



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 10:18 PM EDT

PDB ID : 1F52 / pdb_00001f52
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM
SALMONELLA TYPHIMURIUM CO-CRYSTALLIZED WITH ADP
Authors : Gill, H.S.; Pfluegl, G.M.U.; Eisenberg, D.
Deposited on : 2000-06-12
Resolution : 2.49 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

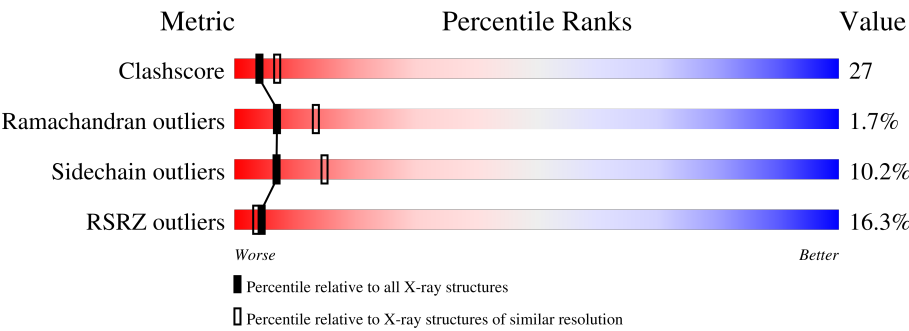
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	468	
1	B	468	
1	C	468	
1	D	468	
1	E	468	
1	F	468	
1	G	468	

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Mol	Chain	Length	Quality of chain
1	H	468	
1	I	468	
1	J	468	
1	K	468	
1	L	468	

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	MPD	A	5472	-	X	X	X
4	MPD	A	5481	-	-	X	-
4	MPD	B	5471	-	-	X	-
4	MPD	B	5474	-	X	X	-
4	MPD	C	5473	-	-	X	-
4	MPD	C	5476	-	X	X	-
4	MPD	D	5475	-	-	X	-
4	MPD	D	5478	-	X	X	-
4	MPD	E	5477	-	-	X	-
4	MPD	E	5480	-	X	X	-
4	MPD	F	5479	-	-	X	-
4	MPD	F	5482	-	X	X	-
4	MPD	G	5484	-	X	X	-
4	MPD	G	5485	-	-	X	-
4	MPD	H	5486	-	X	X	-
4	MPD	H	5487	-	-	X	-
4	MPD	I	5488	-	X	X	X
4	MPD	I	5489	-	-	X	-
4	MPD	J	5490	-	X	X	-
4	MPD	J	5491	-	-	X	-
4	MPD	K	5492	-	X	X	X
4	MPD	K	5493	-	-	X	-
4	MPD	L	5483	-	-	X	-
4	MPD	L	5494	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47688 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
1	A	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	B	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	C	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	D	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	E	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	F	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	G	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	H	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	I	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	J	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	K	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	L	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			

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

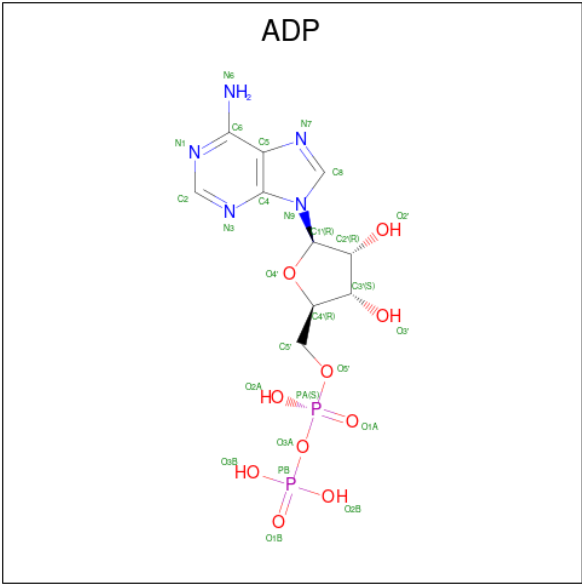
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

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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: C₁₀H₁₅N₅O₁₀P₂).



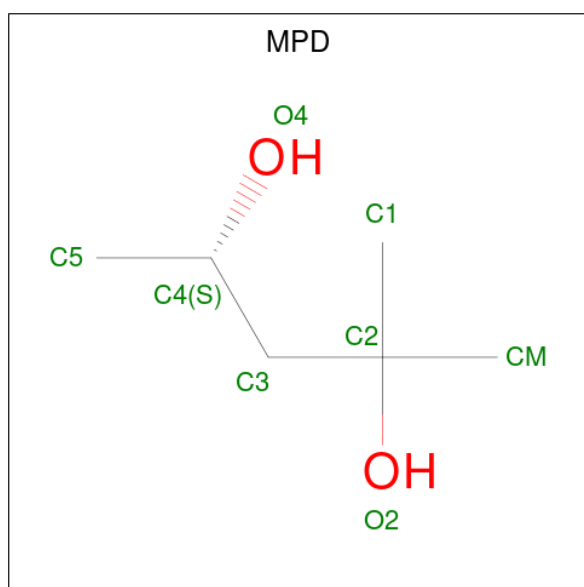
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O P	0	0
			27	10	5	10 2		

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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	F	1	Total C O 8 6 2	0	0
4	F	1	Total C O 8 6 2	0	0
4	G	1	Total C O 8 6 2	0	0
4	G	1	Total C O 8 6 2	0	0
4	H	1	Total C O 8 6 2	0	0
4	H	1	Total C O 8 6 2	0	0
4	I	1	Total C O 8 6 2	0	0
4	I	1	Total C O 8 6 2	0	0
4	J	1	Total C O 8 6 2	0	0
4	J	1	Total C O 8 6 2	0	0
4	K	1	Total C O 8 6 2	0	0
4	K	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			8	6	2		
4	L	1	Total	C	O	0	0
			8	6	2		

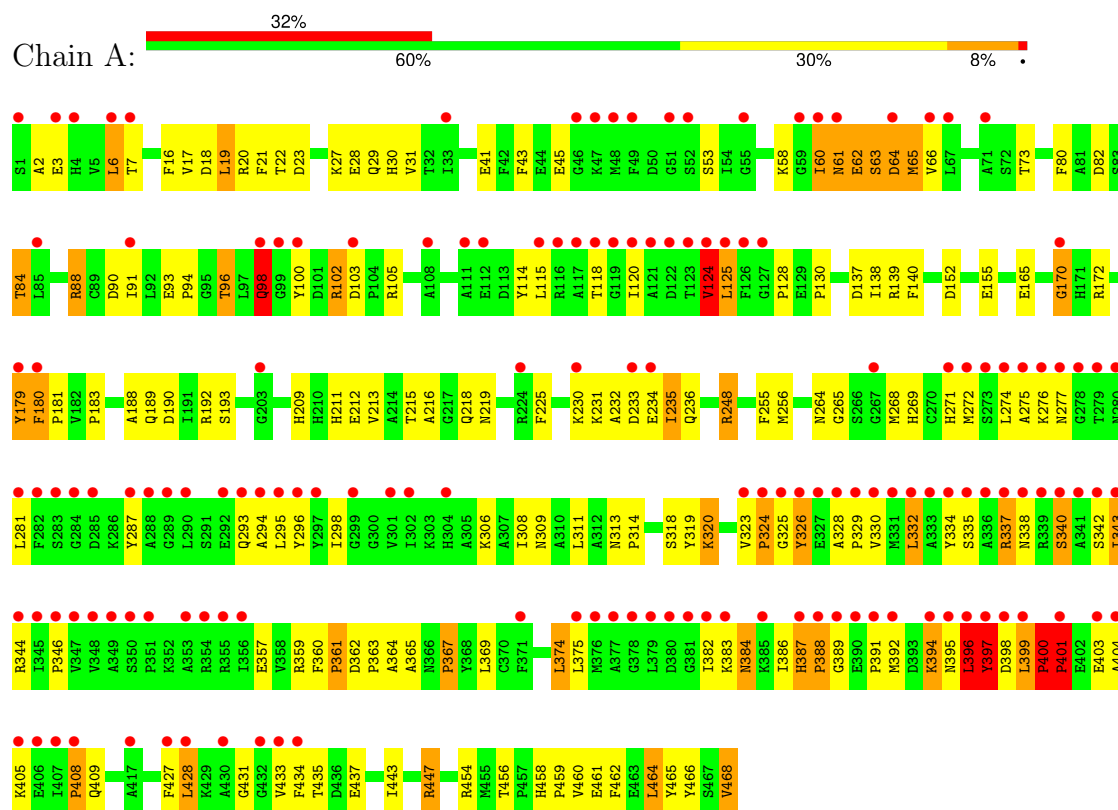
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	294	Total	O		0	0
			294	294			
5	B	297	Total	O		0	0
			297	297			
5	C	293	Total	O		0	0
			293	293			
5	D	295	Total	O		0	0
			295	295			
5	E	294	Total	O		0	0
			294	294			
5	F	293	Total	O		0	0
			293	293			
5	G	288	Total	O		0	0
			288	288			
5	H	288	Total	O		0	0
			288	288			
5	I	295	Total	O		0	0
			295	295			
5	J	287	Total	O		0	0
			287	287			
5	K	288	Total	O		0	0
			288	288			
5	L	292	Total	O		0	0
			292	292			

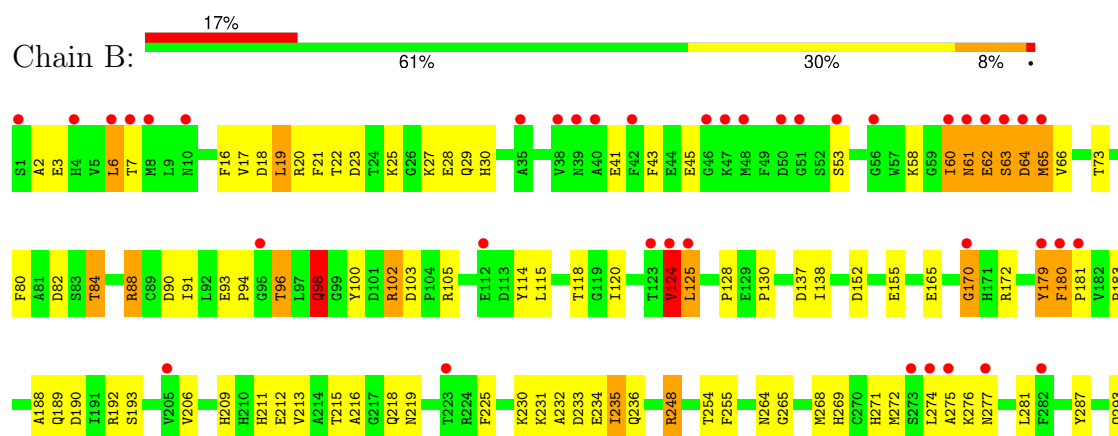
3 Residue-property plots

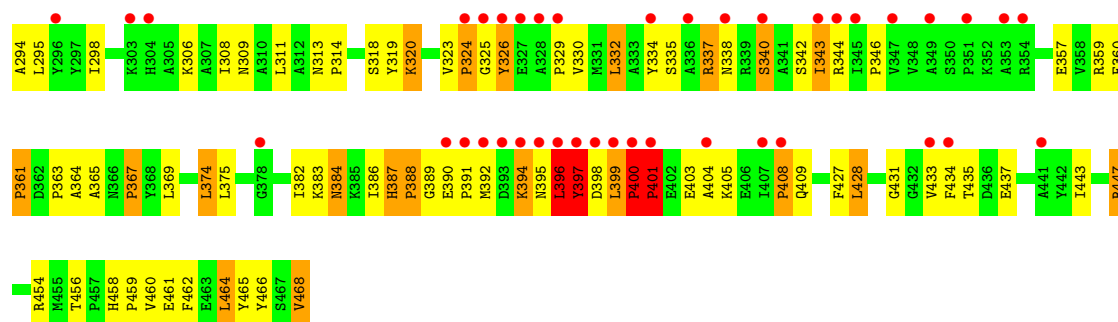
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

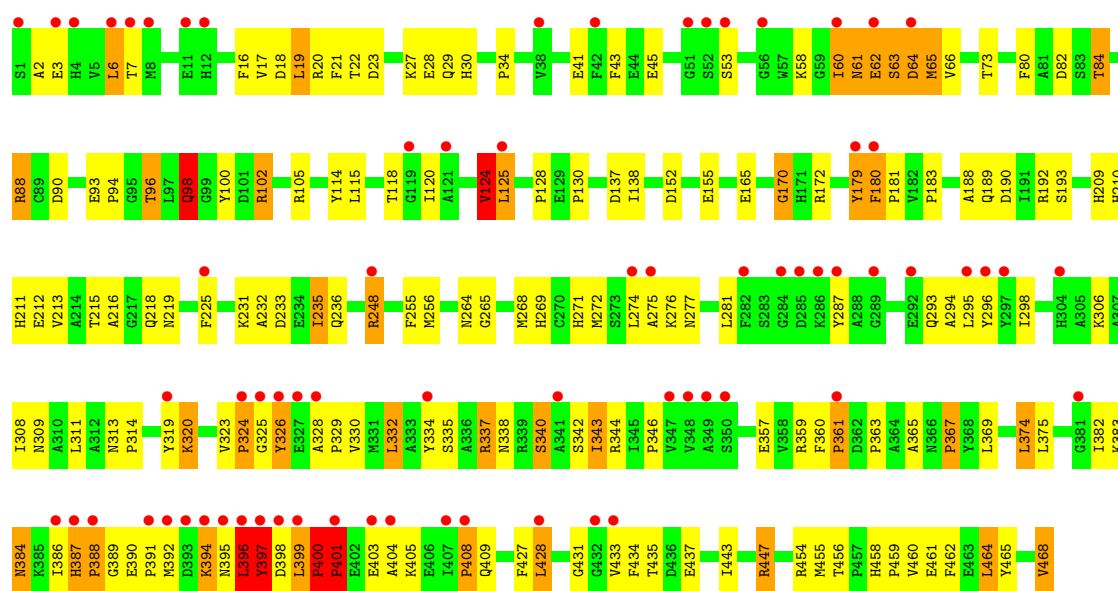


• Molecule 1: GLUTAMINE SYNTHETASE

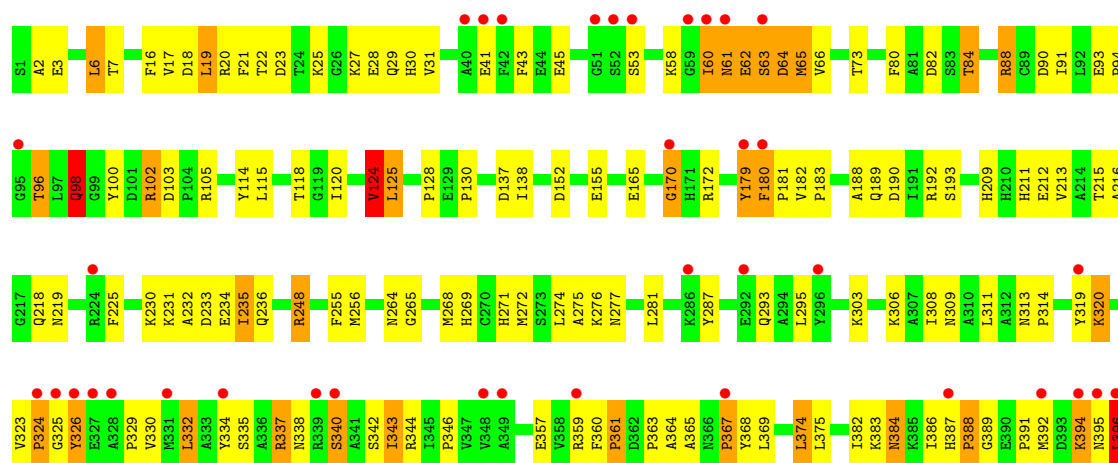


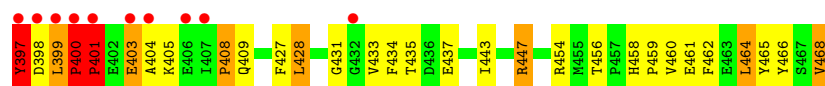


• Molecule 1: GLUTAMINE SYNTHETASE

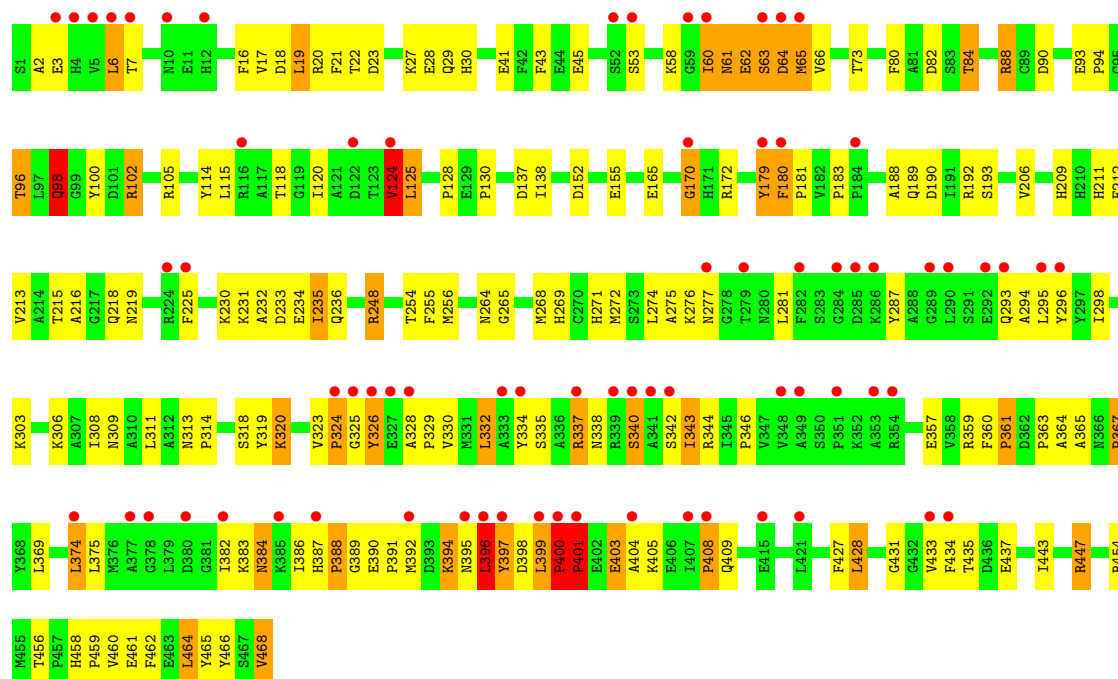


• Molecule 1: GLUTAMINE SYNTHETASE

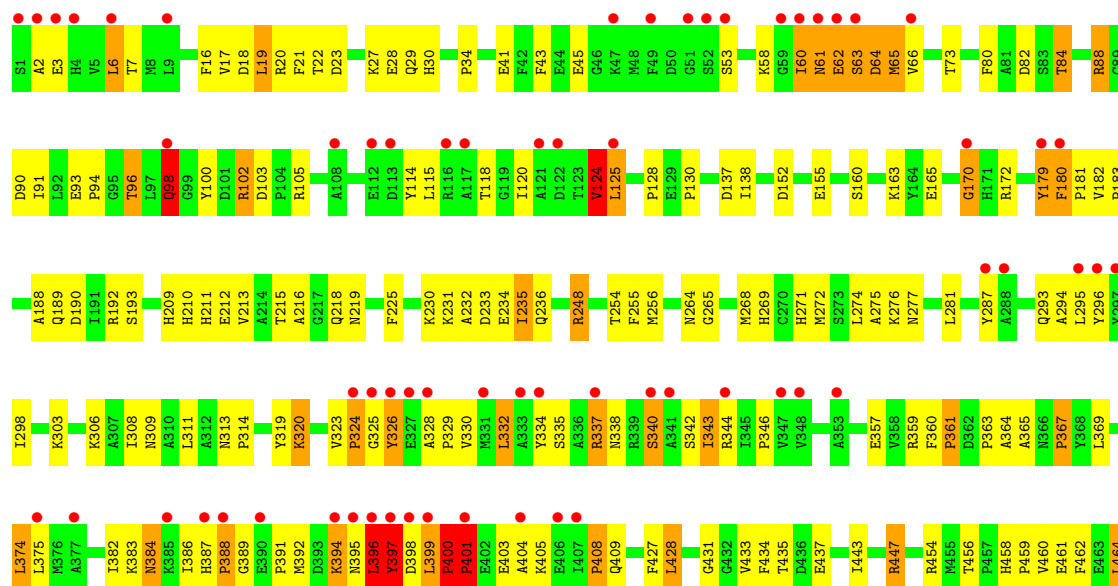




• Molecule 1: GLUTAMINE SYNTHETASE

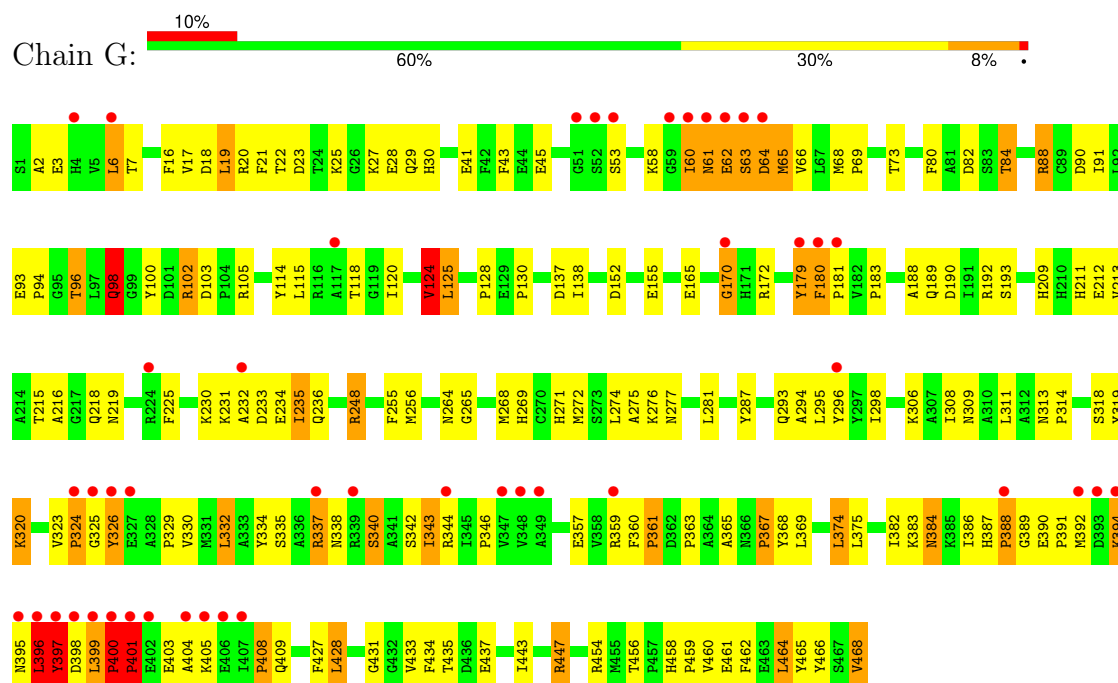


• Molecule 1: GLUTAMINE SYNTHETASE

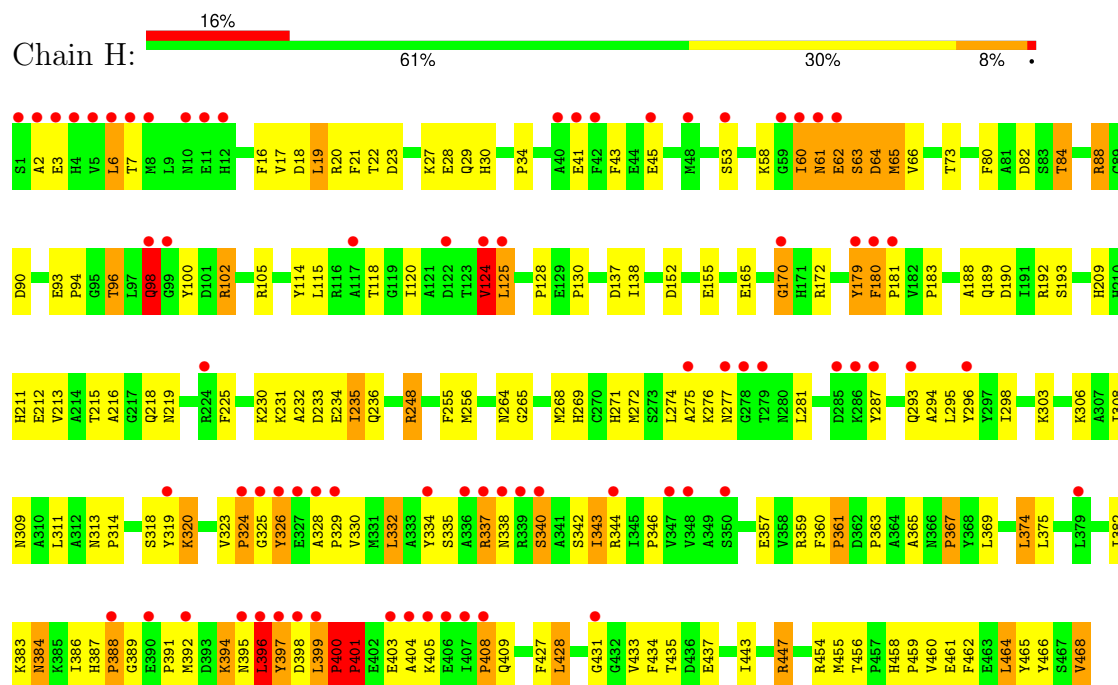




• Molecule 1: GLUTAMINE SYNTHETASE

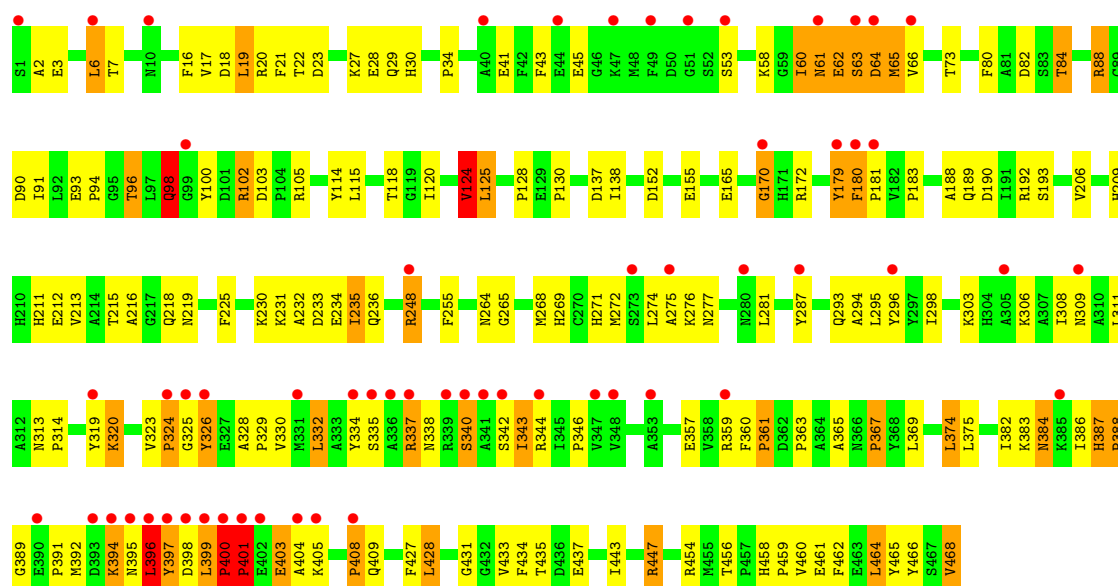


• Molecule 1: GLUTAMINE SYNTHETASE

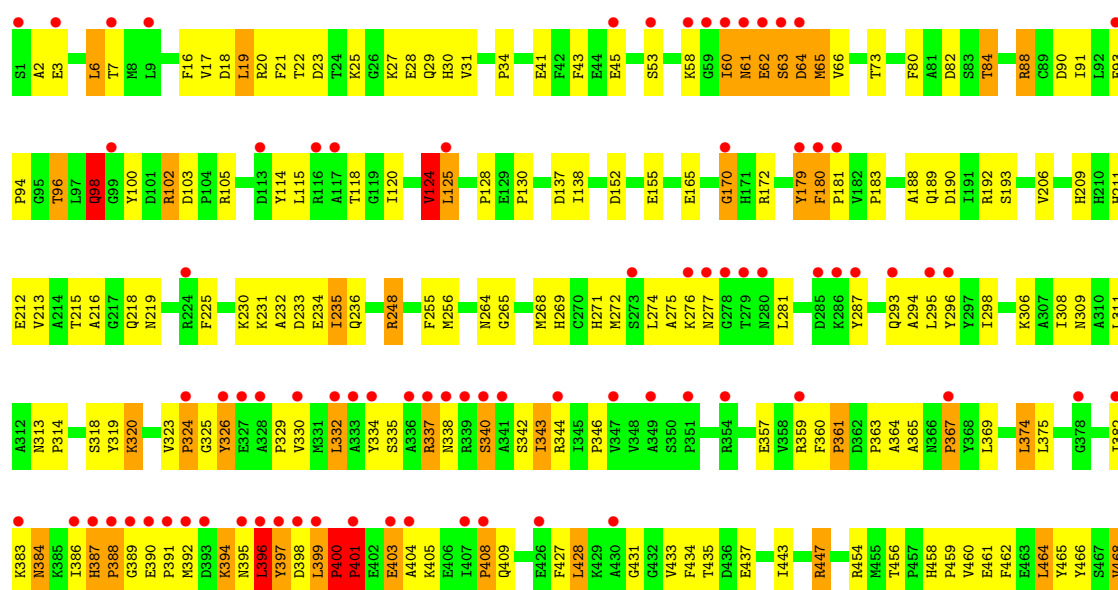


• Molecule 1: GLUTAMINE SYNTHETASE

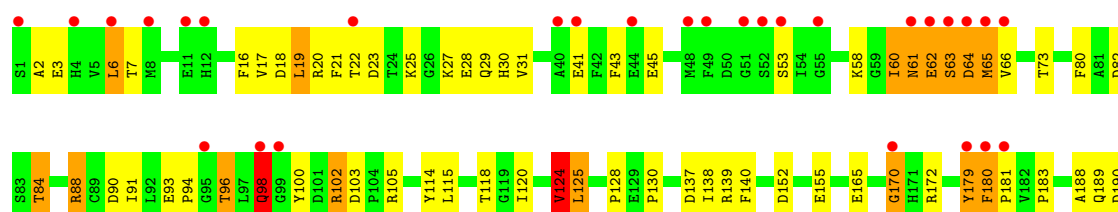


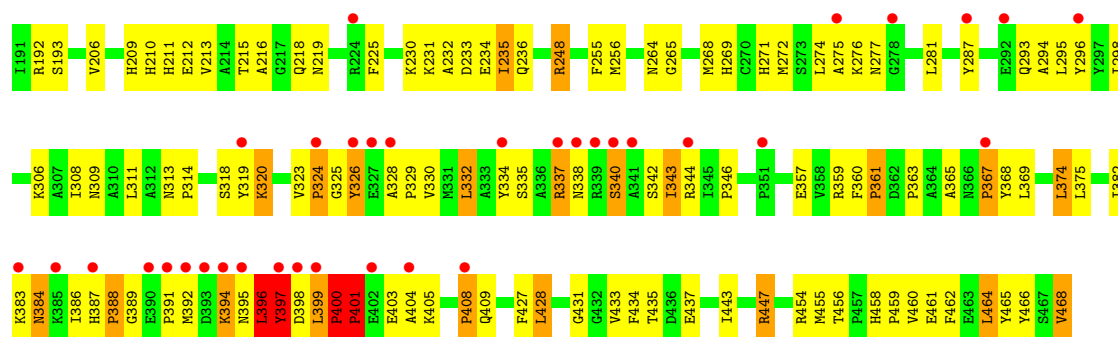


• Molecule 1: GLUTAMINE SYNTHETASE

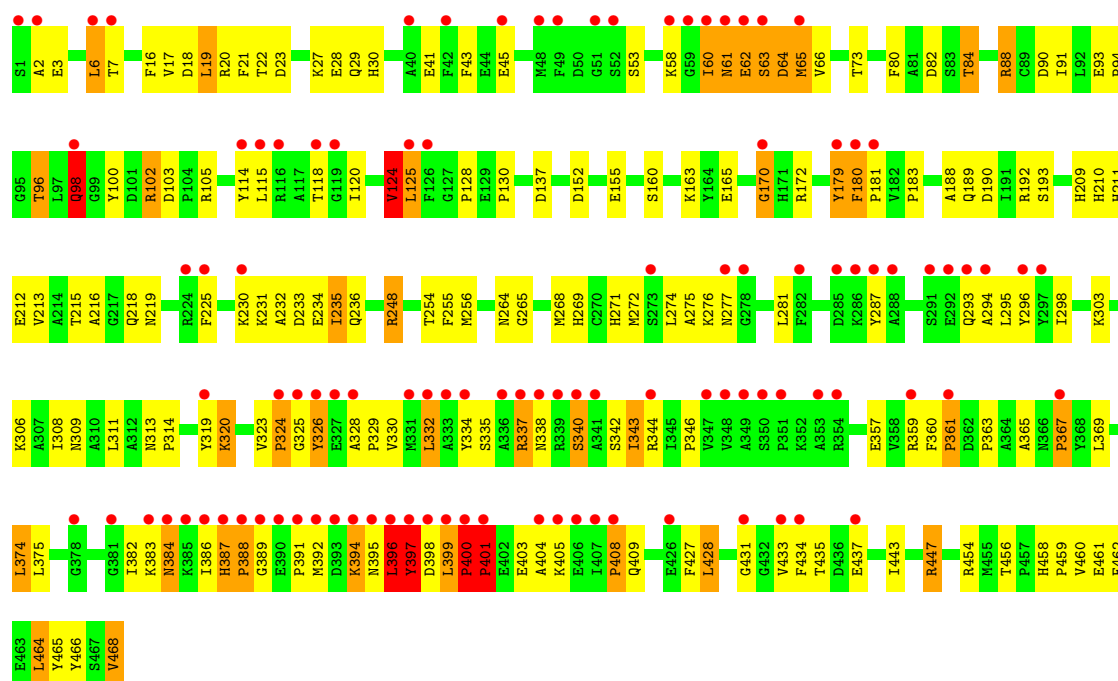


• Molecule 1: GLUTAMINE SYNTHETASE





● 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)	34.90 – 2.49 34.90 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.90-2.49) 97.9 (34.90-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.67 (at 2.48Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.243 , 0.257 0.244 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47688	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: MPD, MN, ADP

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	0.66	0/3724	1.24	41/5043 (0.8%)
1	B	0.66	0/3724	1.24	41/5043 (0.8%)
1	C	0.66	0/3724	1.24	41/5043 (0.8%)
1	D	0.66	0/3724	1.24	42/5043 (0.8%)
1	E	0.66	0/3724	1.25	42/5043 (0.8%)
1	F	0.66	0/3724	1.24	41/5043 (0.8%)
1	G	0.66	0/3724	1.25	41/5043 (0.8%)
1	H	0.66	0/3724	1.24	41/5043 (0.8%)
1	I	0.66	0/3724	1.24	42/5043 (0.8%)
1	J	0.66	0/3724	1.24	42/5043 (0.8%)
1	K	0.66	0/3724	1.24	41/5043 (0.8%)
1	L	0.66	0/3724	1.24	41/5043 (0.8%)
All	All	0.66	0/44688	1.24	496/60516 (0.8%)

There are no bond length outliers.

All (496) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	340	SER	N-CA-C	-9.69	101.97	113.88
1	E	98	GLN	OE1-CD-NE2	-9.68	112.92	122.60
1	L	340	SER	N-CA-C	-9.68	101.97	113.88
1	I	98	GLN	OE1-CD-NE2	-9.68	112.92	122.60
1	I	340	SER	N-CA-C	-9.67	101.99	113.88
1	J	340	SER	N-CA-C	-9.67	101.99	113.88
1	E	340	SER	N-CA-C	-9.67	101.99	113.88
1	J	98	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	B	98	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	A	340	SER	N-CA-C	-9.65	102.01	113.88
1	C	340	SER	N-CA-C	-9.65	102.00	113.88
1	B	340	SER	N-CA-C	-9.65	102.02	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	98	GLN	OE1-CD-NE2	-9.64	112.96	122.60
1	A	98	GLN	OE1-CD-NE2	-9.64	112.96	122.60
1	D	340	SER	N-CA-C	-9.64	102.03	113.88
1	K	98	GLN	OE1-CD-NE2	-9.64	112.96	122.60
1	G	340	SER	N-CA-C	-9.63	102.03	113.88
1	K	340	SER	N-CA-C	-9.63	102.03	113.88
1	F	340	SER	N-CA-C	-9.63	102.03	113.88
1	L	98	GLN	OE1-CD-NE2	-9.62	112.98	122.60
1	H	98	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	C	98	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	F	98	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	G	98	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	G	400	PRO	CA-C-N	9.28	131.44	119.84
1	G	400	PRO	C-N-CA	9.28	131.44	119.84
1	H	400	PRO	CA-C-N	9.28	131.44	119.84
1	H	400	PRO	C-N-CA	9.28	131.44	119.84
1	J	400	PRO	CA-C-N	9.27	131.42	119.84
1	J	400	PRO	C-N-CA	9.27	131.42	119.84
1	E	400	PRO	CA-C-N	9.26	131.41	119.84
1	E	400	PRO	C-N-CA	9.26	131.41	119.84
1	A	400	PRO	CA-C-N	9.24	131.39	119.84
1	A	400	PRO	C-N-CA	9.24	131.39	119.84
1	B	400	PRO	CA-C-N	9.22	131.37	119.84
1	B	400	PRO	C-N-CA	9.22	131.37	119.84
1	L	400	PRO	CA-C-N	9.21	131.36	119.84
1	L	400	PRO	C-N-CA	9.21	131.36	119.84
1	C	400	PRO	CA-C-N	9.21	131.35	119.84
1	C	400	PRO	C-N-CA	9.21	131.35	119.84
1	K	400	PRO	CA-C-N	9.21	131.35	119.84
1	K	400	PRO	C-N-CA	9.21	131.35	119.84
1	D	400	PRO	CA-C-N	9.20	131.34	119.84
1	D	400	PRO	C-N-CA	9.20	131.34	119.84
1	I	400	PRO	CA-C-N	9.20	131.34	119.84
1	I	400	PRO	C-N-CA	9.20	131.34	119.84
1	F	400	PRO	CA-C-N	9.19	131.33	119.84
1	F	400	PRO	C-N-CA	9.19	131.33	119.84
1	L	218	GLN	OE1-CD-NE2	-9.08	113.52	122.60
1	K	218	GLN	OE1-CD-NE2	-9.07	113.53	122.60
1	J	218	GLN	OE1-CD-NE2	-9.07	113.53	122.60
1	E	218	GLN	OE1-CD-NE2	-9.06	113.54	122.60
1	F	218	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	C	218	GLN	OE1-CD-NE2	-9.05	113.55	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	GLN	OE1-CD-NE2	-9.04	113.56	122.60
1	G	218	GLN	OE1-CD-NE2	-9.04	113.56	122.60
1	I	218	GLN	OE1-CD-NE2	-9.03	113.57	122.60
1	H	218	GLN	OE1-CD-NE2	-9.02	113.58	122.60
1	B	218	GLN	OE1-CD-NE2	-9.02	113.58	122.60
1	D	218	GLN	OE1-CD-NE2	-9.00	113.60	122.60
1	F	387	HIS	CA-C-N	8.72	129.59	119.47
1	F	387	HIS	C-N-CA	8.72	129.59	119.47
1	J	387	HIS	CA-C-N	8.71	129.57	119.47
1	J	387	HIS	C-N-CA	8.71	129.57	119.47
1	K	387	HIS	CA-C-N	8.71	129.57	119.47
1	K	387	HIS	C-N-CA	8.71	129.57	119.47
1	I	387	HIS	CA-C-N	8.71	129.57	119.47
1	I	387	HIS	C-N-CA	8.71	129.57	119.47
1	G	387	HIS	CA-C-N	8.70	129.56	119.47
1	G	387	HIS	C-N-CA	8.70	129.56	119.47
1	B	387	HIS	CA-C-N	8.70	129.56	119.47
1	B	387	HIS	C-N-CA	8.70	129.56	119.47
1	A	387	HIS	CA-C-N	8.69	129.55	119.47
1	A	387	HIS	C-N-CA	8.69	129.55	119.47
1	E	387	HIS	CA-C-N	8.69	129.55	119.47
1	E	387	HIS	C-N-CA	8.69	129.55	119.47
1	C	387	HIS	CA-C-N	8.67	129.52	119.47
1	C	387	HIS	C-N-CA	8.67	129.52	119.47
1	L	387	HIS	CA-C-N	8.66	129.52	119.47
1	L	387	HIS	C-N-CA	8.66	129.52	119.47
1	D	387	HIS	CA-C-N	8.66	129.52	119.47
1	D	387	HIS	C-N-CA	8.66	129.52	119.47
1	H	387	HIS	CA-C-N	8.66	129.52	119.47
1	H	387	HIS	C-N-CA	8.66	129.52	119.47
1	H	61	ASN	CA-CB-CG	-8.64	103.96	112.60
1	B	61	ASN	CA-CB-CG	-8.64	103.96	112.60
1	G	61	ASN	CA-CB-CG	-8.64	103.96	112.60
1	E	61	ASN	CA-CB-CG	-8.63	103.97	112.60
1	F	61	ASN	CA-CB-CG	-8.63	103.97	112.60
1	L	61	ASN	CA-CB-CG	-8.62	103.98	112.60
1	C	61	ASN	CA-CB-CG	-8.62	103.98	112.60
1	A	61	ASN	CA-CB-CG	-8.60	104.00	112.60
1	I	61	ASN	CA-CB-CG	-8.60	104.00	112.60
1	D	61	ASN	CA-CB-CG	-8.58	104.02	112.60
1	J	61	ASN	CA-CB-CG	-8.58	104.02	112.60
1	K	61	ASN	CA-CB-CG	-8.56	104.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	213	VAL	N-CA-C	7.98	118.03	110.53
1	G	213	VAL	N-CA-C	7.98	118.03	110.53
1	L	397	TYR	CA-C-N	-7.78	112.26	123.00
1	L	397	TYR	C-N-CA	-7.78	112.26	123.00
1	B	397	TYR	CA-C-N	-7.77	112.28	123.00
1	B	397	TYR	C-N-CA	-7.77	112.28	123.00
1	D	397	TYR	CA-C-N	-7.77	112.28	123.00
1	D	397	TYR	C-N-CA	-7.77	112.28	123.00
1	K	397	TYR	CA-C-N	-7.76	112.29	123.00
1	K	397	TYR	C-N-CA	-7.76	112.29	123.00
1	J	397	TYR	CA-C-N	-7.76	112.29	123.00
1	J	397	TYR	C-N-CA	-7.76	112.29	123.00
1	I	397	TYR	CA-C-N	-7.76	112.30	123.00
1	I	397	TYR	C-N-CA	-7.76	112.30	123.00
1	A	397	TYR	CA-C-N	-7.75	112.30	123.00
1	A	397	TYR	C-N-CA	-7.75	112.30	123.00
1	E	397	TYR	CA-C-N	-7.75	112.30	123.00
1	E	397	TYR	C-N-CA	-7.75	112.30	123.00
1	C	397	TYR	CA-C-N	-7.75	112.30	123.00
1	C	397	TYR	C-N-CA	-7.75	112.30	123.00
1	G	397	TYR	CA-C-N	-7.74	112.31	123.00
1	G	397	TYR	C-N-CA	-7.74	112.31	123.00
1	H	397	TYR	CA-C-N	-7.74	112.31	123.00
1	H	397	TYR	C-N-CA	-7.74	112.31	123.00
1	F	397	TYR	CA-C-N	-7.74	112.32	123.00
1	F	397	TYR	C-N-CA	-7.74	112.32	123.00
1	H	213	VAL	N-CA-C	7.31	118.10	110.72
1	J	213	VAL	N-CA-C	7.28	118.08	110.72
1	C	213	VAL	N-CA-C	7.28	118.07	110.72
1	B	213	VAL	N-CA-C	7.27	118.06	110.72
1	A	213	VAL	N-CA-C	7.27	118.06	110.72
1	L	213	VAL	N-CA-C	7.27	118.06	110.72
1	E	401	PRO	CA-N-CD	-7.26	101.83	112.00
1	I	213	VAL	N-CA-C	7.26	118.06	110.72
1	F	213	VAL	N-CA-C	7.26	118.05	110.72
1	K	213	VAL	N-CA-C	7.26	118.05	110.72
1	E	213	VAL	N-CA-C	7.25	118.05	110.72
1	J	401	PRO	CA-N-CD	-7.25	101.84	112.00
1	I	401	PRO	CA-N-CD	-7.25	101.86	112.00
1	L	401	PRO	CA-N-CD	-7.24	101.86	112.00
1	F	401	PRO	CA-N-CD	-7.24	101.86	112.00
1	H	401	PRO	CA-N-CD	-7.24	101.87	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	PRO	CA-N-CD	-7.23	101.87	112.00
1	G	401	PRO	CA-N-CD	-7.23	101.88	112.00
1	D	401	PRO	CA-N-CD	-7.22	101.89	112.00
1	C	401	PRO	CA-N-CD	-7.22	101.89	112.00
1	B	401	PRO	CA-N-CD	-7.20	101.92	112.00
1	K	401	PRO	CA-N-CD	-7.20	101.92	112.00
1	J	66	VAL	N-CA-C	7.14	118.89	108.53
1	E	66	VAL	N-CA-C	7.14	118.88	108.53
1	I	66	VAL	N-CA-C	7.12	118.85	108.53
1	L	66	VAL	N-CA-C	7.12	118.85	108.53
1	C	66	VAL	N-CA-C	7.11	118.84	108.53
1	F	66	VAL	N-CA-C	7.11	118.83	108.53
1	A	66	VAL	N-CA-C	7.10	118.83	108.53
1	D	66	VAL	N-CA-C	7.10	118.82	108.53
1	B	66	VAL	N-CA-C	7.09	118.81	108.53
1	G	66	VAL	N-CA-C	7.09	118.81	108.53
1	K	66	VAL	N-CA-C	7.09	118.81	108.53
1	H	66	VAL	N-CA-C	7.08	118.80	108.53
1	D	387	HIS	O-C-N	7.01	128.85	121.42
1	B	387	HIS	O-C-N	7.00	128.84	121.42
1	H	387	HIS	O-C-N	7.00	128.84	121.42
1	L	387	HIS	O-C-N	6.99	128.83	121.42
1	J	387	HIS	O-C-N	6.98	128.82	121.42
1	A	387	HIS	O-C-N	6.98	128.82	121.42
1	E	387	HIS	O-C-N	6.98	128.82	121.42
1	C	387	HIS	O-C-N	6.97	128.81	121.42
1	I	387	HIS	O-C-N	6.95	128.79	121.42
1	G	387	HIS	O-C-N	6.94	128.77	121.42
1	K	387	HIS	O-C-N	6.94	128.77	121.42
1	F	387	HIS	O-C-N	6.92	128.76	121.42
1	G	64	ASP	N-CA-C	6.60	120.04	110.28
1	E	64	ASP	N-CA-C	6.59	120.04	110.28
1	B	64	ASP	N-CA-C	6.59	120.03	110.28
1	I	64	ASP	N-CA-C	6.59	120.03	110.28
1	K	64	ASP	N-CA-C	6.58	120.02	110.28
1	C	64	ASP	N-CA-C	6.58	120.02	110.28
1	F	64	ASP	N-CA-C	6.58	120.02	110.28
1	A	64	ASP	N-CA-C	6.57	120.01	110.28
1	J	64	ASP	N-CA-C	6.57	120.00	110.28
1	H	64	ASP	N-CA-C	6.56	119.99	110.28
1	D	64	ASP	N-CA-C	6.56	119.98	110.28
1	B	63	SER	N-CA-C	6.55	118.97	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	98	GLN	CG-CD-NE2	6.55	126.22	116.40
1	J	98	GLN	CG-CD-NE2	6.55	126.22	116.40
1	L	64	ASP	N-CA-C	6.55	119.97	110.28
1	I	98	GLN	CG-CD-NE2	6.53	126.20	116.40
1	E	63	SER	N-CA-C	6.53	118.94	111.11
1	L	98	GLN	CG-CD-NE2	6.53	126.19	116.40
1	B	98	GLN	CG-CD-NE2	6.52	126.19	116.40
1	H	98	GLN	CG-CD-NE2	6.52	126.19	116.40
1	A	98	GLN	CG-CD-NE2	6.52	126.19	116.40
1	C	98	GLN	CG-CD-NE2	6.52	126.18	116.40
1	F	63	SER	N-CA-C	6.52	118.93	111.11
1	I	63	SER	N-CA-C	6.51	118.92	111.11
1	K	98	GLN	CG-CD-NE2	6.51	126.16	116.40
1	H	63	SER	N-CA-C	6.50	118.91	111.11
1	L	63	SER	N-CA-C	6.50	118.91	111.11
1	A	63	SER	N-CA-C	6.50	118.91	111.11
1	D	98	GLN	CG-CD-NE2	6.50	126.15	116.40
1	G	98	GLN	CG-CD-NE2	6.50	126.14	116.40
1	D	63	SER	N-CA-C	6.49	118.90	111.11
1	G	63	SER	N-CA-C	6.49	118.90	111.11
1	K	63	SER	N-CA-C	6.49	118.90	111.11
1	J	63	SER	N-CA-C	6.49	118.90	111.11
1	C	63	SER	N-CA-C	6.49	118.89	111.11
1	F	98	GLN	CG-CD-NE2	6.49	126.13	116.40
1	L	367	PRO	O-C-N	6.41	131.29	122.64
1	D	367	PRO	O-C-N	6.40	131.28	122.64
1	K	367	PRO	O-C-N	6.37	131.25	122.64
1	A	367	PRO	O-C-N	6.37	131.23	122.64
1	I	367	PRO	O-C-N	6.36	131.23	122.64
1	C	367	PRO	O-C-N	6.35	131.22	122.64
1	G	367	PRO	O-C-N	6.35	131.21	122.64
1	B	367	PRO	O-C-N	6.35	131.21	122.64
1	H	367	PRO	O-C-N	6.34	131.20	122.64
1	E	367	PRO	O-C-N	6.33	131.18	122.64
1	F	367	PRO	O-C-N	6.32	131.18	122.64
1	J	367	PRO	O-C-N	6.32	131.18	122.64
1	C	408	PRO	CA-C-N	-6.26	112.07	122.21
1	C	408	PRO	C-N-CA	-6.26	112.07	122.21
1	B	408	PRO	CA-C-N	-6.24	112.10	122.21
1	B	408	PRO	C-N-CA	-6.24	112.10	122.21
1	L	218	GLN	CG-CD-NE2	6.24	125.76	116.40
1	E	188	ALA	N-CA-C	6.24	120.49	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	408	PRO	CA-C-N	-6.23	112.12	122.21
1	K	408	PRO	C-N-CA	-6.23	112.12	122.21
1	B	218	GLN	CG-CD-NE2	6.23	125.74	116.40
1	J	218	GLN	CG-CD-NE2	6.23	125.74	116.40
1	H	218	GLN	CG-CD-NE2	6.22	125.74	116.40
1	J	408	PRO	CA-C-N	-6.22	112.13	122.21
1	J	408	PRO	C-N-CA	-6.22	112.13	122.21
1	K	218	GLN	CG-CD-NE2	6.22	125.74	116.40
1	C	218	GLN	CG-CD-NE2	6.22	125.73	116.40
1	H	408	PRO	CA-C-N	-6.22	112.13	122.21
1	H	408	PRO	C-N-CA	-6.22	112.13	122.21
1	L	408	PRO	CA-C-N	-6.22	112.13	122.21
1	L	408	PRO	C-N-CA	-6.22	112.13	122.21
1	K	188	ALA	N-CA-C	6.22	120.47	112.26
1	A	218	GLN	CG-CD-NE2	6.22	125.73	116.40
1	E	218	GLN	CG-CD-NE2	6.22	125.73	116.40
1	E	408	PRO	CA-C-N	-6.22	112.14	122.21
1	E	408	PRO	C-N-CA	-6.22	112.14	122.21
1	L	188	ALA	N-CA-C	6.22	120.47	112.26
1	A	408	PRO	CA-C-N	-6.22	112.14	122.21
1	A	408	PRO	C-N-CA	-6.22	112.14	122.21
1	G	408	PRO	CA-C-N	-6.22	112.14	122.21
1	G	408	PRO	C-N-CA	-6.22	112.14	122.21
1	B	188	ALA	N-CA-C	6.21	120.46	112.26
1	I	218	GLN	CG-CD-NE2	6.21	125.72	116.40
1	D	218	GLN	CG-CD-NE2	6.21	125.72	116.40
1	L	124	VAL	CB-CA-C	-6.21	101.37	110.81
1	G	124	VAL	CB-CA-C	-6.21	101.38	110.81
1	F	218	GLN	CG-CD-NE2	6.20	125.70	116.40
1	A	188	ALA	N-CA-C	6.20	120.44	112.26
1	C	124	VAL	CB-CA-C	-6.20	101.39	110.81
1	F	408	PRO	CA-C-N	-6.20	112.17	122.21
1	F	408	PRO	C-N-CA	-6.20	112.17	122.21
1	G	218	GLN	CG-CD-NE2	6.20	125.70	116.40
1	D	188	ALA	N-CA-C	6.20	120.44	112.26
1	D	408	PRO	CA-C-N	-6.20	112.17	122.21
1	D	408	PRO	C-N-CA	-6.20	112.17	122.21
1	I	408	PRO	CA-C-N	-6.20	112.17	122.21
1	I	408	PRO	C-N-CA	-6.20	112.17	122.21
1	E	124	VAL	CB-CA-C	-6.20	101.39	110.81
1	B	124	VAL	CB-CA-C	-6.19	101.39	110.81
1	H	124	VAL	CB-CA-C	-6.19	101.40	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	188	ALA	N-CA-C	6.19	120.43	112.26
1	A	124	VAL	CB-CA-C	-6.19	101.40	110.81
1	C	188	ALA	N-CA-C	6.18	120.42	112.26
1	J	188	ALA	N-CA-C	6.18	120.42	112.26
1	D	124	VAL	CB-CA-C	-6.17	101.42	110.81
1	I	188	ALA	N-CA-C	6.17	120.41	112.26
1	G	188	ALA	N-CA-C	6.17	120.41	112.26
1	F	188	ALA	N-CA-C	6.17	120.41	112.26
1	I	124	VAL	CB-CA-C	-6.17	101.43	110.81
1	F	124	VAL	CB-CA-C	-6.17	101.44	110.81
1	K	124	VAL	CB-CA-C	-6.16	101.44	110.81
1	J	124	VAL	CB-CA-C	-6.16	101.45	110.81
1	F	361	PRO	CB-CA-C	5.84	118.87	111.39
1	K	361	PRO	CB-CA-C	5.84	118.87	111.39
1	I	265	GLY	N-CA-C	-5.83	103.36	112.58
1	L	361	PRO	CB-CA-C	5.83	118.86	111.39
1	B	361	PRO	CB-CA-C	5.83	118.85	111.39
1	B	265	GLY	N-CA-C	-5.83	103.38	112.58
1	D	361	PRO	CB-CA-C	5.83	118.85	111.39
1	C	408	PRO	N-CA-C	5.82	120.75	111.26
1	G	361	PRO	CB-CA-C	5.82	118.84	111.39
1	B	408	PRO	N-CA-C	5.82	120.75	111.26
1	C	265	GLY	N-CA-C	-5.82	103.39	112.58
1	H	265	GLY	N-CA-C	-5.82	103.38	112.58
1	F	265	GLY	N-CA-C	-5.82	103.39	112.58
1	I	361	PRO	CB-CA-C	5.82	118.84	111.39
1	A	361	PRO	CB-CA-C	5.82	118.83	111.39
1	D	265	GLY	N-CA-C	-5.82	103.39	112.58
1	E	408	PRO	N-CA-C	5.82	120.74	111.26
1	E	265	GLY	N-CA-C	-5.81	103.39	112.58
1	A	265	GLY	N-CA-C	-5.81	103.40	112.58
1	L	265	GLY	N-CA-C	-5.81	103.41	112.58
1	H	361	PRO	CB-CA-C	5.80	118.82	111.39
1	G	265	GLY	N-CA-C	-5.80	103.41	112.58
1	L	408	PRO	N-CA-C	5.80	120.71	111.26
1	A	408	PRO	N-CA-C	5.80	120.71	111.26
1	E	361	PRO	CB-CA-C	5.80	118.81	111.39
1	K	408	PRO	N-CA-C	5.80	120.71	111.26
1	J	265	GLY	N-CA-C	-5.79	103.43	112.58
1	J	408	PRO	N-CA-C	5.79	120.70	111.26
1	I	408	PRO	N-CA-C	5.79	120.70	111.26
1	C	361	PRO	CB-CA-C	5.79	118.80	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	408	PRO	N-CA-C	5.79	120.70	111.26
1	J	361	PRO	CB-CA-C	5.79	118.80	111.39
1	H	408	PRO	N-CA-C	5.79	120.69	111.26
1	K	265	GLY	N-CA-C	-5.79	103.44	112.58
1	F	408	PRO	N-CA-C	5.78	120.68	111.26
1	D	408	PRO	N-CA-C	5.78	120.68	111.26
1	H	359	ARG	N-CA-C	5.71	120.31	113.23
1	L	359	ARG	N-CA-C	5.71	120.31	113.23
1	F	359	ARG	N-CA-C	5.71	120.31	113.23
1	I	359	ARG	N-CA-C	5.70	120.30	113.23
1	B	359	ARG	N-CA-C	5.70	120.30	113.23
1	D	359	ARG	N-CA-C	5.70	120.30	113.23
1	K	359	ARG	N-CA-C	5.70	120.29	113.23
1	A	359	ARG	N-CA-C	5.69	120.29	113.23
1	C	359	ARG	N-CA-C	5.69	120.28	113.23
1	E	359	ARG	N-CA-C	5.67	120.26	113.23
1	G	359	ARG	N-CA-C	5.66	120.25	113.23
1	J	359	ARG	N-CA-C	5.65	120.24	113.23
1	J	233	ASP	N-CA-C	-5.62	105.05	111.07
1	K	389	GLY	N-CA-C	-5.62	102.64	112.53
1	J	389	GLY	N-CA-C	-5.61	102.66	112.53
1	K	462	PHE	CA-CB-CG	-5.61	108.19	113.80
1	B	389	GLY	N-CA-C	-5.61	102.66	112.53
1	C	233	ASP	N-CA-C	-5.61	105.07	111.07
1	H	462	PHE	CA-CB-CG	-5.60	108.20	113.80
1	C	462	PHE	CA-CB-CG	-5.60	108.20	113.80
1	D	389	GLY	N-CA-C	-5.60	102.67	112.53
1	G	389	GLY	N-CA-C	-5.60	102.67	112.53
1	L	462	PHE	CA-CB-CG	-5.60	108.20	113.80
1	F	389	GLY	N-CA-C	-5.60	102.68	112.53
1	L	233	ASP	N-CA-C	-5.60	105.08	111.07
1	D	233	ASP	N-CA-C	-5.59	105.08	111.07
1	E	389	GLY	N-CA-C	-5.59	102.68	112.53
1	G	233	ASP	N-CA-C	-5.59	105.08	111.07
1	A	389	GLY	N-CA-C	-5.59	102.69	112.53
1	I	389	GLY	N-CA-C	-5.59	102.69	112.53
1	I	462	PHE	CA-CB-CG	-5.59	108.21	113.80
1	C	389	GLY	N-CA-C	-5.59	102.70	112.53
1	D	462	PHE	CA-CB-CG	-5.59	108.21	113.80
1	E	233	ASP	N-CA-C	-5.59	105.09	111.07
1	G	462	PHE	CA-CB-CG	-5.59	108.21	113.80
1	H	389	GLY	N-CA-C	-5.59	102.70	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASP	N-CA-C	-5.58	105.10	111.07
1	I	233	ASP	N-CA-C	-5.58	105.10	111.07
1	B	233	ASP	N-CA-C	-5.58	105.10	111.07
1	A	462	PHE	CA-CB-CG	-5.58	108.22	113.80
1	J	462	PHE	CA-CB-CG	-5.58	108.22	113.80
1	K	233	ASP	N-CA-C	-5.57	105.11	111.07
1	L	389	GLY	N-CA-C	-5.57	102.73	112.53
1	F	233	ASP	N-CA-C	-5.56	105.12	111.07
1	F	462	PHE	CA-CB-CG	-5.56	108.24	113.80
1	H	233	ASP	N-CA-C	-5.56	105.12	111.07
1	B	462	PHE	CA-CB-CG	-5.55	108.25	113.80
1	E	462	PHE	CA-CB-CG	-5.54	108.26	113.80
1	E	319	TYR	CA-CB-CG	-5.54	103.93	113.90
1	F	319	TYR	CA-CB-CG	-5.54	103.93	113.90
1	K	319	TYR	CA-CB-CG	-5.53	103.94	113.90
1	B	319	TYR	CA-CB-CG	-5.53	103.95	113.90
1	H	319	TYR	CA-CB-CG	-5.53	103.95	113.90
1	A	319	TYR	CA-CB-CG	-5.53	103.95	113.90
1	J	319	TYR	CA-CB-CG	-5.52	103.96	113.90
1	C	319	TYR	CA-CB-CG	-5.52	103.96	113.90
1	L	319	TYR	CA-CB-CG	-5.52	103.96	113.90
1	G	319	TYR	CA-CB-CG	-5.52	103.96	113.90
1	I	319	TYR	CA-CB-CG	-5.52	103.96	113.90
1	D	319	TYR	CA-CB-CG	-5.51	103.98	113.90
1	K	314	PRO	N-CA-C	5.37	120.26	114.68
1	D	314	PRO	N-CA-C	5.36	120.25	114.68
1	G	314	PRO	N-CA-C	5.33	120.23	114.68
1	E	314	PRO	N-CA-C	5.33	120.22	114.68
1	A	314	PRO	N-CA-C	5.33	120.22	114.68
1	L	314	PRO	N-CA-C	5.33	120.22	114.68
1	C	314	PRO	N-CA-C	5.33	120.22	114.68
1	B	314	PRO	N-CA-C	5.32	120.22	114.68
1	F	314	PRO	N-CA-C	5.32	120.21	114.68
1	H	314	PRO	N-CA-C	5.32	120.21	114.68
1	F	20	ARG	N-CA-C	5.29	118.18	109.72
1	H	20	ARG	N-CA-C	5.28	118.17	109.72
1	F	404	ALA	N-CA-C	-5.28	105.69	113.72
1	J	314	PRO	N-CA-C	5.28	120.17	114.68
1	L	20	ARG	N-CA-C	5.28	118.17	109.72
1	I	20	ARG	N-CA-C	5.28	118.17	109.72
1	I	314	PRO	N-CA-C	5.28	120.17	114.68
1	J	404	ALA	N-CA-C	-5.28	105.70	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	20	ARG	N-CA-C	5.28	118.16	109.72
1	I	404	ALA	N-CA-C	-5.27	105.71	113.72
1	B	20	ARG	N-CA-C	5.27	118.15	109.72
1	E	43	PHE	N-CA-C	5.27	117.93	111.82
1	D	404	ALA	N-CA-C	-5.27	105.71	113.72
1	A	20	ARG	N-CA-C	5.26	118.14	109.72
1	D	20	ARG	N-CA-C	5.26	118.14	109.72
1	E	330	VAL	N-CA-C	5.26	119.69	113.22
1	A	404	ALA	N-CA-C	-5.26	105.72	113.72
1	C	330	VAL	N-CA-C	5.26	119.69	113.22
1	C	404	ALA	N-CA-C	-5.26	105.73	113.72
1	E	20	ARG	N-CA-C	5.26	118.13	109.72
1	C	43	PHE	N-CA-C	5.26	117.92	111.82
1	K	330	VAL	N-CA-C	5.26	119.69	113.22
1	C	20	ARG	N-CA-C	5.26	118.13	109.72
1	G	330	VAL	N-CA-C	5.26	119.69	113.22
1	J	43	PHE	N-CA-C	5.25	117.91	111.82
1	B	404	ALA	N-CA-C	-5.25	105.74	113.72
1	D	43	PHE	N-CA-C	5.25	117.91	111.82
1	G	404	ALA	N-CA-C	-5.25	105.74	113.72
1	K	20	ARG	N-CA-C	5.25	118.12	109.72
1	E	404	ALA	N-CA-C	-5.25	105.75	113.72
1	H	43	PHE	N-CA-C	5.25	117.91	111.82
1	I	43	PHE	N-CA-C	5.25	117.91	111.82
1	L	404	ALA	N-CA-C	-5.25	105.75	113.72
1	G	43	PHE	N-CA-C	5.24	117.90	111.82
1	L	43	PHE	N-CA-C	5.24	117.90	111.82
1	G	20	ARG	N-CA-C	5.24	118.11	109.72
1	I	330	VAL	N-CA-C	5.24	119.67	113.22
1	H	404	ALA	N-CA-C	-5.24	105.76	113.72
1	G	98	GLN	N-CA-C	5.24	117.99	111.24
1	A	43	PHE	N-CA-C	5.23	117.89	111.82
1	K	404	ALA	N-CA-C	-5.23	105.77	113.72
1	A	330	VAL	N-CA-C	5.23	119.65	113.22
1	F	43	PHE	N-CA-C	5.23	117.89	111.82
1	J	330	VAL	N-CA-C	5.23	119.65	113.22
1	B	43	PHE	N-CA-C	5.23	117.88	111.82
1	B	330	VAL	N-CA-C	5.23	119.65	113.22
1	F	98	GLN	N-CA-C	5.22	117.97	111.24
1	F	330	VAL	N-CA-C	5.22	119.64	113.22
1	B	98	GLN	N-CA-C	5.21	117.96	111.24
1	D	330	VAL	N-CA-C	5.21	119.63	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	43	PHE	N-CA-C	5.21	117.87	111.82
1	L	330	VAL	N-CA-C	5.21	119.63	113.22
1	H	330	VAL	N-CA-C	5.21	119.62	113.22
1	E	98	GLN	N-CA-C	5.20	117.95	111.24
1	J	98	GLN	N-CA-C	5.20	117.95	111.24
1	H	98	GLN	N-CA-C	5.20	117.94	111.24
1	A	98	GLN	N-CA-C	5.19	117.93	111.24
1	I	98	GLN	N-CA-C	5.19	117.93	111.24
1	B	388	PRO	CA-N-CD	-5.18	104.75	112.00
1	C	98	GLN	N-CA-C	5.17	117.91	111.24
1	D	98	GLN	N-CA-C	5.17	117.91	111.24
1	E	388	PRO	CA-N-CD	-5.17	104.76	112.00
1	K	98	GLN	N-CA-C	5.17	117.91	111.24
1	F	388	PRO	CA-N-CD	-5.16	104.78	112.00
1	J	388	PRO	CA-N-CD	-5.16	104.78	112.00
1	L	98	GLN	N-CA-C	5.16	117.89	111.24
1	H	388	PRO	CA-N-CD	-5.16	104.78	112.00
1	L	90	ASP	N-CA-C	-5.15	102.16	110.14
1	A	388	PRO	CA-N-CD	-5.14	104.80	112.00
1	D	388	PRO	CA-N-CD	-5.14	104.80	112.00
1	G	287	TYR	N-CA-C	5.14	117.93	110.42
1	I	287	TYR	N-CA-C	5.14	117.92	110.42
1	I	388	PRO	CA-N-CD	-5.14	104.80	112.00
1	K	90	ASP	N-CA-C	-5.14	102.17	110.14
1	K	388	PRO	CA-N-CD	-5.14	104.81	112.00
1	L	388	PRO	CA-N-CD	-5.13	104.81	112.00
1	C	388	PRO	CA-N-CD	-5.13	104.82	112.00
1	C	90	ASP	N-CA-C	-5.12	102.20	110.14
1	G	388	PRO	CA-N-CD	-5.12	104.83	112.00
1	D	93	GLU	N-CA-C	-5.12	103.33	109.83
1	B	287	TYR	N-CA-C	5.12	117.89	110.42
1	J	287	TYR	N-CA-C	5.11	117.89	110.42
1	E	93	GLU	N-CA-C	-5.11	103.34	109.83
1	G	93	GLU	N-CA-C	-5.11	103.34	109.83
1	A	90	ASP	N-CA-C	-5.11	102.22	110.14
1	E	90	ASP	N-CA-C	-5.11	102.22	110.14
1	H	287	TYR	N-CA-C	5.11	117.88	110.42
1	F	287	TYR	N-CA-C	5.11	117.88	110.42
1	I	90	ASP	N-CA-C	-5.11	102.22	110.14
1	A	287	TYR	N-CA-C	5.11	117.87	110.42
1	E	287	TYR	N-CA-C	5.11	117.87	110.42
1	G	90	ASP	N-CA-C	-5.11	102.23	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	90	ASP	N-CA-C	-5.11	102.23	110.14
1	C	287	TYR	N-CA-C	5.10	117.87	110.42
1	H	90	ASP	N-CA-C	-5.10	102.24	110.14
1	L	287	TYR	N-CA-C	5.10	117.87	110.42
1	D	90	ASP	N-CA-C	-5.10	102.24	110.14
1	J	93	GLU	N-CA-C	-5.10	103.36	109.83
1	B	90	ASP	N-CA-C	-5.09	102.24	110.14
1	F	90	ASP	N-CA-C	-5.09	102.24	110.14
1	I	93	GLU	N-CA-C	-5.09	103.37	109.83
1	K	287	TYR	N-CA-C	5.09	117.85	110.42
1	C	93	GLU	N-CA-C	-5.08	103.37	109.83
1	A	93	GLU	N-CA-C	-5.08	103.37	109.83
1	F	93	GLU	N-CA-C	-5.08	103.38	109.83
1	H	93	GLU	N-CA-C	-5.08	103.39	109.83
1	K	93	GLU	N-CA-C	-5.08	103.38	109.83
1	D	287	TYR	N-CA-C	5.07	117.83	110.42
1	L	93	GLU	N-CA-C	-5.07	103.39	109.83
1	B	93	GLU	N-CA-C	-5.06	103.40	109.83
1	E	403	GLU	N-CA-C	-5.03	107.64	112.97
1	I	403	GLU	N-CA-C	-5.02	107.64	112.97
1	J	403	GLU	N-CA-C	-5.02	107.64	112.97
1	D	403	GLU	N-CA-C	-5.00	107.67	112.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3637	0	3544	212	0
1	B	3637	0	3544	208	0
1	C	3637	0	3544	209	0
1	D	3637	0	3544	207	0
1	E	3637	0	3544	198	0
1	F	3637	0	3544	216	0
1	G	3637	0	3544	206	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3637	0	3544	213	0
1	I	3637	0	3544	212	0
1	J	3637	0	3544	223	0
1	K	3637	0	3544	222	0
1	L	3637	0	3544	217	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	1	0
3	B	27	0	10	1	0
3	C	27	0	10	1	0
3	D	27	0	10	1	0
3	E	27	0	10	1	0
3	F	27	0	10	1	0
3	G	27	0	10	1	0
3	H	27	0	10	1	0
3	I	27	0	10	1	0
3	J	27	0	10	1	0
3	K	27	0	10	1	0
3	L	27	0	10	1	0
4	A	16	0	27	52	0
4	B	16	0	27	57	0
4	C	16	0	27	60	0
4	D	16	0	27	58	0
4	E	16	0	27	51	0
4	F	16	0	27	59	0
4	G	16	0	27	57	0
4	H	16	0	27	61	0
4	I	16	0	27	59	0
4	J	16	0	27	64	0
4	K	16	0	27	62	0
4	L	16	0	27	61	0
5	A	294	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	297	0	0	7	0
5	C	293	0	0	7	0
5	D	295	0	0	8	0
5	E	294	0	0	7	0
5	F	293	0	0	7	0
5	G	288	0	0	8	0
5	H	288	0	0	6	0
5	I	295	0	0	7	0
5	J	287	0	0	8	0
5	K	288	0	0	7	0
5	L	292	0	0	7	0
All	All	47688	0	42972	2391	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 27.

All (2391) 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)
1:J:84:THR:HG21	4:J:5491:MPD:C5	1.53	1.36
1:F:84:THR:HG21	4:F:5479:MPD:C5	1.57	1.32
1:J:84:THR:CG2	4:J:5491:MPD:H52	1.60	1.32
1:L:84:THR:HG21	4:L:5483:MPD:C5	1.60	1.31
1:I:61:ASN:O	1:J:337:ARG:HB2	1.29	1.29
1:H:80:PHE:CB	4:H:5487:MPD:H12	1.63	1.28
1:F:84:THR:CG2	4:F:5479:MPD:H52	1.63	1.28
1:B:84:THR:HG21	4:B:5471:MPD:C5	1.63	1.27
1:G:84:THR:HG21	4:G:5485:MPD:C5	1.65	1.27
1:I:84:THR:HG21	4:I:5489:MPD:C5	1.64	1.26
1:L:80:PHE:CB	4:L:5483:MPD:H12	1.65	1.25
1:G:61:ASN:O	1:H:337:ARG:HB2	1.35	1.25
1:K:84:THR:HG21	4:K:5493:MPD:C5	1.65	1.25
1:E:84:THR:HG21	4:E:5477:MPD:C5	1.66	1.24
1:J:80:PHE:CB	4:J:5491:MPD:H12	1.66	1.24
1:D:84:THR:HG21	4:D:5475:MPD:C5	1.66	1.23
1:E:84:THR:CG2	4:E:5477:MPD:H52	1.68	1.23
1:A:337:ARG:HB2	1:B:61:ASN:O	1.36	1.22
1:C:337:ARG:HB2	1:D:61:ASN:O	1.37	1.22
1:L:84:THR:CG2	4:L:5483:MPD:H52	1.66	1.22
1:F:80:PHE:CB	4:F:5479:MPD:H12	1.69	1.22
1:C:84:THR:HG21	4:C:5473:MPD:C5	1.68	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:THR:CG2	4:B:5471:MPD:H52	1.68	1.22
1:H:84:THR:HG21	4:H:5487:MPD:C5	1.69	1.21
1:G:84:THR:CG2	4:G:5485:MPD:H52	1.69	1.21
1:D:84:THR:CG2	4:D:5475:MPD:H52	1.70	1.20
1:A:84:THR:HG21	4:A:5481:MPD:C5	1.70	1.20
1:K:84:THR:CG2	4:K:5493:MPD:H52	1.70	1.20
1:C:80:PHE:CB	4:C:5473:MPD:H12	1.71	1.19
1:I:84:THR:CG2	4:I:5489:MPD:H52	1.70	1.19
1:K:80:PHE:CB	4:K:5493:MPD:H12	1.71	1.19
1:C:190:ASP:HA	4:D:5475:MPD:HM3	1.19	1.19
1:A:84:THR:CG2	4:A:5481:MPD:H52	1.72	1.19
4:K:5493:MPD:HM1	1:L:193:SER:HB2	1.25	1.18
1:J:61:ASN:O	1:K:337:ARG:HB2	1.41	1.18
1:A:60:ILE:HD13	1:A:60:ILE:H	1.08	1.18
1:C:84:THR:CG2	4:C:5473:MPD:H52	1.74	1.18
1:L:80:PHE:HB3	4:L:5483:MPD:C1	1.74	1.17
1:J:60:ILE:H	1:J:60:ILE:HD13	1.08	1.17
4:G:5485:MPD:HM1	1:H:193:SER:HB2	1.25	1.16
1:G:360:PHE:CD2	1:G:361:PRO:HD3	1.81	1.16
1:I:80:PHE:CB	4:I:5489:MPD:H12	1.73	1.16
1:B:360:PHE:CD2	1:B:361:PRO:HD3	1.81	1.16
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.81	1.16
1:K:360:PHE:CD2	1:K:361:PRO:HD3	1.81	1.16
1:J:360:PHE:CD2	1:J:361:PRO:HD3	1.81	1.16
1:E:193:SER:HB2	4:F:5479:MPD:HM1	1.25	1.15
1:G:337:ARG:HB2	1:L:61:ASN:O	1.46	1.15
1:H:84:THR:CG2	4:H:5487:MPD:H52	1.76	1.15
1:J:80:PHE:HB3	4:J:5491:MPD:C1	1.73	1.15
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.81	1.15
4:A:5481:MPD:HM1	1:F:193:SER:HB2	1.25	1.15
1:B:80:PHE:CB	4:B:5471:MPD:H12	1.77	1.15
1:F:360:PHE:CD2	1:F:361:PRO:HD3	1.81	1.14
1:I:360:PHE:CD2	1:I:361:PRO:HD3	1.81	1.14
1:B:193:SER:HB2	4:C:5473:MPD:HM1	1.25	1.14
1:C:193:SER:HB2	4:D:5475:MPD:HM1	1.25	1.14
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.81	1.14
1:F:80:PHE:HB3	4:F:5479:MPD:C1	1.77	1.14
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.81	1.14
4:I:5489:MPD:HM1	1:J:193:SER:HB2	1.25	1.14
1:L:360:PHE:CD2	1:L:361:PRO:HD3	1.81	1.14
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.81	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:5485:MPD:HM3	1:H:190:ASP:HA	1.19	1.13
1:A:193:SER:HB2	4:B:5471:MPD:HM1	1.25	1.13
1:B:60:ILE:H	1:B:60:ILE:HD13	1.08	1.13
1:H:399:LEU:N	1:H:401:PRO:HG2	1.64	1.13
4:H:5487:MPD:HM3	1:I:190:ASP:HA	1.19	1.13
1:J:399:LEU:N	1:J:401:PRO:HG2	1.64	1.13
1:C:399:LEU:N	1:C:401:PRO:HG2	1.64	1.12
1:D:193:SER:HB2	4:E:5477:MPD:HM1	1.25	1.13
1:E:60:ILE:HD13	1:E:60:ILE:H	1.08	1.12
4:I:5489:MPD:HM3	1:J:190:ASP:HA	1.19	1.12
1:E:190:ASP:HA	4:F:5479:MPD:HM3	1.19	1.12
1:G:193:SER:HB2	4:L:5483:MPD:HM1	1.25	1.12
1:L:399:LEU:N	1:L:401:PRO:HG2	1.64	1.12
1:A:190:ASP:HA	4:B:5471:MPD:HM3	1.19	1.12
1:H:60:ILE:HD13	1:H:60:ILE:H	1.08	1.12
1:K:60:ILE:HD13	1:K:60:ILE:H	1.08	1.12
1:F:60:ILE:HD13	1:F:60:ILE:H	1.08	1.12
1:H:80:PHE:HB3	4:H:5487:MPD:C1	1.77	1.12
4:J:5491:MPD:HM3	1:K:190:ASP:HA	1.19	1.12
4:K:5493:MPD:HM3	1:L:190:ASP:HA	1.19	1.12
1:E:399:LEU:N	1:E:401:PRO:HG2	1.64	1.12
1:G:399:LEU:N	1:G:401:PRO:HG2	1.64	1.12
1:B:399:LEU:N	1:B:401:PRO:HG2	1.64	1.11
1:F:399:LEU:H	1:F:401:PRO:HG2	0.95	1.11
1:F:399:LEU:N	1:F:401:PRO:HG2	1.64	1.11
1:G:60:ILE:H	1:G:60:ILE:HD13	1.08	1.11
1:I:399:LEU:N	1:I:401:PRO:HG2	1.64	1.11
4:A:5481:MPD:HM3	1:F:190:ASP:HA	1.19	1.11
1:A:399:LEU:N	1:A:401:PRO:HG2	1.64	1.11
1:D:80:PHE:CB	4:D:5475:MPD:H12	1.79	1.11
1:D:399:LEU:N	1:D:401:PRO:HG2	1.64	1.11
1:E:399:LEU:H	1:E:401:PRO:HG2	0.95	1.11
1:K:80:PHE:HB3	4:K:5493:MPD:C1	1.81	1.10
1:A:399:LEU:H	1:A:401:PRO:HG2	0.95	1.10
4:J:5491:MPD:HM1	1:K:193:SER:HB2	1.25	1.10
1:K:399:LEU:N	1:K:401:PRO:HG2	1.64	1.10
1:C:400:PRO:HB3	1:C:405:LYS:HE3	1.34	1.09
1:G:22:THR:N	4:G:5484:MPD:H52	1.67	1.09
1:G:190:ASP:HA	4:L:5483:MPD:HM3	1.19	1.09
1:B:190:ASP:HA	4:C:5473:MPD:HM3	1.19	1.09
1:C:60:ILE:HD13	1:C:60:ILE:H	1.08	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ILE:HD13	1:L:60:ILE:H	1.08	1.09
1:A:400:PRO:HB3	1:A:405:LYS:HE3	1.35	1.09
1:E:22:THR:N	4:E:5480:MPD:H52	1.67	1.09
4:H:5487:MPD:HM1	1:I:193:SER:HB2	1.25	1.09
1:B:22:THR:N	4:B:5474:MPD:H52	1.67	1.09
1:D:190:ASP:HA	4:E:5477:MPD:HM3	1.19	1.09
1:E:400:PRO:HB3	1:E:405:LYS:HE3	1.35	1.09
1:F:22:THR:N	4:F:5482:MPD:H52	1.67	1.09
1:I:22:THR:N	4:I:5488:MPD:H52	1.67	1.09
1:K:400:PRO:HB3	1:K:405:LYS:HE3	1.35	1.09
1:D:22:THR:N	4:D:5478:MPD:H52	1.67	1.09
1:K:22:THR:N	4:K:5492:MPD:H52	1.67	1.09
1:G:400:PRO:HB3	1:G:405:LYS:HE3	1.35	1.08
1:I:60:ILE:HD13	1:I:60:ILE:H	1.08	1.08
1:J:22:THR:N	4:J:5490:MPD:H52	1.67	1.08
1:C:399:LEU:H	1:C:401:PRO:HG2	0.95	1.08
1:C:22:THR:N	4:C:5476:MPD:H52	1.67	1.08
1:H:22:THR:N	4:H:5486:MPD:H52	1.67	1.08
1:J:399:LEU:H	1:J:401:PRO:HG2	0.95	1.08
1:I:400:PRO:HB3	1:I:405:LYS:HE3	1.35	1.08
1:D:60:ILE:H	1:D:60:ILE:HD13	1.08	1.08
1:G:399:LEU:H	1:G:401:PRO:HG2	0.95	1.07
1:L:399:LEU:H	1:L:401:PRO:HG2	0.95	1.07
1:J:400:PRO:HB3	1:J:405:LYS:HE3	1.35	1.07
1:A:22:THR:N	4:A:5472:MPD:H52	1.67	1.07
1:A:61:ASN:O	1:F:337:ARG:HB2	1.54	1.07
1:H:400:PRO:HB3	1:H:405:LYS:HE3	1.35	1.07
1:I:399:LEU:H	1:I:401:PRO:HG2	0.95	1.07
1:L:22:THR:N	4:L:5494:MPD:H52	1.67	1.07
1:B:400:PRO:HB3	1:B:405:LYS:HE3	1.35	1.06
1:C:80:PHE:HB3	4:C:5473:MPD:C1	1.84	1.06
1:F:400:PRO:HB3	1:F:405:LYS:HE3	1.35	1.06
1:I:80:PHE:HB3	4:I:5489:MPD:C1	1.84	1.06
1:A:21:PHE:HB2	4:A:5472:MPD:H53	1.38	1.06
1:D:21:PHE:HB2	4:D:5478:MPD:H53	1.38	1.06
1:D:399:LEU:H	1:D:401:PRO:HG2	0.95	1.06
1:H:21:PHE:HB2	4:H:5486:MPD:H53	1.38	1.06
1:H:399:LEU:H	1:H:401:PRO:HG2	0.95	1.06
1:K:21:PHE:HB2	4:K:5492:MPD:H53	1.38	1.06
1:B:399:LEU:H	1:B:401:PRO:HG2	0.95	1.06
1:H:22:THR:OG1	4:H:5486:MPD:H13	1.56	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:399:LEU:H	1:K:401:PRO:HG2	0.95	1.05
1:B:21:PHE:HB2	4:B:5474:MPD:H53	1.38	1.05
1:E:22:THR:OG1	4:E:5480:MPD:H13	1.56	1.05
1:G:80:PHE:CB	4:G:5485:MPD:H12	1.85	1.05
1:L:21:PHE:HB2	4:L:5494:MPD:H53	1.38	1.05
1:L:400:PRO:HB3	1:L:405:LYS:HE3	1.35	1.05
1:A:22:THR:OG1	4:A:5472:MPD:H13	1.56	1.05
1:B:80:PHE:HB3	4:B:5471:MPD:C1	1.86	1.05
1:E:21:PHE:HB2	4:E:5480:MPD:H53	1.38	1.05
1:I:21:PHE:HB2	4:I:5488:MPD:H53	1.38	1.05
1:A:80:PHE:CB	4:A:5481:MPD:H12	1.86	1.05
1:C:22:THR:OG1	4:C:5476:MPD:H13	1.56	1.05
1:F:22:THR:OG1	4:F:5482:MPD:H13	1.56	1.04
1:D:80:PHE:HB3	4:D:5475:MPD:C1	1.88	1.04
1:F:21:PHE:HB2	4:F:5482:MPD:H53	1.38	1.04
1:K:22:THR:OG1	4:K:5492:MPD:H13	1.56	1.04
1:A:22:THR:H	4:A:5472:MPD:C5	1.71	1.04
1:D:22:THR:OG1	4:D:5478:MPD:H13	1.56	1.04
1:G:80:PHE:HB3	4:G:5485:MPD:H12	1.05	1.04
1:B:22:THR:H	4:B:5474:MPD:C5	1.71	1.03
1:I:22:THR:H	4:I:5488:MPD:C5	1.71	1.03
1:J:21:PHE:HB2	4:J:5490:MPD:H53	1.38	1.03
1:J:22:THR:OG1	4:J:5490:MPD:H13	1.56	1.03
1:K:22:THR:H	4:K:5492:MPD:C5	1.71	1.03
1:G:22:THR:H	4:G:5484:MPD:C5	1.71	1.03
1:L:22:THR:OG1	4:L:5494:MPD:H13	1.56	1.03
1:C:21:PHE:HB2	4:C:5476:MPD:H53	1.38	1.03
1:D:400:PRO:HB3	1:D:405:LYS:HE3	1.35	1.03
1:E:22:THR:H	4:E:5480:MPD:C5	1.71	1.03
1:I:22:THR:OG1	4:I:5488:MPD:H13	1.56	1.03
1:L:22:THR:H	4:L:5494:MPD:C5	1.71	1.03
1:C:22:THR:H	4:C:5476:MPD:C5	1.71	1.02
1:B:22:THR:OG1	4:B:5474:MPD:H13	1.56	1.02
1:D:22:THR:H	4:D:5478:MPD:C5	1.71	1.02
1:J:22:THR:H	4:J:5490:MPD:C5	1.71	1.02
1:G:21:PHE:HB2	4:G:5484:MPD:H53	1.38	1.02
1:B:337:ARG:HB2	1:C:61:ASN:O	1.60	1.02
1:H:22:THR:H	4:H:5486:MPD:C5	1.71	1.02
1:G:22:THR:OG1	4:G:5484:MPD:H13	1.56	1.01
1:E:80:PHE:CB	4:E:5477:MPD:H12	1.89	1.01
1:E:80:PHE:HB3	4:E:5477:MPD:H12	1.04	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:THR:H	4:F:5482:MPD:C5	1.71	1.01
1:I:22:THR:HG1	4:I:5488:MPD:H13	1.23	1.01
1:K:61:ASN:O	1:L:337:ARG:HB2	1.61	1.01
1:H:61:ASN:O	1:I:337:ARG:HB2	1.61	1.00
1:D:337:ARG:HB2	1:E:61:ASN:O	1.60	1.00
1:A:80:PHE:HB3	4:A:5481:MPD:C1	1.93	0.99
1:A:80:PHE:HB3	4:A:5481:MPD:H12	1.00	0.99
1:G:80:PHE:HB3	4:G:5485:MPD:C1	1.93	0.98
1:C:22:THR:H	4:C:5476:MPD:H52	0.82	0.98
1:L:22:THR:H	4:L:5494:MPD:H52	0.81	0.98
1:E:80:PHE:HB3	4:E:5477:MPD:C1	1.94	0.97
1:E:337:ARG:HB2	1:F:61:ASN:O	1.61	0.97
1:A:22:THR:H	4:A:5472:MPD:H52	0.82	0.97
1:B:80:PHE:HB3	4:B:5471:MPD:H12	0.97	0.97
1:D:22:THR:H	4:D:5478:MPD:H52	0.82	0.97
1:E:22:THR:H	4:E:5480:MPD:H52	0.82	0.97
1:K:22:THR:H	4:K:5492:MPD:H52	0.82	0.97
1:B:22:THR:H	4:B:5474:MPD:H52	0.81	0.96
1:F:22:THR:H	4:F:5482:MPD:H52	0.81	0.96
1:D:80:PHE:HB3	4:D:5475:MPD:H12	0.97	0.96
1:J:22:THR:H	4:J:5490:MPD:H52	0.81	0.96
1:C:80:PHE:HB3	4:C:5473:MPD:H12	0.96	0.95
1:H:22:THR:H	4:H:5486:MPD:H52	0.82	0.95
1:I:22:THR:H	4:I:5488:MPD:H52	0.81	0.95
1:I:80:PHE:HB3	4:I:5489:MPD:H12	0.97	0.95
1:C:235:ILE:HG21	1:C:367:PRO:HG3	1.49	0.95
1:G:22:THR:H	4:G:5484:MPD:H52	0.82	0.95
1:K:235:ILE:HG21	1:K:367:PRO:HG3	1.49	0.94
1:B:235:ILE:HG21	1:B:367:PRO:HG3	1.49	0.94
1:I:235:ILE:HG21	1:I:367:PRO:HG3	1.49	0.94
1:H:80:PHE:CD1	4:H:5487:MPD:C5	2.51	0.94
1:J:235:ILE:HG21	1:J:367:PRO:HG3	1.49	0.94
1:G:190:ASP:OD2	4:L:5483:MPD:H13	1.68	0.94
4:A:5481:MPD:H13	1:F:190:ASP:OD2	1.68	0.94
1:C:190:ASP:OD2	4:D:5475:MPD:H13	1.68	0.94
1:F:235:ILE:HG21	1:F:367:PRO:HG3	1.49	0.93
1:G:235:ILE:HG21	1:G:367:PRO:HG3	1.49	0.93
1:L:235:ILE:HG21	1:L:367:PRO:HG3	1.49	0.93
1:A:398:ASP:O	1:A:399:LEU:C	2.11	0.93
1:I:398:ASP:O	1:I:399:LEU:C	2.11	0.93
1:H:84:THR:HG21	4:H:5487:MPD:H52	0.93	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:ILE:H	1:J:60:ILE:CD1	1.82	0.93
1:E:190:ASP:OD2	4:F:5479:MPD:H13	1.68	0.92
4:I:5489:MPD:H13	1:J:190:ASP:OD2	1.68	0.92
4:K:5493:MPD:H13	1:L:190:ASP:OD2	1.68	0.92
1:A:235:ILE:HG21	1:A:367:PRO:HG3	1.49	0.92
1:E:398:ASP:O	1:E:399:LEU:C	2.11	0.92
1:L:398:ASP:O	1:L:399:LEU:C	2.11	0.92
1:G:60:ILE:H	1:G:60:ILE:CD1	1.82	0.92
1:B:190:ASP:OD2	4:C:5473:MPD:H13	1.68	0.92
1:H:80:PHE:CD1	4:H:5487:MPD:H53	2.05	0.92
4:H:5487:MPD:H13	1:I:190:ASP:OD2	1.68	0.92
1:A:190:ASP:OD2	4:B:5471:MPD:H13	1.68	0.92
1:D:398:ASP:O	1:D:399:LEU:C	2.11	0.92
1:D:235:ILE:HG21	1:D:367:PRO:HG3	1.49	0.92
1:H:235:ILE:HG21	1:H:367:PRO:HG3	1.49	0.92
1:H:398:ASP:O	1:H:399:LEU:C	2.11	0.92
1:E:235:ILE:HG21	1:E:367:PRO:HG3	1.49	0.91
1:B:398:ASP:O	1:B:399:LEU:C	2.11	0.91
1:C:60:ILE:H	1:C:60:ILE:CD1	1.82	0.91
4:G:5485:MPD:H13	1:H:190:ASP:OD2	1.68	0.91
1:H:60:ILE:H	1:H:60:ILE:CD1	1.82	0.91
4:J:5491:MPD:H13	1:K:190:ASP:OD2	1.68	0.91
1:K:60:ILE:H	1:K:60:ILE:CD1	1.82	0.91
1:D:190:ASP:OD2	4:E:5477:MPD:H13	1.68	0.91
1:B:395:ASN:HB3	1:B:400:PRO:HD2	1.54	0.90
1:G:60:ILE:HD13	1:G:60:ILE:N	1.87	0.90
1:I:60:ILE:HD13	1:I:60:ILE:N	1.87	0.90
1:K:60:ILE:HD13	1:K:60:ILE:N	1.87	0.90
1:D:60:ILE:HD13	1:D:60:ILE:N	1.87	0.90
1:E:60:ILE:HD13	1:E:60:ILE:N	1.87	0.90
1:H:60:ILE:HD13	1:H:60:ILE:N	1.87	0.90
1:I:395:ASN:HB3	1:I:400:PRO:HD2	1.54	0.90
1:J:395:ASN:HB3	1:J:400:PRO:HD2	1.54	0.90
4:K:5493:MPD:HM1	1:L:193:SER:CB	2.02	0.90
1:K:395:ASN:HB3	1:K:400:PRO:HD2	1.54	0.89
1:K:398:ASP:O	1:K:399:LEU:C	2.11	0.89
1:D:395:ASN:HB3	1:D:400:PRO:HD2	1.54	0.89
1:B:60:ILE:HD13	1:B:60:ILE:N	1.87	0.89
1:G:395:ASN:HB3	1:G:400:PRO:HD2	1.54	0.89
1:H:395:ASN:HB3	1:H:400:PRO:HD2	1.54	0.89
1:J:60:ILE:HD13	1:J:60:ILE:N	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ILE:H	1:L:60:ILE:CD1	1.82	0.89
1:I:60:ILE:H	1:I:60:ILE:CD1	1.82	0.89
1:A:193:SER:CB	4:B:5471:MPD:HM1	2.02	0.89
4:A:5481:MPD:HM1	1:F:193:SER:CB	2.02	0.89
1:B:60:ILE:H	1:B:60:ILE:CD1	1.82	0.89
1:C:395:ASN:HB3	1:C:400:PRO:HD2	1.54	0.89
1:I:80:PHE:CD1	4:I:5489:MPD:C5	2.55	0.89
1:J:398:ASP:O	1:J:399:LEU:C	2.11	0.89
1:D:193:SER:CB	4:E:5477:MPD:HM1	2.02	0.89
1:L:60:ILE:HD13	1:L:60:ILE:N	1.87	0.89
1:C:60:ILE:HD13	1:C:60:ILE:N	1.87	0.89
1:C:80:PHE:CD1	4:C:5473:MPD:C5	2.56	0.89
4:H:5487:MPD:HM1	1:I:193:SER:CB	2.02	0.89
1:J:80:PHE:CD1	4:J:5491:MPD:C5	2.56	0.89
1:A:60:ILE:H	1:A:60:ILE:CD1	1.82	0.88
1:B:193:SER:CB	4:C:5473:MPD:HM1	2.02	0.88
1:F:60:ILE:HD13	1:F:60:ILE:N	1.87	0.88
1:F:82:ASP:HB2	4:F:5479:MPD:H31	1.55	0.88
1:F:60:ILE:H	1:F:60:ILE:CD1	1.82	0.88
1:F:395:ASN:HB3	1:F:400:PRO:HD2	1.54	0.88
1:A:60:ILE:HD13	1:A:60:ILE:N	1.87	0.88
1:F:398:ASP:O	1:F:399:LEU:C	2.11	0.88
1:L:80:PHE:CD1	4:L:5483:MPD:H53	2.08	0.88
1:E:193:SER:CB	4:F:5479:MPD:HM1	2.02	0.88
4:I:5489:MPD:HM1	1:J:193:SER:CB	2.02	0.88
1:L:80:PHE:CD1	4:L:5483:MPD:C5	2.57	0.88
4:J:5491:MPD:HM1	1:K:193:SER:CB	2.02	0.88
1:F:80:PHE:HB3	4:F:5479:MPD:H12	0.89	0.88
1:G:193:SER:CB	4:L:5483:MPD:HM1	2.02	0.88
1:J:80:PHE:CD1	4:J:5491:MPD:H53	2.09	0.88
1:A:395:ASN:HB3	1:A:400:PRO:HD2	1.54	0.88
1:L:395:ASN:HB3	1:L:400:PRO:HD2	1.54	0.87
1:C:193:SER:CB	4:D:5475:MPD:HM1	2.02	0.87
4:G:5485:MPD:HM1	1:H:193:SER:CB	2.02	0.87
1:J:21:PHE:HA	4:J:5490:MPD:H31	1.56	0.87
1:F:21:PHE:HA	4:F:5482:MPD:H31	1.56	0.87
1:L:21:PHE:HA	4:L:5494:MPD:H31	1.56	0.87
1:H:80:PHE:HB3	4:H:5487:MPD:H12	0.87	0.87
1:J:84:THR:HG21	4:J:5491:MPD:C4	2.05	0.87
1:C:21:PHE:HA	4:C:5476:MPD:H31	1.57	0.87
1:E:395:ASN:HB3	1:E:400:PRO:HD2	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:ASP:HB2	4:J:5491:MPD:H31	1.55	0.86
1:K:21:PHE:CA	4:K:5492:MPD:HM2	2.06	0.86
1:K:80:PHE:HB3	4:K:5493:MPD:H12	0.90	0.86
1:B:21:PHE:HA	4:B:5474:MPD:H31	1.56	0.86
1:E:22:THR:OG1	4:E:5480:MPD:C1	2.24	0.86
1:G:21:PHE:CA	4:G:5484:MPD:HM2	2.05	0.86
1:G:22:THR:OG1	4:G:5484:MPD:C1	2.24	0.86
1:L:22:THR:N	4:L:5494:MPD:H11	1.91	0.86
1:A:21:PHE:HA	4:A:5472:MPD:H31	1.56	0.86
1:B:21:PHE:CA	4:B:5474:MPD:HM2	2.05	0.86
1:C:22:THR:OG1	4:C:5476:MPD:C1	2.24	0.86
1:E:21:PHE:CA	4:E:5480:MPD:HM2	2.05	0.86
1:E:22:THR:N	4:E:5480:MPD:H11	1.91	0.86
1:H:21:PHE:CA	4:H:5486:MPD:HM2	2.05	0.86
1:K:22:THR:N	4:K:5492:MPD:H11	1.91	0.86
1:K:22:THR:OG1	4:K:5492:MPD:C1	2.24	0.86
1:D:21:PHE:HA	4:D:5478:MPD:H31	1.56	0.86
1:H:22:THR:N	4:H:5486:MPD:H11	1.91	0.86
1:A:22:THR:N	4:A:5472:MPD:H11	1.91	0.86
1:C:22:THR:N	4:C:5476:MPD:H11	1.91	0.86
1:C:82:ASP:O	1:C:84:THR:HG22	1.76	0.86
1:E:82:ASP:O	1:E:84:THR:HG22	1.76	0.86
1:J:22:THR:OG1	4:J:5490:MPD:C1	2.24	0.86
1:C:21:PHE:CA	4:C:5476:MPD:HM2	2.06	0.85
1:F:22:THR:N	4:F:5482:MPD:H11	1.91	0.85
1:G:82:ASP:O	1:G:84:THR:HG22	1.76	0.85
1:H:22:THR:OG1	4:H:5486:MPD:C1	2.24	0.85
1:I:21:PHE:CA	4:I:5488:MPD:HM2	2.05	0.85
1:I:22:THR:N	4:I:5488:MPD:H11	1.91	0.85
1:B:22:THR:OG1	4:B:5474:MPD:C1	2.24	0.85
1:G:21:PHE:HA	4:G:5484:MPD:H31	1.57	0.85
1:H:82:ASP:O	1:H:84:THR:HG22	1.76	0.85
1:I:80:PHE:CD1	4:I:5489:MPD:H53	2.12	0.85
1:B:82:ASP:O	1:B:84:THR:HG22	1.76	0.85
1:F:82:ASP:O	1:F:84:THR:HG22	1.76	0.85
1:C:80:PHE:CD1	4:C:5473:MPD:H53	2.12	0.85
1:C:398:ASP:O	1:C:399:LEU:C	2.11	0.85
1:D:21:PHE:CA	4:D:5478:MPD:HM2	2.06	0.85
1:J:22:THR:N	4:J:5490:MPD:H11	1.91	0.85
1:J:82:ASP:O	1:J:84:THR:HG22	1.76	0.85
1:K:21:PHE:HA	4:K:5492:MPD:H31	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:PHE:CA	4:L:5494:MPD:HM2	2.05	0.85
1:A:22:THR:OG1	4:A:5472:MPD:C1	2.24	0.85
1:F:22:THR:OG1	4:F:5482:MPD:C1	2.24	0.85
1:K:82:ASP:O	1:K:84:THR:HG22	1.76	0.85
1:A:458:HIS:HD2	1:A:460:VAL:H	1.25	0.85
1:G:22:THR:N	4:G:5484:MPD:H11	1.91	0.85
1:I:21:PHE:HA	4:I:5488:MPD:H31	1.56	0.85
1:I:82:ASP:O	1:I:84:THR:HG22	1.76	0.85
1:D:458:HIS:HD2	1:D:460:VAL:H	1.25	0.85
1:E:21:PHE:HA	4:E:5480:MPD:H31	1.57	0.85
1:A:82:ASP:O	1:A:84:THR:HG22	1.76	0.85
1:D:22:THR:OG1	4:D:5478:MPD:C1	2.24	0.85
1:F:21:PHE:CA	4:F:5482:MPD:HM2	2.05	0.85
1:A:21:PHE:CA	4:A:5472:MPD:HM2	2.05	0.84
1:A:130:PRO:HB3	1:A:268:MET:HE3	1.59	0.84
1:D:82:ASP:O	1:D:84:THR:HG22	1.76	0.84
1:I:22:THR:OG1	4:I:5488:MPD:C1	2.24	0.84
1:B:22:THR:N	4:B:5474:MPD:H11	1.91	0.84
1:D:22:THR:N	4:D:5478:MPD:H11	1.91	0.84
1:J:80:PHE:HB3	4:J:5491:MPD:H12	0.86	0.84
1:L:22:THR:OG1	4:L:5494:MPD:C1	2.24	0.84
1:G:398:ASP:O	1:G:399:LEU:C	2.11	0.84
1:D:130:PRO:HB3	1:D:268:MET:HE3	1.59	0.84
1:J:21:PHE:CA	4:J:5490:MPD:HM2	2.05	0.84
1:H:21:PHE:HA	4:H:5486:MPD:H31	1.57	0.84
1:H:130:PRO:HB3	1:H:268:MET:HE3	1.59	0.84
1:C:84:THR:HG21	4:C:5473:MPD:H52	0.87	0.84
1:F:80:PHE:CD1	4:F:5479:MPD:C5	2.61	0.84
1:H:458:HIS:HD2	1:H:460:VAL:H	1.25	0.84
1:K:130:PRO:HB3	1:K:268:MET:HE3	1.59	0.84
1:I:458:HIS:HD2	1:I:460:VAL:H	1.25	0.84
1:L:458:HIS:HD2	1:L:460:VAL:H	1.25	0.84
1:I:130:PRO:HB3	1:I:268:MET:HE3	1.59	0.83
1:L:130:PRO:HB3	1:L:268:MET:HE3	1.59	0.83
1:I:22:THR:CB	4:I:5488:MPD:H11	2.09	0.83
1:B:22:THR:CB	4:B:5474:MPD:H11	2.09	0.83
1:K:458:HIS:HD2	1:K:460:VAL:H	1.25	0.83
1:C:22:THR:CB	4:C:5476:MPD:H11	2.09	0.83
1:E:22:THR:CB	4:E:5480:MPD:H11	2.09	0.83
1:L:22:THR:CB	4:L:5494:MPD:H11	2.09	0.83
1:L:82:ASP:O	1:L:84:THR:HG22	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:PHE:C	4:C:5476:MPD:HM2	2.04	0.83
1:E:60:ILE:H	1:E:60:ILE:CD1	1.82	0.83
1:I:61:ASN:O	1:J:337:ARG:CB	2.21	0.83
1:A:22:THR:CB	4:A:5472:MPD:H11	2.09	0.83
1:F:21:PHE:C	4:F:5482:MPD:HM2	2.04	0.83
1:L:21:PHE:C	4:L:5494:MPD:HM2	2.04	0.83
1:B:458:HIS:HD2	1:B:460:VAL:H	1.25	0.82
1:D:22:THR:CB	4:D:5478:MPD:H11	2.09	0.82
1:F:22:THR:CB	4:F:5482:MPD:H11	2.09	0.82
1:G:22:THR:CB	4:G:5484:MPD:H11	2.09	0.82
1:G:130:PRO:HB3	1:G:268:MET:HE3	1.59	0.82
1:H:22:THR:CB	4:H:5486:MPD:H11	2.09	0.82
1:B:21:PHE:C	4:B:5474:MPD:HM2	2.04	0.82
1:C:130:PRO:HB3	1:C:268:MET:HE3	1.59	0.82
1:D:21:PHE:C	4:D:5478:MPD:HM2	2.04	0.82
1:E:130:PRO:HB3	1:E:268:MET:HE3	1.59	0.82
1:H:21:PHE:C	4:H:5486:MPD:HM2	2.04	0.82
1:J:21:PHE:C	4:J:5490:MPD:HM2	2.04	0.82
1:F:130:PRO:HB3	1:F:268:MET:HE3	1.59	0.82
1:G:21:PHE:C	4:G:5484:MPD:HM2	2.04	0.82
1:I:21:PHE:C	4:I:5488:MPD:HM2	2.04	0.82
1:J:130:PRO:HB3	1:J:268:MET:HE3	1.59	0.82
1:B:130:PRO:HB3	1:B:268:MET:HE3	1.59	0.82
1:F:80:PHE:CD1	4:F:5479:MPD:H53	2.14	0.82
1:K:22:THR:CB	4:K:5492:MPD:H11	2.09	0.82
1:K:80:PHE:CD1	4:K:5493:MPD:C5	2.63	0.82
1:C:458:HIS:HD2	1:C:460:VAL:H	1.25	0.82
1:E:82:ASP:HB2	4:E:5477:MPD:H31	1.61	0.82
1:J:22:THR:CB	4:J:5490:MPD:H11	2.09	0.82
1:K:21:PHE:C	4:K:5492:MPD:HM2	2.04	0.82
1:F:105:ARG:HB2	4:F:5482:MPD:H4	1.62	0.82
1:E:458:HIS:HD2	1:E:460:VAL:H	1.25	0.81
1:K:22:THR:CB	4:K:5492:MPD:C1	2.58	0.81
1:K:80:PHE:CD1	4:K:5493:MPD:H53	2.15	0.81
1:D:21:PHE:HA	4:D:5478:MPD:HM2	1.62	0.81
1:J:22:THR:CB	4:J:5490:MPD:C1	2.58	0.81
1:L:84:THR:HG21	4:L:5483:MPD:C4	2.08	0.81
1:A:22:THR:CB	4:A:5472:MPD:C1	2.58	0.81
1:C:22:THR:CB	4:C:5476:MPD:C1	2.58	0.81
1:E:21:PHE:C	4:E:5480:MPD:HM2	2.04	0.81
1:F:22:THR:CB	4:F:5482:MPD:C1	2.58	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:458:HIS:HD2	1:G:460:VAL:H	1.25	0.81
1:I:105:ARG:HB2	4:I:5488:MPD:H4	1.62	0.81
1:A:21:PHE:C	4:A:5472:MPD:HM2	2.04	0.81
1:B:21:PHE:HA	4:B:5474:MPD:HM2	1.62	0.81
1:E:399:LEU:HA	1:E:400:PRO:C	2.06	0.81
1:A:399:LEU:HA	1:A:400:PRO:C	2.06	0.81
1:G:21:PHE:HA	4:G:5484:MPD:HM2	1.62	0.81
1:G:399:LEU:HA	1:G:400:PRO:C	2.06	0.81
1:H:84:THR:HG21	4:H:5487:MPD:C4	2.11	0.81
1:I:21:PHE:HA	4:I:5488:MPD:HM2	1.62	0.81
1:B:80:PHE:CD1	4:B:5471:MPD:C5	2.63	0.81
1:J:458:HIS:HD2	1:J:460:VAL:H	1.25	0.81
1:D:105:ARG:HB2	4:D:5478:MPD:H4	1.62	0.81
1:D:399:LEU:HA	1:D:400:PRO:C	2.06	0.81
1:F:458:HIS:HD2	1:F:460:VAL:H	1.25	0.81
1:G:22:THR:CB	4:G:5484:MPD:C1	2.58	0.81
1:I:399:LEU:HA	1:I:400:PRO:C	2.06	0.81
1:J:21:PHE:HA	4:J:5490:MPD:HM2	1.62	0.81
1:G:105:ARG:HB2	4:G:5484:MPD:H4	1.62	0.81
1:J:398:ASP:O	1:J:399:LEU:O	1.99	0.81
1:L:22:THR:CB	4:L:5494:MPD:C1	2.58	0.81
1:B:105:ARG:HB2	4:B:5474:MPD:H4	1.62	0.81
1:C:21:PHE:HA	4:C:5476:MPD:HM2	1.62	0.81
1:D:22:THR:CB	4:D:5478:MPD:C1	2.58	0.81
1:F:21:PHE:HA	4:F:5482:MPD:HM2	1.62	0.81
1:F:399:LEU:HA	1:F:400:PRO:C	2.06	0.81
1:H:399:LEU:HA	1:H:400:PRO:C	2.06	0.81
1:I:84:THR:HG21	4:I:5489:MPD:H52	0.83	0.81
1:E:398:ASP:O	1:E:399:LEU:O	1.99	0.80
1:K:84:THR:HG21	4:K:5493:MPD:H52	0.85	0.80
1:L:84:THR:HG21	4:L:5483:MPD:H52	0.82	0.80
1:G:82:ASP:HB2	4:G:5485:MPD:H31	1.62	0.80
1:K:105:ARG:HB2	4:K:5492:MPD:H4	1.62	0.80
1:L:82:ASP:HB2	4:L:5483:MPD:H31	1.62	0.80
1:A:84:THR:HG21	4:A:5481:MPD:H52	0.84	0.80
1:B:22:THR:CB	4:B:5474:MPD:C1	2.58	0.80
1:E:22:THR:CB	4:E:5480:MPD:C1	2.58	0.80
1:G:398:ASP:O	1:G:399:LEU:O	1.99	0.80
1:J:399:LEU:HA	1:J:400:PRO:C	2.06	0.80
1:L:105:ARG:HB2	4:L:5494:MPD:H4	1.62	0.80
1:L:399:LEU:HA	1:L:400:PRO:C	2.06	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:PHE:HA	4:L:5494:MPD:HM2	1.62	0.80
1:L:398:ASP:O	1:L:399:LEU:O	1.99	0.80
1:C:398:ASP:O	1:C:399:LEU:O	1.99	0.80
1:C:399:LEU:HA	1:C:400:PRO:C	2.06	0.80
1:B:398:ASP:O	1:B:399:LEU:O	1.99	0.80
1:H:398:ASP:O	1:H:399:LEU:O	1.99	0.80
1:I:22:THR:CB	4:I:5488:MPD:C1	2.58	0.80
1:A:398:ASP:O	1:A:399:LEU:O	1.99	0.80
1:I:82:ASP:HB2	4:I:5489:MPD:H31	1.64	0.80
1:B:82:ASP:HB2	4:B:5471:MPD:H31	1.61	0.80
1:E:21:PHE:HA	4:E:5480:MPD:HM2	1.62	0.80
1:H:21:PHE:HA	4:H:5486:MPD:HM2	1.62	0.80
1:H:22:THR:CB	4:H:5486:MPD:C1	2.58	0.80
1:H:105:ARG:HB2	4:H:5486:MPD:H4	1.62	0.80
1:B:399:LEU:HA	1:B:400:PRO:C	2.06	0.80
1:K:21:PHE:HA	4:K:5492:MPD:HM2	1.62	0.80
1:K:399:LEU:HA	1:K:400:PRO:C	2.06	0.80
1:A:105:ARG:HB2	4:A:5472:MPD:H4	1.62	0.79
1:L:80:PHE:HB3	4:L:5483:MPD:H12	0.84	0.79
1:A:21:PHE:HA	4:A:5472:MPD:HM2	1.62	0.79
1:C:105:ARG:HB2	4:C:5476:MPD:H4	1.62	0.79
1:F:84:THR:HG21	4:F:5479:MPD:C4	2.11	0.79
1:J:105:ARG:HB2	4:J:5490:MPD:H4	1.62	0.79
1:D:60:ILE:H	1:D:60:ILE:CD1	1.82	0.79
1:C:337:ARG:CB	1:D:61:ASN:O	2.27	0.79
1:F:398:ASP:O	1:F:399:LEU:O	1.99	0.78
1:E:105:ARG:HB2	4:E:5480:MPD:H4	1.62	0.78
1:I:398:ASP:O	1:I:399:LEU:O	1.99	0.78
1:K:398:ASP:O	1:K:399:LEU:O	1.99	0.78
1:A:337:ARG:CB	1:B:61:ASN:O	2.26	0.78
1:D:84:THR:HG21	4:D:5475:MPD:H52	0.83	0.78
1:A:193:SER:HB2	4:B:5471:MPD:CM	2.11	0.78
1:D:193:SER:HB2	4:E:5477:MPD:CM	2.11	0.78
1:D:398:ASP:O	1:D:399:LEU:O	1.99	0.78
4:H:5487:MPD:CM	1:I:193:SER:HB2	2.11	0.78
1:K:82:ASP:HB2	4:K:5493:MPD:H31	1.66	0.78
1:B:80:PHE:CD1	4:B:5471:MPD:H53	2.18	0.78
1:G:193:SER:HB2	4:L:5483:MPD:CM	2.11	0.77
1:C:82:ASP:HB2	4:C:5473:MPD:H31	1.66	0.77
1:B:58:LYS:HD2	1:B:62:GLU:HB2	1.67	0.77
1:D:58:LYS:HD2	1:D:62:GLU:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:LYS:HD2	1:F:62:GLU:HB2	1.67	0.77
1:G:61:ASN:O	1:H:337:ARG:CB	2.28	0.77
1:I:84:THR:HG21	4:I:5489:MPD:C4	2.15	0.77
1:J:58:LYS:HD2	1:J:62:GLU:HB2	1.67	0.77
1:L:58:LYS:HD2	1:L:62:GLU:HB2	1.67	0.77
1:I:58:LYS:HD2	1:I:62:GLU:HB2	1.67	0.76
4:G:5485:MPD:CM	1:H:193:SER:HB2	2.11	0.76
1:C:58:LYS:HD2	1:C:62:GLU:HB2	1.67	0.76
1:C:193:SER:HB2	4:D:5475:MPD:CM	2.11	0.76
1:H:58:LYS:HD2	1:H:62:GLU:HB2	1.67	0.76
1:G:58:LYS:HD2	1:G:62:GLU:HB2	1.67	0.76
1:I:395:ASN:HB3	1:I:400:PRO:CD	2.16	0.76
1:D:82:ASP:HB2	4:D:5475:MPD:H31	1.68	0.76
1:E:395:ASN:HB3	1:E:400:PRO:CD	2.16	0.76
1:G:395:ASN:HB3	1:G:400:PRO:CD	2.16	0.76
1:D:80:PHE:CD1	4:D:5475:MPD:C5	2.68	0.76
1:D:80:PHE:CD1	4:D:5475:MPD:H53	2.21	0.76
1:G:80:PHE:CD1	4:G:5485:MPD:C5	2.68	0.76
1:K:395:ASN:HB3	1:K:400:PRO:CD	2.16	0.76
4:I:5489:MPD:CM	1:J:193:SER:HB2	2.11	0.76
1:L:395:ASN:HB3	1:L:400:PRO:CD	2.16	0.76
1:A:395:ASN:HB3	1:A:400:PRO:CD	2.16	0.76
1:B:395:ASN:HB3	1:B:400:PRO:CD	2.16	0.75
1:D:395:ASN:HB3	1:D:400:PRO:CD	2.16	0.75
1:A:58:LYS:HD2	1:A:62:GLU:HB2	1.67	0.75
1:C:84:THR:HG21	4:C:5473:MPD:C4	2.16	0.75
1:K:58:LYS:HD2	1:K:62:GLU:HB2	1.67	0.75
4:K:5493:MPD:CM	1:L:193:SER:HB2	2.11	0.75
1:C:395:ASN:HB3	1:C:400:PRO:CD	2.16	0.75
1:J:395:ASN:HB3	1:J:400:PRO:CD	2.16	0.75
1:A:27:LYS:HA	5:A:5743:HOH:O	1.87	0.75
1:G:190:ASP:CA	4:L:5483:MPD:HM3	2.11	0.75
1:K:84:THR:HG21	4:K:5493:MPD:C4	2.16	0.75
1:E:193:SER:HB2	4:F:5479:MPD:CM	2.11	0.75
1:G:27:LYS:HA	5:G:5754:HOH:O	1.87	0.75
1:I:27:LYS:HA	5:I:5769:HOH:O	1.87	0.75
1:J:248:ARG:HH21	1:J:248:ARG:CG	2.00	0.75
1:I:248:ARG:HH21	1:I:248:ARG:CG	2.00	0.75
1:B:248:ARG:HH21	1:B:248:ARG:CG	2.00	0.74
1:E:27:LYS:HA	5:E:1454:HOH:O	1.87	0.74
1:E:58:LYS:HD2	1:E:62:GLU:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:5489:MPD:HM3	1:J:190:ASP:CA	2.11	0.74
1:C:248:ARG:HH21	1:C:248:ARG:CG	2.00	0.74
1:D:27:LYS:HA	5:D:1162:HOH:O	1.87	0.74
1:F:248:ARG:HH21	1:F:248:ARG:CG	2.00	0.74
1:J:27:LYS:HA	5:J:2914:HOH:O	1.87	0.74
1:B:193:SER:HB2	4:C:5473:MPD:CM	2.11	0.74
1:H:395:ASN:HB3	1:H:400:PRO:CD	2.16	0.74
1:B:84:THR:HG21	4:B:5471:MPD:H52	0.80	0.74
1:B:192:ARG:HH21	1:B:219:ASN:ND2	1.86	0.74
1:L:248:ARG:CG	1:L:248:ARG:HH21	2.00	0.74
1:B:27:LYS:HA	5:B:5744:HOH:O	1.87	0.74
1:F:395:ASN:HB3	1:F:400:PRO:CD	2.16	0.74
1:G:192:ARG:HH21	1:G:219:ASN:ND2	1.86	0.74
4:A:5481:MPD:CM	1:F:193:SER:HB2	2.11	0.74
1:B:84:THR:HG21	4:B:5471:MPD:C4	2.18	0.74
1:D:248:ARG:HH21	1:D:248:ARG:CG	2.00	0.74
1:H:27:LYS:HA	5:H:5762:HOH:O	1.87	0.74
1:K:27:LYS:HA	5:K:3206:HOH:O	1.87	0.74
1:K:248:ARG:HH21	1:K:248:ARG:CG	2.00	0.74
1:F:27:LYS:HA	5:F:5756:HOH:O	1.87	0.74
1:L:27:LYS:HA	5:L:3498:HOH:O	1.87	0.74
1:E:248:ARG:HH21	1:E:248:ARG:CG	2.00	0.74
1:H:248:ARG:HH21	1:H:248:ARG:CG	2.00	0.74
1:I:192:ARG:HH21	1:I:219:ASN:ND2	1.86	0.74
1:D:192:ARG:HH21	1:D:219:ASN:ND2	1.86	0.73
1:J:192:ARG:HH21	1:J:219:ASN:ND2	1.86	0.73
1:K:192:ARG:HH21	1:K:219:ASN:ND2	1.86	0.73
1:A:248:ARG:HH21	1:A:248:ARG:CG	2.00	0.73
1:E:192:ARG:HH21	1:E:219:ASN:ND2	1.86	0.73
4:K:5493:MPD:HM3	1:L:190:ASP:CA	2.11	0.73
1:G:248:ARG:HH21	1:G:248:ARG:CG	2.00	0.73
1:C:27:LYS:HA	5:C:5744:HOH:O	1.87	0.73
1:C:192:ARG:HH21	1:C:219:ASN:ND2	1.86	0.73
4:A:5481:MPD:HM3	1:F:190:ASP:CA	2.11	0.73
1:C:88:ARG:HE	4:C:5476:MPD:CM	2.02	0.73
1:E:82:ASP:HB2	4:E:5477:MPD:C3	2.18	0.73
1:F:88:ARG:HE	4:F:5482:MPD:CM	2.02	0.73
1:J:88:ARG:HE	4:J:5490:MPD:CM	2.02	0.73
1:L:88:ARG:HE	4:L:5494:MPD:CM	2.02	0.73
1:A:192:ARG:HH21	1:A:219:ASN:ND2	1.86	0.72
1:D:88:ARG:HE	4:D:5478:MPD:CM	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:ARG:HH21	1:F:219:ASN:ND2	1.86	0.72
1:H:88:ARG:HE	4:H:5486:MPD:CM	2.02	0.72
1:C:190:ASP:CA	4:D:5475:MPD:HM3	2.11	0.72
1:H:192:ARG:HH21	1:H:219:ASN:ND2	1.86	0.72
1:L:192:ARG:HH21	1:L:219:ASN:ND2	1.86	0.72
1:A:82:ASP:HB2	4:A:5481:MPD:H31	1.70	0.72
1:H:82:ASP:HB2	4:H:5487:MPD:H31	1.71	0.72
4:J:5491:MPD:CM	1:K:193:SER:HB2	2.11	0.72
1:I:88:ARG:HE	4:I:5488:MPD:CM	2.02	0.72
1:A:88:ARG:HE	4:A:5472:MPD:CM	2.02	0.72
1:B:88:ARG:HE	4:B:5474:MPD:CM	2.02	0.72
1:E:88:ARG:HE	4:E:5480:MPD:CM	2.02	0.72
1:A:96:THR:OG1	1:A:98:GLN:HB2	1.90	0.72
1:E:96:THR:OG1	1:E:98:GLN:HB2	1.90	0.72
1:G:88:ARG:HE	4:G:5484:MPD:CM	2.02	0.72
1:J:96:THR:OG1	1:J:98:GLN:HB2	1.90	0.71
1:K:88:ARG:HE	4:K:5492:MPD:CM	2.02	0.71
1:C:96:THR:OG1	1:C:98:GLN:HB2	1.90	0.71
1:G:96:THR:OG1	1:G:98:GLN:HB2	1.90	0.71
1:L:96:THR:OG1	1:L:98:GLN:HB2	1.90	0.71
1:F:96:THR:OG1	1:F:98:GLN:HB2	1.90	0.71
1:G:80:PHE:CD1	4:G:5485:MPD:H53	2.24	0.71
1:K:96:THR:OG1	1:K:98:GLN:HB2	1.90	0.71
1:D:96:THR:OG1	1:D:98:GLN:HB2	1.90	0.71
1:F:22:THR:HB	4:F:5482:MPD:C1	2.21	0.71
1:F:84:THR:HG21	4:F:5479:MPD:H52	0.76	0.71
1:H:22:THR:HB	4:H:5486:MPD:C1	2.21	0.71
1:I:96:THR:OG1	1:I:98:GLN:HB2	1.90	0.71
1:B:22:THR:HB	4:B:5474:MPD:C1	2.21	0.70
1:E:190:ASP:CA	4:F:5479:MPD:HM3	2.11	0.70
1:J:84:THR:HG21	4:J:5491:MPD:H52	0.75	0.70
1:K:384:ASN:HD22	1:K:384:ASN:N	1.89	0.70
1:L:22:THR:HB	4:L:5494:MPD:C1	2.21	0.70
1:A:22:THR:HB	4:A:5472:MPD:C1	2.21	0.70
1:D:22:THR:HB	4:D:5478:MPD:C1	2.21	0.70
1:L:399:LEU:H	1:L:401:PRO:CG	1.90	0.70
1:F:82:ASP:HB2	4:F:5479:MPD:C3	2.21	0.70
1:H:384:ASN:HD22	1:H:384:ASN:N	1.89	0.70
1:I:22:THR:HB	4:I:5488:MPD:C1	2.21	0.70
1:A:384:ASN:HD22	1:A:384:ASN:N	1.89	0.70
1:E:22:THR:HB	4:E:5480:MPD:C1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:ASN:HD22	1:E:384:ASN:N	1.89	0.70
1:J:22:THR:HB	4:J:5490:MPD:C1	2.21	0.70
1:H:96:THR:OG1	1:H:98:GLN:HB2	1.90	0.70
1:L:384:ASN:HD22	1:L:384:ASN:N	1.89	0.70
1:C:384:ASN:HD22	1:C:384:ASN:N	1.89	0.70
1:E:21:PHE:HA	4:E:5480:MPD:CM	2.22	0.70
1:K:22:THR:HB	4:K:5492:MPD:C1	2.21	0.70
4:G:5485:MPD:HM3	1:H:190:ASP:CA	2.11	0.69
1:G:22:THR:HB	4:G:5484:MPD:C1	2.21	0.69
1:G:82:ASP:HB2	4:G:5485:MPD:C3	2.22	0.69
1:H:21:PHE:HA	4:H:5486:MPD:CM	2.22	0.69
1:B:96:THR:OG1	1:B:98:GLN:HB2	1.90	0.69
1:G:21:PHE:HA	4:G:5484:MPD:CM	2.22	0.69
1:K:21:PHE:HA	4:K:5492:MPD:CM	2.22	0.69
1:I:384:ASN:N	1:I:384:ASN:HD22	1.89	0.69
1:G:84:THR:HG21	4:G:5485:MPD:H52	0.78	0.69
1:G:337:ARG:CB	1:L:61:ASN:O	2.34	0.69
1:G:384:ASN:HD22	1:G:384:ASN:N	1.89	0.69
1:A:190:ASP:CA	4:B:5471:MPD:HM3	2.11	0.69
1:C:21:PHE:HA	4:C:5476:MPD:CM	2.22	0.69
1:C:22:THR:HB	4:C:5476:MPD:C1	2.21	0.69
1:C:22:THR:HB	4:C:5476:MPD:H11	1.75	0.69
1:E:399:LEU:H	1:E:401:PRO:CG	1.90	0.69
1:J:384:ASN:HD22	1:J:384:ASN:N	1.89	0.69
1:L:21:PHE:HA	4:L:5494:MPD:CM	2.22	0.69
1:L:22:THR:HB	4:L:5494:MPD:H11	1.75	0.69
1:A:21:PHE:HA	4:A:5472:MPD:CM	2.22	0.69
1:I:22:THR:HB	4:I:5488:MPD:H11	1.75	0.69
1:D:22:THR:HB	4:D:5478:MPD:H11	1.75	0.69
1:J:82:ASP:HB2	4:J:5491:MPD:C3	2.22	0.69
1:I:21:PHE:HA	4:I:5488:MPD:CM	2.22	0.68
1:E:22:THR:HB	4:E:5480:MPD:H11	1.75	0.68
1:F:21:PHE:HA	4:F:5482:MPD:CM	2.22	0.68
1:H:22:THR:HB	4:H:5486:MPD:H11	1.75	0.68
1:D:399:LEU:HA	1:D:400:PRO:O	1.94	0.68
1:B:21:PHE:HA	4:B:5474:MPD:CM	2.22	0.68
1:D:21:PHE:HA	4:D:5478:MPD:CM	2.22	0.68
1:H:399:LEU:HA	1:H:400:PRO:O	1.94	0.68
4:H:5487:MPD:HM3	1:I:190:ASP:CA	2.11	0.68
1:A:399:LEU:HA	1:A:400:PRO:O	1.94	0.68
1:B:190:ASP:CA	4:C:5473:MPD:HM3	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:THR:HG21	4:D:5475:MPD:C4	2.22	0.68
1:E:399:LEU:HA	1:E:400:PRO:O	1.94	0.68
1:B:399:LEU:HA	1:B:400:PRO:O	1.94	0.68
4:J:5491:MPD:HM3	1:K:190:ASP:CA	2.11	0.68
1:B:384:ASN:HD22	1:B:384:ASN:N	1.89	0.68
1:D:384:ASN:HD22	1:D:384:ASN:N	1.89	0.68
1:F:384:ASN:N	1:F:384:ASN:HD22	1.89	0.68
1:I:88:ARG:HE	4:I:5488:MPD:HM1	1.60	0.68
1:L:88:ARG:HE	4:L:5494:MPD:HM1	1.59	0.68
1:A:22:THR:HB	4:A:5472:MPD:H11	1.75	0.67
1:G:84:THR:HG21	4:G:5485:MPD:C4	2.24	0.67
1:I:399:LEU:HA	1:I:400:PRO:O	1.94	0.67
1:K:399:LEU:HA	1:K:400:PRO:O	1.94	0.67
1:C:399:LEU:HA	1:C:400:PRO:O	1.94	0.67
1:A:88:ARG:HE	4:A:5472:MPD:HM1	1.60	0.67
1:A:399:LEU:N	1:A:401:PRO:CG	2.52	0.67
1:E:458:HIS:CD2	1:E:460:VAL:H	2.11	0.67
1:J:21:PHE:HA	4:J:5490:MPD:CM	2.22	0.67
1:J:399:LEU:HA	1:J:400:PRO:O	1.94	0.67
1:L:399:LEU:HA	1:L:400:PRO:O	1.94	0.67
1:C:399:LEU:N	1:C:401:PRO:CG	2.52	0.67
1:G:295:LEU:O	1:G:388:PRO:CG	2.43	0.67
1:G:399:LEU:HA	1:G:400:PRO:O	1.94	0.67
1:K:22:THR:HB	4:K:5492:MPD:H11	1.75	0.67
1:D:295:LEU:O	1:D:388:PRO:CG	2.43	0.67
1:L:399:LEU:N	1:L:401:PRO:CG	2.52	0.67
4:D:5478:MPD:H52	4:D:5478:MPD:H11	1.77	0.67
1:K:295:LEU:O	1:K:388:PRO:CG	2.43	0.67
4:K:5492:MPD:H52	4:K:5492:MPD:H11	1.77	0.67
1:C:295:LEU:O	1:C:388:PRO:CG	2.43	0.67
1:F:88:ARG:HE	4:F:5482:MPD:HM1	1.60	0.67
4:H:5486:MPD:H52	4:H:5486:MPD:H11	1.77	0.67
1:H:88:ARG:HE	4:H:5486:MPD:HM1	1.60	0.67
1:H:295:LEU:O	1:H:388:PRO:CG	2.43	0.67
1:H:399:LEU:N	1:H:401:PRO:CG	2.52	0.67
1:I:458:HIS:CD2	1:I:460:VAL:H	2.12	0.67
1:J:88:ARG:HE	4:J:5490:MPD:HM1	1.60	0.67
1:L:80:PHE:CB	4:L:5483:MPD:C1	2.53	0.67
1:B:295:LEU:O	1:B:388:PRO:CG	2.43	0.67
1:B:399:LEU:N	1:B:401:PRO:CG	2.52	0.67
4:B:5474:MPD:H52	4:B:5474:MPD:H11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:LEU:O	1:F:388:PRO:CG	2.43	0.67
1:A:295:LEU:O	1:A:388:PRO:CG	2.43	0.67
1:D:190:ASP:CA	4:E:5477:MPD:HM3	2.11	0.67
1:D:461:GLU:OE1	1:J:320:LYS:NZ	2.26	0.67
1:J:30:HIS:H	1:K:180:PHE:HB3	1.58	0.67
1:E:295:LEU:O	1:E:388:PRO:CG	2.43	0.66
1:G:88:ARG:HE	4:G:5484:MPD:HM1	1.59	0.66
1:G:458:HIS:CD2	1:G:460:VAL:H	2.11	0.66
1:H:80:PHE:CB	4:H:5487:MPD:C1	2.53	0.66
1:J:80:PHE:HD1	4:J:5491:MPD:C5	2.09	0.66
1:D:88:ARG:HE	4:D:5478:MPD:HM1	1.59	0.66
1:I:295:LEU:O	1:I:388:PRO:CG	2.43	0.66
1:L:295:LEU:O	1:L:388:PRO:CG	2.43	0.66
1:A:53:SER:HB2	1:F:179:TYR:CD2	2.30	0.66
1:A:80:PHE:CD1	4:A:5481:MPD:H53	2.30	0.66
4:A:5472:MPD:H52	4:A:5472:MPD:H11	1.77	0.66
1:C:105:ARG:HB2	4:C:5476:MPD:C4	2.26	0.66
1:D:399:LEU:H	1:D:401:PRO:CG	1.90	0.66
4:F:5482:MPD:H52	4:F:5482:MPD:H11	1.77	0.66
1:F:399:LEU:HA	1:F:400:PRO:O	1.94	0.66
1:J:295:LEU:O	1:J:388:PRO:CG	2.43	0.66
1:B:82:ASP:HB2	4:B:5471:MPD:C3	2.24	0.66
1:C:88:ARG:HE	4:C:5476:MPD:HM1	1.59	0.66
1:J:80:PHE:CB	4:J:5491:MPD:C1	2.53	0.66
1:A:29:GLN:OE1	1:F:181:PRO:HD3	1.96	0.66
1:G:22:THR:HB	4:G:5484:MPD:H11	1.75	0.66
1:I:399:LEU:N	1:I:401:PRO:CG	2.52	0.66
1:A:82:ASP:HB2	4:A:5481:MPD:C3	2.25	0.66
1:G:105:ARG:HB2	4:G:5484:MPD:C4	2.26	0.66
1:J:22:THR:HB	4:J:5490:MPD:H11	1.75	0.66
4:J:5490:MPD:H52	4:J:5490:MPD:H11	1.77	0.66
1:A:365:ALA:O	1:A:367:PRO:HD3	1.96	0.66
1:J:105:ARG:HB2	4:J:5490:MPD:C4	2.26	0.66
1:L:365:ALA:O	1:L:367:PRO:HD3	1.96	0.66
1:B:105:ARG:HB2	4:B:5474:MPD:C4	2.26	0.66
4:G:5484:MPD:H52	4:G:5484:MPD:H11	1.77	0.66
1:J:458:HIS:CD2	1:J:460:VAL:H	2.11	0.66
1:D:105:ARG:HB2	4:D:5478:MPD:C4	2.26	0.65
1:E:88:ARG:HE	4:E:5480:MPD:HM1	1.60	0.65
1:F:320:LYS:NZ	1:L:461:GLU:OE1	2.27	0.65
1:G:30:HIS:H	1:H:180:PHE:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:ARG:HB2	4:H:5486:MPD:C4	2.26	0.65
4:E:5480:MPD:H52	4:E:5480:MPD:H11	1.77	0.65
1:I:30:HIS:H	1:J:180:PHE:HB3	1.62	0.65
1:I:365:ALA:O	1:I:367:PRO:HD3	1.96	0.65
4:I:5488:MPD:H52	4:I:5488:MPD:H11	1.77	0.65
4:L:5494:MPD:H52	4:L:5494:MPD:H11	1.77	0.65
1:B:88:ARG:HE	4:B:5474:MPD:HM1	1.59	0.65
1:D:365:ALA:O	1:D:367:PRO:HD3	1.96	0.65
1:I:105:ARG:HB2	4:I:5488:MPD:C4	2.26	0.65
4:C:5476:MPD:H52	4:C:5476:MPD:H11	1.77	0.65
1:K:88:ARG:HE	4:K:5492:MPD:HM1	1.59	0.65
1:L:458:HIS:CD2	1:L:460:VAL:H	2.11	0.65
1:A:320:LYS:NZ	1:G:461:GLU:OE1	2.24	0.65
1:C:365:ALA:O	1:C:367:PRO:HD3	1.96	0.65
1:F:105:ARG:HB2	4:F:5482:MPD:C4	2.26	0.65
1:H:80:PHE:HD1	4:H:5487:MPD:H52	1.61	0.65
1:H:365:ALA:O	1:H:367:PRO:HD3	1.96	0.65
1:D:320:LYS:NZ	1:J:461:GLU:OE1	2.28	0.65
1:F:22:THR:HB	4:F:5482:MPD:H11	1.75	0.65
1:H:53:SER:HB2	1:I:179:TYR:CD2	2.32	0.65
1:A:80:PHE:CD1	4:A:5481:MPD:C5	2.80	0.65
1:C:399:LEU:H	1:C:401:PRO:CG	1.90	0.65
1:K:105:ARG:HB2	4:K:5492:MPD:C4	2.26	0.65
1:L:105:ARG:HB2	4:L:5494:MPD:C4	2.26	0.65
1:A:105:ARG:HB2	4:A:5472:MPD:C4	2.26	0.65
1:B:22:THR:HB	4:B:5474:MPD:H11	1.75	0.65
1:E:105:ARG:HB2	4:E:5480:MPD:C4	2.26	0.65
1:C:179:TYR:CD2	1:D:53:SER:HB2	2.32	0.64
1:G:399:LEU:N	1:G:401:PRO:CG	2.52	0.64
1:F:365:ALA:O	1:F:367:PRO:HD3	1.96	0.64
1:K:458:HIS:CD2	1:K:460:VAL:H	2.11	0.64
1:I:170:GLY:HA2	1:I:172:ARG:NH2	2.13	0.64
1:J:80:PHE:CA	4:J:5491:MPD:H12	2.28	0.64
1:D:458:HIS:CD2	1:D:460:VAL:H	2.11	0.64
1:E:399:LEU:N	1:E:401:PRO:CG	2.52	0.64
1:D:82:ASP:HB2	4:D:5475:MPD:C3	2.28	0.64
1:K:365:ALA:O	1:K:367:PRO:HD3	1.96	0.64
1:G:211:HIS:HD2	1:G:212:GLU:O	1.81	0.64
1:I:211:HIS:HD2	1:I:212:GLU:O	1.81	0.64
1:J:170:GLY:HA2	1:J:172:ARG:NH2	2.13	0.64
1:F:170:GLY:HA2	1:F:172:ARG:NH2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:399:LEU:N	1:F:401:PRO:CG	2.52	0.64
1:J:399:LEU:N	1:J:401:PRO:CG	2.52	0.64
1:K:170:GLY:HA2	1:K:172:ARG:NH2	2.13	0.64
1:L:211:HIS:HD2	1:L:212:GLU:O	1.81	0.64
1:A:170:GLY:HA2	1:A:172:ARG:NH2	2.13	0.64
1:D:170:GLY:HA2	1:D:172:ARG:NH2	2.13	0.64
1:G:399:LEU:H	1:G:401:PRO:CG	1.90	0.64
1:J:211:HIS:HD2	1:J:212:GLU:O	1.81	0.64
1:B:365:ALA:O	1:B:367:PRO:HD3	1.96	0.64
1:E:80:PHE:CD1	4:E:5477:MPD:C5	2.81	0.64
1:G:365:ALA:O	1:G:367:PRO:HD3	1.96	0.64
1:J:365:ALA:O	1:J:367:PRO:HD3	1.96	0.64
1:E:80:PHE:CD1	4:E:5477:MPD:H53	2.34	0.63
1:E:365:ALA:O	1:E:367:PRO:HD3	1.96	0.63
1:F:211:HIS:HD2	1:F:212:GLU:O	1.81	0.63
1:B:170:GLY:HA2	1:B:172:ARG:NH2	2.13	0.63
1:C:458:HIS:CD2	1:C:460:VAL:H	2.11	0.63
1:H:170:GLY:HA2	1:H:172:ARG:NH2	2.13	0.63
1:H:211:HIS:HD2	1:H:212:GLU:O	1.81	0.63
1:K:399:LEU:N	1:K:401:PRO:CG	2.52	0.63
1:C:211:HIS:HD2	1:C:212:GLU:O	1.81	0.63
1:H:80:PHE:CA	4:H:5487:MPD:H12	2.29	0.63
1:H:458:HIS:CD2	1:H:460:VAL:H	2.11	0.63
1:K:211:HIS:HD2	1:K:212:GLU:O	1.81	0.63
1:L:386:ILE:O	1:L:388:PRO:HD3	1.99	0.63
1:B:386:ILE:O	1:B:388:PRO:HD3	1.99	0.63
1:G:170:GLY:HA2	1:G:172:ARG:NH2	2.13	0.63
1:E:386:ILE:O	1:E:388:PRO:HD3	1.99	0.63
1:C:170:GLY:HA2	1:C:172:ARG:NH2	2.13	0.63
1:A:211:HIS:HD2	1:A:212:GLU:O	1.81	0.63
1:A:461:GLU:OE1	1:G:320:LYS:NZ	2.25	0.63
1:E:211:HIS:HD2	1:E:212:GLU:O	1.81	0.63
1:L:170:GLY:HA2	1:L:172:ARG:NH2	2.13	0.63
1:B:399:LEU:H	1:B:401:PRO:CG	1.90	0.63
1:F:396:LEU:HD12	1:F:398:ASP:H	1.64	0.63
1:G:386:ILE:O	1:G:388:PRO:HD3	1.99	0.63
1:D:211:HIS:HD2	1:D:212:GLU:O	1.81	0.62
1:E:170:GLY:HA2	1:E:172:ARG:NH2	2.13	0.62
1:F:386:ILE:O	1:F:388:PRO:HD3	1.99	0.62
1:F:437:GLU:HG3	5:F:5724:HOH:O	1.99	0.62
1:H:386:ILE:O	1:H:388:PRO:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:82:ASP:HB2	4:I:5489:MPD:C3	2.29	0.62
1:I:386:ILE:O	1:I:388:PRO:HD3	1.99	0.62
1:L:82:ASP:HB2	4:L:5483:MPD:C3	2.28	0.62
1:A:396:LEU:HD12	1:A:398:ASP:H	1.64	0.62
1:B:211:HIS:HD2	1:B:212:GLU:O	1.81	0.62
1:C:386:ILE:O	1:C:388:PRO:HD3	1.99	0.62
1:D:386:ILE:O	1:D:388:PRO:HD3	1.99	0.62
1:J:386:ILE:O	1:J:388:PRO:HD3	1.99	0.62
1:A:458:HIS:CD2	1:A:460:VAL:H	2.11	0.62
1:D:399:LEU:N	1:D:401:PRO:CG	2.52	0.62
1:I:396:LEU:HD12	1:I:398:ASP:H	1.64	0.62
1:J:437:GLU:HG3	5:J:2881:HOH:O	1.99	0.62
1:L:396:LEU:HD12	1:L:398:ASP:H	1.64	0.62
1:A:386:ILE:O	1:A:388:PRO:HD3	1.99	0.62
1:C:396:LEU:HD12	1:C:398:ASP:H	1.64	0.62
1:F:80:PHE:CA	4:F:5479:MPD:H12	2.29	0.62
1:H:235:ILE:CG2	1:H:367:PRO:HG3	2.28	0.62
1:I:80:PHE:HD1	4:I:5489:MPD:C5	2.12	0.62
1:E:84:THR:HG21	4:E:5477:MPD:H52	0.77	0.62
1:F:458:HIS:CD2	1:F:460:VAL:H	2.11	0.62
1:J:396:LEU:HD12	1:J:398:ASP:H	1.64	0.62
1:L:437:GLU:HG3	5:L:3465:HOH:O	1.99	0.62
1:C:437:GLU:HG3	5:C:5712:HOH:O	1.99	0.62
1:J:235:ILE:CG2	1:J:367:PRO:HG3	2.28	0.62
1:K:386:ILE:O	1:K:388:PRO:HD3	1.99	0.62
1:K:396:LEU:HD12	1:K:398:ASP:H	1.64	0.62
1:A:155:GLU:OE1	1:A:211:HIS:HE1	1.83	0.62
1:E:396:LEU:HD12	1:E:398:ASP:H	1.64	0.62
1:H:396:LEU:HD12	1:H:398:ASP:H	1.64	0.62
1:B:383:LYS:C	1:B:384:ASN:HD22	2.08	0.62
1:G:383:LYS:C	1:G:384:ASN:HD22	2.08	0.62
1:G:437:GLU:HG3	5:G:5723:HOH:O	1.99	0.62
1:K:82:ASP:HB2	4:K:5493:MPD:C3	2.30	0.62
1:B:437:GLU:HG3	5:B:5712:HOH:O	1.99	0.62
1:D:235:ILE:CG2	1:D:367:PRO:HG3	2.28	0.62
1:H:399:LEU:H	1:H:401:PRO:CG	1.90	0.62
1:J:383:LYS:C	1:J:384:ASN:HD22	2.08	0.62
1:D:155:GLU:OE1	1:D:211:HIS:HE1	1.83	0.62
1:G:396:LEU:HD12	1:G:398:ASP:H	1.64	0.62
1:I:437:GLU:HG3	5:I:5738:HOH:O	1.99	0.62
1:B:360:PHE:CG	1:B:361:PRO:HD3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:235:ILE:CG2	1:I:367:PRO:HG3	2.27	0.61
1:A:180:PHE:HB3	1:B:30:HIS:H	1.65	0.61
1:B:155:GLU:OE1	1:B:211:HIS:HE1	1.83	0.61
1:H:383:LYS:C	1:H:384:ASN:HD22	2.08	0.61
1:A:84:THR:HG21	4:A:5481:MPD:C4	2.30	0.61
1:A:437:GLU:HG3	5:A:5711:HOH:O	1.99	0.61
1:B:248:ARG:HH21	1:B:248:ARG:HG2	1.66	0.61
1:B:427:PHE:CE1	1:B:428:LEU:HD13	2.36	0.61
1:C:427:PHE:CE1	1:C:428:LEU:HD13	2.36	0.61
1:D:360:PHE:CG	1:D:361:PRO:HD3	2.35	0.61
1:D:383:LYS:C	1:D:384:ASN:HD22	2.08	0.61
1:D:437:GLU:HG3	5:D:1129:HOH:O	1.99	0.61
1:E:383:LYS:C	1:E:384:ASN:HD22	2.08	0.61
1:H:437:GLU:HG3	5:H:5731:HOH:O	1.99	0.61
1:L:155:GLU:OE1	1:L:211:HIS:HE1	1.83	0.61
1:E:155:GLU:OE1	1:E:211:HIS:HE1	1.83	0.61
1:J:248:ARG:HH21	1:J:248:ARG:HG2	1.65	0.61
1:J:427:PHE:CE1	1:J:428:LEU:HD13	2.36	0.61
1:K:53:SER:HB2	1:L:179:TYR:CD2	2.35	0.61
1:K:155:GLU:OE1	1:K:211:HIS:HE1	1.83	0.61
1:K:437:GLU:HG3	5:K:3173:HOH:O	1.99	0.61
1:C:248:ARG:HH21	1:C:248:ARG:HG2	1.66	0.61
1:D:396:LEU:HD12	1:D:398:ASP:H	1.64	0.61
1:F:383:LYS:C	1:F:384:ASN:HD22	2.08	0.61
1:I:427:PHE:CE1	1:I:428:LEU:HD13	2.35	0.61
1:A:427:PHE:CE1	1:A:428:LEU:HD13	2.36	0.61
1:B:396:LEU:HD12	1:B:398:ASP:H	1.64	0.61
1:E:437:GLU:HG3	5:E:1421:HOH:O	1.99	0.61
1:H:155:GLU:OE1	1:H:211:HIS:HE1	1.83	0.61
1:J:155:GLU:OE1	1:J:211:HIS:HE1	1.83	0.61
1:E:461:GLU:OE1	1:K:320:LYS:NZ	2.27	0.61
1:F:155:GLU:OE1	1:F:211:HIS:HE1	1.83	0.61
1:H:248:ARG:HH21	1:H:248:ARG:HG2	1.66	0.61
1:A:383:LYS:C	1:A:384:ASN:HD22	2.08	0.61
1:D:427:PHE:CE1	1:D:428:LEU:HD13	2.36	0.61
1:E:22:THR:H	4:E:5480:MPD:H11	1.66	0.61
1:E:427:PHE:CE1	1:E:428:LEU:HD13	2.36	0.61
1:G:155:GLU:OE1	1:G:211:HIS:HE1	1.83	0.61
1:G:248:ARG:HH21	1:G:248:ARG:HG2	1.66	0.61
1:I:155:GLU:OE1	1:I:211:HIS:HE1	1.83	0.61
1:I:248:ARG:HH21	1:I:248:ARG:HG2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:PHE:CA	4:C:5473:MPD:H12	2.30	0.61
1:G:427:PHE:CE1	1:G:428:LEU:HD13	2.36	0.61
1:I:80:PHE:CA	4:I:5489:MPD:H12	2.30	0.61
1:K:427:PHE:CE1	1:K:428:LEU:HD13	2.35	0.61
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.36	0.60
1:B:458:HIS:CD2	1:B:460:VAL:H	2.11	0.60
1:C:235:ILE:CG2	1:C:367:PRO:HG3	2.28	0.60
1:F:235:ILE:CG2	1:F:367:PRO:HG3	2.28	0.60
1:G:22:THR:H	4:G:5484:MPD:H11	1.66	0.60
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.36	0.60
1:L:427:PHE:CE1	1:L:428:LEU:HD13	2.36	0.60
1:F:248:ARG:HH21	1:F:248:ARG:HG2	1.66	0.60
1:K:383:LYS:C	1:K:384:ASN:HD22	2.08	0.60
1:L:383:LYS:C	1:L:384:ASN:HD22	2.08	0.60
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.36	0.60
1:C:155:GLU:OE1	1:C:211:HIS:HE1	1.83	0.60
1:F:427:PHE:CE1	1:F:428:LEU:HD13	2.35	0.60
1:G:21:PHE:HB2	4:G:5484:MPD:C5	2.25	0.60
1:H:427:PHE:CE1	1:H:428:LEU:HD13	2.36	0.60
1:I:383:LYS:C	1:I:384:ASN:HD22	2.08	0.60
1:J:360:PHE:CG	1:J:361:PRO:HD3	2.35	0.60
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.36	0.60
1:A:235:ILE:CG2	1:A:367:PRO:HG3	2.28	0.60
1:B:323:VAL:O	1:B:325:GLY:N	2.35	0.60
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.36	0.60
1:E:248:ARG:HH21	1:E:248:ARG:HG2	1.65	0.60
1:K:22:THR:H	4:K:5492:MPD:H11	1.66	0.60
1:C:360:PHE:CG	1:C:361:PRO:HD3	2.35	0.60
1:E:323:VAL:O	1:E:325:GLY:N	2.35	0.60
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.36	0.60
1:I:399:LEU:H	1:I:401:PRO:CG	1.90	0.60
1:E:320:LYS:NZ	1:K:461:GLU:OE1	2.27	0.60
1:F:323:VAL:O	1:F:325:GLY:N	2.35	0.60
1:K:29:GLN:OE1	1:L:181:PRO:HD3	2.01	0.60
1:K:248:ARG:HH21	1:K:248:ARG:HG2	1.65	0.60
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.36	0.60
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.36	0.60
1:L:80:PHE:CA	4:L:5483:MPD:H12	2.30	0.60
1:A:248:ARG:HH21	1:A:248:ARG:HG2	1.66	0.60
1:A:360:PHE:CG	1:A:361:PRO:HD3	2.35	0.60
1:C:383:LYS:C	1:C:384:ASN:HD22	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:VAL:O	1:D:325:GLY:N	2.35	0.60
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.35	0.60
1:H:323:VAL:O	1:H:325:GLY:N	2.35	0.60
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.36	0.60
1:K:323:VAL:O	1:K:325:GLY:N	2.35	0.60
1:C:80:PHE:HD1	4:C:5473:MPD:H52	1.67	0.59
1:J:323:VAL:O	1:J:325:GLY:N	2.35	0.59
1:L:323:VAL:O	1:L:325:GLY:N	2.35	0.59
1:A:22:THR:H	4:A:5472:MPD:H11	1.66	0.59
1:A:399:LEU:H	1:A:401:PRO:CG	1.90	0.59
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.36	0.59
1:A:323:VAL:O	1:A:325:GLY:N	2.35	0.59
1:E:84:THR:HG21	4:E:5477:MPD:C4	2.30	0.59
1:F:80:PHE:HD1	4:F:5479:MPD:C5	2.14	0.59
1:I:323:VAL:O	1:I:325:GLY:N	2.35	0.59
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.36	0.59
1:K:332:LEU:HB2	1:K:408:PRO:HB2	1.85	0.59
1:L:80:PHE:HD1	4:L:5483:MPD:C5	2.10	0.59
1:C:320:LYS:NZ	1:I:461:GLU:OE1	2.30	0.59
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.36	0.59
1:A:332:LEU:HB2	1:A:408:PRO:HB2	1.85	0.59
1:B:332:LEU:HB2	1:B:408:PRO:HB2	1.85	0.59
1:C:80:PHE:CB	4:C:5473:MPD:C1	2.60	0.59
1:D:181:PRO:HD3	1:E:29:GLN:OE1	2.03	0.59
1:F:22:THR:H	4:F:5482:MPD:H11	1.66	0.59
1:C:181:PRO:HD3	1:D:29:GLN:OE1	2.01	0.59
1:D:248:ARG:HH21	1:D:248:ARG:HG2	1.65	0.59
1:G:323:VAL:O	1:G:325:GLY:N	2.35	0.59
1:I:332:LEU:HB2	1:I:408:PRO:HB2	1.85	0.59
1:L:80:PHE:HD1	4:L:5483:MPD:H52	1.68	0.59
1:C:360:PHE:CE2	1:C:361:PRO:HD3	2.36	0.59
1:E:360:PHE:CG	1:E:361:PRO:HD3	2.35	0.59
1:E:180:PHE:HB3	1:F:30:HIS:H	1.66	0.59
5:H:5633:HOH:O	1:I:181:PRO:HG3	2.01	0.59
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.36	0.59
1:J:399:LEU:H	1:J:401:PRO:CG	1.90	0.59
1:K:235:ILE:CG2	1:K:367:PRO:HG3	2.28	0.59
1:C:21:PHE:HB2	4:C:5476:MPD:C5	2.25	0.59
1:C:332:LEU:HB2	1:C:408:PRO:HB2	1.85	0.59
1:E:235:ILE:CG2	1:E:367:PRO:HG3	2.28	0.59
1:H:18:ASP:OD2	1:H:30:HIS:HD2	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:PHE:HB2	4:I:5488:MPD:C5	2.25	0.59
1:I:80:PHE:HD1	4:I:5489:MPD:H52	1.68	0.59
1:K:18:ASP:OD2	1:K:30:HIS:HD2	1.86	0.59
1:L:248:ARG:HH21	1:L:248:ARG:HG2	1.66	0.59
1:C:180:PHE:HB3	1:D:30:HIS:H	1.66	0.58
1:D:332:LEU:HB2	1:D:408:PRO:HB2	1.85	0.58
1:G:235:ILE:CG2	1:G:367:PRO:HG3	2.28	0.58
1:L:22:THR:H	4:L:5494:MPD:H11	1.66	0.58
1:B:18:ASP:OD2	1:B:30:HIS:HD2	1.86	0.58
1:B:22:THR:H	4:B:5474:MPD:H11	1.66	0.58
1:C:80:PHE:CD1	4:C:5473:MPD:H52	2.38	0.58
1:E:18:ASP:OD2	1:E:30:HIS:HD2	1.86	0.58
1:H:118:THR:OG1	1:H:120:ILE:HG13	2.04	0.58
1:I:22:THR:H	4:I:5488:MPD:H11	1.66	0.58
1:A:18:ASP:OD2	1:A:30:HIS:HD2	1.86	0.58
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.36	0.58
1:C:82:ASP:HB2	4:C:5473:MPD:C3	2.33	0.58
1:L:18:ASP:OD2	1:L:30:HIS:HD2	1.86	0.58
1:L:332:LEU:HB2	1:L:408:PRO:HB2	1.85	0.58
1:B:179:TYR:CD2	1:C:53:SER:HB2	2.38	0.58
1:C:323:VAL:O	1:C:325:GLY:N	2.35	0.58
1:C:461:GLU:OE1	1:I:320:LYS:NZ	2.33	0.58
1:F:80:PHE:CB	4:F:5479:MPD:C1	2.56	0.58
1:G:332:LEU:HB2	1:G:408:PRO:HB2	1.85	0.58
1:H:360:PHE:CG	1:H:361:PRO:HD3	2.35	0.58
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.36	0.58
1:D:22:THR:H	4:D:5478:MPD:H11	1.66	0.58
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.04	0.58
1:G:360:PHE:CE2	1:G:361:PRO:HD3	2.36	0.58
1:I:53:SER:HB2	1:J:179:TYR:CD2	2.38	0.58
1:J:21:PHE:HB2	4:J:5490:MPD:C5	2.25	0.58
1:C:18:ASP:OD2	1:C:30:HIS:HD2	1.86	0.58
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.04	0.58
1:H:332:LEU:HB2	1:H:408:PRO:HB2	1.85	0.58
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.03	0.58
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.03	0.58
1:L:235:ILE:CG2	1:L:367:PRO:HG3	2.28	0.58
1:L:360:PHE:CG	1:L:361:PRO:HD3	2.35	0.58
1:B:21:PHE:HB2	4:B:5474:MPD:C5	2.25	0.58
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.36	0.58
1:C:22:THR:H	4:C:5476:MPD:H11	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.86	0.58
1:G:443:ILE:O	1:G:447:ARG:HG3	2.04	0.58
1:I:18:ASP:OD2	1:I:30:HIS:HD2	1.86	0.58
1:J:332:LEU:HB2	1:J:408:PRO:HB2	1.85	0.58
1:J:443:ILE:O	1:J:447:ARG:HG3	2.04	0.58
1:K:308:ILE:HG21	1:K:374:LEU:HD13	1.86	0.58
1:A:21:PHE:HB2	4:A:5472:MPD:C5	2.25	0.58
1:A:118:THR:OG1	1:A:120:ILE:HG13	2.03	0.58
1:F:443:ILE:O	1:F:447:ARG:HG3	2.04	0.58
1:J:22:THR:H	4:J:5490:MPD:H11	1.66	0.58
1:J:82:ASP:O	1:J:84:THR:CG2	2.51	0.58
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.86	0.58
1:D:18:ASP:OD2	1:D:30:HIS:HD2	1.86	0.58
1:D:443:ILE:O	1:D:447:ARG:HG3	2.04	0.58
1:L:118:THR:OG1	1:L:120:ILE:HG13	2.03	0.58
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.04	0.57
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.04	0.57
1:E:82:ASP:O	1:E:84:THR:CG2	2.51	0.57
1:F:332:LEU:HB2	1:F:408:PRO:HB2	1.85	0.57
1:J:18:ASP:OD2	1:J:30:HIS:HD2	1.86	0.57
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.35	0.57
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.04	0.57
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.86	0.57
1:K:360:PHE:CG	1:K:361:PRO:HD3	2.35	0.57
1:B:443:ILE:O	1:B:447:ARG:HG3	2.04	0.57
1:K:443:ILE:O	1:K:447:ARG:HG3	2.04	0.57
1:C:443:ILE:O	1:C:447:ARG:HG3	2.04	0.57
1:E:332:LEU:HB2	1:E:408:PRO:HB2	1.85	0.57
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.36	0.57
1:A:332:LEU:CB	1:A:408:PRO:HB2	2.35	0.57
1:F:435:THR:HG23	5:F:5531:HOH:O	2.05	0.57
1:H:443:ILE:O	1:H:447:ARG:HG3	2.04	0.57
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.36	0.57
1:K:21:PHE:HB2	4:K:5492:MPD:C5	2.25	0.57
1:G:435:THR:HG23	5:G:5529:HOH:O	2.05	0.57
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.04	0.57
1:C:435:THR:HG23	5:C:5518:HOH:O	2.05	0.57
1:E:435:THR:HG23	5:E:1210:HOH:O	2.05	0.57
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.04	0.57
1:F:120:ILE:HD13	1:F:382:ILE:HG21	1.87	0.57
1:G:180:PHE:HB3	1:L:30:HIS:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:332:LEU:CB	1:G:408:PRO:HB2	2.35	0.57
1:I:82:ASP:O	1:I:84:THR:CG2	2.51	0.57
1:I:120:ILE:HD13	1:I:382:ILE:HG21	1.87	0.57
1:K:332:LEU:CB	1:K:408:PRO:HB2	2.35	0.57
1:L:435:THR:HG23	5:L:3254:HOH:O	2.05	0.57
1:B:332:LEU:CB	1:B:408:PRO:HB2	2.35	0.57
1:G:53:SER:HB2	1:H:179:TYR:CD2	2.40	0.57
1:G:82:ASP:O	1:G:84:THR:CG2	2.51	0.57
1:G:120:ILE:HD13	1:G:382:ILE:HG21	1.87	0.57
1:H:192:ARG:HH21	1:H:219:ASN:HD22	1.52	0.57
1:I:80:PHE:CD1	4:I:5489:MPD:H52	2.39	0.57
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.86	0.57
1:A:443:ILE:O	1:A:447:ARG:HG3	2.04	0.57
1:B:235:ILE:CG2	1:B:367:PRO:HG3	2.28	0.57
1:F:192:ARG:HH21	1:F:219:ASN:HD22	1.52	0.57
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.86	0.57
1:I:360:PHE:CG	1:I:361:PRO:HD3	2.35	0.57
1:K:399:LEU:H	1:K:401:PRO:CG	1.90	0.57
4:K:5493:MPD:H11	1:L:189:GLN:HG3	1.87	0.57
1:A:179:TYR:CD2	1:B:53:SER:HB2	2.40	0.57
1:C:180:PHE:O	1:D:29:GLN:HA	2.04	0.57
1:C:192:ARG:HH21	1:C:219:ASN:HD22	1.52	0.57
1:D:120:ILE:HD13	1:D:382:ILE:HG21	1.87	0.57
1:D:180:PHE:HB3	1:E:30:HIS:H	1.70	0.57
1:D:192:ARG:HH21	1:D:219:ASN:HD22	1.52	0.57
1:D:399:LEU:CA	1:D:400:PRO:C	2.78	0.57
1:E:443:ILE:O	1:E:447:ARG:HG3	2.04	0.57
1:F:21:PHE:HB2	4:F:5482:MPD:C5	2.25	0.57
1:H:22:THR:H	4:H:5486:MPD:H11	1.66	0.57
1:K:399:LEU:CA	1:K:400:PRO:C	2.78	0.57
1:L:332:LEU:CB	1:L:408:PRO:HB2	2.35	0.57
1:C:120:ILE:HD13	1:C:382:ILE:HG21	1.87	0.56
1:C:189:GLN:HG3	4:D:5475:MPD:H11	1.87	0.56
1:J:326:TYR:HA	1:J:396:LEU:HD13	1.87	0.56
1:K:120:ILE:HD13	1:K:382:ILE:HG21	1.87	0.56
1:A:189:GLN:HG3	4:B:5471:MPD:H11	1.87	0.56
1:G:460:VAL:HG12	1:G:464:LEU:HD22	1.88	0.56
1:H:435:THR:HG23	5:H:5540:HOH:O	2.05	0.56
1:I:435:THR:HG23	5:I:5542:HOH:O	2.05	0.56
1:K:80:PHE:CB	4:K:5493:MPD:C1	2.60	0.56
1:L:443:ILE:O	1:L:447:ARG:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PHE:HD1	4:B:5471:MPD:C5	2.18	0.56
1:B:120:ILE:HD13	1:B:382:ILE:HG21	1.87	0.56
1:B:399:LEU:CA	1:B:400:PRO:C	2.78	0.56
1:C:340:SER:HB3	1:C:396:LEU:HA	1.88	0.56
1:D:332:LEU:CB	1:D:408:PRO:HB2	2.35	0.56
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.36	0.56
1:F:18:ASP:OD2	1:F:30:HIS:HD2	1.86	0.56
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.86	0.56
1:F:326:TYR:HA	1:F:396:LEU:HD13	1.87	0.56
1:G:18:ASP:OD2	1:G:30:HIS:HD2	1.86	0.56
4:H:5487:MPD:H11	1:I:189:GLN:HG3	1.87	0.56
1:L:120:ILE:HD13	1:L:382:ILE:HG21	1.87	0.56
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.86	0.56
1:L:399:LEU:CA	1:L:400:PRO:C	2.78	0.56
1:B:435:THR:HG23	5:B:5518:HOH:O	2.05	0.56
1:C:460:VAL:HG12	1:C:464:LEU:HD22	1.88	0.56
1:F:460:VAL:HG12	1:F:464:LEU:HD22	1.88	0.56
1:D:179:TYR:CD2	1:E:53:SER:HB2	2.41	0.56
1:E:332:LEU:CB	1:E:408:PRO:HB2	2.35	0.56
1:G:340:SER:HB3	1:G:396:LEU:HA	1.88	0.56
1:H:332:LEU:CB	1:H:408:PRO:HB2	2.35	0.56
4:I:5489:MPD:H11	1:J:189:GLN:HG3	1.87	0.56
1:J:340:SER:HB3	1:J:396:LEU:HA	1.87	0.56
1:K:80:PHE:HD1	4:K:5493:MPD:C5	2.17	0.56
1:K:192:ARG:HH21	1:K:219:ASN:HD22	1.52	0.56
1:K:435:THR:HG23	5:K:2962:HOH:O	2.05	0.56
1:L:326:TYR:HA	1:L:396:LEU:HD13	1.87	0.56
1:A:120:ILE:HD13	1:A:382:ILE:HG21	1.87	0.56
1:E:192:ARG:HH21	1:E:219:ASN:HD22	1.52	0.56
1:L:82:ASP:O	1:L:84:THR:CG2	2.51	0.56
1:B:82:ASP:O	1:B:84:THR:CG2	2.51	0.56
1:B:326:TYR:HA	1:B:396:LEU:HD13	1.88	0.56
1:E:189:GLN:HG3	4:F:5479:MPD:H11	1.87	0.56
1:F:248:ARG:CG	1:F:248:ARG:NH2	2.67	0.56
1:F:332:LEU:CB	1:F:408:PRO:HB2	2.35	0.56
1:G:326:TYR:HA	1:G:396:LEU:HD13	1.87	0.56
1:I:443:ILE:O	1:I:447:ARG:HG3	2.04	0.56
1:I:460:VAL:HG12	1:I:464:LEU:HD22	1.88	0.56
1:J:120:ILE:HD13	1:J:382:ILE:HG21	1.87	0.56
1:J:435:THR:HG23	5:J:2670:HOH:O	2.05	0.56
1:L:192:ARG:HH21	1:L:219:ASN:HD22	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:THR:HG23	5:A:5515:HOH:O	2.05	0.56
1:C:326:TYR:HA	1:C:396:LEU:HD13	1.87	0.56
1:C:399:LEU:CA	1:C:400:PRO:C	2.78	0.56
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.86	0.56
1:D:398:ASP:O	1:D:399:LEU:HG	2.06	0.56
1:E:340:SER:HB3	1:E:396:LEU:HA	1.88	0.56
1:H:398:ASP:O	1:H:399:LEU:HG	2.06	0.56
1:I:332:LEU:CB	1:I:408:PRO:HB2	2.35	0.56
1:J:399:LEU:CA	1:J:400:PRO:C	2.78	0.56
1:K:82:ASP:O	1:K:84:THR:CG2	2.51	0.56
1:A:326:TYR:HA	1:A:396:LEU:HD13	1.87	0.56
1:C:332:LEU:CB	1:C:408:PRO:HB2	2.35	0.56
1:D:21:PHE:HB2	4:D:5478:MPD:C5	2.25	0.56
1:J:61:ASN:O	1:K:337:ARG:CB	2.34	0.56
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.86	0.56
1:G:179:TYR:CD2	1:L:53:SER:HB2	2.40	0.56
1:G:192:ARG:HH21	1:G:219:ASN:HD22	1.52	0.56
4:J:5491:MPD:H11	1:K:189:GLN:HG3	1.87	0.56
1:K:398:ASP:O	1:K:399:LEU:HG	2.06	0.56
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.41	0.55
1:B:189:GLN:HG3	4:C:5473:MPD:H11	1.87	0.55
1:B:398:ASP:O	1:B:399:LEU:HG	2.06	0.55
1:E:120:ILE:HD13	1:E:382:ILE:HG21	1.87	0.55
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.41	0.55
1:H:340:SER:HB3	1:H:396:LEU:HA	1.88	0.55
1:I:340:SER:HB3	1:I:396:LEU:HA	1.87	0.55
1:K:326:TYR:HA	1:K:396:LEU:HD13	1.87	0.55
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.41	0.55
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.74	0.55
1:E:460:VAL:HG12	1:E:464:LEU:HD22	1.88	0.55
1:F:340:SER:HB3	1:F:396:LEU:HA	1.88	0.55
1:G:403:GLU:C	1:G:405:LYS:H	2.14	0.55
1:H:114:TYR:CD2	1:H:431:GLY:HA3	2.41	0.55
1:J:332:LEU:CB	1:J:408:PRO:HB2	2.35	0.55
1:J:460:VAL:HG12	1:J:464:LEU:HD22	1.88	0.55
4:A:5481:MPD:H11	1:F:189:GLN:HG3	1.87	0.55
1:B:181:PRO:HG3	5:C:5611:HOH:O	2.07	0.55
1:B:360:PHE:CD2	1:B:361:PRO:CD	2.74	0.55
1:E:326:TYR:HA	1:E:396:LEU:HD13	1.87	0.55
1:H:326:TYR:HA	1:H:396:LEU:HD13	1.87	0.55
1:H:399:LEU:CA	1:H:400:PRO:C	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:399:LEU:CA	1:I:400:PRO:C	2.78	0.55
1:J:192:ARG:HH21	1:J:219:ASN:HD22	1.52	0.55
1:A:340:SER:HB3	1:A:396:LEU:HA	1.88	0.55
1:A:460:VAL:HG12	1:A:464:LEU:HD22	1.88	0.55
1:C:82:ASP:O	1:C:84:THR:CG2	2.51	0.55
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.86	0.55
1:E:399:LEU:CA	1:E:400:PRO:C	2.78	0.55
1:J:398:ASP:O	1:J:399:LEU:HG	2.06	0.55
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.41	0.55
1:L:340:SER:HB3	1:L:396:LEU:HA	1.88	0.55
1:D:435:THR:HG23	5:D:918:HOH:O	2.05	0.55
1:F:403:GLU:C	1:F:405:LYS:H	2.14	0.55
1:F:461:GLU:OE1	1:L:320:LYS:NZ	2.30	0.55
1:G:189:GLN:HG3	4:L:5483:MPD:H11	1.87	0.55
1:H:120:ILE:HD13	1:H:382:ILE:HG21	1.87	0.55
1:J:80:PHE:HD1	4:J:5491:MPD:H52	1.69	0.55
1:D:189:GLN:HG3	4:E:5477:MPD:H11	1.87	0.55
1:D:340:SER:HB3	1:D:396:LEU:HA	1.88	0.55
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.86	0.55
1:L:398:ASP:O	1:L:399:LEU:HG	2.06	0.55
1:A:398:ASP:O	1:A:399:LEU:HG	2.06	0.55
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.41	0.55
1:D:82:ASP:O	1:D:84:THR:CG2	2.51	0.55
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.41	0.55
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.74	0.55
1:I:398:ASP:O	1:I:399:LEU:HG	2.06	0.55
1:B:80:PHE:CA	4:B:5471:MPD:H12	2.36	0.55
1:E:21:PHE:HB2	4:E:5480:MPD:C5	2.25	0.55
4:G:5485:MPD:H11	1:H:189:GLN:HG3	1.87	0.55
1:H:84:THR:CG2	4:H:5487:MPD:H32	2.37	0.55
1:H:460:VAL:HG12	1:H:464:LEU:HD22	1.88	0.55
1:I:29:GLN:HA	1:J:180:PHE:O	2.06	0.55
1:A:399:LEU:CA	1:A:400:PRO:C	2.78	0.55
1:B:340:SER:HB3	1:B:396:LEU:HA	1.88	0.55
1:B:460:VAL:HG12	1:B:464:LEU:HD22	1.88	0.55
1:D:326:TYR:HA	1:D:396:LEU:HD13	1.87	0.55
1:I:403:GLU:C	1:I:405:LYS:H	2.14	0.55
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.41	0.55
1:K:460:VAL:HG12	1:K:464:LEU:HD22	1.87	0.55
1:A:82:ASP:O	1:A:84:THR:CG2	2.51	0.55
1:D:460:VAL:HG12	1:D:464:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:PRO:HD2	1:L:231:LYS:HE2	1.89	0.55
1:C:398:ASP:O	1:C:399:LEU:HG	2.06	0.54
1:F:399:LEU:CA	1:F:400:PRO:C	2.78	0.54
1:G:29:GLN:OE1	1:H:181:PRO:HD3	2.07	0.54
1:G:398:ASP:O	1:G:399:LEU:HG	2.06	0.54
1:H:248:ARG:CG	1:H:248:ARG:NH2	2.67	0.54
1:I:114:TYR:CD2	1:I:431:GLY:HA3	2.41	0.54
1:K:340:SER:HB3	1:K:396:LEU:HA	1.88	0.54
1:B:192:ARG:HH21	1:B:219:ASN:HD22	1.52	0.54
1:C:181:PRO:HG3	5:D:1020:HOH:O	2.07	0.54
1:C:403:GLU:C	1:C:405:LYS:H	2.14	0.54
1:E:398:ASP:O	1:E:399:LEU:HG	2.06	0.54
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.37	0.54
1:I:22:THR:HG1	4:I:5488:MPD:C1	2.08	0.54
1:I:192:ARG:HH21	1:I:219:ASN:HD22	1.52	0.54
1:J:29:GLN:HA	1:K:180:PHE:O	2.07	0.54
1:J:105:ARG:HD2	4:J:5490:MPD:H32	1.90	0.54
1:J:128:PRO:HD2	1:J:231:LYS:HE2	1.89	0.54
1:J:248:ARG:HG2	1:J:248:ARG:NH2	2.23	0.54
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.74	0.54
1:L:460:VAL:HG12	1:L:464:LEU:HD22	1.88	0.54
1:B:128:PRO:HD2	1:B:231:LYS:HE2	1.89	0.54
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.41	0.54
1:E:248:ARG:HG2	1:E:248:ARG:NH2	2.23	0.54
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.41	0.54
1:K:114:TYR:CD2	1:K:431:GLY:HA3	2.41	0.54
1:K:403:GLU:C	1:K:405:LYS:H	2.14	0.54
1:L:21:PHE:HB2	4:L:5494:MPD:C5	2.25	0.54
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.36	0.54
1:F:128:PRO:HD2	1:F:231:LYS:HE2	1.89	0.54
1:F:398:ASP:O	1:F:399:LEU:HG	2.06	0.54
1:H:128:PRO:HD2	1:H:231:LYS:HE2	1.89	0.54
1:K:29:GLN:HA	1:L:180:PHE:O	2.08	0.54
1:K:30:HIS:H	1:L:180:PHE:HB3	1.73	0.54
1:B:456:THR:O	1:H:458:HIS:HE1	1.91	0.54
1:D:128:PRO:HD2	1:D:231:LYS:HE2	1.89	0.54
1:G:248:ARG:HG2	1:G:248:ARG:NH2	2.23	0.54
1:G:399:LEU:CA	1:G:400:PRO:C	2.78	0.54
1:H:248:ARG:HG2	1:H:248:ARG:NH2	2.23	0.54
1:L:84:THR:CG2	4:L:5483:MPD:H32	2.37	0.54
1:B:320:LYS:NZ	1:H:461:GLU:OE1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ARG:HG2	1:C:248:ARG:NH2	2.23	0.54
1:H:82:ASP:O	1:H:84:THR:CG2	2.51	0.54
1:A:61:ASN:O	1:F:337:ARG:CB	2.44	0.54
1:H:21:PHE:HB2	4:H:5486:MPD:C5	2.25	0.54
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.36	0.54
1:J:403:GLU:C	1:J:405:LYS:H	2.14	0.54
1:B:403:GLU:C	1:B:405:LYS:H	2.14	0.54
1:C:105:ARG:HD2	4:C:5476:MPD:H32	1.90	0.54
1:D:403:GLU:C	1:D:405:LYS:H	2.14	0.54
1:J:29:GLN:OE1	1:K:181:PRO:HD3	2.08	0.54
1:L:248:ARG:HG2	1:L:248:ARG:NH2	2.23	0.54
1:B:105:ARG:HD2	4:B:5474:MPD:H32	1.90	0.54
1:B:180:PHE:HB3	1:C:30:HIS:H	1.73	0.54
1:E:403:GLU:C	1:E:405:LYS:H	2.14	0.54
1:I:326:TYR:HA	1:I:396:LEU:HD13	1.88	0.54
1:K:80:PHE:HD1	4:K:5493:MPD:H52	1.73	0.54
1:A:403:GLU:C	1:A:405:LYS:H	2.14	0.54
1:E:128:PRO:HD2	1:E:231:LYS:HE2	1.89	0.54
5:K:3064:HOH:O	1:L:181:PRO:HG3	2.07	0.54
1:H:105:ARG:HD2	4:H:5486:MPD:H32	1.90	0.53
1:H:403:GLU:C	1:H:405:LYS:H	2.14	0.53
1:L:105:ARG:HD2	4:L:5494:MPD:H32	1.90	0.53
1:A:128:PRO:HD2	1:A:231:LYS:HE2	1.89	0.53
1:A:192:ARG:HH21	1:A:219:ASN:HD22	1.52	0.53
1:D:105:ARG:HD2	4:D:5478:MPD:H32	1.90	0.53
1:H:80:PHE:CG	4:H:5487:MPD:H12	2.37	0.53
1:B:248:ARG:HG2	1:B:248:ARG:NH2	2.23	0.53
1:H:80:PHE:CG	4:H:5487:MPD:C1	2.92	0.53
5:I:5635:HOH:O	1:J:181:PRO:HG3	2.07	0.53
1:D:248:ARG:HG2	1:D:248:ARG:NH2	2.23	0.53
1:H:80:PHE:CD1	4:H:5487:MPD:H52	2.33	0.53
1:K:105:ARG:HD2	4:K:5492:MPD:H32	1.90	0.53
1:A:105:ARG:HD2	4:A:5472:MPD:H32	1.90	0.53
1:E:105:ARG:HD2	4:E:5480:MPD:H32	1.90	0.53
1:I:80:PHE:CB	4:I:5489:MPD:C1	2.61	0.53
1:I:128:PRO:HD2	1:I:231:LYS:HE2	1.89	0.53
1:A:29:GLN:HA	1:F:180:PHE:O	2.08	0.53
1:C:128:PRO:HD2	1:C:231:LYS:HE2	1.89	0.53
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.74	0.53
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.74	0.53
1:B:461:GLU:OE1	1:H:320:LYS:NZ	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:ARG:HD2	4:F:5482:MPD:H32	1.90	0.53
1:F:399:LEU:H	1:F:401:PRO:CG	1.90	0.53
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.74	0.53
1:K:128:PRO:HD2	1:K:231:LYS:HE2	1.89	0.53
1:B:295:LEU:O	1:B:388:PRO:HG3	2.09	0.53
1:F:82:ASP:O	1:F:84:THR:CG2	2.51	0.53
1:G:105:ARG:HD2	4:G:5484:MPD:H32	1.90	0.53
1:H:29:GLN:HA	1:I:180:PHE:O	2.09	0.53
1:L:403:GLU:C	1:L:405:LYS:H	2.14	0.53
1:D:295:LEU:O	1:D:388:PRO:HG3	2.09	0.52
1:F:80:PHE:HD1	4:F:5479:MPD:H52	1.74	0.52
1:F:256:MET:HG3	1:L:466:TYR:HA	1.91	0.52
1:A:248:ARG:HH21	1:A:248:ARG:HG3	1.75	0.52
1:G:21:PHE:HA	4:G:5484:MPD:C3	2.36	0.52
1:G:128:PRO:HD2	1:G:231:LYS:HE2	1.89	0.52
1:H:360:PHE:CD2	1:H:361:PRO:CD	2.74	0.52
1:K:248:ARG:HG2	1:K:248:ARG:NH2	2.23	0.52
1:K:295:LEU:O	1:K:388:PRO:HG3	2.09	0.52
1:B:80:PHE:HD1	4:B:5471:MPD:H52	1.75	0.52
1:I:29:GLN:HB3	1:J:180:PHE:HB2	1.91	0.52
1:I:105:ARG:HD2	4:I:5488:MPD:H32	1.90	0.52
1:J:16:PHE:HB2	1:J:84:THR:HB	1.92	0.52
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.74	0.52
1:A:88:ARG:HH11	4:A:5472:MPD:HM3	1.75	0.52
1:B:16:PHE:HB2	1:B:84:THR:HB	1.92	0.52
1:H:16:PHE:HB2	1:H:84:THR:HB	1.92	0.52
1:H:295:LEU:O	1:H:388:PRO:HG3	2.09	0.52
1:J:295:LEU:O	1:J:388:PRO:HG3	2.09	0.52
1:L:295:LEU:O	1:L:388:PRO:HG3	2.09	0.52
1:A:30:HIS:H	1:F:180:PHE:HB3	1.73	0.52
1:A:248:ARG:HG2	1:A:248:ARG:NH2	2.23	0.52
1:C:88:ARG:HH11	4:C:5476:MPD:HM3	1.75	0.52
1:I:29:GLN:HB3	1:J:180:PHE:CB	2.40	0.52
1:J:88:ARG:HH11	4:J:5490:MPD:HM3	1.75	0.52
1:K:80:PHE:CA	4:K:5493:MPD:H12	2.38	0.52
1:A:256:MET:HG3	1:G:466:TYR:HA	1.91	0.52
1:D:80:PHE:HD1	4:D:5475:MPD:C5	2.23	0.52
1:F:88:ARG:HH11	4:F:5482:MPD:HM3	1.75	0.52
1:I:295:LEU:O	1:I:388:PRO:HG3	2.09	0.52
1:B:248:ARG:HH21	1:B:248:ARG:HG3	1.75	0.52
1:D:456:THR:O	1:J:458:HIS:HE1	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:PHE:HB2	1:E:84:THR:HB	1.92	0.52
1:J:29:GLN:HB3	1:K:180:PHE:HB2	1.92	0.52
1:B:88:ARG:HH11	4:B:5474:MPD:HM3	1.75	0.52
1:B:181:PRO:HD3	1:C:29:GLN:OE1	2.10	0.52
1:D:16:PHE:HB2	1:D:84:THR:HB	1.92	0.52
1:H:88:ARG:HH11	4:H:5486:MPD:HM3	1.75	0.52
1:I:248:ARG:HH21	1:I:248:ARG:HG3	1.75	0.52
1:C:16:PHE:HB2	1:C:84:THR:HB	1.92	0.51
1:I:311:LEU:HD22	1:I:369:LEU:HB3	1.93	0.51
1:F:248:ARG:HG2	1:F:248:ARG:NH2	2.23	0.51
1:I:88:ARG:HH11	4:I:5488:MPD:HM3	1.75	0.51
1:L:311:LEU:HD22	1:L:369:LEU:HB3	1.93	0.51
1:A:295:LEU:O	1:A:388:PRO:HG3	2.09	0.51
5:A:5609:HOH:O	1:F:181:PRO:HG3	2.10	0.51
1:E:295:LEU:O	1:E:388:PRO:HG3	2.09	0.51
1:I:21:PHE:HA	4:I:5488:MPD:C3	2.36	0.51
1:I:29:GLN:OE1	1:J:181:PRO:HD3	2.10	0.51
1:A:311:LEU:HD22	1:A:369:LEU:HB3	1.93	0.51
1:B:311:LEU:HD22	1:B:369:LEU:HB3	1.93	0.51
1:D:88:ARG:HH11	4:D:5478:MPD:HM3	1.75	0.51
1:E:311:LEU:HD22	1:E:369:LEU:HB3	1.93	0.51
1:H:84:THR:HG21	4:H:5487:MPD:H32	1.92	0.51
1:I:248:ARG:HG2	1:I:248:ARG:NH2	2.23	0.51
1:C:295:LEU:O	1:C:388:PRO:HG3	2.09	0.51
1:C:180:PHE:CB	1:D:29:GLN:HB3	2.41	0.51
1:D:458:HIS:HE1	1:J:456:THR:O	1.94	0.51
1:I:16:PHE:HB2	1:I:84:THR:HB	1.92	0.51
1:F:16:PHE:HB2	1:F:84:THR:HB	1.92	0.51
1:G:29:GLN:HA	1:H:180:PHE:O	2.11	0.51
1:J:84:THR:CG2	4:J:5491:MPD:H32	2.40	0.51
1:K:311:LEU:HD22	1:K:369:LEU:HB3	1.93	0.51
1:B:458:HIS:HE1	1:H:456:THR:O	1.93	0.51
1:F:295:LEU:O	1:F:388:PRO:HG3	2.09	0.51
1:G:295:LEU:O	1:G:388:PRO:HG3	2.09	0.51
1:A:248:ARG:CG	1:A:248:ARG:NH2	2.67	0.51
1:C:311:LEU:HD22	1:C:369:LEU:HB3	1.93	0.51
1:F:311:LEU:HD22	1:F:369:LEU:HB3	1.93	0.51
1:G:396:LEU:O	1:G:400:PRO:HG2	2.11	0.51
1:H:29:GLN:OE1	1:I:181:PRO:HD3	2.10	0.51
1:K:88:ARG:HH11	4:K:5492:MPD:HM3	1.75	0.51
1:G:248:ARG:HH21	1:G:248:ARG:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:248:ARG:HH21	1:J:248:ARG:HG3	1.75	0.51
1:K:16:PHE:HB2	1:K:84:THR:HB	1.92	0.51
1:L:88:ARG:HH11	4:L:5494:MPD:HM3	1.75	0.51
1:C:248:ARG:HH21	1:C:248:ARG:HG3	1.75	0.50
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.74	0.50
1:G:16:PHE:HB2	1:G:84:THR:HB	1.92	0.50
1:G:180:PHE:O	1:L:29:GLN:HA	2.10	0.50
1:J:53:SER:HB2	1:K:179:TYR:CD2	2.46	0.50
1:C:21:PHE:CB	4:C:5476:MPD:H53	2.27	0.50
1:G:88:ARG:HH11	4:G:5484:MPD:HM3	1.75	0.50
1:J:82:ASP:N	4:J:5491:MPD:O2	2.39	0.50
1:B:124:VAL:HG13	1:B:274:LEU:HD21	1.94	0.50
1:E:124:VAL:HG13	1:E:274:LEU:HD21	1.94	0.50
1:F:335:SER:HB2	1:F:392:MET:O	2.12	0.50
1:C:396:LEU:O	1:C:400:PRO:HG2	2.11	0.50
1:D:124:VAL:HG13	1:D:274:LEU:HD21	1.94	0.50
1:D:335:SER:HB2	1:D:392:MET:O	2.12	0.50
1:E:88:ARG:HH11	4:E:5480:MPD:HM3	1.75	0.50
1:E:396:LEU:O	1:E:400:PRO:HG2	2.11	0.50
1:H:192:ARG:HD3	1:H:219:ASN:HD22	1.77	0.50
1:I:28:GLU:OE1	1:I:88:ARG:NH1	2.45	0.50
1:I:124:VAL:HG13	1:I:274:LEU:HD21	1.94	0.50
1:L:16:PHE:HB2	1:L:84:THR:HB	1.92	0.50
1:L:124:VAL:HG13	1:L:274:LEU:HD21	1.94	0.50
1:A:16:PHE:HB2	1:A:84:THR:HB	1.92	0.50
1:A:124:VAL:HG13	1:A:274:LEU:HD21	1.94	0.50
1:B:396:LEU:O	1:B:400:PRO:HG2	2.12	0.50
1:C:180:PHE:HB2	1:D:29:GLN:HB3	1.92	0.50
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.77	0.50
1:C:458:HIS:HE1	1:I:456:THR:O	1.95	0.50
1:D:255:PHE:HB3	1:D:363:PRO:HB2	1.94	0.50
1:D:311:LEU:HD22	1:D:369:LEU:HB3	1.93	0.50
1:H:124:VAL:HG13	1:H:274:LEU:HD21	1.94	0.50
1:J:335:SER:HB2	1:J:392:MET:O	2.12	0.50
1:K:124:VAL:HG13	1:K:274:LEU:HD21	1.94	0.50
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.77	0.50
1:L:335:SER:HB2	1:L:392:MET:O	2.12	0.50
1:A:255:PHE:HB3	1:A:363:PRO:HB2	1.94	0.50
1:F:22:THR:CA	4:F:5482:MPD:H11	2.42	0.50
1:F:82:ASP:N	4:F:5479:MPD:O2	2.40	0.50
1:G:29:GLN:HB3	1:H:180:PHE:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:255:PHE:HB3	1:H:363:PRO:HB2	1.94	0.50
1:B:22:THR:CA	4:B:5474:MPD:H11	2.42	0.50
1:D:396:LEU:O	1:D:400:PRO:HG2	2.12	0.50
1:E:256:MET:HG3	1:K:466:TYR:HA	1.94	0.50
1:G:335:SER:HB2	1:G:392:MET:O	2.12	0.50
1:H:248:ARG:HH21	1:H:248:ARG:HG3	1.75	0.50
1:H:311:LEU:HD22	1:H:369:LEU:HB3	1.93	0.50
1:J:396:LEU:O	1:J:400:PRO:HG2	2.12	0.50
1:K:84:THR:CG2	4:K:5493:MPD:H32	2.42	0.50
1:K:255:PHE:HB3	1:K:363:PRO:HB2	1.94	0.50
1:L:22:THR:CA	4:L:5494:MPD:H11	2.42	0.50
1:B:25:LYS:NZ	5:B:5734:HOH:O	2.44	0.50
1:B:255:PHE:HB3	1:B:363:PRO:HB2	1.94	0.50
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.77	0.50
1:H:335:SER:HB2	1:H:392:MET:O	2.12	0.50
1:J:311:LEU:HD22	1:J:369:LEU:HB3	1.93	0.50
1:B:335:SER:HB2	1:B:392:MET:O	2.12	0.49
1:C:22:THR:HG1	4:C:5476:MPD:H13	1.73	0.49
1:D:248:ARG:HH21	1:D:248:ARG:HG3	1.75	0.49
1:F:21:PHE:HA	4:F:5482:MPD:C3	2.36	0.49
1:F:255:PHE:HB3	1:F:363:PRO:HB2	1.94	0.49
1:I:396:LEU:O	1:I:400:PRO:HG2	2.11	0.49
1:L:255:PHE:HB3	1:L:363:PRO:HB2	1.94	0.49
1:A:335:SER:HB2	1:A:392:MET:O	2.12	0.49
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.74	0.49
1:C:21:PHE:HA	4:C:5476:MPD:C3	2.36	0.49
1:C:80:PHE:HD1	4:C:5473:MPD:C5	2.13	0.49
1:D:28:GLU:OE1	1:D:88:ARG:NH1	2.45	0.49
1:E:22:THR:CA	4:E:5480:MPD:H11	2.42	0.49
1:F:80:PHE:CD1	4:F:5479:MPD:H52	2.46	0.49
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.77	0.49
1:G:80:PHE:HD1	4:G:5485:MPD:C5	2.25	0.49
1:H:396:LEU:O	1:H:400:PRO:HG2	2.11	0.49
1:I:22:THR:CA	4:I:5488:MPD:H11	2.42	0.49
1:J:124:VAL:HG13	1:J:274:LEU:HD21	1.94	0.49
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.77	0.49
1:B:80:PHE:CD1	4:B:5471:MPD:H52	2.46	0.49
1:E:255:PHE:HB3	1:E:363:PRO:HB2	1.94	0.49
1:F:396:LEU:O	1:F:400:PRO:HG2	2.11	0.49
1:G:25:LYS:NZ	5:G:5744:HOH:O	2.44	0.49
1:G:124:VAL:HG13	1:G:274:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:LEU:HD22	1:G:369:LEU:HB3	1.93	0.49
1:H:84:THR:HG21	4:H:5487:MPD:C3	2.41	0.49
1:I:255:PHE:HB3	1:I:363:PRO:HB2	1.94	0.49
1:J:255:PHE:HB3	1:J:363:PRO:HB2	1.94	0.49
1:K:28:GLU:OE1	1:K:88:ARG:NH1	2.45	0.49
1:L:84:THR:CB	4:L:5483:MPD:H52	2.38	0.49
1:A:84:THR:CB	4:A:5481:MPD:H52	2.38	0.49
1:B:180:PHE:O	1:C:29:GLN:HA	2.13	0.49
1:E:88:ARG:HD2	5:E:1252:HOH:O	2.13	0.49
1:G:384:ASN:N	1:G:384:ASN:ND2	2.60	0.49
1:I:335:SER:HB2	1:I:392:MET:O	2.12	0.49
1:J:21:PHE:HA	4:J:5490:MPD:C3	2.36	0.49
1:K:396:LEU:O	1:K:400:PRO:HG2	2.11	0.49
1:A:88:ARG:HD2	5:A:5553:HOH:O	2.13	0.49
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.77	0.49
1:C:335:SER:HB2	1:C:392:MET:O	2.12	0.49
1:C:454:ARG:O	1:I:320:LYS:HG3	2.11	0.49
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.77	0.49
1:I:248:ARG:CG	1:I:248:ARG:NH2	2.67	0.49
1:K:84:THR:CB	4:K:5493:MPD:H52	2.40	0.49
1:K:335:SER:HB2	1:K:392:MET:O	2.12	0.49
1:A:22:THR:CA	4:A:5472:MPD:H11	2.42	0.49
1:A:396:LEU:O	1:A:400:PRO:HG2	2.11	0.49
1:L:28:GLU:OE1	1:L:88:ARG:NH1	2.45	0.49
1:F:456:THR:O	1:L:458:HIS:HE1	1.96	0.49
1:G:88:ARG:HD2	5:G:5566:HOH:O	2.13	0.49
1:H:22:THR:CA	4:H:5486:MPD:H11	2.42	0.49
1:K:22:THR:CA	4:K:5492:MPD:H11	2.42	0.49
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.77	0.49
1:C:22:THR:CA	4:C:5476:MPD:H11	2.42	0.49
1:E:181:PRO:HD3	1:F:29:GLN:OE1	2.12	0.49
1:E:335:SER:HB2	1:E:392:MET:O	2.12	0.49
1:F:124:VAL:HG13	1:F:274:LEU:HD21	1.94	0.49
1:F:364:ALA:HA	1:L:468:VAL:HG13	1.95	0.49
1:G:181:PRO:HD3	1:L:29:GLN:OE1	2.13	0.49
1:H:21:PHE:HA	4:H:5486:MPD:C3	2.36	0.49
1:H:82:ASP:HB2	4:H:5487:MPD:C3	2.39	0.49
1:L:88:ARG:HD2	5:L:3296:HOH:O	2.13	0.49
1:L:396:LEU:O	1:L:400:PRO:HG2	2.11	0.49
1:D:22:THR:CA	4:D:5478:MPD:H11	2.42	0.49
1:G:181:PRO:HG3	5:L:3356:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ARG:O	1:G:320:LYS:HG3	2.12	0.49
1:C:124:VAL:HG13	1:C:274:LEU:HD21	1.94	0.49
1:E:248:ARG:HH21	1:E:248:ARG:HG3	1.75	0.49
1:E:466:TYR:HA	1:K:256:MET:HG3	1.94	0.49
1:F:88:ARG:HD2	5:F:5568:HOH:O	2.13	0.49
1:F:180:PHE:O	1:F:181:PRO:C	2.54	0.49
1:I:88:ARG:HD2	5:I:5579:HOH:O	2.13	0.49
1:A:384:ASN:N	1:A:384:ASN:ND2	2.60	0.48
1:C:180:PHE:O	1:C:181:PRO:C	2.54	0.48
1:C:387:HIS:HA	1:C:388:PRO:HD2	1.73	0.48
1:G:22:THR:CA	4:G:5484:MPD:H11	2.42	0.48
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.77	0.48
1:K:88:ARG:HD2	5:K:3004:HOH:O	2.13	0.48
1:L:248:ARG:HH21	1:L:248:ARG:HG3	1.75	0.48
1:B:306:LYS:HE2	5:B:5572:HOH:O	2.13	0.48
1:B:396:LEU:HB2	1:B:397:TYR:H	1.36	0.48
1:C:384:ASN:N	1:C:384:ASN:ND2	2.60	0.48
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.77	0.48
1:J:306:LYS:HE2	5:J:2729:HOH:O	2.13	0.48
1:K:21:PHE:CB	4:K:5492:MPD:H53	2.27	0.48
1:C:255:PHE:HB3	1:C:363:PRO:HB2	1.94	0.48
1:D:21:PHE:HA	4:D:5478:MPD:C3	2.36	0.48
1:D:22:THR:HG22	1:D:23:ASP:O	2.14	0.48
1:D:396:LEU:HB2	1:D:397:TYR:H	1.36	0.48
1:G:306:LYS:HE2	5:G:5583:HOH:O	2.13	0.48
1:H:88:ARG:HD2	5:H:5577:HOH:O	2.13	0.48
1:J:22:THR:CA	4:J:5490:MPD:H11	2.42	0.48
1:J:88:ARG:HD2	5:J:2712:HOH:O	2.13	0.48
1:J:384:ASN:N	1:J:384:ASN:ND2	2.60	0.48
1:D:84:THR:CB	4:D:5475:MPD:H52	2.41	0.48
1:E:22:THR:HG22	1:E:23:ASP:O	2.14	0.48
1:G:22:THR:HG22	1:G:23:ASP:O	2.14	0.48
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.77	0.48
4:K:5493:MPD:CM	1:L:193:SER:CB	2.84	0.48
1:L:84:THR:HG21	4:L:5483:MPD:H32	1.96	0.48
1:E:179:TYR:CD2	1:F:53:SER:HB2	2.49	0.48
1:G:21:PHE:CB	4:G:5484:MPD:H53	2.27	0.48
1:I:96:THR:HG1	1:I:98:GLN:HB2	1.76	0.48
1:J:398:ASP:OD1	1:J:399:LEU:HD23	2.14	0.48
1:K:329:PRO:O	1:K:342:SER:HB3	2.14	0.48
1:G:255:PHE:HB3	1:G:363:PRO:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:THR:HG22	1:I:23:ASP:O	2.14	0.48
1:B:329:PRO:O	1:B:342:SER:HB3	2.14	0.48
1:C:22:THR:HG22	1:C:23:ASP:O	2.14	0.48
1:C:329:PRO:O	1:C:342:SER:HB3	2.14	0.48
1:E:306:LYS:HE2	5:E:1269:HOH:O	2.13	0.48
1:E:398:ASP:OD1	1:E:399:LEU:HD23	2.14	0.48
1:F:458:HIS:HE1	1:L:456:THR:O	1.96	0.48
4:G:5485:MPD:CM	1:H:193:SER:CB	2.84	0.48
1:J:329:PRO:O	1:J:342:SER:HB3	2.14	0.48
1:K:22:THR:HG22	1:K:23:ASP:O	2.14	0.48
1:L:398:ASP:OD1	1:L:399:LEU:HD23	2.14	0.48
1:A:28:GLU:OE1	1:A:88:ARG:NH1	2.45	0.48
1:A:329:PRO:O	1:A:342:SER:HB3	2.14	0.48
1:B:22:THR:HG22	1:B:23:ASP:O	2.14	0.48
1:H:22:THR:HG22	1:H:23:ASP:O	2.14	0.48
1:J:29:GLN:HB3	1:K:180:PHE:CB	2.44	0.48
1:A:180:PHE:O	1:B:29:GLN:HA	2.13	0.48
1:A:398:ASP:OD1	1:A:399:LEU:HD23	2.14	0.48
1:D:329:PRO:O	1:D:342:SER:HB3	2.14	0.48
1:F:329:PRO:O	1:F:342:SER:HB3	2.14	0.48
1:F:364:ALA:HA	1:L:468:VAL:CG1	2.44	0.48
1:H:30:HIS:H	1:I:180:PHE:HB3	1.78	0.48
1:H:329:PRO:O	1:H:342:SER:HB3	2.14	0.48
1:L:329:PRO:O	1:L:342:SER:HB3	2.14	0.48
1:A:22:THR:HG22	1:A:23:ASP:O	2.14	0.48
1:C:398:ASP:OD1	1:C:399:LEU:HD23	2.14	0.48
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.74	0.48
1:J:84:THR:CB	4:J:5491:MPD:H52	2.37	0.48
1:L:84:THR:HG21	4:L:5483:MPD:C3	2.43	0.48
1:L:180:PHE:O	1:L:181:PRO:C	2.54	0.48
1:A:181:PRO:HD3	1:B:29:GLN:OE1	2.14	0.47
1:B:396:LEU:H	1:B:396:LEU:HG	1.46	0.47
1:C:88:ARG:HD2	5:C:5555:HOH:O	2.13	0.47
1:F:22:THR:HG22	1:F:23:ASP:O	2.14	0.47
1:K:328:ALA:HA	1:K:329:PRO:HD3	1.73	0.47
4:K:5493:MPD:O4	1:L:193:SER:OG	2.28	0.47
1:L:306:LYS:HE2	5:L:3313:HOH:O	2.13	0.47
1:D:88:ARG:HD2	5:D:960:HOH:O	2.13	0.47
1:F:306:LYS:HE2	5:F:5585:HOH:O	2.13	0.47
1:G:398:ASP:OD1	1:G:399:LEU:HD23	2.14	0.47
1:J:124:VAL:HG13	1:J:274:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ASP:OD1	1:B:399:LEU:HD23	2.14	0.47
1:D:124:VAL:HG13	1:D:274:LEU:CD2	2.45	0.47
1:D:384:ASN:N	1:D:384:ASN:ND2	2.60	0.47
1:E:232:ALA:HB1	1:E:367:PRO:HB2	1.97	0.47
1:E:329:PRO:O	1:E:342:SER:HB3	2.14	0.47
1:G:124:VAL:HG13	1:G:274:LEU:CD2	2.45	0.47
1:J:82:ASP:O	4:J:5491:MPD:H32	2.14	0.47
1:K:271:HIS:CD2	1:K:357:GLU:HG3	2.50	0.47
1:K:306:LYS:HE2	5:K:3021:HOH:O	2.14	0.47
1:B:21:PHE:HA	4:B:5474:MPD:C3	2.36	0.47
1:D:100:TYR:CE2	1:D:102:ARG:HB2	2.50	0.47
1:F:124:VAL:HG13	1:F:274:LEU:CD2	2.45	0.47
1:G:271:HIS:CD2	1:G:357:GLU:HG3	2.50	0.47
1:G:329:PRO:O	1:G:342:SER:HB3	2.14	0.47
1:H:180:PHE:O	1:H:181:PRO:C	2.54	0.47
1:I:124:VAL:HG13	1:I:274:LEU:CD2	2.45	0.47
1:I:271:HIS:CD2	1:I:357:GLU:HG3	2.50	0.47
1:J:22:THR:HG22	1:J:23:ASP:O	2.13	0.47
1:C:320:LYS:HG3	1:I:454:ARG:O	2.15	0.47
1:C:396:LEU:HB2	1:C:397:TYR:H	1.36	0.47
1:C:465:TYR:O	1:C:468:VAL:HB	2.15	0.47
1:E:193:SER:CB	4:F:5479:MPD:CM	2.84	0.47
1:E:271:HIS:CD2	1:E:357:GLU:HG3	2.50	0.47
1:E:320:LYS:HG3	1:K:454:ARG:O	2.13	0.47
1:G:232:ALA:HB1	1:G:367:PRO:HB2	1.97	0.47
1:K:465:TYR:O	1:K:468:VAL:HB	2.15	0.47
1:L:21:PHE:CB	4:L:5494:MPD:H53	2.27	0.47
1:A:124:VAL:HG13	1:A:274:LEU:CD2	2.45	0.47
1:A:271:HIS:CD2	1:A:357:GLU:HG3	2.50	0.47
1:B:271:HIS:CD2	1:B:357:GLU:HG3	2.50	0.47
1:F:21:PHE:CB	4:F:5482:MPD:H53	2.27	0.47
1:H:28:GLU:OE1	1:H:88:ARG:NH1	2.45	0.47
1:H:306:LYS:HE2	5:H:5594:HOH:O	2.13	0.47
1:J:232:ALA:HB1	1:J:367:PRO:HB2	1.97	0.47
1:K:124:VAL:HG13	1:K:274:LEU:CD2	2.45	0.47
1:A:21:PHE:CB	4:A:5472:MPD:H53	2.27	0.47
1:A:100:TYR:CE2	1:A:102:ARG:HB2	2.50	0.47
1:B:232:ALA:HB1	1:B:367:PRO:HB2	1.97	0.47
1:C:100:TYR:CE2	1:C:102:ARG:HB2	2.50	0.47
1:C:124:VAL:HG13	1:C:274:LEU:CD2	2.45	0.47
1:C:456:THR:O	1:I:458:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ALA:HB1	1:D:367:PRO:HB2	1.97	0.47
1:D:306:LYS:HE2	5:D:977:HOH:O	2.14	0.47
1:D:465:TYR:O	1:D:468:VAL:HB	2.15	0.47
1:E:454:ARG:O	1:K:320:LYS:HG3	2.13	0.47
1:F:248:ARG:HH21	1:F:248:ARG:HG3	1.75	0.47
1:H:232:ALA:HB1	1:H:367:PRO:HB2	1.97	0.47
1:J:180:PHE:O	1:J:181:PRO:C	2.54	0.47
1:J:248:ARG:CG	1:J:248:ARG:NH2	2.66	0.47
1:L:22:THR:HG22	1:L:23:ASP:O	2.14	0.47
1:L:80:PHE:CG	4:L:5483:MPD:C1	2.97	0.47
1:A:193:SER:CB	4:B:5471:MPD:CM	2.84	0.47
1:A:306:LYS:HE2	5:A:5570:HOH:O	2.13	0.47
1:B:28:GLU:OE1	1:B:88:ARG:NH1	2.45	0.47
1:C:232:ALA:HB1	1:C:367:PRO:HB2	1.97	0.47
1:C:455:MET:HG2	1:I:323:VAL:HG11	1.97	0.47
1:E:180:PHE:O	1:E:181:PRO:C	2.54	0.47
1:F:232:ALA:HB1	1:F:367:PRO:HB2	1.97	0.47
1:G:80:PHE:CA	4:G:5485:MPD:H12	2.42	0.47
1:H:398:ASP:OD1	1:H:399:LEU:HD23	2.14	0.47
1:H:465:TYR:O	1:H:468:VAL:HB	2.15	0.47
1:L:21:PHE:HA	4:L:5494:MPD:C3	2.36	0.47
1:L:100:TYR:CE2	1:L:102:ARG:HB2	2.50	0.47
1:B:88:ARG:HD2	5:B:5555:HOH:O	2.13	0.47
1:E:21:PHE:CB	4:E:5480:MPD:H53	2.27	0.47
1:E:124:VAL:HG13	1:E:274:LEU:CD2	2.45	0.47
1:F:100:TYR:CE2	1:F:102:ARG:HB2	2.50	0.47
1:F:398:ASP:OD1	1:F:399:LEU:HD23	2.14	0.47
1:G:28:GLU:OE1	1:G:88:ARG:NH1	2.45	0.47
1:G:100:TYR:CE2	1:G:102:ARG:HB2	2.50	0.47
1:G:465:TYR:O	1:G:468:VAL:HB	2.15	0.47
1:H:328:ALA:HA	1:H:329:PRO:HD3	1.73	0.47
1:I:306:LYS:HE2	5:I:5596:HOH:O	2.13	0.47
1:I:329:PRO:O	1:I:342:SER:HB3	2.14	0.47
1:K:295:LEU:O	1:K:388:PRO:HG2	2.15	0.47
1:L:271:HIS:CD2	1:L:357:GLU:HG3	2.50	0.47
1:A:31:VAL:HG23	1:F:210:HIS:HB3	1.97	0.47
1:A:320:LYS:HG3	1:G:454:ARG:O	2.15	0.47
1:B:100:TYR:CE2	1:B:102:ARG:HB2	2.50	0.47
1:C:193:SER:OG	4:D:5475:MPD:O4	2.28	0.47
1:C:256:MET:HG3	1:I:466:TYR:HA	1.97	0.47
1:E:28:GLU:OE1	1:E:88:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:398:ASP:OD1	1:I:399:LEU:HD23	2.14	0.47
1:J:28:GLU:OE1	1:J:88:ARG:NH1	2.45	0.47
1:J:84:THR:HG21	4:J:5491:MPD:C3	2.45	0.47
1:L:465:TYR:O	1:L:468:VAL:HB	2.15	0.47
1:A:41:GLU:OE2	1:A:45:GLU:OE2	2.34	0.46
1:A:465:TYR:O	1:A:468:VAL:HB	2.15	0.46
1:C:306:LYS:HE2	5:C:5572:HOH:O	2.13	0.46
1:D:80:PHE:HD1	4:D:5475:MPD:H52	1.80	0.46
1:D:398:ASP:OD1	1:D:399:LEU:HD23	2.14	0.46
1:D:466:TYR:HA	1:J:256:MET:HG3	1.97	0.46
1:F:271:HIS:CD2	1:F:357:GLU:HG3	2.50	0.46
1:K:41:GLU:OE2	1:K:45:GLU:OE2	2.34	0.46
1:K:398:ASP:OD1	1:K:399:LEU:HD23	2.14	0.46
1:L:384:ASN:N	1:L:384:ASN:ND2	2.60	0.46
1:A:181:PRO:HG3	5:B:5611:HOH:O	2.14	0.46
1:E:100:TYR:CE2	1:E:102:ARG:HB2	2.50	0.46
5:G:5622:HOH:O	1:H:181:PRO:HG3	2.13	0.46
1:J:80:PHE:CG	4:J:5491:MPD:H53	2.50	0.46
1:J:100:TYR:CE2	1:J:102:ARG:HB2	2.50	0.46
1:K:232:ALA:HB1	1:K:367:PRO:HB2	1.97	0.46
1:L:41:GLU:OE2	1:L:45:GLU:OE2	2.34	0.46
1:F:465:TYR:O	1:F:468:VAL:HB	2.15	0.46
1:G:368:TYR:OH	4:G:5484:MPD:O2	2.26	0.46
1:I:465:TYR:O	1:I:468:VAL:HB	2.15	0.46
1:K:80:PHE:CD1	4:K:5493:MPD:H52	2.46	0.46
1:K:248:ARG:HH21	1:K:248:ARG:HG3	1.75	0.46
1:A:318:SER:OG	1:A:362:ASP:OD2	2.27	0.46
1:B:41:GLU:OE2	1:B:45:GLU:OE2	2.34	0.46
1:B:295:LEU:O	1:B:388:PRO:HG2	2.15	0.46
1:B:465:TYR:O	1:B:468:VAL:HB	2.15	0.46
1:C:271:HIS:CD2	1:C:357:GLU:HG3	2.50	0.46
1:D:41:GLU:OE2	1:D:45:GLU:OE2	2.34	0.46
1:E:41:GLU:OE2	1:E:45:GLU:OE2	2.34	0.46
1:E:396:LEU:H	1:E:396:LEU:HG	1.46	0.46
1:H:41:GLU:OE2	1:H:45:GLU:OE2	2.34	0.46
1:H:271:HIS:CD2	1:H:357:GLU:HG3	2.50	0.46
1:H:295:LEU:O	1:H:388:PRO:HG2	2.15	0.46
1:I:41:GLU:OE2	1:I:45:GLU:OE2	2.34	0.46
4:I:5489:MPD:CM	1:J:193:SER:CB	2.84	0.46
1:J:25:LYS:NZ	5:J:2904:HOH:O	2.44	0.46
1:J:271:HIS:CD2	1:J:357:GLU:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:465:TYR:O	1:J:468:VAL:HB	2.15	0.46
1:L:328:ALA:HA	1:L:329:PRO:HD3	1.73	0.46
1:A:21:PHE:HA	4:A:5472:MPD:C3	2.36	0.46
1:A:180:PHE:O	1:A:181:PRO:C	2.54	0.46
1:I:3:GLU:O	1:I:7:THR:HG23	2.16	0.46
1:K:25:LYS:NZ	5:K:3196:HOH:O	2.44	0.46
1:L:232:ALA:HB1	1:L:367:PRO:HB2	1.97	0.46
1:B:124:VAL:HG13	1:B:274:LEU:CD2	2.44	0.46
1:E:128:PRO:HA	1:E:269:HIS:O	2.16	0.46
1:E:465:TYR:O	1:E:468:VAL:HB	2.15	0.46
1:G:41:GLU:OE2	1:G:45:GLU:OE2	2.34	0.46
1:H:100:TYR:CE2	1:H:102:ARG:HB2	2.50	0.46
1:K:180:PHE:O	1:K:181:PRO:C	2.54	0.46
1:K:403:GLU:C	1:K:405:LYS:N	2.74	0.46
1:A:128:PRO:HA	1:A:269:HIS:O	2.16	0.46
1:A:387:HIS:HA	1:A:388:PRO:HD2	1.73	0.46
1:A:403:GLU:C	1:A:405:LYS:N	2.74	0.46
1:C:88:ARG:NE	4:C:5476:MPD:HM1	2.30	0.46
1:D:271:HIS:CD2	1:D:357:GLU:HG3	2.50	0.46
1:F:454:ARG:O	1:L:320:LYS:HG3	2.16	0.46
1:G:3:GLU:O	1:G:7:THR:HG23	2.16	0.46
1:I:100:TYR:CE2	1:I:102:ARG:HB2	2.50	0.46
1:J:41:GLU:OE2	1:J:45:GLU:OE2	2.34	0.46
1:A:232:ALA:HB1	1:A:367:PRO:HB2	1.97	0.46
1:B:320:LYS:HG3	1:H:454:ARG:O	2.16	0.46
1:F:328:ALA:HA	1:F:329:PRO:HD3	1.73	0.46
1:H:124:VAL:HG13	1:H:274:LEU:CD2	2.45	0.46
1:H:128:PRO:HA	1:H:269:HIS:O	2.16	0.46
1:I:21:PHE:CB	4:I:5488:MPD:H53	2.27	0.46
1:I:384:ASN:N	1:I:384:ASN:ND2	2.60	0.46
1:J:295:LEU:O	1:J:388:PRO:HG2	2.15	0.46
1:B:88:ARG:NE	4:B:5474:MPD:HM1	2.30	0.46
1:C:403:GLU:C	1:C:405:LYS:N	2.74	0.46
1:D:3:GLU:O	1:D:7:THR:HG23	2.16	0.46
1:E:295:LEU:O	1:E:388:PRO:HG2	2.15	0.46
1:F:254:THR:HB	1:L:466:TYR:CE1	2.51	0.46
1:F:384:ASN:N	1:F:384:ASN:ND2	2.60	0.46
1:J:84:THR:CG2	4:J:5491:MPD:C5	2.48	0.46
1:K:100:TYR:CE2	1:K:102:ARG:HB2	2.50	0.46
1:B:80:PHE:CB	4:B:5471:MPD:C1	2.65	0.46
1:C:128:PRO:HA	1:C:269:HIS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:PHE:O	1:D:181:PRO:C	2.54	0.46
1:F:3:GLU:O	1:F:7:THR:HG23	2.16	0.46
1:G:128:PRO:HA	1:G:269:HIS:O	2.16	0.46
1:G:396:LEU:HB2	1:G:397:TYR:H	1.36	0.46
1:I:232:ALA:HB1	1:I:367:PRO:HB2	1.97	0.46
1:J:128:PRO:HA	1:J:269:HIS:O	2.16	0.46
1:L:3:GLU:O	1:L:7:THR:HG23	2.16	0.46
1:A:3:GLU:O	1:A:7:THR:HG23	2.16	0.45
1:B:313:ASN:HD21	1:B:360:PHE:HD2	1.65	0.45
1:G:80:PHE:HD1	4:G:5485:MPD:H52	1.81	0.45
1:J:3:GLU:O	1:J:7:THR:HG23	2.16	0.45
5:J:2772:HOH:O	1:K:181:PRO:HG3	2.15	0.45
1:L:124:VAL:HG13	1:L:274:LEU:CD2	2.45	0.45
1:A:396:LEU:H	1:A:396:LEU:HG	1.46	0.45
1:A:466:TYR:HA	1:G:256:MET:HG3	1.97	0.45
1:C:41:GLU:OE2	1:C:45:GLU:OE2	2.34	0.45
1:D:80:PHE:CA	4:D:5475:MPD:H12	2.45	0.45
1:E:3:GLU:O	1:E:7:THR:HG23	2.16	0.45
1:F:84:THR:CG2	4:F:5479:MPD:H32	2.46	0.45
1:F:313:ASN:HD21	1:F:360:PHE:HD2	1.65	0.45
1:G:313:ASN:HD21	1:G:360:PHE:HD2	1.65	0.45
1:G:403:GLU:C	1:G:405:LYS:N	2.74	0.45
1:B:128:PRO:HA	1:B:269:HIS:O	2.16	0.45
1:C:210:HIS:HB3	1:D:31:VAL:HG23	1.99	0.45
1:D:180:PHE:O	1:E:29:GLN:HA	2.16	0.45
1:F:41:GLU:OE2	1:F:45:GLU:OE2	2.34	0.45
1:G:29:GLN:HB3	1:H:180:PHE:CB	2.46	0.45
1:J:21:PHE:CB	4:J:5490:MPD:H53	2.27	0.45
1:J:84:THR:CG2	4:J:5491:MPD:C4	2.88	0.45
1:K:128:PRO:HA	1:K:269:HIS:O	2.16	0.45
1:K:231:LYS:HD2	1:K:231:LYS:HA	1.74	0.45
1:K:368:TYR:OH	4:K:5492:MPD:O2	2.27	0.45
1:C:3:GLU:O	1:C:7:THR:HG23	2.16	0.45
1:C:28:GLU:OE1	1:C:88:ARG:NH1	2.45	0.45
1:E:180:PHE:O	1:F:29:GLN:HA	2.16	0.45
1:G:80:PHE:CD1	4:G:5485:MPD:H52	2.51	0.45
1:J:313:ASN:HD21	1:J:360:PHE:HD2	1.65	0.45
1:D:128:PRO:HA	1:D:269:HIS:O	2.16	0.45
1:I:128:PRO:HA	1:I:269:HIS:O	2.16	0.45
1:I:328:ALA:HA	1:I:329:PRO:HD3	1.73	0.45
1:J:403:GLU:C	1:J:405:LYS:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:248:ARG:CG	1:K:248:ARG:NH2	2.66	0.45
1:K:313:ASN:HD21	1:K:360:PHE:HD2	1.65	0.45
1:A:193:SER:OG	4:B:5471:MPD:O4	2.28	0.45
1:B:180:PHE:O	1:B:181:PRO:C	2.54	0.45
1:B:323:VAL:HG11	1:H:455:MET:HG2	1.98	0.45
1:D:403:GLU:C	1:D:405:LYS:N	2.74	0.45
1:H:3:GLU:O	1:H:7:THR:HG23	2.16	0.45
1:H:170:GLY:HA2	1:H:172:ARG:HH22	1.81	0.45
1:L:295:LEU:O	1:L:388:PRO:HG2	2.15	0.45
1:B:320:LYS:HG2	1:H:455:MET:C	2.42	0.45
1:H:403:GLU:C	1:H:405:LYS:N	2.74	0.45
1:I:80:PHE:CG	4:I:5489:MPD:H53	2.50	0.45
1:K:3:GLU:O	1:K:7:THR:HG23	2.16	0.45
1:B:403:GLU:C	1:B:405:LYS:N	2.74	0.45
1:C:80:PHE:CG	4:C:5473:MPD:H12	2.48	0.45
1:D:25:LYS:NZ	5:D:1152:HOH:O	2.44	0.45
1:H:21:PHE:CB	4:H:5486:MPD:H53	2.27	0.45
1:I:180:PHE:O	1:I:181:PRO:C	2.54	0.45
1:J:31:VAL:HG23	1:K:210:HIS:HB3	1.98	0.45
1:J:34:PRO:HG2	1:K:206:VAL:O	2.17	0.45
1:A:180:PHE:HB2	1:B:29:GLN:HB3	1.99	0.45
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.82	0.45
1:A:458:HIS:CD2	1:A:459:PRO:HD2	2.52	0.45
1:B:387:HIS:HA	1:B:388:PRO:HD2	1.73	0.45
1:B:454:ARG:O	1:H:320:LYS:HG3	2.17	0.45
1:C:340:SER:HB3	1:C:396:LEU:HB3	1.99	0.45
1:E:84:THR:CB	4:E:5477:MPD:H52	2.41	0.45
1:F:28:GLU:OE1	1:F:88:ARG:NH1	2.45	0.45
1:F:128:PRO:HA	1:F:269:HIS:O	2.16	0.45
1:H:84:THR:CB	4:H:5487:MPD:H52	2.45	0.45
1:I:170:GLY:HA2	1:I:172:ARG:HH22	1.81	0.45
1:K:21:PHE:HA	4:K:5492:MPD:C3	2.36	0.45
1:K:340:SER:HB3	1:K:396:LEU:HB3	1.99	0.45
1:B:340:SER:HB3	1:B:396:LEU:HB3	1.99	0.45
1:D:65:MET:HA	1:D:94:PRO:HG3	1.99	0.45
1:E:340:SER:HB3	1:E:396:LEU:HB3	1.99	0.45
1:F:403:GLU:C	1:F:405:LYS:N	2.74	0.45
1:G:340:SER:HB3	1:G:396:LEU:HB3	1.99	0.45
1:I:276:LYS:HG2	1:I:277:ASN:ND2	2.33	0.45
1:I:340:SER:HB3	1:I:396:LEU:HB3	1.99	0.45
1:K:84:THR:HG21	4:K:5493:MPD:H32	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:458:HIS:CD2	1:K:459:PRO:HD2	2.52	0.45
1:L:128:PRO:HA	1:L:269:HIS:O	2.16	0.45
1:A:276:LYS:HG2	1:A:277:ASN:ND2	2.33	0.44
1:A:295:LEU:O	1:A:388:PRO:HG2	2.15	0.44
1:A:340:SER:HB3	1:A:396:LEU:HB3	1.99	0.44
1:D:88:ARG:NE	4:D:5478:MPD:HM1	2.30	0.44
1:D:276:LYS:HG2	1:D:277:ASN:ND2	2.33	0.44
1:E:181:PRO:HG3	5:F:5624:HOH:O	2.18	0.44
1:L:276:LYS:HG2	1:L:277:ASN:ND2	2.32	0.44
1:B:3:GLU:O	1:B:7:THR:HG23	2.16	0.44
1:C:22:THR:HG1	4:C:5476:MPD:C1	2.29	0.44
1:C:328:ALA:HA	1:C:329:PRO:HD3	1.73	0.44
1:E:403:GLU:C	1:E:405:LYS:N	2.74	0.44
1:E:458:HIS:CD2	1:E:459:PRO:HD2	2.52	0.44
1:G:276:LYS:HG2	1:G:277:ASN:ND2	2.33	0.44
1:L:313:ASN:HD21	1:L:360:PHE:HD2	1.65	0.44
1:A:65:MET:HA	1:A:94:PRO:HG3	2.00	0.44
1:D:295:LEU:O	1:D:388:PRO:HG2	2.15	0.44
1:D:320:LYS:HG3	1:J:454:ARG:O	2.18	0.44
1:D:458:HIS:CD2	1:D:459:PRO:HD2	2.52	0.44
1:E:313:ASN:HD21	1:E:360:PHE:HD2	1.65	0.44
1:J:88:ARG:NE	4:J:5490:MPD:HM1	2.30	0.44
1:J:340:SER:HB3	1:J:396:LEU:HB3	1.99	0.44
1:A:328:ALA:HA	1:A:329:PRO:HD3	1.73	0.44
1:C:80:PHE:CG	4:C:5473:MPD:H53	2.51	0.44
1:E:215:THR:O	1:E:216:ALA:HB3	2.18	0.44
1:I:295:LEU:O	1:I:388:PRO:HG2	2.15	0.44
1:K:65:MET:HA	1:K:94:PRO:HG3	2.00	0.44
1:A:215:THR:O	1:A:216:ALA:HB3	2.18	0.44
1:A:313:ASN:HD21	1:A:360:PHE:HD2	1.65	0.44
1:B:170:GLY:HA2	1:B:172:ARG:HH22	1.81	0.44
1:B:276:LYS:HG2	1:B:277:ASN:ND2	2.33	0.44
1:B:458:HIS:CD2	1:B:459:PRO:HD2	2.52	0.44
1:C:17:VAL:HG12	1:C:19:LEU:HD13	2.00	0.44
1:F:88:ARG:NE	4:F:5482:MPD:HM1	2.30	0.44
1:H:458:HIS:CD2	1:H:459:PRO:HD2	2.52	0.44
1:L:215:THR:O	1:L:216:ALA:HB3	2.18	0.44
1:L:403:GLU:C	1:L:405:LYS:N	2.74	0.44
1:A:17:VAL:HG12	1:A:19:LEU:HD13	2.00	0.44
1:A:396:LEU:HB2	1:A:397:TYR:H	1.36	0.44
1:C:313:ASN:HD21	1:C:360:PHE:HD2	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ASP:C	1:C:399:LEU:HG	2.43	0.44
1:C:455:MET:C	1:I:320:LYS:HG2	2.43	0.44
1:E:21:PHE:HA	4:E:5480:MPD:C3	2.36	0.44
1:F:295:LEU:O	1:F:388:PRO:HG2	2.15	0.44
1:G:180:PHE:O	1:G:181:PRO:C	2.54	0.44
1:G:398:ASP:C	1:G:399:LEU:HG	2.43	0.44
1:H:61:ASN:O	1:I:337:ARG:CB	2.50	0.44
1:H:88:ARG:NE	4:H:5486:MPD:HM1	2.30	0.44
1:I:309:ASN:HD22	1:I:313:ASN:HD22	1.66	0.44
1:J:73:THR:HG21	1:J:88:ARG:HB3	2.00	0.44
1:J:80:PHE:CG	4:J:5491:MPD:C1	3.00	0.44
1:C:275:ALA:HA	1:C:281:LEU:HD13	2.00	0.44
1:D:84:THR:CG2	4:D:5475:MPD:H32	2.48	0.44
1:D:193:SER:CB	4:E:5477:MPD:CM	2.84	0.44
1:F:275:ALA:HA	1:F:281:LEU:HD13	2.00	0.44
1:F:340:SER:HB3	1:F:396:LEU:HB3	1.99	0.44
1:G:275:ALA:HA	1:G:281:LEU:HD13	2.00	0.44
1:G:458:HIS:CD2	1:G:459:PRO:HD2	2.52	0.44
4:G:5485:MPD:O4	1:H:193:SER:OG	2.28	0.44
1:H:215:THR:O	1:H:216:ALA:HB3	2.18	0.44
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.74	0.44
1:I:65:MET:HA	1:I:94:PRO:HG3	2.00	0.44
1:I:231:LYS:HD2	1:I:231:LYS:HA	1.74	0.44
1:I:275:ALA:HA	1:I:281:LEU:HD13	2.00	0.44
1:K:17:VAL:HG12	1:K:19:LEU:HD13	2.00	0.44
1:K:276:LYS:HG2	1:K:277:ASN:ND2	2.32	0.44
1:L:458:HIS:CD2	1:L:459:PRO:HD2	2.53	0.44
1:B:73:THR:HG21	1:B:88:ARG:HB3	2.00	0.44
1:C:458:HIS:CD2	1:C:459:PRO:HD2	2.53	0.44
1:D:398:ASP:C	1:D:399:LEU:HG	2.43	0.44
1:E:276:LYS:HG2	1:E:277:ASN:ND2	2.33	0.44
1:F:231:LYS:HD2	1:F:231:LYS:HA	1.74	0.44
1:F:398:ASP:C	1:F:399:LEU:HG	2.43	0.44
1:G:17:VAL:HG12	1:G:19:LEU:HD13	2.00	0.44
1:G:180:PHE:CB	1:L:29:GLN:HB3	2.48	0.44
1:G:309:ASN:HD22	1:G:313:ASN:HD22	1.66	0.44
1:I:398:ASP:C	1:I:399:LEU:HG	2.43	0.44
1:K:215:THR:O	1:K:216:ALA:HB3	2.18	0.44
1:A:139:ARG:HD3	1:F:163:LYS:HG2	1.99	0.44
1:B:231:LYS:HD2	1:B:231:LYS:HA	1.74	0.44
1:C:295:LEU:O	1:C:388:PRO:HG2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:ASN:HD22	1:D:313:ASN:HD22	1.66	0.44
1:E:17:VAL:HG12	1:E:19:LEU:HD13	2.00	0.44
1:E:309:ASN:HD22	1:E:313:ASN:HD22	1.66	0.44
1:H:340:SER:HB3	1:H:396:LEU:HB3	1.99	0.44
1:H:398:ASP:C	1:H:399:LEU:HG	2.43	0.44
1:I:215:THR:O	1:I:216:ALA:HB3	2.18	0.44
1:I:313:ASN:HD21	1:I:360:PHE:HD2	1.64	0.44
1:I:403:GLU:C	1:I:405:LYS:N	2.74	0.44
1:C:276:LYS:HG2	1:C:277:ASN:ND2	2.32	0.43
1:D:215:THR:O	1:D:216:ALA:HB3	2.18	0.43
1:D:468:VAL:HG13	1:J:364:ALA:HA	1.99	0.43
1:F:82:ASP:O	4:F:5479:MPD:H32	2.18	0.43
1:F:125:LEU:O	1:F:272:MET:HA	2.18	0.43
1:F:458:HIS:CD2	1:F:459:PRO:HD2	2.52	0.43
1:G:65:MET:HA	1:G:94:PRO:HG3	2.00	0.43
1:H:65:MET:HA	1:H:94:PRO:HG3	2.00	0.43
1:H:313:ASN:HD21	1:H:360:PHE:HD2	1.65	0.43
1:I:458:HIS:CD2	1:I:459:PRO:HD2	2.52	0.43
1:L:398:ASP:C	1:L:399:LEU:HG	2.43	0.43
1:B:125:LEU:O	1:B:272:MET:HA	2.19	0.43
1:B:344:ARG:NH1	1:B:346:PRO:HA	2.34	0.43
1:C:215:THR:O	1:C:216:ALA:HB3	2.18	0.43
1:E:344:ARG:NH1	1:E:346:PRO:HA	2.34	0.43
1:F:73:THR:HG21	1:F:88:ARG:HB3	2.00	0.43
1:F:396:LEU:HB2	1:F:397:TYR:H	1.36	0.43
4:G:5485:MPD:H11	1:H:189:GLN:CG	2.48	0.43
1:H:17:VAL:HG12	1:H:19:LEU:HD13	2.00	0.43
1:H:137:ASP:HB3	1:H:152:ASP:HB3	2.01	0.43
1:J:170:GLY:HA2	1:J:172:ARG:HH22	1.81	0.43
1:J:215:THR:O	1:J:216:ALA:HB3	2.18	0.43
1:J:398:ASP:C	1:J:399:LEU:HG	2.43	0.43
1:J:458:HIS:CD2	1:J:459:PRO:HD2	2.52	0.43
1:K:235:ILE:HD13	1:K:235:ILE:HA	1.82	0.43
1:A:125:LEU:O	1:A:272:MET:HA	2.19	0.43
1:A:189:GLN:CG	4:B:5471:MPD:H11	2.48	0.43
1:A:344:ARG:NH1	1:A:346:PRO:HA	2.34	0.43
1:B:21:PHE:CB	4:B:5474:MPD:H53	2.27	0.43
1:C:235:ILE:HD13	1:C:235:ILE:HA	1.82	0.43
1:D:189:GLN:CG	4:E:5477:MPD:H11	2.48	0.43
1:D:468:VAL:CG1	1:J:364:ALA:HA	2.49	0.43
1:F:17:VAL:HG12	1:F:19:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:GLN:OE1	1:F:236:GLN:HA	2.19	0.43
1:F:256:MET:CG	1:L:466:TYR:HA	2.49	0.43
1:G:236:GLN:OE1	1:G:236:GLN:HA	2.19	0.43
1:G:332:LEU:HD22	1:G:409:GLN:C	2.44	0.43
1:H:344:ARG:NH1	1:H:346:PRO:HA	2.34	0.43
1:I:88:ARG:NE	4:I:5488:MPD:HM1	2.30	0.43
1:J:17:VAL:HG12	1:J:19:LEU:HD13	2.00	0.43
1:J:125:LEU:O	1:J:272:MET:HA	2.19	0.43
1:J:276:LYS:HG2	1:J:277:ASN:ND2	2.33	0.43
1:K:236:GLN:HA	1:K:236:GLN:OE1	2.19	0.43
1:A:398:ASP:C	1:A:399:LEU:HG	2.43	0.43
1:B:65:MET:HA	1:B:94:PRO:HG3	2.00	0.43
1:C:65:MET:HA	1:C:94:PRO:HG3	2.00	0.43
1:C:125:LEU:O	1:C:272:MET:HA	2.19	0.43
1:D:313:ASN:HD21	1:D:360:PHE:HD2	1.65	0.43
1:D:332:LEU:HD22	1:D:409:GLN:C	2.44	0.43
1:D:344:ARG:NH1	1:D:346:PRO:HA	2.34	0.43
1:F:276:LYS:HG2	1:F:277:ASN:ND2	2.33	0.43
1:H:236:GLN:OE1	1:H:236:GLN:HA	2.19	0.43
1:H:276:LYS:HG2	1:H:277:ASN:ND2	2.33	0.43
1:H:309:ASN:HD22	1:H:313:ASN:HD22	1.66	0.43
1:I:344:ARG:NH1	1:I:346:PRO:HA	2.34	0.43
1:J:236:GLN:OE1	1:J:236:GLN:HA	2.19	0.43
4:J:5491:MPD:H11	1:K:189:GLN:CG	2.48	0.43
1:K:275:ALA:HA	1:K:281:LEU:HD13	2.00	0.43
1:K:332:LEU:HD22	1:K:409:GLN:C	2.44	0.43
1:L:65:MET:HA	1:L:94:PRO:HG3	2.00	0.43
1:L:344:ARG:NH1	1:L:346:PRO:HA	2.34	0.43
1:L:396:LEU:HB2	1:L:397:TYR:H	1.36	0.43
1:A:180:PHE:CB	1:B:29:GLN:HB3	2.49	0.43
1:A:309:ASN:HD22	1:A:313:ASN:HD22	1.66	0.43
1:B:215:THR:O	1:B:216:ALA:HB3	2.18	0.43
1:B:309:ASN:HD22	1:B:313:ASN:HD22	1.66	0.43
1:B:332:LEU:HD22	1:B:409:GLN:C	2.44	0.43
1:C:236:GLN:HA	1:C:236:GLN:OE1	2.19	0.43
1:D:73:THR:HG21	1:D:88:ARG:HB3	2.00	0.43
1:D:170:GLY:HA2	1:D:172:ARG:HH22	1.81	0.43
1:D:275:ALA:HA	1:D:281:LEU:HD13	2.00	0.43
1:J:387:HIS:HA	1:J:388:PRO:HD2	1.73	0.43
1:K:309:ASN:HD22	1:K:313:ASN:HD22	1.66	0.43
4:K:5493:MPD:H11	1:L:189:GLN:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ASP:C	1:B:399:LEU:HG	2.43	0.43
1:D:125:LEU:O	1:D:272:MET:HA	2.19	0.43
1:D:137:ASP:HB3	1:D:152:ASP:HB3	2.01	0.43
1:E:125:LEU:O	1:E:272:MET:HA	2.19	0.43
1:E:398:ASP:C	1:E:399:LEU:HG	2.43	0.43
1:F:215:THR:O	1:F:216:ALA:HB3	2.18	0.43
1:G:231:LYS:HA	1:G:231:LYS:HD2	1.74	0.43
1:I:73:THR:HG21	1:I:88:ARG:HB3	2.00	0.43
1:J:332:LEU:HD22	1:J:409:GLN:C	2.44	0.43
1:L:125:LEU:O	1:L:272:MET:HA	2.19	0.43
1:A:29:GLN:HB3	1:F:180:PHE:HB2	2.00	0.43
1:A:80:PHE:CB	4:A:5481:MPD:C1	2.75	0.43
1:A:236:GLN:OE1	1:A:236:GLN:HA	2.19	0.43
1:B:320:LYS:HG2	1:H:455:MET:O	2.19	0.43
1:D:368:TYR:OH	4:D:5478:MPD:O2	2.27	0.43
1:E:231:LYS:HA	1:E:231:LYS:HD2	1.74	0.43
1:E:275:ALA:HA	1:E:281:LEU:HD13	2.00	0.43
1:F:65:MET:HA	1:F:94:PRO:HG3	2.00	0.43
1:F:309:ASN:HD22	1:F:313:ASN:HD22	1.66	0.43
1:H:396:LEU:H	1:H:396:LEU:HG	1.46	0.43
4:I:5489:MPD:H11	1:J:189:GLN:CG	2.48	0.43
1:J:65:MET:HA	1:J:94:PRO:HG3	1.99	0.43
1:J:80:PHE:CD1	4:J:5491:MPD:H52	2.44	0.43
4:A:5481:MPD:CM	1:F:193:SER:CB	2.84	0.43
1:B:193:SER:OG	4:C:5473:MPD:O4	2.28	0.43
1:B:236:GLN:OE1	1:B:236:GLN:HA	2.19	0.43
1:D:340:SER:HB3	1:D:396:LEU:HB3	1.99	0.43
1:E:137:ASP:HB3	1:E:152:ASP:HB3	2.01	0.43
1:F:137:ASP:HB3	1:F:152:ASP:HB3	2.01	0.43
1:G:73:THR:HG21	1:G:88:ARG:HB3	2.00	0.43
1:G:344:ARG:NH1	1:G:346:PRO:HA	2.34	0.43
1:H:29:GLN:HB3	1:I:180:PHE:CB	2.49	0.43
1:H:332:LEU:HD22	1:H:409:GLN:C	2.44	0.43
4:H:5487:MPD:CM	1:I:193:SER:CB	2.84	0.43
1:I:17:VAL:HG12	1:I:19:LEU:HD13	2.00	0.43
1:J:275:ALA:HA	1:J:281:LEU:HD13	2.00	0.43
1:K:398:ASP:C	1:K:399:LEU:HG	2.43	0.43
1:L:2:ALA:O	1:L:6:LEU:HD12	2.19	0.43
1:L:88:ARG:NE	4:L:5494:MPD:HM1	2.30	0.43
1:L:137:ASP:HB3	1:L:152:ASP:HB3	2.01	0.43
1:L:275:ALA:HA	1:L:281:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:334:TYR:HA	1:L:343:ILE:O	2.19	0.43
1:A:275:ALA:HA	1:A:281:LEU:HD13	2.00	0.43
1:B:275:ALA:HA	1:B:281:LEU:HD13	2.00	0.43
1:C:189:GLN:CG	4:D:5475:MPD:H11	2.48	0.43
1:C:231:LYS:HD2	1:C:231:LYS:HA	1.74	0.43
1:D:2:ALA:O	1:D:6:LEU:HD12	2.19	0.43
1:D:21:PHE:CB	4:D:5478:MPD:H53	2.27	0.43
1:E:332:LEU:HD22	1:E:409:GLN:C	2.44	0.43
1:I:236:GLN:OE1	1:I:236:GLN:HA	2.19	0.43
1:K:396:LEU:H	1:K:396:LEU:HG	1.46	0.43
1:L:73:THR:HG21	1:L:88:ARG:HB3	2.00	0.43
1:L:340:SER:HB3	1:L:396:LEU:HB3	1.99	0.43
1:C:2:ALA:O	1:C:6:LEU:HD12	2.19	0.43
1:C:73:THR:HG21	1:C:88:ARG:HB3	2.00	0.43
1:C:309:ASN:HD22	1:C:313:ASN:HD22	1.66	0.43
1:F:2:ALA:O	1:F:6:LEU:HD12	2.19	0.43
1:F:466:TYR:HA	1:L:256:MET:HG3	2.01	0.43
1:G:88:ARG:NE	4:G:5484:MPD:HM1	2.29	0.43
1:G:125:LEU:O	1:G:272:MET:HA	2.19	0.43
1:G:189:GLN:CG	4:L:5483:MPD:H11	2.48	0.43
1:H:2:ALA:O	1:H:6:LEU:HD12	2.19	0.43
1:H:22:THR:HG1	4:H:5486:MPD:C1	2.31	0.43
1:H:334:TYR:HA	1:H:343:ILE:O	2.19	0.43
1:I:2:ALA:O	1:I:6:LEU:HD12	2.19	0.43
1:K:80:PHE:CG	4:K:5493:MPD:H12	2.48	0.43
1:K:125:LEU:O	1:K:272:MET:HA	2.19	0.43
1:K:139:ARG:HD3	1:L:163:LYS:HG2	2.01	0.43
1:L:332:LEU:HD22	1:L:409:GLN:C	2.44	0.43
1:A:2:ALA:O	1:A:6:LEU:HD12	2.19	0.42
1:A:332:LEU:HD22	1:A:409:GLN:C	2.44	0.42
1:B:466:TYR:HA	1:H:256:MET:HG3	2.02	0.42
1:C:80:PHE:CG	4:C:5473:MPD:C1	3.01	0.42
1:C:334:TYR:HA	1:C:343:ILE:O	2.19	0.42
1:D:80:PHE:CB	4:D:5475:MPD:C1	2.68	0.42
1:D:80:PHE:CD1	4:D:5475:MPD:H52	2.51	0.42
1:E:2:ALA:O	1:E:6:LEU:HD12	2.19	0.42
1:E:334:TYR:HA	1:E:343:ILE:O	2.19	0.42
1:F:170:GLY:HA2	1:F:172:ARG:HH22	1.81	0.42
1:G:215:THR:O	1:G:216:ALA:HB3	2.18	0.42
1:I:387:HIS:HA	1:I:388:PRO:HD2	1.73	0.42
1:J:84:THR:HG21	4:J:5491:MPD:H32	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:390:GLU:HA	1:J:391:PRO:HD3	1.89	0.42
1:K:29:GLN:HB3	1:L:180:PHE:CB	2.49	0.42
1:K:31:VAL:HG23	1:L:210:HIS:HB3	2.01	0.42
1:K:344:ARG:NH1	1:K:346:PRO:HA	2.34	0.42
1:A:29:GLN:HB3	1:F:180:PHE:CB	2.49	0.42
1:A:30:HIS:HB3	1:F:182:VAL:HG12	2.01	0.42
1:A:73:THR:HG21	1:A:88:ARG:HB3	2.00	0.42
1:B:390:GLU:HA	1:B:391:PRO:HD3	1.89	0.42
1:C:170:GLY:HA2	1:C:172:ARG:HH22	1.81	0.42
1:E:65:MET:HA	1:E:94:PRO:HG3	2.00	0.42
1:F:332:LEU:HD22	1:F:409:GLN:C	2.44	0.42
1:H:125:LEU:O	1:H:272:MET:HA	2.19	0.42
1:J:334:TYR:HA	1:J:343:ILE:O	2.19	0.42
1:J:344:ARG:NH1	1:J:346:PRO:HA	2.33	0.42
1:K:73:THR:HG21	1:K:88:ARG:HB3	2.00	0.42
1:K:396:LEU:HB2	1:K:397:TYR:H	1.36	0.42
1:A:88:ARG:NE	4:A:5472:MPD:HM1	2.30	0.42
4:A:5481:MPD:H11	1:F:189:GLN:CG	2.49	0.42
1:D:334:TYR:HA	1:D:343:ILE:O	2.19	0.42
1:E:458:HIS:HE1	1:K:456:THR:O	2.03	0.42
1:H:73:THR:HG21	1:H:88:ARG:HB3	2.00	0.42
1:H:275:ALA:HA	1:H:281:LEU:HD13	2.00	0.42
1:I:137:ASP:HB3	1:I:152:ASP:HB3	2.01	0.42
1:I:332:LEU:HB2	1:I:408:PRO:CB	2.50	0.42
1:I:332:LEU:HD22	1:I:409:GLN:C	2.44	0.42
1:J:2:ALA:O	1:J:6:LEU:HD12	2.19	0.42
1:J:137:ASP:HB3	1:J:152:ASP:HB3	2.01	0.42
1:K:2:ALA:O	1:K:6:LEU:HD12	2.19	0.42
1:A:138:ILE:HG23	1:A:138:ILE:O	2.20	0.42
1:E:88:ARG:NE	4:E:5480:MPD:HM1	2.30	0.42
1:F:334:TYR:HA	1:F:343:ILE:O	2.19	0.42
1:G:138:ILE:O	1:G:138:ILE:HG23	2.20	0.42
1:G:193:SER:CB	4:L:5483:MPD:CM	2.84	0.42
1:G:334:TYR:HA	1:G:343:ILE:O	2.19	0.42
1:I:125:LEU:O	1:I:272:MET:HA	2.19	0.42
1:K:80:PHE:CG	4:K:5493:MPD:C1	3.01	0.42
1:L:17:VAL:HG12	1:L:19:LEU:HD13	2.00	0.42
1:A:364:ALA:HA	1:G:468:VAL:HG13	2.01	0.42
1:B:332:LEU:HB2	1:B:408:PRO:CB	2.50	0.42
1:B:384:ASN:N	1:B:384:ASN:ND2	2.60	0.42
1:C:344:ARG:NH1	1:C:346:PRO:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:LEU:HB2	1:F:408:PRO:CB	2.50	0.42
1:F:396:LEU:H	1:F:396:LEU:HG	1.46	0.42
1:K:29:GLN:HB3	1:L:180:PHE:HB2	2.01	0.42
1:K:138:ILE:HG23	1:K:138:ILE:O	2.20	0.42
1:K:170:GLY:HA2	1:K:172:ARG:HH22	1.81	0.42
1:L:309:ASN:HD22	1:L:313:ASN:HD22	1.66	0.42
1:B:17:VAL:HG12	1:B:19:LEU:HD13	2.00	0.42
1:B:334:TYR:HA	1:B:343:ILE:O	2.19	0.42
1:C:137:ASP:HB3	1:C:152:ASP:HB3	2.01	0.42
1:C:281:LEU:HB3	1:C:293:GLN:OE1	2.20	0.42
1:C:332:LEU:HD22	1:C:409:GLN:C	2.44	0.42
1:E:138:ILE:HG23	1:E:138:ILE:O	2.20	0.42
1:E:236:GLN:OE1	1:E:236:GLN:HA	2.19	0.42
1:F:344:ARG:NH1	1:F:346:PRO:HA	2.34	0.42
1:I:138:ILE:HG23	1:I:138:ILE:O	2.20	0.42
1:I:334:TYR:HA	1:I:343:ILE:O	2.19	0.42
1:K:137:ASP:HB3	1:K:152:ASP:HB3	2.01	0.42
1:A:137:ASP:HB3	1:A:152:ASP:HB3	2.01	0.42
1:A:256:MET:CG	1:G:466:TYR:HA	2.49	0.42
1:B:281:LEU:HB3	1:B:293:GLN:OE1	2.20	0.42
1:D:192:ARG:NH2	1:D:219:ASN:ND2	2.63	0.42
1:D:454:ARG:O	1:J:320:LYS:HG3	2.20	0.42
1:G:170:GLY:HA2	1:G:172:ARG:HH22	1.81	0.42
1:J:309:ASN:HD22	1:J:313:ASN:HD22	1.66	0.42
1:K:84:THR:HG21	4:K:5493:MPD:C3	2.48	0.42
1:L:80:PHE:CG	4:L:5483:MPD:H53	2.53	0.42
1:L:236:GLN:OE1	1:L:236:GLN:HA	2.19	0.42
1:A:53:SER:CB	1:F:179:TYR:CD2	3.01	0.42
1:A:170:GLY:HA2	1:A:172:ARG:HH22	1.81	0.42
1:A:281:LEU:HB3	1:A:293:GLN:OE1	2.20	0.42
1:B:137:ASP:HB3	1:B:152:ASP:HB3	2.01	0.42
1:B:189:GLN:CG	4:C:5473:MPD:H11	2.49	0.42
1:B:272:MET:HE3	1:B:272:MET:HB2	1.97	0.42
1:D:17:VAL:HG12	1:D:19:LEU:HD13	2.00	0.42
1:D:332:LEU:HB2	1:D:408:PRO:CB	2.50	0.42
1:E:281:LEU:HB3	1:E:293:GLN:OE1	2.20	0.42
1:E:456:THR:O	1:K:458:HIS:HE1	2.02	0.42
1:G:137:ASP:HB3	1:G:152:ASP:HB3	2.01	0.42
1:G:180:PHE:HB2	1:L:29:GLN:HB3	2.00	0.42
1:H:281:LEU:HB3	1:H:293:GLN:OE1	2.20	0.42
1:I:281:LEU:HB3	1:I:293:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:GLY:HA2	1:L:172:ARG:HH22	1.81	0.42
1:D:181:PRO:HG3	5:E:1312:HOH:O	2.19	0.42
1:D:256:MET:HG3	1:J:466:TYR:HA	2.02	0.42
1:G:295:LEU:O	1:G:388:PRO:HG2	2.15	0.42
1:J:138:ILE:O	1:J:138:ILE:HG23	2.20	0.42
1:K:130:PRO:HB3	1:K:268:MET:CE	2.42	0.42
1:L:231:LYS:HA	1:L:231:LYS:HD2	1.74	0.42
1:L:281:LEU:HB3	1:L:293:GLN:OE1	2.20	0.42
1:L:332:LEU:HD12	1:L:332:LEU:HA	1.90	0.42
1:L:387:HIS:HA	1:L:388:PRO:HD2	1.73	0.42
1:A:84:THR:CG2	4:A:5481:MPD:H32	2.50	0.42
1:B:138:ILE:O	1:B:138:ILE:HG23	2.20	0.42
4:B:5474:MPD:H4	4:B:5474:MPD:H12	1.82	0.42
1:C:84:THR:CG2	4:C:5473:MPD:H32	2.49	0.42
1:C:396:LEU:H	1:C:396:LEU:HG	1.46	0.42
1:E:73:THR:HG21	1:E:88:ARG:HB3	2.00	0.42
1:F:192:ARG:NH2	1:F:219:ASN:ND2	2.63	0.42
1:H:332:LEU:HB2	1:H:408:PRO:CB	2.50	0.42
1:A:130:PRO:HB3	1:A:268:MET:CE	2.41	0.41
1:C:225:PHE:HD1	3:C:4473:ADP:O2'	2.03	0.41
1:C:332:LEU:HB2	1:C:408:PRO:CB	2.50	0.41
1:D:281:LEU:HB3	1:D:293:GLN:OE1	2.20	0.41
1:E:170:GLY:HA2	1:E:172:ARG:HH22	1.81	0.41
1:E:272:MET:HE3	1:E:272:MET:HB2	1.97	0.41
1:G:68:MET:HA	1:G:69:PRO:HD2	1.95	0.41
1:J:332:LEU:HD12	1:J:332:LEU:HA	1.90	0.41
1:K:281:LEU:HB3	1:K:293:GLN:OE1	2.20	0.41
1:K:334:TYR:HA	1:K:343:ILE:O	2.19	0.41
1:A:296:TYR:HB3	1:A:382:ILE:HA	2.03	0.41
1:A:334:TYR:HA	1:A:343:ILE:O	2.19	0.41
1:A:364:ALA:HA	1:G:468:VAL:CG1	2.50	0.41
1:A:456:THR:O	1:G:458:HIS:HE1	2.02	0.41
1:B:91:ILE:HB	1:B:103:ASP:HB2	2.02	0.41
1:C:433:VAL:HG12	1:C:434:PHE:CD2	2.55	0.41
1:D:130:PRO:HB3	1:D:268:MET:CE	2.41	0.41
1:D:138:ILE:HG23	1:D:138:ILE:O	2.20	0.41
1:G:91:ILE:HB	1:G:103:ASP:HB2	2.02	0.41
1:I:84:THR:CG2	4:I:5489:MPD:H32	2.50	0.41
4:J:5491:MPD:CM	1:K:193:SER:CB	2.84	0.41
1:K:192:ARG:NH2	1:K:219:ASN:ND2	2.63	0.41
1:K:272:MET:HE3	1:K:272:MET:HB2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:230:LYS:O	1:L:234:GLU:HG3	2.20	0.41
1:L:433:VAL:HG12	1:L:434:PHE:CD2	2.55	0.41
1:E:296:TYR:HB3	1:E:382:ILE:HA	2.03	0.41
1:F:433:VAL:HG12	1:F:434:PHE:CD2	2.55	0.41
1:G:281:LEU:HB3	1:G:293:GLN:OE1	2.20	0.41
1:G:433:VAL:HG12	1:G:434:PHE:CD2	2.56	0.41
4:H:5487:MPD:H11	1:I:189:GLN:CG	2.48	0.41
1:K:88:ARG:NE	4:K:5492:MPD:HM1	2.30	0.41
1:L:225:PHE:HD1	3:L:4482:ADP:O2'	2.03	0.41
1:B:130:PRO:HB3	1:B:268:MET:CE	2.41	0.41
1:C:296:TYR:HB3	1:C:382:ILE:HA	2.03	0.41
1:G:2:ALA:O	1:G:6:LEU:HD12	2.19	0.41
1:H:80:PHE:CG	4:H:5487:MPD:H53	2.50	0.41
1:F:91:ILE:HB	1:F:103:ASP:HB2	2.03	0.41
1:F:230:LYS:O	1:F:234:GLU:HG3	2.21	0.41
1:H:433:VAL:HG12	1:H:434:PHE:CD2	2.55	0.41
1:K:225:PHE:HD1	3:K:4481:ADP:O2'	2.03	0.41
1:K:332:LEU:HB2	1:K:408:PRO:CB	2.50	0.41
1:A:225:PHE:HD1	3:A:4471:ADP:O2'	2.03	0.41
1:B:254:THR:HB	1:H:466:TYR:CE1	2.56	0.41
1:C:138:ILE:O	1:C:138:ILE:HG23	2.20	0.41
1:C:390:GLU:HA	1:C:391:PRO:HD3	1.89	0.41
1:D:236:GLN:OE1	1:D:236:GLN:HA	2.19	0.41
1:F:281:LEU:HB3	1:F:293:GLN:OE1	2.20	0.41
1:G:231:LYS:HE2	5:G:5504:HOH:O	2.21	0.41
1:I:231:LYS:HE2	5:I:5517:HOH:O	2.21	0.41
1:I:396:LEU:H	1:I:396:LEU:HG	1.46	0.41
1:I:433:VAL:HG12	1:I:434:PHE:CD2	2.55	0.41
1:K:91:ILE:HB	1:K:103:ASP:HB2	2.03	0.41
1:L:332:LEU:HB2	1:L:408:PRO:CB	2.50	0.41
1:A:458:HIS:HE1	1:G:456:THR:O	2.03	0.41
1:E:80:PHE:CB	4:E:5477:MPD:C1	2.76	0.41
1:E:225:PHE:HD1	3:E:4475:ADP:O2'	2.03	0.41
1:F:296:TYR:HB3	1:F:382:ILE:HA	2.03	0.41
1:F:320:LYS:HG3	1:L:454:ARG:O	2.21	0.41
1:H:138:ILE:O	1:H:138:ILE:HG23	2.20	0.41
1:H:230:LYS:O	1:H:234:GLU:HG3	2.20	0.41
1:H:384:ASN:N	1:H:384:ASN:ND2	2.60	0.41
1:I:296:TYR:HB3	1:I:382:ILE:HA	2.03	0.41
1:J:91:ILE:HB	1:J:103:ASP:HB2	2.03	0.41
1:J:230:LYS:O	1:J:234:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:281:LEU:HB3	1:J:293:GLN:OE1	2.20	0.41
1:J:396:LEU:H	1:J:396:LEU:HG	1.46	0.41
1:J:433:VAL:HG12	1:J:434:PHE:CD2	2.55	0.41
1:L:91:ILE:HB	1:L:103:ASP:HB2	2.02	0.41
1:B:206:VAL:O	1:C:34:PRO:HG2	2.20	0.41
1:B:230:LYS:O	1:B:234:GLU:HG3	2.20	0.41
1:C:231:LYS:HE2	5:C:5493:HOH:O	2.21	0.41
1:D:225:PHE:HD1	3:D:4474:ADP:O2'	2.03	0.41
1:G:296:TYR:HB3	1:G:382:ILE:HA	2.03	0.41
1:H:114:TYR:O	1:H:118:THR:HG23	2.21	0.41
1:H:296:TYR:HB3	1:H:382:ILE:HA	2.03	0.41
1:I:225:PHE:HD1	3:I:4479:ADP:O2'	2.03	0.41
1:J:231:LYS:HE2	5:J:2640:HOH:O	2.21	0.41
1:J:296:TYR:HB3	1:J:382:ILE:HA	2.03	0.41
1:K:433:VAL:HG12	1:K:434:PHE:CD2	2.55	0.41
1:A:230:LYS:O	1:A:234:GLU:HG3	2.21	0.41
1:A:433:VAL:HG12	1:A:434:PHE:CD2	2.55	0.41
1:B:2:ALA:O	1:B:6:LEU:HD12	2.19	0.41
1:B:313:ASN:HB3	1:B:318:SER:HB3	2.03	0.41
1:C:193:SER:CB	4:D:5475:MPD:CM	2.84	0.41
1:C:294:ALA:O	1:C:298:ILE:HG13	2.21	0.41
1:D:91:ILE:HB	1:D:103:ASP:HB2	2.03	0.41
1:D:114:TYR:O	1:D:118:THR:HG23	2.21	0.41
1:D:332:LEU:HD12	1:D:332:LEU:HA	1.90	0.41
1:D:364:ALA:HA	1:J:468:VAL:HG13	2.03	0.41
1:E:206:VAL:O	1:F:34:PRO:HG2	2.20	0.41
1:E:230:LYS:O	1:E:234:GLU:HG3	2.21	0.41
1:E:231:LYS:HE2	5:E:1180:HOH:O	2.21	0.41
1:E:323:VAL:HG11	1:K:455:MET:HG2	2.03	0.41
1:E:390:GLU:HA	1:E:391:PRO:HD3	1.89	0.41
1:E:433:VAL:HG12	1:E:434:PHE:CD2	2.56	0.41
1:F:138:ILE:HG23	1:F:138:ILE:O	2.20	0.41
1:G:114:TYR:O	1:G:118:THR:HG23	2.21	0.41
1:G:230:LYS:O	1:G:234:GLU:HG3	2.21	0.41
4:G:5484:MPD:C5	4:G:5484:MPD:H11	2.45	0.41
1:I:34:PRO:HG2	1:J:206:VAL:O	2.20	0.41
1:J:272:MET:HE3	1:J:272:MET:HB2	1.97	0.41
1:L:114:TYR:O	1:L:118:THR:HG23	2.21	0.41
1:L:296:TYR:HB3	1:L:382:ILE:HA	2.03	0.41
1:A:91:ILE:HB	1:A:103:ASP:HB2	2.03	0.41
1:B:114:TYR:O	1:B:118:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:HD1	3:B:4472:ADP:O2'	2.03	0.41
1:D:231:LYS:HE2	5:D:888:HOH:O	2.21	0.41
1:D:303:LYS:HD2	1:D:386:ILE:HD13	2.04	0.41
1:E:254:THR:HB	1:K:466:TYR:CE1	2.56	0.41
1:F:294:ALA:O	1:F:298:ILE:HG13	2.21	0.41
1:H:294:ALA:O	1:H:298:ILE:HG13	2.21	0.41
1:I:114:TYR:O	1:I:118:THR:HG23	2.21	0.41
1:K:114:TYR:O	1:K:118:THR:HG23	2.21	0.41
1:K:140:PHE:CE1	1:L:160:SER:HB2	2.56	0.41
1:L:231:LYS:HE2	5:L:3224:HOH:O	2.21	0.41
1:A:114:TYR:O	1:A:118:THR:HG23	2.21	0.40
1:B:84:THR:CG2	4:B:5471:MPD:H32	2.51	0.40
1:C:272:MET:HE3	1:C:272:MET:HB2	1.97	0.40
1:D:433:VAL:HG12	1:D:434:PHE:CD2	2.55	0.40
1:E:294:ALA:O	1:E:298:ILE:HG13	2.21	0.40
1:E:313:ASN:HB3	1:E:318:SER:HB3	2.03	0.40
1:F:80:PHE:CG	4:F:5479:MPD:C1	3.04	0.40
1:F:225:PHE:HD1	3:F:4476:ADP:O2'	2.03	0.40
1:F:466:TYR:CE1	1:L:254:THR:HB	2.56	0.40
1:G:294:ALA:O	1:G:298:ILE:HG13	2.21	0.40
1:G:313:ASN:HB3	1:G:318:SER:HB3	2.03	0.40
1:G:332:LEU:HD12	1:G:332:LEU:HA	1.90	0.40
1:H:303:LYS:HD2	1:H:386:ILE:HD13	2.03	0.40
1:I:80:PHE:CG	4:I:5489:MPD:C1	3.04	0.40
1:J:114:TYR:O	1:J:118:THR:HG23	2.21	0.40
1:J:313:ASN:HB3	1:J:318:SER:HB3	2.03	0.40
1:K:294:ALA:O	1:K:298:ILE:HG13	2.22	0.40
1:K:296:TYR:HB3	1:K:382:ILE:HA	2.03	0.40
1:L:82:ASP:O	4:L:5483:MPD:H32	2.20	0.40
1:L:248:ARG:CG	1:L:248:ARG:NH2	2.67	0.40
1:L:294:ALA:O	1:L:298:ILE:HG13	2.21	0.40
1:A:294:ALA:O	1:A:298:ILE:HG13	2.21	0.40
1:B:235:ILE:HA	1:B:235:ILE:HD13	1.82	0.40
1:B:294:ALA:O	1:B:298:ILE:HG13	2.21	0.40
1:D:230:LYS:O	1:D:234:GLU:HG3	2.21	0.40
1:E:189:GLN:CG	4:F:5479:MPD:H11	2.48	0.40
1:F:231:LYS:HE2	5:F:5506:HOH:O	2.21	0.40
1:F:332:LEU:HD12	1:F:332:LEU:HA	1.90	0.40
1:G:390:GLU:HA	1:G:391:PRO:HD3	1.89	0.40
1:H:34:PRO:HG2	1:I:206:VAL:O	2.21	0.40
1:I:230:LYS:O	1:I:234:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:PHE:HD1	3:J:4480:ADP:O2'	2.03	0.40
1:J:235:ILE:HD13	1:J:235:ILE:HA	1.82	0.40
1:K:105:ARG:HH21	1:K:105:ARG:HD3	1.76	0.40
1:A:140:PHE:CE1	1:F:160:SER:HB2	2.56	0.40
1:B:364:ALA:HA	1:H:468:VAL:CG1	2.51	0.40
1:B:433:VAL:HG12	1:B:434:PHE:CD2	2.55	0.40
1:D:182:VAL:HG12	1:E:30:HIS:HB3	2.03	0.40
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.82	0.40
1:E:114:TYR:O	1:E:118:THR:HG23	2.21	0.40
1:E:328:ALA:HA	1:E:329:PRO:HD3	1.73	0.40
1:E:364:ALA:HA	1:K:468:VAL:HG13	2.03	0.40
1:G:225:PHE:HD1	3:G:4477:ADP:O2'	2.03	0.40
1:I:91:ILE:HB	1:I:103:ASP:HB2	2.02	0.40
1:K:230:LYS:O	1:K:234:GLU:HG3	2.21	0.40
1:K:313:ASN:HB3	1:K:318:SER:HB3	2.03	0.40
1:L:303:LYS:HD2	1:L:386:ILE:HD13	2.04	0.40
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.90	0.40
1:E:303:LYS:HD2	1:E:386:ILE:HD13	2.03	0.40
1:I:294:ALA:O	1:I:298:ILE:HG13	2.22	0.40
1:I:303:LYS:HD2	1:I:386:ILE:HD13	2.04	0.40
1:I:332:LEU:HD12	1:I:332:LEU:HA	1.90	0.40
1:J:332:LEU:HB2	1:J:408:PRO:CB	2.50	0.40
1:A:332:LEU:HB3	1:A:408:PRO:HB2	2.04	0.40
1:E:193:SER:OG	4:F:5479:MPD:O4	2.28	0.40
1:F:303:LYS:HD2	1:F:386:ILE:HD13	2.04	0.40
4:G:5484:MPD:H4	4:G:5484:MPD:H12	1.82	0.40
1:H:225:PHE:HD1	3:H:4478:ADP:O2'	2.03	0.40
1:H:313:ASN:HB3	1:H:318:SER:HB3	2.03	0.40
1:J:125:LEU:HD12	1:J:125:LEU:HA	1.91	0.40
1:J:294:ALA:O	1:J:298:ILE:HG13	2.21	0.40
1:K:384:ASN:N	1:K:384:ASN:ND2	2.60	0.40
4:L:5494:MPD:C5	4:L:5494:MPD:H11	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
1	B	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
1	C	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
1	D	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
1	E	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
1	F	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
1	G	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
1	H	466/468 (100%)	427 (92%)	31 (7%)	8 (2%)	7	13
1	I	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
1	J	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
1	K	466/468 (100%)	427 (92%)	31 (7%)	8 (2%)	7	13
1	L	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	7	13
All	All	5592/5616 (100%)	5114 (92%)	382 (7%)	96 (2%)	7	13

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	A	400	PRO
1	A	401	PRO
1	B	180	PHE
1	B	400	PRO
1	B	401	PRO
1	C	180	PHE
1	C	400	PRO
1	C	401	PRO
1	D	180	PHE
1	D	400	PRO
1	D	401	PRO
1	E	180	PHE
1	E	400	PRO
1	E	401	PRO
1	F	180	PHE
1	F	400	PRO
1	F	401	PRO

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Mol	Chain	Res	Type
1	G	180	PHE
1	G	400	PRO
1	G	401	PRO
1	H	180	PHE
1	H	400	PRO
1	H	401	PRO
1	I	180	PHE
1	I	400	PRO
1	I	401	PRO
1	J	180	PHE
1	J	400	PRO
1	J	401	PRO
1	K	180	PHE
1	K	400	PRO
1	K	401	PRO
1	L	180	PHE
1	L	400	PRO
1	L	401	PRO
1	A	170	GLY
1	B	170	GLY
1	C	170	GLY
1	D	170	GLY
1	E	170	GLY
1	F	170	GLY
1	G	170	GLY
1	H	170	GLY
1	I	170	GLY
1	J	170	GLY
1	K	170	GLY
1	L	170	GLY
1	A	324	PRO
1	A	338	ASN
1	A	394	LYS
1	B	324	PRO
1	B	338	ASN
1	B	394	LYS
1	C	324	PRO
1	C	338	ASN
1	C	394	LYS
1	D	324	PRO
1	D	338	ASN
1	D	394	LYS

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Mol	Chain	Res	Type
1	E	324	PRO
1	E	338	ASN
1	E	394	LYS
1	F	324	PRO
1	F	338	ASN
1	F	394	LYS
1	G	324	PRO
1	G	338	ASN
1	G	394	LYS
1	H	324	PRO
1	H	338	ASN
1	H	394	LYS
1	I	324	PRO
1	I	338	ASN
1	I	394	LYS
1	J	324	PRO
1	J	338	ASN
1	J	394	LYS
1	K	324	PRO
1	K	338	ASN
1	K	394	LYS
1	L	324	PRO
1	L	338	ASN
1	L	394	LYS
1	A	396	LEU
1	B	396	LEU
1	C	396	LEU
1	D	396	LEU
1	E	396	LEU
1	F	396	LEU
1	G	396	LEU
1	H	396	LEU
1	I	396	LEU
1	J	396	LEU
1	K	396	LEU
1	L	396	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	B	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	C	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	D	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	E	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	F	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	G	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	H	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	I	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	J	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	K	384/384 (100%)	345 (90%)	39 (10%)	7	15
1	L	384/384 (100%)	345 (90%)	39 (10%)	7	15
All	All	4608/4608 (100%)	4140 (90%)	468 (10%)	7	15

All (468) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	19	LEU
1	A	60	ILE
1	A	62	GLU
1	A	63	SER
1	A	64	ASP
1	A	65	MET
1	A	84	THR
1	A	88	ARG
1	A	96	THR
1	A	98	GLN
1	A	102	ARG
1	A	115	LEU
1	A	124	VAL
1	A	125	LEU
1	A	165	GLU
1	A	179	TYR
1	A	183	PRO
1	A	209	HIS

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Mol	Chain	Res	Type
1	A	235	ILE
1	A	248	ARG
1	A	264	ASN
1	A	320	LYS
1	A	324	PRO
1	A	326	TYR
1	A	332	LEU
1	A	337	ARG
1	A	343	ILE
1	A	374	LEU
1	A	375	LEU
1	A	384	ASN
1	A	394	LYS
1	A	396	LEU
1	A	397	TYR
1	A	399	LEU
1	A	428	LEU
1	A	447	ARG
1	A	464	LEU
1	A	468	VAL
1	B	6	LEU
1	B	19	LEU
1	B	60	ILE
1	B	62	GLU
1	B	63	SER
1	B	64	ASP
1	B	65	MET
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	165	GLU
1	B	179	TYR
1	B	183	PRO
1	B	209	HIS
1	B	235	ILE
1	B	248	ARG
1	B	264	ASN

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Mol	Chain	Res	Type
1	B	320	LYS
1	B	324	PRO
1	B	326	TYR
1	B	332	LEU
1	B	337	ARG
1	B	343	ILE
1	B	374	LEU
1	B	375	LEU
1	B	384	ASN
1	B	394	LYS
1	B	396	LEU
1	B	397	TYR
1	B	399	LEU
1	B	428	LEU
1	B	447	ARG
1	B	464	LEU
1	B	468	VAL
1	C	6	LEU
1	C	19	LEU
1	C	60	ILE
1	C	62	GLU
1	C	63	SER
1	C	64	ASP
1	C	65	MET
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	165	GLU
1	C	179	TYR
1	C	183	PRO
1	C	209	HIS
1	C	235	ILE
1	C	248	ARG
1	C	264	ASN
1	C	320	LYS
1	C	324	PRO
1	C	326	TYR

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Mol	Chain	Res	Type
1	C	332	LEU
1	C	337	ARG
1	C	343	ILE
1	C	374	LEU
1	C	375	LEU
1	C	384	ASN
1	C	394	LYS
1	C	396	LEU
1	C	397	TYR
1	C	399	LEU
1	C	428	LEU
1	C	447	ARG
1	C	464	LEU
1	C	468	VAL
1	D	6	LEU
1	D	19	LEU
1	D	60	ILE
1	D	62	GLU
1	D	63	SER
1	D	64	ASP
1	D	65	MET
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	165	GLU
1	D	179	TYR
1	D	183	PRO
1	D	209	HIS
1	D	235	ILE
1	D	248	ARG
1	D	264	ASN
1	D	320	LYS
1	D	324	PRO
1	D	326	TYR
1	D	332	LEU
1	D	337	ARG
1	D	343	ILE

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Mol	Chain	Res	Type
1	D	374	LEU
1	D	375	LEU
1	D	384	ASN
1	D	394	LYS
1	D	396	LEU
1	D	397	TYR
1	D	399	LEU
1	D	428	LEU
1	D	447	ARG
1	D	464	LEU
1	D	468	VAL
1	E	6	LEU
1	E	19	LEU
1	E	60	ILE
1	E	62	GLU
1	E	63	SER
1	E	64	ASP
1	E	65	MET
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	165	GLU
1	E	179	TYR
1	E	183	PRO
1	E	209	HIS
1	E	235	ILE
1	E	248	ARG
1	E	264	ASN
1	E	320	LYS
1	E	324	PRO
1	E	326	TYR
1	E	332	LEU
1	E	337	ARG
1	E	343	ILE
1	E	374	LEU
1	E	375	LEU
1	E	384	ASN

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Mol	Chain	Res	Type
1	E	394	LYS
1	E	396	LEU
1	E	397	TYR
1	E	399	LEU
1	E	428	LEU
1	E	447	ARG
1	E	464	LEU
1	E	468	VAL
1	F	6	LEU
1	F	19	LEU
1	F	60	ILE
1	F	62	GLU
1	F	63	SER
1	F	64	ASP
1	F	65	MET
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	165	GLU
1	F	179	TYR
1	F	183	PRO
1	F	209	HIS
1	F	235	ILE
1	F	248	ARG
1	F	264	ASN
1	F	320	LYS
1	F	324	PRO
1	F	326	TYR
1	F	332	LEU
1	F	337	ARG
1	F	343	ILE
1	F	374	LEU
1	F	375	LEU
1	F	384	ASN
1	F	394	LYS
1	F	396	LEU
1	F	397	TYR

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Mol	Chain	Res	Type
1	F	399	LEU
1	F	428	LEU
1	F	447	ARG
1	F	464	LEU
1	F	468	VAL
1	G	6	LEU
1	G	19	LEU
1	G	60	ILE
1	G	62	GLU
1	G	63	SER
1	G	64	ASP
1	G	65	MET
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	165	GLU
1	G	179	TYR
1	G	183	PRO
1	G	209	HIS
1	G	235	ILE
1	G	248	ARG
1	G	264	ASN
1	G	320	LYS
1	G	324	PRO
1	G	326	TYR
1	G	332	LEU
1	G	337	ARG
1	G	343	ILE
1	G	374	LEU
1	G	375	LEU
1	G	384	ASN
1	G	394	LYS
1	G	396	LEU
1	G	397	TYR
1	G	399	LEU
1	G	428	LEU
1	G	447	ARG

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Mol	Chain	Res	Type
1	G	464	LEU
1	G	468	VAL
1	H	6	LEU
1	H	19	LEU
1	H	60	ILE
1	H	62	GLU
1	H	63	SER
1	H	64	ASP
1	H	65	MET
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	165	GLU
1	H	179	TYR
1	H	183	PRO
1	H	209	HIS
1	H	235	ILE
1	H	248	ARG
1	H	264	ASN
1	H	320	LYS
1	H	324	PRO
1	H	326	TYR
1	H	332	LEU
1	H	337	ARG
1	H	343	ILE
1	H	374	LEU
1	H	375	LEU
1	H	384	ASN
1	H	394	LYS
1	H	396	LEU
1	H	397	TYR
1	H	399	LEU
1	H	428	LEU
1	H	447	ARG
1	H	464	LEU
1	H	468	VAL
1	I	6	LEU

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Mol	Chain	Res	Type
1	I	19	LEU
1	I	60	ILE
1	I	62	GLU
1	I	63	SER
1	I	64	ASP
1	I	65	MET
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	165	GLU
1	I	179	TYR
1	I	183	PRO
1	I	209	HIS
1	I	235	ILE
1	I	248	ARG
1	I	264	ASN
1	I	320	LYS
1	I	324	PRO
1	I	326	TYR
1	I	332	LEU
1	I	337	ARG
1	I	343	ILE
1	I	374	LEU
1	I	375	LEU
1	I	384	ASN
1	I	394	LYS
1	I	396	LEU
1	I	397	TYR
1	I	399	LEU
1	I	428	LEU
1	I	447	ARG
1	I	464	LEU
1	I	468	VAL
1	J	6	LEU
1	J	19	LEU
1	J	60	ILE
1	J	62	GLU

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Mol	Chain	Res	Type
1	J	63	SER
1	J	64	ASP
1	J	65	MET
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	165	GLU
1	J	179	TYR
1	J	183	PRO
1	J	209	HIS
1	J	235	ILE
1	J	248	ARG
1	J	264	ASN
1	J	320	LYS
1	J	324	PRO
1	J	326	TYR
1	J	332	LEU
1	J	337	ARG
1	J	343	ILE
1	J	374	LEU
1	J	375	LEU
1	J	384	ASN
1	J	394	LYS
1	J	396	LEU
1	J	397	TYR
1	J	399	LEU
1	J	428	LEU
1	J	447	ARG
1	J	464	LEU
1	J	468	VAL
1	K	6	LEU
1	K	19	LEU
1	K	60	ILE
1	K	62	GLU
1	K	63	SER
1	K	64	ASP
1	K	65	MET

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Mol	Chain	Res	Type
1	K	84	THR
1	K	88	ARG
1	K	96	THR
1	K	98	GLN
1	K	102	ARG
1	K	115	LEU
1	K	124	VAL
1	K	125	LEU
1	K	165	GLU
1	K	179	TYR
1	K	183	PRO
1	K	209	HIS
1	K	235	ILE
1	K	248	ARG
1	K	264	ASN
1	K	320	LYS
1	K	324	PRO
1	K	326	TYR
1	K	332	LEU
1	K	337	ARG
1	K	343	ILE
1	K	374	LEU
1	K	375	LEU
1	K	384	ASN
1	K	394	LYS
1	K	396	LEU
1	K	397	TYR
1	K	399	LEU
1	K	428	LEU
1	K	447	ARG
1	K	464	LEU
1	K	468	VAL
1	L	6	LEU
1	L	19	LEU
1	L	60	ILE
1	L	62	GLU
1	L	63	SER
1	L	64	ASP
1	L	65	MET
1	L	84	THR
1	L	88	ARG
1	L	96	THR

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Mol	Chain	Res	Type
1	L	98	GLN
1	L	102	ARG
1	L	115	LEU
1	L	124	VAL
1	L	125	LEU
1	L	165	GLU
1	L	179	TYR
1	L	183	PRO
1	L	209	HIS
1	L	235	ILE
1	L	248	ARG
1	L	264	ASN
1	L	320	LYS
1	L	324	PRO
1	L	326	TYR
1	L	332	LEU
1	L	337	ARG
1	L	343	ILE
1	L	374	LEU
1	L	375	LEU
1	L	384	ASN
1	L	394	LYS
1	L	396	LEU
1	L	397	TYR
1	L	399	LEU
1	L	428	LEU
1	L	447	ARG
1	L	464	LEU
1	L	468	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	30	HIS
1	A	61	ASN
1	A	211	HIS
1	A	218	GLN
1	A	219	ASN
1	A	244	ASN
1	A	264	ASN
1	A	277	ASN

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Mol	Chain	Res	Type
1	A	313	ASN
1	A	384	ASN
1	A	409	GLN
1	A	458	HIS
1	B	10	ASN
1	B	30	HIS
1	B	61	ASN
1	B	211	HIS
1	B	218	GLN
1	B	219	ASN
1	B	244	ASN
1	B	264	ASN
1	B	277	ASN
1	B	313	ASN
1	B	384	ASN
1	B	409	GLN
1	B	458	HIS
1	C	10	ASN
1	C	30	HIS
1	C	211	HIS
1	C	218	GLN
1	C	219	ASN
1	C	244	ASN
1	C	264	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	HIS
1	D	61	ASN
1	D	211	HIS
1	D	218	GLN
1	D	219	ASN
1	D	244	ASN
1	D	264	ASN
1	D	277	ASN
1	D	313	ASN
1	D	384	ASN
1	D	409	GLN
1	D	458	HIS

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Mol	Chain	Res	Type
1	E	10	ASN
1	E	30	HIS
1	E	61	ASN
1	E	211	HIS
1	E	218	GLN
1	E	219	ASN
1	E	244	ASN
1	E	264	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	HIS
1	F	211	HIS
1	F	218	GLN
1	F	219	ASN
1	F	244	ASN
1	F	264	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	HIS
1	G	61	ASN
1	G	211	HIS
1	G	218	GLN
1	G	219	ASN
1	G	244	ASN
1	G	264	ASN
1	G	277	ASN
1	G	313	ASN
1	G	384	ASN
1	G	409	GLN
1	G	458	HIS
1	H	10	ASN
1	H	30	HIS
1	H	211	HIS
1	H	218	GLN

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Mol	Chain	Res	Type
1	H	219	ASN
1	H	244	ASN
1	H	264	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	HIS
1	I	61	ASN
1	I	211	HIS
1	I	218	GLN
1	I	219	ASN
1	I	244	ASN
1	I	264	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	HIS
1	J	61	ASN
1	J	211	HIS
1	J	218	GLN
1	J	219	ASN
1	J	244	ASN
1	J	264	ASN
1	J	277	ASN
1	J	313	ASN
1	J	384	ASN
1	J	409	GLN
1	J	458	HIS
1	K	10	ASN
1	K	30	HIS
1	K	211	HIS
1	K	218	GLN
1	K	219	ASN
1	K	244	ASN
1	K	264	ASN
1	K	277	ASN

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Mol	Chain	Res	Type
1	K	313	ASN
1	K	384	ASN
1	K	409	GLN
1	K	458	HIS
1	L	10	ASN
1	L	30	HIS
1	L	61	ASN
1	L	211	HIS
1	L	218	GLN
1	L	219	ASN
1	L	244	ASN
1	L	264	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 24 are monoatomic - leaving 36 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
4	MPD	J	5490	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
4	MPD	D	5478	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
3	ADP	J	4480	2	28,29,29	3.36	12 (42%)	43,45,45	2.98	17 (39%)
4	MPD	H	5486	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
3	ADP	G	4477	2	28,29,29	3.36	12 (42%)	43,45,45	2.98	17 (39%)
4	MPD	L	5483	-	7,7,7	1.61	2 (28%)	9,10,10	1.01	0
4	MPD	H	5487	-	7,7,7	1.62	2 (28%)	9,10,10	1.01	0
4	MPD	I	5488	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
4	MPD	D	5475	-	7,7,7	1.61	2 (28%)	9,10,10	1.01	0
4	MPD	C	5473	-	7,7,7	1.61	2 (28%)	9,10,10	1.01	0
4	MPD	B	5471	-	7,7,7	1.62	2 (28%)	9,10,10	1.01	0
4	MPD	C	5476	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
4	MPD	A	5472	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
4	MPD	A	5481	-	7,7,7	1.62	2 (28%)	9,10,10	1.01	0
3	ADP	K	4481	2	28,29,29	3.36	12 (42%)	43,45,45	2.98	17 (39%)
4	MPD	F	5479	-	7,7,7	1.62	2 (28%)	9,10,10	1.02	0
4	MPD	I	5489	-	7,7,7	1.62	2 (28%)	9,10,10	1.01	0
4	MPD	G	5484	-	7,7,7	3.44	4 (57%)	9,10,10	1.60	1 (11%)
3	ADP	B	4472	2	28,29,29	3.36	12 (42%)	43,45,45	2.99	17 (39%)
4	MPD	B	5474	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
3	ADP	F	4476	2	28,29,29	3.36	12 (42%)	43,45,45	2.98	17 (39%)
3	ADP	I	4479	2	28,29,29	3.37	12 (42%)	43,45,45	2.98	17 (39%)
3	ADP	E	4475	2	28,29,29	3.36	12 (42%)	43,45,45	2.98	17 (39%)
3	ADP	A	4471	2	28,29,29	3.36	12 (42%)	43,45,45	2.98	17 (39%)
4	MPD	E	5477	-	7,7,7	1.62	2 (28%)	9,10,10	1.01	0
3	ADP	D	4474	2	28,29,29	3.36	12 (42%)	43,45,45	2.98	17 (39%)
3	ADP	L	4482	2	28,29,29	3.36	12 (42%)	43,45,45	2.99	17 (39%)
4	MPD	K	5492	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
4	MPD	E	5480	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
4	MPD	J	5491	-	7,7,7	1.61	2 (28%)	9,10,10	1.01	0
4	MPD	F	5482	-	7,7,7	3.45	4 (57%)	9,10,10	1.60	1 (11%)
4	MPD	L	5494	-	7,7,7	3.46	4 (57%)	9,10,10	1.60	1 (11%)
4	MPD	G	5485	-	7,7,7	1.62	2 (28%)	9,10,10	1.01	0
4	MPD	K	5493	-	7,7,7	1.61	2 (28%)	9,10,10	1.01	0
3	ADP	C	4473	2	28,29,29	3.36	12 (42%)	43,45,45	2.98	17 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	H	4478	2	28,29,29	3.36	12 (42%)	43,45,45	2.99	17 (39%)

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
4	MPD	J	5490	-	-	5/5/5/5	-
4	MPD	D	5478	-	-	5/5/5/5	-
3	ADP	J	4480	2	-	2/16/32/32	0/3/3/3
4	MPD	H	5486	-	-	5/5/5/5	-
3	ADP	G	4477	2	-	2/16/32/32	0/3/3/3
4	MPD	L	5483	-	-	2/5/5/5	-
4	MPD	H	5487	-	-	2/5/5/5	-
4	MPD	I	5488	-	-	5/5/5/5	-
4	MPD	D	5475	-	-	2/5/5/5	-
4	MPD	C	5473	-	-	2/5/5/5	-
4	MPD	B	5471	-	-	2/5/5/5	-
4	MPD	C	5476	-	-	5/5/5/5	-
4	MPD	A	5472	-	-	5/5/5/5	-
4	MPD	A	5481	-	-	2/5/5/5	-
3	ADP	K	4481	2	-	2/16/32/32	0/3/3/3
4	MPD	F	5479	-	-	2/5/5/5	-
4	MPD	I	5489	-	-	2/5/5/5	-
4	MPD	G	5484	-	-	5/5/5/5	-
3	ADP	B	4472	2	-	2/16/32/32	0/3/3/3
4	MPD	B	5474	-	-	5/5/5/5	-
3	ADP	F	4476	2	-	2/16/32/32	0/3/3/3
3	ADP	I	4479	2	-	2/16/32/32	0/3/3/3
3	ADP	E	4475	2	-	2/16/32/32	0/3/3/3
3	ADP	A	4471	2	-	2/16/32/32	0/3/3/3
4	MPD	E	5477	-	-	2/5/5/5	-
3	ADP	D	4474	2	-	2/16/32/32	0/3/3/3
3	ADP	L	4482	2	-	2/16/32/32	0/3/3/3
4	MPD	K	5492	-	-	5/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	E	5480	-	-	5/5/5/5	-
4	MPD	J	5491	-	-	2/5/5/5	-
4	MPD	F	5482	-	-	5/5/5/5	-
4	MPD	L	5494	-	-	5/5/5/5	-
4	MPD	G	5485	-	-	2/5/5/5	-
4	MPD	K	5493	-	-	2/5/5/5	-
3	ADP	C	4473	2	-	2/16/32/32	0/3/3/3
3	ADP	H	4478	2	-	2/16/32/32	0/3/3/3

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4476	ADP	PA-O3A	8.88	1.69	1.59
3	I	4479	ADP	PA-O3A	8.87	1.69	1.59
3	J	4480	ADP	PA-O3A	8.87	1.69	1.59
3	K	4481	ADP	PA-O3A	8.87	1.69	1.59
3	A	4471	ADP	PA-O3A	8.86	1.69	1.59
3	B	4472	ADP	PA-O3A	8.85	1.69	1.59
3	D	4474	ADP	PA-O3A	8.85	1.69	1.59
3	G	4477	ADP	PA-O3A	8.85	1.69	1.59
3	H	4478	ADP	PA-O3A	8.83	1.69	1.59
3	C	4473	ADP	PA-O3A	8.83	1.69	1.59
3	E	4475	ADP	PA-O3A	8.81	1.69	1.59
3	L	4482	ADP	PA-O3A	8.81	1.69	1.59
3	D	4474	ADP	C1'-N9	7.45	1.66	1.46
3	I	4479	ADP	C1'-N9	7.45	1.66	1.46
3	J	4480	ADP	C1'-N9	7.44	1.66	1.46
3	G	4477	ADP	C1'-N9	7.44	1.66	1.46
3	C	4473	ADP	C1'-N9	7.44	1.66	1.46
3	A	4471	ADP	C1'-N9	7.43	1.66	1.46
3	B	4472	ADP	C1'-N9	7.43	1.66	1.46
3	K	4481	ADP	C1'-N9	7.42	1.66	1.46
3	E	4475	ADP	C1'-N9	7.42	1.66	1.46
3	F	4476	ADP	C1'-N9	7.42	1.66	1.46
3	H	4478	ADP	C1'-N9	7.41	1.66	1.46
3	L	4482	ADP	C1'-N9	7.41	1.66	1.46
4	L	5494	MPD	C1-C2	-7.07	1.31	1.52
4	E	5480	MPD	C1-C2	-7.05	1.31	1.52
4	C	5476	MPD	C1-C2	-7.05	1.31	1.52
4	B	5474	MPD	C1-C2	-7.05	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5472	MPD	C1-C2	-7.04	1.31	1.52
4	K	5492	MPD	C1-C2	-7.03	1.31	1.52
4	D	5478	MPD	C1-C2	-7.03	1.31	1.52
4	I	5488	MPD	C1-C2	-7.03	1.31	1.52
4	G	5484	MPD	C1-C2	-7.03	1.31	1.52
4	H	5486	MPD	C1-C2	-7.03	1.31	1.52
4	J	5490	MPD	C1-C2	-7.02	1.31	1.52
4	F	5482	MPD	C1-C2	-7.02	1.31	1.52
3	E	4475	ADP	O4'-C4'	5.81	1.57	1.45
3	I	4479	ADP	O4'-C4'	5.78	1.57	1.45
3	D	4474	ADP	O4'-C4'	5.77	1.57	1.45
3	F	4476	ADP	O4'-C4'	5.77	1.57	1.45
3	J	4480	ADP	O4'-C4'	5.77	1.57	1.45
3	A	4471	ADP	O4'-C4'	5.76	1.57	1.45
3	G	4477	ADP	O4'-C4'	5.76	1.57	1.45
3	L	4482	ADP	O4'-C4'	5.75	1.57	1.45
3	B	4472	ADP	O4'-C4'	5.75	1.57	1.45
3	K	4481	ADP	O4'-C4'	5.75	1.57	1.45
3	C	4473	ADP	O4'-C4'	5.74	1.57	1.45
3	H	4478	ADP	O4'-C4'	5.74	1.57	1.45
3	K	4481	ADP	O4'-C1'	4.94	1.53	1.42
3	L	4482	ADP	O4'-C1'	4.94	1.53	1.42
3	F	4476	ADP	O4'-C1'	4.93	1.53	1.42
3	C	4473	ADP	O4'-C1'	4.92	1.53	1.42
3	D	4474	ADP	O4'-C1'	4.92	1.53	1.42
3	H	4478	ADP	O4'-C1'	4.91	1.53	1.42
3	A	4471	ADP	O4'-C1'	4.91	1.53	1.42
3	J	4480	ADP	O4'-C1'	4.91	1.53	1.42
3	G	4477	ADP	O4'-C1'	4.91	1.53	1.42
3	E	4475	ADP	O4'-C1'	4.90	1.53	1.42
3	I	4479	ADP	O4'-C1'	4.90	1.53	1.42
3	B	4472	ADP	O4'-C1'	4.88	1.53	1.42
3	B	4472	ADP	C6-N6	-4.68	1.22	1.34
3	D	4474	ADP	C6-N6	-4.67	1.22	1.34
3	I	4479	ADP	C6-N6	-4.67	1.22	1.34
3	J	4480	ADP	C6-N6	-4.66	1.22	1.34
3	A	4471	ADP	C6-N6	-4.66	1.22	1.34
3	F	4476	ADP	C6-N6	-4.65	1.22	1.34
3	H	4478	ADP	C6-N6	-4.65	1.22	1.34
3	K	4481	ADP	C6-N6	-4.65	1.22	1.34
3	L	4482	ADP	C6-N6	-4.65	1.22	1.34
3	C	4473	ADP	C6-N6	-4.64	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4475	ADP	C6-N6	-4.64	1.22	1.34
3	C	4473	ADP	C8-N9	4.64	1.45	1.37
3	I	4479	ADP	C8-N9	4.63	1.45	1.37
3	E	4475	ADP	C8-N9	4.63	1.45	1.37
3	G	4477	ADP	C6-N6	-4.63	1.22	1.34
3	L	4482	ADP	C8-N9	4.62	1.45	1.37
3	K	4481	ADP	C8-N9	4.62	1.45	1.37
3	J	4480	ADP	C8-N9	4.61	1.45	1.37
3	F	4476	ADP	C8-N9	4.60	1.45	1.37
3	A	4471	ADP	C8-N9	4.60	1.45	1.37
4	B	5474	MPD	O2-C2	-4.59	1.33	1.44
4	F	5482	MPD	O2-C2	-4.59	1.33	1.44
3	H	4478	ADP	C8-N9	4.59	1.45	1.37
4	A	5472	MPD	O2-C2	-4.58	1.33	1.44
4	J	5490	MPD	O2-C2	-4.58	1.33	1.44
4	L	5494	MPD	O2-C2	-4.58	1.33	1.44
4	K	5492	MPD	O2-C2	-4.58	1.33	1.44
3	B	4472	ADP	C8-N9	4.57	1.45	1.37
4	I	5488	MPD	O2-C2	-4.57	1.33	1.44
4	H	5486	MPD	O2-C2	-4.57	1.33	1.44
4	E	5480	MPD	O2-C2	-4.57	1.33	1.44
4	G	5484	MPD	O2-C2	-4.57	1.33	1.44
4	C	5476	MPD	O2-C2	-4.57	1.33	1.44
3	D	4474	ADP	C8-N9	4.56	1.45	1.37
4	D	5478	MPD	O2-C2	-4.56	1.33	1.44
3	G	4477	ADP	C8-N9	4.55	1.45	1.37
3	L	4482	ADP	C4-N3	4.37	1.42	1.34
3	H	4478	ADP	C4-N3	4.36	1.42	1.34
3	F	4476	ADP	C4-N3	4.36	1.42	1.34
3	D	4474	ADP	C4-N3	4.34	1.42	1.34
3	G	4477	ADP	C4-N3	4.33	1.42	1.34
3	A	4471	ADP	C4-N3	4.33	1.42	1.34
3	J	4480	ADP	C4-N3	4.33	1.42	1.34
3	C	4473	ADP	C4-N3	4.33	1.42	1.34
3	K	4481	ADP	C4-N3	4.32	1.42	1.34
3	E	4475	ADP	C4-N3	4.32	1.42	1.34
3	B	4472	ADP	C4-N3	4.31	1.42	1.34
3	I	4479	ADP	C4-N3	4.31	1.42	1.34
3	E	4475	ADP	C5-C4	3.95	1.46	1.39
3	G	4477	ADP	C5-C4	3.93	1.46	1.39
3	D	4474	ADP	C5-C4	3.92	1.46	1.39
3	K	4481	ADP	C5-C4	3.91	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4480	ADP	C5-C4	3.91	1.46	1.39
3	A	4471	ADP	C5-C4	3.91	1.46	1.39
3	F	4476	ADP	C5-C4	3.91	1.46	1.39
3	I	4479	ADP	C5-C4	3.91	1.46	1.39
3	C	4473	ADP	C5-C4	3.90	1.46	1.39
3	L	4482	ADP	C5-C4	3.89	1.46	1.39
3	B	4472	ADP	C5-C4	3.87	1.46	1.39
3	H	4478	ADP	C5-C4	3.87	1.46	1.39
3	D	4474	ADP	PB-O3B	3.47	1.67	1.54
3	H	4478	ADP	PB-O3B	3.47	1.67	1.54
3	I	4479	ADP	PB-O3B	3.46	1.67	1.54
3	A	4471	ADP	PB-O3B	3.46	1.67	1.54
3	G	4477	ADP	PB-O3B	3.46	1.67	1.54
3	L	4482	ADP	PB-O3B	3.46	1.67	1.54
3	E	4475	ADP	PB-O3B	3.46	1.67	1.54
3	C	4473	ADP	PB-O3B	3.46	1.67	1.54
3	B	4472	ADP	PB-O3B	3.45	1.67	1.54
3	J	4480	ADP	PB-O3B	3.44	1.67	1.54
3	K	4481	ADP	PB-O3B	3.44	1.67	1.54
3	F	4476	ADP	PB-O3B	3.44	1.67	1.54
4	H	5487	MPD	CM-C2	-3.14	1.43	1.52
4	E	5477	MPD	CM-C2	-3.14	1.43	1.52
4	F	5479	MPD	CM-C2	-3.14	1.43	1.52
4	L	5483	MPD	CM-C2	-3.13	1.43	1.52
4	I	5489	MPD	CM-C2	-3.13	1.43	1.52
4	G	5485	MPD	CM-C2	-3.12	1.43	1.52
4	B	5471	MPD	CM-C2	-3.12	1.43	1.52
4	K	5493	MPD	CM-C2	-3.12	1.43	1.52
4	A	5481	MPD	CM-C2	-3.12	1.43	1.52
4	C	5473	MPD	CM-C2	-3.11	1.43	1.52
4	J	5491	MPD	CM-C2	-3.10	1.43	1.52
4	D	5475	MPD	CM-C2	-3.10	1.43	1.52
3	B	4472	ADP	C4-N9	2.63	1.43	1.37
4	F	5482	MPD	C3-C2	-2.62	1.46	1.54
4	I	5488	MPD	C3-C2	-2.62	1.46	1.54
3	H	4478	ADP	C4-N9	2.62	1.43	1.37
4	H	5486	MPD	C3-C2	-2.62	1.46	1.54
3	E	4475	ADP	C4-N9	2.61	1.43	1.37
4	K	5492	MPD	C3-C2	-2.61	1.46	1.54
4	E	5480	MPD	C3-C2	-2.61	1.46	1.54
4	J	5490	MPD	C3-C2	-2.61	1.46	1.54
4	C	5476	MPD	C3-C2	-2.61	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5472	MPD	C3-C2	-2.61	1.46	1.54
3	G	4477	ADP	C4-N9	2.60	1.43	1.37
4	L	5494	MPD	C3-C2	-2.60	1.46	1.54
4	D	5478	MPD	C3-C2	-2.60	1.46	1.54
4	B	5474	MPD	C3-C2	-2.60	1.46	1.54
3	A	4471	ADP	C4-N9	2.60	1.43	1.37
3	J	4480	ADP	C4-N9	2.60	1.43	1.37
3	F	4476	ADP	C4-N9	2.59	1.43	1.37
3	L	4482	ADP	C4-N9	2.59	1.43	1.37
4	G	5484	MPD	C3-C2	-2.59	1.46	1.54
3	C	4473	ADP	C4-N9	2.58	1.43	1.37
3	I	4479	ADP	C4-N9	2.58	1.43	1.37
3	D	4474	ADP	C4-N9	2.57	1.43	1.37
3	K	4481	ADP	C4-N9	2.57	1.43	1.37
3	F	4476	ADP	C3'-C4'	-2.51	1.46	1.53
3	K	4481	ADP	C2-N3	2.51	1.38	1.33
3	J	4480	ADP	C2-N3	2.50	1.38	1.33
3	I	4479	ADP	C2-N3	2.50	1.38	1.33
3	J	4480	ADP	C3'-C4'	-2.50	1.46	1.53
3	G	4477	ADP	C2-N3	2.50	1.38	1.33
3	I	4479	ADP	C3'-C4'	-2.50	1.46	1.53
3	C	4473	ADP	C2-N3	2.50	1.38	1.33
3	D	4474	ADP	C3'-C4'	-2.49	1.46	1.53
3	A	4471	ADP	C2-N3	2.49	1.38	1.33
3	L	4482	ADP	C3'-C4'	-2.49	1.46	1.53
3	C	4473	ADP	C3'-C4'	-2.49	1.46	1.53
3	H	4478	ADP	C2-N3	2.49	1.38	1.33
3	A	4471	ADP	C3'-C4'	-2.49	1.46	1.53
3	E	4475	ADP	C3'-C4'	-2.49	1.46	1.53
3	D	4474	ADP	C2-N3	2.48	1.38	1.33
3	H	4478	ADP	C3'-C4'	-2.48	1.46	1.53
3	B	4472	ADP	C3'-C4'	-2.48	1.46	1.53
3	B	4472	ADP	C2-N3	2.47	1.38	1.33
3	E	4475	ADP	C2-N3	2.47	1.38	1.33
3	K	4481	ADP	C3'-C4'	-2.47	1.46	1.53
3	G	4477	ADP	C3'-C4'	-2.47	1.46	1.53
3	F	4476	ADP	C2-N3	2.46	1.38	1.33
3	L	4482	ADP	C2-N3	2.44	1.38	1.33
4	D	5478	MPD	CM-C2	-2.23	1.45	1.52
4	H	5486	MPD	CM-C2	-2.22	1.45	1.52
4	G	5484	MPD	CM-C2	-2.21	1.45	1.52
4	E	5480	MPD	CM-C2	-2.20	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5490	MPD	CM-C2	-2.20	1.45	1.52
4	I	5488	MPD	CM-C2	-2.20	1.45	1.52
4	A	5472	MPD	CM-C2	-2.20	1.45	1.52
4	B	5474	MPD	CM-C2	-2.19	1.45	1.52
4	L	5494	MPD	CM-C2	-2.18	1.45	1.52
4	F	5482	MPD	CM-C2	-2.18	1.45	1.52
4	K	5492	MPD	CM-C2	-2.18	1.45	1.52
4	C	5476	MPD	CM-C2	-2.17	1.46	1.52
4	C	5473	MPD	C1-C2	-2.12	1.46	1.52
4	I	5489	MPD	C1-C2	-2.12	1.46	1.52
4	J	5491	MPD	C1-C2	-2.12	1.46	1.52
4	B	5471	MPD	C1-C2	-2.12	1.46	1.52
4	D	5475	MPD	C1-C2	-2.12	1.46	1.52
4	H	5487	MPD	C1-C2	-2.12	1.46	1.52
4	A	5481	MPD	C1-C2	-2.11	1.46	1.52
4	F	5479	MPD	C1-C2	-2.10	1.46	1.52
4	G	5485	MPD	C1-C2	-2.10	1.46	1.52
4	E	5477	MPD	C1-C2	-2.10	1.46	1.52
4	L	5483	MPD	C1-C2	-2.10	1.46	1.52
4	K	5493	MPD	C1-C2	-2.09	1.46	1.52

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	4482	ADP	O5'-C5'-C4'	8.44	137.73	108.99
3	J	4480	ADP	O5'-C5'-C4'	8.44	137.73	108.99
3	I	4479	ADP	O5'-C5'-C4'	8.43	137.71	108.99
3	F	4476	ADP	O5'-C5'-C4'	8.43	137.70	108.99
3	D	4474	ADP	O5'-C5'-C4'	8.43	137.69	108.99
3	C	4473	ADP	O5'-C5'-C4'	8.43	137.69	108.99
3	E	4475	ADP	O5'-C5'-C4'	8.43	137.69	108.99
3	H	4478	ADP	O5'-C5'-C4'	8.43	137.69	108.99
3	A	4471	ADP	O5'-C5'-C4'	8.43	137.68	108.99
3	K	4481	ADP	O5'-C5'-C4'	8.42	137.66	108.99
3	G	4477	ADP	O5'-C5'-C4'	8.42	137.66	108.99
3	B	4472	ADP	O5'-C5'-C4'	8.41	137.64	108.99
3	G	4477	ADP	O4'-C1'-C2'	-6.89	91.87	106.62
3	H	4478	ADP	O4'-C1'-C2'	-6.89	91.87	106.62
3	K	4481	ADP	O4'-C1'-C2'	-6.88	91.89	106.62
3	J	4480	ADP	O4'-C1'-C2'	-6.88	91.89	106.62
3	A	4471	ADP	O4'-C1'-C2'	-6.88	91.89	106.62
3	B	4472	ADP	O4'-C1'-N9	6.88	121.30	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	4479	ADP	O4'-C1'-C2'	-6.88	91.90	106.62
3	L	4482	ADP	O4'-C1'-C2'	-6.88	91.90	106.62
3	B	4472	ADP	O4'-C1'-C2'	-6.88	91.90	106.62
3	D	4474	ADP	O4'-C1'-C2'	-6.87	91.91	106.62
3	C	4473	ADP	O4'-C1'-N9	6.87	121.29	108.09
3	L	4482	ADP	O4'-C1'-N9	6.87	121.29	108.09
3	C	4473	ADP	O4'-C1'-C2'	-6.87	91.92	106.62
3	F	4476	ADP	O4'-C1'-C2'	-6.87	91.92	106.62
3	E	4475	ADP	O4'-C1'-C2'	-6.86	91.93	106.62
3	F	4476	ADP	O4'-C1'-N9	6.86	121.26	108.09
3	H	4478	ADP	O4'-C1'-N9	6.86	121.26	108.09
3	K	4481	ADP	O4'-C1'-N9	6.86	121.26	108.09
3	A	4471	ADP	O4'-C1'-N9	6.86	121.26	108.09
3	I	4479	ADP	O4'-C1'-N9	6.85	121.25	108.09
3	G	4477	ADP	O4'-C1'-N9	6.85	121.25	108.09
3	D	4474	ADP	O4'-C1'-N9	6.85	121.24	108.09
3	J	4480	ADP	O4'-C1'-N9	6.84	121.23	108.09
3	E	4475	ADP	O4'-C1'-N9	6.84	121.23	108.09
3	H	4478	ADP	C4-N9-C8	-5.77	99.68	105.74
3	L	4482	ADP	C4-N9-C8	-5.74	99.71	105.74
3	J	4480	ADP	C4-N9-C8	-5.73	99.72	105.74
3	K	4481	ADP	C4-N9-C8	-5.72	99.73	105.74
3	A	4471	ADP	C4-N9-C8	-5.72	99.73	105.74
3	F	4476	ADP	C4-N9-C8	-5.72	99.73	105.74
3	C	4473	ADP	C4-N9-C8	-5.72	99.74	105.74
3	I	4479	ADP	C4-N9-C8	-5.71	99.74	105.74
3	E	4475	ADP	C4-N9-C8	-5.71	99.75	105.74
3	B	4472	ADP	C4-N9-C8	-5.70	99.75	105.74
3	G	4477	ADP	C4-N9-C8	-5.68	99.77	105.74
3	D	4474	ADP	C4-N9-C8	-5.68	99.77	105.74
3	J	4480	ADP	C4'-O4'-C1'	-4.82	98.82	109.47
3	F	4476	ADP	C4'-O4'-C1'	-4.82	98.82	109.47
3	D	4474	ADP	C4'-O4'-C1'	-4.82	98.82	109.47
3	C	4473	ADP	C4'-O4'-C1'	-4.82	98.83	109.47
3	I	4479	ADP	C4'-O4'-C1'	-4.82	98.83	109.47
3	E	4475	ADP	C4'-O4'-C1'	-4.81	98.85	109.47
3	H	4478	ADP	C4'-O4'-C1'	-4.81	98.86	109.47
3	A	4471	ADP	C4'-O4'-C1'	-4.81	98.86	109.47
3	K	4481	ADP	C4'-O4'-C1'	-4.80	98.86	109.47
3	G	4477	ADP	C4'-O4'-C1'	-4.80	98.86	109.47
3	L	4482	ADP	C4'-O4'-C1'	-4.80	98.87	109.47
3	B	4472	ADP	C4'-O4'-C1'	-4.79	98.88	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4478	ADP	N9-C8-N7	4.34	120.09	113.94
3	L	4482	ADP	N9-C8-N7	4.31	120.05	113.94
3	G	4477	ADP	C5'-C4'-C3'	-4.31	99.71	115.21
3	K	4481	ADP	N9-C8-N7	4.31	120.05	113.94
3	D	4474	ADP	C5'-C4'-C3'	-4.31	99.71	115.21
3	B	4472	ADP	C5'-C4'-C3'	-4.30	99.72	115.21
3	A	4471	ADP	N9-C8-N7	4.30	120.03	113.94
3	B	4472	ADP	N9-C8-N7	4.30	120.03	113.94
3	C	4473	ADP	C5'-C4'-C3'	-4.30	99.74	115.21
3	L	4482	ADP	C5'-C4'-C3'	-4.30	99.74	115.21
3	K	4481	ADP	C5'-C4'-C3'	-4.30	99.74	115.21
3	A	4471	ADP	C5'-C4'-C3'	-4.30	99.75	115.21
3	H	4478	ADP	C5'-C4'-C3'	-4.29	99.76	115.21
3	F	4476	ADP	C5'-C4'-C3'	-4.29	99.77	115.21
3	J	4480	ADP	C5'-C4'-C3'	-4.29	99.77	115.21
3	E	4475	ADP	C5'-C4'-C3'	-4.29	99.78	115.21
3	I	4479	ADP	C5'-C4'-C3'	-4.29	99.78	115.21
3	J	4480	ADP	N9-C8-N7	4.28	120.02	113.94
3	I	4479	ADP	N9-C8-N7	4.28	120.01	113.94
3	C	4473	ADP	N9-C8-N7	4.28	120.01	113.94
3	G	4477	ADP	N9-C8-N7	4.28	120.01	113.94
3	E	4475	ADP	N9-C8-N7	4.28	120.01	113.94
3	F	4476	ADP	N9-C8-N7	4.28	120.01	113.94
3	D	4474	ADP	N9-C8-N7	4.28	120.00	113.94
3	J	4480	ADP	C3'-C2'-C1'	-3.91	94.07	101.46
3	E	4475	ADP	C3'-C2'-C1'	-3.90	94.08	101.46
3	I	4479	ADP	C3'-C2'-C1'	-3.90	94.09	101.46
3	C	4473	ADP	C3'-C2'-C1'	-3.90	94.09	101.46
3	L	4482	ADP	C3'-C2'-C1'	-3.89	94.11	101.46
3	A	4471	ADP	C3'-C2'-C1'	-3.89	94.11	101.46
3	H	4478	ADP	C3'-C2'-C1'	-3.89	94.11	101.46
3	F	4476	ADP	C3'-C2'-C1'	-3.88	94.12	101.46
3	K	4481	ADP	C3'-C2'-C1'	-3.88	94.12	101.46
3	B	4472	ADP	C3'-C2'-C1'	-3.88	94.13	101.46
3	G	4477	ADP	C3'-C2'-C1'	-3.87	94.13	101.46
3	D	4474	ADP	C3'-C2'-C1'	-3.87	94.15	101.46
3	H	4478	ADP	C4-N9-C1'	3.84	135.61	126.63
3	L	4482	ADP	C4-N9-C1'	3.84	135.60	126.63
3	J	4480	ADP	C4-N9-C1'	3.83	135.59	126.63
3	C	4473	ADP	C4-N9-C1'	3.83	135.59	126.63
3	I	4479	ADP	C4-N9-C1'	3.83	135.59	126.63
3	A	4471	ADP	C4-N9-C1'	3.83	135.58	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	4481	ADP	C4-N9-C1'	3.82	135.57	126.63
3	E	4475	ADP	C4-N9-C1'	3.82	135.56	126.63
3	D	4474	ADP	C4-N9-C1'	3.81	135.55	126.63
3	F	4476	ADP	C4-N9-C1'	3.81	135.55	126.63
3	G	4477	ADP	C4-N9-C1'	3.81	135.54	126.63
3	B	4472	ADP	C4-N9-C1'	3.81	135.54	126.63
3	B	4472	ADP	O4'-C4'-C5'	3.55	120.71	109.33
4	J	5490	MPD	O2-C2-C1	-3.55	96.93	107.99
4	I	5488	MPD	O2-C2-C1	-3.55	96.93	107.99
4	E	5480	MPD	O2-C2-C1	-3.54	96.94	107.99
3	J	4480	ADP	O4'-C4'-C5'	3.54	120.68	109.33
3	K	4481	ADP	O4'-C4'-C5'	3.54	120.68	109.33
3	L	4482	ADP	O4'-C4'-C5'	3.54	120.68	109.33
3	H	4478	ADP	O4'-C4'-C5'	3.54	120.68	109.33
3	A	4471	ADP	O4'-C4'-C5'	3.54	120.67	109.33
4	F	5482	MPD	O2-C2-C1	-3.54	96.96	107.99
3	D	4474	ADP	O4'-C4'-C5'	3.54	120.66	109.33
4	C	5476	MPD	O2-C2-C1	-3.54	96.96	107.99
3	G	4477	ADP	O4'-C4'-C5'	3.54	120.66	109.33
3	E	4475	ADP	O4'-C4'-C5'	3.54	120.66	109.33
4	A	5472	MPD	O2-C2-C1	-3.54	96.97	107.99
4	G	5484	MPD	O2-C2-C1	-3.53	96.97	107.99
4	H	5486	MPD	O2-C2-C1	-3.53	96.97	107.99
3	F	4476	ADP	O4'-C4'-C5'	3.53	120.65	109.33
3	C	4473	ADP	O4'-C4'-C5'	3.53	120.64	109.33
3	I	4479	ADP	O4'-C4'-C5'	3.53	120.64	109.33
4	D	5478	MPD	O2-C2-C1	-3.53	96.98	107.99
4	B	5474	MPD	O2-C2-C1	-3.53	96.99	107.99
4	L	5494	MPD	O2-C2-C1	-3.53	96.99	107.99
4	K	5492	MPD	O2-C2-C1	-3.52	97.00	107.99
3	B	4472	ADP	C4-C5-N7	3.39	114.46	110.58
3	E	4475	ADP	C4-C5-N7	3.37	114.43	110.58
3	I	4479	ADP	C4-C5-N7	3.35	114.42	110.58
3	H	4478	ADP	C4-C5-N7	3.35	114.41	110.58
3	L	4482	ADP	C4-C5-N7	3.35	114.41	110.58
3	A	4471	ADP	C4-C5-N7	3.34	114.40	110.58
3	C	4473	ADP	C4-C5-N7	3.34	114.40	110.58
3	J	4480	ADP	C4-C5-N7	3.33	114.39	110.58
3	F	4476	ADP	C4-C5-N7	3.33	114.39	110.58
3	K	4481	ADP	C4-C5-N7	3.33	114.38	110.58
3	G	4477	ADP	C4-C5-N7	3.32	114.38	110.58
3	D	4474	ADP	C4-C5-N7	3.31	114.36	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4475	ADP	O2'-C2'-C1'	3.09	120.75	110.10
3	C	4473	ADP	O2'-C2'-C1'	3.08	120.71	110.10
3	K	4481	ADP	O2'-C2'-C1'	3.08	120.70	110.10
3	D	4474	ADP	O2'-C2'-C1'	3.08	120.70	110.10
3	F	4476	ADP	O2'-C2'-C1'	3.08	120.70	110.10
3	L	4482	ADP	O2'-C2'-C1'	3.08	120.70	110.10
3	G	4477	ADP	O2'-C2'-C1'	3.08	120.69	110.10
3	A	4471	ADP	O2'-C2'-C1'	3.07	120.69	110.10
3	H	4478	ADP	O2'-C2'-C1'	3.07	120.68	110.10
3	I	4479	ADP	O2'-C2'-C1'	3.07	120.68	110.10
3	B	4472	ADP	O2'-C2'-C1'	3.07	120.66	110.10
3	J	4480	ADP	O2'-C2'-C1'	3.06	120.66	110.10
3	B	4472	ADP	PA-O5'-C5'	2.97	138.37	121.35
3	E	4475	ADP	PA-O5'-C5'	2.97	138.37	121.35
3	C	4473	ADP	PA-O5'-C5'	2.97	138.36	121.35
3	H	4478	ADP	PA-O5'-C5'	2.97	138.36	121.35
3	J	4480	ADP	PA-O5'-C5'	2.97	138.34	121.35
3	G	4477	ADP	PA-O5'-C5'	2.96	138.32	121.35
3	A	4471	ADP	PA-O5'-C5'	2.96	138.32	121.35
3	I	4479	ADP	PA-O5'-C5'	2.96	138.32	121.35
3	D	4474	ADP	PA-O5'-C5'	2.96	138.32	121.35
3	K	4481	ADP	PA-O5'-C5'	2.96	138.32	121.35
3	F	4476	ADP	PA-O5'-C5'	2.96	138.31	121.35
3	L	4482	ADP	PA-O5'-C5'	2.96	138.30	121.35
3	E	4475	ADP	C5-C6-N6	-2.42	117.29	123.29
3	I	4479	ADP	C5-C6-N6	-2.42	117.30	123.29
3	K	4481	ADP	C5-C6-N6	-2.41	117.33	123.29
3	G	4477	ADP	C5-C6-N6	-2.40	117.33	123.29
3	A	4471	ADP	C5-C6-N6	-2.40	117.34	123.29
3	B	4472	ADP	C5-C6-N6	-2.40	117.35	123.29
3	H	4478	ADP	C5-C6-N6	-2.40	117.35	123.29
3	F	4476	ADP	C5-C6-N6	-2.40	117.35	123.29
3	L	4482	ADP	C5-C6-N6	-2.39	117.36	123.29
3	D	4474	ADP	C5-C6-N6	-2.39	117.36	123.29
3	C	4473	ADP	C5-C6-N6	-2.39	117.37	123.29
3	J	4480	ADP	C5-C6-N6	-2.39	117.37	123.29
3	H	4478	ADP	C5-N7-C8	-2.35	99.75	103.45
3	B	4472	ADP	C5-N7-C8	-2.35	99.76	103.45
3	L	4482	ADP	C5-N7-C8	-2.34	99.77	103.45
3	K	4481	ADP	C5-N7-C8	-2.34	99.78	103.45
3	A	4471	ADP	C5-N7-C8	-2.32	99.80	103.45
3	C	4473	ADP	C5-N7-C8	-2.32	99.80	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	4479	ADP	C5-N7-C8	-2.31	99.82	103.45
3	E	4475	ADP	O2B-PB-O3A	2.31	112.38	104.64
3	H	4478	ADP	O3'-C3'-C2'	2.31	119.22	111.82
3	I	4479	ADP	O3'-C3'-C2'	2.31	119.22	111.82
3	E	4475	ADP	C5-N7-C8	-2.31	99.82	103.45
3	B	4472	ADP	O3'-C3'-C2'	2.31	119.21	111.82
3	G	4477	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	D	4474	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	L	4482	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	D	4474	ADP	C5-N7-C8	-2.30	99.83	103.45
3	J	4480	ADP	C5-N7-C8	-2.30	99.83	103.45
3	K	4481	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	H	4478	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	E	4475	ADP	O3'-C3'-C2'	2.30	119.20	111.82
3	A	4471	ADP	O2B-PB-O3A	2.30	112.35	104.64
3	B	4472	ADP	O2B-PB-O3A	2.30	112.35	104.64
3	J	4480	ADP	O3'-C3'-C2'	2.30	119.19	111.82
3	I	4479	ADP	O2B-PB-O3A	2.30	112.35	104.64
3	A	4471	ADP	O3'-C3'-C2'	2.30	119.19	111.82
3	K	4481	ADP	O3'-C3'-C2'	2.30	119.18	111.82
3	G	4477	ADP	O3'-C3'-C2'	2.30	119.18	111.82
3	C	4473	ADP	O2B-PB-O3A	2.30	112.34	104.64
3	G	4477	ADP	C5-N7-C8	-2.30	99.84	103.45
3	F	4476	ADP	C5-N7-C8	-2.29	99.84	103.45
3	C	4473	ADP	O3'-C3'-C2'	2.29	119.17	111.82
3	F	4476	ADP	O3'-C3'-C2'	2.29	119.16	111.82
3	F	4476	ADP	O2B-PB-O3A	2.29	112.32	104.64
3	D	4474	ADP	O3'-C3'-C2'	2.29	119.16	111.82
3	J	4480	ADP	O2B-PB-O3A	2.29	112.31	104.64
3	L	4482	ADP	O3'-C3'-C2'	2.28	119.13	111.82

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4471	ADP	C4'-C5'-O5'-PA
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

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Mol	Chain	Res	Type	Atoms
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
4	A	5472	MPD	C1-C2-C3-C4
4	A	5472	MPD	O2-C2-C3-C4
4	A	5472	MPD	C2-C3-C4-O4
4	A	5472	MPD	C2-C3-C4-C5
4	A	5481	MPD	C2-C3-C4-C5
4	B	5471	MPD	C2-C3-C4-C5
4	B	5474	MPD	C1-C2-C3-C4
4	B	5474	MPD	O2-C2-C3-C4
4	B	5474	MPD	C2-C3-C4-O4
4	B	5474	MPD	C2-C3-C4-C5
4	C	5473	MPD	C2-C3-C4-C5
4	C	5476	MPD	C1-C2-C3-C4
4	C	5476	MPD	O2-C2-C3-C4
4	C	5476	MPD	C2-C3-C4-O4
4	C	5476	MPD	C2-C3-C4-C5
4	D	5475	MPD	C2-C3-C4-C5
4	D	5478	MPD	C1-C2-C3-C4
4	D	5478	MPD	O2-C2-C3-C4
4	D	5478	MPD	C2-C3-C4-O4
4	D	5478	MPD	C2-C3-C4-C5
4	E	5477	MPD	C2-C3-C4-C5
4	E	5480	MPD	C1-C2-C3-C4
4	E	5480	MPD	O2-C2-C3-C4
4	E	5480	MPD	C2-C3-C4-O4
4	E	5480	MPD	C2-C3-C4-C5
4	F	5479	MPD	C2-C3-C4-C5
4	F	5482	MPD	C1-C2-C3-C4
4	F	5482	MPD	O2-C2-C3-C4
4	F	5482	MPD	C2-C3-C4-O4
4	F	5482	MPD	C2-C3-C4-C5
4	G	5484	MPD	C1-C2-C3-C4
4	G	5484	MPD	O2-C2-C3-C4
4	G	5484	MPD	C2-C3-C4-O4
4	G	5484	MPD	C2-C3-C4-C5
4	G	5485	MPD	C2-C3-C4-C5
4	H	5486	MPD	C1-C2-C3-C4
4	H	5486	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	H	5486	MPD	C2-C3-C4-O4
4	H	5486	MPD	C2-C3-C4-C5
4	H	5487	MPD	C2-C3-C4-C5
4	I	5488	MPD	C1-C2-C3-C4
4	I	5488	MPD	O2-C2-C3-C4
4	I	5488	MPD	C2-C3-C4-O4
4	I	5488	MPD	C2-C3-C4-C5
4	I	5489	MPD	C2-C3-C4-C5
4	J	5490	MPD	C1-C2-C3-C4
4	J	5490	MPD	O2-C2-C3-C4
4	J	5490	MPD	C2-C3-C4-O4
4	J	5490	MPD	C2-C3-C4-C5
4	J	5491	MPD	C2-C3-C4-C5
4	K	5492	MPD	C1-C2-C3-C4
4	K	5492	MPD	O2-C2-C3-C4
4	K	5492	MPD	C2-C3-C4-O4
4	K	5492	MPD	C2-C3-C4-C5
4	K	5493	MPD	C2-C3-C4-C5
4	L	5483	MPD	C2-C3-C4-C5
4	L	5494	MPD	C1-C2-C3-C4
4	L	5494	MPD	O2-C2-C3-C4
4	L	5494	MPD	C2-C3-C4-O4
4	L	5494	MPD	C2-C3-C4-C5
4	A	5481	MPD	O2-C2-C3-C4
4	B	5471	MPD	O2-C2-C3-C4
4	C	5473	MPD	O2-C2-C3-C4
4	D	5475	MPD	O2-C2-C3-C4
4	E	5477	MPD	O2-C2-C3-C4
4	F	5479	MPD	O2-C2-C3-C4
4	G	5485	MPD	O2-C2-C3-C4
4	H	5487	MPD	O2-C2-C3-C4
4	I	5489	MPD	O2-C2-C3-C4
4	J	5491	MPD	O2-C2-C3-C4
4	K	5493	MPD	O2-C2-C3-C4
4	L	5483	MPD	O2-C2-C3-C4
3	A	4471	ADP	C5'-O5'-PA-O1A
3	B	4472	ADP	C5'-O5'-PA-O1A
3	C	4473	ADP	C5'-O5'-PA-O1A
3	D	4474	ADP	C5'-O5'-PA-O1A
3	E	4475	ADP	C5'-O5'-PA-O1A
3	F	4476	ADP	C5'-O5'-PA-O1A
3	G	4477	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	H	4478	ADP	C5'-O5'-PA-O1A
3	I	4479	ADP	C5'-O5'-PA-O1A
3	J	4480	ADP	C5'-O5'-PA-O1A
3	K	4481	ADP	C5'-O5'-PA-O1A
3	L	4482	ADP	C5'-O5'-PA-O1A
4	A	5472	MPD	CM-C2-C3-C4
4	B	5474	MPD	CM-C2-C3-C4
4	C	5476	MPD	CM-C2-C3-C4
4	D	5478	MPD	CM-C2-C3-C4
4	E	5480	MPD	CM-C2-C3-C4
4	F	5482	MPD	CM-C2-C3-C4
4	G	5484	MPD	CM-C2-C3-C4
4	H	5486	MPD	CM-C2-C3-C4
4	I	5488	MPD	CM-C2-C3-C4
4	J	5490	MPD	CM-C2-C3-C4
4	K	5492	MPD	CM-C2-C3-C4
4	L	5494	MPD	CM-C2-C3-C4

There are no ring outliers.

36 monomers are involved in 713 short contacts:

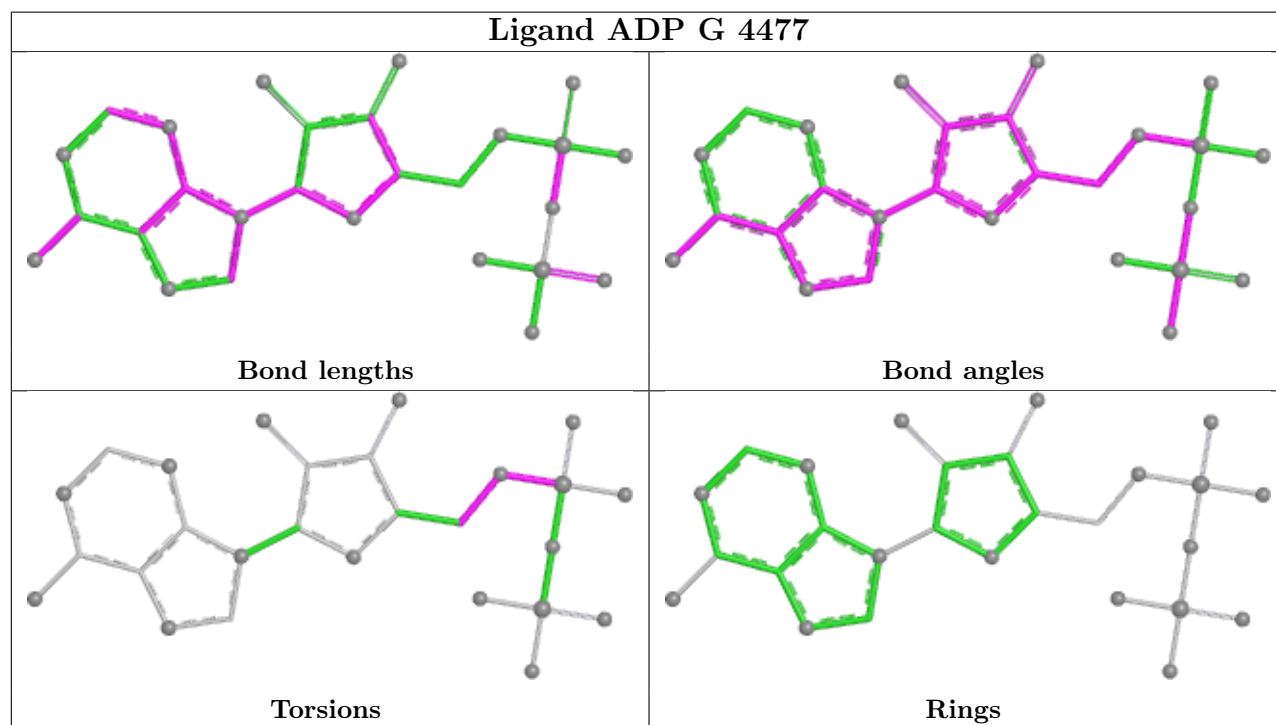
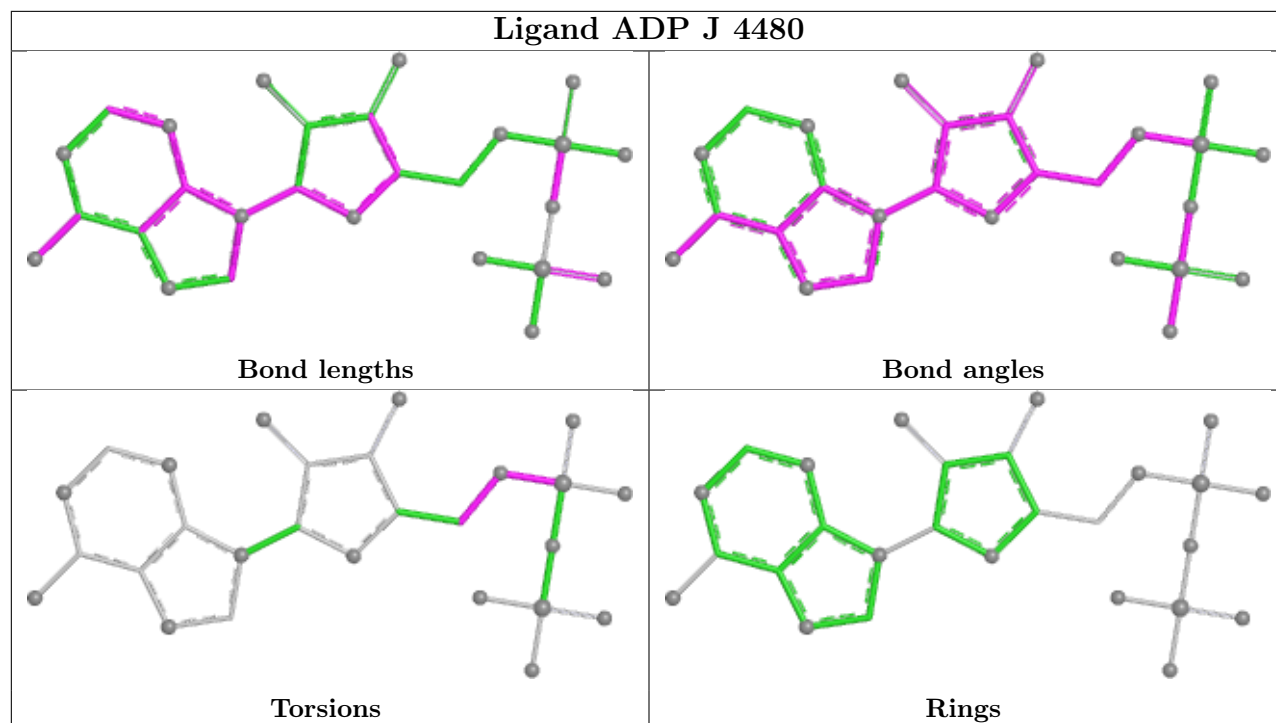
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	5490	MPD	29	0
4	D	5478	MPD	30	0
3	J	4480	ADP	1	0
4	H	5486	MPD	30	0
3	G	4477	ADP	1	0
4	L	5483	MPD	31	0
4	H	5487	MPD	31	0
4	I	5488	MPD	31	0
4	D	5475	MPD	28	0
4	C	5473	MPD	29	0
4	B	5471	MPD	27	0
4	C	5476	MPD	31	0
4	A	5472	MPD	29	0
4	A	5481	MPD	23	0
3	K	4481	ADP	1	0
4	F	5479	MPD	30	0
4	I	5489	MPD	28	0
4	G	5484	MPD	32	0
3	B	4472	ADP	1	0
4	B	5474	MPD	30	0

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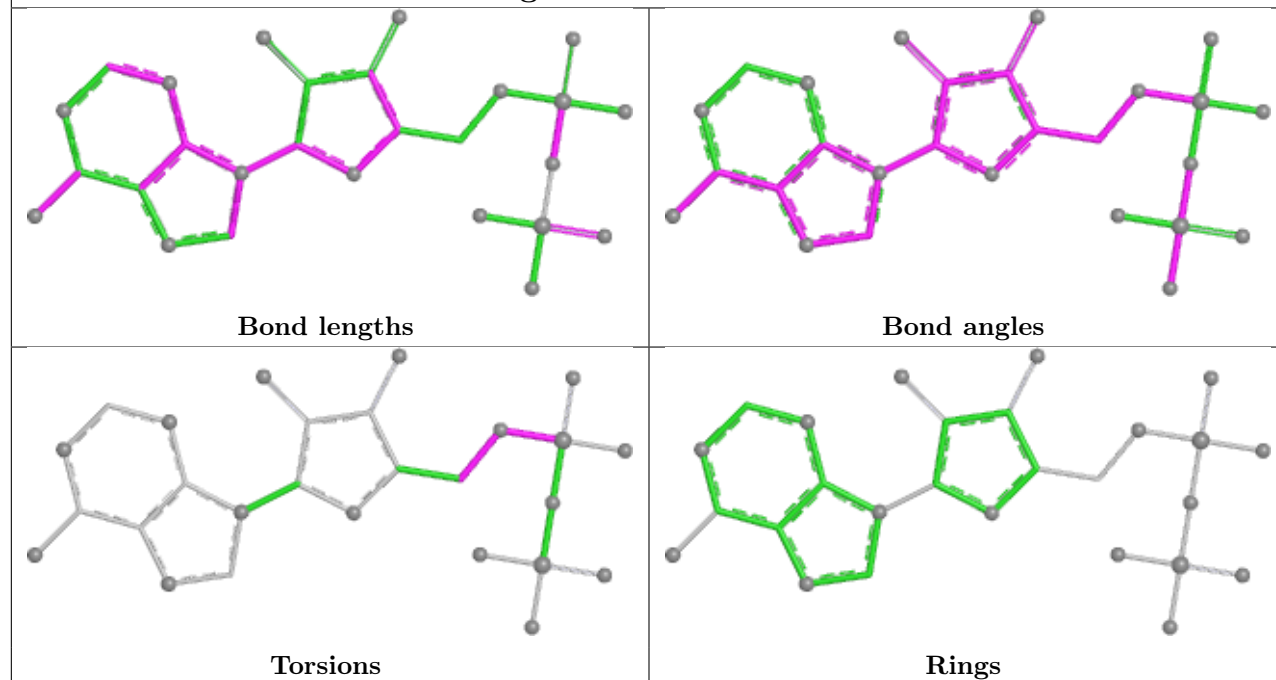
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4476	ADP	1	0
3	I	4479	ADP	1	0
3	E	4475	ADP	1	0
3	A	4471	ADP	1	0
4	E	5477	MPD	22	0
3	D	4474	ADP	1	0
3	L	4482	ADP	1	0
4	K	5492	MPD	30	0
4	E	5480	MPD	29	0
4	J	5491	MPD	35	0
4	F	5482	MPD	29	0
4	L	5494	MPD	30	0
4	G	5485	MPD	25	0
4	K	5493	MPD	32	0
3	C	4473	ADP	1	0
3	H	4478	ADP	1	0

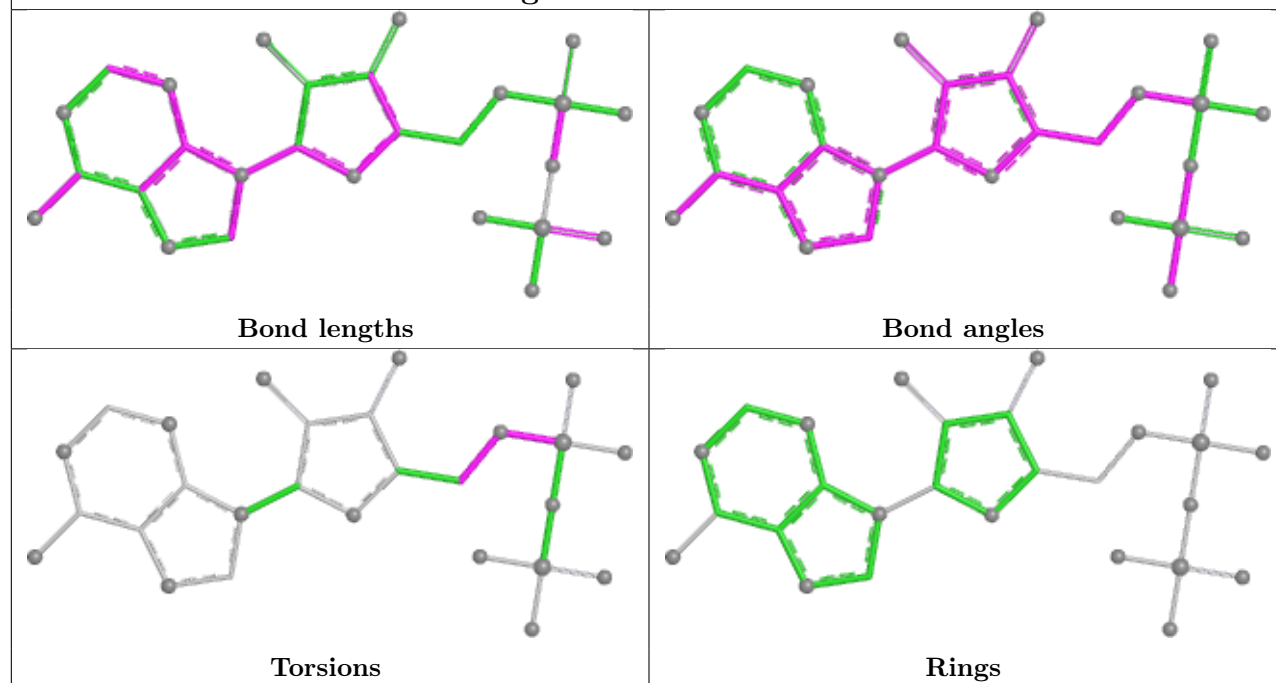
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



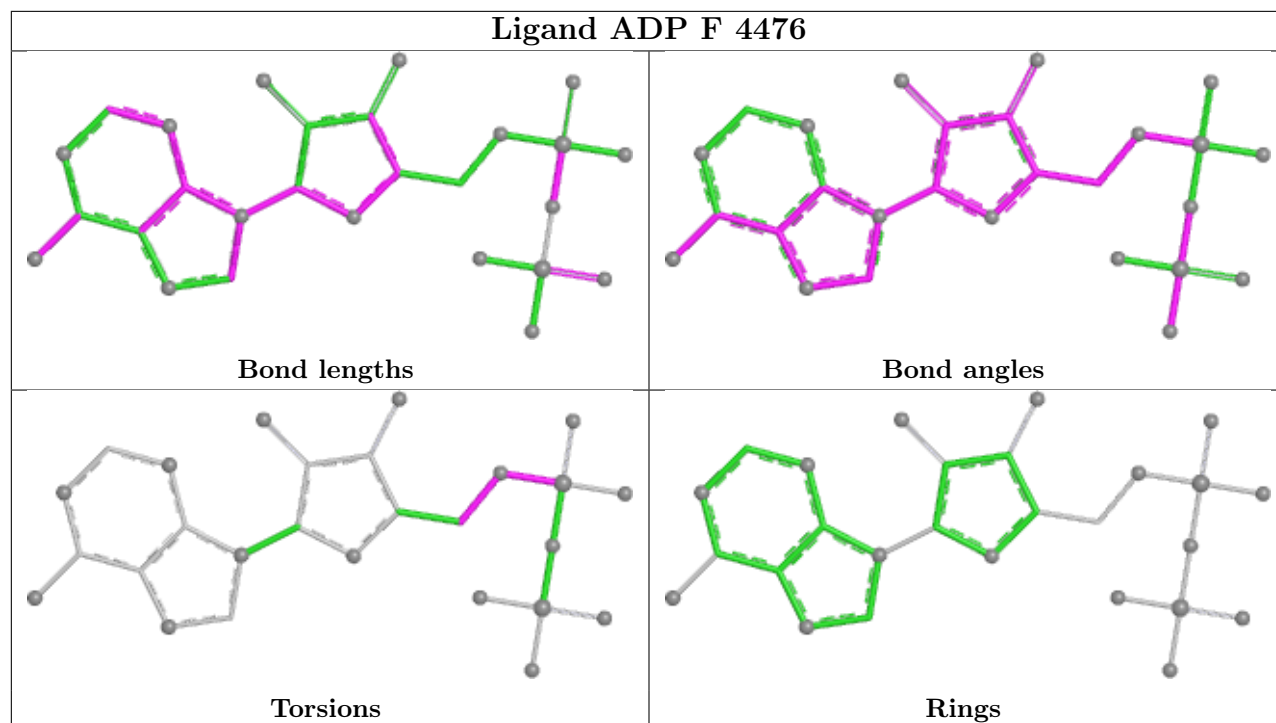
Ligand ADP K 4481



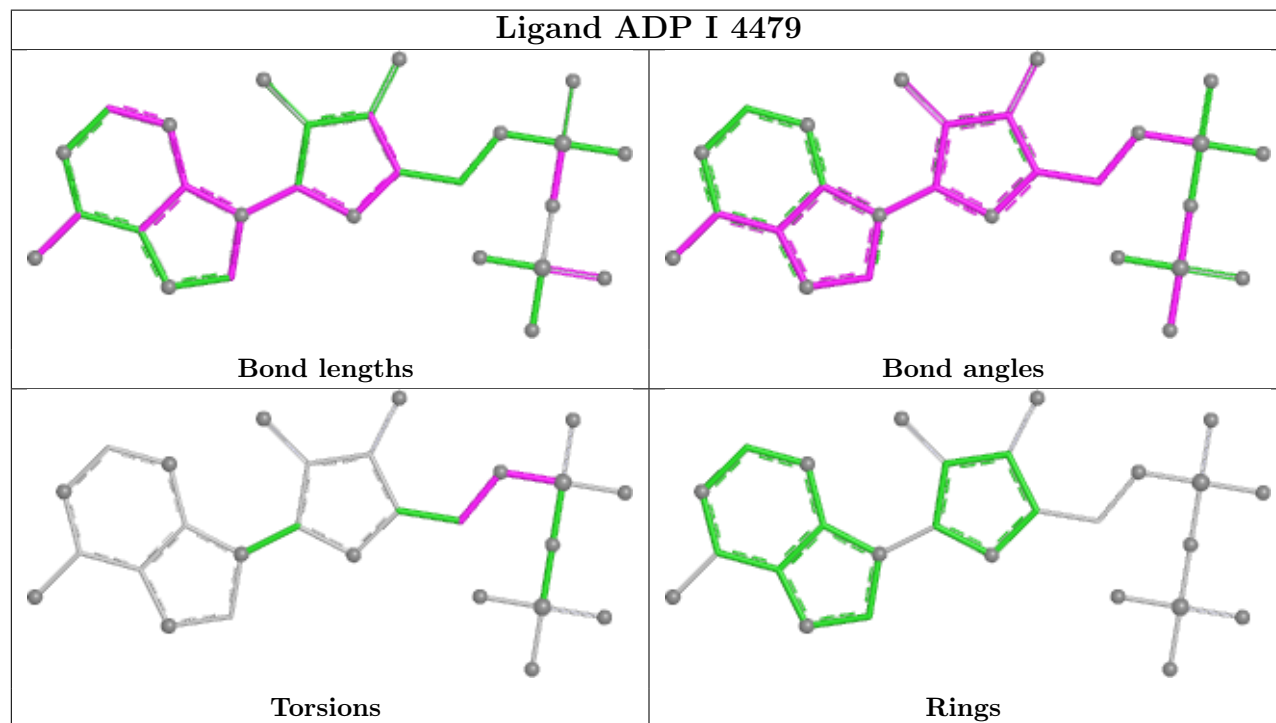
Ligand ADP B 4472

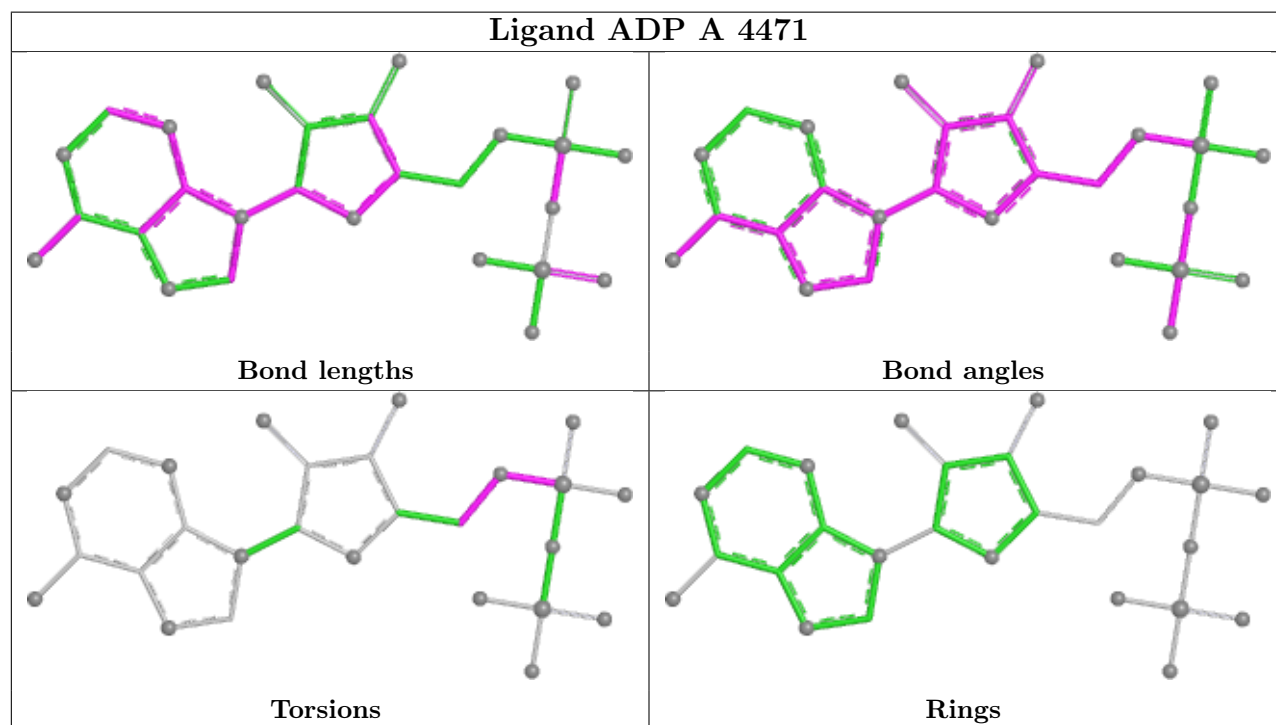
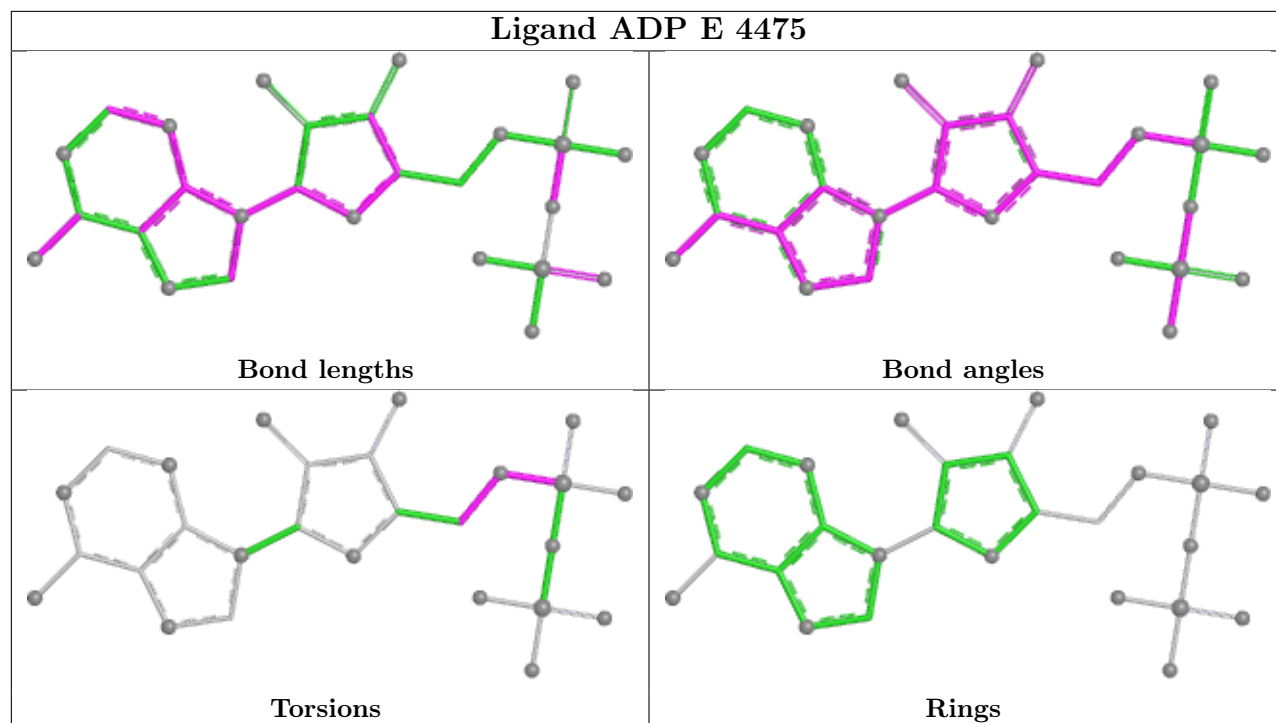


Ligand ADP F 4476

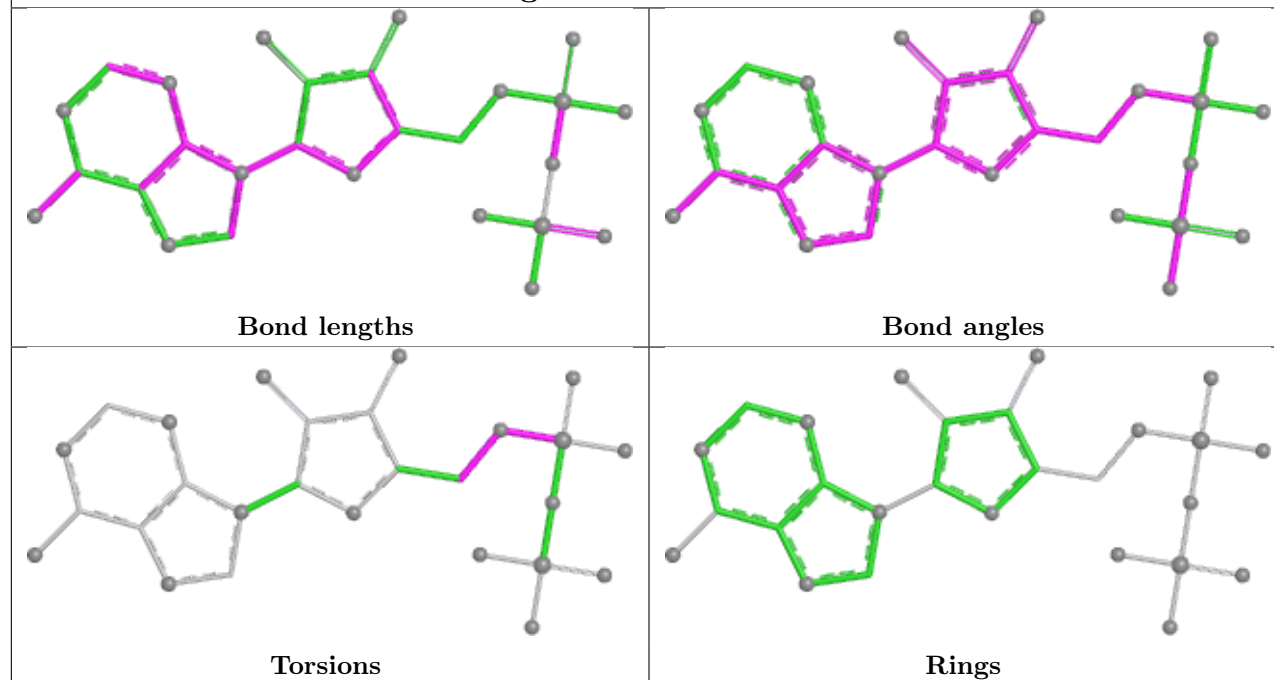


Ligand ADP I 4479

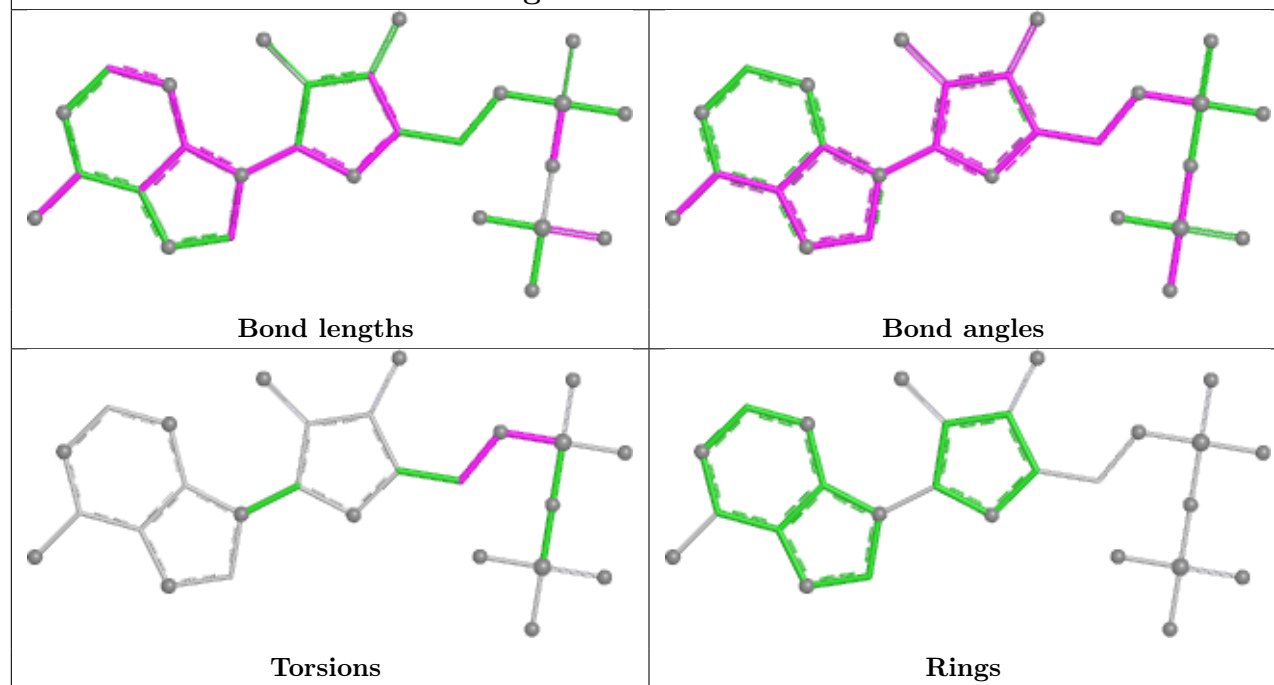


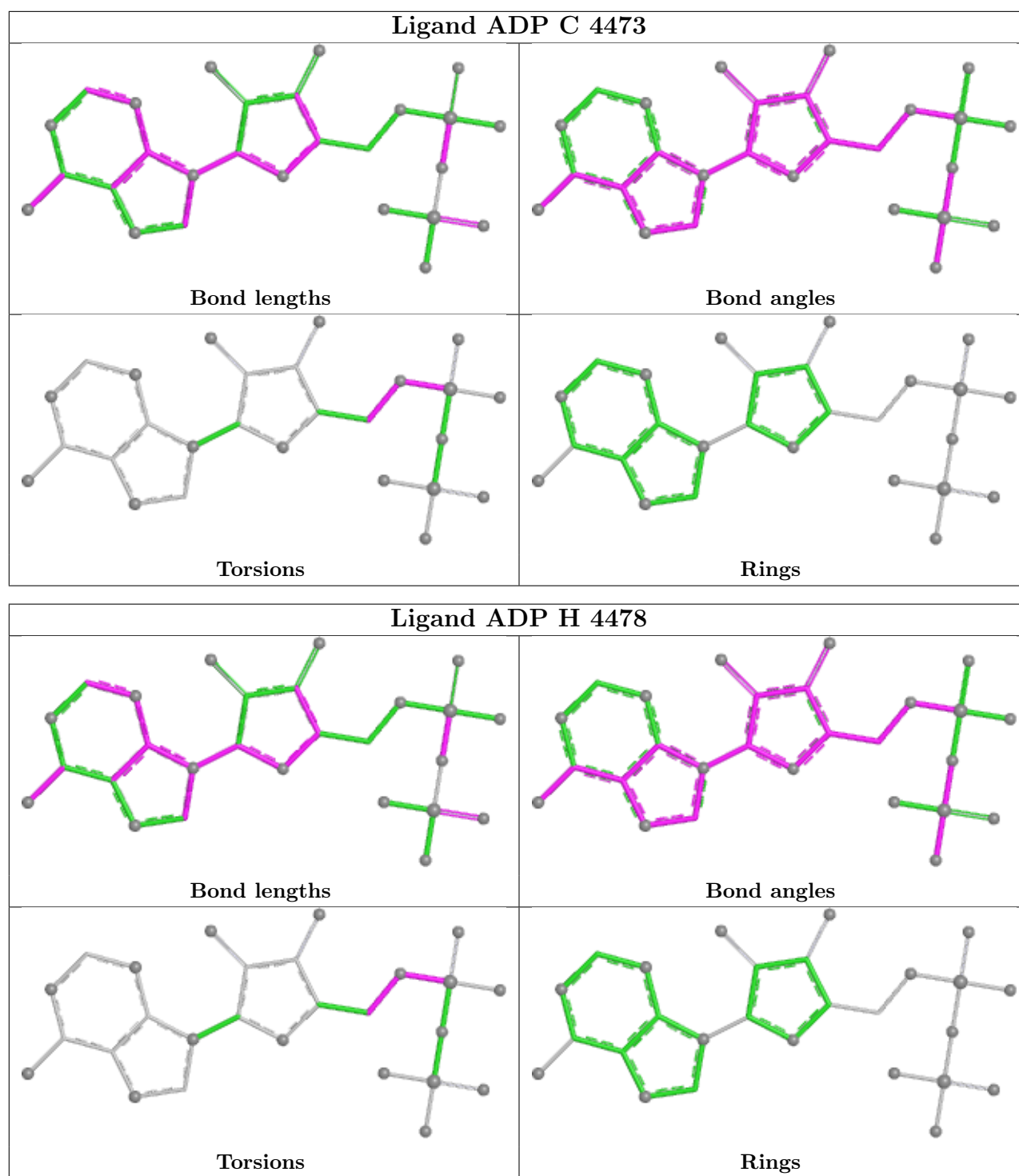


Ligand ADP D 4474



Ligand ADP L 4482





5.7 Other polymers ⓘ

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	468/468 (100%)	1.61	150 (32%) 1 1	28, 48, 90, 100	19 (4%)
1	B	468/468 (100%)	1.14	80 (17%) 4 3	28, 48, 90, 100	19 (4%)
1	C	468/468 (100%)	1.03	71 (15%) 5 4	28, 48, 90, 100	19 (4%)
1	D	468/468 (100%)	0.74	47 (10%) 12 10	28, 48, 90, 100	19 (4%)
1	E	468/468 (100%)	0.98	73 (15%) 5 4	28, 48, 90, 100	19 (4%)
1	F	468/468 (100%)	1.03	66 (14%) 6 5	28, 48, 90, 100	19 (4%)
1	G	468/468 (100%)	0.81	46 (9%) 13 11	28, 48, 90, 100	19 (4%)
1	H	468/468 (100%)	0.98	74 (15%) 5 4	28, 48, 90, 100	19 (4%)
1	I	468/468 (100%)	0.89	59 (12%) 8 6	28, 48, 90, 100	19 (4%)
1	J	468/468 (100%)	1.01	80 (17%) 4 3	28, 48, 90, 100	19 (4%)
1	K	468/468 (100%)	0.87	64 (13%) 6 5	28, 48, 90, 100	19 (4%)
1	L	468/468 (100%)	1.25	105 (22%) 2 2	28, 48, 90, 100	19 (4%)
All	All	5616/5616 (100%)	1.03	915 (16%) 4 3	28, 48, 91, 100	228 (4%)

All (915) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	ASN	6.4
1	A	334	TYR	6.3
1	J	397	TYR	6.2
1	I	397	TYR	6.0
1	L	397	TYR	5.9
1	A	333	ALA	5.8
1	H	397	TYR	5.7
1	H	7	THR	5.6
1	J	277	ASN	5.5
1	H	324	PRO	5.3
1	A	296	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	273	SER	5.2
1	A	326	TYR	5.2
1	L	399	LEU	5.1
1	B	53	SER	5.0
1	A	275	ALA	4.9
1	L	398	ASP	4.9
1	B	61	ASN	4.9
1	G	179	TYR	4.9
1	L	408	PRO	4.8
1	L	170	GLY	4.7
1	A	279	THR	4.7
1	H	179	TYR	4.7
1	A	348	VAL	4.7
1	L	388	PRO	4.7
1	L	393	ASP	4.7
1	L	179	TYR	4.6
1	B	399	LEU	4.6
1	A	351	PRO	4.5
1	J	179	TYR	4.5
1	H	5	VAL	4.5
1	H	12	HIS	4.5
1	A	122	ASP	4.5
1	D	324	PRO	4.4
1	A	299	GLY	4.4
1	C	399	LEU	4.4
1	A	288	ALA	4.4
1	A	126	PHE	4.4
1	A	328	ALA	4.4
1	A	274	LEU	4.3
1	B	407	ILE	4.3
1	A	347	VAL	4.3
1	A	324	PRO	4.3
1	A	179	TYR	4.3
1	A	391	PRO	4.3
1	A	407	ILE	4.3
1	A	404	ALA	4.3
1	A	116	ARG	4.3
1	H	1	SER	4.3
1	A	123	THR	4.2
1	L	347	VAL	4.2
1	C	398	ASP	4.2
1	J	390	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	282	PHE	4.2
1	A	121	ALA	4.2
1	A	280	ASN	4.2
1	B	326	TYR	4.1
1	B	51	GLY	4.1
1	A	345	ILE	4.1
1	J	324	PRO	4.1
1	A	125	LEU	4.1
1	E	395	ASN	4.1
1	J	391	PRO	4.1
1	C	326	TYR	4.1
1	A	278	GLY	4.1
1	A	124	VAL	4.1
1	A	340	SER	4.0
1	G	404	ALA	4.0
1	A	395	ASN	4.0
1	A	285	ASP	4.0
1	I	325	GLY	4.0
1	D	326	TYR	4.0
1	H	399	LEU	4.0
1	K	399	LEU	4.0
1	F	398	ASP	4.0
1	I	399	LEU	4.0
1	L	359	ARG	4.0
1	G	326	TYR	4.0
1	A	344	ARG	4.0
1	G	397	TYR	3.9
1	L	334	TYR	3.9
1	L	288	ALA	3.9
1	I	398	ASP	3.9
1	A	396	LEU	3.9
1	L	180	PHE	3.9
1	H	10	ASN	3.9
1	H	4	HIS	3.9
1	F	326	TYR	3.9
1	L	331	MET	3.9
1	L	61	ASN	3.9
1	A	382	ILE	3.8
1	G	398	ASP	3.8
1	L	390	GLU	3.8
1	A	282	PHE	3.8
1	C	325	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	290	LEU	3.8
1	G	399	LEU	3.8
1	E	7	THR	3.8
1	B	179	TYR	3.8
1	L	326	TYR	3.8
1	L	391	PRO	3.8
1	K	326	TYR	3.8
1	G	64	ASP	3.8
1	F	324	PRO	3.8
1	A	349	ALA	3.7
1	L	62	GLU	3.7
1	C	179	TYR	3.7
1	E	326	TYR	3.7
1	I	326	TYR	3.7
1	J	326	TYR	3.7
1	G	63	SER	3.7
1	L	404	ALA	3.7
1	J	278	GLY	3.7
1	J	395	ASN	3.7
1	B	397	TYR	3.7
1	L	405	LYS	3.7
1	F	328	ALA	3.7
1	K	397	TYR	3.7
1	B	180	PHE	3.6
1	K	44	GLU	3.6
1	I	385	LYS	3.6
1	A	378	GLY	3.6
1	A	48	MET	3.6
1	B	396	LEU	3.6
1	L	392	MET	3.6
1	A	354	ARG	3.6
1	H	398	ASP	3.6
1	A	287	TYR	3.6
1	L	292	GLU	3.6
1	K	40	ALA	3.6
1	D	325	GLY	3.6
1	E	325	GLY	3.6
1	K	398	ASP	3.6
1	E	399	LEU	3.6
1	G	61	ASN	3.6
1	A	276	LYS	3.5
1	B	327	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	L	394	LYS	3.5
1	L	7	THR	3.5
1	L	296	TYR	3.5
1	B	325	GLY	3.5
1	L	327	GLU	3.5
1	D	348	VAL	3.5
1	A	325	GLY	3.5
1	A	353	ALA	3.5
1	B	328	ALA	3.5
1	B	404	ALA	3.5
1	F	399	LEU	3.5
1	A	91	ILE	3.5
1	C	7	THR	3.5
1	C	296	TYR	3.5
1	C	397	TYR	3.5
1	J	399	LEU	3.5
1	I	170	GLY	3.5
1	L	324	PRO	3.5
1	J	180	PHE	3.5
1	L	286	LYS	3.5
1	L	348	VAL	3.5
1	H	326	TYR	3.5
1	B	40	ALA	3.5
1	J	408	PRO	3.5
1	A	398	ASP	3.4
1	G	62	GLU	3.4
1	L	395	ASN	3.4
1	B	6	LEU	3.4
1	A	230	LYS	3.4
1	F	353	ALA	3.4
1	H	328	ALA	3.4
1	K	179	TYR	3.4
1	C	180	PHE	3.4
1	H	42	PHE	3.4
1	F	327	GLU	3.4
1	H	8	MET	3.4
1	E	404	ALA	3.4
1	J	1	SER	3.4
1	K	63	SER	3.4
1	A	112	GLU	3.4
1	E	327	GLU	3.4
1	J	339	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	45	GLU	3.4
1	A	338	ASN	3.4
1	A	332	LEU	3.4
1	C	404	ALA	3.4
1	A	1	SER	3.4
1	J	387	HIS	3.4
1	A	371	PHE	3.4
1	C	282	PHE	3.4
1	A	295	LEU	3.4
1	H	347	VAL	3.4
1	C	324	PRO	3.4
1	J	170	GLY	3.4
1	L	389	GLY	3.4
1	D	349	ALA	3.4
1	D	404	ALA	3.4
1	G	117	ALA	3.4
1	E	179	TYR	3.3
1	H	180	PHE	3.3
1	B	324	PRO	3.3
1	K	344	ARG	3.3
1	L	325	GLY	3.3
1	F	60	ILE	3.3
1	J	60	ILE	3.3
1	H	286	LYS	3.3
1	J	61	ASN	3.3
1	G	348	VAL	3.3
1	L	328	ALA	3.3
1	I	61	ASN	3.3
1	A	408	PRO	3.3
1	L	339	ARG	3.3
1	A	397	TYR	3.3
1	A	337	ARG	3.3
1	L	354	ARG	3.3
1	A	327	GLU	3.3
1	A	381	GLY	3.3
1	C	51	GLY	3.3
1	B	60	ILE	3.3
1	B	35	ALA	3.3
1	I	340	SER	3.2
1	J	340	SER	3.2
1	D	399	LEU	3.2
1	A	392	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	394	LYS	3.2
1	E	180	PHE	3.2
1	I	63	SER	3.2
1	K	180	PHE	3.2
1	A	346	PRO	3.2
1	B	400	PRO	3.2
1	E	324	PRO	3.2
1	J	296	TYR	3.2
1	F	348	VAL	3.2
1	J	7	THR	3.2
1	L	341	ALA	3.2
1	J	398	ASP	3.2
1	K	62	GLU	3.2
1	E	397	TYR	3.2
1	L	433	VAL	3.2
1	K	337	ARG	3.2
1	F	1	SER	3.2
1	A	399	LEU	3.2
1	H	6	LEU	3.2
1	H	62	GLU	3.2
1	J	332	LEU	3.2
1	D	179	TYR	3.2
1	I	179	TYR	3.2
1	E	59	GLY	3.2
1	F	407	ILE	3.2
1	H	404	ALA	3.1
1	I	339	ARG	3.1
1	A	427	PHE	3.1
1	D	286	LYS	3.1
1	A	387	HIS	3.1
1	B	4	HIS	3.1
1	K	4	HIS	3.1
1	L	396	LEU	3.1
1	D	60	ILE	3.1
1	G	60	ILE	3.1
1	A	355	ARG	3.1
1	I	404	ALA	3.1
1	A	330	VAL	3.1
1	A	356	ILE	3.1
1	F	397	TYR	3.1
1	J	334	TYR	3.1
1	E	400	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	64	ASP	3.1
1	A	284	GLY	3.1
1	C	287	TYR	3.1
1	H	117	ALA	3.1
1	B	273	SER	3.1
1	I	53	SER	3.1
1	K	61	ASN	3.1
1	G	51	GLY	3.1
1	A	323	VAL	3.1
1	L	118	THR	3.0
1	E	6	LEU	3.0
1	B	39	ASN	3.0
1	B	395	ASN	3.0
1	J	359	ARG	3.0
1	L	338	ASN	3.0
1	A	170	GLY	3.0
1	G	325	GLY	3.0
1	H	431	GLY	3.0
1	K	51	GLY	3.0
1	A	302	ILE	3.0
1	F	98	GLN	3.0
1	F	62	GLU	3.0
1	I	324	PRO	3.0
1	G	6	LEU	3.0
1	L	332	LEU	3.0
1	K	224	ARG	3.0
1	K	340	SER	3.0
1	C	388	PRO	3.0
1	L	125	LEU	3.0
1	D	432	GLY	3.0
1	C	349	ALA	3.0
1	D	397	TYR	3.0
1	D	224	ARG	3.0
1	K	6	LEU	3.0
1	L	224	ARG	3.0
1	A	405	LYS	3.0
1	D	394	LYS	3.0
1	H	405	LYS	3.0
1	H	53	SER	3.0
1	A	99	GLY	3.0
1	G	170	GLY	3.0
1	L	381	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	120	ILE	2.9
1	K	327	GLU	2.9
1	E	339	ARG	2.9
1	G	339	ARG	2.9
1	K	324	PRO	2.9
1	A	100	TYR	2.9
1	A	297	TYR	2.9
1	E	286	LYS	2.9
1	A	127	GLY	2.9
1	H	325	GLY	2.9
1	D	41	GLU	2.9
1	H	407	ILE	2.9
1	B	7	THR	2.9
1	F	404	ALA	2.9
1	J	351	PRO	2.9
1	A	180	PHE	2.9
1	L	126	PHE	2.9
1	A	389	GLY	2.9
1	L	52	SER	2.9
1	C	8	MET	2.9
1	L	2	ALA	2.9
1	E	396	LEU	2.9
1	A	434	PHE	2.9
1	C	1	SER	2.9
1	J	407	ILE	2.9
1	I	348	VAL	2.9
1	L	387	HIS	2.9
1	L	385	LYS	2.9
1	A	401	PRO	2.9
1	I	40	ALA	2.9
1	L	351	PRO	2.9
1	A	115	LEU	2.9
1	C	295	LEU	2.9
1	A	233	ASP	2.9
1	L	285	ASP	2.9
1	G	180	PHE	2.9
1	J	287	TYR	2.9
1	L	287	TYR	2.9
1	C	327	GLU	2.9
1	J	389	GLY	2.9
1	A	4	HIS	2.8
1	C	60	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	395	ASN	2.8
1	G	401	PRO	2.8
1	C	328	ALA	2.8
1	F	333	ALA	2.8
1	A	428	LEU	2.8
1	B	42	PHE	2.8
1	L	49	PHE	2.8
1	F	325	GLY	2.8
1	G	405	LYS	2.8
1	J	383	LYS	2.8
1	F	52	SER	2.8
1	F	66	VAL	2.8
1	G	400	PRO	2.8
1	F	341	ALA	2.8
1	L	333	ALA	2.8
1	K	390	GLU	2.8
1	J	286	LYS	2.8
1	L	225	PHE	2.8
1	L	230	LYS	2.8
1	B	378	GLY	2.8
1	I	51	GLY	2.8
1	L	319	TYR	2.8
1	E	60	ILE	2.8
1	H	60	ILE	2.8
1	C	53	SER	2.8
1	D	53	SER	2.8
1	J	327	GLU	2.8
1	H	224	ARG	2.8
1	L	282	PHE	2.8
1	F	179	TYR	2.8
1	I	273	SER	2.8
1	A	301	VAL	2.8
1	C	347	VAL	2.8
1	L	401	PRO	2.8
1	B	392	MET	2.8
1	K	392	MET	2.8
1	A	224	ARG	2.8
1	B	398	ASP	2.8
1	C	42	PHE	2.8
1	F	180	PHE	2.8
1	C	395	ASN	2.7
1	F	296	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	391	PRO	2.7
1	L	291	SER	2.7
1	B	38	VAL	2.7
1	J	349	ALA	2.7
1	B	48	MET	2.7
1	H	11	GLU	2.7
1	J	3	GLU	2.7
1	B	304	HIS	2.7
1	F	170	GLY	2.7
1	C	386	ILE	2.7
1	G	395	ASN	2.7
1	H	334	TYR	2.7
1	I	6	LEU	2.7
1	A	336	ALA	2.7
1	A	376	MET	2.7
1	J	392	MET	2.7
1	A	339	ARG	2.7
1	J	62	GLU	2.7
1	K	292	GLU	2.7
1	B	393	ASP	2.7
1	G	393	ASP	2.7
1	A	289	GLY	2.7
1	I	99	GLY	2.7
1	D	401	PRO	2.7
1	L	181	PRO	2.7
1	B	124	VAL	2.7
1	J	330	VAL	2.7
1	G	296	TYR	2.7
1	H	319	TYR	2.7
1	L	1	SER	2.7
1	J	279	THR	2.7
1	J	341	ALA	2.7
1	J	404	ALA	2.7
1	L	336	ALA	2.7
1	L	344	ARG	2.7
1	A	3	GLU	2.7
1	D	327	GLU	2.7
1	A	64	ASP	2.7
1	B	50	ASP	2.7
1	K	48	MET	2.7
1	A	335	SER	2.7
1	K	1	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	273	SER	2.7
1	A	108	ALA	2.7
1	B	353	ALA	2.7
1	C	121	ALA	2.7
1	I	336	ALA	2.7
1	K	41	GLU	2.7
1	B	64	ASP	2.6
1	A	59	GLY	2.6
1	E	284	GLY	2.6
1	H	170	GLY	2.6
1	L	431	GLY	2.6
1	A	388	PRO	2.6
1	I	181	PRO	2.6
1	I	401	PRO	2.6
1	A	331	MET	2.6
1	E	354	ARG	2.6
1	I	10	ASN	2.6
1	I	337	ARG	2.6
1	B	274	LEU	2.6
1	C	396	LEU	2.6
1	E	348	VAL	2.6
1	F	396	LEU	2.6
1	H	125	LEU	2.6
1	G	232	ALA	2.6
1	J	293	GLN	2.6
1	L	294	ALA	2.6
1	D	59	GLY	2.6
1	L	59	GLY	2.6
1	B	282	PHE	2.6
1	C	274	LEU	2.6
1	J	347	VAL	2.6
1	A	350	SER	2.6
1	F	63	SER	2.6
1	A	377	ALA	2.6
1	E	64	ASP	2.6
1	K	393	ASP	2.6
1	D	359	ARG	2.6
1	F	49	PHE	2.6
1	H	48	MET	2.6
1	E	290	LEU	2.6
1	E	295	LEU	2.6
1	H	45	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	396	LEU	2.6
1	D	395	ASN	2.6
1	H	61	ASN	2.6
1	J	117	ALA	2.6
1	K	385	LYS	2.6
1	C	284	GLY	2.6
1	E	401	PRO	2.6
1	G	59	GLY	2.6
1	K	55	GLY	2.6
1	L	65	MET	2.6
1	C	62	GLU	2.6
1	D	292	GLU	2.6
1	A	433	VAL	2.6
1	L	277	ASN	2.6
1	L	384	ASN	2.6
1	A	117	ALA	2.6
1	A	283	SER	2.6
1	A	341	ALA	2.6
1	J	63	SER	2.6
1	K	275	ALA	2.6
1	J	58	LYS	2.6
1	F	334	TYR	2.6
1	D	339	ARG	2.5
1	G	181	PRO	2.5
1	K	170	GLY	2.5
1	A	292	GLU	2.5
1	B	434	PHE	2.5
1	H	403	GLU	2.5
1	A	281	LEU	2.5
1	A	304	HIS	2.5
1	C	387	HIS	2.5
1	I	275	ALA	2.5
1	L	353	ALA	2.5
1	B	334	TYR	2.5
1	B	170	GLY	2.5
1	D	400	PRO	2.5
1	K	278	GLY	2.5
1	K	367	PRO	2.5
1	C	64	ASP	2.5
1	C	292	GLU	2.5
1	A	6	LEU	2.5
1	L	293	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	61	ASN	2.5
1	F	4	HIS	2.5
1	H	124	VAL	2.5
1	E	53	SER	2.5
1	H	340	SER	2.5
1	L	63	SER	2.5
1	B	296	TYR	2.5
1	J	181	PRO	2.5
1	L	400	PRO	2.5
1	H	3	GLU	2.5
1	I	390	GLU	2.5
1	K	11	GLU	2.5
1	L	386	ILE	2.5
1	I	180	PHE	2.5
1	A	394	LYS	2.5
1	C	286	LYS	2.5
1	I	280	ASN	2.5
1	G	349	ALA	2.5
1	L	116	ARG	2.5
1	B	340	SER	2.5
1	D	331	MET	2.5
1	E	392	MET	2.5
1	C	401	PRO	2.5
1	H	408	PRO	2.5
1	A	390	GLU	2.5
1	B	46	GLY	2.5
1	H	59	GLY	2.5
1	K	296	TYR	2.5
1	C	394	LYS	2.5
1	F	6	LEU	2.5
1	F	295	LEU	2.5
1	J	295	LEU	2.5
1	K	383	LYS	2.5
1	E	293	GLN	2.5
1	L	98	GLN	2.5
1	G	4	HIS	2.5
1	J	280	ASN	2.5
1	K	341	ALA	2.5
1	C	52	SER	2.5
1	B	408	PRO	2.4
1	H	181	PRO	2.4
1	J	388	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	51	GLY	2.4
1	F	406	GLU	2.4
1	A	380	ASP	2.4
1	A	383	LYS	2.4
1	E	407	ILE	2.4
1	I	334	TYR	2.4
1	J	276	LYS	2.4
1	L	114	TYR	2.4
1	C	6	LEU	2.4
1	G	396	LEU	2.4
1	A	49	PHE	2.4
1	I	49	PHE	2.4
1	H	337	ARG	2.4
1	B	338	ASN	2.4
1	I	395	ASN	2.4
1	A	430	ALA	2.4
1	B	65	MET	2.4
1	E	341	ALA	2.4
1	H	40	ALA	2.4
1	L	349	ALA	2.4
1	B	181	PRO	2.4
1	G	388	PRO	2.4
1	A	60	ILE	2.4
1	C	428	LEU	2.4
1	E	296	TYR	2.4
1	F	287	TYR	2.4
1	F	375	LEU	2.4
1	H	293	GLN	2.4
1	C	4	HIS	2.4
1	G	344	ARG	2.4
1	B	433	VAL	2.4
1	K	8	MET	2.4
1	F	117	ALA	2.4
1	A	403	GLU	2.4
1	A	406	GLU	2.4
1	B	391	PRO	2.4
1	D	367	PRO	2.4
1	D	406	GLU	2.4
1	F	112	GLU	2.4
1	G	327	GLU	2.4
1	G	406	GLU	2.4
1	H	327	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	394	LYS	2.4
1	A	119	GLY	2.4
1	I	64	ASP	2.4
1	L	407	ILE	2.4
1	A	379	LEU	2.4
1	B	125	LEU	2.4
1	B	354	ARG	2.4
1	G	337	ARG	2.4
1	I	359	ARG	2.4
1	J	224	ARG	2.4
1	C	348	VAL	2.4
1	G	392	MET	2.4
1	E	10	ASN	2.4
1	A	294	ALA	2.4
1	A	329	PRO	2.4
1	C	408	PRO	2.4
1	E	3	GLU	2.4
1	E	408	PRO	2.4
1	K	181	PRO	2.4
1	E	63	SER	2.4
1	A	203	GLY	2.4
1	F	59	GLY	2.4
1	J	99	GLY	2.4
1	H	379	LEU	2.4
1	J	354	ARG	2.4
1	E	225	PHE	2.4
1	I	287	TYR	2.4
1	J	338	ASN	2.4
1	E	353	ALA	2.4
1	J	328	ALA	2.4
1	C	3	GLU	2.4
1	H	388	PRO	2.3
1	B	1	SER	2.3
1	I	1	SER	2.3
1	E	337	ARG	2.3
1	G	407	ILE	2.3
1	L	337	ARG	2.3
1	A	271	HIS	2.3
1	J	9	LEU	2.3
1	J	125	LEU	2.3
1	E	334	TYR	2.3
1	C	433	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	394	LYS	2.3
1	B	441	ALA	2.3
1	C	11	GLU	2.3
1	J	45	GLU	2.3
1	J	333	ALA	2.3
1	J	430	ALA	2.3
1	B	329	PRO	2.3
1	B	123	THR	2.3
1	D	52	SER	2.3
1	E	340	SER	2.3
1	B	56	GLY	2.3
1	B	95	GLY	2.3
1	C	56	GLY	2.3
1	F	337	ARG	2.3
1	H	99	GLY	2.3
1	K	95	GLY	2.3
1	E	4	HIS	2.3
1	I	396	LEU	2.3
1	K	387	HIS	2.3
1	C	285	ASP	2.3
1	A	272	MET	2.3
1	B	47	LYS	2.3
1	E	385	LYS	2.3
1	H	287	TYR	2.3
1	B	62	GLU	2.3
1	B	10	ASN	2.3
1	H	277	ASN	2.3
1	K	395	ASN	2.3
1	F	121	ALA	2.3
1	F	377	ALA	2.3
1	H	275	ALA	2.3
1	K	328	ALA	2.3
1	A	7	THR	2.3
1	G	359	ARG	2.3
1	B	63	SER	2.3
1	J	378	GLY	2.3
1	L	340	SER	2.3
1	C	12	HIS	2.3
1	E	374	LEU	2.3
1	H	285	ASP	2.3
1	J	285	ASP	2.3
1	L	48	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	47	LYS	2.3
1	B	390	GLU	2.3
1	G	347	VAL	2.3
1	G	402	GLU	2.3
1	B	351	PRO	2.3
1	B	401	PRO	2.3
1	C	391	PRO	2.3
1	H	336	ALA	2.3
1	J	367	PRO	2.3
1	K	404	ALA	2.3
1	C	248	ARG	2.3
1	H	98	GLN	2.3
1	G	52	SER	2.3
1	G	53	SER	2.3
1	K	12	HIS	2.3
1	B	345	ILE	2.3
1	C	125	LEU	2.3
1	E	65	MET	2.3
1	E	285	ASP	2.3
1	L	383	LYS	2.3
1	C	225	PHE	2.3
1	C	403	GLU	2.3
1	G	224	ARG	2.3
1	A	118	THR	2.2
1	K	22	THR	2.2
1	D	387	HIS	2.2
1	J	59	GLY	2.2
1	A	343	ILE	2.2
1	E	52	SER	2.2
1	F	331	MET	2.2
1	F	340	SER	2.2
1	H	122	ASP	2.2
1	J	393	ASP	2.2
1	H	406	GLU	2.2
1	L	406	GLU	2.2
1	K	49	PHE	2.2
1	E	124	VAL	2.2
1	E	351	PRO	2.2
1	I	347	VAL	2.2
1	J	116	ARG	2.2
1	L	367	PRO	2.2
1	D	328	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	288	ALA	2.2
1	I	341	ALA	2.2
1	C	304	HIS	2.2
1	H	279	THR	2.2
1	A	385	LYS	2.2
1	C	119	GLY	2.2
1	C	289	GLY	2.2
1	C	381	GLY	2.2
1	C	432	GLY	2.2
1	D	392	MET	2.2
1	K	65	MET	2.2
1	L	6	LEU	2.2
1	A	52	SER	2.2
1	L	60	ILE	2.2
1	C	393	ASP	2.2
1	B	112	GLU	2.2
1	H	339	ARG	2.2
1	J	344	ARG	2.2
1	A	66	VAL	2.2
1	F	347	VAL	2.2
1	A	61	ASN	2.2
1	A	111	ALA	2.2
1	D	40	ALA	2.2
1	I	353	ALA	2.2
1	B	8	MET	2.2
1	D	170	GLY	2.2
1	H	392	MET	2.2
1	H	396	LEU	2.2
1	E	382	ILE	2.2
1	J	386	ILE	2.2
1	D	340	SER	2.2
1	K	52	SER	2.2
1	I	402	GLU	2.2
1	J	93	GLU	2.2
1	I	248	ARG	2.2
1	G	324	PRO	2.2
1	H	329	PRO	2.2
1	E	5	VAL	2.2
1	I	66	VAL	2.2
1	A	417	ALA	2.2
1	E	377	ALA	2.2
1	J	336	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	279	THR	2.2
1	I	296	TYR	2.2
1	L	278	GLY	2.2
1	C	350	SER	2.2
1	E	342	SER	2.2
1	I	335	SER	2.2
1	E	122	ASP	2.2
1	E	292	GLU	2.2
1	I	400	PRO	2.2
1	K	351	PRO	2.2
1	B	303	LYS	2.2
1	G	394	LYS	2.2
1	L	58	LYS	2.2
1	B	205	VAL	2.1
1	A	71	ALA	2.1
1	B	275	ALA	2.1
1	L	378	GLY	2.1
1	F	297	TYR	2.1
1	F	465	TYR	2.1
1	A	342	SER	2.1
1	D	63	SER	2.1
1	F	116	ARG	2.1
1	H	390	GLU	2.1
1	J	401	PRO	2.1
1	K	394	LYS	2.1
1	D	42	PHE	2.1
1	A	98	GLN	2.1
1	C	275	ALA	2.1
1	F	108	ALA	2.1
1	I	305	ALA	2.1
1	I	309	ASN	2.1
1	K	338	ASN	2.1
1	A	267	GLY	2.1
1	A	432	GLY	2.1
1	F	51	GLY	2.1
1	J	382	ILE	2.1
1	A	234	GLU	2.1
1	C	297	TYR	2.1
1	D	403	GLU	2.1
1	E	116	ARG	2.1
1	E	224	ARG	2.1
1	F	3	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	344	ARG	2.1
1	K	319	TYR	2.1
1	L	297	TYR	2.1
1	L	426	GLU	2.1
1	D	398	ASP	2.1
1	I	393	ASP	2.1
1	L	361	PRO	2.1
1	D	180	PHE	2.1
1	E	387	HIS	2.1
1	E	434	PHE	2.1
1	F	387	HIS	2.1
1	E	433	VAL	2.1
1	H	348	VAL	2.1
1	B	336	ALA	2.1
1	B	349	ALA	2.1
1	C	341	ALA	2.1
1	E	328	ALA	2.1
1	F	2	ALA	2.1
1	B	277	ASN	2.1
1	F	395	ASN	2.1
1	A	55	GLY	2.1
1	E	421	LEU	2.1
1	H	278	GLY	2.1
1	L	119	GLY	2.1
1	B	344	ARG	2.1
1	F	344	ARG	2.1
1	J	337	ARG	2.1
1	C	407	ILE	2.1
1	D	407	ILE	2.1
1	L	437	GLU	2.1
1	D	296	TYR	2.1
1	K	287	TYR	2.1
1	K	334	TYR	2.1
1	E	380	ASP	2.1
1	I	47	LYS	2.1
1	H	350	SER	2.1
1	I	342	SER	2.1
1	C	361	PRO	2.1
1	E	12	HIS	2.1
1	A	293	GLN	2.1
1	B	347	VAL	2.1
1	C	38	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	66	VAL	2.1
1	L	42	PHE	2.1
1	L	434	PHE	2.1
1	H	2	ALA	2.1
1	E	277	ASN	2.1
1	F	9	LEU	2.1
1	H	338	ASN	2.1
1	A	51	GLY	2.1
1	D	95	GLY	2.1
1	K	99	GLY	2.1
1	E	415	GLU	2.1
1	F	390	GLU	2.1
1	H	41	GLU	2.1
1	F	47	LYS	2.1
1	I	405	LYS	2.1
1	I	319	TYR	2.1
1	F	401	PRO	2.1
1	I	331	MET	2.1
1	K	98	GLN	2.0
1	K	339	ARG	2.0
1	A	67	LEU	2.0
1	F	61	ASN	2.0
1	F	125	LEU	2.0
1	L	115	LEU	2.0
1	A	46	GLY	2.0
1	E	289	GLY	2.0
1	E	378	GLY	2.0
1	A	33	ILE	2.0
1	B	223	THR	2.0
1	F	385	LYS	2.0
1	A	103	ASP	2.0
1	C	319	TYR	2.0
1	C	334	TYR	2.0
1	D	334	TYR	2.0
1	F	113	ASP	2.0
1	F	122	ASP	2.0
1	F	388	PRO	2.0
1	H	296	TYR	2.0
1	I	408	PRO	2.0
1	J	53	SER	2.0
1	J	273	SER	2.0
1	K	408	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	392	MET	2.0
1	L	350	SER	2.0
1	I	344	ARG	2.0
1	A	85	LEU	2.0
1	A	375	LEU	2.0
1	D	396	LEU	2.0
1	E	333	ALA	2.0
1	E	349	ALA	2.0
1	L	40	ALA	2.0
1	I	44	GLU	2.0
1	J	403	GLU	2.0
1	J	426	GLU	2.0
1	K	402	GLU	2.0
1	E	170	GLY	2.0
1	L	51	GLY	2.0
1	B	343	ILE	2.0
1	E	184	PRO	2.0
1	J	64	ASP	2.0
1	J	113	ASP	2.0
1	D	319	TYR	2.0
1	F	53	SER	2.0
1	K	53	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	A	4471	27/27	0.53	0.32	38,77,100,100	27

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	B	4472	27/27	0.63	0.25	38,77,100,100	27
3	ADP	F	4476	27/27	0.63	0.20	38,77,100,100	27
3	ADP	L	4482	27/27	0.68	0.27	38,77,100,100	27
4	MPD	A	5472	8/8	0.69	0.44	63,68,75,98	8
4	MPD	H	5486	8/8	0.71	0.39	63,68,75,98	8
4	MPD	B	5474	8/8	0.72	0.37	63,68,75,98	8
3	ADP	E	4475	27/27	0.72	0.19	38,77,100,100	27
3	ADP	I	4479	27/27	0.73	0.24	38,77,100,100	27
3	ADP	K	4481	27/27	0.73	0.25	38,77,100,100	27
3	ADP	C	4473	27/27	0.73	0.19	38,77,100,100	27
4	MPD	B	5471	8/8	0.74	0.40	37,50,65,66	8
3	ADP	G	4477	27/27	0.75	0.25	38,77,100,100	27
4	MPD	A	5481	8/8	0.76	0.32	37,50,65,66	8
3	ADP	D	4474	27/27	0.77	0.20	38,77,100,100	27
3	ADP	J	4480	27/27	0.77	0.26	38,77,100,100	27
3	ADP	H	4478	27/27	0.77	0.21	38,77,100,100	27
4	MPD	I	5488	8/8	0.79	0.43	63,68,75,98	8
4	MPD	K	5492	8/8	0.79	0.50	63,68,75,98	8
4	MPD	F	5482	8/8	0.80	0.31	63,68,75,98	8
4	MPD	C	5476	8/8	0.80	0.39	63,68,75,98	8
4	MPD	E	5480	8/8	0.83	0.35	63,68,75,98	8
4	MPD	J	5490	8/8	0.83	0.45	63,68,75,98	8
4	MPD	F	5479	8/8	0.83	0.35	37,50,65,66	8
4	MPD	D	5478	8/8	0.84	0.33	63,68,75,98	8
4	MPD	L	5494	8/8	0.84	0.44	63,68,75,98	8
4	MPD	G	5484	8/8	0.86	0.43	63,68,75,98	8
4	MPD	E	5477	8/8	0.87	0.25	37,50,65,66	8
4	MPD	C	5473	8/8	0.87	0.28	37,50,65,66	8
4	MPD	D	5475	8/8	0.88	0.27	37,50,65,66	8
4	MPD	H	5487	8/8	0.89	0.29	37,50,65,66	8
4	MPD	I	5489	8/8	0.91	0.28	37,50,65,66	8
4	MPD	J	5491	8/8	0.91	0.37	37,50,65,66	8
4	MPD	K	5493	8/8	0.92	0.37	37,50,65,66	8
4	MPD	L	5483	8/8	0.92	0.35	37,50,65,66	8
4	MPD	G	5485	8/8	0.92	0.34	37,50,65,66	8
2	MN	A	470	1/1	0.95	0.09	46,46,46,46	0
2	MN	C	469	1/1	0.96	0.06	47,47,47,47	0
2	MN	D	470	1/1	0.96	0.07	46,46,46,46	0
2	MN	E	470	1/1	0.96	0.09	46,46,46,46	0
2	MN	F	469	1/1	0.96	0.07	47,47,47,47	0
2	MN	B	470	1/1	0.97	0.11	46,46,46,46	0
2	MN	A	469	1/1	0.97	0.08	47,47,47,47	0

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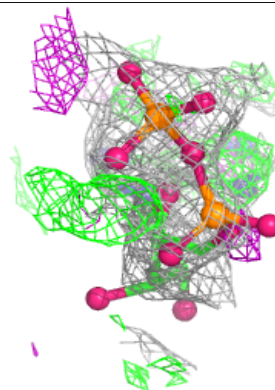
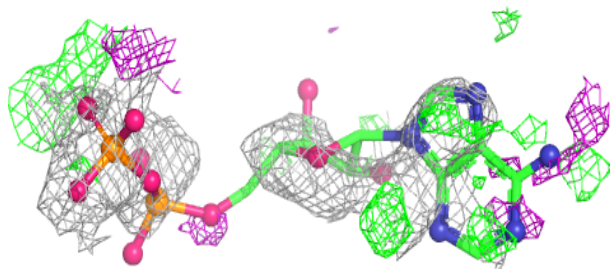
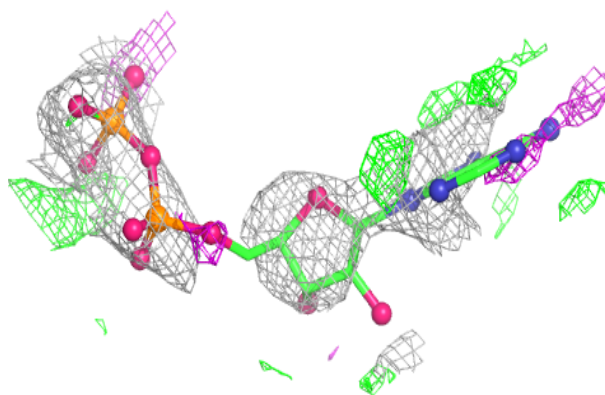
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	H	470	1/1	0.97	0.04	46,46,46,46	0
2	MN	L	469	1/1	0.97	0.09	47,47,47,47	0
2	MN	B	469	1/1	0.97	0.06	47,47,47,47	0
2	MN	H	469	1/1	0.98	0.07	47,47,47,47	0
2	MN	C	470	1/1	0.98	0.07	46,46,46,46	0
2	MN	J	469	1/1	0.98	0.09	47,47,47,47	0
2	MN	K	469	1/1	0.98	0.08	47,47,47,47	0
2	MN	G	470	1/1	0.98	0.04	46,46,46,46	0
2	MN	L	470	1/1	0.98	0.08	46,46,46,46	0
2	MN	D	469	1/1	0.99	0.04	47,47,47,47	0
2	MN	K	470	1/1	0.99	0.04	46,46,46,46	0
2	MN	E	469	1/1	0.99	0.05	47,47,47,47	0
2	MN	F	470	1/1	0.99	0.08	46,46,46,46	0
2	MN	I	469	1/1	0.99	0.04	47,47,47,47	0
2	MN	I	470	1/1	0.99	0.03	46,46,46,46	0
2	MN	G	469	1/1	0.99	0.04	47,47,47,47	0
2	MN	J	470	1/1	0.99	0.05	46,46,46,46	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.

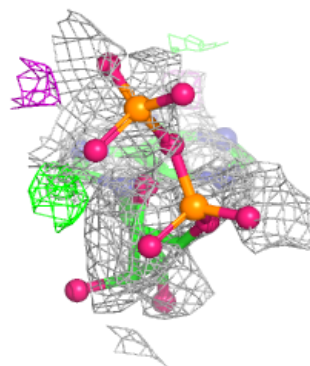
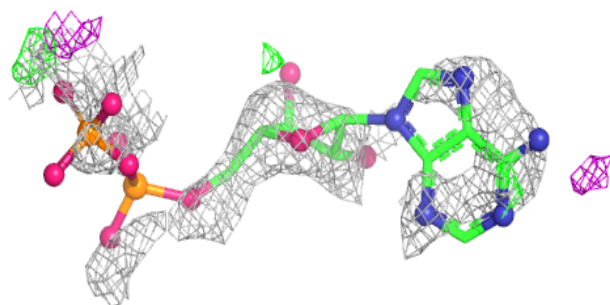
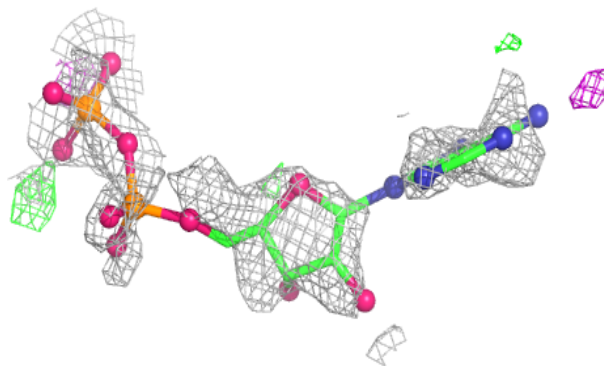
Electron density around ADP A 4471:

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

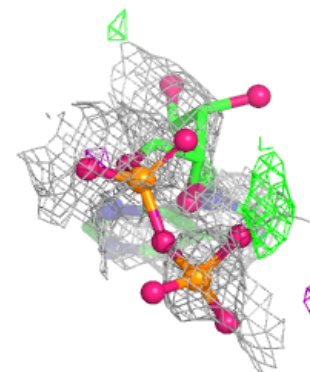
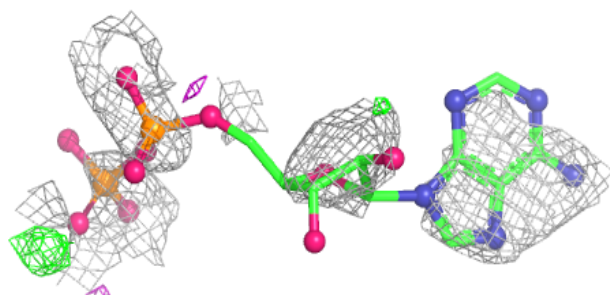
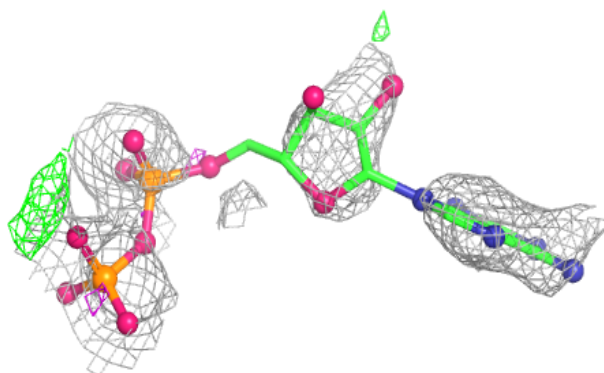


Electron density around ADP B 4472:

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

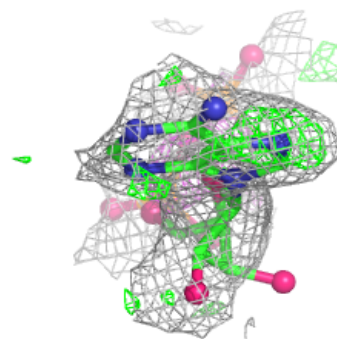
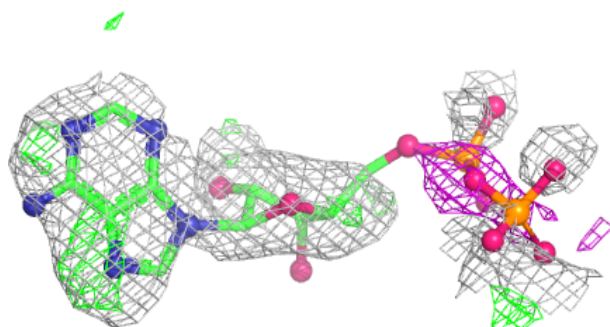
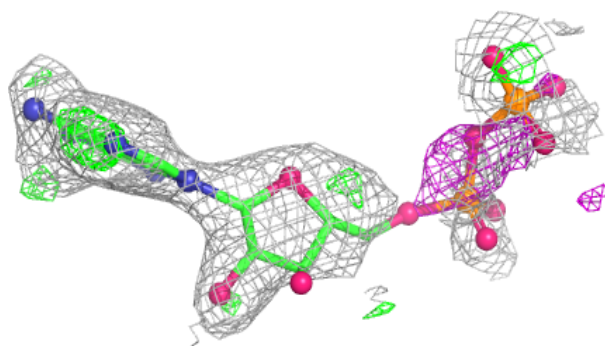
**Electron density around ADP F 4476:**

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

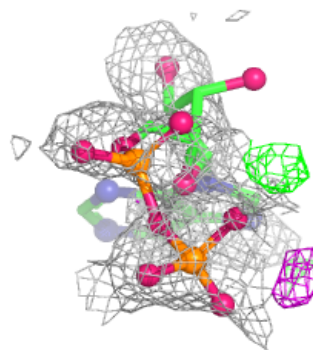
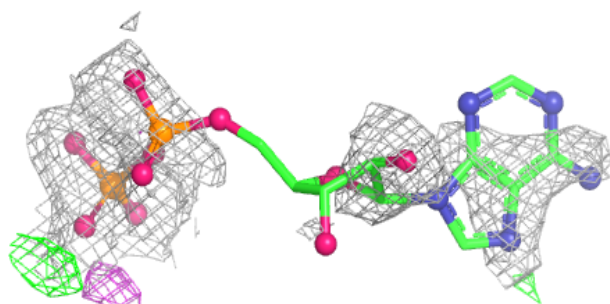
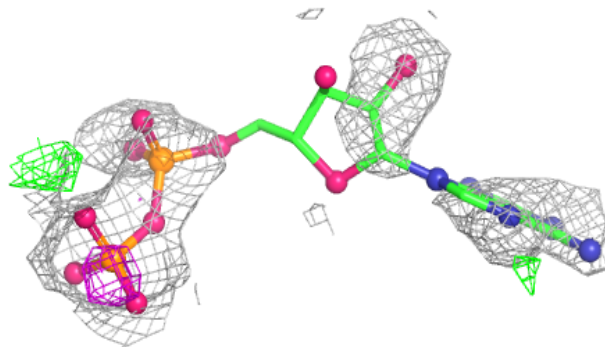


Electron density around ADP L 4482:

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

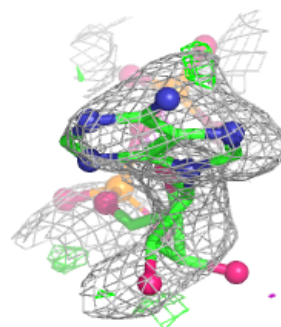
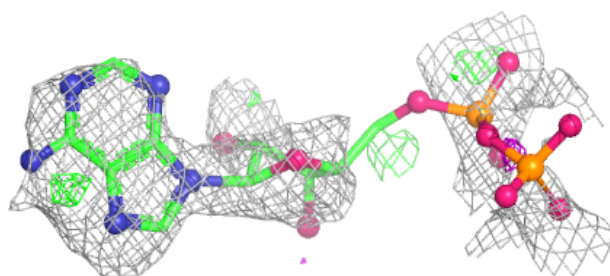
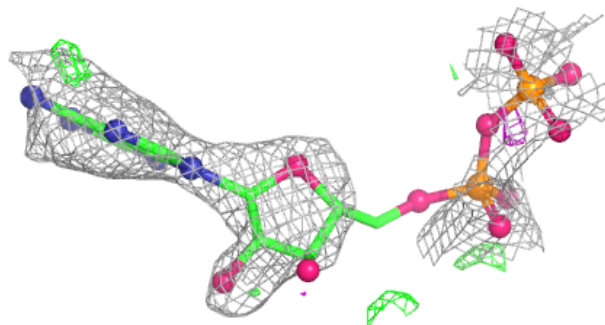
**Electron density around ADP E 4475:**

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

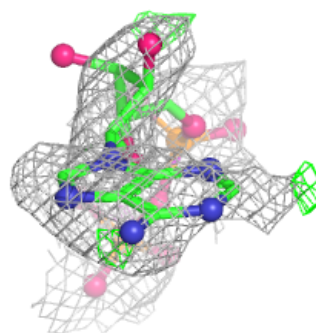
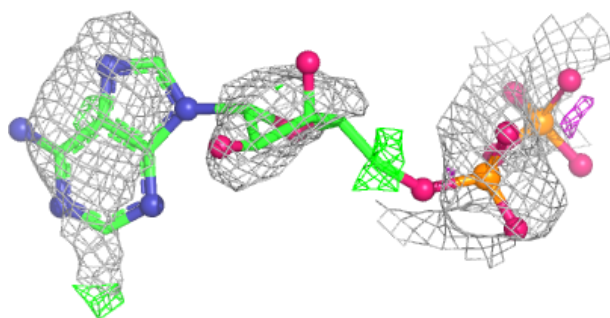
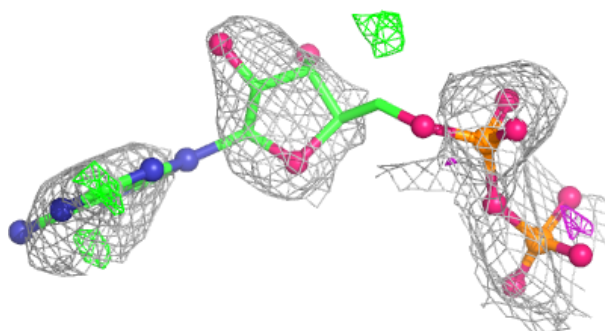


Electron density around ADP I 4479:

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

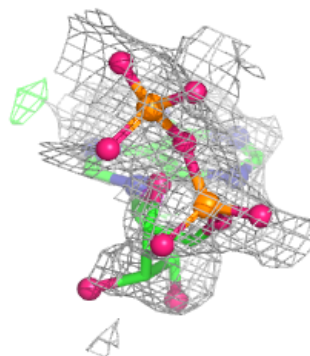
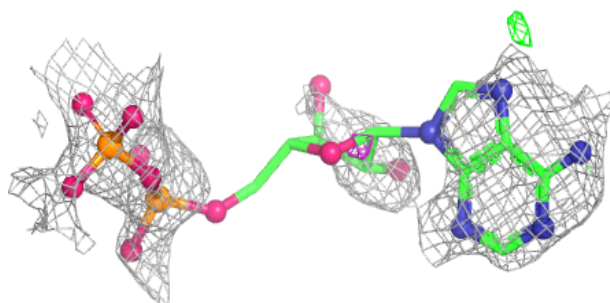
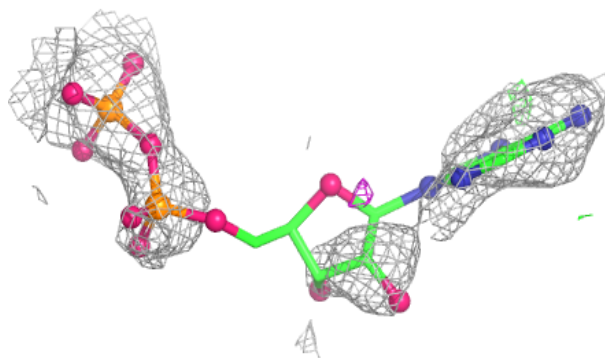
**Electron density around ADP K 4481:**

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

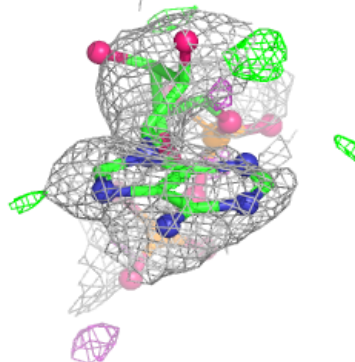
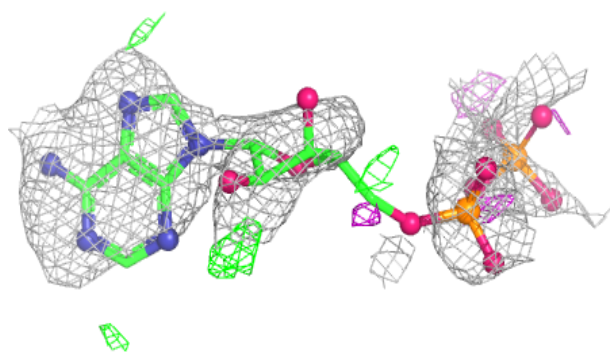
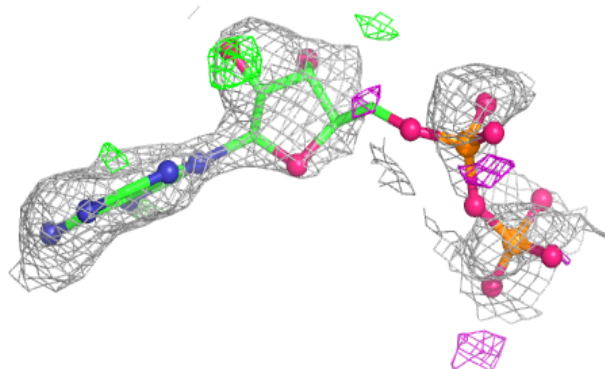


Electron density around ADP C 4473:

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

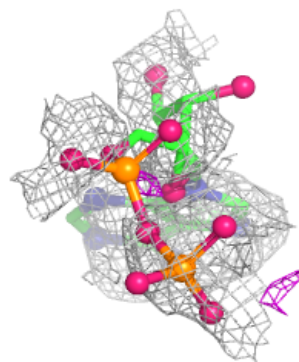
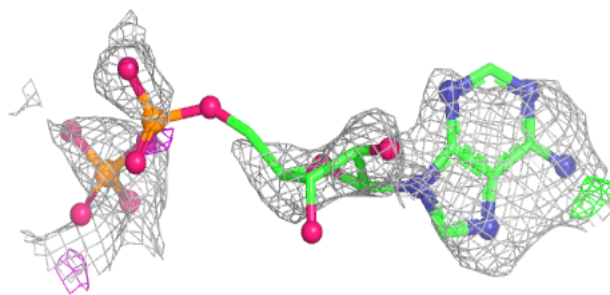
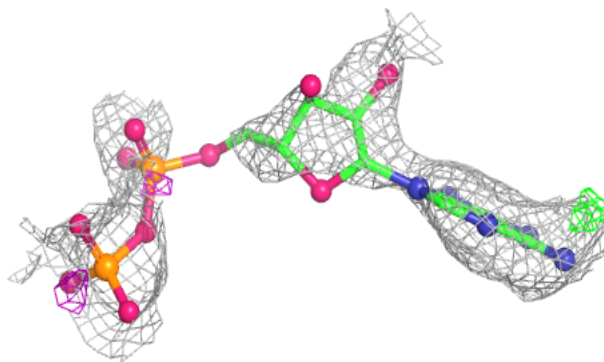
**Electron density around ADP G 4477:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

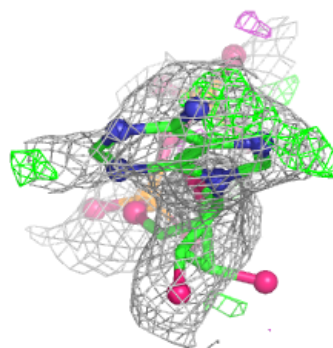
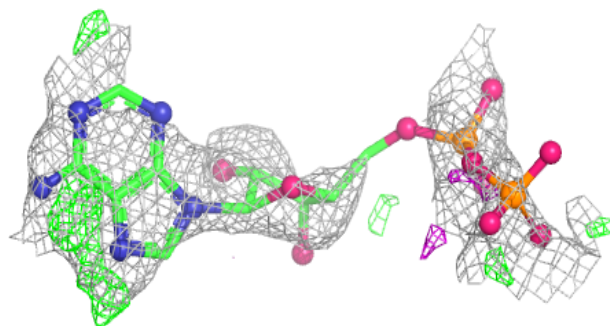
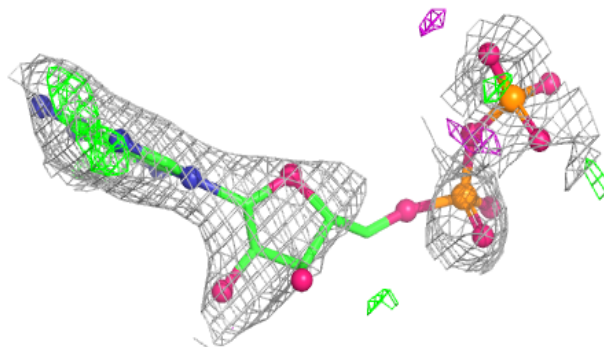


Electron density around ADP D 4474:

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

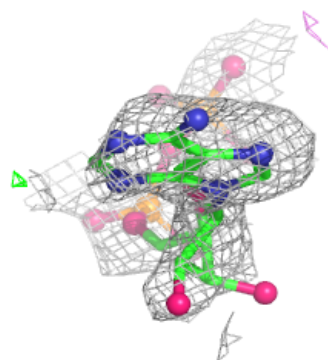
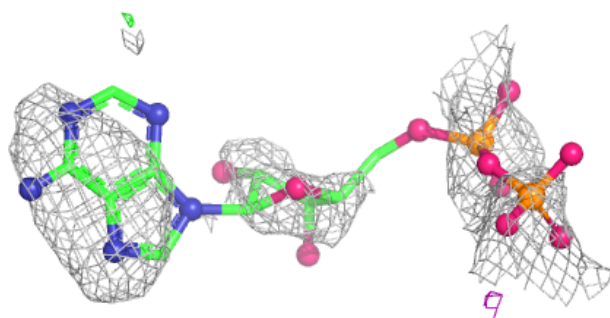
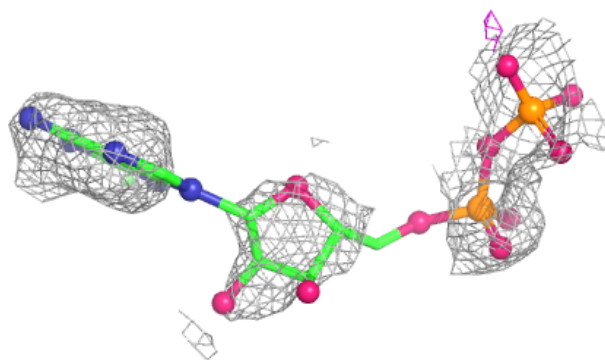
**Electron density around ADP J 4480:**

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



Electron density around ADP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.