3.2
2	B	54	VAL	3.1
2	B	21(A)	LYS	3.1
3	C	242	GLU	3.1
2	P	21(D)	GLY	3.1
1	O	56	SER	3.1
8	V	223	ASP	3.1
7	U	239	GLN	3.0
13	M	-8	THR	3.0
1	O	4	MET	3.0
3	C	207	ALA	3.0
5	E	127	TYR	3.0
3	Q	241	GLN	3.0
7	G	7	GLY	3.0
3	Q	236	ILE	2.9
8	H	199	GLU	2.9
5	S	18(B)	THR	2.9
5	S	127	TYR	2.9
3	Q	55	THR	2.9
1	O	21(P)	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	241	GLN	2.9
3	C	208	LYS	2.9
1	A	235	ALA	2.9
5	S	230	ALA	2.9
2	P	21(C)	ASP	2.9
2	P	21(A)	LYS	2.8
9	I	-8	SER	2.8
2	P	61	GLN	2.8
5	E	33	GLN	2.8
9	W	-8	SER	2.8
5	E	5	ARG	2.8
6	T	18(B)	HIS	2.8
5	S	18(C)	PHE	2.8
3	C	59	GLN	2.7
3	Q	54	SER	2.7
6	T	20(C)	LYS	2.7
8	V	221	ILE	2.7
3	Q	201	VAL	2.7
1	O	235	ALA	2.7
6	T	240	ILE	2.6
6	T	203	GLU	2.6
7	G	237	ALA	2.6
5	S	56	ASP	2.6
2	P	202	THR	2.6
14	2	116	GLY	2.6
10	J	-1	MET	2.6
5	S	18(F)	ILE	2.6
2	B	219	GLU	2.6
6	T	205	ASN	2.6
14	2	18(I)	GLN	2.5
3	C	52	ARG	2.5
1	A	4	MET	2.5
14	2	105	ASP	2.5
3	Q	208	LYS	2.5
5	E	63	TYR	2.5
6	T	199	LEU	2.5
2	B	61	GLN	2.5
6	T	232	ALA	2.5
3	Q	203	THR	2.5
1	O	203	GLU	2.5
5	E	204	GLU	2.5
11	Y	211	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	21(C)	ASP	2.5
2	P	62	ASP	2.5
1	A	203	GLU	2.4
5	S	188	GLU	2.4
7	U	18(H)	GLU	2.4
3	C	240	LYS	2.4
4	R	9	ASP	2.4
5	E	56	ASP	2.4
6	T	43	ASN	2.4
13	M	61	ASP	2.4
2	B	220	TYR	2.4
4	R	158	TYR	2.4
5	S	201	LEU	2.4
5	S	54	ASN	2.4
3	Q	207	ALA	2.4
4	R	12(G)	GLU	2.4
8	H	221	ILE	2.4
10	J	190	PHE	2.4
11	K	208	ASN	2.4
3	Q	202	GLN	2.4
5	S	175	TYR	2.4
14	2	149	GLU	2.4
6	T	5	GLY	2.3
1	O	236	LEU	2.3
5	S	51	LEU	2.3
6	F	180	VAL	2.3
3	Q	210	ILE	2.3
5	E	58	LEU	2.3
12	L	14(W)	LYS	2.3
4	R	242	ALA	2.3
3	C	206	GLY	2.3
11	Y	145	ASP	2.3
5	E	2(E)	ASN	2.3
2	B	20(B)	ALA	2.2
2	P	220	TYR	2.3
6	T	198	TYR	2.3
5	S	60	SER	2.2
12	L	1(I)	ASN	2.2
3	C	243	GLN	2.2
7	U	7	GLY	2.2
2	B	63(A)	SER	2.2
5	E	6	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
5	S	192	ALA	2.2
1	O	5	THR	2.2
3	Q	238	GLN	2.2
3	Q	243	GLN	2.2
5	S	222	THR	2.2
2	B	238	ILE	2.2
5	S	233	ILE	2.2
3	Q	174	GLU	2.2
5	E	57	GLU	2.2
4	R	10	ARG	2.2
6	F	63	LYS	2.2
6	F	241	ASN	2.2
7	G	8	TYR	2.2
1	A	200	SER	2.2
3	C	239	GLU	2.1
4	D	35	SER	2.1
3	Q	57	LYS	2.1
14	2	107	LYS	2.1
6	T	164	ALA	2.1
3	C	33	ARG	2.1
3	C	211	GLU	2.1
3	Q	242	GLU	2.1
9	I	182	ASP	2.1
3	Q	233	VAL	2.1
6	T	170	GLN	2.1
11	Y	208	ASN	2.1
4	D	168	GLY	2.1
4	D	12(G)	GLU	2.1
7	U	236	ILE	2.1
8	V	199	GLU	2.1
5	E	2(C)	VAL	2.1
4	R	121	LEU	2.1
5	S	174	THR	2.1
6	F	240	ILE	2.1
3	C	232	TYR	2.1
10	X	189	ASP	2.1
6	T	215	CYS	2.1
3	Q	206	GLY	2.0
3	Q	225	SER	2.0
10	X	190	PHE	2.0
3	C	57	LYS	2.0
12	Z	1(I)	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
3	Q	185	THR	2.0
7	G	240	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

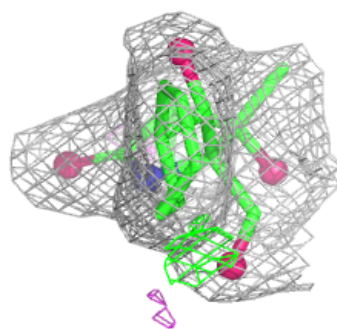
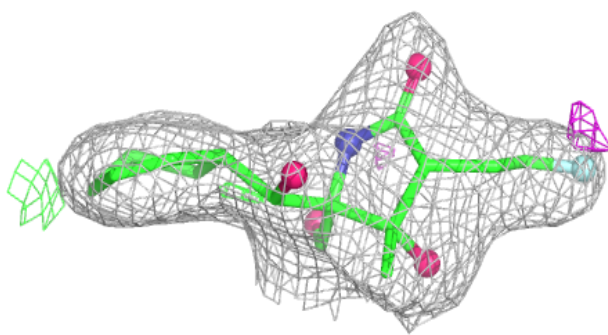
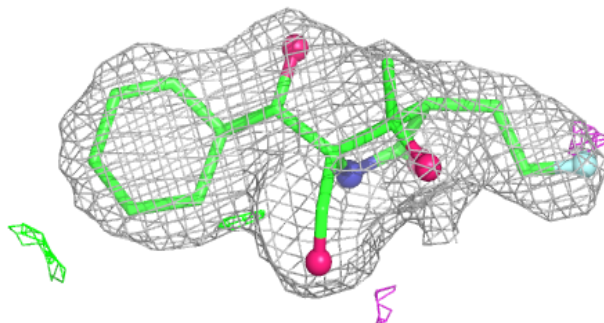
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	GPT	V	224	21/21	0.91	0.10	41,43,48,54	0
15	GPT	H	224	21/21	0.92	0.10	37,41,45,53	0
15	GPT	2	224	21/21	0.92	0.09	33,36,44,54	0
15	GPT	N	224	21/21	0.93	0.09	30,32,41,53	0
15	GPT	Y	224	21/21	0.94	0.08	32,36,39,49	0
15	GPT	K	224	21/21	0.94	0.09	29,32,36,44	0

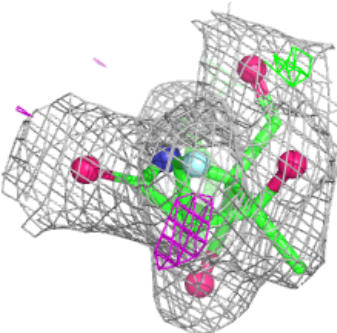
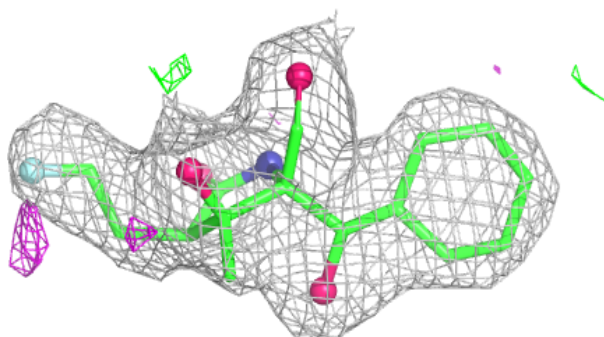
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GPT V 224:

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

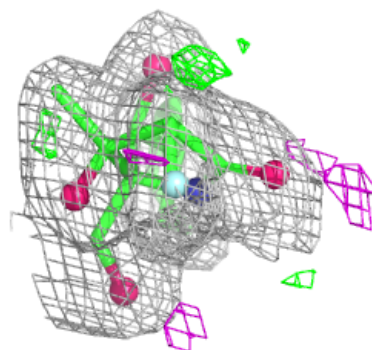
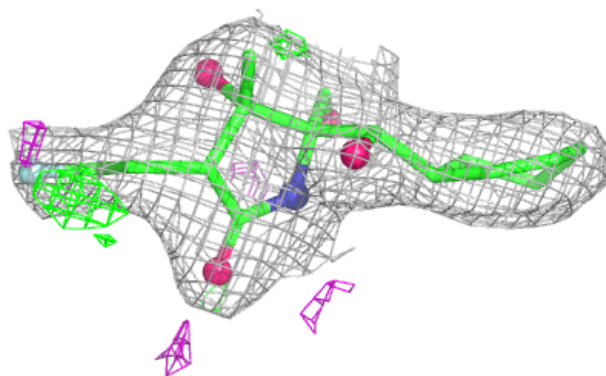
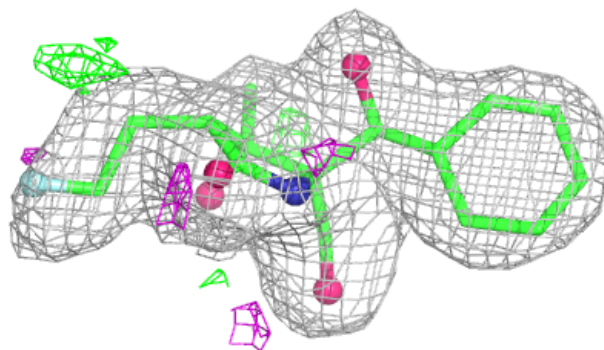
**Electron density around GPT H 224:**

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

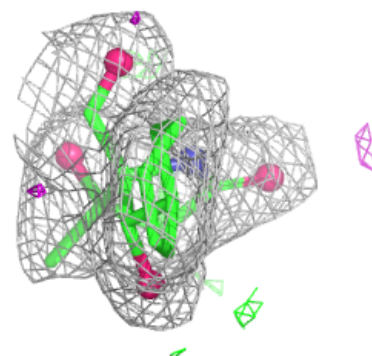
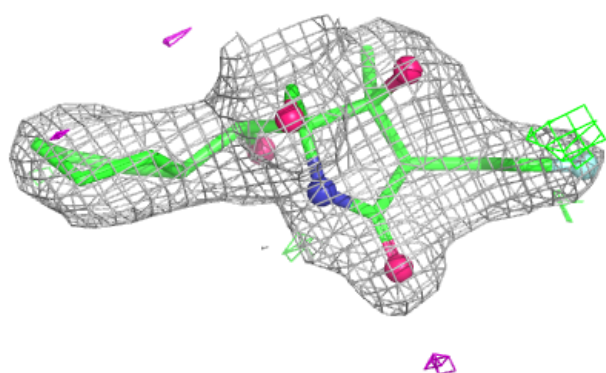
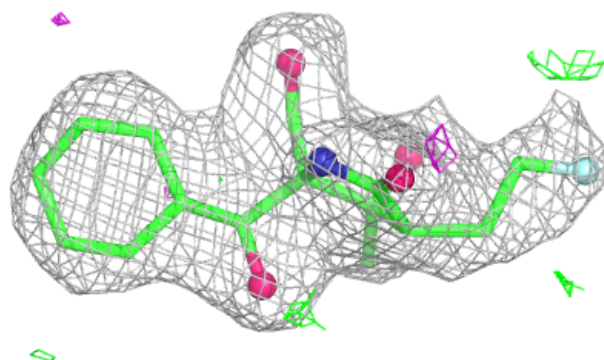


Electron density around GPT 2 224:

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

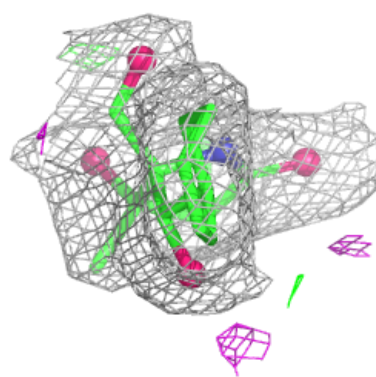
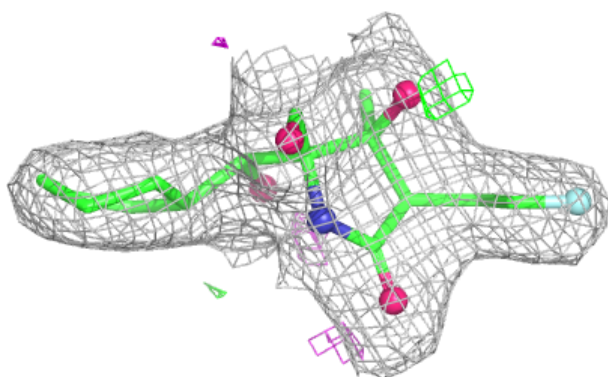
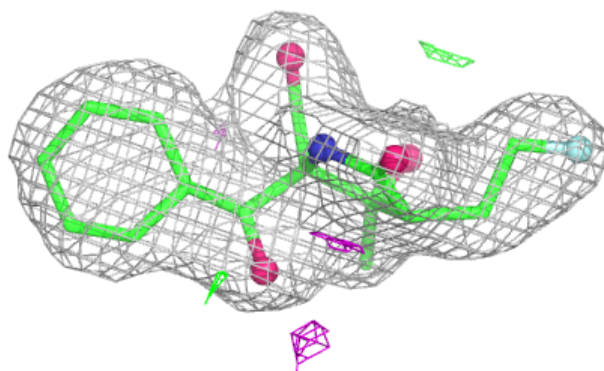
**Electron density around GPT N 224:**

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

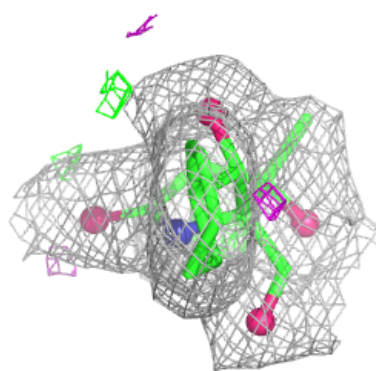
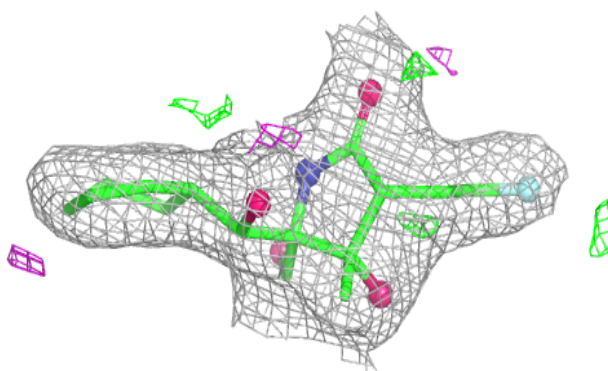
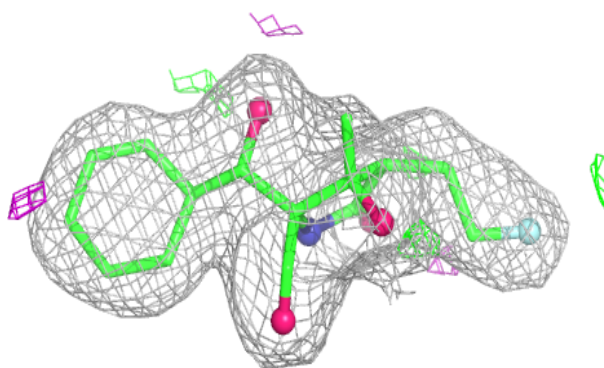


Electron density around GPT Y 224:

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

**Electron density around GPT K 224:**

$2mF_o-DF_c$ (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.