



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:29 AM UTC

PDB ID : 3HYE / pdb_00003hye
Title : Crystal structure of 20S proteasome in complex with hydroxylated salinosporamide
Authors : Groll, M.; Arthur, K.A.M.; Macherla, V.R.; Manam, R.R.; Potts, B.C.
Deposited on : 2009-06-22
Resolution : 2.50 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

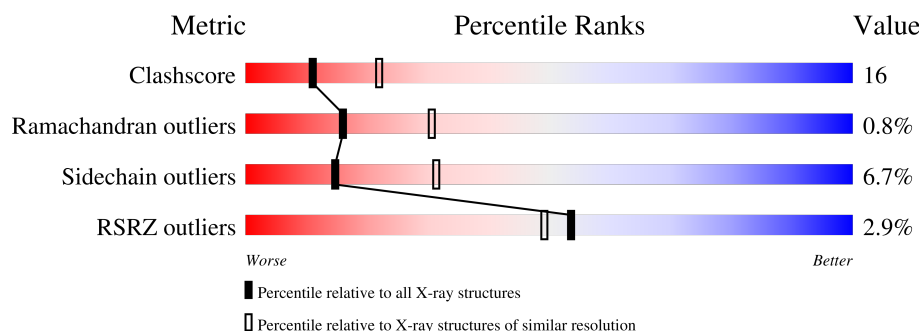
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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% 74% 22% .
1	O	250	3% 73% 22% .
2	B	244	4% 62% 33% 5%
2	P	244	9% 62% 33% 5%
3	C	241	7% 61% 34% .
3	Q	241	8% 60% 34% 5%

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

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

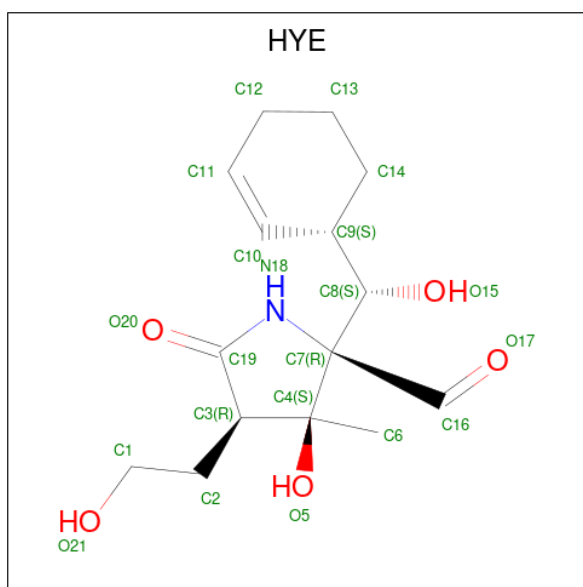
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is (2R,3S,4R)-2-[(S)-(1S)-cyclohex-2-en-1-yl(hydroxy)methyl]-3-hydroxy-4-(2-hydroxyethyl)-3-methyl-5-oxopyrrolidine-2-carbaldehyde (CCD ID: HYE) (formula: C₁₅H₂₃NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			21	15	1	5		
15	K	1	Total	C	N	O	0	0
			21	15	1	5		
15	N	1	Total	C	N	O	0	0
			21	15	1	5		
15	V	1	Total	C	N	O	0	0
			21	15	1	5		
15	Y	1	Total	C	N	O	0	0
			21	15	1	5		
15	2	1	Total	C	N	O	0	0
			21	15	1	5		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	58	Total	O	0	0
			58	58		
16	B	38	Total	O	0	0
			38	38		
16	C	42	Total	O	0	0
			42	42		
16	D	40	Total	O	0	0
			40	40		
16	E	23	Total	O	0	0
			23	23		
16	F	47	Total	O	0	0
			47	47		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	62	Total O 62 62	0	0
16	H	51	Total O 51 51	0	0
16	I	67	Total O 67 67	0	0
16	J	52	Total O 52 52	0	0
16	K	45	Total O 45 45	0	0
16	L	55	Total O 55 55	0	0
16	M	74	Total O 74 74	0	0
16	N	54	Total O 54 54	0	0
16	O	34	Total O 34 34	0	0
16	P	30	Total O 30 30	0	0
16	Q	27	Total O 27 27	0	0
16	R	32	Total O 32 32	0	0
16	S	20	Total O 20 20	0	0
16	T	39	Total O 39 39	0	0
16	U	62	Total O 62 62	0	0
16	V	47	Total O 47 47	0	0
16	W	59	Total O 59 59	0	0
16	X	48	Total O 48 48	0	0
16	Y	47	Total O 47 47	0	0
16	Z	50	Total O 50 50	0	0
16	1	75	Total O 75 75	0	0

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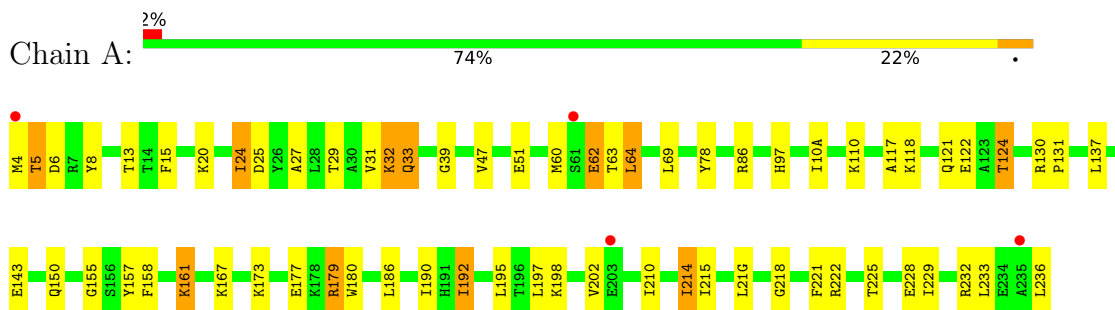
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	56	Total	O	0	0
			56	56		

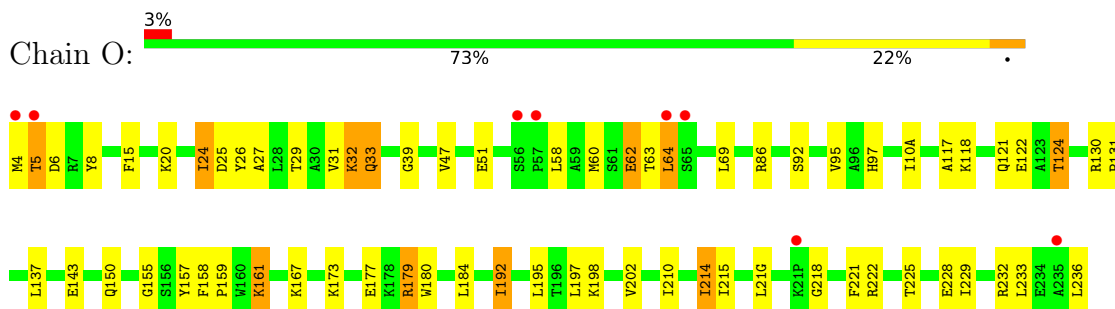
3 Residue-property plots [i](#)

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.

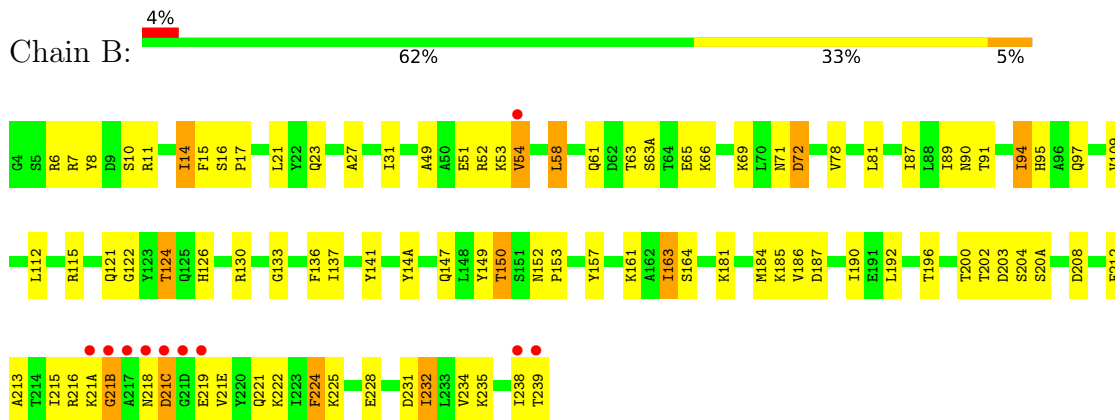
- Molecule 1: Proteasome component Y7



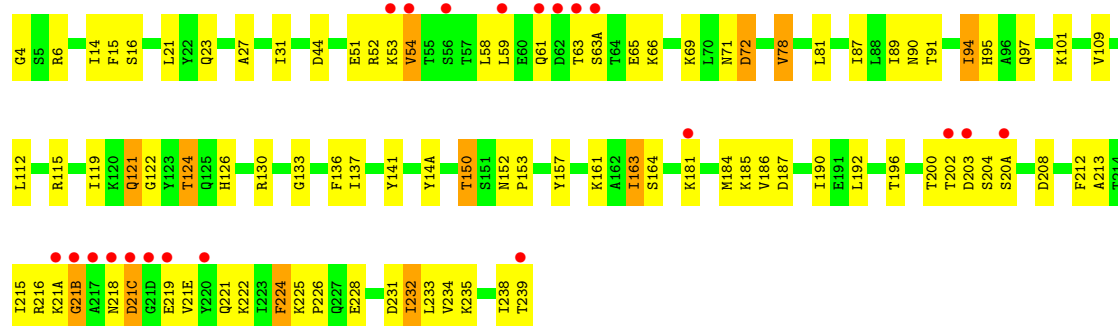
- Molecule 1: Proteasome component Y7



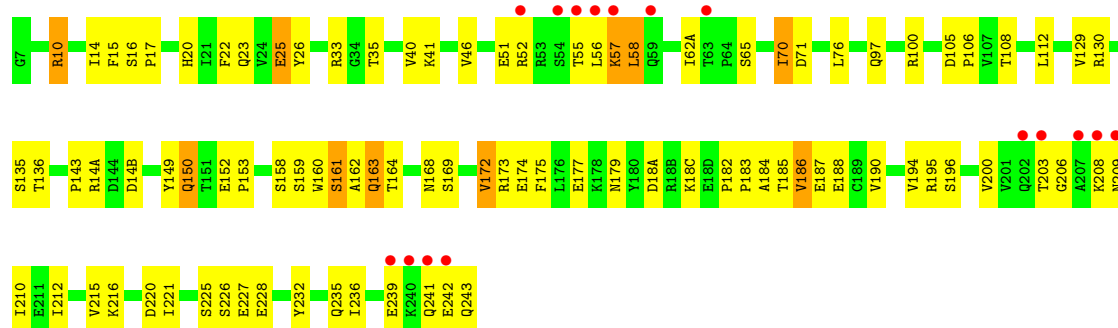
- Molecule 2: Proteasome component Y13



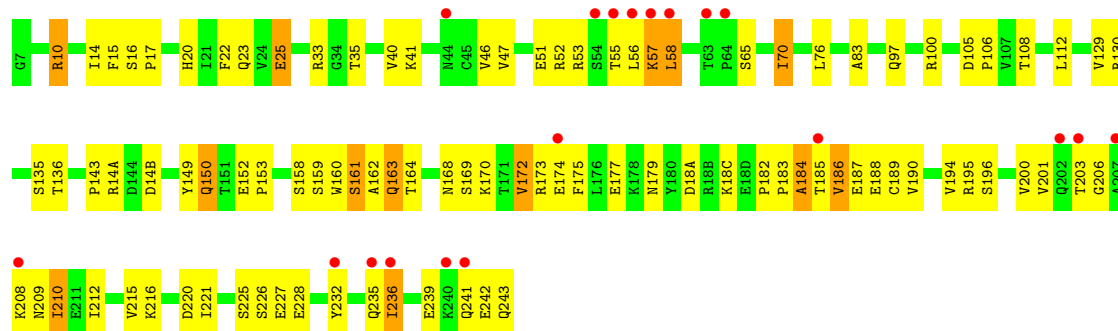
- Molecule 2: Proteasome component Y13



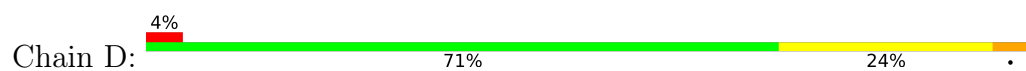
• Molecule 3: Proteasome component PRE6

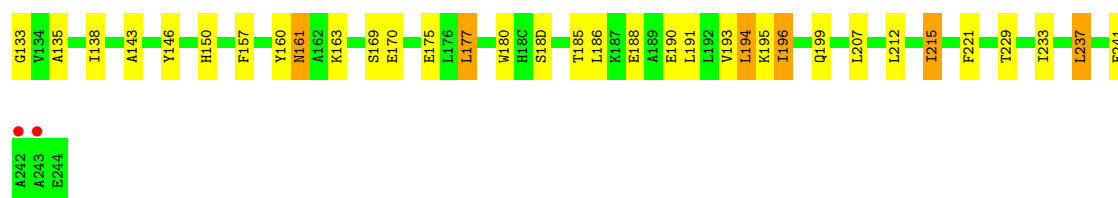


• Molecule 3: Proteasome component PRE6

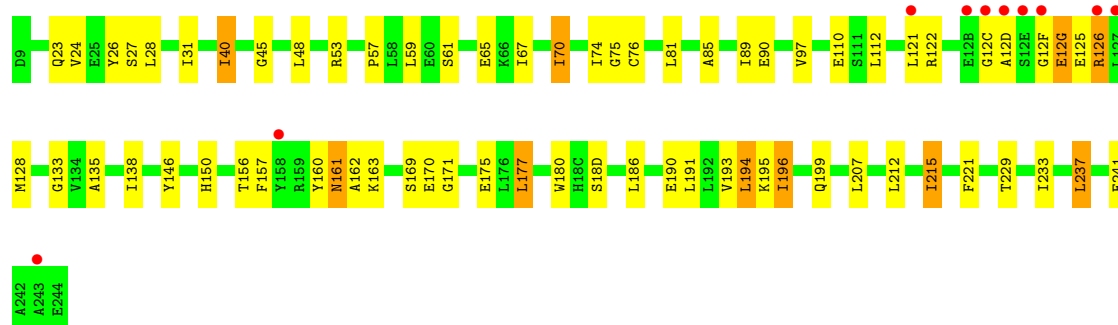
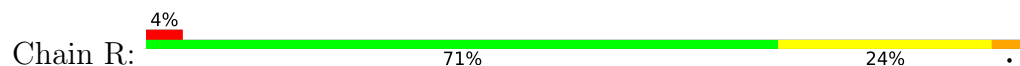


• Molecule 4: Proteasome component PUP2

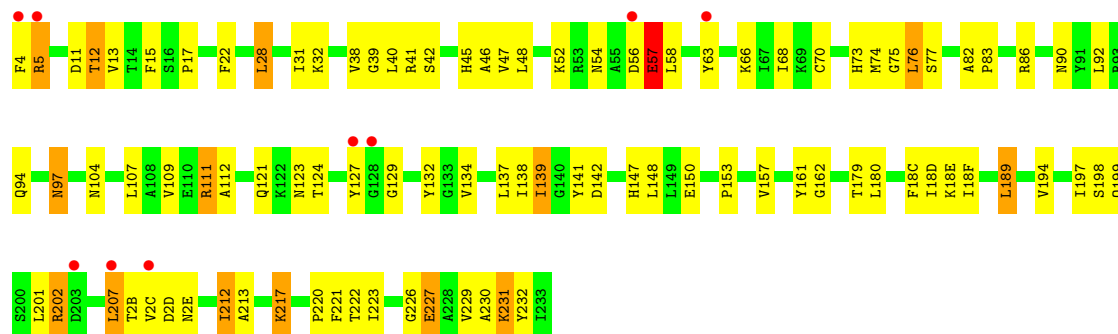




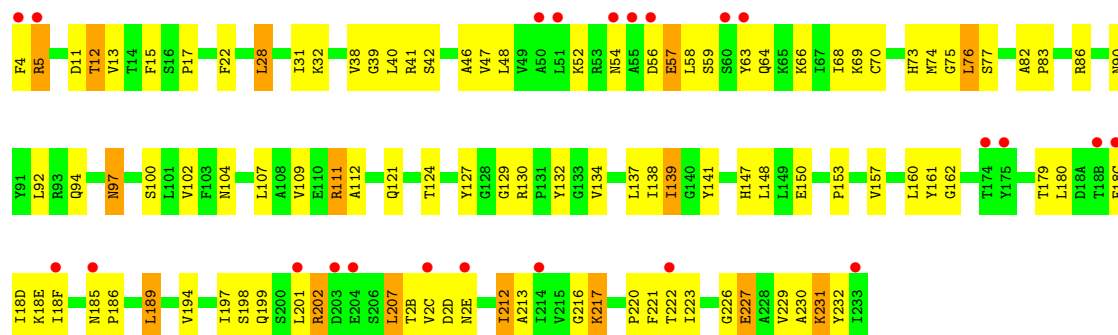
• Molecule 4: Proteasome component PUP2



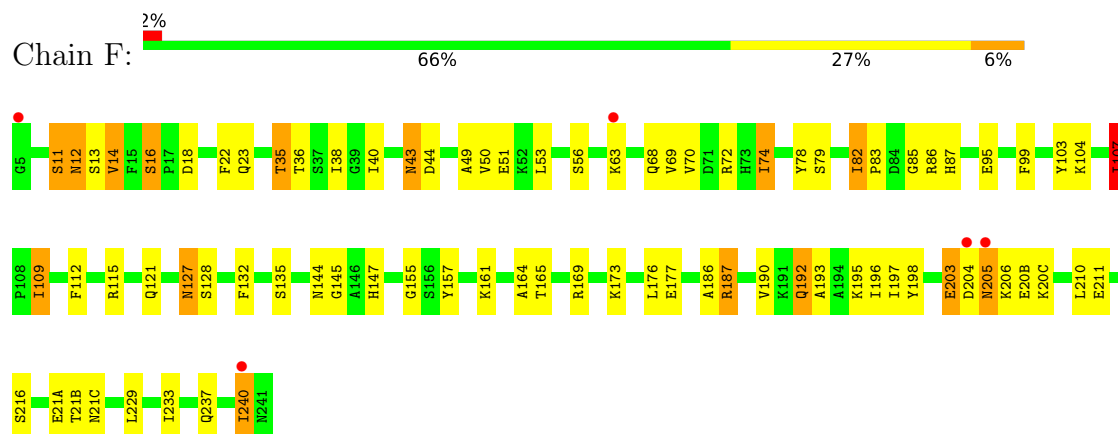
• Molecule 5: Proteasome component PRE5



• Molecule 5: Proteasome component PRE5



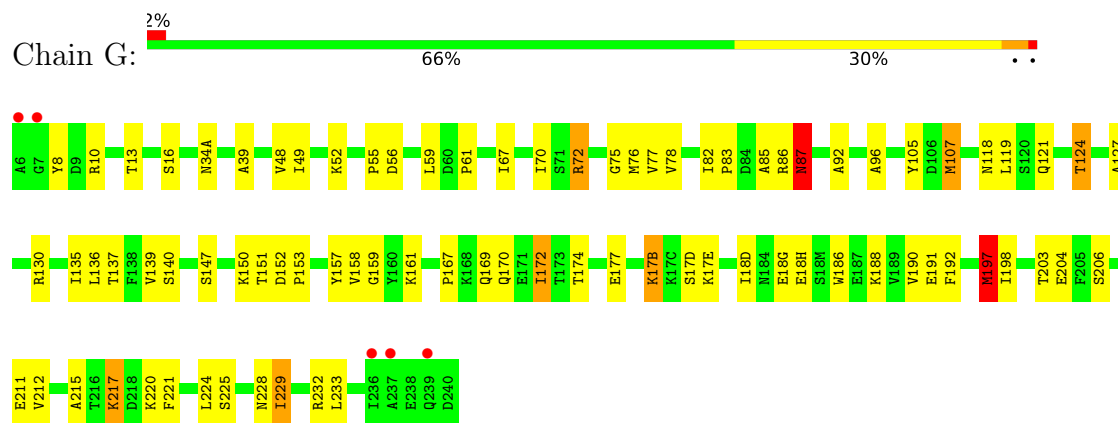
- Molecule 6: Proteasome component C1



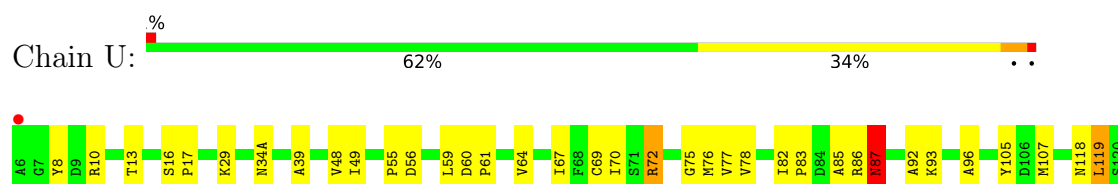
- Molecule 6: Proteasome component C1

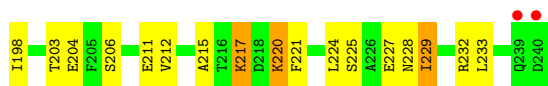


- Molecule 7: Proteasome component C7-alpha

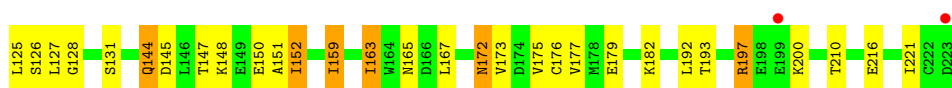


- Molecule 7: Proteasome component C7-alpha





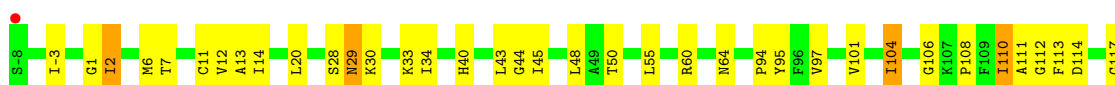
• Molecule 8: Proteasome component PUP1



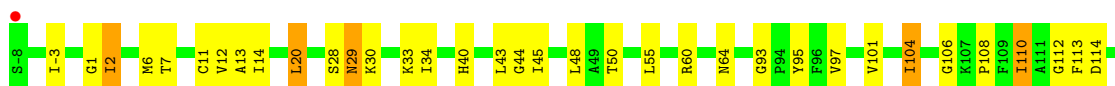
• Molecule 8: Proteasome component PUP1



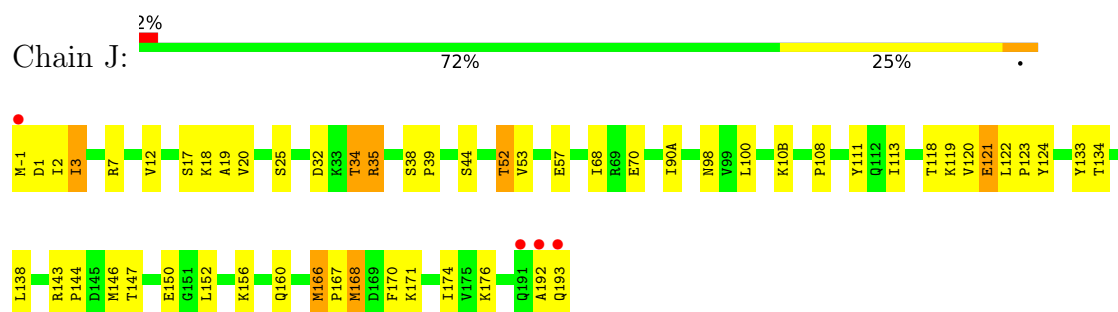
• Molecule 9: Proteasome component PUP3



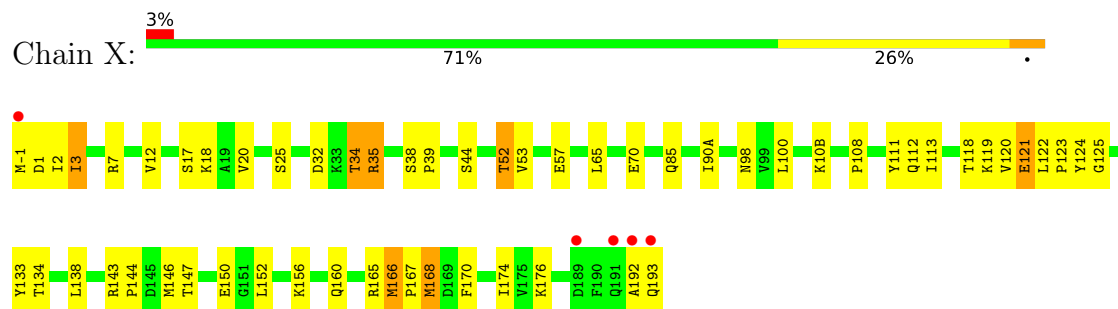
• Molecule 9: Proteasome component PUP3



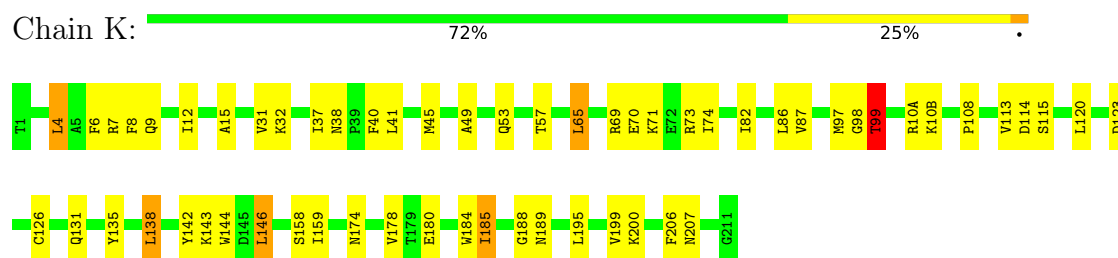
• Molecule 10: Proteasome component C11



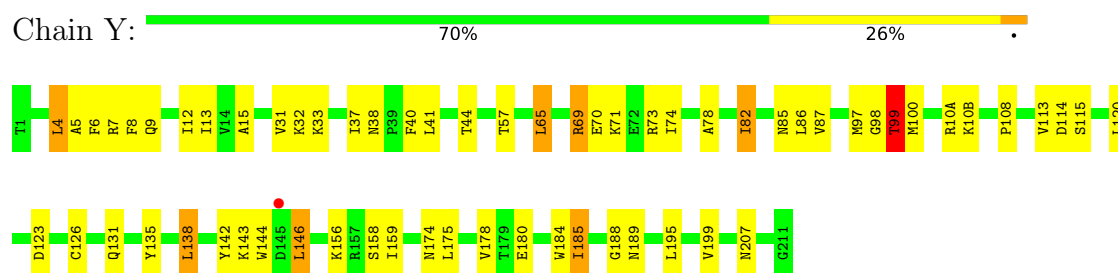
- Molecule 10: Proteasome component C11



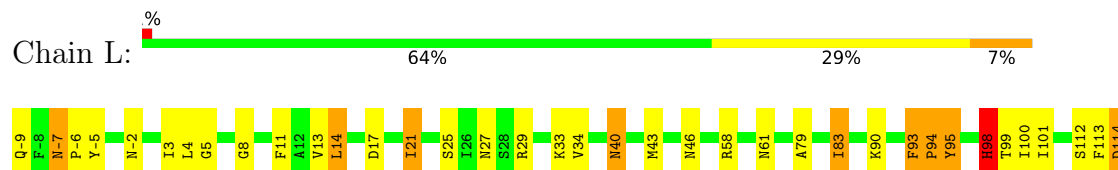
- Molecule 11: Proteasome component PRE2

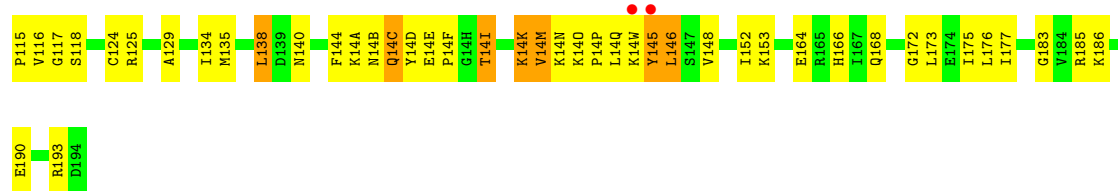


- Molecule 11: Proteasome component PRE2

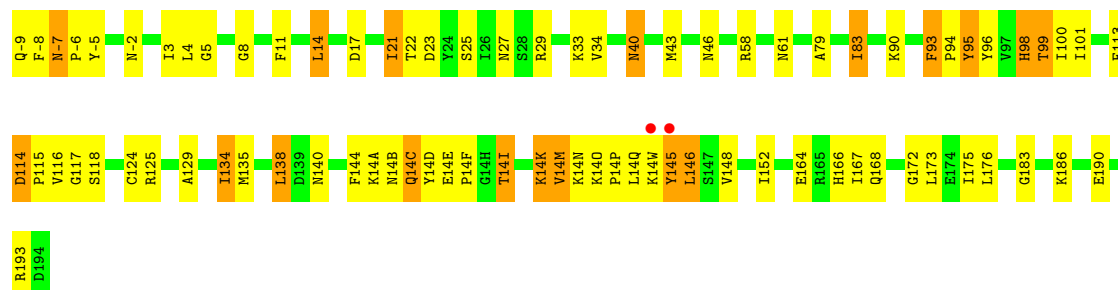


- Molecule 12: Proteasome component C5

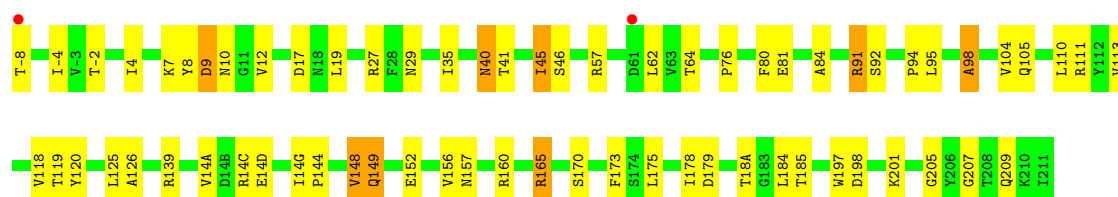




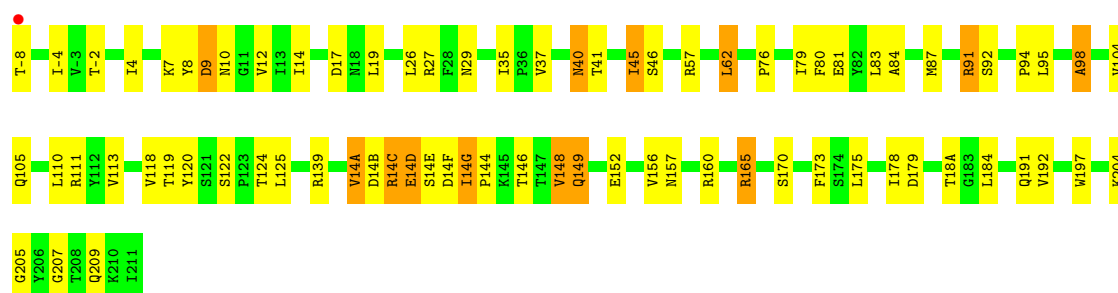
• Molecule 12: Proteasome component C5



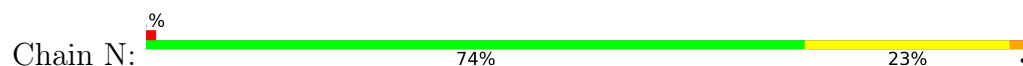
• Molecule 13: Proteasome component PRE4

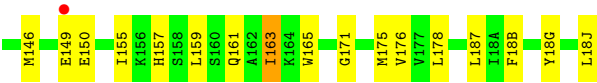


• Molecule 13: Proteasome component PRE4

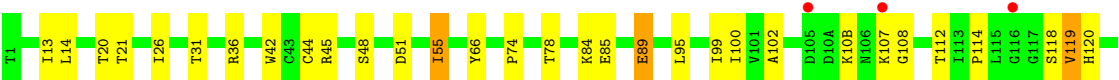


• Molecule 14: Proteasome component PRE3





● 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	135.83Å 300.93Å 144.65Å 90.00° 113.11° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.50) 99.2 (15.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.242 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51008	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: HYE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/1952	0.94	6/2642 (0.2%)
1	O	0.43	0/1952	0.93	5/2642 (0.2%)
2	B	0.43	0/1935	0.91	6/2618 (0.2%)
2	P	0.44	0/1935	0.91	7/2618 (0.3%)
3	C	0.41	0/1920	0.92	6/2598 (0.2%)
3	Q	0.40	0/1920	0.92	6/2598 (0.2%)
4	D	0.42	0/1887	0.90	6/2541 (0.2%)
4	R	0.41	0/1887	0.90	5/2541 (0.2%)
5	E	0.39	0/1823	0.89	3/2463 (0.1%)
5	S	0.40	0/1823	0.90	4/2463 (0.2%)
6	F	0.43	0/1937	0.97	12/2614 (0.5%)
6	T	0.44	0/1937	0.98	12/2614 (0.5%)
7	G	0.48	1/1959 (0.1%)	0.96	8/2652 (0.3%)
7	U	0.46	0/1959	0.96	9/2652 (0.3%)
8	H	0.45	0/1716	0.96	3/2326 (0.1%)
8	V	0.43	0/1716	0.96	3/2326 (0.1%)
9	I	0.44	0/1611	1.00	6/2174 (0.3%)
9	W	0.45	0/1611	1.00	9/2174 (0.4%)
10	J	0.45	0/1613	0.95	6/2173 (0.3%)
10	X	0.46	0/1613	0.96	5/2173 (0.2%)
11	K	0.46	0/1681	0.91	5/2274 (0.2%)
11	Y	0.43	0/1681	0.91	5/2274 (0.2%)
12	L	0.42	0/1795	1.05	14/2420 (0.6%)
12	Z	0.41	0/1795	1.05	14/2420 (0.6%)
13	1	0.46	0/1855	0.97	10/2514 (0.4%)
13	M	0.44	0/1855	0.95	10/2514 (0.4%)
14	2	0.45	0/1541	0.94	2/2087 (0.1%)
14	N	0.46	0/1541	0.94	3/2087 (0.1%)
All	All	0.44	1/50450 (0.0%)	0.95	190/68192 (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	-5.16	1.66	1.79

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	27	ARG	N-CA-C	10.54	122.46	110.97
6	T	12	ASN	N-CA-C	10.37	122.16	111.07
6	F	12	ASN	N-CA-C	10.15	121.94	111.07
13	M	27	ARG	N-CA-C	10.05	122.18	111.03
11	Y	188	GLY	N-CA-C	9.07	124.44	112.65
11	K	188	GLY	N-CA-C	9.06	124.43	112.65
12	Z	93	PHE	CA-C-N	8.79	128.86	119.89
12	Z	93	PHE	C-N-CA	8.79	128.86	119.89
12	L	93	PHE	CA-C-N	8.76	128.82	119.89
12	L	93	PHE	C-N-CA	8.76	128.82	119.89
8	H	37	ILE	N-CA-C	-8.45	103.59	111.45
12	L	95	TYR	N-CA-C	-8.29	96.56	109.25
3	Q	108	THR	N-CA-C	-8.20	99.96	110.53
2	B	161	LYS	N-CA-C	-8.15	103.46	113.41
7	G	161	LYS	N-CA-C	-8.04	102.10	112.23
7	U	161	LYS	N-CA-C	-7.87	102.31	112.23
13	1	95	LEU	N-CA-C	-7.85	95.78	108.41
4	R	161	ASN	N-CA-C	-7.78	102.71	112.90
8	V	37	ILE	N-CA-C	-7.77	104.22	111.45
2	P	161	LYS	N-CA-C	-7.70	104.01	113.41
4	D	161	ASN	N-CA-C	-7.63	102.91	112.90
6	T	107	ILE	N-CA-C	7.62	117.26	108.96
3	C	108	THR	N-CA-C	-7.60	100.73	110.53
13	M	95	LEU	N-CA-C	-7.59	96.20	108.41
6	F	107	ILE	N-CA-C	7.55	117.19	108.96
1	A	161	LYS	N-CA-C	-7.53	101.99	112.45
12	Z	95	TYR	N-CA-C	-7.51	97.03	108.67
1	O	161	LYS	N-CA-C	-7.42	102.14	112.45
10	X	122	LEU	N-CA-C	7.26	116.49	108.14
10	J	122	LEU	N-CA-C	7.18	116.58	108.25
6	F	161	LYS	N-CA-C	-7.09	102.59	112.45
6	T	161	LYS	N-CA-C	-7.06	102.64	112.45
4	R	169	SER	N-CA-C	7.05	119.04	111.36
3	Q	161	SER	N-CA-C	-7.04	103.03	111.69
7	U	16	SER	N-CA-C	-7.04	101.17	110.40
4	D	169	SER	N-CA-C	7.04	119.04	111.36
6	T	14	VAL	N-CA-C	6.99	118.12	108.89
6	T	135	SER	N-CA-C	-6.99	98.01	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	16	SER	N-CA-C	-6.94	101.30	110.40
3	C	161	SER	N-CA-C	-6.89	103.21	111.69
4	D	70	ILE	N-CA-C	-6.84	105.93	111.81
6	F	135	SER	N-CA-C	-6.80	98.31	109.40
12	L	116	VAL	N-CA-C	6.66	118.69	111.77
4	R	70	ILE	N-CA-C	-6.55	106.17	111.81
6	F	14	VAL	N-CA-C	6.47	117.43	108.89
12	L	146	LEU	N-CA-C	6.46	119.60	110.50
3	Q	70	ILE	N-CA-C	-6.45	104.74	111.58
9	W	60	ARG	N-CA-C	-6.44	104.18	111.07
12	Z	146	LEU	N-CA-C	6.43	119.56	110.50
14	N	99	ILE	N-CA-C	6.30	116.93	108.11
9	I	117	GLY	N-CA-C	6.24	123.03	114.92
9	W	117	GLY	N-CA-C	6.22	123.01	114.92
8	H	172	ASN	N-CA-C	6.22	118.90	109.95
7	G	127	ALA	N-CA-C	6.21	118.85	111.71
2	P	16	SER	N-CA-C	-6.20	103.00	110.13
2	B	203	ASP	N-CA-C	-6.20	105.47	113.16
13	1	9	ASP	N-CA-C	6.17	118.79	111.33
5	S	57	GLU	N-CA-C	-6.15	105.64	113.02
12	Z	116	VAL	N-CA-C	6.14	118.16	111.77
9	I	142	TYR	N-CA-C	6.13	119.35	110.28
2	P	72	ASP	N-CA-C	-6.09	105.85	113.28
1	O	143	GLU	N-CA-C	6.09	118.42	111.11
2	P	203	ASP	N-CA-C	-6.06	105.64	113.16
1	A	143	GLU	N-CA-C	6.05	118.38	111.11
9	W	95	TYR	N-CA-C	-6.05	100.63	110.20
13	M	9	ASP	N-CA-C	6.04	118.64	111.33
7	U	127	ALA	N-CA-C	6.02	118.63	111.71
13	M	94	PRO	N-CA-C	5.98	120.38	111.41
14	2	99	ILE	N-CA-C	5.96	117.06	108.48
2	B	137	ILE	N-CA-C	-5.96	99.06	107.75
5	E	161	TYR	N-CA-C	-5.94	105.12	112.90
1	A	137	LEU	N-CA-C	-5.93	98.61	108.34
9	W	142	TYR	N-CA-C	5.92	119.05	110.28
1	O	137	LEU	N-CA-C	-5.91	98.65	108.34
10	J	123	PRO	N-CA-C	-5.89	105.51	113.40
12	Z	134	ILE	N-CA-C	5.87	117.81	111.58
10	X	123	PRO	N-CA-C	-5.87	105.88	113.57
8	V	172	ASN	N-CA-C	5.86	118.38	109.95
3	C	22	PHE	N-CA-C	5.85	118.41	111.33
5	S	161	TYR	N-CA-C	-5.85	105.23	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	61	SER	N-CA-C	5.85	118.41	111.33
13	1	98	ALA	N-CA-C	-5.84	98.75	108.34
12	L	134	ILE	N-CA-C	5.83	117.76	111.58
12	L	21	ILE	N-CA-C	5.83	117.31	108.80
12	Z	117	GLY	N-CA-C	5.80	122.46	114.92
13	M	98	ALA	N-CA-C	-5.80	98.83	108.34
9	I	60	ARG	N-CA-C	-5.79	104.87	111.07
5	E	57	GLU	N-CA-C	-5.79	106.07	113.02
12	L	117	GLY	N-CA-C	5.79	122.44	114.92
6	F	22	PHE	N-CA-C	5.75	118.29	111.33
13	1	94	PRO	N-CA-C	5.75	120.04	111.41
9	I	95	TYR	N-CA-C	-5.75	101.12	110.20
6	T	22	PHE	N-CA-C	5.73	118.26	111.33
13	1	45	ILE	N-CA-C	5.73	116.72	108.48
4	D	61	SER	N-CA-C	5.72	118.25	111.33
12	Z	21	ILE	N-CA-C	5.71	117.14	108.80
12	L	114	ASP	CA-C-N	-5.71	113.74	119.56
12	L	114	ASP	C-N-CA	-5.71	113.74	119.56
13	M	-2	THR	N-CA-C	5.71	118.52	109.50
1	A	10(A)	ILE	CB-CA-C	-5.69	106.04	111.44
6	F	107	ILE	CA-C-N	5.69	125.59	119.85
6	F	107	ILE	C-N-CA	5.69	125.59	119.85
13	M	29	ASN	N-CA-C	5.66	120.89	113.30
6	T	63	LYS	N-CA-C	5.65	118.64	111.69
8	V	99	LEU	N-CA-C	5.65	118.43	109.50
2	P	137	ILE	N-CA-C	-5.64	99.51	107.75
2	B	109	VAL	N-CA-C	5.64	116.28	110.36
12	Z	145	TYR	N-CA-C	5.63	119.42	109.96
9	I	178	ILE	N-CA-C	5.62	115.98	108.11
7	G	87	ASN	N-CA-C	-5.61	105.08	111.14
10	X	25	SER	N-CA-C	5.60	118.69	109.72
2	B	72	ASP	N-CA-C	-5.58	106.47	113.28
13	M	45	ILE	N-CA-C	5.58	116.51	108.48
7	U	87	ASN	N-CA-C	-5.57	105.12	111.14
13	1	-2	THR	N-CA-C	5.57	118.30	109.50
3	Q	22	PHE	N-CA-C	5.57	118.06	111.33
7	U	17(B)	LYS	N-CA-C	-5.56	105.38	111.82
12	Z	114	ASP	CA-C-N	-5.55	113.90	119.56
12	Z	114	ASP	C-N-CA	-5.55	113.90	119.56
2	B	16	SER	N-CA-C	-5.55	103.75	110.13
6	F	63	LYS	N-CA-C	5.53	118.50	111.69
7	G	206	SER	N-CA-C	-5.53	101.81	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	13	THR	N-CA-C	5.51	118.16	109.39
12	L	145	TYR	N-CA-C	5.50	119.19	109.96
3	Q	186	VAL	N-CA-C	-5.50	105.02	110.62
11	K	131	GLN	N-CA-C	5.49	117.69	111.11
1	O	10(A)	ILE	CB-CA-C	-5.45	106.26	111.44
7	U	206	SER	N-CA-C	-5.44	101.96	110.17
7	G	17(B)	LYS	N-CA-C	-5.42	105.53	111.82
11	Y	131	GLN	N-CA-C	5.42	117.61	111.11
3	C	186	VAL	N-CA-C	-5.42	105.09	110.62
7	U	13	THR	N-CA-C	5.41	117.99	109.39
5	S	22	PHE	N-CA-C	5.40	117.16	111.28
4	D	143	ALA	N-CA-C	5.38	117.90	111.71
11	Y	98	GLY	N-CA-C	-5.36	100.47	113.18
13	I	29	ASN	N-CA-C	5.36	120.48	113.30
11	K	98	GLY	N-CA-C	-5.35	100.50	113.18
6	T	155	GLY	N-CA-C	-5.34	107.98	114.92
12	L	98	HIS	N-CA-C	-5.32	98.57	107.99
14	N	141	ASN	N-CA-C	5.32	119.93	113.38
11	Y	99	THR	N-CA-C	5.31	117.25	109.24
10	X	165	ARG	N-CA-C	5.29	119.80	113.23
5	S	102	VAL	N-CA-C	5.29	116.77	111.00
6	F	145	GLY	N-CA-C	5.29	119.32	111.76
7	U	220	LYS	N-CA-C	5.28	116.44	108.46
6	T	107	ILE	CA-C-N	5.26	125.16	119.85
6	T	107	ILE	C-N-CA	5.26	125.16	119.85
10	J	25	SER	N-CA-C	5.24	118.10	109.72
10	J	122	LEU	CA-C-N	5.23	124.55	118.85
10	J	122	LEU	C-N-CA	5.23	124.55	118.85
14	2	141	ASN	N-CA-C	5.22	119.80	113.38
1	A	215	ILE	N-CA-C	-5.21	98.99	107.28
11	Y	57	THR	N-CA-C	-5.21	105.51	111.14
7	G	197	MET	N-CA-C	-5.20	105.51	111.07
11	K	57	THR	N-CA-C	-5.18	105.54	111.14
12	Z	98	HIS	N-CA-C	-5.17	98.83	107.99
4	D	128	MET	N-CA-C	-5.17	99.79	110.80
12	L	115	PRO	N-CA-C	-5.17	107.12	113.84
8	H	99	LEU	N-CA-C	5.16	117.66	109.50
9	W	93	GLY	CA-C-N	5.16	125.14	120.03
9	W	93	GLY	C-N-CA	5.16	125.14	120.03
6	T	16	SER	N-CA-C	-5.16	104.20	110.13
2	P	78	VAL	N-CA-C	5.15	116.00	108.53
3	C	70	ILE	N-CA-C	-5.15	105.09	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	197	MET	N-CA-C	-5.14	105.58	111.14
6	F	16	SER	N-CA-C	-5.14	104.22	110.13
2	P	109	VAL	N-CA-C	5.14	115.76	110.36
3	Q	16	SER	N-CA-C	-5.14	102.69	110.50
10	J	134	THR	N-CA-C	5.14	119.68	113.41
10	X	134	THR	N-CA-C	5.13	119.67	113.41
5	E	22	PHE	N-CA-C	5.13	116.87	111.28
9	W	178	ILE	N-CA-C	5.13	115.29	108.11
13	1	35	ILE	N-CA-C	5.11	113.07	107.60
12	L	94	PRO	N-CA-C	5.10	119.22	111.11
13	M	35	ILE	N-CA-C	5.10	113.05	107.60
3	C	16	SER	N-CA-C	-5.09	102.76	110.50
13	M	165	ARG	N-CA-C	5.09	120.34	113.72
11	K	99	THR	N-CA-C	5.09	117.12	109.23
6	F	155	GLY	N-CA-C	-5.08	108.31	114.92
1	O	215	ILE	N-CA-C	-5.07	99.22	107.28
9	W	93	GLY	N-CA-C	-5.06	102.01	112.34
9	I	94	PRO	N-CA-C	5.05	118.99	111.41
4	R	128	MET	N-CA-C	-5.04	100.06	110.80
13	1	165	ARG	N-CA-C	5.04	120.27	113.72
14	N	19	ARG	N-CA-C	5.04	117.18	109.07
6	T	145	GLY	N-CA-C	5.04	118.97	111.76
12	Z	115	PRO	N-CA-C	-5.04	107.29	113.84
1	A	78	TYR	N-CA-C	5.03	114.79	108.45
9	W	114	ASP	N-CA-C	-5.02	103.03	110.46
12	Z	129	ALA	N-CA-C	5.01	117.14	111.02

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	54	0
1	O	1915	0	1926	59	0
2	B	1905	0	1901	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1905	0	1901	90	0
3	C	1891	0	1900	92	0
3	Q	1891	0	1900	94	0
4	D	1862	0	1836	52	0
4	R	1862	0	1836	57	0
5	E	1795	0	1797	98	0
5	S	1795	0	1797	103	0
6	F	1897	0	1886	61	0
6	T	1897	0	1886	72	0
7	G	1921	0	1910	75	0
7	U	1921	0	1910	88	0
8	H	1685	0	1687	50	0
8	V	1685	0	1687	52	0
9	I	1581	0	1574	45	0
9	W	1581	0	1574	43	0
10	J	1585	0	1590	59	0
10	X	1585	0	1590	63	0
11	K	1644	0	1594	50	0
11	Y	1644	0	1594	54	0
12	L	1757	0	1711	55	0
12	Z	1757	0	1711	57	0
13	1	1824	0	1832	58	0
13	M	1824	0	1832	52	0
14	2	1512	0	1480	48	0
14	N	1512	0	1480	46	0
15	2	21	0	22	3	0
15	H	21	0	22	0	0
15	K	21	0	22	1	0
15	N	21	0	22	1	0
15	V	21	0	22	0	0
15	Y	21	0	22	2	0
16	1	75	0	0	2	0
16	2	56	0	0	2	0
16	A	58	0	0	2	0
16	B	38	0	0	2	0
16	C	42	0	0	2	0
16	D	40	0	0	2	0
16	E	23	0	0	0	0
16	F	47	0	0	2	0
16	G	62	0	0	1	0
16	H	51	0	0	1	0
16	I	67	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	J	52	0	0	0	0
16	K	45	0	0	0	0
16	L	55	0	0	1	0
16	M	74	0	0	1	0
16	N	54	0	0	1	0
16	O	34	0	0	1	0
16	P	30	0	0	0	0
16	Q	27	0	0	4	0
16	R	32	0	0	2	0
16	S	20	0	0	2	0
16	T	39	0	0	4	0
16	U	62	0	0	3	0
16	V	47	0	0	5	0
16	W	59	0	0	1	0
16	X	48	0	0	0	0
16	Y	47	0	0	1	0
16	Z	50	0	0	2	0
All	All	51008	0	49380	1627	0

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

All (1627) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:168:MET:HE3	10:X:168:MET:HE3	1.29	1.12
7:U:96:ALA:HA	7:U:107:MET:HE2	1.33	1.10
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.12	1.09
7:G:96:ALA:HA	7:G:107:MET:HE2	1.35	1.08
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.12	1.05
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.22	1.04
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.22	1.00
2:P:202:THR:HG22	2:P:204:SER:H	1.29	0.97
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.03	0.96
5:S:207:LEU:HD23	5:S:207:LEU:H	1.29	0.96
5:E:207:LEU:HD23	5:E:207:LEU:H	1.30	0.94
2:B:202:THR:HG22	2:B:204:SER:H	1.30	0.93
3:C:185:THR:HG22	3:C:187:GLU:H	1.33	0.93
2:B:15:PHE:H	3:C:23:GLN:HE22	1.09	0.93
3:C:185:THR:HB	3:C:188:GLU:HG2	1.50	0.92
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.49	0.92
5:E:15:PHE:H	6:F:23:GLN:HE22	1.16	0.91
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.04	0.91
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.31	0.91
3:Q:65:SER:HB2	16:Q:303:HOH:O	1.71	0.90
5:S:15:PHE:H	6:T:23:GLN:HE22	1.12	0.90
1:O:15:PHE:H	2:P:23:GLN:HE22	1.14	0.90
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.86	0.89
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.38	0.88
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.38	0.88
10:J:168:MET:CE	10:X:168:MET:HE3	2.04	0.88
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.36	0.87
1:A:15:PHE:H	2:B:23:GLN:HE22	1.22	0.87
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.56	0.87
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.74	0.86
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.56	0.86
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.23	0.85
10:J:168:MET:HE3	10:X:168:MET:CE	2.06	0.85
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.74	0.85
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.58	0.84
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.59	0.84
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.24	0.84
1:A:124:THR:CG2	2:B:130:ARG:HH21	1.90	0.84
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	1.89	0.84
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.42	0.83
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.59	0.83
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.59	0.83
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.60	0.83
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.61	0.83
7:U:96:ALA:HA	7:U:107:MET:CE	2.07	0.83
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.61	0.83
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.93	0.82
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.79	0.82
14:2:126:ILE:HD13	14:2:126:ILE:H	1.44	0.82
7:G:96:ALA:HA	7:G:107:MET:CE	2.09	0.82
9:I:7:THR:HG23	9:I:110:ILE:HD13	1.62	0.82
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.94	0.82
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.80	0.82
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.62	0.82
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.93	0.81
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.44	0.81
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.61	0.81
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.63	0.81
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.46	0.81
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.78	0.81
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.81	0.80
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.82	0.79
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.79	0.79
9:W:7:THR:HG23	9:W:110:ILE:HD13	1.65	0.79
3:C:163:GLN:NE2	3:C:164:THR:H	1.81	0.79
14:N:126:ILE:HD13	14:N:126:ILE:H	1.44	0.79
3:C:232:TYR:O	3:C:236:ILE:HG13	1.84	0.78
11:Y:184:TRP:C	11:Y:185:ILE:HD13	2.09	0.78
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.49	0.78
3:C:15:PHE:H	4:D:23:GLN:HE22	1.32	0.77
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.85	0.77
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.96	0.77
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.19	0.77
3:C:163:GLN:HE21	3:C:164:THR:H	1.33	0.77
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.85	0.77
5:S:221:PHE:CE1	5:S:223:ILE:HD11	2.20	0.77
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.49	0.77
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.31	0.77
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.66	0.77
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.65	0.76
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.67	0.76
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.49	0.75
11:K:184:TRP:C	11:K:185:ILE:HD13	2.11	0.75
14:N:107:LYS:HG2	14:N:108:GLY:H	1.49	0.75
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.86	0.75
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.84	0.75
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.68	0.75
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.87	0.75
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.35	0.74
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.69	0.74
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.68	0.74
14:2:107:LYS:HG2	14:2:108:GLY:H	1.51	0.74
5:S:207:LEU:H	5:S:207:LEU:CD2	2.00	0.74
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.51	0.74
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.35	0.74
5:E:207:LEU:H	5:E:207:LEU:CD2	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:99:THR:HG22	11:K:113:VAL:O	1.88	0.74
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.00	0.74
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.67	0.74
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.36	0.74
9:I:43:LEU:HG	9:I:45:ILE:HD11	1.70	0.74
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.70	0.74
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.69	0.73
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.70	0.73
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.68	0.73
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.68	0.73
5:S:221:PHE:HE1	5:S:223:ILE:HD11	1.53	0.73
2:B:121:GLN:O	2:B:124:THR:HB	1.89	0.73
5:E:221:PHE:HE1	5:E:223:ILE:HD11	1.53	0.73
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.02	0.73
9:W:192:ARG:HG3	16:W:200:HOH:O	1.88	0.73
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.03	0.72
4:D:207:LEU:HD21	4:D:233:ILE:HD12	1.71	0.72
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.18	0.72
6:F:35:THR:HG21	6:F:51:GLU:O	1.89	0.72
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.71	0.72
3:C:185:THR:HG22	3:C:187:GLU:N	2.04	0.72
4:R:207:LEU:HD21	4:R:233:ILE:HD12	1.72	0.72
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.72	0.72
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.20	0.72
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.89	0.72
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.70	0.71
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.33	0.71
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.71	0.71
1:O:159:PRO:O	2:P:59:LEU:HD12	1.90	0.71
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.73	0.71
7:U:59:LEU:O	7:U:61:PRO:HD3	1.89	0.71
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.71	0.71
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.73	0.71
14:N:20:THR:HG22	15:N:300:HYE:H10	1.73	0.71
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.56	0.71
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.26	0.71
3:C:65:SER:HB2	16:C:274:HOH:O	1.91	0.70
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.06	0.70
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.74	0.70
12:L:166:HIS:HD2	12:L:168:GLN:H	1.38	0.70
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.36	0.70
2:P:121:GLN:O	2:P:124:THR:HB	1.89	0.70
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.72	0.70
7:G:217:LYS:HE3	7:G:217:LYS:HA	1.72	0.70
5:E:198:SER:HA	5:E:201:LEU:HG	1.74	0.70
7:G:59:LEU:O	7:G:61:PRO:HD3	1.91	0.70
9:W:6:MET:HE3	9:W:155:ILE:HD12	1.73	0.70
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.72	0.70
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.27	0.70
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.56	0.70
9:W:43:LEU:HG	9:W:45:ILE:HD11	1.74	0.70
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.27	0.70
14:2:20:THR:HG22	15:2:300:HYE:H10	1.74	0.70
2:B:15:PHE:H	3:C:23:GLN:NE2	1.87	0.70
3:Q:70:ILE:HD11	3:Q:76:LEU:HB3	1.73	0.70
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.08	0.69
5:S:198:SER:HA	5:S:201:LEU:HG	1.74	0.69
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.74	0.69
6:T:35:THR:HG21	6:T:51:GLU:O	1.92	0.69
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.23	0.69
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.28	0.69
13:M:40:ASN:H	13:M:40:ASN:HD22	1.38	0.69
13:1:40:ASN:H	13:1:40:ASN:HD22	1.39	0.69
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.75	0.69
1:O:60:MET:HE3	1:O:63:THR:HG21	1.73	0.69
1:A:4:MET:SD	1:A:5:THR:N	2.58	0.69
3:C:70:ILE:HD11	3:C:76:LEU:HB3	1.75	0.69
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.57	0.69
6:F:237:GLN:O	6:F:240:ILE:HG22	1.93	0.69
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.23	0.69
16:B:565:HOH:O	3:C:33:ARG:HD2	1.92	0.69
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.73	0.69
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.23	0.69
9:W:112:GLY:N	9:W:125:ILE:HD12	2.08	0.69
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.75	0.68
6:T:237:GLN:O	6:T:240:ILE:HG22	1.94	0.68
8:H:159:ILE:HG22	8:H:163:ILE:CD1	2.24	0.68
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.76	0.68
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.75	0.68
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.23	0.68
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:6:MET:HE3	9:I:155:ILE:HD12	1.73	0.68
1:O:4:MET:SD	1:O:5:THR:N	2.60	0.68
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.42	0.68
3:Q:241:GLN:C	3:Q:243:GLN:H	2.01	0.68
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.23	0.68
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.24	0.68
1:A:60:MET:HE3	1:A:63:THR:HG21	1.75	0.68
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.74	0.68
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.29	0.68
11:K:142:TYR:O	11:K:143:LYS:HD2	1.93	0.67
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.07	0.67
8:V:172:ASN:HD22	8:V:193:THR:HA	1.58	0.67
2:B:163:ILE:HD13	2:B:164:SER:N	2.09	0.67
6:T:109:ILE:N	6:T:109:ILE:HD13	2.09	0.67
3:C:241:GLN:C	3:C:243:GLN:H	2.01	0.67
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.76	0.67
7:U:198:ILE:HG23	7:U:203:THR:O	1.94	0.67
14:2:20:THR:HG23	14:2:31:THR:OG1	1.95	0.67
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.60	0.67
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.28	0.67
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.76	0.67
6:T:186:ALA:O	6:T:190:VAL:HG23	1.95	0.67
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.77	0.67
5:E:28:LEU:HA	5:E:31:ILE:HD12	1.76	0.67
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.43	0.66
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.94	0.66
5:E:226:GLY:O	5:E:229:VAL:HG22	1.96	0.66
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.10	0.66
7:G:121:GLN:O	7:G:124:THR:HB	1.95	0.66
8:V:221:ILE:HD12	9:W:40:HIS:HA	1.77	0.66
10:X:143:ARG:O	10:X:146:MET:HG3	1.95	0.66
2:P:163:ILE:HD13	2:P:164:SER:N	2.10	0.66
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.07	0.66
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.78	0.66
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.96	0.66
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.96	0.66
7:G:198:ILE:HG23	7:G:203:THR:O	1.94	0.66
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.77	0.66
7:U:121:GLN:O	7:U:124:THR:HB	1.95	0.66
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.59	0.66
14:N:20:THR:HG23	14:N:31:THR:OG1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.59	0.65
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.61	0.65
5:S:226:GLY:O	5:S:229:VAL:HG22	1.96	0.65
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.93	0.65
10:X:156:LYS:O	10:X:160:GLN:HG3	1.95	0.65
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.27	0.65
10:J:156:LYS:O	10:J:160:GLN:HG3	1.97	0.65
5:S:207:LEU:HD23	5:S:207:LEU:N	2.08	0.65
5:S:28:LEU:HA	5:S:31:ILE:HD12	1.77	0.65
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.45	0.65
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.96	0.65
9:I:112:GLY:N	9:I:125:ILE:HD12	2.11	0.64
10:J:168:MET:HG2	10:X:168:MET:HE3	1.79	0.64
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.12	0.64
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.10	0.64
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.79	0.64
6:F:186:ALA:O	6:F:190:VAL:HG23	1.97	0.64
2:P:112:LEU:C	2:P:112:LEU:HD23	2.23	0.64
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.33	0.64
6:F:109:ILE:N	6:F:109:ILE:HD13	2.12	0.64
10:J:143:ARG:O	10:J:146:MET:HG3	1.97	0.64
3:C:163:GLN:HE21	3:C:164:THR:N	1.95	0.64
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.11	0.64
1:A:97:HIS:HD2	8:H:61:SER:OG	1.82	0.63
8:H:172:ASN:HD22	8:H:193:THR:HA	1.61	0.63
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.79	0.63
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.94	0.63
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.10	0.63
4:R:121:LEU:HB2	16:R:853:HOH:O	1.98	0.63
4:R:207:LEU:C	4:R:207:LEU:HD23	2.23	0.63
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.14	0.63
4:D:40:ILE:HG13	4:D:193:VAL:HG23	1.80	0.63
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.78	0.63
10:J:147:THR:OG1	10:J:150:GLU:HG3	1.98	0.63
1:A:179:ARG:HH11	1:A:179:ARG:HB3	1.62	0.63
13:M:14(C):ARG:HH11	13:M:14(C):ARG:CG	2.10	0.63
2:B:112:LEU:HD23	2:B:112:LEU:C	2.24	0.63
2:P:185:LYS:HD3	2:P:186:VAL:N	2.14	0.63
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.34	0.63
6:F:127:ASN:C	6:F:127:ASN:HD22	2.06	0.63
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	1.98	0.63
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.81	0.63
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.98	0.63
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.14	0.63
4:R:40:ILE:HG13	4:R:193:VAL:HG23	1.81	0.63
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.44	0.62
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.29	0.62
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.81	0.62
14:2:126:ILE:HD13	14:2:126:ILE:N	2.14	0.62
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.35	0.62
10:J:90(A):ILE:HD13	10:J:90(A):ILE:O	1.99	0.62
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.64	0.62
10:X:90(A):ILE:HD13	10:X:90(A):ILE:O	2.00	0.62
5:E:207:LEU:HD23	5:E:207:LEU:N	2.09	0.62
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.81	0.62
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.00	0.62
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.34	0.62
3:Q:52:ARG:HD2	3:Q:208:LYS:O	1.99	0.62
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.81	0.62
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.29	0.62
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.47	0.62
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.80	0.62
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.82	0.62
8:H:221:ILE:HD12	9:I:40:HIS:HA	1.82	0.62
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.30	0.62
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.81	0.62
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.00	0.62
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.81	0.62
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.30	0.62
5:E:12:THR:HG21	5:E:124:THR:HA	1.82	0.62
6:T:127:ASN:C	6:T:127:ASN:HD22	2.08	0.62
7:U:8:TYR:C	7:U:10:ARG:H	2.08	0.62
13:1:14(C):ARG:HH11	13:1:14(C):ARG:CG	2.10	0.62
6:T:203:GLU:O	6:T:206:LYS:HD2	2.00	0.61
12:Z:3:ILE:CD1	12:Z:100:ILE:HD12	2.29	0.61
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.65	0.61
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.15	0.61
5:E:15:PHE:H	6:F:23:GLN:NE2	1.95	0.61
10:J:168:MET:HE3	10:X:168:MET:HG2	1.81	0.61
10:J:168:MET:CE	10:X:168:MET:HG2	2.31	0.61
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:190:ILE:HG21	2:P:232:ILE:HD11	1.81	0.61
2:B:185:LYS:HD3	2:B:186:VAL:N	2.15	0.61
4:D:207:LEU:CD2	4:D:233:ILE:HD12	2.29	0.61
6:F:69:VAL:HG12	16:F:319:HOH:O	1.99	0.61
4:R:207:LEU:CD2	4:R:233:ILE:HD12	2.30	0.61
3:C:52:ARG:HD2	3:C:208:LYS:O	2.01	0.61
5:S:15:PHE:H	6:T:23:GLN:NE2	1.92	0.61
4:D:207:LEU:HD23	4:D:207:LEU:C	2.25	0.61
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.82	0.61
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.29	0.61
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.49	0.61
10:J:168:MET:HG2	10:X:168:MET:CE	2.30	0.61
13:1:46:SER:OG	13:1:98:ALA:HB3	2.00	0.61
8:H:34:LEU:HB2	16:H:540:HOH:O	2.01	0.61
9:I:33:LYS:O	9:I:44:GLY:HA2	2.01	0.61
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.14	0.61
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.30	0.60
5:S:12:THR:HG21	5:S:124:THR:HA	1.83	0.60
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	1.83	0.60
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.48	0.60
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.83	0.60
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.83	0.60
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.67	0.60
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.36	0.60
7:G:8:TYR:C	7:G:10:ARG:H	2.07	0.60
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.65	0.60
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.83	0.60
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.48	0.60
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.83	0.60
13:M:4:ILE:O	13:M:4:ILE:HD12	2.02	0.60
2:P:190:ILE:HG21	2:P:232:ILE:CD1	2.32	0.60
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.84	0.60
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.82	0.60
6:F:203:GLU:O	6:F:206:LYS:HD2	2.02	0.60
12:L:3:ILE:CD1	12:L:100:ILE:HD12	2.31	0.60
8:V:159:ILE:HG22	8:V:163:ILE:HD12	1.83	0.60
3:C:41:LYS:HG2	3:C:161:SER:O	2.01	0.60
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.36	0.60
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.02	0.60
4:D:112:LEU:C	4:D:112:LEU:HD13	2.26	0.60
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:HIS:CB	8:H:56:THR:HG21	2.32	0.60
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.14	0.60
9:I:34:ILE:HB	16:I:955:HOH:O	2.01	0.60
11:K:185:ILE:HD13	11:K:185:ILE:N	2.16	0.60
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.98	0.60
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.15	0.59
14:N:126:ILE:HD13	14:N:126:ILE:N	2.15	0.59
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.15	0.59
6:F:109:ILE:N	6:F:109:ILE:CD1	2.64	0.59
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.84	0.59
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.31	0.59
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.83	0.59
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.29	0.59
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.85	0.59
9:W:6:MET:CE	9:W:155:ILE:HA	2.33	0.59
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.83	0.59
12:L:175:ILE:N	12:L:175:ILE:HD12	2.18	0.59
14:N:107:LYS:HG2	14:N:108:GLY:N	2.17	0.59
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.84	0.59
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.84	0.59
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.27	0.59
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.83	0.59
9:I:6:MET:CE	9:I:155:ILE:HA	2.32	0.59
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.84	0.59
7:G:49:ILE:HD12	7:G:212:VAL:HG22	1.83	0.59
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.17	0.59
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.03	0.59
13:M:46:SER:OG	13:M:98:ALA:HB3	2.02	0.59
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.30	0.59
2:B:186:VAL:O	2:B:190:ILE:HG13	2.03	0.59
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.49	0.59
9:W:33:LYS:O	9:W:44:GLY:HA2	2.03	0.59
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.67	0.59
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.85	0.59
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.84	0.59
10:J:-1:MET:HG2	10:J:1:ASP:N	2.18	0.58
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	1.85	0.58
14:N:175:MET:HE3	14:N:18(B):PHE:CE2	2.37	0.58
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.85	0.58
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.84	0.58
8:V:34:LEU:HB2	16:V:578:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.28	0.58
1:A:121:GLN:O	1:A:124:THR:HB	2.03	0.58
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.85	0.58
5:S:132:TYR:O	5:S:153:PRO:HB3	2.03	0.58
13:1:152:GLU:O	13:1:156:VAL:HG23	2.04	0.58
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.32	0.58
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.85	0.58
2:P:186:VAL:O	2:P:190:ILE:HG13	2.02	0.58
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.39	0.58
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.86	0.58
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.85	0.58
11:K:31:VAL:HG11	15:K:300:HYE:H11	1.85	0.58
8:V:35:HIS:CB	8:V:56:THR:HG21	2.33	0.58
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.50	0.58
1:O:97:HIS:HD2	8:V:61:SER:OG	1.86	0.58
6:T:109:ILE:N	6:T:109:ILE:CD1	2.66	0.58
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.69	0.58
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.86	0.58
1:O:121:GLN:O	1:O:124:THR:HB	2.04	0.58
11:Y:31:VAL:HG11	15:Y:300:HYE:H11	1.84	0.58
5:E:132:TYR:O	5:E:153:PRO:HB3	2.04	0.57
13:M:152:GLU:O	13:M:156:VAL:HG23	2.04	0.57
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.87	0.57
5:S:73:HIS:HE1	5:S:107:LEU:O	1.85	0.57
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.85	0.57
8:V:196:VAL:HG23	16:V:652:HOH:O	2.03	0.57
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.69	0.57
11:Y:185:ILE:HD13	11:Y:185:ILE:N	2.18	0.57
14:2:107:LYS:HG2	14:2:108:GLY:N	2.19	0.57
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.02	0.57
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.86	0.57
3:Q:41:LYS:HG2	3:Q:161:SER:O	2.03	0.57
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.85	0.57
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.20	0.57
5:E:227:GLU:N	5:E:227:GLU:CD	2.63	0.57
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.87	0.57
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.03	0.57
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.03	0.57
13:1:14(A):VAL:HG23	13:1:14(A):VAL:O	2.04	0.57
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.68	0.57
8:V:128:GLY:O	8:V:131:SER:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.87	0.57
8:H:159:ILE:HG22	8:H:163:ILE:HD12	1.86	0.57
10:J:167:PRO:O	10:X:168:MET:HE2	2.04	0.57
11:K:99:THR:HG22	11:K:113:VAL:HB	1.87	0.57
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.03	0.57
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.86	0.57
3:C:57:LYS:O	3:C:58:LEU:HB2	2.05	0.56
3:Q:170:LYS:HB2	16:Q:833:HOH:O	2.04	0.56
4:R:112:LEU:HD13	4:R:112:LEU:C	2.30	0.56
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.30	0.56
12:Z:175:ILE:HD12	12:Z:175:ILE:N	2.18	0.56
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.87	0.56
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.02	0.56
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.20	0.56
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.40	0.56
5:E:73:HIS:HE1	5:E:107:LEU:O	1.88	0.56
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.86	0.56
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.21	0.56
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.86	0.56
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.88	0.56
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.39	0.56
11:K:99:THR:CG2	11:K:113:VAL:HB	2.36	0.56
5:S:227:GLU:N	5:S:227:GLU:CD	2.63	0.56
2:B:181:LYS:O	2:B:184:MET:HG3	2.05	0.56
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.88	0.56
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.87	0.56
8:V:172:ASN:ND2	8:V:193:THR:HA	2.21	0.56
10:X:-1:MET:HG2	10:X:1:ASP:N	2.19	0.56
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.05	0.56
14:2:159:LEU:O	14:2:163:ILE:HD12	2.04	0.56
7:G:72:ARG:HB2	7:G:72:ARG:NH1	2.21	0.56
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.71	0.56
2:B:190:ILE:HG21	2:B:232:ILE:HD11	1.86	0.56
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.87	0.56
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.06	0.56
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.71	0.56
9:I:43:LEU:CG	9:I:45:ILE:HD11	2.35	0.56
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.21	0.56
14:N:159:LEU:O	14:N:163:ILE:HD12	2.05	0.56
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.88	0.56
2:B:31:ILE:HD11	2:B:133:GLY:C	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.70	0.56
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.98	0.56
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.40	0.56
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.87	0.55
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.21	0.55
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.87	0.55
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.41	0.55
3:C:41:LYS:HD3	3:C:161:SER:HA	1.87	0.55
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.70	0.55
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.02	0.55
6:F:109:ILE:HD13	6:F:109:ILE:H	1.71	0.55
8:H:22:GLN:CG	8:H:27:ALA:HB2	2.36	0.55
5:E:86:ARG:HG3	5:E:86:ARG:HH11	1.71	0.55
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.21	0.55
12:Z:-7:ASN:C	12:Z:-7:ASN:HD22	2.14	0.55
8:H:200:LYS:HE3	9:I:140:SER:O	2.06	0.55
1:O:214:ILE:HD13	1:O:214:ILE:H	1.72	0.55
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.36	0.55
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.72	0.55
8:H:172:ASN:ND2	8:H:193:THR:HA	2.22	0.55
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.42	0.55
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.88	0.55
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.90	0.55
10:J:-1:MET:HG2	10:J:1:ASP:H	1.72	0.55
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.89	0.55
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.21	0.55
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.22	0.55
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.88	0.55
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.87	0.55
1:O:150:GLN:O	1:O:157:TYR:HA	2.07	0.55
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.07	0.55
5:S:86:ARG:HG3	5:S:86:ARG:HH11	1.72	0.55
14:2:176:VAL:HG12	14:2:178:LEU:CD1	2.37	0.55
1:A:150:GLN:O	1:A:157:TYR:HA	2.07	0.55
2:P:239:THR:OXT	2:P:239:THR:HG22	2.06	0.55
9:W:43:LEU:CD2	9:W:45:ILE:HD11	2.37	0.55
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.06	0.55
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.88	0.55
10:J:168:MET:HE2	10:X:167:PRO:O	2.07	0.55
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.89	0.55
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:ILE:HG21	2:B:232:ILE:CD1	2.37	0.54
2:P:31:ILE:HD11	2:P:133:GLY:C	2.31	0.54
8:V:22:GLN:CG	8:V:27:ALA:HB2	2.37	0.54
9:W:43:LEU:CG	9:W:45:ILE:HD11	2.36	0.54
2:B:202:THR:HG22	2:B:204:SER:N	2.12	0.54
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.88	0.54
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.72	0.54
3:C:175:PHE:O	3:C:179:ASN:HB2	2.08	0.54
3:C:190:VAL:O	3:C:194:VAL:HG23	2.08	0.54
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.71	0.54
10:X:-1:MET:HG2	10:X:1:ASP:H	1.73	0.54
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.08	0.54
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.72	0.54
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.90	0.54
11:K:10(A):ARG:HH11	11:K:10(A):ARG:HG2	1.71	0.54
5:S:77:SER:OG	5:S:137:LEU:HB2	2.08	0.54
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.38	0.54
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.37	0.54
7:G:87:ASN:C	7:G:87:ASN:HD22	2.16	0.54
12:L:3:ILE:O	12:L:3:ILE:HD12	2.07	0.54
12:L:100:ILE:HD11	12:L:125:ARG:HG3	1.90	0.54
3:Q:163:GLN:NE2	3:Q:163:GLN:HA	2.22	0.54
13:1:40:ASN:HD22	13:1:40:ASN:N	2.00	0.54
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.89	0.54
9:I:6:MET:HE1	9:I:155:ILE:HA	1.88	0.54
11:Y:85:ASN:ND2	16:Y:215:HOH:O	2.41	0.54
13:1:4:ILE:HD12	13:1:4:ILE:O	2.07	0.54
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.08	0.54
9:I:43:LEU:HG	9:I:45:ILE:CD1	2.35	0.54
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	1.90	0.54
5:S:227:GLU:CD	5:S:227:GLU:H	2.15	0.54
8:V:41:ILE:HG12	8:V:76:VAL:HG22	1.89	0.54
3:C:163:GLN:NE2	3:C:163:GLN:HA	2.22	0.54
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.89	0.54
4:R:186:LEU:O	4:R:190:GLU:HG3	2.08	0.54
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.08	0.54
7:U:197:MET:HE3	7:U:197:MET:HA	1.90	0.54
11:Y:97:MET:HG2	11:Y:115:SER:HB3	1.90	0.54
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.89	0.54
7:G:55:PRO:HG2	7:G:56:ASP:H	1.72	0.53
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:HD22	11:K:4:LEU:C	2.33	0.53
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.38	0.53
10:X:44:SER:OG	10:X:100:LEU:HB2	2.08	0.53
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.90	0.53
14:N:176:VAL:HG12	14:N:178:LEU:CD1	2.38	0.53
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.06	0.53
6:T:109:ILE:HD13	6:T:109:ILE:H	1.73	0.53
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.05	0.53
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.09	0.53
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.43	0.53
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.21	0.53
9:W:43:LEU:HG	9:W:45:ILE:CD1	2.38	0.53
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.43	0.53
8:H:128:GLY:O	8:H:131:SER:HB2	2.08	0.53
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.90	0.53
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.91	0.53
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.90	0.53
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.90	0.53
6:T:69:VAL:HG12	16:T:811:HOH:O	2.08	0.53
7:U:49:ILE:HD12	7:U:212:VAL:HG22	1.90	0.53
3:C:46:VAL:O	3:C:215:VAL:HG12	2.09	0.53
3:C:225:SER:OG	3:C:228:GLU:HG3	2.08	0.53
8:H:210:THR:HG21	12:Z:14(C):GLN:HG2	1.91	0.53
11:K:195:LEU:O	11:K:199:VAL:HG23	2.09	0.53
7:U:55:PRO:HG2	7:U:56:ASP:H	1.73	0.53
1:A:110:LYS:HG2	16:A:285:HOH:O	2.08	0.53
1:A:214:ILE:HD13	1:A:214:ILE:H	1.73	0.53
3:C:35:THR:HB	3:C:51:GLU:HG3	1.90	0.53
14:N:14:LEU:O	14:N:175:MET:HA	2.08	0.53
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.74	0.53
3:Q:182:PRO:O	3:Q:184:ALA:N	2.42	0.53
5:S:194:VAL:O	5:S:197:ILE:HG22	2.08	0.53
7:U:151:THR:HG22	7:U:157:TYR:CB	2.38	0.53
14:2:44:CYS:HB2	14:2:100:ILE:HB	1.90	0.53
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.21	0.53
8:H:41:ILE:HG12	8:H:76:VAL:HG22	1.90	0.53
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.09	0.53
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.16	0.53
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.44	0.53
2:P:228:GLU:O	2:P:232:ILE:HG22	2.08	0.53
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:6:MET:HE1	9:W:155:ILE:HA	1.90	0.53
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.91	0.53
7:G:151:THR:HG22	7:G:157:TYR:CB	2.38	0.53
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.91	0.53
2:P:202:THR:HG22	2:P:204:SER:N	2.11	0.53
4:D:207:LEU:HD21	4:D:233:ILE:CD1	2.39	0.53
5:E:194:VAL:O	5:E:197:ILE:HG22	2.09	0.53
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.39	0.53
11:K:97:MET:HG2	11:K:115:SER:HB3	1.91	0.53
1:O:179:ARG:HB3	1:O:192:ILE:HD13	1.90	0.53
8:V:200:LYS:HE3	9:W:140:SER:O	2.08	0.53
2:B:239:THR:HG22	2:B:239:THR:OXT	2.08	0.53
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.38	0.53
2:P:122:GLY:C	2:P:124:THR:H	2.17	0.53
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.92	0.53
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.91	0.53
1:A:69:LEU:C	1:A:69:LEU:HD23	2.33	0.52
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.09	0.52
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.44	0.52
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.90	0.52
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.89	0.52
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.09	0.52
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.39	0.52
4:D:186:LEU:O	4:D:190:GLU:HG3	2.08	0.52
5:E:227:GLU:CD	5:E:227:GLU:H	2.15	0.52
14:2:14:LEU:O	14:2:175:MET:HA	2.10	0.52
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.09	0.52
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.74	0.52
10:J:167:PRO:C	10:X:168:MET:HE2	2.35	0.52
7:U:87:ASN:C	7:U:87:ASN:HD22	2.17	0.52
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.09	0.52
9:W:29:ASN:HD22	9:W:29:ASN:C	2.17	0.52
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.74	0.52
6:F:127:ASN:C	6:F:127:ASN:ND2	2.67	0.52
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.74	0.52
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.74	0.52
4:R:207:LEU:HD21	4:R:233:ILE:CD1	2.39	0.52
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.36	0.52
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.09	0.52
3:C:186:VAL:O	3:C:190:VAL:HG23	2.10	0.52
7:G:197:MET:HE3	7:G:197:MET:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.74	0.52
5:S:134:VAL:O	5:S:153:PRO:HG3	2.08	0.52
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.44	0.52
2:P:231:ASP:O	2:P:235:LYS:HG2	2.10	0.52
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.10	0.52
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.74	0.52
1:A:197:LEU:HD23	1:A:210:ILE:HD12	1.92	0.52
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.44	0.52
12:L:93:PHE:N	12:L:94:PRO:HD3	2.23	0.52
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.40	0.52
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.74	0.52
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.91	0.52
3:C:182:PRO:O	3:C:184:ALA:N	2.42	0.52
7:G:77:VAL:CG1	7:G:137:THR:HB	2.40	0.52
8:H:84:LYS:HG3	8:H:85:GLN:N	2.24	0.52
3:Q:225:SER:OG	3:Q:228:GLU:HG3	2.09	0.52
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.10	0.52
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.91	0.52
10:X:10(B):LYS:HB2	10:X:10(B):LYS:NZ	2.25	0.52
2:B:224:PHE:H	2:B:224:PHE:HD2	1.58	0.52
3:C:173:ARG:O	3:C:177:GLU:HG3	2.09	0.52
14:N:114:PRO:HD2	14:N:118:SER:O	2.10	0.52
1:O:69:LEU:C	1:O:69:LEU:HD23	2.35	0.52
8:V:84:LYS:HG3	8:V:85:GLN:N	2.25	0.52
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.34	0.52
2:B:163:ILE:HD13	2:B:164:SER:H	1.74	0.52
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.40	0.52
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.91	0.52
2:P:190:ILE:CG2	2:P:232:ILE:HD11	2.40	0.52
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.92	0.52
4:D:122:ARG:HH11	4:D:122:ARG:HG2	1.75	0.51
10:J:168:MET:HE2	10:X:167:PRO:C	2.35	0.51
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.41	0.51
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	2.10	0.51
12:L:185:ARG:NH1	16:L:1161:HOH:O	2.34	0.51
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.74	0.51
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.10	0.51
4:R:85:ALA:O	4:R:89:ILE:HG12	2.09	0.51
7:G:8:TYR:C	7:G:10:ARG:N	2.68	0.51
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.76	0.51
2:P:181:LYS:O	2:P:184:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.93	0.51
6:F:173:LYS:O	6:F:177:GLU:HG3	2.10	0.51
9:I:29:ASN:HD22	9:I:29:ASN:C	2.18	0.51
13:M:17:ASP:HA	13:M:173:PHE:CB	2.41	0.51
3:Q:195:ARG:HG3	3:Q:236:ILE:CD1	2.33	0.51
5:S:179:THR:O	5:S:179:THR:HG22	2.10	0.51
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.41	0.51
8:V:148:LYS:O	8:V:152:ILE:HD12	2.10	0.51
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.92	0.51
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.25	0.51
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.25	0.51
12:L:145:TYR:CD1	12:L:146:LEU:N	2.78	0.51
2:B:228:GLU:O	2:B:232:ILE:HG22	2.11	0.51
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.75	0.51
10:J:52:THR:CG2	10:J:53:VAL:N	2.73	0.51
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.09	0.51
12:Z:3:ILE:HD12	12:Z:3:ILE:O	2.11	0.51
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.78	0.51
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.93	0.51
6:T:173:LYS:O	6:T:177:GLU:HG3	2.11	0.51
7:U:77:VAL:CG1	7:U:137:THR:HB	2.40	0.51
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.20	0.51
2:B:231:ASP:O	2:B:235:LYS:HG2	2.11	0.51
2:B:232:ILE:HG13	2:B:232:ILE:O	2.11	0.51
10:J:44:SER:OG	10:J:100:LEU:HB2	2.11	0.51
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.10	0.51
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.41	0.51
7:U:83:PRO:HG2	16:U:557:HOH:O	2.09	0.51
1:A:214:ILE:HD13	1:A:222:ARG:O	2.11	0.51
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.93	0.51
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.07	0.51
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.93	0.51
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.93	0.51
7:U:227:GLU:HG2	16:U:1255:HOH:O	2.09	0.51
14:2:51:ASP:O	14:2:55:ILE:HG13	2.11	0.51
14:2:114:PRO:HD2	14:2:118:SER:O	2.09	0.51
5:E:179:THR:HG22	5:E:179:THR:O	2.11	0.51
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.08	0.51
3:Q:241:GLN:C	3:Q:243:GLN:N	2.68	0.51
4:R:53:ARG:O	4:R:53:ARG:HG2	2.11	0.51
6:T:127:ASN:C	6:T:127:ASN:ND2	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:172:ILE:HD13	7:U:197:MET:CE	2.41	0.51
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.93	0.51
9:I:111:ALA:C	9:I:125:ILE:HD12	2.36	0.51
6:T:210:LEU:HD23	6:T:233:ILE:HD13	1.93	0.51
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.92	0.51
10:X:2:ILE:O	10:X:3:ILE:HD13	2.11	0.51
12:Z:3:ILE:HD12	12:Z:3:ILE:C	2.36	0.51
3:C:241:GLN:C	3:C:243:GLN:N	2.68	0.50
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.46	0.50
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.46	0.50
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.46	0.50
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.76	0.50
11:K:86:LEU:C	11:K:86:LEU:HD13	2.36	0.50
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.26	0.50
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.18	0.50
1:O:197:LEU:HD23	1:O:210:ILE:HD12	1.93	0.50
4:R:138:ILE:HD12	4:R:138:ILE:N	2.26	0.50
10:X:52:THR:CG2	10:X:53:VAL:N	2.74	0.50
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.46	0.50
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.76	0.50
1:A:173:LYS:O	1:A:177:GLU:HG3	2.12	0.50
2:B:224:PHE:N	2:B:224:PHE:CD2	2.80	0.50
4:D:177:LEU:CD2	5:E:58:LEU:HD13	2.39	0.50
5:E:77:SER:OG	5:E:137:LEU:HB2	2.10	0.50
5:E:134:VAL:O	5:E:153:PRO:HG3	2.10	0.50
6:F:127:ASN:HD22	6:F:128:SER:N	2.09	0.50
12:L:79:ALA:O	12:L:83:ILE:HG13	2.12	0.50
13:M:149:GLN:NE2	13:M:149:GLN:H	2.09	0.50
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.42	0.50
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.42	0.50
2:B:122:GLY:C	2:B:124:THR:H	2.19	0.50
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.93	0.50
3:C:70:ILE:HD11	3:C:76:LEU:CB	2.41	0.50
7:G:158:VAL:HG22	7:G:159:GLY:N	2.26	0.50
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.93	0.50
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.26	0.50
3:Q:70:ILE:HD11	3:Q:76:LEU:CB	2.40	0.50
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.94	0.50
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.47	0.50
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.41	0.50
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.41	0.50
2:P:224:PHE:N	2:P:224:PHE:CD2	2.80	0.50
9:I:43:LEU:CD2	9:I:45:ILE:HD11	2.41	0.50
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.42	0.50
2:P:224:PHE:H	2:P:224:PHE:HD2	1.57	0.50
1:A:117:ALA:HB1	1:A:155:GLY:O	2.12	0.50
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.27	0.50
13:M:40:ASN:HD22	13:M:40:ASN:N	1.99	0.50
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.71	0.50
4:R:65:GLU:HA	16:R:750:HOH:O	2.12	0.50
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.94	0.50
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.42	0.50
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.93	0.50
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.92	0.50
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.94	0.50
13:1:149:GLN:H	13:1:149:GLN:NE2	2.10	0.50
4:D:53:ARG:O	4:D:53:ARG:HG2	2.12	0.49
1:O:117:ALA:HB1	1:O:155:GLY:O	2.12	0.49
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.77	0.49
2:B:234:VAL:HA	2:B:239:THR:HA	1.93	0.49
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.94	0.49
7:U:49:ILE:CD1	7:U:212:VAL:HG22	2.42	0.49
7:U:192:PHE:CD1	7:U:192:PHE:C	2.89	0.49
2:B:225:LYS:HB2	2:B:228:GLU:HG3	1.94	0.49
8:H:4:VAL:HG13	8:H:159:ILE:CD1	2.43	0.49
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.48	0.49
1:O:58:LEU:HB3	7:U:162:ALA:O	2.12	0.49
2:P:234:VAL:HA	2:P:239:THR:HA	1.93	0.49
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.94	0.49
16:V:1181:HOH:O	9:W:150:ASP:HA	2.11	0.49
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.94	0.49
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.12	0.49
7:G:172:ILE:HD13	7:G:197:MET:CE	2.43	0.49
4:R:70:ILE:HG13	4:R:74:ILE:HG22	1.94	0.49
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.95	0.49
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.94	0.49
4:D:229:THR:O	4:D:233:ILE:HG12	2.13	0.49
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.94	0.49
7:G:49:ILE:CD1	7:G:212:VAL:HG22	2.42	0.49
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.12	0.49
12:L:3:ILE:HD12	12:L:3:ILE:C	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.76	0.49
2:P:224:PHE:N	2:P:224:PHE:HD2	2.10	0.49
6:T:127:ASN:HD22	6:T:128:SER:N	2.10	0.49
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.12	0.49
13:1:184:LEU:C	13:1:184:LEU:HD23	2.38	0.49
9:I:113:PHE:HA	9:I:118:CYS:O	2.12	0.49
7:U:158:VAL:HG22	7:U:159:GLY:N	2.28	0.49
9:W:14:ILE:HG12	9:W:34:ILE:HD12	1.95	0.49
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.95	0.49
2:B:190:ILE:HG23	2:B:212:PHE:HE2	1.76	0.49
2:B:224:PHE:HD2	2:B:224:PHE:N	2.10	0.49
3:C:70:ILE:N	3:C:70:ILE:HD12	2.27	0.49
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.13	0.49
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.78	0.49
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.77	0.49
7:U:82:ILE:N	7:U:83:PRO:HD2	2.28	0.49
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.13	0.49
12:Z:99:THR:HG23	16:Z:231:HOH:O	2.13	0.49
4:D:170:GLU:OE1	4:D:170:GLU:N	2.44	0.49
5:E:4:PHE:CG	5:E:5:ARG:N	2.79	0.49
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.47	0.49
2:P:87:ILE:O	2:P:91:THR:HG23	2.12	0.49
3:Q:70:ILE:N	3:Q:70:ILE:HD12	2.28	0.49
7:U:8:TYR:C	7:U:10:ARG:N	2.69	0.49
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.94	0.49
13:1:7:LYS:HB3	13:1:12:VAL:HG12	1.95	0.49
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.48	0.49
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.94	0.49
12:L:166:HIS:CD2	12:L:168:GLN:H	2.25	0.49
2:P:112:LEU:HD23	2:P:112:LEU:O	2.12	0.49
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.37	0.49
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.78	0.49
5:S:162:GLY:O	6:T:58:LEU:HD13	2.13	0.49
9:W:113:PHE:HA	9:W:118:CYS:O	2.12	0.49
12:Z:100:ILE:HD11	12:Z:125:ARG:HG3	1.93	0.49
3:C:227:GLU:OE1	3:C:227:GLU:N	2.46	0.49
4:D:194:LEU:HG	4:D:233:ILE:HD13	1.95	0.49
14:N:94:ASN:ND2	16:N:946:HOH:O	2.43	0.49
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.13	0.48
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.93	0.48
7:U:228:ASN:HB3	16:U:242:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:128:GLY:O	8:V:131:SER:CB	2.60	0.48
12:Z:79:ALA:O	12:Z:83:ILE:HG13	2.13	0.48
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.12	0.48
4:D:17:PRO:HD2	16:D:1171:HOH:O	2.12	0.48
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.96	0.48
1:O:24:ILE:CD1	1:O:24:ILE:N	2.76	0.48
1:O:173:LYS:O	1:O:177:GLU:HG3	2.13	0.48
2:P:101:LYS:HZ2	10:X:85:GLN:HE21	1.60	0.48
4:R:170:GLU:OE1	4:R:170:GLU:N	2.43	0.48
5:S:4:PHE:CG	5:S:5:ARG:N	2.79	0.48
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.95	0.48
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.95	0.48
8:V:53:GLU:HB2	16:V:1327:HOH:O	2.12	0.48
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.94	0.48
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.27	0.48
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.11	0.48
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.95	0.48
1:A:97:HIS:CD2	8:H:61:SER:OG	2.64	0.48
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.13	0.48
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.76	0.48
1:O:214:ILE:HD13	1:O:222:ARG:O	2.13	0.48
7:U:70:ILE:HD12	7:U:92:ALA:HB3	1.95	0.48
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.13	0.48
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.95	0.48
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.77	0.48
4:D:85:ALA:O	4:D:89:ILE:HG12	2.13	0.48
6:F:35:THR:CG2	6:F:51:GLU:O	2.59	0.48
7:G:192:PHE:CD1	7:G:192:PHE:C	2.90	0.48
8:H:128:GLY:O	8:H:131:SER:CB	2.61	0.48
9:I:14:ILE:HG12	9:I:34:ILE:HD12	1.94	0.48
4:R:59:LEU:C	4:R:59:LEU:HD13	2.38	0.48
5:S:41:ARG:NH1	5:S:42:SER:O	2.45	0.48
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.14	0.48
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.43	0.48
2:B:185:LYS:CD	2:B:187:ASP:H	2.26	0.48
4:D:138:ILE:N	4:D:138:ILE:HD12	2.28	0.48
13:M:7:LYS:HB3	13:M:12:VAL:HG12	1.94	0.48
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.96	0.48
5:E:38:VAL:HG12	5:E:39:GLY:N	2.27	0.48
5:E:223:ILE:N	5:E:223:ILE:HD12	2.29	0.48
7:G:82:ILE:N	7:G:83:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:HD13	11:K:15:ALA:O	2.13	0.48
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.14	0.48
2:P:185:LYS:CD	2:P:187:ASP:H	2.27	0.48
4:R:194:LEU:HG	4:R:233:ILE:HD13	1.95	0.48
16:T:244:HOH:O	7:U:86:ARG:HD2	2.12	0.48
12:Z:99:THR:CG2	16:Z:231:HOH:O	2.61	0.48
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.25	0.48
13:1:17:ASP:HA	13:1:173:PHE:CB	2.43	0.48
6:F:210:LEU:HD23	6:F:233:ILE:HD13	1.96	0.48
7:G:18(D):ILE:HD13	7:G:18(D):ILE:N	2.27	0.48
11:K:138:LEU:HD13	11:K:158:SER:OG	2.13	0.48
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.76	0.48
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.49	0.48
5:S:221:PHE:CE1	5:S:223:ILE:CD1	2.94	0.48
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.95	0.48
8:V:4:VAL:HG13	8:V:159:ILE:CD1	2.44	0.48
9:W:48:LEU:HG	9:W:50:THR:HG22	1.95	0.48
1:A:24:ILE:CD1	1:A:24:ILE:N	2.76	0.48
2:B:87:ILE:O	2:B:91:THR:HG23	2.12	0.48
8:H:175:VAL:HG12	8:H:176:CYS:N	2.29	0.48
11:K:37:ILE:HB	11:K:41:LEU:HB2	1.95	0.48
14:N:107:LYS:CG	14:N:108:GLY:H	2.19	0.48
2:P:163:ILE:HD13	2:P:164:SER:H	1.77	0.48
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.14	0.48
7:U:78:VAL:HG11	7:U:85:ALA:HB2	1.96	0.48
10:X:-1:MET:HE1	10:X:98:ASN:ND2	2.28	0.48
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.48	0.48
2:B:112:LEU:HD23	2:B:112:LEU:O	2.13	0.48
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.14	0.48
5:E:54:ASN:ND2	5:E:56:ASP:O	2.47	0.48
4:D:59:LEU:HD13	4:D:59:LEU:C	2.38	0.48
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.49	0.48
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.42	0.48
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.96	0.48
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.29	0.48
12:L:140:ASN:O	12:L:144:PHE:HA	2.14	0.48
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.49	0.48
1:O:62:GLU:H	1:O:62:GLU:CD	2.21	0.48
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.44	0.48
3:C:235:GLN:O	3:C:239:GLU:HG2	2.14	0.47
6:F:99:PHE:CD2	6:F:107:ILE:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.59	0.47
16:A:244:HOH:O	2:B:10:SER:HB2	2.14	0.47
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.09	0.47
4:D:70:ILE:HG13	4:D:74:ILE:HG22	1.96	0.47
5:E:221:PHE:CE1	5:E:223:ILE:CD1	2.94	0.47
7:G:203:THR:HG22	7:G:204:GLU:N	2.29	0.47
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.14	0.47
7:U:172:ILE:CD1	7:U:197:MET:HE1	2.44	0.47
12:Z:3:ILE:HD13	12:Z:100:ILE:HD12	1.96	0.47
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.15	0.47
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.96	0.47
11:K:12:ILE:HB	11:K:178:VAL:HB	1.96	0.47
11:K:207:ASN:ND2	10:X:144:PRO:HG3	2.29	0.47
13:M:184:LEU:HD23	13:M:184:LEU:C	2.38	0.47
5:S:38:VAL:HG12	5:S:39:GLY:N	2.28	0.47
7:U:203:THR:HG22	7:U:204:GLU:N	2.30	0.47
10:X:133:TYR:CZ	10:X:166:MET:HG3	2.48	0.47
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.50	0.47
2:P:190:ILE:HG23	2:P:212:PHE:HE2	1.77	0.47
5:S:18(C):PHE:CA	5:S:18(F):ILE:HG13	2.38	0.47
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.15	0.47
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.14	0.47
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.15	0.47
7:G:225:SER:OG	7:G:228:ASN:ND2	2.47	0.47
5:S:223:ILE:N	5:S:223:ILE:HD12	2.30	0.47
6:T:147:HIS:HD2	16:T:242:HOH:O	1.96	0.47
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.63	0.47
7:U:139:VAL:HA	7:U:147:SER:O	2.15	0.47
7:U:203:THR:HG22	7:U:204:GLU:O	2.15	0.47
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.45	0.47
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.95	0.47
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.27	0.47
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.61	0.47
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.30	0.47
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.50	0.47
2:B:150:THR:O	2:B:157:TYR:HA	2.14	0.47
2:B:202:THR:CG2	2:B:204:SER:HB2	2.44	0.47
3:C:168:ASN:O	3:C:172:VAL:HG12	2.15	0.47
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.96	0.47
8:H:159:ILE:N	8:H:159:ILE:HD13	2.30	0.47
9:I:48:LEU:HG	9:I:50:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.97	0.47
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.40	0.47
14:N:51:ASP:O	14:N:55:ILE:HG13	2.15	0.47
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.97	0.47
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.49	0.47
4:R:229:THR:O	4:R:233:ILE:HG12	2.13	0.47
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.44	0.47
7:U:225:SER:OG	7:U:228:ASN:ND2	2.48	0.47
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.61	0.47
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.27	0.47
3:C:55:THR:C	3:C:56:LEU:HD22	2.40	0.47
4:D:24:VAL:O	4:D:27:SER:HB3	2.14	0.47
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.45	0.47
8:V:175:VAL:HG12	8:V:176:CYS:N	2.29	0.47
1:A:179:ARG:HB3	1:A:192:ILE:HD13	1.96	0.47
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.96	0.47
3:C:195:ARG:HG3	3:C:236:ILE:CD1	2.37	0.47
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.11	0.47
10:J:133:TYR:CZ	10:J:166:MET:HG3	2.50	0.47
13:M:139:ARG:NH1	8:V:165:ASN:HD22	2.05	0.47
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.50	0.47
9:W:101:VAL:O	9:W:110:ILE:HA	2.15	0.47
13:1:14(D):GLU:O	13:1:14(G):ILE:HD12	2.14	0.47
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.15	0.47
7:G:151:THR:HG22	7:G:157:TYR:HB3	1.97	0.47
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.15	0.47
6:T:13:SER:HB2	7:U:130:ARG:HD3	1.97	0.47
11:Y:37:ILE:HB	11:Y:41:LEU:HB2	1.96	0.47
1:A:62:GLU:CD	1:A:62:GLU:H	2.22	0.46
10:J:-1:MET:HE1	10:J:98:ASN:ND2	2.30	0.46
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.97	0.46
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.97	0.46
10:X:10(B):LYS:HB2	10:X:10(B):LYS:HZ2	1.79	0.46
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.44	0.46
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.30	0.46
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.47	0.46
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.15	0.46
4:D:175:GLU:CG	4:D:196:ILE:HD13	2.46	0.46
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.97	0.46
2:P:196:THR:O	2:P:200:THR:HG23	2.16	0.46
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:53:LEU:HD13	6:T:20(C):LYS:HD2	1.98	0.46
14:2:126:ILE:N	14:2:126:ILE:CD1	2.79	0.46
1:A:24:ILE:HD12	1:A:131:PRO:HG2	1.97	0.46
1:A:233:LEU:O	1:A:236:LEU:HB2	2.15	0.46
2:B:185:LYS:HD2	2:B:187:ASP:H	1.79	0.46
3:C:169:SER:HA	3:C:172:VAL:CG1	2.45	0.46
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.97	0.46
6:F:43:ASN:HD22	6:F:44:ASP:N	2.14	0.46
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.62	0.46
2:P:185:LYS:HD2	2:P:187:ASP:H	1.80	0.46
2:P:225:LYS:HB2	2:P:228:GLU:HG3	1.97	0.46
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.97	0.46
7:U:136:LEU:O	7:U:150:LYS:HA	2.14	0.46
10:X:2:ILE:HD12	10:X:2:ILE:N	2.30	0.46
8:H:148:LYS:O	8:H:152:ILE:HD12	2.16	0.46
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.97	0.46
10:J:2:ILE:O	10:J:3:ILE:HD13	2.15	0.46
10:J:113:ILE:HA	10:J:118:THR:O	2.16	0.46
1:O:233:LEU:O	1:O:236:LEU:HB2	2.15	0.46
3:Q:57:LYS:NZ	16:Q:434:HOH:O	2.48	0.46
7:U:87:ASN:C	7:U:87:ASN:ND2	2.72	0.46
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.97	0.46
13:1:113:VAL:HA	13:1:118:VAL:O	2.16	0.46
14:2:107:LYS:CG	14:2:108:GLY:H	2.21	0.46
9:I:44:GLY:O	9:I:45:ILE:HD13	2.16	0.46
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.46	0.46
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.11	0.46
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.97	0.46
11:K:10(A):ARG:HD3	11:K:180:GLU:OE1	2.16	0.46
13:M:113:VAL:HA	13:M:118:VAL:O	2.16	0.46
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.97	0.46
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.80	0.46
5:E:18(C):PHE:CA	5:E:18(F):ILE:HG13	2.39	0.46
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.50	0.46
2:P:232:ILE:HG13	2:P:232:ILE:O	2.15	0.46
6:T:99:PHE:CD2	6:T:107:ILE:HD12	2.50	0.46
13:1:57:ARG:HH11	13:1:57:ARG:HG2	1.81	0.46
5:S:76:LEU:O	5:S:76:LEU:HD23	2.15	0.46
7:U:225:SER:O	7:U:229:ILE:HG13	2.16	0.46
2:B:122:GLY:C	2:B:124:THR:N	2.75	0.46
10:J:2:ILE:N	10:J:2:ILE:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:122:GLY:C	2:P:124:THR:N	2.73	0.46
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.51	0.46
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.31	0.46
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.97	0.46
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.98	0.46
12:Z:173:LEU:HG	12:Z:175:ILE:HD11	1.98	0.46
1:A:39:GLY:HA2	1:A:47:VAL:O	2.17	0.45
2:B:141:TYR:CD1	2:B:141:TYR:C	2.94	0.45
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.98	0.45
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.98	0.45
13:M:4:ILE:HD12	13:M:4:ILE:C	2.41	0.45
2:P:150:THR:O	2:P:157:TYR:HA	2.16	0.45
7:U:82:ILE:HG22	7:U:83:PRO:HD3	1.98	0.45
8:V:81:GLN:O	8:V:85:GLN:HG3	2.16	0.45
8:V:172:ASN:HB3	8:V:192:LEU:O	2.16	0.45
11:Y:4:LEU:HD13	11:Y:15:ALA:O	2.16	0.45
11:Y:10(A):ARG:HD3	11:Y:180:GLU:OE1	2.17	0.45
5:E:230:ALA:C	5:E:232:TYR:H	2.24	0.45
8:H:144:GLN:O	8:H:145:ASP:HB2	2.16	0.45
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.99	0.45
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	2.31	0.45
2:P:202:THR:CG2	2:P:204:SER:HB2	2.46	0.45
5:S:201:LEU:O	5:S:202:ARG:HB2	2.16	0.45
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.46	0.45
8:V:159:ILE:HD13	8:V:159:ILE:N	2.30	0.45
9:W:29:ASN:ND2	9:W:29:ASN:H	2.14	0.45
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.16	0.45
3:C:158:SER:CB	4:D:59:LEU:HD21	2.46	0.45
6:F:82:ILE:HD13	6:F:82:ILE:N	2.30	0.45
13:M:40:ASN:N	13:M:40:ASN:ND2	2.64	0.45
5:S:54:ASN:ND2	5:S:56:ASP:O	2.49	0.45
5:S:68:ILE:HB	5:S:76:LEU:HD21	1.99	0.45
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.16	0.45
4:D:12(D):ALA:HA	5:E:129:GLY:CA	2.42	0.45
6:F:229:LEU:O	6:F:233:ILE:HG12	2.16	0.45
7:G:70:ILE:HD12	7:G:92:ALA:HB3	1.96	0.45
9:I:11:CYS:HA	9:I:104:ILE:HD11	1.98	0.45
12:L:3:ILE:HD13	12:L:100:ILE:HD12	1.99	0.45
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.44	0.45
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.16	0.45
5:E:41:ARG:NH1	5:E:42:SER:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:222:THR:C	5:E:223:ILE:HD12	2.41	0.45
7:G:136:LEU:O	7:G:150:LYS:HA	2.16	0.45
8:H:148:LYS:HE3	8:H:177:VAL:HG11	1.97	0.45
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.75	0.45
1:O:39:GLY:HA2	1:O:47:VAL:O	2.16	0.45
6:T:35:THR:CG2	6:T:51:GLU:O	2.61	0.45
7:U:18(H):GLU:N	7:U:18(H):GLU:CD	2.74	0.45
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.97	0.45
8:V:148:LYS:HE3	8:V:177:VAL:HG11	1.97	0.45
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.30	0.45
12:Z:27:ASN:HB3	13:1:120:TYR:CE1	2.52	0.45
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.16	0.45
5:E:220:PRO:O	5:E:222:THR:HG23	2.16	0.45
7:G:172:ILE:CD1	7:G:197:MET:HE1	2.46	0.45
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.98	0.45
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.99	0.45
12:L:-2:ASN:HA	12:L:21:ILE:O	2.16	0.45
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.46	0.45
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.80	0.45
5:S:138:ILE:N	5:S:138:ILE:HD12	2.32	0.45
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.52	0.45
7:G:52:LYS:HA	16:G:414:HOH:O	2.17	0.45
10:X:113:ILE:HA	10:X:118:THR:O	2.15	0.45
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.98	0.45
7:G:212:VAL:HG23	7:G:229:ILE:HD13	1.97	0.45
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.51	0.45
1:O:24:ILE:HD12	1:O:131:PRO:HG2	1.99	0.45
3:Q:112:LEU:O	3:Q:112:LEU:HD13	2.17	0.45
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.31	0.45
6:T:107:ILE:HG12	6:T:112:PHE:HB2	1.99	0.45
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.52	0.45
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.57	0.45
12:L:-9:GLN:HG2	13:M:-8:THR:HG21	1.98	0.45
2:P:44:ASP:OD2	2:P:44:ASP:N	2.49	0.45
3:Q:136:THR:O	3:Q:150:GLN:HA	2.17	0.45
4:R:237:LEU:O	4:R:241:GLU:HG3	2.17	0.45
5:S:40:LEU:N	5:S:40:LEU:HD23	2.32	0.45
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.31	0.45
11:Y:32:LYS:HD2	11:Y:32:LYS:N	2.32	0.45
11:K:6:PHE:HA	11:K:123:ASP:O	2.17	0.45
14:N:10(B):LYS:HD3	14:N:10(B):LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.13	0.45
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.47	0.45
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.17	0.45
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.60	0.45
3:C:227:GLU:H	3:C:227:GLU:CD	2.26	0.44
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.44	0.44
7:G:139:VAL:HA	7:G:147:SER:O	2.16	0.44
7:G:203:THR:HG22	7:G:204:GLU:O	2.17	0.44
5:S:222:THR:C	5:S:223:ILE:HD12	2.42	0.44
7:U:140:SER:HA	7:U:215:ALA:HB1	1.99	0.44
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.62	0.44
7:G:87:ASN:C	7:G:87:ASN:ND2	2.72	0.44
9:I:29:ASN:ND2	9:I:29:ASN:H	2.14	0.44
9:I:101:VAL:O	9:I:110:ILE:HA	2.17	0.44
13:M:91:ARG:HG3	13:M:92:SER:N	2.31	0.44
14:N:126:ILE:N	14:N:126:ILE:CD1	2.79	0.44
1:O:24:ILE:N	1:O:24:ILE:HD13	2.32	0.44
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.18	0.44
3:Q:18(A):ASP:OD2	3:Q:18(C):LYS:HG2	2.16	0.44
5:S:220:PRO:O	5:S:222:THR:HG23	2.17	0.44
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.81	0.44
8:V:144:GLN:O	8:V:145:ASP:HB2	2.17	0.44
12:Z:22:THR:O	12:Z:23:ASP:HB2	2.17	0.44
14:2:144:GLU:HG2	16:2:1115:HOH:O	2.16	0.44
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.18	0.44
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.51	0.44
5:E:138:ILE:HD12	5:E:138:ILE:N	2.33	0.44
6:F:53:LEU:HD13	6:F:20(C):LYS:HD2	1.98	0.44
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.47	0.44
9:I:44:GLY:C	9:I:45:ILE:HD13	2.42	0.44
10:J:20:VAL:HG11	11:K:120:LEU:HD11	2.00	0.44
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.32	0.44
13:M:14(C):ARG:CG	13:M:14(C):ARG:NH1	2.75	0.44
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.18	0.44
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.57	0.44
7:U:18(D):ILE:N	7:U:18(D):ILE:HD13	2.33	0.44
2:B:11:ARG:O	2:B:14:ILE:HD13	2.17	0.44
5:E:18(D):ILE:HG12	5:E:18(D):ILE:O	2.16	0.44
6:F:50:VAL:HG22	6:F:51:GLU:N	2.32	0.44
7:G:140:SER:HA	7:G:215:ALA:HB1	1.99	0.44
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:141:TYR:CD1	2:P:141:TYR:C	2.96	0.44
4:R:175:GLU:CG	4:R:196:ILE:HD13	2.47	0.44
5:S:15:PHE:N	6:T:23:GLN:HE22	1.95	0.44
6:T:192:GLN:O	6:T:196:ILE:HG13	2.17	0.44
9:W:6:MET:HE3	9:W:155:ILE:HA	1.99	0.44
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.73	0.44
3:C:57:LYS:HD2	3:C:58:LEU:N	2.32	0.44
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.53	0.44
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.47	0.44
6:F:16:SER:OG	6:F:18:ASP:OD2	2.31	0.44
7:G:78:VAL:HG11	7:G:85:ALA:HB2	2.00	0.44
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.42	0.44
6:T:203:GLU:C	6:T:205:ASN:H	2.25	0.44
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.00	0.44
13:1:4:ILE:HD12	13:1:4:ILE:C	2.42	0.44
13:1:175:LEU:HD23	13:1:175:LEU:C	2.43	0.44
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.47	0.44
4:D:237:LEU:O	4:D:241:GLU:HG3	2.18	0.44
6:F:13:SER:HB2	7:G:130:ARG:HD3	1.99	0.44
6:F:107:ILE:HG12	6:F:112:PHE:HB2	1.99	0.44
9:I:6:MET:HG2	9:I:124:PHE:HB3	1.99	0.44
11:K:38:ASN:C	11:K:38:ASN:OD1	2.60	0.44
1:O:195:LEU:HD23	1:O:236:LEU:HD21	2.00	0.44
6:T:157:TYR:CD1	6:T:157:TYR:C	2.96	0.44
7:U:151:THR:HG22	7:U:157:TYR:HB3	1.98	0.44
5:E:76:LEU:HD23	5:E:76:LEU:O	2.17	0.44
5:E:201:LEU:O	5:E:202:ARG:HB2	2.17	0.44
7:G:82:ILE:HG22	7:G:83:PRO:HD3	1.99	0.44
13:M:165:ARG:HA	14:2:26:ILE:HB	2.00	0.44
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.48	0.44
4:R:24:VAL:O	4:R:27:SER:HB3	2.17	0.44
5:S:4:PHE:O	5:S:5:ARG:C	2.60	0.44
7:U:96:ALA:CA	7:U:107:MET:CE	2.89	0.44
2:B:27:ALA:O	2:B:31:ILE:HG12	2.18	0.44
2:B:196:THR:O	2:B:200:THR:HG23	2.17	0.44
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.33	0.44
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.35	0.44
12:L:5:GLY:O	12:L:124:CYS:HA	2.18	0.44
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.18	0.44
5:S:230:ALA:C	5:S:232:TYR:H	2.25	0.44
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:THR:HG22	2:B:63:THR:O	2.18	0.44
2:B:81:LEU:HD23	2:B:133:GLY:HA3	2.00	0.44
6:F:203:GLU:C	6:F:205:ASN:H	2.25	0.44
11:K:32:LYS:HD2	11:K:32:LYS:N	2.32	0.44
11:K:142:TYR:C	11:K:143:LYS:HD2	2.43	0.44
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.53	0.44
6:T:43:ASN:HD22	6:T:44:ASP:N	2.15	0.44
6:T:78:TYR:CE1	6:T:85:GLY:HA3	2.53	0.44
6:T:87:HIS:HD2	6:T:132:PHE:CE2	2.36	0.44
7:U:18(H):GLU:CD	7:U:18(H):GLU:H	2.26	0.44
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.99	0.44
12:Z:-9:GLN:HG2	13:1:-8:THR:HG21	2.00	0.44
13:1:113:VAL:HG23	13:1:119:THR:HG22	1.99	0.44
13:1:157:ASN:HB3	16:1:558:HOH:O	2.17	0.44
13:1:205:GLY:HA3	13:1:209:GLN:HB3	2.00	0.44
4:D:215:ILE:C	4:D:215:ILE:HD13	2.43	0.43
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.48	0.43
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.18	0.43
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.53	0.43
5:S:76:LEU:HD23	5:S:76:LEU:C	2.43	0.43
6:T:82:ILE:HB	6:T:83:PRO:HD3	2.00	0.43
8:V:172:ASN:ND2	16:V:1000:HOH:O	2.50	0.43
10:X:35:ARG:HH11	10:X:57:GLU:HG2	1.83	0.43
11:Y:70:GLU:O	11:Y:71:LYS:C	2.60	0.43
14:2:84:LYS:HZ3	14:2:119:VAL:HG23	1.83	0.43
16:D:1143:HOH:O	5:E:86:ARG:HD3	2.18	0.43
5:E:4:PHE:O	5:E:5:ARG:C	2.61	0.43
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.39	0.43
13:M:9:ASP:OD1	13:M:10:ASN:N	2.51	0.43
13:M:14(D):GLU:HA	13:M:14(G):ILE:HD12	2.00	0.43
1:O:97:HIS:CD2	8:V:61:SER:OG	2.68	0.43
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.27	0.43
5:S:39:GLY:O	5:S:162:GLY:HA2	2.18	0.43
4:D:195:LYS:HE2	4:D:199:GLN:OE1	2.19	0.43
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.99	0.43
2:P:27:ALA:O	2:P:31:ILE:HG12	2.19	0.43
2:P:63:THR:HG22	2:P:63:THR:O	2.18	0.43
6:T:12:ASN:OD1	6:T:12:ASN:C	2.61	0.43
9:W:11:CYS:HA	9:W:104:ILE:HD11	1.99	0.43
9:W:12:VAL:HG13	9:W:108:PRO:HB3	2.00	0.43
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:212:ILE:HG22	5:E:213:ALA:N	2.33	0.43
7:G:186:TRP:O	7:G:190:VAL:HG23	2.19	0.43
10:J:3:ILE:HD13	10:J:3:ILE:HA	1.80	0.43
6:T:229:LEU:O	6:T:233:ILE:HG12	2.19	0.43
7:U:186:TRP:O	7:U:190:VAL:HG23	2.18	0.43
9:W:43:LEU:HD21	9:W:45:ILE:HD11	1.99	0.43
7:G:18(D):ILE:N	7:G:18(D):ILE:CD1	2.81	0.43
10:J:124:TYR:CD2	10:J:138:LEU:HD13	2.54	0.43
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.48	0.43
3:Q:215:VAL:HG23	3:Q:221:ILE:HG13	2.00	0.43
5:S:69:LYS:HB3	16:S:528:HOH:O	2.18	0.43
12:Z:176:LEU:CD1	12:Z:186:LYS:HG2	2.48	0.43
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.84	0.43
2:B:213:ALA:HA	2:B:222:LYS:O	2.19	0.43
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.53	0.43
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.19	0.43
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.33	0.43
7:U:18(D):ILE:N	7:U:18(D):ILE:CD1	2.81	0.43
13:1:104:VAL:CG2	13:1:178:ILE:HG22	2.44	0.43
13:1:14(D):GLU:HA	13:1:14(G):ILE:HD12	2.01	0.43
3:C:112:LEU:HD13	3:C:112:LEU:O	2.18	0.43
3:C:18(A):ASP:OD2	3:C:18(C):LYS:HG2	2.18	0.43
5:E:40:LEU:N	5:E:40:LEU:HD23	2.34	0.43
5:E:139:ILE:HG22	5:E:148:LEU:HD13	2.00	0.43
7:G:228:ASN:N	7:G:228:ASN:HD22	2.17	0.43
8:H:3:ILE:O	8:H:126:SER:HA	2.19	0.43
8:H:165:ASN:HD22	13:1:139:ARG:NH1	2.06	0.43
8:H:167:LEU:HD22	12:Z:167:ILE:O	2.19	0.43
8:H:172:ASN:HB3	8:H:192:LEU:O	2.18	0.43
1:O:92:SER:O	1:O:95:VAL:HG12	2.19	0.43
3:Q:159:SER:HB2	16:Q:1140:HOH:O	2.19	0.43
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	2.01	0.43
1:A:32:LYS:HA	1:A:32:LYS:HE2	2.00	0.43
1:A:186:LEU:O	1:A:190:ILE:HG13	2.19	0.43
2:B:15:PHE:N	3:C:23:GLN:HE22	1.92	0.43
3:C:97:GLN:NE2	16:C:6:HOH:O	2.51	0.43
5:E:90:ASN:O	5:E:94:GLN:HG3	2.18	0.43
6:F:12:ASN:OD1	6:F:12:ASN:C	2.62	0.43
6:F:157:TYR:C	6:F:157:TYR:CD1	2.96	0.43
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.81	0.43
5:S:104:ASN:HB2	13:1:81:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.16	0.43
2:B:90:ASN:O	2:B:94:ILE:HD12	2.19	0.43
5:E:68:ILE:HB	5:E:76:LEU:HD21	2.01	0.43
7:G:225:SER:O	7:G:229:ILE:HG13	2.19	0.43
13:M:57:ARG:HG2	13:M:57:ARG:HH11	1.84	0.43
3:Q:215:VAL:HG23	3:Q:221:ILE:CG1	2.48	0.43
5:S:231:LYS:H	5:S:231:LYS:HD2	1.84	0.43
7:U:212:VAL:HG23	7:U:229:ILE:HD13	2.00	0.43
10:X:166:MET:HA	10:X:167:PRO:HD3	1.82	0.43
14:2:155:ILE:HG22	14:2:175:MET:HE2	2.01	0.43
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.73	0.43
4:D:12(E):SER:O	5:E:123:ASN:OD1	2.37	0.43
5:E:52:LYS:HB3	5:E:63:TYR:HB3	2.00	0.43
9:I:12:VAL:HG23	9:I:178:ILE:HB	2.01	0.43
11:K:8:PHE:HA	11:K:144:TRP:CE3	2.53	0.43
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	2.01	0.43
4:R:215:ILE:HD13	4:R:215:ILE:C	2.43	0.43
9:W:6:MET:HG2	9:W:124:PHE:HB3	2.00	0.43
10:X:35:ARG:HH11	10:X:57:GLU:CG	2.31	0.43
12:Z:27:ASN:HB3	13:1:120:TYR:CZ	2.54	0.43
5:E:104:ASN:HB2	13:M:81:GLU:HG2	2.00	0.42
5:E:231:LYS:H	5:E:231:LYS:HD2	1.84	0.42
10:J:18:LYS:HG2	10:J:174:ILE:HG13	2.01	0.42
13:M:14(D):GLU:O	13:M:14(G):ILE:HD12	2.18	0.42
1:O:124:THR:CG2	2:P:130:ARG:NH2	2.69	0.42
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.24	0.42
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.48	0.42
9:W:137:MET:HE3	9:W:141:LEU:HD11	2.01	0.42
2:B:71:ASN:ND2	2:B:72:ASP:H	2.17	0.42
3:C:136:THR:O	3:C:150:GLN:HA	2.19	0.42
7:G:96:ALA:CA	7:G:107:MET:CE	2.91	0.42
8:H:81:GLN:O	8:H:85:GLN:HG3	2.19	0.42
10:J:52:THR:HG22	10:J:53:VAL:N	2.34	0.42
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	2.01	0.42
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.53	0.42
4:R:90:GLU:OE1	11:Y:69:ARG:HD2	2.19	0.42
6:T:82:ILE:N	6:T:82:ILE:HD13	2.33	0.42
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.55	0.42
8:V:72:ARG:HG3	8:V:72:ARG:HH11	1.83	0.42
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.19	0.42
11:Y:114:ASP:OD1	11:Y:114:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:O	1:A:33:GLN:HG2	2.19	0.42
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.54	0.42
9:I:114:ASP:HB2	16:I:851:HOH:O	2.20	0.42
13:M:113:VAL:HG23	13:M:119:THR:HG22	1.99	0.42
13:M:205:GLY:HA3	13:M:209:GLN:HB3	2.01	0.42
14:N:146:MET:CE	14:N:150:GLU:HB3	2.44	0.42
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.19	0.42
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.38	0.42
7:U:188:LYS:HD3	7:U:188:LYS:HA	1.85	0.42
10:X:52:THR:HG22	10:X:53:VAL:H	1.83	0.42
13:1:191:GLN:HE21	13:1:191:GLN:HB3	1.63	0.42
14:2:85:GLU:O	14:2:89:GLU:HB2	2.19	0.42
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	2.01	0.42
12:L:173:LEU:HG	12:L:175:ILE:HD11	2.00	0.42
1:O:29:THR:O	1:O:33:GLN:HG2	2.18	0.42
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.34	0.42
6:T:210:LEU:HD12	6:T:211:GLU:H	1.84	0.42
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.34	0.42
13:1:146:THR:HA	16:1:323:HOH:O	2.19	0.42
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.63	0.42
7:G:77:VAL:HG12	7:G:137:THR:HB	2.01	0.42
7:G:18(H):GLU:CD	7:G:18(H):GLU:N	2.77	0.42
3:Q:187:GLU:HG3	3:Q:232:TYR:OH	2.20	0.42
7:U:77:VAL:HG12	7:U:137:THR:HB	2.00	0.42
7:U:172:ILE:HD13	7:U:197:MET:HE1	2.01	0.42
9:W:13:ALA:HA	9:W:176:TYR:O	2.20	0.42
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.20	0.42
1:A:195:LEU:HD23	1:A:236:LEU:HD21	2.01	0.42
5:E:76:LEU:HD23	5:E:76:LEU:C	2.45	0.42
9:I:6:MET:HE3	9:I:155:ILE:HA	1.99	0.42
9:I:106:GLY:HA2	9:I:181:LYS:HD3	2.00	0.42
9:I:130:ALA:HB2	9:I:166:ASP:HB2	2.01	0.42
10:J:19:ALA:HB2	10:J:171:LYS:HG2	2.01	0.42
12:L:176:LEU:CD1	12:L:186:LYS:HG2	2.49	0.42
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.19	0.42
1:O:236:LEU:HD13	1:O:236:LEU:C	2.45	0.42
4:R:170:GLU:H	4:R:170:GLU:CD	2.28	0.42
5:S:52:LYS:HB3	5:S:63:TYR:HB3	2.01	0.42
10:X:-1:MET:HE1	10:X:98:ASN:HD22	1.85	0.42
10:X:35:ARG:NH1	10:X:57:GLU:CG	2.83	0.42
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:40:ASN:N	13:1:40:ASN:ND2	2.66	0.42
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.14	0.42
3:C:20:HIS:HB3	3:C:25:GLU:OE1	2.19	0.42
5:E:4:PHE:CE1	5:E:17:PRO:HD2	2.55	0.42
9:I:151:LEU:O	9:I:155:ILE:HG22	2.20	0.42
11:K:70:GLU:O	11:K:71:LYS:C	2.63	0.42
7:G:169:GLN:HE21	7:G:169:GLN:HB3	1.70	0.42
9:I:12:VAL:HG13	9:I:108:PRO:HB3	2.01	0.42
10:J:52:THR:HG22	10:J:53:VAL:H	1.84	0.42
10:J:166:MET:HA	10:J:167:PRO:HD3	1.82	0.42
11:K:10(B):LYS:CD	11:K:10(B):LYS:N	2.69	0.42
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.35	0.42
3:Q:57:LYS:HD2	3:Q:57:LYS:C	2.45	0.42
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.84	0.42
5:S:139:ILE:HA	5:S:147:HIS:O	2.20	0.42
5:S:139:ILE:HG22	5:S:148:LEU:HD13	2.01	0.42
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	2.19	0.42
9:W:20:LEU:HD13	9:W:20:LEU:C	2.44	0.42
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.92	0.42
2:B:53:LYS:HG2	2:B:54:VAL:HG23	2.01	0.42
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.20	0.42
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.01	0.42
13:M:175:LEU:C	13:M:175:LEU:HD23	2.44	0.42
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.49	0.42
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.62	0.42
5:S:74:MET:HE2	5:S:109:VAL:HA	2.02	0.42
8:V:3:ILE:O	8:V:126:SER:HA	2.20	0.42
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.49	0.42
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.19	0.42
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.55	0.42
4:D:150:HIS:O	4:D:157:PHE:HA	2.20	0.42
5:E:150:GLU:O	5:E:157:VAL:HA	2.19	0.42
10:J:35:ARG:HH11	10:J:57:GLU:CG	2.32	0.42
11:K:7:ARG:HD2	11:K:108:PRO:O	2.20	0.42
11:K:32:LYS:O	11:K:45:MET:CE	2.68	0.42
12:L:17:ASP:HA	12:L:172:GLY:O	2.20	0.42
12:L:113:PHE:N	12:L:113:PHE:CD1	2.87	0.42
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.42
2:P:121:GLN:NE2	2:P:121:GLN:C	2.78	0.42
5:S:4:PHE:CE1	5:S:17:PRO:HD2	2.55	0.42
6:T:79:SER:OG	6:T:165:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:33:LYS:HE2	15:Y:300:HYE:H14	2.01	0.42
12:Z:11:PHE:CE1	12:Z:148:VAL:HA	2.54	0.42
1:A:221:PHE:CD2	1:A:221:PHE:C	2.97	0.41
2:B:11:ARG:HD2	3:C:10:ARG:NH1	2.34	0.41
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.49	0.41
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.02	0.41
3:C:215:VAL:HG23	3:C:221:ILE:CG1	2.50	0.41
4:D:112:LEU:HD13	4:D:112:LEU:O	2.20	0.41
14:N:26:ILE:HB	13:1:165:ARG:HA	2.01	0.41
1:O:62:GLU:C	1:O:64:LEU:H	2.27	0.41
2:P:233:LEU:HD12	2:P:233:LEU:HA	1.85	0.41
4:R:81:LEU:HD12	4:R:133:GLY:HA3	2.02	0.41
5:S:160:LEU:HD22	6:T:59:LEU:HD12	2.01	0.41
6:T:176:LEU:O	6:T:180:VAL:HG23	2.20	0.41
6:T:204:ASP:OD1	6:T:204:ASP:N	2.52	0.41
7:U:60:ASP:OD2	7:U:60:ASP:C	2.62	0.41
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.19	0.41
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.01	0.41
9:W:130:ALA:HB2	9:W:166:ASP:HB2	2.02	0.41
13:1:62:LEU:HD23	13:1:62:LEU:HA	1.88	0.41
13:1:91:ARG:HG3	13:1:92:SER:N	2.33	0.41
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	2.02	0.41
1:A:236:LEU:HD13	1:A:236:LEU:C	2.45	0.41
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.55	0.41
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.50	0.41
5:E:18(C):PHE:CD1	5:E:18(C):PHE:C	2.98	0.41
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.20	0.41
1:O:27:ALA:O	1:O:31:VAL:HG23	2.19	0.41
2:P:136:PHE:O	2:P:150:THR:HA	2.21	0.41
5:S:226:GLY:O	5:S:227:GLU:C	2.63	0.41
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.20	0.41
3:C:215:VAL:HG23	3:C:221:ILE:HG13	2.02	0.41
5:E:11:ASP:OD1	5:E:13:VAL:HG12	2.20	0.41
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.62	0.41
6:F:68:GLN:NE2	6:F:86:ARG:NH1	2.69	0.41
10:J:35:ARG:HH11	10:J:57:GLU:HG2	1.84	0.41
12:L:13:VAL:HG12	12:L:177:ILE:HG13	2.01	0.41
14:N:84:LYS:HZ3	14:N:119:VAL:HG23	1.85	0.41
2:P:53:LYS:HG2	2:P:54:VAL:HG23	2.01	0.41
2:P:225:LYS:O	2:P:226:PRO:C	2.62	0.41
4:R:150:HIS:O	4:R:157:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:143:GLU:CG	9:W:146:LEU:HD21	2.51	0.41
13:1:9:ASP:OD1	13:1:10:ASN:N	2.54	0.41
2:B:78:VAL:HG22	2:B:136:PHE:CE2	2.56	0.41
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.21	0.41
7:G:158:VAL:HG22	7:G:159:GLY:H	1.85	0.41
8:H:72:ARG:HG3	8:H:72:ARG:HH11	1.85	0.41
12:L:98:HIS:HE1	12:L:112:SER:HB2	1.85	0.41
12:L:153:LYS:HG2	8:V:201:GLN:HG3	2.02	0.41
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.34	0.41
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.54	0.41
4:R:170:GLU:HG2	4:R:171:GLY:N	2.35	0.41
5:S:216:GLY:O	5:S:217:LYS:C	2.63	0.41
7:U:171:GLU:OE1	7:U:171:GLU:N	2.53	0.41
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.85	0.41
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.20	0.41
4:D:81:LEU:HD12	4:D:133:GLY:HA3	2.03	0.41
5:E:18(C):PHE:O	5:E:18(F):ILE:HG13	2.21	0.41
6:F:82:ILE:HB	6:F:83:PRO:HD3	2.01	0.41
1:O:4:MET:CG	1:O:5:THR:H	2.31	0.41
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.44	0.41
5:S:11:ASP:OD1	5:S:13:VAL:HG12	2.20	0.41
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.50	0.41
5:S:18(C):PHE:CD1	5:S:18(C):PHE:C	2.99	0.41
7:U:69:CYS:O	7:U:93:LYS:HE2	2.20	0.41
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.85	0.41
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.51	0.41
12:Z:-5:TYR:CE2	12:Z:96:TYR:HB2	2.56	0.41
13:1:19:LEU:HD21	13:1:26:LEU:HD22	2.03	0.41
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.55	0.41
3:C:76:LEU:HD23	3:C:76:LEU:C	2.46	0.41
5:E:74:MET:HE2	5:E:109:VAL:HA	2.03	0.41
6:F:40:ILE:HD12	6:F:193:ALA:HB2	2.02	0.41
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.86	0.41
10:J:35:ARG:NH1	10:J:57:GLU:CG	2.84	0.41
1:O:198:LYS:HE3	1:O:236:LEU:HD11	2.03	0.41
2:P:213:ALA:HA	2:P:222:LYS:O	2.20	0.41
4:R:12(D):ALA:HA	5:S:129:GLY:HA2	2.03	0.41
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.36	0.41
6:T:12:ASN:HB2	16:T:656:HOH:O	2.20	0.41
7:U:29:LYS:HD2	7:U:29:LYS:HA	1.79	0.41
10:X:52:THR:HG22	10:X:53:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	2.01	0.41
9:I:13:ALA:HA	9:I:176:TYR:O	2.19	0.41
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.47	0.41
5:S:100:SER:O	5:S:104:ASN:HA	2.21	0.41
5:S:150:GLU:O	5:S:157:VAL:HA	2.21	0.41
5:S:185:ASN:HA	5:S:186:PRO:HD2	1.93	0.41
6:T:50:VAL:HG22	6:T:51:GLU:N	2.34	0.41
6:T:120:VAL:HG21	6:T:151:LEU:HD21	2.03	0.41
6:T:142:ASP:OD2	6:T:142:ASP:C	2.64	0.41
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.45	0.41
13:1:37:VAL:HG11	13:1:79:ILE:CD1	2.50	0.41
10:J:7:ARG:HH11	10:J:7:ARG:HG2	1.85	0.41
10:J:168:MET:HE3	10:X:168:MET:CG	2.49	0.41
3:Q:47:VAL:HG23	3:Q:189:CYS:SG	2.61	0.41
3:Q:76:LEU:C	3:Q:76:LEU:HD23	2.46	0.41
4:R:175:GLU:OE1	4:R:175:GLU:HA	2.20	0.41
5:S:66:LYS:O	5:S:77:SER:HA	2.20	0.41
6:T:136:THR:O	6:T:150:MET:HA	2.21	0.41
6:T:172:ALA:O	6:T:176:LEU:CD2	2.69	0.41
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	2.03	0.41
7:U:158:VAL:HG22	7:U:159:GLY:H	1.86	0.41
14:2:146:MET:CE	14:2:150:GLU:HB3	2.44	0.41
1:A:13:THR:O	2:B:130:ARG:HD3	2.21	0.41
1:A:62:GLU:C	1:A:64:LEU:H	2.29	0.41
2:B:7:ARG:HD2	2:B:8:TYR:CZ	2.56	0.41
4:D:185:THR:HG23	4:D:188:GLU:OE1	2.21	0.41
5:E:66:LYS:O	5:E:77:SER:HA	2.20	0.41
5:E:142:ASP:HB2	16:M:885:HOH:O	2.20	0.41
5:E:226:GLY:O	5:E:227:GLU:C	2.63	0.41
6:F:70:VAL:HB	6:F:74:ILE:HB	2.03	0.41
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.21	0.41
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.21	0.41
11:K:49:ALA:O	11:K:53:GLN:HB2	2.21	0.41
11:K:200:LYS:HE3	11:K:206:PHE:O	2.20	0.41
12:L:11:PHE:CE1	12:L:148:VAL:HA	2.56	0.41
13:M:4:ILE:HG22	13:M:126:ALA:HB1	2.02	0.41
13:M:184:LEU:HD23	13:M:185:THR:N	2.35	0.41
14:N:85:GLU:O	14:N:89:GLU:HB2	2.20	0.41
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.19	0.41
1:O:221:PHE:CD2	1:O:221:PHE:C	2.98	0.41
2:P:71:ASN:ND2	2:P:72:ASP:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	2.03	0.41
3:Q:18(A):ASP:OD1	3:Q:18(C):LYS:HB2	2.21	0.41
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	2.02	0.41
5:S:212:ILE:HG22	5:S:213:ALA:N	2.35	0.41
6:T:36:THR:HB	6:T:168:GLY:H	1.86	0.41
6:T:40:ILE:HD12	6:T:193:ALA:HB2	2.03	0.41
7:U:119:LEU:HD12	7:U:119:LEU:HA	1.92	0.41
7:U:220:LYS:HG2	7:U:221:PHE:N	2.36	0.41
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.21	0.41
13:1:160:ARG:HB2	13:1:192:VAL:HG13	2.02	0.41
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.56	0.41
5:E:139:ILE:HA	5:E:147:HIS:O	2.20	0.41
16:F:306:HOH:O	7:G:86:ARG:HD2	2.19	0.41
9:I:28:SER:CB	10:J:120:VAL:HG21	2.50	0.41
1:O:197:LEU:CD2	1:O:210:ILE:HD12	2.51	0.41
2:P:21(A):LYS:HG3	2:P:219:GLU:O	2.21	0.41
3:Q:20:HIS:HB3	3:Q:25:GLU:OE1	2.20	0.41
4:R:175:GLU:HB3	4:R:196:ILE:HD13	2.02	0.41
5:S:46:ALA:HB1	5:S:139:ILE:HB	2.02	0.41
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.35	0.41
6:T:68:GLN:NE2	6:T:86:ARG:NH1	2.69	0.41
9:W:151:LEU:O	9:W:155:ILE:HG22	2.20	0.41
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.21	0.41
13:1:104:VAL:HG23	13:1:178:ILE:CG2	2.48	0.41
14:2:45:ARG:NH1	15:2:300:HYE:H12A	2.36	0.41
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.21	0.40
1:A:197:LEU:CD2	1:A:210:ILE:HD12	2.50	0.40
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.56	0.40
5:E:45:HIS:HB2	5:E:189:LEU:HD12	2.03	0.40
6:F:11:SER:HB3	6:F:14:VAL:HG23	2.03	0.40
7:G:220:LYS:HG2	7:G:221:PHE:N	2.36	0.40
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.51	0.40
14:N:155:ILE:HG22	14:N:175:MET:HE2	2.03	0.40
3:Q:160:TRP:CZ2	4:R:59:LEU:HD23	2.56	0.40
6:T:194:ALA:O	6:T:198:TYR:HD1	2.04	0.40
7:U:194:ILE:O	7:U:197:MET:HB3	2.21	0.40
10:X:112:GLN:HE21	10:X:125:GLY:HA3	1.85	0.40
11:Y:8:PHE:HA	11:Y:144:TRP:CE3	2.55	0.40
11:Y:78:ALA:O	11:Y:82:ILE:HG13	2.21	0.40
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.89	0.40
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:PHE:N	6:F:23:GLN:HE22	1.97	0.40
6:F:204:ASP:OD1	6:F:204:ASP:N	2.54	0.40
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	2.03	0.40
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.19	0.40
14:N:175:MET:HE3	14:N:18(B):PHE:CD2	2.55	0.40
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	2.03	0.40
2:P:90:ASN:O	2:P:94:ILE:HD12	2.20	0.40
2:P:181:LYS:CG	2:P:184:MET:HG3	2.52	0.40
4:R:195:LYS:HE2	4:R:199:GLN:OE1	2.21	0.40
1:A:198:LYS:HE3	1:A:236:LEU:HD11	2.03	0.40
2:B:121:GLN:NE2	16:B:328:HOH:O	2.55	0.40
3:C:71:ASP:HA	10:J:68:ILE:HD12	2.04	0.40
5:E:39:GLY:O	5:E:162:GLY:HA2	2.21	0.40
5:E:57:GLU:C	5:E:58:LEU:HD12	2.47	0.40
6:F:79:SER:OG	6:F:165:THR:HG23	2.22	0.40
8:H:68:LEU:HD12	8:H:68:LEU:HA	1.95	0.40
12:L:27:ASN:HB3	13:M:120:TYR:CE1	2.56	0.40
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.57	0.40
1:O:184:LEU:HB2	16:O:486:HOH:O	2.20	0.40
3:Q:97:GLN:HG3	10:X:65:LEU:HB2	2.03	0.40
5:S:64:GLN:HA	16:S:660:HOH:O	2.21	0.40
5:S:90:ASN:O	5:S:94:GLN:HG3	2.22	0.40
8:V:52:THR:O	8:V:56:THR:HB	2.22	0.40
2:B:126:HIS:CB	3:C:129:VAL:HG12	2.47	0.40
3:C:163:GLN:NE2	3:C:163:GLN:CA	2.80	0.40
6:F:49:ALA:HA	6:F:211:GLU:O	2.21	0.40
6:F:103:TYR:O	6:F:104:LYS:HB3	2.22	0.40
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.57	0.40
8:H:52:THR:O	8:H:56:THR:HB	2.21	0.40
12:L:33:LYS:HB3	12:L:33:LYS:HE2	1.98	0.40
13:M:198:ASP:O	13:M:201:LYS:HG2	2.22	0.40
2:P:69:LYS:HE3	2:P:69:LYS:HB2	1.94	0.40
5:S:18(C):PHE:O	5:S:18(F):ILE:HG13	2.21	0.40
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.85	0.40
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.79	0.40
7:U:75:GLY:HA3	7:U:221:PHE:CE2	2.56	0.40
10:X:44:SER:HG	10:X:100:LEU:HB2	1.85	0.40
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	2.03	0.40
14:2:156:LYS:HE3	16:2:1010:HOH:O	2.22	0.40
1:A:27:ALA:O	1:A:31:VAL:HG23	2.22	0.40
3:C:57:LYS:HD2	3:C:57:LYS:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:46:ALA:HB1	5:E:139:ILE:HB	2.02	0.40
6:F:210:LEU:HD12	6:F:211:GLU:H	1.87	0.40
11:K:114:ASP:OD1	11:K:114:ASP:C	2.65	0.40
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.36	0.40
13:M:40:ASN:H	13:M:40:ASN:ND2	2.13	0.40
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.56	0.40
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.21	0.40
6:T:212:ILE:HG22	6:T:213:SER:N	2.37	0.40
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	2.04	0.40
13:1:83:LEU:O	13:1:87:MET:HG2	2.21	0.40
13:1:122:SER:HB3	13:1:124:THR:O	2.21	0.40
14:2:21:THR:OG1	15:2:300:HYE:H2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	233 (94%)	13 (5%)	2 (1%)	16	31
1	O	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	16	31
2	B	242/244 (99%)	221 (91%)	17 (7%)	4 (2%)	7	13
2	P	242/244 (99%)	222 (92%)	16 (7%)	4 (2%)	7	13
3	C	239/241 (99%)	222 (93%)	13 (5%)	4 (2%)	7	13
3	Q	239/241 (99%)	222 (93%)	11 (5%)	6 (2%)	4	7
4	D	240/242 (99%)	232 (97%)	4 (2%)	4 (2%)	7	13
4	R	240/242 (99%)	230 (96%)	6 (2%)	4 (2%)	7	13
5	E	231/233 (99%)	213 (92%)	13 (6%)	5 (2%)	5	9
5	S	231/233 (99%)	212 (92%)	14 (6%)	5 (2%)	5	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	242/244 (99%)	226 (93%)	15 (6%)	1 (0%)	30	49
6	T	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	10	20
7	G	241/243 (99%)	229 (95%)	12 (5%)	0	100	100
7	U	241/243 (99%)	229 (95%)	12 (5%)	0	100	100
8	H	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
8	V	220/222 (99%)	210 (96%)	10 (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%)	188 (96%)	7 (4%)	1 (0%)	24	43
10	X	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	24	43
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	1	231/233 (99%)	223 (96%)	7 (3%)	1 (0%)	30	49
13	M	231/233 (99%)	222 (96%)	8 (4%)	1 (0%)	30	49
14	2	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6312/6368 (99%)	6006 (95%)	258 (4%)	48 (1%)	16	31

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	LEU
4	D	12(G)	GLU
3	Q	58	LEU
4	R	12(G)	GLU
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
5	E	5	ARG
5	E	202	ARG
2	P	54	VAL
2	P	21(B)	GLY

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Mol	Chain	Res	Type
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
5	S	5	ARG
5	S	202	ARG
1	A	5	THR
1	A	167	LYS
2	B	20(A)	SER
4	D	12(F)	GLY
5	E	231	LYS
10	J	192	ALA
1	O	5	THR
1	O	167	LYS
2	P	20(A)	SER
4	R	12(F)	GLY
5	S	217	LYS
5	S	231	LYS
10	X	192	ALA
3	C	242	GLU
4	D	18(D)	SER
5	E	217	LYS
3	Q	242	GLU
4	R	18(D)	SER
6	T	143	LYS
5	E	180	LEU
6	F	205	ASN
5	S	180	LEU
6	T	205	ASN
3	Q	53	ARG
3	Q	184	ALA
6	T	206	LYS
4	D	12(C)	GLY
4	R	12(C)	GLY
13	M	207	GLY
13	1	207	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	198 (95%)	11 (5%)	20	42
1	O	209/209 (100%)	198 (95%)	11 (5%)	20	42
2	B	203/203 (100%)	191 (94%)	12 (6%)	18	37
2	P	203/203 (100%)	189 (93%)	14 (7%)	14	30
3	C	213/213 (100%)	200 (94%)	13 (6%)	17	35
3	Q	213/213 (100%)	199 (93%)	14 (7%)	15	32
4	D	198/198 (100%)	185 (93%)	13 (7%)	15	32
4	R	198/198 (100%)	186 (94%)	12 (6%)	17	35
5	E	192/192 (100%)	178 (93%)	14 (7%)	13	27
5	S	192/192 (100%)	178 (93%)	14 (7%)	13	27
6	F	201/201 (100%)	182 (90%)	19 (10%)	8	17
6	T	201/201 (100%)	182 (90%)	19 (10%)	8	17
7	G	207/207 (100%)	196 (95%)	11 (5%)	20	42
7	U	207/207 (100%)	196 (95%)	11 (5%)	20	42
8	H	181/181 (100%)	168 (93%)	13 (7%)	13	28
8	V	181/181 (100%)	168 (93%)	13 (7%)	13	28
9	I	172/172 (100%)	163 (95%)	9 (5%)	21	42
9	W	172/172 (100%)	163 (95%)	9 (5%)	21	42
10	J	175/175 (100%)	167 (95%)	8 (5%)	24	48
10	X	175/175 (100%)	167 (95%)	8 (5%)	24	48
11	K	169/169 (100%)	158 (94%)	11 (6%)	15	32
11	Y	169/169 (100%)	158 (94%)	11 (6%)	15	32
12	L	185/185 (100%)	160 (86%)	25 (14%)	4	8
12	Z	185/185 (100%)	160 (86%)	25 (14%)	4	8
13	1	199/199 (100%)	183 (92%)	16 (8%)	11	24
13	M	199/199 (100%)	192 (96%)	7 (4%)	32	58
14	2	162/162 (100%)	154 (95%)	8 (5%)	22	45
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	51
All	All	5332/5332 (100%)	4974 (93%)	358 (7%)	15	31

All (358) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	32	LYS
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
1	A	192	ILE
1	A	214	ILE
1	A	229	ILE
2	B	14	ILE
2	B	58	LEU
2	B	89	ILE
2	B	94	ILE
2	B	124	THR
2	B	14(A)	TYR
2	B	150	THR
2	B	163	ILE
2	B	192	LEU
2	B	224	PHE
2	B	232	ILE
2	B	238	ILE
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU
3	C	57	LYS
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	40	ILE
4	D	48	LEU
4	D	52	LYS
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG

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Mol	Chain	Res	Type
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	196	ILE
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	111	ARG
5	E	121	GLN
5	E	139	ILE
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	212	ILE
5	E	227	GLU
6	F	11	SER
6	F	35	THR
6	F	43	ASN
6	F	56	SER
6	F	74	ILE
6	F	82	ILE
6	F	107	ILE
6	F	109	ILE
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	169	ARG
6	F	176	LEU
6	F	187	ARG
6	F	192	GLN
6	F	196	ILE
6	F	197	ILE
6	F	203	GLU
6	F	240	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU

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Mol	Chain	Res	Type
7	G	124	THR
7	G	135	ILE
7	G	172	ILE
7	G	197	MET
7	G	217	LYS
7	G	229	ILE
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	37	ILE
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	100	ILE
8	H	121	VAL
8	H	144	GLN
8	H	152	ILE
8	H	159	ILE
8	H	163	ILE
8	H	197	ARG
9	I	-3	ILE
9	I	2	ILE
9	I	20	LEU
9	I	29	ASN
9	I	104	ILE
9	I	110	ILE
9	I	125	ILE
9	I	155	ILE
9	I	160	LEU
10	J	3	ILE
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	121	GLU
10	J	166	MET
10	J	168	MET
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG

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Mol	Chain	Res	Type
11	K	74	ILE
11	K	82	ILE
11	K	87	VAL
11	K	99	THR
11	K	138	LEU
11	K	146	LEU
11	K	185	ILE
12	L	-7	ASN
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	83	ILE
12	L	98	HIS
12	L	99	THR
12	L	138	LEU
12	L	14(A)	LYS
12	L	14(B)	ASN
12	L	14(C)	GLN
12	L	14(D)	TYR
12	L	14(E)	GLU
12	L	14(F)	PRO
12	L	14(I)	THR
12	L	14(K)	LYS
12	L	14(M)	VAL
12	L	14(N)	LYS
12	L	14(O)	LYS
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS
12	L	152	ILE
12	L	190	GLU
13	M	-4	ILE
13	M	40	ASN
13	M	45	ILE
13	M	62	LEU
13	M	91	ARG
13	M	148	VAL
13	M	149	GLN
14	N	13	ILE
14	N	55	ILE
14	N	89	GLU

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Mol	Chain	Res	Type
14	N	119	VAL
14	N	126	ILE
14	N	149	GLU
14	N	163	ILE
1	O	24	ILE
1	O	32	LYS
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
1	O	192	ILE
1	O	214	ILE
1	O	229	ILE
2	P	14	ILE
2	P	58	LEU
2	P	89	ILE
2	P	94	ILE
2	P	119	ILE
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	224	PHE
2	P	232	ILE
2	P	238	ILE
3	Q	10	ARG
3	Q	14	ILE
3	Q	25	GLU
3	Q	57	LYS
3	Q	135	SER
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

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Mol	Chain	Res	Type
3	Q	236	ILE
4	R	28	LEU
4	R	40	ILE
4	R	48	LEU
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	196	ILE
4	R	215	ILE
4	R	237	LEU
5	S	12	THR
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	121	GLN
5	S	139	ILE
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	212	ILE
5	S	227	GLU
6	T	11	SER
6	T	35	THR
6	T	43	ASN
6	T	56	SER
6	T	74	ILE
6	T	82	ILE
6	T	107	ILE
6	T	109	ILE
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	169	ARG
6	T	176	LEU
6	T	187	ARG
6	T	192	GLN

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Mol	Chain	Res	Type
6	T	196	ILE
6	T	197	ILE
6	T	203	GLU
6	T	240	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	135	ILE
7	U	172	ILE
7	U	197	MET
7	U	217	LYS
7	U	229	ILE
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	37	ILE
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	100	ILE
8	V	121	VAL
8	V	144	GLN
8	V	152	ILE
8	V	159	ILE
8	V	163	ILE
8	V	197	ARG
9	W	-3	ILE
9	W	2	ILE
9	W	20	LEU
9	W	29	ASN
9	W	104	ILE
9	W	110	ILE
9	W	125	ILE
9	W	155	ILE
9	W	160	LEU
10	X	3	ILE
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	70	GLU

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Mol	Chain	Res	Type
10	X	121	GLU
10	X	166	MET
10	X	168	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	69	ARG
11	Y	74	ILE
11	Y	82	ILE
11	Y	87	VAL
11	Y	99	THR
11	Y	138	LEU
11	Y	146	LEU
11	Y	185	ILE
12	Z	-7	ASN
12	Z	14	LEU
12	Z	25	SER
12	Z	40	ASN
12	Z	58	ARG
12	Z	83	ILE
12	Z	98	HIS
12	Z	99	THR
12	Z	138	LEU
12	Z	14(A)	LYS
12	Z	14(B)	ASN
12	Z	14(C)	GLN
12	Z	14(D)	TYR
12	Z	14(E)	GLU
12	Z	14(F)	PRO
12	Z	14(I)	THR
12	Z	14(K)	LYS
12	Z	14(M)	VAL
12	Z	14(N)	LYS
12	Z	14(O)	LYS
12	Z	14(P)	PRO
12	Z	14(Q)	LEU
12	Z	14(W)	LYS
12	Z	152	ILE
12	Z	190	GLU
13	1	-4	ILE
13	1	14	ILE
13	1	40	ASN

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Mol	Chain	Res	Type
13	1	45	ILE
13	1	62	LEU
13	1	91	ARG
13	1	14(A)	VAL
13	1	14(B)	ASP
13	1	14(C)	ARG
13	1	14(D)	GLU
13	1	14(E)	SER
13	1	14(F)	ASP
13	1	14(G)	ILE
13	1	148	VAL
13	1	149	GLN
13	1	204	LYS
14	2	13	ILE
14	2	55	ILE
14	2	78	THR
14	2	89	GLU
14	2	119	VAL
14	2	126	ILE
14	2	149	GLU
14	2	163	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (234) 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	156	ASN
2	B	177	GLN
2	B	218	ASN
2	B	227	GLN
3	C	23	GLN
3	C	59	GLN
3	C	82	ASN
3	C	121	GLN

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Mol	Chain	Res	Type
3	C	125	GLN
3	C	163	GLN
3	C	179	ASN
3	C	209	ASN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	95	GLN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	152	GLN
5	E	156	ASN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	87	HIS
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
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

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Mol	Chain	Res	Type
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	56	ASN
9	I	81	GLN
9	I	157	GLN
10	J	9	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	141	ASN
11	K	174	ASN
11	K	207	ASN
11	K	208	ASN
12	L	-7	ASN
12	L	27	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	98	HIS
12	L	1(I)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	40	ASN
13	M	54	HIS
13	M	89	GLN

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Mol	Chain	Res	Type
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	38	HIS
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	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	156	ASN
2	P	177	GLN
2	P	218	ASN
2	P	227	GLN
3	Q	23	GLN
3	Q	59	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	163	GLN
3	Q	179	ASN
3	Q	209	ASN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	226	ASN
5	S	7	ASN
5	S	64	GLN

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Mol	Chain	Res	Type
5	S	73	HIS
5	S	95	GLN
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	152	GLN
5	S	156	ASN
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	87	HIS
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
6	T	241	ASN
7	U	11	HIS
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	35	HIS
8	V	66	HIS
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	36	HIS
9	W	56	ASN
9	W	81	GLN
9	W	161	ASN

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Mol	Chain	Res	Type
10	X	9	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	186	GLN
10	X	193	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	70(A)	ASN
12	Z	82	ASN
12	Z	98	HIS
12	Z	140	ASN
12	Z	141	GLN
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
12	Z	168	GLN
13	1	-7	GLN
13	1	40	ASN
13	1	54	HIS
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN

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Mol	Chain	Res	Type
13	1	189	ASN
13	1	191	GLN
14	2	38	HIS
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	HYE	2	300	14	17,22,22	1.90	5 (29%)	21,33,33	2.30	4 (19%)
15	HYE	K	300	11	17,22,22	1.66	5 (29%)	21,33,33	1.63	3 (14%)
15	HYE	V	300	8	17,22,22	1.82	4 (23%)	21,33,33	1.68	7 (33%)
15	HYE	Y	300	11	17,22,22	1.68	2 (11%)	21,33,33	1.55	3 (14%)
15	HYE	H	300	8	17,22,22	1.74	4 (23%)	21,33,33	1.64	3 (14%)
15	HYE	N	300	14	17,22,22	1.72	5 (29%)	21,33,33	2.25	4 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HYE	2	300	14	-	0/7/48/48	0/2/2/2
15	HYE	K	300	11	-	0/7/48/48	0/2/2/2
15	HYE	V	300	8	-	0/7/48/48	0/2/2/2
15	HYE	Y	300	11	-	0/7/48/48	0/2/2/2
15	HYE	H	300	8	-	0/7/48/48	0/2/2/2
15	HYE	N	300	14	-	0/7/48/48	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	300	HYE	C9-C8	4.65	1.61	1.54
15	K	300	HYE	C6-C4	3.85	1.57	1.52
15	Y	300	HYE	C6-C4	3.84	1.57	1.52
15	2	300	HYE	C6-C4	3.61	1.57	1.52
15	H	300	HYE	C6-C4	3.37	1.56	1.52
15	H	300	HYE	C9-C8	3.37	1.59	1.54
15	N	300	HYE	C6-C4	3.24	1.56	1.52
15	Y	300	HYE	C9-C8	3.18	1.59	1.54
15	V	300	HYE	C6-C4	3.04	1.56	1.52
15	2	300	HYE	C14-C9	2.85	1.59	1.54
15	N	300	HYE	C14-C9	2.85	1.59	1.54
15	K	300	HYE	C9-C8	2.76	1.58	1.54
15	2	300	HYE	C19-N18	2.74	1.37	1.34
15	H	300	HYE	C14-C9	2.72	1.59	1.54
15	V	300	HYE	C9-C10	2.62	1.54	1.50
15	2	300	HYE	C9-C10	2.61	1.54	1.50
15	N	300	HYE	C9-C10	2.51	1.54	1.50
15	H	300	HYE	C9-C10	2.44	1.54	1.50
15	K	300	HYE	C14-C9	2.38	1.58	1.54
15	K	300	HYE	C9-C10	2.29	1.54	1.50
15	2	300	HYE	O20-C19	-2.21	1.19	1.23
15	V	300	HYE	C14-C9	2.19	1.58	1.54
15	K	300	HYE	C13-C12	2.10	1.58	1.51
15	N	300	HYE	O15-C8	2.09	1.46	1.42
15	N	300	HYE	C13-C12	2.09	1.58	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	300	HYE	C4-C3-C19	-7.40	97.96	104.23
15	N	300	HYE	C4-C3-C19	-7.27	98.07	104.23
15	N	300	HYE	C7-C8-C9	5.05	120.43	114.09
15	2	300	HYE	C7-C8-C9	5.01	120.39	114.09
15	K	300	HYE	C7-C8-C9	4.35	119.56	114.09
15	Y	300	HYE	C7-C8-C9	4.12	119.27	114.09
15	H	300	HYE	C7-C8-C9	3.93	119.02	114.09
15	K	300	HYE	C4-C3-C19	-3.76	101.05	104.23
15	V	300	HYE	C7-C8-C9	3.74	118.79	114.09
15	Y	300	HYE	C4-C3-C19	-3.19	101.52	104.23
15	K	300	HYE	O15-C8-C9	-3.02	103.16	109.98
15	V	300	HYE	O15-C8-C9	-3.00	103.20	109.98
15	2	300	HYE	O15-C8-C9	-2.90	103.45	109.98
15	Y	300	HYE	O15-C8-C9	-2.89	103.46	109.98
15	N	300	HYE	O15-C8-C9	-2.83	103.59	109.98
15	H	300	HYE	O15-C8-C9	-2.80	103.67	109.98
15	V	300	HYE	C4-C3-C19	-2.70	101.94	104.23
15	2	300	HYE	C2-C3-C19	2.63	118.55	112.66
15	N	300	HYE	C2-C3-C19	2.61	118.50	112.66
15	H	300	HYE	C4-C3-C19	-2.35	102.24	104.23
15	V	300	HYE	O15-C8-C7	2.22	112.36	107.15
15	V	300	HYE	C7-C4-C3	2.18	107.56	104.13
15	V	300	HYE	O20-C19-N18	-2.15	123.05	125.72
15	V	300	HYE	C3-C19-N18	2.13	111.77	108.74

There are no chirality outliers.

There are no torsion outliers.

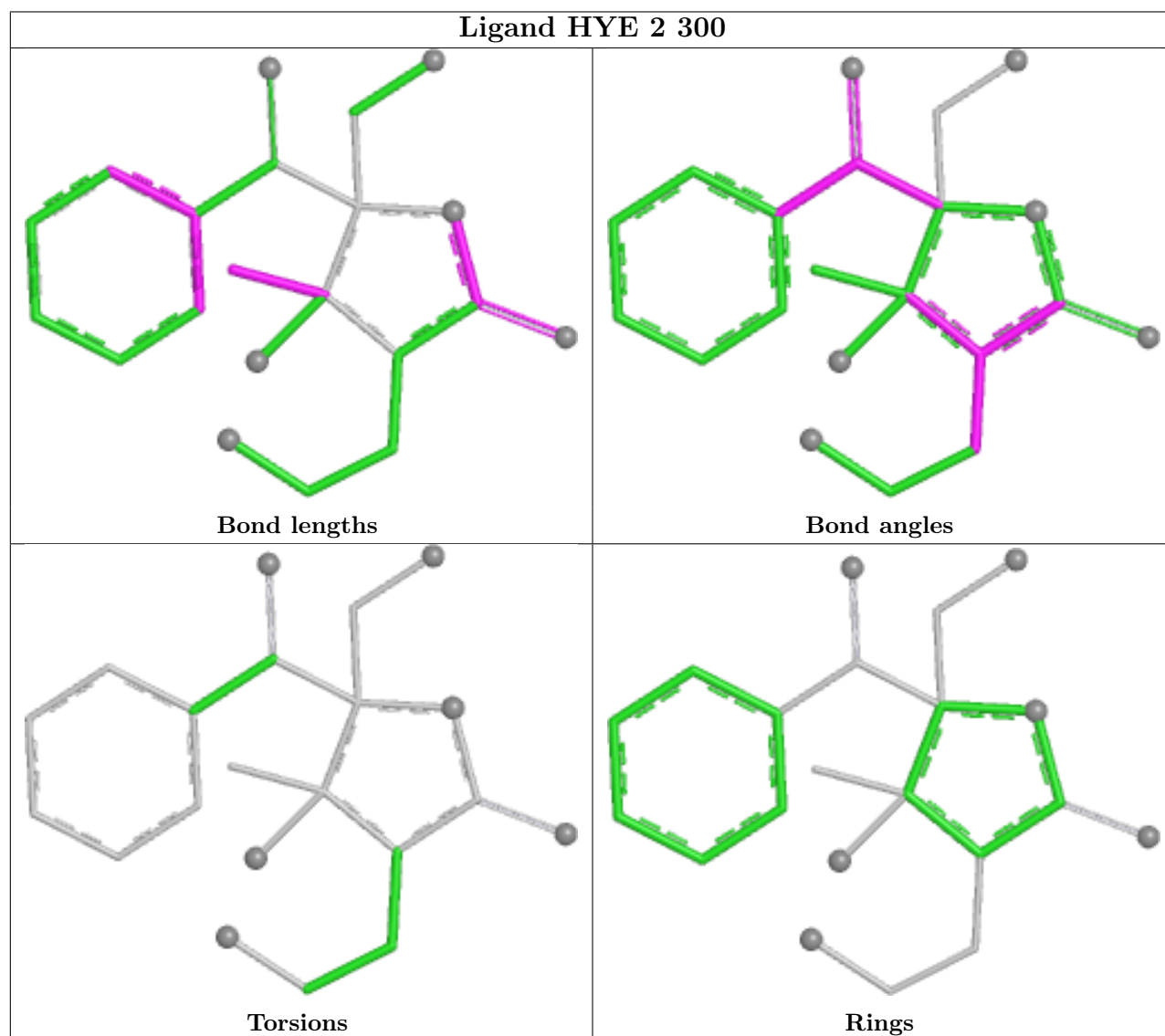
There are no ring outliers.

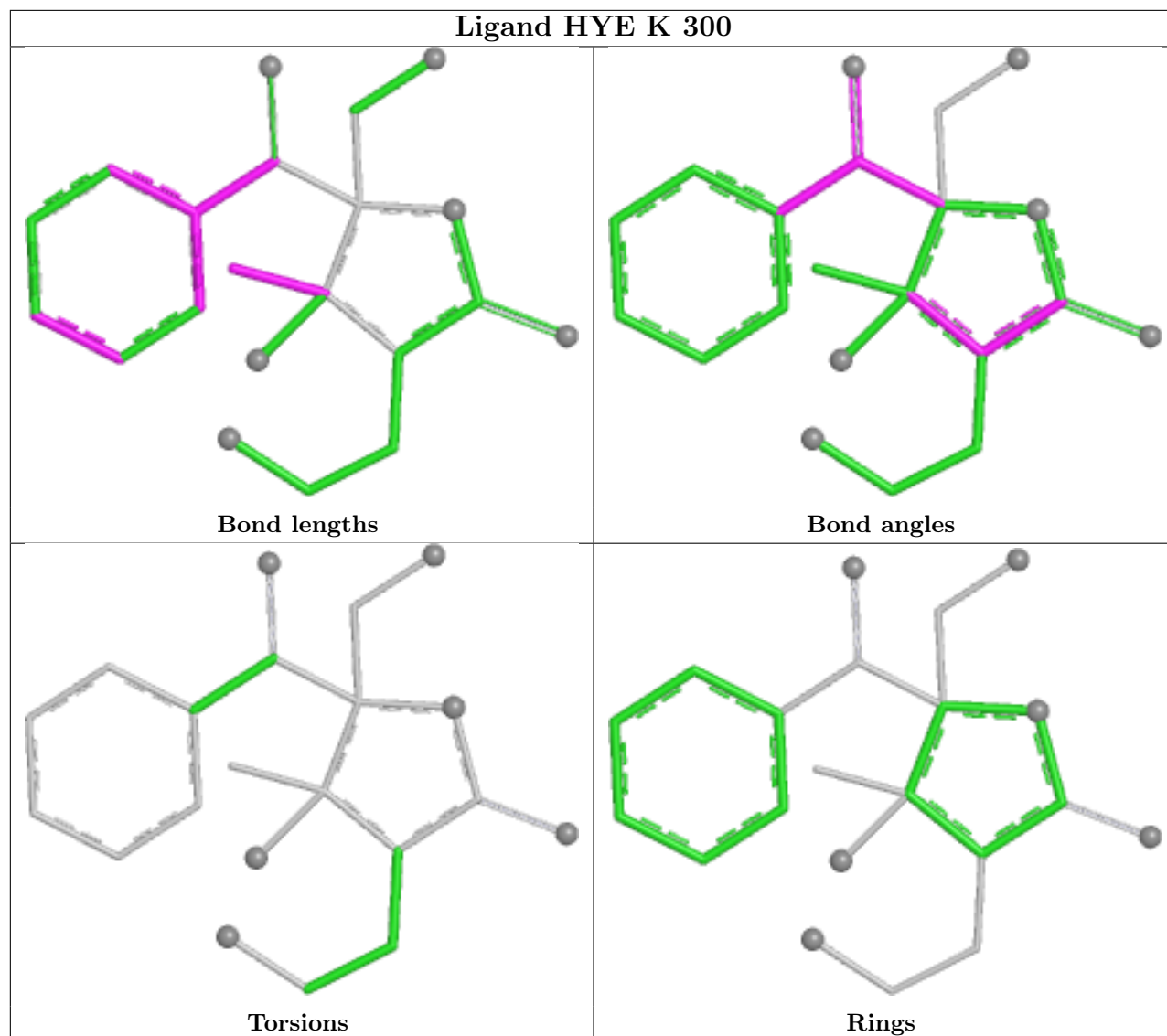
4 monomers are involved in 7 short contacts:

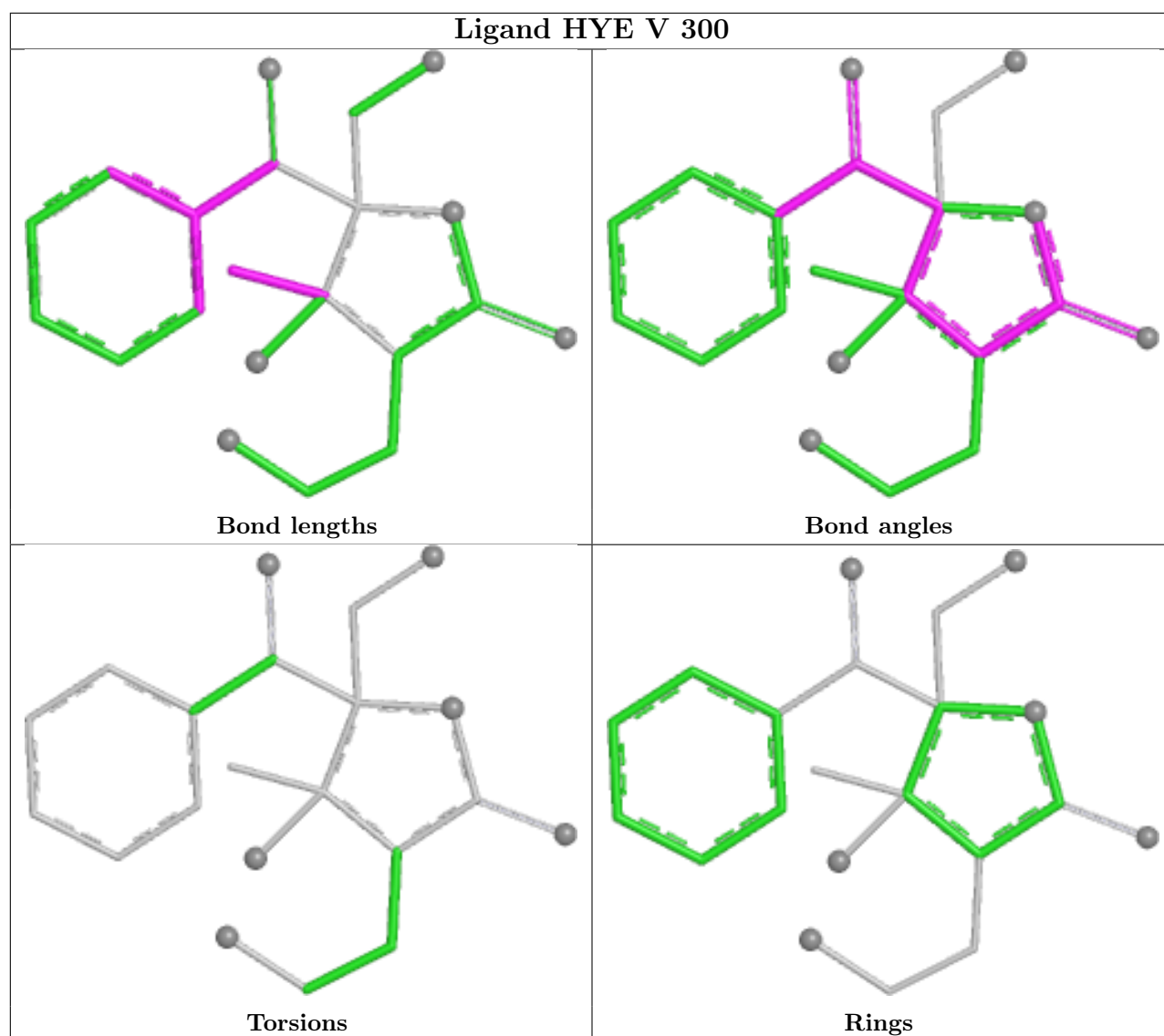
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	2	300	HYE	3	0
15	K	300	HYE	1	0
15	Y	300	HYE	2	0
15	N	300	HYE	1	0

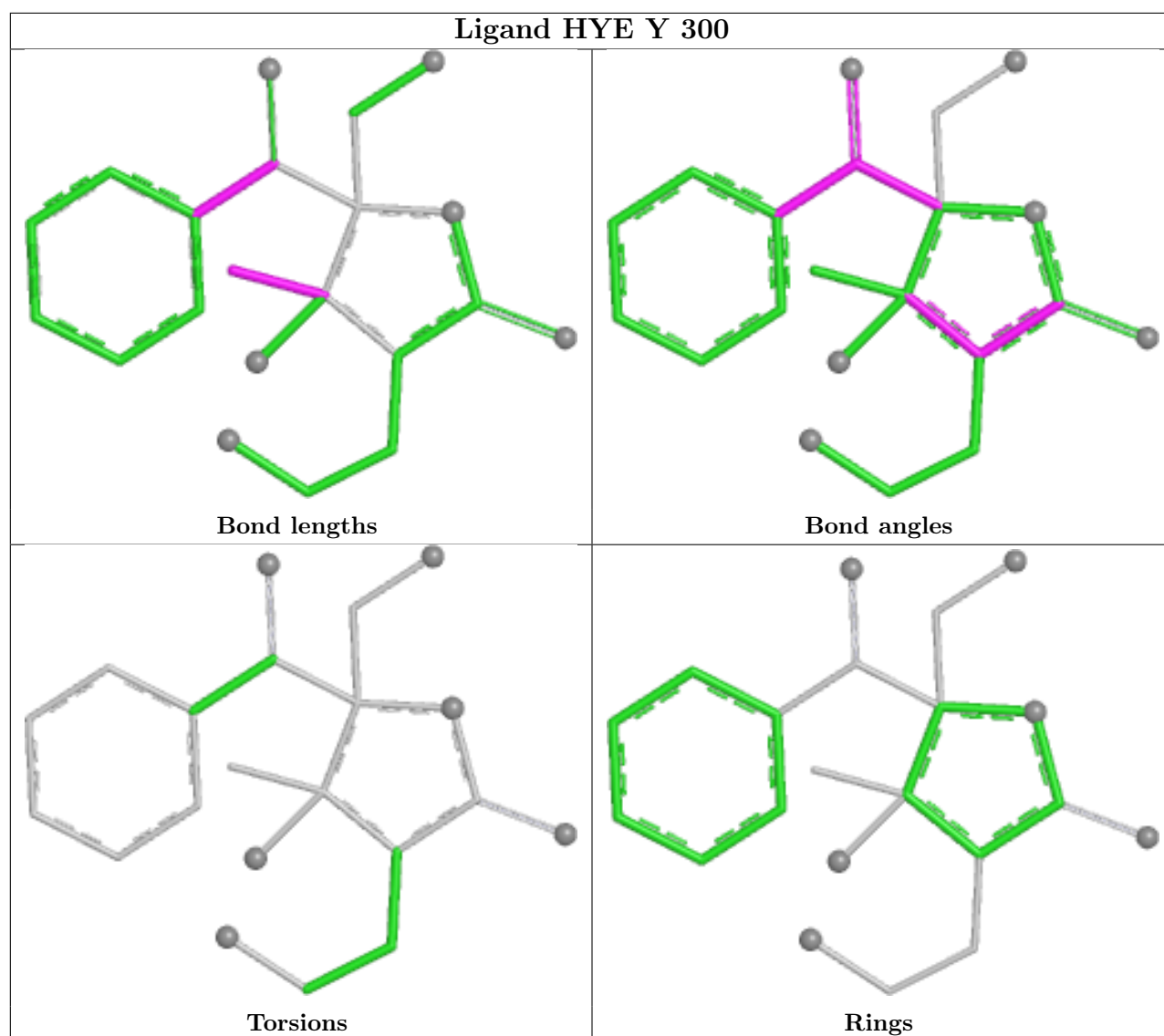
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

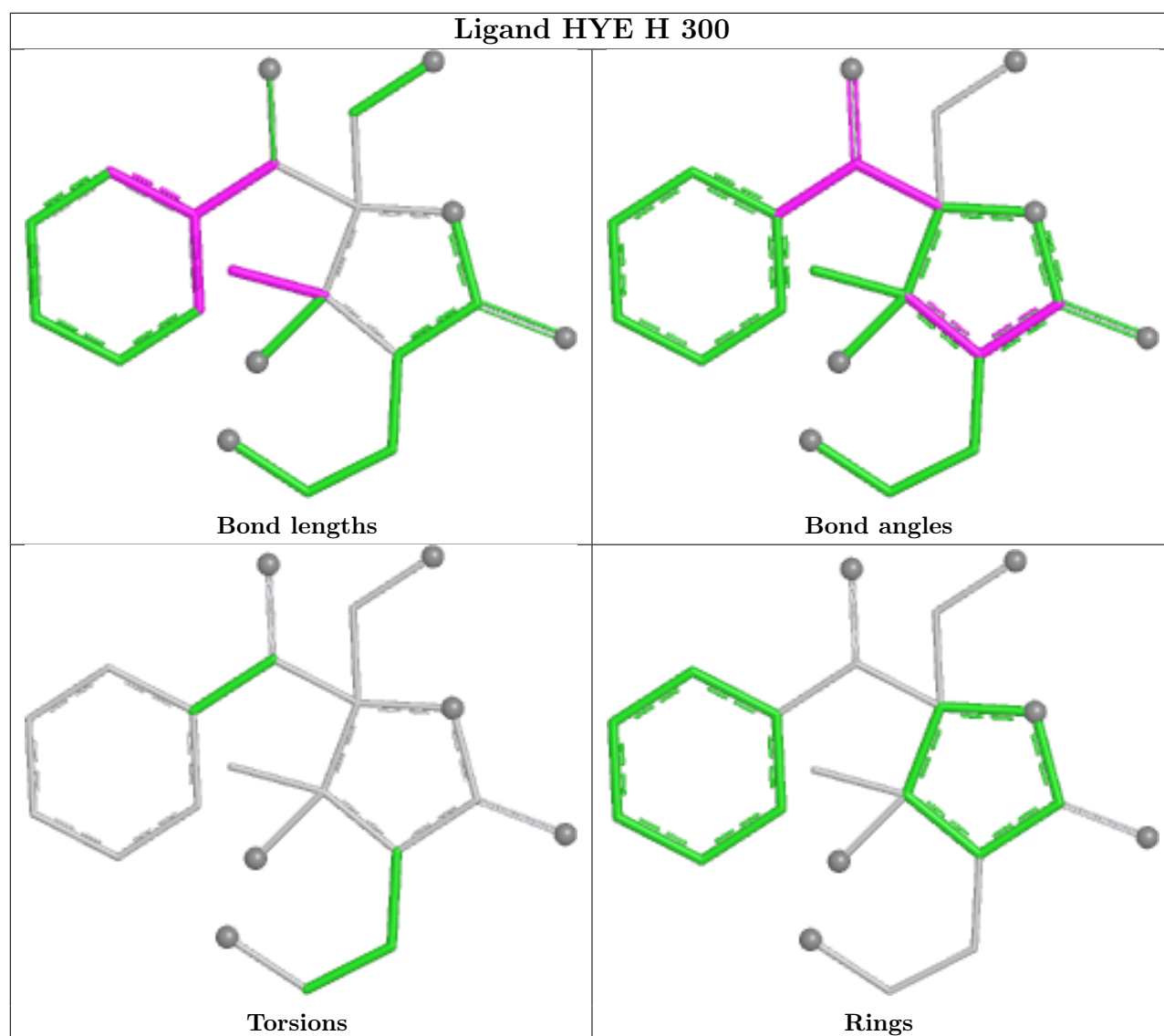
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

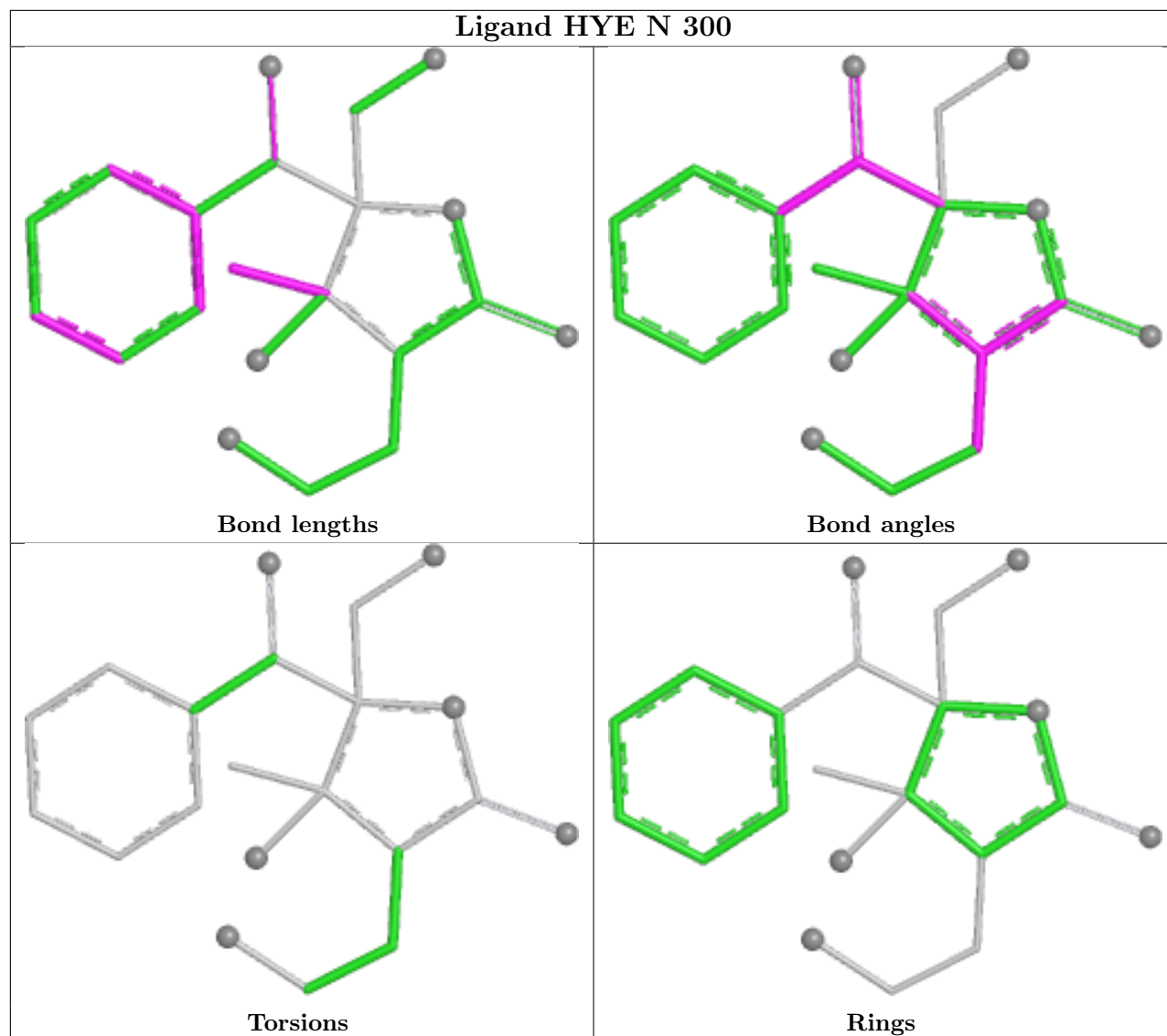












5.7 Other polymers [i](#)

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	39, 51, 78, 108	0
1	O	250/250 (100%)	0.06	8 (3%) 50 46	42, 57, 84, 110	0
2	B	244/244 (100%)	0.24	10 (4%) 41 37	39, 56, 93, 121	0
2	P	244/244 (100%)	0.38	21 (8%) 16 14	41, 59, 95, 121	0
3	C	241/241 (100%)	0.27	16 (6%) 24 21	37, 58, 112, 126	0
3	Q	241/241 (100%)	0.54	19 (7%) 18 16	42, 65, 114, 126	0
4	D	242/242 (100%)	0.25	9 (3%) 45 40	41, 59, 93, 124	0
4	R	242/242 (100%)	0.38	10 (4%) 41 37	42, 62, 94, 125	0
5	E	233/233 (100%)	0.35	9 (3%) 43 38	45, 62, 88, 114	0
5	S	233/233 (100%)	0.75	23 (9%) 13 11	44, 68, 93, 112	0
6	F	244/244 (100%)	0.09	5 (2%) 65 61	38, 57, 93, 108	0
6	T	244/244 (100%)	0.44	13 (5%) 32 28	39, 60, 95, 112	0
7	G	243/243 (100%)	-0.05	5 (2%) 63 59	36, 50, 78, 117	0
7	U	243/243 (100%)	0.07	3 (1%) 76 73	36, 54, 79, 119	0
8	H	222/222 (100%)	-0.22	2 (0%) 81 78	32, 47, 67, 93	0
8	V	222/222 (100%)	-0.24	2 (0%) 81 78	36, 50, 69, 98	0
9	I	204/204 (100%)	-0.34	2 (0%) 79 76	34, 47, 65, 80	0
9	W	204/204 (100%)	-0.31	1 (0%) 87 85	36, 48, 67, 82	0
10	J	198/198 (100%)	-0.23	4 (2%) 65 61	35, 50, 68, 124	0
10	X	198/198 (100%)	-0.15	5 (2%) 58 54	38, 52, 67, 124	0
11	K	212/212 (100%)	-0.32	0 100 100	32, 48, 65, 76	0
11	Y	212/212 (100%)	-0.23	1 (0%) 87 85	37, 50, 69, 77	0
12	L	222/222 (100%)	-0.21	2 (0%) 81 78	34, 49, 71, 93	0
12	Z	222/222 (100%)	-0.18	2 (0%) 81 78	37, 50, 72, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.25	1 (0%)	88 86	35, 49, 64, 71	0
13	M	233/233 (100%)	-0.23	2 (0%)	81 78	35, 50, 67, 71	0
14	2	196/196 (100%)	-0.20	4 (2%)	65 61	31, 47, 67, 83	0
14	N	196/196 (100%)	-0.28	1 (0%)	87 85	36, 46, 67, 80	0
All	All	6368/6368 (100%)	0.03	184 (2%)	53 49	31, 53, 87, 126	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(D)	ALA	8.3
3	Q	56	LEU	7.8
2	B	21(B)	GLY	7.4
4	D	12(C)	GLY	7.1
4	R	12(D)	ALA	6.8
7	U	240	ASP	6.6
4	D	12(E)	SER	6.4
2	P	217	ALA	6.3
2	B	217	ALA	6.2
3	Q	58	LEU	6.2
3	C	56	LEU	5.6
10	J	192	ALA	5.6
4	R	12(E)	SER	5.3
7	U	6	ALA	5.2
5	S	4	PHE	5.1
4	R	12(C)	GLY	5.0
7	G	6	ALA	4.9
3	C	55	THR	4.8
5	E	4	PHE	4.7
3	C	54	SER	4.4
2	B	21(D)	GLY	4.4
4	D	126	ARG	4.4
10	J	193	GLN	4.3
5	S	55	ALA	4.3
4	R	126	ARG	4.2
2	B	218	ASN	4.2
2	B	239	THR	4.1
13	1	-8	THR	4.1
12	L	145	TYR	4.1
2	P	54	VAL	4.0
10	X	193	GLN	3.9
2	P	21(B)	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
12	Z	145	TYR	3.9
3	C	59	GLN	3.9
1	O	235	ALA	3.8
6	F	204	ASP	3.8
13	M	-8	THR	3.8
3	Q	57	LYS	3.7
2	B	54	VAL	3.7
3	C	208	LYS	3.7
1	O	56	SER	3.6
4	D	242	ALA	3.6
5	S	2(E)	ASN	3.6
5	S	63	TYR	3.6
4	R	127	LEU	3.6
10	X	192	ALA	3.5
5	E	5	ARG	3.5
3	Q	54	SER	3.5
4	D	127	LEU	3.4
2	B	21(A)	LYS	3.4
10	X	-1	MET	3.4
3	C	240	LYS	3.3
3	Q	174	GLU	3.3
5	E	203	ASP	3.3
2	P	62	ASP	3.3
3	Q	240	LYS	3.3
2	P	21(C)	ASP	3.2
3	Q	55	THR	3.2
4	D	12(F)	GLY	3.1
2	P	63	THR	3.1
2	P	239	THR	3.1
3	C	207	ALA	3.1
3	Q	64	PRO	3.1
4	R	12(F)	GLY	3.1
3	Q	236	ILE	3.1
1	A	203	GLU	3.1
12	L	14(W)	LYS	3.0
2	P	219	GLU	3.0
13	M	61	ASP	3.0
3	Q	63	THR	3.0
2	P	21(D)	GLY	3.0
10	X	191	GLN	3.0
3	C	242	GLU	3.0
9	I	182	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	243	ALA	2.9
5	S	54	ASN	2.9
7	G	236	ILE	2.9
2	P	53	LYS	2.9
2	B	219	GLU	2.9
7	G	7	GLY	2.9
5	S	203	ASP	2.9
4	R	158	TYR	2.9
2	P	56	SER	2.8
5	S	5	ARG	2.8
9	I	-8	SER	2.8
6	T	240	ILE	2.8
2	P	59	LEU	2.8
10	J	191	GLN	2.8
14	2	116	GLY	2.8
2	P	63(A)	SER	2.8
6	T	205	ASN	2.8
1	O	4	MET	2.8
5	S	56	ASP	2.8
6	F	5	GLY	2.8
2	P	218	ASN	2.8
3	Q	241	GLN	2.8
1	O	64	LEU	2.7
5	S	60	SER	2.7
8	H	199	GLU	2.7
8	V	223	ASP	2.7
3	Q	203	THR	2.7
2	B	238	ILE	2.7
5	S	233	ILE	2.7
14	2	107	LYS	2.7
4	R	121	LEU	2.6
3	C	203	THR	2.6
3	Q	202	GLN	2.6
4	R	243	ALA	2.6
6	T	5	GLY	2.6
5	E	127	TYR	2.6
1	O	21(P)	LYS	2.6
3	C	239	GLU	2.6
5	S	18(C)	PHE	2.5
1	A	61	SER	2.5
10	X	189	ASP	2.5
8	V	221	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
12	Z	14(W)	LYS	2.5
1	O	57	PRO	2.5
6	T	184	LEU	2.5
2	P	21(A)	LYS	2.5
10	J	-1	MET	2.5
6	T	204	ASP	2.5
5	S	174	THR	2.5
2	P	220	TYR	2.4
6	T	20(C)	LYS	2.4
8	H	223	ASP	2.4
3	C	241	GLN	2.4
7	G	239	GLN	2.4
1	A	4	MET	2.4
6	F	240	ILE	2.4
3	Q	208	LYS	2.4
14	2	105	ASP	2.4
5	S	214	ILE	2.3
2	B	21(C)	ASP	2.3
5	E	63	TYR	2.3
4	R	12(B)	GLU	2.3
6	T	18(B)	HIS	2.3
7	U	239	GLN	2.3
5	E	56	ASP	2.3
2	P	181	LYS	2.3
3	C	57	LYS	2.3
2	P	61	GLN	2.3
5	E	128	GLY	2.3
14	2	149	GLU	2.3
11	Y	145	ASP	2.3
4	D	12(G)	GLU	2.3
5	S	2(C)	VAL	2.3
6	T	215	CYS	2.3
5	S	18(B)	THR	2.2
2	P	20(A)	SER	2.2
5	E	207	LEU	2.2
6	T	207	ASP	2.2
3	C	202	GLN	2.2
3	Q	235	GLN	2.2
3	Q	207	ALA	2.2
1	O	5	THR	2.2
5	S	222	THR	2.2
9	W	-8	SER	2.2

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Mol	Chain	Res	Type	RSRZ
6	T	36	THR	2.2
5	S	201	LEU	2.2
6	T	198	TYR	2.2
3	C	52	ARG	2.2
5	S	185	ASN	2.1
6	F	205	ASN	2.1
5	S	18(F)	ILE	2.1
5	S	50	ALA	2.1
7	G	237	ALA	2.1
3	Q	185	THR	2.1
5	S	51	LEU	2.1
1	O	65	SER	2.1
2	P	203	ASP	2.1
5	E	2(C)	VAL	2.1
3	C	209	ASN	2.1
14	N	149	GLU	2.1
6	T	206	LYS	2.1
3	Q	232	TYR	2.1
5	S	175	TYR	2.1
5	S	204	GLU	2.0
2	P	202	THR	2.0
3	C	63	THR	2.0
1	A	235	ALA	2.0
6	F	63	LYS	2.0
6	T	203	GLU	2.0
3	Q	44	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

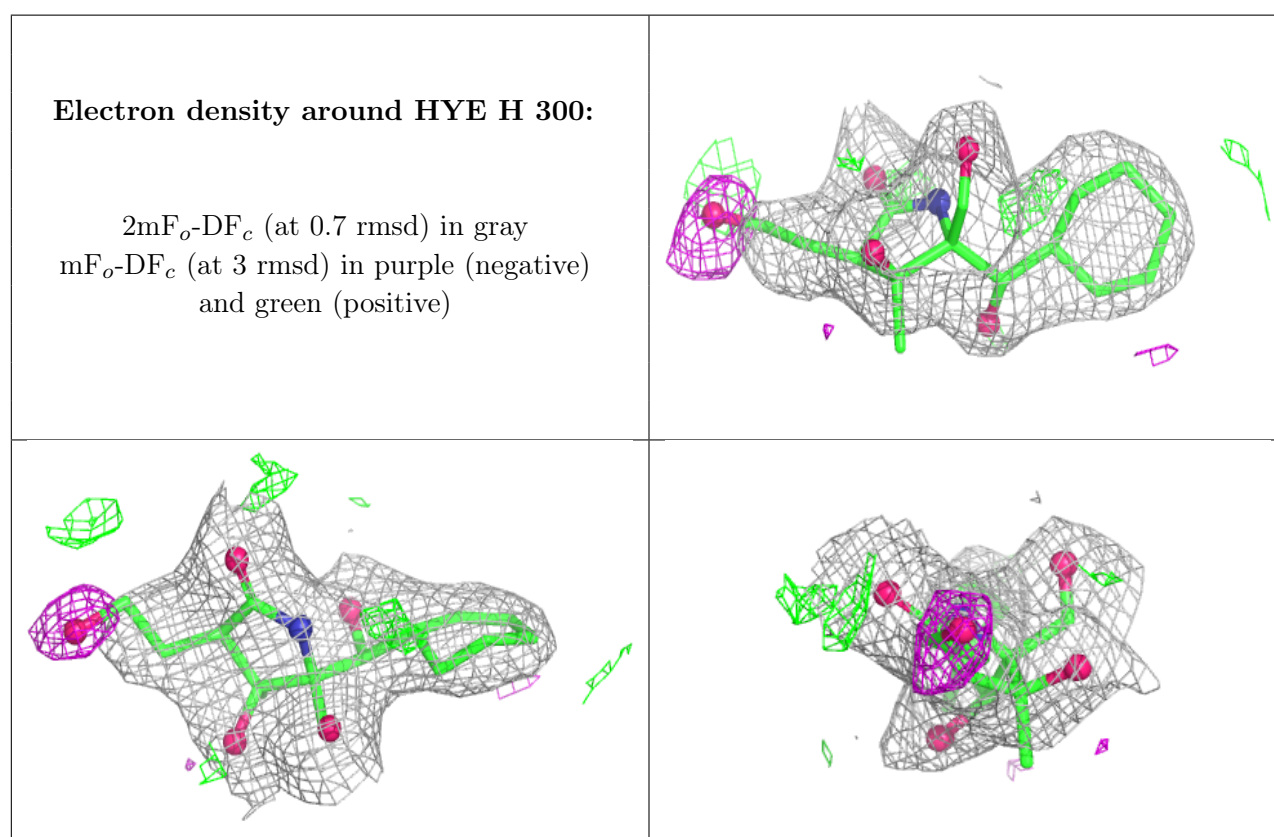
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

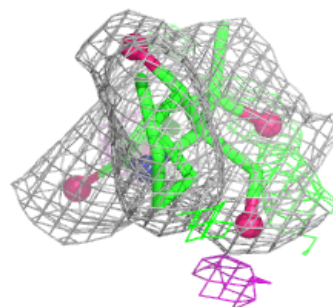
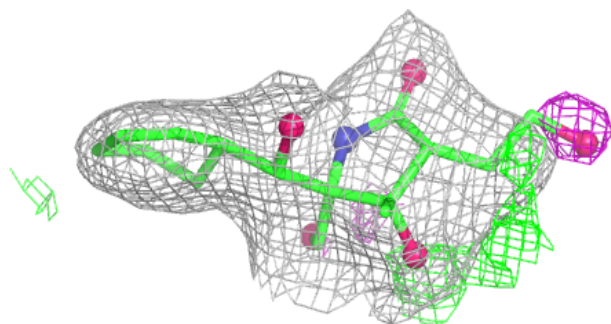
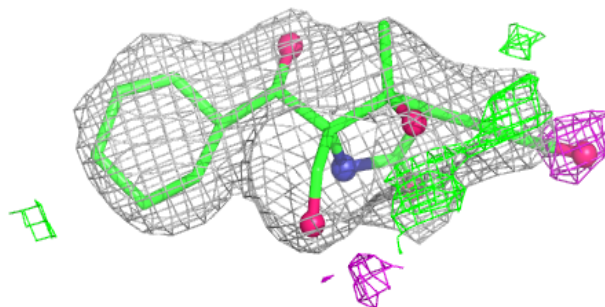
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	HYE	H	300	21/21	0.91	0.11	44,49,56,69	0
15	HYE	V	300	21/21	0.91	0.11	49,53,58,71	0
15	HYE	2	300	21/21	0.92	0.09	40,43,49,60	0
15	HYE	N	300	21/21	0.93	0.09	38,44,51,60	0
15	HYE	Y	300	21/21	0.94	0.09	40,44,48,54	0
15	HYE	K	300	21/21	0.95	0.07	37,44,49,57	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.

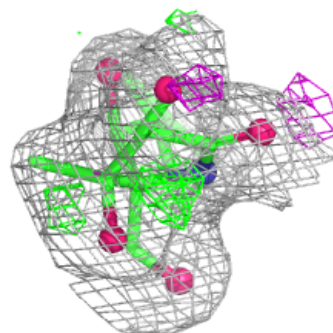
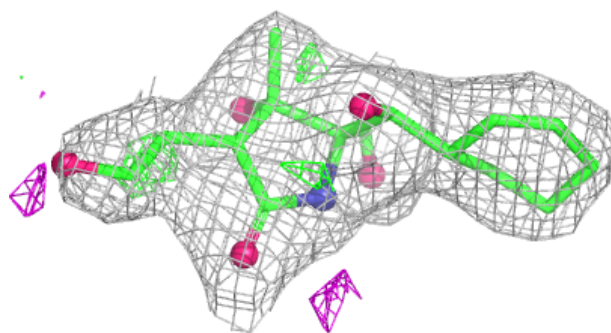
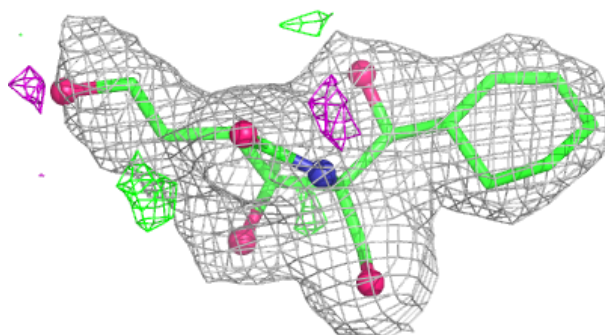


Electron density around HYE V 300:

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

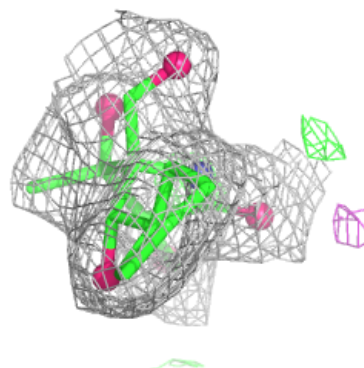
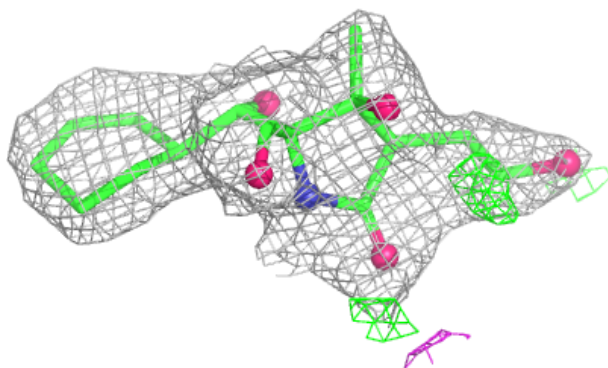
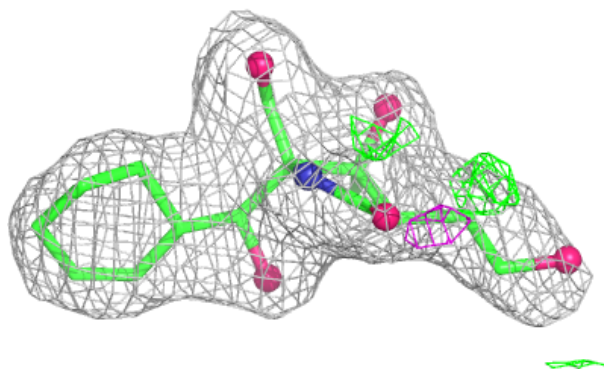
**Electron density around HYE 2 300:**

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

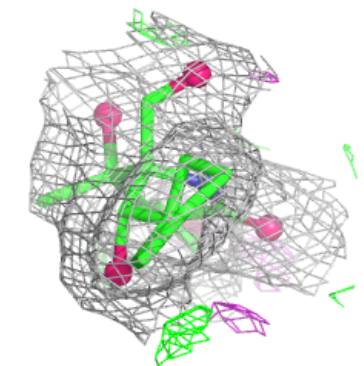
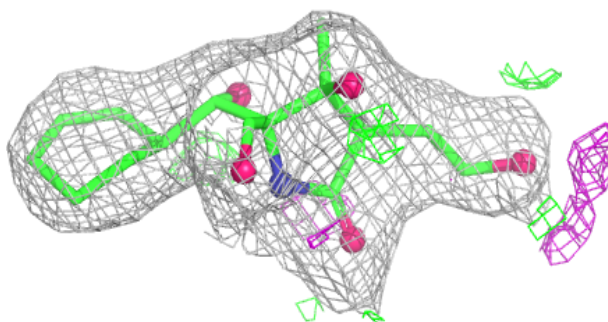
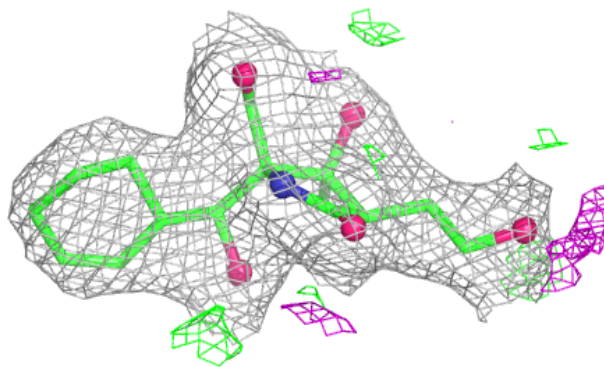


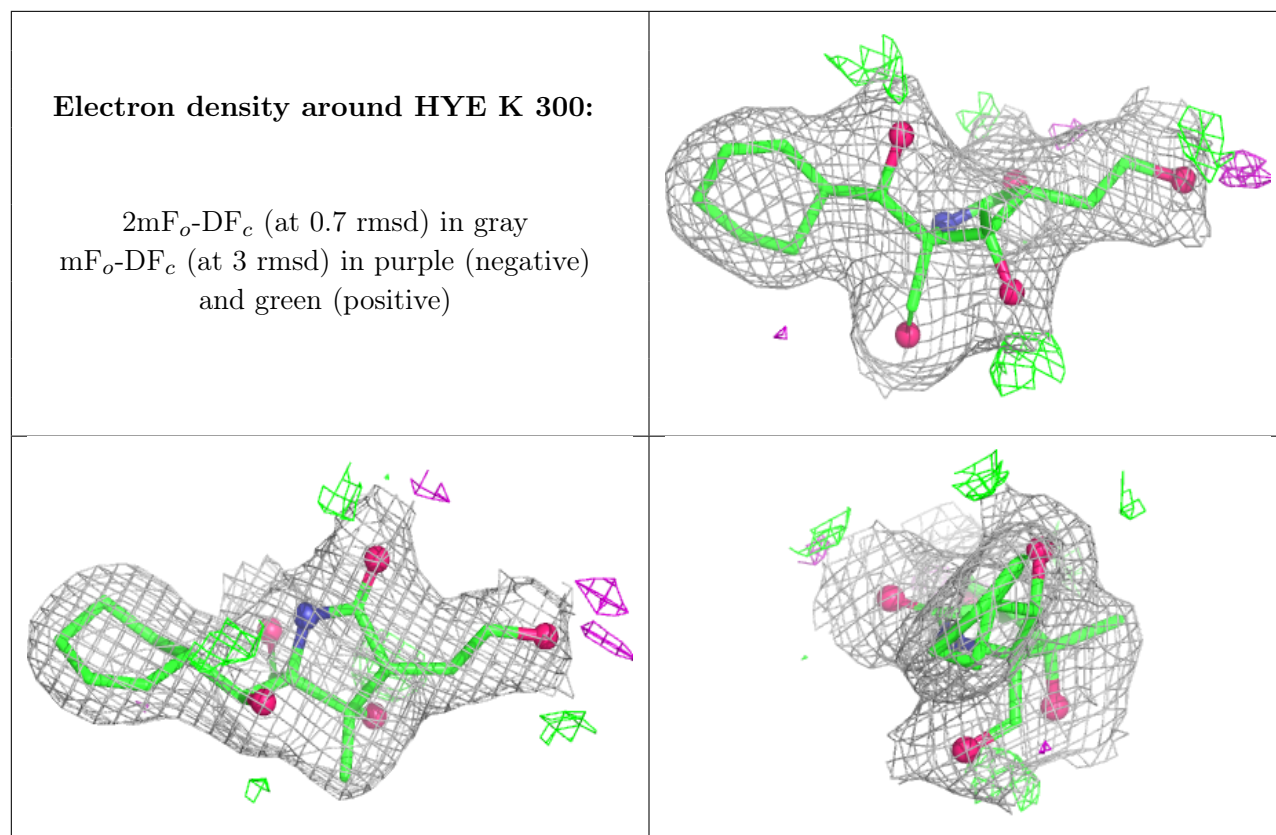
Electron density around HYE N 300:

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

**Electron density around HYE Y 300:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.