



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:11 AM GMT

PDB ID : 1F1H
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM
SALMONELLA TYPHIMURIUM WITH THALLIUM IONS
Authors : Gill, H.S.; Eisenberg, D.
Deposited on : 2000-05-19
Resolution : 2.67 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

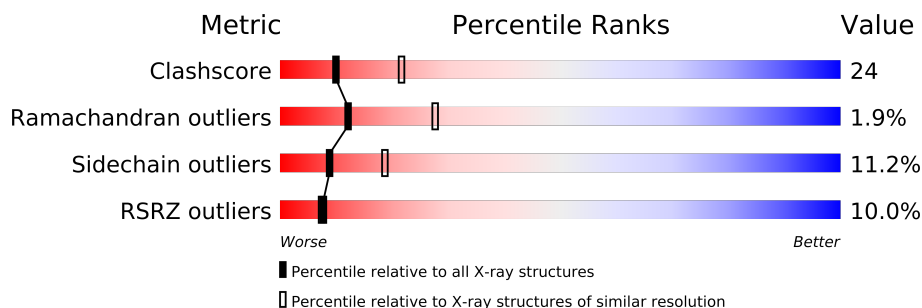
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.67 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	79885	2450 (2.70-2.66)
Ramachandran outliers	78287	2410 (2.70-2.66)
Sidechain outliers	78261	2410 (2.70-2.66)
RSRZ outliers	66119	2013 (2.70-2.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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	
1	H	468	
1	I	468	
1	J	468	
1	K	468	
1	L	468	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ADP	B	1472	-	X
3	ADP	D	1474	-	X
3	ADP	F	1476	-	X
3	ADP	I	1479	-	X
3	ADP	L	1482	-	X
5	MPD	A	1483	-	X
5	MPD	B	1484	-	X
5	MPD	C	1485	-	X
5	MPD	D	1486	-	X
5	MPD	E	1487	-	X
5	MPD	F	1488	-	X
5	MPD	G	1489	-	X
5	MPD	H	1490	-	X
5	MPD	I	1491	-	X
5	MPD	J	1492	-	X
5	MPD	K	1493	-	X
5	MPD	L	1494	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45564 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (GLUTAMINE SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	B	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	C	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	D	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	E	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	F	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	G	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	H	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	I	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	J	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	K	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	L	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

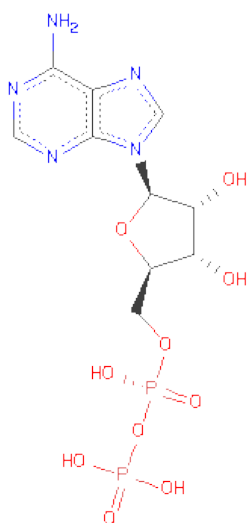
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 THALLIUM (I) ION (three-letter code: Tl) (formula: Tl).

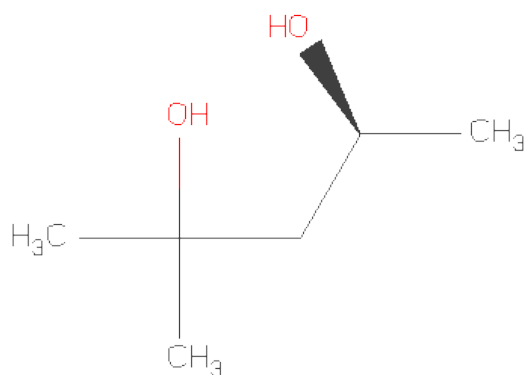
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Tl	0	0
			2	2		
4	J	2	Total	Tl	0	0
			2	2		
4	D	2	Total	Tl	0	0
			2	2		
4	K	2	Total	Tl	0	0
			2	2		
4	E	2	Total	Tl	0	0
			2	2		
4	H	2	Total	Tl	0	0
			2	2		
4	B	2	Total	Tl	0	0
			2	2		
4	I	2	Total	Tl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Tl 2	0	0
4	A	2	Total 2	Tl 2	0	0
4	L	2	Total 2	Tl 2	0	0
4	F	2	Total 2	Tl 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 8	C 6	O 2	0	0
5	B	1	Total 8	C 6	O 2	0	0
5	C	1	Total 8	C 6	O 2	0	0
5	D	1	Total 8	C 6	O 2	0	0
5	E	1	Total 8	C 6	O 2	0	0
5	F	1	Total 8	C 6	O 2	0	0
5	G	1	Total 8	C 6	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			8	6	2		
5	I	1	Total	C	O	0	0
			8	6	2		
5	J	1	Total	C	O	0	0
			8	6	2		
5	K	1	Total	C	O	0	0
			8	6	2		
5	L	1	Total	C	O	0	0
			8	6	2		

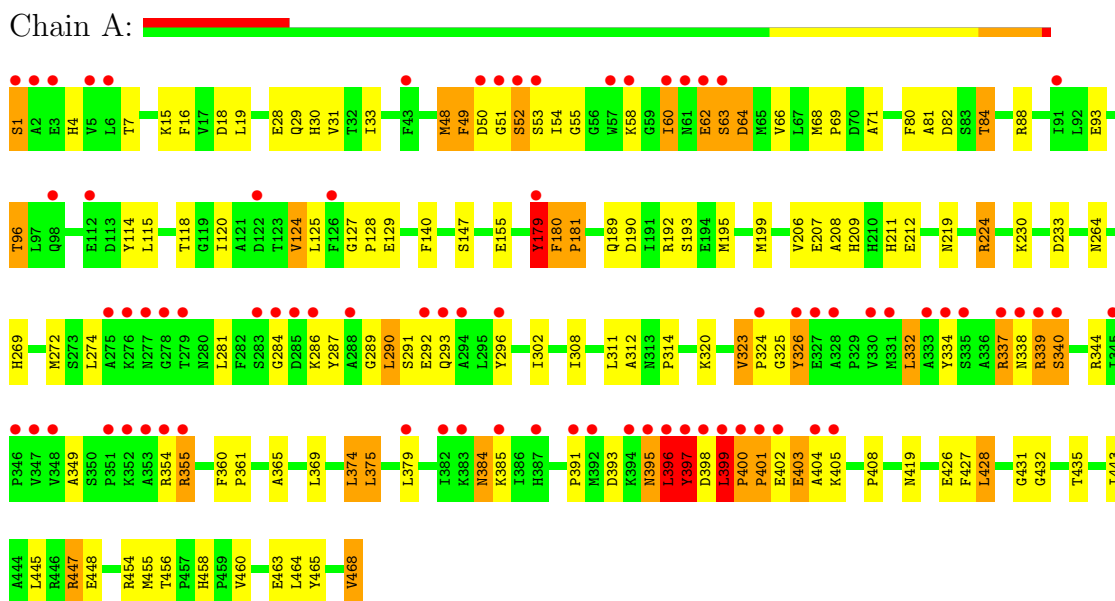
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	121	Total	O	0	0
			121	121		
6	C	119	Total	O	0	0
			119	119		
6	D	122	Total	O	0	0
			122	122		
6	E	122	Total	O	0	0
			122	122		
6	F	121	Total	O	0	0
			121	121		
6	G	122	Total	O	0	0
			122	122		
6	H	121	Total	O	0	0
			121	121		
6	I	122	Total	O	0	0
			122	122		
6	J	120	Total	O	0	0
			120	120		
6	K	123	Total	O	0	0
			123	123		
6	L	119	Total	O	0	0
			119	119		

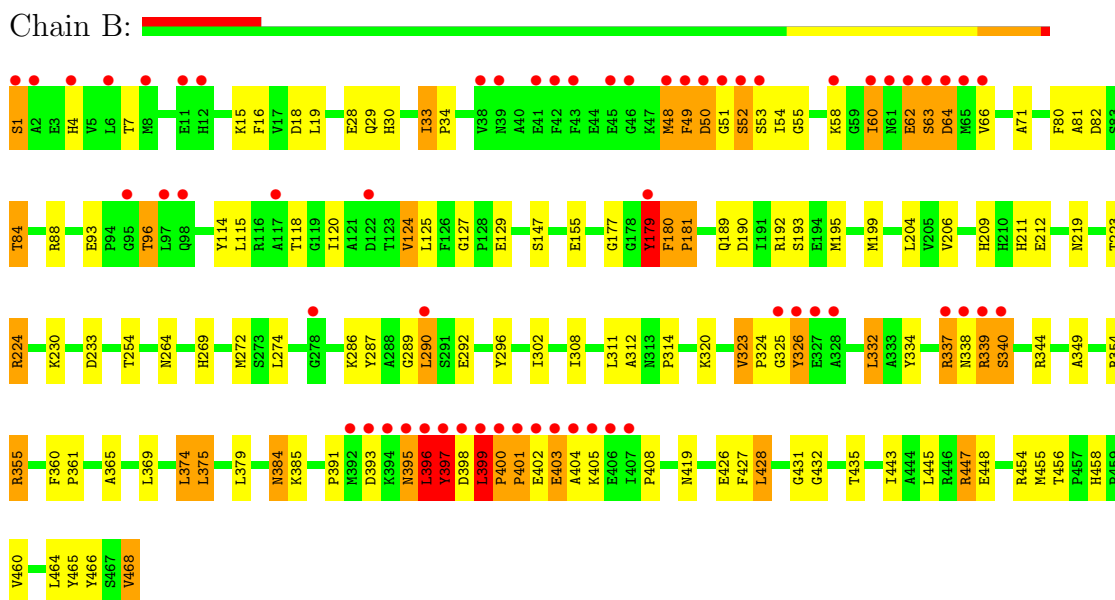
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: PROTEIN (GLUTAMINE SYNTHETASE)

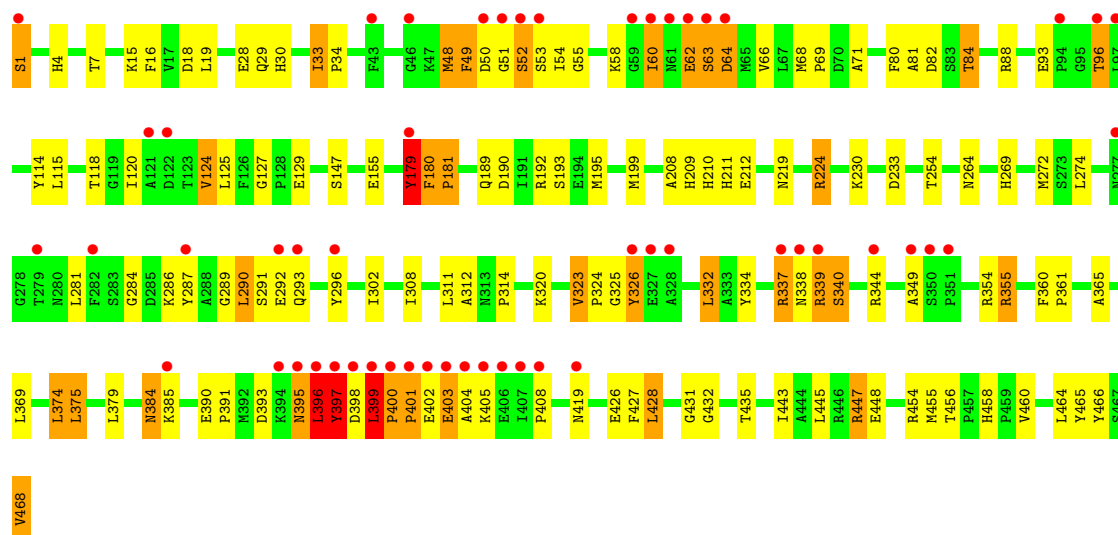


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



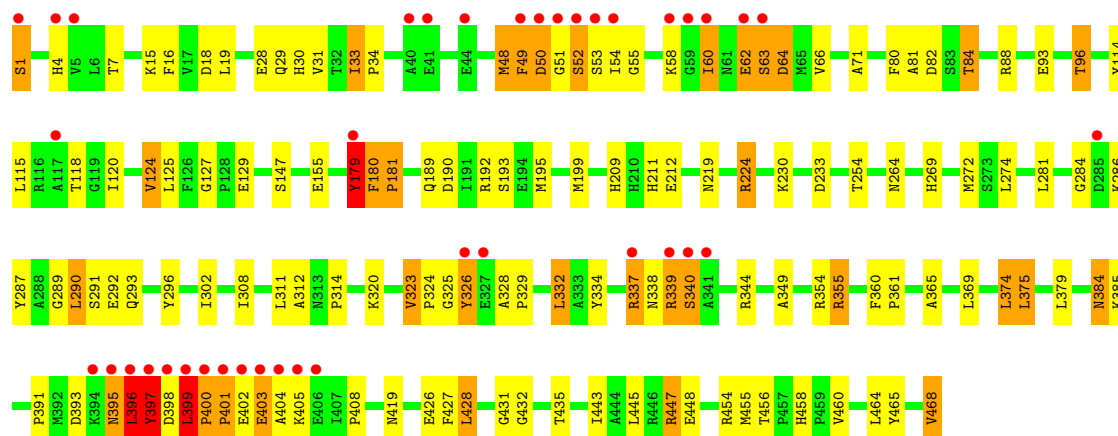
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain C: 



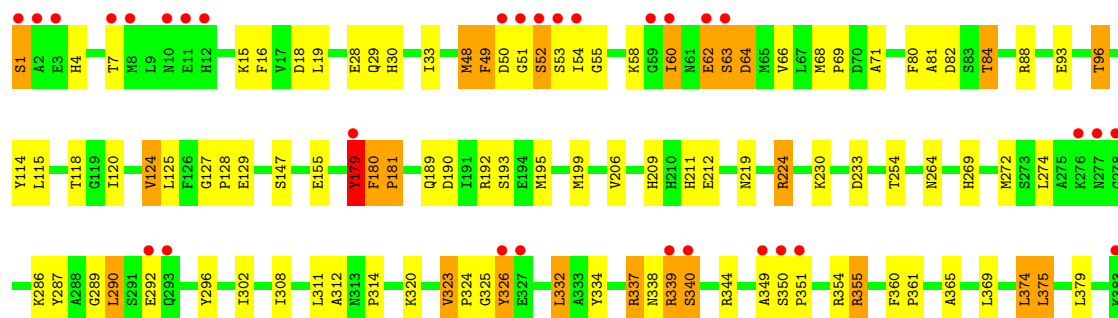
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

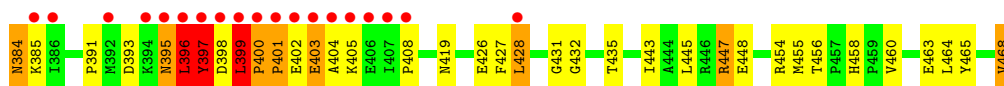
Chain D: 



• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

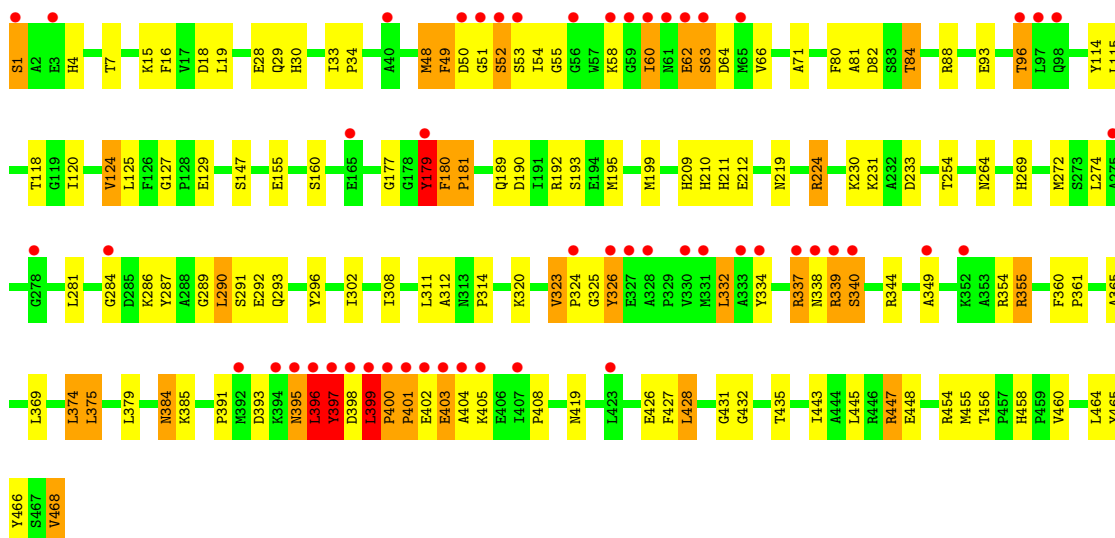
Chain E: 





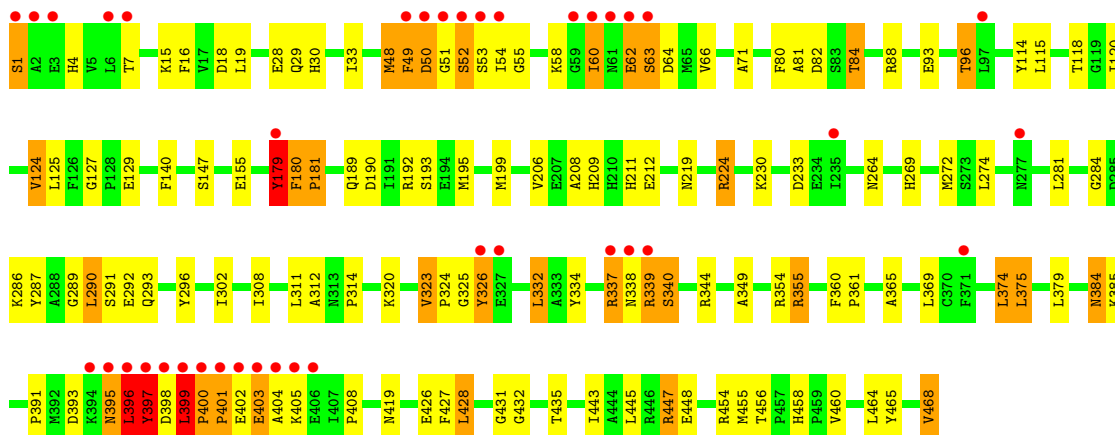
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain F:



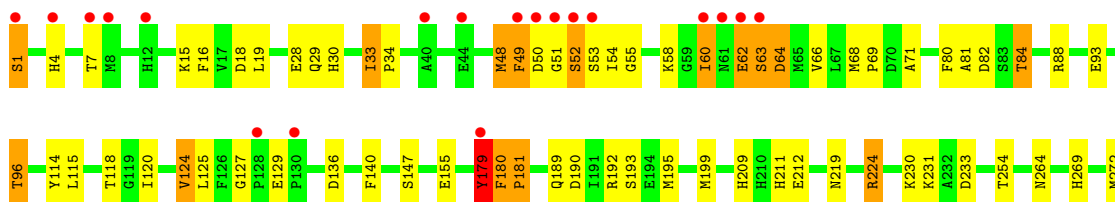
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

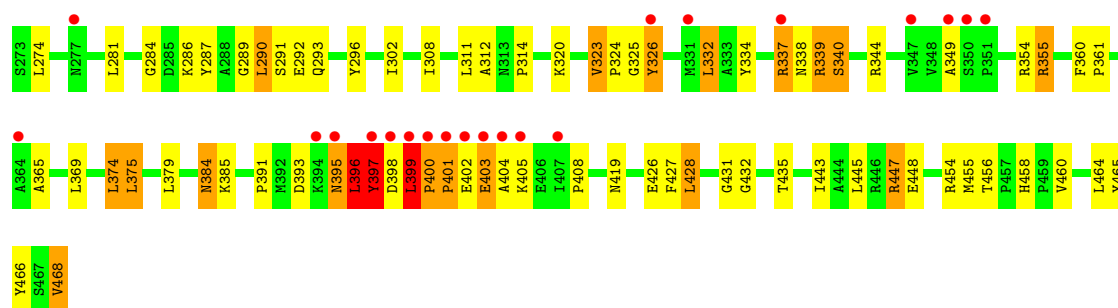
Chain G:



• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

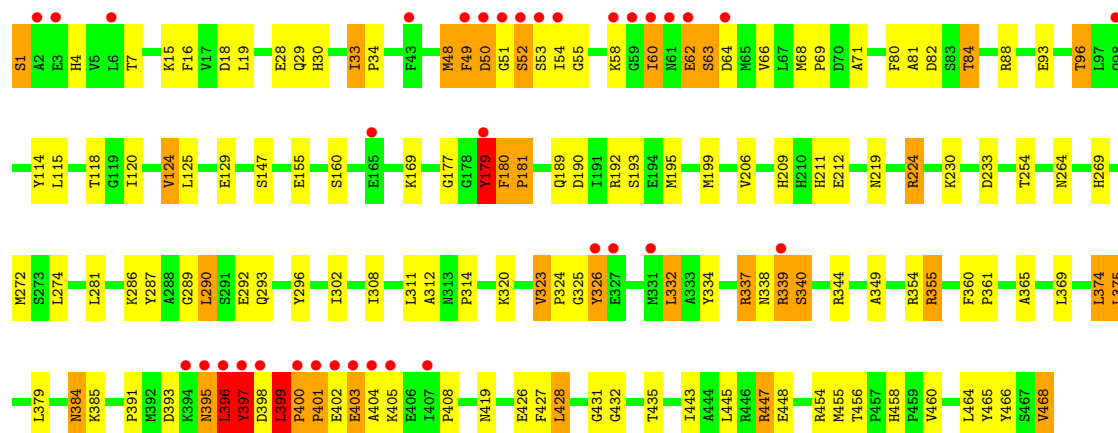
Chain H:





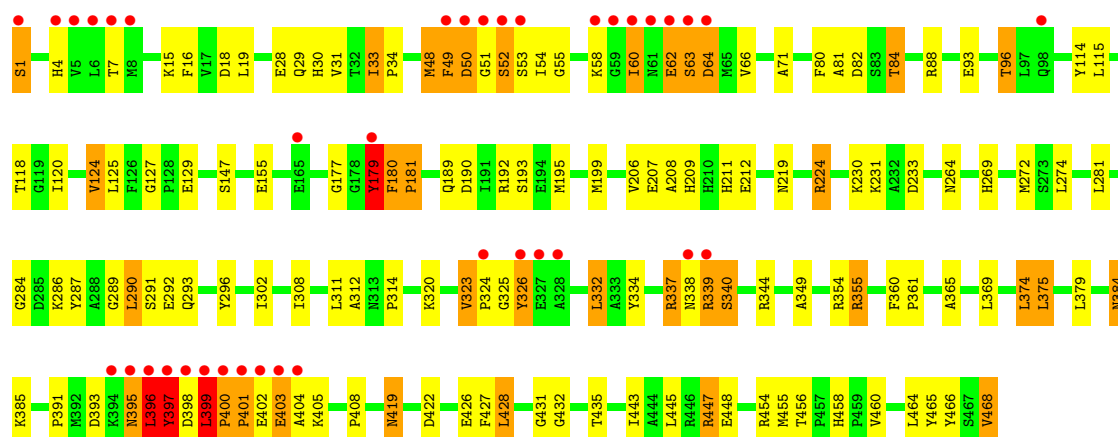
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain I:



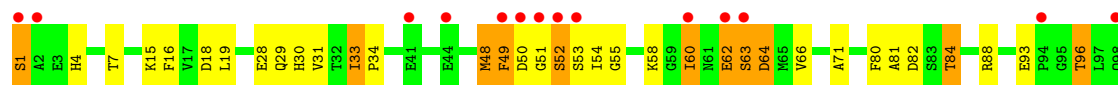
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

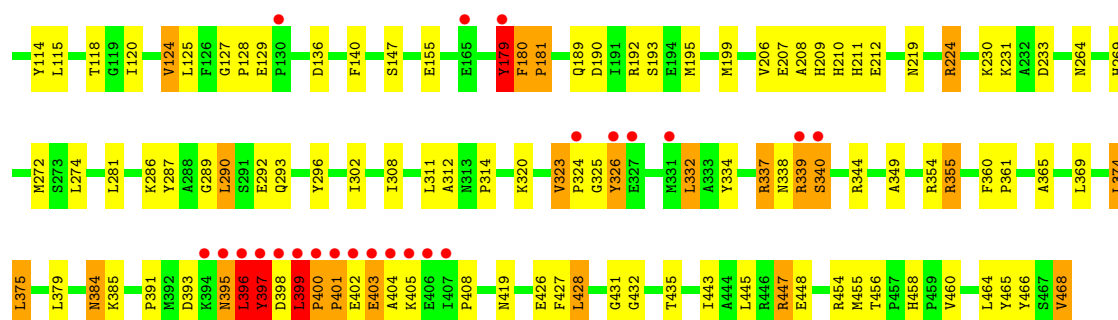
Chain J:



• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

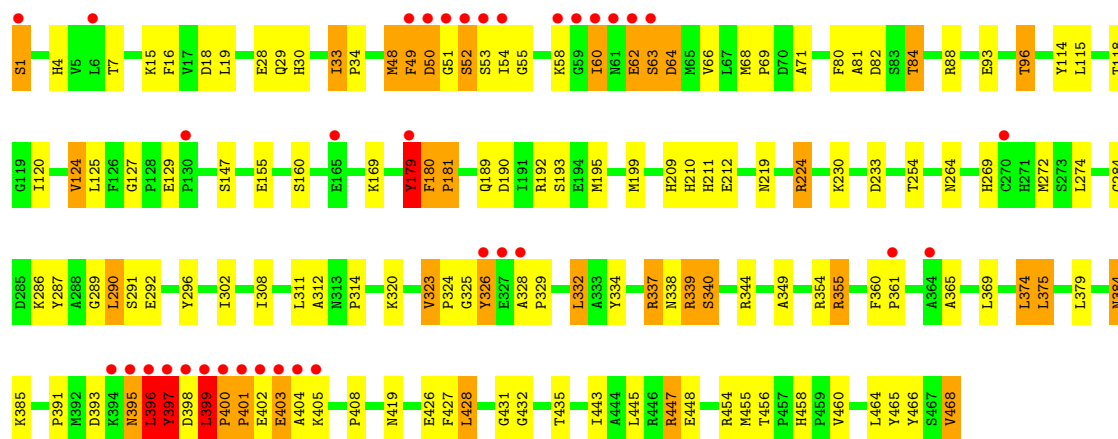
Chain K:





• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.13Å 132.79Å 196.78Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	32.00 – 2.67 36.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.0 (32.00-2.67) 82.0 (36.87-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.232 , 0.263 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 130547 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	45564	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, TL, 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	0.52	0/3724	0.85	4/5043 (0.1%)
1	B	0.52	0/3724	0.85	4/5043 (0.1%)
1	C	0.52	0/3724	0.85	4/5043 (0.1%)
1	D	0.52	0/3724	0.85	4/5043 (0.1%)
1	E	0.52	0/3724	0.85	4/5043 (0.1%)
1	F	0.52	0/3724	0.85	4/5043 (0.1%)
1	G	0.52	0/3724	0.85	4/5043 (0.1%)
1	H	0.52	0/3724	0.85	4/5043 (0.1%)
1	I	0.52	0/3724	0.85	4/5043 (0.1%)
1	J	0.52	0/3724	0.85	4/5043 (0.1%)
1	K	0.52	0/3724	0.85	4/5043 (0.1%)
1	L	0.52	0/3724	0.85	4/5043 (0.1%)
All	All	0.52	0/44688	0.85	48/60516 (0.1%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	TYR	CB-CG-CD1	6.17	124.70	121.00
1	K	179	TYR	CB-CG-CD1	6.14	124.69	121.00
1	J	179	TYR	CB-CG-CD1	6.12	124.67	121.00
1	D	179	TYR	CB-CG-CD1	6.11	124.67	121.00
1	I	179	TYR	CB-CG-CD1	6.10	124.66	121.00
1	B	179	TYR	CB-CG-CD1	6.10	124.66	121.00
1	L	179	TYR	CB-CG-CD1	6.09	124.66	121.00
1	A	179	TYR	CB-CG-CD1	6.08	124.65	121.00
1	C	179	TYR	CB-CG-CD1	6.05	124.63	121.00
1	H	179	TYR	CB-CG-CD1	6.04	124.62	121.00
1	E	179	TYR	CB-CG-CD1	6.02	124.61	121.00
1	G	179	TYR	CB-CG-CD1	5.96	124.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	J	179	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	I	179	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	K	179	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	E	179	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	F	399	LEU	O-C-N	5.44	131.44	121.10
1	D	179	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	B	179	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	K	399	LEU	O-C-N	5.43	131.41	121.10
1	A	179	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	399	LEU	O-C-N	5.42	131.39	121.10
1	E	399	LEU	O-C-N	5.42	131.39	121.10
1	H	179	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	J	399	LEU	O-C-N	5.42	131.39	121.10
1	B	399	LEU	O-C-N	5.42	131.39	121.10
1	L	399	LEU	O-C-N	5.42	131.39	121.10
1	H	399	LEU	O-C-N	5.41	131.38	121.10
1	D	399	LEU	O-C-N	5.40	131.37	121.10
1	C	399	LEU	O-C-N	5.40	131.37	121.10
1	I	399	LEU	O-C-N	5.39	131.35	121.10
1	G	399	LEU	O-C-N	5.39	131.35	121.10
1	C	179	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	L	179	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	G	179	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	F	397	TYR	CA-CB-CG	5.30	123.47	113.40
1	C	397	TYR	CA-CB-CG	5.30	123.46	113.40
1	I	397	TYR	CA-CB-CG	5.29	123.46	113.40
1	H	397	TYR	CA-CB-CG	5.29	123.45	113.40
1	J	397	TYR	CA-CB-CG	5.29	123.45	113.40
1	A	397	TYR	CA-CB-CG	5.29	123.45	113.40
1	E	397	TYR	CA-CB-CG	5.28	123.44	113.40
1	K	397	TYR	CA-CB-CG	5.28	123.44	113.40
1	B	397	TYR	CA-CB-CG	5.28	123.43	113.40
1	L	397	TYR	CA-CB-CG	5.28	123.42	113.40
1	D	397	TYR	CA-CB-CG	5.27	123.42	113.40
1	G	397	TYR	CA-CB-CG	5.27	123.41	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3637	0	3542	186	0
1	B	3637	0	3543	185	0
1	C	3637	0	3543	188	0
1	D	3637	0	3542	180	0
1	E	3637	0	3543	175	0
1	F	3637	0	3543	176	0
1	G	3637	0	3542	176	0
1	H	3637	0	3543	180	0
1	I	3637	0	3542	189	0
1	J	3637	0	3543	193	0
1	K	3637	0	3543	189	0
1	L	3637	0	3543	179	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	4	0
3	B	27	0	10	4	0
3	C	27	0	10	4	0
3	D	27	0	10	4	0
3	E	27	0	10	4	0
3	F	27	0	10	4	0
3	G	27	0	10	4	0
3	H	27	0	10	4	0
3	I	27	0	10	3	0
3	J	27	0	10	4	0
3	K	27	0	10	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	27	0	10	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	8	0	14	29	0
5	B	8	0	14	34	0
5	C	8	0	14	33	0
5	D	8	0	14	34	0
5	E	8	0	14	29	0
5	F	8	0	14	34	0
5	G	8	0	14	31	0
5	H	8	0	14	33	0
5	I	8	0	14	35	0
5	J	8	0	14	34	0
5	K	8	0	14	33	0
5	L	8	0	14	32	0
6	A	120	0	0	6	0
6	B	121	0	0	6	0
6	C	119	0	0	5	0
6	D	122	0	0	6	0
6	E	122	0	0	6	0
6	F	121	0	0	5	0
6	G	122	0	0	6	0
6	H	121	0	0	5	0
6	I	122	0	0	6	0
6	J	120	0	0	6	0
6	K	123	0	0	6	0
6	L	119	0	0	6	0
All	All	45564	0	42800	2077	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (2077) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:K:1481:ADP:C1'	3:K:1481:ADP:N9	1.71	1.54
3:I:1479:ADP:C1'	3:I:1479:ADP:N9	1.71	1.54
3:B:1472:ADP:C1'	3:B:1472:ADP:N9	1.71	1.52
3:F:1476:ADP:N9	3:F:1476:ADP:C1'	1.71	1.52
3:E:1475:ADP:N9	3:E:1475:ADP:C1'	1.71	1.51
3:H:1478:ADP:N9	3:H:1478:ADP:C1'	1.71	1.51
3:G:1477:ADP:N9	3:G:1477:ADP:C1'	1.71	1.51
3:C:1473:ADP:C1'	3:C:1473:ADP:N9	1.71	1.50
3:J:1480:ADP:C1'	3:J:1480:ADP:N9	1.71	1.50
3:D:1474:ADP:N9	3:D:1474:ADP:C1'	1.71	1.50
3:L:1482:ADP:C1'	3:L:1482:ADP:N9	1.71	1.49
3:A:1471:ADP:N9	3:A:1471:ADP:C1'	1.71	1.47
1:E:398:ASP:O	1:E:400:PRO:HD3	1.29	1.33
1:J:398:ASP:O	1:J:400:PRO:HD3	1.29	1.33
1:A:398:ASP:O	1:A:400:PRO:HD3	1.29	1.33
1:B:398:ASP:O	1:B:400:PRO:HD3	1.29	1.31
1:D:398:ASP:O	1:D:400:PRO:HD3	1.29	1.30
1:L:398:ASP:O	1:L:400:PRO:HD3	1.29	1.29
1:H:398:ASP:O	1:H:400:PRO:HD3	1.29	1.27
1:K:398:ASP:O	1:K:400:PRO:HD3	1.29	1.27
1:I:398:ASP:O	1:I:400:PRO:HD3	1.29	1.26
1:C:398:ASP:O	1:C:400:PRO:HD3	1.29	1.26
1:F:398:ASP:O	1:F:400:PRO:HD3	1.29	1.24
1:G:398:ASP:O	1:G:400:PRO:HD3	1.29	1.23
1:I:395:ASN:HB3	1:I:399:LEU:CD1	1.69	1.23
1:B:395:ASN:HB3	1:B:399:LEU:CD1	1.69	1.22
1:E:395:ASN:HB3	1:E:399:LEU:CD1	1.69	1.22
1:C:395:ASN:HB3	1:C:399:LEU:CD1	1.69	1.22
1:L:395:ASN:HB3	1:L:399:LEU:CD1	1.69	1.22
1:K:395:ASN:HB3	1:K:399:LEU:CD1	1.69	1.22
1:F:395:ASN:HB3	1:F:399:LEU:CD1	1.70	1.22
1:A:395:ASN:HB3	1:A:399:LEU:CD1	1.69	1.21
1:D:395:ASN:HB3	1:D:399:LEU:CD1	1.69	1.21
1:J:395:ASN:HB3	1:J:399:LEU:CD1	1.69	1.21
1:H:395:ASN:HB3	1:H:399:LEU:CD1	1.69	1.20
1:G:395:ASN:HB3	1:G:399:LEU:CD1	1.70	1.20
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.78	1.19
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.78	1.19
1:I:360:PHE:CD2	1:I:361:PRO:HD3	1.78	1.19
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.78	1.18
1:E:51:GLY:O	1:E:53:SER:N	1.76	1.18
1:L:51:GLY:O	1:L:53:SER:N	1.76	1.18
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.78	1.18

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:51:GLY:O	1:K:53:SER:N	1.76	1.18
1:L:360:PHE:CD2	1:L:361:PRO:HD3	1.78	1.18
1:I:51:GLY:O	1:I:53:SER:N	1.76	1.18
1:F:360:PHE:CD2	1:F:361:PRO:HD3	1.78	1.18
1:F:51:GLY:O	1:F:53:SER:N	1.77	1.18
1:H:51:GLY:O	1:H:53:SER:N	1.76	1.18
1:K:360:PHE:CD2	1:K:361:PRO:HD3	1.78	1.18
1:A:51:GLY:O	1:A:53:SER:N	1.76	1.18
1:B:51:GLY:O	1:B:53:SER:N	1.76	1.17
1:J:51:GLY:O	1:J:53:SER:N	1.76	1.17
1:G:51:GLY:O	1:G:53:SER:N	1.76	1.17
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.78	1.17
1:D:51:GLY:O	1:D:53:SER:N	1.77	1.17
1:G:360:PHE:CD2	1:G:361:PRO:HD3	1.78	1.17
1:J:360:PHE:CD2	1:J:361:PRO:HD3	1.78	1.17
1:C:51:GLY:O	1:C:53:SER:N	1.77	1.17
1:B:360:PHE:CD2	1:B:361:PRO:HD3	1.78	1.16
1:I:60:ILE:CG2	1:J:395:ASN:HD21	1.58	1.14
1:G:60:ILE:CG2	1:H:395:ASN:HD21	1.63	1.12
1:A:395:ASN:HD21	1:B:60:ILE:HG21	1.15	1.10
1:A:395:ASN:HD21	1:B:60:ILE:CG2	1.65	1.08
1:I:60:ILE:HG21	1:J:395:ASN:HD21	1.10	1.08
1:C:395:ASN:HD21	1:D:60:ILE:CG2	1.67	1.07
1:L:395:ASN:HB3	1:L:399:LEU:HD11	1.36	1.06
1:F:82:ASP:H	5:F:1488:MPD:C1	1.69	1.06
1:J:395:ASN:HB3	1:J:399:LEU:HD11	1.36	1.06
1:G:60:ILE:HG21	1:H:395:ASN:HD21	1.19	1.06
1:H:82:ASP:H	5:H:1490:MPD:C1	1.69	1.06
1:B:82:ASP:H	5:B:1484:MPD:C1	1.69	1.06
1:E:82:ASP:H	5:E:1487:MPD:C1	1.69	1.06
1:D:82:ASP:H	5:D:1486:MPD:C1	1.69	1.05
1:K:82:ASP:H	5:K:1493:MPD:C1	1.69	1.05
1:C:82:ASP:H	5:C:1485:MPD:C1	1.69	1.05
1:G:82:ASP:H	5:G:1489:MPD:C1	1.69	1.05
1:H:395:ASN:HB3	1:H:399:LEU:HD11	1.36	1.05
1:C:395:ASN:HD21	1:D:60:ILE:HG21	1.20	1.05
1:B:395:ASN:HB3	1:B:399:LEU:HD11	1.36	1.05
1:J:82:ASP:H	5:J:1492:MPD:C1	1.69	1.05
1:I:395:ASN:HB3	1:I:399:LEU:HD11	1.36	1.04
1:I:82:ASP:H	5:I:1491:MPD:C1	1.69	1.04
1:L:82:ASP:H	5:L:1494:MPD:C1	1.69	1.04
1:D:395:ASN:HB3	1:D:399:LEU:HD11	1.36	1.04

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:ASP:H	5:A:1483:MPD:C1	1.69	1.04
1:C:395:ASN:HB3	1:C:399:LEU:HD11	1.36	1.03
1:F:395:ASN:HB3	1:F:399:LEU:HD11	1.36	1.03
1:A:395:ASN:HB3	1:A:399:LEU:HD11	1.36	1.03
1:K:395:ASN:HB3	1:K:399:LEU:HD11	1.36	1.03
1:G:395:ASN:HB3	1:G:399:LEU:HD11	1.36	1.02
1:E:395:ASN:HB3	1:E:399:LEU:HD11	1.36	1.02
1:J:60:ILE:CG2	1:K:395:ASN:HD21	1.74	1.00
1:K:51:GLY:C	1:K:53:SER:H	1.64	1.00
1:H:51:GLY:C	1:H:53:SER:H	1.65	0.99
1:J:51:GLY:C	1:J:53:SER:H	1.64	0.99
1:I:51:GLY:C	1:I:53:SER:H	1.65	0.97
1:E:51:GLY:C	1:E:53:SER:H	1.65	0.97
1:D:395:ASN:HD21	1:E:60:ILE:CG2	1.77	0.97
1:B:51:GLY:C	1:B:53:SER:H	1.65	0.97
1:L:51:GLY:C	1:L:53:SER:H	1.65	0.96
1:D:51:GLY:C	1:D:53:SER:H	1.64	0.95
1:G:395:ASN:HD21	1:L:60:ILE:HG21	1.28	0.95
1:A:51:GLY:C	1:A:53:SER:H	1.65	0.95
1:C:51:GLY:C	1:C:53:SER:H	1.65	0.94
5:H:1490:MPD:H32	1:I:193:SER:CB	1.97	0.94
1:C:82:ASP:O	1:C:84:THR:HG22	1.68	0.94
1:A:82:ASP:O	1:A:84:THR:HG22	1.68	0.94
1:E:82:ASP:O	1:E:84:THR:HG22	1.68	0.94
1:J:82:ASP:O	1:J:84:THR:HG22	1.68	0.94
1:G:82:ASP:O	1:G:84:THR:HG22	1.68	0.94
1:C:80:PHE:HB3	5:C:1485:MPD:H11	1.50	0.94
1:I:82:ASP:O	1:I:84:THR:HG22	1.68	0.94
1:L:82:ASP:O	1:L:84:THR:HG22	1.68	0.94
1:K:80:PHE:HB3	5:K:1493:MPD:H11	1.50	0.94
1:J:60:ILE:HG21	1:K:395:ASN:HD21	1.32	0.93
1:A:80:PHE:HB3	5:A:1483:MPD:H11	1.50	0.93
1:D:395:ASN:HD21	1:E:60:ILE:HG21	1.33	0.93
1:I:80:PHE:HB3	5:I:1491:MPD:H11	1.50	0.93
1:F:80:PHE:HB3	5:F:1488:MPD:H11	1.50	0.93
1:K:82:ASP:O	1:K:84:THR:HG22	1.68	0.93
1:D:80:PHE:HB3	5:D:1486:MPD:H11	1.50	0.93
1:H:80:PHE:HB3	5:H:1490:MPD:H11	1.50	0.93
1:J:80:PHE:HB3	5:J:1492:MPD:H11	1.50	0.93
1:A:395:ASN:HB3	1:A:399:LEU:HD12	1.50	0.93
1:L:395:ASN:HB3	1:L:399:LEU:HD12	1.50	0.92
1:C:395:ASN:HB3	1:C:399:LEU:HD12	1.50	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:82:ASP:O	1:H:84:THR:HG22	1.68	0.92
1:G:80:PHE:HB3	5:G:1489:MPD:H11	1.50	0.92
1:C:52:SER:HB3	1:C:63:SER:HB3	1.51	0.92
1:F:82:ASP:O	1:F:84:THR:HG22	1.68	0.92
1:E:80:PHE:HB3	5:E:1487:MPD:H11	1.50	0.92
1:I:395:ASN:HB3	1:I:399:LEU:HD12	1.50	0.92
1:J:52:SER:HB3	1:J:63:SER:HB3	1.51	0.92
1:E:52:SER:HB3	1:E:63:SER:HB3	1.51	0.92
1:B:82:ASP:O	1:B:84:THR:HG22	1.68	0.92
1:A:52:SER:HB3	1:A:63:SER:HB3	1.51	0.92
5:J:1492:MPD:H32	1:K:193:SER:CB	1.99	0.92
1:L:52:SER:HB3	1:L:63:SER:HB3	1.51	0.92
1:H:52:SER:HB3	1:H:63:SER:HB3	1.51	0.92
1:L:80:PHE:HB3	5:L:1494:MPD:H11	1.50	0.92
1:C:1:SER:HA	1:C:71:ALA:CB	2.00	0.92
1:C:82:ASP:H	5:C:1485:MPD:H13	1.34	0.92
1:G:82:ASP:H	5:G:1489:MPD:H13	1.34	0.92
1:D:1:SER:HA	1:D:71:ALA:CB	2.00	0.92
1:L:1:SER:HA	1:L:71:ALA:CB	2.00	0.92
1:H:1:SER:HA	1:H:71:ALA:CB	2.00	0.92
1:D:82:ASP:O	1:D:84:THR:HG22	1.68	0.91
1:K:1:SER:HA	1:K:71:ALA:CB	2.00	0.91
1:K:395:ASN:HB3	1:K:399:LEU:HD12	1.50	0.91
1:D:395:ASN:HB3	1:D:399:LEU:HD12	1.50	0.91
1:F:1:SER:HA	1:F:71:ALA:CB	2.00	0.91
1:G:395:ASN:HD21	1:L:60:ILE:CG2	1.82	0.91
1:B:395:ASN:HB3	1:B:399:LEU:HD12	1.50	0.91
1:H:395:ASN:HB3	1:H:399:LEU:HD12	1.50	0.91
1:F:395:ASN:HB3	1:F:399:LEU:HD12	1.50	0.91
1:B:52:SER:HB3	1:B:63:SER:HB3	1.51	0.91
1:G:51:GLY:C	1:G:53:SER:H	1.65	0.91
1:B:80:PHE:HB3	5:B:1484:MPD:H11	1.50	0.91
1:I:1:SER:HA	1:I:71:ALA:CB	2.00	0.91
1:J:395:ASN:HB3	1:J:399:LEU:HD12	1.50	0.91
1:K:52:SER:HB3	1:K:63:SER:HB3	1.51	0.91
1:F:51:GLY:C	1:F:53:SER:H	1.65	0.91
5:I:1491:MPD:H32	1:J:193:SER:CB	2.00	0.91
1:L:82:ASP:H	5:L:1494:MPD:H13	1.34	0.91
1:B:1:SER:HA	1:B:71:ALA:CB	2.00	0.91
1:J:1:SER:HA	1:J:71:ALA:CB	2.00	0.91
1:B:82:ASP:H	5:B:1484:MPD:H13	1.34	0.91
1:D:52:SER:HB3	1:D:63:SER:HB3	1.51	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:193:SER:CB	5:C:1485:MPD:H32	2.00	0.90
1:A:1:SER:HA	1:A:71:ALA:CB	2.00	0.90
1:G:52:SER:HB3	1:G:63:SER:HB3	1.51	0.90
1:H:82:ASP:H	5:H:1490:MPD:H13	1.34	0.90
1:D:82:ASP:H	5:D:1486:MPD:H13	1.34	0.90
1:E:1:SER:HA	1:E:71:ALA:CB	2.00	0.90
1:G:395:ASN:HB3	1:G:399:LEU:HD12	1.50	0.90
1:G:1:SER:HA	1:G:71:ALA:CB	2.00	0.90
1:G:193:SER:CB	5:L:1494:MPD:H32	2.02	0.90
1:F:458:HIS:HD2	1:F:460:VAL:H	1.20	0.90
1:E:458:HIS:HD2	1:E:460:VAL:H	1.20	0.89
1:F:82:ASP:H	5:F:1488:MPD:H13	1.34	0.89
1:J:458:HIS:HD2	1:J:460:VAL:H	1.20	0.89
1:C:458:HIS:HD2	1:C:460:VAL:H	1.20	0.89
1:E:395:ASN:HB3	1:E:399:LEU:HD12	1.50	0.89
1:E:193:SER:CB	5:F:1488:MPD:H32	2.01	0.89
1:A:82:ASP:H	5:A:1483:MPD:H13	1.34	0.89
1:A:60:ILE:CG2	1:F:395:ASN:HD21	1.85	0.89
1:J:82:ASP:H	5:J:1492:MPD:H13	1.34	0.89
1:E:82:ASP:H	5:E:1487:MPD:H13	1.34	0.89
1:K:82:ASP:H	5:K:1493:MPD:H13	1.34	0.89
1:I:82:ASP:H	5:I:1491:MPD:H13	1.34	0.89
1:H:458:HIS:HD2	1:H:460:VAL:H	1.20	0.89
1:L:458:HIS:HD2	1:L:460:VAL:H	1.20	0.89
1:G:458:HIS:HD2	1:G:460:VAL:H	1.20	0.89
1:I:52:SER:HB3	1:I:63:SER:HB3	1.51	0.89
1:B:458:HIS:HD2	1:B:460:VAL:H	1.20	0.89
1:D:401:PRO:HB3	1:D:404:ALA:HA	1.56	0.88
1:F:52:SER:HB3	1:F:63:SER:HB3	1.51	0.88
1:A:401:PRO:HB3	1:A:404:ALA:HA	1.56	0.88
1:I:401:PRO:HB3	1:I:404:ALA:HA	1.56	0.87
1:K:401:PRO:HB3	1:K:404:ALA:HA	1.56	0.87
1:I:458:HIS:HD2	1:I:460:VAL:H	1.20	0.87
1:A:193:SER:CB	5:B:1484:MPD:H32	2.05	0.87
1:K:458:HIS:HD2	1:K:460:VAL:H	1.20	0.87
1:B:401:PRO:HB3	1:B:404:ALA:HA	1.56	0.86
1:B:395:ASN:HD21	1:C:60:ILE:CG2	1.88	0.86
5:H:1490:MPD:HM3	1:I:190:ASP:OD2	1.75	0.86
1:D:458:HIS:HD2	1:D:460:VAL:H	1.20	0.86
1:G:401:PRO:HB3	1:G:404:ALA:HA	1.56	0.86
1:H:401:PRO:HB3	1:H:404:ALA:HA	1.56	0.86
1:C:401:PRO:HB3	1:C:404:ALA:HA	1.56	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:401:PRO:HB3	1:E:404:ALA:HA	1.56	0.86
1:L:401:PRO:HB3	1:L:404:ALA:HA	1.56	0.86
1:G:190:ASP:OD2	5:L:1494:MPD:HM3	1.76	0.85
1:A:458:HIS:HD2	1:A:460:VAL:H	1.20	0.85
1:A:224:ARG:HG2	1:A:224:ARG:HH21	1.41	0.85
1:L:224:ARG:HG2	1:L:224:ARG:HH21	1.41	0.85
1:H:224:ARG:HH21	1:H:224:ARG:HG2	1.41	0.85
5:K:1493:MPD:HM3	1:L:190:ASP:OD2	1.74	0.85
1:J:401:PRO:HB3	1:J:404:ALA:HA	1.56	0.85
1:J:16:PHE:CD1	5:J:1492:MPD:H52	2.12	0.85
1:F:16:PHE:CD1	5:F:1488:MPD:H52	2.12	0.85
1:E:16:PHE:CD1	5:E:1487:MPD:H52	2.12	0.85
1:L:16:PHE:CD1	5:L:1494:MPD:H52	2.12	0.85
1:B:224:ARG:HH21	1:B:224:ARG:HG2	1.42	0.85
1:F:224:ARG:HH21	1:F:224:ARG:HG2	1.41	0.85
1:I:60:ILE:HG21	1:J:395:ASN:ND2	1.89	0.85
1:I:398:ASP:O	1:I:400:PRO:CD	2.22	0.85
1:D:16:PHE:CD1	5:D:1486:MPD:H52	2.12	0.85
1:B:16:PHE:CD1	5:B:1484:MPD:H52	2.12	0.85
1:G:224:ARG:HG2	1:G:224:ARG:HH21	1.41	0.85
1:E:224:ARG:HG2	1:E:224:ARG:HH21	1.41	0.85
1:C:224:ARG:HH21	1:C:224:ARG:HG2	1.41	0.84
1:F:398:ASP:O	1:F:400:PRO:CD	2.22	0.84
1:G:16:PHE:CD1	5:G:1489:MPD:H52	2.12	0.84
1:J:224:ARG:HH21	1:J:224:ARG:HG2	1.42	0.84
1:H:16:PHE:CD1	5:H:1490:MPD:H52	2.12	0.84
1:C:16:PHE:CD1	5:C:1485:MPD:H52	2.12	0.84
1:D:224:ARG:HH21	1:D:224:ARG:HG2	1.42	0.84
1:A:398:ASP:O	1:A:400:PRO:CD	2.22	0.84
1:F:401:PRO:HB3	1:F:404:ALA:HA	1.56	0.84
1:J:51:GLY:C	1:J:53:SER:N	2.26	0.84
1:K:16:PHE:CD1	5:K:1493:MPD:H52	2.12	0.84
1:A:16:PHE:CD1	5:A:1483:MPD:H52	2.12	0.84
1:I:224:ARG:HG2	1:I:224:ARG:HH21	1.41	0.84
1:E:51:GLY:C	1:E:53:SER:N	2.26	0.83
1:A:60:ILE:HG21	1:F:395:ASN:HD21	1.39	0.83
1:I:16:PHE:CD1	5:I:1491:MPD:H52	2.12	0.83
1:E:398:ASP:O	1:E:400:PRO:CD	2.22	0.83
1:L:51:GLY:C	1:L:53:SER:N	2.26	0.83
1:K:398:ASP:O	1:K:400:PRO:CD	2.22	0.83
1:K:224:ARG:HH21	1:K:224:ARG:HG2	1.41	0.83
1:L:398:ASP:O	1:L:400:PRO:CD	2.22	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:82:ASP:H	5:H:1490:MPD:H12	1.44	0.83
5:A:1483:MPD:HM3	1:F:190:ASP:OD2	1.78	0.83
1:B:398:ASP:O	1:B:400:PRO:CD	2.22	0.83
1:A:395:ASN:ND2	1:B:60:ILE:HG21	1.94	0.82
1:A:82:ASP:H	5:A:1483:MPD:H12	1.44	0.82
1:J:398:ASP:O	1:J:400:PRO:CD	2.22	0.82
1:G:398:ASP:O	1:G:400:PRO:CD	2.22	0.82
5:H:1490:MPD:H32	1:I:193:SER:HB2	1.61	0.82
1:E:323:VAL:HG21	1:K:455:MET:HG2	1.60	0.82
1:D:398:ASP:O	1:D:400:PRO:CD	2.22	0.82
5:K:1493:MPD:H32	1:L:193:SER:CB	2.08	0.82
1:K:340:SER:HB3	1:K:396:LEU:HB3	1.62	0.82
1:G:340:SER:HB3	1:G:396:LEU:HB3	1.62	0.81
1:A:340:SER:HB3	1:A:396:LEU:HB3	1.62	0.81
1:D:395:ASN:CB	1:D:399:LEU:HD11	2.11	0.81
1:G:395:ASN:CB	1:G:399:LEU:HD11	2.11	0.81
1:A:81:ALA:N	5:A:1483:MPD:H13	1.96	0.81
1:E:340:SER:HB3	1:E:396:LEU:HB3	1.62	0.81
1:K:395:ASN:CB	1:K:399:LEU:HD11	2.10	0.81
1:C:81:ALA:N	5:C:1485:MPD:H13	1.96	0.81
5:J:1492:MPD:O2	1:K:190:ASP:HA	1.80	0.81
1:J:81:ALA:N	5:J:1492:MPD:H13	1.96	0.81
1:I:82:ASP:H	5:I:1491:MPD:H12	1.44	0.81
1:L:82:ASP:H	5:L:1494:MPD:H12	1.44	0.81
1:A:395:ASN:CB	1:A:399:LEU:HD11	2.10	0.81
1:E:81:ALA:N	5:E:1487:MPD:H13	1.96	0.81
1:K:81:ALA:N	5:K:1493:MPD:H13	1.96	0.81
1:G:82:ASP:H	5:G:1489:MPD:H12	1.44	0.81
1:J:395:ASN:CB	1:J:399:LEU:HD11	2.10	0.81
1:E:190:ASP:HA	5:F:1488:MPD:O2	1.81	0.81
1:H:81:ALA:N	5:H:1490:MPD:H13	1.96	0.81
1:K:82:ASP:H	5:K:1493:MPD:H12	1.44	0.81
1:L:340:SER:HB3	1:L:396:LEU:HB3	1.62	0.81
1:H:340:SER:HB3	1:H:396:LEU:HB3	1.62	0.81
1:I:81:ALA:N	5:I:1491:MPD:H13	1.96	0.81
1:H:395:ASN:CB	1:H:399:LEU:HD11	2.10	0.81
1:J:82:ASP:H	5:J:1492:MPD:H12	1.44	0.81
1:H:398:ASP:O	1:H:400:PRO:CD	2.22	0.81
1:I:395:ASN:CB	1:I:399:LEU:HD11	2.10	0.81
1:F:395:ASN:CB	1:F:399:LEU:HD11	2.10	0.81
5:J:1492:MPD:H32	1:K:193:SER:HB2	1.62	0.81
1:F:455:MET:HG2	1:L:323:VAL:HG21	1.62	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:395:ASN:CB	1:C:399:LEU:HD11	2.10	0.81
1:C:398:ASP:O	1:C:400:PRO:CD	2.22	0.80
1:C:193:SER:CB	5:D:1486:MPD:H32	2.10	0.80
1:L:81:ALA:N	5:L:1494:MPD:H13	1.96	0.80
1:F:82:ASP:H	5:F:1488:MPD:H12	1.44	0.80
1:L:395:ASN:CB	1:L:399:LEU:HD11	2.10	0.80
1:C:340:SER:HB3	1:C:396:LEU:HB3	1.62	0.80
1:D:82:ASP:H	5:D:1486:MPD:H12	1.44	0.80
1:C:190:ASP:OD2	5:D:1486:MPD:HM3	1.81	0.80
1:B:395:ASN:CB	1:B:399:LEU:HD11	2.10	0.80
1:F:340:SER:HB3	1:F:396:LEU:HB3	1.62	0.80
1:F:81:ALA:N	5:F:1488:MPD:H13	1.96	0.80
1:B:81:ALA:N	5:B:1484:MPD:H13	1.96	0.80
1:G:190:ASP:HA	5:L:1494:MPD:O2	1.81	0.80
1:I:340:SER:HB3	1:I:396:LEU:HB3	1.62	0.80
1:B:340:SER:HB3	1:B:396:LEU:HB3	1.62	0.80
1:D:340:SER:HB3	1:D:396:LEU:HB3	1.62	0.80
1:F:402:GLU:HB2	1:F:405:LYS:HD3	1.64	0.80
1:E:82:ASP:H	5:E:1487:MPD:H12	1.44	0.80
1:D:81:ALA:N	5:D:1486:MPD:H13	1.96	0.80
1:C:82:ASP:H	5:C:1485:MPD:H12	1.44	0.79
1:G:193:SER:HB2	5:L:1494:MPD:H32	1.62	0.79
1:L:402:GLU:HB2	1:L:405:LYS:HD3	1.64	0.79
1:A:402:GLU:HB2	1:A:405:LYS:HD3	1.64	0.79
1:B:82:ASP:H	5:B:1484:MPD:H12	1.44	0.79
1:E:395:ASN:CB	1:E:399:LEU:HD11	2.10	0.79
1:J:340:SER:HB3	1:J:396:LEU:HB3	1.62	0.79
1:G:81:ALA:N	5:G:1489:MPD:H13	1.96	0.79
1:G:402:GLU:HB2	1:G:405:LYS:HD3	1.64	0.78
1:A:323:VAL:HG21	1:G:455:MET:HG2	1.64	0.78
1:I:60:ILE:CG2	1:J:395:ASN:ND2	2.42	0.78
1:A:51:GLY:C	1:A:53:SER:N	2.26	0.78
1:J:402:GLU:HB2	1:J:405:LYS:HD3	1.64	0.78
1:K:402:GLU:HB2	1:K:405:LYS:HD3	1.64	0.78
1:L:52:SER:CB	1:L:63:SER:HB3	2.13	0.78
5:I:1491:MPD:H32	1:J:193:SER:HB2	1.65	0.78
1:K:60:ILE:CG2	1:L:395:ASN:HD21	1.96	0.78
1:K:52:SER:CB	1:K:63:SER:HB3	2.13	0.78
1:J:52:SER:CB	1:J:63:SER:HB3	2.13	0.78
1:D:52:SER:CB	1:D:63:SER:HB3	2.13	0.78
1:B:52:SER:CB	1:B:63:SER:HB3	2.13	0.78
1:H:60:ILE:CG2	1:I:395:ASN:HD21	1.96	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:395:ASN:CB	1:H:399:LEU:CD1	2.60	0.78
1:I:402:GLU:HB2	1:I:405:LYS:HD3	1.64	0.78
1:K:51:GLY:C	1:K:53:SER:N	2.26	0.78
1:I:52:SER:CB	1:I:63:SER:HB3	2.13	0.78
1:B:190:ASP:HA	5:C:1485:MPD:O2	1.84	0.77
1:K:1:SER:HA	1:K:71:ALA:HB1	1.66	0.77
1:C:402:GLU:HB2	1:C:405:LYS:HD3	1.64	0.77
1:D:402:GLU:HB2	1:D:405:LYS:HD3	1.64	0.77
1:E:402:GLU:HB2	1:E:405:LYS:HD3	1.64	0.77
1:F:395:ASN:CB	1:F:399:LEU:CD1	2.60	0.77
1:G:52:SER:CB	1:G:63:SER:HB3	2.13	0.77
5:J:1492:MPD:HM3	1:K:190:ASP:OD2	1.82	0.77
1:A:1:SER:HA	1:A:71:ALA:HB1	1.66	0.77
1:E:395:ASN:HD21	1:F:60:ILE:CG2	1.98	0.77
1:F:52:SER:CB	1:F:63:SER:HB3	2.13	0.77
1:F:1:SER:HA	1:F:71:ALA:HB1	1.66	0.77
1:B:395:ASN:HD21	1:C:60:ILE:HG21	1.48	0.77
1:B:402:GLU:HB2	1:B:405:LYS:HD3	1.64	0.77
1:B:323:VAL:HG21	1:H:455:MET:HG2	1.66	0.77
1:H:52:SER:CB	1:H:63:SER:HB3	2.13	0.77
1:A:52:SER:CB	1:A:63:SER:HB3	2.13	0.77
1:B:51:GLY:C	1:B:53:SER:N	2.26	0.77
1:H:1:SER:HA	1:H:71:ALA:HB1	1.66	0.77
1:H:402:GLU:HB2	1:H:405:LYS:HD3	1.64	0.77
1:I:1:SER:HA	1:I:71:ALA:HB3	1.67	0.77
1:A:190:ASP:HA	5:B:1484:MPD:O2	1.84	0.77
1:E:1:SER:HA	1:E:71:ALA:HB1	1.66	0.77
1:I:1:SER:HA	1:I:71:ALA:HB1	1.66	0.77
1:J:395:ASN:CB	1:J:399:LEU:CD1	2.60	0.77
1:E:52:SER:CB	1:E:63:SER:HB3	2.13	0.77
1:B:1:SER:HA	1:B:71:ALA:HB3	1.67	0.77
1:L:1:SER:HA	1:L:71:ALA:HB3	1.67	0.76
1:J:1:SER:HA	1:J:71:ALA:HB1	1.66	0.76
1:G:1:SER:HA	1:G:71:ALA:HB3	1.67	0.76
1:I:395:ASN:CB	1:I:399:LEU:CD1	2.60	0.76
1:C:52:SER:CB	1:C:63:SER:HB3	2.13	0.76
5:G:1489:MPD:H32	1:H:193:SER:CB	2.14	0.76
1:L:1:SER:HA	1:L:71:ALA:HB1	1.66	0.76
1:A:52:SER:HB3	1:A:63:SER:CB	2.16	0.76
1:C:455:MET:HG2	1:I:323:VAL:HG21	1.66	0.76
1:E:395:ASN:CB	1:E:399:LEU:CD1	2.60	0.76
1:B:395:ASN:CB	1:B:399:LEU:CD1	2.60	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:52:SER:HB3	1:C:63:SER:CB	2.16	0.76
1:B:1:SER:HA	1:B:71:ALA:HB1	1.66	0.76
1:J:1:SER:HA	1:J:71:ALA:HB3	1.67	0.76
1:G:1:SER:HA	1:G:71:ALA:HB1	1.66	0.76
1:K:52:SER:HB3	1:K:63:SER:CB	2.16	0.76
1:G:52:SER:HB3	1:G:63:SER:CB	2.16	0.76
1:E:52:SER:HB3	1:E:63:SER:CB	2.16	0.76
1:C:1:SER:HA	1:C:71:ALA:HB3	1.67	0.76
1:B:190:ASP:OD2	5:C:1485:MPD:HM3	1.86	0.76
1:B:193:SER:HB2	5:C:1485:MPD:H32	1.67	0.76
1:D:1:SER:HA	1:D:71:ALA:HB1	1.66	0.76
1:D:323:VAL:HG21	1:J:455:MET:HG2	1.68	0.76
1:C:395:ASN:ND2	1:D:60:ILE:HG21	2.00	0.76
1:E:189:GLN:HG3	5:F:1488:MPD:HM1	1.68	0.76
1:A:189:GLN:HG3	5:B:1484:MPD:HM1	1.68	0.75
1:C:1:SER:HA	1:C:71:ALA:HB1	1.66	0.75
3:A:1471:ADP:H1'	3:A:1471:ADP:N9	1.99	0.75
3:H:1478:ADP:N9	3:H:1478:ADP:H1'	1.99	0.75
1:G:60:ILE:HG21	1:H:395:ASN:ND2	1.97	0.75
1:K:80:PHE:HB3	5:K:1493:MPD:C1	2.17	0.75
5:I:1491:MPD:O2	1:J:190:ASP:HA	1.85	0.75
3:K:1481:ADP:N9	3:K:1481:ADP:H1'	1.98	0.75
1:I:52:SER:HB3	1:I:63:SER:CB	2.16	0.75
1:F:52:SER:HB3	1:F:63:SER:CB	2.16	0.75
1:A:80:PHE:HB3	5:A:1483:MPD:C1	2.17	0.75
1:L:52:SER:HB3	1:L:63:SER:CB	2.16	0.75
1:B:52:SER:HB3	1:B:63:SER:CB	2.16	0.75
1:D:1:SER:HA	1:D:71:ALA:HB3	1.67	0.75
1:F:1:SER:HA	1:F:71:ALA:HB3	1.67	0.75
1:G:323:VAL:O	1:G:325:GLY:N	2.20	0.75
1:A:395:ASN:ND2	1:B:60:ILE:CG2	2.48	0.75
1:J:52:SER:HB3	1:J:63:SER:CB	2.16	0.75
1:F:80:PHE:HB3	5:F:1488:MPD:C1	2.17	0.75
5:I:1491:MPD:HM3	1:J:190:ASP:OD2	1.87	0.75
1:L:80:PHE:HB3	5:L:1494:MPD:C1	2.17	0.75
1:E:193:SER:HB2	5:F:1488:MPD:H32	1.67	0.75
1:D:190:ASP:OD2	5:E:1487:MPD:HM3	1.85	0.75
1:I:80:PHE:HB3	5:I:1491:MPD:C1	2.17	0.75
1:A:323:VAL:O	1:A:325:GLY:N	2.20	0.75
1:C:323:VAL:O	1:C:325:GLY:N	2.20	0.75
1:D:80:PHE:HB3	5:D:1486:MPD:C1	2.17	0.75
1:A:1:SER:HA	1:A:71:ALA:HB3	1.67	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1:SER:HA	1:E:71:ALA:HB3	1.67	0.75
1:D:323:VAL:O	1:D:325:GLY:N	2.20	0.75
1:D:52:SER:HB3	1:D:63:SER:CB	2.16	0.74
5:K:1493:MPD:H32	1:L:193:SER:HB2	1.69	0.74
1:C:80:PHE:HB3	5:C:1485:MPD:C1	2.17	0.74
1:I:323:VAL:O	1:I:325:GLY:N	2.20	0.74
1:H:52:SER:HB3	1:H:63:SER:CB	2.16	0.74
1:B:189:GLN:HG3	5:C:1485:MPD:HM1	1.69	0.74
1:K:1:SER:HA	1:K:71:ALA:HB3	1.67	0.74
3:C:1473:ADP:HI'	3:C:1473:ADP:N9	1.99	0.74
1:H:80:PHE:HB3	5:H:1490:MPD:C1	2.17	0.74
1:B:80:PHE:HB3	5:B:1484:MPD:C1	2.17	0.74
1:C:190:ASP:HA	5:D:1486:MPD:O2	1.87	0.74
1:L:323:VAL:O	1:L:325:GLY:N	2.20	0.74
1:J:323:VAL:O	1:J:325:GLY:N	2.20	0.74
1:K:323:VAL:O	1:K:325:GLY:N	2.20	0.74
1:K:395:ASN:CB	1:K:399:LEU:CD1	2.60	0.74
1:H:179:TYR:O	1:H:181:PRO:CD	2.36	0.74
1:H:323:VAL:O	1:H:325:GLY:N	2.20	0.74
1:G:60:ILE:CG2	1:H:395:ASN:ND2	2.47	0.74
1:L:179:TYR:O	1:L:181:PRO:CD	2.36	0.74
1:E:323:VAL:O	1:E:325:GLY:N	2.20	0.74
1:E:179:TYR:O	1:E:181:PRO:CD	2.36	0.74
1:H:1:SER:HA	1:H:71:ALA:HB3	1.67	0.74
1:B:455:MET:HG2	1:H:323:VAL:HG21	1.69	0.74
1:A:179:TYR:O	1:A:181:PRO:CD	2.36	0.74
1:J:80:PHE:HB3	5:J:1492:MPD:C1	2.17	0.74
1:E:190:ASP:OD2	5:F:1488:MPD:HM3	1.86	0.74
1:D:179:TYR:O	1:D:181:PRO:CD	2.36	0.73
1:G:179:TYR:O	1:G:181:PRO:CD	2.36	0.73
1:F:323:VAL:O	1:F:325:GLY:N	2.20	0.73
1:C:179:TYR:O	1:C:181:PRO:CD	2.36	0.73
1:E:80:PHE:HB3	5:E:1487:MPD:C1	2.17	0.73
1:H:60:ILE:HG21	1:I:395:ASN:HD21	1.53	0.73
1:F:51:GLY:C	1:F:53:SER:N	2.26	0.73
1:A:455:MET:HG2	1:G:323:VAL:HG21	1.69	0.73
1:I:179:TYR:O	1:I:181:PRO:CD	2.36	0.73
1:A:340:SER:CB	1:A:396:LEU:HB3	2.19	0.73
5:K:1493:MPD:O2	1:L:190:ASP:HA	1.87	0.73
1:K:179:TYR:O	1:K:181:PRO:CD	2.36	0.73
5:G:1489:MPD:HM1	1:H:189:GLN:HG3	1.71	0.73
1:B:323:VAL:O	1:B:325:GLY:N	2.20	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:1475:ADP:H1'	3:E:1475:ADP:N9	1.98	0.73
1:B:179:TYR:O	1:B:181:PRO:CD	2.36	0.73
1:E:340:SER:CB	1:E:396:LEU:HB3	2.19	0.73
1:B:340:SER:CB	1:B:396:LEU:HB3	2.19	0.73
1:H:340:SER:CB	1:H:396:LEU:HB3	2.19	0.73
1:K:340:SER:CB	1:K:396:LEU:HB3	2.19	0.73
1:E:189:GLN:HG3	5:F:1488:MPD:CM	2.19	0.73
1:C:51:GLY:C	1:C:53:SER:N	2.26	0.73
1:G:80:PHE:HB3	5:G:1489:MPD:C1	2.17	0.73
1:F:323:VAL:HG21	1:L:455:MET:HG2	1.71	0.73
1:A:395:ASN:CB	1:A:399:LEU:CD1	2.60	0.72
1:J:179:TYR:O	1:J:181:PRO:CD	2.36	0.72
1:D:340:SER:CB	1:D:396:LEU:HB3	2.19	0.72
1:F:179:TYR:O	1:F:181:PRO:CD	2.36	0.72
5:H:1490:MPD:O2	1:I:190:ASP:HA	1.87	0.72
1:C:340:SER:CB	1:C:396:LEU:HB3	2.19	0.72
1:C:180:PHE:HB3	1:D:29:GLN:HB3	1.72	0.72
1:A:193:SER:HB2	5:B:1484:MPD:H32	1.70	0.72
1:I:29:GLN:HB3	1:J:180:PHE:HB3	1.71	0.72
1:E:395:ASN:HD21	1:F:60:ILE:HG21	1.55	0.72
1:L:395:ASN:CB	1:L:399:LEU:CD1	2.60	0.72
1:I:340:SER:CB	1:I:396:LEU:HB3	2.19	0.72
1:F:340:SER:CB	1:F:396:LEU:HB3	2.19	0.72
1:G:340:SER:CB	1:G:396:LEU:HB3	2.19	0.72
1:A:189:GLN:HG3	5:B:1484:MPD:CM	2.20	0.72
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.25	0.72
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.25	0.72
1:L:340:SER:CB	1:L:396:LEU:HB3	2.19	0.71
1:B:189:GLN:HG3	5:C:1485:MPD:CM	2.20	0.71
3:J:1480:ADP:H1'	3:J:1480:ADP:N9	1.99	0.71
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.25	0.71
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.25	0.71
1:C:395:ASN:CB	1:C:399:LEU:CD1	2.60	0.71
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.25	0.71
1:C:323:VAL:HG21	1:I:455:MET:HG2	1.70	0.71
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.25	0.71
1:J:340:SER:CB	1:J:396:LEU:HB3	2.19	0.71
1:C:193:SER:HB2	5:D:1486:MPD:H32	1.72	0.71
5:I:1491:MPD:HM1	1:J:189:GLN:HG3	1.71	0.71
1:K:60:ILE:HG21	1:L:395:ASN:HD21	1.55	0.71
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.25	0.71
5:J:1492:MPD:HM1	1:K:189:GLN:HG3	1.73	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.25	0.71
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.25	0.71
1:G:395:ASN:CB	1:G:399:LEU:CD1	2.60	0.71
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.25	0.71
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.25	0.70
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.25	0.70
5:I:1491:MPD:CM	1:J:189:GLN:HG3	2.21	0.70
1:A:190:ASP:OD2	5:B:1484:MPD:HM3	1.89	0.70
1:D:455:MET:HG2	1:J:323:VAL:HG21	1.73	0.70
5:G:1489:MPD:HM3	1:H:190:ASP:OD2	1.91	0.70
3:I:1479:ADP:H1'	3:I:1479:ADP:N9	1.99	0.70
5:G:1489:MPD:O2	1:H:190:ASP:HA	1.90	0.70
3:F:1476:ADP:H1'	3:F:1476:ADP:N9	1.98	0.70
1:D:190:ASP:HA	5:E:1487:MPD:O2	1.91	0.70
1:E:455:MET:HG2	1:K:323:VAL:HG21	1.72	0.69
1:A:398:ASP:C	1:A:400:PRO:HD3	2.13	0.69
5:A:1483:MPD:O2	1:F:190:ASP:HA	1.92	0.69
1:D:1:SER:CA	1:D:71:ALA:HB1	2.23	0.69
1:F:1:SER:CA	1:F:71:ALA:HB1	2.23	0.69
1:A:1:SER:CA	1:A:71:ALA:HB1	2.23	0.69
5:A:1483:MPD:H32	1:F:193:SER:CB	2.23	0.69
1:H:1:SER:CA	1:H:71:ALA:HB1	2.23	0.69
1:B:1:SER:CA	1:B:71:ALA:HB1	2.23	0.69
1:A:211:HIS:HD2	1:A:212:GLU:O	1.76	0.69
1:J:211:HIS:HD2	1:J:212:GLU:O	1.76	0.69
1:G:211:HIS:HD2	1:G:212:GLU:O	1.76	0.69
3:B:1472:ADP:H1'	3:B:1472:ADP:N9	1.99	0.69
5:J:1492:MPD:CM	1:K:189:GLN:HG3	2.22	0.69
1:E:211:HIS:HD2	1:E:212:GLU:O	1.76	0.69
1:I:398:ASP:C	1:I:400:PRO:HD3	2.13	0.69
1:J:1:SER:CA	1:J:71:ALA:HB1	2.23	0.69
1:H:211:HIS:HD2	1:H:212:GLU:O	1.76	0.69
1:F:211:HIS:HD2	1:F:212:GLU:O	1.76	0.69
1:K:211:HIS:HD2	1:K:212:GLU:O	1.76	0.69
1:C:1:SER:CA	1:C:71:ALA:HB1	2.23	0.68
1:L:1:SER:CA	1:L:71:ALA:HB1	2.23	0.68
1:K:1:SER:CA	1:K:71:ALA:HB1	2.23	0.68
1:C:398:ASP:C	1:C:400:PRO:HD3	2.13	0.68
1:I:1:SER:CA	1:I:71:ALA:HB1	2.23	0.68
1:G:1:SER:CA	1:G:71:ALA:HB1	2.23	0.68
1:J:397:TYR:CE1	1:J:401:PRO:HD3	2.29	0.68
1:A:397:TYR:CE1	1:A:401:PRO:HD3	2.29	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:211:HIS:HD2	1:C:212:GLU:O	1.76	0.68
1:D:395:ASN:CB	1:D:399:LEU:CD1	2.60	0.68
1:D:397:TYR:CE1	1:D:401:PRO:HD3	2.29	0.68
1:C:397:TYR:CE1	1:C:401:PRO:HD3	2.29	0.68
1:G:397:TYR:CE1	1:G:401:PRO:HD3	2.29	0.68
1:D:193:SER:CB	5:E:1487:MPD:H32	2.22	0.68
1:E:224:ARG:CG	1:E:224:ARG:HH21	2.07	0.68
1:B:211:HIS:HD2	1:B:212:GLU:O	1.76	0.68
1:I:211:HIS:HD2	1:I:212:GLU:O	1.76	0.68
1:I:397:TYR:CE1	1:I:401:PRO:HD3	2.29	0.68
1:K:458:HIS:CD2	1:K:460:VAL:H	2.09	0.68
1:L:211:HIS:HD2	1:L:212:GLU:O	1.76	0.68
1:L:398:ASP:C	1:L:400:PRO:HD3	2.13	0.68
1:K:224:ARG:HH21	1:K:224:ARG:CG	2.07	0.68
1:E:398:ASP:C	1:E:400:PRO:HD3	2.13	0.68
1:K:397:TYR:CE1	1:K:401:PRO:HD3	2.29	0.68
5:G:1489:MPD:CM	1:H:189:GLN:HG3	2.24	0.68
1:L:397:TYR:CE1	1:L:401:PRO:HD3	2.29	0.67
1:E:1:SER:CA	1:E:71:ALA:HB1	2.23	0.67
3:L:1482:ADP:N9	3:L:1482:ADP:H1'	1.99	0.67
1:L:458:HIS:CD2	1:L:460:VAL:H	2.09	0.67
1:D:211:HIS:HD2	1:D:212:GLU:O	1.76	0.67
1:D:129:GLU:OE2	1:D:269:HIS:HB2	1.95	0.67
1:E:397:TYR:CE1	1:E:401:PRO:HD3	2.29	0.67
1:F:398:ASP:C	1:F:400:PRO:HD3	2.13	0.67
1:K:129:GLU:OE2	1:K:269:HIS:HB2	1.95	0.67
1:J:398:ASP:C	1:J:400:PRO:HD3	2.13	0.67
3:D:1474:ADP:N9	3:D:1474:ADP:H1'	1.99	0.67
1:I:129:GLU:OE2	1:I:269:HIS:HB2	1.95	0.67
1:A:224:ARG:CG	1:A:224:ARG:HH21	2.07	0.67
1:B:224:ARG:HH21	1:B:224:ARG:CG	2.07	0.67
1:G:129:GLU:OE2	1:G:269:HIS:HB2	1.95	0.67
1:F:397:TYR:CE1	1:F:401:PRO:HD3	2.29	0.67
1:F:1:SER:C	1:F:71:ALA:HB1	2.15	0.67
1:G:458:HIS:CD2	1:G:460:VAL:H	2.10	0.67
1:J:224:ARG:HH21	1:J:224:ARG:CG	2.07	0.67
1:L:129:GLU:OE2	1:L:269:HIS:HB2	1.95	0.67
1:B:129:GLU:OE2	1:B:269:HIS:HB2	1.95	0.67
1:J:129:GLU:OE2	1:J:269:HIS:HB2	1.95	0.67
1:F:224:ARG:HH21	1:F:224:ARG:CG	2.07	0.67
1:D:224:ARG:HH21	1:D:224:ARG:CG	2.07	0.67
1:F:129:GLU:OE2	1:F:269:HIS:HB2	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:82:ASP:HB2	5:H:1490:MPD:H12	1.77	0.67
1:H:224:ARG:HH21	1:H:224:ARG:CG	2.07	0.67
1:H:397:TYR:CE1	1:H:401:PRO:HD3	2.29	0.67
1:J:82:ASP:HB2	5:J:1492:MPD:H12	1.77	0.67
1:H:1:SER:C	1:H:71:ALA:HB1	2.15	0.67
1:A:1:SER:C	1:A:71:ALA:HB1	2.15	0.67
1:E:1:SER:C	1:E:71:ALA:HB1	2.15	0.67
1:G:1:SER:C	1:G:71:ALA:HB1	2.15	0.67
1:C:129:GLU:OE2	1:C:269:HIS:HB2	1.95	0.67
1:H:458:HIS:CD2	1:H:460:VAL:H	2.09	0.66
1:E:129:GLU:OE2	1:E:269:HIS:HB2	1.95	0.66
1:B:82:ASP:HB2	5:B:1484:MPD:H12	1.77	0.66
1:D:82:ASP:HB2	5:D:1486:MPD:H12	1.77	0.66
1:I:1:SER:C	1:I:71:ALA:HB1	2.15	0.66
1:B:397:TYR:CE1	1:B:401:PRO:HD3	2.29	0.66
1:F:82:ASP:HB2	5:F:1488:MPD:H12	1.77	0.66
1:L:1:SER:C	1:L:71:ALA:HB1	2.15	0.66
1:C:458:HIS:CD2	1:C:460:VAL:H	2.09	0.66
1:H:129:GLU:OE2	1:H:269:HIS:HB2	1.95	0.66
1:G:180:PHE:HB3	1:L:29:GLN:HB3	1.77	0.66
3:G:1477:ADP:N9	3:G:1477:ADP:H1'	1.98	0.66
1:B:398:ASP:C	1:B:400:PRO:HD3	2.13	0.66
1:L:403:GLU:HG2	1:L:403:GLU:O	1.96	0.66
1:E:458:HIS:CD2	1:E:460:VAL:H	2.10	0.66
1:C:224:ARG:HH21	1:C:224:ARG:CG	2.07	0.66
1:B:1:SER:C	1:B:71:ALA:HB1	2.15	0.66
1:A:129:GLU:OE2	1:A:269:HIS:HB2	1.95	0.66
1:J:29:GLN:HB3	1:K:180:PHE:HB3	1.77	0.66
1:D:1:SER:C	1:D:71:ALA:HB1	2.15	0.66
1:G:224:ARG:HH21	1:G:224:ARG:CG	2.07	0.66
1:E:82:ASP:HB2	5:E:1487:MPD:H12	1.77	0.66
1:J:1:SER:C	1:J:71:ALA:HB1	2.15	0.66
1:K:1:SER:C	1:K:71:ALA:HB1	2.15	0.66
1:J:397:TYR:HE1	1:J:401:PRO:HD3	1.61	0.66
1:L:397:TYR:HE1	1:L:401:PRO:HD3	1.61	0.66
1:I:397:TYR:HE1	1:I:401:PRO:HD3	1.61	0.66
1:C:82:ASP:HB2	5:C:1485:MPD:H12	1.77	0.66
1:F:458:HIS:CD2	1:F:460:VAL:H	2.10	0.66
1:L:224:ARG:HH21	1:L:224:ARG:CG	2.07	0.66
1:B:397:TYR:HE1	1:B:401:PRO:HD3	1.61	0.66
1:F:397:TYR:HE1	1:F:401:PRO:HD3	1.61	0.66
1:I:82:ASP:HB2	5:I:1491:MPD:H12	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1:SER:C	1:C:71:ALA:HB1	2.15	0.66
1:F:403:GLU:HG2	1:F:403:GLU:O	1.96	0.65
1:D:403:GLU:HG2	1:D:403:GLU:O	1.96	0.65
1:L:82:ASP:HB2	5:L:1494:MPD:H12	1.77	0.65
1:I:224:ARG:HH21	1:I:224:ARG:CG	2.07	0.65
1:I:403:GLU:HG2	1:I:403:GLU:O	1.96	0.65
1:B:403:GLU:HG2	1:B:403:GLU:O	1.96	0.65
1:J:60:ILE:HG21	1:K:395:ASN:ND2	2.08	0.65
1:A:82:ASP:HB2	5:A:1483:MPD:H12	1.77	0.65
1:E:403:GLU:HG2	1:E:403:GLU:O	1.96	0.65
1:D:84:THR:HG21	5:D:1486:MPD:O4	1.97	0.65
1:J:403:GLU:O	1:J:403:GLU:HG2	1.96	0.65
1:A:403:GLU:O	1:A:403:GLU:HG2	1.96	0.65
1:I:84:THR:HG21	5:I:1491:MPD:O4	1.97	0.65
1:H:403:GLU:O	1:H:403:GLU:HG2	1.96	0.65
1:C:397:TYR:HE1	1:C:401:PRO:HD3	1.61	0.65
1:C:403:GLU:O	1:C:403:GLU:HG2	1.96	0.65
1:K:82:ASP:HB2	5:K:1493:MPD:H12	1.77	0.65
1:G:155:GLU:OE1	1:G:211:HIS:HE1	1.80	0.65
1:H:397:TYR:HE1	1:H:401:PRO:HD3	1.61	0.65
1:B:84:THR:HG21	5:B:1484:MPD:O4	1.97	0.65
1:D:398:ASP:C	1:D:400:PRO:HD3	2.13	0.64
1:E:84:THR:HG21	5:E:1487:MPD:O4	1.97	0.64
1:C:180:PHE:O	1:D:29:GLN:HA	1.97	0.64
1:D:189:GLN:HG3	5:E:1487:MPD:HM1	1.79	0.64
1:L:84:THR:HG21	5:L:1494:MPD:O4	1.97	0.64
1:C:155:GLU:OE1	1:C:211:HIS:HE1	1.80	0.64
1:D:397:TYR:HE1	1:D:401:PRO:HD3	1.61	0.64
1:G:395:ASN:ND2	1:L:60:ILE:HG21	2.07	0.64
1:B:193:SER:OG	5:C:1485:MPD:H32	1.97	0.64
1:G:84:THR:HG21	5:G:1489:MPD:O4	1.97	0.64
1:D:155:GLU:OE1	1:D:211:HIS:HE1	1.80	0.64
1:A:84:THR:HG21	5:A:1483:MPD:O4	1.97	0.64
1:G:398:ASP:C	1:G:400:PRO:HD3	2.13	0.64
1:G:403:GLU:O	1:G:403:GLU:HG2	1.96	0.64
1:A:180:PHE:HB3	1:B:29:GLN:HB3	1.80	0.64
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.71	0.64
1:G:82:ASP:HB2	5:G:1489:MPD:H12	1.77	0.64
1:J:84:THR:HG21	5:J:1492:MPD:O4	1.97	0.64
1:A:155:GLU:OE1	1:A:211:HIS:HE1	1.80	0.64
1:A:397:TYR:HE1	1:A:401:PRO:HD3	1.61	0.64
1:F:84:THR:HG21	5:F:1488:MPD:O4	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:189:GLN:HG3	5:D:1486:MPD:HM1	1.79	0.64
1:B:458:HIS:CD2	1:B:460:VAL:H	2.10	0.64
1:I:155:GLU:OE1	1:I:211:HIS:HE1	1.80	0.64
1:J:155:GLU:OE1	1:J:211:HIS:HE1	1.80	0.64
1:F:155:GLU:OE1	1:F:211:HIS:HE1	1.80	0.64
1:K:397:TYR:HE1	1:K:401:PRO:HD3	1.61	0.64
1:F:179:TYR:C	1:F:181:PRO:HD2	2.19	0.64
1:H:84:THR:HG21	5:H:1490:MPD:O4	1.97	0.64
1:K:84:THR:HG21	5:K:1493:MPD:O4	1.97	0.64
1:C:84:THR:HG21	5:C:1485:MPD:O4	1.97	0.64
1:H:29:GLN:HB3	1:I:180:PHE:HB3	1.79	0.64
1:H:398:ASP:C	1:H:400:PRO:HD3	2.13	0.63
1:D:179:TYR:C	1:D:181:PRO:HD2	2.19	0.63
1:E:155:GLU:OE1	1:E:211:HIS:HE1	1.80	0.63
1:C:395:ASN:ND2	1:D:60:ILE:CG2	2.51	0.63
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.71	0.63
1:G:397:TYR:HE1	1:G:401:PRO:HD3	1.61	0.63
1:H:179:TYR:C	1:H:181:PRO:HD2	2.19	0.63
1:B:155:GLU:OE1	1:B:211:HIS:HE1	1.80	0.63
1:G:29:GLN:HB3	1:H:180:PHE:HB3	1.78	0.63
1:K:403:GLU:HG2	1:K:403:GLU:O	1.96	0.63
5:G:1489:MPD:H32	1:H:193:SER:HB2	1.78	0.63
1:D:458:HIS:CD2	1:D:460:VAL:H	2.09	0.63
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.71	0.63
1:H:155:GLU:OE1	1:H:211:HIS:HE1	1.80	0.63
1:A:458:HIS:CD2	1:A:460:VAL:H	2.10	0.63
1:D:51:GLY:C	1:D:53:SER:N	2.26	0.63
1:G:179:TYR:C	1:G:181:PRO:HD2	2.19	0.63
1:K:179:TYR:C	1:K:181:PRO:HD2	2.19	0.63
1:K:155:GLU:OE1	1:K:211:HIS:HE1	1.80	0.63
1:D:384:ASN:N	1:D:384:ASN:HD22	1.97	0.63
1:E:384:ASN:N	1:E:384:ASN:HD22	1.97	0.63
1:A:384:ASN:HD22	1:A:384:ASN:N	1.97	0.63
1:E:397:TYR:HE1	1:E:401:PRO:HD3	1.61	0.63
1:L:179:TYR:C	1:L:181:PRO:HD2	2.19	0.63
1:J:51:GLY:O	1:J:52:SER:C	2.37	0.63
1:B:179:TYR:C	1:B:181:PRO:HD2	2.19	0.63
1:J:179:TYR:C	1:J:181:PRO:HD2	2.19	0.63
1:A:29:GLN:HB3	1:F:180:PHE:HB3	1.81	0.63
1:C:179:TYR:C	1:C:181:PRO:HD2	2.19	0.63
1:G:189:GLN:HG3	5:L:1494:MPD:CM	2.28	0.63
1:G:189:GLN:HG3	5:L:1494:MPD:HM1	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:384:ASN:HD22	1:K:384:ASN:N	1.97	0.63
1:F:384:ASN:N	1:F:384:ASN:HD22	1.97	0.63
1:H:384:ASN:HD22	1:H:384:ASN:N	1.97	0.63
1:E:51:GLY:O	1:E:52:SER:C	2.37	0.62
1:I:179:TYR:C	1:I:181:PRO:HD2	2.19	0.62
1:E:179:TYR:C	1:E:181:PRO:HD2	2.19	0.62
1:I:384:ASN:N	1:I:384:ASN:HD22	1.97	0.62
1:B:384:ASN:N	1:B:384:ASN:HD22	1.97	0.62
1:E:396:LEU:O	1:E:399:LEU:HB2	2.00	0.62
1:K:396:LEU:O	1:K:399:LEU:HB2	2.00	0.62
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.71	0.62
1:C:179:TYR:O	1:C:181:PRO:HD2	2.00	0.62
1:I:29:GLN:HA	1:J:180:PHE:O	1.98	0.62
1:L:155:GLU:OE1	1:L:211:HIS:HE1	1.80	0.62
1:C:384:ASN:N	1:C:384:ASN:HD22	1.97	0.62
1:A:396:LEU:O	1:A:399:LEU:HB2	2.00	0.62
1:K:398:ASP:C	1:K:400:PRO:HD3	2.13	0.62
1:I:396:LEU:O	1:I:399:LEU:HB2	2.00	0.62
1:A:179:TYR:C	1:A:181:PRO:HD2	2.19	0.62
1:K:29:GLN:HB3	1:L:180:PHE:HB3	1.81	0.62
1:D:396:LEU:O	1:D:399:LEU:HB2	2.00	0.62
1:C:396:LEU:O	1:C:399:LEU:HB2	2.00	0.62
1:K:51:GLY:O	1:K:52:SER:C	2.37	0.62
1:F:179:TYR:O	1:F:181:PRO:HD2	2.00	0.62
1:E:193:SER:OG	5:F:1488:MPD:H32	1.99	0.62
1:J:179:TYR:O	1:J:181:PRO:HD2	2.00	0.62
1:J:60:ILE:CG2	1:K:395:ASN:ND2	2.57	0.62
1:F:179:TYR:O	1:F:181:PRO:HD3	2.00	0.62
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.71	0.62
5:H:1490:MPD:HM1	1:I:189:GLN:HG3	1.81	0.62
1:G:179:TYR:O	1:G:181:PRO:HD3	2.00	0.62
1:G:384:ASN:N	1:G:384:ASN:HD22	1.97	0.62
1:H:396:LEU:O	1:H:399:LEU:HB2	2.00	0.62
1:F:396:LEU:O	1:F:399:LEU:HB2	2.00	0.62
1:C:189:GLN:HG3	5:D:1486:MPD:CM	2.30	0.62
1:K:179:TYR:O	1:K:181:PRO:HD3	2.00	0.62
1:C:179:TYR:O	1:C:181:PRO:HD3	2.00	0.62
1:G:179:TYR:O	1:G:181:PRO:HD2	2.00	0.62
1:L:384:ASN:N	1:L:384:ASN:HD22	1.97	0.62
1:A:179:TYR:O	1:A:181:PRO:HD3	2.00	0.61
1:J:384:ASN:N	1:J:384:ASN:HD22	1.97	0.61
1:H:51:GLY:C	1:H:53:SER:N	2.26	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:51:GLY:O	1:B:52:SER:C	2.37	0.61
5:A:1483:MPD:H32	1:F:193:SER:HB2	1.82	0.61
1:J:396:LEU:O	1:J:399:LEU:HB2	2.00	0.61
1:L:396:LEU:O	1:L:399:LEU:HB2	2.00	0.61
1:G:396:LEU:O	1:G:399:LEU:HB2	2.00	0.61
1:B:396:LEU:O	1:B:399:LEU:HB2	2.00	0.61
1:I:179:TYR:O	1:I:181:PRO:HD3	2.00	0.61
5:H:1490:MPD:C3	1:I:193:SER:CB	2.77	0.61
1:G:224:ARG:NH2	1:G:224:ARG:HG2	2.15	0.61
1:J:179:TYR:O	1:J:181:PRO:HD3	2.00	0.61
5:A:1483:MPD:CM	1:F:190:ASP:OD2	2.48	0.61
3:H:1478:ADP:C1'	3:H:1478:ADP:C8	2.81	0.61
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.71	0.61
1:E:48:MET:CE	1:E:66:VAL:HG22	2.31	0.61
1:L:48:MET:CE	1:L:66:VAL:HG22	2.31	0.61
1:F:48:MET:CE	1:F:66:VAL:HG22	2.31	0.61
5:I:1491:MPD:H32	1:J:193:SER:OG	2.00	0.61
1:B:179:TYR:O	1:B:181:PRO:HD2	2.00	0.61
1:D:179:TYR:O	1:D:181:PRO:HD2	2.00	0.61
1:D:48:MET:CE	1:D:66:VAL:HG22	2.31	0.61
1:H:48:MET:CE	1:H:66:VAL:HG22	2.31	0.61
1:B:193:SER:OG	5:C:1485:MPD:C3	2.48	0.61
1:H:51:GLY:O	1:H:52:SER:C	2.37	0.61
1:C:82:ASP:N	5:C:1485:MPD:H13	2.13	0.61
1:H:179:TYR:O	1:H:181:PRO:HD2	2.00	0.61
1:E:179:TYR:O	1:E:181:PRO:HD3	2.00	0.61
1:C:48:MET:CE	1:C:66:VAL:HG22	2.31	0.61
1:D:179:TYR:O	1:D:181:PRO:HD3	2.00	0.60
1:I:179:TYR:O	1:I:181:PRO:HD2	2.00	0.60
5:H:1490:MPD:CM	1:I:189:GLN:HG3	2.31	0.60
1:A:179:TYR:O	1:A:181:PRO:HD2	2.00	0.60
1:D:180:PHE:HB3	1:E:29:GLN:HB3	1.83	0.60
1:A:48:MET:CE	1:A:66:VAL:HG22	2.31	0.60
1:L:179:TYR:O	1:L:181:PRO:HD3	2.00	0.60
1:K:179:TYR:O	1:K:181:PRO:HD2	2.00	0.60
1:I:48:MET:CE	1:I:66:VAL:HG22	2.31	0.60
1:I:395:ASN:CB	1:I:399:LEU:HD12	2.29	0.60
1:D:193:SER:HB2	5:E:1487:MPD:H32	1.84	0.60
1:H:179:TYR:O	1:H:181:PRO:HD3	2.00	0.60
1:E:179:TYR:O	1:E:181:PRO:HD2	2.00	0.60
1:B:179:TYR:O	1:B:181:PRO:HD3	2.00	0.60
1:B:48:MET:CE	1:B:66:VAL:HG22	2.31	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:82:ASP:CB	5:G:1489:MPD:H12	2.32	0.60
1:G:48:MET:CE	1:G:66:VAL:HG22	2.31	0.60
1:L:179:TYR:O	1:L:181:PRO:HD2	2.00	0.60
1:B:82:ASP:CB	5:B:1484:MPD:H12	2.32	0.60
1:G:82:ASP:N	5:G:1489:MPD:H12	2.17	0.60
1:J:82:ASP:CB	5:J:1492:MPD:H12	2.32	0.60
1:A:82:ASP:CB	5:A:1483:MPD:H12	2.32	0.60
1:I:458:HIS:CD2	1:I:460:VAL:H	2.09	0.60
1:L:51:GLY:O	1:L:52:SER:C	2.37	0.60
1:F:82:ASP:CB	5:F:1488:MPD:H12	2.32	0.60
5:K:1493:MPD:HM1	1:L:189:GLN:HG3	1.84	0.60
1:A:82:ASP:N	5:A:1483:MPD:H13	2.13	0.60
1:J:29:GLN:HA	1:K:180:PHE:O	2.01	0.60
1:D:395:ASN:ND2	1:E:60:ILE:HG21	2.11	0.60
1:F:51:GLY:O	1:F:52:SER:C	2.37	0.60
5:I:1491:MPD:C3	1:J:193:SER:OG	2.49	0.60
1:F:82:ASP:N	5:F:1488:MPD:H12	2.17	0.60
1:H:82:ASP:N	5:H:1490:MPD:C1	2.54	0.60
5:H:1490:MPD:C3	1:I:193:SER:OG	2.50	0.60
1:J:48:MET:CE	1:J:66:VAL:HG22	2.31	0.60
3:L:1482:ADP:C1'	3:L:1482:ADP:C8	2.81	0.60
1:H:360:PHE:CD2	1:H:361:PRO:CD	2.71	0.60
1:E:82:ASP:N	5:E:1487:MPD:H12	2.17	0.59
1:C:82:ASP:CB	5:C:1485:MPD:H12	2.32	0.59
1:I:82:ASP:CB	5:I:1491:MPD:H12	2.32	0.59
1:L:395:ASN:CB	1:L:399:LEU:HD12	2.30	0.59
1:F:82:ASP:N	5:F:1488:MPD:H13	2.13	0.59
1:K:224:ARG:NH2	1:K:224:ARG:HG2	2.15	0.59
1:E:193:SER:OG	5:F:1488:MPD:C3	2.50	0.59
1:D:189:GLN:HG3	5:E:1487:MPD:CM	2.32	0.59
1:D:82:ASP:CB	5:D:1486:MPD:H12	2.32	0.59
1:J:82:ASP:N	5:J:1492:MPD:H12	2.17	0.59
1:D:180:PHE:CD1	1:D:180:PHE:N	2.70	0.59
1:K:48:MET:CE	1:K:66:VAL:HG22	2.31	0.59
1:B:180:PHE:N	1:B:180:PHE:CD1	2.70	0.59
1:E:82:ASP:CB	5:E:1487:MPD:H12	2.32	0.59
1:D:456:THR:O	1:J:458:HIS:HE1	1.86	0.59
1:L:58:LYS:HZ1	1:L:60:ILE:HD11	1.67	0.59
1:K:82:ASP:N	5:K:1493:MPD:H13	2.13	0.59
1:C:82:ASP:N	5:C:1485:MPD:C1	2.54	0.59
1:L:82:ASP:CB	5:L:1494:MPD:H12	2.32	0.59
1:K:180:PHE:N	1:K:180:PHE:CD1	2.70	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:180:PHE:CD1	1:F:180:PHE:N	2.70	0.59
1:E:180:PHE:N	1:E:180:PHE:CD1	2.70	0.59
1:K:48:MET:HE2	1:K:66:VAL:HG22	1.83	0.59
5:J:1492:MPD:H32	1:K:193:SER:OG	2.01	0.59
1:E:179:TYR:HB2	6:E:1524:HOH:O	2.03	0.59
3:D:1474:ADP:C1'	3:D:1474:ADP:C8	2.81	0.59
5:J:1492:MPD:C3	1:K:193:SER:OG	2.50	0.59
1:K:179:TYR:HB2	6:K:1534:HOH:O	2.03	0.59
1:H:82:ASP:N	5:H:1490:MPD:H12	2.17	0.59
1:B:179:TYR:HB2	6:B:1521:HOH:O	2.03	0.59
1:H:82:ASP:CB	5:H:1490:MPD:H12	2.32	0.59
1:D:82:ASP:N	5:D:1486:MPD:H13	2.13	0.59
3:C:1473:ADP:C8	3:C:1473:ADP:C1'	2.81	0.58
1:D:51:GLY:O	1:D:52:SER:C	2.37	0.58
1:F:82:ASP:N	5:F:1488:MPD:C1	2.54	0.58
1:L:82:ASP:N	5:L:1494:MPD:H12	2.17	0.58
1:J:458:HIS:CD2	1:J:460:VAL:H	2.10	0.58
1:H:179:TYR:HB2	6:H:1528:HOH:O	2.03	0.58
1:A:179:TYR:HB2	6:A:1514:HOH:O	2.03	0.58
1:C:180:PHE:CD1	1:C:180:PHE:N	2.70	0.58
1:A:193:SER:OG	5:B:1484:MPD:H32	2.03	0.58
1:K:82:ASP:CB	5:K:1493:MPD:H12	2.32	0.58
1:G:82:ASP:N	5:G:1489:MPD:C1	2.54	0.58
1:H:180:PHE:CD1	1:H:180:PHE:N	2.70	0.58
1:D:179:TYR:HB2	6:D:1525:HOH:O	2.03	0.58
1:H:82:ASP:N	5:H:1490:MPD:H13	2.13	0.58
1:E:82:ASP:N	5:E:1487:MPD:C1	2.54	0.58
1:G:180:PHE:N	1:G:180:PHE:CD1	2.70	0.58
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.86	0.58
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.71	0.58
1:A:29:GLN:HA	1:F:180:PHE:O	2.02	0.58
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.86	0.58
1:K:308:ILE:HG21	1:K:374:LEU:HD13	1.86	0.58
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.86	0.58
1:I:63:SER:HB2	1:J:339:ARG:HH22	1.69	0.58
1:A:16:PHE:HB2	5:A:1483:MPD:H51	1.86	0.58
1:B:48:MET:HE2	1:B:66:VAL:HG22	1.85	0.58
1:B:224:ARG:NH2	1:B:224:ARG:HG2	2.15	0.58
1:I:180:PHE:CD1	1:I:180:PHE:N	2.70	0.58
1:G:326:TYR:N	1:G:326:TYR:CD2	2.72	0.58
1:F:179:TYR:HB2	6:F:1527:HOH:O	2.03	0.58
5:H:1490:MPD:C3	1:I:193:SER:HB2	2.32	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:179:TYR:HB2	6:J:1530:HOH:O	2.03	0.58
3:A:1471:ADP:C8	3:A:1471:ADP:C1'	2.81	0.58
1:D:16:PHE:HB2	5:D:1486:MPD:H51	1.86	0.58
1:F:395:ASN:CB	1:F:399:LEU:HD12	2.30	0.57
1:I:51:GLY:O	1:I:52:SER:C	2.37	0.57
1:F:16:PHE:CD1	5:F:1488:MPD:C5	2.87	0.57
1:A:395:ASN:CB	1:A:399:LEU:HD12	2.30	0.57
1:G:180:PHE:O	1:L:29:GLN:HA	2.03	0.57
1:G:29:GLN:HA	1:H:180:PHE:O	2.03	0.57
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.86	0.57
1:K:326:TYR:CD2	1:K:326:TYR:N	2.72	0.57
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.86	0.57
1:C:326:TYR:CD2	1:C:326:TYR:N	2.72	0.57
1:C:179:TYR:HB2	6:C:1523:HOH:O	2.03	0.57
1:K:16:PHE:HB2	5:K:1493:MPD:H51	1.86	0.57
1:A:82:ASP:N	5:A:1483:MPD:H12	2.17	0.57
1:G:179:TYR:HB2	6:G:1528:HOH:O	2.03	0.57
1:H:29:GLN:HA	1:I:180:PHE:O	2.03	0.57
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.86	0.57
1:I:16:PHE:HB2	5:I:1491:MPD:H51	1.86	0.57
1:L:16:PHE:CD1	5:L:1494:MPD:C5	2.87	0.57
1:J:180:PHE:N	1:J:180:PHE:CD1	2.70	0.57
1:L:179:TYR:HB2	6:L:1365:HOH:O	2.03	0.57
1:B:82:ASP:N	5:B:1484:MPD:H12	2.17	0.57
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.86	0.57
5:H:1490:MPD:H32	1:I:193:SER:OG	2.04	0.57
5:K:1493:MPD:CM	1:L:190:ASP:OD2	2.49	0.57
1:L:16:PHE:HB2	5:L:1494:MPD:H51	1.86	0.57
1:C:224:ARG:NH2	1:C:224:ARG:HG2	2.15	0.57
1:B:180:PHE:HB3	1:C:29:GLN:HB3	1.85	0.57
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.70	0.57
1:D:326:TYR:N	1:D:326:TYR:CD2	2.72	0.57
1:E:395:ASN:CB	1:E:399:LEU:HD12	2.30	0.57
1:C:51:GLY:O	1:C:52:SER:C	2.37	0.57
1:K:82:ASP:N	5:K:1493:MPD:C1	2.54	0.57
1:I:82:ASP:N	5:I:1491:MPD:H13	2.13	0.57
5:A:1483:MPD:HM1	1:F:189:GLN:HG3	1.86	0.57
1:E:48:MET:HE2	1:E:66:VAL:HG22	1.86	0.57
1:D:180:PHE:O	1:E:29:GLN:HA	2.05	0.57
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.70	0.57
1:E:326:TYR:CD2	1:E:326:TYR:N	2.72	0.57
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:K:1481:ADP:C1'	3:K:1481:ADP:C8	2.81	0.57
3:J:1480:ADP:C1'	3:J:1480:ADP:C8	2.81	0.57
1:C:395:ASN:CB	1:C:399:LEU:HD12	2.30	0.57
1:I:179:TYR:HB2	6:I:1530:HOH:O	2.03	0.57
1:A:193:SER:OG	5:B:1484:MPD:C3	2.53	0.57
1:E:16:PHE:CD1	5:E:1487:MPD:C5	2.87	0.57
1:J:16:PHE:HB2	5:J:1492:MPD:H51	1.86	0.57
1:E:1:SER:CA	1:E:71:ALA:CB	2.80	0.57
1:L:180:PHE:N	1:L:180:PHE:CD1	2.70	0.57
1:K:29:GLN:HA	1:L:180:PHE:O	2.04	0.57
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.70	0.57
3:B:1472:ADP:C8	3:B:1472:ADP:C1'	2.81	0.57
1:A:16:PHE:CD1	5:A:1483:MPD:C5	2.87	0.57
1:D:458:HIS:HE1	1:J:456:THR:O	1.87	0.57
1:J:58:LYS:HZ1	1:J:60:ILE:HD11	1.70	0.56
1:H:16:PHE:HB2	5:H:1490:MPD:H51	1.86	0.56
1:A:82:ASP:N	5:A:1483:MPD:C1	2.54	0.56
1:L:48:MET:HE2	1:L:66:VAL:HG22	1.86	0.56
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.86	0.56
1:A:326:TYR:CD2	1:A:326:TYR:N	2.72	0.56
3:E:1475:ADP:C8	3:E:1475:ADP:C1'	2.81	0.56
3:G:1477:ADP:C1'	3:G:1477:ADP:C8	2.81	0.56
1:B:360:PHE:CD2	1:B:361:PRO:CD	2.71	0.56
1:H:16:PHE:CD1	5:H:1490:MPD:C5	2.87	0.56
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.86	0.56
1:I:63:SER:OG	1:J:339:ARG:NH2	2.39	0.56
1:B:82:ASP:N	5:B:1484:MPD:H13	2.13	0.56
1:D:82:ASP:N	5:D:1486:MPD:H12	2.17	0.56
5:K:1493:MPD:CM	1:L:189:GLN:HG3	2.35	0.56
1:C:82:ASP:N	5:C:1485:MPD:H12	2.17	0.56
1:A:180:PHE:N	1:A:180:PHE:CD1	2.70	0.56
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.70	0.56
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.86	0.56
1:J:326:TYR:CD2	1:J:326:TYR:N	2.72	0.56
1:B:16:PHE:HB2	5:B:1484:MPD:H51	1.86	0.56
1:E:16:PHE:HB2	5:E:1487:MPD:H51	1.86	0.56
1:C:16:PHE:HB2	5:C:1485:MPD:H51	1.86	0.56
1:G:82:ASP:N	5:G:1489:MPD:H13	2.13	0.56
1:G:16:PHE:HB2	5:G:1489:MPD:H51	1.86	0.56
1:G:193:SER:CB	5:L:1494:MPD:C3	2.82	0.56
1:D:399:LEU:O	1:D:400:PRO:O	2.24	0.56
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.71	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:193:SER:HB2	5:L:1494:MPD:C3	2.35	0.56
1:F:48:MET:HE2	1:F:66:VAL:HG22	1.86	0.56
1:D:48:MET:HE2	1:D:66:VAL:HG22	1.87	0.56
1:I:48:MET:HE2	1:I:66:VAL:HG22	1.87	0.56
1:H:192:ARG:HD3	1:H:219:ASN:HD22	1.70	0.56
1:B:399:LEU:O	1:B:400:PRO:O	2.24	0.56
1:F:399:LEU:O	1:F:400:PRO:O	2.24	0.56
1:I:82:ASP:N	5:I:1491:MPD:C1	2.54	0.56
1:L:1:SER:CA	1:L:71:ALA:CB	2.80	0.56
1:B:456:THR:O	1:H:458:HIS:HE1	1.88	0.56
1:K:399:LEU:O	1:K:400:PRO:O	2.24	0.56
1:A:58:LYS:HZ1	1:A:60:ILE:HD11	1.70	0.56
1:J:16:PHE:CD1	5:J:1492:MPD:C5	2.87	0.56
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.70	0.56
1:K:82:ASP:N	5:K:1493:MPD:H12	2.17	0.56
1:C:48:MET:HE2	1:C:66:VAL:HG22	1.86	0.56
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.06	0.56
1:B:458:HIS:HE1	1:H:456:THR:O	1.89	0.56
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.70	0.56
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.70	0.56
1:H:399:LEU:O	1:H:400:PRO:O	2.24	0.56
1:G:51:GLY:O	1:G:52:SER:C	2.37	0.56
1:G:16:PHE:CD1	5:G:1489:MPD:C5	2.87	0.56
1:E:224:ARG:HG2	1:E:224:ARG:NH2	2.15	0.56
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.70	0.56
1:F:16:PHE:HB2	5:F:1488:MPD:H51	1.86	0.55
1:K:16:PHE:CD1	5:K:1493:MPD:C5	2.87	0.55
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.70	0.55
1:H:118:THR:OG1	1:H:120:ILE:HG13	2.06	0.55
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.06	0.55
1:F:326:TYR:CD2	1:F:326:TYR:N	2.72	0.55
1:H:395:ASN:CB	1:H:399:LEU:HD12	2.30	0.55
1:F:1:SER:CA	1:F:71:ALA:CB	2.80	0.55
1:L:224:ARG:HG2	1:L:224:ARG:NH2	2.15	0.55
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.06	0.55
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.70	0.55
1:G:395:ASN:CB	1:G:399:LEU:HD12	2.30	0.55
1:D:16:PHE:CD1	5:D:1486:MPD:C5	2.87	0.55
1:A:180:PHE:O	1:B:29:GLN:HA	2.06	0.55
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.70	0.55
1:C:400:PRO:CB	1:C:401:PRO:HD2	2.37	0.55
1:I:326:TYR:N	1:I:326:TYR:CD2	2.72	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.06	0.55
1:B:395:ASN:CB	1:B:399:LEU:HD12	2.29	0.55
1:C:16:PHE:CD1	5:C:1485:MPD:C5	2.87	0.55
1:J:1:SER:CA	1:J:71:ALA:CB	2.80	0.55
1:L:118:THR:OG1	1:L:120:ILE:HG13	2.06	0.55
1:B:326:TYR:N	1:B:326:TYR:CD2	2.72	0.55
1:E:399:LEU:O	1:E:400:PRO:O	2.24	0.55
1:L:399:LEU:O	1:L:400:PRO:O	2.24	0.55
1:J:82:ASP:N	5:J:1492:MPD:H13	2.13	0.55
3:I:1479:ADP:C1'	3:I:1479:ADP:C8	2.81	0.55
1:J:395:ASN:CB	1:J:399:LEU:HD12	2.30	0.55
1:D:397:TYR:C	1:D:399:LEU:N	2.60	0.55
1:L:400:PRO:CB	1:L:401:PRO:HD2	2.37	0.55
1:K:397:TYR:C	1:K:399:LEU:N	2.60	0.55
1:K:395:ASN:CB	1:K:399:LEU:HD12	2.29	0.55
1:I:397:TYR:C	1:I:399:LEU:N	2.60	0.55
1:F:400:PRO:CB	1:F:401:PRO:HD2	2.37	0.55
1:G:400:PRO:CB	1:G:401:PRO:HD2	2.37	0.55
1:G:395:ASN:ND2	1:L:60:ILE:CG2	2.63	0.55
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.71	0.55
1:G:193:SER:OG	5:L:1494:MPD:C3	2.55	0.55
1:A:118:THR:OG1	1:A:120:ILE:HG13	2.06	0.55
1:L:326:TYR:N	1:L:326:TYR:CD2	2.72	0.55
1:I:50:ASP:CG	6:I:1613:HOH:O	2.44	0.55
1:J:399:LEU:O	1:J:400:PRO:O	2.24	0.55
1:D:400:PRO:CB	1:D:401:PRO:HD2	2.37	0.55
1:I:400:PRO:CB	1:I:401:PRO:HD2	2.37	0.55
1:B:180:PHE:O	1:C:29:GLN:HA	2.06	0.55
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.06	0.55
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.06	0.55
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.06	0.55
1:H:326:TYR:N	1:H:326:TYR:CD2	2.72	0.55
1:E:400:PRO:CB	1:E:401:PRO:HD2	2.37	0.55
1:K:400:PRO:CB	1:K:401:PRO:HD2	2.37	0.55
1:C:399:LEU:O	1:C:400:PRO:O	2.24	0.55
1:G:399:LEU:O	1:G:400:PRO:O	2.24	0.55
1:A:399:LEU:O	1:A:400:PRO:O	2.24	0.54
1:J:400:PRO:CB	1:J:401:PRO:HD2	2.37	0.54
1:L:397:TYR:C	1:L:399:LEU:N	2.60	0.54
1:J:82:ASP:N	5:J:1492:MPD:C1	2.54	0.54
1:G:48:MET:HE2	1:G:66:VAL:HG22	1.89	0.54
1:I:399:LEU:O	1:I:400:PRO:O	2.24	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.71	0.54
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.06	0.54
1:F:58:LYS:HZ1	1:F:60:ILE:HD11	1.73	0.54
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.39	0.54
1:I:16:PHE:CD1	5:I:1491:MPD:C5	2.87	0.54
1:B:400:PRO:CB	1:B:401:PRO:HD2	2.37	0.54
1:A:51:GLY:O	1:A:52:SER:C	2.37	0.54
1:D:82:ASP:N	5:D:1486:MPD:C1	2.54	0.54
3:F:1476:ADP:C8	3:F:1476:ADP:C1'	2.81	0.54
5:I:1491:MPD:C3	1:J:193:SER:HB2	2.37	0.54
1:G:190:ASP:OD2	5:L:1494:MPD:CM	2.53	0.54
1:B:82:ASP:N	5:B:1484:MPD:C1	2.54	0.54
5:J:1492:MPD:C3	1:K:193:SER:HB2	2.36	0.54
1:C:458:HIS:HE1	1:I:456:THR:O	1.90	0.54
1:A:400:PRO:CB	1:A:401:PRO:HD2	2.37	0.54
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.39	0.54
1:I:82:ASP:N	5:I:1491:MPD:H12	2.17	0.54
1:F:458:HIS:HE1	1:L:456:THR:O	1.90	0.54
1:C:58:LYS:HZ1	1:C:60:ILE:HD11	1.73	0.53
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.06	0.53
5:H:1490:MPD:CM	1:I:190:ASP:OD2	2.53	0.53
1:B:16:PHE:CD1	5:B:1484:MPD:C5	2.87	0.53
1:B:193:SER:CB	5:C:1485:MPD:C3	2.81	0.53
1:E:454:ARG:O	1:K:320:LYS:HG2	2.08	0.53
1:E:397:TYR:C	1:E:399:LEU:N	2.60	0.53
1:H:400:PRO:CB	1:H:401:PRO:HD2	2.37	0.53
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.39	0.53
1:H:48:MET:HE1	1:H:66:VAL:HG22	1.90	0.53
1:J:397:TYR:C	1:J:399:LEU:N	2.60	0.53
1:E:58:LYS:HZ1	1:E:60:ILE:HD11	1.73	0.53
1:C:456:THR:O	1:I:458:HIS:HE1	1.91	0.53
1:D:302:ILE:HG23	1:D:332:LEU:HB3	1.91	0.53
1:I:58:LYS:HZ1	1:I:60:ILE:HD11	1.74	0.53
1:A:397:TYR:C	1:A:399:LEU:N	2.60	0.53
5:I:1491:MPD:C3	1:J:193:SER:CB	2.80	0.53
1:G:427:PHE:CE1	1:G:428:LEU:HD13	2.44	0.53
1:E:82:ASP:N	5:E:1487:MPD:H13	2.13	0.53
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.39	0.53
5:A:1483:MPD:CM	1:F:189:GLN:HG3	2.39	0.53
1:H:302:ILE:HG23	1:H:332:LEU:HB3	1.91	0.53
1:G:337:ARG:HG2	1:G:338:ASN:H	1.74	0.53
1:D:80:PHE:CG	5:D:1486:MPD:HM2	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:80:PHE:CG	5:L:1494:MPD:HM2	2.44	0.53
1:I:224:ARG:NH2	1:I:224:ARG:HG2	2.15	0.53
1:H:427:PHE:CE1	1:H:428:LEU:HD13	2.44	0.53
1:I:337:ARG:HG2	1:I:338:ASN:H	1.74	0.53
1:J:427:PHE:CE1	1:J:428:LEU:HD13	2.44	0.53
1:B:397:TYR:C	1:B:399:LEU:N	2.60	0.53
1:D:395:ASN:CB	1:D:399:LEU:HD12	2.30	0.53
1:E:312:ALA:HB1	1:E:361:PRO:HG3	1.91	0.53
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.39	0.53
1:K:80:PHE:CG	5:K:1493:MPD:HM2	2.44	0.53
1:A:80:PHE:CG	5:A:1483:MPD:HM2	2.44	0.53
1:H:337:ARG:HG2	1:H:338:ASN:H	1.74	0.53
1:K:58:LYS:HZ1	1:K:60:ILE:HD11	1.73	0.53
1:J:312:ALA:HB1	1:J:361:PRO:HG3	1.91	0.53
1:F:80:PHE:CG	5:F:1488:MPD:HM2	2.44	0.53
1:G:80:PHE:CG	5:G:1489:MPD:HM2	2.44	0.53
5:J:1492:MPD:C3	1:K:193:SER:CB	2.81	0.53
1:B:337:ARG:HG2	1:B:338:ASN:H	1.74	0.53
1:I:427:PHE:CE1	1:I:428:LEU:HD13	2.44	0.53
1:C:427:PHE:CE1	1:C:428:LEU:HD13	2.44	0.53
1:F:337:ARG:HG2	1:F:338:ASN:H	1.74	0.53
1:C:312:ALA:HB1	1:C:361:PRO:HG3	1.91	0.52
1:C:339:ARG:NH2	1:D:63:SER:OG	2.42	0.52
1:H:80:PHE:CG	5:H:1490:MPD:HM2	2.44	0.52
1:G:193:SER:OG	5:L:1494:MPD:H32	2.08	0.52
1:J:302:ILE:HG23	1:J:332:LEU:HB3	1.91	0.52
1:A:302:ILE:HG23	1:A:332:LEU:HB3	1.91	0.52
1:D:427:PHE:CE1	1:D:428:LEU:HD13	2.44	0.52
1:L:427:PHE:CE1	1:L:428:LEU:HD13	2.44	0.52
1:A:312:ALA:HB1	1:A:361:PRO:HG3	1.91	0.52
1:L:312:ALA:HB1	1:L:361:PRO:HG3	1.91	0.52
1:C:1:SER:CA	1:C:71:ALA:CB	2.80	0.52
1:B:427:PHE:CE1	1:B:428:LEU:HD13	2.44	0.52
1:F:427:PHE:CE1	1:F:428:LEU:HD13	2.44	0.52
1:E:80:PHE:CG	5:E:1487:MPD:HM2	2.44	0.52
1:A:48:MET:HE1	1:A:66:VAL:HG22	1.91	0.52
1:E:180:PHE:HB3	1:F:29:GLN:HB3	1.92	0.52
1:E:320:LYS:HG2	1:K:454:ARG:O	2.09	0.52
1:C:124:VAL:HG11	1:C:375:LEU:HG	1.92	0.52
1:K:337:ARG:HG2	1:K:338:ASN:H	1.74	0.52
1:F:124:VAL:HG11	1:F:375:LEU:HG	1.92	0.52
1:E:427:PHE:CE1	1:E:428:LEU:HD13	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:397:TYR:C	1:C:399:LEU:N	2.60	0.52
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.39	0.52
1:D:312:ALA:HB1	1:D:361:PRO:HG3	1.91	0.52
1:F:80:PHE:CD1	5:F:1488:MPD:O4	2.63	0.52
1:H:80:PHE:CD1	5:H:1490:MPD:O4	2.63	0.52
1:B:80:PHE:CG	5:B:1484:MPD:HM2	2.44	0.52
1:C:337:ARG:HG2	1:C:338:ASN:H	1.74	0.52
1:L:302:ILE:HG23	1:L:332:LEU:HB3	1.91	0.52
1:K:427:PHE:CE1	1:K:428:LEU:HD13	2.44	0.52
1:H:312:ALA:HB1	1:H:361:PRO:HG3	1.91	0.52
1:B:80:PHE:CD1	5:B:1484:MPD:O4	2.63	0.52
1:J:80:PHE:CG	5:J:1492:MPD:HM2	2.44	0.52
1:I:80:PHE:CG	5:I:1491:MPD:HM2	2.44	0.52
1:J:48:MET:HE1	1:J:66:VAL:HG22	1.91	0.52
1:B:302:ILE:HG23	1:B:332:LEU:HB3	1.91	0.52
1:G:124:VAL:HG11	1:G:375:LEU:HG	1.92	0.52
1:F:302:ILE:HG23	1:F:332:LEU:HB3	1.91	0.52
1:H:397:TYR:C	1:H:399:LEU:N	2.60	0.52
1:K:80:PHE:CD1	5:K:1493:MPD:O4	2.63	0.52
1:C:80:PHE:CD1	5:C:1485:MPD:O4	2.63	0.52
1:G:80:PHE:CD1	5:G:1489:MPD:O4	2.63	0.52
1:L:82:ASP:N	5:L:1494:MPD:H13	2.13	0.52
1:A:80:PHE:CD1	5:A:1483:MPD:O4	2.63	0.52
1:C:465:TYR:O	1:C:468:VAL:HB	2.10	0.52
1:E:124:VAL:HG11	1:E:375:LEU:HG	1.92	0.52
1:A:465:TYR:O	1:A:468:VAL:HB	2.10	0.52
1:L:124:VAL:HG11	1:L:375:LEU:HG	1.92	0.52
1:B:465:TYR:O	1:B:468:VAL:HB	2.10	0.52
1:I:465:TYR:O	1:I:468:VAL:HB	2.10	0.52
1:G:360:PHE:CE2	1:G:361:PRO:HD3	2.39	0.52
1:E:16:PHE:HB2	1:E:84:THR:HB	1.92	0.52
1:L:82:ASP:N	5:L:1494:MPD:C1	2.54	0.52
1:F:456:THR:O	1:L:458:HIS:HE1	1.93	0.52
1:I:124:VAL:HG11	1:I:375:LEU:HG	1.92	0.52
1:C:302:ILE:HG23	1:C:332:LEU:HB3	1.91	0.52
1:B:124:VAL:HG11	1:B:375:LEU:HG	1.92	0.52
1:J:340:SER:OG	1:J:396:LEU:HB3	2.10	0.52
1:A:60:ILE:HG21	1:F:395:ASN:ND2	2.18	0.52
1:I:312:ALA:HB1	1:I:361:PRO:HG3	1.91	0.52
1:F:312:ALA:HB1	1:F:361:PRO:HG3	1.91	0.52
1:B:312:ALA:HB1	1:B:361:PRO:HG3	1.91	0.52
1:K:16:PHE:HB2	1:K:84:THR:HB	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:180:PHE:HD1	1:L:180:PHE:N	2.08	0.52
1:I:302:ILE:HG23	1:I:332:LEU:HB3	1.91	0.52
1:L:340:SER:OG	1:L:396:LEU:HB3	2.10	0.52
1:F:340:SER:OG	1:F:396:LEU:HB3	2.10	0.52
1:C:80:PHE:CG	5:C:1485:MPD:HM2	2.44	0.52
1:L:80:PHE:CD1	5:L:1494:MPD:O4	2.63	0.52
1:D:465:TYR:O	1:D:468:VAL:HB	2.10	0.52
1:H:136:ASP:O	1:I:169:LYS:NZ	2.35	0.52
1:A:337:ARG:HG2	1:A:338:ASN:H	1.74	0.52
1:K:124:VAL:HG11	1:K:375:LEU:HG	1.92	0.52
1:D:337:ARG:HG2	1:D:338:ASN:H	1.74	0.52
1:E:337:ARG:HG2	1:E:338:ASN:H	1.74	0.52
1:G:397:TYR:C	1:G:399:LEU:N	2.60	0.52
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.39	0.52
1:I:80:PHE:CD1	5:I:1491:MPD:O4	2.63	0.52
1:J:180:PHE:HD1	1:J:180:PHE:N	2.08	0.52
1:F:465:TYR:O	1:F:468:VAL:HB	2.10	0.52
1:D:340:SER:OG	1:D:396:LEU:HB3	2.10	0.51
1:K:312:ALA:HB1	1:K:361:PRO:HG3	1.91	0.51
1:D:80:PHE:CD1	5:D:1486:MPD:O4	2.63	0.51
1:K:465:TYR:O	1:K:468:VAL:HB	2.10	0.51
1:K:302:ILE:HG23	1:K:332:LEU:HB3	1.91	0.51
1:J:337:ARG:HG2	1:J:338:ASN:H	1.74	0.51
1:B:340:SER:OG	1:B:396:LEU:HB3	2.10	0.51
1:B:16:PHE:HB2	1:B:84:THR:HB	1.92	0.51
1:E:80:PHE:CD1	5:E:1487:MPD:O4	2.63	0.51
5:G:1489:MPD:H32	1:H:193:SER:OG	2.09	0.51
1:J:80:PHE:CD1	5:J:1492:MPD:O4	2.63	0.51
1:H:180:PHE:HD1	1:H:180:PHE:N	2.08	0.51
1:H:124:VAL:HG11	1:H:375:LEU:HG	1.92	0.51
1:E:465:TYR:O	1:E:468:VAL:HB	2.10	0.51
1:G:312:ALA:HB1	1:G:361:PRO:HG3	1.91	0.51
1:H:16:PHE:HB2	1:H:84:THR:HB	1.92	0.51
1:A:340:SER:OG	1:A:396:LEU:HB3	2.10	0.51
1:C:340:SER:OG	1:C:396:LEU:HB3	2.10	0.51
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.39	0.51
1:C:180:PHE:HD1	1:C:180:PHE:N	2.08	0.51
1:A:427:PHE:CE1	1:A:428:LEU:HD13	2.44	0.51
1:L:465:TYR:O	1:L:468:VAL:HB	2.10	0.51
1:G:302:ILE:HG23	1:G:332:LEU:HB3	1.91	0.51
1:L:337:ARG:HG2	1:L:338:ASN:H	1.74	0.51
1:J:465:TYR:O	1:J:468:VAL:HB	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:193:SER:HB2	5:C:1485:MPD:C3	2.39	0.51
1:G:16:PHE:HB2	1:G:84:THR:HB	1.92	0.51
1:I:375:LEU:HD22	1:I:379:LEU:HG	1.93	0.51
1:D:50:ASP:CG	6:D:1493:HOH:O	2.48	0.51
1:G:465:TYR:O	1:G:468:VAL:HB	2.10	0.51
1:H:465:TYR:O	1:H:468:VAL:HB	2.10	0.51
1:I:340:SER:OG	1:I:396:LEU:HB3	2.10	0.51
1:I:16:PHE:HB2	1:I:84:THR:HB	1.92	0.51
1:A:224:ARG:HG2	1:A:224:ARG:NH2	2.15	0.51
1:F:124:VAL:HG13	1:F:274:LEU:CD2	2.41	0.51
1:I:124:VAL:HG13	1:I:274:LEU:CD2	2.41	0.51
1:K:49:PHE:CD2	1:K:49:PHE:N	2.79	0.51
1:F:49:PHE:CD2	1:F:49:PHE:N	2.79	0.51
1:H:58:LYS:HZ1	1:H:60:ILE:HD11	1.74	0.51
1:A:180:PHE:N	1:A:180:PHE:HD1	2.08	0.51
1:L:49:PHE:N	1:L:49:PHE:CD2	2.79	0.51
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.39	0.51
1:A:16:PHE:HB2	1:A:84:THR:HB	1.92	0.51
1:I:180:PHE:HD1	1:I:180:PHE:N	2.08	0.51
1:G:124:VAL:HG13	1:G:274:LEU:CD2	2.41	0.51
1:A:124:VAL:HG11	1:A:375:LEU:HG	1.92	0.51
1:J:124:VAL:HG11	1:J:375:LEU:HG	1.92	0.51
1:F:397:TYR:C	1:F:399:LEU:N	2.60	0.51
1:G:340:SER:OG	1:G:396:LEU:HB3	2.10	0.51
1:D:360:PHE:CG	1:D:361:PRO:HD3	2.42	0.51
1:C:16:PHE:HB2	1:C:84:THR:HB	1.92	0.51
1:A:48:MET:HE2	1:A:66:VAL:HG22	1.93	0.51
1:B:180:PHE:N	1:B:180:PHE:HD1	2.08	0.51
1:C:124:VAL:HG13	1:C:274:LEU:CD2	2.41	0.51
1:K:124:VAL:HG13	1:K:274:LEU:CD2	2.41	0.51
1:H:49:PHE:CD2	1:H:49:PHE:N	2.79	0.51
1:G:180:PHE:N	1:G:180:PHE:HD1	2.08	0.51
1:J:124:VAL:HG13	1:J:274:LEU:CD2	2.41	0.51
1:D:375:LEU:HD22	1:D:379:LEU:HG	1.93	0.51
1:E:302:ILE:HG23	1:E:332:LEU:HB3	1.91	0.51
1:J:58:LYS:O	1:J:58:LYS:HG2	2.12	0.50
5:K:1493:MPD:C3	1:L:193:SER:HB2	2.41	0.50
1:J:16:PHE:HB2	1:J:84:THR:HB	1.92	0.50
1:F:375:LEU:HD22	1:F:379:LEU:HG	1.93	0.50
1:D:124:VAL:HG13	1:D:274:LEU:CD2	2.41	0.50
1:E:49:PHE:N	1:E:49:PHE:CD2	2.79	0.50
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.43	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:339:ARG:HH22	1:B:63:SER:HB2	1.76	0.50
1:F:16:PHE:HB2	1:F:84:THR:HB	1.92	0.50
1:E:124:VAL:HG13	1:E:274:LEU:CD2	2.41	0.50
1:L:124:VAL:HG13	1:L:274:LEU:CD2	2.41	0.50
1:H:124:VAL:HG13	1:H:274:LEU:CD2	2.41	0.50
1:A:124:VAL:HG13	1:A:274:LEU:CD2	2.41	0.50
1:A:49:PHE:N	1:A:49:PHE:CD2	2.79	0.50
1:B:375:LEU:HD22	1:B:379:LEU:HG	1.93	0.50
1:D:124:VAL:HG11	1:D:375:LEU:HG	1.92	0.50
1:H:340:SER:OG	1:H:396:LEU:HB3	2.10	0.50
1:H:58:LYS:O	1:H:58:LYS:HG2	2.12	0.50
1:B:49:PHE:CD2	1:B:49:PHE:N	2.79	0.50
1:I:49:PHE:N	1:I:49:PHE:CD2	2.79	0.50
1:E:58:LYS:HG2	1:E:58:LYS:O	2.12	0.50
1:D:16:PHE:HB2	1:D:84:THR:HB	1.92	0.50
1:G:375:LEU:HD22	1:G:379:LEU:HG	1.93	0.50
1:K:375:LEU:HD22	1:K:379:LEU:HG	1.93	0.50
1:G:49:PHE:CD2	1:G:49:PHE:N	2.79	0.50
1:D:401:PRO:CB	1:D:404:ALA:HA	2.37	0.50
1:L:58:LYS:O	1:L:58:LYS:HG2	2.12	0.50
1:A:360:PHE:CG	1:A:361:PRO:HD3	2.43	0.50
1:E:189:GLN:OE1	5:F:1488:MPD:H4	2.12	0.50
1:L:16:PHE:HB2	1:L:84:THR:HB	1.92	0.50
1:F:224:ARG:HG2	1:F:224:ARG:NH2	2.15	0.50
1:B:124:VAL:HG13	1:B:274:LEU:CD2	2.41	0.50
1:B:49:PHE:HD2	1:B:49:PHE:N	2.10	0.50
1:K:340:SER:OG	1:K:396:LEU:HB3	2.10	0.50
1:G:84:THR:HG21	5:G:1489:MPD:C5	2.42	0.50
1:I:84:THR:HG21	5:I:1491:MPD:C5	2.42	0.50
1:K:435:THR:HG23	6:K:1518:HOH:O	2.12	0.50
1:A:454:ARG:O	1:G:320:LYS:HG2	2.11	0.50
1:B:58:LYS:HG2	1:B:58:LYS:O	2.12	0.50
1:B:395:ASN:ND2	1:C:60:ILE:HG21	2.22	0.50
1:D:395:ASN:ND2	1:E:60:ILE:CG2	2.61	0.50
1:D:84:THR:HG21	5:D:1486:MPD:C5	2.42	0.50
1:K:84:THR:HG21	5:K:1493:MPD:C5	2.42	0.50
1:H:49:PHE:HD2	1:H:49:PHE:N	2.10	0.50
1:J:49:PHE:CD2	1:J:49:PHE:N	2.79	0.50
1:D:49:PHE:N	1:D:49:PHE:CD2	2.79	0.50
1:E:340:SER:OG	1:E:396:LEU:HB3	2.10	0.50
1:C:360:PHE:CE2	1:C:361:PRO:HD3	2.39	0.50
1:J:48:MET:HE2	1:J:66:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:375:LEU:HD22	1:C:379:LEU:HG	1.93	0.50
1:A:49:PHE:N	1:A:49:PHE:HD2	2.10	0.50
1:C:49:PHE:CD2	1:C:49:PHE:N	2.79	0.50
1:E:84:THR:HG21	5:E:1487:MPD:C5	2.42	0.49
5:G:1489:MPD:H4	1:H:189:GLN:OE1	2.12	0.49
1:D:180:PHE:N	1:D:180:PHE:HD1	2.08	0.49
1:H:375:LEU:HD22	1:H:379:LEU:HG	1.93	0.49
1:K:49:PHE:HD2	1:K:49:PHE:N	2.10	0.49
1:F:49:PHE:N	1:F:49:PHE:HD2	2.10	0.49
1:A:58:LYS:HG2	1:A:58:LYS:O	2.12	0.49
1:I:179:TYR:C	1:I:181:PRO:CD	2.81	0.49
1:A:339:ARG:NH2	1:B:63:SER:OG	2.46	0.49
1:J:375:LEU:HD22	1:J:379:LEU:HG	1.93	0.49
1:J:435:THR:HG23	6:J:1514:HOH:O	2.12	0.49
1:F:84:THR:HG21	5:F:1488:MPD:C5	2.42	0.49
5:K:1493:MPD:C3	1:L:193:SER:CB	2.88	0.49
5:G:1489:MPD:C3	1:H:193:SER:OG	2.60	0.49
1:L:375:LEU:HD22	1:L:379:LEU:HG	1.93	0.49
1:I:34:PRO:HG2	1:J:206:VAL:O	2.12	0.49
1:L:84:THR:HG21	5:L:1494:MPD:C5	2.42	0.49
1:I:29:GLN:HB3	1:J:180:PHE:CB	2.41	0.49
1:F:180:PHE:N	1:F:180:PHE:HD1	2.08	0.49
1:E:375:LEU:HD22	1:E:379:LEU:HG	1.93	0.49
1:A:435:THR:HG23	6:A:1498:HOH:O	2.12	0.49
1:B:435:THR:HG23	6:B:1505:HOH:O	2.12	0.49
1:G:58:LYS:O	1:G:58:LYS:HG2	2.12	0.49
1:C:190:ASP:OD2	5:D:1486:MPD:CM	2.54	0.49
1:C:193:SER:OG	5:D:1486:MPD:H32	2.13	0.49
1:A:84:THR:HG21	5:A:1483:MPD:C5	2.42	0.49
1:A:375:LEU:HD22	1:A:379:LEU:HG	1.93	0.49
1:I:49:PHE:N	1:I:49:PHE:HD2	2.10	0.49
1:I:33:ILE:CD1	1:J:208:ALA:HB2	2.42	0.49
1:B:84:THR:HG21	5:B:1484:MPD:C5	2.42	0.49
1:D:1:SER:CA	1:D:71:ALA:CB	2.80	0.49
1:I:1:SER:CA	1:I:71:ALA:CB	2.80	0.49
1:G:179:TYR:C	1:G:181:PRO:CD	2.81	0.49
1:L:49:PHE:N	1:L:49:PHE:HD2	2.10	0.49
1:I:33:ILE:HD11	1:J:208:ALA:HB2	1.94	0.49
1:B:58:LYS:HZ1	1:B:60:ILE:HD11	1.77	0.49
1:D:190:ASP:OD2	5:E:1487:MPD:CM	2.55	0.49
1:E:179:TYR:C	1:E:181:PRO:CD	2.81	0.49
1:H:48:MET:HE2	1:H:66:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:49:PHE:N	1:E:49:PHE:HD2	2.10	0.49
1:J:49:PHE:N	1:J:49:PHE:HD2	2.10	0.49
1:D:49:PHE:N	1:D:49:PHE:HD2	2.10	0.49
1:D:58:LYS:HG2	1:D:58:LYS:O	2.12	0.49
1:C:84:THR:HG21	5:C:1485:MPD:C5	2.42	0.49
1:K:58:LYS:O	1:K:58:LYS:HG2	2.12	0.49
1:I:401:PRO:CB	1:I:404:ALA:HA	2.37	0.49
1:G:48:MET:HE1	1:G:66:VAL:HG22	1.95	0.49
1:A:192:ARG:HH21	1:A:219:ASN:ND2	2.11	0.49
1:I:435:THR:HG23	6:I:1514:HOH:O	2.12	0.49
1:J:60:ILE:HA	1:J:60:ILE:HD13	1.62	0.49
1:C:193:SER:OG	5:D:1486:MPD:C3	2.61	0.49
1:J:192:ARG:HH21	1:J:219:ASN:ND2	2.11	0.49
1:F:435:THR:HG23	6:F:1511:HOH:O	2.12	0.49
1:K:401:PRO:CB	1:K:404:ALA:HA	2.37	0.48
1:F:179:TYR:C	1:F:181:PRO:CD	2.81	0.48
1:H:84:THR:HG21	5:H:1490:MPD:C5	2.42	0.48
1:J:84:THR:HG21	5:J:1492:MPD:C5	2.42	0.48
1:I:192:ARG:HH21	1:I:219:ASN:ND2	2.11	0.48
1:C:454:ARG:O	1:I:320:LYS:HG2	2.13	0.48
1:H:435:THR:HG23	6:H:1512:HOH:O	2.12	0.48
1:D:435:THR:HG23	6:D:1509:HOH:O	2.12	0.48
1:D:58:LYS:HZ1	1:D:60:ILE:HD11	1.78	0.48
1:L:360:PHE:CG	1:L:361:PRO:HD3	2.43	0.48
1:B:189:GLN:OE1	5:C:1485:MPD:H4	2.13	0.48
1:C:192:ARG:HH21	1:C:219:ASN:ND2	2.11	0.48
1:K:192:ARG:HH21	1:K:219:ASN:ND2	2.11	0.48
1:L:435:THR:HG23	6:L:1348:HOH:O	2.12	0.48
1:G:435:THR:HG23	6:G:1512:HOH:O	2.12	0.48
1:F:287:TYR:O	1:F:290:LEU:HB2	2.14	0.48
1:F:58:LYS:HG2	1:F:58:LYS:O	2.12	0.48
5:K:1493:MPD:H32	1:L:193:SER:OG	2.13	0.48
1:E:180:PHE:O	1:F:29:GLN:HA	2.13	0.48
1:D:287:TYR:O	1:D:290:LEU:HB2	2.14	0.48
1:A:320:LYS:HG2	1:G:454:ARG:O	2.13	0.48
1:L:287:TYR:O	1:L:290:LEU:HB2	2.14	0.48
1:C:435:THR:HG23	6:C:1507:HOH:O	2.12	0.48
1:E:435:THR:HG23	6:E:1508:HOH:O	2.12	0.48
1:A:193:SER:CB	5:B:1484:MPD:C3	2.86	0.48
1:G:49:PHE:N	1:G:49:PHE:HD2	2.10	0.48
1:C:49:PHE:HD2	1:C:49:PHE:N	2.10	0.48
1:G:287:TYR:O	1:G:290:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:287:TYR:O	1:I:290:LEU:HB2	2.14	0.48
1:G:58:LYS:HZ1	1:G:60:ILE:HD11	1.78	0.48
1:J:224:ARG:HG2	1:J:224:ARG:NH2	2.15	0.48
1:K:179:TYR:C	1:K:181:PRO:CD	2.81	0.48
1:L:192:ARG:HH21	1:L:219:ASN:ND2	2.11	0.48
1:D:192:ARG:HH21	1:D:219:ASN:ND2	2.11	0.48
1:I:58:LYS:O	1:I:58:LYS:HG2	2.12	0.48
1:C:58:LYS:HG2	1:C:58:LYS:O	2.12	0.48
1:F:332:LEU:HB2	1:F:408:PRO:O	2.14	0.48
1:J:287:TYR:O	1:J:290:LEU:HB2	2.14	0.48
1:K:136:ASP:O	1:L:169:LYS:NZ	2.42	0.48
5:K:1493:MPD:C3	1:L:193:SER:OG	2.61	0.48
1:K:1:SER:CA	1:K:71:ALA:CB	2.80	0.48
1:B:179:TYR:C	1:B:181:PRO:CD	2.81	0.48
1:H:192:ARG:HH21	1:H:219:ASN:ND2	2.11	0.48
1:I:332:LEU:HB2	1:I:408:PRO:O	2.14	0.48
1:B:1:SER:CA	1:B:71:ALA:CB	2.80	0.48
1:C:332:LEU:HB2	1:C:408:PRO:O	2.14	0.48
1:C:287:TYR:O	1:C:290:LEU:HB2	2.14	0.48
1:C:179:TYR:C	1:C:181:PRO:CD	2.81	0.48
1:E:180:PHE:N	1:E:180:PHE:HD1	2.08	0.48
1:B:192:ARG:HH21	1:B:219:ASN:ND2	2.11	0.48
1:L:332:LEU:HB2	1:L:408:PRO:O	2.14	0.48
1:G:60:ILE:HA	1:G:60:ILE:HD13	1.62	0.48
1:H:332:LEU:HB2	1:H:408:PRO:O	2.14	0.48
1:G:332:LEU:HB2	1:G:408:PRO:O	2.14	0.48
1:E:287:TYR:O	1:E:290:LEU:HB2	2.14	0.48
1:D:443:ILE:O	1:D:447:ARG:HB2	2.14	0.48
1:D:395:ASN:HD22	1:D:395:ASN:HA	1.53	0.47
1:K:180:PHE:N	1:K:180:PHE:HD1	2.08	0.47
1:F:192:ARG:HH21	1:F:219:ASN:ND2	2.11	0.47
1:A:332:LEU:HB2	1:A:408:PRO:O	2.14	0.47
1:E:332:LEU:HB2	1:E:408:PRO:O	2.14	0.47
1:B:287:TYR:O	1:B:290:LEU:HB2	2.14	0.47
1:E:395:ASN:ND2	1:F:60:ILE:HG21	2.28	0.47
1:C:339:ARG:HH22	1:D:63:SER:HB2	1.78	0.47
1:J:311:LEU:HD22	1:J:369:LEU:HB3	1.97	0.47
1:G:63:SER:HB2	1:H:339:ARG:HH22	1.79	0.47
1:A:189:GLN:OE1	5:B:1484:MPD:H4	2.13	0.47
1:D:189:GLN:OE1	5:E:1487:MPD:H4	2.13	0.47
1:D:224:ARG:NH2	1:D:224:ARG:HG2	2.15	0.47
1:D:332:LEU:HB2	1:D:408:PRO:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:443:ILE:O	1:A:447:ARG:HB2	2.14	0.47
1:C:397:TYR:OH	1:C:404:ALA:O	2.29	0.47
1:G:63:SER:OG	1:H:339:ARG:NH2	2.47	0.47
1:I:48:MET:HE1	1:I:66:VAL:HG22	1.96	0.47
1:F:18:ASP:OD2	1:F:30:HIS:HD2	1.98	0.47
1:L:443:ILE:O	1:L:447:ARG:HB2	2.14	0.47
1:G:311:LEU:HD22	1:G:369:LEU:HB3	1.97	0.47
1:A:287:TYR:O	1:A:290:LEU:HB2	2.14	0.47
1:L:401:PRO:CB	1:L:404:ALA:HA	2.37	0.47
1:G:401:PRO:CB	1:G:404:ALA:HA	2.37	0.47
1:A:53:SER:HB2	1:F:179:TYR:HE2	1.79	0.47
1:A:179:TYR:C	1:A:181:PRO:CD	2.81	0.47
1:J:34:PRO:HG2	1:K:206:VAL:O	2.14	0.47
1:G:18:ASP:OD2	1:G:30:HIS:HD2	1.98	0.47
1:I:443:ILE:O	1:I:447:ARG:HB2	2.14	0.47
1:J:18:ASP:OD2	1:J:30:HIS:HD2	1.98	0.47
1:L:179:TYR:C	1:L:181:PRO:CD	2.81	0.47
1:A:339:ARG:HD3	1:A:339:ARG:HA	1.71	0.47
1:J:332:LEU:HB2	1:J:408:PRO:O	2.14	0.47
1:K:332:LEU:HB2	1:K:408:PRO:O	2.14	0.47
1:F:443:ILE:O	1:F:447:ARG:HB2	2.14	0.47
1:H:287:TYR:O	1:H:290:LEU:HB2	2.14	0.47
1:J:443:ILE:O	1:J:447:ARG:HB2	2.14	0.47
1:K:60:ILE:HD13	1:K:60:ILE:HA	1.62	0.47
1:D:179:TYR:C	1:D:181:PRO:CD	2.81	0.47
1:E:193:SER:CB	5:F:1488:MPD:C3	2.84	0.47
1:H:1:SER:CA	1:H:71:ALA:CB	2.81	0.47
1:G:443:ILE:O	1:G:447:ARG:HB2	2.14	0.47
1:B:443:ILE:O	1:B:447:ARG:HB2	2.14	0.47
1:G:50:ASP:CG	6:G:1609:HOH:O	2.53	0.47
1:F:311:LEU:HD22	1:F:369:LEU:HB3	1.97	0.47
1:D:18:ASP:OD2	1:D:30:HIS:HD2	1.98	0.47
1:C:18:ASP:OD2	1:C:30:HIS:HD2	1.98	0.47
1:B:360:PHE:CG	1:B:361:PRO:HD3	2.43	0.47
1:C:193:SER:HB2	5:D:1486:MPD:C3	2.44	0.47
1:E:456:THR:O	1:K:458:HIS:HE1	1.97	0.47
1:G:192:ARG:HH21	1:G:219:ASN:ND2	2.11	0.47
1:B:332:LEU:HB2	1:B:408:PRO:O	2.14	0.47
1:B:311:LEU:HD22	1:B:369:LEU:HB3	1.97	0.47
1:B:18:ASP:OD2	1:B:30:HIS:HD2	1.98	0.47
1:A:400:PRO:HB3	1:A:401:PRO:HD2	1.97	0.47
1:F:401:PRO:CB	1:F:404:ALA:HA	2.37	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:53:SER:HB2	1:F:179:TYR:CE2	2.50	0.47
5:J:1492:MPD:H4	1:K:189:GLN:OE1	2.15	0.47
1:C:180:PHE:CB	1:D:29:GLN:HB3	2.43	0.47
1:E:192:ARG:HH21	1:E:219:ASN:ND2	2.11	0.47
1:K:287:TYR:O	1:K:290:LEU:HB2	2.14	0.47
1:C:311:LEU:HD22	1:C:369:LEU:HB3	1.97	0.47
1:C:443:ILE:O	1:C:447:ARG:HB2	2.15	0.47
1:C:208:ALA:HB2	1:D:33:ILE:HD11	1.97	0.47
1:E:401:PRO:CB	1:E:404:ALA:HA	2.37	0.46
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.43	0.46
1:G:81:ALA:H	5:G:1489:MPD:H13	1.80	0.46
1:H:179:TYR:C	1:H:181:PRO:CD	2.80	0.46
1:K:443:ILE:O	1:K:447:ARG:HB2	2.14	0.46
1:E:443:ILE:O	1:E:447:ARG:HB2	2.14	0.46
1:D:397:TYR:OH	1:D:404:ALA:O	2.29	0.46
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.39	0.46
1:A:456:THR:O	1:G:458:HIS:HE1	1.98	0.46
1:I:286:LYS:HE2	1:I:292:GLU:HB3	1.98	0.46
1:K:311:LEU:HD22	1:K:369:LEU:HB3	1.97	0.46
1:I:18:ASP:OD2	1:I:30:HIS:HD2	1.98	0.46
1:E:311:LEU:HD22	1:E:369:LEU:HB3	1.96	0.46
1:K:360:PHE:CG	1:K:361:PRO:HD3	2.43	0.46
1:I:337:ARG:HD3	1:I:393:ASP:OD2	2.15	0.46
1:F:337:ARG:HD3	1:F:393:ASP:OD2	2.15	0.46
1:L:311:LEU:HD22	1:L:369:LEU:HB3	1.97	0.46
1:H:443:ILE:O	1:H:447:ARG:HB2	2.14	0.46
1:C:286:LYS:HE2	1:C:292:GLU:HB3	1.98	0.46
1:C:400:PRO:HB3	1:C:401:PRO:HD2	1.97	0.46
1:K:18:ASP:OD2	1:K:30:HIS:HD2	1.98	0.46
1:I:311:LEU:HD22	1:I:369:LEU:HB3	1.97	0.46
1:F:286:LYS:HE2	1:F:292:GLU:HB3	1.98	0.46
1:G:286:LYS:HE2	1:G:292:GLU:HB3	1.98	0.46
1:J:395:ASN:HD22	1:J:395:ASN:HA	1.53	0.46
1:L:400:PRO:HB3	1:L:401:PRO:HD2	1.97	0.46
5:I:1491:MPD:O4	5:I:1491:MPD:HM2	2.16	0.46
1:E:48:MET:HE1	1:E:66:VAL:HG22	1.98	0.46
1:G:124:VAL:HG13	1:G:274:LEU:HD21	1.98	0.46
1:F:454:ARG:O	1:L:320:LYS:HG2	2.15	0.46
1:D:286:LYS:HE2	1:D:292:GLU:HB3	1.98	0.46
1:A:18:ASP:OD2	1:A:30:HIS:HD2	1.98	0.46
1:E:400:PRO:HB3	1:E:401:PRO:HD2	1.97	0.46
1:B:60:ILE:HD13	1:B:60:ILE:HA	1.62	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:395:ASN:ND2	1:C:60:ILE:CG2	2.69	0.46
1:I:400:PRO:HB3	1:I:401:PRO:HD2	1.97	0.46
1:G:400:PRO:HB3	1:G:401:PRO:HD2	1.97	0.46
1:I:33:ILE:HG13	1:J:207:GLU:O	2.14	0.46
1:L:18:ASP:OD2	1:L:30:HIS:HD2	1.98	0.46
1:L:28:GLU:OE1	1:L:88:ARG:NH1	2.48	0.46
1:K:296:TYR:CE2	1:K:385:LYS:HD3	2.51	0.46
1:J:179:TYR:C	1:J:181:PRO:CD	2.81	0.46
1:B:337:ARG:HD3	1:B:393:ASP:OD2	2.16	0.46
1:C:124:VAL:HG13	1:C:274:LEU:HD21	1.98	0.46
1:H:18:ASP:OD2	1:H:30:HIS:HD2	1.98	0.46
1:L:296:TYR:CE2	1:L:385:LYS:HD3	2.51	0.46
5:E:1487:MPD:HM2	5:E:1487:MPD:O4	2.16	0.46
5:A:1483:MPD:O4	5:A:1483:MPD:HM2	2.16	0.46
1:L:48:MET:HE1	1:L:66:VAL:HG22	1.98	0.46
1:J:286:LYS:HE2	1:J:292:GLU:HB3	1.98	0.46
1:F:466:TYR:CE1	1:L:254:THR:HB	2.51	0.46
1:H:296:TYR:CE2	1:H:385:LYS:HD3	2.51	0.46
1:E:18:ASP:OD2	1:E:30:HIS:HD2	1.98	0.46
1:C:296:TYR:CE2	1:C:385:LYS:HD3	2.51	0.46
1:E:193:SER:HB2	5:F:1488:MPD:C3	2.40	0.46
5:D:1486:MPD:O4	5:D:1486:MPD:HM2	2.16	0.46
1:G:1:SER:CA	1:G:71:ALA:CB	2.80	0.46
1:C:337:ARG:HD3	1:C:393:ASP:OD2	2.15	0.46
1:D:93:GLU:HB3	1:D:96:THR:HG23	1.98	0.46
1:D:311:LEU:HD22	1:D:369:LEU:HB3	1.97	0.46
1:A:311:LEU:HD22	1:A:369:LEU:HB3	1.97	0.46
1:C:401:PRO:CB	1:C:404:ALA:HA	2.37	0.46
5:F:1488:MPD:HM2	5:F:1488:MPD:O4	2.16	0.46
5:G:1489:MPD:O4	5:G:1489:MPD:HM2	2.16	0.46
1:F:48:MET:HE1	1:F:66:VAL:HG22	1.98	0.46
1:A:463:GLU:HA	1:G:140:PHE:CE1	2.51	0.46
1:I:93:GLU:HB3	1:I:96:THR:HG23	1.98	0.46
1:L:286:LYS:HE2	1:L:292:GLU:HB3	1.98	0.46
1:A:296:TYR:CE2	1:A:385:LYS:HD3	2.51	0.46
1:B:296:TYR:CE2	1:B:385:LYS:HD3	2.51	0.46
1:I:296:TYR:CE2	1:I:385:LYS:HD3	2.51	0.46
1:I:397:TYR:OH	1:I:404:ALA:O	2.29	0.45
5:B:1484:MPD:HM2	5:B:1484:MPD:O4	2.16	0.45
1:K:337:ARG:HD3	1:K:393:ASP:OD2	2.15	0.45
1:A:337:ARG:HD3	1:A:393:ASP:OD2	2.15	0.45
1:K:124:VAL:HG13	1:K:274:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:337:ARG:HD3	1:L:393:ASP:OD2	2.15	0.45
1:A:93:GLU:HB3	1:A:96:THR:HG23	1.98	0.45
1:J:296:TYR:CE2	1:J:385:LYS:HD3	2.51	0.45
1:B:320:LYS:HG2	1:H:454:ARG:O	2.16	0.45
1:F:296:TYR:CE2	1:F:385:LYS:HD3	2.51	0.45
1:A:286:LYS:HE2	1:A:292:GLU:HB3	1.98	0.45
1:B:206:VAL:O	1:C:34:PRO:HG2	2.16	0.45
1:B:401:PRO:CB	1:B:404:ALA:HA	2.37	0.45
1:K:400:PRO:HB3	1:K:401:PRO:HD2	1.97	0.45
1:F:400:PRO:HB3	1:F:401:PRO:HD2	1.97	0.45
1:G:339:ARG:NH2	1:L:63:SER:OG	2.49	0.45
5:H:1490:MPD:HM2	5:H:1490:MPD:O4	2.16	0.45
1:I:124:VAL:HG13	1:I:274:LEU:HD21	1.98	0.45
1:J:337:ARG:HD3	1:J:393:ASP:OD2	2.16	0.45
1:A:124:VAL:HG13	1:A:274:LEU:HD21	1.98	0.45
1:K:93:GLU:HB3	1:K:96:THR:HG23	1.98	0.45
1:I:60:ILE:HA	1:I:60:ILE:HD13	1.62	0.45
1:J:401:PRO:CB	1:J:404:ALA:HA	2.37	0.45
1:E:124:VAL:HG13	1:E:274:LEU:HD21	1.98	0.45
1:D:124:VAL:HG13	1:D:274:LEU:HD21	1.98	0.45
1:E:296:TYR:CE2	1:E:385:LYS:HD3	2.51	0.45
1:D:432:GLY:HA2	6:D:1602:HOH:O	2.17	0.45
1:H:286:LYS:HE2	1:H:292:GLU:HB3	1.98	0.45
5:C:1485:MPD:HM2	5:C:1485:MPD:O4	2.16	0.45
1:G:337:ARG:HD3	1:G:393:ASP:OD2	2.15	0.45
1:J:33:ILE:HD11	1:K:208:ALA:HB2	1.98	0.45
1:E:286:LYS:HE2	1:E:292:GLU:HB3	1.98	0.45
1:L:195:MET:O	1:L:199:MET:HG3	2.17	0.45
1:L:339:ARG:HA	1:L:339:ARG:HD3	1.71	0.45
1:J:400:PRO:HB3	1:J:401:PRO:HD2	1.98	0.45
5:I:1491:MPD:H4	1:J:189:GLN:OE1	2.17	0.45
1:F:124:VAL:HG13	1:F:274:LEU:HD21	1.98	0.45
1:L:432:GLY:HA2	6:L:1452:HOH:O	2.17	0.45
1:H:311:LEU:HD22	1:H:369:LEU:HB3	1.97	0.45
1:K:395:ASN:HA	1:K:395:ASN:HD22	1.53	0.45
5:J:1492:MPD:HM2	5:J:1492:MPD:O4	2.16	0.45
1:C:48:MET:HE1	1:C:66:VAL:HG22	1.98	0.45
1:A:195:MET:O	1:A:199:MET:HG3	2.17	0.45
1:H:395:ASN:HD22	1:H:395:ASN:HA	1.53	0.45
5:L:1494:MPD:O4	5:L:1494:MPD:HM2	2.16	0.45
1:H:337:ARG:HD3	1:H:393:ASP:OD2	2.15	0.45
1:D:337:ARG:HD3	1:D:393:ASP:OD2	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:93:GLU:HB3	1:G:96:THR:HG23	1.98	0.45
1:D:289:GLY:O	1:D:354:ARG:HD2	2.17	0.45
1:D:195:MET:O	1:D:199:MET:HG3	2.17	0.45
1:I:195:MET:O	1:I:199:MET:HG3	2.17	0.45
1:I:432:GLY:HA2	6:I:1606:HOH:O	2.17	0.45
1:A:289:GLY:O	1:A:354:ARG:HD2	2.17	0.45
1:B:50:ASP:CG	6:B:1490:HOH:O	2.54	0.45
1:B:84:THR:CG2	5:B:1484:MPD:C5	2.95	0.45
1:C:193:SER:CB	5:D:1486:MPD:C3	2.90	0.45
1:B:124:VAL:HG13	1:B:274:LEU:HD21	1.98	0.45
1:H:124:VAL:HG13	1:H:274:LEU:HD21	1.98	0.45
1:J:33:ILE:CD1	1:K:208:ALA:HB2	2.47	0.45
1:J:289:GLY:O	1:J:354:ARG:HD2	2.17	0.45
1:D:296:TYR:CE2	1:D:385:LYS:HD3	2.51	0.45
1:G:289:GLY:O	1:G:354:ARG:HD2	2.17	0.45
1:H:272:MET:O	1:H:355:ARG:HB2	2.17	0.45
1:D:339:ARG:HA	1:D:339:ARG:HD3	1.71	0.45
1:J:432:GLY:HA2	6:J:1605:HOH:O	2.17	0.45
1:A:206:VAL:O	1:B:34:PRO:HG2	2.17	0.45
1:D:272:MET:O	1:D:355:ARG:HB2	2.17	0.45
1:K:272:MET:O	1:K:355:ARG:HB2	2.17	0.45
1:F:432:GLY:HA2	6:F:1604:HOH:O	2.17	0.45
1:F:254:THR:HB	1:L:466:TYR:CE1	2.52	0.45
1:E:289:GLY:O	1:E:354:ARG:HD2	2.17	0.45
1:C:93:GLU:HB3	1:C:96:THR:HG23	1.98	0.45
1:B:432:GLY:HA2	6:B:1597:HOH:O	2.17	0.45
1:J:396:LEU:HG	1:J:396:LEU:H	1.54	0.45
1:D:400:PRO:HB3	1:D:401:PRO:HD2	1.97	0.45
1:H:400:PRO:HB3	1:H:401:PRO:HD2	1.97	0.45
1:H:339:ARG:HD3	6:H:1602:HOH:O	2.17	0.45
5:K:1493:MPD:HM2	5:K:1493:MPD:O4	2.16	0.45
1:I:84:THR:CG2	5:I:1491:MPD:C5	2.95	0.45
1:G:190:ASP:N	5:L:1494:MPD:HM1	2.32	0.45
1:K:289:GLY:O	1:K:354:ARG:HD2	2.17	0.45
1:B:93:GLU:HB3	1:B:96:THR:HG23	1.98	0.45
1:A:432:GLY:HA2	6:A:1590:HOH:O	2.17	0.45
1:G:296:TYR:CE2	1:G:385:LYS:HD3	2.51	0.45
1:B:289:GLY:O	1:B:354:ARG:HD2	2.17	0.45
1:L:93:GLU:HB3	1:L:96:THR:HG23	1.98	0.45
1:G:339:ARG:HD3	6:G:1602:HOH:O	2.17	0.44
1:E:84:THR:CG2	5:E:1487:MPD:C5	2.95	0.44
1:E:337:ARG:HD3	1:E:393:ASP:OD2	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:28:GLU:OE1	1:D:88:ARG:NH1	2.48	0.44
1:F:195:MET:O	1:F:199:MET:HG3	2.17	0.44
1:H:34:PRO:HG2	1:I:206:VAL:O	2.17	0.44
1:I:405:LYS:HA	1:I:405:LYS:HD2	1.84	0.44
1:D:84:THR:CG2	5:D:1486:MPD:C5	2.95	0.44
1:G:84:THR:CG2	5:G:1489:MPD:C5	2.95	0.44
1:L:124:VAL:HG13	1:L:274:LEU:HD21	1.98	0.44
1:K:28:GLU:OE1	1:K:88:ARG:NH1	2.48	0.44
1:I:289:GLY:O	1:I:354:ARG:HD2	2.17	0.44
1:H:93:GLU:HB3	1:H:96:THR:HG23	1.98	0.44
1:K:286:LYS:HE2	1:K:292:GLU:HB3	1.98	0.44
1:E:339:ARG:HD3	6:E:1597:HOH:O	2.17	0.44
1:E:458:HIS:HE1	1:K:456:THR:O	2.00	0.44
1:A:458:HIS:HE1	1:G:456:THR:O	2.00	0.44
1:A:140:PHE:CE1	1:F:160:SER:HB2	2.53	0.44
1:E:272:MET:O	1:E:355:ARG:HB2	2.17	0.44
1:H:432:GLY:HA2	6:H:1604:HOH:O	2.17	0.44
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.53	0.44
1:B:195:MET:O	1:B:199:MET:HG3	2.17	0.44
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.53	0.44
1:B:286:LYS:HE2	1:B:292:GLU:HB3	1.98	0.44
1:G:405:LYS:HD2	1:G:405:LYS:HA	1.84	0.44
1:L:54:ILE:HG22	1:L:55:GLY:N	2.33	0.44
1:E:360:PHE:CG	1:E:361:PRO:HD3	2.42	0.44
1:H:54:ILE:HG22	1:H:55:GLY:N	2.33	0.44
1:B:54:ILE:HG22	1:B:55:GLY:N	2.33	0.44
1:B:230:LYS:O	1:B:233:ASP:HB2	2.18	0.44
1:F:272:MET:O	1:F:355:ARG:HB2	2.17	0.44
1:G:272:MET:O	1:G:355:ARG:HB2	2.17	0.44
1:C:432:GLY:HA2	6:C:1597:HOH:O	2.17	0.44
1:B:4:HIS:O	1:B:7:THR:HB	2.18	0.44
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.53	0.44
1:L:400:PRO:CB	1:L:401:PRO:CD	2.96	0.44
1:E:54:ILE:HG22	1:E:55:GLY:N	2.33	0.44
1:F:84:THR:CG2	5:F:1488:MPD:C5	2.95	0.44
5:J:1492:MPD:HM1	1:K:190:ASP:N	2.33	0.44
1:A:84:THR:CG2	5:A:1483:MPD:C5	2.95	0.44
1:J:4:HIS:O	1:J:7:THR:HB	2.18	0.44
1:K:195:MET:O	1:K:199:MET:HG3	2.17	0.44
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.53	0.44
1:B:28:GLU:OE1	1:B:88:ARG:NH1	2.48	0.44
1:B:454:ARG:O	1:H:320:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:272:MET:O	1:B:355:ARG:HB2	2.17	0.44
1:H:289:GLY:O	1:H:354:ARG:HD2	2.17	0.44
1:C:400:PRO:CB	1:C:401:PRO:CD	2.96	0.44
1:H:360:PHE:CG	1:H:361:PRO:HD3	2.43	0.44
1:K:54:ILE:HG22	1:K:55:GLY:N	2.33	0.44
1:F:54:ILE:HG22	1:F:55:GLY:N	2.33	0.44
1:J:54:ILE:HG22	1:J:55:GLY:N	2.33	0.44
5:G:1489:MPD:CM	1:H:190:ASP:OD2	2.64	0.44
1:J:84:THR:CG2	5:J:1492:MPD:C5	2.95	0.44
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.53	0.44
1:A:272:MET:O	1:A:355:ARG:HB2	2.17	0.44
1:G:28:GLU:OE1	1:G:88:ARG:NH1	2.48	0.44
1:A:28:GLU:OE1	1:A:88:ARG:NH1	2.48	0.44
1:L:68:MET:HA	1:L:69:PRO:HD2	1.89	0.44
1:B:400:PRO:CB	1:B:401:PRO:CD	2.96	0.44
1:B:400:PRO:HB3	1:B:401:PRO:HD2	1.97	0.44
1:I:51:GLY:C	1:I:53:SER:N	2.26	0.44
1:C:54:ILE:HG22	1:C:55:GLY:N	2.33	0.44
1:D:81:ALA:H	5:D:1486:MPD:H13	1.79	0.44
1:L:84:THR:CG2	5:L:1494:MPD:C5	2.95	0.44
1:D:339:ARG:HD3	6:D:1600:HOH:O	2.17	0.44
1:J:195:MET:O	1:J:199:MET:HG3	2.17	0.44
1:G:230:LYS:O	1:G:233:ASP:HB2	2.18	0.44
1:D:4:HIS:O	1:D:7:THR:HB	2.18	0.44
1:C:195:MET:O	1:C:199:MET:HG3	2.17	0.44
1:F:230:LYS:O	1:F:233:ASP:HB2	2.18	0.44
1:J:93:GLU:HB3	1:J:96:THR:HG23	1.98	0.44
1:G:195:MET:O	1:G:199:MET:HG3	2.17	0.44
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.53	0.44
1:K:230:LYS:O	1:K:233:ASP:HB2	2.18	0.44
1:K:339:ARG:HD3	6:K:1607:HOH:O	2.17	0.44
1:J:400:PRO:CB	1:J:401:PRO:CD	2.96	0.44
1:I:400:PRO:CB	1:I:401:PRO:CD	2.96	0.44
1:H:224:ARG:NH2	1:H:224:ARG:HG2	2.15	0.44
1:L:339:ARG:HD3	6:L:1450:HOH:O	2.17	0.44
1:E:195:MET:O	1:E:199:MET:HG3	2.17	0.44
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.53	0.44
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.53	0.44
1:L:289:GLY:O	1:L:354:ARG:HD2	2.17	0.44
1:F:60:ILE:HD13	1:F:60:ILE:HA	1.62	0.44
1:K:53:SER:HB2	1:L:179:TYR:HE2	1.83	0.44
1:I:51:GLY:O	1:I:54:ILE:N	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:84:THR:CG2	5:K:1493:MPD:C5	2.95	0.44
1:I:80:PHE:CE2	1:J:189:GLN:HG2	2.53	0.44
1:I:337:ARG:HG2	1:I:338:ASN:N	2.33	0.44
1:J:124:VAL:HG13	1:J:274:LEU:HD21	1.98	0.44
1:G:432:GLY:HA2	6:G:1604:HOH:O	2.17	0.44
1:F:320:LYS:HG2	1:L:454:ARG:O	2.17	0.44
1:B:339:ARG:HD3	6:B:1595:HOH:O	2.17	0.44
1:F:289:GLY:O	1:F:354:ARG:HD2	2.17	0.44
1:I:230:LYS:O	1:I:233:ASP:HB2	2.18	0.44
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.53	0.44
1:F:4:HIS:O	1:F:7:THR:HB	2.18	0.44
1:D:230:LYS:O	1:D:233:ASP:HB2	2.18	0.44
1:A:4:HIS:O	1:A:7:THR:HB	2.18	0.44
1:E:93:GLU:HB3	1:E:96:THR:HG23	1.98	0.44
1:H:195:MET:O	1:H:199:MET:HG3	2.17	0.44
1:I:272:MET:O	1:I:355:ARG:HB2	2.17	0.44
1:F:339:ARG:HD3	6:F:1602:HOH:O	2.17	0.44
1:L:398:ASP:C	1:L:400:PRO:CD	2.82	0.43
1:L:51:GLY:O	1:L:54:ILE:N	2.51	0.43
1:I:54:ILE:HG22	1:I:55:GLY:N	2.33	0.43
1:C:84:THR:CG2	5:C:1485:MPD:C5	2.95	0.43
1:L:337:ARG:HG2	1:L:338:ASN:N	2.33	0.43
1:F:93:GLU:HB3	1:F:96:THR:HG23	1.98	0.43
1:D:54:ILE:HG22	1:D:55:GLY:N	2.33	0.43
1:L:272:MET:O	1:L:355:ARG:HB2	2.17	0.43
1:K:432:GLY:HA2	6:K:1609:HOH:O	2.17	0.43
1:L:4:HIS:O	1:L:7:THR:HB	2.18	0.43
1:E:432:GLY:HA2	6:E:1599:HOH:O	2.17	0.43
1:G:4:HIS:O	1:G:7:THR:HB	2.18	0.43
1:E:463:GLU:HA	1:K:140:PHE:CE1	2.53	0.43
1:C:4:HIS:O	1:C:7:THR:HB	2.18	0.43
1:A:400:PRO:CB	1:A:401:PRO:CD	2.96	0.43
1:B:395:ASN:HD22	1:B:395:ASN:HA	1.53	0.43
1:I:398:ASP:C	1:I:400:PRO:CD	2.82	0.43
1:H:84:THR:CG2	5:H:1490:MPD:C5	2.95	0.43
1:D:48:MET:HE1	1:D:66:VAL:HG22	1.96	0.43
1:D:337:ARG:HG2	1:D:338:ASN:N	2.33	0.43
1:I:339:ARG:HD3	6:I:1604:HOH:O	2.17	0.43
1:C:289:GLY:O	1:C:354:ARG:HD2	2.17	0.43
1:J:272:MET:O	1:J:355:ARG:HB2	2.17	0.43
1:J:339:ARG:HD3	6:J:1603:HOH:O	2.17	0.43
1:C:339:ARG:HD3	6:C:1595:HOH:O	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:384:ASN:N	1:A:384:ASN:ND2	2.66	0.43
1:F:337:ARG:HG2	1:F:338:ASN:N	2.33	0.43
1:L:230:LYS:O	1:L:233:ASP:HB2	2.18	0.43
1:A:230:LYS:O	1:A:233:ASP:HB2	2.18	0.43
1:C:320:LYS:HG2	1:I:454:ARG:O	2.18	0.43
1:C:254:THR:HB	1:I:466:TYR:CE1	2.54	0.43
1:I:4:HIS:O	1:I:7:THR:HB	2.18	0.43
1:K:400:PRO:CB	1:K:401:PRO:CD	2.96	0.43
1:C:189:GLN:OE1	5:D:1486:MPD:H4	2.18	0.43
1:J:33:ILE:HG13	1:K:207:GLU:O	2.19	0.43
1:D:33:ILE:HA	1:D:34:PRO:HD3	1.92	0.43
1:G:445:LEU:O	1:G:448:GLU:HG2	2.19	0.43
1:H:28:GLU:OE1	1:H:88:ARG:NH1	2.48	0.43
1:C:210:HIS:HB3	1:D:31:VAL:HG23	2.01	0.43
1:G:400:PRO:CB	1:G:401:PRO:CD	2.96	0.43
1:J:81:ALA:H	5:J:1492:MPD:H13	1.79	0.43
1:G:337:ARG:HG2	1:G:338:ASN:N	2.33	0.43
1:E:4:HIS:O	1:E:7:THR:HB	2.18	0.43
1:A:445:LEU:O	1:A:448:GLU:HG2	2.19	0.43
1:C:272:MET:O	1:C:355:ARG:HB2	2.17	0.43
1:E:230:LYS:O	1:E:233:ASP:HB2	2.18	0.43
1:H:4:HIS:O	1:H:7:THR:HB	2.18	0.43
1:H:400:PRO:CB	1:H:401:PRO:CD	2.96	0.43
1:J:360:PHE:CG	1:J:361:PRO:HD3	2.43	0.43
1:K:81:ALA:H	5:K:1493:MPD:H13	1.79	0.43
1:H:114:TYR:CD2	1:H:431:GLY:HA3	2.53	0.43
1:J:230:LYS:O	1:J:233:ASP:HB2	2.18	0.43
1:G:54:ILE:HG22	1:G:55:GLY:N	2.33	0.43
1:J:28:GLU:OE1	1:J:88:ARG:NH1	2.48	0.43
1:H:401:PRO:CB	1:H:404:ALA:HA	2.37	0.43
1:C:360:PHE:CG	1:C:361:PRO:HD3	2.43	0.43
1:A:54:ILE:HG22	1:A:55:GLY:N	2.33	0.43
1:A:193:SER:HB2	5:B:1484:MPD:C3	2.43	0.43
5:I:1491:MPD:HM2	1:J:189:GLN:HG3	2.00	0.43
1:B:337:ARG:HG2	1:B:338:ASN:N	2.33	0.43
1:E:337:ARG:HG2	1:E:338:ASN:N	2.33	0.43
1:B:339:ARG:HA	1:B:339:ARG:HD3	1.71	0.43
1:F:445:LEU:O	1:F:448:GLU:HG2	2.19	0.43
1:H:230:LYS:O	1:H:233:ASP:HB2	2.18	0.43
1:D:445:LEU:O	1:D:448:GLU:HG2	2.19	0.43
1:F:400:PRO:CB	1:F:401:PRO:CD	2.96	0.43
1:E:189:GLN:HG3	5:F:1488:MPD:HM2	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:384:ASN:N	1:E:384:ASN:ND2	2.66	0.43
1:C:384:ASN:ND2	1:C:384:ASN:N	2.66	0.43
1:K:314:PRO:HG3	1:K:365:ALA:HA	2.01	0.43
1:L:445:LEU:O	1:L:448:GLU:HG2	2.19	0.43
1:B:445:LEU:O	1:B:448:GLU:HG2	2.19	0.43
1:A:208:ALA:HB2	1:B:33:ILE:HD11	2.01	0.43
1:I:445:LEU:O	1:I:448:GLU:HG2	2.19	0.43
1:E:396:LEU:O	1:E:399:LEU:CB	2.67	0.43
1:E:400:PRO:CB	1:E:401:PRO:CD	2.96	0.43
1:E:398:ASP:C	1:E:400:PRO:CD	2.82	0.43
1:D:400:PRO:CB	1:D:401:PRO:CD	2.96	0.43
1:A:339:ARG:HD3	6:A:1588:HOH:O	2.17	0.43
1:K:114:TYR:CD2	1:K:431:GLY:HA3	2.53	0.43
1:K:4:HIS:O	1:K:7:THR:HB	2.18	0.43
1:H:445:LEU:O	1:H:448:GLU:HG2	2.19	0.43
1:I:114:TYR:CD2	1:I:431:GLY:HA3	2.53	0.43
1:D:454:ARG:O	1:J:320:LYS:HG2	2.19	0.43
1:K:445:LEU:O	1:K:448:GLU:HG2	2.19	0.43
1:A:398:ASP:C	1:A:400:PRO:CD	2.82	0.43
1:G:339:ARG:HA	1:G:339:ARG:HD3	1.71	0.43
5:A:1483:MPD:H4	1:F:189:GLN:OE1	2.19	0.43
1:C:337:ARG:HG2	1:C:338:ASN:N	2.33	0.43
1:A:337:ARG:HG2	1:A:338:ASN:N	2.33	0.43
1:H:33:ILE:HA	1:H:34:PRO:HD3	1.92	0.43
1:E:339:ARG:HD3	1:E:339:ARG:HA	1.71	0.43
1:A:208:ALA:HB2	1:B:33:ILE:CD1	2.49	0.43
1:E:28:GLU:OE1	1:E:88:ARG:NH1	2.48	0.43
1:E:206:VAL:O	1:F:34:PRO:HG2	2.19	0.43
1:J:405:LYS:HA	1:J:405:LYS:HD2	1.84	0.42
1:B:396:LEU:O	1:B:399:LEU:CB	2.67	0.42
1:K:337:ARG:HG2	1:K:338:ASN:N	2.34	0.42
1:H:314:PRO:HG3	1:H:365:ALA:HA	2.01	0.42
1:A:426:GLU:HG2	6:A:1563:HOH:O	2.20	0.42
1:G:208:ALA:HB2	1:L:33:ILE:HD11	2.01	0.42
1:G:314:PRO:HG3	1:G:365:ALA:HA	2.01	0.42
1:C:445:LEU:O	1:C:448:GLU:HG2	2.19	0.42
1:F:231:LYS:HA	1:F:231:LYS:HD2	1.82	0.42
1:F:405:LYS:HD2	1:F:405:LYS:HA	1.85	0.42
1:I:63:SER:CB	1:J:339:ARG:NH2	2.82	0.42
1:A:51:GLY:O	1:A:54:ILE:N	2.51	0.42
1:K:48:MET:HE1	1:K:66:VAL:HG22	2.01	0.42
1:E:254:THR:HB	1:K:466:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:426:GLU:HG2	6:H:1577:HOH:O	2.20	0.42
1:H:140:PHE:CE1	1:I:160:SER:HB2	2.54	0.42
1:E:314:PRO:HG3	1:E:365:ALA:HA	2.01	0.42
1:K:53:SER:HB2	1:L:179:TYR:CE2	2.55	0.42
1:B:314:PRO:HG3	1:B:365:ALA:HA	2.01	0.42
1:K:398:ASP:C	1:K:400:PRO:CD	2.82	0.42
1:H:58:LYS:NZ	1:H:60:ILE:HD11	2.35	0.42
1:F:397:TYR:OH	1:F:404:ALA:O	2.29	0.42
1:E:68:MET:HA	1:E:69:PRO:HD2	1.89	0.42
1:J:314:PRO:HG3	1:J:365:ALA:HA	2.01	0.42
1:C:28:GLU:OE1	1:C:88:ARG:NH1	2.48	0.42
1:A:405:LYS:HD2	1:A:405:LYS:HA	1.84	0.42
1:C:81:ALA:H	5:C:1485:MPD:H13	1.79	0.42
5:I:1491:MPD:CM	1:J:190:ASP:OD2	2.63	0.42
1:K:458:HIS:HD2	1:K:460:VAL:N	2.02	0.42
1:C:208:ALA:HB2	1:D:33:ILE:CD1	2.50	0.42
1:C:33:ILE:HA	1:C:34:PRO:HD3	1.92	0.42
1:F:28:GLU:OE1	1:F:88:ARG:NH1	2.48	0.42
1:K:231:LYS:HD2	1:K:231:LYS:HA	1.82	0.42
1:D:398:ASP:C	1:D:400:PRO:CD	2.82	0.42
1:K:397:TYR:OH	1:K:404:ALA:O	2.29	0.42
1:C:396:LEU:O	1:C:399:LEU:CB	2.67	0.42
1:D:426:GLU:HG2	6:D:1575:HOH:O	2.20	0.42
1:E:426:GLU:HG2	6:E:1572:HOH:O	2.19	0.42
1:E:127:GLY:HA3	3:E:1475:ADP:H1'	2.02	0.42
1:D:58:LYS:HZ2	1:D:60:ILE:HD13	1.84	0.42
1:F:396:LEU:O	1:F:399:LEU:CB	2.67	0.42
1:B:48:MET:HE1	1:B:66:VAL:HG22	1.99	0.42
1:C:230:LYS:O	1:C:233:ASP:HB2	2.18	0.42
1:D:320:LYS:HG2	1:J:454:ARG:O	2.18	0.42
1:A:401:PRO:CB	1:A:404:ALA:HA	2.37	0.42
1:E:58:LYS:NZ	1:E:60:ILE:HD11	2.35	0.42
1:H:337:ARG:HG2	1:H:338:ASN:N	2.33	0.42
1:C:68:MET:HA	1:C:69:PRO:HD2	1.89	0.42
1:L:426:GLU:HG2	6:L:1421:HOH:O	2.20	0.42
1:K:127:GLY:HA3	3:K:1481:ADP:H1'	2.02	0.42
1:K:403:GLU:C	1:K:405:LYS:H	2.23	0.42
1:G:403:GLU:O	1:G:404:ALA:HB3	2.20	0.42
1:J:339:ARG:HD3	1:J:339:ARG:HA	1.71	0.42
1:A:190:ASP:OD2	5:B:1484:MPD:CM	2.65	0.42
1:K:384:ASN:N	1:K:384:ASN:ND2	2.66	0.42
1:C:426:GLU:HG2	6:C:1571:HOH:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:28:GLU:OE1	1:I:88:ARG:NH1	2.48	0.42
1:J:445:LEU:O	1:J:448:GLU:HG2	2.19	0.42
1:B:127:GLY:HA3	3:B:1472:ADP:H1'	2.02	0.42
1:J:403:GLU:O	1:J:404:ALA:HB3	2.20	0.42
1:C:58:LYS:NZ	1:C:60:ILE:HD11	2.35	0.42
1:H:80:PHE:CZ	1:I:189:GLN:HG2	2.55	0.42
1:L:405:LYS:HD2	1:L:405:LYS:HA	1.84	0.42
1:A:230:LYS:HB2	1:A:230:LYS:HE3	1.89	0.42
1:E:445:LEU:O	1:E:448:GLU:HG2	2.19	0.42
1:A:31:VAL:HG23	1:F:210:HIS:HB3	2.02	0.42
1:H:68:MET:HA	1:H:69:PRO:HD2	1.89	0.42
1:I:314:PRO:HG3	1:I:365:ALA:HA	2.01	0.42
1:K:426:GLU:HG2	6:K:1582:HOH:O	2.20	0.42
1:F:426:GLU:HG2	6:F:1577:HOH:O	2.19	0.42
1:H:127:GLY:HA3	3:H:1478:ADP:H1'	2.02	0.41
1:D:396:LEU:O	1:D:399:LEU:CB	2.67	0.41
1:K:58:LYS:NZ	1:K:60:ILE:HD11	2.35	0.41
1:G:58:LYS:NZ	1:G:60:ILE:HD11	2.35	0.41
1:H:51:GLY:O	1:H:54:ILE:N	2.51	0.41
1:A:53:SER:CB	1:F:179:TYR:CE2	3.03	0.41
1:C:339:ARG:HA	1:C:339:ARG:HD3	1.71	0.41
1:B:81:ALA:H	5:B:1484:MPD:H13	1.79	0.41
5:J:1492:MPD:CM	1:K:190:ASP:OD2	2.59	0.41
1:A:82:ASP:O	1:A:84:THR:CG2	2.55	0.41
1:G:426:GLU:HG2	6:G:1577:HOH:O	2.19	0.41
1:C:314:PRO:HG3	1:C:365:ALA:HA	2.01	0.41
1:D:328:ALA:HA	1:D:329:PRO:HD2	1.93	0.41
1:A:314:PRO:HG3	1:A:365:ALA:HA	2.01	0.41
1:A:396:LEU:O	1:A:399:LEU:CB	2.67	0.41
1:B:403:GLU:C	1:B:405:LYS:H	2.24	0.41
1:C:403:GLU:O	1:C:404:ALA:HB3	2.20	0.41
1:D:58:LYS:NZ	1:D:60:ILE:HD11	2.35	0.41
1:G:396:LEU:O	1:G:399:LEU:CB	2.67	0.41
1:J:51:GLY:O	1:J:54:ILE:N	2.51	0.41
1:C:390:GLU:HA	1:C:391:PRO:HD3	1.95	0.41
1:L:230:LYS:HB2	1:L:230:LYS:HE3	1.89	0.41
1:G:127:GLY:HA3	3:G:1477:ADP:H1'	2.02	0.41
1:A:127:GLY:HA3	3:A:1471:ADP:H1'	2.02	0.41
1:F:340:SER:OG	1:F:396:LEU:CB	2.69	0.41
1:F:403:GLU:C	1:F:405:LYS:H	2.23	0.41
1:B:189:GLN:HG3	5:C:1485:MPD:HM2	2.00	0.41
1:J:80:PHE:CE2	1:K:189:GLN:HG2	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:337:ARG:HG2	1:J:338:ASN:N	2.33	0.41
1:L:328:ALA:HA	1:L:329:PRO:HD2	1.93	0.41
1:J:426:GLU:HG2	6:J:1578:HOH:O	2.20	0.41
1:K:31:VAL:HG23	1:L:210:HIS:HB3	2.03	0.41
1:I:58:LYS:NZ	1:I:60:ILE:HD11	2.35	0.41
1:G:58:LYS:HZ2	1:G:60:ILE:HD13	1.84	0.41
1:K:403:GLU:O	1:K:404:ALA:HB3	2.20	0.41
1:A:58:LYS:NZ	1:A:60:ILE:HD11	2.35	0.41
1:G:340:SER:OG	1:G:396:LEU:CB	2.69	0.41
1:I:81:ALA:H	5:I:1491:MPD:H13	1.79	0.41
1:K:339:ARG:HA	1:K:339:ARG:HD3	1.71	0.41
1:F:339:ARG:HA	1:F:339:ARG:HD3	1.71	0.41
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.82	0.41
1:J:340:SER:OG	1:J:396:LEU:CB	2.69	0.41
1:K:405:LYS:HD2	1:K:405:LYS:HA	1.84	0.41
1:F:398:ASP:C	1:F:400:PRO:CD	2.82	0.41
1:E:51:GLY:O	1:E:54:ILE:N	2.51	0.41
1:D:179:TYR:HE2	1:E:53:SER:HB2	1.86	0.41
5:H:1490:MPD:HM1	1:I:190:ASP:N	2.35	0.41
1:D:16:PHE:CG	5:D:1486:MPD:H52	2.55	0.41
1:L:49:PHE:O	1:L:64:ASP:OD2	2.39	0.41
1:H:49:PHE:O	1:H:64:ASP:OD2	2.39	0.41
1:B:426:GLU:HG2	6:B:1570:HOH:O	2.20	0.41
1:B:254:THR:HB	1:H:466:TYR:CE1	2.55	0.41
1:C:127:GLY:HA3	3:C:1473:ADP:H1'	2.02	0.41
1:J:396:LEU:O	1:J:399:LEU:CB	2.67	0.41
1:B:403:GLU:O	1:B:404:ALA:HB3	2.20	0.41
1:H:403:GLU:O	1:H:404:ALA:HB3	2.20	0.41
1:A:16:PHE:CG	5:A:1483:MPD:H52	2.55	0.41
1:A:1:SER:CA	1:A:71:ALA:CB	2.80	0.41
1:H:405:LYS:HA	1:H:405:LYS:HD2	1.85	0.41
1:A:49:PHE:O	1:A:64:ASP:OD2	2.39	0.41
1:D:314:PRO:HG3	1:D:365:ALA:HA	2.01	0.41
1:K:396:LEU:HG	1:K:396:LEU:H	1.54	0.41
1:I:396:LEU:H	1:I:396:LEU:HG	1.54	0.41
1:C:340:SER:OG	1:C:396:LEU:CB	2.69	0.41
1:B:51:GLY:O	1:B:54:ILE:N	2.51	0.41
1:C:82:ASP:O	1:C:84:THR:CG2	2.55	0.41
1:B:384:ASN:N	1:B:384:ASN:ND2	2.66	0.41
1:J:49:PHE:O	1:J:64:ASP:OD2	2.39	0.41
1:C:49:PHE:O	1:C:64:ASP:OD2	2.39	0.41
1:K:140:PHE:CE1	1:L:160:SER:HB2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:284:GLY:HA3	1:F:291:SER:HA	2.03	0.41
1:G:206:VAL:O	1:L:34:PRO:HG2	2.21	0.41
1:F:314:PRO:HG3	1:F:365:ALA:HA	2.01	0.41
1:J:403:GLU:C	1:J:405:LYS:H	2.23	0.41
1:C:396:LEU:H	1:C:396:LEU:HG	1.54	0.41
1:G:403:GLU:C	1:G:405:LYS:H	2.23	0.41
1:C:51:GLY:O	1:C:54:ILE:N	2.51	0.41
1:E:190:ASP:N	5:F:1488:MPD:HM1	2.36	0.41
1:E:81:ALA:H	5:E:1487:MPD:H13	1.79	0.41
1:B:177:GLY:C	1:B:179:TYR:H	2.25	0.41
1:H:384:ASN:ND2	1:H:384:ASN:N	2.66	0.41
1:D:284:GLY:HA3	1:D:291:SER:HA	2.03	0.41
1:I:426:GLU:HG2	6:I:1579:HOH:O	2.20	0.41
1:C:466:TYR:CE1	1:I:254:THR:HB	2.56	0.41
1:L:314:PRO:HG3	1:L:365:ALA:HA	2.01	0.41
1:L:127:GLY:HA3	3:L:1482:ADP:H1'	2.02	0.41
1:F:58:LYS:NZ	1:F:60:ILE:HD11	2.35	0.41
1:E:340:SER:OG	1:E:396:LEU:CB	2.69	0.41
1:A:403:GLU:O	1:A:404:ALA:HB3	2.20	0.41
1:B:58:LYS:NZ	1:B:60:ILE:HD11	2.35	0.41
1:B:58:LYS:HZ2	1:B:60:ILE:HD13	1.85	0.41
1:L:403:GLU:O	1:L:404:ALA:HB3	2.20	0.41
1:H:398:ASP:C	1:H:400:PRO:CD	2.82	0.41
1:I:396:LEU:O	1:I:399:LEU:CB	2.67	0.41
1:I:340:SER:OG	1:I:396:LEU:CB	2.69	0.41
1:I:403:GLU:O	1:I:404:ALA:HB3	2.20	0.41
1:C:403:GLU:C	1:C:405:LYS:H	2.23	0.41
1:C:398:ASP:C	1:C:400:PRO:CD	2.82	0.41
1:F:403:GLU:O	1:F:404:ALA:HB3	2.20	0.41
1:F:51:GLY:O	1:F:54:ILE:N	2.51	0.41
1:I:177:GLY:C	1:I:179:TYR:H	2.25	0.41
1:F:177:GLY:C	1:F:179:TYR:H	2.25	0.41
1:C:179:TYR:HE2	1:D:53:SER:HB2	1.86	0.41
1:H:80:PHE:CE2	1:I:189:GLN:HG2	2.55	0.41
1:C:458:HIS:HD2	1:C:460:VAL:N	2.02	0.41
1:J:177:GLY:C	1:J:179:TYR:H	2.24	0.41
1:B:49:PHE:O	1:B:64:ASP:OD2	2.39	0.41
1:D:49:PHE:O	1:D:64:ASP:OD2	2.39	0.41
1:A:281:LEU:HD23	1:A:293:GLN:OE1	2.21	0.41
1:G:284:GLY:HA3	1:G:291:SER:HA	2.03	0.41
1:H:281:LEU:HD23	1:H:293:GLN:OE1	2.21	0.41
1:A:68:MET:HA	1:A:69:PRO:HD2	1.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:68:MET:HA	1:I:69:PRO:HD2	1.89	0.41
1:K:128:PRO:HD2	6:K:1507:HOH:O	2.21	0.41
1:J:31:VAL:HG23	1:K:210:HIS:HB3	2.03	0.41
1:E:350:SER:HA	1:E:351:PRO:HD3	1.98	0.41
1:D:127:GLY:HA3	3:D:1474:ADP:H1'	2.02	0.41
1:E:403:GLU:C	1:E:405:LYS:H	2.24	0.41
1:E:403:GLU:O	1:E:404:ALA:HB3	2.20	0.41
1:A:403:GLU:C	1:A:405:LYS:H	2.23	0.41
1:B:340:SER:OG	1:B:396:LEU:CB	2.69	0.41
1:I:360:PHE:CG	1:I:361:PRO:HD3	2.43	0.41
1:H:16:PHE:CG	5:H:1490:MPD:H52	2.55	0.41
1:I:16:PHE:CG	5:I:1491:MPD:H52	2.55	0.41
1:F:384:ASN:N	1:F:384:ASN:ND2	2.66	0.41
1:A:207:GLU:O	1:B:33:ILE:HG13	2.20	0.41
1:J:284:GLY:HA3	1:J:291:SER:HA	2.03	0.41
1:C:281:LEU:HD23	1:C:293:GLN:OE1	2.21	0.41
1:C:284:GLY:HA3	1:C:291:SER:HA	2.03	0.41
1:L:284:GLY:HA3	1:L:291:SER:HA	2.03	0.41
1:G:281:LEU:HD23	1:G:293:GLN:OE1	2.21	0.41
1:K:396:LEU:O	1:K:399:LEU:CB	2.67	0.40
1:K:51:GLY:O	1:K:54:ILE:N	2.51	0.40
1:F:16:PHE:CG	5:F:1488:MPD:H52	2.55	0.40
1:J:33:ILE:HA	1:J:34:PRO:HD3	1.92	0.40
1:K:33:ILE:HA	1:K:34:PRO:HD3	1.92	0.40
1:J:50:ASP:CG	6:J:1612:HOH:O	2.59	0.40
1:B:466:TYR:CE1	1:H:254:THR:HB	2.56	0.40
1:L:50:ASP:CG	6:L:838:HOH:O	2.60	0.40
1:J:231:LYS:HA	1:J:231:LYS:HD2	1.82	0.40
1:I:281:LEU:HD23	1:I:293:GLN:OE1	2.21	0.40
1:F:127:GLY:HA3	3:F:1476:ADP:H1'	2.02	0.40
1:J:127:GLY:HA3	3:J:1480:ADP:H1'	2.02	0.40
1:D:403:GLU:O	1:D:404:ALA:HB3	2.20	0.40
1:L:340:SER:OG	1:L:396:LEU:CB	2.69	0.40
1:H:340:SER:OG	1:H:396:LEU:CB	2.69	0.40
1:B:16:PHE:CG	5:B:1484:MPD:H52	2.55	0.40
1:B:189:GLN:HG2	1:C:80:PHE:CE2	2.57	0.40
1:E:49:PHE:O	1:E:64:ASP:OD2	2.39	0.40
1:A:128:PRO:HD2	6:A:1487:HOH:O	2.21	0.40
1:E:128:PRO:HD2	6:E:1497:HOH:O	2.21	0.40
1:H:396:LEU:O	1:H:399:LEU:CB	2.67	0.40
1:H:53:SER:HB2	1:I:179:TYR:HE2	1.86	0.40
1:H:339:ARG:HD3	1:H:339:ARG:HA	1.71	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:82:ASP:O	1:D:84:THR:CG2	2.55	0.40
1:G:189:GLN:HG2	1:L:80:PHE:CE2	2.57	0.40
1:I:230:LYS:HB2	1:I:230:LYS:HE3	1.89	0.40
1:K:281:LEU:HD23	1:K:293:GLN:OE1	2.21	0.40
1:B:204:LEU:HD23	1:B:223:THR:HG21	2.04	0.40
5:K:1493:MPD:H4	1:L:189:GLN:OE1	2.21	0.40
1:D:230:LYS:HE3	1:D:230:LYS:HB2	1.89	0.40
1:D:281:LEU:HD23	1:D:293:GLN:OE1	2.21	0.40
1:J:281:LEU:HD23	1:J:293:GLN:OE1	2.21	0.40
1:F:281:LEU:HD23	1:F:293:GLN:OE1	2.21	0.40
1:A:284:GLY:HA3	1:A:291:SER:HA	2.03	0.40
1:I:403:GLU:C	1:I:405:LYS:H	2.24	0.40
1:A:180:PHE:CB	1:B:29:GLN:HB3	2.50	0.40
1:L:384:ASN:N	1:L:384:ASN:ND2	2.66	0.40
1:K:49:PHE:O	1:K:64:ASP:OD2	2.39	0.40
1:J:419:ASN:O	1:J:422:ASP:HB3	2.22	0.40
1:H:284:GLY:HA3	1:H:291:SER:HA	2.03	0.40
1:D:254:THR:HB	1:J:466:TYR:CE1	2.57	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%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	B	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	C	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	D	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	E	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	F	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	G	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	H	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	J	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	K	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	L	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
All	All	5592/5616 (100%)	5148 (92%)	336 (6%)	108 (2%)	12	28

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	62	GLU
1	A	180	PHE
1	A	399	LEU
1	A	400	PRO
1	A	401	PRO
1	B	52	SER
1	B	62	GLU
1	B	180	PHE
1	B	399	LEU
1	B	400	PRO
1	B	401	PRO
1	C	52	SER
1	C	62	GLU
1	C	180	PHE
1	C	399	LEU
1	C	400	PRO
1	C	401	PRO
1	D	52	SER
1	D	62	GLU
1	D	180	PHE
1	D	399	LEU
1	D	400	PRO
1	D	401	PRO
1	E	52	SER
1	E	62	GLU
1	E	180	PHE
1	E	399	LEU
1	E	400	PRO
1	E	401	PRO
1	F	52	SER
1	F	62	GLU

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Mol	Chain	Res	Type
1	F	180	PHE
1	F	399	LEU
1	F	400	PRO
1	F	401	PRO
1	G	52	SER
1	G	62	GLU
1	G	180	PHE
1	G	399	LEU
1	G	400	PRO
1	G	401	PRO
1	H	52	SER
1	H	62	GLU
1	H	180	PHE
1	H	399	LEU
1	H	400	PRO
1	H	401	PRO
1	I	52	SER
1	I	62	GLU
1	I	180	PHE
1	I	399	LEU
1	I	400	PRO
1	I	401	PRO
1	J	52	SER
1	J	62	GLU
1	J	180	PHE
1	J	399	LEU
1	J	400	PRO
1	J	401	PRO
1	K	52	SER
1	K	62	GLU
1	K	180	PHE
1	K	399	LEU
1	K	400	PRO
1	K	401	PRO
1	L	52	SER
1	L	62	GLU
1	L	180	PHE
1	L	399	LEU
1	L	400	PRO
1	L	401	PRO
1	A	324	PRO
1	A	396	LEU

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Mol	Chain	Res	Type
1	B	324	PRO
1	B	396	LEU
1	C	324	PRO
1	C	396	LEU
1	D	324	PRO
1	D	396	LEU
1	E	324	PRO
1	E	396	LEU
1	F	324	PRO
1	F	396	LEU
1	G	324	PRO
1	G	396	LEU
1	H	324	PRO
1	H	396	LEU
1	I	324	PRO
1	I	396	LEU
1	J	324	PRO
1	J	396	LEU
1	K	324	PRO
1	K	396	LEU
1	L	324	PRO
1	L	396	LEU
1	A	349	ALA
1	B	349	ALA
1	C	349	ALA
1	D	349	ALA
1	E	349	ALA
1	F	349	ALA
1	G	349	ALA
1	H	349	ALA
1	I	349	ALA
1	J	349	ALA
1	K	349	ALA
1	L	349	ALA

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%)	341 (89%)	43 (11%)	9	19
1	B	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	C	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	D	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	E	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	F	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	G	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	H	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	I	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	J	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	K	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	L	384/384 (100%)	341 (89%)	43 (11%)	9	19
All	All	4608/4608 (100%)	4092 (89%)	516 (11%)	9	19

All (516) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	15	LYS
1	A	19	LEU
1	A	33	ILE
1	A	48	MET
1	A	49	PHE
1	A	50	ASP
1	A	60	ILE
1	A	62	GLU
1	A	63	SER
1	A	64	ASP
1	A	84	THR
1	A	96	THR
1	A	115	LEU
1	A	124	VAL
1	A	125	LEU
1	A	147	SER
1	A	179	TYR
1	A	181	PRO
1	A	209	HIS
1	A	224	ARG
1	A	264	ASN

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Mol	Chain	Res	Type
1	A	290	LEU
1	A	323	VAL
1	A	326	TYR
1	A	332	LEU
1	A	337	ARG
1	A	339	ARG
1	A	340	SER
1	A	344	ARG
1	A	355	ARG
1	A	374	LEU
1	A	375	LEU
1	A	384	ASN
1	A	395	ASN
1	A	396	LEU
1	A	397	TYR
1	A	403	GLU
1	A	419	ASN
1	A	428	LEU
1	A	447	ARG
1	A	464	LEU
1	A	468	VAL
1	B	1	SER
1	B	15	LYS
1	B	19	LEU
1	B	33	ILE
1	B	48	MET
1	B	49	PHE
1	B	50	ASP
1	B	60	ILE
1	B	62	GLU
1	B	63	SER
1	B	64	ASP
1	B	84	THR
1	B	96	THR
1	B	115	LEU
1	B	124	VAL
1	B	125	LEU
1	B	147	SER
1	B	179	TYR
1	B	181	PRO
1	B	209	HIS
1	B	224	ARG

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Mol	Chain	Res	Type
1	B	264	ASN
1	B	290	LEU
1	B	323	VAL
1	B	326	TYR
1	B	332	LEU
1	B	337	ARG
1	B	339	ARG
1	B	340	SER
1	B	344	ARG
1	B	355	ARG
1	B	374	LEU
1	B	375	LEU
1	B	384	ASN
1	B	395	ASN
1	B	396	LEU
1	B	397	TYR
1	B	403	GLU
1	B	419	ASN
1	B	428	LEU
1	B	447	ARG
1	B	464	LEU
1	B	468	VAL
1	C	1	SER
1	C	15	LYS
1	C	19	LEU
1	C	33	ILE
1	C	48	MET
1	C	49	PHE
1	C	50	ASP
1	C	60	ILE
1	C	62	GLU
1	C	63	SER
1	C	64	ASP
1	C	84	THR
1	C	96	THR
1	C	115	LEU
1	C	124	VAL
1	C	125	LEU
1	C	147	SER
1	C	179	TYR
1	C	181	PRO
1	C	209	HIS

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Mol	Chain	Res	Type
1	C	224	ARG
1	C	264	ASN
1	C	290	LEU
1	C	323	VAL
1	C	326	TYR
1	C	332	LEU
1	C	337	ARG
1	C	339	ARG
1	C	340	SER
1	C	344	ARG
1	C	355	ARG
1	C	374	LEU
1	C	375	LEU
1	C	384	ASN
1	C	395	ASN
1	C	396	LEU
1	C	397	TYR
1	C	403	GLU
1	C	419	ASN
1	C	428	LEU
1	C	447	ARG
1	C	464	LEU
1	C	468	VAL
1	D	1	SER
1	D	15	LYS
1	D	19	LEU
1	D	33	ILE
1	D	48	MET
1	D	49	PHE
1	D	50	ASP
1	D	60	ILE
1	D	62	GLU
1	D	63	SER
1	D	64	ASP
1	D	84	THR
1	D	96	THR
1	D	115	LEU
1	D	124	VAL
1	D	125	LEU
1	D	147	SER
1	D	179	TYR
1	D	181	PRO

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Mol	Chain	Res	Type
1	D	209	HIS
1	D	224	ARG
1	D	264	ASN
1	D	290	LEU
1	D	323	VAL
1	D	326	TYR
1	D	332	LEU
1	D	337	ARG
1	D	339	ARG
1	D	340	SER
1	D	344	ARG
1	D	355	ARG
1	D	374	LEU
1	D	375	LEU
1	D	384	ASN
1	D	395	ASN
1	D	396	LEU
1	D	397	TYR
1	D	403	GLU
1	D	419	ASN
1	D	428	LEU
1	D	447	ARG
1	D	464	LEU
1	D	468	VAL
1	E	1	SER
1	E	15	LYS
1	E	19	LEU
1	E	33	ILE
1	E	48	MET
1	E	49	PHE
1	E	50	ASP
1	E	60	ILE
1	E	62	GLU
1	E	63	SER
1	E	64	ASP
1	E	84	THR
1	E	96	THR
1	E	115	LEU
1	E	124	VAL
1	E	125	LEU
1	E	147	SER
1	E	179	TYR

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Mol	Chain	Res	Type
1	E	181	PRO
1	E	209	HIS
1	E	224	ARG
1	E	264	ASN
1	E	290	LEU
1	E	323	VAL
1	E	326	TYR
1	E	332	LEU
1	E	337	ARG
1	E	339	ARG
1	E	340	SER
1	E	344	ARG
1	E	355	ARG
1	E	374	LEU
1	E	375	LEU
1	E	384	ASN
1	E	395	ASN
1	E	396	LEU
1	E	397	TYR
1	E	403	GLU
1	E	419	ASN
1	E	428	LEU
1	E	447	ARG
1	E	464	LEU
1	E	468	VAL
1	F	1	SER
1	F	15	LYS
1	F	19	LEU
1	F	33	ILE
1	F	48	MET
1	F	49	PHE
1	F	50	ASP
1	F	60	ILE
1	F	62	GLU
1	F	63	SER
1	F	64	ASP
1	F	84	THR
1	F	96	THR
1	F	115	LEU
1	F	124	VAL
1	F	125	LEU
1	F	147	SER

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Mol	Chain	Res	Type
1	F	179	TYR
1	F	181	PRO
1	F	209	HIS
1	F	224	ARG
1	F	264	ASN
1	F	290	LEU
1	F	323	VAL
1	F	326	TYR
1	F	332	LEU
1	F	337	ARG
1	F	339	ARG
1	F	340	SER
1	F	344	ARG
1	F	355	ARG
1	F	374	LEU
1	F	375	LEU
1	F	384	ASN
1	F	395	ASN
1	F	396	LEU
1	F	397	TYR
1	F	403	GLU
1	F	419	ASN
1	F	428	LEU
1	F	447	ARG
1	F	464	LEU
1	F	468	VAL
1	G	1	SER
1	G	15	LYS
1	G	19	LEU
1	G	33	ILE
1	G	48	MET
1	G	49	PHE
1	G	50	ASP
1	G	60	ILE
1	G	62	GLU
1	G	63	SER
1	G	64	ASP
1	G	84	THR
1	G	96	THR
1	G	115	LEU
1	G	124	VAL
1	G	125	LEU

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Mol	Chain	Res	Type
1	G	147	SER
1	G	179	TYR
1	G	181	PRO
1	G	209	HIS
1	G	224	ARG
1	G	264	ASN
1	G	290	LEU
1	G	323	VAL
1	G	326	TYR
1	G	332	LEU
1	G	337	ARG
1	G	339	ARG
1	G	340	SER
1	G	344	ARG
1	G	355	ARG
1	G	374	LEU
1	G	375	LEU
1	G	384	ASN
1	G	395	ASN
1	G	396	LEU
1	G	397	TYR
1	G	403	GLU
1	G	419	ASN
1	G	428	LEU
1	G	447	ARG
1	G	464	LEU
1	G	468	VAL
1	H	1	SER
1	H	15	LYS
1	H	19	LEU
1	H	33	ILE
1	H	48	MET
1	H	49	PHE
1	H	50	ASP
1	H	60	ILE
1	H	62	GLU
1	H	63	SER
1	H	64	ASP
1	H	84	THR
1	H	96	THR
1	H	115	LEU
1	H	124	VAL

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Mol	Chain	Res	Type
1	H	125	LEU
1	H	147	SER
1	H	179	TYR
1	H	181	PRO
1	H	209	HIS
1	H	224	ARG
1	H	264	ASN
1	H	290	LEU
1	H	323	VAL
1	H	326	TYR
1	H	332	LEU
1	H	337	ARG
1	H	339	ARG
1	H	340	SER
1	H	344	ARG
1	H	355	ARG
1	H	374	LEU
1	H	375	LEU
1	H	384	ASN
1	H	395	ASN
1	H	396	LEU
1	H	397	TYR
1	H	403	GLU
1	H	419	ASN
1	H	428	LEU
1	H	447	ARG
1	H	464	LEU
1	H	468	VAL
1	I	1	SER
1	I	15	LYS
1	I	19	LEU
1	I	33	ILE
1	I	48	MET
1	I	49	PHE
1	I	50	ASP
1	I	60	ILE
1	I	62	GLU
1	I	63	SER
1	I	64	ASP
1	I	84	THR
1	I	96	THR
1	I	115	LEU

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Mol	Chain	Res	Type
1	I	124	VAL
1	I	125	LEU
1	I	147	SER
1	I	179	TYR
1	I	181	PRO
1	I	209	HIS
1	I	224	ARG
1	I	264	ASN
1	I	290	LEU
1	I	323	VAL
1	I	326	TYR
1	I	332	LEU
1	I	337	ARG
1	I	339	ARG
1	I	340	SER
1	I	344	ARG
1	I	355	ARG
1	I	374	LEU
1	I	375	LEU
1	I	384	ASN
1	I	395	ASN
1	I	396	LEU
1	I	397	TYR
1	I	403	GLU
1	I	419	ASN
1	I	428	LEU
1	I	447	ARG
1	I	464	LEU
1	I	468	VAL
1	J	1	SER
1	J	15	LYS
1	J	19	LEU
1	J	33	ILE
1	J	48	MET
1	J	49	PHE
1	J	50	ASP
1	J	60	ILE
1	J	62	GLU
1	J	63	SER
1	J	64	ASP
1	J	84	THR
1	J	96	THR

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Mol	Chain	Res	Type
1	J	115	LEU
1	J	124	VAL
1	J	125	LEU
1	J	147	SER
1	J	179	TYR
1	J	181	PRO
1	J	209	HIS
1	J	224	ARG
1	J	264	ASN
1	J	290	LEU
1	J	323	VAL
1	J	326	TYR
1	J	332	LEU
1	J	337	ARG
1	J	339	ARG
1	J	340	SER
1	J	344	ARG
1	J	355	ARG
1	J	374	LEU
1	J	375	LEU
1	J	384	ASN
1	J	395	ASN
1	J	396	LEU
1	J	397	TYR
1	J	403	GLU
1	J	419	ASN
1	J	428	LEU
1	J	447	ARG
1	J	464	LEU
1	J	468	VAL
1	K	1	SER
1	K	15	LYS
1	K	19	LEU
1	K	33	ILE
1	K	48	MET
1	K	49	PHE
1	K	50	ASP
1	K	60	ILE
1	K	62	GLU
1	K	63	SER
1	K	64	ASP
1	K	84	THR

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Mol	Chain	Res	Type
1	K	96	THR
1	K	115	LEU
1	K	124	VAL
1	K	125	LEU
1	K	147	SER
1	K	179	TYR
1	K	181	PRO
1	K	209	HIS
1	K	224	ARG
1	K	264	ASN
1	K	290	LEU
1	K	323	VAL
1	K	326	TYR
1	K	332	LEU
1	K	337	ARG
1	K	339	ARG
1	K	340	SER
1	K	344	ARG
1	K	355	ARG
1	K	374	LEU
1	K	375	LEU
1	K	384	ASN
1	K	395	ASN
1	K	396	LEU
1	K	397	TYR
1	K	403	GLU
1	K	419	ASN
1	K	428	LEU
1	K	447	ARG
1	K	464	LEU
1	K	468	VAL
1	L	1	SER
1	L	15	LYS
1	L	19	LEU
1	L	33	ILE
1	L	48	MET
1	L	49	PHE
1	L	50	ASP
1	L	60	ILE
1	L	62	GLU
1	L	63	SER
1	L	64	ASP

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Mol	Chain	Res	Type
1	L	84	THR
1	L	96	THR
1	L	115	LEU
1	L	124	VAL
1	L	125	LEU
1	L	147	SER
1	L	179	TYR
1	L	181	PRO
1	L	209	HIS
1	L	224	ARG
1	L	264	ASN
1	L	290	LEU
1	L	323	VAL
1	L	326	TYR
1	L	332	LEU
1	L	337	ARG
1	L	339	ARG
1	L	340	SER
1	L	344	ARG
1	L	355	ARG
1	L	374	LEU
1	L	375	LEU
1	L	384	ASN
1	L	395	ASN
1	L	396	LEU
1	L	397	TYR
1	L	403	GLU
1	L	419	ASN
1	L	428	LEU
1	L	447	ARG
1	L	464	LEU
1	L	468	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	211	HIS
1	A	218	GLN
1	A	219	ASN
1	A	244	ASN
1	A	313	ASN

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Mol	Chain	Res	Type
1	A	338	ASN
1	A	384	ASN
1	A	395	ASN
1	A	409	GLN
1	A	458	HIS
1	B	61	ASN
1	B	211	HIS
1	B	218	GLN
1	B	219	ASN
1	B	244	ASN
1	B	313	ASN
1	B	338	ASN
1	B	384	ASN
1	B	395	ASN
1	B	409	GLN
1	B	458	HIS
1	C	61	ASN
1	C	211	HIS
1	C	218	GLN
1	C	219	ASN
1	C	236	GLN
1	C	244	ASN
1	C	313	ASN
1	C	338	ASN
1	C	384	ASN
1	C	395	ASN
1	C	409	GLN
1	C	458	HIS
1	D	61	ASN
1	D	211	HIS
1	D	218	GLN
1	D	219	ASN
1	D	244	ASN
1	D	313	ASN
1	D	338	ASN
1	D	384	ASN
1	D	395	ASN
1	D	409	GLN
1	D	458	HIS
1	E	61	ASN
1	E	211	HIS
1	E	218	GLN

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Mol	Chain	Res	Type
1	E	219	ASN
1	E	236	GLN
1	E	244	ASN
1	E	313	ASN
1	E	338	ASN
1	E	384	ASN
1	E	395	ASN
1	E	409	GLN
1	E	458	HIS
1	F	61	ASN
1	F	211	HIS
1	F	218	GLN
1	F	219	ASN
1	F	236	GLN
1	F	244	ASN
1	F	313	ASN
1	F	338	ASN
1	F	384	ASN
1	F	395	ASN
1	F	409	GLN
1	F	458	HIS
1	G	61	ASN
1	G	211	HIS
1	G	218	GLN
1	G	219	ASN
1	G	244	ASN
1	G	313	ASN
1	G	338	ASN
1	G	384	ASN
1	G	395	ASN
1	G	409	GLN
1	G	458	HIS
1	H	61	ASN
1	H	211	HIS
1	H	218	GLN
1	H	219	ASN
1	H	236	GLN
1	H	244	ASN
1	H	313	ASN
1	H	338	ASN
1	H	384	ASN
1	H	395	ASN

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Mol	Chain	Res	Type
1	H	409	GLN
1	H	458	HIS
1	I	61	ASN
1	I	211	HIS
1	I	218	GLN
1	I	219	ASN
1	I	244	ASN
1	I	313	ASN
1	I	338	ASN
1	I	384	ASN
1	I	395	ASN
1	I	409	GLN
1	I	458	HIS
1	J	61	ASN
1	J	211	HIS
1	J	218	GLN
1	J	219	ASN
1	J	244	ASN
1	J	313	ASN
1	J	338	ASN
1	J	384	ASN
1	J	395	ASN
1	J	409	GLN
1	J	458	HIS
1	K	61	ASN
1	K	211	HIS
1	K	218	GLN
1	K	219	ASN
1	K	236	GLN
1	K	244	ASN
1	K	313	ASN
1	K	338	ASN
1	K	384	ASN
1	K	395	ASN
1	K	409	GLN
1	K	458	HIS
1	L	61	ASN
1	L	211	HIS
1	L	218	GLN
1	L	219	ASN
1	L	236	GLN
1	L	244	ASN

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Mol	Chain	Res	Type
1	L	313	ASN
1	L	338	ASN
1	L	384	ASN
1	L	395	ASN
1	L	409	GLN
1	L	458	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 72 ligands modelled in this entry, 48 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	1471	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	A	1483	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	B	1472	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	B	1484	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	C	1473	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	C	1485	-	7,7,7	1.02	0	10,10,10	0.63	0
3	ADP	D	1474	-	29,29,29	3.33	13 (44%)	45,45,45	3.92	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	D	1486	-	7,7,7	1.00	0	10,10,10	0.63	0
3	ADP	E	1475	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	E	1487	-	7,7,7	1.00	0	10,10,10	0.63	0
3	ADP	F	1476	-	29,29,29	3.33	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	F	1488	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	G	1477	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	G	1489	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	H	1478	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	H	1490	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	I	1479	-	29,29,29	3.34	13 (44%)	45,45,45	3.91	15 (33%)
5	MPD	I	1491	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	J	1480	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	J	1492	-	7,7,7	1.00	0	10,10,10	0.63	0
3	ADP	K	1481	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	K	1493	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	L	1482	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	L	1494	-	7,7,7	1.01	0	10,10,10	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1471	-	-	0/16/32/32	0/1/3/3
5	MPD	A	1483	-	-	0/5/5/5	0/0/0/0
3	ADP	B	1472	-	-	0/16/32/32	0/1/3/3
5	MPD	B	1484	-	-	0/5/5/5	0/0/0/0
3	ADP	C	1473	-	-	0/16/32/32	0/1/3/3
5	MPD	C	1485	-	-	0/5/5/5	0/0/0/0
3	ADP	D	1474	-	-	0/16/32/32	0/1/3/3
5	MPD	D	1486	-	-	0/5/5/5	0/0/0/0
3	ADP	E	1475	-	-	0/16/32/32	0/1/3/3
5	MPD	E	1487	-	-	0/5/5/5	0/0/0/0
3	ADP	F	1476	-	-	0/16/32/32	0/1/3/3
5	MPD	F	1488	-	-	0/5/5/5	0/0/0/0
3	ADP	G	1477	-	-	0/16/32/32	0/1/3/3
5	MPD	G	1489	-	-	0/5/5/5	0/0/0/0
3	ADP	H	1478	-	-	0/16/32/32	0/1/3/3
5	MPD	H	1490	-	-	0/5/5/5	0/0/0/0
3	ADP	I	1479	-	-	0/16/32/32	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	I	1491	-	-	0/5/5/5	0/0/0/0
3	ADP	J	1480	-	-	0/16/32/32	0/1/3/3
5	MPD	J	1492	-	-	0/5/5/5	0/0/0/0
3	ADP	K	1481	-	-	0/16/32/32	0/1/3/3
5	MPD	K	1493	-	-	0/5/5/5	0/0/0/0
3	ADP	L	1482	-	-	0/16/32/32	0/1/3/3
5	MPD	L	1494	-	-	0/5/5/5	0/0/0/0

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1479	ADP	C1'-N9	7.21	1.71	1.48
3	L	1482	ADP	C1'-N9	7.20	1.71	1.48
3	D	1474	ADP	C1'-N9	7.19	1.71	1.48
3	C	1473	ADP	C1'-N9	7.19	1.71	1.48
3	H	1478	ADP	C1'-N9	7.19	1.71	1.48
3	A	1471	ADP	C1'-N9	7.19	1.71	1.48
3	B	1472	ADP	C1'-N9	7.19	1.71	1.48
3	F	1476	ADP	C1'-N9	7.18	1.71	1.48
3	E	1475	ADP	C1'-N9	7.18	1.71	1.48
3	G	1477	ADP	C8-N9	7.18	1.47	1.36
3	J	1480	ADP	C1'-N9	7.18	1.71	1.48
3	G	1477	ADP	C1'-N9	7.17	1.71	1.48
3	K	1481	ADP	C1'-N9	7.16	1.71	1.48
3	L	1482	ADP	C8-N9	7.16	1.47	1.36
3	C	1473	ADP	C8-N9	7.16	1.47	1.36
3	H	1478	ADP	C8-N9	7.14	1.47	1.36
3	E	1475	ADP	C8-N9	7.14	1.47	1.36
3	K	1481	ADP	C8-N9	7.13	1.47	1.36
3	I	1479	ADP	C8-N9	7.12	1.47	1.36
3	F	1476	ADP	C8-N9	7.12	1.47	1.36
3	B	1472	ADP	C8-N9	7.12	1.47	1.36
3	D	1474	ADP	C8-N9	7.11	1.47	1.36
3	A	1471	ADP	C8-N9	7.11	1.47	1.36
3	J	1480	ADP	C8-N9	7.11	1.47	1.36
3	K	1481	ADP	O4'-C1'	6.80	1.51	1.41
3	G	1477	ADP	O4'-C1'	6.79	1.51	1.41
3	H	1478	ADP	O4'-C1'	6.79	1.51	1.41
3	I	1479	ADP	O4'-C1'	6.79	1.51	1.41
3	L	1482	ADP	O4'-C1'	6.78	1.51	1.41
3	E	1475	ADP	O4'-C1'	6.77	1.51	1.41
3	D	1474	ADP	O4'-C1'	6.76	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1472	ADP	O4'-C1'	6.77	1.51	1.41
3	A	1471	ADP	O4'-C1'	6.76	1.51	1.41
3	J	1480	ADP	O4'-C1'	6.75	1.51	1.41
3	C	1473	ADP	O4'-C1'	6.74	1.51	1.41
3	F	1476	ADP	O4'-C1'	6.72	1.51	1.41
3	E	1475	ADP	C4-N9	5.54	1.45	1.37
3	F	1476	ADP	C4-N9	5.53	1.45	1.37
3	H	1478	ADP	C4-N9	5.52	1.45	1.37
3	I	1479	ADP	C4-N9	5.51	1.45	1.37
3	K	1481	ADP	C4-N9	5.51	1.45	1.37
3	J	1480	ADP	C4-N9	5.51	1.45	1.37
3	B	1472	ADP	C4-N9	5.50	1.45	1.37
3	A	1471	ADP	C4-N9	5.50	1.45	1.37
3	C	1473	ADP	C4-N9	5.50	1.45	1.37
3	G	1477	ADP	C4-N9	5.49	1.45	1.37
3	L	1482	ADP	C4-N9	5.48	1.45	1.37
3	D	1474	ADP	C4-N9	5.47	1.45	1.37
3	L	1482	ADP	C4-N3	4.96	1.43	1.35
3	K	1481	ADP	C4-N3	4.92	1.43	1.35
3	B	1472	ADP	C4-N3	4.92	1.43	1.35
3	D	1474	ADP	C4-N3	4.91	1.43	1.35
3	A	1471	ADP	C4-N3	4.91	1.43	1.35
3	H	1478	ADP	C4-N3	4.90	1.43	1.35
3	E	1475	ADP	C4-N3	4.89	1.43	1.35
3	G	1477	ADP	C4-N3	4.89	1.43	1.35
3	F	1476	ADP	C4-N3	4.88	1.43	1.35
3	C	1473	ADP	C4-N3	4.88	1.43	1.35
3	J	1480	ADP	C4-N3	4.88	1.43	1.35
3	I	1479	ADP	C4-N3	4.87	1.43	1.35
3	J	1480	ADP	PA-O3A	4.79	1.68	1.59
3	I	1479	ADP	PA-O3A	4.78	1.68	1.59
3	D	1474	ADP	PA-O3A	4.77	1.68	1.59
3	B	1472	ADP	PA-O3A	4.77	1.68	1.59
3	L	1482	ADP	PA-O3A	4.76	1.68	1.59
3	A	1471	ADP	PA-O3A	4.76	1.68	1.59
3	C	1473	ADP	PA-O3A	4.75	1.68	1.59
3	F	1476	ADP	PA-O3A	4.74	1.68	1.59
3	G	1477	ADP	PA-O3A	4.74	1.68	1.59
3	E	1475	ADP	PA-O3A	4.74	1.68	1.59
3	K	1481	ADP	PA-O3A	4.74	1.68	1.59
3	H	1478	ADP	PA-O3A	4.72	1.68	1.59
3	F	1476	ADP	PB-O3A	4.60	1.68	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1481	ADP	PB-O3A	4.59	1.68	1.60
3	H	1478	ADP	PB-O3A	4.59	1.68	1.60
3	L	1482	ADP	PB-O3A	4.58	1.68	1.60
3	D	1474	ADP	PB-O3A	4.57	1.68	1.60
3	A	1471	ADP	PB-O3A	4.57	1.68	1.60
3	B	1472	ADP	PB-O3A	4.56	1.68	1.60
3	J	1480	ADP	PB-O3A	4.56	1.68	1.60
3	I	1479	ADP	PB-O3A	4.55	1.68	1.60
3	E	1475	ADP	PB-O3A	4.55	1.68	1.60
3	G	1477	ADP	PB-O3A	4.55	1.68	1.60
3	C	1473	ADP	PB-O3A	4.53	1.68	1.60
3	B	1472	ADP	O4'-C4'	3.83	1.54	1.45
3	C	1473	ADP	O4'-C4'	3.83	1.54	1.45
3	I	1479	ADP	O4'-C4'	3.82	1.54	1.45
3	J	1480	ADP	O4'-C4'	3.82	1.54	1.45
3	K	1481	ADP	O4'-C4'	3.81	1.54	1.45
3	F	1476	ADP	O4'-C4'	3.81	1.54	1.45
3	H	1478	ADP	O4'-C4'	3.81	1.53	1.45
3	A	1471	ADP	O4'-C4'	3.80	1.53	1.45
3	G	1477	ADP	O4'-C4'	3.80	1.53	1.45
3	E	1475	ADP	O4'-C4'	3.79	1.53	1.45
3	L	1482	ADP	O4'-C4'	3.79	1.53	1.45
3	D	1474	ADP	O4'-C4'	3.77	1.53	1.45
3	G	1477	ADP	PB-O3B	3.69	1.68	1.54
3	J	1480	ADP	PB-O3B	3.68	1.68	1.54
3	B	1472	ADP	PB-O3B	3.67	1.68	1.54
3	A	1471	ADP	PB-O3B	3.66	1.68	1.54
3	K	1481	ADP	PB-O3B	3.66	1.68	1.54
3	F	1476	ADP	PB-O3B	3.66	1.68	1.54
3	D	1474	ADP	PB-O3B	3.66	1.68	1.54
3	L	1482	ADP	PB-O3B	3.66	1.68	1.54
3	H	1478	ADP	PB-O3B	3.66	1.68	1.54
3	I	1479	ADP	PB-O3B	3.66	1.68	1.54
3	E	1475	ADP	PB-O3B	3.65	1.68	1.54
3	C	1473	ADP	PB-O3B	3.65	1.68	1.54
3	K	1481	ADP	C6-N6	-3.62	1.23	1.35
3	I	1479	ADP	C6-N6	-3.62	1.23	1.35
3	D	1474	ADP	C6-N6	-3.61	1.23	1.35
3	C	1473	ADP	C6-N6	-3.61	1.23	1.35
3	G	1477	ADP	C6-N6	-3.61	1.23	1.35
3	A	1471	ADP	C6-N6	-3.60	1.23	1.35
3	J	1480	ADP	C6-N6	-3.60	1.23	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1475	ADP	C6-N6	-3.59	1.23	1.35
3	H	1478	ADP	C6-N6	-3.59	1.23	1.35
3	L	1482	ADP	C6-N6	-3.59	1.23	1.35
3	B	1472	ADP	C6-N6	-3.59	1.23	1.35
3	F	1476	ADP	C6-N6	-3.58	1.23	1.35
3	J	1480	ADP	C2-N3	3.38	1.38	1.32
3	K	1481	ADP	C2-N3	3.38	1.38	1.32
3	E	1475	ADP	C2-N3	3.38	1.38	1.32
3	I	1479	ADP	C2-N3	3.37	1.38	1.32
3	C	1473	ADP	C2-N3	3.37	1.38	1.32
3	F	1476	ADP	C2-N3	3.36	1.38	1.32
3	G	1477	ADP	C2-N3	3.36	1.38	1.32
3	A	1471	ADP	C2-N3	3.36	1.38	1.32
3	L	1482	ADP	C2-N3	3.36	1.38	1.32
3	B	1472	ADP	C2-N3	3.36	1.38	1.32
3	H	1478	ADP	C2-N3	3.35	1.38	1.32
3	D	1474	ADP	C2-N3	3.35	1.38	1.32
3	H	1478	ADP	C3'-C4'	-2.54	1.46	1.53
3	K	1481	ADP	C3'-C4'	-2.53	1.46	1.53
3	J	1480	ADP	C3'-C4'	-2.53	1.46	1.53
3	G	1477	ADP	C3'-C4'	-2.53	1.46	1.53
3	L	1482	ADP	C3'-C4'	-2.52	1.46	1.53
3	E	1475	ADP	C3'-C4'	-2.52	1.46	1.53
3	F	1476	ADP	C3'-C4'	-2.52	1.46	1.53
3	A	1471	ADP	C3'-C4'	-2.52	1.46	1.53
3	I	1479	ADP	C3'-C4'	-2.52	1.46	1.53
3	D	1474	ADP	C3'-C4'	-2.51	1.46	1.53
3	B	1472	ADP	C3'-C4'	-2.50	1.46	1.53
3	C	1473	ADP	C3'-C4'	-2.50	1.46	1.53
3	K	1481	ADP	C5-C4	2.39	1.45	1.40
3	E	1475	ADP	C5-C4	2.39	1.45	1.40
3	G	1477	ADP	C5-C4	2.39	1.45	1.40
3	F	1476	ADP	C5-C4	2.38	1.45	1.40
3	D	1474	ADP	C5-C4	2.36	1.45	1.40
3	C	1473	ADP	C5-C4	2.37	1.45	1.40
3	A	1471	ADP	C5-C4	2.37	1.45	1.40
3	I	1479	ADP	C5-C4	2.36	1.45	1.40
3	J	1480	ADP	C5-C4	2.36	1.45	1.40
3	L	1482	ADP	C5-C4	2.35	1.45	1.40
3	B	1472	ADP	C5-C4	2.35	1.45	1.40
3	H	1478	ADP	C5-C4	2.35	1.45	1.40

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1475	ADP	O4'-C1'-N9	12.75	120.30	108.44
3	D	1474	ADP	O4'-C1'-N9	12.74	120.29	108.44
3	K	1481	ADP	O4'-C1'-N9	12.73	120.28	108.44
3	G	1477	ADP	O4'-C1'-N9	12.73	120.28	108.44
3	B	1472	ADP	O4'-C1'-N9	12.72	120.27	108.44
3	F	1476	ADP	O4'-C1'-N9	12.72	120.27	108.44
3	A	1471	ADP	O4'-C1'-N9	12.70	120.26	108.44
3	J	1480	ADP	O4'-C1'-N9	12.70	120.26	108.44
3	H	1478	ADP	O4'-C1'-N9	12.68	120.24	108.44
3	L	1482	ADP	O4'-C1'-N9	12.68	120.23	108.44
3	C	1473	ADP	O4'-C1'-N9	12.68	120.23	108.44
3	I	1479	ADP	O4'-C1'-N9	12.66	120.22	108.44
3	D	1474	ADP	O4'-C1'-C2'	-11.36	89.36	106.77
3	G	1477	ADP	O4'-C1'-C2'	-11.35	89.38	106.77
3	K	1481	ADP	O4'-C1'-C2'	-11.34	89.38	106.77
3	B	1472	ADP	O4'-C1'-C2'	-11.34	89.39	106.77
3	E	1475	ADP	O4'-C1'-C2'	-11.34	89.40	106.77
3	I	1479	ADP	O4'-C1'-C2'	-11.33	89.40	106.77
3	J	1480	ADP	O4'-C1'-C2'	-11.33	89.40	106.77
3	F	1476	ADP	O4'-C1'-C2'	-11.33	89.41	106.77
3	A	1471	ADP	O4'-C1'-C2'	-11.32	89.41	106.77
3	C	1473	ADP	O4'-C1'-C2'	-11.32	89.42	106.77
3	H	1478	ADP	O4'-C1'-C2'	-11.32	89.42	106.77
3	L	1482	ADP	O4'-C1'-C2'	-11.31	89.43	106.77
3	H	1478	ADP	C8-N9-C4	-9.86	99.38	106.90
3	K	1481	ADP	C8-N9-C4	-9.83	99.40	106.90
3	L	1482	ADP	C8-N9-C4	-9.82	99.40	106.90
3	G	1477	ADP	C8-N9-C4	-9.82	99.40	106.90
3	J	1480	ADP	C8-N9-C4	-9.82	99.41	106.90
3	C	1473	ADP	C8-N9-C4	-9.81	99.41	106.90
3	E	1475	ADP	C8-N9-C4	-9.80	99.42	106.90
3	A	1471	ADP	C8-N9-C4	-9.79	99.42	106.90
3	D	1474	ADP	C8-N9-C4	-9.78	99.43	106.90
3	F	1476	ADP	C8-N9-C4	-9.78	99.43	106.90
3	B	1472	ADP	C8-N9-C4	-9.78	99.44	106.90
3	I	1479	ADP	C8-N9-C4	-9.76	99.45	106.90
3	H	1478	ADP	C4'-O4'-C1'	-8.77	100.22	109.75
3	L	1482	ADP	C4'-O4'-C1'	-8.76	100.24	109.75
3	I	1479	ADP	C4'-O4'-C1'	-8.75	100.24	109.75
3	J	1480	ADP	C4'-O4'-C1'	-8.73	100.27	109.75
3	B	1472	ADP	C4'-O4'-C1'	-8.72	100.28	109.75
3	K	1481	ADP	C4'-O4'-C1'	-8.72	100.28	109.75
3	A	1471	ADP	C4'-O4'-C1'	-8.71	100.28	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1473	ADP	C4'-O4'-C1'	-8.71	100.29	109.75
3	F	1476	ADP	C4'-O4'-C1'	-8.70	100.30	109.75
3	E	1475	ADP	C4'-O4'-C1'	-8.70	100.30	109.75
3	G	1477	ADP	C4'-O4'-C1'	-8.70	100.30	109.75
3	D	1474	ADP	C4'-O4'-C1'	-8.66	100.34	109.75
3	K	1481	ADP	O5'-C5'-C4'	7.53	136.58	108.94
3	E	1475	ADP	O5'-C5'-C4'	7.53	136.56	108.94
3	J	1480	ADP	O5'-C5'-C4'	7.53	136.56	108.94
3	L	1482	ADP	O5'-C5'-C4'	7.52	136.56	108.94
3	D	1474	ADP	O5'-C5'-C4'	7.52	136.56	108.94
3	A	1471	ADP	O5'-C5'-C4'	7.52	136.54	108.94
3	C	1473	ADP	O5'-C5'-C4'	7.52	136.53	108.94
3	H	1478	ADP	O5'-C5'-C4'	7.52	136.53	108.94
3	I	1479	ADP	O5'-C5'-C4'	7.52	136.52	108.94
3	F	1476	ADP	O5'-C5'-C4'	7.51	136.52	108.94
3	B	1472	ADP	O5'-C5'-C4'	7.51	136.51	108.94
3	G	1477	ADP	O5'-C5'-C4'	7.51	136.50	108.94
3	L	1482	ADP	C1'-N9-C4	5.59	136.30	126.64
3	C	1473	ADP	C1'-N9-C4	5.59	136.29	126.64
3	G	1477	ADP	C1'-N9-C4	5.59	136.29	126.64
3	H	1478	ADP	C1'-N9-C4	5.58	136.28	126.64
3	D	1474	ADP	C1'-N9-C4	5.57	136.26	126.64
3	B	1472	ADP	C1'-N9-C4	5.57	136.26	126.64
3	J	1480	ADP	C1'-N9-C4	5.57	136.26	126.64
3	K	1481	ADP	C1'-N9-C4	5.57	136.26	126.64
3	E	1475	ADP	C1'-N9-C4	5.56	136.25	126.64
3	A	1471	ADP	C1'-N9-C4	5.56	136.25	126.64
3	I	1479	ADP	C1'-N9-C4	5.56	136.24	126.64
3	F	1476	ADP	C1'-N9-C4	5.54	136.21	126.64
3	H	1478	ADP	C4-C5-N7	5.54	114.26	109.52
3	B	1472	ADP	C4-C5-N7	5.52	114.25	109.52
3	J	1480	ADP	C4-C5-N7	5.51	114.24	109.52
3	I	1479	ADP	C4-C5-N7	5.51	114.24	109.52
3	C	1473	ADP	C4-C5-N7	5.49	114.23	109.52
3	A	1471	ADP	C4-C5-N7	5.49	114.22	109.52
3	G	1477	ADP	C4-C5-N7	5.49	114.22	109.52
3	D	1474	ADP	C4-C5-N7	5.49	114.22	109.52
3	F	1476	ADP	C4-C5-N7	5.49	114.22	109.52
3	L	1482	ADP	C4-C5-N7	5.47	114.20	109.52
3	E	1475	ADP	C4-C5-N7	5.46	114.19	109.52
3	K	1481	ADP	C4-C5-N7	5.45	114.19	109.52
3	D	1474	ADP	O4'-C4'-C5'	4.46	125.27	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1473	ADP	O4'-C4'-C5'	4.45	125.25	109.36
3	E	1475	ADP	O4'-C4'-C5'	4.45	125.25	109.36
3	F	1476	ADP	O4'-C4'-C5'	4.45	125.24	109.36
3	B	1472	ADP	O4'-C4'-C5'	4.44	125.22	109.36
3	A	1471	ADP	O4'-C4'-C5'	4.44	125.22	109.36
3	G	1477	ADP	O4'-C4'-C5'	4.44	125.22	109.36
3	J	1480	ADP	O4'-C4'-C5'	4.44	125.20	109.36
3	K	1481	ADP	O4'-C4'-C5'	4.44	125.19	109.36
3	L	1482	ADP	O4'-C4'-C5'	4.43	125.19	109.36
3	I	1479	ADP	O4'-C4'-C5'	4.43	125.18	109.36
3	H	1478	ADP	O4'-C4'-C5'	4.43	125.18	109.36
3	C	1473	ADP	O2'-C2'-C1'	3.63	122.20	111.23
3	B	1472	ADP	O2'-C2'-C1'	3.62	122.19	111.23
3	G	1477	ADP	O2'-C2'-C1'	3.62	122.19	111.23
3	L	1482	ADP	O2'-C2'-C1'	3.62	122.19	111.23
3	H	1478	ADP	O2'-C2'-C1'	3.62	122.19	111.23
3	A	1471	ADP	O2'-C2'-C1'	3.62	122.19	111.23
3	I	1479	ADP	O2'-C2'-C1'	3.62	122.18	111.23
3	J	1480	ADP	O2'-C2'-C1'	3.62	122.17	111.23
3	D	1474	ADP	O2'-C2'-C1'	3.62	122.17	111.23
3	K	1481	ADP	O2'-C2'-C1'	3.61	122.16	111.23
3	F	1476	ADP	O2'-C2'-C1'	3.61	122.15	111.23
3	E	1475	ADP	O2'-C2'-C1'	3.61	122.14	111.23
3	I	1479	ADP	C5'-C4'-C3'	-3.55	101.00	115.21
3	G	1477	ADP	C5'-C4'-C3'	-3.54	101.01	115.21
3	L	1482	ADP	C5'-C4'-C3'	-3.54	101.03	115.21
3	A	1471	ADP	C5'-C4'-C3'	-3.54	101.02	115.21
3	F	1476	ADP	C5'-C4'-C3'	-3.54	101.03	115.21
3	B	1472	ADP	C5'-C4'-C3'	-3.54	101.03	115.21
3	H	1478	ADP	C5'-C4'-C3'	-3.54	101.03	115.21
3	D	1474	ADP	C5'-C4'-C3'	-3.54	101.05	115.21
3	J	1480	ADP	C5'-C4'-C3'	-3.54	101.04	115.21
3	C	1473	ADP	C5'-C4'-C3'	-3.54	101.05	115.21
3	K	1481	ADP	C5'-C4'-C3'	-3.53	101.08	115.21
3	E	1475	ADP	C5'-C4'-C3'	-3.53	101.08	115.21
3	J	1480	ADP	O3'-C3'-C2'	2.93	121.38	111.83
3	K	1481	ADP	O3'-C3'-C2'	2.93	121.36	111.83
3	E	1475	ADP	O3'-C3'-C2'	2.93	121.36	111.83
3	D	1474	ADP	O3'-C3'-C2'	2.93	121.35	111.83
3	I	1479	ADP	O3'-C3'-C2'	2.93	121.35	111.83
3	F	1476	ADP	O3'-C3'-C2'	2.93	121.35	111.83
3	L	1482	ADP	O3'-C3'-C2'	2.92	121.34	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1472	ADP	O3'-C3'-C2'	2.92	121.34	111.83
3	C	1473	ADP	O3'-C3'-C2'	2.92	121.33	111.83
3	A	1471	ADP	O3'-C3'-C2'	2.92	121.33	111.83
3	G	1477	ADP	O3'-C3'-C2'	2.91	121.30	111.83
3	H	1478	ADP	O3'-C3'-C2'	2.91	121.29	111.83
3	F	1476	ADP	N3-C4-N9	2.81	130.50	125.43
3	B	1472	ADP	N3-C4-N9	2.80	130.49	125.43
3	D	1474	ADP	N3-C4-N9	2.80	130.49	125.43
3	K	1481	ADP	N3-C4-N9	2.79	130.48	125.43
3	G	1477	ADP	N3-C4-N9	2.79	130.48	125.43
3	A	1471	ADP	N3-C4-N9	2.79	130.47	125.43
3	J	1480	ADP	N3-C4-N9	2.79	130.47	125.43
3	I	1479	ADP	N3-C4-N9	2.79	130.46	125.43
3	E	1475	ADP	N3-C4-N9	2.79	130.46	125.43
3	C	1473	ADP	N3-C4-N9	2.79	130.46	125.43
3	H	1478	ADP	N3-C4-N9	2.78	130.46	125.43
3	L	1482	ADP	N3-C4-N9	2.78	130.45	125.43
3	I	1479	ADP	PA-O5'-C5'	2.25	138.19	122.03
3	J	1480	ADP	PA-O5'-C5'	2.25	138.20	122.03
3	K	1481	ADP	PA-O5'-C5'	2.25	138.19	122.03
3	D	1474	ADP	PA-O5'-C5'	2.25	138.18	122.03
3	F	1476	ADP	PA-O5'-C5'	2.25	138.18	122.03
3	B	1472	ADP	PA-O5'-C5'	2.25	138.18	122.03
3	E	1475	ADP	PA-O5'-C5'	2.25	138.17	122.03
3	C	1473	ADP	PA-O5'-C5'	2.25	138.17	122.03
3	A	1471	ADP	PA-O5'-C5'	2.25	138.18	122.03
3	L	1482	ADP	PA-O5'-C5'	2.24	138.15	122.03
3	G	1477	ADP	PA-O5'-C5'	2.24	138.16	122.03
3	H	1478	ADP	PA-O5'-C5'	2.24	138.14	122.03
3	G	1477	ADP	O3A-PA-O5'	2.07	112.67	103.41
3	F	1476	ADP	O3A-PA-O5'	2.07	112.64	103.41
3	E	1475	ADP	O3A-PA-O5'	2.07	112.65	103.41
3	K	1481	ADP	O3A-PA-O5'	2.06	112.63	103.41
3	C	1473	ADP	O3A-PA-O5'	2.06	112.63	103.41
3	H	1478	ADP	O3A-PA-O5'	2.06	112.64	103.41
3	D	1474	ADP	O3A-PA-O5'	2.06	112.62	103.41
3	A	1471	ADP	O3A-PA-O5'	2.06	112.62	103.41
3	I	1479	ADP	O3A-PA-O5'	2.06	112.61	103.41
3	B	1472	ADP	O3A-PA-O5'	2.06	112.61	103.41
3	J	1480	ADP	O3A-PA-O5'	2.06	112.61	103.41
3	C	1473	ADP	O5'-PA-O1A	-2.06	101.32	109.37
3	L	1482	ADP	O3A-PA-O5'	2.06	112.60	103.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1478	ADP	O5'-PA-O1A	-2.06	101.32	109.37
3	E	1475	ADP	O5'-PA-O1A	-2.05	101.33	109.37
3	L	1482	ADP	O5'-PA-O1A	-2.05	101.35	109.37
3	D	1474	ADP	O5'-PA-O1A	-2.05	101.35	109.37
3	K	1481	ADP	O5'-PA-O1A	-2.05	101.35	109.37
3	A	1471	ADP	O5'-PA-O1A	-2.05	101.36	109.37
3	J	1480	ADP	O5'-PA-O1A	-2.05	101.36	109.37
3	G	1477	ADP	O5'-PA-O1A	-2.05	101.36	109.37
3	I	1479	ADP	O5'-PA-O1A	-2.04	101.38	109.37
3	F	1476	ADP	O5'-PA-O1A	-2.04	101.40	109.37
3	B	1472	ADP	O5'-PA-O1A	-2.04	101.39	109.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.75	76 (16%)	2 2	18, 39, 91, 100	29 (6%)
1	B	468/468 (100%)	0.50	60 (12%)	4 4	18, 39, 91, 100	29 (6%)
1	C	468/468 (100%)	0.35	53 (11%)	6 5	18, 39, 91, 100	29 (6%)
1	D	468/468 (100%)	0.20	39 (8%)	11 11	18, 39, 91, 100	29 (6%)
1	E	468/468 (100%)	0.39	50 (10%)	6 6	18, 39, 91, 100	29 (6%)
1	F	468/468 (100%)	0.37	52 (11%)	6 6	18, 39, 91, 100	29 (6%)
1	G	468/468 (100%)	0.29	39 (8%)	11 11	18, 39, 91, 100	29 (6%)
1	H	468/468 (100%)	0.36	40 (8%)	11 10	18, 39, 91, 100	29 (6%)
1	I	468/468 (100%)	0.23	35 (7%)	14 14	18, 39, 91, 100	29 (6%)
1	J	468/468 (100%)	0.29	38 (8%)	12 12	18, 39, 91, 100	29 (6%)
1	K	468/468 (100%)	0.25	37 (7%)	13 13	18, 39, 91, 100	29 (6%)
1	L	468/468 (100%)	0.37	35 (7%)	14 14	18, 39, 91, 100	29 (6%)
All	All	5616/5616 (100%)	0.36	554 (9%)	8 7	18, 39, 92, 100	348 (6%)

All (554) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	TYR	15.5
1	L	397	TYR	14.9
1	A	397	TYR	14.0
1	A	395	ASN	14.0
1	K	397	TYR	12.3
1	E	397	TYR	12.2
1	K	326	TYR	12.1
1	L	51	GLY	11.9
1	J	397	TYR	11.9
1	J	62	GLU	11.6
1	D	326	TYR	11.1

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Mol	Chain	Res	Type	RSRZ
1	H	402	GLU	11.0
1	C	397	TYR	10.5
1	K	398	ASP	10.3
1	F	400	PRO	10.2
1	F	398	ASP	9.7
1	A	396	LEU	9.5
1	A	398	ASP	9.4
1	B	404	ALA	9.2
1	H	397	TYR	9.1
1	F	397	TYR	9.0
1	E	51	GLY	8.9
1	G	397	TYR	8.7
1	G	395	ASN	8.7
1	A	51	GLY	8.6
1	I	326	TYR	8.5
1	D	51	GLY	8.3
1	E	398	ASP	8.2
1	J	398	ASP	8.2
1	J	51	GLY	8.1
1	B	400	PRO	8.1
1	J	326	TYR	8.1
1	F	326	TYR	7.9
1	E	395	ASN	7.9
1	D	60	ILE	7.8
1	A	58	LYS	7.7
1	B	398	ASP	7.7
1	A	326	TYR	7.6
1	B	326	TYR	7.6
1	H	395	ASN	7.6
1	L	400	PRO	7.6
1	K	400	PRO	7.5
1	B	396	LEU	7.4
1	A	52	SER	7.3
1	H	51	GLY	7.3
1	I	60	ILE	7.3
1	A	60	ILE	7.2
1	D	398	ASP	7.2
1	K	394	LYS	7.2
1	G	51	GLY	7.2
1	D	403	GLU	7.1
1	K	51	GLY	7.0
1	L	50	ASP	7.0

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Mol	Chain	Res	Type	RSRZ
1	G	398	ASP	6.9
1	J	50	ASP	6.9
1	H	62	GLU	6.9
1	H	403	GLU	6.9
1	B	405	LYS	6.8
1	A	296	TYR	6.8
1	L	60	ILE	6.8
1	F	51	GLY	6.8
1	J	396	LEU	6.8
1	J	395	ASN	6.8
1	C	403	GLU	6.7
1	I	397	TYR	6.7
1	J	400	PRO	6.6
1	J	60	ILE	6.6
1	A	394	LYS	6.6
1	K	402	GLU	6.5
1	D	395	ASN	6.5
1	C	51	GLY	6.5
1	B	64	ASP	6.5
1	D	405	LYS	6.5
1	F	401	PRO	6.4
1	L	405	LYS	6.3
1	G	60	ILE	6.2
1	E	403	GLU	6.2
1	E	396	LEU	6.2
1	G	52	SER	6.2
1	L	403	GLU	6.2
1	F	50	ASP	6.2
1	C	52	SER	6.2
1	L	52	SER	6.2
1	G	402	GLU	6.2
1	F	52	SER	6.1
1	E	326	TYR	6.0
1	A	399	LEU	6.0
1	C	326	TYR	6.0
1	L	402	GLU	6.0
1	F	396	LEU	6.0
1	G	394	LYS	5.9
1	I	62	GLU	5.9
1	I	51	GLY	5.9
1	H	50	ASP	5.9
1	L	394	LYS	5.9

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Mol	Chain	Res	Type	RSRZ
1	L	398	ASP	5.9
1	E	406	GLU	5.8
1	D	404	ALA	5.8
1	D	1	SER	5.8
1	A	285	ASP	5.8
1	B	63	SER	5.8
1	G	1	SER	5.8
1	L	401	PRO	5.7
1	I	405	LYS	5.7
1	K	52	SER	5.7
1	G	401	PRO	5.7
1	E	399	LEU	5.7
1	A	400	PRO	5.7
1	B	51	GLY	5.7
1	I	327	GLU	5.7
1	A	334	TYR	5.6
1	G	326	TYR	5.6
1	F	395	ASN	5.6
1	D	401	PRO	5.6
1	J	63	SER	5.6
1	H	60	ILE	5.6
1	C	398	ASP	5.6
1	G	400	PRO	5.6
1	E	50	ASP	5.5
1	K	395	ASN	5.5
1	C	61	ASN	5.5
1	E	405	LYS	5.5
1	H	52	SER	5.5
1	K	396	LEU	5.5
1	K	403	GLU	5.5
1	D	394	LYS	5.4
1	E	400	PRO	5.4
1	I	50	ASP	5.4
1	G	50	ASP	5.3
1	K	399	LEU	5.3
1	E	404	ALA	5.3
1	C	62	GLU	5.3
1	F	399	LEU	5.3
1	D	52	SER	5.3
1	B	62	GLU	5.3
1	H	349	ALA	5.3
1	A	327	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	400	PRO	5.2
1	H	179	TYR	5.1
1	A	63	SER	5.1
1	I	403	GLU	5.1
1	H	351	PRO	5.1
1	L	179	TYR	5.1
1	I	52	SER	5.0
1	H	394	LYS	5.0
1	C	405	LYS	5.0
1	D	397	TYR	5.0
1	I	404	ALA	5.0
1	A	50	ASP	5.0
1	F	61	ASN	5.0
1	J	52	SER	4.9
1	G	61	ASN	4.9
1	D	402	GLU	4.9
1	D	396	LEU	4.9
1	C	53	SER	4.9
1	E	60	ILE	4.9
1	A	338	ASN	4.8
1	A	339	ARG	4.8
1	I	394	LYS	4.8
1	E	394	LYS	4.8
1	K	401	PRO	4.8
1	H	398	ASP	4.8
1	B	1	SER	4.8
1	A	345	ILE	4.8
1	I	396	LEU	4.8
1	A	392	MET	4.7
1	F	403	GLU	4.7
1	J	61	ASN	4.7
1	H	326	TYR	4.7
1	A	53	SER	4.7
1	F	60	ILE	4.7
1	B	53	SER	4.7
1	I	3	GLU	4.7
1	H	61	ASN	4.7
1	A	354	ARG	4.7
1	L	395	ASN	4.7
1	C	337	ARG	4.7
1	K	50	ASP	4.7
1	A	277	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	62	GLU	4.6
1	F	394	LYS	4.6
1	B	407	ILE	4.6
1	A	347	VAL	4.5
1	A	340	SER	4.5
1	I	398	ASP	4.5
1	B	61	ASN	4.5
1	A	402	GLU	4.5
1	K	406	GLU	4.5
1	B	395	ASN	4.5
1	D	400	PRO	4.5
1	C	50	ASP	4.5
1	A	62	GLU	4.4
1	E	327	GLU	4.4
1	G	396	LEU	4.4
1	G	405	LYS	4.4
1	J	53	SER	4.4
1	B	339	ARG	4.4
1	B	394	LYS	4.4
1	C	395	ASN	4.3
1	B	399	LEU	4.3
1	C	404	ALA	4.3
1	J	394	LYS	4.3
1	B	403	GLU	4.3
1	B	52	SER	4.3
1	B	401	PRO	4.3
1	C	401	PRO	4.3
1	C	394	LYS	4.3
1	A	404	ALA	4.2
1	E	350	SER	4.2
1	G	339	ARG	4.2
1	E	386	ILE	4.2
1	I	98	GLN	4.2
1	H	1	SER	4.2
1	H	53	SER	4.1
1	G	399	LEU	4.1
1	A	351	PRO	4.1
1	F	331	MET	4.1
1	C	402	GLU	4.1
1	E	7	THR	4.1
1	K	179	TYR	4.1
1	F	179	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	46	GLY	4.0
1	B	60	ILE	4.0
1	H	12	HIS	4.0
1	L	61	ASN	4.0
1	F	53	SER	4.0
1	I	53	SER	4.0
1	B	50	ASP	4.0
1	B	328	ALA	4.0
1	E	52	SER	3.9
1	F	340	SER	3.9
1	I	395	ASN	3.9
1	B	327	GLU	3.9
1	F	327	GLU	3.9
1	F	402	GLU	3.9
1	K	405	LYS	3.9
1	L	59	GLY	3.9
1	E	292	GLU	3.9
1	J	403	GLU	3.9
1	K	340	SER	3.9
1	A	324	PRO	3.8
1	J	339	ARG	3.8
1	L	53	SER	3.8
1	B	2	ALA	3.8
1	D	62	GLU	3.8
1	B	392	MET	3.7
1	G	2	ALA	3.7
1	A	91	ILE	3.7
1	A	348	VAL	3.7
1	E	1	SER	3.7
1	J	1	SER	3.7
1	C	63	SER	3.7
1	C	179	TYR	3.7
1	I	179	TYR	3.7
1	C	60	ILE	3.7
1	C	351	PRO	3.7
1	F	392	MET	3.7
1	G	49	PHE	3.6
1	L	404	ALA	3.6
1	B	393	ASP	3.6
1	D	4	HIS	3.6
1	C	293	GLN	3.6
1	I	59	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	179	TYR	3.6
1	J	59	GLY	3.6
1	B	12	HIS	3.6
1	D	285	ASP	3.6
1	E	62	GLU	3.6
1	G	3	GLU	3.6
1	K	327	GLU	3.6
1	D	179	TYR	3.6
1	A	279	THR	3.6
1	C	349	ALA	3.5
1	H	400	PRO	3.5
1	J	327	GLU	3.5
1	A	293	GLN	3.5
1	J	5	VAL	3.5
1	E	407	ILE	3.5
1	A	333	ALA	3.5
1	I	61	ASN	3.5
1	F	404	ALA	3.5
1	J	179	TYR	3.5
1	F	405	LYS	3.5
1	C	339	ARG	3.4
1	G	63	SER	3.4
1	H	8	MET	3.4
1	C	59	GLY	3.4
1	A	98	GLN	3.4
1	E	179	TYR	3.4
1	B	406	GLU	3.4
1	L	327	GLU	3.4
1	E	385	LYS	3.4
1	B	65	MET	3.4
1	A	335	SER	3.4
1	C	396	LEU	3.4
1	B	95	GLY	3.4
1	A	179	TYR	3.3
1	C	296	TYR	3.3
1	D	50	ASP	3.4
1	L	62	GLU	3.3
1	C	327	GLU	3.3
1	A	382	ILE	3.3
1	I	54	ILE	3.3
1	D	53	SER	3.3
1	E	12	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	339	ARG	3.3
1	D	63	SER	3.3
1	B	325	GLY	3.3
1	F	278	GLY	3.3
1	K	1	SER	3.3
1	K	165	GLU	3.2
1	A	292	GLU	3.2
1	B	8	MET	3.2
1	E	349	ALA	3.2
1	L	63	SER	3.2
1	L	326	TYR	3.2
1	A	379	LEU	3.2
1	B	98	GLN	3.2
1	I	64	ASP	3.1
1	K	53	SER	3.1
1	F	407	ILE	3.1
1	J	98	GLN	3.1
1	I	58	LYS	3.1
1	A	278	GLY	3.1
1	A	405	LYS	3.0
1	B	39	ASN	3.0
1	F	349	ALA	3.0
1	F	352	LYS	3.0
1	H	350	SER	3.0
1	L	399	LEU	3.0
1	B	179	TYR	3.0
1	D	117	ALA	3.0
1	A	337	ARG	3.0
1	F	284	GLY	3.0
1	D	399	LEU	3.0
1	B	278	GLY	3.0
1	E	53	SER	3.0
1	F	63	SER	2.9
1	A	43	PHE	2.9
1	I	49	PHE	2.9
1	I	331	MET	2.9
1	H	405	LYS	2.9
1	A	346	PRO	2.9
1	E	277	ASN	2.9
1	K	98	GLN	2.9
1	B	66	VAL	2.9
1	A	353	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	63	SER	2.9
1	J	401	PRO	2.9
1	L	58	LYS	2.9
1	J	404	ALA	2.9
1	H	399	LEU	2.9
1	H	7	THR	2.9
1	H	4	HIS	2.9
1	B	402	GLU	2.9
1	F	338	ASN	2.9
1	A	391	PRO	2.9
1	H	331	MET	2.9
1	C	1	SER	2.8
1	A	122	ASP	2.8
1	E	11	GLU	2.8
1	A	275	ALA	2.8
1	C	399	LEU	2.8
1	I	401	PRO	2.8
1	L	328	ALA	2.8
1	F	59	GLY	2.8
1	H	337	ARG	2.8
1	D	49	PHE	2.8
1	L	396	LEU	2.7
1	L	49	PHE	2.7
1	E	63	SER	2.7
1	B	97	LEU	2.7
1	G	62	GLU	2.7
1	A	276	LYS	2.7
1	A	387	HIS	2.7
1	A	5	VAL	2.7
1	H	40	ALA	2.7
1	F	98	GLN	2.7
1	K	49	PHE	2.6
1	H	347	VAL	2.6
1	C	406	GLU	2.6
1	F	337	ARG	2.6
1	K	41	GLU	2.6
1	C	43	PHE	2.6
1	C	277	ASN	2.6
1	K	2	ALA	2.6
1	H	130	PRO	2.6
1	C	407	ILE	2.6
1	B	58	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	401	PRO	2.6
1	K	331	MET	2.6
1	G	404	ALA	2.6
1	I	2	ALA	2.6
1	L	270	CYS	2.6
1	D	44	GLU	2.6
1	G	277	ASN	2.6
1	A	288	ALA	2.6
1	E	2	ALA	2.6
1	D	339	ARG	2.6
1	A	331	MET	2.6
1	B	290	LEU	2.5
1	A	61	ASN	2.5
1	C	96	THR	2.5
1	F	65	MET	2.5
1	E	351	PRO	2.5
1	D	406	GLU	2.5
1	G	403	GLU	2.5
1	B	337	ARG	2.5
1	F	40	ALA	2.5
1	G	53	SER	2.5
1	I	400	PRO	2.5
1	J	324	PRO	2.5
1	A	286	LYS	2.5
1	I	402	GLU	2.5
1	G	337	ARG	2.5
1	J	8	MET	2.5
1	A	328	ALA	2.5
1	D	59	GLY	2.5
1	E	293	GLN	2.5
1	E	392	MET	2.5
1	J	338	ASN	2.5
1	E	3	GLU	2.5
1	C	419	ASN	2.5
1	I	43	PHE	2.5
1	D	40	ALA	2.5
1	E	339	ARG	2.5
1	B	49	PHE	2.5
1	F	328	ALA	2.5
1	G	406	GLU	2.4
1	H	364	ALA	2.4
1	K	62	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	2.4
1	F	330	VAL	2.4
1	F	56	GLY	2.4
1	F	275	ALA	2.4
1	C	46	GLY	2.4
1	H	49	PHE	2.4
1	L	6	LEU	2.4
1	A	352	LYS	2.4
1	B	4	HIS	2.4
1	F	165	GLU	2.4
1	H	277	ASN	2.4
1	G	54	ILE	2.4
1	A	401	PRO	2.4
1	E	10	ASN	2.4
1	A	283	SER	2.4
1	E	278	GLY	2.4
1	F	334	TYR	2.4
1	L	361	PRO	2.4
1	A	330	VAL	2.3
1	B	117	ALA	2.3
1	C	328	ALA	2.3
1	H	407	ILE	2.3
1	L	165	GLU	2.3
1	B	122	ASP	2.3
1	J	49	PHE	2.3
1	D	41	GLU	2.3
1	F	97	LEU	2.3
1	E	401	PRO	2.3
1	K	94	PRO	2.3
1	D	337	ARG	2.3
1	J	7	THR	2.3
1	K	339	ARG	2.3
1	A	284	GLY	2.3
1	D	341	ALA	2.3
1	F	333	ALA	2.3
1	J	165	GLU	2.3
1	E	340	SER	2.3
1	K	63	SER	2.3
1	B	6	LEU	2.3
1	G	6	LEU	2.3
1	C	64	ASP	2.3
1	L	54	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	43	PHE	2.3
1	A	294	ALA	2.3
1	C	122	ASP	2.3
1	A	3	GLU	2.3
1	C	338	ASN	2.3
1	J	64	ASP	2.2
1	E	383	LYS	2.2
1	C	344	ARG	2.2
1	E	8	MET	2.2
1	F	3	GLU	2.2
1	J	6	LEU	2.2
1	E	408	PRO	2.2
1	H	44	GLU	2.2
1	K	44	GLU	2.2
1	C	408	PRO	2.2
1	I	407	ILE	2.2
1	K	60	ILE	2.2
1	C	121	ALA	2.2
1	C	385	LYS	2.2
1	A	57	TRP	2.2
1	G	97	LEU	2.2
1	I	6	LEU	2.2
1	H	404	ALA	2.2
1	E	54	ILE	2.2
1	J	402	GLU	2.2
1	E	276	LYS	2.2
1	F	423	LEU	2.2
1	C	279	THR	2.2
1	C	287	TYR	2.2
1	G	59	GLY	2.2
1	E	402	GLU	2.2
1	K	324	PRO	2.2
1	B	48	MET	2.1
1	G	7	THR	2.1
1	A	355	ARG	2.1
1	A	383	LYS	2.1
1	G	327	GLU	2.1
1	A	6	LEU	2.1
1	C	97	LEU	2.1
1	B	338	ASN	2.1
1	C	94	PRO	2.1
1	B	340	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	340	SER	2.1
1	F	1	SER	2.1
1	C	282	PHE	2.1
1	E	428	LEU	2.1
1	B	45	GLU	2.1
1	A	1	SER	2.1
1	H	128	PRO	2.1
1	D	327	GLU	2.1
1	I	165	GLU	2.1
1	J	4	HIS	2.1
1	L	130	PRO	2.1
1	A	126	PHE	2.1
1	A	112	GLU	2.1
1	B	11	GLU	2.1
1	J	328	ALA	2.1
1	L	364	ALA	2.1
1	J	58	LYS	2.1
1	B	42	PHE	2.1
1	J	399	LEU	2.1
1	D	58	LYS	2.1
1	F	324	PRO	2.1
1	B	41	GLU	2.1
1	C	292	GLU	2.1
1	K	407	ILE	2.1
1	I	339	ARG	2.1
1	B	38	VAL	2.0
1	K	130	PRO	2.0
1	G	371	PHE	2.0
1	A	385	LYS	2.0
1	K	404	ALA	2.0
1	L	1	SER	2.0
1	E	59	GLY	2.0
1	G	338	ASN	2.0
1	D	54	ILE	2.0
1	G	235	ILE	2.0
1	C	350	SER	2.0
1	F	58	LYS	2.0
1	F	96	THR	2.0
1	D	5	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MPD	L	1494	8/8	0.44	15.98	16,43,64,74	8
5	MPD	K	1493	8/8	0.39	13.14	16,43,64,74	8
5	MPD	G	1489	8/8	0.33	12.24	16,43,64,74	8
5	MPD	F	1488	8/8	0.42	11.79	16,43,64,74	8
5	MPD	C	1485	8/8	0.45	11.24	16,43,64,74	8
5	MPD	H	1490	8/8	0.38	9.98	16,43,64,74	8
5	MPD	I	1491	8/8	0.33	7.96	16,43,64,74	8
5	MPD	J	1492	8/8	0.35	7.76	16,43,64,74	8
5	MPD	B	1484	8/8	0.40	7.69	16,43,64,74	8
5	MPD	D	1486	8/8	0.36	7.17	16,43,64,74	8
5	MPD	E	1487	8/8	0.39	4.73	16,43,64,74	8
5	MPD	A	1483	8/8	0.32	4.25	16,43,64,74	8
3	ADP	L	1482	27/27	0.48	3.43	20,78,100,100	27
3	ADP	D	1474	27/27	0.47	2.97	20,78,100,100	27
3	ADP	I	1479	27/27	0.49	2.91	20,78,100,100	27
3	ADP	F	1476	27/27	0.49	2.86	20,78,100,100	27
3	ADP	B	1472	27/27	0.41	2.57	20,78,100,100	27
3	ADP	K	1481	27/27	0.41	1.78	20,78,100,100	27
3	ADP	C	1473	27/27	0.34	1.67	20,78,100,100	27
3	ADP	J	1480	27/27	0.35	1.65	20,78,100,100	27
3	ADP	H	1478	27/27	0.35	1.41	20,78,100,100	27
3	ADP	A	1471	27/27	0.38	1.15	20,78,100,100	27
3	ADP	E	1475	27/27	0.34	1.13	20,78,100,100	27
3	ADP	G	1477	27/27	0.33	1.06	20,78,100,100	27
4	TL	I	474	1/1	0.14	-0.44	75,75,75,75	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	TL	J	473	1/1	0.24	-0.51	67,67,67,67	1
4	TL	L	473	1/1	0.24	-0.65	67,67,67,67	1
4	TL	I	473	1/1	0.19	-0.73	67,67,67,67	1
2	MN	D	469	1/1	0.11	-0.75	34,34,34,34	0
4	TL	A	473	1/1	0.18	-0.77	67,67,67,67	1
4	TL	D	474	1/1	0.11	-0.79	75,75,75,75	1
4	TL	G	473	1/1	0.16	-0.80	67,67,67,67	1
4	TL	H	473	1/1	0.18	-0.82	67,67,67,67	1
2	MN	I	469	1/1	0.09	-0.97	34,34,34,34	0
2	MN	G	469	1/1	0.08	-0.98	34,34,34,34	0
4	TL	G	474	1/1	0.12	-1.00	75,75,75,75	1
2	MN	K	469	1/1	0.14	-1.00	34,34,34,34	0
2	MN	J	469	1/1	0.13	-1.01	34,34,34,34	0
2	MN	H	469	1/1	0.09	-1.04	34,34,34,34	0
2	MN	E	469	1/1	0.05	-1.06	34,34,34,34	0
2	MN	C	469	1/1	0.12	-1.07	34,34,34,34	0
2	MN	L	469	1/1	0.13	-1.08	34,34,34,34	0
4	TL	C	473	1/1	0.16	-1.08	67,67,67,67	1
2	MN	J	470	1/1	0.10	-1.10	41,41,41,41	0
2	MN	H	470	1/1	0.09	-1.20	41,41,41,41	0
4	TL	E	473	1/1	0.07	-1.20	67,67,67,67	1
4	TL	L	474	1/1	0.12	-1.20	75,75,75,75	1
4	TL	E	474	1/1	0.10	-1.21	75,75,75,75	1
2	MN	F	469	1/1	0.06	-1.23	34,34,34,34	0
4	TL	K	473	1/1	0.12	-1.34	67,67,67,67	1
2	MN	B	469	1/1	0.07	-1.34	34,34,34,34	0
2	MN	A	469	1/1	0.05	-1.35	34,34,34,34	0
4	TL	F	473	1/1	0.10	-1.40	67,67,67,67	1
4	TL	J	474	1/1	0.11	-1.53	75,75,75,75	1
4	TL	D	473	1/1	0.04	-1.57	67,67,67,67	1
2	MN	A	470	1/1	0.06	-1.57	41,41,41,41	0
4	TL	B	473	1/1	0.05	-1.60	67,67,67,67	1
2	MN	I	470	1/1	0.14	-1.74	41,41,41,41	0
2	MN	D	470	1/1	0.11	-1.77	41,41,41,41	0
4	TL	K	474	1/1	0.13	-1.78	75,75,75,75	1
2	MN	C	470	1/1	0.04	-1.98	41,41,41,41	0
4	TL	A	474	1/1	0.07	-2.77	75,75,75,75	1
4	TL	H	474	1/1	0.04	-2.83	75,75,75,75	1
2	MN	L	470	1/1	0.18	-2.88	41,41,41,41	0
2	MN	F	470	1/1	0.05	-3.60	41,41,41,41	0
2	MN	K	470	1/1	0.16	-3.91	41,41,41,41	0
4	TL	F	474	1/1	0.03	-3.93	75,75,75,75	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	E	470	1/1	0.09	-4.10	41,41,41,41	0
2	MN	B	470	1/1	0.04	-4.14	41,41,41,41	0
2	MN	G	470	1/1	0.13	-4.49	41,41,41,41	0
4	TL	B	474	1/1	0.09	-4.71	75,75,75,75	1
4	TL	C	474	1/1	0.04	-4.89	75,75,75,75	1

6.5 Other polymers

There are no such residues in this entry.