



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 PM UTC

PDB ID : 1FPY / pdb_00001fpy
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM
SALMONELLA TYPHIMURIUM WITH INHIBITOR PHOS-
PHINOTHRICIN
Authors : Gill, H.S.; Eisenberg, D.
Deposited on : 2000-08-31
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

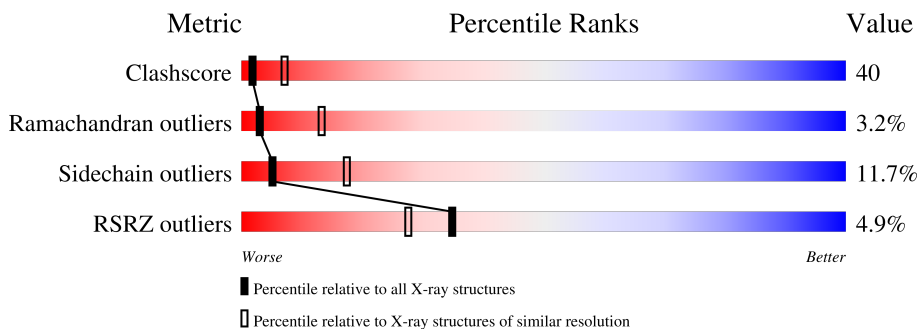
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	468	 9% 46% 42% 12%
1	B	468	 6% 47% 41% 11%
1	C	468	 4% 45% 43% 11%
1	D	468	 4% 46% 42% 11%
1	E	468	 3% 45% 43% 11%
1	F	468	 4% 46% 42% 11%

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Mol	Chain	Length	Quality of chain
1	G	468	 3% 46% 42% 11%
1	H	468	 6% 47% 42% 11%
1	I	468	 4% 45% 43% 11%
1	J	468	 6% 47% 42% 11%
1	K	468	 4% 45% 43% 11%
1	L	468	 6% 46% 43% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PPQ	A	5900	-	-	X	-
4	PPQ	B	5901	-	-	X	-
4	PPQ	C	5902	-	-	X	-
4	PPQ	D	5903	-	-	X	-
4	PPQ	E	5904	-	-	X	-
4	PPQ	F	5905	-	-	X	-
4	PPQ	G	5906	-	-	X	-
4	PPQ	H	5907	-	-	X	-
4	PPQ	I	5908	-	-	X	-
4	PPQ	J	5909	-	-	X	-
4	PPQ	L	5911	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 47280 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 GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	468	3747	2371	643	713	20	0	26	0
1	B	468	3747	2371	643	713	20	0	26	0
1	C	468	3747	2371	643	713	20	0	26	0
1	D	468	3747	2371	643	713	20	0	26	0
1	E	468	3747	2371	643	713	20	0	26	0
1	F	468	3747	2371	643	713	20	0	26	0
1	G	468	3747	2371	643	713	20	0	26	0
1	H	468	3747	2371	643	713	20	0	26	0
1	I	468	3747	2371	643	713	20	0	26	0
1	J	468	3747	2371	643	713	20	0	26	0
1	K	468	3747	2371	643	713	20	0	26	0
1	L	468	3747	2371	643	713	20	0	26	0

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

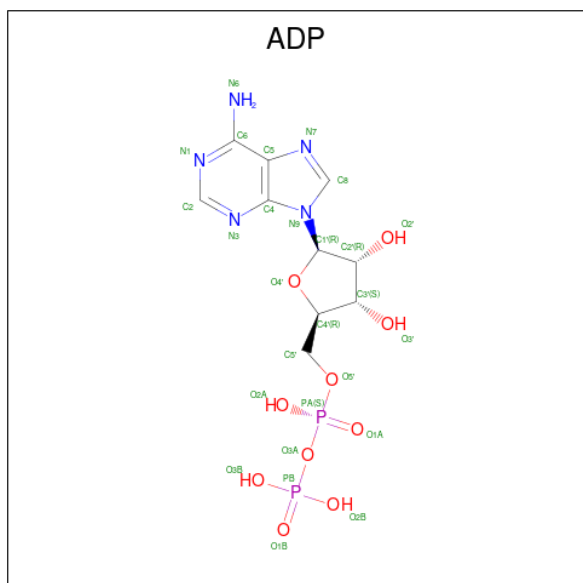
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		
2	G	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	I	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		
2	K	2	Total	Mn	0	0
			2	2		
2	L	2	Total	Mn	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



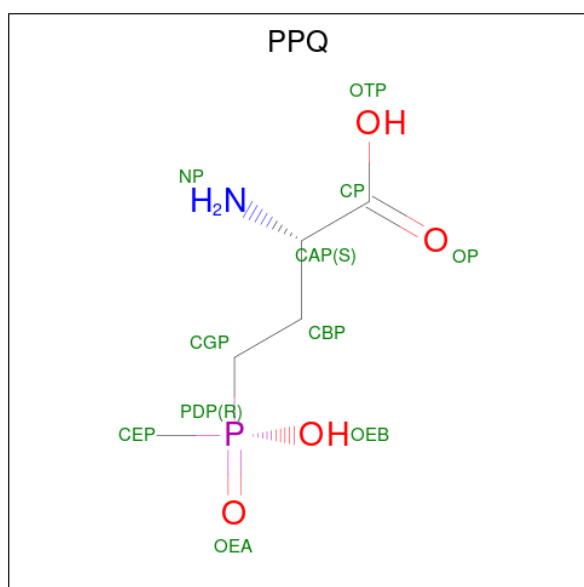
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is PHOSPHINOTHRICIN (CCD ID: PPQ) (formula: C₅H₁₂NO₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	I	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	J	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	L	1	Total	C	N	O	P	0	0
			11	5	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		
5	B	155	Total	O	0	0
			155	155		
5	C	152	Total	O	0	0
			152	152		
5	D	153	Total	O	0	0
			153	153		
5	E	154	Total	O	0	0
			154	154		
5	F	152	Total	O	0	0
			152	152		
5	G	155	Total	O	0	0
			155	155		
5	H	150	Total	O	0	0
			150	150		

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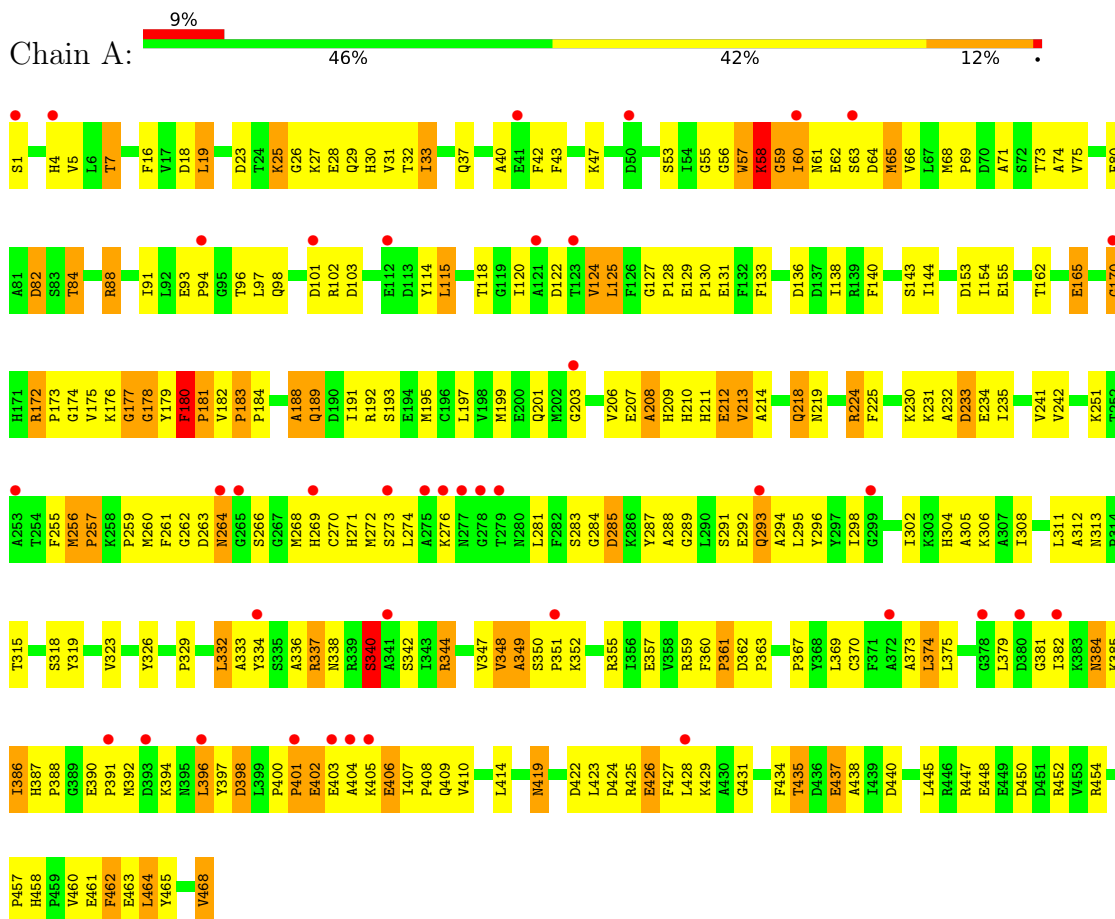
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	156	Total 156	O 156	0	0
5	J	151	Total 151	O 151	0	0
5	K	153	Total 153	O 153	0	0
5	L	153	Total 153	O 153	0	0

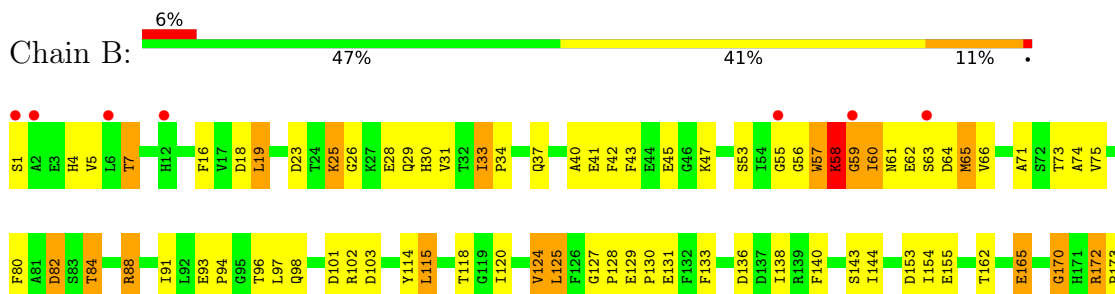
3 Residue-property plots [i](#)

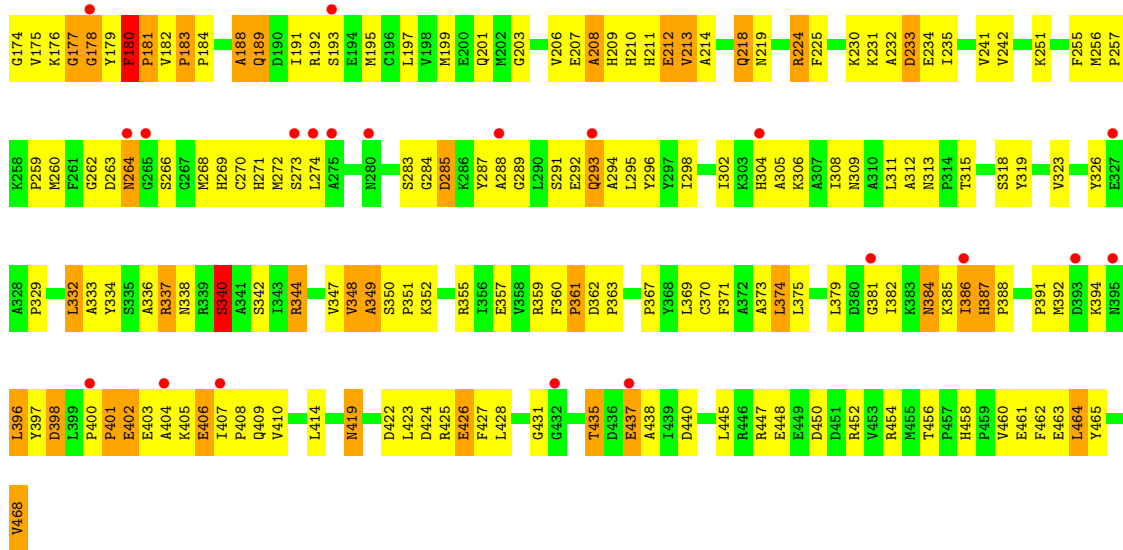
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: GLUTAMINE SYNTHETASE

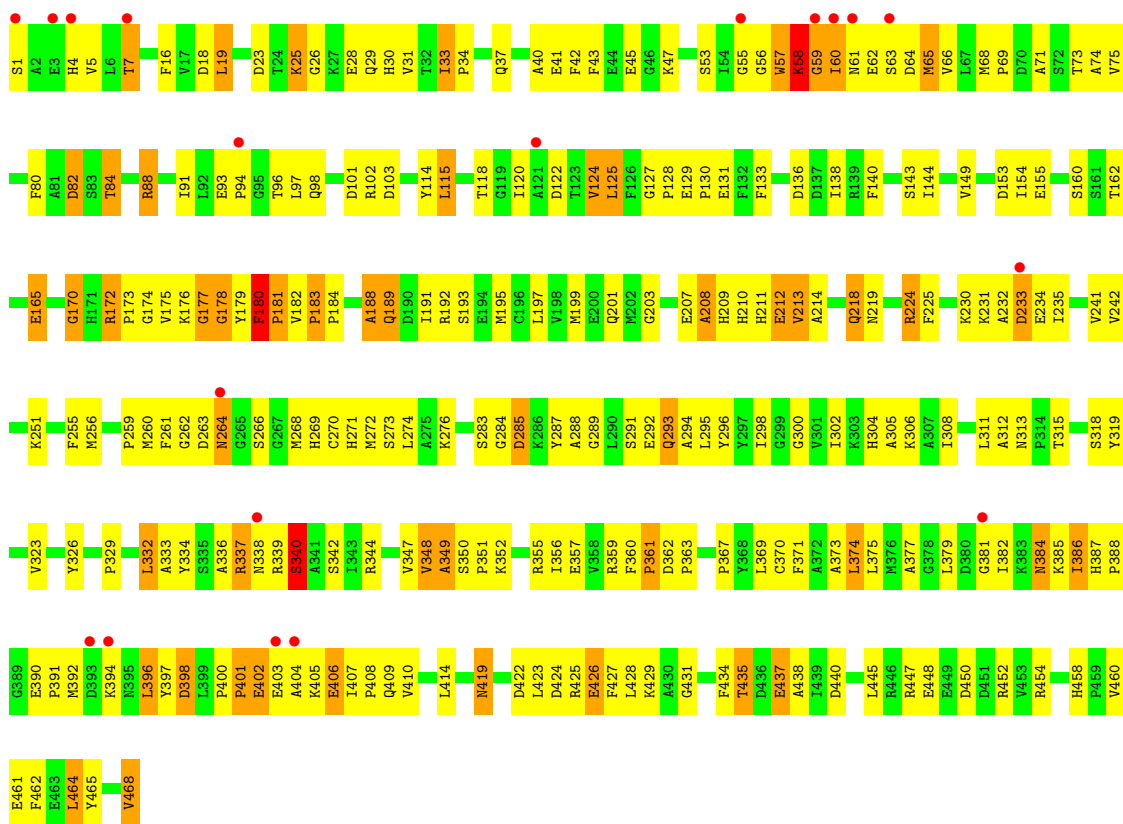
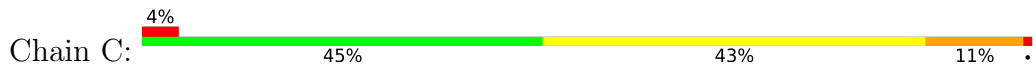


- Molecule 1: GLUTAMINE SYNTHETASE



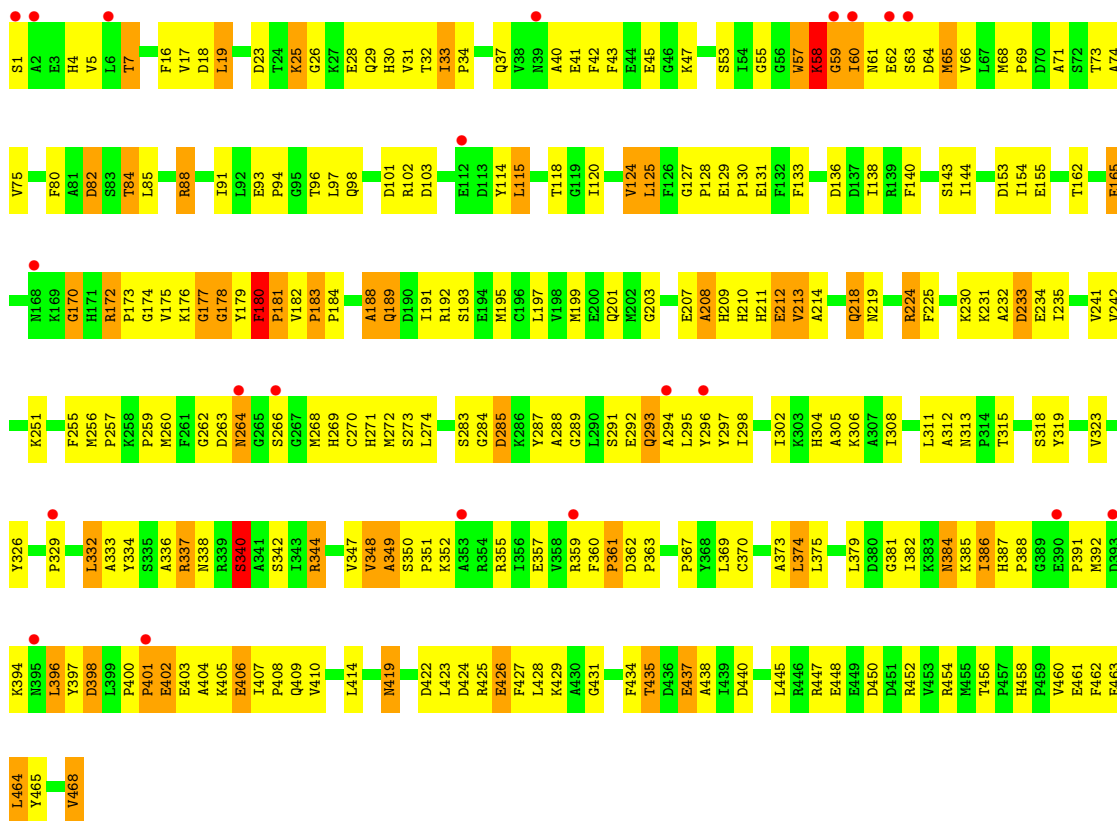


• Molecule 1: GLUTAMINE SYNTHETASE

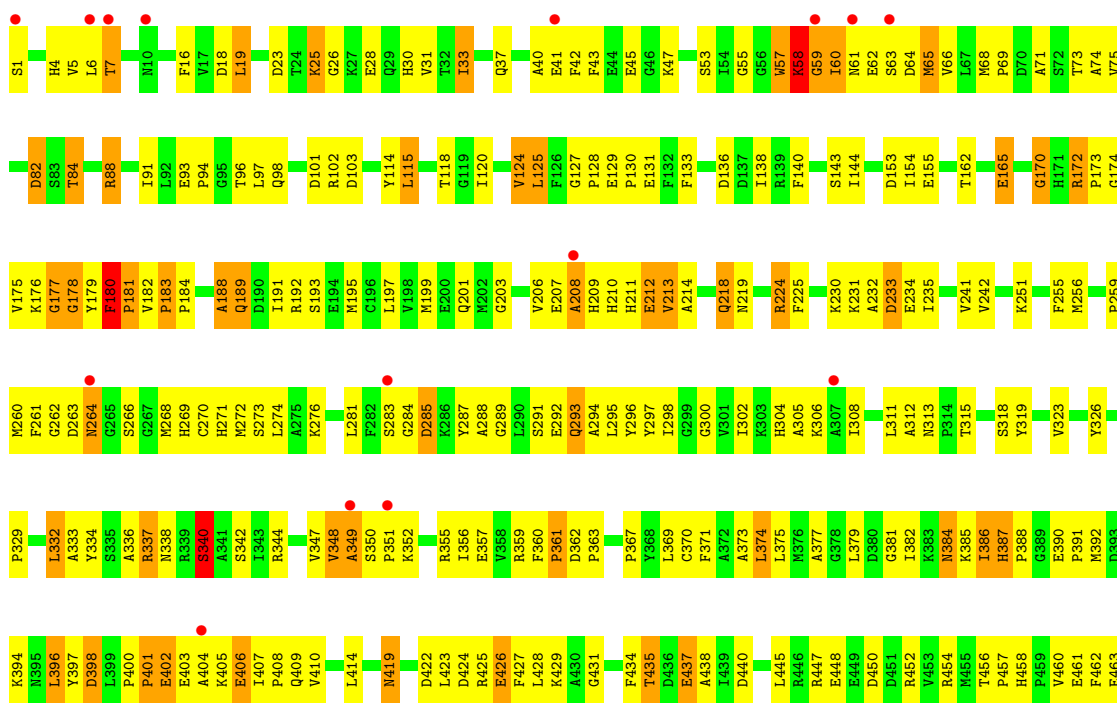


• Molecule 1: GLUTAMINE SYNTHETASE



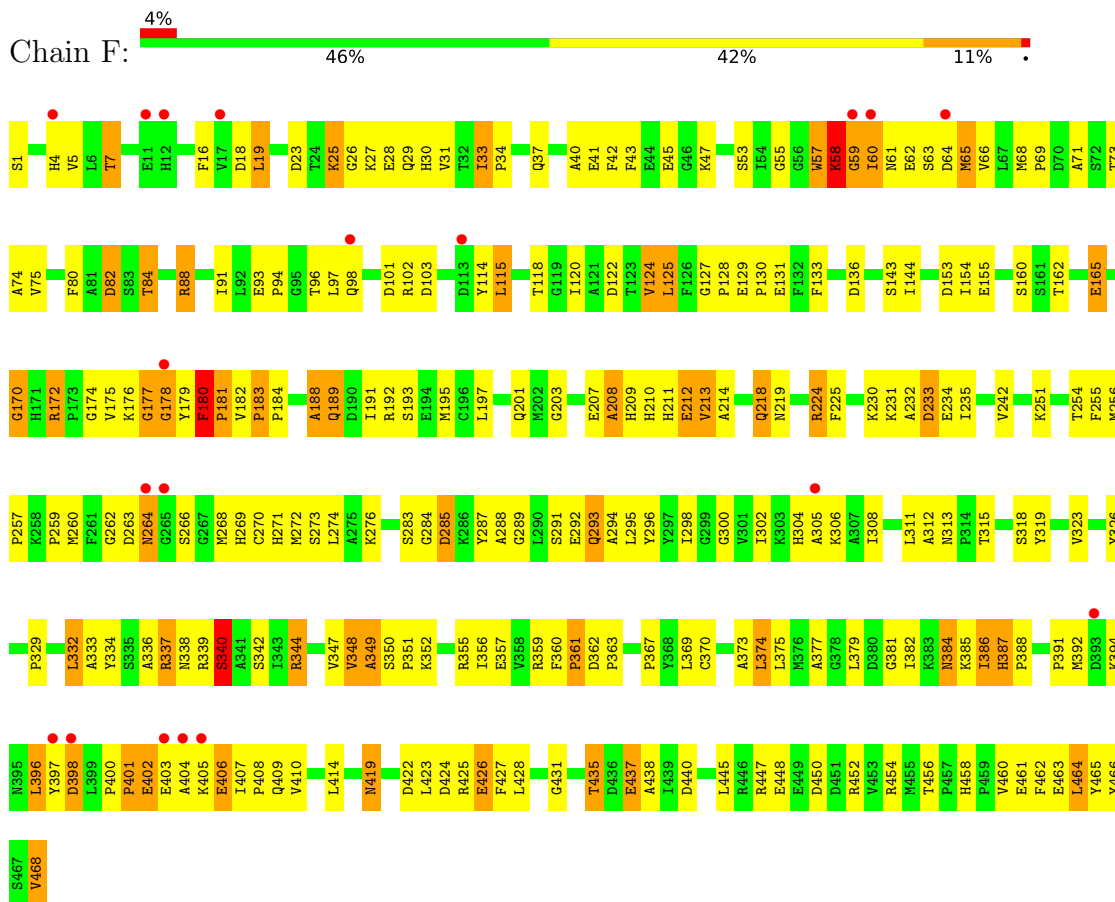


• Molecule 1: GLUTAMINE SYNTHETASE

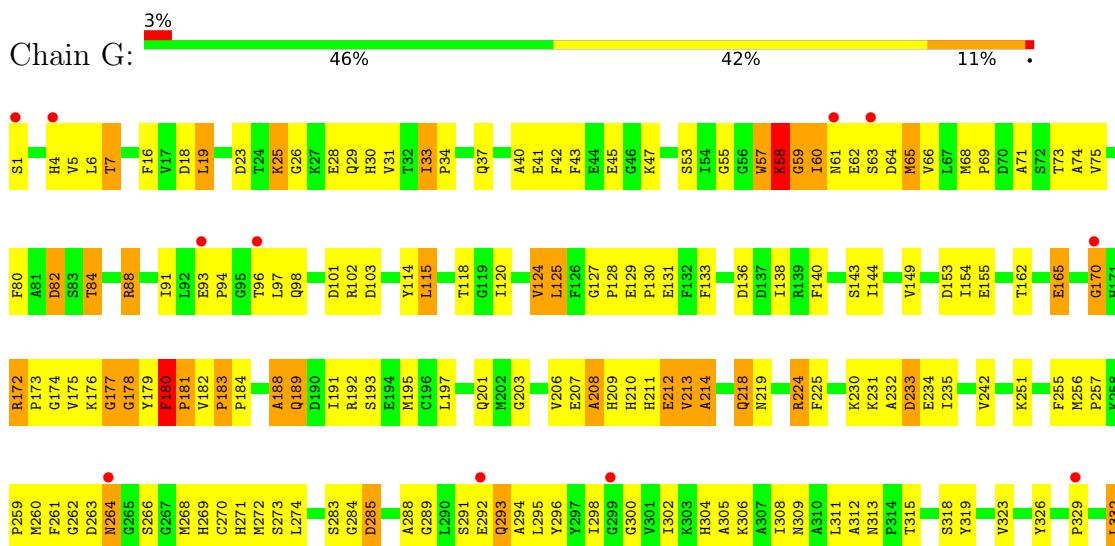


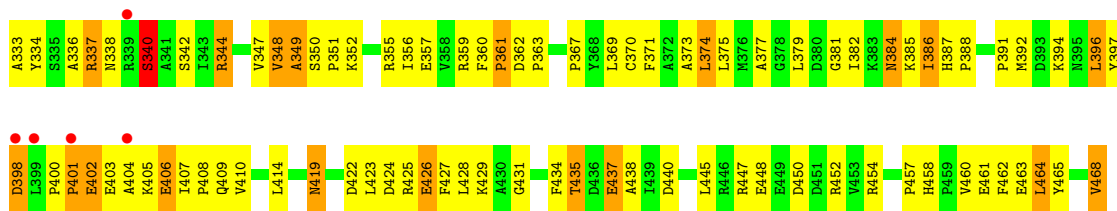


• Molecule 1: GLUTAMINE SYNTHETASE

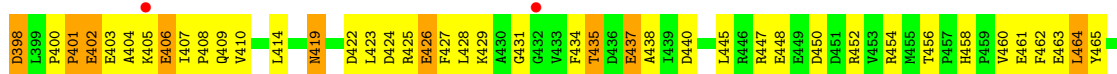
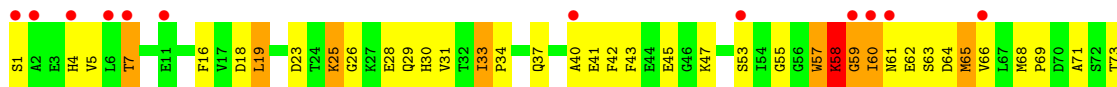


• Molecule 1: GLUTAMINE SYNTHETASE

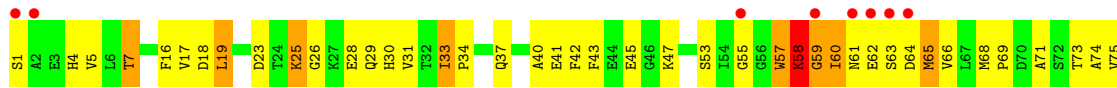


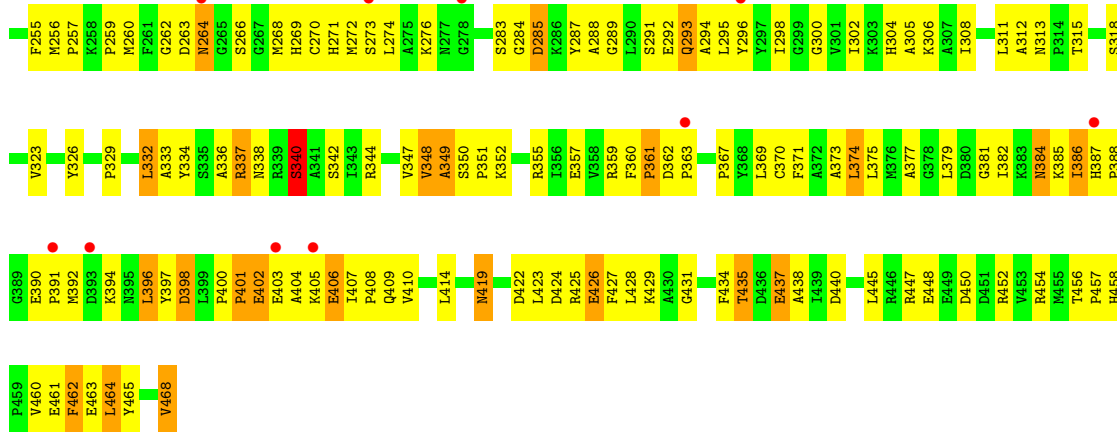


• Molecule 1: GLUTAMINE SYNTHETASE

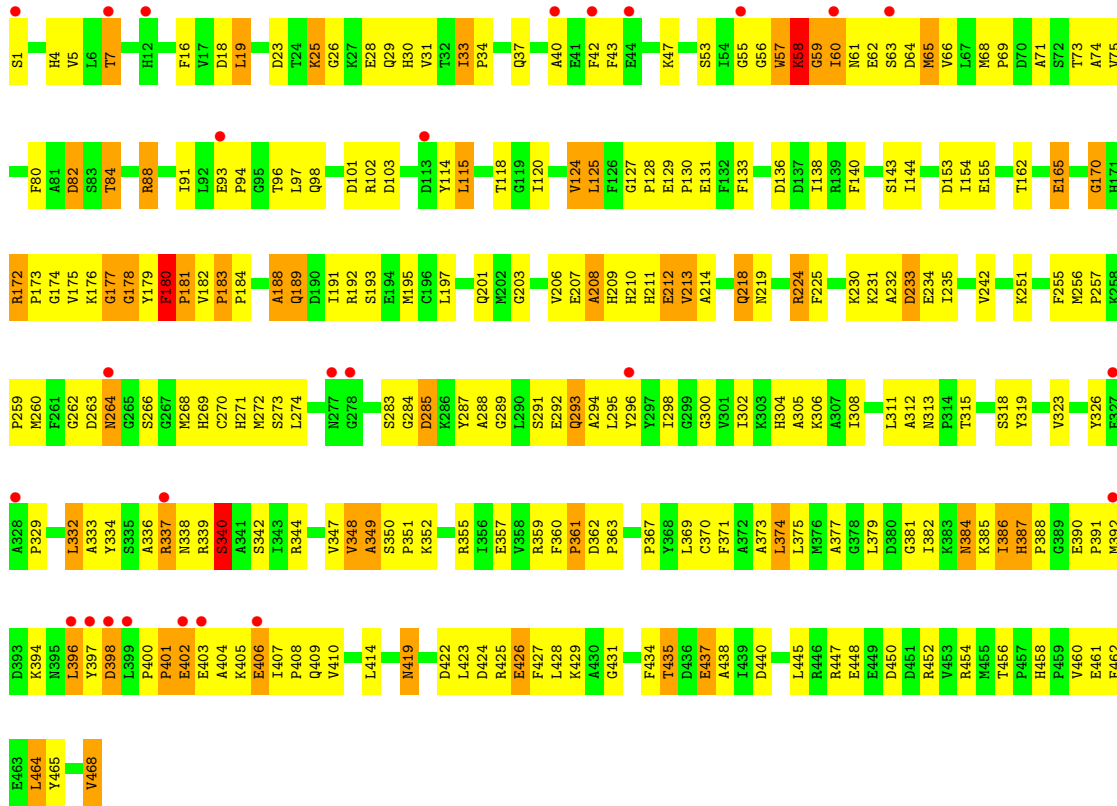


• Molecule 1: GLUTAMINE SYNTHETASE



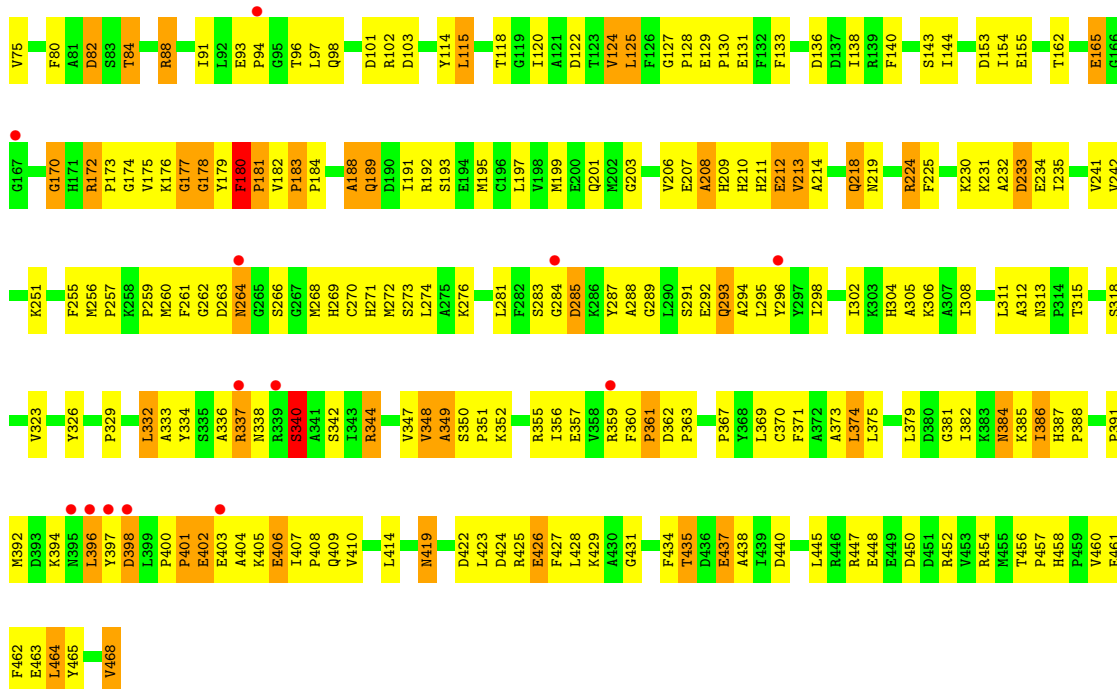


• Molecule 1: GLUTAMINE SYNTHETASE

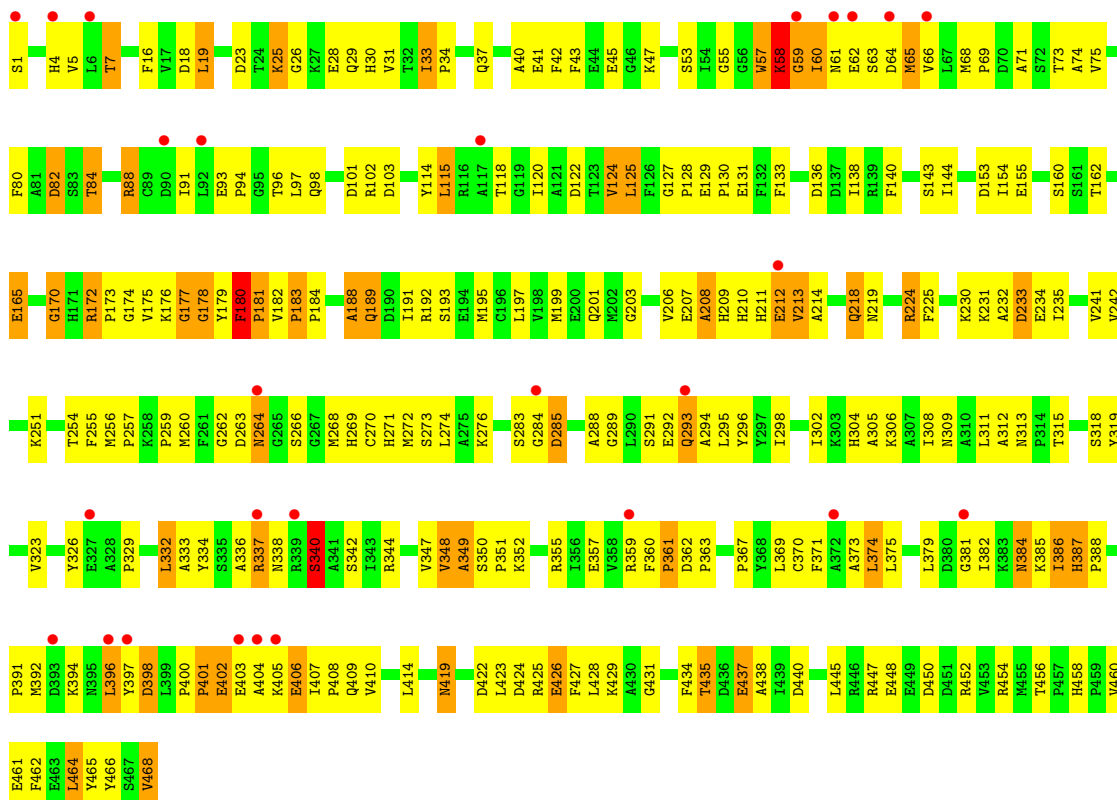


• Molecule 1: GLUTAMINE SYNTHETASE





• Molecule 1: GLUTAMINE SYNTHETASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	230.60Å 132.50Å 195.90Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	15.00 – 2.89 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	70.0 (15.00-2.89) 68.1 (15.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.91Å)	Xtrriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.248 , 0.263 0.246 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtrriage
Anisotropy	0.455	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47280	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, ADP, PPQ

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	0.74	0/3850	1.27	51/5212 (1.0%)
1	B	0.74	0/3850	1.27	51/5212 (1.0%)
1	C	0.74	0/3850	1.27	50/5212 (1.0%)
1	D	0.74	0/3850	1.27	52/5212 (1.0%)
1	E	0.74	0/3850	1.27	51/5212 (1.0%)
1	F	0.74	0/3850	1.27	51/5212 (1.0%)
1	G	0.74	0/3850	1.27	52/5212 (1.0%)
1	H	0.74	0/3850	1.27	50/5212 (1.0%)
1	I	0.74	0/3850	1.27	50/5212 (1.0%)
1	J	0.74	0/3850	1.27	51/5212 (1.0%)
1	K	0.74	0/3850	1.27	50/5212 (1.0%)
1	L	0.74	0/3850	1.27	51/5212 (1.0%)
All	All	0.74	0/46200	1.27	610/62544 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1

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

There are no bond length outliers.

All (610) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	189	GLN	OE1-CD-NE2	-10.06	112.54	122.60
1	B	189	GLN	OE1-CD-NE2	-10.04	112.56	122.60
1	G	189	GLN	OE1-CD-NE2	-10.03	112.57	122.60
1	L	189	GLN	OE1-CD-NE2	-10.03	112.57	122.60
1	H	189	GLN	OE1-CD-NE2	-10.01	112.59	122.60
1	C	189	GLN	OE1-CD-NE2	-10.00	112.60	122.60
1	A	189	GLN	OE1-CD-NE2	-10.00	112.60	122.60
1	D	189	GLN	OE1-CD-NE2	-9.99	112.61	122.60
1	F	189	GLN	OE1-CD-NE2	-9.98	112.62	122.60
1	E	189	GLN	OE1-CD-NE2	-9.97	112.63	122.60
1	I	189	GLN	OE1-CD-NE2	-9.96	112.64	122.60
1	K	189	GLN	OE1-CD-NE2	-9.95	112.65	122.60
1	F	218	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	H	218	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	G	218	GLN	OE1-CD-NE2	-9.90	112.70	122.60
1	D	218	GLN	OE1-CD-NE2	-9.89	112.70	122.60
1	L	218	GLN	OE1-CD-NE2	-9.89	112.71	122.60
1	K	218	GLN	OE1-CD-NE2	-9.89	112.71	122.60
1	I	218	GLN	OE1-CD-NE2	-9.88	112.72	122.60
1	J	218	GLN	OE1-CD-NE2	-9.88	112.72	122.60
1	E	218	GLN	OE1-CD-NE2	-9.88	112.72	122.60
1	A	218	GLN	OE1-CD-NE2	-9.88	112.72	122.60
1	B	218	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	C	218	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	E	398	ASP	N-CA-C	7.68	120.06	109.54
1	B	398	ASP	N-CA-C	7.66	120.04	109.54
1	A	398	ASP	N-CA-C	7.64	120.01	109.54
1	D	398	ASP	N-CA-C	7.64	120.01	109.54
1	L	398	ASP	N-CA-C	7.64	120.01	109.54
1	K	398	ASP	N-CA-C	7.64	120.00	109.54
1	C	398	ASP	N-CA-C	7.63	120.00	109.54
1	J	398	ASP	N-CA-C	7.63	119.99	109.54
1	H	398	ASP	N-CA-C	7.63	119.99	109.54
1	G	398	ASP	N-CA-C	7.62	119.99	109.54
1	I	398	ASP	N-CA-C	7.62	119.98	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	398	ASP	N-CA-C	7.61	119.97	109.54
1	F	426	GLU	N-CA-C	7.15	118.72	111.07
1	B	426	GLU	N-CA-C	7.12	118.69	111.07
1	C	426	GLU	N-CA-C	7.12	118.69	111.07
1	A	426	GLU	N-CA-C	7.11	118.68	111.07
1	D	426	GLU	N-CA-C	7.11	118.68	111.07
1	G	426	GLU	N-CA-C	7.10	118.67	111.07
1	H	426	GLU	N-CA-C	7.10	118.67	111.07
1	J	426	GLU	N-CA-C	7.10	118.67	111.07
1	I	426	GLU	N-CA-C	7.10	118.66	111.07
1	E	426	GLU	N-CA-C	7.09	118.66	111.07
1	L	426	GLU	N-CA-C	7.09	118.65	111.07
1	G	340	SER	N-CA-C	-7.08	104.64	113.28
1	E	340	SER	N-CA-C	-7.08	104.64	113.28
1	D	340	SER	N-CA-C	-7.08	104.64	113.28
1	C	340	SER	N-CA-C	-7.07	104.65	113.28
1	A	340	SER	N-CA-C	-7.07	104.66	113.28
1	H	340	SER	N-CA-C	-7.07	104.66	113.28
1	I	340	SER	N-CA-C	-7.06	104.66	113.28
1	K	426	GLU	N-CA-C	7.06	118.63	111.07
1	K	340	SER	N-CA-C	-7.06	104.66	113.28
1	L	340	SER	N-CA-C	-7.06	104.66	113.28
1	B	340	SER	N-CA-C	-7.06	104.67	113.28
1	F	340	SER	N-CA-C	-7.05	104.68	113.28
1	J	340	SER	N-CA-C	-7.04	104.69	113.28
1	G	136	ASP	N-CA-C	-6.66	105.69	113.88
1	K	136	ASP	N-CA-C	-6.66	105.69	113.88
1	E	136	ASP	N-CA-C	-6.65	105.70	113.88
1	B	136	ASP	N-CA-C	-6.65	105.70	113.88
1	L	136	ASP	N-CA-C	-6.65	105.70	113.88
1	D	136	ASP	N-CA-C	-6.65	105.70	113.88
1	A	136	ASP	N-CA-C	-6.63	105.72	113.88
1	I	136	ASP	N-CA-C	-6.63	105.72	113.88
1	C	136	ASP	N-CA-C	-6.63	105.73	113.88
1	F	136	ASP	N-CA-C	-6.62	105.73	113.88
1	J	136	ASP	N-CA-C	-6.61	105.76	113.88
1	H	136	ASP	N-CA-C	-6.58	105.78	113.88
1	I	256	MET	CA-C-N	6.45	126.21	119.05
1	I	256	MET	C-N-CA	6.45	126.21	119.05
1	L	256	MET	CA-C-N	6.45	126.20	119.05
1	L	256	MET	C-N-CA	6.45	126.20	119.05
1	L	403	GLU	N-CA-C	-6.41	103.64	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	403	GLU	N-CA-C	-6.41	103.64	112.03
1	K	403	GLU	N-CA-C	-6.40	103.65	112.03
1	F	403	GLU	N-CA-C	-6.39	103.66	112.03
1	J	403	GLU	N-CA-C	-6.39	103.66	112.03
1	C	403	GLU	N-CA-C	-6.39	103.67	112.03
1	D	403	GLU	N-CA-C	-6.39	103.66	112.03
1	G	403	GLU	N-CA-C	-6.39	103.67	112.03
1	H	403	GLU	N-CA-C	-6.38	103.67	112.03
1	A	403	GLU	N-CA-C	-6.38	103.67	112.03
1	B	403	GLU	N-CA-C	-6.38	103.67	112.03
1	I	403	GLU	N-CA-C	-6.38	103.67	112.03
1	C	400	PRO	N-CA-C	6.36	118.46	110.70
1	F	313	ASN	CA-C-N	6.36	127.17	120.12
1	F	313	ASN	C-N-CA	6.36	127.17	120.12
1	C	313	ASN	CA-C-N	6.35	127.17	120.12
1	C	313	ASN	C-N-CA	6.35	127.17	120.12
1	L	189	GLN	CG-CD-NE2	6.35	125.92	116.40
1	I	400	PRO	N-CA-C	6.35	118.44	110.70
1	B	189	GLN	CG-CD-NE2	6.34	125.91	116.40
1	B	313	ASN	CA-C-N	6.34	127.16	120.12
1	B	313	ASN	C-N-CA	6.34	127.16	120.12
1	C	189	GLN	CG-CD-NE2	6.34	125.91	116.40
1	D	400	PRO	N-CA-C	6.34	118.43	110.70
1	E	313	ASN	CA-C-N	6.34	127.16	120.12
1	E	313	ASN	C-N-CA	6.34	127.16	120.12
1	G	189	GLN	CG-CD-NE2	6.34	125.91	116.40
1	J	189	GLN	CG-CD-NE2	6.34	125.91	116.40
1	D	313	ASN	CA-C-N	6.34	127.16	120.12
1	D	313	ASN	C-N-CA	6.34	127.16	120.12
1	F	400	PRO	N-CA-C	6.34	118.43	110.70
1	K	400	PRO	N-CA-C	6.33	118.43	110.70
1	L	400	PRO	N-CA-C	6.33	118.42	110.70
1	J	313	ASN	CA-C-N	6.33	127.15	120.12
1	J	313	ASN	C-N-CA	6.33	127.15	120.12
1	A	189	GLN	CG-CD-NE2	6.33	125.89	116.40
1	A	313	ASN	CA-C-N	6.33	127.14	120.12
1	A	313	ASN	C-N-CA	6.33	127.14	120.12
1	H	189	GLN	CG-CD-NE2	6.33	125.89	116.40
1	H	313	ASN	CA-C-N	6.33	127.14	120.12
1	H	313	ASN	C-N-CA	6.33	127.14	120.12
1	J	400	PRO	N-CA-C	6.32	118.42	110.70
1	D	189	GLN	CG-CD-NE2	6.32	125.88	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	189	GLN	CG-CD-NE2	6.32	125.88	116.40
1	K	189	GLN	CG-CD-NE2	6.32	125.88	116.40
1	A	400	PRO	N-CA-C	6.32	118.41	110.70
1	H	400	PRO	N-CA-C	6.32	118.41	110.70
1	E	400	PRO	N-CA-C	6.32	118.40	110.70
1	I	313	ASN	CA-C-N	6.31	127.13	120.12
1	I	313	ASN	C-N-CA	6.31	127.13	120.12
1	L	313	ASN	CA-C-N	6.31	127.13	120.12
1	L	313	ASN	C-N-CA	6.31	127.13	120.12
1	I	189	GLN	CG-CD-NE2	6.31	125.87	116.40
1	G	400	PRO	N-CA-C	6.31	118.39	110.70
1	K	313	ASN	CA-C-N	6.30	127.12	120.12
1	K	313	ASN	C-N-CA	6.30	127.12	120.12
1	F	189	GLN	CG-CD-NE2	6.30	125.86	116.40
1	B	400	PRO	N-CA-C	6.30	118.38	110.70
1	J	57	TRP	N-CA-C	-6.30	104.17	113.61
1	G	57	TRP	N-CA-C	-6.29	104.18	113.61
1	G	313	ASN	CA-C-N	6.29	127.10	120.12
1	G	313	ASN	C-N-CA	6.29	127.10	120.12
1	C	57	TRP	N-CA-C	-6.29	104.18	113.61
1	D	57	TRP	N-CA-C	-6.29	104.18	113.61
1	E	57	TRP	N-CA-C	-6.29	104.18	113.61
1	A	57	TRP	N-CA-C	-6.28	104.18	113.61
1	B	57	TRP	N-CA-C	-6.28	104.19	113.61
1	F	218	GLN	CG-CD-NE2	6.28	125.81	116.40
1	K	57	TRP	N-CA-C	-6.28	104.20	113.61
1	I	57	TRP	N-CA-C	-6.27	104.20	113.61
1	L	57	TRP	N-CA-C	-6.27	104.20	113.61
1	E	218	GLN	CG-CD-NE2	6.26	125.80	116.40
1	F	57	TRP	N-CA-C	-6.26	104.22	113.61
1	H	57	TRP	N-CA-C	-6.26	104.22	113.61
1	C	218	GLN	CG-CD-NE2	6.25	125.78	116.40
1	D	218	GLN	CG-CD-NE2	6.25	125.78	116.40
1	L	218	GLN	CG-CD-NE2	6.25	125.78	116.40
1	K	218	GLN	CG-CD-NE2	6.25	125.77	116.40
1	A	218	GLN	CG-CD-NE2	6.24	125.76	116.40
1	I	218	GLN	CG-CD-NE2	6.24	125.76	116.40
1	B	218	GLN	CG-CD-NE2	6.24	125.75	116.40
1	H	218	GLN	CG-CD-NE2	6.23	125.75	116.40
1	J	218	GLN	CG-CD-NE2	6.23	125.75	116.40
1	E	387	HIS	CA-C-N	6.22	127.03	120.12
1	E	387	HIS	C-N-CA	6.22	127.03	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	218	GLN	CG-CD-NE2	6.22	125.74	116.40
1	D	188	ALA	N-CA-C	6.22	120.14	111.56
1	I	188	ALA	N-CA-C	6.22	120.14	111.56
1	H	188	ALA	N-CA-C	6.22	120.14	111.56
1	J	188	ALA	N-CA-C	6.22	120.14	111.56
1	J	362	ASP	CA-C-N	6.22	125.95	119.05
1	J	362	ASP	C-N-CA	6.22	125.95	119.05
1	A	188	ALA	N-CA-C	6.21	120.13	111.56
1	B	362	ASP	CA-C-N	6.21	125.94	119.05
1	B	362	ASP	C-N-CA	6.21	125.94	119.05
1	E	188	ALA	N-CA-C	6.21	120.13	111.56
1	F	362	ASP	CA-C-N	6.21	125.94	119.05
1	F	362	ASP	C-N-CA	6.21	125.94	119.05
1	B	188	ALA	N-CA-C	6.21	120.13	111.56
1	K	188	ALA	N-CA-C	6.21	120.13	111.56
1	H	387	HIS	CA-C-N	6.20	127.00	120.12
1	H	387	HIS	C-N-CA	6.20	127.00	120.12
1	L	188	ALA	N-CA-C	6.20	120.12	111.56
1	F	188	ALA	N-CA-C	6.20	120.11	111.56
1	L	387	HIS	CA-C-N	6.20	127.00	120.12
1	L	387	HIS	C-N-CA	6.20	127.00	120.12
1	C	362	ASP	CA-C-N	6.19	125.93	119.05
1	C	362	ASP	C-N-CA	6.19	125.93	119.05
1	G	188	ALA	N-CA-C	6.19	120.11	111.56
1	I	362	ASP	CA-C-N	6.19	125.92	119.05
1	I	362	ASP	C-N-CA	6.19	125.92	119.05
1	A	387	HIS	CA-C-N	6.19	126.99	120.12
1	A	387	HIS	C-N-CA	6.19	126.99	120.12
1	C	188	ALA	N-CA-C	6.19	120.10	111.56
1	C	387	HIS	CA-C-N	6.19	126.99	120.12
1	C	387	HIS	C-N-CA	6.19	126.99	120.12
1	A	362	ASP	CA-C-N	6.18	125.91	119.05
1	A	362	ASP	C-N-CA	6.18	125.91	119.05
1	B	387	HIS	CA-C-N	6.18	126.98	120.12
1	B	387	HIS	C-N-CA	6.18	126.98	120.12
1	F	387	HIS	CA-C-N	6.18	126.98	120.12
1	F	387	HIS	C-N-CA	6.18	126.98	120.12
1	G	387	HIS	CA-C-N	6.18	126.98	120.12
1	G	387	HIS	C-N-CA	6.18	126.98	120.12
1	H	362	ASP	CA-C-N	6.18	125.91	119.05
1	H	362	ASP	C-N-CA	6.18	125.91	119.05
1	L	402	GLU	N-CA-C	-6.18	105.90	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	GLU	N-CA-C	-6.17	105.91	113.50
1	D	362	ASP	CA-C-N	6.17	125.90	119.05
1	D	362	ASP	C-N-CA	6.17	125.90	119.05
1	D	387	HIS	CA-C-N	6.17	126.97	120.12
1	D	387	HIS	C-N-CA	6.17	126.97	120.12
1	E	402	GLU	N-CA-C	-6.17	105.91	113.50
1	G	362	ASP	CA-C-N	6.17	125.90	119.05
1	G	362	ASP	C-N-CA	6.17	125.90	119.05
1	E	362	ASP	CA-C-N	6.17	125.90	119.05
1	E	362	ASP	C-N-CA	6.17	125.90	119.05
1	J	387	HIS	CA-C-N	6.17	126.97	120.12
1	J	387	HIS	C-N-CA	6.17	126.97	120.12
1	C	402	GLU	N-CA-C	-6.17	105.91	113.50
1	F	402	GLU	N-CA-C	-6.17	105.91	113.50
1	I	387	HIS	CA-C-N	6.17	126.97	120.12
1	I	387	HIS	C-N-CA	6.17	126.97	120.12
1	K	362	ASP	CA-C-N	6.17	125.89	119.05
1	K	362	ASP	C-N-CA	6.17	125.89	119.05
1	L	362	ASP	CA-C-N	6.16	125.89	119.05
1	L	362	ASP	C-N-CA	6.16	125.89	119.05
1	H	402	GLU	N-CA-C	-6.16	105.92	113.50
1	K	387	HIS	CA-C-N	6.16	126.96	120.12
1	K	387	HIS	C-N-CA	6.16	126.96	120.12
1	A	402	GLU	N-CA-C	-6.15	105.93	113.50
1	J	402	GLU	N-CA-C	-6.15	105.93	113.50
1	D	402	GLU	N-CA-C	-6.15	105.94	113.50
1	K	402	GLU	N-CA-C	-6.15	105.94	113.50
1	I	402	GLU	N-CA-C	-6.14	105.94	113.50
1	G	402	GLU	N-CA-C	-6.12	105.97	113.50
1	I	438	ALA	N-CA-C	-6.11	104.53	111.07
1	F	438	ALA	N-CA-C	-6.11	104.54	111.07
1	J	438	ALA	N-CA-C	-6.09	104.56	111.07
1	F	256	MET	CA-C-N	6.09	126.26	119.32
1	F	256	MET	C-N-CA	6.09	126.26	119.32
1	G	438	ALA	N-CA-C	-6.07	104.57	111.07
1	E	256	MET	CA-C-N	6.07	126.24	119.32
1	E	256	MET	C-N-CA	6.07	126.24	119.32
1	J	256	MET	CA-C-N	6.07	126.23	119.32
1	J	256	MET	C-N-CA	6.07	126.23	119.32
1	C	256	MET	CA-C-N	6.06	126.23	119.32
1	C	256	MET	C-N-CA	6.06	126.23	119.32
1	A	438	ALA	N-CA-C	-6.06	104.59	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	438	ALA	N-CA-C	-6.06	104.59	111.07
1	A	256	MET	CA-C-N	6.05	126.22	119.32
1	A	256	MET	C-N-CA	6.05	126.22	119.32
1	C	438	ALA	N-CA-C	-6.05	104.59	111.07
1	D	438	ALA	N-CA-C	-6.05	104.59	111.07
1	K	256	MET	CA-C-N	6.05	126.22	119.32
1	K	256	MET	C-N-CA	6.05	126.22	119.32
1	L	438	ALA	N-CA-C	-6.05	104.59	111.07
1	E	438	ALA	N-CA-C	-6.05	104.60	111.07
1	K	438	ALA	N-CA-C	-6.05	104.60	111.07
1	B	438	ALA	N-CA-C	-6.04	104.61	111.07
1	B	256	MET	CA-C-N	6.04	126.20	119.32
1	B	256	MET	C-N-CA	6.04	126.20	119.32
1	G	256	MET	CA-C-N	6.03	126.20	119.32
1	G	256	MET	C-N-CA	6.03	126.20	119.32
1	D	256	MET	CA-C-N	6.03	126.20	119.32
1	D	256	MET	C-N-CA	6.03	126.20	119.32
1	H	256	MET	CA-C-N	6.03	126.19	119.32
1	H	256	MET	C-N-CA	6.03	126.19	119.32
1	B	74	ALA	N-CA-C	5.96	118.98	110.10
1	H	74	ALA	N-CA-C	5.96	118.97	110.10
1	F	74	ALA	N-CA-C	5.96	118.97	110.10
1	C	74	ALA	N-CA-C	5.95	118.96	110.10
1	K	74	ALA	N-CA-C	5.94	118.95	110.10
1	I	74	ALA	N-CA-C	5.94	118.94	110.10
1	D	74	ALA	N-CA-C	5.93	118.94	110.10
1	A	74	ALA	N-CA-C	5.93	118.94	110.10
1	J	74	ALA	N-CA-C	5.93	118.94	110.10
1	E	74	ALA	N-CA-C	5.93	118.93	110.10
1	G	74	ALA	N-CA-C	5.92	118.93	110.10
1	L	74	ALA	N-CA-C	5.92	118.92	110.10
1	K	462	PHE	CA-CB-CG	-5.91	107.89	113.80
1	H	462	PHE	CA-CB-CG	-5.90	107.90	113.80
1	C	462	PHE	CA-CB-CG	-5.89	107.91	113.80
1	F	462	PHE	CA-CB-CG	-5.88	107.92	113.80
1	D	462	PHE	CA-CB-CG	-5.88	107.92	113.80
1	I	462	PHE	CA-CB-CG	-5.87	107.93	113.80
1	A	462	PHE	CA-CB-CG	-5.87	107.93	113.80
1	H	97	LEU	N-CA-C	5.86	119.74	112.24
1	C	97	LEU	N-CA-C	5.86	119.74	112.24
1	L	462	PHE	CA-CB-CG	-5.86	107.94	113.80
1	B	462	PHE	CA-CB-CG	-5.85	107.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	462	PHE	CA-CB-CG	-5.85	107.95	113.80
1	K	97	LEU	N-CA-C	5.85	119.72	112.24
1	D	97	LEU	N-CA-C	5.84	119.72	112.24
1	E	462	PHE	CA-CB-CG	-5.84	107.96	113.80
1	A	97	LEU	N-CA-C	5.84	119.71	112.24
1	J	97	LEU	N-CA-C	5.83	119.71	112.24
1	B	97	LEU	N-CA-C	5.83	119.71	112.24
1	L	97	LEU	N-CA-C	5.83	119.70	112.24
1	G	97	LEU	N-CA-C	5.83	119.70	112.24
1	F	97	LEU	N-CA-C	5.83	119.70	112.24
1	I	97	LEU	N-CA-C	5.83	119.70	112.24
1	J	462	PHE	CA-CB-CG	-5.82	107.98	113.80
1	E	97	LEU	N-CA-C	5.79	119.65	112.24
1	C	184	PRO	CA-C-N	-5.74	112.60	120.46
1	C	184	PRO	C-N-CA	-5.74	112.60	120.46
1	B	184	PRO	CA-C-N	-5.73	112.60	120.46
1	B	184	PRO	C-N-CA	-5.73	112.60	120.46
1	L	184	PRO	CA-C-N	-5.73	112.61	120.46
1	L	184	PRO	C-N-CA	-5.73	112.61	120.46
1	G	292	GLU	N-CA-C	-5.72	104.95	111.07
1	D	184	PRO	CA-C-N	-5.72	112.62	120.46
1	D	184	PRO	C-N-CA	-5.72	112.62	120.46
1	J	184	PRO	CA-C-N	-5.71	112.63	120.46
1	J	184	PRO	C-N-CA	-5.71	112.63	120.46
1	K	184	PRO	CA-C-N	-5.71	112.63	120.46
1	K	184	PRO	C-N-CA	-5.71	112.63	120.46
1	B	292	GLU	N-CA-C	-5.71	104.96	111.07
1	E	180[A]	PHE	CA-C-N	-5.71	114.06	119.89
1	E	180[A]	PHE	C-N-CA	-5.71	114.06	119.89
1	E	180[B]	PHE	CA-C-N	-5.71	114.06	119.89
1	E	180[B]	PHE	C-N-CA	-5.71	114.06	119.89
1	I	184	PRO	CA-C-N	-5.71	112.64	120.46
1	I	184	PRO	C-N-CA	-5.71	112.64	120.46
1	F	184	PRO	CA-C-N	-5.71	112.64	120.46
1	F	184	PRO	C-N-CA	-5.71	112.64	120.46
1	H	184	PRO	CA-C-N	-5.71	112.64	120.46
1	H	184	PRO	C-N-CA	-5.71	112.64	120.46
1	E	184	PRO	CA-C-N	-5.71	112.64	120.46
1	E	184	PRO	C-N-CA	-5.71	112.64	120.46
1	G	184	PRO	CA-C-N	-5.71	112.64	120.46
1	G	184	PRO	C-N-CA	-5.71	112.64	120.46
1	L	292	GLU	N-CA-C	-5.70	104.97	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	PRO	CA-C-N	-5.70	112.65	120.46
1	A	184	PRO	C-N-CA	-5.70	112.65	120.46
1	D	292	GLU	N-CA-C	-5.70	104.97	111.07
1	J	180[A]	PHE	CA-C-N	-5.69	114.08	119.89
1	J	180[A]	PHE	C-N-CA	-5.69	114.08	119.89
1	J	180[B]	PHE	CA-C-N	-5.69	114.08	119.89
1	J	180[B]	PHE	C-N-CA	-5.69	114.08	119.89
1	L	180[A]	PHE	CA-C-N	-5.69	114.09	119.89
1	L	180[A]	PHE	C-N-CA	-5.69	114.09	119.89
1	L	180[B]	PHE	CA-C-N	-5.69	114.09	119.89
1	L	180[B]	PHE	C-N-CA	-5.69	114.09	119.89
1	I	180[A]	PHE	CA-C-N	-5.69	114.09	119.89
1	I	180[A]	PHE	C-N-CA	-5.69	114.09	119.89
1	I	180[B]	PHE	CA-C-N	-5.69	114.09	119.89
1	I	180[B]	PHE	C-N-CA	-5.69	114.09	119.89
1	C	292	GLU	N-CA-C	-5.69	104.99	111.07
1	H	180[A]	PHE	CA-C-N	-5.68	114.10	119.89
1	H	180[A]	PHE	C-N-CA	-5.68	114.10	119.89
1	H	180[B]	PHE	CA-C-N	-5.68	114.10	119.89
1	H	180[B]	PHE	C-N-CA	-5.68	114.10	119.89
1	A	292	GLU	N-CA-C	-5.68	105.00	111.07
1	J	292	GLU	N-CA-C	-5.68	105.00	111.07
1	F	57	TRP	CA-C-O	5.67	125.88	119.18
1	K	180[A]	PHE	CA-C-N	-5.67	114.10	119.89
1	K	180[A]	PHE	C-N-CA	-5.67	114.10	119.89
1	K	180[B]	PHE	CA-C-N	-5.67	114.10	119.89
1	K	180[B]	PHE	C-N-CA	-5.67	114.10	119.89
1	G	400	PRO	CB-CA-C	5.67	117.83	110.92
1	A	180[A]	PHE	CA-C-N	-5.67	114.11	119.89
1	A	180[A]	PHE	C-N-CA	-5.67	114.11	119.89
1	A	180[B]	PHE	CA-C-N	-5.67	114.11	119.89
1	A	180[B]	PHE	C-N-CA	-5.67	114.11	119.89
1	G	180[A]	PHE	CA-C-N	-5.67	114.11	119.89
1	G	180[A]	PHE	C-N-CA	-5.67	114.11	119.89
1	G	180[B]	PHE	CA-C-N	-5.67	114.11	119.89
1	G	180[B]	PHE	C-N-CA	-5.67	114.11	119.89
1	I	292	GLU	N-CA-C	-5.67	105.01	111.07
1	C	180[A]	PHE	CA-C-N	-5.67	114.11	119.89
1	C	180[A]	PHE	C-N-CA	-5.67	114.11	119.89
1	C	180[B]	PHE	CA-C-N	-5.67	114.11	119.89
1	C	180[B]	PHE	C-N-CA	-5.67	114.11	119.89
1	H	292	GLU	N-CA-C	-5.67	105.01	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	VAL	N-CA-C	5.66	116.10	108.17
1	I	400	PRO	CB-CA-C	5.66	117.83	110.92
1	F	400	PRO	CB-CA-C	5.66	117.82	110.92
1	B	180[A]	PHE	CA-C-N	-5.65	114.12	119.89
1	B	180[A]	PHE	C-N-CA	-5.65	114.12	119.89
1	B	180[B]	PHE	CA-C-N	-5.65	114.12	119.89
1	B	180[B]	PHE	C-N-CA	-5.65	114.12	119.89
1	D	400	PRO	CB-CA-C	5.65	117.81	110.92
1	G	66	VAL	N-CA-C	5.65	116.08	108.17
1	J	400	PRO	CB-CA-C	5.65	117.81	110.92
1	L	57	TRP	CA-C-O	5.65	125.84	119.18
1	D	180[A]	PHE	CA-C-N	-5.65	114.13	119.89
1	D	180[A]	PHE	C-N-CA	-5.65	114.13	119.89
1	D	180[B]	PHE	CA-C-N	-5.65	114.13	119.89
1	D	180[B]	PHE	C-N-CA	-5.65	114.13	119.89
1	E	292	GLU	N-CA-C	-5.65	105.03	111.07
1	F	66	VAL	N-CA-C	5.65	116.07	108.17
1	H	57	TRP	CA-C-O	5.65	125.84	119.18
1	A	400	PRO	CB-CA-C	5.64	117.81	110.92
1	F	292	GLU	N-CA-C	-5.64	105.03	111.07
1	B	66	VAL	N-CA-C	5.64	116.07	108.17
1	K	400	PRO	CB-CA-C	5.64	117.80	110.92
1	E	400	PRO	CB-CA-C	5.64	117.80	110.92
1	H	66	VAL	N-CA-C	5.64	116.06	108.17
1	B	57	TRP	CA-C-O	5.64	125.83	119.18
1	D	66	VAL	N-CA-C	5.64	116.06	108.17
1	E	66	VAL	N-CA-C	5.64	116.06	108.17
1	L	400	PRO	CB-CA-C	5.63	117.79	110.92
1	C	400	PRO	CB-CA-C	5.63	117.79	110.92
1	G	43	PHE	N-CA-C	5.63	117.50	111.36
1	A	66	VAL	N-CA-C	5.63	116.05	108.17
1	I	57	TRP	CA-C-O	5.63	125.82	119.18
1	H	400	PRO	CB-CA-C	5.63	117.78	110.92
1	F	180[A]	PHE	CA-C-N	-5.62	114.15	119.89
1	F	180[A]	PHE	C-N-CA	-5.62	114.15	119.89
1	F	180[B]	PHE	CA-C-N	-5.62	114.15	119.89
1	F	180[B]	PHE	C-N-CA	-5.62	114.15	119.89
1	B	400	PRO	CB-CA-C	5.62	117.78	110.92
1	C	57	TRP	CA-C-O	5.62	125.81	119.18
1	J	66	VAL	N-CA-C	5.62	116.04	108.17
1	D	57	TRP	CA-C-O	5.62	125.81	119.18
1	G	57	TRP	CA-C-O	5.62	125.81	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	TRP	CA-C-O	5.62	125.81	119.18
1	K	292	GLU	N-CA-C	-5.62	105.06	111.07
1	L	66	VAL	N-CA-C	5.61	116.03	108.17
1	I	66	VAL	N-CA-C	5.61	116.03	108.17
1	K	66	VAL	N-CA-C	5.61	116.03	108.17
1	L	43	PHE	N-CA-C	5.61	117.47	111.36
1	E	43	PHE	N-CA-C	5.61	117.47	111.36
1	E	57	TRP	CA-C-O	5.60	125.79	119.18
1	A	43	PHE	N-CA-C	5.60	117.46	111.36
1	K	43	PHE	N-CA-C	5.60	117.46	111.36
1	K	57	TRP	CA-C-O	5.60	125.78	119.18
1	B	43	PHE	N-CA-C	5.59	117.45	111.36
1	D	43	PHE	N-CA-C	5.59	117.45	111.36
1	J	57	TRP	CA-C-O	5.58	125.77	119.18
1	H	43	PHE	N-CA-C	5.58	117.44	111.36
1	J	43	PHE	N-CA-C	5.58	117.44	111.36
1	L	65	MET	N-CA-C	5.57	118.71	110.46
1	B	65	MET	N-CA-C	5.57	118.71	110.46
1	C	43	PHE	N-CA-C	5.57	117.43	111.36
1	G	65	MET	N-CA-C	5.56	118.69	110.46
1	F	65	MET	N-CA-C	5.56	118.69	110.46
1	F	43	PHE	N-CA-C	5.56	117.42	111.36
1	I	43	PHE	N-CA-C	5.56	117.42	111.36
1	H	65	MET	N-CA-C	5.55	118.68	110.46
1	L	257	PRO	N-CA-C	5.55	121.25	113.53
1	D	65	MET	N-CA-C	5.55	118.67	110.46
1	G	172	ARG	CA-C-N	5.55	125.72	119.90
1	G	172	ARG	C-N-CA	5.55	125.72	119.90
1	H	348	VAL	N-CA-C	5.55	115.16	108.06
1	A	65	MET	N-CA-C	5.54	118.67	110.46
1	J	348	VAL	N-CA-C	5.54	115.16	108.06
1	C	65	MET	N-CA-C	5.54	118.66	110.46
1	I	348	VAL	N-CA-C	5.54	115.16	108.06
1	L	348	VAL	N-CA-C	5.54	115.16	108.06
1	F	348	VAL	N-CA-C	5.54	115.15	108.06
1	G	348	VAL	N-CA-C	5.54	115.15	108.06
1	I	257	PRO	N-CA-C	5.54	121.23	113.53
1	B	172	ARG	CA-C-N	5.54	125.71	119.90
1	B	172	ARG	C-N-CA	5.54	125.71	119.90
1	H	172	ARG	CA-C-N	5.54	125.71	119.90
1	H	172	ARG	C-N-CA	5.54	125.71	119.90
1	A	348	VAL	N-CA-C	5.54	115.15	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	65	MET	N-CA-C	5.54	118.65	110.46
1	K	65	MET	N-CA-C	5.53	118.65	110.46
1	D	172	ARG	CA-C-N	5.53	125.71	119.90
1	D	172	ARG	C-N-CA	5.53	125.71	119.90
1	B	348	VAL	N-CA-C	5.53	115.13	108.06
1	I	172	ARG	CA-C-N	5.53	125.70	119.90
1	I	172	ARG	C-N-CA	5.53	125.70	119.90
1	E	65	MET	N-CA-C	5.52	118.64	110.46
1	A	172	ARG	CA-C-N	5.52	125.70	119.90
1	A	172	ARG	C-N-CA	5.52	125.70	119.90
1	C	172	ARG	CA-C-N	5.52	125.70	119.90
1	C	172	ARG	C-N-CA	5.52	125.70	119.90
1	D	348	VAL	N-CA-C	5.52	115.12	108.06
1	J	65	MET	N-CA-C	5.52	118.63	110.46
1	J	172	ARG	CA-C-N	5.52	125.70	119.90
1	J	172	ARG	C-N-CA	5.52	125.70	119.90
1	K	348	VAL	N-CA-C	5.52	115.13	108.06
1	C	348	VAL	N-CA-C	5.52	115.12	108.06
1	F	172	ARG	CA-C-N	5.51	125.69	119.90
1	F	172	ARG	C-N-CA	5.51	125.69	119.90
1	E	348	VAL	N-CA-C	5.51	115.11	108.06
1	K	172	ARG	CA-C-N	5.50	125.68	119.90
1	K	172	ARG	C-N-CA	5.50	125.68	119.90
1	L	172	ARG	CA-C-N	5.50	125.68	119.90
1	L	172	ARG	C-N-CA	5.50	125.68	119.90
1	E	172	ARG	CA-C-N	5.50	125.68	119.90
1	E	172	ARG	C-N-CA	5.50	125.68	119.90
1	I	397	TYR	N-CA-C	5.42	119.85	111.56
1	K	397	TYR	N-CA-C	5.41	119.84	111.56
1	G	397	TYR	N-CA-C	5.41	119.84	111.56
1	J	397	TYR	N-CA-C	5.41	119.84	111.56
1	D	397	TYR	N-CA-C	5.40	119.82	111.56
1	H	397	TYR	N-CA-C	5.40	119.82	111.56
1	A	397	TYR	N-CA-C	5.40	119.82	111.56
1	F	397	TYR	N-CA-C	5.40	119.82	111.56
1	L	397	TYR	N-CA-C	5.39	119.81	111.56
1	B	397	TYR	N-CA-C	5.38	119.80	111.56
1	E	397	TYR	N-CA-C	5.37	119.78	111.56
1	C	213[A]	VAL	N-CA-C	5.37	120.51	109.34
1	E	213[A]	VAL	N-CA-C	5.37	120.51	109.34
1	C	397	TYR	N-CA-C	5.37	119.77	111.56
1	L	213[A]	VAL	N-CA-C	5.37	120.50	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	213[A]	VAL	N-CA-C	5.36	120.49	109.34
1	I	203	GLY	N-CA-C	5.36	121.46	115.08
1	D	213[A]	VAL	N-CA-C	5.35	120.48	109.34
1	A	213[A]	VAL	N-CA-C	5.35	120.47	109.34
1	B	213[A]	VAL	N-CA-C	5.35	120.46	109.34
1	G	213[A]	VAL	N-CA-C	5.35	120.46	109.34
1	H	213[A]	VAL	N-CA-C	5.35	120.46	109.34
1	F	213[A]	VAL	N-CA-C	5.35	120.46	109.34
1	J	213[A]	VAL	N-CA-C	5.35	120.46	109.34
1	B	203	GLY	N-CA-C	5.34	121.44	115.08
1	K	213[A]	VAL	N-CA-C	5.34	120.44	109.34
1	E	203	GLY	N-CA-C	5.33	121.42	115.08
1	K	203	GLY	N-CA-C	5.32	121.41	115.08
1	A	203	GLY	N-CA-C	5.32	121.41	115.08
1	L	203	GLY	N-CA-C	5.32	121.41	115.08
1	J	203	GLY	N-CA-C	5.32	121.41	115.08
1	F	203	GLY	N-CA-C	5.31	121.40	115.08
1	H	203	GLY	N-CA-C	5.31	121.40	115.08
1	G	203	GLY	N-CA-C	5.30	121.38	115.08
1	C	203	GLY	N-CA-C	5.29	121.38	115.08
1	D	203	GLY	N-CA-C	5.29	121.38	115.08
1	C	162	THR	N-CA-C	5.25	117.85	110.23
1	G	162	THR	N-CA-C	5.25	117.84	110.23
1	K	270	CYS	N-CA-C	5.25	117.21	108.02
1	B	162	THR	N-CA-C	5.24	117.83	110.23
1	L	162	THR	N-CA-C	5.24	117.83	110.23
1	A	162	THR	N-CA-C	5.24	117.83	110.23
1	I	162	THR	N-CA-C	5.24	117.83	110.23
1	B	270	CYS	N-CA-C	5.24	117.19	108.02
1	D	162	THR	N-CA-C	5.24	117.82	110.23
1	D	270	CYS	N-CA-C	5.24	117.18	108.02
1	K	162	THR	N-CA-C	5.24	117.82	110.23
1	J	270	CYS	N-CA-C	5.23	117.17	108.02
1	H	162	THR	N-CA-C	5.23	117.81	110.23
1	E	270	CYS	N-CA-C	5.23	117.17	108.02
1	F	162	THR	N-CA-C	5.23	117.81	110.23
1	L	270	CYS	N-CA-C	5.23	117.17	108.02
1	J	162	THR	N-CA-C	5.22	117.80	110.23
1	A	270	CYS	N-CA-C	5.22	117.16	108.02
1	E	162	THR	N-CA-C	5.22	117.80	110.23
1	C	270	CYS	N-CA-C	5.21	117.15	108.02
1	F	270	CYS	N-CA-C	5.21	117.13	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	270	CYS	N-CA-C	5.21	117.13	108.02
1	I	270	CYS	N-CA-C	5.20	117.12	108.02
1	G	270	CYS	N-CA-C	5.19	117.10	108.02
1	E	336	ALA	N-CA-C	-5.19	107.12	113.50
1	L	336	ALA	N-CA-C	-5.18	107.13	113.50
1	B	336	ALA	N-CA-C	-5.17	107.13	113.50
1	I	336	ALA	N-CA-C	-5.17	107.14	113.50
1	H	336	ALA	N-CA-C	-5.17	107.14	113.50
1	A	336	ALA	N-CA-C	-5.16	107.15	113.50
1	J	336	ALA	N-CA-C	-5.15	107.16	113.50
1	F	336	ALA	N-CA-C	-5.15	107.17	113.50
1	D	336	ALA	N-CA-C	-5.15	107.17	113.50
1	C	336	ALA	N-CA-C	-5.14	107.17	113.50
1	G	336	ALA	N-CA-C	-5.14	107.18	113.50
1	K	336	ALA	N-CA-C	-5.13	107.19	113.50
1	K	288	ALA	N-CA-C	5.11	118.81	112.47
1	L	288	ALA	N-CA-C	5.11	118.81	112.47
1	E	288	ALA	N-CA-C	5.10	118.80	112.47
1	G	233	ASP	N-CA-C	-5.10	105.42	110.97
1	G	288	ALA	N-CA-C	5.09	118.79	112.47
1	B	288	ALA	N-CA-C	5.09	118.78	112.47
1	F	288	ALA	N-CA-C	5.09	118.78	112.47
1	A	288	ALA	N-CA-C	5.09	118.78	112.47
1	J	288	ALA	N-CA-C	5.09	118.78	112.47
1	C	288	ALA	N-CA-C	5.08	118.78	112.47
1	D	288	ALA	N-CA-C	5.08	118.77	112.47
1	C	233	ASP	N-CA-C	-5.08	105.44	110.97
1	K	233	ASP	N-CA-C	-5.08	105.44	110.97
1	F	181[A]	PRO	CB-CA-C	5.07	117.88	111.39
1	J	181[A]	PRO	CB-CA-C	5.07	117.88	111.39
1	J	233	ASP	N-CA-C	-5.07	105.45	110.97
1	A	233	ASP	N-CA-C	-5.06	105.45	110.97
1	B	233	ASP	N-CA-C	-5.06	105.45	110.97
1	I	288	ALA	N-CA-C	5.06	118.75	112.47
1	H	288	ALA	N-CA-C	5.06	118.74	112.47
1	G	181[A]	PRO	CB-CA-C	5.06	117.86	111.39
1	G	214	ALA	N-CA-C	5.06	117.23	110.35
1	D	233	ASP	N-CA-C	-5.06	105.46	110.97
1	I	233	ASP	N-CA-C	-5.06	105.46	110.97
1	D	181[A]	PRO	CB-CA-C	5.05	117.86	111.39
1	H	233	ASP	N-CA-C	-5.05	105.46	110.97
1	K	181[A]	PRO	CB-CA-C	5.05	117.85	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	233	ASP	N-CA-C	-5.04	105.47	110.97
1	L	233	ASP	N-CA-C	-5.04	105.47	110.97
1	L	181[A]	PRO	CB-CA-C	5.04	117.84	111.39
1	J	257	PRO	N-CA-C	5.04	121.26	113.75
1	A	181[A]	PRO	CB-CA-C	5.04	117.84	111.39
1	F	233	ASP	N-CA-C	-5.04	105.48	110.97
1	B	181[A]	PRO	CB-CA-C	5.03	117.83	111.39
1	C	319	TYR	CA-CB-CG	-5.03	104.84	113.90
1	C	181[A]	PRO	CB-CA-C	5.03	117.83	111.39
1	D	257	PRO	N-CA-C	5.03	121.24	113.75
1	B	319	TYR	CA-CB-CG	-5.03	104.85	113.90
1	G	319	TYR	CA-CB-CG	-5.03	104.85	113.90
1	E	181[A]	PRO	CB-CA-C	5.03	117.82	111.39
1	I	181[A]	PRO	CB-CA-C	5.02	117.82	111.39
1	D	319	TYR	CA-CB-CG	-5.02	104.86	113.90
1	F	257	PRO	N-CA-C	5.02	121.23	113.75
1	H	181[A]	PRO	CB-CA-C	5.02	117.82	111.39
1	K	257	PRO	N-CA-C	5.02	121.23	113.75
1	B	257	PRO	N-CA-C	5.02	121.23	113.75
1	G	257	PRO	N-CA-C	5.02	121.23	113.75
1	E	297	TYR	N-CA-C	-5.01	105.70	111.07
1	L	319	TYR	CA-CB-CG	-5.01	104.87	113.90
1	A	257	PRO	N-CA-C	5.01	121.22	113.75
1	F	319	TYR	CA-CB-CG	-5.01	104.88	113.90
1	J	319	TYR	CA-CB-CG	-5.01	104.88	113.90
1	A	319	TYR	CA-CB-CG	-5.01	104.89	113.90
1	H	257	PRO	N-CA-C	5.01	121.21	113.75
1	E	319	TYR	CA-CB-CG	-5.00	104.89	113.90
1	D	297	TYR	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ALA	Mainchain
1	B	208	ALA	Mainchain
1	C	208	ALA	Mainchain
1	D	208	ALA	Mainchain
1	E	208	ALA	Mainchain
1	F	208	ALA	Mainchain
1	G	208	ALA	Mainchain
1	H	208	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	I	208	ALA	Mainchain
1	J	208	ALA	Mainchain
1	K	208	ALA	Mainchain
1	L	208	ALA	Mainchain

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	3747	0	3621	304	0
1	B	3747	0	3621	298	0
1	C	3747	0	3621	299	0
1	D	3747	0	3621	293	0
1	E	3747	0	3621	294	0
1	F	3747	0	3621	297	0
1	G	3747	0	3621	299	0
1	H	3747	0	3621	298	0
1	I	3747	0	3621	304	0
1	J	3747	0	3621	303	0
1	K	3747	0	3621	304	0
1	L	3747	0	3621	297	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	27	0	10	8	0
3	B	27	0	10	8	0
3	C	27	0	10	8	0
3	D	27	0	10	8	0
3	E	27	0	10	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	27	0	10	8	0
3	G	27	0	10	8	0
3	H	27	0	10	8	0
3	I	27	0	10	8	0
3	J	27	0	10	8	0
3	K	27	0	10	8	0
3	L	27	0	10	8	0
4	A	11	0	10	7	0
4	B	11	0	10	7	0
4	C	11	0	10	6	0
4	D	11	0	10	6	0
4	E	11	0	10	6	0
4	F	11	0	10	7	0
4	G	11	0	10	6	0
4	H	11	0	10	7	0
4	I	11	0	10	6	0
4	J	11	0	10	6	0
4	K	11	0	10	5	0
4	L	11	0	10	7	0
5	A	152	0	0	83	0
5	B	155	0	0	83	0
5	C	152	0	0	83	0
5	D	153	0	0	79	0
5	E	154	0	0	83	0
5	F	152	0	0	81	0
5	G	155	0	0	82	0
5	H	150	0	0	80	0
5	I	156	0	0	85	0
5	J	151	0	0	82	0
5	K	153	0	0	79	0
5	L	153	0	0	82	0
All	All	47280	0	43692	3535	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 40.

All (3535) 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)
3:L:4482:ADP:N9	3:L:4482:ADP:C1'	1.70	1.54
3:C:4473:ADP:N9	3:C:4473:ADP:C1'	1.70	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4479:ADP:N9	3:I:4479:ADP:C1'	1.70	1.53
3:H:4478:ADP:N9	3:H:4478:ADP:C1'	1.70	1.52
3:B:4472:ADP:N9	3:B:4472:ADP:C1'	1.70	1.52
3:J:4480:ADP:N9	3:J:4480:ADP:C1'	1.70	1.51
3:K:4481:ADP:N9	3:K:4481:ADP:C1'	1.70	1.51
3:A:4471:ADP:N9	3:A:4471:ADP:C1'	1.70	1.50
3:F:4476:ADP:N9	3:F:4476:ADP:C1'	1.70	1.50
3:G:4477:ADP:N9	3:G:4477:ADP:C1'	1.70	1.49
3:D:4474:ADP:N9	3:D:4474:ADP:C1'	1.70	1.49
3:E:4475:ADP:N9	3:E:4475:ADP:C1'	1.70	1.49
1:D:211[B]:HIS:O	1:D:212[B]:GLU:HG2	1.07	1.25
1:K:211[B]:HIS:O	1:K:212[B]:GLU:HG2	1.07	1.24
1:G:211[B]:HIS:O	1:G:212[B]:GLU:HG2	1.07	1.23
1:A:211[B]:HIS:O	1:A:212[B]:GLU:HG2	1.07	1.23
1:I:211[B]:HIS:O	1:I:212[B]:GLU:HG2	1.07	1.23
1:F:211[B]:HIS:O	1:F:212[B]:GLU:HG2	1.07	1.23
1:C:211[B]:HIS:O	1:C:212[B]:GLU:HG2	1.07	1.22
1:L:211[B]:HIS:O	1:L:212[B]:GLU:HG2	1.07	1.22
1:E:211[B]:HIS:O	1:E:212[B]:GLU:HG2	1.07	1.21
1:H:211[B]:HIS:O	1:H:212[B]:GLU:HG2	1.07	1.21
1:A:337:ARG:HG3	1:A:338:ASN:N	1.31	1.20
1:B:211[B]:HIS:O	1:B:212[B]:GLU:HG2	1.07	1.20
1:J:211[B]:HIS:O	1:J:212[B]:GLU:HG2	1.07	1.20
1:K:337:ARG:HG3	1:K:338:ASN:N	1.32	1.19
1:F:337:ARG:HG3	1:F:338:ASN:N	1.31	1.19
1:L:329:PRO:HG2	1:L:359:ARG:HD2	1.24	1.19
1:F:323:VAL:HG12	5:F:6047:HOH:O	1.44	1.18
1:C:323:VAL:HG12	5:C:6037:HOH:O	1.44	1.17
1:G:323:VAL:HG12	5:G:6047:HOH:O	1.44	1.17
1:F:179[A]:TYR:OH	5:F:5911:HOH:O	1.59	1.17
1:H:337:ARG:CG	1:H:338:ASN:N	2.07	1.17
1:L:337:ARG:CG	1:L:338:ASN:N	2.07	1.17
1:I:323:VAL:HG12	5:I:6058:HOH:O	1.44	1.17
1:A:337:ARG:CG	1:A:338:ASN:N	2.07	1.16
1:H:337:ARG:HG3	1:H:338:ASN:N	1.32	1.16
1:C:337:ARG:HG3	1:C:338:ASN:N	1.31	1.16
1:E:337:ARG:CG	1:E:338:ASN:N	2.07	1.15
1:J:337:ARG:CG	1:J:338:ASN:N	2.07	1.15
1:F:329:PRO:HG2	1:F:359:ARG:HD2	1.24	1.15
1:K:323:VAL:HG12	5:K:1677:HOH:O	1.44	1.15
1:F:337:ARG:CG	1:F:338:ASN:N	2.07	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:323:VAL:HG12	5:J:6054:HOH:O	1.44	1.15
1:H:323:VAL:HG12	5:H:6051:HOH:O	1.44	1.15
1:L:323:VAL:HG12	5:L:1830:HOH:O	1.44	1.15
1:I:337:ARG:HG3	1:I:338:ASN:N	1.31	1.15
1:E:337:ARG:HG3	1:E:338:ASN:N	1.31	1.14
1:A:323:VAL:HG12	5:A:6037:HOH:O	1.44	1.14
1:H:211[B]:HIS:O	1:H:212[B]:GLU:CG	1.96	1.14
1:L:179[A]:TYR:OH	5:L:1632:HOH:O	1.65	1.14
1:D:323:VAL:HG12	5:D:6040:HOH:O	1.44	1.14
1:C:179[A]:TYR:OH	5:C:6049:HOH:O	1.61	1.14
1:I:329:PRO:HG2	1:I:359:ARG:HD2	1.24	1.14
1:A:211[B]:HIS:O	1:A:212[B]:GLU:CG	1.96	1.14
1:B:211[B]:HIS:O	1:B:212[B]:GLU:CG	1.96	1.14
1:D:211[B]:HIS:O	1:D:212[B]:GLU:CG	1.96	1.14
1:G:337:ARG:HG3	1:G:338:ASN:N	1.31	1.14
1:C:329:PRO:HG2	1:C:359:ARG:HD2	1.24	1.13
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.83	1.13
1:F:211[B]:HIS:O	1:F:212[B]:GLU:CG	1.96	1.13
1:H:329:PRO:HG2	1:H:359:ARG:HD2	1.24	1.13
1:L:211[B]:HIS:O	1:L:212[B]:GLU:CG	1.96	1.13
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.83	1.13
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.83	1.13
1:K:360:PHE:CD2	1:K:361:PRO:HD3	1.83	1.13
1:E:323:VAL:HG12	5:E:759:HOH:O	1.44	1.13
1:G:211[B]:HIS:O	1:G:212[B]:GLU:CG	1.96	1.13
1:B:337:ARG:CG	1:B:338:ASN:N	2.07	1.13
1:E:211[B]:HIS:O	1:E:212[B]:GLU:CG	1.96	1.12
1:G:360:PHE:CD2	1:G:361:PRO:HD3	1.83	1.13
1:J:211[B]:HIS:O	1:J:212[B]:GLU:CG	1.96	1.12
1:K:211[B]:HIS:O	1:K:212[B]:GLU:CG	1.96	1.13
1:E:293:GLN:HB2	5:E:752:HOH:O	1.49	1.12
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.83	1.12
1:I:211[B]:HIS:O	1:I:212[B]:GLU:CG	1.96	1.12
1:J:337:ARG:HG3	1:J:338:ASN:N	1.31	1.12
1:L:360:PHE:CD2	1:L:361:PRO:HD3	1.83	1.12
1:C:211[B]:HIS:O	1:C:212[B]:GLU:CG	1.96	1.12
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.84	1.12
1:E:211[B]:HIS:C	1:E:212[B]:GLU:HG2	1.75	1.12
1:E:329:PRO:HG2	1:E:359:ARG:HD2	1.24	1.12
1:F:211[B]:HIS:C	1:F:212[B]:GLU:HG2	1.75	1.12
1:G:211[B]:HIS:C	1:G:212[B]:GLU:HG2	1.75	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:360:PHE:CD2	1:J:361:PRO:HD3	1.83	1.12
1:B:323:VAL:HG12	5:B:6038:HOH:O	1.44	1.12
1:F:360:PHE:CD2	1:F:361:PRO:HD3	1.83	1.12
1:G:293:GLN:HB2	5:G:6041:HOH:O	1.49	1.12
1:B:329:PRO:HG2	1:B:359:ARG:HD2	1.24	1.11
1:B:360:PHE:CD2	1:B:361:PRO:HD3	1.83	1.11
1:A:211[B]:HIS:C	1:A:212[B]:GLU:HG2	1.75	1.11
1:G:337:ARG:CG	1:G:338:ASN:N	2.07	1.11
1:I:360:PHE:CD2	1:I:361:PRO:HD3	1.83	1.11
1:C:293:GLN:HB2	5:C:6031:HOH:O	1.49	1.11
1:D:211[B]:HIS:C	1:D:212[B]:GLU:HG2	1.75	1.11
1:D:337:ARG:HG3	1:D:338:ASN:N	1.31	1.11
1:K:211[B]:HIS:C	1:K:212[B]:GLU:HG2	1.75	1.11
1:I:337:ARG:CG	1:I:338:ASN:N	2.07	1.11
1:J:211[B]:HIS:C	1:J:212[B]:GLU:HG2	1.75	1.11
1:J:329:PRO:HG2	1:J:359:ARG:HD2	1.24	1.11
1:B:211[B]:HIS:C	1:B:212[B]:GLU:HG2	1.75	1.10
1:B:293:GLN:HB2	5:B:6032:HOH:O	1.49	1.10
1:I:211[B]:HIS:C	1:I:212[B]:GLU:HG2	1.75	1.10
1:K:179[A]:TYR:OH	5:K:1479:HOH:O	1.68	1.10
1:D:337:ARG:CG	1:D:338:ASN:N	2.07	1.10
1:H:211[B]:HIS:C	1:H:212[B]:GLU:HG2	1.75	1.10
1:B:337:ARG:HG3	1:B:338:ASN:N	1.32	1.10
1:I:293:GLN:HB2	5:I:6052:HOH:O	1.49	1.10
1:J:293:GLN:HB2	5:J:6048:HOH:O	1.49	1.10
1:L:1:SER:HB2	1:L:4:HIS:HB3	1.34	1.10
1:L:211[B]:HIS:C	1:L:212[B]:GLU:HG2	1.75	1.10
1:D:329:PRO:HG2	1:D:359:ARG:HD2	1.24	1.10
1:H:293:GLN:HB2	5:H:6045:HOH:O	1.49	1.10
1:K:1:SER:HB2	1:K:4:HIS:HB3	1.34	1.10
1:L:293:GLN:HB2	5:L:1823:HOH:O	1.50	1.10
1:A:1:SER:HB2	1:A:4:HIS:HB3	1.34	1.09
1:J:1:SER:HB2	1:J:4:HIS:HB3	1.34	1.09
1:K:293:GLN:HB2	5:K:1670:HOH:O	1.49	1.09
1:A:329:PRO:HG2	1:A:359:ARG:HD2	1.24	1.09
1:B:1:SER:HB2	1:B:4:HIS:HB3	1.34	1.09
1:C:337:ARG:CG	1:C:338:ASN:N	2.07	1.08
1:K:329:PRO:HG2	1:K:359:ARG:HD2	1.24	1.08
1:F:293:GLN:HB2	5:F:6041:HOH:O	1.49	1.08
1:G:329:PRO:HG2	1:G:359:ARG:HD2	1.24	1.08
1:K:337:ARG:CG	1:K:338:ASN:N	2.07	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLN:HB2	5:A:6031:HOH:O	1.49	1.08
1:C:224:ARG:HH21	1:C:224:ARG:HG2	1.19	1.08
1:D:293:GLN:HB2	5:D:6034:HOH:O	1.49	1.08
1:C:211[B]:HIS:C	1:C:212[B]:GLU:HG2	1.75	1.08
1:D:179[A]:TYR:OH	5:D:6052:HOH:O	1.70	1.08
1:J:224:ARG:HG2	1:J:224:ARG:HH21	1.19	1.08
1:D:224:ARG:HG2	1:D:224:ARG:HH21	1.19	1.07
1:F:1:SER:HB2	1:F:4:HIS:HB3	1.34	1.07
1:L:224:ARG:HG2	1:L:224:ARG:HH21	1.19	1.07
1:D:1:SER:HB2	1:D:4:HIS:HB3	1.34	1.07
1:B:211[B]:HIS:CD2	1:B:211[B]:HIS:N	2.22	1.06
1:E:1:SER:HB2	1:E:4:HIS:HB3	1.34	1.06
1:I:224:ARG:HG2	1:I:224:ARG:HH21	1.19	1.06
1:J:211[B]:HIS:CD2	1:J:211[B]:HIS:N	2.22	1.06
1:L:337:ARG:HG3	1:L:338:ASN:N	1.31	1.06
1:A:224:ARG:HG2	1:A:224:ARG:HH21	1.19	1.06
1:I:179[A]:TYR:OH	5:I:5921:HOH:O	1.74	1.06
1:G:179[A]:TYR:OH	5:G:6061:HOH:O	1.74	1.05
1:D:211[B]:HIS:CD2	1:D:211[B]:HIS:N	2.22	1.05
1:G:211[B]:HIS:CD2	1:G:211[B]:HIS:N	2.22	1.05
1:H:1:SER:HB2	1:H:4:HIS:HB3	1.34	1.05
1:A:211[B]:HIS:N	1:A:211[B]:HIS:CD2	2.22	1.05
1:H:176[B]:LYS:O	1:H:178[B]:GLY:N	1.90	1.05
1:E:179[A]:TYR:OH	5:E:867:HOH:O	1.73	1.05
1:F:176[B]:LYS:O	1:F:178[B]:GLY:N	1.90	1.05
1:G:176[B]:LYS:O	1:G:178[B]:GLY:N	1.90	1.05
1:C:176[B]:LYS:O	1:C:178[B]:GLY:N	1.90	1.04
1:E:176[B]:LYS:O	1:E:178[B]:GLY:N	1.90	1.04
1:G:224:ARG:HG2	1:G:224:ARG:HH21	1.19	1.04
1:H:179[A]:TYR:OH	5:H:5917:HOH:O	1.73	1.04
1:K:176[B]:LYS:O	1:K:178[B]:GLY:N	1.90	1.04
1:G:1:SER:HB2	1:G:4:HIS:HB3	1.34	1.04
1:A:176[B]:LYS:O	1:A:178[B]:GLY:N	1.90	1.04
1:C:1:SER:HB2	1:C:4:HIS:HB3	1.34	1.04
1:I:176[B]:LYS:O	1:I:178[B]:GLY:N	1.90	1.04
1:B:176[B]:LYS:O	1:B:178[B]:GLY:N	1.90	1.04
1:I:1:SER:HB2	1:I:4:HIS:HB3	1.34	1.04
1:C:211[B]:HIS:N	1:C:211[B]:HIS:CD2	2.22	1.03
1:D:179[B]:TYR:CD1	1:D:212[B]:GLU:HA	1.93	1.03
1:L:179[B]:TYR:CD1	1:L:212[B]:GLU:HA	1.93	1.03
1:E:179[B]:TYR:CD1	1:E:212[B]:GLU:HA	1.93	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179[B]:TYR:CD1	1:H:212[B]:GLU:HA	1.93	1.03
1:D:176[B]:LYS:O	1:D:178[B]:GLY:N	1.90	1.03
1:J:179[B]:TYR:CD1	1:J:212[B]:GLU:HA	1.93	1.03
1:K:211[B]:HIS:N	1:K:211[B]:HIS:CD2	2.22	1.03
1:C:179[B]:TYR:CD1	1:C:212[B]:GLU:HA	1.93	1.03
1:F:224:ARG:HH21	1:F:224:ARG:HG2	1.19	1.03
1:G:179[B]:TYR:CD1	1:G:212[B]:GLU:HA	1.93	1.03
1:J:176[B]:LYS:O	1:J:178[B]:GLY:N	1.90	1.03
1:F:179[B]:TYR:CD1	1:F:212[B]:GLU:HA	1.93	1.02
1:H:224:ARG:HH21	1:H:224:ARG:HG2	1.19	1.02
1:J:329:PRO:CG	1:J:359:ARG:HD2	1.89	1.02
1:B:179[A]:TYR:OH	5:B:6052:HOH:O	1.76	1.02
1:E:211[B]:HIS:CD2	1:E:211[B]:HIS:N	2.22	1.02
1:F:211[B]:HIS:N	1:F:211[B]:HIS:CD2	2.22	1.02
1:H:329:PRO:CG	1:H:359:ARG:HD2	1.90	1.02
1:L:329:PRO:CG	1:L:359:ARG:HD2	1.89	1.02
1:A:329:PRO:CG	1:A:359:ARG:HD2	1.90	1.02
1:C:329:PRO:CG	1:C:359:ARG:HD2	1.89	1.02
1:D:329:PRO:CG	1:D:359:ARG:HD2	1.90	1.02
1:B:179[B]:TYR:CD1	1:B:212[B]:GLU:HA	1.93	1.02
1:K:224:ARG:HH21	1:K:224:ARG:HG2	1.19	1.02
1:L:176[B]:LYS:O	1:L:178[B]:GLY:N	1.90	1.02
1:L:211[B]:HIS:CD2	1:L:211[B]:HIS:N	2.22	1.02
1:A:179[B]:TYR:CD1	1:A:212[B]:GLU:HA	1.93	1.02
1:F:329:PRO:CG	1:F:359:ARG:HD2	1.90	1.02
1:H:211[B]:HIS:CD2	1:H:211[B]:HIS:N	2.22	1.02
1:I:179[B]:TYR:CD1	1:I:212[B]:GLU:HA	1.93	1.02
1:E:224:ARG:HG2	1:E:224:ARG:HH21	1.19	1.01
1:K:329:PRO:CG	1:K:359:ARG:HD2	1.90	1.01
1:B:329:PRO:CG	1:B:359:ARG:HD2	1.90	1.01
1:B:224:ARG:HG2	1:B:224:ARG:HH21	1.18	1.01
1:K:179[B]:TYR:CD1	1:K:212[B]:GLU:HA	1.93	1.01
1:L:285:ASP:HA	5:L:1816:HOH:O	1.60	1.01
1:D:211[B]:HIS:C	1:D:212[B]:GLU:CG	2.33	1.01
1:I:211[B]:HIS:N	1:I:211[B]:HIS:CD2	2.22	1.00
1:I:329:PRO:CG	1:I:359:ARG:HD2	1.90	1.00
1:J:285:ASP:HA	5:J:6041:HOH:O	1.60	1.00
1:E:329:PRO:CG	1:E:359:ARG:HD2	1.89	1.00
1:I:285:ASP:HA	5:I:6045:HOH:O	1.60	1.00
1:G:329:PRO:CG	1:G:359:ARG:HD2	1.90	1.00
1:A:179[A]:TYR:OH	5:A:6048:HOH:O	1.78	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASP:HA	5:A:6024:HOH:O	1.60	1.00
1:H:285:ASP:HA	5:H:6038:HOH:O	1.61	0.99
1:B:285:ASP:HA	5:B:6025:HOH:O	1.60	0.99
1:J:211[B]:HIS:C	1:J:212[B]:GLU:CG	2.33	0.99
1:C:285:ASP:HA	5:C:6024:HOH:O	1.60	0.99
1:G:285:ASP:HA	5:G:6034:HOH:O	1.60	0.99
1:D:285:ASP:HA	5:D:6027:HOH:O	1.60	0.98
1:L:337:ARG:CG	1:L:338:ASN:H	1.73	0.98
1:J:179[A]:TYR:OH	5:J:5919:HOH:O	1.79	0.98
1:C:211[B]:HIS:C	1:C:212[B]:GLU:CG	2.33	0.98
1:E:285:ASP:HA	5:E:745:HOH:O	1.60	0.98
1:K:285:ASP:HA	5:K:1663:HOH:O	1.60	0.98
1:B:211[B]:HIS:C	1:B:212[B]:GLU:CG	2.33	0.98
1:F:285:ASP:HA	5:F:6034:HOH:O	1.60	0.98
1:J:337:ARG:HG3	1:J:338:ASN:H	0.87	0.97
1:K:211[B]:HIS:C	1:K:212[B]:GLU:CG	2.33	0.97
1:F:337:ARG:CG	1:F:338:ASN:H	1.73	0.97
1:I:211[B]:HIS:C	1:I:212[B]:GLU:CG	2.33	0.97
1:G:211[B]:HIS:C	1:G:212[B]:GLU:CG	2.33	0.96
1:C:406:GLU:HA	5:C:5984:HOH:O	1.66	0.96
1:L:337:ARG:HG3	1:L:338:ASN:H	0.87	0.96
1:D:192[A]:ARG:HD3	1:D:219:ASN:HD22	1.31	0.96
1:F:211[B]:HIS:C	1:F:212[B]:GLU:CG	2.33	0.96
1:L:406:GLU:HA	5:L:1771:HOH:O	1.66	0.96
1:L:192[A]:ARG:HD3	1:L:219:ASN:HD22	1.31	0.96
1:A:192[A]:ARG:HD3	1:A:219:ASN:HD22	1.31	0.96
1:A:406:GLU:HA	5:A:5984:HOH:O	1.66	0.96
1:F:406:GLU:HA	5:F:5994:HOH:O	1.66	0.96
1:B:406:GLU:HA	5:B:5985:HOH:O	1.66	0.95
1:G:337:ARG:HG3	1:G:338:ASN:H	0.87	0.95
1:J:406:GLU:HA	5:J:6001:HOH:O	1.66	0.95
1:I:192[A]:ARG:HD3	1:I:219:ASN:HD22	1.31	0.95
1:E:337:ARG:CG	1:E:338:ASN:H	1.73	0.95
1:J:192[A]:ARG:HD3	1:J:219:ASN:HD22	1.31	0.95
1:C:409:GLN:HB3	5:C:6026:HOH:O	1.67	0.95
1:L:409:GLN:HB3	5:L:1818:HOH:O	1.67	0.95
1:F:192[A]:ARG:HD3	1:F:219:ASN:HD22	1.31	0.94
1:H:406:GLU:HA	5:H:5998:HOH:O	1.66	0.94
1:I:337:ARG:HG3	1:I:338:ASN:H	0.87	0.94
1:K:406:GLU:HA	5:K:1618:HOH:O	1.66	0.94
1:A:337:ARG:CG	1:A:338:ASN:H	1.73	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLN:HB3	5:A:6026:HOH:O	1.67	0.94
1:J:409:GLN:HB3	5:J:6043:HOH:O	1.67	0.94
1:B:192[A]:ARG:HD3	1:B:219:ASN:HD22	1.31	0.94
1:H:211[B]:HIS:C	1:H:212[B]:GLU:CG	2.33	0.94
1:H:409:GLN:HB3	5:H:6040:HOH:O	1.67	0.94
1:I:406:GLU:HA	5:I:6005:HOH:O	1.66	0.94
1:D:406:GLU:HA	5:D:5987:HOH:O	1.66	0.94
1:E:406:GLU:HA	5:E:700:HOH:O	1.66	0.94
1:A:211[B]:HIS:C	1:A:212[B]:GLU:CG	2.33	0.94
1:G:192[A]:ARG:HD3	1:G:219:ASN:HD22	1.31	0.94
1:J:337:ARG:CG	1:J:338:ASN:H	1.73	0.94
1:H:192[A]:ARG:HD3	1:H:219:ASN:HD22	1.31	0.93
1:D:409:GLN:HB3	5:D:6029:HOH:O	1.67	0.93
1:H:337:ARG:HG3	1:H:338:ASN:H	0.87	0.93
1:C:177[B]:GLY:O	1:C:178[B]:GLY:C	2.12	0.93
1:G:406:GLU:HA	5:G:5994:HOH:O	1.66	0.93
1:L:177[B]:GLY:O	1:L:178[B]:GLY:C	2.12	0.93
1:K:192[A]:ARG:HD3	1:K:219:ASN:HD22	1.31	0.93
1:C:192[A]:ARG:HD3	1:C:219:ASN:HD22	1.31	0.93
1:I:409:GLN:HB3	5:I:6047:HOH:O	1.67	0.93
1:E:192[A]:ARG:HD3	1:E:219:ASN:HD22	1.31	0.92
1:F:409:GLN:HB3	5:F:6036:HOH:O	1.67	0.92
1:K:409:GLN:HB3	5:K:1665:HOH:O	1.67	0.92
1:E:177[B]:GLY:O	1:E:178[B]:GLY:C	2.12	0.92
1:H:211[B]:HIS:CD2	1:H:211[B]:HIS:H	1.87	0.92
1:K:337:ARG:CG	1:K:338:ASN:H	1.73	0.92
1:I:177[B]:GLY:O	1:I:178[B]:GLY:C	2.12	0.92
1:D:426:GLU:HB2	5:D:5963:HOH:O	1.70	0.92
1:E:211[B]:HIS:C	1:E:212[B]:GLU:CG	2.33	0.92
1:E:409:GLN:HB3	5:E:747:HOH:O	1.67	0.92
1:B:177[B]:GLY:O	1:B:178[B]:GLY:C	2.12	0.92
1:H:426:GLU:HB2	5:H:5974:HOH:O	1.70	0.92
1:I:337:ARG:CG	1:I:338:ASN:H	1.73	0.92
1:K:177[B]:GLY:O	1:K:178[B]:GLY:C	2.12	0.92
1:B:409:GLN:HB3	5:B:6027:HOH:O	1.67	0.92
1:F:337:ARG:HG3	1:F:338:ASN:H	0.87	0.92
1:H:177[B]:GLY:O	1:H:178[B]:GLY:C	2.12	0.91
1:A:177[B]:GLY:O	1:A:178[B]:GLY:C	2.12	0.91
1:D:337:ARG:HG3	1:D:338:ASN:H	0.87	0.91
1:A:426:GLU:HB2	5:A:5960:HOH:O	1.70	0.91
1:D:177[B]:GLY:O	1:D:178[B]:GLY:C	2.12	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177[B]:GLY:O	1:F:178[B]:GLY:C	2.12	0.91
1:K:211[B]:HIS:CD2	1:K:211[B]:HIS:H	1.87	0.91
1:D:179[B]:TYR:CE2	1:D:211[B]:HIS:HB2	2.06	0.91
1:J:426:GLU:HB2	5:J:5977:HOH:O	1.70	0.91
1:K:179[B]:TYR:CE2	1:K:211[B]:HIS:HB2	2.06	0.91
1:F:211[B]:HIS:CD2	1:F:211[B]:HIS:H	1.87	0.91
1:L:211[B]:HIS:C	1:L:212[B]:GLU:CG	2.33	0.91
1:A:179[B]:TYR:CE2	1:A:211[B]:HIS:HB2	2.06	0.91
1:G:179[B]:TYR:CE2	1:G:211[B]:HIS:HB2	2.06	0.91
1:G:409:GLN:HB3	5:G:6036:HOH:O	1.67	0.91
1:I:179[B]:TYR:CE2	1:I:211[B]:HIS:HB2	2.06	0.91
1:C:179[B]:TYR:CE2	1:C:211[B]:HIS:HB2	2.06	0.90
1:C:211[B]:HIS:CD2	1:C:211[B]:HIS:H	1.87	0.90
1:I:426:GLU:HB2	5:I:5981:HOH:O	1.70	0.90
1:J:179[B]:TYR:CE2	1:J:211[B]:HIS:HB2	2.06	0.90
1:A:337:ARG:HG3	1:A:338:ASN:H	0.87	0.90
1:B:337:ARG:HG3	1:B:338:ASN:H	0.87	0.90
1:C:426:GLU:HB2	5:C:5960:HOH:O	1.70	0.90
1:H:323:VAL:HA	5:H:6051:HOH:O	1.72	0.90
1:L:179[B]:TYR:CE2	1:L:211[B]:HIS:HB2	2.06	0.90
1:B:179[B]:TYR:CE2	1:B:211[B]:HIS:HB2	2.06	0.90
1:B:426:GLU:HB2	5:B:5961:HOH:O	1.70	0.90
1:H:179[B]:TYR:CE2	1:H:211[B]:HIS:HB2	2.06	0.90
1:A:323:VAL:HA	5:A:6037:HOH:O	1.72	0.90
1:D:211[B]:HIS:CD2	1:D:211[B]:HIS:H	1.87	0.90
1:E:426:GLU:HB2	5:E:675:HOH:O	1.70	0.90
1:K:426:GLU:HB2	5:K:1593:HOH:O	1.70	0.90
1:B:337:ARG:CG	1:B:338:ASN:H	1.73	0.90
1:C:302:ILE:HD13	5:C:5998:HOH:O	1.72	0.90
1:E:211[B]:HIS:CD2	1:E:211[B]:HIS:H	1.87	0.90
1:L:426:GLU:HB2	5:L:1746:HOH:O	1.70	0.90
1:E:179[B]:TYR:CE2	1:E:211[B]:HIS:HB2	2.06	0.90
1:F:179[B]:TYR:CE2	1:F:211[B]:HIS:HB2	2.06	0.90
1:A:302:ILE:HD13	5:A:5998:HOH:O	1.72	0.89
1:H:302:ILE:HD13	5:H:6012:HOH:O	1.72	0.89
1:D:302:ILE:HD13	5:D:6001:HOH:O	1.72	0.89
1:G:426:GLU:HB2	5:G:5970:HOH:O	1.70	0.89
1:E:302:ILE:HD13	5:E:717:HOH:O	1.73	0.89
1:I:302:ILE:HD13	5:I:6019:HOH:O	1.72	0.89
1:F:302:ILE:HD13	5:F:6008:HOH:O	1.72	0.89
1:D:323:VAL:HA	5:D:6040:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211[B]:HIS:CD2	1:G:211[B]:HIS:H	1.87	0.89
1:K:323:VAL:HA	5:K:1677:HOH:O	1.72	0.89
1:F:323:VAL:HA	5:F:6047:HOH:O	1.72	0.89
1:J:302:ILE:HD13	5:J:6015:HOH:O	1.72	0.89
1:L:302:ILE:HD13	5:L:1788:HOH:O	1.72	0.89
3:A:4471:ADP:H3'	5:A:5976:HOH:O	1.73	0.89
3:E:4475:ADP:H3'	5:E:691:HOH:O	1.73	0.89
1:J:177[B]:GLY:O	1:J:178[B]:GLY:C	2.12	0.89
1:C:337:ARG:CG	1:C:338:ASN:H	1.73	0.88
1:G:177[B]:GLY:O	1:G:178[B]:GLY:C	2.12	0.88
3:K:4481:ADP:H3'	5:K:1609:HOH:O	1.73	0.88
1:B:211[B]:HIS:CD2	1:B:211[B]:HIS:H	1.87	0.88
1:B:323:VAL:HA	5:B:6038:HOH:O	1.72	0.88
3:H:4478:ADP:H3'	5:H:5990:HOH:O	1.73	0.88
1:K:177[B]:GLY:O	1:K:178[B]:GLY:O	1.92	0.88
1:I:177[B]:GLY:O	1:I:178[B]:GLY:O	1.92	0.88
1:F:426:GLU:HB2	5:F:5970:HOH:O	1.70	0.88
1:G:177[B]:GLY:O	1:G:178[B]:GLY:O	1.92	0.88
1:J:323:VAL:HA	5:J:6054:HOH:O	1.72	0.88
1:C:177[B]:GLY:O	1:C:178[B]:GLY:O	1.92	0.88
1:C:323:VAL:HA	5:C:6037:HOH:O	1.72	0.88
1:J:211[B]:HIS:CD2	1:J:211[B]:HIS:H	1.87	0.88
1:A:211[B]:HIS:CD2	1:A:211[B]:HIS:H	1.87	0.88
1:D:177[B]:GLY:O	1:D:178[B]:GLY:O	1.92	0.88
1:H:340:SER:OG	1:H:396:LEU:HA	1.74	0.88
1:I:323:VAL:HA	5:I:6058:HOH:O	1.72	0.88
1:A:177[B]:GLY:O	1:A:178[B]:GLY:O	1.92	0.88
1:B:177[B]:GLY:O	1:B:178[B]:GLY:O	1.92	0.88
1:I:340:SER:OG	1:I:396:LEU:HA	1.74	0.88
1:C:337:ARG:HG3	1:C:338:ASN:H	0.87	0.87
1:D:180[B]:PHE:CD1	1:E:31:VAL:HB	2.09	0.87
1:E:177[B]:GLY:O	1:E:178[B]:GLY:O	1.92	0.87
3:L:4482:ADP:H3'	5:L:1762:HOH:O	1.73	0.87
1:K:302:ILE:HD13	5:K:1635:HOH:O	1.72	0.87
1:L:323:VAL:HA	5:L:1830:HOH:O	1.72	0.87
1:F:177[B]:GLY:O	1:F:178[B]:GLY:O	1.92	0.87
1:B:302:ILE:HD13	5:B:5999:HOH:O	1.72	0.87
1:G:302:ILE:HD13	5:G:6008:HOH:O	1.72	0.87
1:G:323:VAL:HA	5:G:6047:HOH:O	1.72	0.87
1:B:340:SER:OG	1:B:396:LEU:HA	1.74	0.87
1:E:340:SER:OG	1:E:396:LEU:HA	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:4480:ADP:H3'	5:J:5993:HOH:O	1.73	0.87
1:L:211[B]:HIS:CD2	1:L:211[B]:HIS:H	1.87	0.87
3:F:4476:ADP:H3'	5:F:5986:HOH:O	1.73	0.87
3:C:4473:ADP:H3'	5:C:5976:HOH:O	1.73	0.87
1:E:323:VAL:HA	5:E:759:HOH:O	1.72	0.87
3:I:4479:ADP:H3'	5:I:5997:HOH:O	1.73	0.87
1:H:337:ARG:CG	1:H:338:ASN:H	1.73	0.87
1:L:177[B]:GLY:O	1:L:178[B]:GLY:O	1.92	0.87
1:D:340:SER:OG	1:D:396:LEU:HA	1.74	0.87
3:D:4474:ADP:H3'	5:D:5979:HOH:O	1.73	0.86
3:G:4477:ADP:H3'	5:G:5986:HOH:O	1.73	0.86
1:L:340:SER:OG	1:L:396:LEU:HA	1.74	0.86
3:B:4472:ADP:H3'	5:B:5977:HOH:O	1.73	0.86
1:C:340:SER:OG	1:C:396:LEU:HA	1.74	0.86
1:J:177[B]:GLY:O	1:J:178[B]:GLY:O	1.92	0.86
1:K:340:SER:OG	1:K:396:LEU:HA	1.74	0.86
1:H:177[B]:GLY:O	1:H:178[B]:GLY:O	1.92	0.86
1:A:340:SER:OG	1:A:396:LEU:HA	1.74	0.86
1:G:340:SER:OG	1:G:396:LEU:HA	1.74	0.86
1:I:211[B]:HIS:CD2	1:I:211[B]:HIS:H	1.87	0.86
1:D:435:THR:HG23	5:D:5960:HOH:O	1.76	0.86
1:E:180[B]:PHE:CD1	1:F:31:VAL:HB	2.10	0.86
1:J:340:SER:OG	1:J:396:LEU:HA	1.74	0.86
1:A:435:THR:HG23	5:A:5957:HOH:O	1.76	0.85
1:J:435:THR:HG23	5:J:5974:HOH:O	1.76	0.85
1:L:435:THR:HG23	5:L:1742:HOH:O	1.76	0.85
1:D:337:ARG:CG	1:D:338:ASN:H	1.73	0.85
1:H:435:THR:HG23	5:H:5971:HOH:O	1.76	0.85
1:B:435:THR:HG23	5:B:5958:HOH:O	1.76	0.85
1:F:340:SER:OG	1:F:396:LEU:HA	1.74	0.85
1:I:435:THR:HG23	5:I:5978:HOH:O	1.76	0.85
1:E:435:THR:HG23	5:E:671:HOH:O	1.76	0.84
1:G:165:GLU:HB2	5:G:5971:HOH:O	1.78	0.84
1:K:165:GLU:HB2	5:K:1594:HOH:O	1.78	0.84
1:K:435:THR:HG23	5:K:1589:HOH:O	1.76	0.84
1:E:165:GLU:HB2	5:E:676:HOH:O	1.78	0.84
1:A:165:GLU:HB2	5:A:5961:HOH:O	1.78	0.83
1:I:165:GLU:HB2	5:I:5982:HOH:O	1.78	0.83
1:C:435:THR:HG23	5:C:5957:HOH:O	1.76	0.83
1:C:458:HIS:HD2	1:C:460:VAL:H	1.26	0.83
1:C:165:GLU:HB2	5:C:5961:HOH:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:ARG:HG3	1:E:338:ASN:H	0.87	0.83
1:F:435:THR:HG23	5:F:5967:HOH:O	1.76	0.83
1:K:458:HIS:HD2	1:K:460:VAL:H	1.26	0.83
1:B:165:GLU:HB2	5:B:5962:HOH:O	1.78	0.83
1:J:458:HIS:HD2	1:J:460:VAL:H	1.26	0.83
1:B:458:HIS:HD2	1:B:460:VAL:H	1.26	0.83
1:G:435:THR:HG23	5:G:5967:HOH:O	1.76	0.83
1:A:458:HIS:HD2	1:A:460:VAL:H	1.26	0.83
1:E:458:HIS:HD2	1:E:460:VAL:H	1.26	0.82
1:J:165:GLU:HB2	5:J:5978:HOH:O	1.78	0.82
1:H:165:GLU:HB2	5:H:5975:HOH:O	1.78	0.82
1:L:165:GLU:HB2	5:L:1747:HOH:O	1.78	0.82
1:G:458:HIS:HD2	1:G:460:VAL:H	1.26	0.82
1:I:458:HIS:HD2	1:I:460:VAL:H	1.26	0.82
1:B:180[B]:PHE:CE1	1:C:31:VAL:HB	2.13	0.82
1:D:165:GLU:HB2	5:D:5964:HOH:O	1.78	0.82
1:H:176[B]:LYS:C	1:H:178[B]:GLY:H	1.88	0.82
1:A:176[B]:LYS:C	1:A:178[B]:GLY:H	1.88	0.81
1:E:180[B]:PHE:CE1	1:F:31:VAL:HB	2.14	0.81
1:L:458:HIS:HD2	1:L:460:VAL:H	1.26	0.81
1:B:176[B]:LYS:C	1:B:178[B]:GLY:H	1.88	0.81
1:F:165:GLU:HB2	5:F:5971:HOH:O	1.78	0.81
1:I:176[B]:LYS:C	1:I:178[B]:GLY:H	1.88	0.81
1:B:40:ALA:CB	5:B:5982:HOH:O	2.29	0.81
3:D:4474:ADP:N9	3:D:4474:ADP:HI ¹	1.96	0.81
1:L:40:ALA:CB	5:L:1768:HOH:O	2.29	0.81
3:A:4471:ADP:N9	3:A:4471:ADP:HI ¹	1.96	0.80
1:G:337:ARG:CG	1:G:338:ASN:H	1.73	0.80
1:J:176[B]:LYS:C	1:J:178[B]:GLY:H	1.88	0.80
1:K:40:ALA:CB	5:K:1615:HOH:O	2.29	0.80
1:A:40:ALA:CB	5:A:5981:HOH:O	2.29	0.80
1:G:176[B]:LYS:C	1:G:178[B]:GLY:H	1.88	0.80
3:B:4472:ADP:N9	3:B:4472:ADP:HI ¹	1.96	0.80
1:L:176[B]:LYS:C	1:L:178[B]:GLY:H	1.88	0.80
1:C:40:ALA:CB	5:C:5981:HOH:O	2.29	0.80
1:E:170:GLY:HA2	1:E:172:ARG:HH22	1.47	0.80
1:I:170:GLY:HA2	1:I:172:ARG:HH22	1.47	0.80
1:K:170:GLY:HA2	1:K:172:ARG:HH22	1.47	0.80
1:L:347:VAL:HB	5:L:1792:HOH:O	1.82	0.80
1:B:347:VAL:HB	5:B:6003:HOH:O	1.82	0.80
1:D:176[B]:LYS:C	1:D:178[B]:GLY:H	1.88	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4475:ADP:N9	3:E:4475:ADP:H1'	1.96	0.80
1:D:458:HIS:HD2	1:D:460:VAL:H	1.26	0.80
1:F:176[B]:LYS:C	1:F:178[B]:GLY:H	1.88	0.80
1:J:31:VAL:HB	1:K:180[B]:PHE:CD1	2.17	0.80
1:B:170:GLY:HA2	1:B:172:ARG:HH22	1.46	0.80
1:C:176[B]:LYS:C	1:C:178[B]:GLY:H	1.88	0.80
1:H:170:GLY:HA2	1:H:172:ARG:HH22	1.47	0.80
1:J:347:VAL:HB	5:J:6019:HOH:O	1.82	0.80
1:L:170:GLY:HA2	1:L:172:ARG:HH22	1.47	0.80
1:A:347:VAL:HB	5:A:6002:HOH:O	1.82	0.79
3:I:4479:ADP:N9	3:I:4479:ADP:H1'	1.96	0.79
1:J:170:GLY:HA2	1:J:172:ARG:HH22	1.47	0.79
1:E:176[B]:LYS:C	1:E:178[B]:GLY:H	1.88	0.79
1:G:40:ALA:CB	5:G:5991:HOH:O	2.29	0.79
1:H:40:ALA:HB3	5:H:5995:HOH:O	1.83	0.79
1:A:170:GLY:HA2	1:A:172:ARG:HH22	1.47	0.79
1:B:40:ALA:HB3	5:B:5982:HOH:O	1.83	0.79
1:D:40:ALA:HB3	5:D:5984:HOH:O	1.83	0.79
1:E:40:ALA:HB3	5:E:697:HOH:O	1.83	0.79
1:H:347:VAL:HB	5:H:6016:HOH:O	1.82	0.79
1:I:40:ALA:CB	5:I:6002:HOH:O	2.29	0.79
1:K:347:VAL:HB	5:K:1639:HOH:O	1.82	0.79
1:H:458:HIS:HD2	1:H:460:VAL:H	1.26	0.79
1:J:40:ALA:CB	5:J:5998:HOH:O	2.29	0.79
1:J:40:ALA:HB3	5:J:5998:HOH:O	1.83	0.79
1:D:347:VAL:HB	5:D:6005:HOH:O	1.82	0.79
1:F:458:HIS:HD2	1:F:460:VAL:H	1.26	0.79
1:I:347:VAL:HB	5:I:6023:HOH:O	1.82	0.79
1:J:31:VAL:HB	1:K:180[B]:PHE:CE1	2.17	0.79
1:B:180[B]:PHE:CD1	1:C:31:VAL:HB	2.16	0.79
1:F:40:ALA:CB	5:F:5991:HOH:O	2.29	0.79
3:L:4482:ADP:N9	3:L:4482:ADP:H1'	1.96	0.79
1:A:40:ALA:HB3	5:A:5981:HOH:O	1.83	0.79
1:I:40:ALA:HB3	5:I:6002:HOH:O	1.83	0.79
1:K:176[B]:LYS:C	1:K:178[B]:GLY:H	1.88	0.79
1:D:40:ALA:CB	5:D:5984:HOH:O	2.29	0.79
1:D:170:GLY:HA2	1:D:172:ARG:HH22	1.47	0.79
1:E:40:ALA:CB	5:E:697:HOH:O	2.29	0.79
1:F:170:GLY:HA2	1:F:172:ARG:HH22	1.47	0.79
1:F:347:VAL:HB	5:F:6012:HOH:O	1.82	0.79
1:K:337:ARG:HG3	1:K:338:ASN:H	0.87	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:ARG:HD3	5:E:698:HOH:O	1.84	0.78
1:I:447:ARG:HD3	5:I:6003:HOH:O	1.83	0.78
1:G:170:GLY:HA2	1:G:172:ARG:HH22	1.47	0.78
1:H:40:ALA:CB	5:H:5995:HOH:O	2.29	0.78
1:L:447:ARG:HD3	5:L:1769:HOH:O	1.84	0.78
1:K:40:ALA:HB3	5:K:1615:HOH:O	1.83	0.78
1:J:447:ARG:HD3	5:J:5999:HOH:O	1.83	0.78
3:K:4481:ADP:N9	3:K:4481:ADP:H1'	1.96	0.78
1:C:347:VAL:HB	5:C:6002:HOH:O	1.82	0.78
1:F:447:ARG:HD3	5:F:5992:HOH:O	1.83	0.78
1:G:40:ALA:HB3	5:G:5991:HOH:O	1.83	0.78
1:C:170:GLY:HA2	1:C:172:ARG:HH22	1.47	0.78
1:L:75:VAL:HG23	5:L:1701:HOH:O	1.84	0.78
1:B:75:VAL:HG23	5:B:5917:HOH:O	1.84	0.78
1:C:75:VAL:HG23	5:C:5917:HOH:O	1.84	0.78
1:J:75:VAL:HG23	5:J:5934:HOH:O	1.84	0.78
1:A:75:VAL:HG23	5:A:5916:HOH:O	1.84	0.78
1:C:40:ALA:HB3	5:C:5981:HOH:O	1.83	0.78
1:E:347:VAL:HB	5:E:721:HOH:O	1.82	0.78
1:K:224:ARG:HG2	1:K:224:ARG:NH2	1.97	0.77
1:C:170:GLY:HA2	1:C:172:ARG:NH2	2.00	0.77
1:H:75:VAL:HG23	5:H:5932:HOH:O	1.84	0.77
1:H:170:GLY:HA2	1:H:172:ARG:NH2	1.99	0.77
1:H:447:ARG:HD3	5:H:5996:HOH:O	1.83	0.77
1:L:40:ALA:HB3	5:L:1768:HOH:O	1.83	0.77
1:G:447:ARG:HD3	5:G:5992:HOH:O	1.84	0.77
1:J:170:GLY:HA2	1:J:172:ARG:NH2	1.99	0.77
1:B:170:GLY:HA2	1:B:172:ARG:NH2	2.00	0.77
1:F:75:VAL:HG23	5:F:5927:HOH:O	1.84	0.77
1:K:75:VAL:HG23	5:K:1548:HOH:O	1.84	0.77
1:D:180[B]:PHE:CE1	1:E:31:VAL:HB	2.20	0.77
1:D:170:GLY:HA2	1:D:172:ARG:NH2	2.00	0.77
1:G:170:GLY:HA2	1:G:172:ARG:NH2	2.00	0.77
3:H:4478:ADP:N9	3:H:4478:ADP:H1'	1.96	0.77
1:A:447:ARG:HD3	5:A:5982:HOH:O	1.83	0.77
1:F:170:GLY:HA2	1:F:172:ARG:NH2	2.00	0.77
1:B:447:ARG:HD3	5:B:5983:HOH:O	1.83	0.77
1:E:75:VAL:HG23	5:E:630:HOH:O	1.84	0.77
1:J:251:LYS:HE3	5:J:5940:HOH:O	1.85	0.77
1:L:170:GLY:HA2	1:L:172:ARG:NH2	1.99	0.77
1:B:251:LYS:HE3	5:B:5923:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:VAL:HG23	5:D:5919:HOH:O	1.84	0.77
1:E:170:GLY:HA2	1:E:172:ARG:NH2	2.00	0.77
1:C:447:ARG:HD3	5:C:5982:HOH:O	1.83	0.77
1:F:251:LYS:HE3	5:F:5933:HOH:O	1.85	0.77
1:G:31:VAL:HB	1:H:180[B]:PHE:CD1	2.20	0.77
1:L:191:ILE:HG13	5:L:1743:HOH:O	1.85	0.77
1:C:1:SER:HB2	1:C:4:HIS:CB	2.15	0.76
1:G:180[B]:PHE:CD1	1:L:31:VAL:HB	2.20	0.76
1:I:170:GLY:HA2	1:I:172:ARG:NH2	2.00	0.76
1:K:191:ILE:HG13	5:K:1590:HOH:O	1.85	0.76
1:F:191:ILE:HG13	5:F:5968:HOH:O	1.85	0.76
1:F:251:LYS:CE	5:F:5933:HOH:O	2.34	0.76
1:G:251:LYS:HE3	5:G:5932:HOH:O	1.85	0.76
1:G:347:VAL:HB	5:G:6012:HOH:O	1.82	0.76
1:H:251:LYS:HE3	5:H:5938:HOH:O	1.85	0.76
1:D:447:ARG:HD3	5:D:5985:HOH:O	1.83	0.76
1:K:170:GLY:HA2	1:K:172:ARG:NH2	2.00	0.76
1:C:251:LYS:HE3	5:C:5923:HOH:O	1.85	0.76
1:G:191:ILE:HG13	5:G:5968:HOH:O	1.85	0.76
1:J:191:ILE:HG13	5:J:5975:HOH:O	1.85	0.76
1:K:251:LYS:CE	5:K:1554:HOH:O	2.34	0.76
1:K:447:ARG:HD3	5:K:1616:HOH:O	1.84	0.76
1:B:191:ILE:HG13	5:B:5959:HOH:O	1.85	0.76
1:E:251:LYS:HE3	5:E:636:HOH:O	1.85	0.76
1:E:349:ALA:HB3	5:E:648:HOH:O	1.86	0.76
1:G:251:LYS:CE	5:G:5932:HOH:O	2.34	0.76
1:I:251:LYS:HE3	5:I:5943:HOH:O	1.85	0.76
1:K:349:ALA:HB3	5:K:1566:HOH:O	1.86	0.76
1:F:40:ALA:HB3	5:F:5991:HOH:O	1.83	0.76
1:H:251:LYS:CE	5:H:5938:HOH:O	2.34	0.76
1:D:191:ILE:HG13	5:D:5961:HOH:O	1.85	0.76
1:I:75:VAL:HG23	5:I:5937:HOH:O	1.84	0.76
1:B:251:LYS:CE	5:B:5923:HOH:O	2.34	0.76
1:E:1:SER:CB	1:E:4:HIS:HB3	2.16	0.76
1:G:75:VAL:HG23	5:G:5926:HOH:O	1.84	0.76
1:L:251:LYS:HE3	5:L:1707:HOH:O	1.85	0.76
1:C:311:LEU:HD13	1:C:369:LEU:HB3	1.68	0.76
1:A:191:ILE:HG13	5:A:5958:HOH:O	1.85	0.75
1:D:251:LYS:HE3	5:D:5925:HOH:O	1.85	0.75
1:I:31:VAL:HB	1:J:180[B]:PHE:CE1	2.21	0.75
1:K:251:LYS:HE3	5:K:1554:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ILE:HG13	5:C:5958:HOH:O	1.85	0.75
1:H:349:ALA:HB3	5:H:5949:HOH:O	1.86	0.75
1:I:191:ILE:HG13	5:I:5979:HOH:O	1.85	0.75
1:K:1:SER:HB2	1:K:4:HIS:CB	2.15	0.75
1:E:179[A]:TYR:O	1:E:181[A]:PRO:CD	2.35	0.75
1:G:1:SER:HB2	1:G:4:HIS:CB	2.15	0.75
3:G:4477:ADP:N9	3:G:4477:ADP:H1'	1.96	0.75
1:H:179[A]:TYR:O	1:H:181[A]:PRO:CD	2.34	0.75
1:I:251:LYS:CE	5:I:5943:HOH:O	2.34	0.75
1:L:251:LYS:CE	5:L:1707:HOH:O	2.34	0.75
1:C:179[A]:TYR:O	1:C:181[A]:PRO:CD	2.35	0.75
1:E:191:ILE:HG13	5:E:672:HOH:O	1.85	0.75
1:E:251:LYS:CE	5:E:636:HOH:O	2.34	0.75
1:G:180[B]:PHE:CE1	1:L:31:VAL:HB	2.22	0.75
1:G:349:ALA:HB3	5:G:5944:HOH:O	1.86	0.75
1:K:1:SER:CB	1:K:4:HIS:HB3	2.15	0.75
1:L:179[A]:TYR:O	1:L:181[A]:PRO:CD	2.35	0.75
1:A:251:LYS:HE3	5:A:5922:HOH:O	1.85	0.75
1:A:349:ALA:HB3	5:A:5934:HOH:O	1.86	0.75
1:A:170:GLY:HA2	1:A:172:ARG:NH2	2.00	0.75
1:B:224:ARG:HG2	1:B:224:ARG:NH2	1.97	0.75
1:F:179[A]:TYR:O	1:F:181[A]:PRO:CD	2.35	0.75
1:F:189:GLN:NE2	1:F:209[A]:HIS:HE1	1.85	0.75
1:G:189:GLN:NE2	1:G:209[A]:HIS:HE1	1.85	0.75
1:G:311:LEU:HD13	1:G:369:LEU:HB3	1.69	0.75
1:H:311:LEU:HD13	1:H:369:LEU:HB3	1.69	0.75
1:K:179[A]:TYR:O	1:K:181[A]:PRO:CD	2.35	0.75
1:L:311:LEU:HD13	1:L:369:LEU:HB3	1.69	0.75
1:A:1:SER:HB2	1:A:4:HIS:CB	2.15	0.75
1:B:179[A]:TYR:O	1:B:181[A]:PRO:CD	2.34	0.75
1:B:189:GLN:NE2	1:B:209[A]:HIS:HE1	1.85	0.75
1:E:311:LEU:HD13	1:E:369:LEU:HB3	1.69	0.75
1:G:31:VAL:HB	1:H:180[B]:PHE:CE1	2.21	0.75
1:I:311:LEU:HD13	1:I:369:LEU:HB3	1.68	0.75
1:A:311:LEU:HD13	1:A:369:LEU:HB3	1.68	0.75
1:C:1:SER:CB	1:C:4:HIS:HB3	2.16	0.75
1:G:179[A]:TYR:O	1:G:181[A]:PRO:CD	2.34	0.75
1:J:179[A]:TYR:O	1:J:181[A]:PRO:CD	2.35	0.75
1:J:311:LEU:HD13	1:J:369:LEU:HB3	1.68	0.75
1:A:179[A]:TYR:O	1:A:181[A]:PRO:CD	2.35	0.74
1:D:349:ALA:HB3	5:D:5937:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:ILE:HG13	5:H:5972:HOH:O	1.85	0.74
1:J:189:GLN:NE2	1:J:209[A]:HIS:HE1	1.85	0.74
3:J:4480:ADP:N9	3:J:4480:ADP:HI'	1.96	0.74
1:B:349:ALA:HB3	5:B:5935:HOH:O	1.86	0.74
1:A:31:VAL:HB	1:F:180[B]:PHE:CD1	2.22	0.74
1:C:180[B]:PHE:CD1	1:D:31:VAL:HB	2.22	0.74
1:C:251:LYS:CE	5:C:5923:HOH:O	2.34	0.74
1:D:311:LEU:HD13	1:D:369:LEU:HB3	1.69	0.74
1:L:349:ALA:HB3	5:L:1719:HOH:O	1.86	0.74
1:H:224:ARG:HG2	1:H:224:ARG:NH2	1.97	0.74
1:K:189:GLN:NE2	1:K:209[A]:HIS:HE1	1.85	0.74
1:A:251:LYS:CE	5:A:5922:HOH:O	2.34	0.74
1:D:251:LYS:CE	5:D:5925:HOH:O	2.34	0.74
1:E:189:GLN:NE2	1:E:209[A]:HIS:HE1	1.85	0.74
1:F:1:SER:CB	1:F:4:HIS:HB3	2.15	0.74
1:F:349:ALA:HB3	5:F:5944:HOH:O	1.86	0.74
1:I:179[A]:TYR:O	1:I:181[A]:PRO:CD	2.35	0.74
1:J:1:SER:HB2	1:J:4:HIS:CB	2.15	0.74
1:D:179[A]:TYR:O	1:D:181[A]:PRO:CD	2.34	0.74
1:I:1:SER:CB	1:I:4:HIS:HB3	2.16	0.74
1:I:189:GLN:NE2	1:I:209[A]:HIS:HE1	1.85	0.74
1:L:189:GLN:NE2	1:L:209[A]:HIS:HE1	1.85	0.74
1:B:1:SER:HB2	1:B:4:HIS:CB	2.15	0.74
1:J:251:LYS:CE	5:J:5940:HOH:O	2.34	0.74
1:H:1:SER:CB	1:H:4:HIS:HB3	2.16	0.74
1:J:349:ALA:HB3	5:J:5951:HOH:O	1.86	0.74
1:G:407:ILE:HB	1:G:408:PRO:HD2	1.70	0.74
1:F:407:ILE:HB	1:F:408:PRO:HD2	1.70	0.74
1:D:1:SER:HB2	1:D:4:HIS:CB	2.15	0.73
1:C:189:GLN:NE2	1:C:209[A]:HIS:HE1	1.85	0.73
1:D:189:GLN:NE2	1:D:209[A]:HIS:HE1	1.85	0.73
1:L:407:ILE:HB	1:L:408:PRO:HD2	1.70	0.73
1:C:349:ALA:HB3	5:C:5934:HOH:O	1.86	0.73
1:D:224:ARG:HH21	1:D:224:ARG:CG	2.01	0.73
1:E:407:ILE:HB	1:E:408:PRO:HD2	1.70	0.73
1:K:311:LEU:HD13	1:K:369:LEU:HB3	1.68	0.73
1:A:189:GLN:NE2	1:A:209[A]:HIS:HE1	1.85	0.73
1:B:311:LEU:HD13	1:B:369:LEU:HB3	1.68	0.73
1:E:1:SER:HB2	1:E:4:HIS:CB	2.15	0.73
1:I:349:ALA:HB3	5:I:5955:HOH:O	1.86	0.73
1:A:1:SER:CB	1:A:4:HIS:HB3	2.15	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:TRP:O	1:C:58:LYS:O	2.07	0.73
1:E:57:TRP:O	1:E:58:LYS:O	2.07	0.73
1:F:311:LEU:HD13	1:F:369:LEU:HB3	1.68	0.73
1:J:1:SER:CB	1:J:4:HIS:HB3	2.15	0.73
1:B:407:ILE:HB	1:B:408:PRO:HD2	1.70	0.73
1:C:269:HIS:HE1	4:C:5902:PPQ:CEP	2.02	0.73
1:F:269:HIS:HE1	4:F:5905:PPQ:CEP	2.02	0.73
1:H:179[B]:TYR:CE1	1:H:212[B]:GLU:CA	2.72	0.73
1:H:189:GLN:NE2	1:H:209[A]:HIS:HE1	1.85	0.73
1:I:407:ILE:HB	1:I:408:PRO:HD2	1.70	0.73
1:D:407:ILE:HB	1:D:408:PRO:HD2	1.70	0.73
1:K:179[B]:TYR:CE1	1:K:212[B]:GLU:CA	2.72	0.73
1:L:1:SER:HB2	1:L:4:HIS:CB	2.15	0.73
1:B:269:HIS:HE1	4:B:5901:PPQ:CEP	2.02	0.72
1:G:57:TRP:O	1:G:58:LYS:O	2.07	0.72
1:J:57:TRP:O	1:J:58:LYS:O	2.07	0.72
1:K:57:TRP:O	1:K:58:LYS:O	2.07	0.72
1:B:57:TRP:O	1:B:58:LYS:O	2.07	0.72
1:F:179[B]:TYR:CE1	1:F:212[B]:GLU:CA	2.72	0.72
1:I:57:TRP:O	1:I:58:LYS:O	2.07	0.72
1:K:269:HIS:HE1	4:K:5910:PPQ:CEP	2.02	0.72
1:A:407:ILE:HB	1:A:408:PRO:HD2	1.70	0.72
1:G:179[B]:TYR:CE1	1:G:212[B]:GLU:CA	2.72	0.72
1:I:269:HIS:HE1	4:I:5908:PPQ:CEP	2.02	0.72
1:J:179[B]:TYR:CE1	1:J:212[B]:GLU:CA	2.72	0.72
1:L:1:SER:CB	1:L:4:HIS:HB3	2.15	0.72
1:A:179[B]:TYR:CE1	1:A:212[B]:GLU:CA	2.72	0.72
1:C:179[B]:TYR:CE1	1:C:212[B]:GLU:CA	2.72	0.72
1:D:269:HIS:HE1	4:D:5903:PPQ:CEP	2.02	0.72
1:E:179[B]:TYR:CE1	1:E:212[B]:GLU:CA	2.72	0.72
1:E:269:HIS:HE1	4:E:5904:PPQ:CEP	2.02	0.72
1:G:269:HIS:HE1	4:G:5906:PPQ:CEP	2.02	0.72
1:I:179[B]:TYR:CE1	1:I:212[B]:GLU:CA	2.72	0.72
1:J:269:HIS:HE1	4:J:5909:PPQ:CEP	2.02	0.72
1:K:407:ILE:HB	1:K:408:PRO:HD2	1.70	0.72
1:D:179[B]:TYR:CE1	1:D:212[B]:GLU:CA	2.72	0.72
1:E:224:ARG:HG2	1:E:224:ARG:NH2	1.97	0.72
1:I:31:VAL:HB	1:J:180[B]:PHE:CD1	2.25	0.72
1:L:57:TRP:O	1:L:58:LYS:O	2.07	0.72
1:B:224:ARG:HH21	1:B:224:ARG:CG	2.01	0.72
1:G:1:SER:CB	1:G:4:HIS:HB3	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:HIS:HE1	4:A:5900:PPQ:CEP	2.02	0.72
1:B:337:ARG:HG3	1:B:338:ASN:CA	2.20	0.72
1:F:337:ARG:HG3	1:F:338:ASN:CA	2.20	0.72
1:G:224:ARG:HH21	1:G:224:ARG:CG	2.01	0.72
1:J:407:ILE:HB	1:J:408:PRO:HD2	1.70	0.72
1:L:179[B]:TYR:CE1	1:L:212[B]:GLU:CA	2.72	0.72
1:B:179[B]:TYR:CE1	1:B:212[B]:GLU:CA	2.72	0.72
1:C:224:ARG:HH21	1:C:224:ARG:CG	2.01	0.72
1:C:407:ILE:HB	1:C:408:PRO:HD2	1.70	0.71
3:C:4473:ADP:N9	3:C:4473:ADP:H1'	1.96	0.71
1:H:57:TRP:O	1:H:58:LYS:O	2.07	0.71
1:H:176[B]:LYS:C	1:H:178[B]:GLY:N	2.47	0.71
1:A:180[B]:PHE:CD1	1:B:31:VAL:HB	2.25	0.71
1:F:57:TRP:O	1:F:58:LYS:O	2.07	0.71
1:G:384:ASN:HD22	1:G:384:ASN:N	1.88	0.71
1:H:407:ILE:HB	1:H:408:PRO:HD2	1.70	0.71
1:B:179[A]:TYR:C	1:B:181[A]:PRO:HD2	2.16	0.71
1:D:57:TRP:O	1:D:58:LYS:O	2.07	0.71
1:G:337:ARG:HG3	1:G:338:ASN:CA	2.20	0.71
1:H:179[A]:TYR:C	1:H:181[A]:PRO:HD2	2.16	0.71
1:H:224:ARG:HH21	1:H:224:ARG:CG	2.01	0.71
1:D:179[A]:TYR:C	1:D:181[A]:PRO:HD2	2.16	0.71
1:E:384:ASN:HD22	1:E:384:ASN:N	1.88	0.71
1:G:179[A]:TYR:C	1:G:181[A]:PRO:HD2	2.16	0.71
1:J:179[A]:TYR:C	1:J:181[A]:PRO:HD2	2.16	0.71
1:L:269:HIS:HE1	4:L:5911:PPQ:CEP	2.02	0.71
1:A:57:TRP:O	1:A:58:LYS:O	2.07	0.71
1:E:179[A]:TYR:C	1:E:181[A]:PRO:HD2	2.16	0.71
1:H:31:VAL:HB	1:I:180[B]:PHE:CD1	2.25	0.71
1:J:337:ARG:HG3	1:J:338:ASN:CA	2.20	0.71
1:F:1:SER:HB2	1:F:4:HIS:CB	2.15	0.71
1:K:31:VAL:HB	1:L:180[B]:PHE:CD1	2.25	0.71
1:K:179[A]:TYR:C	1:K:181[A]:PRO:HD2	2.16	0.71
1:A:179[A]:TYR:O	1:A:181[A]:PRO:HD3	1.91	0.71
1:A:179[A]:TYR:C	1:A:181[A]:PRO:HD2	2.16	0.71
1:C:384:ASN:HD22	1:C:384:ASN:N	1.88	0.71
1:H:269:HIS:HE1	4:H:5907:PPQ:CEP	2.02	0.71
1:I:179[A]:TYR:O	1:I:181[A]:PRO:HD3	1.91	0.70
1:L:176[B]:LYS:C	1:L:178[B]:GLY:N	2.47	0.70
1:L:179[A]:TYR:C	1:L:181[A]:PRO:HD2	2.16	0.70
1:B:176[B]:LYS:C	1:B:178[B]:GLY:N	2.47	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179[A]:TYR:C	1:C:181[A]:PRO:HD2	2.16	0.70
1:F:179[A]:TYR:C	1:F:181[A]:PRO:HD2	2.16	0.70
1:H:384:ASN:HD22	1:H:384:ASN:N	1.88	0.70
1:I:381:GLY:HA2	1:I:386:ILE:HG13	1.74	0.70
1:A:384:ASN:HD22	1:A:384:ASN:N	1.88	0.70
1:K:179[A]:TYR:O	1:K:181[A]:PRO:HD3	1.91	0.70
1:E:337:ARG:HG3	1:E:338:ASN:CA	2.20	0.70
1:I:401:PRO:HA	1:I:404:ALA:HA	1.74	0.70
1:J:384:ASN:HD22	1:J:384:ASN:N	1.89	0.70
1:C:337:ARG:HG3	1:C:338:ASN:CA	2.20	0.70
1:I:1:SER:HB2	1:I:4:HIS:CB	2.15	0.70
1:K:401:PRO:HA	1:K:404:ALA:HA	1.74	0.70
1:C:381:GLY:HA2	1:C:386:ILE:HG13	1.74	0.70
1:E:179[A]:TYR:O	1:E:181[A]:PRO:HD3	1.92	0.70
1:I:179[B]:TYR:CE1	1:I:212[B]:GLU:HA	2.27	0.70
1:I:384:ASN:N	1:I:384:ASN:HD22	1.88	0.70
1:L:179[A]:TYR:O	1:L:181[A]:PRO:HD3	1.92	0.70
1:B:1:SER:CB	1:B:4:HIS:HB3	2.15	0.70
1:D:401:PRO:HA	1:D:404:ALA:HA	1.74	0.70
1:J:179[A]:TYR:O	1:J:181[A]:PRO:HD3	1.91	0.70
1:B:401:PRO:HA	1:B:404:ALA:HA	1.74	0.70
1:D:381:GLY:HA2	1:D:386:ILE:HG13	1.74	0.70
1:E:224:ARG:HH21	1:E:224:ARG:CG	2.01	0.70
1:F:381:GLY:HA2	1:F:386:ILE:HG13	1.74	0.70
1:F:384:ASN:N	1:F:384:ASN:HD22	1.88	0.70
1:G:381:GLY:HA2	1:G:386:ILE:HG13	1.74	0.70
1:A:401:PRO:HA	1:A:404:ALA:HA	1.74	0.69
1:E:381:GLY:HA2	1:E:386:ILE:HG13	1.74	0.69
1:H:1:SER:HB2	1:H:4:HIS:CB	2.15	0.69
1:C:179[B]:TYR:CE1	1:C:212[B]:GLU:HA	2.27	0.69
1:F:179[B]:TYR:CE1	1:F:212[B]:GLU:HA	2.27	0.69
3:F:4476:ADP:N9	3:F:4476:ADP:H1'	1.96	0.69
1:I:179[A]:TYR:C	1:I:181[A]:PRO:HD2	2.16	0.69
1:B:179[A]:TYR:O	1:B:181[A]:PRO:HD3	1.91	0.69
1:B:384:ASN:HD22	1:B:384:ASN:N	1.88	0.69
1:C:179[A]:TYR:O	1:C:181[A]:PRO:HD3	1.91	0.69
1:D:59:GLY:C	1:D:61:ASN:H	2.01	0.69
1:D:426:GLU:HG2	5:D:5936:HOH:O	1.93	0.69
1:F:179[A]:TYR:O	1:F:181[A]:PRO:HD3	1.91	0.69
1:H:179[A]:TYR:O	1:H:181[A]:PRO:HD3	1.91	0.69
1:K:384:ASN:HD22	1:K:384:ASN:N	1.88	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:224:ARG:HG2	1:L:224:ARG:NH2	1.97	0.69
1:D:1:SER:CB	1:D:4:HIS:HB3	2.16	0.69
1:F:59:GLY:C	1:F:61:ASN:H	2.01	0.69
1:I:176[B]:LYS:C	1:I:178[B]:GLY:N	2.47	0.69
1:A:381:GLY:HA2	1:A:386:ILE:HG13	1.74	0.69
1:A:426:GLU:HG2	5:A:5933:HOH:O	1.93	0.69
1:C:59:GLY:C	1:C:61:ASN:H	2.01	0.69
1:C:401:PRO:HA	1:C:404:ALA:HA	1.74	0.69
1:D:179[B]:TYR:CE1	1:D:212[B]:GLU:HA	2.27	0.69
1:F:224:ARG:HH21	1:F:224:ARG:CG	2.01	0.69
1:G:179[B]:TYR:CE1	1:G:212[B]:GLU:HA	2.27	0.69
1:H:381:GLY:HA2	1:H:386:ILE:HG13	1.74	0.69
1:J:401:PRO:HA	1:J:404:ALA:HA	1.74	0.69
1:B:59:GLY:C	1:B:61:ASN:H	2.01	0.69
1:B:381:GLY:HA2	1:B:386:ILE:HG13	1.74	0.69
1:D:384:ASN:HD22	1:D:384:ASN:N	1.88	0.69
1:G:59:GLY:C	1:G:61:ASN:H	2.01	0.69
1:B:179[B]:TYR:CE1	1:B:212[B]:GLU:HA	2.27	0.69
1:D:179[A]:TYR:O	1:D:181[A]:PRO:HD3	1.91	0.69
1:G:179[A]:TYR:O	1:G:181[A]:PRO:HD3	1.91	0.69
1:G:211[A]:HIS:CD2	1:G:212[A]:GLU:H	2.11	0.69
1:G:231:LYS:HE2	5:G:5917:HOH:O	1.93	0.69
1:I:211[A]:HIS:CD2	1:I:212[A]:GLU:H	2.11	0.69
1:J:231:LYS:HE2	5:J:5926:HOH:O	1.93	0.69
1:K:426:GLU:HG2	5:K:1565:HOH:O	1.93	0.69
1:B:426:GLU:HG2	5:B:5934:HOH:O	1.93	0.69
1:F:231:LYS:HE2	5:F:5919:HOH:O	1.93	0.69
1:F:269:HIS:HE1	4:F:5905:PPQ:HEP3	1.58	0.69
1:H:401:PRO:HA	1:H:404:ALA:HA	1.74	0.69
1:I:224:ARG:HH21	1:I:224:ARG:CG	2.01	0.69
1:A:180[B]:PHE:CE1	1:B:31:VAL:HB	2.28	0.69
1:A:211[A]:HIS:CD2	1:A:212[A]:GLU:H	2.11	0.69
1:F:176[B]:LYS:C	1:F:178[B]:GLY:N	2.47	0.69
1:F:426:GLU:HG2	5:F:5943:HOH:O	1.92	0.69
1:G:269:HIS:HE1	4:G:5906:PPQ:HEP3	1.58	0.69
1:H:426:GLU:HG2	5:H:5948:HOH:O	1.92	0.69
1:J:59:GLY:C	1:J:61:ASN:H	2.01	0.69
1:L:381:GLY:HA2	1:L:386:ILE:HG13	1.74	0.69
1:A:337:ARG:HG3	1:A:338:ASN:CA	2.20	0.68
1:J:427:PHE:HB2	5:J:6046:HOH:O	1.93	0.68
1:L:179[B]:TYR:CE1	1:L:212[B]:GLU:HA	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:211[A]:HIS:CD2	1:L:212[A]:GLU:H	2.11	0.68
1:E:179[B]:TYR:CE1	1:E:212[B]:GLU:HA	2.27	0.68
1:K:179[B]:TYR:CE1	1:K:212[B]:GLU:HA	2.27	0.68
1:L:59:GLY:C	1:L:61:ASN:H	2.01	0.68
1:B:231:LYS:HE2	5:B:5908:HOH:O	1.93	0.68
1:H:427:PHE:HB2	5:H:6043:HOH:O	1.94	0.68
1:J:179[B]:TYR:CE1	1:J:212[B]:GLU:HA	2.27	0.68
1:K:329:PRO:HG3	5:K:1655:HOH:O	1.94	0.68
1:K:381:GLY:HA2	1:K:386:ILE:HG13	1.74	0.68
1:A:427:PHE:HB2	5:A:6029:HOH:O	1.94	0.68
1:C:180[B]:PHE:CE1	1:D:31:VAL:HB	2.29	0.68
1:D:427:PHE:HB2	5:D:6032:HOH:O	1.94	0.68
1:E:329:PRO:HG3	5:E:737:HOH:O	1.94	0.68
1:G:224:ARG:HG2	1:G:224:ARG:NH2	1.97	0.68
1:G:426:GLU:HG2	5:G:5943:HOH:O	1.93	0.68
1:I:269:HIS:HE1	4:I:5908:PPQ:HEP3	1.58	0.68
1:K:176[B]:LYS:C	1:K:178[B]:GLY:N	2.47	0.68
1:A:179[B]:TYR:CE1	1:A:212[B]:GLU:HA	2.27	0.68
1:A:269:HIS:HE1	4:A:5900:PPQ:HEP3	1.58	0.68
1:B:329:PRO:HG3	5:B:6017:HOH:O	1.94	0.68
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.29	0.68
1:H:337:ARG:HG3	1:H:338:ASN:CA	2.20	0.68
1:L:427:PHE:HB2	5:L:1821:HOH:O	1.94	0.68
1:A:224:ARG:HH21	1:A:224:ARG:CG	2.01	0.68
1:C:427:PHE:HB2	5:C:6029:HOH:O	1.94	0.68
1:E:211[A]:HIS:CD2	1:E:212[A]:GLU:H	2.11	0.68
1:E:426:GLU:HG2	5:E:647:HOH:O	1.92	0.68
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.29	0.68
1:J:224:ARG:HH21	1:J:224:ARG:CG	2.01	0.68
1:J:381:GLY:HA2	1:J:386:ILE:HG13	1.74	0.68
1:J:426:GLU:HG2	5:J:5950:HOH:O	1.93	0.68
1:K:269:HIS:HE1	4:K:5910:PPQ:HEP3	1.58	0.68
1:A:59:GLY:C	1:A:61:ASN:H	2.01	0.68
1:B:269:HIS:HE1	4:B:5901:PPQ:HEP3	1.58	0.68
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.29	0.68
1:F:401:PRO:HA	1:F:404:ALA:HA	1.74	0.68
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.29	0.68
1:H:31:VAL:HB	1:I:180[B]:PHE:CE1	2.28	0.68
1:H:179[B]:TYR:CE1	1:H:212[B]:GLU:HA	2.27	0.68
1:J:211[A]:HIS:CD2	1:J:212[A]:GLU:H	2.11	0.68
1:K:211[A]:HIS:CD2	1:K:212[A]:GLU:H	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:337:ARG:HG3	1:L:338:ASN:CA	2.20	0.68
1:L:401:PRO:HA	1:L:404:ALA:HA	1.74	0.68
1:D:231:LYS:HE2	5:D:5910:HOH:O	1.93	0.68
1:D:269:HIS:HE1	4:D:5903:PPQ:HEP3	1.58	0.68
1:D:337:ARG:HG3	1:D:338:ASN:CA	2.20	0.68
1:H:211[A]:HIS:CD2	1:H:212[A]:GLU:H	2.11	0.68
1:I:59:GLY:C	1:I:61:ASN:H	2.01	0.68
1:I:231:LYS:HE2	5:I:5928:HOH:O	1.93	0.68
1:I:337:ARG:HG3	1:I:338:ASN:CA	2.20	0.68
1:K:114:TYR:CD2	1:K:431:GLY:HA3	2.29	0.68
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.29	0.68
1:A:231:LYS:HE2	5:A:5907:HOH:O	1.93	0.68
1:G:401:PRO:HA	1:G:404:ALA:HA	1.74	0.68
1:I:224:ARG:HG2	1:I:224:ARG:NH2	1.97	0.68
1:K:59:GLY:C	1:K:61:ASN:H	2.01	0.68
1:K:323:VAL:CG1	5:K:1677:HOH:O	2.20	0.68
1:K:337:ARG:HG3	1:K:338:ASN:CA	2.20	0.68
1:K:427:PHE:HB2	5:K:1668:HOH:O	1.93	0.68
1:E:231:LYS:HE2	5:E:621:HOH:O	1.93	0.68
1:F:427:PHE:HB2	5:F:6039:HOH:O	1.94	0.68
1:I:114:TYR:CD2	1:I:431:GLY:HA3	2.29	0.68
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.29	0.68
1:B:427:PHE:HB2	5:B:6030:HOH:O	1.94	0.67
1:D:211[A]:HIS:CD2	1:D:212[A]:GLU:H	2.11	0.67
1:F:211[A]:HIS:CD2	1:F:212[A]:GLU:H	2.11	0.67
1:G:212[A]:GLU:HG3	1:G:218:GLN:NE2	2.10	0.67
1:C:211[A]:HIS:CD2	1:C:212[A]:GLU:H	2.11	0.67
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.29	0.67
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.29	0.67
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.29	0.67
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.29	0.67
1:L:269:HIS:HE1	4:L:5911:PPQ:HEP3	1.58	0.67
1:A:329:PRO:HG3	5:A:6016:HOH:O	1.94	0.67
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.29	0.67
1:C:231:LYS:HE2	5:C:5909:HOH:O	1.93	0.67
1:C:426:GLU:HG2	5:C:5933:HOH:O	1.93	0.67
1:D:212[A]:GLU:HG3	1:D:218:GLN:NE2	2.10	0.67
1:K:224:ARG:HH21	1:K:224:ARG:CG	2.01	0.67
1:G:329:PRO:HG3	5:G:6026:HOH:O	1.94	0.67
1:H:212[A]:GLU:HG3	1:H:218:GLN:NE2	2.10	0.67
1:L:384:ASN:HD22	1:L:384:ASN:N	1.88	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212[A]:GLU:HG3	1:A:218:GLN:NE2	2.10	0.67
1:A:224:ARG:HG2	1:A:224:ARG:NH2	1.97	0.67
1:E:401:PRO:HA	1:E:404:ALA:HA	1.74	0.67
1:F:329:PRO:HG3	5:F:6026:HOH:O	1.94	0.67
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.29	0.67
1:H:329:PRO:HG3	5:H:6030:HOH:O	1.94	0.67
1:I:426:GLU:HG2	5:I:5954:HOH:O	1.92	0.67
1:J:212[A]:GLU:HG3	1:J:218:GLN:NE2	2.10	0.67
1:K:212[A]:GLU:HG3	1:K:218:GLN:NE2	2.10	0.67
1:K:231:LYS:HE2	5:K:1539:HOH:O	1.93	0.67
1:L:224:ARG:HH21	1:L:224:ARG:CG	2.01	0.67
1:L:231:LYS:HE2	5:L:1692:HOH:O	1.93	0.67
1:G:360:PHE:CE2	1:G:361:PRO:HD3	2.29	0.67
1:H:114:TYR:CD2	1:H:431:GLY:HA3	2.29	0.67
1:H:269:HIS:HE1	4:H:5907:PPQ:HEP3	1.58	0.67
1:I:212[A]:GLU:HG3	1:I:218:GLN:NE2	2.10	0.67
1:B:211[A]:HIS:CD2	1:B:212[A]:GLU:H	2.11	0.67
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.29	0.67
1:C:269:HIS:HE1	4:C:5902:PPQ:HEP3	1.58	0.67
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.29	0.67
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.29	0.67
1:I:427:PHE:HB2	5:I:6050:HOH:O	1.94	0.67
1:L:426:GLU:HG2	5:L:1718:HOH:O	1.93	0.67
1:E:59:GLY:C	1:E:61:ASN:H	2.01	0.67
1:E:212[A]:GLU:HG3	1:E:218:GLN:NE2	2.10	0.67
1:B:212[A]:GLU:HG3	1:B:218:GLN:NE2	2.10	0.67
1:E:269:HIS:HE1	4:E:5904:PPQ:HEP3	1.58	0.67
1:C:212[A]:GLU:HG3	1:C:218:GLN:NE2	2.10	0.66
1:E:315:THR:O	1:E:318:SER:HB2	1.96	0.66
1:E:427:PHE:HB2	5:E:750:HOH:O	1.94	0.66
1:H:59:GLY:C	1:H:61:ASN:H	2.01	0.66
1:I:329:PRO:HG3	5:I:6037:HOH:O	1.94	0.66
1:A:82:ASP:HB3	5:A:5943:HOH:O	1.96	0.66
1:B:323:VAL:CG1	5:B:6038:HOH:O	2.20	0.66
1:C:82:ASP:HB3	5:C:5943:HOH:O	1.96	0.66
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.29	0.66
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.29	0.66
1:I:385:LYS:HE2	5:I:5992:HOH:O	1.95	0.66
1:K:315:THR:O	1:K:318:SER:HB2	1.96	0.66
1:G:385:LYS:HE2	5:G:5981:HOH:O	1.95	0.66
1:J:329:PRO:HG3	5:J:6033:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PRO:HG3	5:C:6016:HOH:O	1.94	0.66
1:C:360:PHE:CE2	1:C:361:PRO:HD3	2.29	0.66
1:D:329:PRO:HG3	5:D:6019:HOH:O	1.94	0.66
1:F:298:ILE:O	1:F:302:ILE:HG13	1.96	0.66
1:A:298:ILE:O	1:A:302:ILE:HG13	1.96	0.66
1:B:55:GLY:HA3	5:B:5947:HOH:O	1.96	0.66
1:B:315:THR:O	1:B:318:SER:HB2	1.96	0.66
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.29	0.66
1:L:82:ASP:HB3	5:L:1728:HOH:O	1.96	0.66
1:L:329:PRO:HG3	5:L:1808:HOH:O	1.94	0.66
1:A:179[B]:TYR:CD1	1:A:212[B]:GLU:CA	2.77	0.66
1:C:385:LYS:HE2	5:C:5971:HOH:O	1.95	0.66
1:F:385:LYS:HE2	5:F:5981:HOH:O	1.95	0.66
1:H:231:LYS:HE2	5:H:5924:HOH:O	1.93	0.66
1:H:315:THR:O	1:H:318:SER:HB2	1.95	0.66
1:I:315:THR:O	1:I:318:SER:HB2	1.96	0.66
1:K:298:ILE:O	1:K:302:ILE:HG13	1.96	0.66
1:C:298:ILE:O	1:C:302:ILE:HG13	1.96	0.66
1:D:25:LYS:HD3	5:D:5949:HOH:O	1.96	0.66
1:K:31:VAL:HB	1:L:180[B]:PHE:CE1	2.31	0.66
1:L:212[A]:GLU:HG3	1:L:218:GLN:NE2	2.10	0.66
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.29	0.66
1:B:82:ASP:HB3	5:B:5944:HOH:O	1.96	0.66
1:F:212[A]:GLU:HG3	1:F:218:GLN:NE2	2.10	0.66
1:J:269:HIS:HE1	4:J:5909:PPQ:HEP3	1.58	0.66
1:K:385:LYS:HE2	5:K:1604:HOH:O	1.95	0.66
1:L:315:THR:O	1:L:318:SER:HB2	1.96	0.66
1:L:385:LYS:HE2	5:L:1757:HOH:O	1.95	0.66
1:G:427:PHE:HB2	5:G:6039:HOH:O	1.94	0.66
1:I:298:ILE:O	1:I:302:ILE:HG13	1.96	0.66
1:L:298:ILE:O	1:L:302:ILE:HG13	1.96	0.66
1:G:315:THR:O	1:G:318:SER:HB2	1.96	0.66
1:I:25:LYS:HD3	5:I:5967:HOH:O	1.96	0.66
1:J:82:ASP:HB3	5:J:5960:HOH:O	1.95	0.66
1:L:334:TYR:CD1	5:L:1764:HOH:O	2.49	0.66
1:A:334:TYR:CD1	5:A:5978:HOH:O	2.49	0.65
1:E:298:ILE:O	1:E:302:ILE:HG13	1.96	0.65
1:G:334:TYR:CD1	5:G:5988:HOH:O	2.49	0.65
1:K:82:ASP:HB3	5:K:1575:HOH:O	1.96	0.65
1:K:308:ILE:HG21	1:K:374:LEU:HD13	1.78	0.65
1:A:315:THR:O	1:A:318:SER:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:O	1:C:34:PRO:HG2	1.97	0.65
1:D:298:ILE:O	1:D:302:ILE:HG13	1.96	0.65
1:F:315:THR:O	1:F:318:SER:HB2	1.96	0.65
1:H:55:GLY:HA3	5:H:5961:HOH:O	1.96	0.65
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.78	0.65
1:J:385:LYS:HE2	5:J:5988:HOH:O	1.96	0.65
1:C:25:LYS:HD3	5:C:5946:HOH:O	1.96	0.65
1:C:315:THR:O	1:C:318:SER:HB2	1.96	0.65
1:E:25:LYS:CD	5:E:660:HOH:O	2.45	0.65
1:E:385:LYS:HE2	5:E:686:HOH:O	1.95	0.65
1:F:82:ASP:HB3	5:F:5953:HOH:O	1.96	0.65
1:J:25:LYS:HD3	5:J:5963:HOH:O	1.96	0.65
1:J:55:GLY:HA3	5:J:5963:HOH:O	1.96	0.65
1:J:315:THR:O	1:J:318:SER:HB2	1.95	0.65
1:A:458:HIS:CD2	1:A:460:VAL:H	2.14	0.65
1:B:25:LYS:HD3	5:B:5947:HOH:O	1.96	0.65
1:B:385:LYS:HE2	5:B:5972:HOH:O	1.95	0.65
1:D:315:THR:O	1:D:318:SER:HB2	1.96	0.65
1:G:298:ILE:O	1:G:302:ILE:HG13	1.96	0.65
1:I:82:ASP:HB3	5:I:5964:HOH:O	1.96	0.65
1:I:334:TYR:CD1	5:I:5999:HOH:O	2.49	0.65
1:K:55:GLY:HA3	5:K:1578:HOH:O	1.96	0.65
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.78	0.65
1:C:25:LYS:CD	5:C:5946:HOH:O	2.45	0.65
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.78	0.65
1:E:179[B]:TYR:CD1	1:E:212[B]:GLU:CA	2.77	0.65
1:F:334:TYR:CD1	5:F:5988:HOH:O	2.49	0.65
1:H:82:ASP:HB3	5:H:5958:HOH:O	1.96	0.65
1:I:458:HIS:CD2	1:I:460:VAL:H	2.14	0.65
1:A:323:VAL:CG1	5:A:6037:HOH:O	2.20	0.65
1:C:334:TYR:CD1	5:C:5978:HOH:O	2.49	0.65
1:F:25:LYS:HD3	5:F:5956:HOH:O	1.96	0.65
1:J:298:ILE:O	1:J:302:ILE:HG13	1.96	0.65
1:F:201:GLN:HA	5:F:6013:HOH:O	1.97	0.65
1:F:224:ARG:HG2	1:F:224:ARG:NH2	1.97	0.65
1:H:298:ILE:O	1:H:302:ILE:HG13	1.96	0.65
1:C:201:GLN:HA	5:C:6003:HOH:O	1.97	0.65
1:G:201:GLN:HA	5:G:6013:HOH:O	1.97	0.65
1:B:298:ILE:O	1:B:302:ILE:HG13	1.96	0.65
1:E:82:ASP:HB3	5:E:657:HOH:O	1.96	0.65
1:H:385:LYS:HE2	5:H:5985:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:GLN:HA	5:I:6024:HOH:O	1.97	0.65
1:J:334:TYR:CD1	5:J:5995:HOH:O	2.49	0.65
1:L:25:LYS:HD3	5:L:1731:HOH:O	1.96	0.65
1:B:334:TYR:CD1	5:B:5979:HOH:O	2.49	0.65
1:D:25:LYS:CD	5:D:5949:HOH:O	2.45	0.65
1:E:55:GLY:HA3	5:E:660:HOH:O	1.96	0.65
1:F:179[B]:TYR:CD1	1:F:212[B]:GLU:CA	2.77	0.65
1:I:323:VAL:CG1	5:I:6058:HOH:O	2.20	0.65
1:J:176[B]:LYS:C	1:J:178[B]:GLY:N	2.47	0.65
1:L:179[B]:TYR:CD1	1:L:212[B]:GLU:CA	2.77	0.65
1:F:25:LYS:CD	5:F:5956:HOH:O	2.45	0.64
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.78	0.64
1:G:82:ASP:HB3	5:G:5953:HOH:O	1.95	0.64
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.78	0.64
1:K:25:LYS:CD	5:K:1578:HOH:O	2.45	0.64
1:A:55:GLY:HA3	5:A:5946:HOH:O	1.96	0.64
1:C:55:GLY:HA3	5:C:5946:HOH:O	1.96	0.64
1:F:55:GLY:HA3	5:F:5956:HOH:O	1.96	0.64
1:G:25:LYS:HD3	5:G:5956:HOH:O	1.96	0.64
1:I:55:GLY:HA3	5:I:5967:HOH:O	1.96	0.64
1:J:25:LYS:CD	5:J:5963:HOH:O	2.45	0.64
1:L:201:GLN:HA	5:L:1793:HOH:O	1.97	0.64
1:A:31:VAL:HB	1:F:180[B]:PHE:CE1	2.31	0.64
1:E:201:GLN:HA	5:E:722:HOH:O	1.97	0.64
1:E:334:TYR:CD1	5:E:693:HOH:O	2.49	0.64
1:H:25:LYS:HD3	5:H:5961:HOH:O	1.96	0.64
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.78	0.64
1:L:25:LYS:CD	5:L:1731:HOH:O	2.45	0.64
1:A:25:LYS:HD3	5:A:5946:HOH:O	1.96	0.64
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.78	0.64
1:D:201:GLN:HA	5:D:6006:HOH:O	1.97	0.64
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.78	0.64
1:G:323:VAL:CG1	5:G:6047:HOH:O	2.20	0.64
1:K:25:LYS:HD3	5:K:1578:HOH:O	1.96	0.64
1:D:55:GLY:HA3	5:D:5949:HOH:O	1.96	0.64
1:D:82:ASP:HB3	5:D:5946:HOH:O	1.96	0.64
1:I:25:LYS:CD	5:I:5967:HOH:O	2.45	0.64
1:L:458:HIS:CD2	1:L:460:VAL:H	2.14	0.64
1:A:385:LYS:HE2	5:A:5971:HOH:O	1.95	0.64
1:D:385:LYS:HE2	5:D:5974:HOH:O	1.95	0.64
1:B:25:LYS:CD	5:B:5947:HOH:O	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:LYS:CD	5:G:5956:HOH:O	2.45	0.64
1:H:334:TYR:CD1	5:H:5992:HOH:O	2.49	0.64
1:A:201:GLN:HA	5:A:6003:HOH:O	1.97	0.64
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.78	0.64
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.78	0.64
1:A:82:ASP:O	1:A:84:THR:HG22	1.98	0.64
1:I:82:ASP:O	1:I:84:THR:HG22	1.98	0.64
1:K:155:GLU:OE1	1:K:211[A]:HIS:HE1	1.81	0.64
1:L:82:ASP:O	1:L:84:THR:HG22	1.98	0.64
1:B:201:GLN:HA	5:B:6004:HOH:O	1.97	0.64
1:F:174[B]:GLY:O	1:F:177[B]:GLY:N	2.31	0.64
1:H:25:LYS:CD	5:H:5961:HOH:O	2.45	0.64
1:H:155:GLU:OE1	1:H:211[A]:HIS:HE1	1.82	0.64
1:J:201:GLN:HA	5:J:6020:HOH:O	1.97	0.64
1:K:458:HIS:CD2	1:K:460:VAL:H	2.14	0.64
1:G:55:GLY:HA3	5:G:5956:HOH:O	1.96	0.63
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.78	0.63
1:L:55:GLY:HA3	5:L:1731:HOH:O	1.96	0.63
1:D:165:GLU:CB	5:D:5964:HOH:O	2.43	0.63
1:D:334:TYR:CD1	5:D:5981:HOH:O	2.49	0.63
1:G:174[B]:GLY:O	1:G:177[B]:GLY:N	2.31	0.63
1:G:179[B]:TYR:CD1	1:G:212[B]:GLU:CA	2.77	0.63
5:I:5969:HOH:O	1:J:182:VAL:HG23	1.97	0.63
1:K:334:TYR:CD1	5:K:1611:HOH:O	2.49	0.63
1:A:176[B]:LYS:C	1:A:178[B]:GLY:N	2.47	0.63
1:C:82:ASP:O	1:C:84:THR:HG22	1.98	0.63
1:C:174[B]:GLY:O	1:C:177[B]:GLY:N	2.31	0.63
1:D:82:ASP:O	1:D:84:THR:HG22	1.98	0.63
1:E:82:ASP:O	1:E:84:THR:HG22	1.98	0.63
1:E:155:GLU:OE1	1:E:211[A]:HIS:HE1	1.81	0.63
1:G:155:GLU:OE1	1:G:211[A]:HIS:HE1	1.81	0.63
1:H:178[A]:GLY:O	1:H:212[A]:GLU:C	2.42	0.63
1:J:224:ARG:HG2	1:J:224:ARG:NH2	1.97	0.63
1:K:174[B]:GLY:O	1:K:177[B]:GLY:N	2.31	0.63
1:C:178[A]:GLY:O	1:C:212[A]:GLU:C	2.42	0.63
1:D:458:HIS:CD2	1:D:460:VAL:H	2.14	0.63
1:J:178[A]:GLY:O	1:J:212[A]:GLU:C	2.42	0.63
1:J:360:PHE:CG	1:J:361:PRO:HD3	2.34	0.63
1:A:155:GLU:OE1	1:A:211[A]:HIS:HE1	1.81	0.63
1:J:155:GLU:OE1	1:J:211[A]:HIS:HE1	1.81	0.63
1:K:178[A]:GLY:O	1:K:212[A]:GLU:C	2.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:CD	5:A:5946:HOH:O	2.45	0.63
1:H:201:GLN:HA	5:H:6017:HOH:O	1.97	0.63
1:I:155:GLU:OE1	1:I:211[A]:HIS:HE1	1.81	0.63
1:I:178[A]:GLY:O	1:I:212[A]:GLU:C	2.42	0.63
1:E:178[A]:GLY:O	1:E:212[A]:GLU:C	2.42	0.63
1:L:155:GLU:OE1	1:L:211[A]:HIS:HE1	1.81	0.63
1:B:155:GLU:OE1	1:B:211[A]:HIS:HE1	1.81	0.62
1:B:165:GLU:CB	5:B:5962:HOH:O	2.43	0.62
1:B:178[A]:GLY:O	1:B:212[A]:GLU:C	2.42	0.62
1:E:360:PHE:CG	1:E:361:PRO:HD3	2.34	0.62
1:F:155:GLU:OE1	1:F:211[A]:HIS:HE1	1.81	0.62
1:D:178[A]:GLY:O	1:D:212[A]:GLU:C	2.42	0.62
1:I:174[B]:GLY:O	1:I:177[B]:GLY:N	2.31	0.62
1:C:155:GLU:OE1	1:C:211[A]:HIS:HE1	1.81	0.62
1:E:25:LYS:HD3	5:E:660:HOH:O	1.96	0.62
1:G:82:ASP:O	1:G:84:THR:HG22	1.98	0.62
1:K:201:GLN:HA	5:K:1640:HOH:O	1.97	0.62
1:F:82:ASP:O	1:F:84:THR:HG22	1.98	0.62
1:J:82:ASP:O	1:J:84:THR:HG22	1.98	0.62
1:J:174[B]:GLY:O	1:J:177[B]:GLY:N	2.32	0.62
1:K:269:HIS:CE1	4:K:5910:PPQ:HEP3	2.35	0.62
1:A:452:ARG:HA	5:A:6015:HOH:O	2.00	0.62
1:B:174[B]:GLY:O	1:B:177[B]:GLY:N	2.31	0.62
1:B:269:HIS:CE1	4:B:5901:PPQ:HEP3	2.35	0.62
1:D:155:GLU:OE1	1:D:211[A]:HIS:HE1	1.82	0.62
1:D:269:HIS:CE1	4:D:5903:PPQ:HEP3	2.35	0.62
1:F:178[A]:GLY:O	1:F:212[A]:GLU:C	2.42	0.62
1:F:269:HIS:CE1	4:F:5905:PPQ:HEP3	2.35	0.62
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.34	0.62
1:I:269:HIS:CE1	4:I:5908:PPQ:HEP3	2.35	0.62
1:A:178[A]:GLY:O	1:A:212[A]:GLU:C	2.42	0.62
1:D:179[B]:TYR:CD1	1:D:212[B]:GLU:CA	2.77	0.62
1:G:178[A]:GLY:O	1:G:212[A]:GLU:C	2.42	0.62
1:H:82:ASP:O	1:H:84:THR:HG22	1.98	0.62
1:J:452:ARG:HA	5:J:6032:HOH:O	2.00	0.62
1:K:82:ASP:O	1:K:84:THR:HG22	1.98	0.62
1:B:82:ASP:O	1:B:84:THR:HG22	1.98	0.62
1:C:165:GLU:CB	5:C:5961:HOH:O	2.43	0.62
1:F:128:PRO:HD2	5:F:5919:HOH:O	2.00	0.62
1:H:360:PHE:CG	1:H:361:PRO:HD3	2.34	0.62
1:L:452:ARG:HA	5:L:1807:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PRO:HD2	5:B:5908:HOH:O	2.00	0.62
1:C:360:PHE:CG	1:C:361:PRO:HD3	2.34	0.62
1:C:452:ARG:HA	5:C:6015:HOH:O	2.00	0.62
1:H:174[B]:GLY:O	1:H:177[B]:GLY:N	2.31	0.62
1:I:329:PRO:CG	1:I:359:ARG:CD	2.75	0.62
1:K:437:GLU:HA	5:K:1656:HOH:O	2.00	0.62
1:E:174[B]:GLY:O	1:E:177[B]:GLY:N	2.31	0.62
1:I:128:PRO:HD2	5:I:5928:HOH:O	2.00	0.62
1:I:437:GLU:HA	5:I:6038:HOH:O	2.00	0.62
1:A:174[B]:GLY:O	1:A:177[B]:GLY:N	2.31	0.62
1:A:437:GLU:HA	5:A:6017:HOH:O	2.00	0.62
1:C:128:PRO:HD2	5:C:5909:HOH:O	2.00	0.62
1:C:437:GLU:HA	5:C:6017:HOH:O	2.00	0.62
1:G:452:ARG:HA	5:G:6025:HOH:O	2.00	0.62
1:I:452:ARG:HA	5:I:6036:HOH:O	2.00	0.62
1:L:178[A]:GLY:O	1:L:212[A]:GLU:C	2.42	0.62
1:D:211[B]:HIS:N	1:D:211[B]:HIS:HD2	1.96	0.61
1:B:452:ARG:HA	5:B:6016:HOH:O	2.00	0.61
1:D:437:GLU:HA	5:D:6020:HOH:O	2.00	0.61
1:F:452:ARG:HA	5:F:6025:HOH:O	2.00	0.61
1:J:269:HIS:CE1	4:J:5909:PPQ:HEP3	2.35	0.61
1:D:174[B]:GLY:O	1:D:177[B]:GLY:N	2.31	0.61
1:D:224:ARG:HG2	1:D:224:ARG:NH2	1.97	0.61
1:E:128:PRO:HD2	5:E:621:HOH:O	2.00	0.61
1:J:437:GLU:HA	5:J:6034:HOH:O	2.00	0.61
1:L:269:HIS:CE1	4:L:5911:PPQ:HEP3	2.35	0.61
1:B:1:SER:C	1:B:71:ALA:HB1	2.25	0.61
1:B:437:GLU:HA	5:B:6018:HOH:O	2.00	0.61
1:F:1:SER:C	1:F:71:ALA:HB1	2.26	0.61
1:K:1:SER:C	1:K:71:ALA:HB1	2.25	0.61
1:L:350:SER:HB2	1:L:351:PRO:HD2	1.83	0.61
1:C:350:SER:HB2	1:C:351:PRO:HD2	1.83	0.61
1:E:269:HIS:CE1	4:E:5904:PPQ:HEP3	2.35	0.61
1:E:437:GLU:HA	5:E:738:HOH:O	2.00	0.61
1:F:57:TRP:C	1:F:58:LYS:O	2.42	0.61
1:G:128:PRO:HD2	5:G:5917:HOH:O	2.00	0.61
1:G:269:HIS:CE1	4:G:5906:PPQ:HEP3	2.35	0.61
1:E:452:ARG:HA	5:E:736:HOH:O	2.00	0.61
1:G:437:GLU:HA	5:G:6027:HOH:O	2.00	0.61
1:H:1:SER:C	1:H:71:ALA:HB1	2.26	0.61
1:H:57:TRP:C	1:H:58:LYS:O	2.42	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:128:PRO:HD2	5:J:5926:HOH:O	2.00	0.61
1:K:57:TRP:C	1:K:58:LYS:O	2.42	0.61
1:K:165:GLU:CB	5:K:1594:HOH:O	2.43	0.61
1:B:182:VAL:HG23	5:C:5948:HOH:O	2.00	0.61
1:D:360:PHE:CG	1:D:361:PRO:HD3	2.34	0.61
1:F:437:GLU:HA	5:F:6027:HOH:O	2.00	0.61
1:F:458:HIS:CD2	1:F:460:VAL:H	2.14	0.61
1:G:1:SER:C	1:G:71:ALA:HB1	2.26	0.61
1:G:458:HIS:CD2	1:G:460:VAL:H	2.14	0.61
1:I:360:PHE:CG	1:I:361:PRO:HD3	2.34	0.61
1:J:165:GLU:CB	5:J:5978:HOH:O	2.43	0.61
1:K:42:PHE:HA	5:K:1622:HOH:O	2.01	0.61
1:L:165:GLU:CB	5:L:1747:HOH:O	2.43	0.61
1:A:1:SER:C	1:A:71:ALA:HB1	2.26	0.61
1:A:128:PRO:HD2	5:A:5907:HOH:O	2.00	0.61
1:C:1:SER:C	1:C:71:ALA:HB1	2.26	0.61
1:E:1:SER:C	1:E:71:ALA:HB1	2.26	0.61
1:H:269:HIS:CE1	4:H:5907:PPQ:HEP3	2.35	0.61
1:K:360:PHE:CG	1:K:361:PRO:HD3	2.34	0.61
1:L:174[B]:GLY:O	1:L:177[B]:GLY:N	2.31	0.61
1:L:329:PRO:CG	1:L:359:ARG:CD	2.75	0.61
1:L:360:PHE:CG	1:L:361:PRO:HD3	2.34	0.61
1:A:269:HIS:CE1	4:A:5900:PPQ:HEP3	2.35	0.61
1:C:269:HIS:CE1	4:C:5902:PPQ:HEP3	2.35	0.61
1:E:42:PHE:HA	5:E:704:HOH:O	2.01	0.61
1:E:458:HIS:CD2	1:E:460:VAL:H	2.14	0.61
1:H:350:SER:HB2	1:H:351:PRO:HD2	1.83	0.61
1:K:128:PRO:HD2	5:K:1539:HOH:O	2.00	0.61
1:A:360:PHE:CG	1:A:361:PRO:HD3	2.34	0.61
1:B:57:TRP:C	1:B:58:LYS:O	2.42	0.61
1:I:1:SER:C	1:I:71:ALA:HB1	2.25	0.61
1:J:192[A]:ARG:HD3	1:J:219:ASN:ND2	2.11	0.61
1:J:350:SER:HB2	1:J:351:PRO:HD2	1.83	0.61
1:K:179[B]:TYR:CD1	1:K:212[B]:GLU:CA	2.77	0.61
1:F:350:SER:HB2	1:F:351:PRO:HD2	1.83	0.60
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.34	0.60
1:J:1:SER:C	1:J:71:ALA:HB1	2.26	0.60
1:J:323:VAL:CG1	5:J:6054:HOH:O	2.20	0.60
1:K:452:ARG:HA	5:K:1654:HOH:O	2.00	0.60
1:L:128:PRO:HD2	5:L:1692:HOH:O	2.00	0.60
1:L:192[A]:ARG:HD3	1:L:219:ASN:ND2	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:437:GLU:HA	5:L:1809:HOH:O	2.00	0.60
1:A:350:SER:HB2	1:A:351:PRO:HD2	1.83	0.60
3:C:4473:ADP:C1'	3:C:4473:ADP:C8	2.81	0.60
3:D:4474:ADP:C1'	3:D:4474:ADP:C8	2.81	0.60
1:E:57:TRP:C	1:E:58:LYS:O	2.42	0.60
1:E:350:SER:HB2	1:E:351:PRO:HD2	1.83	0.60
1:G:57:TRP:C	1:G:58:LYS:O	2.42	0.60
1:I:29[A]:GLN:HB3	1:J:180[A]:PHE:HB3	1.83	0.60
1:B:42:PHE:HA	5:B:5989:HOH:O	2.01	0.60
1:C:211[B]:HIS:N	1:C:211[B]:HIS:HD2	1.96	0.60
1:H:458:HIS:CD2	1:H:460:VAL:H	2.14	0.60
1:A:192[A]:ARG:HD3	1:A:219:ASN:ND2	2.11	0.60
1:D:128:PRO:HD2	5:D:5910:HOH:O	2.00	0.60
1:J:285:ASP:CA	5:J:6041:HOH:O	2.35	0.60
1:K:350:SER:HB2	1:K:351:PRO:HD2	1.83	0.60
1:H:179[B]:TYR:CD1	1:H:212[B]:GLU:CA	2.77	0.60
1:I:57:TRP:C	1:I:58:LYS:O	2.42	0.60
1:L:323:VAL:CG1	5:L:1830:HOH:O	2.20	0.60
1:A:42:PHE:HA	5:A:5988:HOH:O	2.01	0.60
1:B:350:SER:HB2	1:B:351:PRO:HD2	1.83	0.60
1:C:57:TRP:C	1:C:58:LYS:O	2.42	0.60
1:E:329:PRO:CG	1:E:359:ARG:CD	2.75	0.60
1:G:179[A]:TYR:C	1:G:181[A]:PRO:CD	2.75	0.60
1:H:437:GLU:HA	5:H:6031:HOH:O	2.00	0.60
1:L:1:SER:C	1:L:71:ALA:HB1	2.26	0.60
1:B:179[A]:TYR:C	1:B:181[A]:PRO:CD	2.75	0.60
1:D:350:SER:HB2	1:D:351:PRO:HD2	1.83	0.60
1:E:179[A]:TYR:C	1:E:181[A]:PRO:CD	2.75	0.60
1:H:452:ARG:HA	5:H:6029:HOH:O	2.00	0.60
1:J:329:PRO:CG	1:J:359:ARG:CD	2.75	0.60
1:J:458:HIS:CD2	1:J:460:VAL:H	2.14	0.60
1:A:465:TYR:O	1:A:468:VAL:HB	2.02	0.60
1:B:458:HIS:CD2	1:B:460:VAL:H	2.14	0.60
1:D:1:SER:C	1:D:71:ALA:HB1	2.26	0.60
1:D:465:TYR:O	1:D:468:VAL:HB	2.02	0.60
1:E:211[B]:HIS:N	1:E:211[B]:HIS:HD2	1.96	0.60
1:F:42:PHE:HA	5:F:5998:HOH:O	2.01	0.60
1:I:465:TYR:O	1:I:468:VAL:HB	2.02	0.60
1:J:465:TYR:O	1:J:468:VAL:HB	2.02	0.60
1:K:26:GLY:HA3	5:K:1592:HOH:O	2.02	0.60
1:F:465:TYR:O	1:F:468:VAL:HB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:PHE:HA	5:H:6002:HOH:O	2.01	0.60
1:I:350:SER:HB2	1:I:351:PRO:HD2	1.83	0.60
1:J:179[A]:TYR:C	1:J:181[A]:PRO:CD	2.75	0.60
1:E:26:GLY:HA3	5:E:674:HOH:O	2.02	0.60
1:E:465:TYR:O	1:E:468:VAL:HB	2.02	0.60
1:H:128:PRO:HD2	5:H:5924:HOH:O	2.00	0.60
1:H:179[A]:TYR:C	1:H:181[A]:PRO:CD	2.75	0.60
1:K:465:TYR:O	1:K:468:VAL:HB	2.02	0.60
1:A:26:GLY:HA3	5:A:5959:HOH:O	2.02	0.59
1:D:42:PHE:HA	5:D:5991:HOH:O	2.01	0.59
1:G:42:PHE:HA	5:G:5998:HOH:O	2.01	0.59
1:J:42:PHE:HA	5:J:6005:HOH:O	2.01	0.59
1:K:251:LYS:HE2	5:K:1554:HOH:O	2.01	0.59
1:C:179[A]:TYR:C	1:C:181[A]:PRO:CD	2.75	0.59
1:C:465:TYR:O	1:C:468:VAL:HB	2.02	0.59
1:D:452:ARG:HA	5:D:6018:HOH:O	2.00	0.59
1:H:28:GLU:HB2	5:H:5945:HOH:O	2.03	0.59
1:L:26:GLY:HA3	5:L:1745:HOH:O	2.02	0.59
1:A:30[A]:HIS:CE1	1:F:183:PRO:HD3	2.37	0.59
1:B:465:TYR:O	1:B:468:VAL:HB	2.02	0.59
1:G:350:SER:HB2	1:G:351:PRO:HD2	1.83	0.59
3:J:4480:ADP:C3'	5:J:5993:HOH:O	2.43	0.59
1:A:28:GLU:HB2	5:A:5930:HOH:O	2.03	0.59
1:D:183:PRO:HB2	5:E:684:HOH:O	2.01	0.59
1:H:192[A]:ARG:HD3	1:H:219:ASN:ND2	2.11	0.59
1:I:179[A]:TYR:C	1:I:181[A]:PRO:CD	2.75	0.59
1:J:34:PRO:HG2	1:K:206:VAL:O	2.02	0.59
1:B:329:PRO:CG	1:B:359:ARG:CD	2.75	0.59
1:D:179[A]:TYR:C	1:D:181[A]:PRO:CD	2.75	0.59
1:D:329:PRO:CG	1:D:359:ARG:CD	2.75	0.59
3:J:4480:ADP:C1'	3:J:4480:ADP:C8	2.81	0.59
3:K:4481:ADP:C1'	3:K:4481:ADP:C8	2.81	0.59
1:F:26:GLY:HA3	5:F:5969:HOH:O	2.02	0.59
1:G:26:GLY:HA3	5:G:5969:HOH:O	2.02	0.59
3:G:4477:ADP:C3'	5:G:5986:HOH:O	2.43	0.59
1:I:26:GLY:HA3	5:I:5980:HOH:O	2.02	0.59
1:L:42:PHE:HA	5:L:1775:HOH:O	2.01	0.59
1:B:211[B]:HIS:N	1:B:211[B]:HIS:HD2	1.96	0.59
1:K:179[A]:TYR:C	1:K:181[A]:PRO:CD	2.75	0.59
1:L:28:GLU:HB2	5:L:1715:HOH:O	2.03	0.59
1:L:57:TRP:C	1:L:58:LYS:O	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TRP:C	1:A:58:LYS:O	2.42	0.59
1:C:192[A]:ARG:HD3	1:C:219:ASN:ND2	2.11	0.59
1:G:212[A]:GLU:HG3	1:G:218:GLN:HE21	1.68	0.59
1:G:465:TYR:O	1:G:468:VAL:HB	2.02	0.59
1:D:28:GLU:HB2	5:D:5933:HOH:O	2.03	0.59
1:D:57:TRP:O	1:D:58:LYS:C	2.46	0.59
1:D:57:TRP:C	1:D:58:LYS:O	2.42	0.59
1:D:212[A]:GLU:HG3	1:D:218:GLN:HE21	1.68	0.59
1:D:323:VAL:CG1	5:D:6040:HOH:O	2.20	0.59
1:E:176[B]:LYS:C	1:E:178[B]:GLY:N	2.47	0.59
1:H:131:GLU:OE2	4:H:5907:PPQ:NP	2.36	0.59
1:K:28:GLU:HB2	5:K:1562:HOH:O	2.03	0.59
1:L:465:TYR:O	1:L:468:VAL:HB	2.02	0.59
1:A:419:ASN:O	1:A:422:ASP:HB3	2.03	0.59
1:C:419:ASN:O	1:C:422:ASP:HB3	2.03	0.59
1:F:179[A]:TYR:C	1:F:181[A]:PRO:CD	2.75	0.59
1:F:57:TRP:O	1:F:58:LYS:C	2.46	0.58
1:F:212[A]:GLU:HG3	1:F:218:GLN:HE21	1.68	0.58
1:H:329:PRO:CG	1:H:359:ARG:CD	2.75	0.58
1:I:57:TRP:O	1:I:58:LYS:C	2.46	0.58
1:I:165:GLU:CB	5:I:5982:HOH:O	2.43	0.58
1:K:131:GLU:OE2	4:K:5910:PPQ:NP	2.36	0.58
1:L:57:TRP:O	1:L:58:LYS:C	2.46	0.58
1:A:179[A]:TYR:C	1:A:181[A]:PRO:CD	2.75	0.58
1:A:182:VAL:HG23	5:B:5949:HOH:O	2.01	0.58
1:B:57:TRP:O	1:B:58:LYS:C	2.46	0.58
1:D:131:GLU:OE2	4:D:5903:PPQ:NP	2.36	0.58
1:E:131:GLU:OE2	4:E:5904:PPQ:NP	2.36	0.58
1:E:419:ASN:O	1:E:422:ASP:HB3	2.03	0.58
1:F:285:ASP:CA	5:F:6034:HOH:O	2.35	0.58
1:I:42:PHE:HA	5:I:6009:HOH:O	2.01	0.58
1:I:212[A]:GLU:HG3	1:I:218:GLN:HE21	1.68	0.58
1:J:57:TRP:C	1:J:58:LYS:O	2.42	0.58
1:K:285:ASP:CA	5:K:1663:HOH:O	2.35	0.58
1:A:57:TRP:O	1:A:58:LYS:C	2.46	0.58
1:A:285:ASP:CA	5:A:6024:HOH:O	2.35	0.58
3:B:4472:ADP:C1'	3:B:4472:ADP:C8	2.81	0.58
1:C:26:GLY:HA3	5:C:5959:HOH:O	2.02	0.58
1:E:28:GLU:HB2	5:E:644:HOH:O	2.03	0.58
1:G:28:GLU:HB2	5:G:5940:HOH:O	2.03	0.58
1:G:131:GLU:OE2	4:G:5906:PPQ:NP	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:GLU:CB	5:H:5975:HOH:O	2.43	0.58
1:I:419:ASN:O	1:I:422:ASP:HB3	2.03	0.58
1:B:360:PHE:CG	1:B:361:PRO:HD3	2.34	0.58
1:C:212[A]:GLU:HG3	1:C:218:GLN:HE21	1.68	0.58
1:F:28:GLU:HB2	5:F:5940:HOH:O	2.03	0.58
1:H:26:GLY:HA3	5:H:5973:HOH:O	2.02	0.58
1:H:211[B]:HIS:N	1:H:211[B]:HIS:HD2	1.96	0.58
1:H:465:TYR:O	1:H:468:VAL:HB	2.02	0.58
1:J:251:LYS:HE2	5:J:5940:HOH:O	2.00	0.58
1:K:211[B]:HIS:N	1:K:211[B]:HIS:HD2	1.96	0.58
1:L:419:ASN:O	1:L:422:ASP:HB3	2.03	0.58
1:G:332:LEU:HD22	1:G:409:GLN:C	2.29	0.58
1:K:212[A]:GLU:HG3	1:K:218:GLN:HE21	1.68	0.58
1:B:131:GLU:OE2	4:B:5901:PPQ:NP	2.36	0.58
1:B:332:LEU:HD22	1:B:409:GLN:C	2.29	0.58
1:C:131:GLU:OE2	4:C:5902:PPQ:NP	2.36	0.58
1:C:332:LEU:HD22	1:C:409:GLN:C	2.29	0.58
1:D:26:GLY:HA3	5:D:5962:HOH:O	2.02	0.58
1:F:329:PRO:CG	1:F:359:ARG:CD	2.75	0.58
1:G:57:TRP:O	1:G:58:LYS:C	2.46	0.58
1:G:419:ASN:O	1:G:422:ASP:HB3	2.03	0.58
1:J:131:GLU:OE2	4:J:5909:PPQ:NP	2.36	0.58
1:K:419:ASN:O	1:K:422:ASP:HB3	2.03	0.58
1:L:212[A]:GLU:HG3	1:L:218:GLN:HE21	1.68	0.58
1:A:131:GLU:OE2	4:A:5900:PPQ:NP	2.36	0.58
1:B:189:GLN:HG3	1:C:80:PHE:CZ	2.39	0.58
1:B:192[A]:ARG:HD3	1:B:219:ASN:ND2	2.11	0.58
1:C:28:GLU:HB2	5:C:5930:HOH:O	2.03	0.58
1:C:42:PHE:HA	5:C:5988:HOH:O	2.01	0.58
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.75	0.58
1:F:332:LEU:HD22	1:F:409:GLN:C	2.29	0.58
1:G:285:ASP:CA	5:G:6034:HOH:O	2.35	0.58
1:H:419:ASN:O	1:H:422:ASP:HB3	2.03	0.58
1:I:131:GLU:OE2	4:I:5908:PPQ:NP	2.36	0.58
1:I:211[B]:HIS:N	1:I:211[B]:HIS:HD2	1.96	0.58
1:J:57:TRP:O	1:J:58:LYS:C	2.46	0.58
1:J:114:TYR:HD2	1:J:431:GLY:HA3	1.69	0.58
1:J:332:LEU:HD22	1:J:409:GLN:C	2.29	0.58
1:J:419:ASN:O	1:J:422:ASP:HB3	2.03	0.58
1:K:192[A]:ARG:HD3	1:K:219:ASN:ND2	2.11	0.58
1:B:26:GLY:HA3	5:B:5960:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ARG:HG2	1:C:224:ARG:NH2	1.97	0.58
1:E:183:PRO:HB2	5:F:5979:HOH:O	2.03	0.58
1:E:192[A]:ARG:HD3	1:E:219:ASN:ND2	2.11	0.58
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.75	0.58
1:J:28:GLU:HB2	5:J:5947:HOH:O	2.03	0.58
1:L:114:TYR:HD2	1:L:431:GLY:HA3	1.69	0.58
1:L:179[A]:TYR:C	1:L:181[A]:PRO:CD	2.75	0.58
1:L:332:LEU:HD22	1:L:409:GLN:C	2.29	0.58
1:A:212[A]:GLU:HG3	1:A:218:GLN:HE21	1.68	0.58
3:A:4471:ADP:C1'	3:A:4471:ADP:C8	2.81	0.58
1:F:131:GLU:OE2	4:F:5905:PPQ:NP	2.36	0.58
1:H:34:PRO:HG2	1:I:206:VAL:O	2.03	0.58
1:L:131:GLU:OE2	4:L:5911:PPQ:NP	2.36	0.58
1:L:211[B]:HIS:N	1:L:211[B]:HIS:HD2	1.96	0.58
1:B:419:ASN:O	1:B:422:ASP:HB3	2.03	0.58
1:D:192[A]:ARG:HD3	1:D:219:ASN:ND2	2.11	0.58
3:D:4474:ADP:C3'	5:D:5979:HOH:O	2.43	0.58
3:E:4475:ADP:C1'	3:E:4475:ADP:C8	2.81	0.58
1:G:211[B]:HIS:N	1:G:211[B]:HIS:HD2	1.96	0.58
3:G:4477:ADP:C1'	3:G:4477:ADP:C8	2.81	0.58
1:H:57:TRP:O	1:H:58:LYS:C	2.46	0.58
1:I:28:GLU:HB2	5:I:5951:HOH:O	2.03	0.58
1:I:332:LEU:HD22	1:I:409:GLN:C	2.29	0.58
1:K:57:TRP:O	1:K:58:LYS:C	2.46	0.58
1:C:57:TRP:O	1:C:58:LYS:C	2.46	0.57
1:D:114:TYR:HD2	1:D:431:GLY:HA3	1.69	0.57
3:I:4479:ADP:C3'	5:I:5997:HOH:O	2.42	0.57
1:J:26:GLY:HA3	5:J:5976:HOH:O	2.02	0.57
1:B:251:LYS:HE2	5:B:5923:HOH:O	2.00	0.57
1:E:57:TRP:O	1:E:58:LYS:C	2.46	0.57
1:F:458:HIS:HD2	1:F:460:VAL:N	2.01	0.57
1:B:360:PHE:CD2	1:B:361:PRO:CD	2.75	0.57
1:E:332:LEU:HD22	1:E:409:GLN:C	2.29	0.57
1:I:179[B]:TYR:CD1	1:I:212[B]:GLU:CA	2.77	0.57
1:E:347:VAL:HA	5:E:670:HOH:O	2.04	0.57
1:K:291:SER:O	1:K:295:LEU:HD12	2.05	0.57
1:B:28:GLU:HB2	5:B:5931:HOH:O	2.03	0.57
1:B:291:SER:O	1:B:295:LEU:HD12	2.05	0.57
5:B:5946:HOH:O	1:C:84:THR:HG21	2.05	0.57
1:D:332:LEU:HD22	1:D:409:GLN:C	2.29	0.57
1:I:114:TYR:HD2	1:I:431:GLY:HA3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179[B]:TYR:CD1	1:J:212[B]:GLU:CA	2.77	0.57
1:J:212[A]:GLU:HG3	1:J:218:GLN:HE21	1.68	0.57
1:K:29[A]:GLN:HB3	1:L:180[A]:PHE:HB3	1.87	0.57
1:B:312:ALA:HB2	1:B:370:CYS:SG	2.45	0.57
1:F:347:VAL:HA	5:F:5966:HOH:O	2.04	0.57
1:G:291:SER:O	1:G:295:LEU:HD12	2.05	0.57
3:I:4479:ADP:C1'	3:I:4479:ADP:C8	2.81	0.57
1:C:312:ALA:HB2	1:C:370:CYS:SG	2.45	0.57
1:D:311:LEU:HD12	1:D:373:ALA:HB2	1.87	0.57
1:E:323:VAL:CG1	5:E:759:HOH:O	2.20	0.57
1:F:201:GLN:CA	5:F:6013:HOH:O	2.53	0.57
1:G:165:GLU:CB	5:G:5971:HOH:O	2.43	0.57
1:H:285:ASP:CA	5:H:6038:HOH:O	2.35	0.57
1:K:312:ALA:HB2	1:K:370:CYS:SG	2.45	0.57
1:K:332:LEU:HD22	1:K:409:GLN:C	2.29	0.57
3:L:4482:ADP:C3'	5:L:1762:HOH:O	2.43	0.57
1:A:311:LEU:HD12	1:A:373:ALA:HB2	1.87	0.57
1:A:312:ALA:HB2	1:A:370:CYS:SG	2.45	0.57
1:B:212[A]:GLU:HG3	1:B:218:GLN:HE21	1.68	0.57
1:D:419:ASN:O	1:D:422:ASP:HB3	2.03	0.57
1:G:312:ALA:HB2	1:G:370:CYS:SG	2.45	0.57
1:H:291:SER:O	1:H:295:LEU:HD12	2.05	0.57
1:H:311:LEU:HD12	1:H:373:ALA:HB2	1.87	0.57
1:H:458:HIS:HD2	1:H:460:VAL:N	2.01	0.57
1:A:332:LEU:HD22	1:A:409:GLN:C	2.29	0.57
1:B:285:ASP:CA	5:B:6025:HOH:O	2.35	0.57
1:C:180[A]:PHE:HB3	1:D:29[A]:GLN:HB3	1.86	0.57
1:D:312:ALA:HB2	1:D:370:CYS:SG	2.45	0.57
1:E:291:SER:O	1:E:295:LEU:HD12	2.05	0.57
1:F:291:SER:O	1:F:295:LEU:HD12	2.05	0.57
1:F:419:ASN:O	1:F:422:ASP:HB3	2.03	0.57
1:G:114:TYR:HD2	1:G:431:GLY:HA3	1.69	0.57
1:G:347:VAL:HA	5:G:5966:HOH:O	2.04	0.57
1:H:312:ALA:HB2	1:H:370:CYS:SG	2.45	0.57
1:H:332:LEU:HD22	1:H:409:GLN:C	2.29	0.57
1:I:291:SER:O	1:I:295:LEU:HD12	2.05	0.57
1:L:311:LEU:HD12	1:L:373:ALA:HB2	1.87	0.57
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.75	0.57
1:A:114:TYR:HD2	1:A:431:GLY:HA3	1.69	0.57
1:E:165:GLU:CB	5:E:676:HOH:O	2.43	0.57
5:G:5958:HOH:O	1:H:182:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:VAL:HA	5:H:5970:HOH:O	2.04	0.57
1:I:311:LEU:HD12	1:I:373:ALA:HB2	1.87	0.57
1:I:312:ALA:HB2	1:I:370:CYS:SG	2.45	0.57
1:J:84:THR:HG21	5:K:1577:HOH:O	2.05	0.57
1:L:264[B]:ASN:HA	1:L:326:TYR:HB3	1.87	0.57
1:A:347:VAL:HA	5:A:5956:HOH:O	2.04	0.56
3:A:4471:ADP:C3'	5:A:5976:HOH:O	2.43	0.56
1:C:291:SER:O	1:C:295:LEU:HD12	2.05	0.56
1:J:230:LYS:O	1:J:233:ASP:HB2	2.05	0.56
1:K:114:TYR:HD2	1:K:431:GLY:HA3	1.69	0.56
1:K:347:VAL:HA	5:K:1588:HOH:O	2.04	0.56
1:B:180[A]:PHE:HB3	1:C:29[A]:GLN:HB3	1.88	0.56
1:F:264[B]:ASN:HA	1:F:326:TYR:HB3	1.87	0.56
1:H:264[B]:ASN:HA	1:H:326:TYR:HB3	1.87	0.56
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.75	0.56
1:J:291:SER:O	1:J:295:LEU:HD12	2.05	0.56
1:K:311:LEU:HD12	1:K:373:ALA:HB2	1.87	0.56
1:B:230:LYS:O	1:B:233:ASP:HB2	2.05	0.56
1:C:114:TYR:HD2	1:C:431:GLY:HA3	1.69	0.56
1:C:230:LYS:O	1:C:233:ASP:HB2	2.05	0.56
1:C:251:LYS:HE2	5:C:5923:HOH:O	2.01	0.56
1:C:264[B]:ASN:HA	1:C:326:TYR:HB3	1.87	0.56
1:C:347:VAL:HA	5:C:5956:HOH:O	2.04	0.56
1:E:230:LYS:O	1:E:233:ASP:HB2	2.05	0.56
1:E:311:LEU:HD12	1:E:373:ALA:HB2	1.87	0.56
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.75	0.56
1:G:189:GLN:NE2	1:G:209[A]:HIS:CE1	2.72	0.56
1:H:212[A]:GLU:HG3	1:H:218:GLN:HE21	1.68	0.56
1:H:230:LYS:O	1:H:233:ASP:HB2	2.05	0.56
1:J:80:PHE:CZ	1:K:189:GLN:HG3	2.40	0.56
1:J:264[B]:ASN:HA	1:J:326:TYR:HB3	1.87	0.56
1:L:230:LYS:O	1:L:233:ASP:HB2	2.05	0.56
1:L:312:ALA:HB2	1:L:370:CYS:SG	2.45	0.56
1:A:165:GLU:CB	5:A:5961:HOH:O	2.43	0.56
1:B:311:LEU:HD12	1:B:373:ALA:HB2	1.87	0.56
1:E:212[A]:GLU:HG3	1:E:218:GLN:HE21	1.68	0.56
1:E:312:ALA:HB2	1:E:370:CYS:SG	2.45	0.56
3:E:4475:ADP:C3'	5:E:691:HOH:O	2.43	0.56
1:I:61:ASN:O	1:J:337:ARG:O	2.23	0.56
1:I:347:VAL:HA	5:I:5977:HOH:O	2.04	0.56
1:C:458:HIS:CD2	1:C:460:VAL:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:VAL:HA	5:D:5959:HOH:O	2.04	0.56
1:F:311:LEU:HD12	1:F:373:ALA:HB2	1.87	0.56
1:G:192[A]:ARG:HD3	1:G:219:ASN:ND2	2.11	0.56
3:H:4478:ADP:C1'	3:H:4478:ADP:C8	2.81	0.56
1:J:347:VAL:HA	5:J:5973:HOH:O	2.04	0.56
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.75	0.56
1:K:264[B]:ASN:HA	1:K:326:TYR:HB3	1.87	0.56
1:B:264[B]:ASN:HA	1:B:326:TYR:HB3	1.87	0.56
1:C:329:PRO:CG	1:C:359:ARG:CD	2.75	0.56
1:G:201:GLN:CA	5:G:6013:HOH:O	2.53	0.56
1:J:29[A]:GLN:HB3	1:K:180[A]:PHE:HB3	1.87	0.56
1:L:347:VAL:HA	5:L:1741:HOH:O	2.04	0.56
1:F:114:TYR:HD2	1:F:431:GLY:HA3	1.69	0.56
1:F:312:ALA:HB2	1:F:370:CYS:SG	2.45	0.56
1:G:29[A]:GLN:HB3	1:H:180[A]:PHE:HB3	1.88	0.56
1:I:182:VAL:HG23	5:I:5916:HOH:O	2.05	0.56
1:J:312:ALA:HB2	1:J:370:CYS:SG	2.45	0.56
1:L:291:SER:O	1:L:295:LEU:HD12	2.05	0.56
3:L:4482:ADP:C1'	3:L:4482:ADP:C8	2.81	0.56
1:A:291:SER:O	1:A:295:LEU:HD12	2.05	0.56
1:C:311:LEU:HD12	1:C:373:ALA:HB2	1.87	0.56
1:E:285:ASP:CA	5:E:745:HOH:O	2.35	0.56
1:E:458:HIS:HB3	1:E:461:GLU:HG3	1.88	0.56
1:F:230:LYS:O	1:F:233:ASP:HB2	2.05	0.56
1:H:201:GLN:CA	5:H:6017:HOH:O	2.53	0.56
1:C:269:HIS:CD2	1:C:359:ARG:HG3	2.41	0.56
3:F:4476:ADP:C1'	3:F:4476:ADP:C8	2.81	0.56
1:H:251:LYS:HE2	5:H:5938:HOH:O	2.00	0.56
1:K:201:GLN:CA	5:K:1640:HOH:O	2.53	0.56
1:L:211[B]:HIS:O	1:L:212[B]:GLU:CB	2.54	0.56
1:B:347:VAL:HA	5:B:5957:HOH:O	2.04	0.56
1:D:269:HIS:CD2	1:D:359:ARG:HG3	2.41	0.56
1:F:192[A]:ARG:HD3	1:F:219:ASN:ND2	2.11	0.56
1:G:311:LEU:HD12	1:G:373:ALA:HB2	1.87	0.56
1:H:29[A]:GLN:HB3	1:I:180[A]:PHE:HB3	1.88	0.56
3:H:4478:ADP:C3'	5:H:5990:HOH:O	2.43	0.56
1:I:251:LYS:HE2	5:I:5943:HOH:O	2.01	0.56
1:I:458:HIS:HB3	1:I:461:GLU:HG3	1.88	0.56
1:J:269:HIS:CD2	1:J:359:ARG:HG3	2.41	0.56
5:J:5965:HOH:O	1:K:182:VAL:HG23	2.06	0.56
1:K:179[A]:TYR:O	1:K:181[A]:PRO:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:HIS:HB3	1:A:461:GLU:HG3	1.88	0.55
1:C:91:ILE:HB	1:C:103:ASP:HB2	1.88	0.55
1:C:201:GLN:CA	5:C:6003:HOH:O	2.53	0.55
1:I:230:LYS:O	1:I:233:ASP:HB2	2.05	0.55
1:I:264[B]:ASN:HA	1:I:326:TYR:HB3	1.87	0.55
1:I:269:HIS:CD2	1:I:359:ARG:HG3	2.41	0.55
1:A:230:LYS:O	1:A:233:ASP:HB2	2.05	0.55
1:D:251:LYS:HE2	5:D:5925:HOH:O	2.01	0.55
1:D:458:HIS:HB3	1:D:461:GLU:HG3	1.88	0.55
1:E:91:ILE:HB	1:E:103:ASP:HB2	1.89	0.55
1:G:61:ASN:O	1:H:337:ARG:O	2.24	0.55
1:G:269:HIS:CD2	1:G:359:ARG:HG3	2.41	0.55
1:G:334:TYR:HD1	5:G:5988:HOH:O	1.88	0.55
1:G:458:HIS:HD2	1:G:460:VAL:N	2.01	0.55
1:H:360:PHE:CD2	1:H:361:PRO:CD	2.75	0.55
1:I:192[A]:ARG:HD3	1:I:219:ASN:ND2	2.11	0.55
1:J:458:HIS:HB3	1:J:461:GLU:HG3	1.88	0.55
1:L:458:HIS:HB3	1:L:461:GLU:HG3	1.88	0.55
1:A:264[B]:ASN:HA	1:A:326:TYR:HB3	1.87	0.55
1:E:251:LYS:HE2	5:E:636:HOH:O	2.01	0.55
1:G:91:ILE:HB	1:G:103:ASP:HB2	1.88	0.55
1:K:230:LYS:O	1:K:233:ASP:HB2	2.05	0.55
1:C:183:PRO:HD3	1:D:30[A]:HIS:CE1	2.41	0.55
1:H:80:PHE:CZ	1:I:189:GLN:HG3	2.42	0.55
1:I:189:GLN:NE2	1:I:209[A]:HIS:CE1	2.72	0.55
1:I:201:GLN:CA	5:I:6024:HOH:O	2.53	0.55
1:J:189:GLN:NE2	1:J:209[A]:HIS:CE1	2.72	0.55
1:J:458:HIS:HD2	1:J:460:VAL:N	2.01	0.55
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.75	0.55
1:A:29[A]:GLN:HB3	1:F:180[A]:PHE:HB3	1.88	0.55
1:A:179[A]:TYR:O	1:A:181[A]:PRO:HD2	2.05	0.55
1:E:264[B]:ASN:HA	1:E:326:TYR:HB3	1.87	0.55
1:J:91:ILE:HB	1:J:103:ASP:HB2	1.88	0.55
1:K:458:HIS:HD2	1:K:460:VAL:N	2.01	0.55
1:D:264[B]:ASN:HA	1:D:326:TYR:HB3	1.87	0.55
1:D:291:SER:O	1:D:295:LEU:HD12	2.05	0.55
1:E:189:GLN:HG3	1:F:80:PHE:CZ	2.41	0.55
1:F:323:VAL:CG1	5:F:6047:HOH:O	2.20	0.55
1:G:176[B]:LYS:C	1:G:178[B]:GLY:N	2.47	0.55
1:H:323:VAL:CG1	5:H:6051:HOH:O	2.20	0.55
1:B:458:HIS:HD2	1:B:460:VAL:N	2.01	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:GLY:C	1:F:61:ASN:N	2.65	0.55
1:F:269:HIS:CD2	1:F:359:ARG:HG3	2.41	0.55
1:G:59:GLY:C	1:G:61:ASN:N	2.65	0.55
1:G:230:LYS:O	1:G:233:ASP:HB2	2.05	0.55
1:J:201:GLN:CA	5:J:6020:HOH:O	2.53	0.55
1:J:211[B]:HIS:N	1:J:211[B]:HIS:HD2	1.96	0.55
1:L:91:ILE:HB	1:L:103:ASP:HB2	1.88	0.55
1:A:334:TYR:HD1	5:A:5978:HOH:O	1.88	0.55
1:B:458:HIS:HB3	1:B:461:GLU:HG3	1.88	0.55
1:E:269:HIS:CD2	1:E:359:ARG:HG3	2.41	0.55
1:H:91:ILE:HB	1:H:103:ASP:HB2	1.88	0.55
1:H:269:HIS:CD2	1:H:359:ARG:HG3	2.41	0.55
1:K:334:TYR:HD1	5:K:1611:HOH:O	1.88	0.55
1:G:264[B]:ASN:HA	1:G:326:TYR:HB3	1.87	0.55
1:I:34:PRO:HG2	1:J:206:VAL:O	2.06	0.55
1:K:269:HIS:CD2	1:K:359:ARG:HG3	2.41	0.55
1:L:201:GLN:CA	5:L:1793:HOH:O	2.53	0.55
1:A:201:GLN:CA	5:A:6003:HOH:O	2.53	0.55
1:A:454:ARG:NH2	1:A:454:ARG:HB3	2.22	0.55
1:B:59:GLY:C	1:B:61:ASN:N	2.65	0.55
1:B:454:ARG:HB3	1:B:454:ARG:NH2	2.22	0.55
3:C:4473:ADP:C3'	5:C:5976:HOH:O	2.43	0.55
1:E:458:HIS:HD2	1:E:460:VAL:N	2.01	0.55
1:H:59:GLY:C	1:H:61:ASN:N	2.65	0.55
1:I:91:ILE:HB	1:I:103:ASP:HB2	1.89	0.55
1:L:269:HIS:CD2	1:L:359:ARG:HG3	2.41	0.55
1:A:59:GLY:C	1:A:61:ASN:N	2.65	0.54
1:C:454:ARG:NH2	1:C:454:ARG:HB3	2.22	0.54
1:D:201:GLN:CA	5:D:6006:HOH:O	2.53	0.54
1:D:230:LYS:O	1:D:233:ASP:HB2	2.05	0.54
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.75	0.54
1:E:201:GLN:CA	5:E:722:HOH:O	2.53	0.54
1:F:165:GLU:CB	5:F:5971:HOH:O	2.43	0.54
1:G:189:GLN:HG3	1:L:80:PHE:CZ	2.42	0.54
1:K:211[B]:HIS:O	1:K:212[B]:GLU:CB	2.54	0.54
1:K:458:HIS:HB3	1:K:461:GLU:HG3	1.88	0.54
1:A:269:HIS:CD2	1:A:359:ARG:HG3	2.41	0.54
1:B:269:HIS:CD2	1:B:359:ARG:HG3	2.41	0.54
1:D:91:ILE:HB	1:D:103:ASP:HB2	1.89	0.54
1:H:458:HIS:HB3	1:H:461:GLU:HG3	1.88	0.54
1:K:91:ILE:HB	1:K:103:ASP:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:329:PRO:CG	1:K:359:ARG:CD	2.75	0.54
1:L:59:GLY:C	1:L:61:ASN:N	2.65	0.54
1:E:179[A]:TYR:O	1:E:181[A]:PRO:HD2	2.05	0.54
1:G:179[A]:TYR:O	1:G:181[A]:PRO:HD2	2.05	0.54
1:G:458:HIS:HB3	1:G:461:GLU:HG3	1.88	0.54
1:I:179[A]:TYR:O	1:I:181[A]:PRO:HD2	2.05	0.54
1:A:91:ILE:HB	1:A:103:ASP:HB2	1.89	0.54
1:A:189:GLN:NE2	1:A:209[A]:HIS:CE1	2.72	0.54
1:C:59:GLY:C	1:C:61:ASN:N	2.65	0.54
1:C:458:HIS:HB3	1:C:461:GLU:HG3	1.88	0.54
1:E:206:VAL:O	1:F:34:PRO:HG2	2.08	0.54
1:F:334:TYR:HD1	5:F:5988:HOH:O	1.89	0.54
1:F:458:HIS:HB3	1:F:461:GLU:HG3	1.88	0.54
1:G:183:PRO:HB2	5:L:1755:HOH:O	2.06	0.54
1:H:114:TYR:HD2	1:H:431:GLY:HA3	1.69	0.54
1:I:129:GLU:HA	5:I:5925:HOH:O	2.08	0.54
1:J:311:LEU:HD12	1:J:373:ALA:HB2	1.87	0.54
1:D:454:ARG:NH2	1:D:454:ARG:HB3	2.22	0.54
1:E:454:ARG:HB3	1:E:454:ARG:NH2	2.22	0.54
1:F:189:GLN:NE2	1:F:209[A]:HIS:CE1	2.72	0.54
1:F:211[A]:HIS:CD2	1:F:212[A]:GLU:N	2.76	0.54
1:F:454:ARG:NH2	1:F:454:ARG:HB3	2.22	0.54
1:G:182:VAL:HG23	5:L:1733:HOH:O	2.07	0.54
1:J:59:GLY:C	1:J:61:ASN:N	2.65	0.54
1:L:129:GLU:HA	5:L:1689:HOH:O	2.08	0.54
1:L:454:ARG:NH2	1:L:454:ARG:HB3	2.22	0.54
1:B:91:ILE:HB	1:B:103:ASP:HB2	1.88	0.54
1:G:454:ARG:NH2	1:G:454:ARG:HB3	2.23	0.54
1:H:84:THR:HG21	5:I:5966:HOH:O	2.08	0.54
1:H:454:ARG:NH2	1:H:454:ARG:HB3	2.22	0.54
1:I:59:GLY:O	1:I:61:ASN:N	2.41	0.54
1:J:454:ARG:NH2	1:J:454:ARG:HB3	2.22	0.54
1:D:211[A]:HIS:CD2	1:D:212[A]:GLU:N	2.76	0.54
1:D:211[B]:HIS:O	1:D:212[B]:GLU:CB	2.54	0.54
1:G:211[A]:HIS:CD2	1:G:212[A]:GLU:N	2.76	0.54
1:A:211[A]:HIS:CD2	1:A:212[A]:GLU:N	2.76	0.54
1:A:251:LYS:HE2	5:A:5922:HOH:O	2.00	0.54
1:C:211[A]:HIS:CD2	1:C:212[A]:GLU:N	2.76	0.54
1:D:179[A]:TYR:O	1:D:181[A]:PRO:HD2	2.05	0.54
1:D:268:MET:HB2	1:D:363:PRO:HD3	1.90	0.54
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211[B]:HIS:O	1:F:212[B]:GLU:CB	2.54	0.54
1:G:251:LYS:HE2	5:G:5932:HOH:O	2.01	0.54
1:I:268:MET:HB2	1:I:363:PRO:HD3	1.90	0.54
1:I:454:ARG:NH2	1:I:454:ARG:HB3	2.22	0.54
1:K:211[A]:HIS:CD2	1:K:212[A]:GLU:N	2.76	0.54
1:D:59:GLY:O	1:D:61:ASN:N	2.41	0.54
1:F:59:GLY:O	1:F:61:ASN:N	2.41	0.54
1:D:59:GLY:C	1:D:61:ASN:N	2.65	0.54
1:D:189:GLN:HE22	1:D:209[A]:HIS:CE1	2.26	0.54
1:F:268:MET:HB2	1:F:363:PRO:HD3	1.90	0.54
1:G:180[A]:PHE:HB3	1:L:29[A]:GLN:HB3	1.89	0.54
1:H:179[A]:TYR:O	1:H:181[A]:PRO:HD2	2.05	0.54
1:K:189:GLN:NE2	1:K:209[A]:HIS:CE1	2.72	0.54
1:L:268:MET:HB2	1:L:363:PRO:HD3	1.90	0.54
1:E:334:TYR:HD1	5:E:693:HOH:O	1.88	0.53
1:J:308:ILE:HG21	1:J:374:LEU:CD1	2.39	0.53
1:K:454:ARG:NH2	1:K:454:ARG:HB3	2.22	0.53
1:L:334:TYR:HD1	5:L:1764:HOH:O	1.88	0.53
1:B:308:ILE:HG21	1:B:374:LEU:CD1	2.39	0.53
3:B:4472:ADP:C3'	5:B:5977:HOH:O	2.43	0.53
1:F:91:ILE:HB	1:F:103:ASP:HB2	1.89	0.53
1:G:308:ILE:HG21	1:G:374:LEU:CD1	2.39	0.53
1:A:118:THR:OG1	1:A:120:ILE:HG13	2.09	0.53
1:B:179[A]:TYR:O	1:B:181[A]:PRO:HD2	2.05	0.53
1:B:268:MET:HB2	1:B:363:PRO:HD3	1.90	0.53
1:C:189:GLN:NE2	1:C:209[A]:HIS:CE1	2.72	0.53
1:E:189:GLN:NE2	1:E:209[A]:HIS:CE1	2.72	0.53
1:F:129:GLU:HA	5:F:5916:HOH:O	2.08	0.53
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.43	0.53
1:G:129:GLU:HA	5:G:5914:HOH:O	2.08	0.53
5:G:5979:HOH:O	1:H:183:PRO:HB2	2.07	0.53
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.43	0.53
1:K:129:GLU:HA	5:K:1536:HOH:O	2.08	0.53
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.43	0.53
1:B:129:GLU:HA	5:B:5905:HOH:O	2.08	0.53
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.43	0.53
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.09	0.53
1:E:189:GLN:HE22	1:E:209[A]:HIS:CE1	2.26	0.53
1:G:268:MET:HB2	1:G:363:PRO:HD3	1.90	0.53
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.09	0.53
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLN:HE22	1:B:209[A]:HIS:CE1	2.26	0.53
1:B:211[A]:HIS:CD2	1:B:212[A]:GLU:N	2.76	0.53
1:D:308:ILE:HG21	1:D:374:LEU:CD1	2.38	0.53
1:E:114:TYR:HD2	1:E:431:GLY:HA3	1.69	0.53
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.43	0.53
1:H:189:GLN:HE22	1:H:209[A]:HIS:CE1	2.26	0.53
1:H:211[A]:HIS:CD2	1:H:212[A]:GLU:N	2.76	0.53
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.43	0.53
1:J:268:MET:HB2	1:J:363:PRO:HD3	1.90	0.53
1:K:189:GLN:HE22	1:K:209[A]:HIS:CE1	2.26	0.53
1:L:118:THR:OG1	1:L:120:ILE:HG13	2.09	0.53
1:B:337:ARG:CD	1:B:338:ASN:N	2.72	0.53
1:C:308:ILE:HG21	1:C:374:LEU:CD1	2.38	0.53
1:E:59:GLY:C	1:E:61:ASN:N	2.65	0.53
5:E:659:HOH:O	1:F:84:THR:HG21	2.08	0.53
1:F:251:LYS:HE2	5:F:5933:HOH:O	2.01	0.53
1:H:308:ILE:HG21	1:H:374:LEU:CD1	2.39	0.53
1:L:189:GLN:HE22	1:L:209[A]:HIS:CE1	2.26	0.53
1:A:19:LEU:O	1:A:30[A]:HIS:HA	2.09	0.53
1:A:337:ARG:CD	1:A:338:ASN:N	2.72	0.53
1:C:255:PHE:O	1:C:363:PRO:HB2	2.09	0.53
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.43	0.53
1:D:458:HIS:HD2	1:D:460:VAL:N	2.01	0.53
1:E:195:MET:HE2	1:E:242:VAL:HA	1.91	0.53
1:H:63:SER:HB2	1:H:65:MET:HE1	1.91	0.53
1:H:255:PHE:O	1:H:363:PRO:HB2	2.09	0.53
1:I:211[A]:HIS:CD2	1:I:212[A]:GLU:N	2.76	0.53
1:J:19:LEU:O	1:J:30[A]:HIS:HA	2.09	0.53
1:K:59:GLY:C	1:K:61:ASN:N	2.65	0.53
1:K:189:GLN:HE22	1:K:209[A]:HIS:HE1	1.57	0.53
1:L:47:LYS:HD3	5:L:1827:HOH:O	2.09	0.53
1:B:19:LEU:O	1:B:30[A]:HIS:HA	2.09	0.53
1:B:195:MET:HE2	1:B:242:VAL:HA	1.91	0.53
1:D:63:SER:HB2	1:D:65:MET:HE1	1.91	0.53
1:E:129:GLU:HA	5:E:618:HOH:O	2.08	0.53
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.09	0.53
1:F:255:PHE:O	1:F:363:PRO:HB2	2.09	0.53
1:F:337:ARG:CD	1:F:338:ASN:N	2.72	0.53
1:H:130:PRO:HB3	1:H:268:MET:HE3	1.91	0.53
1:I:308:ILE:HG21	1:I:374:LEU:CD1	2.38	0.53
1:K:30[A]:HIS:CE1	1:L:183:PRO:HD3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.09	0.53
1:K:195:MET:HE2	1:K:242:VAL:HA	1.91	0.53
1:K:255:PHE:O	1:K:363:PRO:HB2	2.09	0.53
1:L:130:PRO:HB3	1:L:268:MET:HE3	1.91	0.53
1:A:47:LYS:HD3	5:A:6035:HOH:O	2.09	0.53
1:A:308:ILE:HG21	1:A:374:LEU:CD1	2.39	0.53
1:B:114:TYR:HD2	1:B:431:GLY:HA3	1.69	0.53
1:B:255:PHE:O	1:B:363:PRO:HB2	2.09	0.53
1:C:285:ASP:CA	5:C:6024:HOH:O	2.35	0.53
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.43	0.53
1:E:211[A]:HIS:CD2	1:E:212[A]:GLU:N	2.76	0.53
1:G:195:MET:HE2	1:G:242:VAL:HA	1.91	0.53
1:H:47:LYS:HD3	5:H:6049:HOH:O	2.09	0.53
1:I:189:GLN:HE22	1:I:209[A]:HIS:CE1	2.26	0.53
1:J:211[A]:HIS:CD2	1:J:212[A]:GLU:N	2.76	0.53
1:L:19:LEU:O	1:L:30[A]:HIS:HA	2.09	0.53
1:A:268:MET:HB2	1:A:363:PRO:HD3	1.90	0.53
1:B:201:GLN:CA	5:B:6004:HOH:O	2.53	0.53
1:D:19:LEU:O	1:D:30[A]:HIS:HA	2.09	0.53
1:D:176[B]:LYS:C	1:D:178[B]:GLY:N	2.47	0.53
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.09	0.53
1:F:195:MET:HE2	1:F:242:VAL:HA	1.91	0.53
1:G:189:GLN:HE22	1:G:209[A]:HIS:CE1	2.26	0.53
1:G:255:PHE:O	1:G:363:PRO:HB2	2.09	0.53
1:G:329:PRO:CG	1:G:359:ARG:CD	2.75	0.53
1:H:195:MET:HE2	1:H:242:VAL:HA	1.91	0.53
1:K:59:GLY:O	1:K:61:ASN:N	2.41	0.53
1:C:268:MET:HB2	1:C:363:PRO:HD3	1.90	0.52
1:E:19:LEU:O	1:E:30[A]:HIS:HA	2.09	0.52
1:E:130:PRO:HB3	1:E:268:MET:HE3	1.91	0.52
1:E:255:PHE:O	1:E:363:PRO:HB2	2.09	0.52
1:F:308:ILE:HG21	1:F:374:LEU:CD1	2.39	0.52
1:H:19:LEU:O	1:H:30[A]:HIS:HA	2.09	0.52
1:I:63:SER:HB2	1:I:65:MET:HE1	1.91	0.52
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.09	0.52
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.43	0.52
1:J:255:PHE:O	1:J:363:PRO:HB2	2.09	0.52
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.43	0.52
1:A:130:PRO:HB3	1:A:268:MET:HE3	1.91	0.52
1:C:129:GLU:HA	5:C:5906:HOH:O	2.08	0.52
1:D:47:LYS:HD3	5:D:6038:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:GLU:HA	5:D:5907:HOH:O	2.08	0.52
1:D:189:GLN:HE22	1:D:209[A]:HIS:HE1	1.57	0.52
1:E:47:LYS:HD3	5:E:756:HOH:O	2.09	0.52
1:G:329:PRO:CD	1:G:359:ARG:CD	2.87	0.52
1:I:255:PHE:O	1:I:363:PRO:HB2	2.09	0.52
1:J:195:MET:HE2	1:J:242:VAL:HA	1.91	0.52
1:L:285:ASP:CA	5:L:1816:HOH:O	2.35	0.52
1:B:47:LYS:HD3	5:B:6036:HOH:O	2.09	0.52
1:C:179[A]:TYR:O	1:C:181[A]:PRO:HD2	2.05	0.52
1:C:195:MET:HE2	1:C:242:VAL:HA	1.91	0.52
1:C:329:PRO:CD	1:C:359:ARG:CD	2.87	0.52
1:C:458:HIS:HD2	1:C:460:VAL:N	2.01	0.52
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.09	0.52
1:E:63:SER:HB2	1:E:65:MET:HE1	1.91	0.52
1:E:308:ILE:HG21	1:E:374:LEU:CD1	2.39	0.52
1:F:130:PRO:HB3	1:F:268:MET:HE3	1.91	0.52
1:G:19:LEU:O	1:G:30[A]:HIS:HA	2.09	0.52
1:H:118:THR:OG1	1:H:120:ILE:HG13	2.09	0.52
1:I:295:LEU:HB3	1:I:388:PRO:HG3	1.91	0.52
1:I:334:TYR:HD1	5:I:5999:HOH:O	1.88	0.52
1:K:329:PRO:CD	1:K:359:ARG:CD	2.87	0.52
1:L:255:PHE:O	1:L:363:PRO:HB2	2.09	0.52
1:A:189:GLN:HE22	1:A:209[A]:HIS:CE1	2.26	0.52
1:A:458:HIS:HD2	1:A:460:VAL:N	2.01	0.52
1:C:189:GLN:HE22	1:C:209[A]:HIS:CE1	2.26	0.52
1:D:130:PRO:HB3	1:D:268:MET:HE3	1.91	0.52
1:D:255:PHE:O	1:D:363:PRO:HB2	2.09	0.52
1:E:268:MET:HB2	1:E:363:PRO:HD3	1.90	0.52
1:E:295:LEU:HB3	1:E:388:PRO:HG3	1.92	0.52
1:H:268:MET:HB2	1:H:363:PRO:HD3	1.90	0.52
1:I:59:GLY:C	1:I:61:ASN:N	2.65	0.52
1:L:195:MET:HE2	1:L:242:VAL:HA	1.91	0.52
1:C:63:SER:HB2	1:C:65:MET:HE1	1.91	0.52
1:D:189:GLN:NE2	1:D:209[A]:HIS:CE1	2.72	0.52
1:E:329:PRO:CD	1:E:359:ARG:CD	2.87	0.52
1:E:337:ARG:CD	1:E:338:ASN:N	2.72	0.52
1:F:19:LEU:O	1:F:30[A]:HIS:HA	2.09	0.52
1:F:47:LYS:HD3	5:F:6045:HOH:O	2.09	0.52
1:F:329:PRO:CD	1:F:359:ARG:CD	2.87	0.52
1:H:295:LEU:HB3	1:H:388:PRO:HG3	1.91	0.52
1:H:334:TYR:HD1	5:H:5992:HOH:O	1.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:GLU:HA	5:J:5923:HOH:O	2.08	0.52
1:J:329:PRO:CD	1:J:359:ARG:CD	2.87	0.52
1:L:211[A]:HIS:CD2	1:L:212[A]:GLU:N	2.76	0.52
1:A:129:GLU:HA	5:A:5904:HOH:O	2.08	0.52
1:A:329:PRO:CD	1:A:359:ARG:CD	2.87	0.52
1:B:189:GLN:NE2	1:B:209[A]:HIS:CE1	2.72	0.52
1:B:295:LEU:HB3	1:B:388:PRO:HG3	1.91	0.52
1:B:329:PRO:CD	1:B:359:ARG:CD	2.87	0.52
1:C:47:LYS:HD3	5:C:6035:HOH:O	2.09	0.52
1:F:189:GLN:HE22	1:F:209[A]:HIS:CE1	2.26	0.52
1:F:437:GLU:CA	5:F:6027:HOH:O	2.58	0.52
1:G:59:GLY:O	1:G:61:ASN:N	2.41	0.52
1:G:130:PRO:HB3	1:G:268:MET:HE3	1.91	0.52
1:H:129:GLU:HA	5:H:5921:HOH:O	2.08	0.52
1:J:47:LYS:HD3	5:J:6052:HOH:O	2.09	0.52
1:J:130:PRO:HB3	1:J:268:MET:HE3	1.91	0.52
1:K:308:ILE:HG21	1:K:374:LEU:CD1	2.39	0.52
1:L:295:LEU:HB3	1:L:388:PRO:HG3	1.92	0.52
1:A:59:GLY:O	1:A:61:ASN:N	2.41	0.52
1:C:130:PRO:HB3	1:C:268:MET:HE3	1.91	0.52
1:D:295:LEU:HB3	1:D:388:PRO:HG3	1.92	0.52
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.09	0.52
5:G:5955:HOH:O	1:L:84:THR:HG21	2.09	0.52
1:H:211[B]:HIS:O	1:H:212[B]:GLU:CB	2.54	0.52
1:I:437:GLU:CA	5:I:6038:HOH:O	2.58	0.52
1:J:179[A]:TYR:O	1:J:181[A]:PRO:HD2	2.05	0.52
1:J:334:TYR:HD1	5:J:5995:HOH:O	1.88	0.52
1:K:80:PHE:CZ	1:L:189:GLN:HG3	2.45	0.52
1:D:28:GLU:CB	5:D:5933:HOH:O	2.58	0.52
1:D:329:PRO:CD	1:D:359:ARG:CD	2.87	0.52
1:G:47:LYS:HD3	5:G:6045:HOH:O	2.09	0.52
1:K:19:LEU:O	1:K:30[A]:HIS:HA	2.09	0.52
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.09	0.52
1:C:295:LEU:HB3	1:C:388:PRO:HG3	1.91	0.52
1:H:189:GLN:NE2	1:H:209[A]:HIS:CE1	2.72	0.52
1:H:329:PRO:CD	1:H:359:ARG:CD	2.87	0.52
1:I:285:ASP:CA	5:I:6045:HOH:O	2.35	0.52
1:A:235:ILE:HG21	1:A:367:PRO:HG3	1.92	0.52
1:A:329:PRO:CG	1:A:359:ARG:CD	2.75	0.52
1:A:457:PRO:HD3	1:G:261[A]:PHE:HB2	1.92	0.52
1:C:334:TYR:HD1	5:C:5978:HOH:O	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ILE:HG21	1:D:367:PRO:HG3	1.92	0.52
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.75	0.52
1:G:47:LYS:HA	5:G:6045:HOH:O	2.10	0.52
1:G:295:LEU:HB3	1:G:388:PRO:HG3	1.92	0.52
1:H:337:ARG:CD	1:H:338:ASN:N	2.72	0.52
1:K:63:SER:HB2	1:K:65:MET:HE1	1.91	0.52
1:L:308:ILE:HG21	1:L:374:LEU:CD1	2.39	0.52
1:A:414:LEU:HD23	1:A:450:ASP:HB2	1.93	0.51
1:E:33:ILE:HG23	1:E:37:GLN:HB2	1.92	0.51
1:I:19:LEU:O	1:I:30[A]:HIS:HA	2.09	0.51
1:I:329:PRO:CD	1:I:359:ARG:CD	2.87	0.51
1:I:337:ARG:CD	1:I:338:ASN:N	2.72	0.51
1:L:179[A]:TYR:O	1:L:181[A]:PRO:HD2	2.05	0.51
1:A:255:PHE:O	1:A:363:PRO:HB2	2.09	0.51
1:B:33:ILE:HG23	1:B:37:GLN:HB2	1.92	0.51
1:E:47:LYS:HA	5:E:756:HOH:O	2.10	0.51
1:F:414:LEU:HD23	1:F:450:ASP:HB2	1.92	0.51
1:G:437:GLU:CA	5:G:6027:HOH:O	2.58	0.51
1:H:59:GLY:O	1:H:61:ASN:N	2.41	0.51
1:I:414:LEU:HD23	1:I:450:ASP:HB2	1.93	0.51
1:J:189:GLN:HE22	1:J:209[A]:HIS:HE1	1.57	0.51
1:K:33:ILE:HG23	1:K:37:GLN:HB2	1.92	0.51
1:K:47:LYS:HA	5:K:1674:HOH:O	2.10	0.51
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.75	0.51
1:B:211[B]:HIS:O	1:B:212[B]:GLU:CB	2.54	0.51
1:D:334:TYR:HD1	5:D:5981:HOH:O	1.88	0.51
1:J:189:GLN:HE22	1:J:209[A]:HIS:CE1	2.26	0.51
1:L:63:SER:HB2	1:L:65:MET:HE1	1.91	0.51
1:L:235:ILE:HG21	1:L:367:PRO:HG3	1.92	0.51
1:L:329:PRO:CD	1:L:359:ARG:CD	2.87	0.51
1:L:414:LEU:HD23	1:L:450:ASP:HB2	1.93	0.51
1:A:63:SER:HB2	1:A:65:MET:HE1	1.91	0.51
1:A:195:MET:HE2	1:A:242:VAL:HA	1.91	0.51
1:A:211[B]:HIS:N	1:A:211[B]:HIS:HD2	1.96	0.51
1:A:437:GLU:CA	5:A:6017:HOH:O	2.58	0.51
1:B:63:SER:HB2	1:B:65:MET:HE1	1.91	0.51
1:G:33:ILE:HG23	1:G:37:GLN:HB2	1.92	0.51
1:G:63:SER:HB2	1:G:65:MET:HE1	1.91	0.51
1:J:414:LEU:HD23	1:J:450:ASP:HB2	1.93	0.51
1:K:47:LYS:HD3	5:K:1674:HOH:O	2.09	0.51
1:K:115:LEU:HD23	1:K:379:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:295:LEU:HB3	1:K:388:PRO:HG3	1.92	0.51
1:A:4:HIS:O	1:A:7:THR:HG23	2.11	0.51
1:A:28:GLU:CB	5:A:5930:HOH:O	2.58	0.51
1:A:115:LEU:HD23	1:A:379:LEU:HD21	1.93	0.51
1:C:179[B]:TYR:CE1	1:C:212[B]:GLU:N	2.79	0.51
1:D:195:MET:HE2	1:D:242:VAL:HA	1.91	0.51
1:D:414:LEU:HD23	1:D:450:ASP:HB2	1.93	0.51
1:E:4:HIS:O	1:E:7:THR:HG23	2.11	0.51
1:F:47:LYS:HA	5:F:6045:HOH:O	2.10	0.51
1:F:63:SER:HB2	1:F:65:MET:HE1	1.91	0.51
1:F:115:LEU:HD23	1:F:379:LEU:HD21	1.93	0.51
1:G:206:VAL:O	1:L:34:PRO:HG2	2.11	0.51
1:G:414:LEU:HD23	1:G:450:ASP:HB2	1.93	0.51
1:H:179[B]:TYR:CE1	1:H:212[B]:GLU:N	2.79	0.51
1:I:33:ILE:HG23	1:I:37:GLN:HB2	1.92	0.51
1:I:130:PRO:HB3	1:I:268:MET:HE3	1.91	0.51
1:J:179[B]:TYR:CE1	1:J:212[B]:GLU:N	2.79	0.51
1:K:268:MET:HB2	1:K:363:PRO:HD3	1.90	0.51
1:A:179[B]:TYR:CE1	1:A:212[B]:GLU:N	2.79	0.51
1:A:180[A]:PHE:HB3	1:B:29[A]:GLN:HB3	1.92	0.51
1:A:295:LEU:HB3	1:A:388:PRO:HG3	1.91	0.51
1:B:59:GLY:O	1:B:61:ASN:N	2.41	0.51
1:C:323:VAL:CG1	5:C:6037:HOH:O	2.20	0.51
1:E:179[B]:TYR:CE1	1:E:212[B]:GLU:N	2.79	0.51
1:F:179[B]:TYR:CE1	1:F:212[B]:GLU:N	2.79	0.51
1:H:235:ILE:HG21	1:H:367:PRO:HG3	1.92	0.51
1:J:337:ARG:CD	1:J:338:ASN:N	2.72	0.51
1:K:188:ALA:HA	5:K:1590:HOH:O	2.11	0.51
1:K:414:LEU:HD23	1:K:450:ASP:HB2	1.93	0.51
1:L:4:HIS:O	1:L:7:THR:HG23	2.11	0.51
1:B:130:PRO:HB3	1:B:268:MET:HE3	1.91	0.51
1:B:179[B]:TYR:CE1	1:B:212[B]:GLU:N	2.79	0.51
1:C:19:LEU:O	1:C:30[A]:HIS:HA	2.09	0.51
1:D:115:LEU:HD23	1:D:379:LEU:HD21	1.93	0.51
1:D:183:PRO:HD3	1:E:30[A]:HIS:CE1	2.46	0.51
1:D:384:ASN:N	1:D:384:ASN:ND2	2.59	0.51
1:J:115:LEU:HD23	1:J:379:LEU:HD21	1.93	0.51
1:L:28:GLU:CB	5:L:1715:HOH:O	2.58	0.51
1:L:251:LYS:HE2	5:L:1707:HOH:O	2.01	0.51
1:B:25:LYS:HD2	5:B:5947:HOH:O	2.10	0.51
1:C:115:LEU:HD23	1:C:379:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:HIS:O	1:D:7:THR:HG23	2.11	0.51
1:E:437:GLU:CA	5:E:738:HOH:O	2.58	0.51
1:F:28:GLU:CB	5:F:5940:HOH:O	2.58	0.51
1:G:115:LEU:HD23	1:G:379:LEU:HD21	1.93	0.51
1:I:115:LEU:HD23	1:I:379:LEU:HD21	1.93	0.51
1:I:179[B]:TYR:CE1	1:I:212[B]:GLU:N	2.79	0.51
1:I:445:LEU:O	1:I:448:GLU:HG2	2.11	0.51
1:J:63:SER:HB2	1:J:65:MET:HE1	1.91	0.51
1:J:445:LEU:O	1:J:448:GLU:HG2	2.11	0.51
1:L:47:LYS:HA	5:L:1827:HOH:O	2.10	0.51
1:L:179[B]:TYR:CE1	1:L:212[B]:GLU:N	2.79	0.51
1:L:189:GLN:NE2	1:L:209[A]:HIS:CE1	2.72	0.51
1:A:189:GLN:HE22	1:A:209[A]:HIS:HE1	1.57	0.51
1:C:264[B]:ASN:CA	1:C:326:TYR:HB3	2.41	0.51
1:D:47:LYS:HA	5:D:6038:HOH:O	2.10	0.51
1:G:179[B]:TYR:CE1	1:G:212[B]:GLU:N	2.79	0.51
1:H:445:LEU:O	1:H:448:GLU:HG2	2.11	0.51
1:I:189:GLN:HE22	1:I:209[A]:HIS:HE1	1.57	0.51
1:J:4:HIS:O	1:J:7:THR:HG23	2.11	0.51
1:J:28:GLU:CB	5:J:5947:HOH:O	2.58	0.51
1:J:211[B]:HIS:O	1:J:212[B]:GLU:CB	2.54	0.51
1:K:264[B]:ASN:CA	1:K:326:TYR:HB3	2.41	0.51
1:L:384:ASN:N	1:L:384:ASN:ND2	2.59	0.51
1:A:33:ILE:HG23	1:A:37:GLN:HB2	1.92	0.51
1:B:47:LYS:HA	5:B:6036:HOH:O	2.10	0.51
1:B:179[B]:TYR:CD1	1:B:212[B]:GLU:CA	2.77	0.51
1:B:183:PRO:HB2	5:C:5969:HOH:O	2.10	0.51
1:B:264[B]:ASN:CA	1:B:326:TYR:HB3	2.41	0.51
1:D:33:ILE:HG23	1:D:37:GLN:HB2	1.92	0.51
1:D:73:THR:HG21	1:D:88:ARG:HB3	1.93	0.51
1:D:264[B]:ASN:CA	1:D:326:TYR:HB3	2.41	0.51
1:D:445:LEU:O	1:D:448:GLU:HG2	2.11	0.51
1:G:188:ALA:HA	5:G:5968:HOH:O	2.11	0.51
1:H:188:ALA:HA	5:H:5972:HOH:O	2.11	0.51
1:I:235:ILE:HG21	1:I:367:PRO:HG3	1.92	0.51
5:J:5986:HOH:O	1:K:183:PRO:HB2	2.11	0.51
1:L:445:LEU:O	1:L:448:GLU:HG2	2.11	0.51
1:A:47:LYS:HA	5:A:6035:HOH:O	2.10	0.50
1:B:384:ASN:N	1:B:384:ASN:ND2	2.59	0.50
1:C:33:ILE:HG23	1:C:37:GLN:HB2	1.92	0.50
1:F:33:ILE:HG23	1:F:37:GLN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:445:LEU:O	1:G:448:GLU:HG2	2.11	0.50
1:H:33:ILE:HG23	1:H:37:GLN:HB2	1.92	0.50
1:I:4:HIS:O	1:I:7:THR:HG23	2.11	0.50
1:I:195:MET:HE2	1:I:242:VAL:HA	1.91	0.50
1:I:211[B]:HIS:O	1:I:212[B]:GLU:CB	2.54	0.50
1:I:264[B]:ASN:CA	1:I:326:TYR:HB3	2.41	0.50
1:K:130:PRO:HB3	1:K:268:MET:HE3	1.91	0.50
1:A:445:LEU:O	1:A:448:GLU:HG2	2.11	0.50
1:C:445:LEU:O	1:C:448:GLU:HG2	2.11	0.50
1:D:188:ALA:HA	5:D:5961:HOH:O	2.11	0.50
1:E:125:LEU:O	1:E:272:MET:HA	2.12	0.50
1:F:445:LEU:O	1:F:448:GLU:HG2	2.11	0.50
3:F:4476:ADP:C3'	5:F:5986:HOH:O	2.43	0.50
1:G:264[B]:ASN:CA	1:G:326:TYR:HB3	2.41	0.50
1:H:334:TYR:CZ	1:H:391:PRO:HG3	2.47	0.50
1:H:460:VAL:HG12	1:H:464:LEU:HD22	1.93	0.50
1:K:179[B]:TYR:CE1	1:K:212[B]:GLU:N	2.79	0.50
1:K:460:VAL:HG12	1:K:464:LEU:HD22	1.94	0.50
1:L:337:ARG:CD	1:L:338:ASN:N	2.72	0.50
1:A:264[B]:ASN:CA	1:A:326:TYR:HB3	2.41	0.50
1:C:337:ARG:CD	1:C:338:ASN:N	2.72	0.50
1:D:179[B]:TYR:CE1	1:D:212[B]:GLU:N	2.79	0.50
1:D:337:ARG:CD	1:D:338:ASN:N	2.72	0.50
1:D:460:VAL:HG12	1:D:464:LEU:HD22	1.94	0.50
1:H:73:THR:HG21	1:H:88:ARG:HB3	1.93	0.50
1:I:80:PHE:CZ	1:J:189:GLN:HG3	2.46	0.50
1:J:47:LYS:HA	5:J:6052:HOH:O	2.10	0.50
1:K:235:ILE:HG21	1:K:367:PRO:HG3	1.92	0.50
1:K:334:TYR:CZ	1:K:391:PRO:HG3	2.47	0.50
1:A:210[B]:HIS:C	1:A:211[B]:HIS:CD2	2.89	0.50
1:B:188:ALA:HA	5:B:5959:HOH:O	2.11	0.50
1:D:125:LEU:O	1:D:272:MET:HA	2.12	0.50
1:F:460:VAL:HG12	1:F:464:LEU:HD22	1.94	0.50
1:H:125:LEU:O	1:H:272:MET:HA	2.12	0.50
5:I:5990:HOH:O	1:J:183:PRO:HB2	2.11	0.50
1:J:33:ILE:HG23	1:J:37:GLN:HB2	1.92	0.50
1:J:125:LEU:O	1:J:272:MET:HA	2.12	0.50
1:J:264[B]:ASN:CA	1:J:326:TYR:HB3	2.41	0.50
1:L:188:ALA:HA	5:L:1743:HOH:O	2.11	0.50
1:A:25:LYS:HD2	5:A:5946:HOH:O	2.10	0.50
1:C:28:GLU:CB	5:C:5930:HOH:O	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:O	1:C:272:MET:HA	2.12	0.50
1:E:445:LEU:O	1:E:448:GLU:HG2	2.11	0.50
1:H:4:HIS:O	1:H:7:THR:HG23	2.11	0.50
1:H:25:LYS:HD2	5:H:5961:HOH:O	2.10	0.50
1:H:264[B]:ASN:CA	1:H:326:TYR:HB3	2.41	0.50
1:I:460:VAL:HG12	1:I:464:LEU:HD22	1.94	0.50
1:J:25:LYS:HD2	5:J:5963:HOH:O	2.11	0.50
1:J:235:ILE:HG21	1:J:367:PRO:HG3	1.92	0.50
1:K:28:GLU:CB	5:K:1562:HOH:O	2.58	0.50
1:K:337:ARG:CD	1:K:338:ASN:N	2.72	0.50
1:L:33:ILE:HG23	1:L:37:GLN:HB2	1.92	0.50
1:L:334:TYR:CZ	1:L:391:PRO:HG3	2.46	0.50
1:A:334:TYR:CZ	1:A:391:PRO:HG3	2.47	0.50
1:B:334:TYR:CZ	1:B:391:PRO:HG3	2.47	0.50
1:D:272:MET:O	1:D:355:ARG:HB2	2.12	0.50
1:E:235:ILE:HG21	1:E:367:PRO:HG3	1.92	0.50
1:F:179[A]:TYR:O	1:F:181[A]:PRO:HD2	2.05	0.50
1:F:235:ILE:HG21	1:F:367:PRO:HG3	1.92	0.50
1:G:4:HIS:O	1:G:7:THR:HG23	2.11	0.50
1:G:28:GLU:CB	5:G:5940:HOH:O	2.58	0.50
1:G:235:ILE:HG21	1:G:367:PRO:HG3	1.92	0.50
1:G:337:ARG:CD	1:G:338:ASN:N	2.72	0.50
1:I:73:THR:HG21	1:I:88:ARG:HB3	1.93	0.50
1:L:25:LYS:HD2	5:L:1731:HOH:O	2.10	0.50
1:A:188:ALA:HA	5:A:5958:HOH:O	2.11	0.50
1:A:460:VAL:HG12	1:A:464:LEU:HD22	1.94	0.50
1:C:4:HIS:O	1:C:7:THR:HG23	2.11	0.50
1:C:60:ILE:HG23	1:C:60:ILE:O	2.12	0.50
1:C:235:ILE:HG21	1:C:367:PRO:HG3	1.92	0.50
1:E:183:PRO:CB	5:F:5979:HOH:O	2.59	0.50
1:F:295:LEU:HB3	1:F:388:PRO:HG3	1.91	0.50
1:F:334:TYR:CZ	1:F:391:PRO:HG3	2.47	0.50
1:H:47:LYS:HA	5:H:6049:HOH:O	2.10	0.50
1:H:272:MET:O	1:H:355:ARG:HB2	2.12	0.50
1:I:47:LYS:HD3	5:I:6056:HOH:O	2.09	0.50
1:I:334:TYR:CZ	1:I:391:PRO:HG3	2.46	0.50
1:J:295:LEU:HB3	1:J:388:PRO:HG3	1.91	0.50
1:K:272:MET:O	1:K:355:ARG:HB2	2.12	0.50
1:A:25:LYS:NZ	5:A:5919:HOH:O	2.45	0.50
1:B:414:LEU:HD23	1:B:450:ASP:HB2	1.93	0.50
1:C:334:TYR:CZ	1:C:391:PRO:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:LEU:HD23	1:C:450:ASP:HB2	1.93	0.50
1:E:210[B]:HIS:C	1:E:211[B]:HIS:CD2	2.89	0.50
1:F:4:HIS:O	1:F:7:THR:HG23	2.11	0.50
1:I:47:LYS:HA	5:I:6056:HOH:O	2.10	0.50
1:I:458:HIS:HD2	1:I:460:VAL:N	2.01	0.50
1:K:4:HIS:O	1:K:7:THR:HG23	2.11	0.50
1:K:445:LEU:O	1:K:448:GLU:HG2	2.11	0.50
1:L:115:LEU:HD23	1:L:379:LEU:HD21	1.93	0.50
1:L:460:VAL:HG12	1:L:464:LEU:HD22	1.93	0.50
1:B:125:LEU:O	1:B:272:MET:HA	2.12	0.50
1:E:59:GLY:O	1:E:61:ASN:N	2.41	0.50
1:E:460:VAL:HG12	1:E:464:LEU:HD22	1.94	0.50
1:F:211[B]:HIS:N	1:F:211[B]:HIS:HD2	1.96	0.50
1:F:272:MET:O	1:F:355:ARG:HB2	2.12	0.50
1:I:125:LEU:O	1:I:272:MET:HA	2.12	0.50
1:J:188:ALA:HA	5:J:5975:HOH:O	2.11	0.50
1:K:125:LEU:O	1:K:272:MET:HA	2.12	0.50
1:L:59:GLY:O	1:L:61:ASN:N	2.41	0.50
1:L:264[B]:ASN:CA	1:L:326:TYR:HB3	2.41	0.50
1:B:235:ILE:HG21	1:B:367:PRO:HG3	1.92	0.49
1:D:437:GLU:CA	5:D:6020:HOH:O	2.58	0.49
1:E:414:LEU:HD23	1:E:450:ASP:HB2	1.93	0.49
1:F:188:ALA:HA	5:F:5968:HOH:O	2.11	0.49
1:G:73:THR:HG21	1:G:88:ARG:HB3	1.93	0.49
1:G:272:MET:O	1:G:355:ARG:HB2	2.12	0.49
1:G:334:TYR:CZ	1:G:391:PRO:HG3	2.47	0.49
1:H:179[B]:TYR:CD2	1:H:211[B]:HIS:HB2	2.47	0.49
1:L:125:LEU:O	1:L:272:MET:HA	2.12	0.49
1:C:47:LYS:HA	5:C:6035:HOH:O	2.10	0.49
1:E:73:THR:HG21	1:E:88:ARG:HB3	1.93	0.49
1:E:115:LEU:HD23	1:E:379:LEU:HD21	1.93	0.49
1:H:115:LEU:HD23	1:H:379:LEU:HD21	1.93	0.49
1:I:188:ALA:HA	5:I:5979:HOH:O	2.11	0.49
1:B:175[B]:VAL:O	1:B:175[B]:VAL:HG12	2.13	0.49
1:B:272:MET:O	1:B:355:ARG:HB2	2.12	0.49
1:B:445:LEU:O	1:B:448:GLU:HG2	2.11	0.49
1:B:460:VAL:HG12	1:B:464:LEU:HD22	1.93	0.49
1:C:124:VAL:HA	1:C:274:LEU:HD23	1.95	0.49
1:D:75:VAL:CG2	5:D:5919:HOH:O	2.53	0.49
1:E:188:ALA:HA	5:E:672:HOH:O	2.11	0.49
1:E:334:TYR:CZ	1:E:391:PRO:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:THR:HG21	1:F:88:ARG:HB3	1.93	0.49
1:F:125:LEU:O	1:F:272:MET:HA	2.12	0.49
1:H:414:LEU:HD23	1:H:450:ASP:HB2	1.93	0.49
1:I:210[B]:HIS:C	1:I:211[B]:HIS:CD2	2.90	0.49
1:I:272:MET:O	1:I:355:ARG:HB2	2.12	0.49
1:J:25:LYS:NZ	5:J:5937:HOH:O	2.45	0.49
1:J:178[A]:GLY:O	1:J:212[A]:GLU:O	2.31	0.49
1:J:460:VAL:HG12	1:J:464:LEU:HD22	1.94	0.49
1:K:175[B]:VAL:O	1:K:175[B]:VAL:HG12	2.13	0.49
3:K:4481:ADP:C3'	5:K:1609:HOH:O	2.42	0.49
1:L:178[A]:GLY:O	1:L:212[A]:GLU:O	2.31	0.49
1:L:179[B]:TYR:CD2	1:L:211[B]:HIS:HB2	2.47	0.49
1:B:73:THR:HG21	1:B:88:ARG:HB3	1.93	0.49
1:B:115:LEU:HD23	1:B:379:LEU:HD21	1.93	0.49
1:D:178[A]:GLY:O	1:D:212[A]:GLU:O	2.31	0.49
1:E:25:LYS:HD2	5:E:660:HOH:O	2.10	0.49
1:G:125:LEU:O	1:G:272:MET:HA	2.12	0.49
1:H:175[B]:VAL:HG12	1:H:175[B]:VAL:O	2.13	0.49
1:I:60:ILE:O	1:I:60:ILE:HG23	2.12	0.49
1:J:334:TYR:CZ	1:J:391:PRO:HG3	2.47	0.49
1:K:73:THR:HG21	1:K:88:ARG:HB3	1.93	0.49
1:L:60:ILE:HG23	1:L:60:ILE:O	2.12	0.49
1:L:458:HIS:HD2	1:L:460:VAL:N	2.01	0.49
1:B:4:HIS:O	1:B:7:THR:HG23	2.11	0.49
1:B:259:PRO:HG2	1:B:260[A]:MET:H	1.78	0.49
1:C:178[A]:GLY:O	1:C:212[A]:GLU:O	2.31	0.49
1:C:188:ALA:HA	5:C:5958:HOH:O	2.11	0.49
1:D:179[B]:TYR:CD2	1:D:211[B]:HIS:HB2	2.47	0.49
1:E:28:GLU:CB	5:E:644:HOH:O	2.58	0.49
1:E:272:MET:O	1:E:355:ARG:HB2	2.12	0.49
1:F:178[A]:GLY:O	1:F:212[A]:GLU:O	2.31	0.49
1:F:264[B]:ASN:CA	1:F:326:TYR:HB3	2.41	0.49
1:G:60:ILE:HG23	1:G:60:ILE:O	2.12	0.49
1:G:178[A]:GLY:O	1:G:212[A]:GLU:O	2.31	0.49
1:H:60:ILE:HG23	1:H:60:ILE:O	2.12	0.49
1:J:73:THR:HG21	1:J:88:ARG:HB3	1.93	0.49
1:A:463:GLU:HA	1:G:140:PHE:CE1	2.47	0.49
1:B:178[A]:GLY:O	1:B:212[A]:GLU:O	2.31	0.49
1:C:73:THR:HG21	1:C:88:ARG:HB3	1.93	0.49
1:C:179[B]:TYR:CD2	1:C:211[B]:HIS:HB2	2.47	0.49
1:C:259:PRO:HG2	1:C:260[A]:MET:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:VAL:HG23	5:F:5958:HOH:O	2.11	0.49
1:I:124:VAL:HA	1:I:274:LEU:HD23	1.95	0.49
1:J:33:ILE:CD1	1:K:208:ALA:HB2	2.42	0.49
1:J:59:GLY:O	1:J:61:ASN:N	2.41	0.49
1:K:60:ILE:HG23	1:K:60:ILE:O	2.12	0.49
1:L:73:THR:HG21	1:L:88:ARG:HB3	1.93	0.49
1:B:348:VAL:HG22	5:B:5935:HOH:O	2.13	0.49
1:D:334:TYR:CZ	1:D:391:PRO:HG3	2.47	0.49
1:E:60:ILE:HG23	1:E:60:ILE:O	2.12	0.49
1:E:175[B]:VAL:O	1:E:175[B]:VAL:HG12	2.13	0.49
1:E:264[B]:ASN:CA	1:E:326:TYR:HB3	2.41	0.49
1:F:60:ILE:O	1:F:60:ILE:HG23	2.12	0.49
1:F:179[B]:TYR:CD2	1:F:211[B]:HIS:HB2	2.47	0.49
1:G:25:LYS:NZ	5:G:5929:HOH:O	2.45	0.49
1:G:329:PRO:CD	1:G:359:ARG:HD2	2.42	0.49
1:K:124:VAL:HA	1:K:274:LEU:HD23	1.95	0.49
1:L:75:VAL:CG2	5:L:1701:HOH:O	2.53	0.49
1:A:178[A]:GLY:O	1:A:212[A]:GLU:O	2.31	0.49
1:A:183:PRO:HB2	5:B:5970:HOH:O	2.12	0.49
1:B:28:GLU:CB	5:B:5931:HOH:O	2.58	0.49
1:C:460:VAL:HG12	1:C:464:LEU:HD22	1.94	0.49
1:D:175[B]:VAL:O	1:D:175[B]:VAL:HG12	2.12	0.49
1:D:348:VAL:HG22	5:D:5937:HOH:O	2.13	0.49
1:H:437:GLU:CA	5:H:6031:HOH:O	2.58	0.49
1:I:178[A]:GLY:O	1:I:212[A]:GLU:O	2.31	0.49
1:J:179[B]:TYR:CD2	1:J:211[B]:HIS:HB2	2.47	0.49
1:K:437:GLU:CA	5:K:1656:HOH:O	2.58	0.49
1:A:73:THR:HG21	1:A:88:ARG:HB3	1.93	0.49
1:A:272:MET:O	1:A:355:ARG:HB2	2.12	0.49
1:C:25:LYS:HD2	5:C:5946:HOH:O	2.10	0.49
1:E:75:VAL:CG2	5:E:630:HOH:O	2.53	0.49
1:E:178[A]:GLY:O	1:E:212[A]:GLU:O	2.31	0.49
1:I:179[B]:TYR:CD2	1:I:211[B]:HIS:HB2	2.47	0.49
1:J:259:PRO:HG2	1:J:260[A]:MET:H	1.78	0.49
1:K:25:LYS:NZ	5:K:1551:HOH:O	2.45	0.49
1:L:25:LYS:NZ	5:L:1704:HOH:O	2.45	0.49
1:A:32:THR:OG1	1:F:189:GLN:NE2	2.46	0.49
1:A:60:ILE:O	1:A:60:ILE:HG23	2.12	0.49
1:A:124:VAL:HA	1:A:274:LEU:HD23	1.95	0.49
1:D:25:LYS:HD2	5:D:5949:HOH:O	2.11	0.49
1:E:259:PRO:HG2	1:E:260[A]:MET:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:LYS:NZ	5:H:5935:HOH:O	2.45	0.49
1:I:174[B]:GLY:O	1:I:177[B]:GLY:HA2	2.13	0.49
1:K:348:VAL:HG22	5:K:1566:HOH:O	2.13	0.49
1:A:179[B]:TYR:CD2	1:A:211[B]:HIS:HB2	2.47	0.48
1:B:174[B]:GLY:O	1:B:177[B]:GLY:HA2	2.13	0.48
1:C:25:LYS:NZ	5:C:5920:HOH:O	2.45	0.48
1:D:25:LYS:NZ	5:D:5922:HOH:O	2.45	0.48
1:D:174[B]:GLY:O	1:D:177[B]:GLY:HA2	2.13	0.48
1:F:25:LYS:NZ	5:F:5930:HOH:O	2.45	0.48
1:F:259:PRO:HG2	1:F:260[A]:MET:H	1.78	0.48
1:F:329:PRO:CD	1:F:359:ARG:HD2	2.42	0.48
1:G:460:VAL:HG12	1:G:464:LEU:HD22	1.94	0.48
1:H:231:LYS:CE	5:H:5924:HOH:O	2.59	0.48
1:I:348:VAL:HG22	5:I:5955:HOH:O	2.13	0.48
1:J:60:ILE:HG23	1:J:60:ILE:O	2.12	0.48
5:K:1580:HOH:O	1:L:182:VAL:HG23	2.13	0.48
1:A:175[B]:VAL:O	1:A:175[B]:VAL:HG12	2.13	0.48
1:C:59:GLY:O	1:C:61:ASN:N	2.41	0.48
1:F:348:VAL:HG22	5:F:5944:HOH:O	2.13	0.48
1:H:259:PRO:HG2	1:H:260[A]:MET:H	1.77	0.48
1:K:174[B]:GLY:O	1:K:177[B]:GLY:HA2	2.13	0.48
1:L:437:GLU:CA	5:L:1809:HOH:O	2.58	0.48
1:A:125:LEU:O	1:A:272:MET:HA	2.12	0.48
1:B:25:LYS:NZ	5:B:5920:HOH:O	2.45	0.48
1:B:124:VAL:HA	1:B:274:LEU:HD23	1.95	0.48
1:F:124:VAL:HA	1:F:274:LEU:HD23	1.95	0.48
1:G:124:VAL:HA	1:G:274:LEU:HD23	1.95	0.48
1:G:175[B]:VAL:O	1:G:175[B]:VAL:HG12	2.13	0.48
1:H:178[A]:GLY:O	1:H:212[A]:GLU:O	2.31	0.48
1:H:348:VAL:HG22	5:H:5949:HOH:O	2.13	0.48
1:I:25:LYS:HD2	5:I:5967:HOH:O	2.10	0.48
1:J:272:MET:O	1:J:355:ARG:HB2	2.12	0.48
1:L:174[B]:GLY:O	1:L:177[B]:GLY:HA2	2.13	0.48
1:L:230:LYS:HG2	5:L:1749:HOH:O	2.14	0.48
1:B:334:TYR:HD1	5:B:5979:HOH:O	1.88	0.48
1:C:154:ILE:HG13	5:C:5977:HOH:O	2.14	0.48
1:G:25:LYS:HD2	5:G:5956:HOH:O	2.10	0.48
1:I:25:LYS:NZ	5:I:5940:HOH:O	2.45	0.48
1:J:329:PRO:HG2	1:J:359:ARG:CD	2.18	0.48
1:K:259:PRO:HG2	1:K:260[A]:MET:H	1.78	0.48
1:L:210[B]:HIS:C	1:L:211[B]:HIS:CD2	2.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:348:VAL:HG22	5:L:1719:HOH:O	2.13	0.48
1:D:124:VAL:HA	1:D:274:LEU:HD23	1.95	0.48
1:D:423:LEU:C	1:D:425:ARG:H	2.22	0.48
1:E:360:PHE:CG	1:E:361:PRO:CD	2.97	0.48
3:E:4475:ADP:H5'1	5:E:691:HOH:O	2.14	0.48
1:G:384:ASN:N	1:G:384:ASN:ND2	2.59	0.48
1:H:28:GLU:CB	5:H:5945:HOH:O	2.58	0.48
1:H:154:ILE:HG13	5:H:5991:HOH:O	2.13	0.48
1:I:60:ILE:O	1:J:339:ARG:HB2	2.14	0.48
1:I:259:PRO:HG2	1:I:260[A]:MET:H	1.78	0.48
1:J:410:VAL:HG22	5:J:6043:HOH:O	2.14	0.48
1:K:178[A]:GLY:O	1:K:212[A]:GLU:O	2.31	0.48
1:L:175[B]:VAL:O	1:L:175[B]:VAL:HG12	2.13	0.48
1:L:259:PRO:HG2	1:L:260[A]:MET:H	1.78	0.48
1:L:272:MET:O	1:L:355:ARG:HB2	2.12	0.48
1:B:179[B]:TYR:CD2	1:B:211[B]:HIS:HB2	2.47	0.48
1:B:437:GLU:CA	5:B:6018:HOH:O	2.58	0.48
1:D:60:ILE:HG23	1:D:60:ILE:O	2.12	0.48
1:E:211[B]:HIS:O	1:E:212[B]:GLU:CB	2.54	0.48
1:F:174[B]:GLY:O	1:F:177[B]:GLY:HA2	2.13	0.48
1:F:410:VAL:HG22	5:F:6036:HOH:O	2.14	0.48
1:G:329:PRO:HG2	1:G:359:ARG:CD	2.18	0.48
1:A:174[B]:GLY:O	1:A:177[B]:GLY:HA2	2.13	0.48
1:A:259:PRO:HG2	1:A:260[A]:MET:H	1.78	0.48
1:A:329:PRO:CD	1:A:359:ARG:HD2	2.42	0.48
1:A:423:LEU:C	1:A:425:ARG:H	2.22	0.48
1:B:423:LEU:C	1:B:425:ARG:H	2.22	0.48
1:C:175[B]:VAL:O	1:C:175[B]:VAL:HG12	2.13	0.48
1:C:230:LYS:HG2	5:C:5963:HOH:O	2.14	0.48
1:C:272:MET:O	1:C:355:ARG:HB2	2.12	0.48
1:D:285:ASP:CA	5:D:6027:HOH:O	2.35	0.48
1:F:175[B]:VAL:O	1:F:175[B]:VAL:HG12	2.12	0.48
1:G:211[B]:HIS:O	1:G:212[B]:GLU:CB	2.54	0.48
1:J:124:VAL:HA	1:J:274:LEU:HD23	1.95	0.48
1:J:175[B]:VAL:O	1:J:175[B]:VAL:HG12	2.13	0.48
1:E:179[B]:TYR:CD2	1:E:211[B]:HIS:HB2	2.47	0.48
1:E:348:VAL:HG22	5:E:648:HOH:O	2.13	0.48
1:F:423:LEU:C	1:F:425:ARG:H	2.22	0.48
1:H:75:VAL:CG2	5:H:5932:HOH:O	2.53	0.48
1:C:183:PRO:HB2	5:D:5972:HOH:O	2.14	0.48
1:D:259:PRO:HG2	1:D:260[A]:MET:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:PRO:CD	1:D:359:ARG:HD2	2.42	0.48
1:E:25:LYS:NZ	5:E:633:HOH:O	2.45	0.48
1:E:124:VAL:HA	1:E:274:LEU:HD23	1.95	0.48
1:E:230:LYS:HG2	5:E:678:HOH:O	2.14	0.48
1:G:179[B]:TYR:CD2	1:G:211[B]:HIS:HB2	2.47	0.48
1:G:423:LEU:C	1:G:425:ARG:H	2.22	0.48
1:H:269:HIS:CE1	4:H:5907:PPQ:CEP	2.92	0.48
1:L:410:VAL:HG22	5:L:1818:HOH:O	2.14	0.48
1:A:206:VAL:O	1:B:34:PRO:HG2	2.13	0.48
1:B:410:VAL:HG22	5:B:6027:HOH:O	2.14	0.48
1:C:304:HIS:O	1:C:308:ILE:HG13	2.14	0.48
1:D:456:THR:O	1:J:458:HIS:HE1	1.97	0.48
1:E:180[A]:PHE:HB3	1:F:29[A]:GLN:HB3	1.96	0.48
1:G:174[B]:GLY:O	1:G:177[B]:GLY:HA2	2.13	0.48
1:H:124:VAL:HA	1:H:274:LEU:HD23	1.95	0.48
1:H:174[B]:GLY:O	1:H:177[B]:GLY:HA2	2.13	0.48
1:H:304:HIS:O	1:H:308:ILE:HG13	2.14	0.48
1:H:423:LEU:C	1:H:425:ARG:H	2.22	0.48
1:H:463:GLU:OE1	5:H:5909:HOH:O	2.20	0.48
1:J:154:ILE:HG13	5:J:5994:HOH:O	2.14	0.48
1:K:25:LYS:HD2	5:K:1578:HOH:O	2.11	0.48
1:K:360:PHE:CG	1:K:361:PRO:CD	2.97	0.48
1:L:128:PRO:CD	5:L:1692:HOH:O	2.61	0.48
1:L:360:PHE:CG	1:L:361:PRO:CD	2.97	0.48
1:L:423:LEU:C	1:L:425:ARG:H	2.22	0.48
1:A:304:HIS:O	1:A:308:ILE:HG13	2.14	0.47
1:A:348:VAL:HG22	5:A:5934:HOH:O	2.13	0.47
1:B:60:ILE:HG23	1:B:60:ILE:O	2.12	0.47
1:D:304:HIS:O	1:D:308:ILE:HG13	2.14	0.47
1:D:329:PRO:HB2	1:D:342:SER:HA	1.96	0.47
1:G:189:GLN:HE22	1:G:209[A]:HIS:HE1	1.57	0.47
1:G:230:LYS:HG2	5:G:5973:HOH:O	2.14	0.47
3:G:4477:ADP:H5'1	5:G:5986:HOH:O	2.14	0.47
3:H:4478:ADP:H5'1	5:H:5990:HOH:O	2.14	0.47
1:I:68:MET:HA	1:I:69:PRO:HD2	1.78	0.47
1:I:154:ILE:HG13	5:I:5998:HOH:O	2.14	0.47
1:I:269:HIS:CE1	4:I:5908:PPQ:CEP	2.92	0.47
1:K:423:LEU:C	1:K:425:ARG:H	2.22	0.47
1:L:124:VAL:HA	1:L:274:LEU:HD23	1.95	0.47
1:A:230:LYS:HG2	5:A:5963:HOH:O	2.14	0.47
1:B:210[B]:HIS:C	1:B:211[B]:HIS:CD2	2.90	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:PHE:CG	1:C:361:PRO:CD	2.97	0.47
1:E:154:ILE:HG13	5:E:692:HOH:O	2.14	0.47
1:F:68:MET:HA	1:F:69:PRO:HD2	1.78	0.47
1:F:304:HIS:O	1:F:308:ILE:HG13	2.14	0.47
1:F:329:PRO:HB2	1:F:342:SER:HA	1.97	0.47
1:G:210[B]:HIS:C	1:G:211[B]:HIS:CD2	2.89	0.47
1:G:259:PRO:HG2	1:G:260[A]:MET:H	1.78	0.47
1:H:230:LYS:HG2	5:H:5977:HOH:O	2.14	0.47
1:H:360:PHE:CG	1:H:361:PRO:CD	2.97	0.47
1:I:175[B]:VAL:O	1:I:175[B]:VAL:HG12	2.12	0.47
1:I:224:ARG:CG	1:I:224:ARG:NH2	2.69	0.47
1:I:423:LEU:C	1:I:425:ARG:H	2.22	0.47
1:J:423:LEU:C	1:J:425:ARG:H	2.22	0.47
1:J:437:GLU:CA	5:J:6034:HOH:O	2.58	0.47
1:K:34:PRO:HG2	1:L:206:VAL:O	2.14	0.47
1:B:154:ILE:HG13	5:B:5978:HOH:O	2.14	0.47
1:C:261[A]:PHE:HB2	1:I:457:PRO:HD3	1.97	0.47
1:D:154:ILE:HG13	5:D:5980:HOH:O	2.14	0.47
1:D:410:VAL:HG22	5:D:6029:HOH:O	2.14	0.47
1:E:174[B]:GLY:O	1:E:177[B]:GLY:HA2	2.13	0.47
1:F:230:LYS:HG2	5:F:5973:HOH:O	2.14	0.47
1:G:154:ILE:HG13	5:G:5987:HOH:O	2.14	0.47
1:G:329:PRO:HB2	1:G:342:SER:HA	1.96	0.47
1:H:410:VAL:HG22	5:H:6040:HOH:O	2.14	0.47
1:J:174[B]:GLY:O	1:J:177[B]:GLY:HA2	2.13	0.47
1:K:230:LYS:HG2	5:K:1596:HOH:O	2.14	0.47
1:L:154:ILE:HG13	5:L:1763:HOH:O	2.14	0.47
1:A:360:PHE:CG	1:A:361:PRO:CD	2.97	0.47
1:B:329:PRO:HB2	1:B:342:SER:HA	1.96	0.47
3:B:4472:ADP:H5'1	5:B:5977:HOH:O	2.14	0.47
1:C:174[B]:GLY:O	1:C:177[B]:GLY:HA2	2.13	0.47
1:D:128:PRO:CD	5:D:5910:HOH:O	2.61	0.47
1:F:210[B]:HIS:C	1:F:211[B]:HIS:CD2	2.89	0.47
1:I:231:LYS:CE	5:I:5928:HOH:O	2.59	0.47
1:K:179[B]:TYR:CD2	1:K:211[B]:HIS:HB2	2.47	0.47
1:A:128:PRO:CD	5:A:5907:HOH:O	2.61	0.47
1:A:154:ILE:HG13	5:A:5977:HOH:O	2.14	0.47
1:C:140:PHE:CE1	1:I:463:GLU:HA	2.49	0.47
1:C:232:ALA:HB1	1:C:367:PRO:HB2	1.97	0.47
1:D:68:MET:HA	1:D:69:PRO:HD2	1.78	0.47
1:H:210[B]:HIS:C	1:H:211[B]:HIS:CD2	2.89	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:329:PRO:CD	1:I:359:ARG:HD2	2.42	0.47
1:I:329:PRO:HB2	1:I:342:SER:HA	1.96	0.47
1:J:329:PRO:CD	1:J:359:ARG:HD2	2.42	0.47
1:K:84:THR:HG21	5:L:1730:HOH:O	2.12	0.47
1:K:304:HIS:O	1:K:308:ILE:HG13	2.14	0.47
1:A:296:TYR:HB3	1:A:382:ILE:HA	1.97	0.47
1:B:174[B]:GLY:O	1:B:177[B]:GLY:CA	2.63	0.47
1:C:165:GLU:N	5:C:5961:HOH:O	2.46	0.47
1:C:207:GLU:O	1:C:208:ALA:HB2	2.15	0.47
1:E:329:PRO:HB2	1:E:342:SER:HA	1.96	0.47
1:F:154:ILE:HG13	5:F:5987:HOH:O	2.14	0.47
1:G:165:GLU:N	5:G:5971:HOH:O	2.46	0.47
1:H:207:GLU:O	1:H:208:ALA:HB2	2.15	0.47
1:H:329:PRO:CD	1:H:359:ARG:HD2	2.42	0.47
1:K:231:LYS:CE	5:K:1539:HOH:O	2.59	0.47
1:K:447:ARG:HD2	5:K:1647:HOH:O	2.15	0.47
1:L:304:HIS:O	1:L:308:ILE:HG13	2.14	0.47
1:A:230:LYS:O	1:A:234:GLU:HG3	2.15	0.47
1:A:401:PRO:HA	1:A:404:ALA:CA	2.44	0.47
1:B:230:LYS:HG2	5:B:5964:HOH:O	2.14	0.47
1:C:174[B]:GLY:O	1:C:177[B]:GLY:CA	2.63	0.47
1:C:348:VAL:HG22	5:C:5934:HOH:O	2.13	0.47
1:D:210[B]:HIS:C	1:D:211[B]:HIS:CD2	2.89	0.47
1:D:296:TYR:HB3	1:D:382:ILE:HA	1.97	0.47
1:D:332:LEU:O	5:D:6001:HOH:O	2.20	0.47
1:D:360:PHE:CG	1:D:361:PRO:CD	2.97	0.47
1:E:68:MET:HA	1:E:69:PRO:HD2	1.78	0.47
1:E:232:ALA:HB1	1:E:367:PRO:HB2	1.97	0.47
1:F:1:SER:N	1:F:71:ALA:CB	2.78	0.47
1:F:128:PRO:CD	5:F:5919:HOH:O	2.61	0.47
1:F:174[B]:GLY:O	1:F:177[B]:GLY:CA	2.63	0.47
1:G:1:SER:N	1:G:71:ALA:CB	2.78	0.47
1:G:1:SER:O	1:G:5:VAL:HG23	2.15	0.47
1:G:34:PRO:HG2	1:H:206:VAL:O	2.15	0.47
1:G:60:ILE:O	1:H:339:ARG:HB2	2.15	0.47
1:G:447:ARG:HD2	5:G:6019:HOH:O	2.15	0.47
1:H:230:LYS:O	1:H:234:GLU:HG3	2.15	0.47
1:H:296:TYR:HB3	1:H:382:ILE:HA	1.97	0.47
1:I:28:GLU:CB	5:I:5951:HOH:O	2.58	0.47
1:I:174[B]:GLY:O	1:I:177[B]:GLY:CA	2.63	0.47
1:I:360:PHE:CG	1:I:361:PRO:CD	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:410:VAL:HG22	5:I:6047:HOH:O	2.14	0.47
1:J:75:VAL:CG2	5:J:5934:HOH:O	2.53	0.47
1:J:174[B]:GLY:O	1:J:177[B]:GLY:CA	2.63	0.47
1:J:210[B]:HIS:C	1:J:211[B]:HIS:CD2	2.89	0.47
1:J:304:HIS:O	1:J:308:ILE:HG13	2.14	0.47
1:J:348:VAL:HG22	5:J:5951:HOH:O	2.13	0.47
1:J:360:PHE:CG	1:J:361:PRO:CD	2.97	0.47
3:J:4480:ADP:H5'1	5:J:5993:HOH:O	2.14	0.47
1:K:296:TYR:HB3	1:K:382:ILE:HA	1.97	0.47
1:K:332:LEU:O	5:K:1635:HOH:O	2.20	0.47
3:K:4481:ADP:H5'1	5:K:1609:HOH:O	2.14	0.47
1:L:165:GLU:N	5:L:1747:HOH:O	2.46	0.47
1:L:174[B]:GLY:O	1:L:177[B]:GLY:CA	2.63	0.47
1:A:332:LEU:O	5:A:5998:HOH:O	2.20	0.47
1:D:230:LYS:O	1:D:234:GLU:HG3	2.15	0.47
1:H:1:SER:O	1:H:5:VAL:HG23	2.15	0.47
1:I:207:GLU:O	1:I:208:ALA:HB2	2.15	0.47
1:J:230:LYS:HG2	5:J:5980:HOH:O	2.14	0.47
1:J:329:PRO:HB2	1:J:342:SER:HA	1.96	0.47
1:L:232:ALA:HB1	1:L:367:PRO:HB2	1.97	0.47
1:A:232:ALA:HB1	1:A:367:PRO:HB2	1.97	0.47
1:A:261[A]:PHE:HB2	1:G:457:PRO:HD3	1.96	0.47
1:A:384:ASN:N	1:A:384:ASN:ND2	2.59	0.47
1:B:165:GLU:N	5:B:5962:HOH:O	2.46	0.47
1:B:208:ALA:HB2	1:C:33:ILE:CD1	2.44	0.47
1:C:1:SER:N	1:C:71:ALA:CB	2.78	0.47
1:C:273:SER:OG	3:C:4473:ADP:N6	2.48	0.47
3:C:4473:ADP:H5'1	5:C:5976:HOH:O	2.14	0.47
1:G:174[B]:GLY:O	1:G:177[B]:GLY:CA	2.63	0.47
1:G:232:ALA:HB1	1:G:367:PRO:HB2	1.97	0.47
1:H:329:PRO:HB2	1:H:342:SER:HA	1.97	0.47
1:I:230:LYS:O	1:I:234:GLU:HG3	2.15	0.47
1:I:230:LYS:HG2	5:I:5984:HOH:O	2.14	0.47
1:J:273:SER:OG	3:J:4480:ADP:N6	2.48	0.47
1:K:1:SER:O	1:K:5:VAL:HG23	2.15	0.47
1:L:207:GLU:O	1:L:208:ALA:HB2	2.15	0.47
1:A:211[B]:HIS:O	1:A:212[B]:GLU:CB	2.54	0.47
1:A:410:VAL:HG22	5:A:6026:HOH:O	2.14	0.47
1:A:447:ARG:HD2	5:A:6009:HOH:O	2.15	0.47
1:B:273:SER:OG	3:B:4472:ADP:N6	2.48	0.47
1:B:296:TYR:HB3	1:B:382:ILE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:PHE:CG	1:B:361:PRO:CD	2.97	0.47
1:B:447:ARG:HD2	5:B:6010:HOH:O	2.15	0.47
1:C:1:SER:O	1:C:5:VAL:HG23	2.15	0.47
1:C:329:PRO:CD	1:C:359:ARG:HD2	2.42	0.47
1:C:423:LEU:C	1:C:425:ARG:H	2.22	0.47
1:D:133:PHE:CE2	1:D:218:GLN:HB2	2.50	0.47
1:D:273:SER:OG	3:D:4474:ADP:N6	2.48	0.47
1:E:1:SER:O	1:E:5:VAL:HG23	2.15	0.47
1:F:1:SER:O	1:F:5:VAL:HG23	2.15	0.47
1:G:133:PHE:CE2	1:G:218:GLN:HB2	2.50	0.47
1:G:304:HIS:O	1:G:308:ILE:HG13	2.14	0.47
1:G:348:VAL:HG22	5:G:5944:HOH:O	2.13	0.47
1:G:410:VAL:HG22	5:G:6036:HOH:O	2.14	0.47
1:I:232:ALA:HB1	1:I:367:PRO:HB2	1.97	0.47
1:I:329:PRO:HG2	1:I:359:ARG:CD	2.18	0.47
1:K:1:SER:N	1:K:71:ALA:CB	2.78	0.47
1:L:1:SER:O	1:L:5:VAL:HG23	2.15	0.47
1:A:1:SER:N	1:A:71:ALA:CB	2.78	0.46
1:A:224:ARG:CG	1:A:224:ARG:NH2	2.69	0.46
1:B:1:SER:N	1:B:71:ALA:CB	2.78	0.46
1:B:133:PHE:CE2	1:B:218:GLN:HB2	2.50	0.46
1:D:174[B]:GLY:O	1:D:177[B]:GLY:CA	2.63	0.46
3:D:4474:ADP:H5'1	5:D:5979:HOH:O	2.14	0.46
1:E:273:SER:OG	3:E:4475:ADP:N6	2.48	0.46
1:E:296:TYR:HB3	1:E:382:ILE:HA	1.97	0.46
1:E:304:HIS:O	1:E:308:ILE:HG13	2.14	0.46
1:E:329:PRO:HG2	1:E:359:ARG:CD	2.18	0.46
1:F:207:GLU:O	1:F:208:ALA:HB2	2.15	0.46
1:G:75:VAL:CG2	5:G:5926:HOH:O	2.53	0.46
1:H:232:ALA:HB1	1:H:367:PRO:HB2	1.97	0.46
1:I:128:PRO:CD	5:I:5928:HOH:O	2.61	0.46
1:I:384:ASN:N	1:I:384:ASN:ND2	2.59	0.46
1:J:1:SER:N	1:J:71:ALA:CB	2.78	0.46
1:J:232:ALA:HB1	1:J:367:PRO:HB2	1.97	0.46
1:K:232:ALA:HB1	1:K:367:PRO:HB2	1.97	0.46
1:K:329:PRO:HG2	1:K:359:ARG:CD	2.18	0.46
1:L:230:LYS:O	1:L:234:GLU:HG3	2.15	0.46
1:L:273:SER:OG	3:L:4482:ADP:N6	2.48	0.46
1:L:329:PRO:HB2	1:L:342:SER:HA	1.97	0.46
3:A:4471:ADP:H5'1	5:A:5976:HOH:O	2.14	0.46
5:A:5969:HOH:O	1:F:183:PRO:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:HIS:HE1	1:H:456:THR:O	1.98	0.46
1:C:75:VAL:CG2	5:C:5917:HOH:O	2.53	0.46
1:C:210[B]:HIS:C	1:C:211[B]:HIS:CD2	2.90	0.46
1:E:423:LEU:C	1:E:425:ARG:H	2.22	0.46
1:G:207:GLU:O	1:G:208:ALA:HB2	2.15	0.46
1:G:360:PHE:CG	1:G:361:PRO:CD	2.97	0.46
3:I:4479:ADP:H5'1	5:I:5997:HOH:O	2.14	0.46
1:K:210[B]:HIS:C	1:K:211[B]:HIS:CD2	2.89	0.46
1:K:329:PRO:HB2	1:K:342:SER:HA	1.96	0.46
1:B:1:SER:O	1:B:5:VAL:HG23	2.15	0.46
1:B:304:HIS:O	1:B:308:ILE:HG13	2.14	0.46
1:C:133:PHE:CE2	1:C:218:GLN:HB2	2.50	0.46
1:D:1:SER:N	1:D:71:ALA:CB	2.78	0.46
1:D:230:LYS:HG2	5:D:5966:HOH:O	2.14	0.46
1:D:294:ALA:O	1:D:298:ILE:HG13	2.16	0.46
1:D:447:ARG:HD2	5:D:6012:HOH:O	2.15	0.46
1:E:174[B]:GLY:O	1:E:177[B]:GLY:CA	2.63	0.46
1:F:230:LYS:O	1:F:234:GLU:HG3	2.15	0.46
1:H:133:PHE:CE2	1:H:218:GLN:HB2	2.50	0.46
1:J:384:ASN:N	1:J:384:ASN:ND2	2.59	0.46
1:K:273:SER:OG	3:K:4481:ADP:N6	2.48	0.46
1:L:1:SER:N	1:L:71:ALA:CB	2.78	0.46
1:C:329:PRO:HB2	1:C:342:SER:HA	1.96	0.46
1:E:1:SER:N	1:E:71:ALA:CB	2.78	0.46
1:E:230:LYS:O	1:E:234:GLU:HG3	2.15	0.46
1:F:332:LEU:O	5:F:6008:HOH:O	2.20	0.46
1:G:273:SER:OG	3:G:4477:ADP:N6	2.48	0.46
1:H:447:ARG:HD2	5:H:6023:HOH:O	2.15	0.46
1:I:1:SER:N	1:I:71:ALA:CB	2.78	0.46
1:I:133:PHE:CE2	1:I:218:GLN:HB2	2.50	0.46
1:I:447:ARG:HD2	5:I:6030:HOH:O	2.15	0.46
1:J:1:SER:O	1:J:5:VAL:HG23	2.15	0.46
1:K:133:PHE:CE2	1:K:218:GLN:HB2	2.50	0.46
1:K:174[B]:GLY:O	1:K:177[B]:GLY:CA	2.63	0.46
1:K:207:GLU:O	1:K:208:ALA:HB2	2.15	0.46
1:L:401:PRO:HA	1:L:404:ALA:CA	2.44	0.46
1:C:447:ARG:HD2	5:C:6009:HOH:O	2.15	0.46
1:E:207:GLU:O	1:E:208:ALA:HB2	2.15	0.46
1:E:333:ALA:HB1	1:E:392:MET:HG2	1.97	0.46
1:E:410:VAL:HG22	5:E:747:HOH:O	2.14	0.46
1:F:18:ASP:OD2	1:F:30[A]:HIS:HD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:SER:OG	3:F:4476:ADP:N6	2.48	0.46
1:G:18:ASP:OD2	1:G:30[A]:HIS:HD2	1.99	0.46
1:H:273:SER:OG	3:H:4478:ADP:N6	2.48	0.46
1:I:33:ILE:CD1	1:J:208:ALA:HB2	2.45	0.46
1:I:84:THR:HG21	5:J:5962:HOH:O	2.16	0.46
1:I:332:LEU:O	5:I:6019:HOH:O	2.20	0.46
1:I:333:ALA:HB1	1:I:392:MET:HG2	1.97	0.46
1:J:207:GLU:O	1:J:208:ALA:HB2	2.15	0.46
1:K:401:PRO:HA	1:K:404:ALA:CA	2.44	0.46
3:L:4482:ADP:H5'1	5:L:1762:HOH:O	2.14	0.46
1:A:133:PHE:CE2	1:A:218:GLN:HB2	2.50	0.46
1:A:174[B]:GLY:O	1:A:177[B]:GLY:CA	2.63	0.46
1:B:232:ALA:HB1	1:B:367:PRO:HB2	1.97	0.46
1:C:410:VAL:HG22	5:C:6026:HOH:O	2.14	0.46
1:D:182:VAL:HG23	5:E:662:HOH:O	2.16	0.46
1:D:183:PRO:CB	5:E:684:HOH:O	2.62	0.46
1:E:390:GLU:HA	1:E:391:PRO:HD3	1.84	0.46
1:F:447:ARG:HD2	5:F:6019:HOH:O	2.15	0.46
1:I:304:HIS:O	1:I:308:ILE:HG13	2.14	0.46
1:K:410:VAL:HG22	5:K:1665:HOH:O	2.14	0.46
1:L:296:TYR:HB3	1:L:382:ILE:HA	1.97	0.46
1:L:447:ARG:HD2	5:L:1800:HOH:O	2.15	0.46
1:A:269:HIS:CE1	4:A:5900:PPQ:CEP	2.92	0.46
1:A:333:ALA:HB1	1:A:392:MET:HG2	1.97	0.46
1:C:437:GLU:CA	5:C:6017:HOH:O	2.58	0.46
1:D:1:SER:O	1:D:5:VAL:HG23	2.15	0.46
1:D:232:ALA:HB1	1:D:367:PRO:HB2	1.97	0.46
1:E:306:LYS:HE2	5:E:751:HOH:O	2.16	0.46
1:F:133:PHE:CE2	1:F:218:GLN:HB2	2.51	0.46
3:F:4476:ADP:H5'1	5:F:5986:HOH:O	2.14	0.46
1:J:18:ASP:OD2	1:J:30[A]:HIS:HD2	1.99	0.46
1:J:133:PHE:CE2	1:J:218:GLN:HB2	2.50	0.46
1:J:230:LYS:O	1:J:234:GLU:HG3	2.15	0.46
1:J:447:ARG:HD2	5:J:6026:HOH:O	2.15	0.46
1:L:332:LEU:O	5:L:1788:HOH:O	2.20	0.46
1:A:207:GLU:O	1:A:208:ALA:HB2	2.15	0.46
1:B:294:ALA:O	1:B:298:ILE:HG13	2.16	0.46
1:B:332:LEU:O	5:B:5999:HOH:O	2.20	0.46
1:B:333:ALA:HB1	1:B:392:MET:HG2	1.97	0.46
1:D:333:ALA:HB1	1:D:392:MET:HG2	1.97	0.46
1:E:447:ARG:HD2	5:E:729:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1:SER:O	1:I:5:VAL:HG23	2.15	0.46
1:I:296:TYR:HB3	1:I:382:ILE:HA	1.97	0.46
1:I:401:PRO:HA	1:I:404:ALA:CA	2.44	0.46
1:A:273:SER:OG	3:A:4471:ADP:N6	2.48	0.46
1:B:140:PHE:CE1	1:H:463:GLU:HA	2.51	0.46
1:B:207:GLU:O	1:B:208:ALA:HB2	2.15	0.46
1:C:18:ASP:OD2	1:C:30[A]:HIS:HD2	1.99	0.46
1:D:18:ASP:OD2	1:D:30[A]:HIS:HD2	1.99	0.46
1:F:211[B]:HIS:C	1:F:212[B]:GLU:HG3	2.37	0.46
1:G:230:LYS:O	1:G:234:GLU:HG3	2.15	0.46
1:I:273:SER:OG	3:I:4479:ADP:N6	2.48	0.46
1:I:294:ALA:O	1:I:298:ILE:HG13	2.16	0.46
1:K:18:ASP:OD2	1:K:30[A]:HIS:HD2	1.99	0.46
1:K:154:ILE:HG13	5:K:1610:HOH:O	2.14	0.46
1:A:294:ALA:O	1:A:298:ILE:HG13	2.16	0.46
1:B:344:ARG:HE	1:B:344:ARG:HB3	1.59	0.46
1:C:68:MET:HA	1:C:69:PRO:HD2	1.78	0.46
1:C:189:GLN:NE2	1:D:32:THR:OG1	2.48	0.46
1:C:333:ALA:HB1	1:C:392:MET:HG2	1.97	0.46
1:E:210[A]:HIS:ND1	1:E:211[A]:HIS:O	2.47	0.46
1:G:235:ILE:HD13	1:G:235:ILE:HA	1.80	0.46
1:H:1:SER:N	1:H:71:ALA:CB	2.78	0.46
1:H:172:ARG:HA	1:H:173[A]:PRO:HD3	1.80	0.46
1:H:174[B]:GLY:O	1:H:177[B]:GLY:CA	2.63	0.46
1:A:1:SER:O	1:A:5:VAL:HG23	2.15	0.45
1:A:18:ASP:OD2	1:A:30[A]:HIS:HD2	1.99	0.45
1:B:306:LYS:HE2	5:B:6031:HOH:O	2.16	0.45
1:C:180[A]:PHE:O	1:D:29[A]:GLN:HA	2.16	0.45
1:D:231:LYS:CE	5:D:5910:HOH:O	2.59	0.45
1:E:133:PHE:CE2	1:E:218:GLN:HB2	2.50	0.45
1:E:165:GLU:N	5:E:676:HOH:O	2.46	0.45
1:G:125:LEU:HD12	1:G:125:LEU:HA	1.79	0.45
1:H:294:ALA:O	1:H:298:ILE:HG13	2.16	0.45
1:J:165:GLU:N	5:J:5978:HOH:O	2.46	0.45
1:J:332:LEU:O	5:J:6015:HOH:O	2.20	0.45
1:J:333:ALA:HB1	1:J:392:MET:HG2	1.97	0.45
1:K:230:LYS:O	1:K:234:GLU:HG3	2.15	0.45
1:L:133:PHE:CE2	1:L:218:GLN:HB2	2.51	0.45
1:L:333:ALA:HB1	1:L:392:MET:HG2	1.97	0.45
1:A:211[B]:HIS:C	1:A:212[B]:GLU:HG3	2.36	0.45
1:C:230:LYS:O	1:C:234:GLU:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:ALA:O	1:E:298:ILE:HG13	2.16	0.45
1:F:232:ALA:HB1	1:F:367:PRO:HB2	1.97	0.45
1:G:80:PHE:CZ	1:H:189:GLN:HG3	2.51	0.45
1:I:165:GLU:N	5:I:5982:HOH:O	2.46	0.45
1:J:272:MET:HE3	1:J:272:MET:HB2	1.84	0.45
1:K:210[A]:HIS:ND1	1:K:211[A]:HIS:O	2.47	0.45
1:L:18:ASP:OD2	1:L:30[A]:HIS:HD2	1.99	0.45
1:L:294:ALA:O	1:L:298:ILE:HG13	2.16	0.45
1:A:47:LYS:CD	5:A:6035:HOH:O	2.65	0.45
1:A:329:PRO:HB2	1:A:342:SER:HA	1.96	0.45
1:B:230:LYS:O	1:B:234:GLU:HG3	2.15	0.45
1:C:296:TYR:HB3	1:C:382:ILE:HA	1.97	0.45
1:D:47:LYS:CD	5:D:6038:HOH:O	2.65	0.45
1:E:269:HIS:CE1	4:E:5904:PPQ:CEP	2.92	0.45
1:F:296:TYR:HB3	1:F:382:ILE:HA	1.97	0.45
1:G:155:GLU:OE1	1:G:211[A]:HIS:CE1	2.68	0.45
1:H:333:ALA:HB1	1:H:392:MET:HG2	1.97	0.45
1:H:401:PRO:HA	1:H:404:ALA:CA	2.44	0.45
1:J:47:LYS:CD	5:J:6052:HOH:O	2.65	0.45
1:J:128:PRO:CD	5:J:5926:HOH:O	2.61	0.45
1:J:294:ALA:O	1:J:298:ILE:HG13	2.16	0.45
1:J:296:TYR:HB3	1:J:382:ILE:HA	1.97	0.45
1:K:128:PRO:CD	5:K:1539:HOH:O	2.61	0.45
1:K:294:ALA:O	1:K:298:ILE:HG13	2.16	0.45
1:C:182:VAL:HG23	5:D:5951:HOH:O	2.16	0.45
1:C:285:ASP:C	5:C:6024:HOH:O	2.60	0.45
1:E:18:ASP:OD2	1:E:30[A]:HIS:HD2	1.99	0.45
1:G:172:ARG:HA	1:G:173[A]:PRO:HD3	1.80	0.45
1:G:296:TYR:HB3	1:G:382:ILE:HA	1.97	0.45
1:H:18:ASP:OD2	1:H:30[A]:HIS:HD2	1.99	0.45
1:J:211[B]:HIS:C	1:J:212[B]:GLU:HG3	2.36	0.45
1:A:165:GLU:N	5:A:5961:HOH:O	2.46	0.45
1:A:329:PRO:HD2	1:A:359:ARG:HG2	1.99	0.45
1:D:165:GLU:N	5:D:5964:HOH:O	2.46	0.45
1:F:153:ASP:OD1	1:F:251:LYS:NZ	2.50	0.45
1:F:333:ALA:HB1	1:F:392:MET:HG2	1.97	0.45
1:F:344:ARG:HE	1:F:344:ARG:HB3	1.59	0.45
1:G:153:ASP:OD1	1:G:251:LYS:NZ	2.50	0.45
1:G:333:ALA:HB1	1:G:392:MET:HG2	1.97	0.45
1:H:306:LYS:HE2	5:H:6044:HOH:O	2.16	0.45
1:K:333:ALA:HB1	1:K:392:MET:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:OD1	1:B:251:LYS:NZ	2.50	0.45
1:B:284:GLY:HA3	1:B:291:SER:HA	1.99	0.45
1:C:128:PRO:CD	5:C:5909:HOH:O	2.61	0.45
1:C:153:ASP:OD1	1:C:251:LYS:NZ	2.50	0.45
1:E:172:ARG:HA	1:E:173[A]:PRO:HD3	1.80	0.45
1:A:189:GLN:HG3	1:B:80:PHE:CZ	2.51	0.45
1:C:306:LYS:HE2	5:C:6030:HOH:O	2.16	0.45
1:D:207:GLU:O	1:D:208:ALA:HB2	2.15	0.45
1:F:294:ALA:O	1:F:298:ILE:HG13	2.16	0.45
1:G:183:PRO:CB	5:L:1755:HOH:O	2.62	0.45
1:G:294:ALA:O	1:G:298:ILE:HG13	2.16	0.45
1:G:306:LYS:HE2	5:G:6040:HOH:O	2.16	0.45
1:H:329:PRO:HD2	1:H:359:ARG:HG2	1.99	0.45
1:I:306:LYS:HE2	5:I:6051:HOH:O	2.16	0.45
1:J:306:LYS:HE2	5:J:6047:HOH:O	2.16	0.45
1:K:165:GLU:N	5:K:1594:HOH:O	2.46	0.45
1:K:306:LYS:HE2	5:K:1669:HOH:O	2.16	0.45
1:L:211[B]:HIS:C	1:L:212[B]:GLU:HG3	2.37	0.45
1:L:329:PRO:HD2	1:L:359:ARG:HG2	1.99	0.45
1:A:4:HIS:CE1	5:A:5986:HOH:O	2.70	0.45
1:A:153:ASP:OD1	1:A:251:LYS:NZ	2.50	0.45
1:C:211[B]:HIS:C	1:C:212[B]:GLU:HG3	2.37	0.45
1:D:329:PRO:HD2	1:D:359:ARG:HG2	1.99	0.45
1:E:128:PRO:CD	5:E:621:HOH:O	2.61	0.45
1:E:153:ASP:OD1	1:E:251:LYS:NZ	2.50	0.45
1:G:332:LEU:O	5:G:6008:HOH:O	2.20	0.45
1:I:40:ALA:HB2	5:I:6002:HOH:O	2.10	0.45
1:K:29[A]:GLN:HA	1:L:180[A]:PHE:O	2.17	0.45
1:B:18:ASP:OD2	1:B:30[A]:HIS:HD2	1.99	0.45
1:B:183:PRO:CB	5:C:5969:HOH:O	2.65	0.45
1:C:189:GLN:HG3	1:D:80:PHE:CZ	2.51	0.45
1:D:447:ARG:HH21	1:D:447:ARG:HG3	1.82	0.45
1:F:210[A]:HIS:ND1	1:F:211[A]:HIS:O	2.47	0.45
1:F:306:LYS:HE2	5:F:6040:HOH:O	2.16	0.45
1:F:401:PRO:HA	1:F:404:ALA:CA	2.44	0.45
1:H:284:GLY:HA3	1:H:291:SER:HA	1.99	0.45
1:I:4:HIS:CE1	5:I:6007:HOH:O	2.70	0.45
1:I:18:ASP:OD2	1:I:30[A]:HIS:HD2	1.99	0.45
1:J:401:PRO:CA	1:J:404:ALA:HA	2.46	0.45
1:K:193:SER:O	1:K:197:LEU:HG	2.17	0.45
1:B:269:HIS:HE1	4:B:5901:PPQ:HEP2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ALA:O	1:C:298:ILE:HG13	2.16	0.45
1:D:359:ARG:HH11	1:D:359:ARG:HD3	1.65	0.45
1:D:458:HIS:HE1	1:J:456:THR:O	2.00	0.45
1:E:47:LYS:CD	5:E:756:HOH:O	2.65	0.45
1:H:153:ASP:OD1	1:H:251:LYS:NZ	2.50	0.45
1:H:193:SER:O	1:H:197:LEU:HG	2.17	0.45
1:K:447:ARG:HH21	1:K:447:ARG:HG3	1.83	0.45
1:L:153:ASP:OD1	1:L:251:LYS:NZ	2.50	0.45
1:L:306:LYS:HE2	5:L:1822:HOH:O	2.16	0.45
1:C:149:VAL:HG21	1:I:462:PHE:CE1	2.52	0.44
1:C:268:MET:N	1:C:363:PRO:HD3	2.33	0.44
1:D:284:GLY:HA3	1:D:291:SER:HA	1.99	0.44
1:E:447:ARG:HH21	1:E:447:ARG:HG3	1.82	0.44
1:F:25:LYS:HD2	5:F:5956:HOH:O	2.10	0.44
1:F:155:GLU:OE1	1:F:211[A]:HIS:CE1	2.68	0.44
1:G:47:LYS:CD	5:G:6045:HOH:O	2.65	0.44
1:G:447:ARG:HH21	1:G:447:ARG:HG3	1.82	0.44
1:H:210[A]:HIS:ND1	1:H:211[A]:HIS:O	2.47	0.44
1:J:401:PRO:HA	1:J:404:ALA:CA	2.44	0.44
1:L:387:HIS:HA	1:L:388:PRO:HD2	1.85	0.44
1:A:447:ARG:HG3	1:A:447:ARG:HH21	1.82	0.44
1:A:462:PHE:CE1	1:G:149:VAL:HG21	2.52	0.44
1:B:115:LEU:CD2	1:B:379:LEU:HD21	2.48	0.44
1:B:193:SER:O	1:B:197:LEU:HG	2.17	0.44
1:B:401:PRO:HA	1:B:404:ALA:CA	2.44	0.44
1:C:339:ARG:HB2	1:D:60:ILE:O	2.18	0.44
1:E:115:LEU:CD2	1:E:379:LEU:HD21	2.48	0.44
1:I:268:MET:N	1:I:363:PRO:HD3	2.33	0.44
1:K:153:ASP:OD1	1:K:251:LYS:NZ	2.50	0.44
1:L:210[A]:HIS:ND1	1:L:211[A]:HIS:O	2.47	0.44
1:A:60:ILE:O	1:F:339:ARG:HB2	2.17	0.44
1:A:231:LYS:CE	5:A:5907:HOH:O	2.59	0.44
1:B:401:PRO:CA	1:B:404:ALA:HA	2.47	0.44
1:D:153:ASP:OD1	1:D:251:LYS:NZ	2.50	0.44
1:D:289:GLY:HA2	5:D:6027:HOH:O	2.18	0.44
1:D:401:PRO:HA	1:D:404:ALA:CA	2.44	0.44
1:E:289:GLY:HA2	5:E:745:HOH:O	2.18	0.44
1:F:75:VAL:CG2	5:F:5927:HOH:O	2.53	0.44
1:F:360:PHE:CG	1:F:361:PRO:CD	2.97	0.44
1:H:211[B]:HIS:C	1:H:212[B]:GLU:HG3	2.37	0.44
1:H:268:MET:N	1:H:363:PRO:HD3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:401:PRO:CA	1:H:404:ALA:HA	2.47	0.44
1:I:329:PRO:HD2	1:I:359:ARG:HG2	1.99	0.44
1:I:447:ARG:HG3	1:I:447:ARG:HH21	1.82	0.44
1:J:4:His:CE1	5:J:6003:HOH:O	2.70	0.44
1:J:447:ARG:HG3	1:J:447:ARG:HH21	1.82	0.44
1:K:68:MET:HA	1:K:69:PRO:HD2	1.78	0.44
1:K:329:PRO:HD2	1:K:359:ARG:HG2	1.99	0.44
1:B:268:MET:N	1:B:363:PRO:HD3	2.33	0.44
1:B:447:ARG:HG3	1:B:447:ARG:HH21	1.82	0.44
1:C:210[A]:His:ND1	1:C:211[A]:His:O	2.47	0.44
1:C:332:LEU:O	5:C:5998:HOH:O	2.20	0.44
1:F:268:MET:N	1:F:363:PRO:HD3	2.33	0.44
1:H:4:His:CE1	5:H:6000:HOH:O	2.70	0.44
1:H:447:ARG:HG3	1:H:447:ARG:HH21	1.82	0.44
1:J:284:GLY:HA3	1:J:291:SER:HA	1.99	0.44
1:L:285:ASP:C	5:L:1816:HOH:O	2.60	0.44
1:C:329:PRO:HD2	1:C:359:ARG:HG2	1.99	0.44
1:C:337:ARG:C	1:C:337:ARG:HD3	2.43	0.44
1:D:4:His:CE1	5:D:5989:HOH:O	2.70	0.44
1:E:193:SER:O	1:E:197:LEU:HG	2.18	0.44
1:F:193:SER:O	1:F:197:LEU:HG	2.17	0.44
1:F:284:GLY:HA3	1:F:291:SER:HA	1.99	0.44
1:G:289:GLY:HA2	5:G:6034:HOH:O	2.18	0.44
1:I:153:ASP:OD1	1:I:251:LYS:NZ	2.50	0.44
1:J:153:ASP:OD1	1:J:251:LYS:NZ	2.50	0.44
1:A:268:MET:N	1:A:363:PRO:HD3	2.33	0.44
1:A:306:LYS:HE2	5:A:6030:HOH:O	2.16	0.44
1:C:337:ARG:O	1:D:61:ASN:O	2.35	0.44
1:D:115:LEU:CD2	1:D:379:LEU:HD21	2.48	0.44
1:D:193:SER:O	1:D:197:LEU:HG	2.17	0.44
1:D:306:LYS:HE2	5:D:6033:HOH:O	2.16	0.44
1:G:193:SER:O	1:G:197:LEU:HG	2.17	0.44
1:H:289:GLY:HA2	5:H:6038:HOH:O	2.18	0.44
1:H:337:ARG:C	1:H:337:ARG:HD3	2.43	0.44
1:J:231:LYS:CE	5:J:5926:HOH:O	2.59	0.44
1:K:47:LYS:CD	5:K:1674:HOH:O	2.65	0.44
1:K:284:GLY:HA3	1:K:291:SER:HA	1.99	0.44
1:K:337:ARG:C	1:K:337:ARG:HD3	2.43	0.44
1:K:359:ARG:HH11	1:K:359:ARG:HD3	1.65	0.44
1:L:447:ARG:HH21	1:L:447:ARG:HG3	1.82	0.44
1:A:68:MET:HA	1:A:69:PRO:HD2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:HIS:HE1	4:C:5902:PPQ:HEP2	1.82	0.44
1:D:268:MET:N	1:D:363:PRO:HD3	2.33	0.44
1:E:401:PRO:HA	1:E:404:ALA:CA	2.44	0.44
1:F:4:HIS:CE1	5:F:5996:HOH:O	2.70	0.44
1:F:329:PRO:HD2	1:F:359:ARG:HG2	1.99	0.44
1:F:352:LYS:HA	1:F:352:LYS:HE2	2.00	0.44
1:G:68:MET:HA	1:G:69:PRO:HD2	1.78	0.44
1:G:210[A]:HIS:ND1	1:G:211[A]:HIS:O	2.47	0.44
1:G:268:MET:N	1:G:363:PRO:HD3	2.33	0.44
1:I:193:SER:O	1:I:197:LEU:HG	2.17	0.44
1:J:115:LEU:CD2	1:J:379:LEU:HD21	2.48	0.44
1:K:101:ASP:CG	1:K:435:THR:HG21	2.43	0.44
1:K:178[A]:GLY:O	1:K:211[A]:HIS:HD2	2.01	0.44
1:L:268:MET:N	1:L:363:PRO:HD3	2.33	0.44
1:L:284:GLY:HA3	1:L:291:SER:HA	1.99	0.44
1:A:40:ALA:HB2	5:A:5981:HOH:O	2.10	0.44
1:B:231:LYS:CE	5:B:5908:HOH:O	2.59	0.44
1:F:101:ASP:CG	1:F:435:THR:HG21	2.43	0.44
1:G:208:ALA:HB2	1:L:33:ILE:CD1	2.48	0.44
1:K:4:HIS:CE1	5:K:1620:HOH:O	2.70	0.44
1:K:210[B]:HIS:C	1:K:211[B]:HIS:HD2	2.26	0.44
1:K:344:ARG:HE	1:K:344:ARG:HB3	1.59	0.44
1:A:337:ARG:C	1:A:337:ARG:HD3	2.43	0.44
1:B:337:ARG:HD3	1:B:337:ARG:C	2.43	0.44
1:C:4:HIS:CE1	5:C:5986:HOH:O	2.70	0.44
1:D:337:ARG:C	1:D:337:ARG:HD3	2.43	0.44
1:E:284:GLY:HA3	1:E:291:SER:HA	1.99	0.44
1:E:337:ARG:HD3	1:E:337:ARG:C	2.43	0.44
1:F:128:PRO:HA	1:F:269:HIS:O	2.18	0.44
1:G:230:LYS:CG	5:G:5973:HOH:O	2.66	0.44
1:G:269:HIS:CE1	4:G:5906:PPQ:CEP	2.92	0.44
1:H:115:LEU:CD2	1:H:379:LEU:HD21	2.48	0.44
1:H:180[A]:PHE:O	1:H:181[A]:PRO:C	2.60	0.44
1:H:230:LYS:CG	5:H:5977:HOH:O	2.66	0.44
1:H:323:VAL:O	5:H:5936:HOH:O	2.21	0.44
1:J:210[B]:HIS:C	1:J:211[B]:HIS:HD2	2.26	0.44
1:K:115:LEU:CD2	1:K:379:LEU:HD21	2.48	0.44
1:K:289:GLY:HA2	5:K:1663:HOH:O	2.18	0.44
1:K:401:PRO:CA	1:K:404:ALA:HA	2.47	0.44
1:L:4:HIS:CE1	5:L:1773:HOH:O	2.70	0.44
1:L:128:PRO:HA	1:L:269:HIS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:210[B]:HIS:C	1:L:211[B]:HIS:HD2	2.26	0.44
1:L:231:LYS:CE	5:L:1692:HOH:O	2.59	0.44
1:L:269:HIS:CE1	4:L:5911:PPQ:CEP	2.92	0.44
1:A:193:SER:O	1:A:197:LEU:HG	2.17	0.43
1:B:4:HIS:CE1	5:B:5987:HOH:O	2.70	0.43
1:B:329:PRO:HD2	1:B:359:ARG:HG2	1.99	0.43
1:C:101:ASP:CG	1:C:435:THR:HG21	2.43	0.43
1:C:193:SER:O	1:C:197:LEU:HG	2.18	0.43
1:C:211[B]:HIS:O	1:C:212[B]:GLU:CB	2.54	0.43
1:C:230:LYS:CG	5:C:5963:HOH:O	2.66	0.43
1:D:178[A]:GLY:O	1:D:211[A]:HIS:HD2	2.01	0.43
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.80	0.43
1:E:180[A]:PHE:O	1:E:181[A]:PRO:C	2.60	0.43
1:E:285:ASP:C	5:E:745:HOH:O	2.60	0.43
1:F:230:LYS:CG	5:F:5973:HOH:O	2.66	0.43
1:G:401:PRO:HA	1:G:404:ALA:CA	2.44	0.43
1:J:101:ASP:CG	1:J:435:THR:HG21	2.43	0.43
1:J:268:MET:N	1:J:363:PRO:HD3	2.33	0.43
1:K:16:PHE:HB2	1:K:84:THR:HB	2.00	0.43
1:K:268:MET:N	1:K:363:PRO:HD3	2.33	0.43
1:L:101:ASP:CG	1:L:435:THR:HG21	2.43	0.43
1:L:193:SER:O	1:L:197:LEU:HG	2.18	0.43
1:L:289:GLY:HA2	5:L:1816:HOH:O	2.18	0.43
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.91	0.43
1:B:128:PRO:CD	5:B:5908:HOH:O	2.61	0.43
1:C:128:PRO:HA	1:C:269:HIS:O	2.18	0.43
1:C:178[A]:GLY:O	1:C:211[A]:HIS:HD2	2.01	0.43
1:D:323:VAL:O	5:D:5923:HOH:O	2.21	0.43
1:E:4:HIS:CE1	5:E:702:HOH:O	2.70	0.43
1:E:231:LYS:CE	5:E:621:HOH:O	2.59	0.43
1:E:323:VAL:O	5:E:634:HOH:O	2.21	0.43
1:G:4:HIS:CE1	5:G:5996:HOH:O	2.70	0.43
1:G:16:PHE:HB2	1:G:84:THR:HB	2.00	0.43
1:H:30[A]:HIS:CE1	1:I:183:PRO:HD3	2.54	0.43
1:H:68:MET:HA	1:H:69:PRO:HD2	1.78	0.43
1:I:47:LYS:CD	5:I:6056:HOH:O	2.65	0.43
1:I:128:PRO:HA	1:I:269:HIS:O	2.18	0.43
1:I:285:ASP:C	5:I:6045:HOH:O	2.60	0.43
1:J:337:ARG:HD3	1:J:337:ARG:C	2.43	0.43
1:L:172:ARG:HA	1:L:173[A]:PRO:HD3	1.80	0.43
1:L:323:VAL:O	5:L:1705:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PHE:HB2	1:A:84:THR:HB	2.00	0.43
1:B:323:VAL:O	5:B:5921:HOH:O	2.21	0.43
1:D:155:GLU:OE1	1:D:211[A]:HIS:CE1	2.68	0.43
1:E:101:ASP:CG	1:E:435:THR:HG21	2.43	0.43
1:E:128:PRO:HA	1:E:269:HIS:O	2.18	0.43
1:E:463:GLU:HA	1:K:140:PHE:CE1	2.53	0.43
1:F:47:LYS:CD	5:F:6045:HOH:O	2.65	0.43
1:F:178[A]:GLY:O	1:F:211[A]:HIS:HD2	2.01	0.43
1:G:183:PRO:HD3	1:L:30[A]:HIS:CE1	2.52	0.43
1:H:33:ILE:HA	1:H:34:PRO:HD3	1.90	0.43
1:H:210[B]:HIS:C	1:H:211[B]:HIS:HD2	2.26	0.43
1:I:115:LEU:CD2	1:I:379:LEU:HD21	2.48	0.43
1:I:284:GLY:HA3	1:I:291:SER:HA	1.99	0.43
1:K:127:GLY:HA3	3:K:4481:ADP:H1'	2.00	0.43
1:K:323:VAL:O	5:K:1552:HOH:O	2.21	0.43
1:L:178[A]:GLY:O	1:L:211[A]:HIS:HD2	2.01	0.43
1:L:352:LYS:HE2	1:L:352:LYS:HA	2.00	0.43
1:A:101:ASP:CG	1:A:435:THR:HG21	2.43	0.43
1:A:390:GLU:HA	1:A:391:PRO:HD3	1.84	0.43
1:B:56:GLY:N	5:B:5994:HOH:O	2.40	0.43
1:B:456:THR:O	1:H:458:HIS:HE1	2.00	0.43
1:C:115:LEU:CD2	1:C:379:LEU:HD21	2.48	0.43
1:C:284:GLY:HA3	1:C:291:SER:HA	1.99	0.43
1:D:344:ARG:HE	1:D:344:ARG:HB3	1.58	0.43
1:F:447:ARG:HH21	1:F:447:ARG:HG3	1.82	0.43
1:G:178[A]:GLY:O	1:G:211[A]:HIS:HD2	2.01	0.43
1:G:329:PRO:HD2	1:G:359:ARG:HG2	1.99	0.43
1:G:337:ARG:C	1:G:337:ARG:HD3	2.43	0.43
1:I:289:GLY:HA2	5:I:6045:HOH:O	2.18	0.43
1:J:29[A]:GLN:HA	1:K:180[A]:PHE:O	2.18	0.43
1:J:193:SER:O	1:J:197:LEU:HG	2.17	0.43
1:L:68:MET:HA	1:L:69:PRO:HD2	1.78	0.43
1:L:115:LEU:CD2	1:L:379:LEU:HD21	2.48	0.43
1:A:289:GLY:HA2	5:A:6024:HOH:O	2.18	0.43
1:B:127:GLY:HA3	3:B:4472:ADP:H1'	2.00	0.43
1:B:128:PRO:HA	1:B:269:HIS:O	2.18	0.43
1:B:180[A]:PHE:O	1:C:29[A]:GLN:HA	2.19	0.43
1:D:33:ILE:HA	1:D:34:PRO:HD3	1.90	0.43
1:D:128:PRO:HA	1:D:269:HIS:O	2.18	0.43
1:E:230:LYS:CG	5:E:678:HOH:O	2.66	0.43
1:E:272:MET:HE3	1:E:272:MET:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:PRO:CA	1:E:404:ALA:HA	2.47	0.43
1:G:30[A]:HIS:CE1	1:H:183:PRO:HD3	2.54	0.43
1:G:101:ASP:CG	1:G:435:THR:HG21	2.43	0.43
1:G:284:GLY:HA3	1:G:291:SER:HA	1.99	0.43
1:H:101:ASP:CG	1:H:435:THR:HG21	2.43	0.43
1:H:178[A]:GLY:O	1:H:211[A]:HIS:HD2	2.01	0.43
1:H:269:HIS:HE1	4:H:5907:PPQ:HEP2	1.82	0.43
1:I:16:PHE:HB2	1:I:84:THR:HB	2.00	0.43
1:I:75:VAL:CG2	5:I:5937:HOH:O	2.53	0.43
1:I:178[A]:GLY:O	1:I:211[A]:HIS:HD2	2.01	0.43
1:J:178[A]:GLY:O	1:J:211[A]:HIS:HD2	2.01	0.43
1:J:329:PRO:HD2	1:J:359:ARG:HG2	1.99	0.43
1:K:32:THR:OG1	1:L:189:GLN:NE2	2.50	0.43
1:K:125:LEU:HD12	1:K:125:LEU:HA	1.79	0.43
1:A:140:PHE:CE1	1:G:463:GLU:HA	2.54	0.43
1:A:230:LYS:CG	5:A:5963:HOH:O	2.66	0.43
1:A:284:GLY:HA3	1:A:291:SER:HA	1.99	0.43
1:B:16:PHE:HB2	1:B:84:THR:HB	2.00	0.43
1:B:289:GLY:HA2	5:B:6025:HOH:O	2.18	0.43
1:C:33:ILE:HA	1:C:34:PRO:HD3	1.90	0.43
1:C:230:LYS:HB2	1:C:230:LYS:HE2	1.85	0.43
1:C:231:LYS:CE	5:C:5909:HOH:O	2.59	0.43
1:C:271:HIS:CD2	1:C:357:GLU:HB2	2.54	0.43
1:D:16:PHE:HB2	1:D:84:THR:HB	2.00	0.43
1:D:210[B]:HIS:C	1:D:211[B]:HIS:HD2	2.26	0.43
1:E:1:SER:N	1:E:71:ALA:HB3	2.34	0.43
1:E:140:PHE:CE1	1:K:463:GLU:HA	2.54	0.43
1:E:261[A]:PHE:HB2	1:K:457:PRO:HD3	2.01	0.43
1:E:302:ILE:CD1	5:E:717:HOH:O	2.49	0.43
1:F:16:PHE:HB2	1:F:84:THR:HB	2.00	0.43
1:F:82:ASP:O	1:F:84:THR:CG2	2.67	0.43
1:F:165:GLU:N	5:F:5971:HOH:O	2.46	0.43
1:F:269:HIS:CE1	4:F:5905:PPQ:CEP	2.91	0.43
1:G:40:ALA:HB2	5:G:5991:HOH:O	2.10	0.43
1:G:115:LEU:CD2	1:G:379:LEU:HD21	2.48	0.43
1:G:144:ILE:HG22	5:G:5922:HOH:O	2.19	0.43
1:G:271:HIS:CD2	1:G:357:GLU:HB2	2.54	0.43
1:I:337:ARG:C	1:I:337:ARG:HD3	2.43	0.43
1:J:30[A]:HIS:CE1	1:K:183:PRO:HD3	2.53	0.43
1:J:230:LYS:CG	5:J:5980:HOH:O	2.66	0.43
1:A:29[A]:GLN:HA	1:F:180[A]:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210[B]:HIS:C	1:A:211[B]:HIS:HD2	2.26	0.43
1:B:1:SER:H2	1:B:71:ALA:HB3	1.83	0.43
1:B:101:ASP:CG	1:B:435:THR:HG21	2.43	0.43
1:C:359:ARG:HH12	4:C:5902:PPQ:HEP2	1.84	0.43
1:C:458:HIS:HE1	1:I:456:THR:O	2.02	0.43
1:D:352:LYS:HE2	1:D:352:LYS:HA	2.00	0.43
1:E:16:PHE:HB2	1:E:84:THR:HB	2.00	0.43
1:E:192[A]:ARG:HH21	1:E:219:ASN:ND2	2.17	0.43
1:E:268:MET:N	1:E:363:PRO:HD3	2.33	0.43
1:F:144:ILE:HG22	5:F:5923:HOH:O	2.19	0.43
1:F:359:ARG:HH12	4:F:5905:PPQ:HEP2	1.84	0.43
1:H:128:PRO:HA	1:H:269:HIS:O	2.18	0.43
1:H:272:MET:HE3	1:H:272:MET:HB2	1.84	0.43
1:J:210[A]:HIS:ND1	1:J:211[A]:HIS:O	2.47	0.43
1:J:390:GLU:HA	1:J:391:PRO:HD3	1.84	0.43
1:K:271:HIS:CD2	1:K:357:GLU:HB2	2.54	0.43
1:L:337:ARG:C	1:L:337:ARG:HD3	2.43	0.43
1:A:155:GLU:OE1	1:A:211[A]:HIS:CE1	2.68	0.43
5:A:5945:HOH:O	1:B:84:THR:HG21	2.18	0.43
1:B:180[A]:PHE:O	1:B:181[A]:PRO:C	2.60	0.43
1:C:16:PHE:HB2	1:C:84:THR:HB	2.00	0.43
1:C:144:ILE:HG22	5:C:5913:HOH:O	2.19	0.43
1:D:463:GLU:HA	1:J:140:PHE:CE1	2.54	0.43
1:E:384:ASN:N	1:E:384:ASN:ND2	2.59	0.43
1:F:115:LEU:CD2	1:F:379:LEU:HD21	2.48	0.43
1:G:210[B]:HIS:C	1:G:211[B]:HIS:HD2	2.26	0.43
1:H:1:SER:N	1:H:71:ALA:HB3	2.34	0.43
1:H:201:GLN:N	5:H:6017:HOH:O	2.52	0.43
1:H:305:ALA:CB	1:H:332:LEU:HD21	2.49	0.43
1:I:230:LYS:CG	5:I:5984:HOH:O	2.66	0.43
1:I:323:VAL:O	5:I:5941:HOH:O	2.21	0.43
1:A:115:LEU:CD2	1:A:379:LEU:HD21	2.48	0.43
1:A:140:PHE:CE1	1:F:160:SER:HB2	2.54	0.43
1:A:192[A]:ARG:HH21	1:A:219:ASN:ND2	2.17	0.43
1:B:1:SER:N	1:B:71:ALA:HB3	2.34	0.43
1:B:178[A]:GLY:O	1:B:211[A]:HIS:HD2	2.01	0.43
1:B:305:ALA:CB	1:B:332:LEU:HD21	2.49	0.43
1:C:201:GLN:N	5:C:6003:HOH:O	2.52	0.43
1:C:305:ALA:CB	1:C:332:LEU:HD21	2.49	0.43
1:C:401:PRO:CA	1:C:404:ALA:HA	2.47	0.43
1:C:447:ARG:HH21	1:C:447:ARG:HG3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192[A]:ARG:HH21	1:D:219:ASN:ND2	2.17	0.43
1:E:127:GLY:HA3	3:E:4475:ADP:H1'	2.00	0.43
1:E:329:PRO:HD2	1:E:359:ARG:HG2	1.99	0.43
1:F:401:PRO:CA	1:F:404:ALA:HA	2.46	0.43
1:G:192[A]:ARG:HH21	1:G:219:ASN:ND2	2.17	0.43
1:I:172:ARG:HA	1:I:173[A]:PRO:HD3	1.80	0.43
1:I:305:ALA:CB	1:I:332:LEU:HD21	2.49	0.43
1:J:128:PRO:HA	1:J:269:HIS:O	2.18	0.43
1:J:180[A]:PHE:O	1:J:181[A]:PRO:C	2.60	0.43
5:J:5986:HOH:O	1:K:183:PRO:CB	2.66	0.43
1:K:201:GLN:N	5:K:1640:HOH:O	2.52	0.43
1:K:305:ALA:CB	1:K:332:LEU:HD21	2.49	0.43
1:L:201:GLN:N	5:L:1793:HOH:O	2.52	0.43
1:A:271:HIS:CD2	1:A:357:GLU:HB2	2.54	0.43
1:B:352:LYS:HE2	1:B:352:LYS:HA	2.00	0.43
1:C:40:ALA:HB2	5:C:5981:HOH:O	2.10	0.43
1:C:352:LYS:HE2	1:C:352:LYS:HA	2.00	0.43
1:D:101:ASP:CG	1:D:435:THR:HG21	2.43	0.43
1:D:305:ALA:CB	1:D:332:LEU:HD21	2.49	0.43
1:E:332:LEU:O	5:E:717:HOH:O	2.20	0.43
1:F:127:GLY:HA3	3:F:4476:ADP:H1'	2.00	0.43
1:F:192[A]:ARG:HH21	1:F:219:ASN:ND2	2.17	0.43
1:F:289:GLY:HA2	5:F:6034:HOH:O	2.18	0.43
1:G:128:PRO:HA	1:G:269:HIS:O	2.18	0.43
1:I:144:ILE:HG22	5:I:5933:HOH:O	2.19	0.43
1:I:452:ARG:HG2	5:I:6036:HOH:O	2.19	0.43
1:J:31:VAL:HG23	1:K:210[A]:HIS:HB3	2.00	0.43
1:J:289:GLY:HA2	5:J:6041:HOH:O	2.18	0.43
1:K:192[A]:ARG:HH21	1:K:219:ASN:ND2	2.17	0.43
1:K:197:LEU:O	1:K:201:GLN:HG3	2.19	0.43
1:K:352:LYS:HE2	1:K:352:LYS:HA	2.00	0.43
1:A:180[A]:PHE:O	1:A:181[A]:PRO:C	2.60	0.42
1:B:309:ASN:HD22	1:B:309:ASN:HA	1.71	0.42
1:D:127:GLY:HA3	3:D:4474:ADP:H1'	2.00	0.42
1:D:175[B]:VAL:O	1:D:176[B]:LYS:HB2	2.20	0.42
1:D:180[A]:PHE:O	1:D:181[A]:PRO:C	2.60	0.42
1:D:359:ARG:HH12	4:D:5903:PPQ:HEP2	1.84	0.42
1:E:305:ALA:CB	1:E:332:LEU:HD21	2.49	0.42
1:G:93:GLU:OE2	1:G:94:PRO:HD2	2.20	0.42
1:G:180[A]:PHE:O	1:G:181[A]:PRO:C	2.60	0.42
5:G:5979:HOH:O	1:H:183:PRO:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29[A]:GLN:HA	1:J:180[A]:PHE:O	2.19	0.42
1:I:192[A]:ARG:HH21	1:I:219:ASN:ND2	2.17	0.42
1:I:359:ARG:HH12	4:I:5908:PPQ:HEP2	1.84	0.42
1:K:1:SER:N	1:K:71:ALA:HB3	2.34	0.42
1:L:16:PHE:HB2	1:L:84:THR:HB	2.00	0.42
1:L:127:GLY:HA3	3:L:4482:ADP:H1'	2.00	0.42
1:L:452:ARG:HG2	5:L:1807:HOH:O	2.19	0.42
1:A:128:PRO:HA	1:A:269:HIS:O	2.18	0.42
1:A:178[A]:GLY:O	1:A:211[A]:HIS:HD2	2.01	0.42
1:A:285:ASP:C	5:A:6024:HOH:O	2.60	0.42
1:B:47:LYS:CD	5:B:6036:HOH:O	2.65	0.42
1:B:271:HIS:CD2	1:B:357:GLU:HB2	2.54	0.42
1:B:285:ASP:C	5:B:6025:HOH:O	2.60	0.42
1:C:289:GLY:HA2	5:C:6024:HOH:O	2.18	0.42
1:E:93:GLU:OE2	1:E:94:PRO:HD2	2.19	0.42
1:E:125:LEU:HD12	1:E:125:LEU:HA	1.79	0.42
1:E:178[A]:GLY:O	1:E:211[A]:HIS:HD2	2.01	0.42
1:F:197:LEU:O	1:F:201:GLN:HG3	2.19	0.42
1:H:47:LYS:CD	5:H:6049:HOH:O	2.65	0.42
1:I:101:ASP:CG	1:I:435:THR:HG21	2.43	0.42
1:J:144:ILE:HG22	5:J:5930:HOH:O	2.19	0.42
1:J:197:LEU:O	1:J:201:GLN:HG3	2.20	0.42
1:J:323:VAL:O	5:J:5938:HOH:O	2.21	0.42
1:J:387:HIS:HA	1:J:388:PRO:HD2	1.85	0.42
1:L:230:LYS:CG	5:L:1749:HOH:O	2.66	0.42
1:B:210[B]:HIS:C	1:B:211[B]:HIS:HD2	2.26	0.42
1:B:211[B]:HIS:C	1:B:212[B]:GLU:HG3	2.37	0.42
1:B:359:ARG:HH12	4:B:5901:PPQ:HEP2	1.84	0.42
1:C:160:SER:HB2	1:D:140:PHE:CE1	2.54	0.42
1:D:269:HIS:HE1	4:D:5903:PPQ:HEP2	1.82	0.42
1:E:183:PRO:HD3	1:F:30[A]:HIS:CE1	2.54	0.42
1:F:337:ARG:C	1:F:337:ARG:HD3	2.43	0.42
1:F:374:LEU:HD12	1:F:374:LEU:HA	1.91	0.42
1:F:458:HIS:HE1	1:L:456:THR:O	2.02	0.42
1:G:127:GLY:HA3	3:G:4477:ADP:H1'	2.00	0.42
1:G:175[B]:VAL:O	1:G:176[B]:LYS:HB2	2.20	0.42
1:G:352:LYS:HE2	1:G:352:LYS:HA	2.00	0.42
1:H:271:HIS:CD2	1:H:357:GLU:HB2	2.54	0.42
1:H:352:LYS:HE2	1:H:352:LYS:HA	2.00	0.42
1:I:175[B]:VAL:O	1:I:176[B]:LYS:HB2	2.20	0.42
1:I:201:GLN:N	5:I:6024:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:271:HIS:CD2	1:I:357:GLU:HB2	2.54	0.42
1:J:305:ALA:CB	1:J:332:LEU:HD21	2.49	0.42
1:L:192[A]:ARG:HH21	1:L:219:ASN:ND2	2.17	0.42
1:A:82:ASP:O	1:A:84:THR:CG2	2.67	0.42
1:A:197:LEU:O	1:A:201:GLN:HG3	2.20	0.42
1:B:144:ILE:HG22	5:B:5913:HOH:O	2.19	0.42
1:D:230:LYS:CG	5:D:5966:HOH:O	2.66	0.42
1:D:271:HIS:CD2	1:D:357:GLU:HB2	2.54	0.42
1:E:271:HIS:CD2	1:E:357:GLU:HB2	2.54	0.42
1:F:271:HIS:CD2	1:F:357:GLU:HB2	2.54	0.42
1:G:1:SER:N	1:G:71:ALA:HB3	2.34	0.42
1:G:197:LEU:O	1:G:201:GLN:HG3	2.19	0.42
1:G:309:ASN:HD22	1:G:309:ASN:HA	1.71	0.42
1:H:127:GLY:HA3	3:H:4478:ADP:H1'	2.00	0.42
1:H:285:ASP:C	5:H:6038:HOH:O	2.60	0.42
1:K:128:PRO:HA	1:K:269:HIS:O	2.18	0.42
1:L:47:LYS:CD	5:L:1827:HOH:O	2.65	0.42
1:A:1:SER:N	1:A:71:ALA:HB3	2.34	0.42
1:A:93:GLU:OE2	1:A:94:PRO:HD2	2.19	0.42
1:A:127:GLY:HA3	3:A:4471:ADP:H1'	2.00	0.42
1:A:172:ARG:HA	1:A:173[A]:PRO:HD3	1.80	0.42
1:A:175[B]:VAL:O	1:A:176[B]:LYS:HB2	2.20	0.42
1:A:183:PRO:HD3	1:B:30[A]:HIS:CE1	2.54	0.42
1:A:269:HIS:HE1	4:A:5900:PPQ:HEP2	1.82	0.42
1:A:305:ALA:CB	1:A:332:LEU:HD21	2.49	0.42
1:A:452:ARG:HG2	5:A:6015:HOH:O	2.19	0.42
1:C:155:GLU:OE1	1:C:211[A]:HIS:CE1	2.68	0.42
1:C:192[A]:ARG:HH21	1:C:219:ASN:ND2	2.17	0.42
1:C:323:VAL:O	5:C:5921:HOH:O	2.21	0.42
1:D:374:LEU:HD12	1:D:374:LEU:HA	1.91	0.42
1:E:175[B]:VAL:O	1:E:176[B]:LYS:HB2	2.20	0.42
1:E:201:GLN:N	5:E:722:HOH:O	2.52	0.42
1:E:329:PRO:CD	1:E:359:ARG:HD2	2.42	0.42
1:E:359:ARG:HH12	4:E:5904:PPQ:HEP2	1.84	0.42
1:F:174[B]:GLY:O	1:F:175[B]:VAL:C	2.63	0.42
1:F:210[B]:HIS:C	1:F:211[B]:HIS:HD2	2.26	0.42
1:G:401:PRO:CA	1:G:404:ALA:HA	2.47	0.42
1:H:359:ARG:HH12	4:H:5907:PPQ:HEP2	1.84	0.42
1:I:93:GLU:OE2	1:I:94:PRO:HD2	2.19	0.42
1:I:210[B]:HIS:C	1:I:211[B]:HIS:HD2	2.26	0.42
1:I:272:MET:HE3	1:I:272:MET:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:352:LYS:HA	1:I:352:LYS:HE2	2.00	0.42
1:J:155:GLU:OE1	1:J:211[A]:HIS:CE1	2.68	0.42
1:J:271:HIS:CD2	1:J:357:GLU:HB2	2.54	0.42
1:J:359:ARG:HH12	4:J:5909:PPQ:HEP2	1.84	0.42
1:K:93:GLU:OE2	1:K:94:PRO:HD2	2.19	0.42
1:K:180[A]:PHE:O	1:K:181[A]:PRO:C	2.60	0.42
1:L:144:ILE:HG22	5:L:1697:HOH:O	2.19	0.42
1:L:272:MET:HE3	1:L:272:MET:HB2	1.84	0.42
1:C:1:SER:N	1:C:71:ALA:HB3	2.34	0.42
1:C:93:GLU:OE2	1:C:94:PRO:HD2	2.19	0.42
1:C:127:GLY:HA3	3:C:4473:ADP:H1'	2.00	0.42
1:D:1:SER:N	1:D:71:ALA:HB3	2.34	0.42
1:D:172:ARG:HA	1:D:173[A]:PRO:HD3	1.80	0.42
1:E:197:LEU:O	1:E:201:GLN:HG3	2.20	0.42
1:E:332:LEU:HD12	1:E:332:LEU:HA	1.90	0.42
1:E:352:LYS:HE2	1:E:352:LYS:HA	2.00	0.42
1:F:201:GLN:N	5:F:6013:HOH:O	2.52	0.42
1:F:231:LYS:CE	5:F:5919:HOH:O	2.59	0.42
1:G:174[B]:GLY:O	1:G:175[B]:VAL:C	2.63	0.42
1:H:192[A]:ARG:HH21	1:H:219:ASN:ND2	2.17	0.42
1:I:1:SER:N	1:I:71:ALA:HB3	2.34	0.42
1:I:127:GLY:HA3	3:I:4479:ADP:H1'	2.00	0.42
1:J:33:ILE:HA	1:J:34:PRO:HD3	1.90	0.42
1:J:352:LYS:HE2	1:J:352:LYS:HA	2.00	0.42
1:K:285:ASP:C	5:K:1663:HOH:O	2.60	0.42
1:L:93:GLU:OE2	1:L:94:PRO:HD2	2.19	0.42
1:L:271:HIS:CD2	1:L:357:GLU:HB2	2.54	0.42
1:A:352:LYS:HA	1:A:352:LYS:HE2	2.00	0.42
5:A:5948:HOH:O	1:F:182:VAL:HG23	2.20	0.42
1:B:197:LEU:O	1:B:201:GLN:HG3	2.20	0.42
1:C:47:LYS:CD	5:C:6035:HOH:O	2.65	0.42
1:C:197:LEU:O	1:C:201:GLN:HG3	2.19	0.42
1:C:235:ILE:HD13	1:C:235:ILE:HA	1.80	0.42
1:D:272:MET:HE3	1:D:272:MET:HB2	1.84	0.42
1:E:457:PRO:HD3	1:K:261[A]:PHE:HB2	2.01	0.42
1:G:359:ARG:HH12	4:G:5906:PPQ:HEP2	1.84	0.42
1:H:16:PHE:HB2	1:H:84:THR:HB	2.00	0.42
1:H:197:LEU:O	1:H:201:GLN:HG3	2.19	0.42
1:H:332:LEU:O	5:H:6012:HOH:O	2.20	0.42
1:I:197:LEU:O	1:I:201:GLN:HG3	2.19	0.42
1:J:16:PHE:HB2	1:J:84:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:33:ILE:HD12	1:K:208:ALA:CB	2.49	0.42
1:J:56:GLY:N	5:J:6010:HOH:O	2.40	0.42
1:J:127:GLY:HA3	3:J:4480:ADP:HI'	2.00	0.42
1:J:192[A]:ARG:HH21	1:J:219:ASN:ND2	2.17	0.42
1:K:140:PHE:CE1	1:L:160:SER:HB2	2.55	0.42
1:L:359:ARG:HH12	4:L:5911:PPQ:HEP2	1.84	0.42
1:B:155:GLU:OE1	1:B:211[A]:HIS:CE1	2.68	0.42
1:B:175[B]:VAL:O	1:B:176[B]:LYS:HB2	2.20	0.42
1:B:192[A]:ARG:HH21	1:B:219:ASN:ND2	2.17	0.42
1:C:401:PRO:HA	1:C:404:ALA:CA	2.44	0.42
1:E:155:GLU:OE1	1:E:211[A]:HIS:CE1	2.68	0.42
1:E:452:ARG:HG2	5:E:736:HOH:O	2.19	0.42
1:F:125:LEU:HD12	1:F:125:LEU:HA	1.79	0.42
1:F:456:THR:O	1:L:458:HIS:HE1	2.02	0.42
1:G:305:ALA:CB	1:G:332:LEU:HD21	2.49	0.42
1:H:175[B]:VAL:O	1:H:176[B]:LYS:HB2	2.20	0.42
1:H:447:ARG:CD	5:H:6023:HOH:O	2.68	0.42
1:I:174[B]:GLY:O	1:I:175[B]:VAL:C	2.63	0.42
1:J:125:LEU:HD12	1:J:125:LEU:HA	1.79	0.42
1:K:174[B]:GLY:O	1:K:175[B]:VAL:C	2.63	0.42
1:K:175[B]:VAL:O	1:K:176[B]:LYS:HB2	2.20	0.42
1:K:230:LYS:CG	5:K:1596:HOH:O	2.66	0.42
1:L:175[B]:VAL:O	1:L:176[B]:LYS:HB2	2.20	0.42
1:L:305:ALA:CB	1:L:332:LEU:HD21	2.49	0.42
1:A:272:MET:HE3	1:A:272:MET:HB2	1.84	0.42
1:A:440:ASP:HB2	5:A:6028:HOH:O	2.20	0.42
1:B:210[A]:HIS:ND1	1:B:211[A]:HIS:O	2.47	0.42
1:B:272:MET:HE3	1:B:272:MET:HB2	1.84	0.42
1:B:463:GLU:HA	1:H:140:PHE:CE1	2.54	0.42
1:D:447:ARG:CD	5:D:6012:HOH:O	2.68	0.42
1:E:144:ILE:HG22	5:E:626:HOH:O	2.19	0.42
1:E:387:HIS:HA	1:E:388:PRO:HD2	1.85	0.42
1:E:456:THR:O	1:K:458:HIS:HE1	2.03	0.42
1:F:1:SER:N	1:F:71:ALA:HB3	2.34	0.42
1:F:93:GLU:OE2	1:F:94:PRO:HD2	2.20	0.42
1:F:305:ALA:CB	1:F:332:LEU:HD21	2.49	0.42
1:G:201:GLN:N	5:G:6013:HOH:O	2.52	0.42
1:H:93:GLU:OE2	1:H:94:PRO:HD2	2.20	0.42
1:I:401:PRO:CA	1:I:404:ALA:HA	2.46	0.42
1:J:201:GLN:N	5:J:6020:HOH:O	2.52	0.42
1:L:1:SER:N	1:L:71:ALA:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.90	0.42
1:B:125:LEU:HA	1:B:125:LEU:HD12	1.79	0.42
1:B:201:GLN:N	5:B:6004:HOH:O	2.52	0.42
1:B:208:ALA:CB	1:C:33:ILE:HD12	2.50	0.42
1:C:174[B]:GLY:O	1:C:175[B]:VAL:C	2.63	0.42
1:G:323:VAL:O	5:G:5930:HOH:O	2.21	0.42
1:H:144:ILE:HG22	5:H:5928:HOH:O	2.19	0.42
1:J:129:GLU:O	1:J:268:MET:HA	2.20	0.42
1:L:401:PRO:CA	1:L:404:ALA:HA	2.47	0.42
1:A:61:ASN:O	1:F:337:ARG:O	2.38	0.41
1:A:323:VAL:O	5:A:5920:HOH:O	2.21	0.41
1:C:82:ASP:O	1:C:84:THR:CG2	2.67	0.41
1:C:175[B]:VAL:O	1:C:176[B]:LYS:HB2	2.20	0.41
1:C:390:GLU:HA	1:C:391:PRO:HD3	1.84	0.41
1:C:452:ARG:HG2	5:C:6015:HOH:O	2.19	0.41
1:D:214:ALA:HA	1:D:263[A]:ASP:OD2	2.21	0.41
1:D:452:ARG:HG2	5:D:6018:HOH:O	2.19	0.41
1:E:447:ARG:CD	5:E:729:HOH:O	2.68	0.41
1:F:175[B]:VAL:O	1:F:176[B]:LYS:HB2	2.20	0.41
1:F:452:ARG:HG2	5:F:6025:HOH:O	2.19	0.41
1:H:29[A]:GLN:HA	1:I:180[A]:PHE:O	2.20	0.41
1:H:129:GLU:O	1:H:268:MET:HA	2.20	0.41
1:H:165:GLU:N	5:H:5975:HOH:O	2.46	0.41
1:I:390:GLU:HA	1:I:391:PRO:HD3	1.84	0.41
1:J:172:ARG:HA	1:J:173[A]:PRO:HD3	1.80	0.41
1:J:440:ASP:HB2	5:J:6045:HOH:O	2.20	0.41
1:L:197:LEU:O	1:L:201:GLN:HG3	2.20	0.41
1:L:440:ASP:HB2	5:L:1820:HOH:O	2.20	0.41
1:A:56:GLY:N	5:A:5993:HOH:O	2.40	0.41
1:A:201:GLN:N	5:A:6003:HOH:O	2.52	0.41
1:A:401:PRO:CA	1:A:404:ALA:HA	2.46	0.41
1:C:179[B]:TYR:CD1	1:C:212[B]:GLU:CA	2.77	0.41
1:C:210[B]:HIS:C	1:C:211[B]:HIS:HD2	2.26	0.41
1:D:138:ILE:O	1:D:138:ILE:HG23	2.20	0.41
1:F:129:GLU:O	1:F:268:MET:HA	2.20	0.41
1:G:128:PRO:CD	5:G:5917:HOH:O	2.61	0.41
1:G:129:GLU:O	1:G:268:MET:HA	2.20	0.41
1:G:461:GLU:O	1:G:465:TYR:N	2.50	0.41
1:H:138:ILE:O	1:H:138:ILE:HG23	2.21	0.41
1:H:140:PHE:CE1	1:I:160:SER:HB2	2.55	0.41
1:H:283:SER:O	1:H:291:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:82:ASP:O	1:I:84:THR:CG2	2.67	0.41
1:I:447:ARG:CD	5:I:6030:HOH:O	2.68	0.41
1:I:461:GLU:O	1:I:465:TYR:N	2.50	0.41
1:K:440:ASP:HB2	5:K:1667:HOH:O	2.20	0.41
1:L:82:ASP:O	1:L:84:THR:CG2	2.67	0.41
1:A:80:PHE:CZ	1:F:189:GLN:HG3	2.55	0.41
1:A:144:ILE:HG22	5:A:5912:HOH:O	2.19	0.41
1:B:269:HIS:CE1	4:B:5901:PPQ:CEP	2.92	0.41
1:B:359:ARG:HH11	1:B:359:ARG:HD3	1.65	0.41
1:C:125:LEU:HG	1:C:225:PHE:CD2	2.56	0.41
1:C:129:GLU:O	1:C:268:MET:HA	2.20	0.41
1:E:129:GLU:O	1:E:268:MET:HA	2.20	0.41
1:E:283:SER:O	1:E:291:SER:HB3	2.20	0.41
1:E:440:ASP:HB2	5:E:749:HOH:O	2.20	0.41
1:F:254:THR:HB	1:L:466:TYR:CE1	2.54	0.41
1:F:384:ASN:N	1:F:384:ASN:ND2	2.59	0.41
1:F:440:ASP:HB2	5:F:6038:HOH:O	2.20	0.41
1:G:452:ARG:HG2	5:G:6025:HOH:O	2.19	0.41
1:I:180[A]:PHE:O	1:I:181[A]:PRO:C	2.60	0.41
1:J:1:SER:N	1:J:71:ALA:HB3	2.34	0.41
1:J:93:GLU:OE2	1:J:94:PRO:HD2	2.19	0.41
1:K:359:ARG:HH12	4:K:5910:PPQ:HEP2	1.84	0.41
1:L:125:LEU:HG	1:L:225:PHE:CD2	2.56	0.41
1:A:447:ARG:CD	5:A:6009:HOH:O	2.68	0.41
1:B:138:ILE:O	1:B:138:ILE:HG23	2.20	0.41
1:B:174[B]:GLY:O	1:B:175[B]:VAL:C	2.63	0.41
1:B:214:ALA:HA	1:B:263[A]:ASP:OD2	2.21	0.41
1:B:302:ILE:CD1	5:B:5999:HOH:O	2.49	0.41
1:C:210[A]:HIS:HB3	1:D:31:VAL:HG23	2.02	0.41
1:C:359:ARG:HH11	1:C:359:ARG:HD3	1.65	0.41
1:D:93:GLU:OE2	1:D:94:PRO:HD2	2.19	0.41
1:G:125:LEU:HG	1:G:225:PHE:CD2	2.56	0.41
1:H:125:LEU:HG	1:H:225:PHE:CD2	2.56	0.41
5:I:5990:HOH:O	1:J:183:PRO:CB	2.68	0.41
1:J:175[B]:VAL:O	1:J:176[B]:LYS:HB2	2.20	0.41
1:J:224:ARG:CG	1:J:224:ARG:NH2	2.69	0.41
1:J:283:SER:O	1:J:291:SER:HB3	2.21	0.41
1:J:452:ARG:HG2	5:J:6032:HOH:O	2.19	0.41
1:K:75:VAL:CG2	5:K:1548:HOH:O	2.53	0.41
1:L:129:GLU:O	1:L:268:MET:HA	2.20	0.41
1:A:125:LEU:HG	1:A:225:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ARG:HH12	4:A:5900:PPQ:HEP2	1.84	0.41
1:B:93:GLU:OE2	1:B:94:PRO:HD2	2.19	0.41
1:B:230:LYS:CG	5:B:5964:HOH:O	2.66	0.41
1:B:371:PHE:N	1:B:371:PHE:CD2	2.89	0.41
1:C:429:LYS:HA	1:C:434:PHE:O	2.21	0.41
1:D:175[B]:VAL:O	1:D:176[B]:LYS:CB	2.69	0.41
1:D:197:LEU:O	1:D:201:GLN:HG3	2.20	0.41
1:D:201:GLN:N	5:D:6006:HOH:O	2.52	0.41
1:E:125:LEU:HG	1:E:225:PHE:CD2	2.56	0.41
1:F:125:LEU:HG	1:F:225:PHE:CD2	2.56	0.41
1:F:323:VAL:O	5:F:5931:HOH:O	2.21	0.41
1:F:447:ARG:CD	5:F:6019:HOH:O	2.68	0.41
1:H:214:ALA:HA	1:H:263[A]:ASP:OD2	2.21	0.41
1:I:138:ILE:HG23	1:I:138:ILE:O	2.20	0.41
1:K:129:GLU:O	1:K:268:MET:HA	2.20	0.41
1:K:199:MET:HG3	1:K:241:VAL:HG11	2.03	0.41
1:L:155:GLU:OE1	1:L:211[A]:HIS:CE1	2.68	0.41
1:A:283:SER:O	1:A:291:SER:HB3	2.20	0.41
1:B:129:GLU:O	1:B:268:MET:HA	2.20	0.41
1:C:175[B]:VAL:O	1:C:176[B]:LYS:CB	2.69	0.41
1:D:129:GLU:O	1:D:268:MET:HA	2.20	0.41
1:E:82:ASP:O	1:E:84:THR:CG2	2.67	0.41
1:E:429:LYS:HA	1:E:434:PHE:O	2.21	0.41
1:F:285:ASP:C	5:F:6034:HOH:O	2.60	0.41
1:F:387:HIS:HA	1:F:388:PRO:HD2	1.85	0.41
1:G:344:ARG:HE	1:G:344:ARG:HB3	1.58	0.41
1:H:235:ILE:HD13	1:H:235:ILE:HA	1.80	0.41
1:I:129:GLU:O	1:I:268:MET:HA	2.20	0.41
1:I:199:MET:HG3	1:I:241:VAL:HG11	2.03	0.41
1:J:82:ASP:O	1:J:84:THR:CG2	2.67	0.41
1:J:174[B]:GLY:O	1:J:175[B]:VAL:C	2.63	0.41
1:J:214:ALA:HA	1:J:263[A]:ASP:OD2	2.21	0.41
1:K:138:ILE:O	1:K:138:ILE:HG23	2.20	0.41
1:K:144:ILE:HG22	5:K:1544:HOH:O	2.19	0.41
1:K:175[B]:VAL:O	1:K:176[B]:LYS:CB	2.69	0.41
1:K:461:GLU:O	1:K:465:TYR:N	2.50	0.41
1:L:138:ILE:HG23	1:L:138:ILE:O	2.21	0.41
1:L:214:ALA:HA	1:L:263[A]:ASP:OD2	2.21	0.41
1:A:27:LYS:HD2	1:A:27:LYS:HA	1.95	0.41
1:A:75:VAL:CG2	5:A:5916:HOH:O	2.53	0.41
1:A:138:ILE:HG23	1:A:138:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HA	1:A:235:ILE:HD13	1.80	0.41
1:B:199:MET:HG3	1:B:241:VAL:HG11	2.03	0.41
1:B:452:ARG:HG2	5:B:6016:HOH:O	2.19	0.41
1:C:56:GLY:N	5:C:5993:HOH:O	2.40	0.41
1:C:272:MET:HE3	1:C:272:MET:HB2	1.84	0.41
1:D:401:PRO:CA	1:D:404:ALA:HA	2.47	0.41
1:F:302:ILE:CD1	5:F:6008:HOH:O	2.49	0.41
1:F:466:TYR:CE1	1:L:254:THR:HB	2.56	0.41
1:G:214:ALA:HA	1:G:263[A]:ASP:OD2	2.21	0.41
1:H:429:LYS:HA	1:H:434:PHE:O	2.21	0.41
1:J:1:SER:H3	1:J:71:ALA:CB	2.33	0.41
1:K:33:ILE:HA	1:K:34:PRO:HD3	1.90	0.41
1:K:287:TYR:CD1	1:K:391:PRO:HG2	2.56	0.41
1:L:269:HIS:HE1	4:L:5911:PPQ:HEP2	1.82	0.41
1:A:199:MET:HG3	1:A:241:VAL:HG11	2.03	0.41
1:A:429:LYS:HA	1:A:434:PHE:O	2.21	0.41
1:B:172:ARG:HA	1:B:173[A]:PRO:HD3	1.80	0.41
1:B:387:HIS:HA	1:B:388:PRO:HD2	1.85	0.41
1:C:138:ILE:HG23	1:C:138:ILE:O	2.20	0.41
1:D:179[B]:TYR:HB3	1:D:180[B]:PHE:CD2	2.56	0.41
1:D:199:MET:HG3	1:D:241:VAL:HG11	2.03	0.41
1:E:6:LEU:HD13	1:E:6:LEU:HA	1.93	0.41
1:E:174[B]:GLY:O	1:E:175[B]:VAL:C	2.63	0.41
1:E:199:MET:HG3	1:E:241:VAL:HG11	2.03	0.41
1:E:235:ILE:HD13	1:E:235:ILE:HA	1.80	0.41
1:E:276:LYS:HB3	1:E:281:LEU:HD11	2.03	0.41
1:F:180[A]:PHE:O	1:F:181[A]:PRO:C	2.60	0.41
1:F:269:HIS:HE1	4:F:5905:PPQ:HEP2	1.82	0.41
1:H:82:ASP:CB	5:H:5958:HOH:O	2.64	0.41
1:H:174[B]:GLY:O	1:H:175[B]:VAL:C	2.63	0.41
1:H:199:MET:HG3	1:H:241:VAL:HG11	2.03	0.41
1:H:287:TYR:CD1	1:H:391:PRO:HG2	2.56	0.41
1:I:440:ASP:HB2	5:I:6049:HOH:O	2.20	0.41
1:J:138:ILE:O	1:J:138:ILE:HG23	2.21	0.41
1:K:41:GLU:O	1:K:45:GLU:HG2	2.21	0.41
1:K:283:SER:O	1:K:291:SER:HB3	2.21	0.41
1:L:283:SER:O	1:L:291:SER:HB3	2.21	0.41
1:L:429:LYS:HA	1:L:434:PHE:O	2.21	0.41
1:A:211[A]:HIS:HD2	1:A:212[A]:GLU:O	2.04	0.41
1:A:256:MET:HA	1:A:257:PRO:HD2	1.89	0.41
1:A:264[B]:ASN:N	1:A:326:TYR:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HB2	1:A:408:PRO:O	2.21	0.41
1:B:41:GLU:O	1:B:45:GLU:HG2	2.21	0.41
1:B:283:SER:O	1:B:291:SER:HB3	2.21	0.41
1:B:329:PRO:HG2	1:B:359:ARG:CD	2.18	0.41
1:B:447:ARG:CD	5:B:6010:HOH:O	2.68	0.41
1:C:440:ASP:HB2	5:C:6028:HOH:O	2.20	0.41
1:D:41:GLU:O	1:D:45:GLU:HG2	2.21	0.41
1:D:125:LEU:HG	1:D:225:PHE:CD2	2.56	0.41
1:D:144:ILE:HG22	5:D:5915:HOH:O	2.19	0.41
1:D:174[B]:GLY:O	1:D:175[B]:VAL:C	2.63	0.41
1:D:285:ASP:C	5:D:6027:HOH:O	2.60	0.41
1:D:332:LEU:HB2	1:D:408:PRO:O	2.21	0.41
1:E:41:GLU:O	1:E:45:GLU:HG2	2.21	0.41
1:E:214:ALA:HA	1:E:263[A]:ASP:OD2	2.21	0.41
1:E:371:PHE:N	1:E:371:PHE:CD2	2.89	0.41
1:F:214:ALA:HA	1:F:263[A]:ASP:OD2	2.21	0.41
1:G:33:ILE:CD1	1:H:208:ALA:HB2	2.51	0.41
1:G:138:ILE:O	1:G:138:ILE:HG23	2.20	0.41
1:G:175[B]:VAL:O	1:G:176[B]:LYS:CB	2.69	0.41
1:G:211[B]:HIS:C	1:G:212[B]:GLU:HG3	2.36	0.41
1:G:447:ARG:CD	5:G:5992:HOH:O	2.58	0.41
1:H:128:PRO:CD	5:H:5924:HOH:O	2.61	0.41
1:H:440:ASP:HB2	5:H:6042:HOH:O	2.20	0.41
1:I:125:LEU:HG	1:I:225:PHE:CD2	2.56	0.41
1:I:211[A]:HIS:HD2	1:I:212[A]:GLU:O	2.04	0.41
1:I:264[B]:ASN:N	1:I:326:TYR:HD2	2.19	0.41
1:I:371:PHE:N	1:I:371:PHE:CD2	2.89	0.41
1:I:429:LYS:HA	1:I:434:PHE:O	2.21	0.41
1:J:269:HIS:CE1	4:J:5909:PPQ:CEP	2.92	0.41
1:K:1:SER:O	1:K:1:SER:OG	2.39	0.41
1:K:214:ALA:HA	1:K:263[A]:ASP:OD2	2.21	0.41
1:K:276:LYS:HB3	1:K:281:LEU:HD11	2.03	0.41
1:K:371:PHE:N	1:K:371:PHE:CD2	2.89	0.41
1:K:452:ARG:HG2	5:K:1654:HOH:O	2.20	0.41
5:K:1602:HOH:O	1:L:183:PRO:HB2	2.21	0.41
1:L:174[B]:GLY:O	1:L:175[B]:VAL:C	2.63	0.41
1:L:179[B]:TYR:HB3	1:L:180[B]:PHE:CD2	2.56	0.41
1:L:180[A]:PHE:O	1:L:181[A]:PRO:C	2.60	0.41
1:L:199:MET:HG3	1:L:241:VAL:HG11	2.03	0.41
1:L:211[A]:HIS:HD2	1:L:212[A]:GLU:O	2.04	0.41
1:L:264[B]:ASN:N	1:L:326:TYR:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:309:ASN:HD22	1:L:309:ASN:HA	1.71	0.41
1:L:371:PHE:N	1:L:371:PHE:CD2	2.89	0.41
1:L:426:GLU:CB	5:L:1746:HOH:O	2.49	0.41
1:A:174[B]:GLY:O	1:A:175[B]:VAL:C	2.63	0.41
1:A:276:LYS:HB3	1:A:281:LEU:HD11	2.03	0.41
1:B:80:PHE:HE2	5:B:5970:HOH:O	2.04	0.41
1:B:175[B]:VAL:O	1:B:176[B]:LYS:CB	2.69	0.41
1:B:264[B]:ASN:N	1:B:326:TYR:HD2	2.19	0.41
1:C:271:HIS:HA	1:C:356:ILE:O	2.21	0.41
1:C:287:TYR:CD1	1:C:391:PRO:HG2	2.56	0.41
1:C:371:PHE:N	1:C:371:PHE:CD2	2.89	0.41
1:D:210[A]:HIS:ND1	1:D:211[A]:HIS:O	2.47	0.41
1:D:211[A]:HIS:HD2	1:D:212[A]:GLU:O	2.04	0.41
1:D:283:SER:O	1:D:291:SER:HB3	2.20	0.41
1:D:440:ASP:HB2	5:D:6031:HOH:O	2.20	0.41
1:E:138:ILE:O	1:E:138:ILE:HG23	2.20	0.41
1:E:359:ARG:HH11	1:E:359:ARG:HD3	1.65	0.41
1:F:463:GLU:HA	1:L:140:PHE:CE1	2.56	0.41
1:G:6:LEU:HD13	1:G:6:LEU:HA	1.93	0.41
1:G:271:HIS:HA	1:G:356:ILE:O	2.21	0.41
1:G:283:SER:O	1:G:291:SER:HB3	2.20	0.41
1:G:429:LYS:HA	1:G:434:PHE:O	2.21	0.41
1:H:179[B]:TYR:HB3	1:H:180[B]:PHE:CD2	2.56	0.41
1:I:29[A]:GLN:HB3	1:J:180[A]:PHE:CB	2.49	0.41
1:I:283:SER:O	1:I:291:SER:HB3	2.20	0.41
1:J:287:TYR:CD1	1:J:391:PRO:HG2	2.56	0.41
1:J:302:ILE:CD1	5:J:6015:HOH:O	2.49	0.41
1:K:264[B]:ASN:N	1:K:326:TYR:HD2	2.19	0.41
1:L:175[B]:VAL:O	1:L:176[B]:LYS:CB	2.69	0.41
1:L:447:ARG:CD	5:L:1800:HOH:O	2.68	0.41
1:A:129:GLU:O	1:A:268:MET:HA	2.20	0.40
1:B:1:SER:O	1:B:1:SER:OG	2.39	0.40
1:B:179[B]:TYR:HB3	1:B:180[B]:PHE:CD2	2.56	0.40
1:C:41:GLU:O	1:C:45:GLU:HG2	2.21	0.40
1:C:199:MET:HG3	1:C:241:VAL:HG11	2.03	0.40
1:C:300:GLY:HA3	1:C:377:ALA:O	2.21	0.40
1:D:287:TYR:CD1	1:D:391:PRO:HG2	2.56	0.40
1:D:429:LYS:HA	1:D:434:PHE:O	2.21	0.40
1:E:458:HIS:HE1	1:K:456:THR:O	2.04	0.40
1:F:175[B]:VAL:O	1:F:176[B]:LYS:CB	2.69	0.40
1:G:82:ASP:CB	5:G:5953:HOH:O	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:GLU:OE1	1:H:211[A]:HIS:CE1	2.68	0.40
1:H:461:GLU:O	1:H:465:TYR:N	2.50	0.40
1:I:41:GLU:O	1:I:45:GLU:HG2	2.21	0.40
1:I:214:ALA:HA	1:I:263[A]:ASP:OD2	2.21	0.40
1:I:287:TYR:CD1	1:I:391:PRO:HG2	2.56	0.40
1:J:179[B]:TYR:HB3	1:J:180[B]:PHE:CD2	2.56	0.40
1:J:285:ASP:C	5:J:6041:HOH:O	2.60	0.40
1:K:125:LEU:HG	1:K:225:PHE:CD2	2.56	0.40
1:K:172:ARG:HA	1:K:173[A]:PRO:HD3	1.80	0.40
1:K:211[B]:HIS:C	1:K:212[B]:GLU:HG3	2.37	0.40
1:K:332:LEU:HB2	1:K:408:PRO:O	2.21	0.40
1:K:429:LYS:HA	1:K:434:PHE:O	2.21	0.40
1:A:31:VAL:HG23	1:F:210[A]:HIS:HB3	2.03	0.40
1:A:179[B]:TYR:HB3	1:A:180[B]:PHE:CD2	2.56	0.40
1:B:75:VAL:CG2	5:B:5917:HOH:O	2.53	0.40
1:C:447:ARG:CD	5:C:6009:HOH:O	2.68	0.40
1:E:447:ARG:CD	5:E:698:HOH:O	2.58	0.40
1:F:1:SER:O	1:F:1:SER:OG	2.39	0.40
1:F:332:LEU:HB2	1:F:408:PRO:O	2.21	0.40
1:G:231:LYS:CE	5:G:5917:HOH:O	2.59	0.40
1:G:371:PHE:N	1:G:371:PHE:CD2	2.89	0.40
1:H:371:PHE:N	1:H:371:PHE:CD2	2.89	0.40
1:I:82:ASP:CB	5:I:5964:HOH:O	2.64	0.40
1:J:264[B]:ASN:N	1:J:326:TYR:HD2	2.19	0.40
1:J:429:LYS:HA	1:J:434:PHE:O	2.21	0.40
1:L:230:LYS:HB2	1:L:230:LYS:HE2	1.85	0.40
1:L:332:LEU:HB2	1:L:408:PRO:O	2.21	0.40
1:A:122:ASP:CG	1:A:276:LYS:HA	2.47	0.40
1:A:214:ALA:HA	1:A:263[A]:ASP:OD2	2.21	0.40
1:A:302:ILE:CD1	5:A:5998:HOH:O	2.49	0.40
1:A:344:ARG:HE	1:A:344:ARG:HB3	1.59	0.40
1:B:125:LEU:HG	1:B:225:PHE:CD2	2.56	0.40
1:B:440:ASP:HB2	5:B:6029:HOH:O	2.20	0.40
1:E:300:GLY:HA3	1:E:377:ALA:O	2.21	0.40
1:E:332:LEU:HB2	1:E:408:PRO:O	2.21	0.40
1:F:41:GLU:O	1:F:45:GLU:HG2	2.21	0.40
1:F:122:ASP:CG	1:F:276:LYS:HA	2.47	0.40
1:F:179[B]:TYR:HB3	1:F:180[B]:PHE:CD2	2.56	0.40
1:F:283:SER:O	1:F:291:SER:HB3	2.20	0.40
1:F:287:TYR:CD1	1:F:391:PRO:HG2	2.56	0.40
1:F:300:GLY:HA3	1:F:377:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:MET:HE3	1:G:272:MET:HB2	1.84	0.40
1:G:440:ASP:HB2	5:G:6038:HOH:O	2.20	0.40
1:H:41:GLU:O	1:H:45:GLU:HG2	2.21	0.40
1:H:452:ARG:HG2	5:H:6029:HOH:O	2.19	0.40
1:I:60:ILE:HG12	1:J:339:ARG:HB2	2.03	0.40
1:I:175[B]:VAL:O	1:I:176[B]:LYS:CB	2.69	0.40
1:K:122:ASP:CG	1:K:276:LYS:HA	2.47	0.40
1:L:41:GLU:O	1:L:45:GLU:HG2	2.21	0.40
1:L:122:ASP:CG	1:L:276:LYS:HA	2.47	0.40
1:A:287:TYR:CD1	1:A:391:PRO:HG2	2.56	0.40
1:B:211[A]:HIS:HD2	1:B:212[A]:GLU:O	2.04	0.40
1:C:122:ASP:CG	1:C:276:LYS:HA	2.47	0.40
1:C:179[B]:TYR:HB3	1:C:180[B]:PHE:CD2	2.56	0.40
1:D:17:VAL:HA	1:D:85:LEU:O	2.22	0.40
1:F:271:HIS:HA	1:F:356:ILE:O	2.21	0.40
1:G:29[A]:GLN:HA	1:H:180[A]:PHE:O	2.21	0.40
1:G:41:GLU:O	1:G:45:GLU:HG2	2.21	0.40
1:G:264[B]:ASN:N	1:G:326:TYR:HD2	2.19	0.40
1:G:300:GLY:HA3	1:G:377:ALA:O	2.21	0.40
1:H:82:ASP:O	1:H:84:THR:CG2	2.67	0.40
1:I:80:PHE:HE2	5:I:5990:HOH:O	2.04	0.40
1:I:122:ASP:CG	1:I:276:LYS:HA	2.47	0.40
1:I:210[A]:HIS:ND1	1:I:211[A]:HIS:O	2.47	0.40
1:I:300:GLY:HA3	1:I:377:ALA:O	2.21	0.40
1:J:68:MET:HA	1:J:69:PRO:HD2	1.78	0.40
1:J:125:LEU:HG	1:J:225:PHE:CD2	2.56	0.40
1:J:175[B]:VAL:O	1:J:176[B]:LYS:CB	2.69	0.40
1:J:371:PHE:N	1:J:371:PHE:CD2	2.89	0.40
1:K:329:PRO:CD	1:K:359:ARG:HD2	2.42	0.40
1:B:287:TYR:CD1	1:B:391:PRO:HG2	2.56	0.40
1:C:172:ARG:HA	1:C:173[A]:PRO:HD3	1.80	0.40
1:C:214:ALA:HA	1:C:263[A]:ASP:OD2	2.21	0.40
1:C:283:SER:O	1:C:291:SER:HB3	2.21	0.40
5:C:5945:HOH:O	1:D:84:THR:HG21	2.21	0.40
1:E:271:HIS:HA	1:E:356:ILE:O	2.21	0.40
1:E:287:TYR:CD1	1:E:391:PRO:HG2	2.56	0.40
1:F:27:LYS:HD2	1:F:27:LYS:HA	1.95	0.40
1:H:82:ASP:OD2	5:H:5937:HOH:O	2.22	0.40
1:H:332:LEU:HB2	1:H:408:PRO:O	2.21	0.40
1:I:1:SER:OG	1:I:5:VAL:HG23	2.22	0.40
1:I:17:VAL:HA	1:I:85:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:GLU:OE1	1:I:211[A]:HIS:CE1	2.68	0.40
1:I:179[B]:TYR:HB3	1:I:180[B]:PHE:CD2	2.56	0.40
1:J:300:GLY:HA3	1:J:377:ALA:O	2.21	0.40
1:K:179[B]:TYR:HB3	1:K:180[B]:PHE:CD2	2.56	0.40
1:K:271:HIS:HA	1:K:356:ILE:O	2.22	0.40
1:K:337:ARG:CD	1:K:337:ARG:C	2.94	0.40
1:K:423:LEU:O	1:K:425:ARG:N	2.53	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	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	B	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	C	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	D	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	E	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	F	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	G	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	H	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	I	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	J	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	K	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
1	L	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2 8
All	All	5784/5616 (103%)	4932 (85%)	600 (10%)	252 (4%)	3 8

All (252) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	177[A]	GLY
1	A	177[B]	GLY
1	A	180[A]	PHE
1	A	180[B]	PHE
1	A	212[A]	GLU
1	A	212[B]	GLU
1	A	213[A]	VAL
1	A	262[A]	GLY
1	A	262[B]	GLY
1	A	396	LEU
1	B	58	LYS
1	B	177[A]	GLY
1	B	177[B]	GLY
1	B	180[A]	PHE
1	B	180[B]	PHE
1	B	212[A]	GLU
1	B	212[B]	GLU
1	B	213[A]	VAL
1	B	262[A]	GLY
1	B	262[B]	GLY
1	B	396	LEU
1	C	58	LYS
1	C	177[A]	GLY
1	C	177[B]	GLY
1	C	180[A]	PHE
1	C	180[B]	PHE
1	C	212[A]	GLU
1	C	212[B]	GLU
1	C	213[A]	VAL
1	C	262[A]	GLY
1	C	262[B]	GLY
1	C	396	LEU
1	D	58	LYS
1	D	177[A]	GLY
1	D	177[B]	GLY
1	D	180[A]	PHE
1	D	180[B]	PHE
1	D	212[A]	GLU
1	D	212[B]	GLU
1	D	213[A]	VAL
1	D	262[A]	GLY
1	D	262[B]	GLY

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Mol	Chain	Res	Type
1	D	396	LEU
1	E	58	LYS
1	E	177[A]	GLY
1	E	177[B]	GLY
1	E	180[A]	PHE
1	E	180[B]	PHE
1	E	212[A]	GLU
1	E	212[B]	GLU
1	E	213[A]	VAL
1	E	262[A]	GLY
1	E	262[B]	GLY
1	E	396	LEU
1	F	58	LYS
1	F	177[A]	GLY
1	F	177[B]	GLY
1	F	180[A]	PHE
1	F	180[B]	PHE
1	F	212[A]	GLU
1	F	212[B]	GLU
1	F	213[A]	VAL
1	F	262[A]	GLY
1	F	262[B]	GLY
1	F	396	LEU
1	G	58	LYS
1	G	177[A]	GLY
1	G	177[B]	GLY
1	G	180[A]	PHE
1	G	180[B]	PHE
1	G	212[A]	GLU
1	G	212[B]	GLU
1	G	213[A]	VAL
1	G	262[A]	GLY
1	G	262[B]	GLY
1	G	396	LEU
1	H	58	LYS
1	H	177[A]	GLY
1	H	177[B]	GLY
1	H	180[A]	PHE
1	H	180[B]	PHE
1	H	212[A]	GLU
1	H	212[B]	GLU
1	H	213[A]	VAL

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Mol	Chain	Res	Type
1	H	262[A]	GLY
1	H	262[B]	GLY
1	H	396	LEU
1	I	58	LYS
1	I	177[A]	GLY
1	I	177[B]	GLY
1	I	180[A]	PHE
1	I	180[B]	PHE
1	I	212[A]	GLU
1	I	212[B]	GLU
1	I	213[A]	VAL
1	I	262[A]	GLY
1	I	262[B]	GLY
1	I	396	LEU
1	J	58	LYS
1	J	177[A]	GLY
1	J	177[B]	GLY
1	J	180[A]	PHE
1	J	180[B]	PHE
1	J	212[A]	GLU
1	J	212[B]	GLU
1	J	213[A]	VAL
1	J	262[A]	GLY
1	J	262[B]	GLY
1	J	396	LEU
1	K	58	LYS
1	K	177[A]	GLY
1	K	177[B]	GLY
1	K	180[A]	PHE
1	K	180[B]	PHE
1	K	212[A]	GLU
1	K	212[B]	GLU
1	K	213[A]	VAL
1	K	262[A]	GLY
1	K	262[B]	GLY
1	K	396	LEU
1	L	58	LYS
1	L	177[A]	GLY
1	L	177[B]	GLY
1	L	180[A]	PHE
1	L	180[B]	PHE
1	L	212[A]	GLU

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Mol	Chain	Res	Type
1	L	212[B]	GLU
1	L	213[A]	VAL
1	L	262[A]	GLY
1	L	262[B]	GLY
1	L	396	LEU
1	A	60	ILE
1	A	178[A]	GLY
1	A	178[B]	GLY
1	A	264[A]	ASN
1	A	264[B]	ASN
1	A	349	ALA
1	B	60	ILE
1	B	178[A]	GLY
1	B	178[B]	GLY
1	B	264[A]	ASN
1	B	264[B]	ASN
1	B	349	ALA
1	C	60	ILE
1	C	178[A]	GLY
1	C	178[B]	GLY
1	C	264[A]	ASN
1	C	264[B]	ASN
1	C	349	ALA
1	D	60	ILE
1	D	178[A]	GLY
1	D	178[B]	GLY
1	D	264[A]	ASN
1	D	264[B]	ASN
1	D	349	ALA
1	E	60	ILE
1	E	178[A]	GLY
1	E	178[B]	GLY
1	E	264[A]	ASN
1	E	264[B]	ASN
1	E	349	ALA
1	F	60	ILE
1	F	178[A]	GLY
1	F	178[B]	GLY
1	F	264[A]	ASN
1	F	264[B]	ASN
1	F	349	ALA
1	G	60	ILE

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Mol	Chain	Res	Type
1	G	178[A]	GLY
1	G	178[B]	GLY
1	G	264[A]	ASN
1	G	264[B]	ASN
1	G	349	ALA
1	H	60	ILE
1	H	178[A]	GLY
1	H	178[B]	GLY
1	H	264[A]	ASN
1	H	264[B]	ASN
1	H	349	ALA
1	I	60	ILE
1	I	178[A]	GLY
1	I	178[B]	GLY
1	I	264[A]	ASN
1	I	264[B]	ASN
1	I	349	ALA
1	J	60	ILE
1	J	178[A]	GLY
1	J	178[B]	GLY
1	J	264[A]	ASN
1	J	264[B]	ASN
1	J	349	ALA
1	K	60	ILE
1	K	178[A]	GLY
1	K	178[B]	GLY
1	K	264[A]	ASN
1	K	264[B]	ASN
1	K	349	ALA
1	L	60	ILE
1	L	178[A]	GLY
1	L	178[B]	GLY
1	L	264[A]	ASN
1	L	264[B]	ASN
1	L	349	ALA
1	A	59	GLY
1	A	170	GLY
1	A	424	ASP
1	B	59	GLY
1	B	170	GLY
1	B	424	ASP
1	C	59	GLY

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Mol	Chain	Res	Type
1	C	170	GLY
1	C	424	ASP
1	D	59	GLY
1	D	170	GLY
1	D	424	ASP
1	E	59	GLY
1	E	170	GLY
1	E	424	ASP
1	F	59	GLY
1	F	170	GLY
1	F	424	ASP
1	G	59	GLY
1	G	170	GLY
1	G	424	ASP
1	H	59	GLY
1	H	170	GLY
1	H	424	ASP
1	I	59	GLY
1	I	170	GLY
1	I	424	ASP
1	J	59	GLY
1	J	170	GLY
1	J	424	ASP
1	K	59	GLY
1	K	170	GLY
1	K	424	ASP
1	L	59	GLY
1	L	170	GLY
1	L	424	ASP
1	A	401	PRO
1	B	401	PRO
1	C	401	PRO
1	D	401	PRO
1	E	401	PRO
1	F	401	PRO
1	G	401	PRO
1	H	401	PRO
1	I	401	PRO
1	J	401	PRO
1	K	401	PRO
1	L	401	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	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	B	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	C	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	D	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	E	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	F	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	G	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	H	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	I	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	J	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	K	395/384 (103%)	349 (88%)	46 (12%)	5	18
1	L	395/384 (103%)	349 (88%)	46 (12%)	5	18
All	All	4740/4608 (103%)	4188 (88%)	552 (12%)	5	18

All (552) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	19	LEU
1	A	23	ASP
1	A	25	LYS
1	A	33	ILE
1	A	53	SER
1	A	58	LYS
1	A	62	GLU
1	A	64	ASP
1	A	82	ASP
1	A	84	THR
1	A	88	ARG
1	A	96	THR
1	A	98	GLN

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Mol	Chain	Res	Type
1	A	102	ARG
1	A	115	LEU
1	A	124	VAL
1	A	125	LEU
1	A	143	SER
1	A	165	GLU
1	A	183	PRO
1	A	224	ARG
1	A	266[A]	SER
1	A	266[B]	SER
1	A	285	ASP
1	A	293	GLN
1	A	332	LEU
1	A	337	ARG
1	A	340	SER
1	A	344	ARG
1	A	361	PRO
1	A	374	LEU
1	A	375	LEU
1	A	384	ASN
1	A	386	ILE
1	A	394	LYS
1	A	398	ASP
1	A	402	GLU
1	A	405	LYS
1	A	406	GLU
1	A	419	ASN
1	A	428	LEU
1	A	435	THR
1	A	437	GLU
1	A	464	LEU
1	A	468	VAL
1	B	7	THR
1	B	19	LEU
1	B	23	ASP
1	B	25	LYS
1	B	33	ILE
1	B	53	SER
1	B	58	LYS
1	B	62	GLU
1	B	64	ASP
1	B	82	ASP

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Mol	Chain	Res	Type
1	B	84	THR
1	B	88	ARG
1	B	96	THR
1	B	98	GLN
1	B	102	ARG
1	B	115	LEU
1	B	124	VAL
1	B	125	LEU
1	B	143	SER
1	B	165	GLU
1	B	183	PRO
1	B	224	ARG
1	B	266[A]	SER
1	B	266[B]	SER
1	B	285	ASP
1	B	293	GLN
1	B	332	LEU
1	B	337	ARG
1	B	340	SER
1	B	344	ARG
1	B	361	PRO
1	B	374	LEU
1	B	375	LEU
1	B	384	ASN
1	B	386	ILE
1	B	394	LYS
1	B	398	ASP
1	B	402	GLU
1	B	405	LYS
1	B	406	GLU
1	B	419	ASN
1	B	428	LEU
1	B	435	THR
1	B	437	GLU
1	B	464	LEU
1	B	468	VAL
1	C	7	THR
1	C	19	LEU
1	C	23	ASP
1	C	25	LYS
1	C	33	ILE
1	C	53	SER

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Mol	Chain	Res	Type
1	C	58	LYS
1	C	62	GLU
1	C	64	ASP
1	C	82	ASP
1	C	84	THR
1	C	88	ARG
1	C	96	THR
1	C	98	GLN
1	C	102	ARG
1	C	115	LEU
1	C	124	VAL
1	C	125	LEU
1	C	143	SER
1	C	165	GLU
1	C	183	PRO
1	C	224	ARG
1	C	266[A]	SER
1	C	266[B]	SER
1	C	285	ASP
1	C	293	GLN
1	C	332	LEU
1	C	337	ARG
1	C	340	SER
1	C	344	ARG
1	C	361	PRO
1	C	374	LEU
1	C	375	LEU
1	C	384	ASN
1	C	386	ILE
1	C	394	LYS
1	C	398	ASP
1	C	402	GLU
1	C	405	LYS
1	C	406	GLU
1	C	419	ASN
1	C	428	LEU
1	C	435	THR
1	C	437	GLU
1	C	464	LEU
1	C	468	VAL
1	D	7	THR
1	D	19	LEU

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Mol	Chain	Res	Type
1	D	23	ASP
1	D	25	LYS
1	D	33	ILE
1	D	53	SER
1	D	58	LYS
1	D	62	GLU
1	D	64	ASP
1	D	82	ASP
1	D	84	THR
1	D	88	ARG
1	D	96	THR
1	D	98	GLN
1	D	102	ARG
1	D	115	LEU
1	D	124	VAL
1	D	125	LEU
1	D	143	SER
1	D	165	GLU
1	D	183	PRO
1	D	224	ARG
1	D	266[A]	SER
1	D	266[B]	SER
1	D	285	ASP
1	D	293	GLN
1	D	332	LEU
1	D	337	ARG
1	D	340	SER
1	D	344	ARG
1	D	361	PRO
1	D	374	LEU
1	D	375	LEU
1	D	384	ASN
1	D	386	ILE
1	D	394	LYS
1	D	398	ASP
1	D	402	GLU
1	D	405	LYS
1	D	406	GLU
1	D	419	ASN
1	D	428	LEU
1	D	435	THR
1	D	437	GLU

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Mol	Chain	Res	Type
1	D	464	LEU
1	D	468	VAL
1	E	7	THR
1	E	19	LEU
1	E	23	ASP
1	E	25	LYS
1	E	33	ILE
1	E	53	SER
1	E	58	LYS
1	E	62	GLU
1	E	64	ASP
1	E	82	ASP
1	E	84	THR
1	E	88	ARG
1	E	96	THR
1	E	98	GLN
1	E	102	ARG
1	E	115	LEU
1	E	124	VAL
1	E	125	LEU
1	E	143	SER
1	E	165	GLU
1	E	183	PRO
1	E	224	ARG
1	E	266[A]	SER
1	E	266[B]	SER
1	E	285	ASP
1	E	293	GLN
1	E	332	LEU
1	E	337	ARG
1	E	340	SER
1	E	344	ARG
1	E	361	PRO
1	E	374	LEU
1	E	375	LEU
1	E	384	ASN
1	E	386	ILE
1	E	394	LYS
1	E	398	ASP
1	E	402	GLU
1	E	405	LYS
1	E	406	GLU

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Mol	Chain	Res	Type
1	E	419	ASN
1	E	428	LEU
1	E	435	THR
1	E	437	GLU
1	E	464	LEU
1	E	468	VAL
1	F	7	THR
1	F	19	LEU
1	F	23	ASP
1	F	25	LYS
1	F	33	ILE
1	F	53	SER
1	F	58	LYS
1	F	62	GLU
1	F	64	ASP
1	F	82	ASP
1	F	84	THR
1	F	88	ARG
1	F	96	THR
1	F	98	GLN
1	F	102	ARG
1	F	115	LEU
1	F	124	VAL
1	F	125	LEU
1	F	143	SER
1	F	165	GLU
1	F	183	PRO
1	F	224	ARG
1	F	266[A]	SER
1	F	266[B]	SER
1	F	285	ASP
1	F	293	GLN
1	F	332	LEU
1	F	337	ARG
1	F	340	SER
1	F	344	ARG
1	F	361	PRO
1	F	374	LEU
1	F	375	LEU
1	F	384	ASN
1	F	386	ILE
1	F	394	LYS

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Mol	Chain	Res	Type
1	F	398	ASP
1	F	402	GLU
1	F	405	LYS
1	F	406	GLU
1	F	419	ASN
1	F	428	LEU
1	F	435	THR
1	F	437	GLU
1	F	464	LEU
1	F	468	VAL
1	G	7	THR
1	G	19	LEU
1	G	23	ASP
1	G	25	LYS
1	G	33	ILE
1	G	53	SER
1	G	58	LYS
1	G	62	GLU
1	G	64	ASP
1	G	82	ASP
1	G	84	THR
1	G	88	ARG
1	G	96	THR
1	G	98	GLN
1	G	102	ARG
1	G	115	LEU
1	G	124	VAL
1	G	125	LEU
1	G	143	SER
1	G	165	GLU
1	G	183	PRO
1	G	224	ARG
1	G	266[A]	SER
1	G	266[B]	SER
1	G	285	ASP
1	G	293	GLN
1	G	332	LEU
1	G	337	ARG
1	G	340	SER
1	G	344	ARG
1	G	361	PRO
1	G	374	LEU

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Mol	Chain	Res	Type
1	G	375	LEU
1	G	384	ASN
1	G	386	ILE
1	G	394	LYS
1	G	398	ASP
1	G	402	GLU
1	G	405	LYS
1	G	406	GLU
1	G	419	ASN
1	G	428	LEU
1	G	435	THR
1	G	437	GLU
1	G	464	LEU
1	G	468	VAL
1	H	7	THR
1	H	19	LEU
1	H	23	ASP
1	H	25	LYS
1	H	33	ILE
1	H	53	SER
1	H	58	LYS
1	H	62	GLU
1	H	64	ASP
1	H	82	ASP
1	H	84	THR
1	H	88	ARG
1	H	96	THR
1	H	98	GLN
1	H	102	ARG
1	H	115	LEU
1	H	124	VAL
1	H	125	LEU
1	H	143	SER
1	H	165	GLU
1	H	183	PRO
1	H	224	ARG
1	H	266[A]	SER
1	H	266[B]	SER
1	H	285	ASP
1	H	293	GLN
1	H	332	LEU
1	H	337	ARG

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Mol	Chain	Res	Type
1	H	340	SER
1	H	344	ARG
1	H	361	PRO
1	H	374	LEU
1	H	375	LEU
1	H	384	ASN
1	H	386	ILE
1	H	394	LYS
1	H	398	ASP
1	H	402	GLU
1	H	405	LYS
1	H	406	GLU
1	H	419	ASN
1	H	428	LEU
1	H	435	THR
1	H	437	GLU
1	H	464	LEU
1	H	468	VAL
1	I	7	THR
1	I	19	LEU
1	I	23	ASP
1	I	25	LYS
1	I	33	ILE
1	I	53	SER
1	I	58	LYS
1	I	62	GLU
1	I	64	ASP
1	I	82	ASP
1	I	84	THR
1	I	88	ARG
1	I	96	THR
1	I	98	GLN
1	I	102	ARG
1	I	115	LEU
1	I	124	VAL
1	I	125	LEU
1	I	143	SER
1	I	165	GLU
1	I	183	PRO
1	I	224	ARG
1	I	266[A]	SER
1	I	266[B]	SER

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Mol	Chain	Res	Type
1	I	285	ASP
1	I	293	GLN
1	I	332	LEU
1	I	337	ARG
1	I	340	SER
1	I	344	ARG
1	I	361	PRO
1	I	374	LEU
1	I	375	LEU
1	I	384	ASN
1	I	386	ILE
1	I	394	LYS
1	I	398	ASP
1	I	402	GLU
1	I	405	LYS
1	I	406	GLU
1	I	419	ASN
1	I	428	LEU
1	I	435	THR
1	I	437	GLU
1	I	464	LEU
1	I	468	VAL
1	J	7	THR
1	J	19	LEU
1	J	23	ASP
1	J	25	LYS
1	J	33	ILE
1	J	53	SER
1	J	58	LYS
1	J	62	GLU
1	J	64	ASP
1	J	82	ASP
1	J	84	THR
1	J	88	ARG
1	J	96	THR
1	J	98	GLN
1	J	102	ARG
1	J	115	LEU
1	J	124	VAL
1	J	125	LEU
1	J	143	SER
1	J	165	GLU

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Mol	Chain	Res	Type
1	J	183	PRO
1	J	224	ARG
1	J	266[A]	SER
1	J	266[B]	SER
1	J	285	ASP
1	J	293	GLN
1	J	332	LEU
1	J	337	ARG
1	J	340	SER
1	J	344	ARG
1	J	361	PRO
1	J	374	LEU
1	J	375	LEU
1	J	384	ASN
1	J	386	ILE
1	J	394	LYS
1	J	398	ASP
1	J	402	GLU
1	J	405	LYS
1	J	406	GLU
1	J	419	ASN
1	J	428	LEU
1	J	435	THR
1	J	437	GLU
1	J	464	LEU
1	J	468	VAL
1	K	7	THR
1	K	19	LEU
1	K	23	ASP
1	K	25	LYS
1	K	33	ILE
1	K	53	SER
1	K	58	LYS
1	K	62	GLU
1	K	64	ASP
1	K	82	ASP
1	K	84	THR
1	K	88	ARG
1	K	96	THR
1	K	98	GLN
1	K	102	ARG
1	K	115	LEU

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Mol	Chain	Res	Type
1	K	124	VAL
1	K	125	LEU
1	K	143	SER
1	K	165	GLU
1	K	183	PRO
1	K	224	ARG
1	K	266[A]	SER
1	K	266[B]	SER
1	K	285	ASP
1	K	293	GLN
1	K	332	LEU
1	K	337	ARG
1	K	340	SER
1	K	344	ARG
1	K	361	PRO
1	K	374	LEU
1	K	375	LEU
1	K	384	ASN
1	K	386	ILE
1	K	394	LYS
1	K	398	ASP
1	K	402	GLU
1	K	405	LYS
1	K	406	GLU
1	K	419	ASN
1	K	428	LEU
1	K	435	THR
1	K	437	GLU
1	K	464	LEU
1	K	468	VAL
1	L	7	THR
1	L	19	LEU
1	L	23	ASP
1	L	25	LYS
1	L	33	ILE
1	L	53	SER
1	L	58	LYS
1	L	62	GLU
1	L	64	ASP
1	L	82	ASP
1	L	84	THR
1	L	88	ARG

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Mol	Chain	Res	Type
1	L	96	THR
1	L	98	GLN
1	L	102	ARG
1	L	115	LEU
1	L	124	VAL
1	L	125	LEU
1	L	143	SER
1	L	165	GLU
1	L	183	PRO
1	L	224	ARG
1	L	266[A]	SER
1	L	266[B]	SER
1	L	285	ASP
1	L	293	GLN
1	L	332	LEU
1	L	337	ARG
1	L	340	SER
1	L	344	ARG
1	L	361	PRO
1	L	374	LEU
1	L	375	LEU
1	L	384	ASN
1	L	386	ILE
1	L	394	LYS
1	L	398	ASP
1	L	402	GLU
1	L	405	LYS
1	L	406	GLU
1	L	419	ASN
1	L	428	LEU
1	L	435	THR
1	L	437	GLU
1	L	464	LEU
1	L	468	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30[A]	HIS
1	A	189	GLN
1	A	218	GLN
1	A	219	ASN

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Mol	Chain	Res	Type
1	A	244	ASN
1	A	277	ASN
1	A	313	ASN
1	A	384	ASN
1	A	458	HIS
1	B	10	ASN
1	B	30[A]	HIS
1	B	189	GLN
1	B	218	GLN
1	B	219	ASN
1	B	244	ASN
1	B	277	ASN
1	B	313	ASN
1	B	384	ASN
1	B	458	HIS
1	C	10	ASN
1	C	30[A]	HIS
1	C	189	GLN
1	C	218	GLN
1	C	219	ASN
1	C	244	ASN
1	C	277	ASN
1	C	313	ASN
1	C	384	ASN
1	C	409	GLN
1	C	458	HIS
1	D	10	ASN
1	D	30[A]	HIS
1	D	189	GLN
1	D	218	GLN
1	D	219	ASN
1	D	244	ASN
1	D	277	ASN
1	D	313	ASN
1	D	384	ASN
1	D	458	HIS
1	E	10	ASN
1	E	29[A]	GLN
1	E	30[A]	HIS
1	E	189	GLN
1	E	218	GLN
1	E	219	ASN

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Mol	Chain	Res	Type
1	E	244	ASN
1	E	277	ASN
1	E	313	ASN
1	E	384	ASN
1	E	409	GLN
1	E	458	HIS
1	F	10	ASN
1	F	30[A]	HIS
1	F	189	GLN
1	F	218	GLN
1	F	219	ASN
1	F	244	ASN
1	F	277	ASN
1	F	313	ASN
1	F	384	ASN
1	F	409	GLN
1	F	458	HIS
1	G	10	ASN
1	G	30[A]	HIS
1	G	189	GLN
1	G	218	GLN
1	G	219	ASN
1	G	244	ASN
1	G	277	ASN
1	G	313	ASN
1	G	384	ASN
1	G	458	HIS
1	H	30[A]	HIS
1	H	189	GLN
1	H	218	GLN
1	H	219	ASN
1	H	244	ASN
1	H	277	ASN
1	H	313	ASN
1	H	384	ASN
1	H	409	GLN
1	H	458	HIS
1	I	10	ASN
1	I	30[A]	HIS
1	I	189	GLN
1	I	218	GLN
1	I	219	ASN

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Mol	Chain	Res	Type
1	I	244	ASN
1	I	277	ASN
1	I	313	ASN
1	I	384	ASN
1	I	409	GLN
1	I	458	HIS
1	J	10	ASN
1	J	30[A]	HIS
1	J	189	GLN
1	J	218	GLN
1	J	219	ASN
1	J	244	ASN
1	J	277	ASN
1	J	313	ASN
1	J	384	ASN
1	J	458	HIS
1	K	30[A]	HIS
1	K	189	GLN
1	K	218	GLN
1	K	219	ASN
1	K	244	ASN
1	K	277	ASN
1	K	313	ASN
1	K	384	ASN
1	K	458	HIS
1	L	10	ASN
1	L	30[A]	HIS
1	L	189	GLN
1	L	218	GLN
1	L	219	ASN
1	L	244	ASN
1	L	277	ASN
1	L	313	ASN
1	L	384	ASN
1	L	409	GLN
1	L	458	HIS

5.3.3 RNA

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](#)

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 for Mogul analysis.

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
3	ADP	L	4482	2	28,29,29	3.87	13 (46%)	43,45,45	2.99	18 (41%)
4	PPQ	K	5910	2	7,10,10	1.23	1 (14%)	5,14,14	5.42	2 (40%)
3	ADP	I	4479	2	28,29,29	3.88	13 (46%)	43,45,45	2.99	18 (41%)
4	PPQ	J	5909	2	7,10,10	1.25	1 (14%)	5,14,14	5.42	2 (40%)
4	PPQ	C	5902	2	7,10,10	1.24	1 (14%)	5,14,14	5.42	2 (40%)
3	ADP	B	4472	2	28,29,29	3.86	13 (46%)	43,45,45	2.99	18 (41%)
3	ADP	K	4481	2	28,29,29	3.86	13 (46%)	43,45,45	2.99	18 (41%)
4	PPQ	B	5901	2	7,10,10	1.24	1 (14%)	5,14,14	5.43	2 (40%)
3	ADP	A	4471	2	28,29,29	3.86	13 (46%)	43,45,45	2.99	18 (41%)
4	PPQ	H	5907	2	7,10,10	1.25	1 (14%)	5,14,14	5.43	2 (40%)
4	PPQ	F	5905	2	7,10,10	1.24	1 (14%)	5,14,14	5.42	2 (40%)
4	PPQ	I	5908	2	7,10,10	1.26	1 (14%)	5,14,14	5.43	2 (40%)
3	ADP	G	4477	2	28,29,29	3.86	13 (46%)	43,45,45	2.99	18 (41%)
3	ADP	H	4478	2	28,29,29	3.86	13 (46%)	43,45,45	2.99	18 (41%)
4	PPQ	E	5904	2	7,10,10	1.25	1 (14%)	5,14,14	5.43	2 (40%)
3	ADP	D	4474	2	28,29,29	3.86	13 (46%)	43,45,45	2.99	18 (41%)
4	PPQ	D	5903	2	7,10,10	1.25	1 (14%)	5,14,14	5.42	2 (40%)
4	PPQ	A	5900	2	7,10,10	1.25	1 (14%)	5,14,14	5.42	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PPQ	L	5911	2	7,10,10	1.24	1 (14%)	5,14,14	5.43	2 (40%)
4	PPQ	G	5906	2	7,10,10	1.25	1 (14%)	5,14,14	5.43	2 (40%)
3	ADP	J	4480	2	28,29,29	3.87	13 (46%)	43,45,45	2.99	18 (41%)
3	ADP	C	4473	2	28,29,29	3.86	13 (46%)	43,45,45	2.99	18 (41%)
3	ADP	F	4476	2	28,29,29	3.86	13 (46%)	43,45,45	2.99	18 (41%)
3	ADP	E	4475	2	28,29,29	3.86	13 (46%)	43,45,45	2.99	18 (41%)

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
3	ADP	L	4482	2	-	7/16/32/32	0/3/3/3
4	PPQ	K	5910	2	-	6/10/10/10	-
3	ADP	I	4479	2	-	7/16/32/32	0/3/3/3
4	PPQ	J	5909	2	-	6/10/10/10	-
4	PPQ	C	5902	2	-	6/10/10/10	-
3	ADP	B	4472	2	-	7/16/32/32	0/3/3/3
3	ADP	K	4481	2	-	7/16/32/32	0/3/3/3
4	PPQ	B	5901	2	-	6/10/10/10	-
3	ADP	A	4471	2	-	7/16/32/32	0/3/3/3
4	PPQ	H	5907	2	-	6/10/10/10	-
4	PPQ	F	5905	2	-	6/10/10/10	-
4	PPQ	I	5908	2	-	6/10/10/10	-
3	ADP	G	4477	2	-	7/16/32/32	0/3/3/3
3	ADP	H	4478	2	-	7/16/32/32	0/3/3/3
4	PPQ	E	5904	2	-	6/10/10/10	-
3	ADP	D	4474	2	-	7/16/32/32	0/3/3/3
4	PPQ	D	5903	2	-	6/10/10/10	-
4	PPQ	A	5900	2	-	6/10/10/10	-
4	PPQ	L	5911	2	-	6/10/10/10	-
4	PPQ	G	5906	2	-	6/10/10/10	-
3	ADP	J	4480	2	-	7/16/32/32	0/3/3/3
3	ADP	C	4473	2	-	7/16/32/32	0/3/3/3
3	ADP	F	4476	2	-	7/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	E	4475	2	-	7/16/32/32	0/3/3/3

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4479	ADP	PA-O3A	12.93	1.73	1.59
3	J	4480	ADP	PA-O3A	12.92	1.73	1.59
3	B	4472	ADP	PA-O3A	12.90	1.73	1.59
3	A	4471	ADP	PA-O3A	12.87	1.73	1.59
3	C	4473	ADP	PA-O3A	12.87	1.73	1.59
3	L	4482	ADP	PA-O3A	12.87	1.73	1.59
3	D	4474	ADP	PA-O3A	12.85	1.73	1.59
3	G	4477	ADP	PA-O3A	12.85	1.73	1.59
3	K	4481	ADP	PA-O3A	12.84	1.73	1.59
3	E	4475	ADP	PA-O3A	12.84	1.73	1.59
3	H	4478	ADP	PA-O3A	12.84	1.73	1.59
3	F	4476	ADP	PA-O3A	12.82	1.73	1.59
3	F	4476	ADP	C1'-N9	8.79	1.70	1.46
3	H	4478	ADP	C1'-N9	8.79	1.70	1.46
3	E	4475	ADP	C1'-N9	8.79	1.70	1.46
3	J	4480	ADP	C1'-N9	8.79	1.70	1.46
3	A	4471	ADP	C1'-N9	8.78	1.70	1.46
3	B	4472	ADP	C1'-N9	8.78	1.70	1.46
3	L	4482	ADP	C1'-N9	8.78	1.70	1.46
3	G	4477	ADP	C1'-N9	8.77	1.70	1.46
3	I	4479	ADP	C1'-N9	8.77	1.70	1.46
3	D	4474	ADP	C1'-N9	8.76	1.70	1.46
3	C	4473	ADP	C1'-N9	8.76	1.70	1.46
3	K	4481	ADP	C1'-N9	8.75	1.70	1.46
3	C	4473	ADP	C8-N9	5.69	1.47	1.37
3	E	4475	ADP	C8-N9	5.68	1.47	1.37
3	I	4479	ADP	C8-N9	5.67	1.47	1.37
3	F	4476	ADP	C8-N9	5.65	1.47	1.37
3	L	4482	ADP	C8-N9	5.65	1.47	1.37
3	G	4477	ADP	C8-N9	5.64	1.47	1.37
3	A	4471	ADP	C8-N9	5.64	1.47	1.37
3	K	4481	ADP	C8-N9	5.64	1.47	1.37
3	D	4474	ADP	C8-N9	5.62	1.47	1.37
3	B	4472	ADP	C8-N9	5.62	1.47	1.37
3	H	4478	ADP	C8-N9	5.62	1.47	1.37
3	J	4480	ADP	C8-N9	5.59	1.47	1.37
3	I	4479	ADP	C6-N6	-4.63	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4475	ADP	C6-N6	-4.62	1.22	1.34
3	D	4474	ADP	C6-N6	-4.62	1.22	1.34
3	J	4480	ADP	C6-N6	-4.61	1.22	1.34
3	B	4472	ADP	C6-N6	-4.61	1.22	1.34
3	A	4471	ADP	C6-N6	-4.60	1.22	1.34
3	L	4482	ADP	C6-N6	-4.60	1.22	1.34
3	H	4478	ADP	C6-N6	-4.60	1.22	1.34
3	F	4476	ADP	C6-N6	-4.60	1.22	1.34
3	G	4477	ADP	C6-N6	-4.60	1.22	1.34
3	C	4473	ADP	C6-N6	-4.59	1.22	1.34
3	K	4481	ADP	C6-N6	-4.59	1.22	1.34
3	C	4473	ADP	C4-N3	4.33	1.42	1.34
3	J	4480	ADP	C4-N3	4.33	1.42	1.34
3	G	4477	ADP	C4-N3	4.30	1.42	1.34
3	H	4478	ADP	C4-N3	4.29	1.42	1.34
3	F	4476	ADP	C4-N3	4.29	1.42	1.34
3	L	4482	ADP	C4-N3	4.29	1.42	1.34
3	I	4479	ADP	C4-N3	4.28	1.42	1.34
3	A	4471	ADP	C4-N3	4.28	1.42	1.34
3	E	4475	ADP	C4-N3	4.28	1.42	1.34
3	D	4474	ADP	C4-N3	4.28	1.42	1.34
3	B	4472	ADP	C4-N3	4.26	1.42	1.34
3	K	4481	ADP	C4-N3	4.25	1.42	1.34
3	I	4479	ADP	O4'-C4'	4.18	1.54	1.45
3	L	4482	ADP	O4'-C4'	4.18	1.54	1.45
3	E	4475	ADP	O4'-C4'	4.17	1.54	1.45
3	B	4472	ADP	O4'-C4'	4.17	1.54	1.45
3	K	4481	ADP	O4'-C4'	4.16	1.54	1.45
3	A	4471	ADP	O4'-C4'	4.16	1.54	1.45
3	H	4478	ADP	O4'-C4'	4.16	1.54	1.45
3	F	4476	ADP	O4'-C4'	4.15	1.54	1.45
3	G	4477	ADP	O4'-C4'	4.14	1.54	1.45
3	D	4474	ADP	O4'-C4'	4.14	1.54	1.45
3	C	4473	ADP	O4'-C4'	4.13	1.54	1.45
3	J	4480	ADP	O4'-C4'	4.12	1.54	1.45
3	L	4482	ADP	O4'-C1'	4.11	1.51	1.42
3	K	4481	ADP	O4'-C1'	4.11	1.51	1.42
3	J	4480	ADP	O4'-C1'	4.10	1.51	1.42
3	I	4479	ADP	O4'-C1'	4.09	1.51	1.42
3	G	4477	ADP	O4'-C1'	4.09	1.51	1.42
3	E	4475	ADP	O4'-C1'	4.08	1.51	1.42
3	D	4474	ADP	O4'-C1'	4.08	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4471	ADP	O4'-C1'	4.08	1.51	1.42
3	C	4473	ADP	O4'-C1'	4.08	1.51	1.42
3	H	4478	ADP	O4'-C1'	4.07	1.51	1.42
3	F	4476	ADP	O4'-C1'	4.07	1.51	1.42
3	B	4472	ADP	O4'-C1'	4.06	1.51	1.42
3	H	4478	ADP	PB-O3B	4.01	1.69	1.54
3	I	4479	ADP	PB-O3B	4.00	1.69	1.54
3	J	4480	ADP	PB-O3B	4.00	1.69	1.54
3	C	4473	ADP	PB-O3B	4.00	1.69	1.54
3	L	4482	ADP	PB-O3B	4.00	1.69	1.54
3	B	4472	ADP	PB-O3B	4.00	1.69	1.54
3	K	4481	ADP	PB-O3B	4.00	1.69	1.54
3	A	4471	ADP	PB-O3B	3.99	1.69	1.54
3	D	4474	ADP	PB-O3B	3.99	1.69	1.54
3	G	4477	ADP	PB-O3B	3.99	1.69	1.54
3	E	4475	ADP	PB-O3B	3.98	1.69	1.54
3	F	4476	ADP	PB-O3B	3.97	1.69	1.54
3	K	4481	ADP	C4-N9	3.66	1.45	1.37
3	D	4474	ADP	C4-N9	3.65	1.45	1.37
3	H	4478	ADP	C4-N9	3.64	1.45	1.37
3	G	4477	ADP	C4-N9	3.63	1.45	1.37
3	E	4475	ADP	C4-N9	3.63	1.45	1.37
3	L	4482	ADP	C4-N9	3.63	1.45	1.37
3	A	4471	ADP	C4-N9	3.63	1.45	1.37
3	F	4476	ADP	C4-N9	3.63	1.45	1.37
3	I	4479	ADP	C4-N9	3.63	1.45	1.37
3	J	4480	ADP	C4-N9	3.62	1.45	1.37
3	B	4472	ADP	C4-N9	3.62	1.45	1.37
3	C	4473	ADP	C4-N9	3.61	1.45	1.37
3	I	4479	ADP	C5-C4	3.45	1.45	1.39
3	D	4474	ADP	C5-C4	3.42	1.45	1.39
3	B	4472	ADP	C5-C4	3.42	1.45	1.39
3	H	4478	ADP	C5-C4	3.42	1.45	1.39
3	F	4476	ADP	C5-C4	3.41	1.45	1.39
3	K	4481	ADP	C5-C4	3.41	1.45	1.39
3	L	4482	ADP	C5-C4	3.41	1.45	1.39
3	A	4471	ADP	C5-C4	3.41	1.45	1.39
3	C	4473	ADP	C5-C4	3.41	1.45	1.39
3	G	4477	ADP	C5-C4	3.40	1.45	1.39
3	E	4475	ADP	C5-C4	3.39	1.45	1.39
3	J	4480	ADP	C5-C4	3.39	1.45	1.39
3	L	4482	ADP	C2-N3	2.85	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4472	ADP	C2-N3	2.85	1.39	1.33
3	H	4478	ADP	C2-N3	2.84	1.39	1.33
3	K	4481	ADP	C2-N3	2.84	1.39	1.33
3	A	4471	ADP	C2-N3	2.83	1.39	1.33
3	I	4479	ADP	C2-N3	2.82	1.39	1.33
3	D	4474	ADP	C2-N3	2.82	1.38	1.33
3	E	4475	ADP	C2-N3	2.82	1.38	1.33
3	F	4476	ADP	C2-N3	2.81	1.38	1.33
3	C	4473	ADP	C2-N3	2.80	1.38	1.33
3	J	4480	ADP	C2-N3	2.80	1.38	1.33
3	G	4477	ADP	C2-N3	2.79	1.38	1.33
3	H	4478	ADP	C3'-C4'	-2.33	1.47	1.53
3	L	4482	ADP	C3'-C4'	-2.33	1.47	1.53
3	J	4480	ADP	C3'-C4'	-2.33	1.47	1.53
3	A	4471	ADP	C3'-C4'	-2.31	1.47	1.53
3	B	4472	ADP	C3'-C4'	-2.31	1.47	1.53
3	G	4477	ADP	C3'-C4'	-2.31	1.47	1.53
3	I	4479	ADP	C3'-C4'	-2.30	1.47	1.53
3	D	4474	ADP	C3'-C4'	-2.30	1.47	1.53
3	F	4476	ADP	C3'-C4'	-2.30	1.47	1.53
3	K	4481	ADP	C3'-C4'	-2.30	1.47	1.53
3	E	4475	ADP	C3'-C4'	-2.30	1.47	1.53
3	C	4473	ADP	C3'-C4'	-2.30	1.47	1.53
3	H	4478	ADP	PB-O1B	2.18	1.57	1.50
3	F	4476	ADP	PB-O1B	2.18	1.57	1.50
3	J	4480	ADP	PB-O1B	2.18	1.57	1.50
3	D	4474	ADP	PB-O1B	2.17	1.57	1.50
3	L	4482	ADP	PB-O1B	2.17	1.57	1.50
3	A	4471	ADP	PB-O1B	2.17	1.57	1.50
3	G	4477	ADP	PB-O1B	2.16	1.57	1.50
3	C	4473	ADP	PB-O1B	2.16	1.57	1.50
3	K	4481	ADP	PB-O1B	2.16	1.57	1.50
3	E	4475	ADP	PB-O1B	2.16	1.57	1.50
3	I	4479	ADP	PB-O1B	2.16	1.57	1.50
3	B	4472	ADP	PB-O1B	2.14	1.57	1.50
4	D	5903	PPQ	OTP-CP	-2.04	1.24	1.30
4	G	5906	PPQ	OTP-CP	-2.03	1.24	1.30
4	I	5908	PPQ	OTP-CP	-2.03	1.24	1.30
4	L	5911	PPQ	OTP-CP	-2.03	1.24	1.30
4	A	5900	PPQ	OTP-CP	-2.03	1.24	1.30
4	F	5905	PPQ	OTP-CP	-2.03	1.24	1.30
4	B	5901	PPQ	OTP-CP	-2.02	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5909	PPQ	OTP-CP	-2.02	1.24	1.30
4	K	5910	PPQ	OTP-CP	-2.02	1.24	1.30
4	C	5902	PPQ	OTP-CP	-2.01	1.24	1.30
4	E	5904	PPQ	OTP-CP	-2.01	1.24	1.30
4	H	5907	PPQ	OTP-CP	-2.00	1.24	1.30

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	5907	PPQ	PDP-CGP-CBP	9.93	132.71	114.53
4	G	5906	PPQ	PDP-CGP-CBP	9.93	132.71	114.53
4	F	5905	PPQ	PDP-CGP-CBP	9.92	132.70	114.53
4	I	5908	PPQ	PDP-CGP-CBP	9.92	132.70	114.53
4	E	5904	PPQ	PDP-CGP-CBP	9.91	132.68	114.53
4	L	5911	PPQ	PDP-CGP-CBP	9.91	132.67	114.53
4	A	5900	PPQ	PDP-CGP-CBP	9.90	132.67	114.53
4	B	5901	PPQ	PDP-CGP-CBP	9.90	132.66	114.53
4	D	5903	PPQ	PDP-CGP-CBP	9.90	132.66	114.53
4	C	5902	PPQ	PDP-CGP-CBP	9.89	132.65	114.53
4	K	5910	PPQ	PDP-CGP-CBP	9.89	132.63	114.53
4	J	5909	PPQ	PDP-CGP-CBP	9.88	132.63	114.53
3	I	4479	ADP	O5'-C5'-C4'	8.43	137.70	108.99
3	K	4481	ADP	O5'-C5'-C4'	8.43	137.70	108.99
3	L	4482	ADP	O5'-C5'-C4'	8.43	137.70	108.99
3	D	4474	ADP	O5'-C5'-C4'	8.43	137.69	108.99
3	A	4471	ADP	O5'-C5'-C4'	8.42	137.68	108.99
3	E	4475	ADP	O5'-C5'-C4'	8.42	137.68	108.99
3	F	4476	ADP	O5'-C5'-C4'	8.42	137.67	108.99
3	G	4477	ADP	O5'-C5'-C4'	8.42	137.67	108.99
3	H	4478	ADP	O5'-C5'-C4'	8.42	137.66	108.99
3	C	4473	ADP	O5'-C5'-C4'	8.42	137.65	108.99
3	J	4480	ADP	O5'-C5'-C4'	8.42	137.65	108.99
3	B	4472	ADP	O5'-C5'-C4'	8.41	137.63	108.99
3	J	4480	ADP	O4'-C1'-C2'	-7.24	91.13	106.62
3	L	4482	ADP	O4'-C1'-C2'	-7.24	91.13	106.62
3	C	4473	ADP	O4'-C1'-C2'	-7.23	91.14	106.62
3	B	4472	ADP	O4'-C1'-C2'	-7.23	91.15	106.62
3	D	4474	ADP	O4'-C1'-N9	7.23	121.97	108.09
3	A	4471	ADP	O4'-C1'-C2'	-7.23	91.15	106.62
3	K	4481	ADP	O4'-C1'-C2'	-7.23	91.15	106.62
3	D	4474	ADP	O4'-C1'-C2'	-7.23	91.15	106.62
3	G	4477	ADP	O4'-C1'-C2'	-7.23	91.15	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4472	ADP	O4'-C1'-N9	7.22	121.96	108.09
3	E	4475	ADP	O4'-C1'-C2'	-7.22	91.16	106.62
3	H	4478	ADP	O4'-C1'-C2'	-7.22	91.17	106.62
3	I	4479	ADP	O4'-C1'-C2'	-7.22	91.17	106.62
3	C	4473	ADP	O4'-C1'-N9	7.21	121.94	108.09
3	I	4479	ADP	O4'-C1'-N9	7.21	121.94	108.09
3	F	4476	ADP	O4'-C1'-C2'	-7.21	91.19	106.62
3	F	4476	ADP	O4'-C1'-N9	7.21	121.94	108.09
3	L	4482	ADP	O4'-C1'-N9	7.21	121.93	108.09
3	K	4481	ADP	O4'-C1'-N9	7.21	121.93	108.09
3	A	4471	ADP	O4'-C1'-N9	7.20	121.92	108.09
3	J	4480	ADP	O4'-C1'-N9	7.20	121.92	108.09
3	H	4478	ADP	O4'-C1'-N9	7.20	121.91	108.09
3	G	4477	ADP	O4'-C1'-N9	7.19	121.90	108.09
3	E	4475	ADP	O4'-C1'-N9	7.19	121.90	108.09
4	J	5909	PPQ	CEP-PDP-CGP	6.91	119.81	107.62
4	B	5901	PPQ	CEP-PDP-CGP	6.89	119.78	107.62
4	L	5911	PPQ	CEP-PDP-CGP	6.88	119.76	107.62
4	D	5903	PPQ	CEP-PDP-CGP	6.88	119.75	107.62
4	C	5902	PPQ	CEP-PDP-CGP	6.87	119.75	107.62
4	E	5904	PPQ	CEP-PDP-CGP	6.87	119.75	107.62
4	H	5907	PPQ	CEP-PDP-CGP	6.87	119.75	107.62
4	A	5900	PPQ	CEP-PDP-CGP	6.87	119.75	107.62
4	K	5910	PPQ	CEP-PDP-CGP	6.87	119.74	107.62
4	I	5908	PPQ	CEP-PDP-CGP	6.86	119.73	107.62
4	G	5906	PPQ	CEP-PDP-CGP	6.86	119.73	107.62
4	F	5905	PPQ	CEP-PDP-CGP	6.85	119.70	107.62
3	E	4475	ADP	C4-N9-C8	-5.72	99.73	105.74
3	K	4481	ADP	C4-N9-C8	-5.71	99.74	105.74
3	C	4473	ADP	C4-N9-C8	-5.70	99.75	105.74
3	J	4480	ADP	C4-N9-C8	-5.69	99.76	105.74
3	G	4477	ADP	C4-N9-C8	-5.69	99.76	105.74
3	I	4479	ADP	C4-N9-C8	-5.68	99.77	105.74
3	H	4478	ADP	C4-N9-C8	-5.68	99.78	105.74
3	A	4471	ADP	C4-N9-C8	-5.68	99.78	105.74
3	F	4476	ADP	C4-N9-C8	-5.67	99.78	105.74
3	B	4472	ADP	C4-N9-C8	-5.67	99.78	105.74
3	D	4474	ADP	C4-N9-C8	-5.67	99.79	105.74
3	L	4482	ADP	C4-N9-C8	-5.66	99.79	105.74
3	C	4473	ADP	C5'-C4'-C3'	-4.12	100.39	115.21
3	F	4476	ADP	C5'-C4'-C3'	-4.11	100.41	115.21
3	I	4479	ADP	C5'-C4'-C3'	-4.11	100.42	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	4480	ADP	C5'-C4'-C3'	-4.11	100.42	115.21
3	B	4472	ADP	C5'-C4'-C3'	-4.11	100.42	115.21
3	H	4478	ADP	C5'-C4'-C3'	-4.11	100.42	115.21
3	A	4471	ADP	C5'-C4'-C3'	-4.11	100.43	115.21
3	G	4477	ADP	C5'-C4'-C3'	-4.11	100.43	115.21
3	D	4474	ADP	C5'-C4'-C3'	-4.10	100.45	115.21
3	E	4475	ADP	C5'-C4'-C3'	-4.10	100.45	115.21
3	K	4481	ADP	C5'-C4'-C3'	-4.10	100.46	115.21
3	L	4482	ADP	C5'-C4'-C3'	-4.09	100.47	115.21
3	H	4478	ADP	C4'-O4'-C1'	-3.89	100.87	109.47
3	E	4475	ADP	C4'-O4'-C1'	-3.89	100.88	109.47
3	I	4479	ADP	C4'-O4'-C1'	-3.89	100.88	109.47
3	L	4482	ADP	C4'-O4'-C1'	-3.88	100.89	109.47
3	G	4477	ADP	C4'-O4'-C1'	-3.88	100.90	109.47
3	K	4481	ADP	C4'-O4'-C1'	-3.88	100.90	109.47
3	F	4476	ADP	C4'-O4'-C1'	-3.88	100.90	109.47
3	J	4480	ADP	C4'-O4'-C1'	-3.88	100.90	109.47
3	A	4471	ADP	C4'-O4'-C1'	-3.88	100.91	109.47
3	D	4474	ADP	C4'-O4'-C1'	-3.87	100.93	109.47
3	C	4473	ADP	C4'-O4'-C1'	-3.86	100.94	109.47
3	B	4472	ADP	C4'-O4'-C1'	-3.86	100.95	109.47
3	G	4477	ADP	C4-N9-C1'	3.81	135.53	126.63
3	E	4475	ADP	C4-N9-C1'	3.81	135.53	126.63
3	C	4473	ADP	C4-N9-C1'	3.81	135.53	126.63
3	E	4475	ADP	N9-C8-N7	3.80	119.33	113.94
3	B	4472	ADP	N9-C8-N7	3.80	119.33	113.94
3	K	4481	ADP	C4-N9-C1'	3.80	135.52	126.63
3	H	4478	ADP	N9-C8-N7	3.80	119.32	113.94
3	A	4471	ADP	C4-N9-C1'	3.79	135.50	126.63
3	J	4480	ADP	C4-N9-C1'	3.79	135.50	126.63
3	I	4479	ADP	N9-C8-N7	3.79	119.31	113.94
3	B	4472	ADP	C4-N9-C1'	3.79	135.50	126.63
3	L	4482	ADP	N9-C8-N7	3.79	119.31	113.94
3	K	4481	ADP	N9-C8-N7	3.79	119.31	113.94
3	L	4482	ADP	C4-N9-C1'	3.79	135.49	126.63
3	F	4476	ADP	C4-N9-C1'	3.79	135.48	126.63
3	H	4478	ADP	C4-N9-C1'	3.79	135.48	126.63
3	I	4479	ADP	C4-N9-C1'	3.79	135.48	126.63
3	J	4480	ADP	N9-C8-N7	3.78	119.30	113.94
3	D	4474	ADP	C4-N9-C1'	3.78	135.48	126.63
3	A	4471	ADP	N9-C8-N7	3.78	119.30	113.94
3	C	4473	ADP	N9-C8-N7	3.78	119.29	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4476	ADP	N9-C8-N7	3.77	119.29	113.94
3	G	4477	ADP	N9-C8-N7	3.77	119.28	113.94
3	D	4474	ADP	N9-C8-N7	3.76	119.28	113.94
3	J	4480	ADP	O4'-C4'-C5'	3.75	121.36	109.33
3	B	4472	ADP	O4'-C4'-C5'	3.75	121.35	109.33
3	G	4477	ADP	O4'-C4'-C5'	3.75	121.35	109.33
3	E	4475	ADP	O4'-C4'-C5'	3.75	121.35	109.33
3	F	4476	ADP	O4'-C4'-C5'	3.75	121.34	109.33
3	H	4478	ADP	O4'-C4'-C5'	3.75	121.33	109.33
3	K	4481	ADP	O4'-C4'-C5'	3.75	121.33	109.33
3	A	4471	ADP	O4'-C4'-C5'	3.75	121.33	109.33
3	D	4474	ADP	O4'-C4'-C5'	3.75	121.33	109.33
3	C	4473	ADP	O4'-C4'-C5'	3.74	121.31	109.33
3	L	4482	ADP	O4'-C4'-C5'	3.74	121.31	109.33
3	I	4479	ADP	O4'-C4'-C5'	3.72	121.26	109.33
3	L	4482	ADP	C4-C5-N7	3.35	114.41	110.58
3	K	4481	ADP	C4-C5-N7	3.35	114.41	110.58
3	B	4472	ADP	C4-C5-N7	3.34	114.40	110.58
3	G	4477	ADP	C4-C5-N7	3.33	114.39	110.58
3	A	4471	ADP	C4-C5-N7	3.31	114.37	110.58
3	C	4473	ADP	C4-C5-N7	3.31	114.37	110.58
3	I	4479	ADP	C4-C5-N7	3.30	114.36	110.58
3	J	4480	ADP	C4-C5-N7	3.29	114.34	110.58
3	F	4476	ADP	C4-C5-N7	3.28	114.34	110.58
3	H	4478	ADP	C4-C5-N7	3.28	114.33	110.58
3	B	4472	ADP	PA-O5'-C5'	3.28	140.12	121.35
3	I	4479	ADP	PA-O5'-C5'	3.27	140.11	121.35
3	K	4481	ADP	PA-O5'-C5'	3.27	140.11	121.35
3	L	4482	ADP	PA-O5'-C5'	3.27	140.10	121.35
3	C	4473	ADP	PA-O5'-C5'	3.27	140.10	121.35
3	D	4474	ADP	C4-C5-N7	3.27	114.32	110.58
3	E	4475	ADP	C4-C5-N7	3.27	114.32	110.58
3	D	4474	ADP	PA-O5'-C5'	3.27	140.09	121.35
3	A	4471	ADP	PA-O5'-C5'	3.27	140.08	121.35
3	J	4480	ADP	PA-O5'-C5'	3.27	140.07	121.35
3	G	4477	ADP	PA-O5'-C5'	3.27	140.07	121.35
3	H	4478	ADP	PA-O5'-C5'	3.27	140.06	121.35
3	F	4476	ADP	PA-O5'-C5'	3.27	140.06	121.35
3	E	4475	ADP	PA-O5'-C5'	3.26	140.05	121.35
3	H	4478	ADP	C3'-C2'-C1'	-3.18	95.45	101.46
3	E	4475	ADP	C3'-C2'-C1'	-3.18	95.45	101.46
3	K	4481	ADP	C3'-C2'-C1'	-3.17	95.47	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4476	ADP	C3'-C2'-C1'	-3.16	95.48	101.46
3	D	4474	ADP	C3'-C2'-C1'	-3.16	95.49	101.46
3	A	4471	ADP	C3'-C2'-C1'	-3.16	95.49	101.46
3	B	4472	ADP	C3'-C2'-C1'	-3.16	95.49	101.46
3	G	4477	ADP	C3'-C2'-C1'	-3.16	95.49	101.46
3	J	4480	ADP	C3'-C2'-C1'	-3.15	95.50	101.46
3	C	4473	ADP	C3'-C2'-C1'	-3.15	95.51	101.46
3	I	4479	ADP	C3'-C2'-C1'	-3.15	95.51	101.46
3	L	4482	ADP	C3'-C2'-C1'	-3.14	95.52	101.46
3	K	4481	ADP	O2B-PB-O3A	3.01	114.71	104.64
3	J	4480	ADP	O2B-PB-O3A	3.00	114.70	104.64
3	C	4473	ADP	O2B-PB-O3A	3.00	114.68	104.64
3	I	4479	ADP	O2B-PB-O3A	2.99	114.68	104.64
3	H	4478	ADP	O2B-PB-O3A	2.99	114.68	104.64
3	F	4476	ADP	O2B-PB-O3A	2.99	114.67	104.64
3	L	4482	ADP	O2B-PB-O3A	2.99	114.66	104.64
3	E	4475	ADP	O2B-PB-O3A	2.99	114.66	104.64
3	A	4471	ADP	O2B-PB-O3A	2.99	114.66	104.64
3	B	4472	ADP	O2B-PB-O3A	2.99	114.65	104.64
3	D	4474	ADP	O2B-PB-O3A	2.98	114.63	104.64
3	F	4476	ADP	O2'-C2'-C1'	2.98	120.36	110.10
3	G	4477	ADP	O2B-PB-O3A	2.97	114.61	104.64
3	I	4479	ADP	O2'-C2'-C1'	2.97	120.33	110.10
3	D	4474	ADP	O2'-C2'-C1'	2.97	120.33	110.10
3	A	4471	ADP	O2'-C2'-C1'	2.97	120.33	110.10
3	C	4473	ADP	O2'-C2'-C1'	2.97	120.32	110.10
3	G	4477	ADP	O2'-C2'-C1'	2.96	120.31	110.10
3	H	4478	ADP	O2'-C2'-C1'	2.96	120.31	110.10
3	B	4472	ADP	O2'-C2'-C1'	2.96	120.31	110.10
3	K	4481	ADP	O2'-C2'-C1'	2.96	120.30	110.10
3	E	4475	ADP	O2'-C2'-C1'	2.96	120.29	110.10
3	J	4480	ADP	O2'-C2'-C1'	2.96	120.28	110.10
3	L	4482	ADP	O2'-C2'-C1'	2.95	120.27	110.10
3	E	4475	ADP	O3'-C3'-C2'	2.54	119.97	111.82
3	J	4480	ADP	O3'-C3'-C2'	2.54	119.97	111.82
3	B	4472	ADP	O3'-C3'-C2'	2.54	119.97	111.82
3	H	4478	ADP	O3'-C3'-C2'	2.54	119.97	111.82
3	D	4474	ADP	O3'-C3'-C2'	2.54	119.94	111.82
3	K	4481	ADP	O3'-C3'-C2'	2.53	119.94	111.82
3	L	4482	ADP	O3'-C3'-C2'	2.53	119.94	111.82
3	G	4477	ADP	O3'-C3'-C2'	2.53	119.94	111.82
3	C	4473	ADP	O3'-C3'-C2'	2.53	119.94	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4471	ADP	O3'-C3'-C2'	2.53	119.94	111.82
3	F	4476	ADP	O3'-C3'-C2'	2.53	119.93	111.82
3	I	4479	ADP	O3'-C3'-C2'	2.52	119.91	111.82
3	J	4480	ADP	C5-C4-N3	-2.25	123.62	126.72
3	D	4474	ADP	C5-C4-N3	-2.24	123.63	126.72
3	F	4476	ADP	C5-C4-N3	-2.24	123.64	126.72
3	E	4475	ADP	C5-C4-N3	-2.23	123.65	126.72
3	C	4473	ADP	C5-C4-N3	-2.22	123.65	126.72
3	A	4471	ADP	C5-C4-N3	-2.22	123.66	126.72
3	I	4479	ADP	C5-C4-N3	-2.22	123.66	126.72
3	G	4477	ADP	C5-C4-N3	-2.21	123.67	126.72
3	B	4472	ADP	C5-C4-N3	-2.21	123.68	126.72
3	H	4478	ADP	C5-C4-N3	-2.20	123.69	126.72
3	L	4482	ADP	C5-C4-N3	-2.19	123.69	126.72
3	K	4481	ADP	C5-C4-N3	-2.19	123.70	126.72
3	K	4481	ADP	C5-C6-N6	-2.07	118.16	123.29
3	B	4472	ADP	C5-C6-N6	-2.06	118.18	123.29
3	C	4473	ADP	C5-C6-N6	-2.06	118.19	123.29
3	L	4482	ADP	C5-C6-N6	-2.05	118.20	123.29
3	G	4477	ADP	C5-C6-N6	-2.05	118.21	123.29
3	H	4478	ADP	C5-C6-N6	-2.05	118.21	123.29
3	A	4471	ADP	C5-C6-N6	-2.05	118.22	123.29
3	I	4479	ADP	C5-C6-N6	-2.05	118.22	123.29
3	H	4478	ADP	O5'-PA-O1A	-2.04	100.86	108.94
3	G	4477	ADP	O5'-PA-O1A	-2.04	100.86	108.94
3	J	4480	ADP	C5-C6-N6	-2.04	118.24	123.29
3	D	4474	ADP	C5-C6-N6	-2.04	118.25	123.29
3	K	4481	ADP	O5'-PA-O1A	-2.03	100.88	108.94
3	E	4475	ADP	O5'-PA-O1A	-2.03	100.88	108.94
3	F	4476	ADP	O5'-PA-O1A	-2.03	100.89	108.94
3	A	4471	ADP	O5'-PA-O1A	-2.03	100.89	108.94
3	F	4476	ADP	C5-C6-N6	-2.03	118.26	123.29
3	L	4482	ADP	O5'-PA-O1A	-2.03	100.89	108.94
3	J	4480	ADP	O5'-PA-O1A	-2.03	100.90	108.94
3	E	4475	ADP	C5-C6-N6	-2.03	118.27	123.29
3	D	4474	ADP	O5'-PA-O1A	-2.03	100.91	108.94
3	C	4473	ADP	O5'-PA-O1A	-2.02	100.92	108.94
3	B	4472	ADP	O5'-PA-O1A	-2.02	100.92	108.94
3	I	4479	ADP	O5'-PA-O1A	-2.02	100.93	108.94

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4471	ADP	C5'-O5'-PA-O1A
3	A	4471	ADP	C5'-O5'-PA-O2A
3	A	4471	ADP	C5'-O5'-PA-O3A
3	B	4472	ADP	C5'-O5'-PA-O1A
3	B	4472	ADP	C5'-O5'-PA-O2A
3	B	4472	ADP	C5'-O5'-PA-O3A
3	C	4473	ADP	C5'-O5'-PA-O1A
3	C	4473	ADP	C5'-O5'-PA-O2A
3	C	4473	ADP	C5'-O5'-PA-O3A
3	D	4474	ADP	C5'-O5'-PA-O1A
3	D	4474	ADP	C5'-O5'-PA-O2A
3	D	4474	ADP	C5'-O5'-PA-O3A
3	E	4475	ADP	C5'-O5'-PA-O1A
3	E	4475	ADP	C5'-O5'-PA-O2A
3	E	4475	ADP	C5'-O5'-PA-O3A
3	F	4476	ADP	C5'-O5'-PA-O1A
3	F	4476	ADP	C5'-O5'-PA-O2A
3	F	4476	ADP	C5'-O5'-PA-O3A
3	G	4477	ADP	C5'-O5'-PA-O1A
3	G	4477	ADP	C5'-O5'-PA-O2A
3	G	4477	ADP	C5'-O5'-PA-O3A
3	H	4478	ADP	C5'-O5'-PA-O1A
3	H	4478	ADP	C5'-O5'-PA-O2A
3	H	4478	ADP	C5'-O5'-PA-O3A
3	I	4479	ADP	C5'-O5'-PA-O1A
3	I	4479	ADP	C5'-O5'-PA-O2A
3	I	4479	ADP	C5'-O5'-PA-O3A
3	J	4480	ADP	C5'-O5'-PA-O1A
3	J	4480	ADP	C5'-O5'-PA-O2A
3	J	4480	ADP	C5'-O5'-PA-O3A
3	K	4481	ADP	C5'-O5'-PA-O1A
3	K	4481	ADP	C5'-O5'-PA-O2A
3	K	4481	ADP	C5'-O5'-PA-O3A
3	L	4482	ADP	C5'-O5'-PA-O1A
3	L	4482	ADP	C5'-O5'-PA-O2A
3	L	4482	ADP	C5'-O5'-PA-O3A
4	A	5900	PPQ	CBP-CGP-PDP-CEP
4	A	5900	PPQ	CBP-CGP-PDP-OEA
4	A	5900	PPQ	CBP-CGP-PDP-OEB
4	B	5901	PPQ	CBP-CGP-PDP-CEP
4	B	5901	PPQ	CBP-CGP-PDP-OEA
4	B	5901	PPQ	CBP-CGP-PDP-OEB
4	C	5902	PPQ	CBP-CGP-PDP-CEP

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Mol	Chain	Res	Type	Atoms
4	C	5902	PPQ	CBP-CGP-PDP-OEA
4	C	5902	PPQ	CBP-CGP-PDP-OEB
4	D	5903	PPQ	CBP-CGP-PDP-CEP
4	D	5903	PPQ	CBP-CGP-PDP-OEA
4	D	5903	PPQ	CBP-CGP-PDP-OEB
4	E	5904	PPQ	CBP-CGP-PDP-CEP
4	E	5904	PPQ	CBP-CGP-PDP-OEA
4	E	5904	PPQ	CBP-CGP-PDP-OEB
4	F	5905	PPQ	CBP-CGP-PDP-CEP
4	F	5905	PPQ	CBP-CGP-PDP-OEA
4	F	5905	PPQ	CBP-CGP-PDP-OEB
4	G	5906	PPQ	CBP-CGP-PDP-CEP
4	G	5906	PPQ	CBP-CGP-PDP-OEA
4	G	5906	PPQ	CBP-CGP-PDP-OEB
4	H	5907	PPQ	CBP-CGP-PDP-CEP
4	H	5907	PPQ	CBP-CGP-PDP-OEA
4	H	5907	PPQ	CBP-CGP-PDP-OEB
4	I	5908	PPQ	CBP-CGP-PDP-CEP
4	I	5908	PPQ	CBP-CGP-PDP-OEA
4	I	5908	PPQ	CBP-CGP-PDP-OEB
4	J	5909	PPQ	CBP-CGP-PDP-CEP
4	J	5909	PPQ	CBP-CGP-PDP-OEA
4	J	5909	PPQ	CBP-CGP-PDP-OEB
4	K	5910	PPQ	CBP-CGP-PDP-CEP
4	K	5910	PPQ	CBP-CGP-PDP-OEA
4	K	5910	PPQ	CBP-CGP-PDP-OEB
4	L	5911	PPQ	CBP-CGP-PDP-CEP
4	L	5911	PPQ	CBP-CGP-PDP-OEA
4	L	5911	PPQ	CBP-CGP-PDP-OEB
4	A	5900	PPQ	NP-CAP-CP-OTP
4	B	5901	PPQ	NP-CAP-CP-OTP
4	C	5902	PPQ	NP-CAP-CP-OTP
4	D	5903	PPQ	NP-CAP-CP-OTP
4	E	5904	PPQ	NP-CAP-CP-OTP
4	F	5905	PPQ	NP-CAP-CP-OTP
4	G	5906	PPQ	NP-CAP-CP-OTP
4	H	5907	PPQ	NP-CAP-CP-OTP
4	I	5908	PPQ	NP-CAP-CP-OTP
4	J	5909	PPQ	NP-CAP-CP-OTP
4	K	5910	PPQ	NP-CAP-CP-OTP
4	L	5911	PPQ	NP-CAP-CP-OTP
3	A	4471	ADP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	B	4472	ADP	C4'-C5'-O5'-PA
3	C	4473	ADP	C4'-C5'-O5'-PA
3	D	4474	ADP	C4'-C5'-O5'-PA
3	E	4475	ADP	C4'-C5'-O5'-PA
3	F	4476	ADP	C4'-C5'-O5'-PA
3	G	4477	ADP	C4'-C5'-O5'-PA
3	H	4478	ADP	C4'-C5'-O5'-PA
3	I	4479	ADP	C4'-C5'-O5'-PA
3	J	4480	ADP	C4'-C5'-O5'-PA
3	K	4481	ADP	C4'-C5'-O5'-PA
3	L	4482	ADP	C4'-C5'-O5'-PA
3	A	4471	ADP	PA-O3A-PB-O3B
3	B	4472	ADP	PA-O3A-PB-O3B
3	C	4473	ADP	PA-O3A-PB-O3B
3	D	4474	ADP	PA-O3A-PB-O3B
3	E	4475	ADP	PA-O3A-PB-O3B
3	F	4476	ADP	PA-O3A-PB-O3B
3	G	4477	ADP	PA-O3A-PB-O3B
3	H	4478	ADP	PA-O3A-PB-O3B
3	I	4479	ADP	PA-O3A-PB-O3B
3	J	4480	ADP	PA-O3A-PB-O3B
3	K	4481	ADP	PA-O3A-PB-O3B
3	L	4482	ADP	PA-O3A-PB-O3B
4	A	5900	PPQ	CBP-CAP-CP-OTP
4	B	5901	PPQ	CBP-CAP-CP-OTP
4	C	5902	PPQ	CBP-CAP-CP-OTP
4	D	5903	PPQ	CBP-CAP-CP-OTP
4	E	5904	PPQ	CBP-CAP-CP-OTP
4	F	5905	PPQ	CBP-CAP-CP-OTP
4	G	5906	PPQ	CBP-CAP-CP-OTP
4	H	5907	PPQ	CBP-CAP-CP-OTP
4	I	5908	PPQ	CBP-CAP-CP-OTP
4	J	5909	PPQ	CBP-CAP-CP-OTP
4	K	5910	PPQ	CBP-CAP-CP-OTP
4	L	5911	PPQ	CBP-CAP-CP-OTP
4	A	5900	PPQ	CBP-CAP-CP-OP
4	B	5901	PPQ	CBP-CAP-CP-OP
4	C	5902	PPQ	CBP-CAP-CP-OP
4	D	5903	PPQ	CBP-CAP-CP-OP
4	E	5904	PPQ	CBP-CAP-CP-OP
4	F	5905	PPQ	CBP-CAP-CP-OP
4	G	5906	PPQ	CBP-CAP-CP-OP

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Mol	Chain	Res	Type	Atoms
4	H	5907	PPQ	CBP-CAP-CP-OP
4	I	5908	PPQ	CBP-CAP-CP-OP
4	J	5909	PPQ	CBP-CAP-CP-OP
4	K	5910	PPQ	CBP-CAP-CP-OP
4	L	5911	PPQ	CBP-CAP-CP-OP
3	A	4471	ADP	C2'-C1'-N9-C8
3	B	4472	ADP	C2'-C1'-N9-C8
3	C	4473	ADP	C2'-C1'-N9-C8
3	D	4474	ADP	C2'-C1'-N9-C8
3	E	4475	ADP	C2'-C1'-N9-C8
3	F	4476	ADP	C2'-C1'-N9-C8
3	G	4477	ADP	C2'-C1'-N9-C8
3	H	4478	ADP	C2'-C1'-N9-C8
3	I	4479	ADP	C2'-C1'-N9-C8
3	J	4480	ADP	C2'-C1'-N9-C8
3	K	4481	ADP	C2'-C1'-N9-C8
3	L	4482	ADP	C2'-C1'-N9-C8
3	A	4471	ADP	O4'-C1'-N9-C8
3	B	4472	ADP	O4'-C1'-N9-C8
3	C	4473	ADP	O4'-C1'-N9-C8
3	D	4474	ADP	O4'-C1'-N9-C8
3	E	4475	ADP	O4'-C1'-N9-C8
3	F	4476	ADP	O4'-C1'-N9-C8
3	G	4477	ADP	O4'-C1'-N9-C8
3	H	4478	ADP	O4'-C1'-N9-C8
3	I	4479	ADP	O4'-C1'-N9-C8
3	J	4480	ADP	O4'-C1'-N9-C8
3	K	4481	ADP	O4'-C1'-N9-C8
3	L	4482	ADP	O4'-C1'-N9-C8

There are no ring outliers.

24 monomers are involved in 172 short contacts:

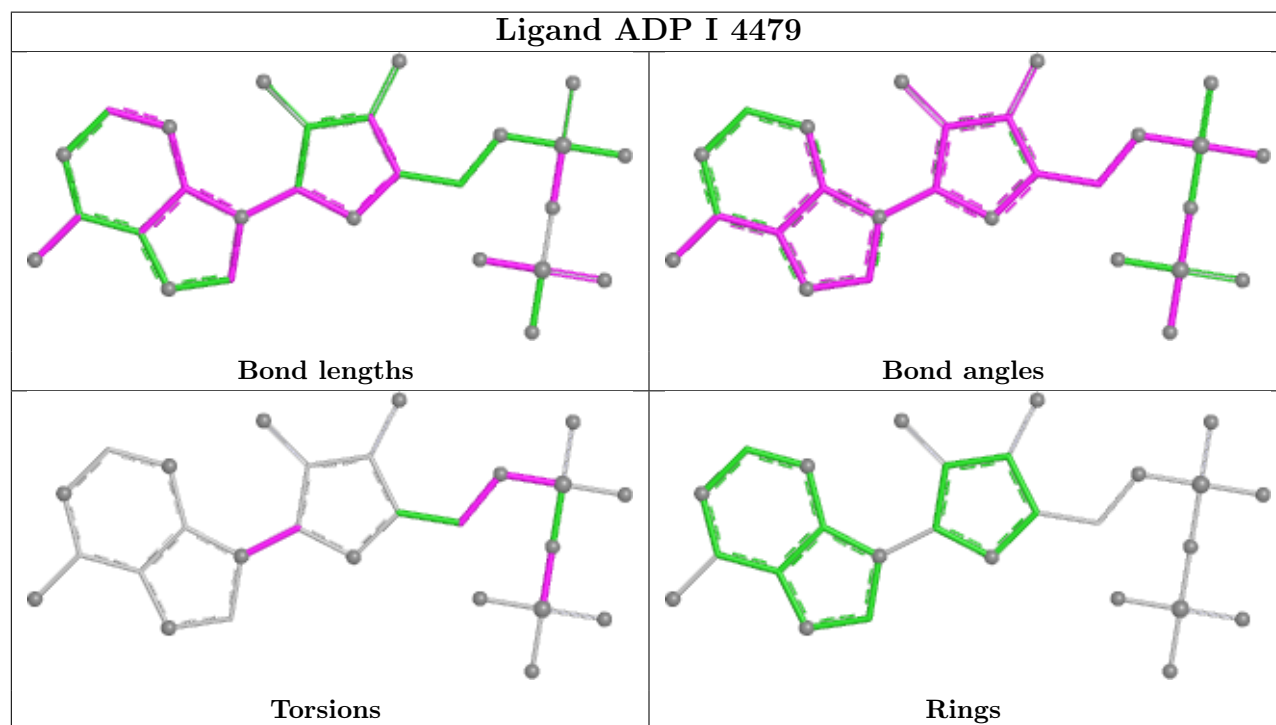
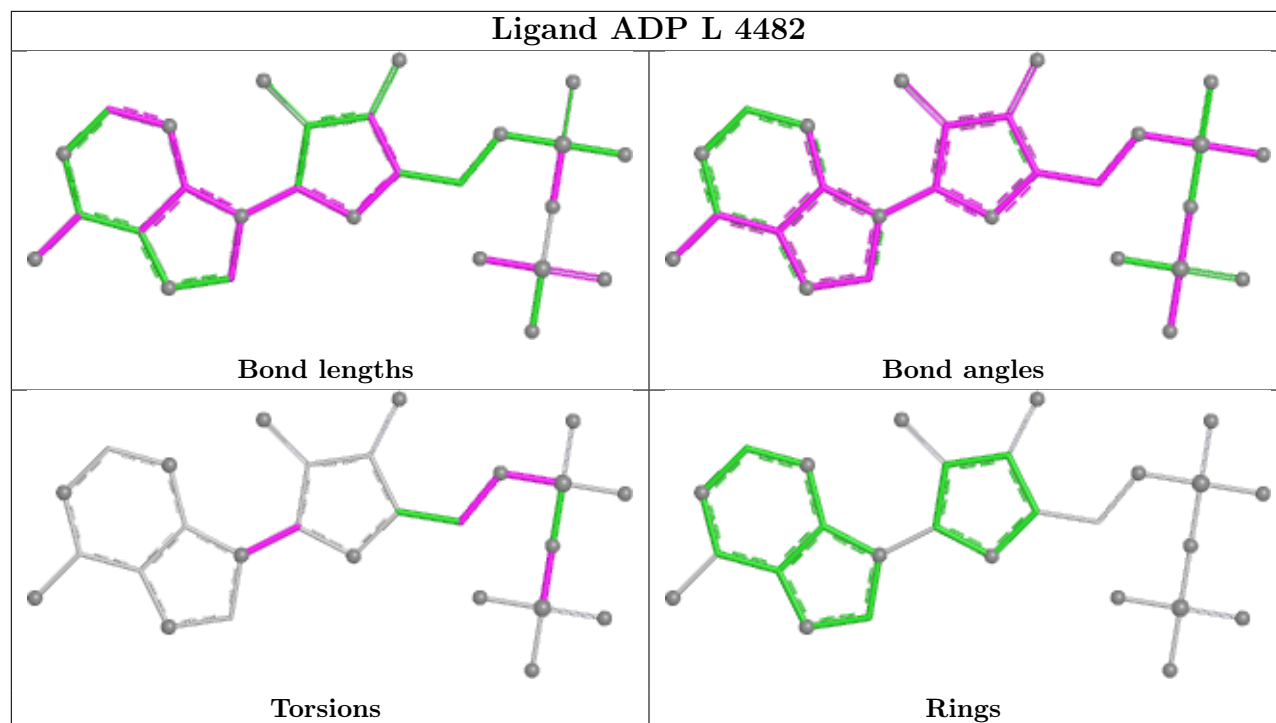
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	4482	ADP	8	0
4	K	5910	PPQ	5	0
3	I	4479	ADP	8	0
4	J	5909	PPQ	6	0
4	C	5902	PPQ	6	0
3	B	4472	ADP	8	0
3	K	4481	ADP	8	0
4	B	5901	PPQ	7	0

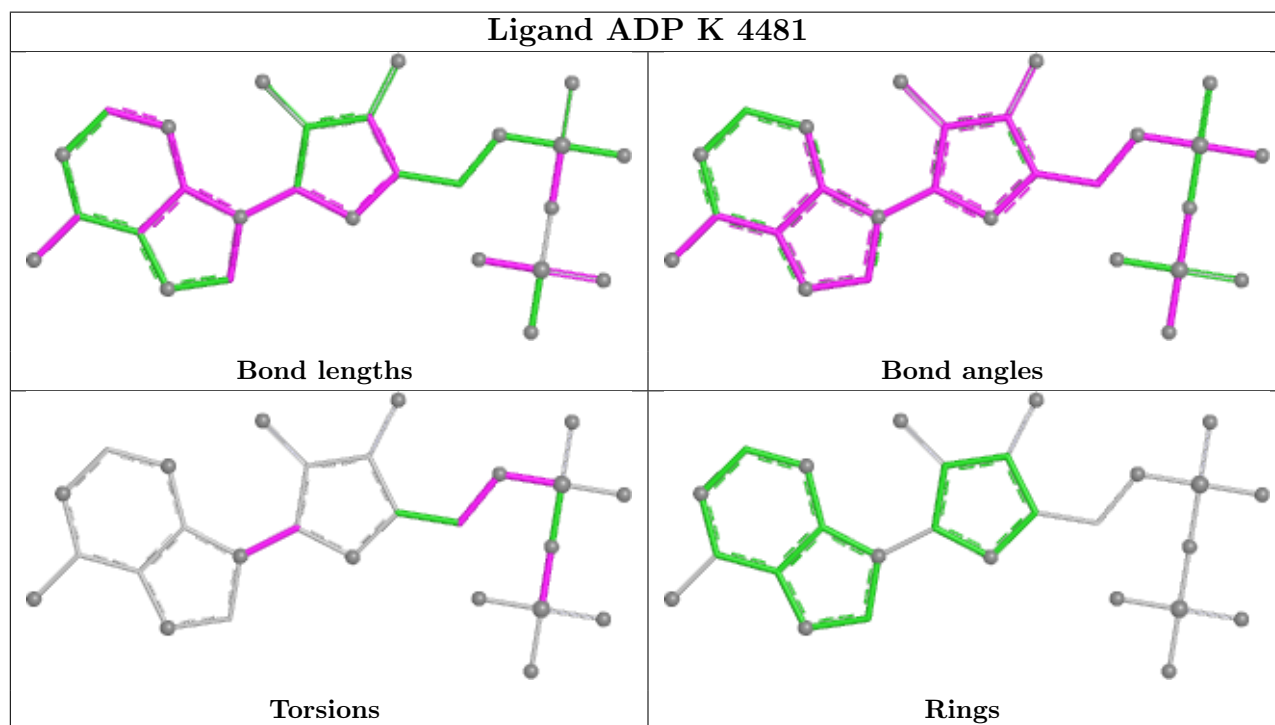
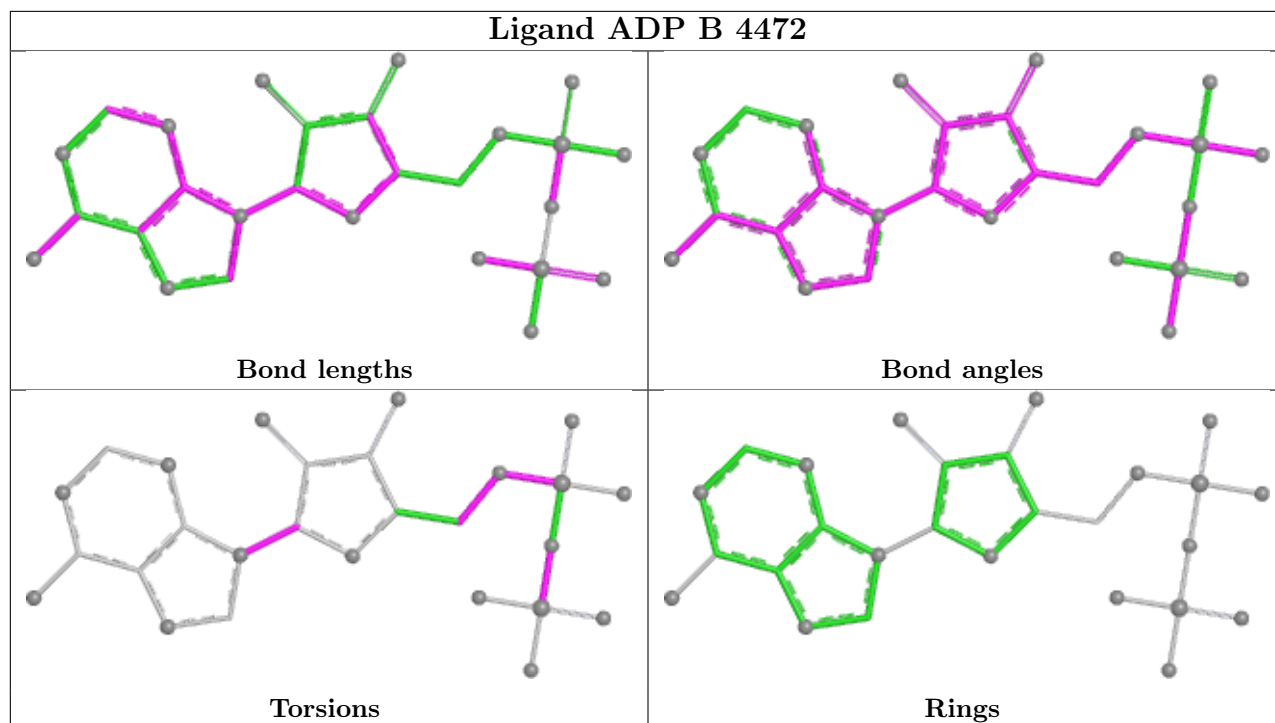
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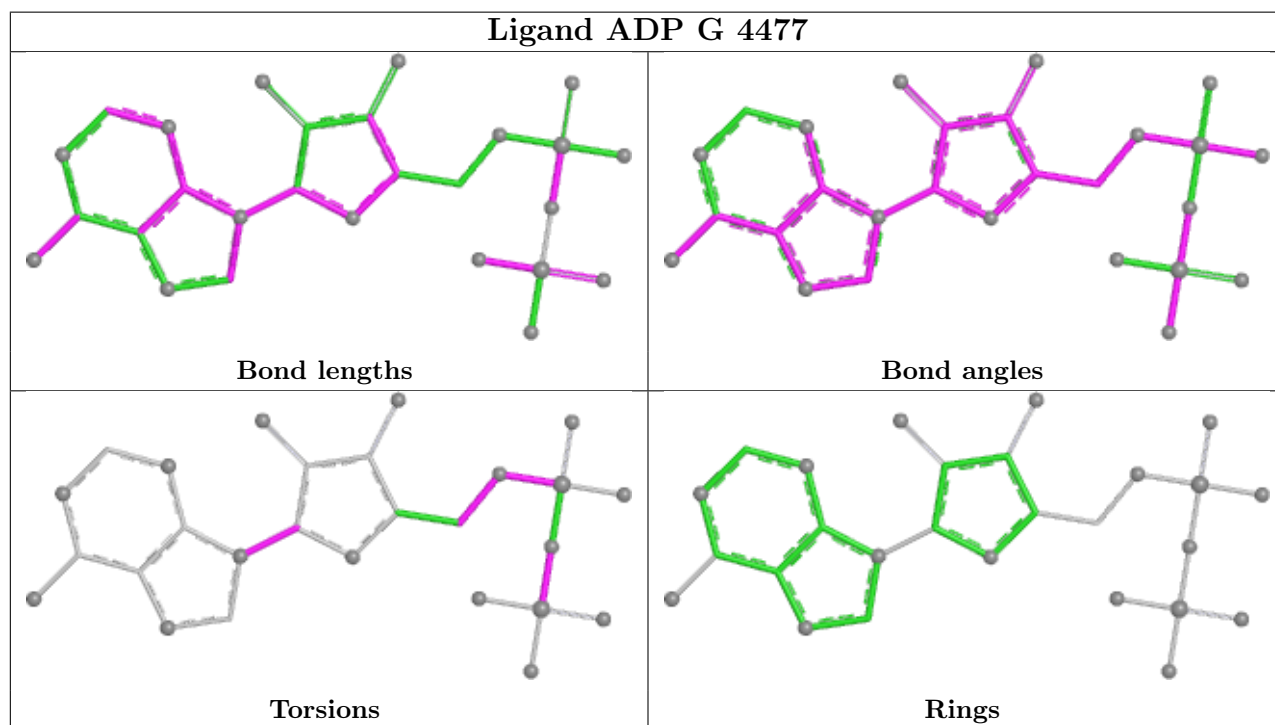
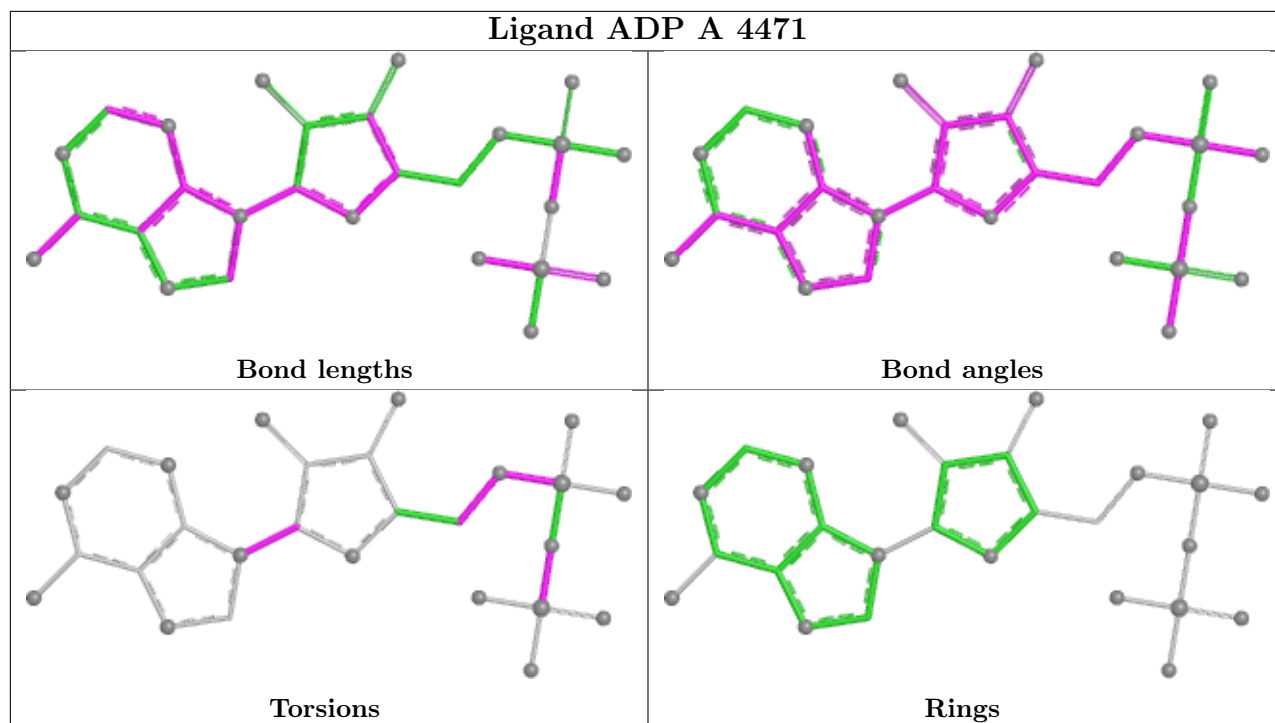
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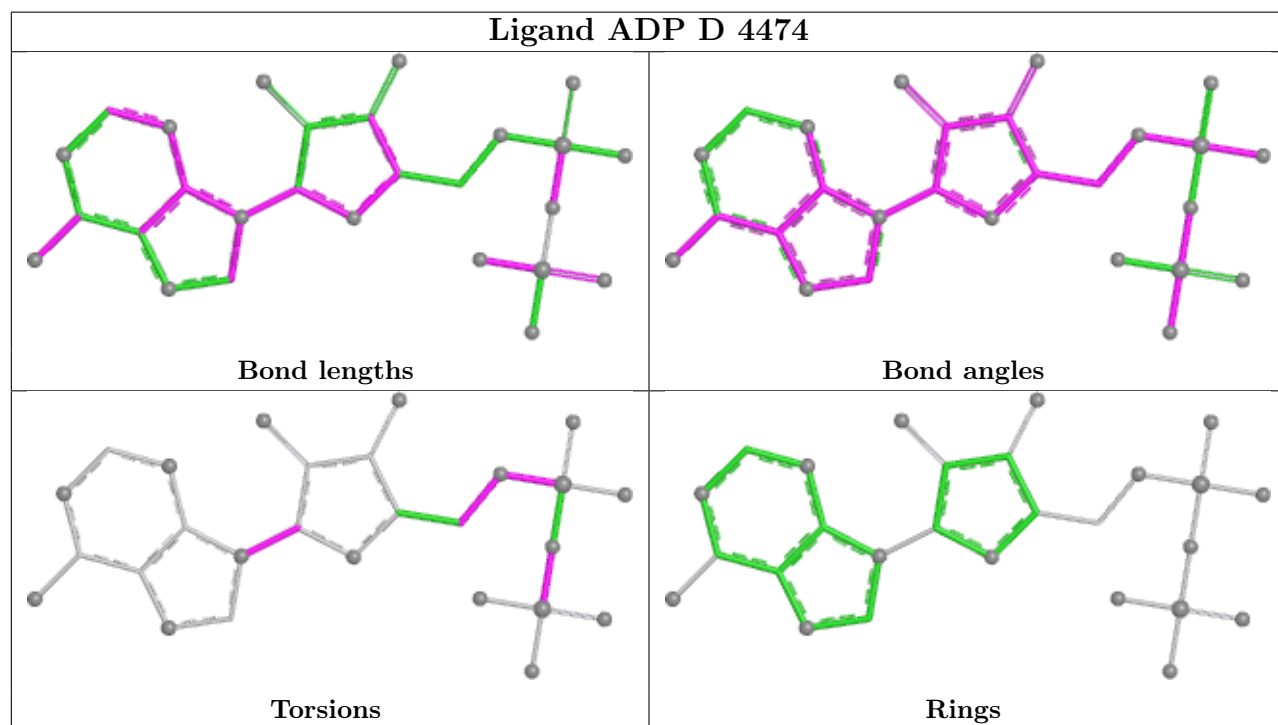
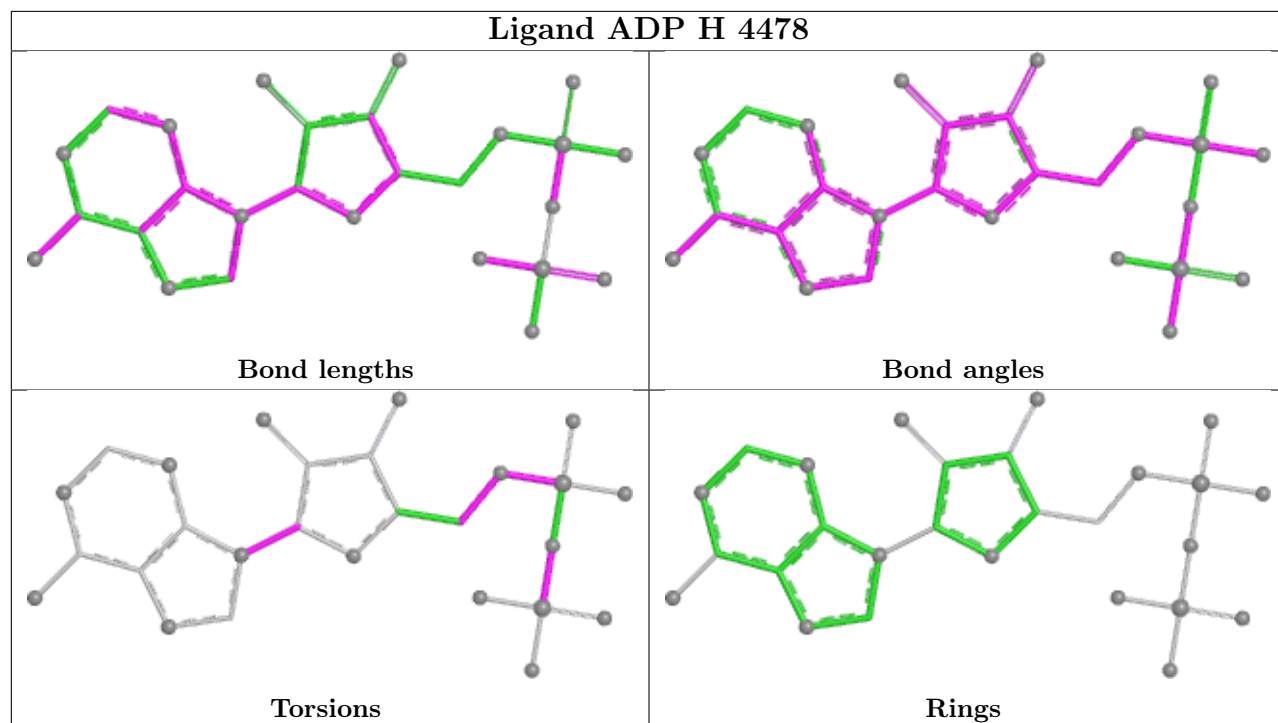
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4471	ADP	8	0
4	H	5907	PPQ	7	0
4	F	5905	PPQ	7	0
4	I	5908	PPQ	6	0
3	G	4477	ADP	8	0
3	H	4478	ADP	8	0
4	E	5904	PPQ	6	0
3	D	4474	ADP	8	0
4	D	5903	PPQ	6	0
4	A	5900	PPQ	7	0
4	L	5911	PPQ	7	0
4	G	5906	PPQ	6	0
3	J	4480	ADP	8	0
3	C	4473	ADP	8	0
3	F	4476	ADP	8	0
3	E	4475	ADP	8	0

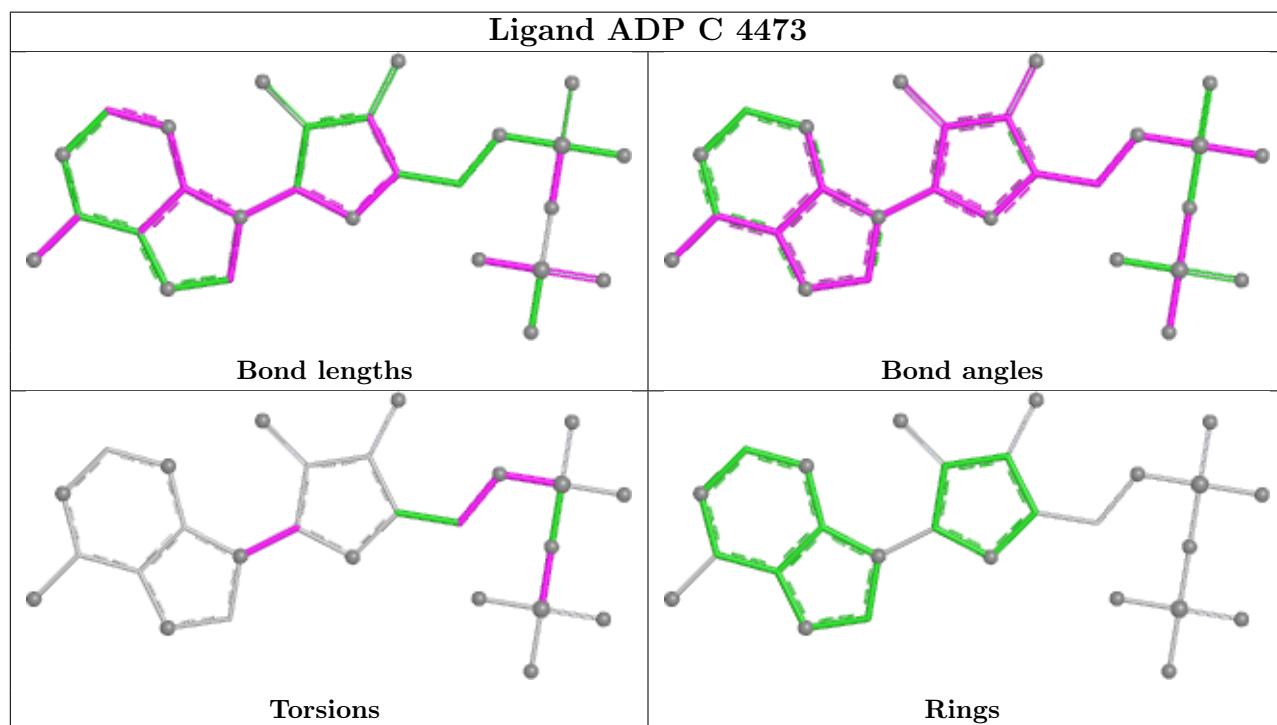
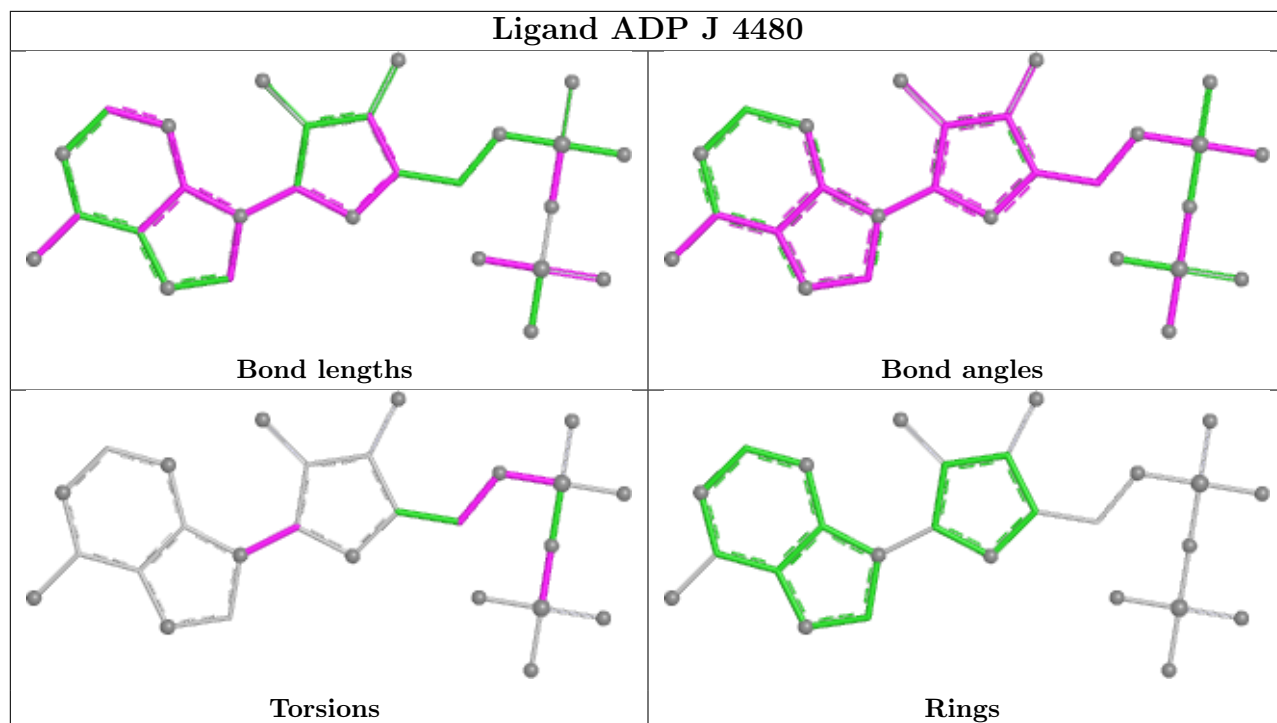
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

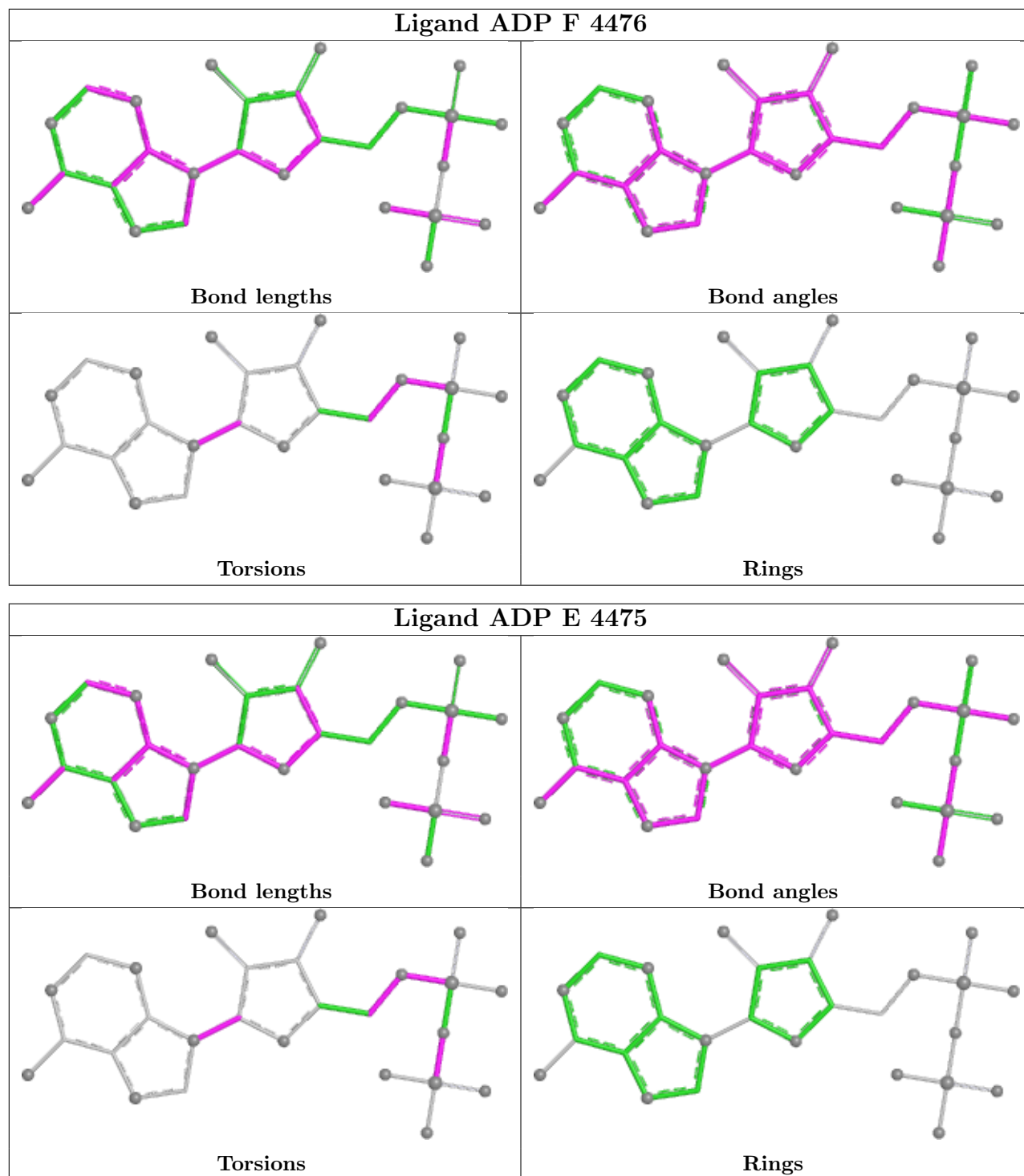












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	468/468 (100%)	0.70	40 (8%) 16 14	12, 44, 74, 100	108 (23%)
1	B	468/468 (100%)	0.45	28 (5%) 27 21	12, 44, 74, 100	108 (23%)
1	C	468/468 (100%)	0.38	19 (4%) 41 33	12, 44, 74, 100	108 (23%)
1	D	468/468 (100%)	0.30	21 (4%) 38 30	12, 44, 74, 100	108 (23%)
1	E	468/468 (100%)	0.38	15 (3%) 50 41	12, 44, 74, 100	108 (23%)
1	F	468/468 (100%)	0.40	19 (4%) 41 33	12, 44, 74, 100	108 (23%)
1	G	468/468 (100%)	0.33	16 (3%) 48 39	12, 44, 74, 100	108 (23%)
1	H	468/468 (100%)	0.38	26 (5%) 30 23	12, 44, 74, 100	108 (23%)
1	I	468/468 (100%)	0.32	19 (4%) 41 33	12, 44, 74, 100	108 (23%)
1	J	468/468 (100%)	0.44	26 (5%) 30 23	12, 44, 74, 100	108 (23%)
1	K	468/468 (100%)	0.38	18 (3%) 44 36	12, 44, 74, 100	108 (23%)
1	L	468/468 (100%)	0.44	27 (5%) 29 22	12, 44, 74, 100	108 (23%)
All	All	5616/5616 (100%)	0.41	274 (4%) 35 27	12, 44, 74, 100	1296 (23%)

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264[A]	ASN	9.1
1	G	264[A]	ASN	8.8
1	I	264[A]	ASN	8.7
1	D	264[A]	ASN	7.2
1	L	264[A]	ASN	6.6
1	A	264[A]	ASN	6.6
1	E	264[A]	ASN	5.7
1	F	264[A]	ASN	5.6
1	J	264[A]	ASN	5.3
1	H	264[A]	ASN	5.3
1	J	1	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	H	11	GLU	5.0
1	J	328	ALA	5.0
1	K	396	LEU	5.0
1	H	4	HIS	4.9
1	A	378	GLY	4.8
1	F	59	GLY	4.5
1	L	405	LYS	4.4
1	I	278	GLY	4.3
1	K	264[A]	ASN	4.3
1	J	63	SER	4.3
1	C	264[A]	ASN	4.2
1	C	393	ASP	4.2
1	A	404	ALA	4.0
1	G	63	SER	4.0
1	H	1	SER	4.0
1	L	1	SER	4.0
1	H	59	GLY	3.8
1	G	1	SER	3.8
1	C	4	HIS	3.8
1	B	404	ALA	3.8
1	A	112	GLU	3.7
1	J	337	ARG	3.6
1	L	396	LEU	3.6
1	K	1	SER	3.6
1	E	59	GLY	3.6
1	K	403	GLU	3.5
1	G	399	LEU	3.5
1	F	265[A]	GLY	3.5
1	A	403	GLU	3.5
1	I	63	SER	3.5
1	G	93	GLU	3.4
1	A	277	ASN	3.4
1	D	329	PRO	3.4
1	I	64	ASP	3.4
1	K	60	ILE	3.4
1	K	284	GLY	3.4
1	H	61	ASN	3.3
1	F	404	ALA	3.3
1	K	397	TYR	3.3
1	A	275	ALA	3.3
1	I	405	LYS	3.2
1	B	437	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	396	LEU	3.2
1	B	2	ALA	3.1
1	B	178[A]	GLY	3.1
1	C	59	GLY	3.1
1	B	400	PRO	3.1
1	J	278	GLY	3.1
1	A	279	THR	3.1
1	A	273	SER	3.0
1	D	59	GLY	3.0
1	I	55	GLY	3.0
1	I	178[A]	GLY	3.0
1	K	167	GLY	3.0
1	A	351	PRO	3.0
1	J	406	GLU	3.0
1	C	7	THR	3.0
1	F	60	ILE	3.0
1	H	344	ARG	3.0
1	C	61	ASN	3.0
1	F	393	ASP	3.0
1	A	253	ALA	3.0
1	H	337	ARG	3.0
1	A	278	GLY	3.0
1	K	61	ASN	3.0
1	B	381	GLY	2.9
1	D	1	SER	2.9
1	C	121	ALA	2.9
1	F	305	ALA	2.9
1	E	63	SER	2.9
1	E	404	ALA	2.9
1	H	60	ILE	2.9
1	F	98	GLN	2.8
1	D	63	SER	2.8
1	G	170	GLY	2.8
1	H	381	GLY	2.8
1	A	391	PRO	2.8
1	A	41	GLU	2.8
1	L	339	ARG	2.8
1	K	398	ASP	2.8
1	C	1	SER	2.8
1	L	403	GLU	2.7
1	D	296	TYR	2.7
1	L	92	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1	SER	2.7
1	L	6	LEU	2.7
1	J	277	ASN	2.7
1	K	94	PRO	2.7
1	L	337	ARG	2.7
1	L	327	GLU	2.7
1	L	61	ASN	2.7
1	L	393	ASP	2.7
1	B	386	ILE	2.7
1	L	359	ARG	2.7
1	A	203	GLY	2.7
1	B	55	GLY	2.7
1	L	293	GLN	2.7
1	E	1	SER	2.7
1	A	121	ALA	2.6
1	F	405	LYS	2.6
1	B	193	SER	2.6
1	F	4	HIS	2.6
1	F	397	TYR	2.6
1	B	288	ALA	2.6
1	A	334	TYR	2.6
1	H	432	GLY	2.6
1	I	59	GLY	2.6
1	A	123	THR	2.6
1	H	7	THR	2.6
1	C	60	ILE	2.6
1	I	61	ASN	2.6
1	D	353	ALA	2.6
1	J	398	ASP	2.6
1	J	113	ASP	2.6
1	L	212[A]	GLU	2.5
1	F	113	ASP	2.5
1	A	1	SER	2.5
1	B	59	GLY	2.5
1	H	284	GLY	2.5
1	D	2	ALA	2.5
1	A	60	ILE	2.5
1	C	3	GLU	2.5
1	B	293	GLN	2.5
1	E	307	ALA	2.5
1	A	50	ASP	2.5
1	D	393	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	428	LEU	2.5
1	A	63	SER	2.5
1	D	401	PRO	2.5
1	J	392	MET	2.5
1	J	44	GLU	2.5
1	A	293	GLN	2.5
1	C	394	LYS	2.5
1	I	393	ASP	2.4
1	G	401	PRO	2.4
1	C	55	GLY	2.4
1	K	44	GLU	2.4
1	J	296	TYR	2.4
1	B	280	ASN	2.4
1	D	39	ASN	2.4
1	F	64	ASP	2.4
1	B	273	SER	2.4
1	F	11	GLU	2.4
1	J	399	LEU	2.4
1	K	10	ASN	2.4
1	A	94	PRO	2.4
1	I	391	PRO	2.4
1	F	178[A]	GLY	2.4
1	H	178[A]	GLY	2.4
1	A	341	ALA	2.4
1	D	294	ALA	2.4
1	J	7	THR	2.4
1	D	60	ILE	2.4
1	J	60	ILE	2.4
1	B	395	ASN	2.4
1	L	66	VAL	2.4
1	C	403	GLU	2.4
1	D	390	GLU	2.4
1	L	62	GLU	2.4
1	B	63	SER	2.4
1	H	340	SER	2.4
1	E	7	THR	2.4
1	J	397	TYR	2.4
1	D	6	LEU	2.4
1	B	407	ILE	2.4
1	D	395	ASN	2.3
1	A	393	ASP	2.3
1	D	112	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	1	SER	2.3
1	A	299	GLY	2.3
1	H	40	ALA	2.3
1	I	403	GLU	2.3
1	B	274	LEU	2.3
1	H	53	SER	2.3
1	E	351	PRO	2.3
1	L	372	ALA	2.3
1	G	4	HIS	2.3
1	C	63	SER	2.3
1	H	339	ARG	2.3
1	A	265[A]	GLY	2.3
1	A	372	ALA	2.2
1	G	404	ALA	2.2
1	J	327	GLU	2.2
1	D	359	ARG	2.2
1	L	397	TYR	2.2
1	E	41	GLU	2.2
1	E	349	ALA	2.2
1	L	404	ALA	2.2
1	D	168	ASN	2.2
1	E	61	ASN	2.2
1	H	405	LYS	2.2
1	A	380	ASP	2.2
1	B	393	ASP	2.2
1	G	329	PRO	2.2
1	J	403	GLU	2.2
1	J	12	HIS	2.2
1	G	398	ASP	2.2
1	H	330	VAL	2.2
1	A	170	GLY	2.2
1	J	42	PHE	2.2
1	E	6	LEU	2.2
1	L	117	ALA	2.2
1	B	12	HIS	2.2
1	A	401	PRO	2.2
1	H	388	PRO	2.2
1	A	276	LYS	2.2
1	A	405	LYS	2.2
1	L	381	GLY	2.2
1	D	266[A]	SER	2.2
1	E	208	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	2	ALA	2.2
1	A	382	ILE	2.1
1	A	269	HIS	2.1
1	C	338	ASN	2.1
1	L	4	HIS	2.1
1	C	94	PRO	2.1
1	A	101	ASP	2.1
1	C	233	ASP	2.1
1	C	381	GLY	2.1
1	G	96	THR	2.1
1	H	6	LEU	2.1
1	B	275	ALA	2.1
1	I	273	SER	2.1
1	A	4	HIS	2.1
1	G	61	ASN	2.1
1	F	17	VAL	2.1
1	L	64	ASP	2.1
1	G	299	GLY	2.1
1	H	2	ALA	2.1
1	G	292	GLU	2.1
1	I	363	PRO	2.1
1	B	6	LEU	2.1
1	B	265[A]	GLY	2.1
1	G	339	ARG	2.1
1	K	359	ARG	2.1
1	B	327	GLU	2.1
1	I	62	GLU	2.1
1	F	12	HIS	2.1
1	A	396	LEU	2.1
1	H	289	GLY	2.1
1	J	55	GLY	2.1
1	L	90	ASP	2.1
1	D	62	GLU	2.1
1	K	296	TYR	2.1
1	I	387	HIS	2.0
1	H	66	VAL	2.0
1	K	395	ASN	2.0
1	F	398	ASP	2.0
1	I	296	TYR	2.0
1	B	304	HIS	2.0
1	E	283	SER	2.0
1	E	10	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	337	ARG	2.0
1	K	339	ARG	2.0
1	B	432	GLY	2.0
1	L	59	GLY	2.0
1	L	284	GLY	2.0
1	C	404	ALA	2.0
1	J	40	ALA	2.0
1	F	403	GLU	2.0
1	J	93	GLU	2.0
1	J	402	GLU	2.0
1	H	179[A]	TYR	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
3	ADP	F	4476	27/27	0.62	0.19	42,80,100,100	27
3	ADP	C	4473	27/27	0.68	0.17	42,80,100,100	27
3	ADP	E	4475	27/27	0.69	0.18	42,80,100,100	27
3	ADP	I	4479	27/27	0.74	0.17	42,80,100,100	27
3	ADP	K	4481	27/27	0.76	0.21	42,80,100,100	27
3	ADP	B	4472	27/27	0.77	0.16	42,80,100,100	27
3	ADP	A	4471	27/27	0.77	0.17	42,80,100,100	27
3	ADP	H	4478	27/27	0.78	0.18	42,80,100,100	27
3	ADP	L	4482	27/27	0.78	0.19	42,80,100,100	27
3	ADP	G	4477	27/27	0.81	0.19	42,80,100,100	27
4	PPQ	B	5901	11/11	0.83	0.17	16,36,70,83	11
3	ADP	J	4480	27/27	0.84	0.15	42,80,100,100	27

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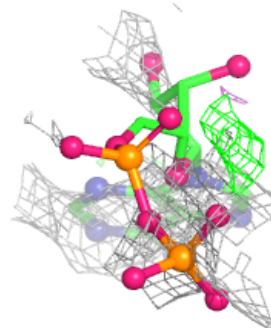
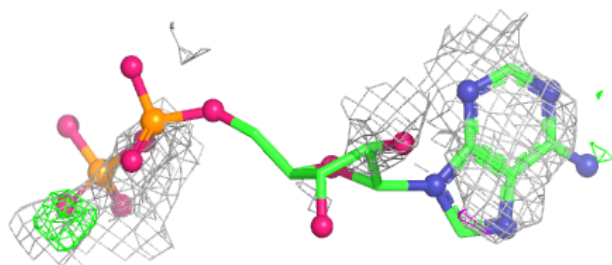
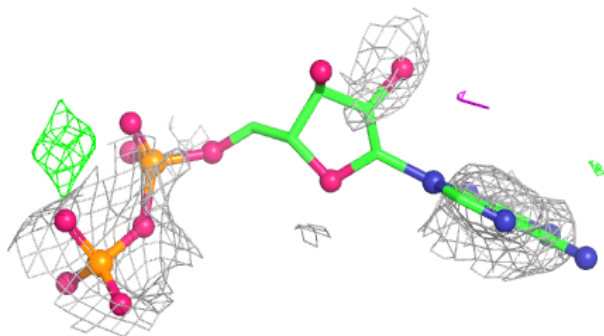
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PPQ	F	5905	11/11	0.84	0.17	16,36,70,83	11
3	ADP	D	4474	27/27	0.85	0.14	42,80,100,100	27
4	PPQ	I	5908	11/11	0.87	0.16	16,36,70,83	11
4	PPQ	H	5907	11/11	0.88	0.14	16,36,70,83	11
4	PPQ	G	5906	11/11	0.89	0.12	16,36,70,83	11
4	PPQ	C	5902	11/11	0.89	0.12	16,36,70,83	11
2	MN	C	469	1/1	0.89	0.07	41,41,41,41	0
4	PPQ	K	5910	11/11	0.89	0.12	16,36,70,83	11
4	PPQ	J	5909	11/11	0.90	0.14	16,36,70,83	11
2	MN	H	470	1/1	0.90	0.06	43,43,43,43	0
2	MN	E	470	1/1	0.91	0.08	43,43,43,43	0
4	PPQ	D	5903	11/11	0.91	0.12	16,36,70,83	11
2	MN	H	469	1/1	0.92	0.10	41,41,41,41	0
4	PPQ	E	5904	11/11	0.92	0.11	16,36,70,83	11
2	MN	F	469	1/1	0.93	0.04	41,41,41,41	0
4	PPQ	A	5900	11/11	0.93	0.12	16,36,70,83	11
2	MN	L	469	1/1	0.94	0.09	41,41,41,41	0
2	MN	C	470	1/1	0.94	0.04	43,43,43,43	0
2	MN	G	469	1/1	0.94	0.05	41,41,41,41	0
2	MN	E	469	1/1	0.95	0.04	41,41,41,41	0
2	MN	D	469	1/1	0.95	0.08	41,41,41,41	0
2	MN	D	470	1/1	0.95	0.07	43,43,43,43	0
2	MN	I	469	1/1	0.95	0.06	41,41,41,41	0
4	PPQ	L	5911	11/11	0.95	0.14	16,36,70,83	11
2	MN	B	469	1/1	0.96	0.04	41,41,41,41	0
2	MN	G	470	1/1	0.96	0.04	43,43,43,43	0
2	MN	I	470	1/1	0.96	0.04	43,43,43,43	0
2	MN	K	469	1/1	0.96	0.10	41,41,41,41	0
2	MN	F	470	1/1	0.96	0.08	43,43,43,43	0
2	MN	L	470	1/1	0.96	0.07	43,43,43,43	0
2	MN	K	470	1/1	0.97	0.04	43,43,43,43	0
2	MN	A	469	1/1	0.97	0.05	41,41,41,41	0
2	MN	A	470	1/1	0.97	0.03	43,43,43,43	0
2	MN	B	470	1/1	0.98	0.04	43,43,43,43	0
2	MN	J	469	1/1	0.99	0.07	41,41,41,41	0
2	MN	J	470	1/1	0.99	0.03	43,43,43,43	0

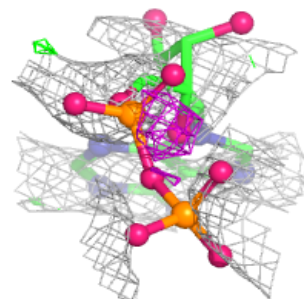
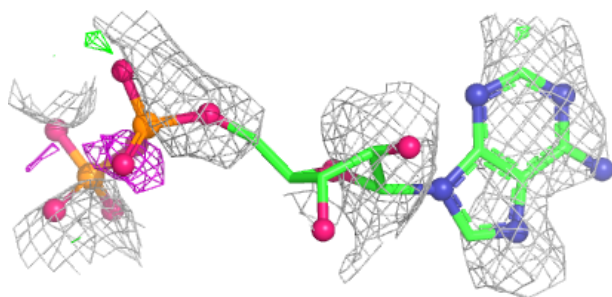
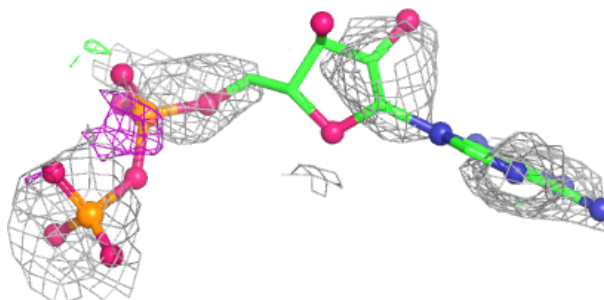
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP F 4476:

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

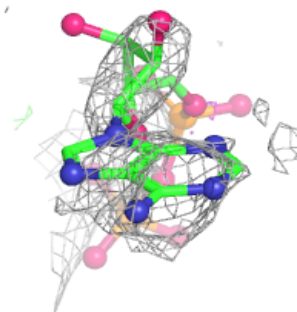
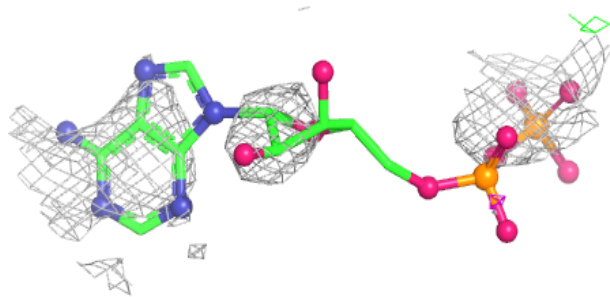
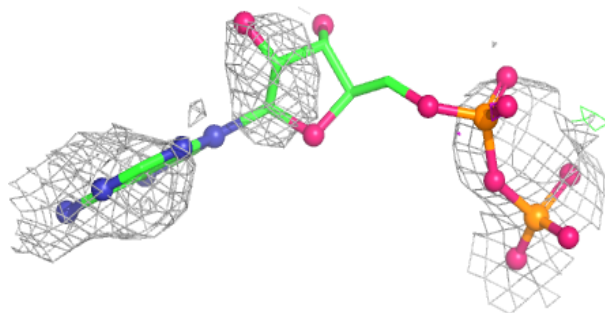
**Electron density around ADP C 4473:**

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

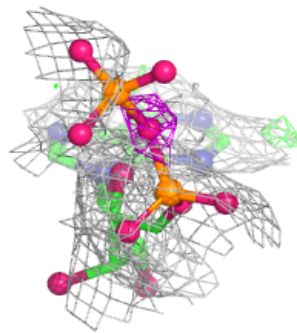
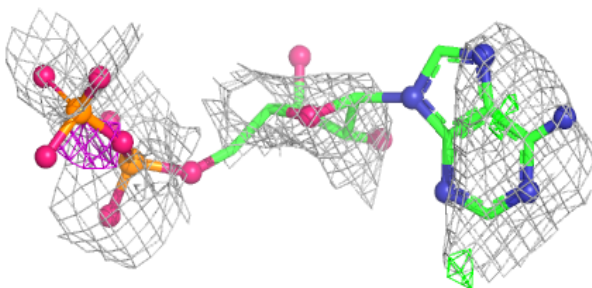
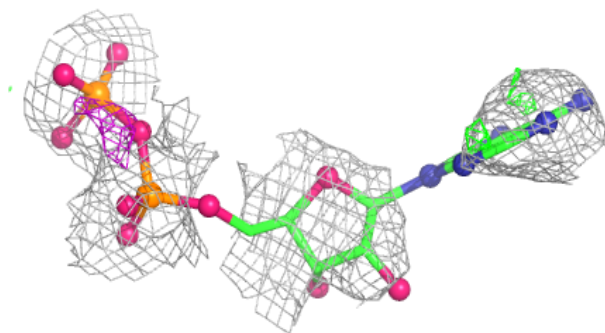


Electron density around ADP E 4475:

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

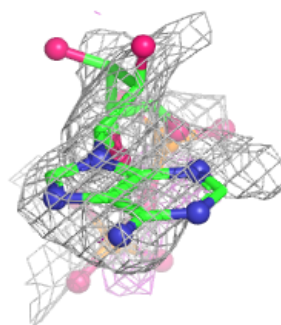
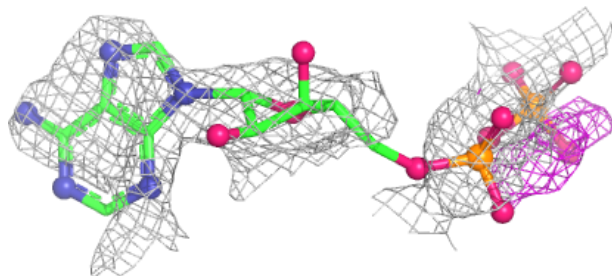
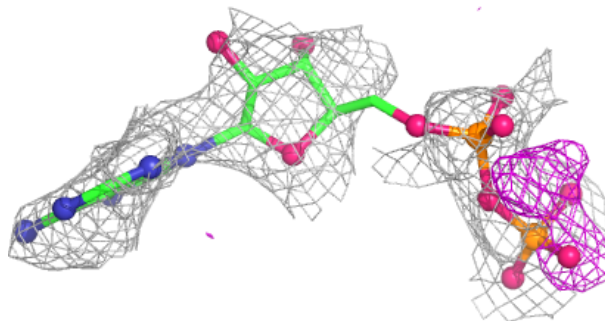
**Electron density around ADP I 4479:**

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

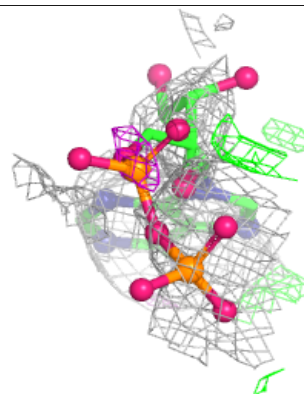
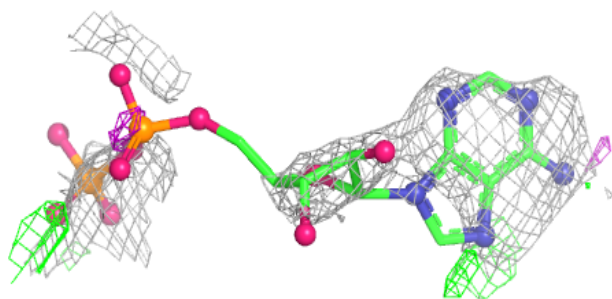
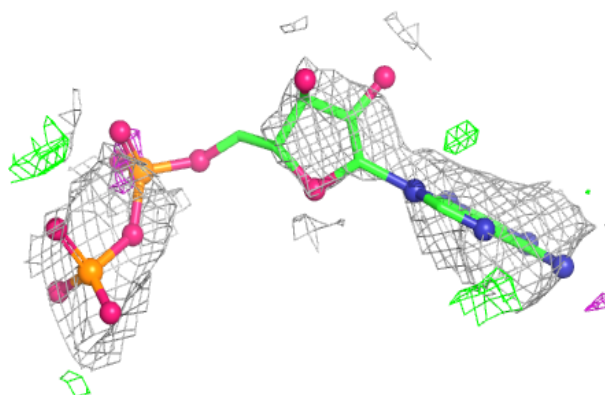


Electron density around ADP K 4481:

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

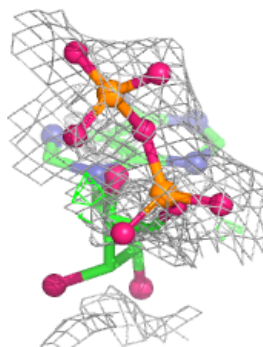
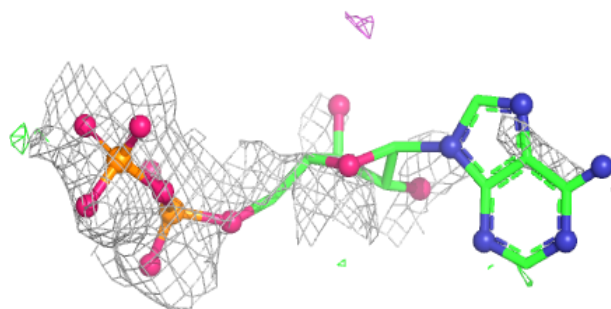
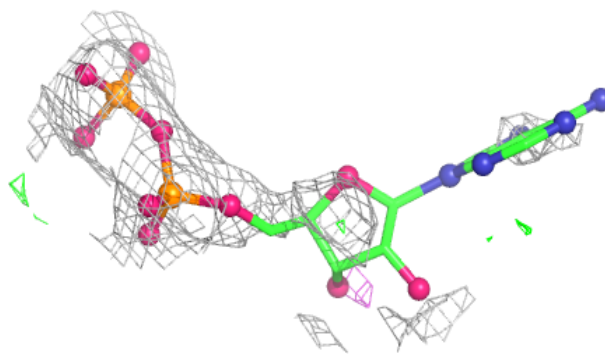
**Electron density around ADP B 4472:**

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

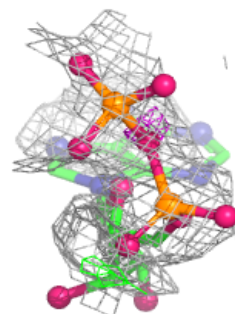
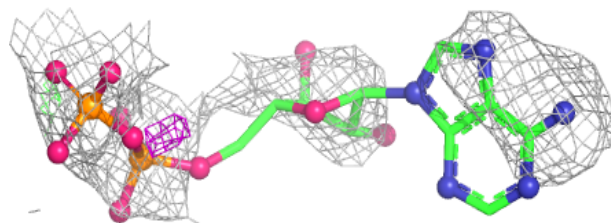
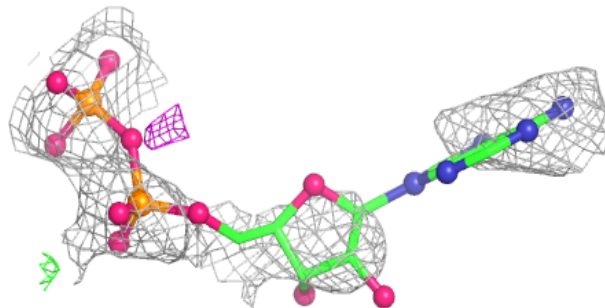


Electron density around ADP A 4471:

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

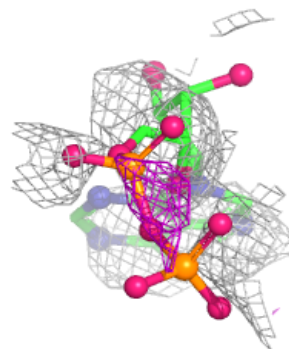
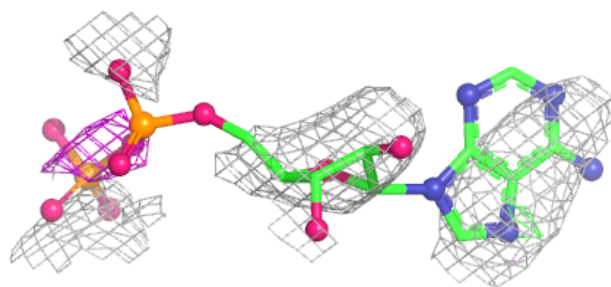
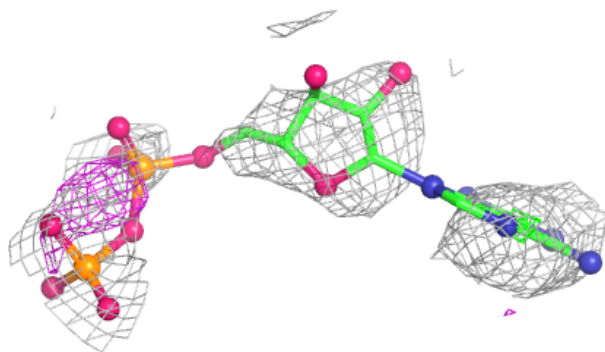
**Electron density around ADP H 4478:**

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

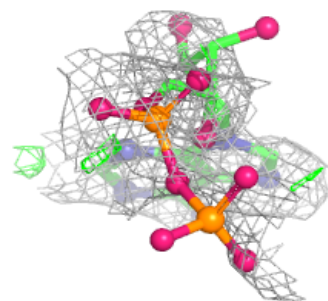
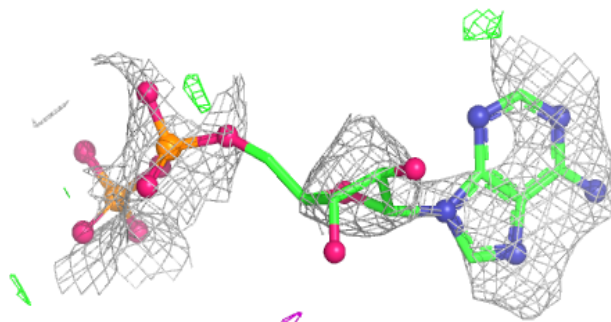
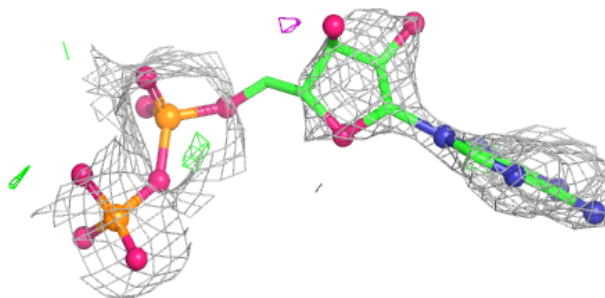


Electron density around ADP L 4482:

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

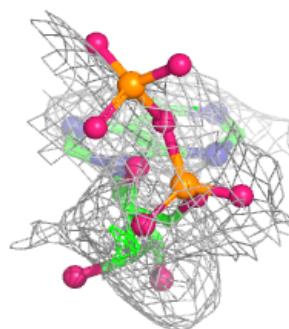
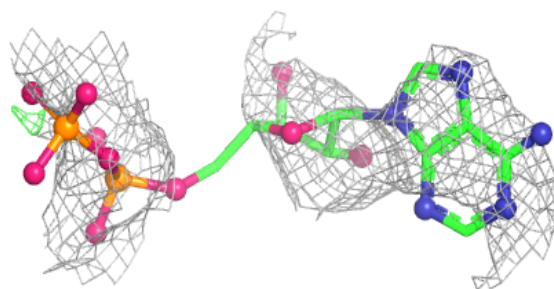
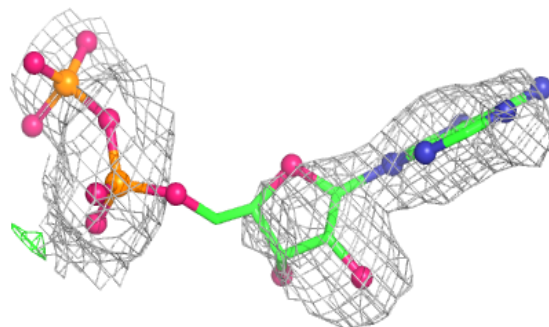
**Electron density around ADP G 4477:**

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

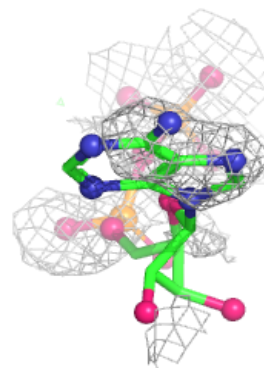
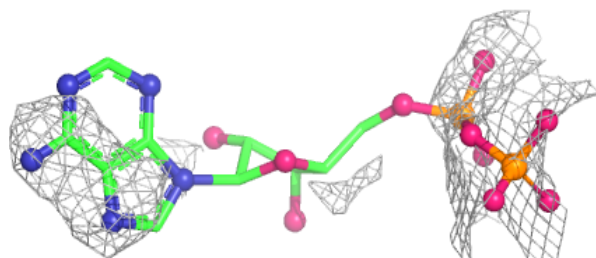
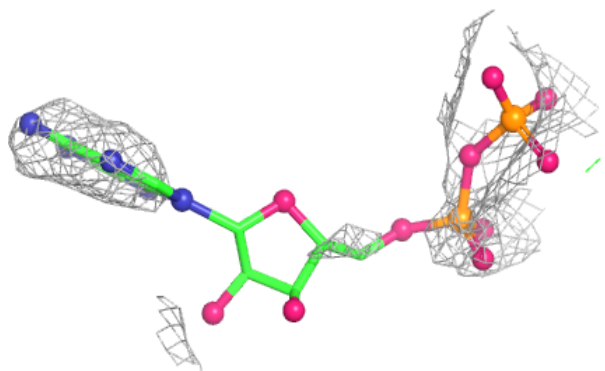


Electron density around ADP J 4480:

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

**Electron density around ADP D 4474:**

$2mF_o-DF_c$ (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.