



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 01:12 AM UTC

PDB ID : 2FAK / pdb_00002fak
Title : Crystal structure of Salinosporamide A in complex with the yeast 20S proteasome
Authors : Groll, M.; Potts, B.C.
Deposited on : 2005-12-07
Resolution : 2.80 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)
Xtrriage (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

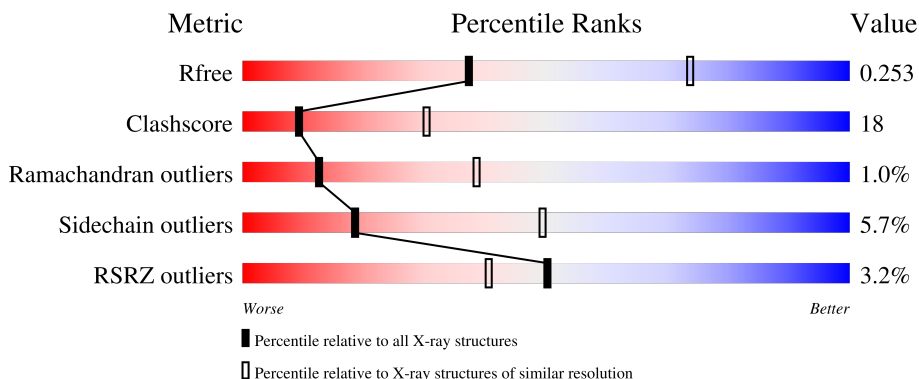
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	 8% 72% 26%
1	O	250	 3% 72% 26%
2	B	244	 6% 55% 40% 5%
2	P	244	 8% 55% 40% 5%
3	C	241	 8% 56% 41%

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Mol	Chain	Length	Quality of chain
3	Q	241	<p>9% 58% 39%</p>
4	D	242	<p>5% 66% 29%</p>
4	R	242	<p>5% 66% 29%</p>
5	E	233	<p>3% 58% 36%</p>
5	S	233	<p>12% 57% 37%</p>
6	F	244	<p>2% 60% 36%</p>
6	T	244	<p>5% 59% 35%</p>
7	G	243	<p>3% 64% 31%</p>
7	U	243	<p>2% 59% 35%</p>
8	H	222	<p>70% 28%</p>
8	V	222	<p>69% 29%</p>
9	I	204	<p>70% 27%</p>
9	W	204	<p>68% 30%</p>
10	J	198	<p>4% 64% 32%</p>
10	X	198	<p>3% 66% 30%</p>
11	K	212	<p>71% 26%</p>
11	Y	212	<p>70% 27%</p>
12	L	222	<p>61% 32%</p>
12	Z	222	<p>60% 33%</p>
13	1	233	<p>64% 32%</p>
13	M	233	<p>2% 63% 34%</p>
14	2	196	<p>64% 34%</p>
14	N	196	<p>66% 31%</p>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50685 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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			

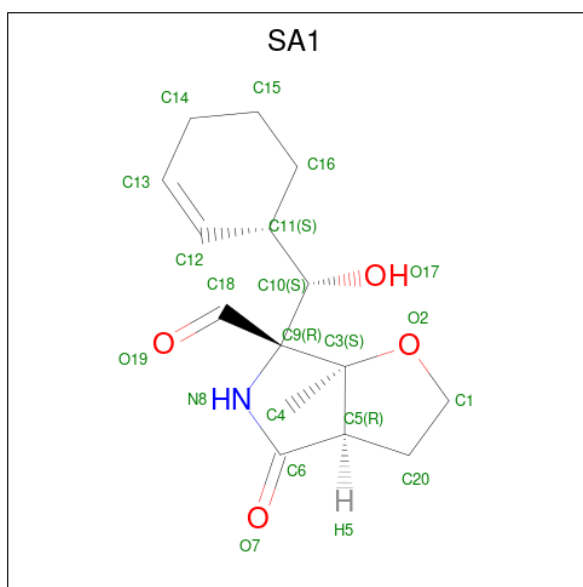
- Molecule 13 is a protein called Proteasome component PRE4.

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 (3AR,6R,6AS)-6-((S)-((S)-CYCLOHEX-2-ENYL)(HYDROXY)METHYL)-6A-METHYL-4-OXO-HEXAHYDRO-2H-FURO[3,2-C]PYRROLE-6-CARBALDEHYDE (CCD ID: SA1) (formula: C₁₅H₂₁NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
15	H	1	20	15	1	4	0	0
15	K	1	20	15	1	4	0	0
15	N	1	20	15	1	4	0	0
15	V	1	20	15	1	4	0	0
15	Y	1	20	15	1	4	0	0
15	2	1	20	15	1	4	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	A	42	42	42	0	0
16	B	29	29	29	0	0
16	C	35	35	35	0	0
16	D	27	27	27	0	0
16	E	10	10	10	0	0
16	F	35	35	35	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	50	Total O 50 50	0	0
16	H	40	Total O 40 40	0	0
16	I	49	Total O 49 49	0	0
16	J	43	Total O 43 43	0	0
16	K	30	Total O 30 30	0	0
16	L	36	Total O 36 36	0	0
16	M	49	Total O 49 49	0	0
16	N	51	Total O 51 51	0	0
16	O	28	Total O 28 28	0	0
16	P	20	Total O 20 20	0	0
16	Q	20	Total O 20 20	0	0
16	R	23	Total O 23 23	0	0
16	S	17	Total O 17 17	0	0
16	T	31	Total O 31 31	0	0
16	U	47	Total O 47 47	0	0
16	V	42	Total O 42 42	0	0
16	W	41	Total O 41 41	0	0
16	X	37	Total O 37 37	0	0
16	Y	34	Total O 34 34	0	0
16	Z	46	Total O 46 46	0	0
16	1	59	Total O 59 59	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	46	Total	O	0	0
			46	46		

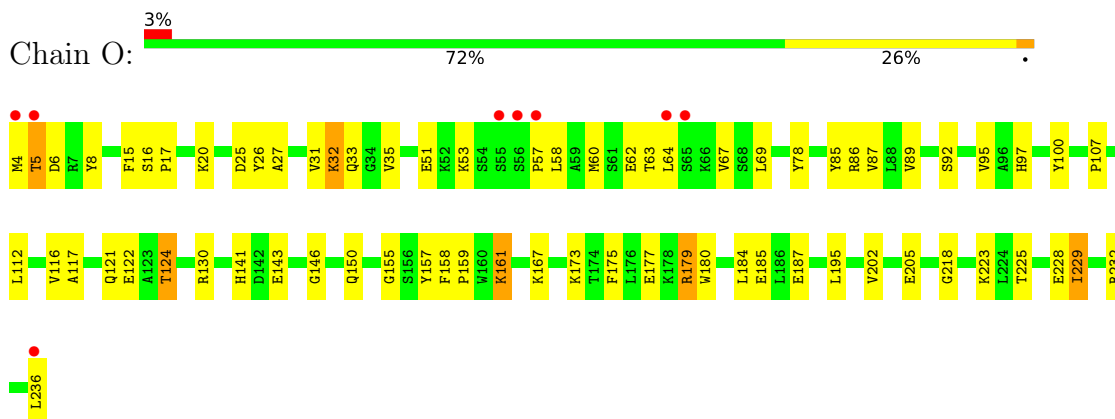
3 Residue-property plots [i](#)

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

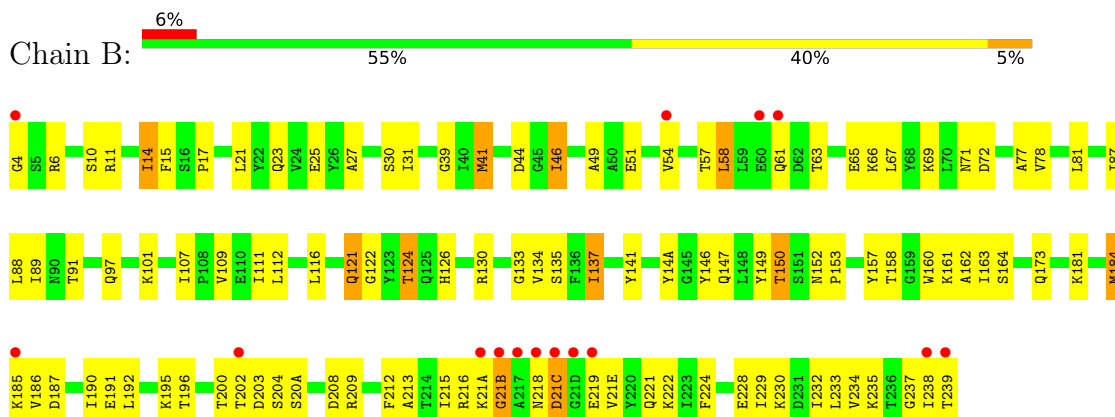
- Molecule 1: Proteasome component Y7



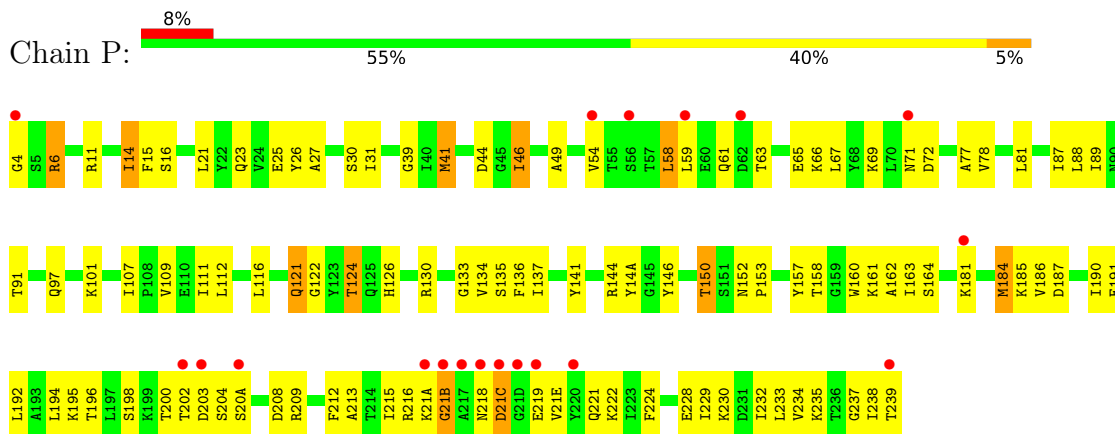
- Molecule 1: Proteasome component Y7



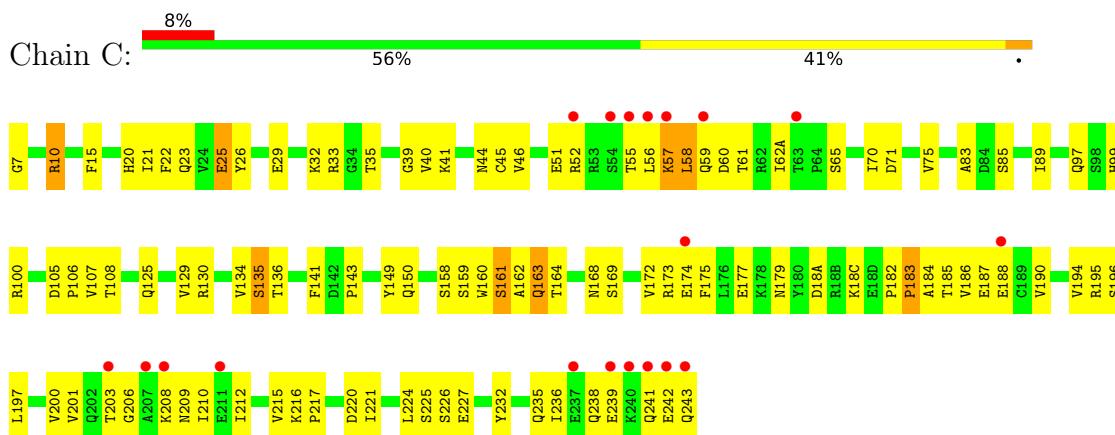
- Molecule 2: Proteasome component Y13



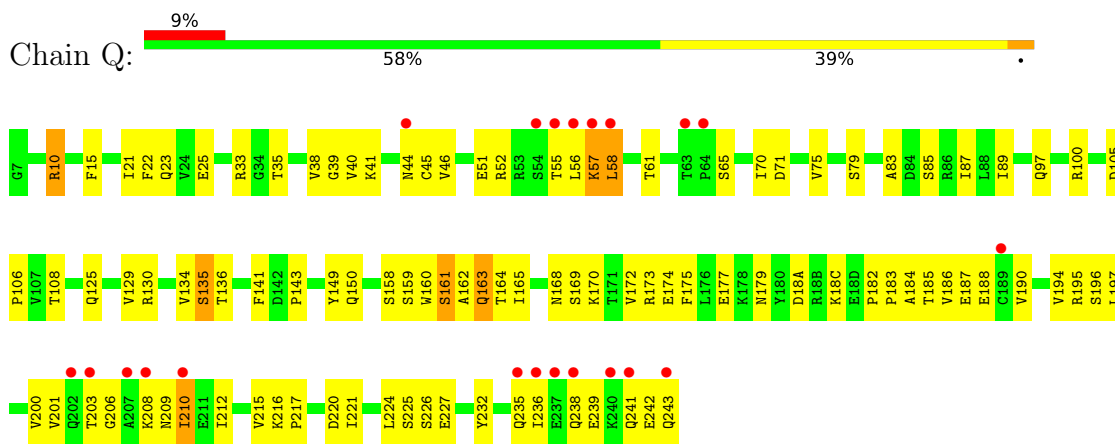
- Molecule 2: Proteasome component Y13



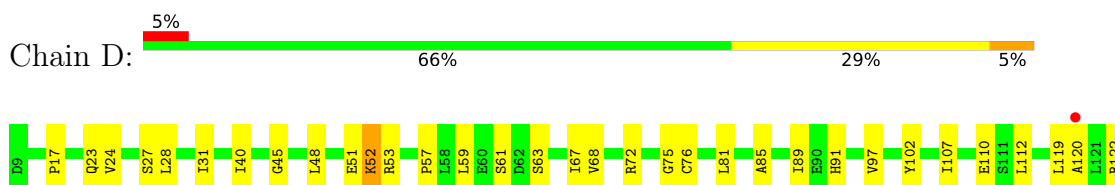
- Molecule 3: Proteasome component PRE6

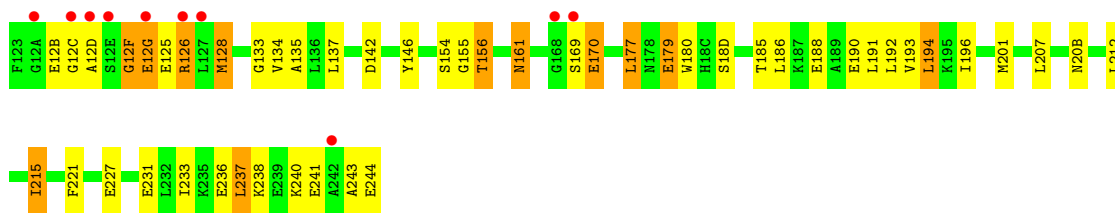


- Molecule 3: Proteasome component PRE6



- Molecule 4: Proteasome component PUP2

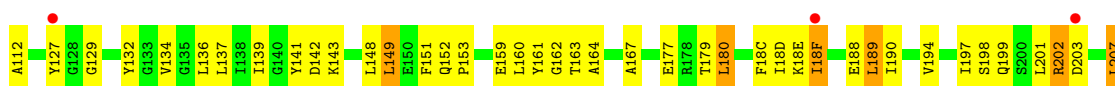




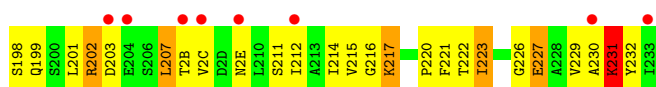
- Molecule 4: Proteasome component PUP2



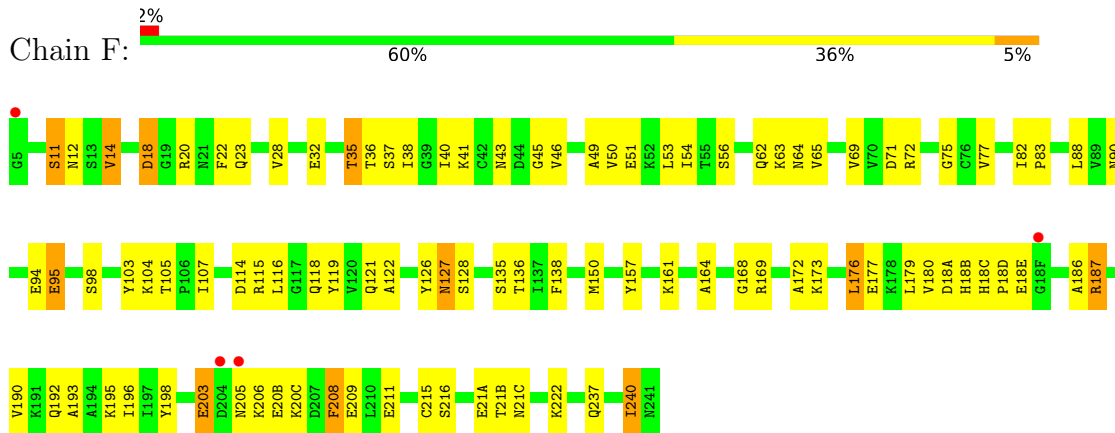
- Molecule 5: Proteasome component PRE5



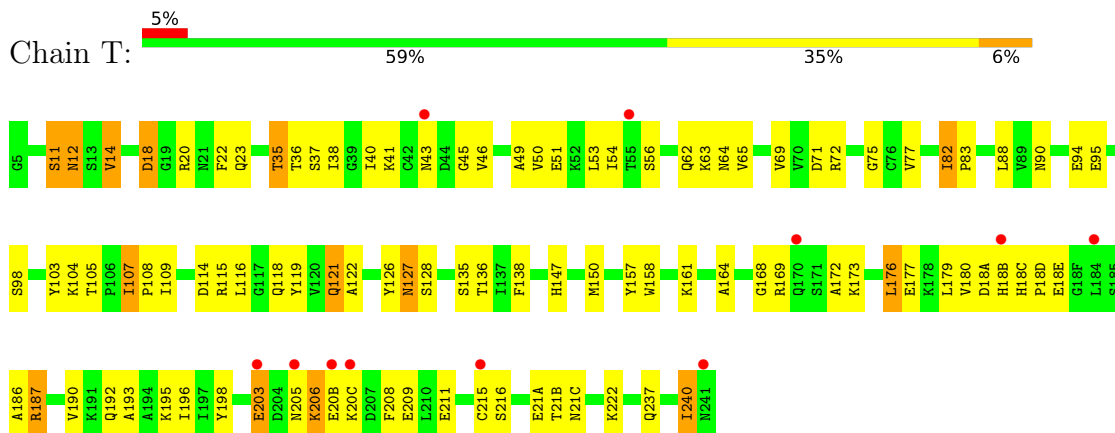
- Molecule 5: Proteasome component PRE5



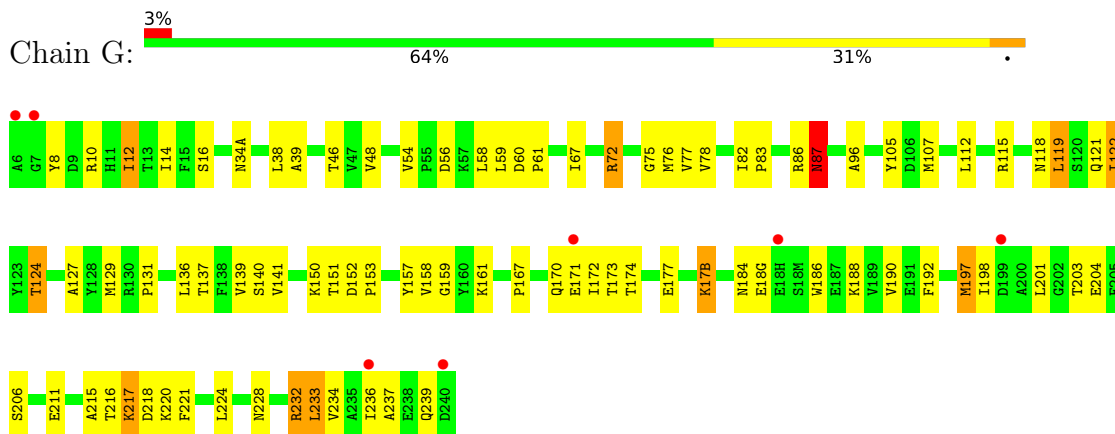
- Molecule 6: Proteasome component C1



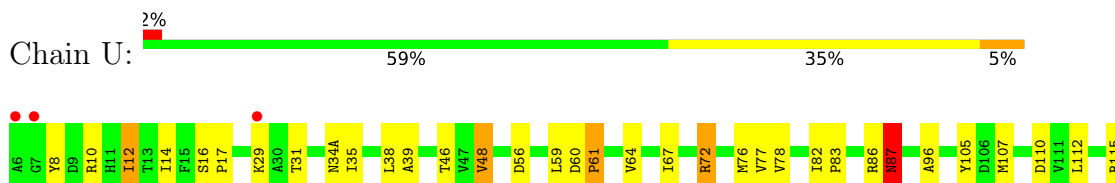
- Molecule 6: Proteasome component C1

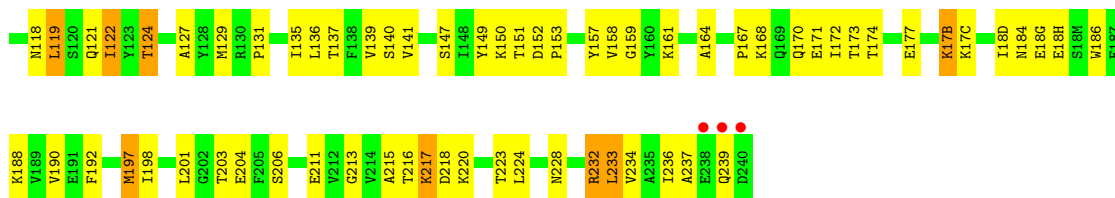


- Molecule 7: Proteasome component C7-alpha



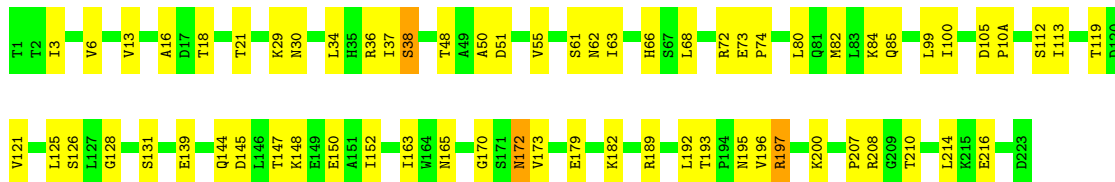
- Molecule 7: Proteasome component C7-alpha





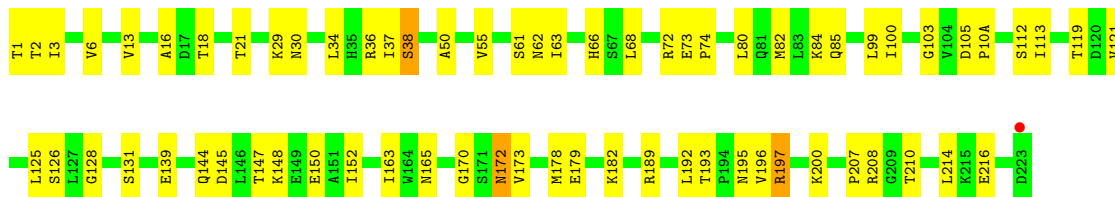
- Molecule 8: Proteasome component PUP1

Chain H: 70% 28%



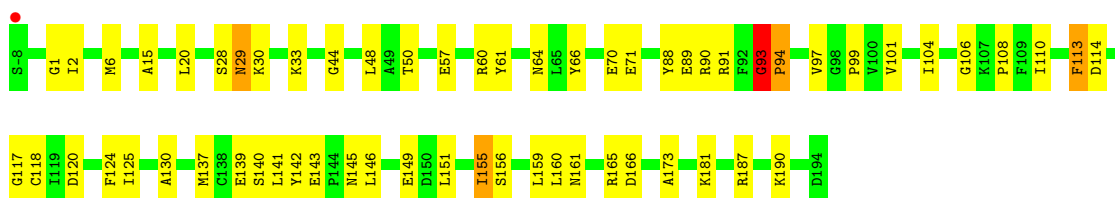
- Molecule 8: Proteasome component PUP1

Chain V: 69% 29%



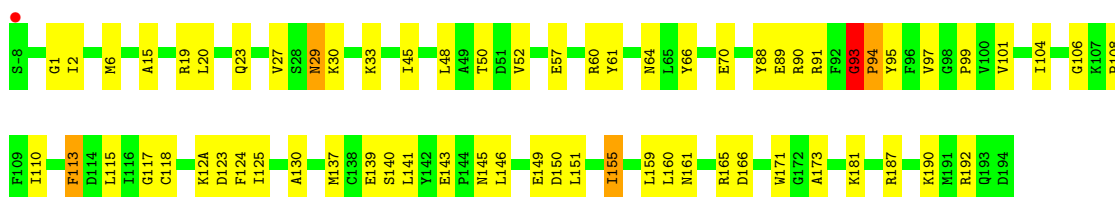
- Molecule 9: Proteasome component PUP3

Chain I: 70% 27%

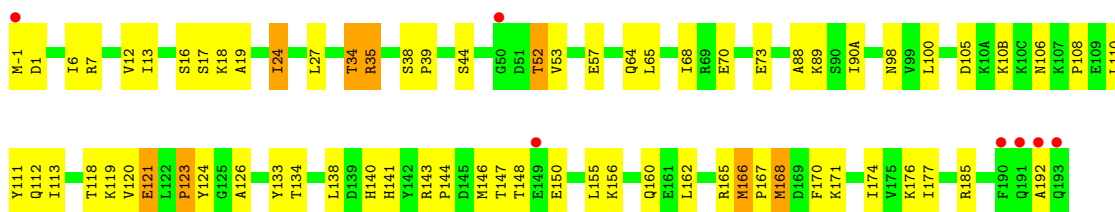


- Molecule 9: Proteasome component PUP3

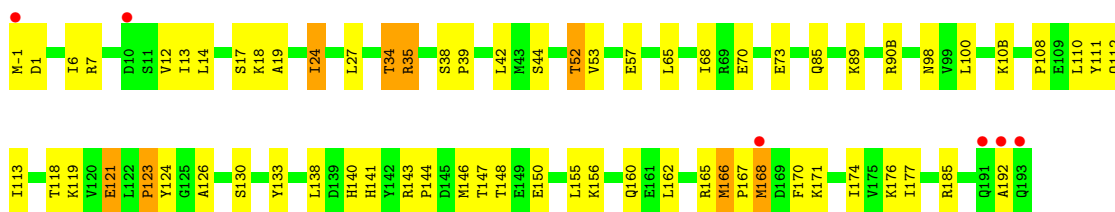
Chain W: 68% 30%



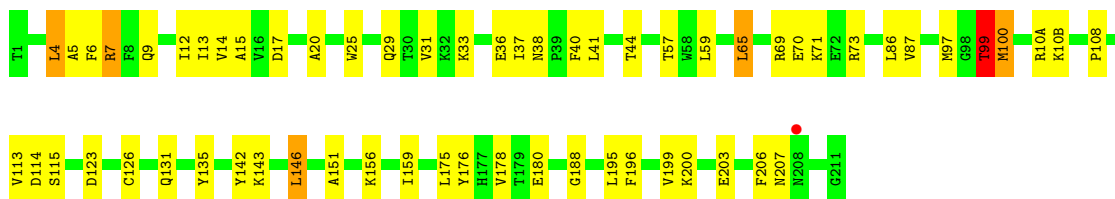
- Molecule 10: Proteasome component C11



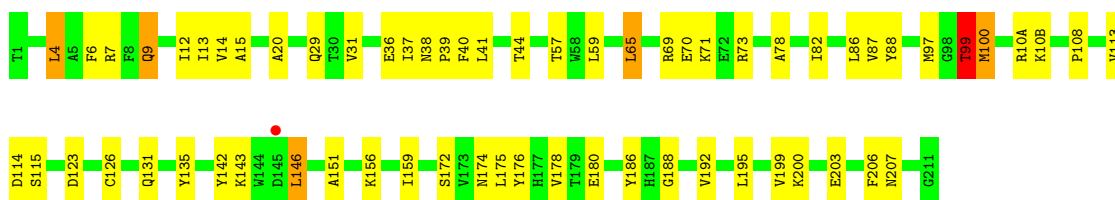
- Molecule 10: Proteasome component C11



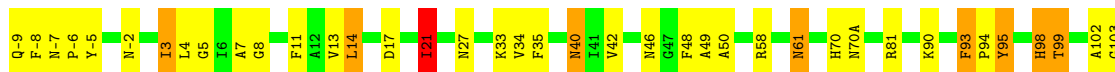
- Molecule 11: Proteasome component PRE2

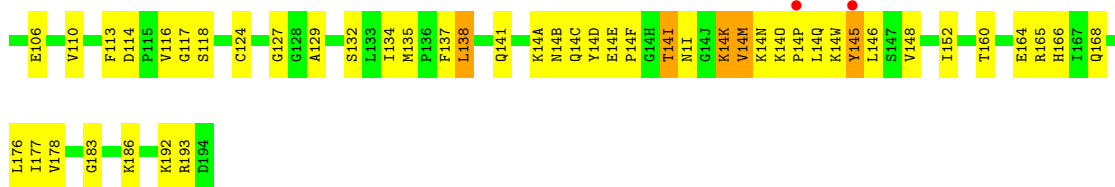


- Molecule 11: Proteasome component PRE2



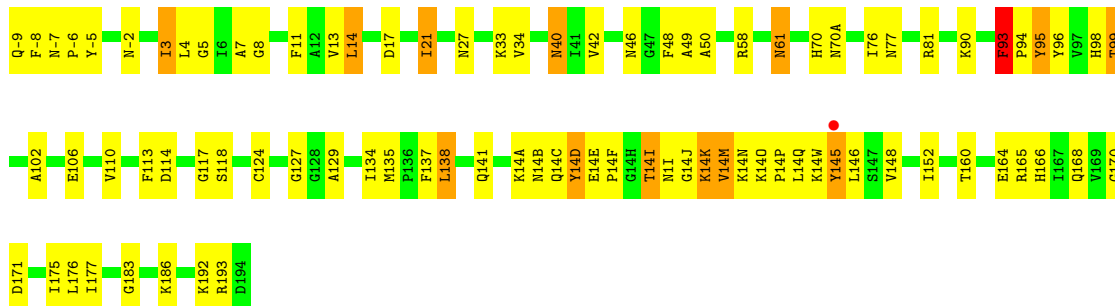
- Molecule 12: Proteasome component C5





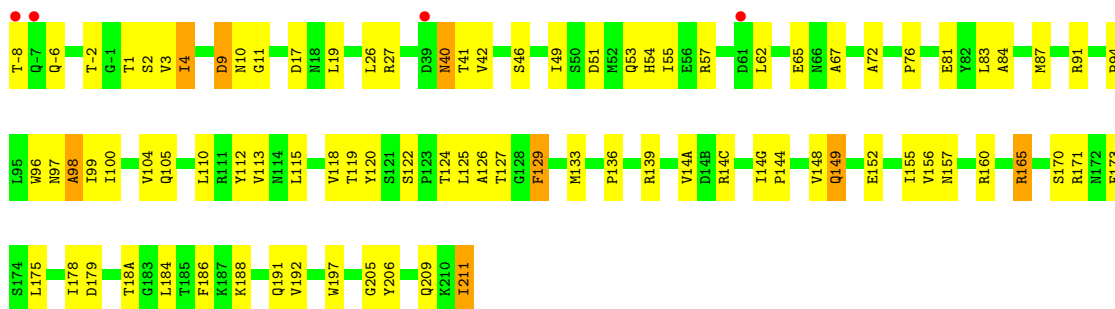
- Molecule 12: Proteasome component C5

Chain Z: 60% 33% 6%



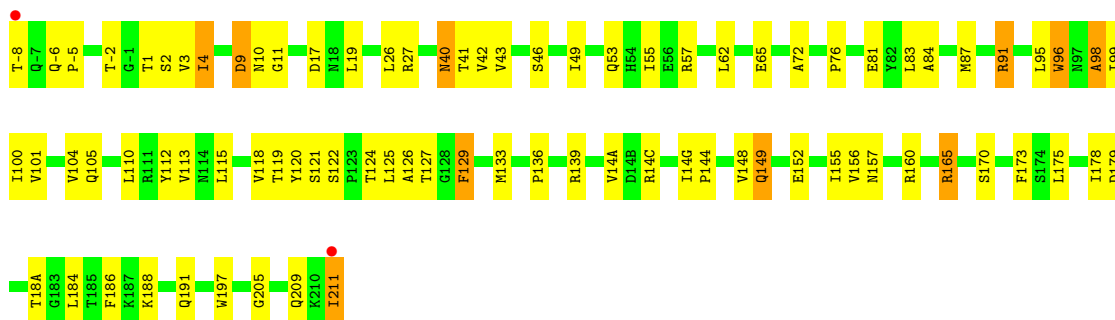
- Molecule 13: Proteasome component PRE4

Chain M: 2% 63% 34%



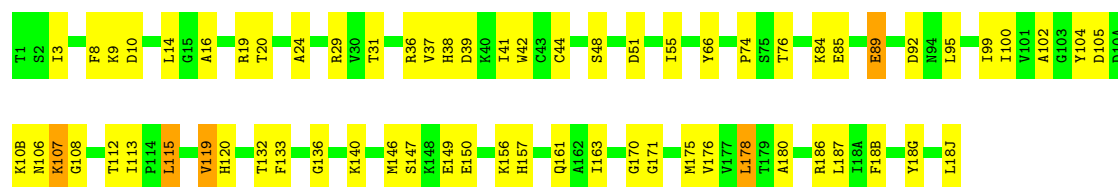
- Molecule 13: Proteasome component PRE4

Chain 1: 64% 32%



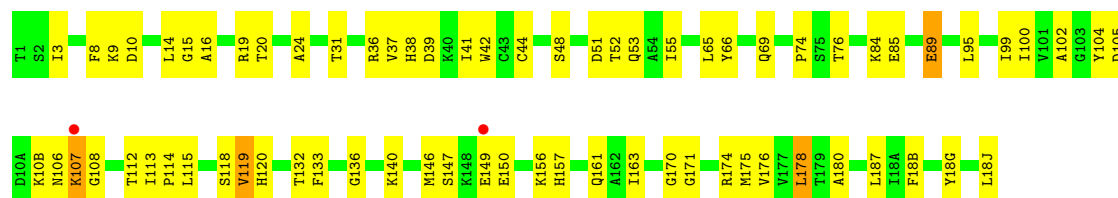
- Molecule 14: Proteasome component PRE3

Chain N:  66% 31%



• Molecule 14: Proteasome component PRE3

Chain 2:  64% 34%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.17Å 301.16Å 144.14Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.80) 98.4 (15.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.75Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.254 0.229 , 0.253	Depositor DCC
R_{free} test set	13425 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtrriage
Anisotropy	0.558	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50685	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SA1

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	0.45	0/1952	0.92	7/2642 (0.3%)
1	O	0.43	0/1952	0.92	6/2642 (0.2%)
2	B	0.45	0/1935	0.94	8/2618 (0.3%)
2	P	0.45	0/1935	0.94	7/2618 (0.3%)
3	C	0.41	0/1920	0.94	5/2598 (0.2%)
3	Q	0.41	0/1920	0.94	5/2598 (0.2%)
4	D	0.45	0/1887	0.93	6/2541 (0.2%)
4	R	0.45	0/1887	0.93	6/2541 (0.2%)
5	E	0.40	0/1823	0.91	4/2463 (0.2%)
5	S	0.40	0/1823	0.92	4/2463 (0.2%)
6	F	0.44	0/1937	0.94	9/2614 (0.3%)
6	T	0.43	0/1937	0.94	9/2614 (0.3%)
7	G	0.47	0/1959	0.96	10/2652 (0.4%)
7	U	0.48	0/1959	0.96	6/2652 (0.2%)
8	H	0.48	0/1716	0.99	6/2326 (0.3%)
8	V	0.47	0/1716	0.98	6/2326 (0.3%)
9	I	0.46	0/1611	0.99	7/2174 (0.3%)
9	W	0.49	0/1611	1.01	7/2174 (0.3%)
10	J	0.47	0/1613	0.97	5/2173 (0.2%)
10	X	0.46	0/1613	0.98	4/2173 (0.2%)
11	K	0.47	0/1681	0.93	5/2274 (0.2%)
11	Y	0.44	0/1681	0.92	5/2274 (0.2%)
12	L	0.44	0/1795	1.03	11/2420 (0.5%)
12	Z	0.44	0/1795	1.02	9/2420 (0.4%)
13	1	0.49	0/1855	0.96	6/2514 (0.2%)
13	M	0.46	0/1855	0.95	7/2514 (0.3%)
14	2	0.48	0/1541	0.96	3/2087 (0.1%)
14	N	0.49	0/1541	0.97	3/2087 (0.1%)
All	All	0.45	0/50450	0.96	176/68192 (0.3%)

There are no bond length outliers.

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	27	ARG	N-CA-C	9.72	121.57	110.97
13	1	27	ARG	N-CA-C	9.53	121.36	110.97
8	H	37	ILE	N-CA-C	-9.42	104.27	111.90
8	V	37	ILE	N-CA-C	-8.62	104.91	111.90
6	T	12	ASN	N-CA-C	8.43	120.08	111.07
1	A	161	LYS	N-CA-C	-8.38	101.92	112.90
4	R	161	ASN	N-CA-C	-8.21	102.14	112.90
6	F	12	ASN	N-CA-C	8.16	119.86	110.97
12	L	95	TYR	N-CA-C	-8.15	96.78	109.25
1	O	161	LYS	N-CA-C	-8.08	102.31	112.90
12	Z	95	TYR	N-CA-C	-7.97	97.06	109.25
10	J	123	PRO	N-CA-C	-7.96	103.14	113.57
4	D	169	SER	N-CA-C	7.95	120.72	111.02
4	R	169	SER	N-CA-C	7.90	120.66	111.02
7	G	161	LYS	N-CA-C	-7.85	102.61	112.90
4	D	161	ASN	N-CA-C	-7.65	102.88	112.90
10	X	123	PRO	N-CA-C	-7.61	103.59	113.57
6	F	107	ILE	N-CA-C	7.57	117.21	108.96
7	U	161	LYS	N-CA-C	-7.57	102.99	112.90
6	F	161	LYS	N-CA-C	-7.46	103.12	112.90
6	T	107	ILE	N-CA-C	7.39	117.02	108.96
9	W	60	ARG	N-CA-C	-7.39	103.17	111.07
6	T	14	VAL	N-CA-C	7.37	118.62	108.89
2	B	161	LYS	N-CA-C	-7.36	104.43	113.41
6	T	161	LYS	N-CA-C	-7.36	103.26	112.90
7	G	127	ALA	N-CA-C	7.32	119.26	111.28
3	C	108	THR	N-CA-C	-7.19	101.25	110.53
11	Y	188	GLY	N-CA-C	7.18	124.10	112.61
3	Q	161	SER	N-CA-C	-7.11	102.94	111.69
6	F	14	VAL	N-CA-C	7.07	118.22	108.89
2	P	161	LYS	N-CA-C	-7.05	104.81	113.41
7	U	16	SER	N-CA-C	-7.01	101.21	110.40
8	H	38	SER	N-CA-C	-7.01	100.08	108.14
11	K	188	GLY	N-CA-C	7.00	123.81	112.61
13	M	165	ARG	N-CA-C	7.00	121.99	113.38
13	1	165	ARG	N-CA-C	6.91	121.88	113.38
3	C	161	SER	N-CA-C	-6.89	103.22	111.69
7	G	16	SER	N-CA-C	-6.84	101.43	110.40
8	V	38	SER	N-CA-C	-6.84	100.28	108.14
7	U	127	ALA	N-CA-C	6.83	118.81	111.36
2	B	238	ILE	N-CA-C	-6.80	106.01	113.43
5	E	161	TYR	N-CA-C	-6.79	104.00	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	78	TYR	N-CA-C	6.76	116.97	108.45
6	F	240	ILE	N-CA-C	-6.73	106.17	112.83
2	P	238	ILE	N-CA-C	-6.73	106.09	113.43
3	Q	108	THR	N-CA-C	-6.71	100.86	110.59
8	V	100	ILE	N-CA-C	-6.70	97.46	107.37
6	F	135	SER	N-CA-C	-6.68	98.51	109.40
9	I	145	ASN	N-CA-C	6.48	120.45	111.90
12	Z	134	ILE	N-CA-C	6.45	118.03	111.00
9	W	145	ASN	N-CA-C	6.41	120.37	111.90
5	S	161	TYR	N-CA-C	-6.36	104.57	112.90
9	I	60	ARG	N-CA-C	-6.33	104.30	111.07
6	T	240	ILE	N-CA-C	-6.22	106.67	112.83
13	1	9	ASP	N-CA-C	6.18	118.81	111.33
8	H	100	ILE	N-CA-C	-6.16	98.26	107.37
6	T	135	SER	N-CA-C	-6.07	99.01	108.90
12	L	134	ILE	N-CA-C	6.05	117.99	111.58
13	M	9	ASP	N-CA-C	6.04	118.64	111.33
4	R	61	SER	N-CA-C	6.04	119.48	111.75
5	S	58	LEU	N-CA-C	-6.01	105.90	113.72
3	Q	70	ILE	N-CA-C	-6.00	105.21	111.58
11	K	131	GLN	N-CA-C	6.00	118.31	111.11
2	B	109	VAL	N-CA-C	5.98	116.64	110.36
13	1	-2	THR	N-CA-C	5.93	119.21	109.72
4	D	61	SER	N-CA-C	5.90	119.31	111.75
8	V	21	THR	N-CA-C	5.88	118.35	109.23
10	J	27	LEU	N-CA-C	5.88	118.47	111.71
13	M	-2	THR	N-CA-C	5.87	119.11	109.72
12	Z	21	ILE	N-CA-C	5.86	117.36	108.80
12	Z	93	PHE	CA-C-N	5.84	127.14	119.84
12	Z	93	PHE	C-N-CA	5.84	127.14	119.84
7	U	17(B)	LYS	N-CA-C	-5.84	104.92	111.28
2	P	109	VAL	N-CA-C	5.83	116.48	110.36
8	H	21	THR	N-CA-C	5.83	118.26	109.23
1	A	78	TYR	N-CA-C	5.79	116.73	108.74
2	B	203	ASP	N-CA-C	-5.76	106.10	113.02
5	E	58	LEU	N-CA-C	-5.76	106.23	113.72
11	Y	131	GLN	N-CA-C	5.74	117.99	111.11
13	1	98	ALA	N-CA-C	-5.73	98.94	108.34
1	O	143	GLU	N-CA-C	5.73	118.26	111.33
7	G	206	SER	N-CA-C	-5.69	101.58	110.17
2	B	137	ILE	N-CA-C	-5.68	99.45	107.75
10	X	27	LEU	N-CA-C	5.68	118.25	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	49	ALA	N-CA-C	5.63	118.14	111.33
2	P	78	VAL	N-CA-C	5.63	117.10	108.71
13	M	98	ALA	N-CA-C	-5.61	98.76	108.69
10	X	89	LYS	N-CA-C	-5.60	105.10	111.14
11	Y	99	THR	N-CA-C	5.59	117.89	109.23
3	C	70	ILE	N-CA-C	-5.58	105.66	111.58
7	G	17(B)	LYS	N-CA-C	-5.58	105.19	111.28
11	K	99	THR	N-CA-C	5.58	117.88	109.23
9	W	93	GLY	CA-C-N	5.58	125.55	120.03
9	W	93	GLY	C-N-CA	5.58	125.55	120.03
9	I	94	PRO	N-CA-C	5.57	119.77	111.41
6	T	71	ASP	CB-CA-C	-5.56	110.19	116.63
11	K	57	THR	N-CA-C	-5.55	105.31	111.36
6	F	71	ASP	CB-CA-C	-5.53	110.21	116.63
12	L	21	ILE	N-CA-C	5.51	116.85	108.80
12	L	93	PHE	CA-C-N	5.51	126.73	119.84
12	L	93	PHE	C-N-CA	5.51	126.73	119.84
4	R	179	GLU	N-CA-C	5.50	117.28	111.28
9	W	95	TYR	N-CA-C	-5.48	101.04	109.76
4	D	63	SER	N-CA-C	-5.48	106.44	113.02
9	I	117	GLY	N-CA-C	5.46	122.02	114.92
8	H	172	ASN	N-CA-C	5.46	118.54	110.46
14	N	19	ARG	N-CA-C	5.44	117.83	109.07
2	P	203	ASP	N-CA-C	-5.44	106.49	113.02
11	Y	57	THR	N-CA-C	-5.44	105.43	111.36
3	Q	136	THR	N-CA-C	5.42	117.92	109.52
1	A	12	LEU	N-CA-C	-5.41	106.69	113.72
2	B	78	VAL	N-CA-C	5.36	116.69	108.71
5	E	152	GLN	CA-C-N	5.35	126.53	119.84
5	E	152	GLN	C-N-CA	5.35	126.53	119.84
12	L	49	ALA	N-CA-C	5.35	117.80	111.33
3	C	136	THR	N-CA-C	5.34	117.80	109.52
9	W	94	PRO	N-CA-C	5.34	119.42	111.41
10	X	165	ARG	N-CA-C	5.34	119.85	113.23
4	R	63	SER	N-CA-C	-5.33	106.55	113.16
2	B	134	VAL	N-CA-C	5.33	116.34	108.45
6	T	22	PHE	N-CA-C	5.31	117.75	111.33
1	A	218	GLY	CA-C-N	5.30	125.06	119.76
1	A	218	GLY	C-N-CA	5.30	125.06	119.76
8	V	99	LEU	N-CA-C	5.30	117.87	109.50
9	W	117	GLY	N-CA-C	5.30	121.80	114.92
1	O	16	SER	N-CA-C	-5.29	103.47	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	93	GLY	CA-C-N	5.28	125.26	120.03
9	I	93	GLY	C-N-CA	5.28	125.26	120.03
10	J	89	LYS	N-CA-C	-5.28	105.44	111.14
11	K	29	GLN	N-CA-C	-5.28	106.23	113.30
7	U	206	SER	N-CA-C	-5.27	102.21	110.17
13	M	94	PRO	N-CA-C	5.26	119.31	111.41
12	L	116	VAL	N-CA-C	5.25	117.23	111.77
2	P	16	SER	N-CA-C	-5.25	103.33	110.36
12	Z	193	ARG	N-CA-C	5.24	118.69	112.72
4	D	128	MET	N-CA-C	-5.24	99.65	110.80
4	D	179	GLU	N-CA-C	5.23	116.98	111.28
5	S	152	GLN	CA-C-N	5.18	126.32	119.84
5	S	152	GLN	C-N-CA	5.18	126.32	119.84
7	G	87	ASN	N-CA-C	-5.18	105.72	111.36
8	H	99	LEU	N-CA-C	5.18	117.68	109.50
4	R	128	MET	N-CA-C	-5.17	99.79	110.80
14	N	99	ILE	N-CA-C	5.16	115.92	108.48
14	2	19	ARG	N-CA-C	5.15	117.36	109.07
10	J	165	ARG	N-CA-C	5.14	119.61	113.23
8	V	172	ASN	N-CA-C	5.13	118.05	110.46
10	J	134	THR	N-CA-C	5.11	119.57	113.23
12	L	35	PHE	N-CA-C	5.11	117.58	109.50
6	T	82	ILE	CB-CA-C	-5.11	108.85	113.70
12	L	193	ARG	N-CA-C	5.11	119.20	112.92
13	1	95	LEU	N-CA-C	-5.10	98.27	107.75
6	F	208	PHE	N-CA-C	5.10	116.05	108.86
3	Q	22	PHE	N-CA-C	5.08	117.48	111.33
7	G	60	ASP	CA-C-N	5.08	126.19	119.84
7	G	60	ASP	C-N-CA	5.08	126.19	119.84
1	A	107	PRO	N-CA-C	5.05	115.99	110.58
14	N	107	LYS	CB-CA-C	-5.05	110.77	116.63
2	P	134	VAL	N-CA-C	5.05	115.93	108.45
12	Z	145	TYR	N-CA-C	5.05	118.04	109.76
14	2	99	ILE	N-CA-C	5.04	115.74	108.48
2	B	57	THR	N-CA-C	-5.04	105.79	111.28
11	Y	29	GLN	N-CA-C	-5.04	106.38	112.88
7	G	54	VAL	CA-C-N	5.03	124.20	118.97
7	G	54	VAL	C-N-CA	5.03	124.20	118.97
12	L	145	TYR	N-CA-C	5.03	118.00	109.76
14	2	107	LYS	CB-CA-C	-5.02	110.81	116.63
12	Z	117	GLY	N-CA-C	5.02	121.67	114.64
6	F	22	PHE	N-CA-C	5.01	117.39	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	I	142	TYR	N-CA-C	5.01	118.12	110.20
13	M	97	ASN	N-CA-C	5.01	116.61	109.14
12	L	117	GLY	N-CA-C	5.00	121.65	114.64
1	A	16	SER	N-CA-C	-5.00	103.85	110.40
3	C	22	PHE	N-CA-C	5.00	117.38	111.33
1	O	218	GLY	CA-C-N	5.00	124.76	119.76
1	O	218	GLY	C-N-CA	5.00	124.76	119.76
7	U	87	ASN	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	56	0
1	O	1915	0	1926	59	0
2	B	1905	0	1901	108	0
2	P	1905	0	1901	98	0
3	C	1891	0	1900	113	0
3	Q	1891	0	1900	100	0
4	D	1862	0	1836	64	0
4	R	1862	0	1836	68	0
5	E	1795	0	1797	95	0
5	S	1795	0	1797	106	0
6	F	1897	0	1886	69	0
6	T	1897	0	1886	78	0
7	G	1921	0	1910	75	0
7	U	1921	0	1910	88	0
8	H	1685	0	1687	47	0
8	V	1685	0	1687	48	0
9	I	1581	0	1574	56	0
9	W	1581	0	1574	55	0
10	J	1585	0	1590	73	0
10	X	1585	0	1590	76	0
11	K	1644	0	1594	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Y	1644	0	1594	53	0
12	L	1757	0	1711	62	0
12	Z	1757	0	1711	67	0
13	1	1824	0	1832	69	0
13	M	1824	0	1832	67	0
14	2	1512	0	1480	56	0
14	N	1512	0	1480	53	0
15	2	20	0	20	0	0
15	H	20	0	20	0	0
15	K	20	0	20	1	0
15	N	20	0	20	0	0
15	V	20	0	20	0	0
15	Y	20	0	20	1	0
16	1	59	0	0	0	0
16	2	46	0	0	0	0
16	A	42	0	0	1	0
16	B	29	0	0	4	0
16	C	35	0	0	3	0
16	D	27	0	0	1	0
16	E	10	0	0	1	0
16	F	35	0	0	6	0
16	G	50	0	0	1	0
16	H	40	0	0	2	0
16	I	49	0	0	2	0
16	J	43	0	0	2	0
16	K	30	0	0	1	0
16	L	36	0	0	2	0
16	M	49	0	0	4	0
16	N	51	0	0	3	0
16	O	28	0	0	1	0
16	P	20	0	0	2	0
16	Q	20	0	0	4	0
16	R	23	0	0	2	0
16	S	17	0	0	4	0
16	T	31	0	0	4	0
16	U	47	0	0	1	0
16	V	42	0	0	2	0
16	W	41	0	0	3	0
16	X	37	0	0	8	0
16	Y	34	0	0	1	0
16	Z	46	0	0	3	0
All	All	50685	0	49368	1791	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 18.

All (1791) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.11	1.11
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.11	1.08
2:P:202:THR:HG22	2:P:204:SER:H	1.23	1.04
2:B:202:THR:HG22	2:B:204:SER:H	1.23	1.02
10:J:168:MET:HE3	10:X:168:MET:HE3	1.40	1.02
7:G:96:ALA:HA	7:G:107:MET:HE2	1.42	1.01
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.20	1.01
7:U:96:ALA:HA	7:U:107:MET:HE2	1.43	1.01
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.20	1.00
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.41	0.97
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.11	0.96
1:O:15:PHE:H	2:P:23:GLN:HE22	1.06	0.93
13:1:14(C):ARG:HH11	13:1:14(C):ARG:HG3	1.31	0.93
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.51	0.92
3:C:163:GLN:HE21	3:C:164:THR:H	1.15	0.92
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.14	0.92
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.18	0.91
3:C:163:GLN:NE2	3:C:164:THR:H	1.69	0.91
3:C:15:PHE:H	4:D:23:GLN:HE22	1.12	0.90
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.15	0.90
1:A:15:PHE:H	2:B:23:GLN:HE22	1.15	0.89
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.35	0.89
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.53	0.89
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.37	0.89
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.73	0.89
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.55	0.88
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.56	0.87
2:B:71:ASN:ND2	2:B:72:ASP:H	1.73	0.87
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.56	0.87
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.56	0.87
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.75	0.87
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.57	0.86
3:C:185:THR:HB	3:C:188:GLU:HG2	1.57	0.86
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.72	0.86
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.41	0.86
5:S:15:PHE:H	6:T:23:GLN:HE22	1.23	0.86
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:THR:HG22	3:C:187:GLU:H	1.40	0.85
2:P:71:ASN:ND2	2:P:72:ASP:H	1.73	0.85
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.38	0.85
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.89	0.84
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.61	0.83
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.76	0.83
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.44	0.83
4:R:243:ALA:O	4:R:244:GLU:HB2	1.80	0.82
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.59	0.82
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.78	0.82
2:B:15:PHE:H	3:C:23:GLN:HE22	1.25	0.82
2:P:190:ILE:CG2	2:P:232:ILE:HD11	2.08	0.81
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.79	0.81
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.92	0.81
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.46	0.81
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.78	0.81
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.80	0.81
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.46	0.80
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.46	0.80
1:O:60:MET:HE3	1:O:63:THR:HG21	1.62	0.80
4:D:243:ALA:O	4:D:244:GLU:HB2	1.79	0.80
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.11	0.80
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.81	0.80
1:O:179:ARG:HB3	1:O:179:ARG:HH11	1.46	0.80
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.45	0.80
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.18	0.79
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.63	0.79
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.18	0.79
3:C:163:GLN:HE21	3:C:164:THR:N	1.80	0.79
2:P:190:ILE:HG21	2:P:232:ILE:HD11	1.65	0.78
1:A:60:MET:HE3	1:A:63:THR:HG21	1.65	0.78
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.46	0.78
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.97	0.78
13:1:211:ILE:HD13	13:1:211:ILE:H	1.49	0.78
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.48	0.78
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.49	0.78
5:E:15:PHE:H	6:F:23:GLN:HE22	1.32	0.78
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.46	0.78
10:J:168:MET:CE	10:X:168:MET:HE3	2.14	0.77
10:J:168:MET:HE3	10:X:168:MET:CE	2.14	0.77
14:2:20:THR:HG23	14:2:31:THR:OG1	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.51	0.76
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.66	0.76
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.51	0.76
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	1.90	0.76
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.68	0.75
3:Q:65:SER:HB2	16:Q:247:HOH:O	1.86	0.75
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.69	0.75
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.86	0.75
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.17	0.75
2:B:190:ILE:HG21	2:B:232:ILE:HD11	1.69	0.74
6:T:18:ASP:OD1	6:T:20:ARG:HD3	1.87	0.74
6:F:18:ASP:OD1	6:F:20:ARG:HD3	1.87	0.74
14:N:20:THR:HG23	14:N:31:THR:OG1	1.87	0.74
13:M:211:ILE:H	13:M:211:ILE:HD13	1.51	0.74
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.83	0.74
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.69	0.74
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.86	0.74
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.53	0.74
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.70	0.74
2:P:185:LYS:HD3	2:P:186:VAL:N	2.03	0.74
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.69	0.74
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.70	0.74
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.02	0.73
5:E:132:TYR:O	5:E:153:PRO:HB3	1.88	0.73
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.01	0.73
16:B:258:HOH:O	3:C:33:ARG:HD2	1.89	0.73
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.18	0.73
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.71	0.73
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.69	0.73
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.88	0.73
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.37	0.73
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	1.97	0.73
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.52	0.73
3:Q:52:ARG:HD2	3:Q:208:LYS:O	1.89	0.72
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.70	0.72
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.71	0.72
9:W:6:MET:HE3	9:W:155:ILE:HD12	1.70	0.72
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.35	0.72
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.55	0.72
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.97	0.72
2:B:185:LYS:HD3	2:B:186:VAL:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.05	0.72
9:W:192:ARG:HG3	16:W:200:HOH:O	1.90	0.72
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.53	0.72
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.72	0.71
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.71	0.71
5:S:132:TYR:O	5:S:153:PRO:HB3	1.89	0.71
2:B:202:THR:HG22	2:B:204:SER:N	2.03	0.71
11:K:142:TYR:O	11:K:143:LYS:HD2	1.89	0.71
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.04	0.71
3:C:41:LYS:HG2	3:C:161:SER:O	1.89	0.71
7:U:59:LEU:O	7:U:61:PRO:HD3	1.89	0.71
7:U:96:ALA:CA	7:U:107:MET:HE2	2.19	0.71
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.90	0.71
3:C:52:ARG:HD2	3:C:208:LYS:O	1.90	0.71
3:C:71:ASP:HA	10:J:68:ILE:HD13	1.72	0.71
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.21	0.71
9:I:6:MET:HE3	9:I:155:ILE:HD12	1.72	0.71
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.06	0.71
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.73	0.70
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.04	0.70
4:R:192:LEU:O	4:R:196:ILE:HG12	1.92	0.70
7:U:87:ASN:C	7:U:87:ASN:HD22	1.98	0.70
7:G:96:ALA:CA	7:G:107:MET:HE2	2.20	0.70
12:Z:21:ILE:C	12:Z:21:ILE:HD12	2.16	0.70
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.37	0.70
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.71	0.70
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.91	0.70
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.92	0.70
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.92	0.70
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.41	0.69
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.72	0.69
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.90	0.69
13:1:14(C):ARG:HH11	13:1:14(C):ARG:CG	2.02	0.69
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.75	0.69
12:L:166:HIS:HD2	12:L:168:GLN:H	1.41	0.69
13:M:14(C):ARG:HH11	13:M:14(C):ARG:CG	2.05	0.69
1:O:121:GLN:O	1:O:124:THR:HB	1.92	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.69
7:G:59:LEU:O	7:G:61:PRO:HD3	1.93	0.68
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.07	0.68
12:L:21:ILE:C	12:L:21:ILE:HD12	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.74	0.68
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.40	0.68
7:G:87:ASN:C	7:G:87:ASN:HD22	2.02	0.68
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.40	0.68
2:P:202:THR:HG22	2:P:204:SER:N	2.03	0.68
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.08	0.68
3:C:65:SER:HB2	16:C:253:HOH:O	1.94	0.68
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.27	0.68
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.58	0.68
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.07	0.67
4:R:207:LEU:CD2	4:R:233:ILE:HD12	2.24	0.67
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.42	0.67
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.09	0.67
5:E:226:GLY:O	5:E:229:VAL:HG22	1.93	0.67
4:D:207:LEU:CD2	4:D:233:ILE:HD12	2.24	0.67
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.09	0.67
10:J:168:MET:HG2	10:X:168:MET:HE3	1.75	0.67
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.94	0.67
5:S:220:PRO:O	5:S:222:THR:HG23	1.95	0.67
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.09	0.67
1:A:4:MET:SD	1:A:5:THR:N	2.60	0.67
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.09	0.67
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.75	0.67
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.77	0.67
10:J:168:MET:HE3	10:X:168:MET:HG2	1.76	0.67
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.77	0.67
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.75	0.67
1:A:121:GLN:O	1:A:124:THR:HB	1.95	0.66
4:D:192:LEU:O	4:D:196:ILE:HG12	1.95	0.66
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	1.96	0.66
2:B:41:MET:HE3	16:B:240:HOH:O	1.95	0.66
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.31	0.66
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.25	0.66
7:G:121:GLN:O	7:G:124:THR:HB	1.96	0.66
1:O:27:ALA:O	1:O:31:VAL:HG23	1.96	0.66
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.78	0.66
2:B:181:LYS:O	2:B:184:MET:HG3	1.95	0.66
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.43	0.66
10:J:168:MET:HG2	10:X:168:MET:CE	2.26	0.66
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.11	0.66
5:S:226:GLY:O	5:S:229:VAL:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.78	0.65
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.26	0.65
2:P:121:GLN:O	2:P:124:THR:HB	1.96	0.65
3:C:105:ASP:OD2	3:C:106:PRO:HD2	1.96	0.65
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.26	0.65
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.78	0.65
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.11	0.65
6:F:35:THR:HG21	6:F:51:GLU:O	1.96	0.65
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.78	0.65
10:J:168:MET:CE	10:X:168:MET:HG2	2.25	0.65
3:C:185:THR:HG22	3:C:187:GLU:N	2.10	0.65
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.42	0.65
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.79	0.65
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.60	0.65
5:E:177:GLU:OE1	6:F:56:SER:HB2	1.96	0.65
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.77	0.65
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.61	0.65
4:R:161:ASN:N	5:S:58:LEU:O	2.30	0.65
13:1:40:ASN:H	13:1:40:ASN:HD22	1.44	0.65
3:Q:170:LYS:HB2	16:Q:254:HOH:O	1.97	0.65
6:T:35:THR:HG21	6:T:51:GLU:O	1.97	0.65
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.79	0.65
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.79	0.65
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.32	0.65
2:P:181:LYS:O	2:P:184:MET:HG3	1.97	0.65
6:T:127:ASN:HD22	6:T:127:ASN:C	2.05	0.65
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.27	0.64
10:J:-1:MET:HG2	10:J:1:ASP:H	1.62	0.64
7:G:198:ILE:HG23	7:G:203:THR:O	1.97	0.64
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.43	0.64
5:S:207:LEU:HD23	5:S:207:LEU:N	2.12	0.64
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.79	0.64
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.62	0.64
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.97	0.64
7:U:121:GLN:O	7:U:124:THR:HB	1.96	0.64
7:U:198:ILE:HG23	7:U:203:THR:O	1.97	0.64
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.80	0.64
4:R:102:TYR:O	12:Z:81:ARG:HG3	1.97	0.64
7:U:236:ILE:HD12	7:U:237:ALA:N	2.13	0.64
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.98	0.64
2:B:228:GLU:O	2:B:232:ILE:HG22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.46	0.64
9:I:48:LEU:HG	9:I:50:THR:HG22	1.80	0.64
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.28	0.63
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.80	0.63
3:C:46:VAL:O	3:C:215:VAL:HG12	1.98	0.63
6:T:186:ALA:O	6:T:190:VAL:HG23	1.97	0.63
9:W:48:LEU:HG	9:W:50:THR:HG22	1.79	0.63
5:E:198:SER:HA	5:E:201:LEU:HG	1.79	0.63
13:M:40:ASN:HD22	13:M:40:ASN:H	1.44	0.63
2:P:97:GLN:NE2	9:W:64:ASN:HD22	1.96	0.63
3:C:175:PHE:O	3:C:179:ASN:HB2	1.98	0.63
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.81	0.63
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.79	0.63
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.34	0.63
5:S:198:SER:HA	5:S:201:LEU:HG	1.79	0.63
10:X:147:THR:OG1	10:X:150:GLU:HG3	1.99	0.63
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.14	0.63
1:A:27:ALA:O	1:A:31:VAL:HG23	1.98	0.63
10:J:147:THR:OG1	10:J:150:GLU:HG3	1.98	0.63
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.78	0.63
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.47	0.63
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.29	0.63
10:X:-1:MET:HG2	10:X:1:ASP:H	1.63	0.63
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.64	0.63
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.63	0.63
5:E:220:PRO:O	5:E:222:THR:HG23	1.97	0.62
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.80	0.62
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.79	0.62
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.80	0.62
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.64	0.62
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.79	0.62
5:S:177:GLU:OE1	6:T:56:SER:HB2	1.99	0.62
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.81	0.62
3:Q:173:ARG:O	3:Q:177:GLU:HG3	1.99	0.62
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.81	0.62
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.81	0.62
12:L:148:VAL:O	12:L:152:ILE:HG12	2.00	0.62
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.00	0.62
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.80	0.62
4:D:102:TYR:O	12:L:81:ARG:HG3	1.99	0.62
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.79	0.62
10:X:156:LYS:O	10:X:160:GLN:HG3	1.98	0.62
5:E:207:LEU:N	5:E:207:LEU:HD23	2.14	0.62
7:G:8:TYR:C	7:G:10:ARG:H	2.07	0.62
1:O:4:MET:SD	1:O:5:THR:N	2.62	0.62
2:B:97:GLN:NE2	9:I:64:ASN:HD22	1.98	0.62
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.15	0.62
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.82	0.62
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.82	0.62
3:C:186:VAL:O	3:C:190:VAL:HG23	2.00	0.61
6:F:127:ASN:HD22	6:F:127:ASN:C	2.07	0.61
4:D:154:SER:OG	4:D:156:THR:HG23	2.00	0.61
4:R:121:LEU:HB2	16:R:853:HOH:O	1.99	0.61
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.35	0.61
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.30	0.61
2:P:71:ASN:ND2	2:P:72:ASP:N	2.47	0.61
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.82	0.61
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.82	0.61
4:R:154:SER:OG	4:R:156:THR:HG23	2.00	0.61
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.82	0.61
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.83	0.61
11:K:99:THR:HG22	11:K:113:VAL:O	2.01	0.61
1:O:159:PRO:O	2:P:59:LEU:HD12	2.00	0.61
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.99	0.61
16:P:248:HOH:O	3:Q:87:ILE:HD11	1.98	0.61
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.00	0.61
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.16	0.61
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.31	0.61
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.83	0.61
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.82	0.61
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.65	0.61
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.82	0.60
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.36	0.60
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.48	0.60
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.31	0.60
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.35	0.60
4:D:207:LEU:C	4:D:207:LEU:HD23	2.27	0.60
7:G:172:ILE:HD12	7:G:197:MET:CE	2.31	0.60
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.82	0.60
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.00	0.60
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:ASN:ND2	2:B:72:ASP:N	2.47	0.60
5:S:207:LEU:HD23	5:S:207:LEU:H	1.65	0.60
2:B:15:PHE:H	3:C:23:GLN:NE2	1.98	0.60
8:V:172:ASN:ND2	8:V:193:THR:HA	2.17	0.60
1:A:58:LEU:HD12	7:G:173:THR:HG23	1.84	0.60
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.83	0.60
2:P:160:TRP:CD2	2:P:163:ILE:HD12	2.37	0.60
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.36	0.60
12:Z:148:VAL:O	12:Z:152:ILE:HG12	2.00	0.60
6:F:186:ALA:O	6:F:190:VAL:HG23	2.00	0.60
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.84	0.60
16:F:246:HOH:O	7:G:86:ARG:HD2	2.01	0.60
10:J:156:LYS:O	10:J:160:GLN:HG3	2.02	0.60
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.50	0.60
7:U:172:ILE:HD12	7:U:197:MET:CE	2.31	0.60
7:U:217:LYS:HA	7:U:217:LYS:HE3	1.84	0.60
10:J:-1:MET:HG2	10:J:1:ASP:N	2.17	0.60
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.50	0.60
6:T:237:GLN:O	6:T:240:ILE:HG22	2.01	0.60
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.36	0.59
7:G:236:ILE:HD12	7:G:237:ALA:N	2.17	0.59
5:S:18(C):PHE:O	5:S:18(F):ILE:HG12	2.02	0.59
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.83	0.59
2:B:160:TRP:CD2	2:B:163:ILE:HD12	2.36	0.59
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.84	0.59
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.83	0.59
6:T:127:ASN:HD22	6:T:128:SER:N	2.00	0.59
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.84	0.59
14:2:89:GLU:OE1	14:2:89:GLU:HA	2.02	0.59
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.37	0.59
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.85	0.59
7:U:8:TYR:C	7:U:10:ARG:H	2.09	0.59
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.84	0.59
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.99	0.59
2:P:228:GLU:O	2:P:232:ILE:HG22	2.01	0.59
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.84	0.59
9:I:137:MET:HE3	9:I:141:LEU:CD1	2.32	0.59
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.17	0.59
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.85	0.59
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.16	0.59
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.33	0.59
10:X:-1:MET:HG2	10:X:1:ASP:N	2.17	0.59
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.85	0.59
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.32	0.59
1:O:184:LEU:HB2	16:O:248:HOH:O	2.02	0.59
8:V:148:LYS:O	8:V:152:ILE:HG12	2.01	0.59
13:1:133:MET:HE1	13:1:165:ARG:HG3	1.83	0.59
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.85	0.59
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.27	0.59
5:E:18(C):PHE:O	5:E:18(F):ILE:HG12	2.02	0.59
4:R:207:LEU:HD23	4:R:207:LEU:C	2.27	0.59
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.84	0.59
6:F:127:ASN:HD22	6:F:128:SER:N	2.01	0.59
6:F:237:GLN:O	6:F:240:ILE:HG22	2.03	0.59
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.85	0.59
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.84	0.59
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.49	0.59
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.33	0.59
1:O:150:GLN:O	1:O:157:TYR:HA	2.03	0.59
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.03	0.59
16:T:244:HOH:O	7:U:86:ARG:HD2	2.02	0.59
12:Z:3:ILE:HD12	12:Z:46:ASN:HB2	1.85	0.59
5:E:207:LEU:HD23	5:E:207:LEU:H	1.68	0.58
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.84	0.58
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.84	0.58
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.02	0.58
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.00	0.58
1:A:173:LYS:O	1:A:177:GLU:HG3	2.03	0.58
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.84	0.58
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.84	0.58
14:N:89:GLU:OE1	14:N:89:GLU:HA	2.02	0.58
3:Q:159:SER:HB2	16:Q:258:HOH:O	2.03	0.58
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.38	0.58
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.37	0.58
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.33	0.58
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.84	0.58
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.68	0.58
14:N:10(B):LYS:C	14:N:10(B):LYS:HD3	2.28	0.58
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.66	0.58
2:P:11:ARG:O	2:P:14:ILE:HD12	2.02	0.58
1:A:69:LEU:HD23	1:A:69:LEU:C	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:GLN:NE2	16:J:215:HOH:O	2.34	0.58
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.39	0.58
5:S:227:GLU:CD	5:S:227:GLU:N	2.62	0.58
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.03	0.58
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.85	0.58
7:U:87:ASN:C	7:U:87:ASN:ND2	2.60	0.58
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.84	0.58
3:C:173:ARG:O	3:C:177:GLU:HG3	2.03	0.58
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.85	0.58
11:K:37:ILE:HD12	11:K:59:LEU:HD23	1.86	0.58
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.34	0.58
7:U:77:VAL:CG1	7:U:137:THR:HB	2.34	0.58
4:R:68:VAL:HG21	4:R:89:ILE:HD13	1.86	0.57
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.87	0.57
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.40	0.57
5:E:227:GLU:N	5:E:227:GLU:CD	2.62	0.57
2:P:87:ILE:O	2:P:91:THR:HG23	2.04	0.57
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.03	0.57
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.17	0.57
11:Y:37:ILE:HD12	11:Y:59:LEU:HD23	1.86	0.57
12:Z:99:THR:HG22	16:Z:203:HOH:O	2.04	0.57
5:E:40:LEU:N	5:E:40:LEU:HD23	2.20	0.57
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.86	0.57
4:D:112:LEU:C	4:D:112:LEU:HD13	2.30	0.57
7:G:77:VAL:CG1	7:G:137:THR:HB	2.34	0.57
8:V:196:VAL:HG23	16:V:246:HOH:O	2.03	0.57
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.35	0.57
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.39	0.57
13:M:133:MET:HE1	13:M:165:ARG:HG3	1.87	0.57
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.40	0.57
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.70	0.57
2:P:46:ILE:HD11	2:P:146:TYR:HB3	1.85	0.57
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.86	0.57
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.86	0.57
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.87	0.57
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.87	0.57
8:V:200:LYS:HE3	9:W:140:SER:O	2.04	0.57
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.12	0.57
12:Z:3:ILE:HD13	12:Z:127:GLY:O	2.05	0.57
1:A:150:GLN:O	1:A:157:TYR:HA	2.05	0.57
3:C:235:GLN:O	3:C:239:GLU:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.40	0.57
5:E:76:LEU:HD12	5:E:136:LEU:HD22	1.86	0.57
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.70	0.57
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.40	0.57
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.40	0.57
6:T:127:ASN:C	6:T:127:ASN:ND2	2.63	0.57
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.05	0.57
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.40	0.57
1:O:69:LEU:C	1:O:69:LEU:HD23	2.30	0.56
2:B:27:ALA:O	2:B:31:ILE:HG12	2.05	0.56
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.86	0.56
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.88	0.56
8:H:144:GLN:O	8:H:145:ASP:HB2	2.04	0.56
14:N:175:MET:HE3	14:N:18(B):PHE:CE2	2.40	0.56
8:V:172:ASN:HD22	8:V:193:THR:HA	1.69	0.56
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.05	0.56
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.03	0.56
1:A:97:HIS:HD2	8:H:61:SER:OG	1.88	0.56
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.18	0.56
4:D:68:VAL:HG21	4:D:89:ILE:HD13	1.88	0.56
5:E:231:LYS:H	5:E:231:LYS:HD2	1.69	0.56
2:P:163:ILE:HG12	2:P:164:SER:N	2.21	0.56
3:Q:241:GLN:C	3:Q:243:GLN:H	2.14	0.56
4:R:243:ALA:O	4:R:244:GLU:CB	2.53	0.56
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.69	0.56
3:C:57:LYS:O	3:C:58:LEU:HB2	2.06	0.56
3:C:241:GLN:C	3:C:243:GLN:H	2.14	0.56
8:H:172:ASN:ND2	8:H:193:THR:HA	2.21	0.56
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.87	0.56
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.30	0.56
13:1:14(A):VAL:HG23	13:1:14(A):VAL:O	2.06	0.56
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.04	0.56
7:U:236:ILE:HD12	7:U:236:ILE:C	2.30	0.56
8:V:144:GLN:O	8:V:145:ASP:HB2	2.06	0.56
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.40	0.56
13:M:175:LEU:HD23	13:M:175:LEU:C	2.30	0.56
4:R:186:LEU:O	4:R:190:GLU:HG3	2.06	0.56
9:W:29:ASN:ND2	9:W:29:ASN:H	2.04	0.56
9:W:137:MET:HE2	9:W:161:ASN:HB2	1.87	0.56
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.70	0.56
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:40:ILE:CD1	4:R:193:VAL:HG23	2.34	0.56
5:E:227:GLU:CD	5:E:227:GLU:H	2.14	0.56
8:H:148:LYS:O	8:H:152:ILE:HG12	2.06	0.56
2:B:87:ILE:O	2:B:91:THR:HG23	2.05	0.56
2:P:122:GLY:C	2:P:124:THR:H	2.14	0.56
5:S:40:LEU:N	5:S:40:LEU:HD23	2.21	0.56
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.71	0.56
6:F:203:GLU:C	6:F:205:ASN:H	2.14	0.56
13:M:4:ILE:HD12	13:M:155:ILE:HD12	1.87	0.56
5:S:231:LYS:H	5:S:231:LYS:HD2	1.71	0.56
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.21	0.55
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.35	0.55
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.86	0.55
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.88	0.55
1:O:173:LYS:O	1:O:177:GLU:HG3	2.05	0.55
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.71	0.55
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.07	0.55
5:S:207:LEU:H	5:S:207:LEU:CD2	2.18	0.55
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.22	0.55
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.36	0.55
2:B:46:ILE:HD11	2:B:146:TYR:HB3	1.87	0.55
4:D:186:LEU:O	4:D:190:GLU:HG3	2.06	0.55
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.42	0.55
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.89	0.55
9:W:137:MET:HE3	9:W:141:LEU:CD1	2.35	0.55
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.89	0.55
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.88	0.55
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.89	0.55
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.36	0.55
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.88	0.55
2:B:21:LEU:O	2:B:25:GLU:HG2	2.06	0.55
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.88	0.55
5:E:67:ILE:CG2	5:E:223:ILE:HD13	2.36	0.55
2:P:14:ILE:HD13	2:P:14:ILE:H	1.71	0.55
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.87	0.55
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.21	0.55
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.07	0.55
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.89	0.55
6:F:21(B):THR:HG22	6:F:222:LYS:HD3	1.89	0.55
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.89	0.55
12:L:3:ILE:HD13	12:L:127:GLY:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:TYR:HA	5:S:59:SER:HA	1.88	0.55
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.88	0.55
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.42	0.55
2:P:27:ALA:O	2:P:31:ILE:HG12	2.07	0.55
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.37	0.55
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.41	0.55
6:T:21(B):THR:HG22	6:T:222:LYS:HD3	1.88	0.55
7:U:197:MET:HA	7:U:197:MET:HE3	1.88	0.55
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.89	0.55
6:T:203:GLU:C	6:T:205:ASN:H	2.14	0.55
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.89	0.55
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.07	0.55
13:1:152:GLU:O	13:1:156:VAL:HG23	2.07	0.55
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.71	0.55
8:H:62:ASN:HB3	8:H:82:MET:HE1	1.89	0.55
11:K:7:ARG:HD2	11:K:108:PRO:O	2.06	0.55
10:X:6:ILE:CG2	10:X:13:ILE:HB	2.36	0.55
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.88	0.55
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.88	0.54
12:Z:8:GLY:HA3	12:Z:11:PHE:CZ	2.42	0.54
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.89	0.54
8:H:200:LYS:HE3	9:I:140:SER:O	2.07	0.54
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.07	0.54
11:K:4:LEU:HD22	11:K:4:LEU:C	2.32	0.54
12:L:3:ILE:HD12	12:L:46:ASN:HB2	1.90	0.54
2:P:112:LEU:HD23	2:P:112:LEU:C	2.32	0.54
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.90	0.54
6:F:127:ASN:C	6:F:127:ASN:ND2	2.65	0.54
12:L:14(I):THR:O	12:L:1(I):ASN:HB3	2.08	0.54
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.89	0.54
5:S:67:ILE:CG2	5:S:223:ILE:HD13	2.37	0.54
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.22	0.54
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.89	0.54
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.32	0.54
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.89	0.54
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.89	0.54
14:N:41:ILE:HD12	14:N:76:THR:HA	1.90	0.54
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.73	0.54
4:R:53:ARG:O	4:R:53:ARG:HG2	2.07	0.54
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.37	0.54
8:V:62:ASN:HB3	8:V:82:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.88	0.54
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.08	0.54
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.43	0.54
6:T:88:LEU:HD11	6:T:116:LEU:HD22	1.89	0.54
13:1:4:ILE:HD12	13:1:155:ILE:HD12	1.90	0.54
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.89	0.54
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.20	0.54
5:S:15:PHE:H	6:T:23:GLN:NE2	2.00	0.54
5:S:227:GLU:CD	5:S:227:GLU:H	2.14	0.54
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.89	0.54
6:F:203:GLU:OE1	6:F:203:GLU:HA	2.08	0.54
7:G:8:TYR:C	7:G:10:ARG:N	2.66	0.54
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.38	0.54
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.42	0.54
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.22	0.54
14:2:14:LEU:O	14:2:175:MET:HA	2.08	0.54
5:E:167:ALA:HB3	16:E:243:HOH:O	2.07	0.54
8:H:196:VAL:HG23	16:H:245:HOH:O	2.08	0.54
10:J:6:ILE:CG2	10:J:13:ILE:HB	2.38	0.54
2:B:163:ILE:HG12	2:B:164:SER:N	2.24	0.53
13:M:57:ARG:NE	16:M:239:HOH:O	2.40	0.53
13:M:149:GLN:NE2	13:M:149:GLN:H	2.05	0.53
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.23	0.53
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.22	0.53
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.90	0.53
8:V:36:ARG:HG3	8:V:38:SER:O	2.08	0.53
2:B:11:ARG:O	2:B:14:ILE:HD12	2.08	0.53
2:B:122:GLY:C	2:B:124:THR:H	2.14	0.53
7:G:197:MET:HA	7:G:197:MET:HE3	1.89	0.53
10:J:168:MET:HE2	10:X:167:PRO:C	2.34	0.53
14:N:92:ASP:HB2	16:N:199:HOH:O	2.08	0.53
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.91	0.53
12:Z:17:ASP:OD2	12:Z:33:LYS:NZ	2.40	0.53
1:A:85:TYR:O	1:A:89:VAL:HG23	2.08	0.53
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.43	0.53
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.90	0.53
6:F:176:LEU:O	6:F:180:VAL:HG23	2.08	0.53
9:I:29:ASN:ND2	9:I:29:ASN:H	2.06	0.53
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.91	0.53
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.24	0.53
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.24	0.53
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.24	0.53
11:Y:10(A):ARG:HD3	11:Y:180:GLU:OE1	2.09	0.53
3:C:190:VAL:O	3:C:194:VAL:HG23	2.08	0.53
7:G:38:LEU:C	7:G:38:LEU:HD12	2.33	0.53
10:J:162:LEU:O	10:J:166:MET:HB2	2.09	0.53
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.39	0.53
13:1:175:LEU:HD23	13:1:175:LEU:C	2.34	0.53
3:C:7:GLY:N	16:C:271:HOH:O	2.41	0.53
3:C:227:GLU:OE1	3:C:227:GLU:N	2.38	0.53
4:D:170:GLU:N	4:D:170:GLU:OE1	2.41	0.53
5:E:207:LEU:H	5:E:207:LEU:CD2	2.21	0.53
7:G:192:PHE:C	7:G:192:PHE:CD1	2.86	0.53
11:K:13:ILE:HG13	11:K:151:ALA:HB1	1.90	0.53
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.91	0.53
4:R:21:LEU:HD21	5:S:130:ARG:HD2	1.89	0.53
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.35	0.53
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.90	0.53
5:S:134:VAL:O	5:S:153:PRO:HG3	2.08	0.53
11:Y:13:ILE:HG13	11:Y:151:ALA:HB1	1.90	0.53
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	1.91	0.53
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.90	0.53
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.74	0.53
7:G:118:ASN:O	7:G:122:ILE:HD12	2.09	0.53
10:J:52:THR:CG2	10:J:53:VAL:N	2.72	0.53
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.38	0.53
14:N:14:LEU:O	14:N:175:MET:HA	2.09	0.53
6:T:41:LYS:HA	6:T:46:VAL:HG12	1.91	0.53
7:G:236:ILE:HD12	7:G:236:ILE:C	2.34	0.53
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.90	0.53
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.90	0.53
14:2:85:GLU:O	14:2:89:GLU:HB2	2.09	0.53
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.22	0.53
8:H:36:ARG:HG3	8:H:38:SER:O	2.09	0.53
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.38	0.53
12:L:61:ASN:ND2	16:L:218:HOH:O	2.41	0.53
2:P:101:LYS:NZ	10:X:85:GLN:HE22	2.06	0.53
2:P:185:LYS:HD3	2:P:186:VAL:H	1.74	0.53
6:T:192:GLN:O	6:T:196:ILE:HG12	2.09	0.53
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.44	0.53
13:1:46:SER:OG	13:1:98:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.23	0.52
13:M:17:ASP:HA	13:M:173:PHE:CB	2.39	0.52
5:S:41:ARG:NH1	5:S:42:SER:O	2.43	0.52
8:V:128:GLY:O	8:V:131:SER:HB2	2.09	0.52
2:P:77:ALA:HB3	2:P:137:ILE:HB	1.90	0.52
6:T:136:THR:O	6:T:150:MET:HA	2.10	0.52
12:Z:27:ASN:HB3	13:1:120:TYR:CZ	2.45	0.52
12:Z:14(I):THR:O	12:Z:1(I):ASN:HB3	2.07	0.52
11:K:196:PHE:HB3	16:K:215:HOH:O	2.09	0.52
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	2.09	0.52
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.38	0.52
7:U:192:PHE:C	7:U:192:PHE:CD1	2.86	0.52
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.90	0.52
1:A:21(A):GLU:HG3	16:A:260:HOH:O	2.10	0.52
5:E:41:ARG:NH1	5:E:42:SER:O	2.43	0.52
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.75	0.52
4:R:227:GLU:O	4:R:231:GLU:HG3	2.09	0.52
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.91	0.52
6:T:176:LEU:O	6:T:180:VAL:HG23	2.08	0.52
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.40	0.52
2:B:15:PHE:N	3:C:23:GLN:HE22	2.02	0.52
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.10	0.52
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.90	0.52
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.10	0.52
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.92	0.52
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.23	0.52
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.90	0.52
5:S:73:HIS:HE1	5:S:107:LEU:O	1.92	0.52
10:X:113:ILE:HA	10:X:118:THR:O	2.10	0.52
2:B:77:ALA:HB3	2:B:137:ILE:HB	1.92	0.52
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	1.92	0.52
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.22	0.52
5:S:201:LEU:O	5:S:202:ARG:HB2	2.09	0.52
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.92	0.52
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.92	0.52
10:X:52:THR:CG2	10:X:53:VAL:N	2.72	0.52
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.17	0.52
3:C:55:THR:C	3:C:56:LEU:HD22	2.35	0.52
6:F:69:VAL:HG12	16:F:249:HOH:O	2.09	0.52
6:F:192:GLN:O	6:F:196:ILE:HG12	2.09	0.52
11:K:4:LEU:HD13	11:K:15:ALA:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:122:GLU:C	1:O:124:THR:H	2.17	0.52
2:P:239:THR:HG22	2:P:239:THR:OXT	2.09	0.52
16:S:242:HOH:O	6:T:12:ASN:HB2	2.09	0.52
6:T:203:GLU:HA	6:T:203:GLU:OE1	2.10	0.52
4:D:243:ALA:O	4:D:244:GLU:CB	2.53	0.52
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ2	1.75	0.52
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.91	0.52
2:P:150:THR:O	2:P:157:TYR:HA	2.09	0.52
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.92	0.52
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.92	0.52
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.91	0.52
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.93	0.52
10:J:113:ILE:HA	10:J:118:THR:O	2.10	0.52
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.75	0.52
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.92	0.52
11:K:199:VAL:O	11:K:203:GLU:HB3	2.10	0.52
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.92	0.52
2:B:112:LEU:HD23	2:B:112:LEU:C	2.34	0.51
3:C:15:PHE:N	4:D:23:GLN:HE22	1.93	0.51
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.45	0.51
5:E:67:ILE:HG22	5:E:223:ILE:HD13	1.92	0.51
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.93	0.51
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.91	0.51
7:G:141:VAL:HG21	7:G:216:THR:HA	1.92	0.51
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.09	0.51
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.92	0.51
7:U:140:SER:HA	7:U:215:ALA:HB1	1.92	0.51
14:2:41:ILE:HD12	14:2:76:THR:HA	1.92	0.51
10:J:167:PRO:C	10:X:168:MET:HE2	2.34	0.51
5:S:190:ILE:HG23	5:S:212:ILE:HD13	1.91	0.51
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.92	0.51
3:C:232:TYR:O	3:C:236:ILE:HG13	2.10	0.51
8:H:172:ASN:HD22	8:H:193:THR:HA	1.74	0.51
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.93	0.51
6:T:147:HIS:HD2	16:T:242:HOH:O	1.94	0.51
13:1:149:GLN:NE2	13:1:149:GLN:H	2.07	0.51
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.91	0.51
4:D:207:LEU:HD21	4:D:233:ILE:HD12	1.93	0.51
6:F:41:LYS:HA	6:F:46:VAL:HG12	1.91	0.51
12:L:93:PHE:N	12:L:94:PRO:HD3	2.25	0.51
13:M:4:ILE:HD11	13:M:155:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:112:LEU:HD13	4:R:112:LEU:C	2.36	0.51
4:D:53:ARG:O	4:D:53:ARG:HG2	2.10	0.51
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.26	0.51
10:J:133:TYR:OH	10:X:24:ILE:HG12	2.10	0.51
11:K:10(A):ARG:HD3	11:K:180:GLU:OE1	2.10	0.51
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.46	0.51
4:R:170:GLU:OE1	4:R:170:GLU:N	2.42	0.51
4:R:237:LEU:O	4:R:241:GLU:HG3	2.10	0.51
5:E:142:ASP:HB2	16:M:247:HOH:O	2.11	0.51
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.17	0.51
12:L:5:GLY:O	12:L:124:CYS:HA	2.10	0.51
1:O:177:GLU:HG2	2:P:58:LEU:HD22	1.91	0.51
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.74	0.51
5:E:190:ILE:HG23	5:E:212:ILE:HD13	1.93	0.51
9:I:137:MET:HE2	9:I:161:ASN:HB2	1.91	0.51
12:L:145:TYR:CD1	12:L:146:LEU:N	2.79	0.51
14:N:85:GLU:O	14:N:89:GLU:HB2	2.10	0.51
3:Q:190:VAL:HG13	3:Q:212:ILE:HG21	1.92	0.51
5:S:67:ILE:HG22	5:S:223:ILE:CD1	2.41	0.51
5:E:4:PHE:CG	5:E:5:ARG:N	2.79	0.51
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.68	0.51
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.46	0.51
10:J:16:SER:HB2	16:J:205:HOH:O	2.10	0.51
5:S:67:ILE:HG22	5:S:223:ILE:HD13	1.93	0.51
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.26	0.51
8:V:214:LEU:HD21	9:W:190:LYS:HD2	1.92	0.51
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.40	0.51
4:D:227:GLU:O	4:D:231:GLU:HG3	2.10	0.51
4:D:237:LEU:O	4:D:241:GLU:HG3	2.10	0.51
5:E:148:LEU:HD23	5:E:162:GLY:HA2	1.93	0.51
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.92	0.51
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.09	0.50
5:E:201:LEU:O	5:E:202:ARG:HB2	2.10	0.50
8:H:214:LEU:HD21	9:I:190:LYS:HD2	1.94	0.50
10:X:143:ARG:O	10:X:146:MET:HG3	2.11	0.50
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.94	0.50
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.93	0.50
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.11	0.50
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.11	0.50
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.92	0.50
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.11	0.50
16:F:246:HOH:O	7:G:83:PRO:HA	2.10	0.50
9:I:114:ASP:HB2	16:I:232:HOH:O	2.11	0.50
1:O:85:TYR:O	1:O:89:VAL:HG23	2.11	0.50
5:S:76:LEU:HD12	5:S:136:LEU:HD22	1.93	0.50
5:S:82:ALA:CB	16:S:237:HOH:O	2.59	0.50
8:V:84:LYS:HG3	8:V:85:GLN:N	2.27	0.50
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.26	0.50
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.12	0.50
5:E:2(C):VAL:O	5:E:226:GLY:HA2	2.12	0.50
7:G:140:SER:HA	7:G:215:ALA:HB1	1.92	0.50
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.08	0.50
7:U:8:TYR:C	7:U:10:ARG:N	2.68	0.50
7:U:38:LEU:C	7:U:38:LEU:HD12	2.37	0.50
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.92	0.50
11:Y:4:LEU:HD13	11:Y:15:ALA:O	2.11	0.50
11:Y:199:VAL:O	11:Y:203:GLU:HB3	2.11	0.50
1:A:225:THR:O	1:A:229:ILE:HG13	2.11	0.50
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.46	0.50
13:1:17:ASP:HA	13:1:173:PHE:CB	2.42	0.50
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.93	0.50
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.93	0.50
3:C:57:LYS:HD2	3:C:58:LEU:N	2.27	0.50
6:F:88:LEU:HD11	6:F:116:LEU:HD22	1.94	0.50
8:H:73:GLU:OE1	8:H:73:GLU:HA	2.10	0.50
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.94	0.50
2:P:191:GLU:O	2:P:195:LYS:HG2	2.12	0.50
7:U:131:PRO:HB3	16:U:257:HOH:O	2.11	0.50
2:B:150:THR:O	2:B:157:TYR:HA	2.11	0.50
6:F:136:THR:O	6:F:150:MET:HA	2.12	0.50
10:J:24:ILE:HG12	10:X:133:TYR:OH	2.11	0.50
10:J:133:TYR:HE1	16:X:220:HOH:O	1.95	0.50
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.46	0.50
2:P:121:GLN:NE2	2:P:121:GLN:C	2.70	0.50
7:U:118:ASN:O	7:U:122:ILE:HD12	2.11	0.50
13:1:4:ILE:HD11	13:1:155:ILE:HG23	1.94	0.50
3:C:35:THR:HB	3:C:51:GLU:HG3	1.93	0.50
14:N:113:ILE:HG12	14:N:119:VAL:HG13	1.93	0.50
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.55	0.50
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.27	0.50
13:M:129:PHE:HE2	14:2:24:ALA:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:141:VAL:HG21	7:U:216:THR:HA	1.93	0.50
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.94	0.50
5:E:194:VAL:HA	5:E:197:ILE:HG22	1.94	0.49
7:G:87:ASN:C	7:G:87:ASN:ND2	2.64	0.49
13:M:46:SER:OG	13:M:98:ALA:HB3	2.12	0.49
2:P:202:THR:CG2	2:P:204:SER:HB2	2.42	0.49
2:P:235:LYS:C	2:P:237:GLY:H	2.20	0.49
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.94	0.49
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.11	0.49
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.09	0.49
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.47	0.49
2:B:191:GLU:O	2:B:195:LYS:HG2	2.12	0.49
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.94	0.49
6:F:90:ASN:O	6:F:94:GLU:HG3	2.12	0.49
7:G:233:LEU:O	7:G:236:ILE:HG13	2.12	0.49
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.93	0.49
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.94	0.49
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.47	0.49
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.12	0.49
5:S:160:LEU:HD13	5:S:163:THR:HB	1.95	0.49
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.11	0.49
5:E:35:SER:O	5:E:66:LYS:NZ	2.45	0.49
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.11	0.49
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.47	0.49
7:U:12:ILE:HD13	7:U:12:ILE:H	1.76	0.49
2:B:202:THR:CG2	2:B:204:SER:HB2	2.42	0.49
3:C:39:GLY:O	3:C:162:ALA:HA	2.13	0.49
9:I:29:ASN:C	9:I:29:ASN:HD22	2.20	0.49
13:M:-6:GLN:HG3	13:M:-6:GLN:O	2.13	0.49
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.94	0.49
4:R:85:ALA:HB2	4:R:134:VAL:HG11	1.94	0.49
5:S:52:LYS:HD3	5:S:211:SER:HB2	1.94	0.49
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.42	0.49
6:T:157:TYR:CD1	6:T:157:TYR:C	2.90	0.49
10:X:162:LEU:O	10:X:166:MET:HB2	2.12	0.49
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.95	0.49
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.80	0.49
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.94	0.49
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.55	0.49
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.37	0.49
1:O:225:THR:O	1:O:229:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.94	0.49
5:S:139:ILE:HG22	5:S:148:LEU:HD13	1.93	0.49
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.94	0.49
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.12	0.49
3:C:97:GLN:HG3	10:J:65:LEU:HB2	1.95	0.49
7:G:12:ILE:HG12	7:G:14:ILE:HG23	1.94	0.49
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.95	0.49
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.94	0.49
6:T:88:LEU:CD1	6:T:116:LEU:HD22	2.42	0.49
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.95	0.49
1:A:117:ALA:HB1	1:A:155:GLY:O	2.12	0.49
1:A:122:GLU:C	1:A:124:THR:H	2.19	0.49
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.48	0.49
2:B:160:TRP:HA	3:C:59:GLN:HA	1.95	0.49
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.93	0.49
5:E:38:VAL:HG12	5:E:39:GLY:N	2.28	0.49
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.93	0.49
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.40	0.49
10:J:148:THR:HG21	10:J:177:ILE:HD13	1.95	0.49
10:J:167:PRO:O	10:X:168:MET:HE2	2.13	0.49
2:P:71:ASN:HD22	2:P:72:ASP:H	1.55	0.49
3:Q:55:THR:HG22	3:Q:56:LEU:CD2	2.40	0.49
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.27	0.49
5:S:15:PHE:N	6:T:23:GLN:HE22	2.03	0.49
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.43	0.49
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.94	0.49
3:C:190:VAL:HG13	3:C:212:ILE:HG21	1.95	0.49
5:E:73:HIS:HE1	5:E:107:LEU:O	1.96	0.49
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.95	0.49
6:F:195:LYS:NZ	16:F:276:HOH:O	2.41	0.49
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.47	0.49
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.28	0.49
7:U:233:LEU:O	7:U:236:ILE:HG13	2.12	0.49
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.95	0.49
2:B:14:ILE:HD13	2:B:14:ILE:H	1.77	0.49
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.78	0.49
8:H:128:GLY:O	8:H:131:SER:HB2	2.12	0.49
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.76	0.49
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.94	0.49
10:X:110:LEU:O	10:X:121:GLU:HG2	2.13	0.49
11:Y:14:VAL:HB	11:Y:176:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:ARG:HD2	3:C:10:ARG:NH1	2.28	0.49
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.95	0.49
5:E:67:ILE:HG22	5:E:223:ILE:CD1	2.43	0.49
6:F:186:ALA:HB3	16:F:264:HOH:O	2.13	0.49
10:J:44:SER:OG	10:J:100:LEU:HB2	2.13	0.49
2:P:141:TYR:CD1	2:P:141:TYR:C	2.91	0.49
2:P:235:LYS:HD3	2:P:235:LYS:N	2.28	0.49
4:R:59:LEU:HD13	4:R:59:LEU:C	2.38	0.49
11:Y:97:MET:HG2	11:Y:115:SER:HB3	1.94	0.49
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.78	0.49
3:C:44:ASN:O	3:C:45:CYS:HB3	2.13	0.48
4:R:24:VAL:O	4:R:27:SER:HB3	2.13	0.48
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.95	0.48
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.43	0.48
10:X:44:SER:OG	10:X:100:LEU:HB2	2.12	0.48
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.95	0.48
13:1:9:ASP:OD1	13:1:10:ASN:N	2.46	0.48
2:B:41:MET:HE1	3:C:60:ASP:OD1	2.12	0.48
4:D:85:ALA:HB2	4:D:134:VAL:HG11	1.95	0.48
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.96	0.48
8:H:18:THR:HB	8:H:30:ASN:HD22	1.78	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.94	0.48
13:M:9:ASP:OD1	13:M:10:ASN:N	2.46	0.48
13:M:100:ILE:HD11	13:M:127:THR:HG23	1.95	0.48
7:U:158:VAL:HG22	7:U:159:GLY:N	2.28	0.48
13:1:122:SER:HB3	13:1:124:THR:O	2.13	0.48
5:E:160:LEU:HD13	5:E:163:THR:HB	1.95	0.48
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.28	0.48
7:G:12:ILE:HD13	7:G:12:ILE:H	1.78	0.48
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.43	0.48
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.13	0.48
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.48	0.48
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.44	0.48
12:L:17:ASP:OD2	12:L:33:LYS:NZ	2.44	0.48
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.48	0.48
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.14	0.48
13:1:99:ILE:C	13:1:100:ILE:HD12	2.38	0.48
2:B:141:TYR:CD1	2:B:141:TYR:C	2.92	0.48
2:B:185:LYS:HD3	2:B:186:VAL:H	1.76	0.48
2:B:239:THR:HG22	2:B:239:THR:OXT	2.13	0.48
10:J:110:LEU:O	10:J:121:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:44:THR:OG1	11:K:100:MET:HB2	2.13	0.48
11:K:195:LEU:O	11:K:199:VAL:HG23	2.13	0.48
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.96	0.48
13:M:133:MET:C	13:M:136:PRO:HD2	2.39	0.48
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.14	0.48
2:P:163:ILE:HG12	2:P:164:SER:H	1.79	0.48
5:S:4:PHE:CG	5:S:5:ARG:N	2.80	0.48
6:T:18:ASP:OD2	6:T:18:ASP:N	2.39	0.48
9:W:29:ASN:H	9:W:29:ASN:HD22	1.61	0.48
11:Y:31:VAL:HG11	15:Y:0:SA1:H13	1.95	0.48
12:Z:3:ILE:HD12	12:Z:46:ASN:CB	2.44	0.48
2:B:234:VAL:HA	2:B:239:THR:HA	1.96	0.48
5:E:52:LYS:HD3	5:E:211:SER:HB2	1.96	0.48
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.95	0.48
13:M:99:ILE:C	13:M:100:ILE:HD12	2.38	0.48
2:P:224:PHE:HD2	2:P:224:PHE:N	2.11	0.48
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.40	0.48
7:U:12:ILE:HG12	7:U:14:ILE:HG23	1.96	0.48
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.14	0.48
6:T:36:THR:HB	6:T:168:GLY:H	1.79	0.48
6:T:69:VAL:HG12	16:T:262:HOH:O	2.12	0.48
2:B:6:ARG:NH1	4:D:12(B):GLU:OE2	2.47	0.48
2:B:71:ASN:HD22	2:B:72:ASP:H	1.54	0.48
5:E:2(B):THR:H	5:E:2(E):ASN:HB3	1.78	0.48
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.13	0.48
7:G:203:THR:HG22	7:G:204:GLU:N	2.28	0.48
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.96	0.48
10:J:168:MET:HE2	10:X:167:PRO:O	2.14	0.48
11:K:14:VAL:HB	11:K:176:TYR:HB2	1.95	0.48
11:K:17:ASP:CG	11:K:33:LYS:HZ2	2.22	0.48
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.96	0.48
3:Q:39:GLY:O	3:Q:162:ALA:HA	2.13	0.48
5:S:2(C):VAL:O	5:S:226:GLY:HA2	2.13	0.48
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.94	0.48
10:X:10(B):LYS:HB2	10:X:10(B):LYS:NZ	2.28	0.48
14:N:147:SER:OG	14:N:150:GLU:HG3	2.14	0.48
2:P:21:LEU:O	2:P:25:GLU:HG2	2.14	0.48
2:P:224:PHE:N	2:P:224:PHE:CD2	2.81	0.48
3:Q:41:LYS:HD3	3:Q:160:TRP:O	2.13	0.48
6:T:172:ALA:O	6:T:176:LEU:HD22	2.14	0.48
8:V:18:THR:HB	8:V:30:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:101:VAL:O	9:W:110:ILE:HA	2.14	0.48
14:2:113:ILE:HG12	14:2:119:VAL:HG13	1.95	0.48
2:B:224:PHE:N	2:B:224:PHE:CD2	2.82	0.48
5:E:76:LEU:CD1	5:E:136:LEU:HD22	2.43	0.48
8:H:84:LYS:HG3	8:H:85:GLN:N	2.27	0.48
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.95	0.48
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.42	0.48
10:J:133:TYR:HD1	16:Y:232:HOH:O	1.96	0.48
4:R:207:LEU:HD21	4:R:233:ILE:HD12	1.96	0.48
5:S:38:VAL:HG12	5:S:39:GLY:N	2.27	0.48
13:1:133:MET:C	13:1:136:PRO:HD2	2.38	0.48
5:E:179:THR:HG22	5:E:179:THR:O	2.14	0.47
2:P:234:VAL:HA	2:P:239:THR:HA	1.96	0.47
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.14	0.47
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.95	0.47
5:E:15:PHE:H	6:F:23:GLN:NE2	2.06	0.47
7:G:151:THR:HG22	7:G:157:TYR:CB	2.44	0.47
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.50	0.47
5:S:179:THR:HG22	5:S:179:THR:O	2.13	0.47
10:X:148:THR:HG21	10:X:177:ILE:HD13	1.97	0.47
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.95	0.47
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.95	0.47
3:C:41:LYS:HD3	3:C:160:TRP:O	2.14	0.47
3:C:224:LEU:HD12	3:C:224:LEU:N	2.29	0.47
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.96	0.47
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.97	0.47
13:1:113:VAL:HA	13:1:118:VAL:O	2.14	0.47
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.74	0.47
6:F:157:TYR:CD1	6:F:157:TYR:C	2.92	0.47
11:K:86:LEU:HD13	11:K:86:LEU:C	2.39	0.47
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.49	0.47
12:L:98:HIS:HD2	16:L:199:HOH:O	1.98	0.47
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.95	0.47
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.77	0.47
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.95	0.47
7:U:82:ILE:N	7:U:83:PRO:HD2	2.30	0.47
13:1:100:ILE:HD11	13:1:127:THR:HG23	1.95	0.47
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.95	0.47
2:B:224:PHE:N	2:B:224:PHE:HD2	2.12	0.47
12:L:42:VAL:HG23	12:L:102:ALA:HB3	1.97	0.47
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:97:HIS:HD2	8:V:61:SER:OG	1.97	0.47
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.49	0.47
13:1:1:THR:OG1	13:1:2:SER:N	2.47	0.47
1:A:13:THR:O	2:B:130:ARG:HD3	2.14	0.47
5:E:134:VAL:O	5:E:153:PRO:HG3	2.14	0.47
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.96	0.47
13:M:40:ASN:HD22	13:M:40:ASN:N	2.06	0.47
2:P:44:ASP:OD2	2:P:44:ASP:N	2.45	0.47
5:S:58:LEU:N	5:S:58:LEU:HD12	2.30	0.47
9:W:29:ASN:HD22	9:W:29:ASN:C	2.23	0.47
10:X:100:LEU:CD2	10:X:112:GLN:HG3	2.44	0.47
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.13	0.47
4:D:59:LEU:HD13	4:D:59:LEU:C	2.40	0.47
6:F:180:VAL:HG21	7:G:58:LEU:HD23	1.95	0.47
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.97	0.47
10:J:143:ARG:O	10:J:146:MET:HG3	2.14	0.47
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.96	0.47
13:M:152:GLU:O	13:M:156:VAL:HG23	2.14	0.47
1:O:67:VAL:HB	1:O:223:LYS:NZ	2.29	0.47
1:O:236:LEU:C	1:O:236:LEU:HD13	2.39	0.47
6:T:114:ASP:O	6:T:118:GLN:HG2	2.14	0.47
7:U:203:THR:HG22	7:U:204:GLU:N	2.30	0.47
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.97	0.47
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.95	0.47
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.40	0.47
13:1:133:MET:O	13:1:136:PRO:HD2	2.14	0.47
1:A:141:HIS:HA	1:A:146:GLY:O	2.15	0.47
2:B:229:ILE:O	2:B:233:LEU:HB2	2.15	0.47
2:B:235:LYS:C	2:B:237:GLY:H	2.22	0.47
4:D:24:VAL:O	4:D:27:SER:HB3	2.15	0.47
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.44	0.47
7:G:158:VAL:HG22	7:G:159:GLY:N	2.30	0.47
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.14	0.47
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.50	0.47
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.12	0.47
2:P:196:THR:O	2:P:200:THR:HG23	2.15	0.47
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.30	0.47
9:W:124:PHE:O	9:W:125:ILE:HD12	2.15	0.47
2:B:6:ARG:HG2	3:C:10:ARG:NH2	2.29	0.47
6:F:53:LEU:HD13	6:F:20(C):LYS:HD2	1.97	0.47
6:F:114:ASP:O	6:F:118:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.13	0.47
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.80	0.47
5:S:149:LEU:HD12	5:S:159:GLU:HA	1.97	0.47
5:S:2(B):THR:H	5:S:2(E):ASN:HB3	1.79	0.47
6:T:45:GLY:HA3	6:T:215:CYS:O	2.14	0.47
11:Y:114:ASP:C	11:Y:114:ASP:OD1	2.57	0.47
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.98	0.47
5:E:188:GLU:OE1	5:E:188:GLU:HA	2.15	0.47
6:F:88:LEU:CD1	6:F:116:LEU:HD22	2.44	0.47
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.30	0.47
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.96	0.47
7:U:46:THR:HG21	7:U:139:VAL:HB	1.96	0.47
9:W:104:ILE:HD13	9:W:108:PRO:HA	1.97	0.47
1:A:236:LEU:C	1:A:236:LEU:HD13	2.40	0.46
2:B:196:THR:O	2:B:200:THR:HG23	2.15	0.46
4:D:17:PRO:HD2	16:D:268:HOH:O	2.15	0.46
12:L:27:ASN:HB3	13:M:120:TYR:CZ	2.50	0.46
1:O:141:HIS:HA	1:O:146:GLY:O	2.15	0.46
9:W:61:TYR:CD1	9:W:61:TYR:C	2.93	0.46
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.29	0.46
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.50	0.46
1:A:67:VAL:HB	1:A:223:LYS:NZ	2.30	0.46
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.50	0.46
3:C:97:GLN:NE2	16:C:244:HOH:O	2.47	0.46
4:D:170:GLU:H	4:D:170:GLU:CD	2.22	0.46
7:G:46:THR:HG21	7:G:139:VAL:HB	1.97	0.46
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.15	0.46
4:R:215:ILE:HD13	4:R:215:ILE:C	2.40	0.46
12:Z:160:THR:O	12:Z:164:GLU:HG2	2.16	0.46
3:C:159:SER:O	4:D:59:LEU:HD22	2.16	0.46
5:E:58:LEU:HD12	5:E:58:LEU:N	2.29	0.46
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.72	0.46
12:L:3:ILE:HD12	12:L:46:ASN:CB	2.46	0.46
2:P:190:ILE:HG21	2:P:232:ILE:CD1	2.41	0.46
3:Q:125:GLN:NE2	16:Q:256:HOH:O	2.48	0.46
6:T:90:ASN:O	6:T:94:GLU:HG3	2.15	0.46
7:U:151:THR:HG22	7:U:157:TYR:CB	2.45	0.46
7:U:234:VAL:O	7:U:237:ALA:HB3	2.15	0.46
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.16	0.46
8:V:208:ARG:HD3	9:W:149:GLU:HB3	1.97	0.46
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.14	0.46
2:B:39:GLY:O	2:B:162:ALA:HA	2.16	0.46
2:B:44:ASP:OD2	2:B:44:ASP:N	2.46	0.46
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.98	0.46
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.45	0.46
11:K:12:ILE:HB	11:K:178:VAL:HB	1.97	0.46
12:L:160:THR:O	12:L:164:GLU:HG2	2.14	0.46
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.97	0.46
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.27	0.46
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.80	0.46
9:W:27:VAL:HG13	16:W:208:HOH:O	2.16	0.46
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.45	0.46
2:P:235:LYS:C	2:P:237:GLY:N	2.73	0.46
4:R:110:GLU:HB2	16:R:828:HOH:O	2.15	0.46
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.46	0.46
5:S:214:ILE:HG12	5:S:215:VAL:N	2.31	0.46
10:X:100:LEU:HD21	10:X:112:GLN:HG3	1.97	0.46
1:A:205:GLU:HA	1:A:205:GLU:OE2	2.15	0.46
11:K:200:LYS:HE3	11:K:206:PHE:O	2.15	0.46
2:P:39:GLY:O	2:P:162:ALA:HA	2.15	0.46
2:P:71:ASN:HD22	2:P:72:ASP:N	2.12	0.46
3:Q:182:PRO:O	3:Q:184:ALA:N	2.49	0.46
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.11	0.46
7:U:152:ASP:HB2	7:U:153:PRO:HD2	1.96	0.46
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.14	0.46
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.97	0.46
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.46	0.46
8:H:6:VAL:O	8:H:13:VAL:HG12	2.16	0.46
1:O:60:MET:HE3	1:O:63:THR:CG2	2.40	0.46
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.46	0.46
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.45	0.46
16:V:261:HOH:O	9:W:150:ASP:HA	2.15	0.46
9:W:137:MET:CE	9:W:141:LEU:HD11	2.39	0.46
13:1:83:LEU:O	13:1:87:MET:HG2	2.16	0.46
5:E:207:LEU:N	5:E:207:LEU:CD2	2.78	0.46
6:F:18:ASP:OD2	6:F:18:ASP:N	2.40	0.46
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.31	0.46
5:S:194:VAL:HA	5:S:197:ILE:HG22	1.96	0.46
10:X:112:GLN:NE2	10:X:126:ALA:H	2.14	0.46
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.51	0.46
10:X:185:ARG:HG2	10:X:185:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.15	0.46
14:2:3:ILE:HG22	14:2:16:ALA:HB2	1.97	0.46
14:2:107:LYS:HG2	14:2:108:GLY:N	2.31	0.46
6:F:36:THR:HB	6:F:168:GLY:H	1.79	0.46
9:I:101:VAL:O	9:I:110:ILE:HA	2.16	0.46
9:I:124:PHE:O	9:I:125:ILE:HD12	2.15	0.46
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.81	0.46
13:M:1:THR:OG1	13:M:2:SER:N	2.49	0.46
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.96	0.46
4:R:170:GLU:CD	4:R:170:GLU:H	2.23	0.46
8:V:73:GLU:OE1	8:V:73:GLU:HA	2.15	0.46
10:X:85:GLN:HB3	16:X:210:HOH:O	2.16	0.46
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	1.98	0.46
3:C:182:PRO:O	3:C:184:ALA:N	2.49	0.46
10:J:100:LEU:CD2	10:J:112:GLN:HG3	2.46	0.46
5:S:35:SER:O	5:S:66:LYS:NZ	2.49	0.46
2:B:122:GLY:C	2:B:124:THR:N	2.74	0.45
3:C:15:PHE:H	4:D:23:GLN:NE2	1.95	0.45
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.81	0.45
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.51	0.45
5:E:214:ILE:HG12	5:E:215:VAL:N	2.32	0.45
9:I:104:ILE:HG21	9:I:181:LYS:HG2	1.98	0.45
9:I:137:MET:CE	9:I:141:LEU:HD11	2.36	0.45
12:L:70:HIS:O	12:L:70(A):ASN:C	2.59	0.45
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.51	0.45
4:D:142:ASP:C	4:D:142:ASP:OD2	2.59	0.45
7:G:152:ASP:HB2	7:G:153:PRO:HD2	1.98	0.45
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.51	0.45
1:O:32:LYS:HA	1:O:32:LYS:CE	2.47	0.45
3:Q:44:ASN:O	3:Q:45:CYS:HB3	2.15	0.45
6:T:62:GLN:HA	6:T:209:GLU:OE2	2.16	0.45
6:T:95:GLU:HG3	6:T:115:ARG:HD2	1.99	0.45
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.17	0.45
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.81	0.45
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.52	0.45
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.98	0.45
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.17	0.45
13:1:14(C):ARG:CG	13:1:14(C):ARG:NH1	2.70	0.45
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.98	0.45
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.98	0.45
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:LEU:HD13	9:I:20:LEU:C	2.41	0.45
9:I:113:PHE:CD2	9:I:113:PHE:N	2.83	0.45
14:N:37:VAL:HG22	14:N:41:ILE:O	2.17	0.45
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.87	0.45
1:A:4:MET:HG2	6:F:126:TYR:CE2	2.51	0.45
3:C:163:GLN:NE2	3:C:163:GLN:HA	2.30	0.45
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.80	0.45
5:E:40:LEU:HD23	5:E:40:LEU:H	1.81	0.45
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.98	0.45
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.98	0.45
10:J:100:LEU:HD21	10:J:112:GLN:HG3	1.98	0.45
11:K:142:TYR:C	11:K:143:LYS:HD2	2.42	0.45
13:M:40:ASN:H	13:M:40:ASN:ND2	2.13	0.45
4:R:120:ALA:CB	4:R:155:GLY:HA2	2.46	0.45
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.11	0.45
11:Y:37:ILE:HB	11:Y:41:LEU:HB2	1.98	0.45
14:2:107:LYS:HG2	14:2:108:GLY:H	1.82	0.45
2:B:163:ILE:HG12	2:B:164:SER:H	1.81	0.45
2:B:235:LYS:HD3	2:B:235:LYS:N	2.30	0.45
7:G:173:THR:O	7:G:177:GLU:HG3	2.16	0.45
11:K:114:ASP:C	11:K:114:ASP:OD1	2.60	0.45
12:L:21:ILE:C	12:L:21:ILE:CD1	2.86	0.45
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.99	0.45
13:M:211:ILE:H	13:M:211:ILE:CD1	2.26	0.45
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.98	0.45
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.98	0.45
10:X:185:ARG:NH1	16:X:218:HOH:O	2.50	0.45
14:2:20:THR:CG2	14:2:31:THR:OG1	2.62	0.45
3:C:169:SER:HA	3:C:172:VAL:CG1	2.47	0.45
14:N:186:ARG:HD2	16:N:229:HOH:O	2.16	0.45
1:O:117:ALA:HB1	1:O:155:GLY:O	2.17	0.45
3:Q:163:GLN:NE2	3:Q:163:GLN:HA	2.30	0.45
4:R:52:LYS:HB2	4:R:20(B):ASN:C	2.42	0.45
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.51	0.45
6:T:75:GLY:O	6:T:138:PHE:HA	2.17	0.45
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.52	0.45
10:X:119:LYS:HE2	16:X:216:HOH:O	2.16	0.45
6:F:103:TYR:O	6:F:104:LYS:HB3	2.17	0.45
6:F:119:TYR:O	6:F:122:ALA:HB3	2.16	0.45
10:J:185:ARG:HG2	10:J:185:ARG:HH11	1.82	0.45
7:U:82:ILE:HG22	7:U:83:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.47	0.45
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.52	0.45
16:Z:209:HOH:O	13:1:121:SER:HB2	2.16	0.45
11:K:97:MET:HG2	11:K:115:SER:HB3	1.97	0.45
13:M:4:ILE:CD1	13:M:155:ILE:HG23	2.47	0.45
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.97	0.45
3:Q:238:GLN:O	3:Q:242:GLU:HG3	2.17	0.45
6:T:173:LYS:O	6:T:177:GLU:HG3	2.17	0.45
7:U:18(D):ILE:O	7:U:18(G):GLU:N	2.50	0.45
12:Z:27:ASN:HB3	13:1:120:TYR:CE1	2.52	0.45
4:D:215:ILE:C	4:D:215:ILE:HD13	2.41	0.45
6:F:62:GLN:HA	6:F:209:GLU:OE2	2.16	0.45
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.32	0.45
14:N:24:ALA:HB3	13:1:129:PHE:HE2	1.81	0.45
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.99	0.45
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.64	0.45
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.69	0.45
7:U:188:LYS:HD3	7:U:188:LYS:HA	1.77	0.45
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.96	0.45
12:L:166:HIS:CD2	12:L:168:GLN:H	2.28	0.45
1:O:57:PRO:HG3	7:U:177:GLU:OE1	2.17	0.45
4:R:142:ASP:OD2	4:R:142:ASP:C	2.60	0.45
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.00	0.45
9:W:89:GLU:HG2	9:W:90:ARG:NH1	2.32	0.45
9:W:113:PHE:CD2	9:W:113:PHE:N	2.85	0.45
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.42	0.45
12:Z:21:ILE:C	12:Z:21:ILE:CD1	2.85	0.45
6:F:45:GLY:HA3	6:F:215:CYS:O	2.17	0.44
8:H:29:LYS:HE2	12:Z:165:ARG:NH2	2.32	0.44
8:H:48:THR:HB	8:H:51:ASP:HB2	2.00	0.44
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.32	0.44
14:N:29:ARG:HG2	16:N:227:HOH:O	2.16	0.44
14:N:10(B):LYS:HD3	14:N:10(B):LYS:O	2.17	0.44
8:V:128:GLY:O	8:V:131:SER:CB	2.65	0.44
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.99	0.44
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.17	0.44
13:1:211:ILE:HD13	13:1:211:ILE:N	2.24	0.44
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.98	0.44
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.52	0.44
3:C:55:THR:HG22	3:C:56:LEU:CD2	2.42	0.44
6:F:54:ILE:HG13	6:F:208:PHE:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.99	0.44
6:T:53:LEU:HD13	6:T:20(C):LYS:HD2	1.98	0.44
6:T:54:ILE:HG13	6:T:208:PHE:HA	1.98	0.44
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.81	0.44
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.17	0.44
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.83	0.44
10:X:7:ARG:NE	16:X:195:HOH:O	2.42	0.44
12:Z:70:HIS:O	12:Z:70(A):ASN:C	2.60	0.44
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.99	0.44
2:B:230:LYS:O	2:B:234:VAL:HG23	2.17	0.44
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.48	0.44
5:E:57:GLU:C	5:E:58:LEU:HD12	2.42	0.44
11:K:36:GLU:O	11:K:37:ILE:C	2.61	0.44
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.99	0.44
5:S:82:ALA:HB1	16:S:237:HOH:O	2.17	0.44
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.47	0.44
13:1:49:ILE:O	13:1:53:GLN:HG3	2.18	0.44
14:2:15:GLY:HA2	14:2:174:ARG:O	2.17	0.44
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.98	0.44
1:A:32:LYS:HA	1:A:32:LYS:CE	2.48	0.44
8:H:147:THR:O	8:H:148:LYS:C	2.61	0.44
11:K:31:VAL:HG11	15:K:0:SA1:H13	1.99	0.44
12:L:103:GLY:HA2	12:L:178:VAL:HG11	1.99	0.44
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.47	0.44
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.18	0.44
10:X:35:ARG:NH1	10:X:57:GLU:CG	2.81	0.44
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.18	0.44
14:2:9:LYS:O	14:2:107:LYS:HD3	2.17	0.44
3:C:85:SER:O	3:C:89:ILE:HD13	2.18	0.44
5:S:57:GLU:C	5:S:58:LEU:HD12	2.43	0.44
6:T:119:TYR:O	6:T:122:ALA:HB3	2.17	0.44
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.31	0.44
12:Z:-8:PHE:HB2	13:1:-8:THR:HG23	2.00	0.44
12:Z:48:PHE:CZ	12:Z:50:ALA:HB3	2.53	0.44
13:1:211:ILE:H	13:1:211:ILE:CD1	2.24	0.44
2:B:101:LYS:HG3	9:I:57:GLU:HB3	2.00	0.44
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.82	0.44
8:H:30:ASN:O	8:H:189:ARG:NH2	2.49	0.44
8:H:128:GLY:O	8:H:131:SER:CB	2.66	0.44
9:I:61:TYR:CD1	9:I:61:TYR:C	2.96	0.44
5:S:40:LEU:HD23	5:S:40:LEU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:172:ALA:HB2	5:S:196:ALA:O	2.17	0.44
7:U:186:TRP:O	7:U:190:VAL:HG23	2.18	0.44
7:U:218:ASP:O	7:U:220:LYS:HB2	2.18	0.44
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.17	0.44
10:X:12:VAL:HG22	10:X:108:PRO:HB2	1.99	0.44
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.32	0.44
6:F:95:GLU:HG3	6:F:115:ARG:HD2	2.00	0.44
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.17	0.44
10:J:124:TYR:CD2	10:J:138:LEU:HD13	2.53	0.44
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.16	0.44
11:K:37:ILE:HB	11:K:41:LEU:HB2	1.99	0.44
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.15	0.44
1:O:205:GLU:HA	1:O:205:GLU:OE2	2.16	0.44
5:S:188:GLU:HA	5:S:188:GLU:OE1	2.17	0.44
8:V:3:ILE:HG22	8:V:16:ALA:HB2	2.00	0.44
7:G:234:VAL:O	7:G:237:ALA:HB3	2.17	0.44
13:M:83:LEU:O	13:M:87:MET:HG2	2.18	0.44
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.52	0.44
6:T:126:TYR:HE1	7:U:129:MET:SD	2.40	0.44
7:U:119:LEU:HD12	7:U:119:LEU:HA	1.87	0.44
12:Z:-8:PHE:HB3	13:1:-8:THR:HG23	1.99	0.44
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.26	0.44
2:B:63:THR:O	2:B:63:THR:HG22	2.18	0.44
2:B:69:LYS:HE3	2:B:69:LYS:HB2	1.77	0.44
3:C:158:SER:CB	4:D:59:LEU:HD21	2.48	0.44
4:D:179:GLU:HG3	4:D:192:LEU:HD11	1.99	0.44
6:F:75:GLY:O	6:F:138:PHE:HA	2.16	0.44
14:N:9:LYS:O	14:N:107:LYS:HD3	2.17	0.44
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.99	0.44
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.79	0.44
2:B:235:LYS:C	2:B:237:GLY:N	2.75	0.43
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.53	0.43
5:E:40:LEU:N	5:E:40:LEU:CD2	2.81	0.43
7:G:218:ASP:O	7:G:220:LYS:HB2	2.17	0.43
10:J:105:ASP:O	10:J:106:ASN:N	2.48	0.43
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.53	0.43
13:M:113:VAL:HA	13:M:118:VAL:O	2.17	0.43
14:N:107:LYS:HG2	14:N:108:GLY:N	2.33	0.43
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.18	0.43
5:S:74:MET:CE	5:S:96:CYS:SG	3.06	0.43
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:203:GLU:O	6:T:206:LYS:HD2	2.18	0.43
4:D:51:GLU:HG2	4:D:53:ARG:HB2	1.99	0.43
13:M:211:ILE:HD11	14:2:36:ARG:HD3	2.00	0.43
1:O:15:PHE:N	2:P:23:GLN:HE22	1.91	0.43
2:P:63:THR:O	2:P:63:THR:HG22	2.18	0.43
2:P:144:ARG:O	2:P:144:ARG:HG2	2.18	0.43
5:S:38:VAL:HG22	5:S:164:ALA:CB	2.47	0.43
10:X:143:ARG:HG2	10:X:143:ARG:HH11	1.83	0.43
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.54	0.43
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.49	0.43
7:G:173:THR:HG22	7:G:177:GLU:OE2	2.17	0.43
9:I:29:ASN:H	9:I:29:ASN:HD22	1.65	0.43
9:I:89:GLU:HG2	9:I:90:ARG:NH1	2.32	0.43
13:M:14(C):ARG:CG	13:M:14(C):ARG:NH1	2.72	0.43
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.48	0.43
4:R:51:GLU:HG2	4:R:53:ARG:HB2	2.00	0.43
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.43	0.43
14:2:156:LYS:HG2	14:2:18(J):LEU:CD1	2.49	0.43
1:A:185:GLU:OE1	1:A:187:GLU:HB2	2.19	0.43
3:C:163:GLN:NE2	3:C:164:THR:N	2.48	0.43
4:D:52:LYS:HB2	4:D:20(B):ASN:C	2.44	0.43
6:F:173:LYS:O	6:F:177:GLU:HG3	2.18	0.43
12:L:176:LEU:HG	12:L:186:LYS:HG2	2.00	0.43
3:Q:206:GLY:CA	3:Q:209:ASN:HB2	2.47	0.43
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.53	0.43
4:R:160:TYR:HA	5:S:58:LEU:O	2.18	0.43
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.53	0.43
5:S:39:GLY:O	5:S:162:GLY:HA2	2.18	0.43
16:X:211:HOH:O	11:Y:88:TYR:HB2	2.18	0.43
14:2:38:HIS:O	14:2:39:ASP:C	2.62	0.43
2:B:71:ASN:HD22	2:B:72:ASP:N	2.12	0.43
11:K:6:PHE:HA	11:K:123:ASP:O	2.19	0.43
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.54	0.43
2:P:229:ILE:O	2:P:233:LEU:HB2	2.18	0.43
10:X:90(B):ARG:NH1	16:X:204:HOH:O	2.49	0.43
10:X:166:MET:HA	10:X:167:PRO:HD3	1.82	0.43
2:B:121:GLN:NE2	2:B:121:GLN:C	2.77	0.43
4:D:201:MET:HE2	4:D:201:MET:HB3	1.91	0.43
5:E:216:GLY:O	5:E:217:LYS:C	2.62	0.43
11:K:200:LYS:HG3	11:K:206:PHE:HB2	2.00	0.43
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.53	0.43
2:P:69:LYS:HE3	2:P:69:LYS:HB2	1.78	0.43
3:Q:159:SER:O	4:R:59:LEU:HD22	2.19	0.43
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.84	0.43
5:S:216:GLY:O	5:S:217:LYS:C	2.61	0.43
7:U:31:THR:HG21	7:U:135:ILE:HG13	2.01	0.43
8:V:30:ASN:O	8:V:189:ARG:NH2	2.45	0.43
8:V:147:THR:O	8:V:148:LYS:C	2.62	0.43
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.54	0.43
5:E:18(D):ILE:HG12	5:E:18(D):ILE:O	2.17	0.43
5:E:190:ILE:O	5:E:194:VAL:HG23	2.18	0.43
7:G:82:ILE:HG22	7:G:83:PRO:HD3	1.99	0.43
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.48	0.43
10:J:171:LYS:HE3	16:X:223:HOH:O	2.19	0.43
13:M:67:ALA:HB3	16:M:254:HOH:O	2.18	0.43
14:N:133:PHE:HA	14:2:132:THR:O	2.18	0.43
2:P:88:LEU:HB3	2:P:116:LEU:HD21	1.99	0.43
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.81	0.43
3:Q:18(A):ASP:OD2	3:Q:18(C):LYS:HG2	2.18	0.43
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.83	0.43
5:S:40:LEU:N	5:S:40:LEU:CD2	2.82	0.43
10:X:19:ALA:HB2	10:X:171:LYS:HG2	2.00	0.43
10:X:39:PRO:HG2	10:X:73:GLU:CD	2.44	0.43
12:Z:99:THR:CG2	16:Z:203:HOH:O	2.65	0.43
4:D:120:ALA:CB	4:D:155:GLY:HA2	2.48	0.43
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.54	0.43
5:E:85:ALA:HB2	5:E:134:VAL:HG21	2.00	0.43
6:F:50:VAL:HB	6:F:77:VAL:HG21	2.01	0.43
8:H:208:ARG:HD3	9:I:149:GLU:HB3	1.99	0.43
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.43
10:J:39:PRO:HG2	10:J:73:GLU:CD	2.44	0.43
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.49	0.43
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	2.01	0.43
13:M:112:TYR:CE1	13:M:127:THR:HG22	2.51	0.43
13:M:113:VAL:HG23	13:M:119:THR:HG22	2.00	0.43
1:O:185:GLU:OE1	1:O:187:GLU:HB2	2.19	0.43
5:S:47:VAL:HG23	5:S:189:LEU:HD13	2.00	0.43
5:S:190:ILE:O	5:S:194:VAL:HG23	2.19	0.43
7:U:213:GLY:HA2	7:U:223:THR:HA	2.01	0.43
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.00	0.43
11:Y:99:THR:HG22	11:Y:113:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:VAL:HG12	3:C:135:SER:N	2.34	0.43
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.66	0.43
9:I:6:MET:CE	9:I:155:ILE:HA	2.48	0.43
10:J:52:THR:HG23	10:J:53:VAL:N	2.34	0.43
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.82	0.43
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.01	0.43
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.16	0.43
1:O:60:MET:HB2	1:O:63:THR:HG23	2.01	0.43
5:S:76:LEU:CD1	5:S:136:LEU:HD22	2.49	0.43
8:V:3:ILE:O	8:V:126:SER:HA	2.19	0.43
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.99	0.43
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.19	0.43
13:1:40:ASN:HD22	13:1:40:ASN:N	2.07	0.43
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.36	0.43
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.18	0.43
3:C:20:HIS:HB3	3:C:25:GLU:OE1	2.19	0.43
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.19	0.43
10:J:166:MET:HA	10:J:167:PRO:HD3	1.83	0.43
11:K:99:THR:HG22	11:K:113:VAL:HB	2.00	0.43
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.34	0.43
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.49	0.43
6:T:103:TYR:O	6:T:104:LYS:HB3	2.18	0.43
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.83	0.43
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.18	0.43
9:W:20:LEU:C	9:W:20:LEU:HD13	2.44	0.43
10:X:24:ILE:HG12	10:X:24:ILE:O	2.18	0.43
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.54	0.43
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.53	0.42
5:E:18(C):PHE:CD1	5:E:18(C):PHE:C	2.97	0.42
7:G:224:LEU:HB3	7:G:228:ASN:HB2	2.01	0.42
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.84	0.42
12:L:-2:ASN:HA	12:L:21:ILE:O	2.18	0.42
13:M:115:LEU:HD23	13:M:115:LEU:N	2.34	0.42
12:Z:129:ALA:HB1	12:Z:166:HIS:NE2	2.34	0.42
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.54	0.42
2:B:41:MET:HE2	2:B:146:TYR:O	2.18	0.42
2:B:213:ALA:HA	2:B:222:LYS:O	2.19	0.42
5:E:143:LYS:HB2	16:M:247:HOH:O	2.19	0.42
7:G:82:ILE:N	7:G:83:PRO:HD2	2.33	0.42
9:I:104:ILE:HD13	9:I:108:PRO:HA	2.00	0.42
2:P:230:LYS:O	2:P:234:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:225:SER:O	3:Q:226:SER:C	2.62	0.42
10:X:140:HIS:HD2	10:X:141:HIS:CE1	2.36	0.42
5:E:15:PHE:N	6:F:23:GLN:HE22	2.09	0.42
5:E:149:LEU:HD12	5:E:159:GLU:HA	2.00	0.42
7:G:186:TRP:O	7:G:190:VAL:HG23	2.19	0.42
9:I:93:GLY:N	9:I:94:PRO:CD	2.83	0.42
2:P:27:ALA:O	2:P:30:SER:HB3	2.19	0.42
2:P:213:ALA:HA	2:P:222:LYS:O	2.19	0.42
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.54	0.42
5:S:18(C):PHE:C	5:S:18(C):PHE:CD1	2.97	0.42
6:T:90:ASN:ND2	16:T:248:HOH:O	2.52	0.42
9:W:23:GLN:HB2	16:W:229:HOH:O	2.18	0.42
13:1:11:GLY:HA3	13:1:178:ILE:O	2.20	0.42
3:C:238:GLN:O	3:C:242:GLU:HG3	2.18	0.42
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	2.01	0.42
7:G:115:ARG:HH12	7:G:119:LEU:HD13	1.85	0.42
7:G:136:LEU:O	7:G:150:LYS:HA	2.19	0.42
10:J:12:VAL:HG22	10:J:108:PRO:HB2	2.02	0.42
12:L:27:ASN:HB3	13:M:120:TYR:CE1	2.54	0.42
1:O:112:LEU:O	1:O:116:VAL:HG23	2.19	0.42
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.92	0.42
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.62	0.42
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:N	2.69	0.42
12:Z:175:ILE:C	12:Z:176:LEU:HD12	2.44	0.42
13:1:40:ASN:H	13:1:40:ASN:ND2	2.14	0.42
1:A:109:THR:O	1:A:113:VAL:HG23	2.20	0.42
3:C:215:VAL:O	3:C:215:VAL:HG13	2.19	0.42
3:C:225:SER:O	3:C:226:SER:C	2.62	0.42
3:C:241:GLN:C	3:C:243:GLN:N	2.75	0.42
4:D:76:CYS:HB2	4:D:137:LEU:O	2.19	0.42
5:E:194:VAL:O	5:E:197:ILE:HG22	2.19	0.42
10:J:24:ILE:HG12	10:J:24:ILE:O	2.19	0.42
14:N:132:THR:O	14:2:133:PHE:HA	2.20	0.42
1:O:33:GLN:HA	1:O:33:GLN:NE2	2.34	0.42
1:O:92:SER:O	1:O:95:VAL:HG12	2.19	0.42
3:Q:85:SER:O	3:Q:89:ILE:HD13	2.19	0.42
5:S:194:VAL:O	5:S:197:ILE:HG22	2.20	0.42
11:Y:36:GLU:O	11:Y:37:ILE:C	2.63	0.42
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.29	0.42
12:Z:176:LEU:HG	12:Z:186:LYS:HG2	2.02	0.42
2:B:202:THR:HG21	2:B:204:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ARG:HG2	2:B:209:ARG:HH11	1.84	0.42
3:C:18(A):ASP:OD2	3:C:18(C):LYS:HG2	2.19	0.42
5:E:74:MET:CE	5:E:96:CYS:SG	3.08	0.42
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.49	0.42
14:N:115:LEU:HD12	14:N:115:LEU:HA	1.77	0.42
1:O:4:MET:HG2	6:T:126:TYR:CE2	2.54	0.42
3:Q:241:GLN:C	3:Q:243:GLN:N	2.75	0.42
5:S:230:ALA:C	5:S:232:TYR:H	2.28	0.42
7:U:115:ARG:HH12	7:U:119:LEU:HD13	1.83	0.42
13:1:4:ILE:CD1	13:1:155:ILE:HG23	2.48	0.42
13:1:57:ARG:HG2	13:1:57:ARG:HH11	1.83	0.42
3:C:125:GLN:O	3:C:125:GLN:HG3	2.20	0.42
4:D:91:HIS:CG	4:D:119:LEU:HD11	2.55	0.42
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.85	0.42
5:E:4:PHE:O	5:E:5:ARG:C	2.62	0.42
10:J:112:GLN:NE2	10:J:126:ALA:H	2.17	0.42
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.55	0.42
1:O:225:THR:HG23	1:O:228:GLU:OE1	2.20	0.42
5:S:109:VAL:HG12	5:S:149:LEU:HD22	2.00	0.42
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	2.02	0.42
14:2:105:ASP:OD2	14:2:106:ASN:N	2.47	0.42
2:B:97:GLN:NE2	16:B:246:HOH:O	2.46	0.42
3:C:182:PRO:O	3:C:183:PRO:C	2.62	0.42
5:E:38:VAL:HG22	5:E:164:ALA:CB	2.50	0.42
6:F:28:VAL:O	6:F:32:GLU:HG3	2.20	0.42
6:F:41:LYS:HD2	16:F:248:HOH:O	2.20	0.42
6:F:172:ALA:O	6:F:176:LEU:HD22	2.20	0.42
9:I:89:GLU:HG2	9:I:90:ARG:HH12	1.85	0.42
10:J:35:ARG:NH1	10:J:57:GLU:CG	2.83	0.42
2:P:185:LYS:HD2	2:P:187:ASP:H	1.84	0.42
3:Q:79:SER:OG	3:Q:165:ILE:HG13	2.20	0.42
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.20	0.42
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.85	0.42
7:U:60:ASP:OD2	7:U:60:ASP:C	2.63	0.42
7:U:110:ASP:HB3	7:U:149:TYR:CE2	2.55	0.42
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.84	0.42
9:W:130:ALA:HB2	9:W:166:ASP:CB	2.50	0.42
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.20	0.42
3:C:75:VAL:HG13	3:C:221:ILE:HD13	2.02	0.42
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.19	0.42
14:N:107:LYS:HG2	14:N:108:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.19	0.42
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.55	0.42
14:2:44:CYS:HB2	14:2:100:ILE:HB	2.01	0.42
4:D:238:LYS:HE2	4:D:238:LYS:HB3	1.81	0.42
7:G:107:MET:CE	7:G:112:LEU:HD13	2.47	0.42
10:J:143:ARG:HG2	10:J:143:ARG:HH11	1.84	0.42
11:K:25:TRP:CH2	12:L:132:SER:HA	2.54	0.42
11:K:38:ASN:C	11:K:38:ASN:OD1	2.63	0.42
13:M:3:VAL:O	13:M:126:ALA:HA	2.20	0.42
3:Q:215:VAL:HG13	3:Q:215:VAL:O	2.19	0.42
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.83	0.42
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.27	0.42
4:R:236:GLU:O	4:R:240:LYS:HG3	2.19	0.42
4:R:238:LYS:HB3	4:R:238:LYS:HE2	1.84	0.42
5:S:4:PHE:O	5:S:5:ARG:C	2.63	0.42
1:A:92:SER:O	1:A:95:VAL:HG12	2.20	0.41
1:A:112:LEU:O	1:A:116:VAL:HG23	2.19	0.41
5:E:230:ALA:C	5:E:232:TYR:H	2.27	0.41
6:F:126:TYR:HE1	7:G:129:MET:SD	2.42	0.41
7:G:232:ARG:NE	7:G:232:ARG:HA	2.35	0.41
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.01	0.41
9:I:155:ILE:HG23	9:I:156:SER:N	2.35	0.41
14:N:14:LEU:HD11	14:N:102:ALA:HB3	2.01	0.41
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.20	0.41
5:S:220:PRO:O	5:S:221:PHE:C	2.62	0.41
7:U:233:LEU:HD12	7:U:233:LEU:HA	1.89	0.41
8:V:80:LEU:HD12	8:V:113:ILE:CD1	2.46	0.41
12:Z:170:GLY:O	12:Z:171:ASP:HB2	2.20	0.41
13:1:3:VAL:O	13:1:126:ALA:HA	2.20	0.41
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.55	0.41
2:B:10:SER:HB2	16:B:248:HOH:O	2.20	0.41
2:B:27:ALA:O	2:B:30:SER:HB3	2.21	0.41
9:I:88:TYR:CE1	9:I:91:ARG:HD3	2.55	0.41
3:Q:97:GLN:HG3	10:X:65:LEU:HB2	2.01	0.41
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.83	0.41
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	2.01	0.41
7:U:168:LYS:O	7:U:172:ILE:HG12	2.19	0.41
7:U:232:ARG:HA	7:U:232:ARG:NE	2.35	0.41
13:1:43:VAL:HG22	13:1:101:VAL:HG22	2.01	0.41
1:A:179:ARG:HH11	1:A:179:ARG:CB	2.25	0.41
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.21	0.41
2:B:181:LYS:HG3	2:B:184:MET:HG3	2.03	0.41
6:F:203:GLU:O	6:F:206:LYS:HD2	2.20	0.41
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.03	0.41
9:I:130:ALA:HB2	9:I:166:ASP:CB	2.51	0.41
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.35	0.41
13:M:100:ILE:CD1	13:M:127:THR:HG23	2.51	0.41
13:M:122:SER:HB3	13:M:124:THR:O	2.20	0.41
2:P:181:LYS:HG3	2:P:184:MET:HG3	2.02	0.41
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.84	0.41
4:R:159:ARG:O	5:S:60:SER:N	2.53	0.41
9:W:19:ARG:HB2	9:W:171:TRP:HB2	2.02	0.41
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.50	0.41
11:Y:172:SER:HA	11:Y:192:VAL:HG23	2.03	0.41
3:C:197:LEU:O	3:C:201:VAL:HG23	2.21	0.41
10:J:168:MET:HE3	10:X:168:MET:CG	2.48	0.41
10:J:168:MET:CG	10:X:168:MET:HE3	2.47	0.41
6:T:203:GLU:C	6:T:205:ASN:N	2.79	0.41
7:U:172:ILE:HD12	7:U:197:MET:HE1	2.01	0.41
8:V:103:GLY:HA2	8:V:178:MET:SD	2.61	0.41
11:Y:174:ASN:ND2	11:Y:186:TYR:OH	2.53	0.41
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.50	0.41
13:1:113:VAL:HG23	13:1:119:THR:HG22	2.01	0.41
14:2:114:PRO:HD2	14:2:118:SER:O	2.20	0.41
5:E:36:VAL:HG22	5:E:37:THR:N	2.35	0.41
5:E:220:PRO:O	5:E:221:PHE:C	2.63	0.41
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.20	0.41
10:J:35:ARG:HD3	10:J:35:ARG:HA	1.79	0.41
11:K:4:LEU:C	11:K:4:LEU:CD2	2.94	0.41
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.56	0.41
2:P:136:PHE:O	2:P:150:THR:HA	2.21	0.41
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.19	0.41
5:S:85:ALA:HB2	5:S:134:VAL:HG21	2.03	0.41
9:W:89:GLU:HG2	9:W:90:ARG:HH12	1.85	0.41
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.50	0.41
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.56	0.41
2:B:185:LYS:HD2	2:B:187:ASP:H	1.84	0.41
3:C:224:LEU:N	3:C:224:LEU:CD1	2.82	0.41
5:E:227:GLU:N	5:E:227:GLU:OE2	2.54	0.41
6:F:187:ARG:HH11	6:F:187:ARG:HG3	1.86	0.41
8:H:3:ILE:O	8:H:126:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:-1:MET:HE1	10:J:98:ASN:ND2	2.35	0.41
10:J:140:HIS:HD2	10:J:141:HIS:CE1	2.39	0.41
2:P:41:MET:HE2	2:P:146:TYR:O	2.20	0.41
2:P:202:THR:HG21	2:P:204:SER:HB2	2.02	0.41
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	2.02	0.41
5:S:36:VAL:HG22	5:S:37:THR:N	2.36	0.41
7:U:164:ALA:CB	7:U:172:ILE:HB	2.50	0.41
9:W:115:LEU:N	9:W:115:LEU:HD23	2.35	0.41
10:X:-1:MET:HE1	10:X:98:ASN:ND2	2.36	0.41
14:2:48:SER:O	14:2:52:THR:HG23	2.21	0.41
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.56	0.41
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.20	0.41
4:D:237:LEU:HD22	4:D:241:GLU:HG3	2.02	0.41
7:G:77:VAL:HG12	7:G:137:THR:HB	2.02	0.41
7:G:171:GLU:N	7:G:171:GLU:OE1	2.53	0.41
13:M:171:ARG:HG3	13:M:192:VAL:HB	2.02	0.41
14:N:36:ARG:HD3	13:1:211:ILE:HD11	2.03	0.41
1:O:175:PHE:O	1:O:179:ARG:HG2	2.20	0.41
2:P:121:GLN:NE2	16:P:248:HOH:O	2.53	0.41
2:P:194:LEU:O	2:P:198:SER:HB2	2.21	0.41
7:U:136:LEU:O	7:U:150:LYS:HA	2.20	0.41
9:W:45:ILE:HB	9:W:52:VAL:HG13	2.02	0.41
12:Z:14(I):THR:O	12:Z:1(I):ASN:CB	2.69	0.41
14:2:37:VAL:HG22	14:2:41:ILE:O	2.19	0.41
14:2:147:SER:OG	14:2:150:GLU:HG3	2.21	0.41
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.28	0.41
3:C:55:THR:O	3:C:56:LEU:HD22	2.21	0.41
3:C:163:GLN:NE2	3:C:163:GLN:CA	2.83	0.41
4:D:185:THR:HG23	4:D:188:GLU:OE1	2.20	0.41
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.56	0.41
1:O:100:TYR:CG	1:O:107:PRO:HB3	2.55	0.41
4:R:107:ILE:CD1	4:R:111:SER:HB2	2.51	0.41
5:S:51:LEU:HD11	5:S:2(E):ASN:HD21	1.85	0.41
6:T:205:ASN:C	6:T:20(B):GLU:H	2.28	0.41
8:V:6:VAL:O	8:V:13:VAL:HG12	2.20	0.41
1:A:15:PHE:N	2:B:23:GLN:HE22	1.98	0.41
1:A:60:MET:HB2	1:A:63:THR:HG23	2.03	0.41
5:E:100:SER:O	5:E:104:ASN:HA	2.21	0.41
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.56	0.41
8:H:63:ILE:HD13	8:H:63:ILE:HA	1.94	0.41
9:I:15:ALA:HB1	9:I:159:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:93:GLY:C	16:I:223:HOH:O	2.63	0.41
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.56	0.41
9:I:120:ASP:OD2	9:I:120:ASP:C	2.64	0.41
12:L:61:ASN:HD22	12:L:61:ASN:HA	1.72	0.41
13:M:11:GLY:HA3	13:M:178:ILE:O	2.21	0.41
13:M:57:ARG:HH11	13:M:57:ARG:HG2	1.86	0.41
14:N:38:HIS:O	14:N:39:ASP:C	2.63	0.41
14:N:105:ASP:HB3	14:N:106:ASN:HB2	2.02	0.41
2:P:101:LYS:HG3	9:W:57:GLU:HB3	2.03	0.41
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.35	0.41
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	2.02	0.41
4:R:68:VAL:HG21	4:R:89:ILE:CD1	2.50	0.41
4:R:99:HIS:CG	4:R:107:ILE:HG12	2.56	0.41
4:R:185:THR:HG23	4:R:188:GLU:OE1	2.21	0.41
5:S:12:THR:HG21	5:S:124:THR:HA	2.03	0.41
5:S:77:SER:OG	5:S:137:LEU:HB2	2.21	0.41
5:S:82:ALA:HB3	16:S:237:HOH:O	2.19	0.41
6:T:50:VAL:HB	6:T:77:VAL:HG21	2.02	0.41
6:T:63:LYS:O	6:T:65:VAL:N	2.54	0.41
6:T:196:ILE:HG12	6:T:196:ILE:H	1.66	0.41
6:T:20(B):GLU:HG3	6:T:20(C):LYS:H	1.85	0.41
9:W:6:MET:CE	9:W:155:ILE:HA	2.50	0.41
9:W:29:ASN:ND2	9:W:29:ASN:N	2.66	0.41
10:X:6:ILE:HG23	10:X:13:ILE:HB	2.02	0.41
10:X:14:LEU:HD12	10:X:42:LEU:HD23	2.03	0.41
10:X:18:LYS:CD	10:X:174:ILE:HG13	2.51	0.41
10:X:126:ALA:HB1	10:X:130:SER:HB2	2.03	0.41
11:Y:70:GLU:O	11:Y:71:LYS:C	2.63	0.41
13:1:100:ILE:CD1	13:1:127:THR:HG23	2.50	0.41
14:2:14:LEU:HD12	14:2:14:LEU:N	2.36	0.41
4:D:68:VAL:HG21	4:D:89:ILE:CD1	2.50	0.41
6:F:49:ALA:HA	6:F:211:GLU:O	2.20	0.41
6:F:63:LYS:O	6:F:65:VAL:N	2.53	0.41
9:I:113:PHE:HA	9:I:118:CYS:O	2.20	0.41
9:I:159:LEU:HD21	9:I:173:ALA:HB1	2.02	0.41
12:L:114:ASP:CB	12:L:118:SER:HB3	2.50	0.41
13:M:49:ILE:O	13:M:53:GLN:HG3	2.21	0.41
13:M:51:ASP:O	13:M:54:HIS:HB3	2.21	0.41
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.35	0.41
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.56	0.41
4:R:237:LEU:HD22	4:R:241:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:76:LEU:HB3	5:S:138:ILE:HG13	2.03	0.41
6:T:95:GLU:CG	6:T:115:ARG:HD2	2.51	0.41
6:T:109:ILE:HG21	6:T:147:HIS:HB2	2.03	0.41
7:U:77:VAL:HG12	7:U:137:THR:HB	2.03	0.41
8:V:1:THR:CG2	8:V:2:THR:N	2.84	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.82	0.41
9:W:12(A):LYS:HG3	9:W:123:ASP:N	2.35	0.41
9:W:159:LEU:HD21	9:W:173:ALA:HB1	2.03	0.41
4:D:177:LEU:HD22	5:E:58:LEU:HD11	2.03	0.40
5:E:76:LEU:HA	5:E:137:LEU:O	2.22	0.40
9:I:29:ASN:ND2	9:I:29:ASN:N	2.68	0.40
10:J:143:ARG:HA	10:J:144:PRO:HD3	1.94	0.40
13:M:206:TYR:CZ	14:2:53:GLN:HG2	2.55	0.40
14:N:156:LYS:HG2	14:N:18(J):LEU:CD1	2.50	0.40
9:W:104:ILE:HG21	9:W:181:LYS:HG2	2.04	0.40
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.51	0.40
1:A:169:SER:O	1:A:173:LYS:HG3	2.21	0.40
1:A:175:PHE:O	1:A:179:ARG:HG2	2.21	0.40
3:C:227:GLU:H	3:C:227:GLU:CD	2.26	0.40
5:E:82:ALA:HB3	5:E:83:PRO:HD3	2.03	0.40
11:K:5:ALA:HA	11:K:13:ILE:O	2.21	0.40
12:L:48:PHE:CE2	12:L:50:ALA:HB3	2.56	0.40
1:O:35:VAL:HG11	1:O:51:GLU:HB3	2.03	0.40
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.36	0.40
5:S:5:ARG:HG3	5:S:22:PHE:CE1	2.56	0.40
7:U:18(H):GLU:N	7:U:18(H):GLU:CD	2.79	0.40
12:Z:14(D):TYR:CG	12:Z:14(J):GLY:HA2	2.57	0.40
13:1:115:LEU:N	13:1:115:LEU:HD23	2.35	0.40
3:C:206:GLY:CA	3:C:209:ASN:HB2	2.49	0.40
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	2.04	0.40
9:I:6:MET:HE1	9:I:155:ILE:HA	2.03	0.40
9:I:70:GLU:O	9:I:71:GLU:HB2	2.22	0.40
12:L:4:LEU:O	12:L:14:LEU:HD23	2.21	0.40
14:N:14:LEU:HD12	14:N:14:LEU:N	2.36	0.40
5:S:130:ARG:HG3	5:S:130:ARG:HH11	1.86	0.40
7:U:35:ILE:HD13	7:U:35:ILE:HA	1.79	0.40
7:U:139:VAL:HA	7:U:147:SER:O	2.21	0.40
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.35	0.40
3:C:29:GLU:OE2	3:C:32:LYS:HE2	2.22	0.40
3:C:241:GLN:O	3:C:243:GLN:N	2.50	0.40
4:D:236:GLU:O	4:D:240:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.56	0.40
9:I:28:SER:HB2	10:J:120:VAL:HG21	2.03	0.40
11:K:70:GLU:O	11:K:71:LYS:C	2.64	0.40
14:N:44:CYS:HB2	14:N:100:ILE:HB	2.03	0.40
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.56	0.40
1:O:32:LYS:HE2	1:O:32:LYS:CA	2.51	0.40
2:P:209:ARG:HG2	2:P:209:ARG:HH11	1.86	0.40
3:Q:206:GLY:HA2	3:Q:209:ASN:HD22	1.86	0.40
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.52	0.40
6:T:49:ALA:HA	6:T:211:GLU:O	2.21	0.40
6:T:121:GLN:HE21	6:T:121:GLN:HB3	1.64	0.40
7:U:107:MET:CE	7:U:112:LEU:HD13	2.49	0.40
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.51	0.40
9:W:88:TYR:CE1	9:W:91:ARG:HD3	2.56	0.40
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.89	0.40
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.87	0.40
14:2:18(G):TYR:CD1	14:2:18(G):TYR:C	3.00	0.40
1:A:52:LYS:HG3	1:A:211:GLU:HB2	2.04	0.40
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.78	0.40
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.72	0.40
5:E:2(C):VAL:HG22	5:E:226:GLY:C	2.47	0.40
6:F:20(B):GLU:HG3	6:F:20(C):LYS:H	1.86	0.40
7:G:131:PRO:HB3	16:G:244:HOH:O	2.20	0.40
8:H:62:ASN:ND2	16:H:227:HOH:O	2.50	0.40
1:O:195:LEU:HD23	1:O:236:LEU:HD21	2.03	0.40
5:S:76:LEU:HA	5:S:137:LEU:O	2.21	0.40
7:U:171:GLU:OE1	7:U:171:GLU:N	2.54	0.40
9:W:15:ALA:HB1	9:W:159:LEU:HD22	2.04	0.40
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.56	0.40
11:Y:9:GLN:CD	11:Y:9:GLN:C	2.90	0.40
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.21	0.40
12:Z:-5:TYR:CE2	12:Z:96:TYR:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	235 (95%)	10 (4%)	3 (1%)	10	34
1	O	248/250 (99%)	236 (95%)	9 (4%)	3 (1%)	10	34
2	B	242/244 (99%)	219 (90%)	18 (7%)	5 (2%)	5	20
2	P	242/244 (99%)	219 (90%)	17 (7%)	6 (2%)	4	16
3	C	239/241 (99%)	220 (92%)	16 (7%)	3 (1%)	9	31
3	Q	239/241 (99%)	219 (92%)	17 (7%)	3 (1%)	9	31
4	D	240/242 (99%)	225 (94%)	10 (4%)	5 (2%)	5	20
4	R	240/242 (99%)	224 (93%)	11 (5%)	5 (2%)	5	20
5	E	231/233 (99%)	211 (91%)	13 (6%)	7 (3%)	3	12
5	S	231/233 (99%)	210 (91%)	14 (6%)	7 (3%)	3	12
6	F	242/244 (99%)	226 (93%)	15 (6%)	1 (0%)	30	60
6	T	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	16	44
7	G	241/243 (99%)	226 (94%)	13 (5%)	2 (1%)	16	44
7	U	241/243 (99%)	225 (93%)	13 (5%)	3 (1%)	10	34
8	H	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
8	V	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
9	I	202/204 (99%)	194 (96%)	7 (4%)	1 (0%)	24	55
9	W	202/204 (99%)	194 (96%)	7 (4%)	1 (0%)	24	55
10	J	196/198 (99%)	185 (94%)	10 (5%)	1 (0%)	24	55
10	X	196/198 (99%)	185 (94%)	10 (5%)	1 (0%)	24	55
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
12	Z	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	24	55
13	1	231/233 (99%)	216 (94%)	13 (6%)	2 (1%)	14	41
13	M	231/233 (99%)	215 (93%)	14 (6%)	2 (1%)	14	41
14	2	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6312/6368 (99%)	5929 (94%)	319 (5%)	64 (1%)	12	38

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20(A)	SER
3	C	58	LEU
4	D	12(G)	GLU
3	Q	58	LEU
4	R	12(G)	GLU
1	A	5	THR
1	A	53	LYS
1	A	167	LYS
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
4	D	18(D)	SER
5	E	5	ARG
5	E	202	ARG
10	J	192	ALA
13	M	96	TRP
1	O	5	THR
1	O	53	LYS
1	O	167	LYS
2	P	54	VAL
2	P	20(A)	SER
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	18(D)	SER
5	S	5	ARG
5	S	202	ARG
10	X	192	ALA
5	E	203	ASP
5	E	231	LYS
6	F	64	ASN
5	S	203	ASP
5	S	231	LYS
6	T	64	ASN
7	U	184	ASN
13	1	96	TRP
2	B	184	MET
4	D	12(F)	GLY
4	D	128	MET

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Mol	Chain	Res	Type
5	E	180	LEU
5	E	217	LYS
9	I	93	GLY
4	R	12(F)	GLY
4	R	128	MET
5	S	180	LEU
5	S	217	LYS
9	W	93	GLY
7	G	184	ASN
7	G	239	GLN
13	M	72	ALA
7	U	239	GLN
13	1	72	ALA
2	P	6	ARG
2	P	184	MET
6	T	206	LYS
12	Z	93	PHE
5	E	18(F)	ILE
5	S	18(F)	ILE
4	D	12(C)	GLY
4	R	12(C)	GLY
7	U	61	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	202 (97%)	7 (3%)	33	69
1	O	209/209 (100%)	201 (96%)	8 (4%)	29	64
2	B	203/203 (100%)	190 (94%)	13 (6%)	16	44
2	P	203/203 (100%)	190 (94%)	13 (6%)	16	44
3	C	213/213 (100%)	204 (96%)	9 (4%)	26	61
3	Q	213/213 (100%)	204 (96%)	9 (4%)	26	61
4	D	198/198 (100%)	184 (93%)	14 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	198/198 (100%)	184 (93%)	14 (7%)	13	39
5	E	192/192 (100%)	180 (94%)	12 (6%)	16	45
5	S	192/192 (100%)	180 (94%)	12 (6%)	16	45
6	F	201/201 (100%)	182 (90%)	19 (10%)	8	26
6	T	201/201 (100%)	183 (91%)	18 (9%)	9	28
7	G	207/207 (100%)	197 (95%)	10 (5%)	23	56
7	U	207/207 (100%)	196 (95%)	11 (5%)	20	52
8	H	181/181 (100%)	176 (97%)	5 (3%)	38	73
8	V	181/181 (100%)	176 (97%)	5 (3%)	38	73
9	I	172/172 (100%)	168 (98%)	4 (2%)	44	78
9	W	172/172 (100%)	168 (98%)	4 (2%)	44	78
10	J	175/175 (100%)	166 (95%)	9 (5%)	21	54
10	X	175/175 (100%)	166 (95%)	9 (5%)	21	54
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	52
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	57
12	L	185/185 (100%)	161 (87%)	24 (13%)	4	14
12	Z	185/185 (100%)	162 (88%)	23 (12%)	4	16
13	1	199/199 (100%)	187 (94%)	12 (6%)	17	47
13	M	199/199 (100%)	187 (94%)	12 (6%)	17	47
14	2	162/162 (100%)	157 (97%)	5 (3%)	35	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	35	70
All	All	5332/5332 (100%)	5029 (94%)	303 (6%)	18	49

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	62	GLU
1	A	64	LEU
1	A	87	VAL
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
2	B	14	ILE
2	B	41	MET

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Mol	Chain	Res	Type
2	B	46	ILE
2	B	58	LEU
2	B	67	LEU
2	B	89	ILE
2	B	121	GLN
2	B	124	THR
2	B	135	SER
2	B	14(A)	TYR
2	B	150	THR
2	B	158	THR
2	B	192	LEU
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	61	THR
3	C	135	SER
3	C	150	GLN
3	C	163	GLN
3	C	174	GLU
3	C	210	ILE
4	D	28	LEU
4	D	48	LEU
4	D	52	LYS
4	D	72	ARG
4	D	107	ILE
4	D	110	GLU
4	D	126	ARG
4	D	156	THR
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	149	LEU
5	E	189	LEU
5	E	199	GLN

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Mol	Chain	Res	Type
5	E	207	LEU
5	E	223	ILE
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	18	ASP
6	F	35	THR
6	F	43	ASN
6	F	72	ARG
6	F	95	GLU
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	169	ARG
6	F	176	LEU
6	F	18(A)	ASP
6	F	18(B)	HIS
6	F	18(C)	HIS
6	F	18(D)	PRO
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
7	G	12	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	122	ILE
7	G	124	THR
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	121	VAL
8	H	197	ARG
9	I	29	ASN
9	I	113	PHE
9	I	155	ILE
9	I	160	LEU

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Mol	Chain	Res	Type
10	J	24	ILE
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	121	GLU
10	J	155	LEU
10	J	166	MET
10	J	168	MET
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	99	THR
11	K	100	MET
11	K	146	LEU
12	L	3	ILE
12	L	14	LEU
12	L	21	ILE
12	L	40	ASN
12	L	58	ARG
12	L	61	ASN
12	L	98	HIS
12	L	99	THR
12	L	106	GLU
12	L	138	LEU
12	L	14(A)	LYS
12	L	14(B)	ASN
12	L	14(C)	GLN
12	L	14(D)	TYR
12	L	14(E)	GLU
12	L	14(F)	PRO
12	L	14(I)	THR
12	L	14(K)	LYS
12	L	14(M)	VAL
12	L	14(N)	LYS
12	L	14(O)	LYS
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS

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Mol	Chain	Res	Type
13	M	4	ILE
13	M	40	ASN
13	M	55	ILE
13	M	62	LEU
13	M	65	GLU
13	M	91	ARG
13	M	129	PHE
13	M	148	VAL
13	M	149	GLN
13	M	184	LEU
13	M	191	GLN
13	M	211	ILE
14	N	89	GLU
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU
14	N	178	LEU
1	O	32	LYS
1	O	62	GLU
1	O	64	LEU
1	O	87	VAL
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
1	O	229	ILE
2	P	14	ILE
2	P	41	MET
2	P	46	ILE
2	P	58	LEU
2	P	67	LEU
2	P	89	ILE
2	P	121	GLN
2	P	124	THR
2	P	135	SER
2	P	14(A)	TYR
2	P	150	THR
2	P	158	THR
2	P	192	LEU
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	61	THR

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Mol	Chain	Res	Type
3	Q	135	SER
3	Q	150	GLN
3	Q	163	GLN
3	Q	174	GLU
3	Q	210	ILE
4	R	28	LEU
4	R	48	LEU
4	R	52	LYS
4	R	72	ARG
4	R	107	ILE
4	R	110	GLU
4	R	126	ARG
4	R	156	THR
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	12	THR
5	S	13	VAL
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	149	LEU
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	223	ILE
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	18	ASP
6	T	35	THR
6	T	43	ASN
6	T	72	ARG
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	169	ARG
6	T	176	LEU

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Mol	Chain	Res	Type
6	T	18(A)	ASP
6	T	18(B)	HIS
6	T	18(C)	HIS
6	T	18(D)	PRO
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
7	U	12	ILE
7	U	48	VAL
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	122	ILE
7	U	124	THR
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	121	VAL
8	V	197	ARG
9	W	29	ASN
9	W	113	PHE
9	W	155	ILE
9	W	160	LEU
10	X	24	ILE
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	121	GLU
10	X	155	LEU
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	87	VAL
11	Y	99	THR

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Mol	Chain	Res	Type
11	Y	100	MET
11	Y	146	LEU
12	Z	3	ILE
12	Z	14	LEU
12	Z	40	ASN
12	Z	58	ARG
12	Z	61	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	106	GLU
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
13	1	4	ILE
13	1	40	ASN
13	1	55	ILE
13	1	62	LEU
13	1	65	GLU
13	1	91	ARG
13	1	129	PHE
13	1	148	VAL
13	1	149	GLN
13	1	184	LEU
13	1	191	GLN
13	1	211	ILE
14	2	89	GLU
14	2	115	LEU
14	2	119	VAL
14	2	149	GLU
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (254) 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
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	120	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	99	HIS
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	20(A)	ASN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	73	HIS
5	E	94	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

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Mol	Chain	Res	Type
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
6	F	221	HIS
6	F	237	GLN
7	G	11	HIS
7	G	32	ASN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	10	ASN
8	H	30	ASN
8	H	35	HIS
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	201	GLN
9	I	29	ASN
9	I	56	ASN
9	I	81	GLN
9	I	157	GLN
9	I	193	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	64	GLN
10	J	77	GLN
10	J	85	GLN

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Mol	Chain	Res	Type
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	160	GLN
10	J	186	GLN
11	K	9	GLN
11	K	24	ASN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	27	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	98	HIS
12	L	123	GLN
12	L	140	ASN
12	L	141	GLN
12	L	14(B)	ASN
12	L	1(I)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	132	HIS
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	189	ASN
13	M	191	GLN
14	N	69	GLN
14	N	145	ASN
14	N	157	HIS

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Mol	Chain	Res	Type
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	121	GLN
1	O	125	GLN
1	O	150	GLN
2	P	23	GLN
2	P	33	HIS
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	120	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	20(A)	ASN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	73	HIS
5	S	94	GLN
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	152	GLN
5	S	156	ASN

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Mol	Chain	Res	Type
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
6	T	202	HIS
6	T	221	HIS
6	T	237	GLN
7	U	11	HIS
7	U	32	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	35	HIS
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	201	GLN
9	W	29	ASN
9	W	56	ASN
9	W	64	ASN
9	W	81	GLN
9	W	157	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN

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Mol	Chain	Res	Type
10	X	64	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	160	GLN
10	X	186	GLN
11	Y	9	GLN
11	Y	24	ASN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	27	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	123	GLN
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	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	132	HIS
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	189	ASN
13	1	191	GLN
14	2	69	GLN
14	2	141	ASN

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Mol	Chain	Res	Type
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	SA1	Y	0	11	18,22,22	1.32	2 (11%)	24,34,34	1.98	4 (16%)
15	SA1	H	0	8	18,22,22	1.49	1 (5%)	24,34,34	1.93	4 (16%)
15	SA1	N	0	14	18,22,22	1.27	2 (11%)	24,34,34	2.10	5 (20%)
15	SA1	2	0	14	18,22,22	1.48	3 (16%)	24,34,34	2.04	5 (20%)
15	SA1	V	0	8	18,22,22	1.49	3 (16%)	24,34,34	2.12	3 (12%)
15	SA1	K	0	11	18,22,22	1.40	3 (16%)	24,34,34	1.92	5 (20%)

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	SA1	Y	0	11	-	0/4/52/52	0/3/3/3
15	SA1	H	0	8	-	0/4/52/52	0/3/3/3
15	SA1	N	0	14	-	0/4/52/52	0/3/3/3
15	SA1	2	0	14	-	0/4/52/52	0/3/3/3
15	SA1	V	0	8	-	0/4/52/52	0/3/3/3
15	SA1	K	0	11	-	0/4/52/52	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	0	SA1	C4-C3	3.93	1.58	1.51
15	V	0	SA1	C4-C3	3.87	1.58	1.51
15	H	0	SA1	C4-C3	3.87	1.58	1.51
15	N	0	SA1	C4-C3	3.20	1.57	1.51
15	V	0	SA1	O17-C10	3.13	1.48	1.42
15	Y	0	SA1	C4-C3	3.00	1.56	1.51
15	K	0	SA1	O2-C3	2.86	1.48	1.45
15	K	0	SA1	C4-C3	2.81	1.56	1.51
15	N	0	SA1	O2-C3	2.51	1.47	1.45
15	2	0	SA1	O2-C3	2.29	1.47	1.45
15	2	0	SA1	O17-C10	2.18	1.47	1.42
15	V	0	SA1	C12-C13	2.18	1.37	1.32
15	Y	0	SA1	O17-C10	2.06	1.46	1.42
15	K	0	SA1	C6-N8	2.06	1.36	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	0	SA1	C9-C10-C11	7.31	123.27	114.09
15	N	0	SA1	C9-C10-C11	6.69	122.49	114.09
15	K	0	SA1	C9-C10-C11	6.64	122.43	114.09
15	H	0	SA1	C9-C10-C11	6.55	122.32	114.09
15	2	0	SA1	C9-C10-C11	6.54	122.30	114.09
15	Y	0	SA1	C9-C10-C11	6.41	122.14	114.09
15	V	0	SA1	C3-C5-C6	-5.31	99.97	104.28
15	N	0	SA1	C3-C5-C6	-5.29	99.99	104.28
15	2	0	SA1	C3-C5-C6	-5.10	100.15	104.28
15	Y	0	SA1	C3-C5-C6	-4.42	100.70	104.28
15	H	0	SA1	C3-C5-C6	-4.23	100.85	104.28
15	Y	0	SA1	O2-C3-C5	-4.03	97.26	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	0	SA1	O2-C3-C5	-3.69	97.73	102.81
15	K	0	SA1	C3-C5-C6	-3.67	101.31	104.28
15	V	0	SA1	O2-C3-C5	-3.62	97.83	102.81
15	2	0	SA1	O2-C3-C5	-3.54	97.94	102.81
15	N	0	SA1	O2-C3-C5	-3.52	97.97	102.81
15	K	0	SA1	O2-C3-C5	-3.48	98.02	102.81
15	Y	0	SA1	O2-C3-C4	2.57	111.92	107.73
15	2	0	SA1	O2-C3-C4	2.50	111.81	107.73
15	N	0	SA1	O7-C6-C5	-2.41	123.58	126.15
15	K	0	SA1	O2-C3-C4	2.34	111.55	107.73
15	2	0	SA1	O7-C6-C5	-2.21	123.79	126.15
15	K	0	SA1	O7-C6-C5	-2.20	123.81	126.15
15	N	0	SA1	O2-C3-C4	2.17	111.27	107.73
15	H	0	SA1	O2-C3-C4	2.14	111.23	107.73

There are no chirality outliers.

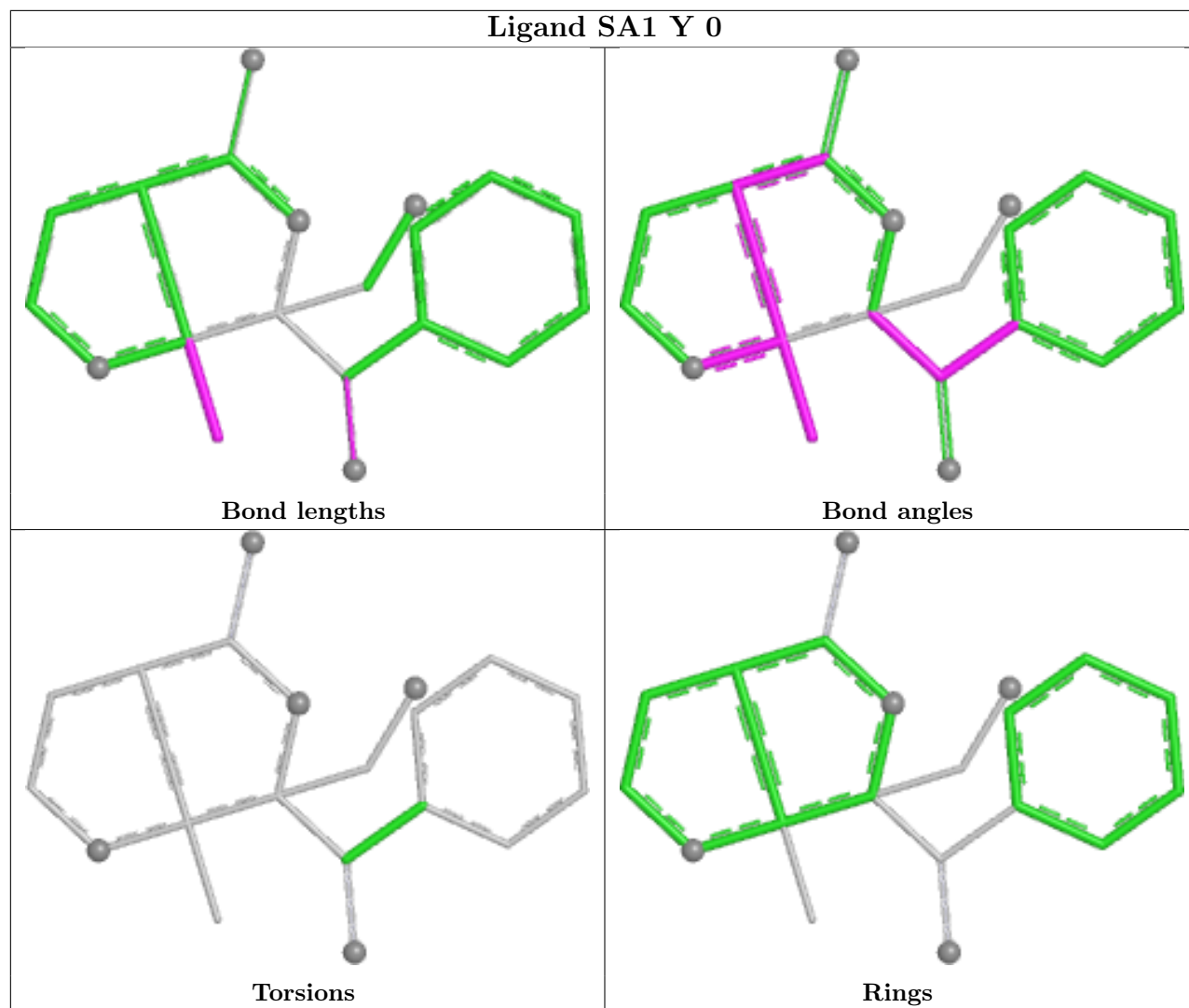
There are no torsion outliers.

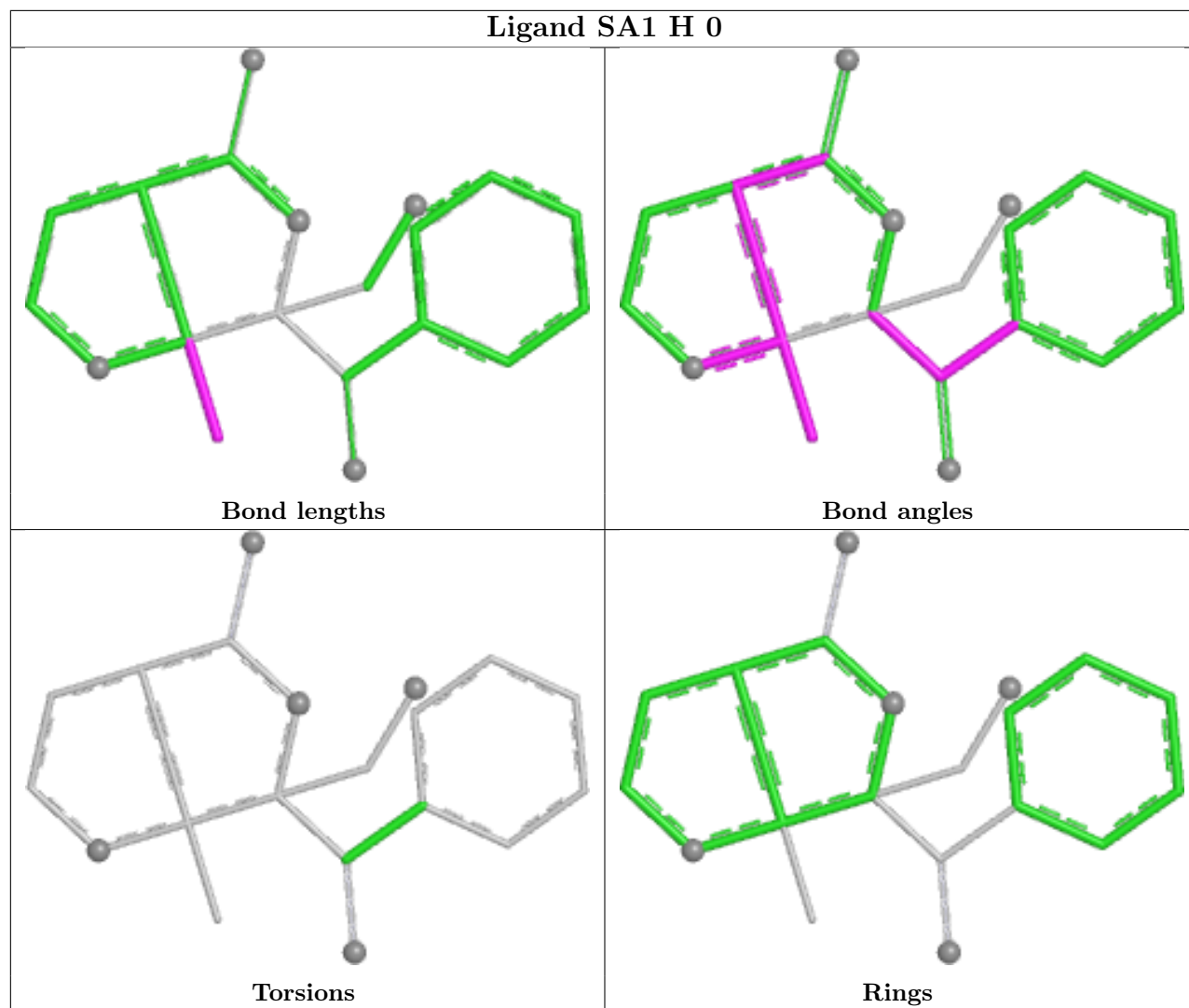
There are no ring outliers.

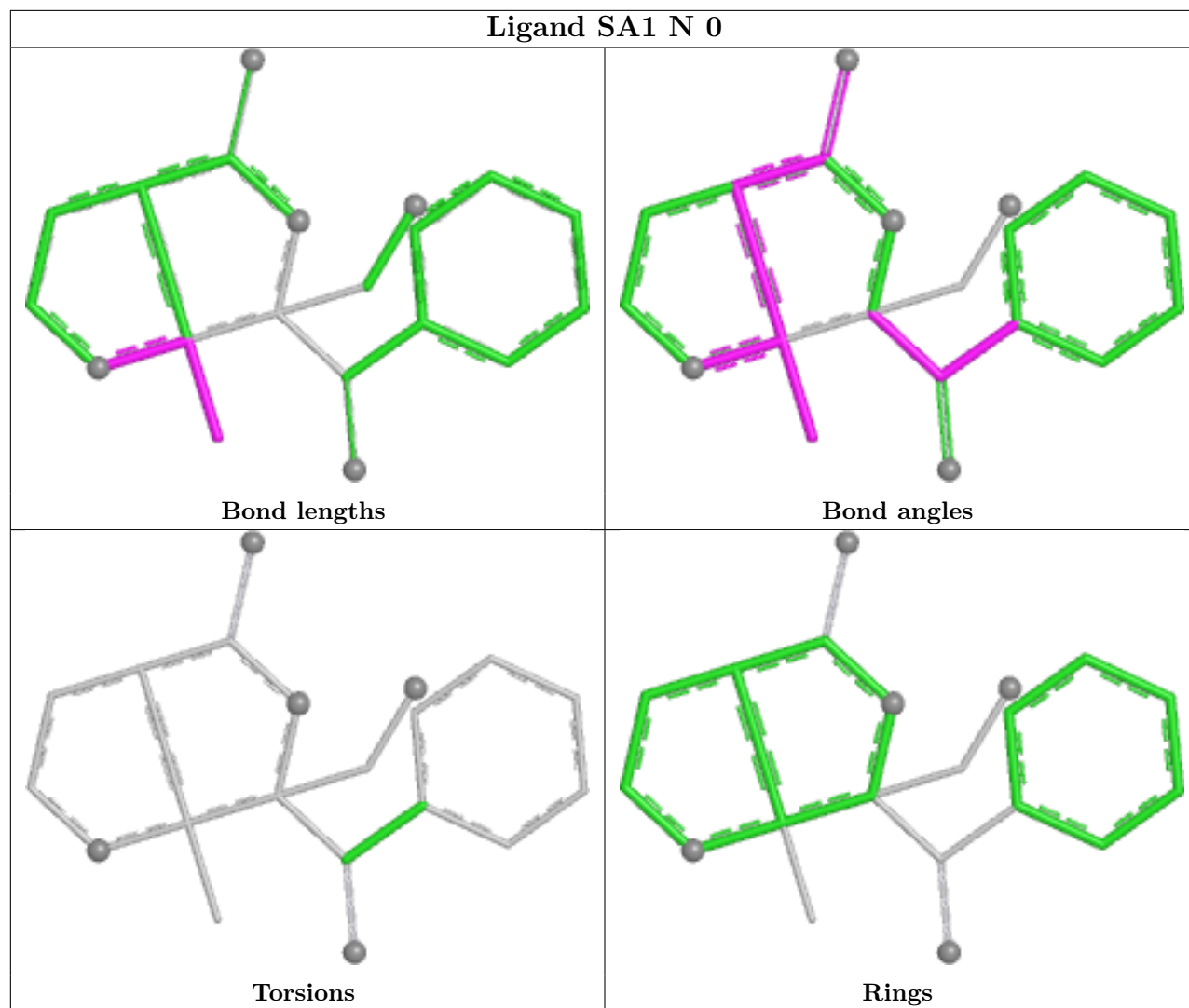
2 monomers are involved in 2 short contacts:

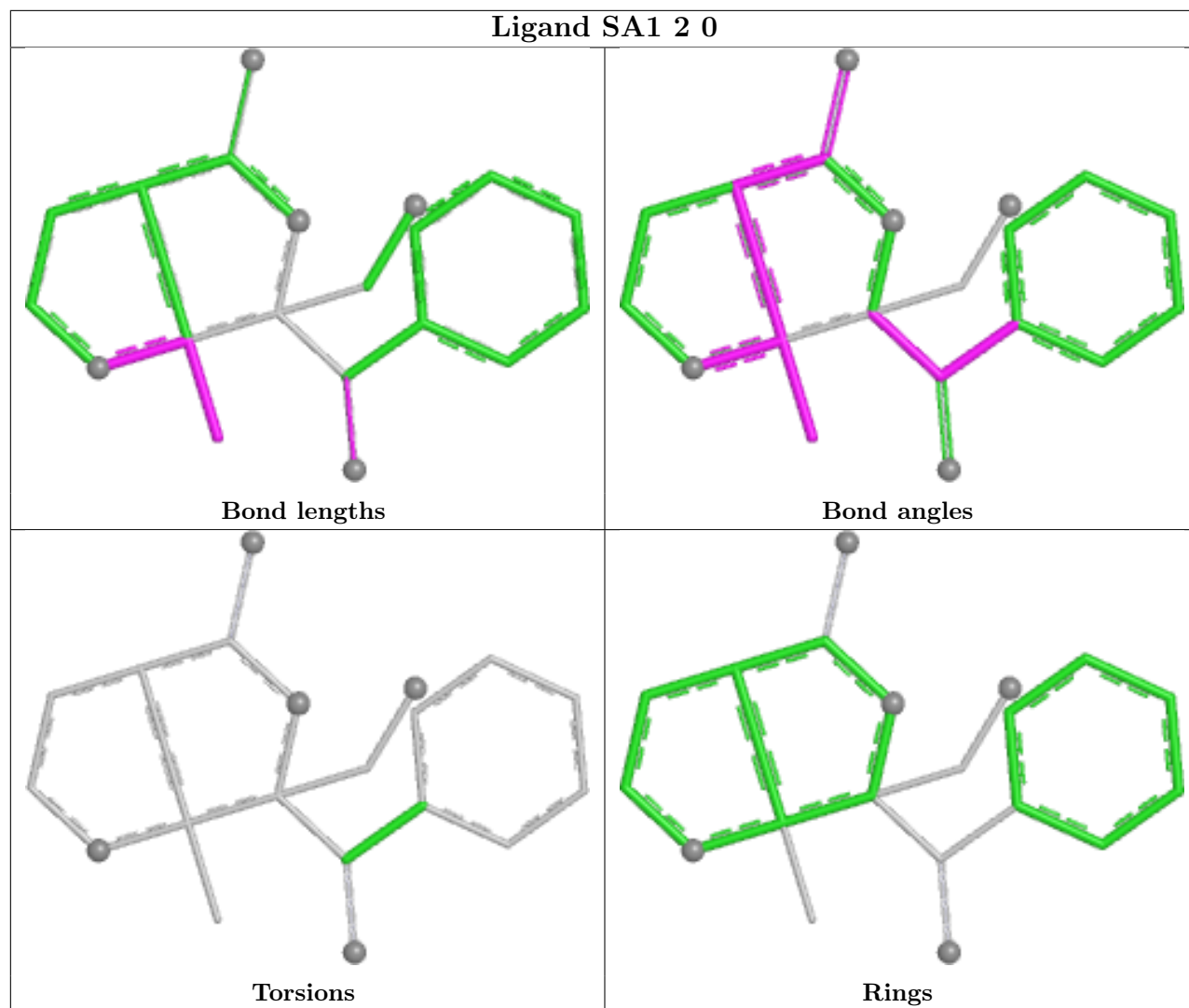
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Y	0	SA1	1	0
15	K	0	SA1	1	0

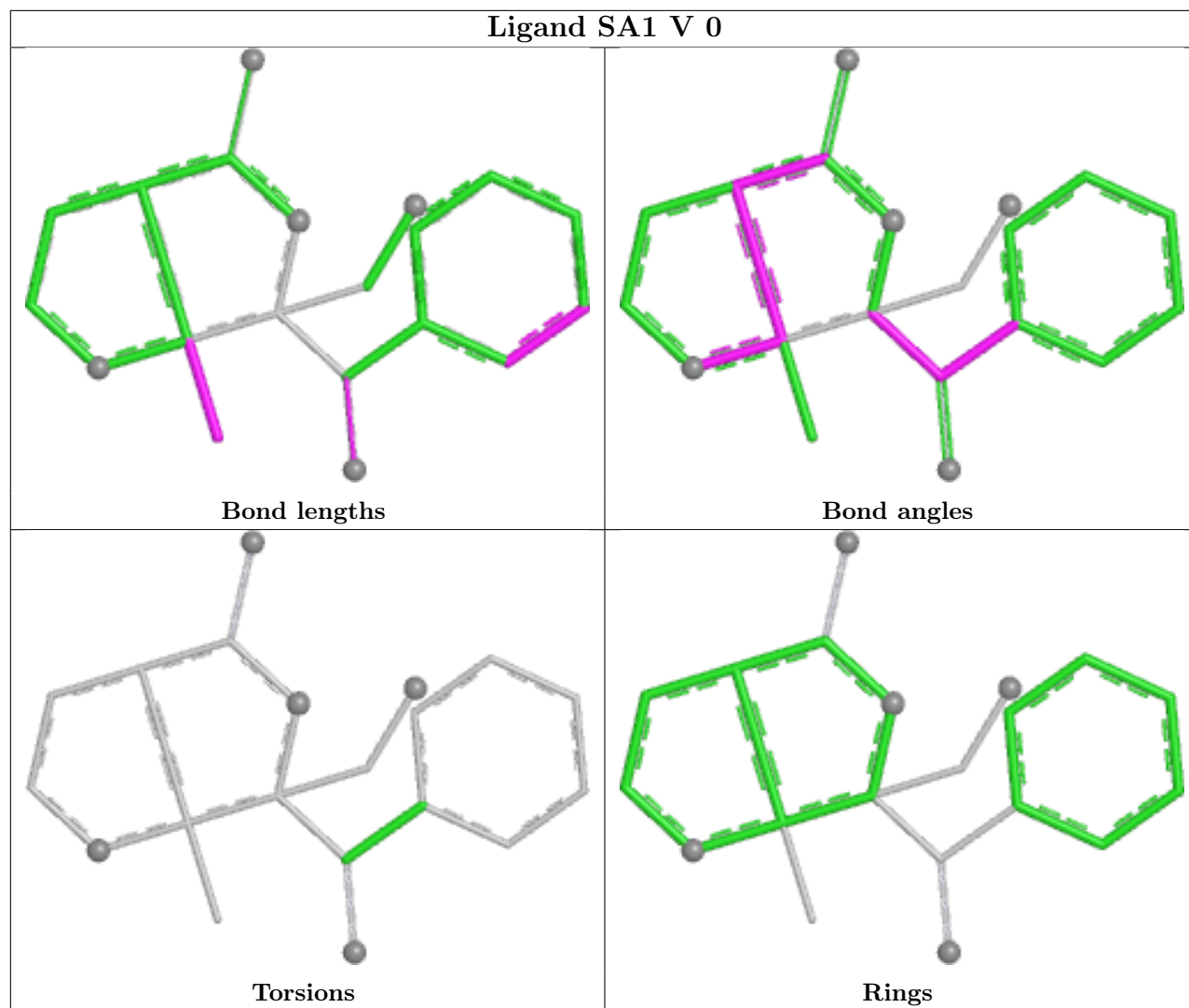
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

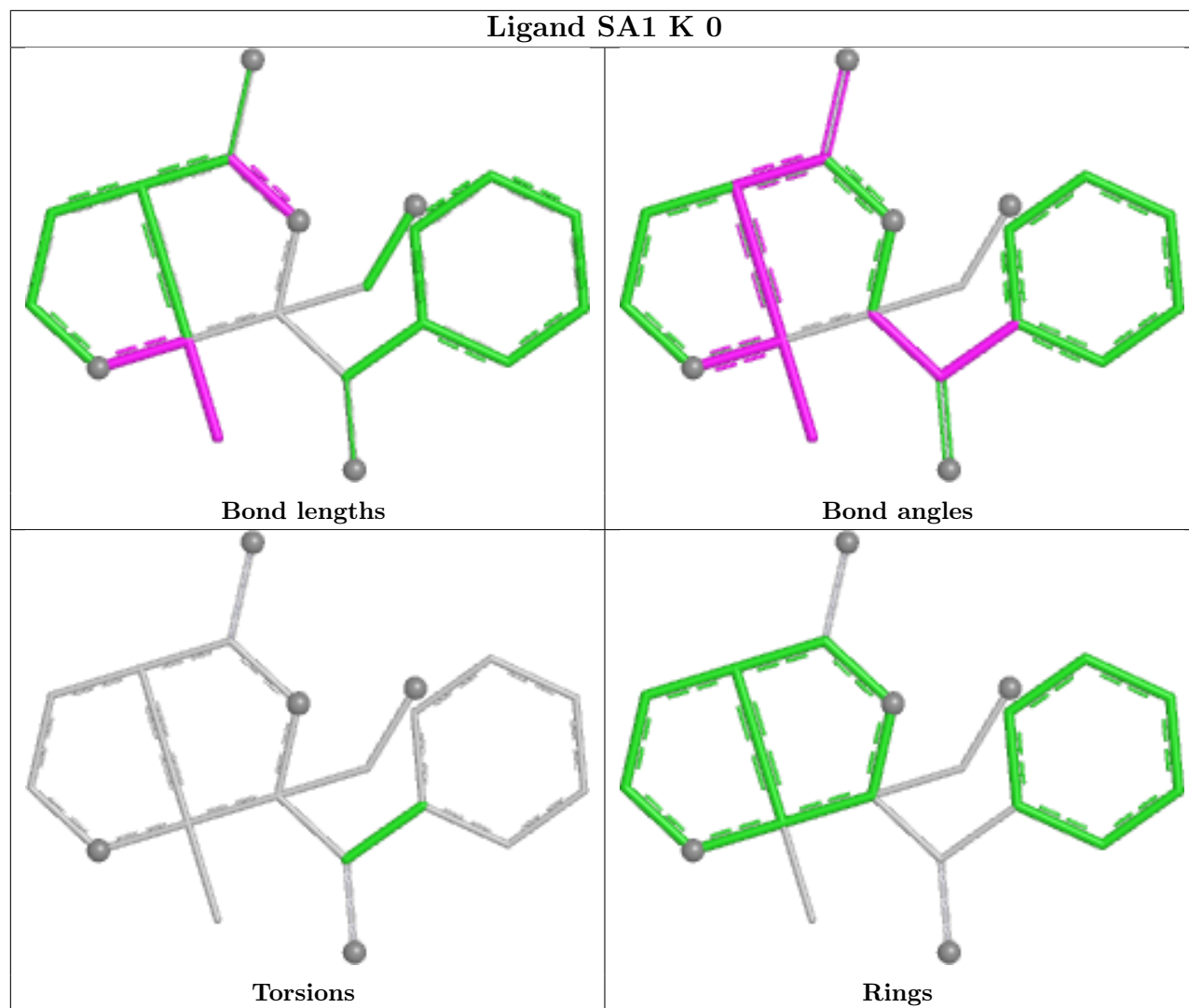












5.7 Other polymers [i](#)

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 i

6.1 Protein, DNA and RNA chains i

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%)	0.02	3 (1%) 76 68	32, 45, 74, 99	0
1	O	250/250 (100%)	0.10	8 (3%) 50 40	35, 51, 80, 100	0
2	B	244/244 (100%)	0.33	15 (6%) 27 20	32, 50, 84, 116	0
2	P	244/244 (100%)	0.35	19 (7%) 19 14	34, 52, 87, 116	0
3	C	241/241 (100%)	0.38	19 (7%) 18 13	30, 54, 105, 122	0
3	Q	241/241 (100%)	0.57	21 (8%) 16 11	36, 59, 109, 121	0
4	D	242/242 (100%)	0.34	11 (4%) 38 30	32, 54, 88, 117	0
4	R	242/242 (100%)	0.46	13 (5%) 31 24	35, 57, 90, 120	0
5	E	233/233 (100%)	0.39	7 (3%) 52 42	39, 58, 82, 109	0
5	S	233/233 (100%)	0.80	28 (12%) 9 6	37, 62, 86, 107	0
6	F	244/244 (100%)	0.23	4 (1%) 70 61	33, 51, 85, 101	0
6	T	244/244 (100%)	0.34	11 (4%) 38 30	31, 53, 89, 102	0
7	G	243/243 (100%)	-0.02	7 (2%) 53 43	28, 44, 72, 106	0
7	U	243/243 (100%)	0.16	6 (2%) 58 48	28, 47, 73, 105	0
8	H	222/222 (100%)	-0.11	0 100 100	23, 41, 61, 91	0
8	V	222/222 (100%)	-0.08	1 (0%) 87 82	30, 44, 61, 89	0
9	I	204/204 (100%)	-0.17	1 (0%) 87 82	29, 42, 57, 75	0
9	W	204/204 (100%)	-0.25	1 (0%) 87 82	29, 41, 61, 78	0
10	J	198/198 (100%)	0.01	7 (3%) 47 38	26, 45, 62, 115	0
10	X	198/198 (100%)	-0.09	6 (3%) 52 42	30, 46, 62, 116	0
11	K	212/212 (100%)	-0.29	1 (0%) 87 82	26, 42, 61, 70	0
11	Y	212/212 (100%)	-0.09	1 (0%) 87 82	30, 44, 63, 73	0
12	L	222/222 (100%)	-0.11	2 (0%) 81 74	26, 44, 64, 85	0
12	Z	222/222 (100%)	-0.09	1 (0%) 87 82	27, 44, 67, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.20	2 (0%) 81 74	28, 43, 57, 64	0
13	M	233/233 (100%)	-0.11	4 (1%) 69 60	28, 44, 58, 66	0
14	2	196/196 (100%)	-0.14	2 (1%) 79 72	23, 41, 61, 74	0
14	N	196/196 (100%)	-0.24	0 100 100	25, 39, 61, 73	0
All	All	6368/6368 (100%)	0.10	201 (3%) 50 40	23, 47, 81, 122	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	56	LEU	8.5
7	U	240	ASP	7.7
7	U	6	ALA	7.0
3	C	56	LEU	6.8
4	D	12(D)	ALA	6.8
2	P	217	ALA	6.5
4	R	12(D)	ALA	6.2
2	B	217	ALA	6.0
2	B	21(B)	GLY	5.8
10	X	193	GLN	5.6
2	B	239	THR	5.6
3	C	55	THR	5.5
4	D	12(C)	GLY	5.3
4	R	12(E)	SER	5.2
7	G	6	ALA	5.0
4	D	12(E)	SER	4.8
2	P	21(B)	GLY	4.8
3	Q	58	LEU	4.8
5	S	2(E)	ASN	4.6
4	R	19	GLY	4.5
3	C	59	GLN	4.5
5	E	4	PHE	4.5
10	J	193	GLN	4.4
3	C	54	SER	4.3
4	R	12(C)	GLY	4.1
3	Q	55	THR	4.1
4	D	126	ARG	4.1
10	J	192	ALA	4.1
6	F	204	ASP	4.1
5	S	59	SER	4.1
4	R	126	ARG	4.1
5	S	63	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	207	ALA	4.0
5	S	55	ALA	4.0
6	F	5	GLY	4.0
1	O	64	LEU	3.9
5	S	56	ASP	3.8
5	S	4	PHE	3.8
10	J	191	GLN	3.8
2	P	21(C)	ASP	3.8
1	O	4	MET	3.7
3	Q	54	SER	3.6
10	X	192	ALA	3.6
2	B	21(C)	ASP	3.6
2	B	54	VAL	3.6
3	Q	240	LYS	3.6
13	1	-8	THR	3.5
12	L	145	TYR	3.5
11	Y	145	ASP	3.5
5	S	54	ASN	3.5
13	M	-8	THR	3.5
5	S	60	SER	3.5
6	T	203	GLU	3.4
4	R	12(F)	GLY	3.4
5	S	5	ARG	3.4
2	P	21(A)	LYS	3.4
2	P	218	ASN	3.3
5	S	230	ALA	3.3
2	P	62	ASP	3.3
2	P	4	GLY	3.2
12	Z	145	TYR	3.2
4	D	242	ALA	3.2
4	D	127	LEU	3.1
5	S	51	LEU	3.1
9	W	-8	SER	3.1
3	Q	63	THR	3.1
2	B	218	ASN	3.1
2	B	219	GLU	3.1
2	P	219	GLU	3.1
2	P	239	THR	3.1
7	G	236	ILE	3.0
3	Q	57	LYS	3.0
2	B	21(D)	GLY	3.0
7	U	239	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
9	I	-8	SER	3.0
5	S	233	ILE	3.0
3	C	242	GLU	3.0
5	S	58	LEU	2.9
4	R	121	LEU	2.9
5	E	127	TYR	2.9
3	C	57	LYS	2.8
5	S	18(C)	PHE	2.8
7	G	240	ASP	2.8
5	S	18(B)	THR	2.8
3	Q	208	LYS	2.8
6	T	241	ASN	2.8
3	Q	243	GLN	2.8
3	Q	203	THR	2.8
2	B	238	ILE	2.8
2	P	21(D)	GLY	2.8
3	Q	64	PRO	2.8
5	E	203	ASP	2.7
3	C	52	ARG	2.7
5	S	204	GLU	2.7
2	P	54	VAL	2.7
3	C	241	GLN	2.7
5	S	188	GLU	2.7
5	S	127	TYR	2.7
2	B	21(A)	LYS	2.7
2	P	181	LYS	2.7
14	2	107	LYS	2.7
4	R	158	TYR	2.7
5	E	56	ASP	2.7
3	C	239	GLU	2.7
1	O	65	SER	2.7
5	S	52	LYS	2.6
1	O	56	SER	2.6
2	B	4	GLY	2.6
6	T	20(C)	LYS	2.6
3	C	211	GLU	2.6
1	O	5	THR	2.6
3	Q	237	GLU	2.6
5	S	203	ASP	2.6
4	D	168	GLY	2.6
4	R	12(B)	GLU	2.6
5	S	2(C)	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
10	J	-1	MET	2.5
13	M	39	ASP	2.5
1	O	57	PRO	2.5
3	Q	236	ILE	2.5
10	X	-1	MET	2.5
3	Q	241	GLN	2.5
3	C	208	LYS	2.5
4	R	127	LEU	2.5
3	Q	238	GLN	2.5
10	J	190	PHE	2.5
3	C	240	LYS	2.5
1	O	236	LEU	2.4
5	S	18(F)	ILE	2.4
4	R	35	SER	2.4
2	P	220	TYR	2.4
3	C	243	GLN	2.4
6	T	18(B)	HIS	2.4
5	S	197	ILE	2.4
7	U	238	GLU	2.4
3	Q	202	GLN	2.4
6	T	55	THR	2.4
2	B	185	LYS	2.4
4	D	120	ALA	2.4
2	P	202	THR	2.4
3	Q	44	ASN	2.4
10	X	10	ASP	2.4
3	C	237	GLU	2.4
4	D	12(G)	GLU	2.4
14	2	149	GLU	2.4
10	X	191	GLN	2.4
4	D	12(A)	GLY	2.3
6	T	215	CYS	2.3
8	V	223	ASP	2.3
5	E	63	TYR	2.3
5	S	2(B)	THR	2.3
11	K	208	ASN	2.3
3	C	188	GLU	2.3
3	C	203	THR	2.3
2	B	61	GLN	2.3
3	C	63	THR	2.3
2	B	60	GLU	2.3
5	S	174	THR	2.3

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Mol	Chain	Res	Type	RSRZ
10	J	50	GLY	2.3
6	T	43	ASN	2.2
6	T	170	GLN	2.2
1	A	5	THR	2.2
7	G	7	GLY	2.2
3	Q	207	ALA	2.2
3	Q	235	GLN	2.2
3	Q	189	CYS	2.2
5	S	171	GLY	2.2
13	M	61	ASP	2.2
1	A	4	MET	2.2
4	D	169	SER	2.2
7	U	7	GLY	2.2
10	J	149	GLU	2.2
2	P	71	ASN	2.2
13	M	-7	GLN	2.2
7	G	199	ASP	2.2
1	O	55	SER	2.2
2	P	56	SER	2.2
7	G	171	GLU	2.2
5	E	18(F)	ILE	2.1
5	E	33	GLN	2.1
4	R	12(G)	GLU	2.1
7	G	18(H)	GLU	2.1
3	Q	210	ILE	2.1
6	T	205	ASN	2.1
10	X	168	MET	2.1
2	P	203	ASP	2.1
3	C	174	GLU	2.1
12	L	14(P)	PRO	2.1
2	P	20(A)	SER	2.1
5	S	212	ILE	2.1
4	R	244	GLU	2.1
6	T	184	LEU	2.0
5	S	53	ARG	2.0
2	B	202	THR	2.0
13	1	211	ILE	2.0
7	U	29	LYS	2.0
2	P	59	LEU	2.0
6	F	205	ASN	2.0
6	F	18(F)	GLY	2.0
1	A	203	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
6	T	20(B)	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

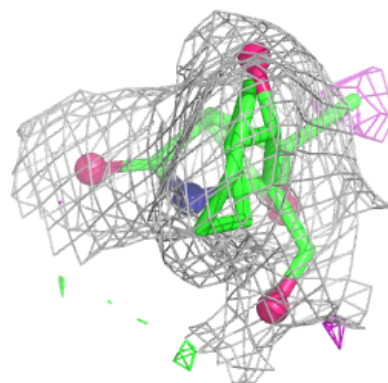
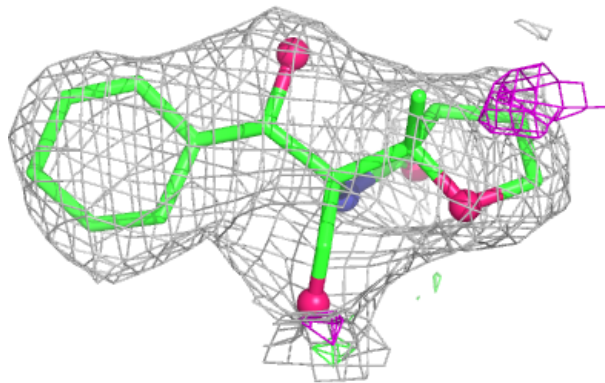
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	SA1	H	0	20/20	0.92	0.10	37,40,42,44	0
15	SA1	2	0	20/20	0.92	0.10	28,33,36,38	0
15	SA1	Y	0	20/20	0.93	0.10	34,36,38,39	0
15	SA1	K	0	20/20	0.93	0.10	26,33,37,37	0
15	SA1	N	0	20/20	0.94	0.10	22,34,37,38	0
15	SA1	V	0	20/20	0.95	0.08	35,39,42,42	0

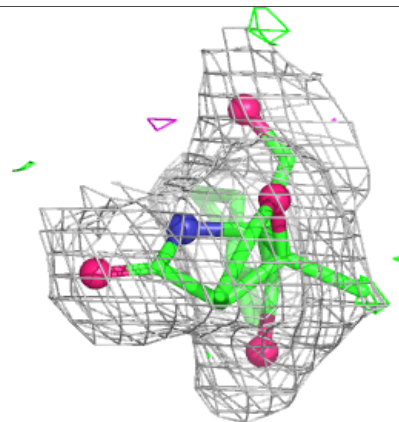
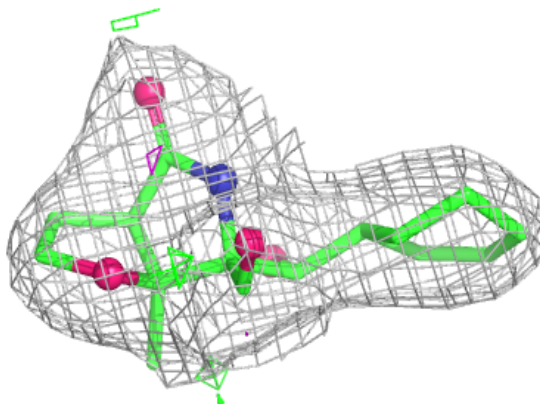
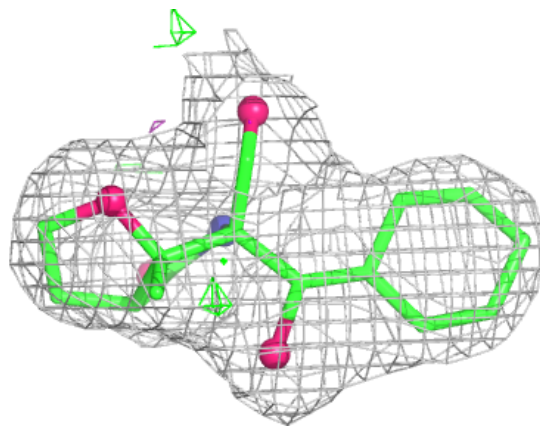
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SA1 H 0:

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

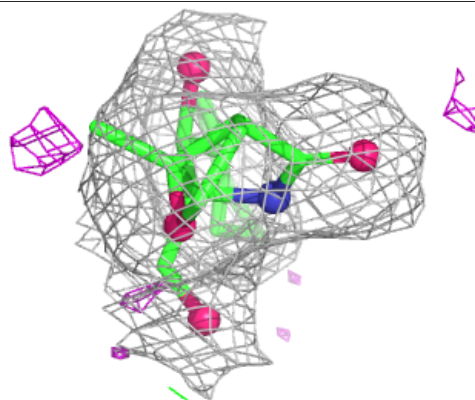
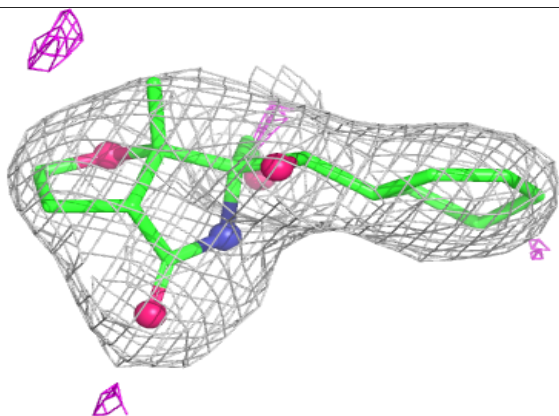
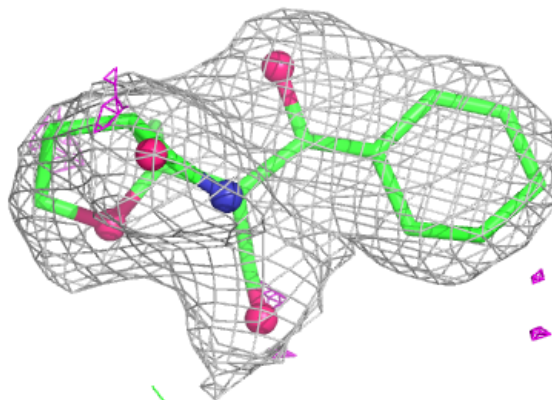
**Electron density around SA1 2 0:**

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



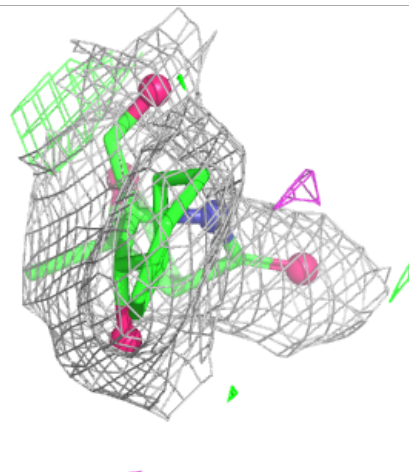
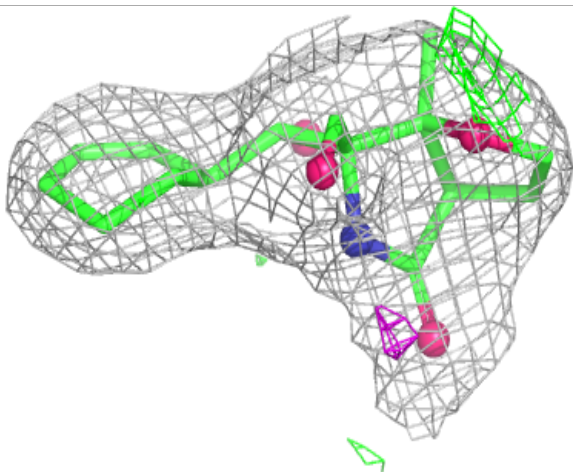
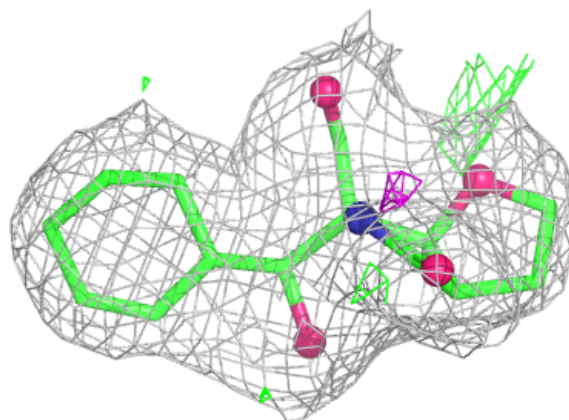
Electron density around SA1 Y 0:

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



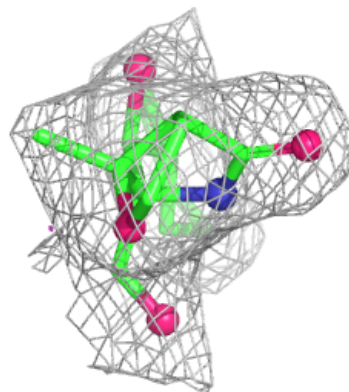
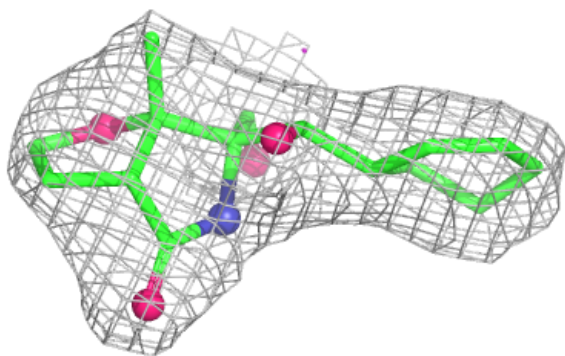
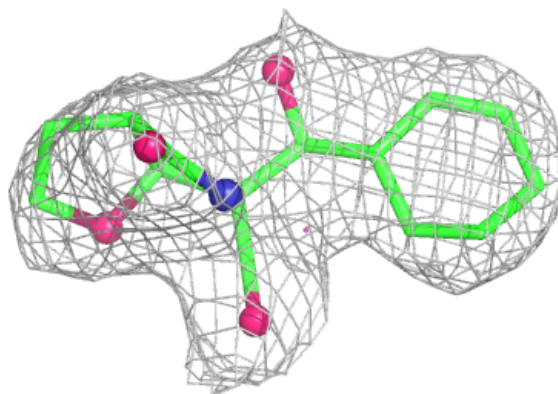
Electron density around SA1 K 0:

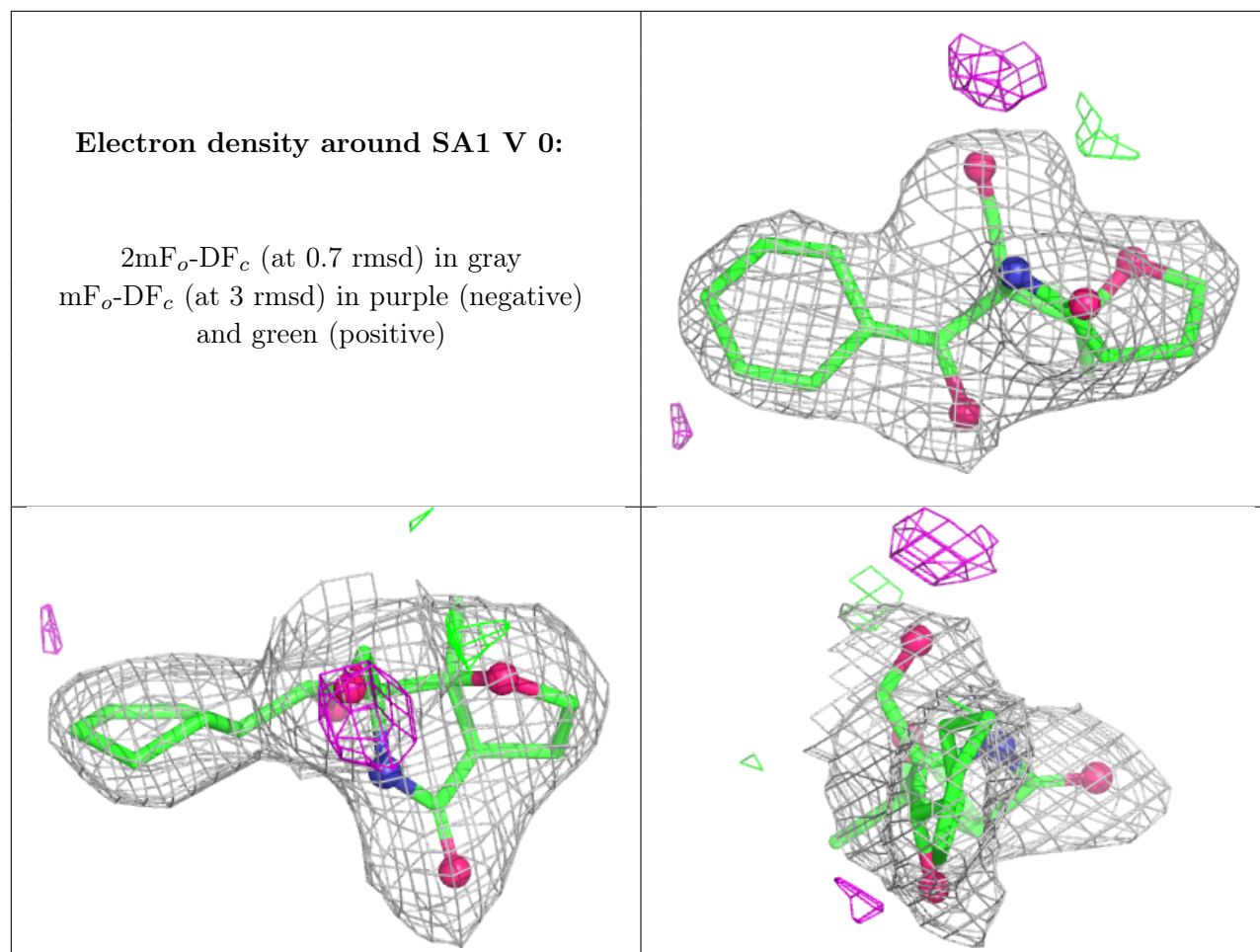
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SA1 N 0:

$2mF_o-DF_c$ (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.