



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:21 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

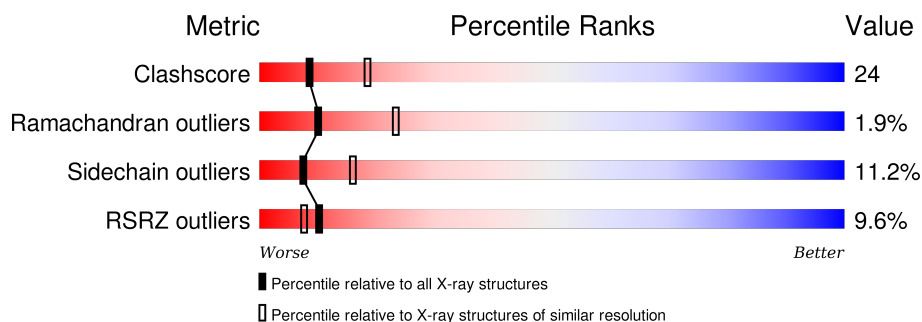
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	B	1472	-	-	-	X
3	ADP	D	1474	-	-	-	X
3	ADP	F	1476	-	-	-	X
3	ADP	I	1479	-	-	-	X
3	ADP	K	1481	-	-	-	X
3	ADP	L	1482	-	-	-	X
5	MPD	A	1483	-	-	X	X
5	MPD	B	1484	-	-	X	X
5	MPD	C	1485	-	-	X	X
5	MPD	D	1486	-	-	X	X
5	MPD	E	1487	-	-	X	X
5	MPD	F	1488	-	-	X	X
5	MPD	G	1489	-	-	X	X
5	MPD	H	1490	-	-	X	X
5	MPD	I	1491	-	-	X	X
5	MPD	J	1492	-	-	X	X
5	MPD	K	1493	-	-	X	X
5	MPD	L	1494	-	-	X	X

2 Entry composition [i](#)

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

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

- Molecule 1 is a protein called 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).

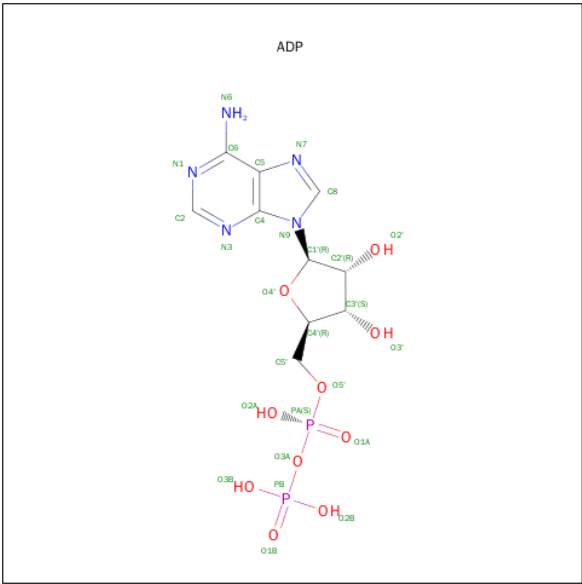
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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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: C₁₀H₁₅N₅O₁₀P₂).



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

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

- Molecule 4 is THALLIUM (I) ION (three-letter code: Tl) (formula: Tl).

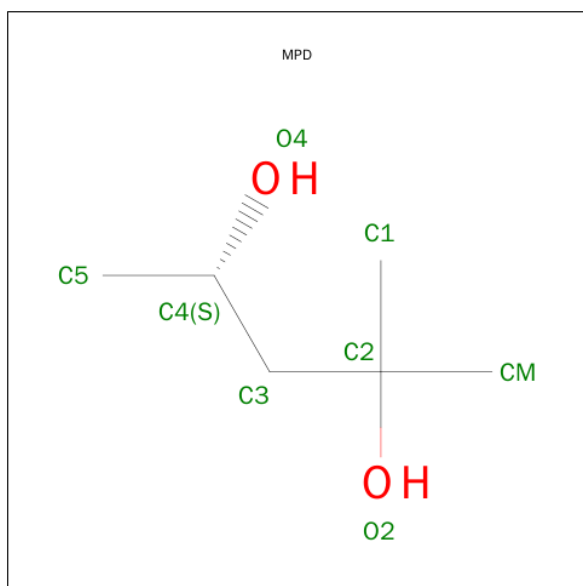
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total 2	Tl 2	0	0
4	J	2	Total 2	Tl 2	0	0
4	D	2	Total 2	Tl 2	0	0
4	K	2	Total 2	Tl 2	0	0
4	E	2	Total 2	Tl 2	0	0
4	H	2	Total 2	Tl 2	0	0
4	B	2	Total 2	Tl 2	0	0
4	I	2	Total 2	Tl 2	0	0

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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		

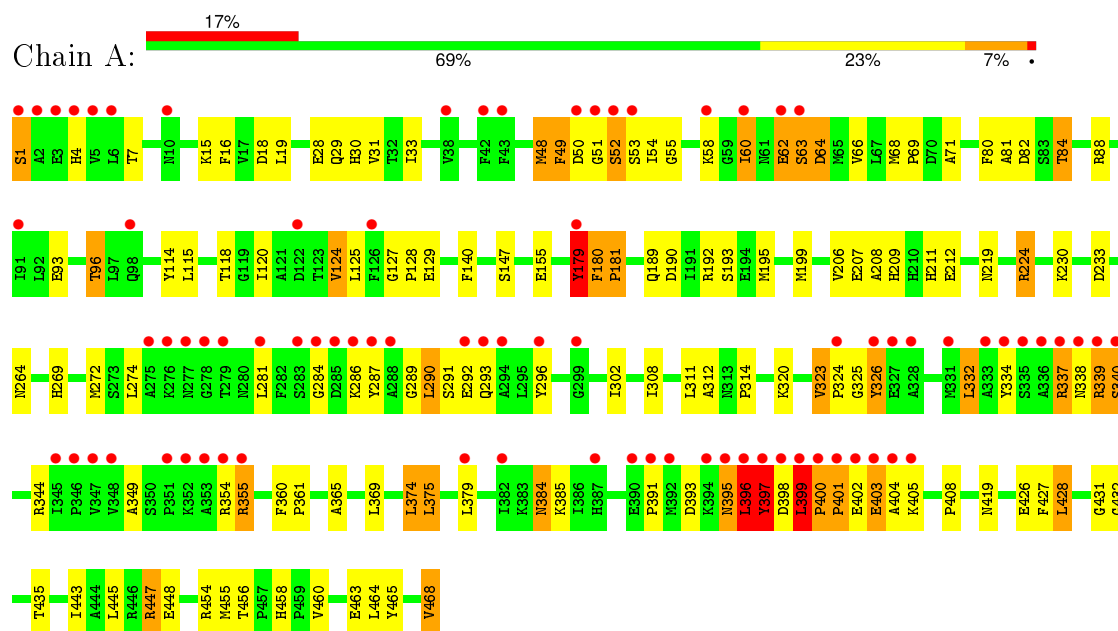
- Molecule 6 is water.

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		

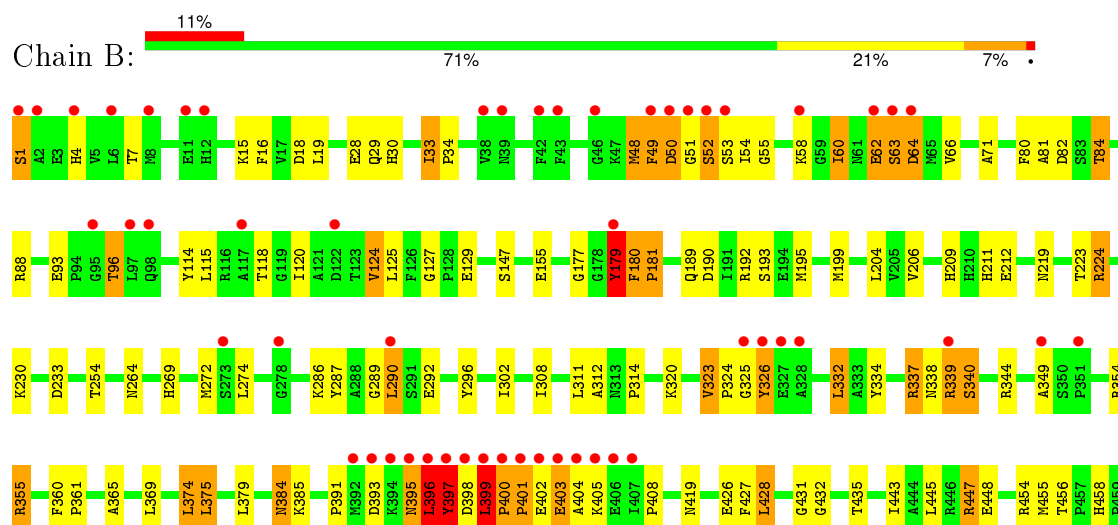
3 Residue-property plots [i](#)

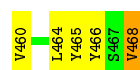
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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)



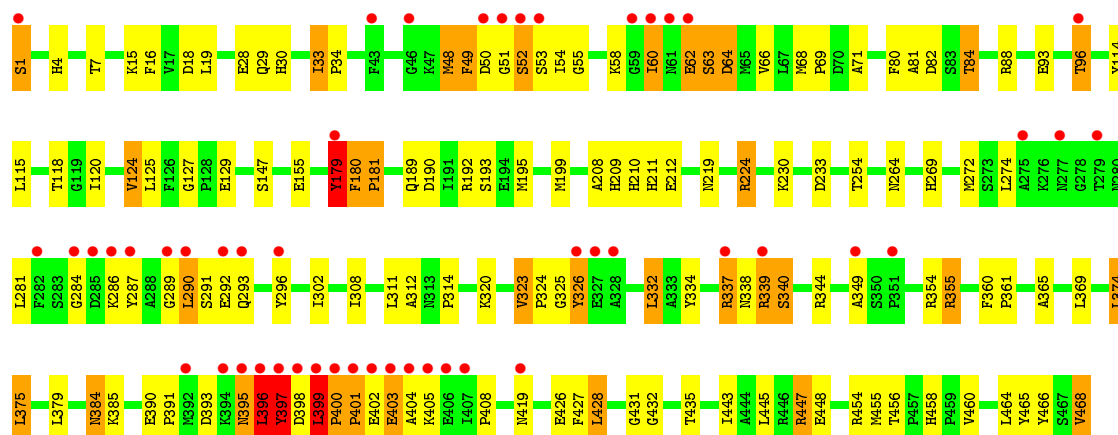
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)





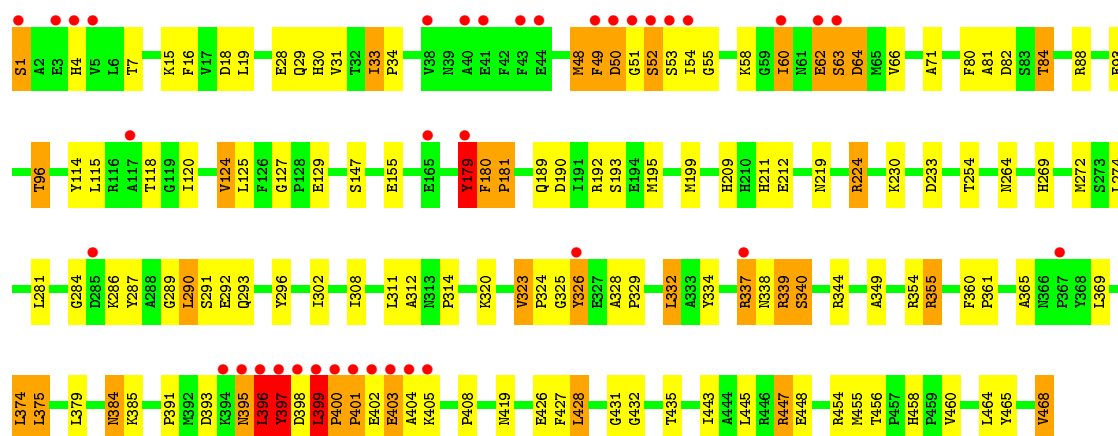
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain C: 10% 69% 23% 7%



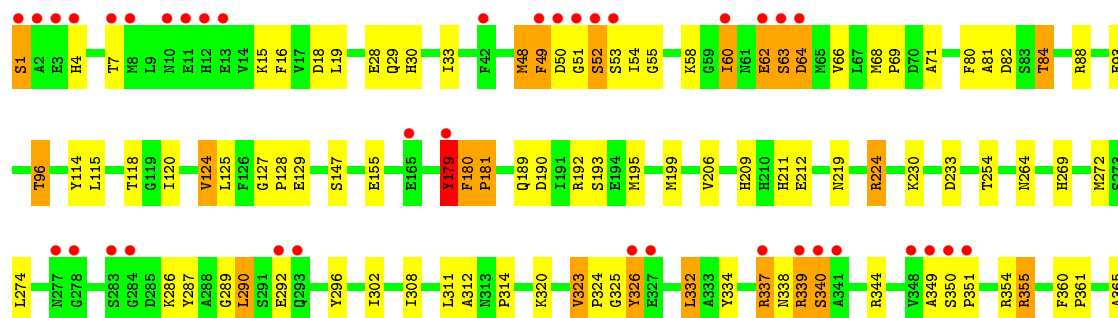
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

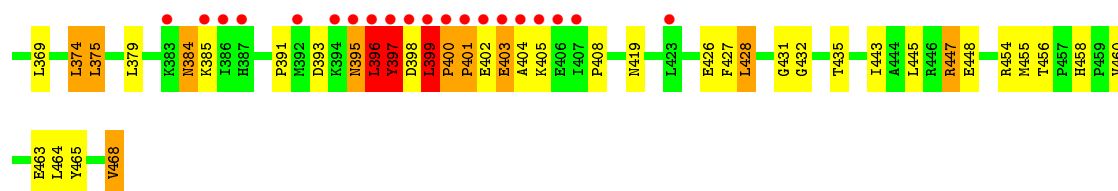
Chain D: 8% 70% 22% 7%



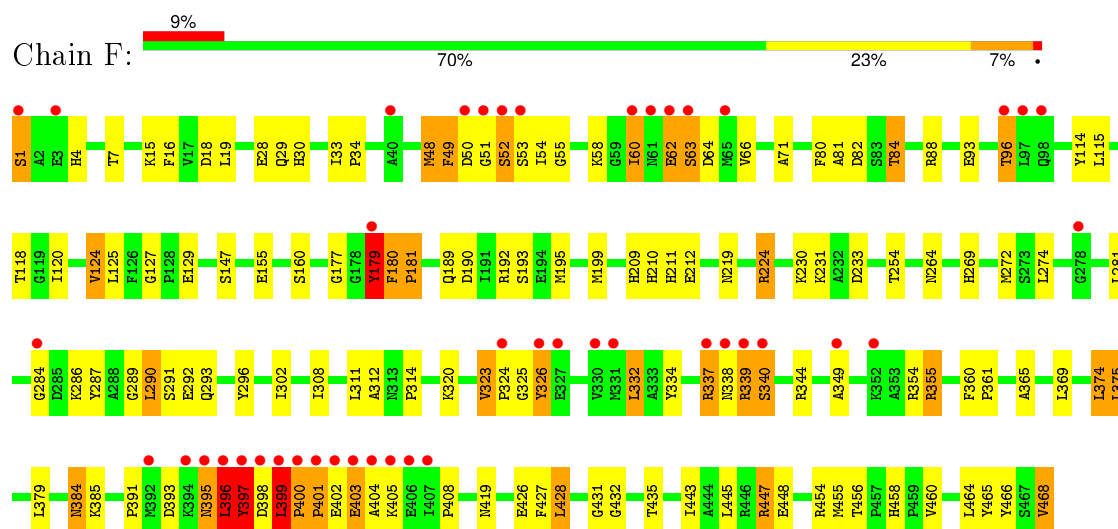
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain E: 12% 70% 22% 7%

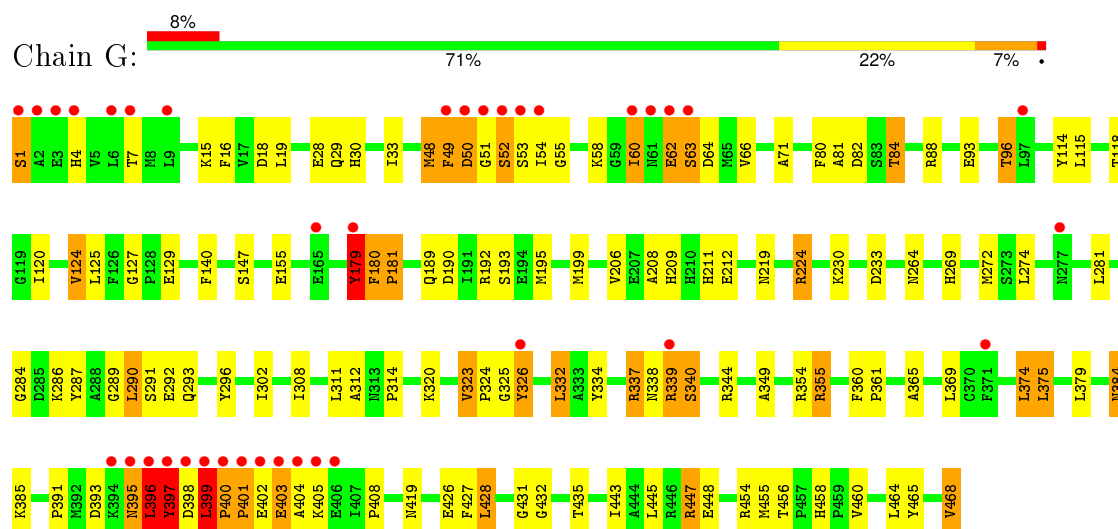




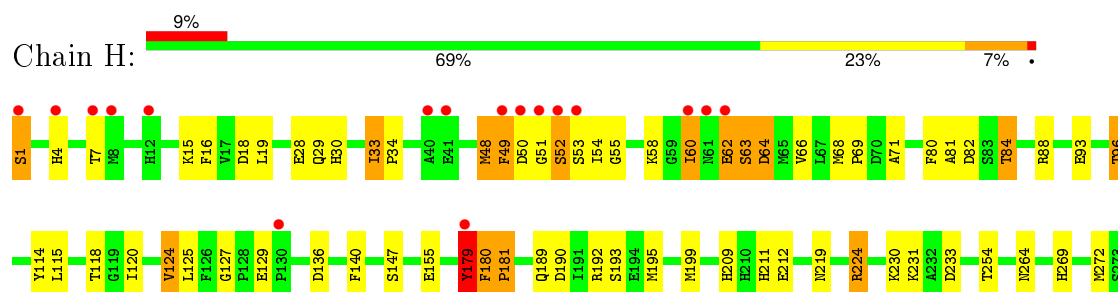
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

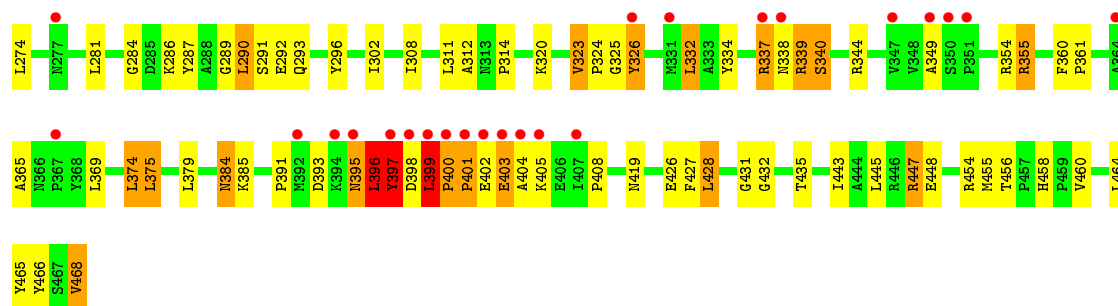


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

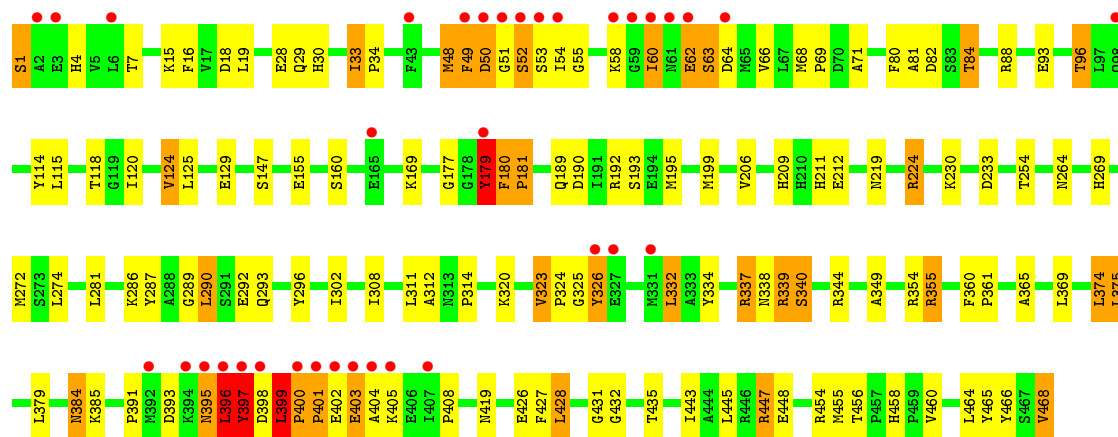


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

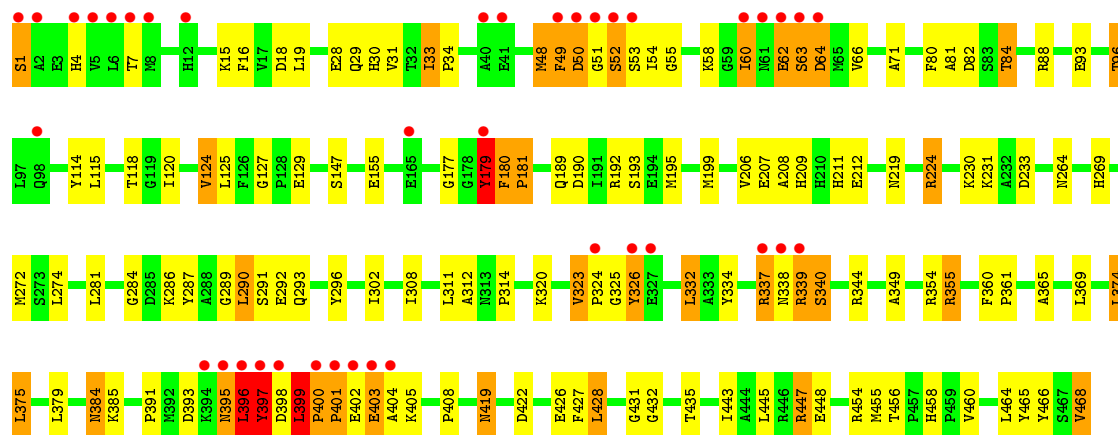




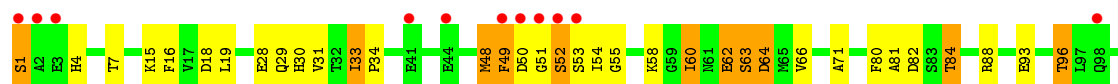
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

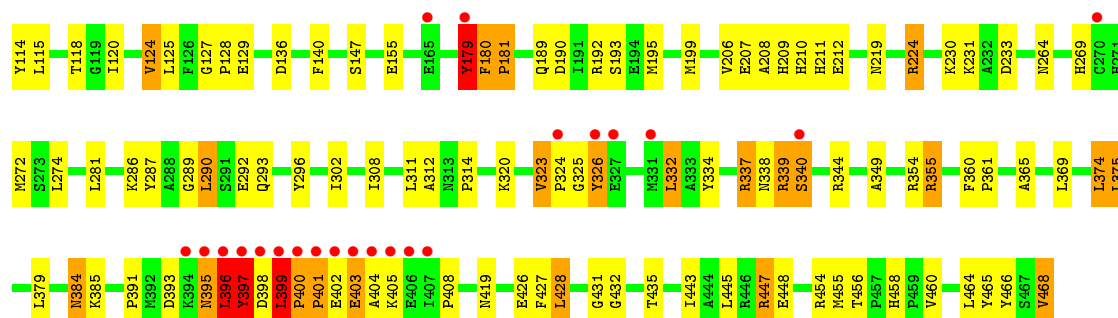


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

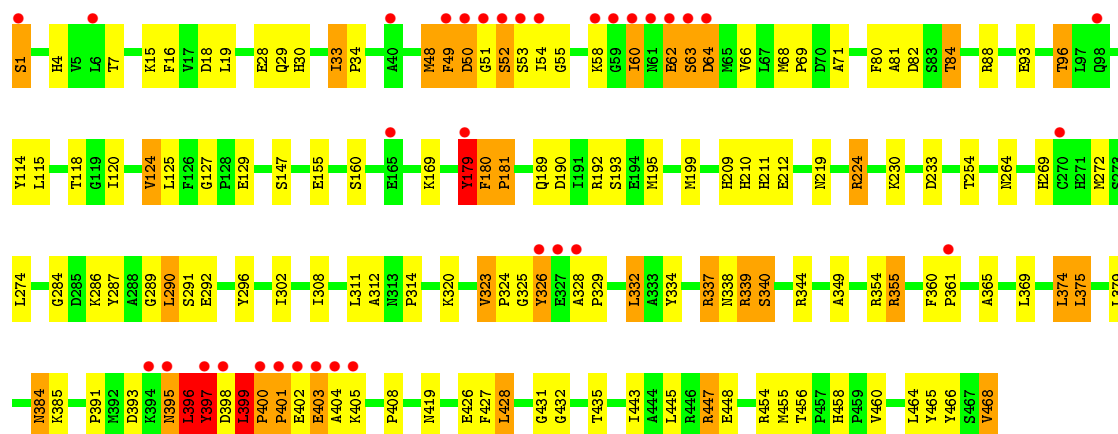


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)





• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, MN, 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 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3637	0	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
3	L	27	0	10	4	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2077) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.78	1.18
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H1'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:272:MET:O	1:B:355:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ARG:HD3	6:C:1595:HOH:O	2.17	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	10	23
1	B	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	C	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	D	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	E	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	F	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	G	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	H	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	I	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	J	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	K	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
1	L	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	10	23
All	All	5592/5616 (100%)	5148 (92%)	336 (6%)	108 (2%)	10	23

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	7	16
1	B	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	C	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	D	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	E	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	F	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	G	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	H	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	I	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	J	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	K	384/384 (100%)	341 (89%)	43 (11%)	7	16
1	L	384/384 (100%)	341 (89%)	43 (11%)	7	16
All	All	4608/4608 (100%)	4092 (89%)	516 (11%)	7	16

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	22,29,29	2.84	9 (40%)	27,45,45	3.40	12 (44%)
5	MPD	A	1483	-	6,7,7	0.96	0	7,10,10	0.68	0
3	ADP	B	1472	-	22,29,29	2.84	8 (36%)	27,45,45	3.40	12 (44%)
5	MPD	B	1484	-	6,7,7	0.96	0	7,10,10	0.67	0
3	ADP	C	1473	-	22,29,29	2.83	9 (40%)	27,45,45	3.40	12 (44%)
5	MPD	C	1485	-	6,7,7	0.97	0	7,10,10	0.68	0
3	ADP	D	1474	-	22,29,29	2.83	9 (40%)	27,45,45	3.39	12 (44%)
5	MPD	D	1486	-	6,7,7	0.96	0	7,10,10	0.67	0
3	ADP	E	1475	-	22,29,29	2.84	9 (40%)	27,45,45	3.40	12 (44%)
5	MPD	E	1487	-	6,7,7	0.95	0	7,10,10	0.68	0
3	ADP	F	1476	-	22,29,29	2.83	8 (36%)	27,45,45	3.39	12 (44%)
5	MPD	F	1488	-	6,7,7	0.96	0	7,10,10	0.68	0
3	ADP	G	1477	-	22,29,29	2.84	9 (40%)	27,45,45	3.40	12 (44%)
5	MPD	G	1489	-	6,7,7	0.96	0	7,10,10	0.68	0
3	ADP	H	1478	-	22,29,29	2.84	9 (40%)	27,45,45	3.40	12 (44%)
5	MPD	H	1490	-	6,7,7	0.96	0	7,10,10	0.68	0
3	ADP	I	1479	-	22,29,29	2.84	9 (40%)	27,45,45	3.40	12 (44%)
5	MPD	I	1491	-	6,7,7	0.96	0	7,10,10	0.68	0
3	ADP	J	1480	-	22,29,29	2.84	9 (40%)	27,45,45	3.40	12 (44%)
5	MPD	J	1492	-	6,7,7	0.96	0	7,10,10	0.67	0
3	ADP	K	1481	-	22,29,29	2.85	9 (40%)	27,45,45	3.40	12 (44%)
5	MPD	K	1493	-	6,7,7	0.96	0	7,10,10	0.67	0
3	ADP	L	1482	-	22,29,29	2.84	9 (40%)	27,45,45	3.40	12 (44%)
5	MPD	L	1494	-	6,7,7	0.97	0	7,10,10	0.68	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	-	-	0/12/32/32	0/3/3/3
5	MPD	A	1483	-	-	0/5/5/5	0/0/0/0
3	ADP	B	1472	-	-	0/12/32/32	0/3/3/3
5	MPD	B	1484	-	-	0/5/5/5	0/0/0/0
3	ADP	C	1473	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	C	1485	-	-	0/5/5/5	0/0/0/0
3	ADP	D	1474	-	-	0/12/32/32	0/3/3/3
5	MPD	D	1486	-	-	0/5/5/5	0/0/0/0
3	ADP	E	1475	-	-	0/12/32/32	0/3/3/3
5	MPD	E	1487	-	-	0/5/5/5	0/0/0/0
3	ADP	F	1476	-	-	0/12/32/32	0/3/3/3
5	MPD	F	1488	-	-	0/5/5/5	0/0/0/0
3	ADP	G	1477	-	-	0/12/32/32	0/3/3/3
5	MPD	G	1489	-	-	0/5/5/5	0/0/0/0
3	ADP	H	1478	-	-	0/12/32/32	0/3/3/3
5	MPD	H	1490	-	-	0/5/5/5	0/0/0/0
3	ADP	I	1479	-	-	0/12/32/32	0/3/3/3
5	MPD	I	1491	-	-	0/5/5/5	0/0/0/0
3	ADP	J	1480	-	-	0/12/32/32	0/3/3/3
5	MPD	J	1492	-	-	0/5/5/5	0/0/0/0
3	ADP	K	1481	-	-	0/12/32/32	0/3/3/3
5	MPD	K	1493	-	-	0/5/5/5	0/0/0/0
3	ADP	L	1482	-	-	0/12/32/32	0/3/3/3
5	MPD	L	1494	-	-	0/5/5/5	0/0/0/0

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1481	ADP	C6-N6	-3.75	1.23	1.34
3	I	1479	ADP	C6-N6	-3.74	1.23	1.34
3	D	1474	ADP	C6-N6	-3.74	1.23	1.34
3	G	1477	ADP	C6-N6	-3.74	1.23	1.34
3	C	1473	ADP	C6-N6	-3.74	1.23	1.34
3	A	1471	ADP	C6-N6	-3.73	1.23	1.34
3	J	1480	ADP	C6-N6	-3.73	1.23	1.34
3	H	1478	ADP	C6-N6	-3.72	1.23	1.34
3	E	1475	ADP	C6-N6	-3.72	1.23	1.34
3	L	1482	ADP	C6-N6	-3.72	1.23	1.34
3	B	1472	ADP	C6-N6	-3.71	1.23	1.34
3	F	1476	ADP	C6-N6	-3.71	1.23	1.34
3	H	1478	ADP	C3'-C4'	-2.59	1.46	1.53
3	J	1480	ADP	C3'-C4'	-2.58	1.46	1.53
3	K	1481	ADP	C3'-C4'	-2.58	1.46	1.53
3	G	1477	ADP	C3'-C4'	-2.58	1.46	1.53
3	L	1482	ADP	C3'-C4'	-2.57	1.46	1.53
3	E	1475	ADP	C3'-C4'	-2.57	1.46	1.53
3	F	1476	ADP	C3'-C4'	-2.57	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1471	ADP	C3'-C4'	-2.57	1.46	1.53
3	I	1479	ADP	C3'-C4'	-2.57	1.46	1.53
3	D	1474	ADP	C3'-C4'	-2.56	1.46	1.53
3	B	1472	ADP	C3'-C4'	-2.55	1.46	1.53
3	C	1473	ADP	C3'-C4'	-2.55	1.46	1.53
3	E	1475	ADP	PB-O2B	-2.02	1.47	1.54
3	J	1480	ADP	PB-O2B	-2.02	1.47	1.54
3	G	1477	ADP	PB-O2B	-2.01	1.47	1.54
3	L	1482	ADP	PB-O2B	-2.01	1.47	1.54
3	D	1474	ADP	PB-O2B	-2.01	1.47	1.54
3	K	1481	ADP	PB-O2B	-2.01	1.47	1.54
3	I	1479	ADP	PB-O2B	-2.01	1.47	1.54
3	H	1478	ADP	PB-O2B	-2.00	1.47	1.54
3	C	1473	ADP	PB-O2B	-2.00	1.47	1.54
3	A	1471	ADP	PB-O2B	-2.00	1.47	1.54
3	B	1472	ADP	C5-C4	2.35	1.45	1.40
3	H	1478	ADP	C5-C4	2.35	1.45	1.40
3	L	1482	ADP	C5-C4	2.35	1.45	1.40
3	J	1480	ADP	C5-C4	2.36	1.45	1.40
3	I	1479	ADP	C5-C4	2.36	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	F	1476	ADP	C5-C4	2.38	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	K	1481	ADP	C5-C4	2.39	1.45	1.40
3	E	1475	ADP	PB-O3B	3.72	1.68	1.54
3	C	1473	ADP	PB-O3B	3.72	1.68	1.54
3	I	1479	ADP	PB-O3B	3.72	1.68	1.54
3	H	1478	ADP	PB-O3B	3.72	1.68	1.54
3	L	1482	ADP	PB-O3B	3.73	1.68	1.54
3	D	1474	ADP	PB-O3B	3.73	1.68	1.54
3	K	1481	ADP	PB-O3B	3.73	1.68	1.54
3	F	1476	ADP	PB-O3B	3.73	1.68	1.54
3	A	1471	ADP	PB-O3B	3.73	1.68	1.54
3	D	1474	ADP	C2-N3	3.73	1.38	1.32
3	B	1472	ADP	PB-O3B	3.73	1.68	1.54
3	H	1478	ADP	C2-N3	3.74	1.38	1.32
3	B	1472	ADP	C2-N3	3.75	1.38	1.32
3	L	1482	ADP	C2-N3	3.75	1.38	1.32
3	A	1471	ADP	C2-N3	3.75	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1477	ADP	C2-N3	3.75	1.38	1.32
3	J	1480	ADP	PB-O3B	3.75	1.68	1.54
3	F	1476	ADP	C2-N3	3.75	1.38	1.32
3	C	1473	ADP	C2-N3	3.75	1.38	1.32
3	G	1477	ADP	PB-O3B	3.76	1.68	1.54
3	I	1479	ADP	C2-N3	3.76	1.38	1.32
3	E	1475	ADP	C2-N3	3.77	1.38	1.32
3	K	1481	ADP	C2-N3	3.77	1.38	1.32
3	J	1480	ADP	C2-N3	3.77	1.38	1.32
3	D	1474	ADP	O4'-C4'	3.83	1.53	1.45
3	L	1482	ADP	O4'-C4'	3.85	1.53	1.45
3	E	1475	ADP	O4'-C4'	3.85	1.53	1.45
3	G	1477	ADP	O4'-C4'	3.86	1.53	1.45
3	A	1471	ADP	O4'-C4'	3.86	1.53	1.45
3	H	1478	ADP	O4'-C4'	3.87	1.53	1.45
3	F	1476	ADP	O4'-C4'	3.87	1.54	1.45
3	K	1481	ADP	O4'-C4'	3.87	1.54	1.45
3	J	1480	ADP	O4'-C4'	3.88	1.54	1.45
3	I	1479	ADP	O4'-C4'	3.88	1.54	1.45
3	C	1473	ADP	O4'-C4'	3.89	1.54	1.45
3	B	1472	ADP	O4'-C4'	3.89	1.54	1.45
3	I	1479	ADP	C4-N3	5.02	1.43	1.35
3	J	1480	ADP	C4-N3	5.03	1.43	1.35
3	F	1476	ADP	C4-N3	5.03	1.43	1.35
3	C	1473	ADP	C4-N3	5.03	1.43	1.35
3	G	1477	ADP	C4-N3	5.04	1.43	1.35
3	E	1475	ADP	C4-N3	5.04	1.43	1.35
3	H	1478	ADP	C4-N3	5.06	1.43	1.35
3	A	1471	ADP	C4-N3	5.06	1.43	1.35
3	D	1474	ADP	C4-N3	5.06	1.43	1.35
3	B	1472	ADP	C4-N3	5.08	1.43	1.35
3	K	1481	ADP	C4-N3	5.08	1.43	1.35
3	L	1482	ADP	C4-N3	5.11	1.43	1.35
3	F	1476	ADP	O4'-C1'	8.30	1.51	1.41
3	C	1473	ADP	O4'-C1'	8.32	1.51	1.41
3	J	1480	ADP	O4'-C1'	8.33	1.51	1.41
3	A	1471	ADP	O4'-C1'	8.34	1.51	1.41
3	D	1474	ADP	O4'-C1'	8.34	1.51	1.41
3	B	1472	ADP	O4'-C1'	8.34	1.51	1.41
3	E	1475	ADP	O4'-C1'	8.35	1.51	1.41
3	L	1482	ADP	O4'-C1'	8.36	1.51	1.41
3	I	1479	ADP	O4'-C1'	8.37	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1478	ADP	O4'-C1'	8.37	1.51	1.41
3	G	1477	ADP	O4'-C1'	8.38	1.51	1.41
3	K	1481	ADP	O4'-C1'	8.38	1.51	1.41

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1478	ADP	C4'-O4'-C1'	-8.64	100.22	109.72
3	L	1482	ADP	C4'-O4'-C1'	-8.63	100.24	109.72
3	I	1479	ADP	C4'-O4'-C1'	-8.62	100.24	109.72
3	J	1480	ADP	C4'-O4'-C1'	-8.60	100.27	109.72
3	B	1472	ADP	C4'-O4'-C1'	-8.59	100.28	109.72
3	K	1481	ADP	C4'-O4'-C1'	-8.59	100.28	109.72
3	A	1471	ADP	C4'-O4'-C1'	-8.59	100.28	109.72
3	C	1473	ADP	C4'-O4'-C1'	-8.58	100.29	109.72
3	E	1475	ADP	C4'-O4'-C1'	-8.57	100.30	109.72
3	F	1476	ADP	C4'-O4'-C1'	-8.57	100.30	109.72
3	G	1477	ADP	C4'-O4'-C1'	-8.57	100.30	109.72
3	D	1474	ADP	C4'-O4'-C1'	-8.54	100.34	109.72
3	I	1479	ADP	C5'-C4'-C3'	-3.58	101.00	115.21
3	G	1477	ADP	C5'-C4'-C3'	-3.58	101.01	115.21
3	A	1471	ADP	C5'-C4'-C3'	-3.57	101.02	115.21
3	L	1482	ADP	C5'-C4'-C3'	-3.57	101.03	115.21
3	B	1472	ADP	C5'-C4'-C3'	-3.57	101.03	115.21
3	F	1476	ADP	C5'-C4'-C3'	-3.57	101.03	115.21
3	H	1478	ADP	C5'-C4'-C3'	-3.57	101.03	115.21
3	J	1480	ADP	C5'-C4'-C3'	-3.57	101.04	115.21
3	D	1474	ADP	C5'-C4'-C3'	-3.57	101.05	115.21
3	C	1473	ADP	C5'-C4'-C3'	-3.57	101.05	115.21
3	E	1475	ADP	C5'-C4'-C3'	-3.56	101.08	115.21
3	K	1481	ADP	C5'-C4'-C3'	-3.56	101.08	115.21
3	C	1473	ADP	O5'-PA-O1A	-2.14	101.32	109.62
3	H	1478	ADP	O5'-PA-O1A	-2.14	101.32	109.62
3	E	1475	ADP	O5'-PA-O1A	-2.14	101.33	109.62
3	L	1482	ADP	O5'-PA-O1A	-2.13	101.35	109.62
3	D	1474	ADP	O5'-PA-O1A	-2.13	101.35	109.62
3	K	1481	ADP	O5'-PA-O1A	-2.13	101.35	109.62
3	A	1471	ADP	O5'-PA-O1A	-2.13	101.36	109.62
3	J	1480	ADP	O5'-PA-O1A	-2.13	101.36	109.62
3	G	1477	ADP	O5'-PA-O1A	-2.13	101.36	109.62
3	I	1479	ADP	O5'-PA-O1A	-2.12	101.38	109.62
3	B	1472	ADP	O5'-PA-O1A	-2.12	101.39	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1476	ADP	O5'-PA-O1A	-2.12	101.40	109.62
3	F	1476	ADP	O2B-PB-O3A	2.04	114.36	105.09
3	H	1478	ADP	O2B-PB-O3A	2.06	114.42	105.09
3	I	1479	ADP	O2B-PB-O3A	2.06	114.43	105.09
3	A	1471	ADP	O2B-PB-O3A	2.06	114.43	105.09
3	K	1481	ADP	O2B-PB-O3A	2.06	114.44	105.09
3	E	1475	ADP	O2B-PB-O3A	2.06	114.44	105.09
3	D	1474	ADP	O2B-PB-O3A	2.06	114.44	105.09
3	G	1477	ADP	O2B-PB-O3A	2.06	114.44	105.09
3	C	1473	ADP	O2B-PB-O3A	2.06	114.45	105.09
3	L	1482	ADP	O2B-PB-O3A	2.07	114.46	105.09
3	B	1472	ADP	O2B-PB-O3A	2.07	114.46	105.09
3	J	1480	ADP	O2B-PB-O3A	2.07	114.47	105.09
3	C	1473	ADP	C2'-C1'-N9	2.36	117.90	114.29
3	L	1482	ADP	C2'-C1'-N9	2.37	117.91	114.29
3	B	1472	ADP	C2'-C1'-N9	2.37	117.92	114.29
3	H	1478	ADP	C2'-C1'-N9	2.38	117.92	114.29
3	G	1477	ADP	C2'-C1'-N9	2.38	117.93	114.29
3	J	1480	ADP	C2'-C1'-N9	2.39	117.94	114.29
3	A	1471	ADP	C2'-C1'-N9	2.39	117.95	114.29
3	I	1479	ADP	C2'-C1'-N9	2.39	117.95	114.29
3	E	1475	ADP	C2'-C1'-N9	2.40	117.96	114.29
3	D	1474	ADP	C2'-C1'-N9	2.40	117.96	114.29
3	K	1481	ADP	C2'-C1'-N9	2.40	117.96	114.29
3	F	1476	ADP	C2'-C1'-N9	2.42	117.99	114.29
3	H	1478	ADP	O3'-C3'-C2'	2.91	121.29	111.83
3	G	1477	ADP	O3'-C3'-C2'	2.91	121.30	111.83
3	A	1471	ADP	O3'-C3'-C2'	2.92	121.33	111.83
3	C	1473	ADP	O3'-C3'-C2'	2.92	121.33	111.83
3	B	1472	ADP	O3'-C3'-C2'	2.92	121.34	111.83
3	L	1482	ADP	O3'-C3'-C2'	2.93	121.34	111.83
3	D	1474	ADP	O3'-C3'-C2'	2.93	121.35	111.83
3	F	1476	ADP	O3'-C3'-C2'	2.93	121.35	111.83
3	I	1479	ADP	O3'-C3'-C2'	2.93	121.35	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	J	1480	ADP	O3'-C3'-C2'	2.94	121.38	111.83
3	L	1482	ADP	O3A-PA-O5'	3.64	112.60	102.94
3	I	1479	ADP	O3A-PA-O5'	3.65	112.61	102.94
3	J	1480	ADP	O3A-PA-O5'	3.65	112.61	102.94
3	B	1472	ADP	O3A-PA-O5'	3.65	112.61	102.94
3	D	1474	ADP	O3A-PA-O5'	3.65	112.62	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1471	ADP	O3A-PA-O5'	3.65	112.62	102.94
3	K	1481	ADP	O3A-PA-O5'	3.66	112.63	102.94
3	C	1473	ADP	O3A-PA-O5'	3.66	112.63	102.94
3	H	1478	ADP	O3A-PA-O5'	3.66	112.64	102.94
3	F	1476	ADP	O3A-PA-O5'	3.66	112.64	102.94
3	E	1475	ADP	O3A-PA-O5'	3.66	112.65	102.94
3	G	1477	ADP	O3A-PA-O5'	3.67	112.67	102.94
3	H	1478	ADP	O4'-C4'-C5'	4.43	125.18	109.32
3	I	1479	ADP	O4'-C4'-C5'	4.43	125.18	109.32
3	L	1482	ADP	O4'-C4'-C5'	4.44	125.19	109.32
3	K	1481	ADP	O4'-C4'-C5'	4.44	125.19	109.32
3	J	1480	ADP	O4'-C4'-C5'	4.44	125.20	109.32
3	G	1477	ADP	O4'-C4'-C5'	4.44	125.22	109.32
3	B	1472	ADP	O4'-C4'-C5'	4.45	125.22	109.32
3	A	1471	ADP	O4'-C4'-C5'	4.45	125.22	109.32
3	F	1476	ADP	O4'-C4'-C5'	4.45	125.24	109.32
3	E	1475	ADP	O4'-C4'-C5'	4.45	125.25	109.32
3	C	1473	ADP	O4'-C4'-C5'	4.45	125.25	109.32
3	D	1474	ADP	O4'-C4'-C5'	4.46	125.27	109.32
3	K	1481	ADP	C4-C5-N7	5.13	114.19	109.48
3	E	1475	ADP	C4-C5-N7	5.13	114.19	109.48
3	L	1482	ADP	C4-C5-N7	5.14	114.20	109.48
3	D	1474	ADP	C4-C5-N7	5.15	114.22	109.48
3	F	1476	ADP	C4-C5-N7	5.15	114.22	109.48
3	A	1471	ADP	C4-C5-N7	5.16	114.22	109.48
3	G	1477	ADP	C4-C5-N7	5.16	114.22	109.48
3	C	1473	ADP	C4-C5-N7	5.16	114.23	109.48
3	I	1479	ADP	C4-C5-N7	5.18	114.24	109.48
3	J	1480	ADP	C4-C5-N7	5.18	114.24	109.48
3	B	1472	ADP	C4-C5-N7	5.19	114.25	109.48
3	H	1478	ADP	C4-C5-N7	5.20	114.26	109.48
3	I	1479	ADP	O4'-C1'-N9	5.79	120.22	108.10
3	L	1482	ADP	O4'-C1'-N9	5.80	120.23	108.10
3	C	1473	ADP	O4'-C1'-N9	5.80	120.23	108.10
3	H	1478	ADP	O4'-C1'-N9	5.80	120.24	108.10
3	A	1471	ADP	O4'-C1'-N9	5.81	120.26	108.10
3	J	1480	ADP	O4'-C1'-N9	5.81	120.26	108.10
3	F	1476	ADP	O4'-C1'-N9	5.82	120.27	108.10
3	B	1472	ADP	O4'-C1'-N9	5.82	120.27	108.10
3	K	1481	ADP	O4'-C1'-N9	5.82	120.28	108.10
3	G	1477	ADP	O4'-C1'-N9	5.82	120.28	108.10
3	D	1474	ADP	O4'-C1'-N9	5.82	120.29	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1475	ADP	O4'-C1'-N9	5.83	120.30	108.10
3	F	1476	ADP	C1'-N9-C4	6.14	136.21	126.94
3	I	1479	ADP	C1'-N9-C4	6.16	136.24	126.94
3	E	1475	ADP	C1'-N9-C4	6.17	136.25	126.94
3	A	1471	ADP	C1'-N9-C4	6.17	136.25	126.94
3	K	1481	ADP	C1'-N9-C4	6.18	136.26	126.94
3	D	1474	ADP	C1'-N9-C4	6.18	136.26	126.94
3	B	1472	ADP	C1'-N9-C4	6.18	136.26	126.94
3	J	1480	ADP	C1'-N9-C4	6.18	136.26	126.94
3	H	1478	ADP	C1'-N9-C4	6.19	136.28	126.94
3	G	1477	ADP	C1'-N9-C4	6.20	136.29	126.94
3	C	1473	ADP	C1'-N9-C4	6.20	136.29	126.94
3	L	1482	ADP	C1'-N9-C4	6.20	136.30	126.94
3	G	1477	ADP	O5'-C5'-C4'	7.43	136.50	109.12
3	B	1472	ADP	O5'-C5'-C4'	7.43	136.51	109.12
3	F	1476	ADP	O5'-C5'-C4'	7.43	136.52	109.12
3	I	1479	ADP	O5'-C5'-C4'	7.43	136.52	109.12
3	C	1473	ADP	O5'-C5'-C4'	7.44	136.53	109.12
3	H	1478	ADP	O5'-C5'-C4'	7.44	136.53	109.12
3	A	1471	ADP	O5'-C5'-C4'	7.44	136.54	109.12
3	L	1482	ADP	O5'-C5'-C4'	7.44	136.56	109.12
3	D	1474	ADP	O5'-C5'-C4'	7.44	136.56	109.12
3	E	1475	ADP	O5'-C5'-C4'	7.44	136.56	109.12
3	J	1480	ADP	O5'-C5'-C4'	7.44	136.56	109.12
3	K	1481	ADP	O5'-C5'-C4'	7.45	136.58	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 438 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1471	ADP	4	0
5	A	1483	MPD	29	0
3	B	1472	ADP	4	0
5	B	1484	MPD	34	0
3	C	1473	ADP	4	0
5	C	1485	MPD	33	0
3	D	1474	ADP	4	0
5	D	1486	MPD	34	0
3	E	1475	ADP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1487	MPD	29	0
3	F	1476	ADP	4	0
5	F	1488	MPD	34	0
3	G	1477	ADP	4	0
5	G	1489	MPD	31	0
3	H	1478	ADP	4	0
5	H	1490	MPD	33	0
3	I	1479	ADP	3	0
5	I	1491	MPD	35	0
3	J	1480	ADP	4	0
5	J	1492	MPD	34	0
3	K	1481	ADP	4	0
5	K	1493	MPD	33	0
3	L	1482	ADP	4	0
5	L	1494	MPD	32	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	468/468 (100%)	0.68	80 (17%) 2 1	18, 39, 91, 100	29 (6%)
1	B	468/468 (100%)	0.44	53 (11%) 7 5	18, 39, 91, 100	29 (6%)
1	C	468/468 (100%)	0.34	49 (10%) 8 6	18, 39, 91, 100	29 (6%)
1	D	468/468 (100%)	0.17	37 (7%) 15 13	18, 39, 91, 100	29 (6%)
1	E	468/468 (100%)	0.39	58 (12%) 5 4	18, 39, 91, 100	29 (6%)
1	F	468/468 (100%)	0.35	44 (9%) 11 8	18, 39, 91, 100	29 (6%)
1	G	468/468 (100%)	0.29	37 (7%) 15 13	18, 39, 91, 100	29 (6%)
1	H	468/468 (100%)	0.36	41 (8%) 12 9	18, 39, 91, 100	29 (6%)
1	I	468/468 (100%)	0.19	35 (7%) 17 14	18, 39, 91, 100	29 (6%)
1	J	468/468 (100%)	0.28	39 (8%) 14 11	18, 39, 91, 100	29 (6%)
1	K	468/468 (100%)	0.26	33 (7%) 19 16	18, 39, 91, 100	29 (6%)
1	L	468/468 (100%)	0.35	34 (7%) 18 15	18, 39, 91, 100	29 (6%)
All	All	5616/5616 (100%)	0.34	540 (9%) 10 7	18, 39, 92, 100	348 (6%)

All (540) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	397	TYR	13.3
1	K	397	TYR	12.9
1	H	402	GLU	12.7
1	B	397	TYR	12.5
1	L	51	GLY	12.1
1	K	326	TYR	11.7
1	J	397	TYR	11.6
1	F	400	PRO	11.4
1	K	398	ASP	10.7
1	C	397	TYR	10.6
1	A	397	TYR	10.4

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Mol	Chain	Res	Type	RSRZ
1	E	397	TYR	10.3
1	J	62	GLU	10.0
1	E	51	GLY	9.9
1	F	397	TYR	9.6
1	F	398	ASP	9.6
1	A	395	ASN	9.5
1	B	400	PRO	9.3
1	H	397	TYR	9.0
1	H	395	ASN	9.0
1	D	51	GLY	8.9
1	A	51	GLY	8.7
1	K	400	PRO	8.7
1	G	397	TYR	8.5
1	J	51	GLY	8.3
1	L	50	ASP	8.2
1	E	395	ASN	8.2
1	G	51	GLY	8.0
1	H	51	GLY	8.0
1	B	398	ASP	7.9
1	D	326	TYR	7.7
1	F	326	TYR	7.5
1	H	403	GLU	7.5
1	A	52	SER	7.5
1	F	51	GLY	7.4
1	G	401	PRO	7.4
1	K	402	GLU	7.3
1	C	403	GLU	7.3
1	K	394	LYS	7.3
1	K	51	GLY	7.2
1	F	401	PRO	7.2
1	L	52	SER	7.0
1	B	404	ALA	7.0
1	L	400	PRO	6.9
1	C	51	GLY	6.9
1	A	326	TYR	6.8
1	E	50	ASP	6.8
1	B	51	GLY	6.8
1	G	50	ASP	6.8
1	G	52	SER	6.7
1	H	50	ASP	6.6
1	H	62	GLU	6.5
1	F	61	ASN	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	403	GLU	6.4
1	G	402	GLU	6.4
1	H	52	SER	6.4
1	J	403	GLU	6.4
1	E	394	LYS	6.3
1	A	285	ASP	6.3
1	B	326	TYR	6.3
1	A	394	LYS	6.3
1	F	52	SER	6.3
1	K	401	PRO	6.2
1	F	50	ASP	6.2
1	F	403	GLU	6.2
1	J	326	TYR	6.2
1	I	51	GLY	6.1
1	A	296	TYR	6.1
1	E	400	PRO	6.1
1	J	50	ASP	6.1
1	I	405	LYS	6.1
1	A	398	ASP	6.1
1	A	334	TYR	6.0
1	A	396	LEU	6.0
1	J	398	ASP	5.9
1	G	60	ILE	5.9
1	C	52	SER	5.9
1	L	394	LYS	5.9
1	K	396	LEU	5.9
1	G	400	PRO	5.9
1	C	400	PRO	5.9
1	D	394	LYS	5.8
1	G	395	ASN	5.8
1	K	395	ASN	5.8
1	I	50	ASP	5.7
1	C	404	ALA	5.6
1	D	60	ILE	5.6
1	E	398	ASP	5.6
1	K	52	SER	5.6
1	H	394	LYS	5.6
1	K	403	GLU	5.5
1	L	401	PRO	5.5
1	C	326	TYR	5.5
1	K	50	ASP	5.5
1	E	399	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	1	SER	5.5
1	B	396	LEU	5.5
1	G	398	ASP	5.4
1	A	354	ARG	5.4
1	J	394	LYS	5.4
1	L	179	TYR	5.4
1	F	399	LEU	5.4
1	L	60	ILE	5.4
1	J	400	PRO	5.3
1	H	179	TYR	5.3
1	I	394	LYS	5.3
1	B	405	LYS	5.3
1	H	398	ASP	5.3
1	D	52	SER	5.3
1	F	62	GLU	5.2
1	C	405	LYS	5.2
1	J	53	SER	5.2
1	I	397	TYR	5.2
1	A	392	MET	5.2
1	K	399	LEU	5.2
1	B	52	SER	5.1
1	B	1	SER	5.1
1	D	405	LYS	5.1
1	G	61	ASN	5.1
1	B	403	GLU	5.1
1	L	402	GLU	5.1
1	A	345	ILE	5.1
1	J	60	ILE	5.1
1	L	398	ASP	5.1
1	B	53	SER	5.1
1	A	277	ASN	5.0
1	I	404	ALA	5.0
1	I	53	SER	5.0
1	G	1	SER	5.0
1	A	53	SER	5.0
1	A	404	ALA	5.0
1	E	7	THR	5.0
1	E	1	SER	4.9
1	B	399	LEU	4.9
1	J	395	ASN	4.9
1	L	53	SER	4.9
1	C	50	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLU	4.9
1	I	52	SER	4.9
1	C	398	ASP	4.9
1	J	63	SER	4.8
1	I	326	TYR	4.8
1	I	62	GLU	4.8
1	A	50	ASP	4.8
1	A	58	LYS	4.8
1	F	395	ASN	4.7
1	H	349	ALA	4.7
1	G	405	LYS	4.7
1	L	405	LYS	4.7
1	G	326	TYR	4.7
1	E	386	ILE	4.6
1	C	401	PRO	4.6
1	C	53	SER	4.6
1	F	53	SER	4.6
1	A	400	PRO	4.6
1	D	402	GLU	4.6
1	D	404	ALA	4.6
1	J	52	SER	4.6
1	D	401	PRO	4.5
1	D	395	ASN	4.5
1	F	396	LEU	4.5
1	J	1	SER	4.5
1	A	351	PRO	4.5
1	K	179	TYR	4.5
1	J	396	LEU	4.5
1	G	3	GLU	4.4
1	G	394	LYS	4.4
1	F	404	ALA	4.4
1	A	347	VAL	4.4
1	C	394	LYS	4.4
1	J	404	ALA	4.4
1	D	398	ASP	4.3
1	L	395	ASN	4.3
1	L	403	GLU	4.3
1	F	60	ILE	4.3
1	I	403	GLU	4.3
1	C	402	GLU	4.3
1	A	278	GLY	4.3
1	A	348	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	395	ASN	4.2
1	I	3	GLU	4.2
1	E	52	SER	4.1
1	H	60	ILE	4.1
1	C	293	GLN	4.1
1	K	406	GLU	4.1
1	H	400	PRO	4.1
1	A	399	LEU	4.1
1	D	285	ASP	4.1
1	A	60	ILE	4.1
1	I	60	ILE	4.1
1	A	333	ALA	4.0
1	A	63	SER	4.0
1	B	64	ASP	4.0
1	B	2	ALA	4.0
1	G	179	TYR	4.0
1	H	61	ASN	4.0
1	K	405	LYS	4.0
1	E	396	LEU	4.0
1	H	8	MET	3.9
1	F	331	MET	3.9
1	J	5	VAL	3.9
1	F	394	LYS	3.9
1	C	296	TYR	3.9
1	H	12	HIS	3.9
1	K	327	GLU	3.9
1	A	98	GLN	3.9
1	C	61	ASN	3.8
1	B	12	HIS	3.8
1	G	53	SER	3.8
1	H	53	SER	3.8
1	K	340	SER	3.8
1	C	179	TYR	3.8
1	L	63	SER	3.8
1	I	327	GLU	3.8
1	H	1	SER	3.8
1	B	46	GLY	3.8
1	E	406	GLU	3.8
1	D	397	TYR	3.8
1	E	179	TYR	3.8
1	H	351	PRO	3.8
1	E	12	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	350	SER	3.8
1	K	1	SER	3.7
1	I	398	ASP	3.7
1	B	401	PRO	3.7
1	B	58	LYS	3.7
1	E	385	LYS	3.7
1	C	337	ARG	3.7
1	A	279	THR	3.7
1	B	50	ASP	3.7
1	H	401	PRO	3.7
1	D	179	TYR	3.7
1	C	62	GLU	3.7
1	F	179	TYR	3.6
1	D	50	ASP	3.6
1	G	2	ALA	3.6
1	B	395	ASN	3.6
1	A	324	PRO	3.6
1	F	407	ILE	3.6
1	I	179	TYR	3.6
1	A	335	SER	3.6
1	G	6	LEU	3.6
1	H	399	LEU	3.6
1	A	62	GLU	3.5
1	J	179	TYR	3.5
1	E	405	LYS	3.5
1	A	293	GLN	3.5
1	J	61	ASN	3.5
1	A	402	GLU	3.5
1	F	402	GLU	3.5
1	B	63	SER	3.5
1	D	53	SER	3.5
1	H	326	TYR	3.5
1	K	98	GLN	3.5
1	A	179	TYR	3.5
1	B	62	GLU	3.5
1	B	327	GLU	3.5
1	D	4	HIS	3.5
1	E	60	ILE	3.4
1	D	400	PRO	3.4
1	F	392	MET	3.4
1	H	7	THR	3.4
1	E	403	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	59	GLY	3.4
1	C	279	THR	3.4
1	C	351	PRO	3.4
1	D	117	ALA	3.4
1	G	339	ARG	3.3
1	C	327	GLU	3.3
1	F	284	GLY	3.3
1	H	337	ARG	3.3
1	B	394	LYS	3.3
1	F	327	GLU	3.3
1	G	49	PHE	3.3
1	A	353	ALA	3.3
1	G	63	SER	3.3
1	B	328	ALA	3.3
1	I	98	GLN	3.3
1	C	1	SER	3.3
1	K	53	SER	3.3
1	G	62	GLU	3.2
1	E	2	ALA	3.2
1	E	63	SER	3.2
1	B	8	MET	3.2
1	C	287	TYR	3.2
1	A	276	LYS	3.2
1	A	391	PRO	3.2
1	J	401	PRO	3.1
1	F	40	ALA	3.1
1	I	395	ASN	3.1
1	D	63	SER	3.1
1	A	43	PHE	3.1
1	A	338	ASN	3.1
1	B	179	TYR	3.1
1	B	402	GLU	3.1
1	I	396	LEU	3.1
1	A	339	ARG	3.1
1	E	351	PRO	3.1
1	A	91	ILE	3.1
1	E	11	GLU	3.1
1	A	288	ALA	3.1
1	G	7	THR	3.1
1	B	407	ILE	3.1
1	C	284	GLY	3.1
1	G	404	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	327	GLU	3.0
1	E	53	SER	3.0
1	A	292	GLU	3.0
1	C	285	ASP	3.0
1	A	5	VAL	3.0
1	L	61	ASN	3.0
1	F	405	LYS	3.0
1	J	402	GLU	3.0
1	F	98	GLN	3.0
1	H	405	LYS	3.0
1	J	98	GLN	2.9
1	B	98	GLN	2.9
1	I	407	ILE	2.9
1	I	59	GLY	2.9
1	J	4	HIS	2.9
1	E	383	LYS	2.9
1	C	59	GLY	2.9
1	A	2	ALA	2.9
1	L	49	PHE	2.9
1	I	54	ILE	2.9
1	F	337	ARG	2.9
1	B	39	ASN	2.9
1	D	38	VAL	2.9
1	E	404	ALA	2.9
1	H	40	ALA	2.9
1	J	8	MET	2.8
1	B	278	GLY	2.8
1	J	7	THR	2.8
1	I	401	PRO	2.8
1	A	405	LYS	2.8
1	F	278	GLY	2.8
1	K	49	PHE	2.8
1	H	4	HIS	2.8
1	H	404	ALA	2.8
1	C	406	GLU	2.8
1	C	419	ASN	2.8
1	A	6	LEU	2.8
1	C	396	LEU	2.8
1	J	6	LEU	2.8
1	I	331	MET	2.8
1	A	387	HIS	2.8
1	I	402	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	8	MET	2.8
1	C	349	ALA	2.8
1	E	277	ASN	2.8
1	A	352	LYS	2.7
1	C	292	GLU	2.7
1	G	399	LEU	2.7
1	K	165	GLU	2.7
1	D	49	PHE	2.7
1	L	58	LYS	2.7
1	L	270	CYS	2.7
1	A	3	GLU	2.7
1	E	62	GLU	2.7
1	G	403	GLU	2.7
1	B	392	MET	2.7
1	I	58	LYS	2.7
1	I	61	ASN	2.7
1	B	393	ASP	2.7
1	E	326	TYR	2.7
1	C	286	LYS	2.7
1	E	3	GLU	2.7
1	F	63	SER	2.7
1	C	289	GLY	2.6
1	A	382	ILE	2.6
1	I	49	PHE	2.6
1	E	10	ASN	2.6
1	G	165	GLU	2.6
1	A	275	ALA	2.6
1	F	340	SER	2.6
1	D	44	GLU	2.6
1	I	400	PRO	2.6
1	C	277	ASN	2.6
1	A	346	PRO	2.6
1	J	49	PHE	2.6
1	L	165	GLU	2.6
1	C	282	PHE	2.6
1	I	43	PHE	2.6
1	B	122	ASP	2.6
1	B	11	GLU	2.6
1	E	292	GLU	2.6
1	C	399	LEU	2.6
1	E	283	SER	2.6
1	D	40	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	2	ALA	2.5
1	K	404	ALA	2.5
1	B	97	LEU	2.5
1	I	392	MET	2.5
1	D	3	GLU	2.5
1	L	1	SER	2.5
1	A	401	PRO	2.5
1	G	396	LEU	2.5
1	C	339	ARG	2.5
1	L	326	TYR	2.5
1	C	290	LEU	2.5
1	B	4	HIS	2.5
1	B	95	GLY	2.5
1	E	401	PRO	2.5
1	K	331	MET	2.5
1	F	349	ALA	2.5
1	H	350	SER	2.5
1	C	407	ILE	2.5
1	L	6	LEU	2.5
1	A	337	ARG	2.5
1	A	390	GLU	2.5
1	H	364	ALA	2.5
1	K	41	GLU	2.5
1	E	337	ARG	2.4
1	G	406	GLU	2.4
1	A	286	LYS	2.4
1	F	324	PRO	2.4
1	F	406	GLU	2.4
1	C	96	THR	2.4
1	A	1	SER	2.4
1	A	340	SER	2.4
1	I	64	ASP	2.4
1	B	290	LEU	2.4
1	K	324	PRO	2.4
1	L	361	PRO	2.4
1	C	60	ILE	2.4
1	A	284	GLY	2.4
1	E	387	HIS	2.4
1	L	98	GLN	2.4
1	E	278	GLY	2.4
1	A	4	HIS	2.4
1	A	283	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	299	GLY	2.4
1	B	6	LEU	2.4
1	D	43	PHE	2.4
1	H	49	PHE	2.4
1	F	1	SER	2.4
1	A	379	LEU	2.3
1	H	331	MET	2.3
1	L	328	ALA	2.3
1	F	65	MET	2.3
1	J	327	GLU	2.3
1	E	340	SER	2.3
1	E	392	MET	2.3
1	K	44	GLU	2.3
1	C	275	ALA	2.3
1	L	327	GLU	2.3
1	K	407	ILE	2.3
1	E	423	LEU	2.3
1	I	6	LEU	2.3
1	E	64	ASP	2.3
1	J	64	ASP	2.3
1	I	165	GLU	2.3
1	A	294	ALA	2.3
1	F	338	ASN	2.3
1	L	404	ALA	2.3
1	J	339	ARG	2.3
1	B	43	PHE	2.3
1	D	41	GLU	2.3
1	A	355	ARG	2.3
1	G	277	ASN	2.3
1	A	122	ASP	2.2
1	H	347	VAL	2.2
1	A	287	TYR	2.2
1	F	3	GLU	2.2
1	E	42	PHE	2.2
1	J	338	ASN	2.2
1	E	348	VAL	2.2
1	J	41	GLU	2.2
1	A	336	ALA	2.2
1	K	3	GLU	2.2
1	F	339	ARG	2.2
1	B	351	PRO	2.2
1	D	165	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	349	ALA	2.2
1	D	396	LEU	2.2
1	B	42	PHE	2.2
1	A	403	GLU	2.2
1	H	392	MET	2.2
1	E	407	ILE	2.2
1	B	49	PHE	2.2
1	L	40	ALA	2.2
1	A	331	MET	2.2
1	D	62	GLU	2.2
1	H	338	ASN	2.2
1	J	12	HIS	2.2
1	J	337	ARG	2.2
1	C	392	MET	2.2
1	G	9	LEU	2.1
1	A	42	PHE	2.1
1	E	341	ALA	2.1
1	E	402	GLU	2.1
1	A	10	ASN	2.1
1	H	277	ASN	2.1
1	E	13	GLU	2.1
1	L	64	ASP	2.1
1	D	5	VAL	2.1
1	E	284	GLY	2.1
1	C	328	ALA	2.1
1	A	126	PHE	2.1
1	F	352	LYS	2.1
1	J	165	GLU	2.1
1	B	117	ALA	2.1
1	A	38	VAL	2.1
1	B	38	VAL	2.1
1	G	54	ILE	2.1
1	E	339	ARG	2.1
1	F	330	VAL	2.1
1	D	54	ILE	2.1
1	E	49	PHE	2.1
1	E	293	GLN	2.1
1	E	4	HIS	2.1
1	G	4	HIS	2.1
1	J	2	ALA	2.1
1	J	324	PRO	2.1
1	B	339	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	337	ARG	2.1
1	A	328	ALA	2.1
1	I	2	ALA	2.1
1	A	281	LEU	2.0
1	G	97	LEU	2.0
1	C	43	PHE	2.0
1	D	367	PRO	2.0
1	G	371	PHE	2.0
1	H	407	ILE	2.0
1	B	273	SER	2.0
1	F	97	LEU	2.0
1	C	46	GLY	2.0
1	D	399	LEU	2.0
1	E	349	ALA	2.0
1	J	40	ALA	2.0
1	E	165	GLU	2.0
1	H	130	PRO	2.0
1	L	54	ILE	2.0
1	B	325	GLY	2.0
1	B	406	GLU	2.0
1	H	41	GLU	2.0
1	L	62	GLU	2.0
1	F	96	THR	2.0
1	H	367	PRO	2.0
1	K	270	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MPD	G	1489	8/8	0.94	0.35	16.70	16,43,64,74	8
5	MPD	L	1494	8/8	0.92	0.45	15.31	16,43,64,74	8
5	MPD	K	1493	8/8	0.91	0.41	12.99	16,43,64,74	8
5	MPD	F	1488	8/8	0.87	0.43	12.70	16,43,64,74	8
5	MPD	C	1485	8/8	0.85	0.48	11.95	16,43,64,74	8
5	MPD	B	1484	8/8	0.75	0.44	10.40	16,43,64,74	8
5	MPD	H	1490	8/8	0.93	0.41	9.67	16,43,64,74	8
5	MPD	J	1492	8/8	0.92	0.35	9.48	16,43,64,74	8
5	MPD	D	1486	8/8	0.86	0.39	8.52	16,43,64,74	8
5	MPD	I	1491	8/8	0.91	0.32	7.49	16,43,64,74	8
5	MPD	E	1487	8/8	0.91	0.45	5.88	16,43,64,74	8
5	MPD	A	1483	8/8	0.84	0.34	4.11	16,43,64,74	8
3	ADP	F	1476	27/27	0.60	0.51	3.47	20,78,100,100	27
3	ADP	L	1482	27/27	0.67	0.48	3.04	20,78,100,100	27
3	ADP	B	1472	27/27	0.66	0.49	2.96	20,78,100,100	27
3	ADP	I	1479	27/27	0.62	0.50	2.89	20,78,100,100	27
3	ADP	D	1474	27/27	0.65	0.49	2.66	20,78,100,100	27
3	ADP	K	1481	27/27	0.71	0.43	2.24	20,78,100,100	27
3	ADP	C	1473	27/27	0.75	0.35	1.95	20,78,100,100	27
3	ADP	J	1480	27/27	0.84	0.35	1.51	20,78,100,100	27
3	ADP	H	1478	27/27	0.74	0.37	1.43	20,78,100,100	27
3	ADP	E	1475	27/27	0.76	0.35	1.20	20,78,100,100	27
3	ADP	A	1471	27/27	0.69	0.39	1.12	20,78,100,100	27
3	ADP	G	1477	27/27	0.83	0.34	0.94	20,78,100,100	27
4	TL	J	473	1/1	0.93	0.26	-0.47	67,67,67,67	1
4	TL	G	474	1/1	0.96	0.13	-0.49	75,75,75,75	1
4	TL	I	473	1/1	0.86	0.22	-0.55	67,67,67,67	1
4	TL	L	473	1/1	0.93	0.23	-0.68	67,67,67,67	1
4	TL	G	473	1/1	0.96	0.17	-0.77	67,67,67,67	1
2	MN	D	469	1/1	0.97	0.10	-0.78	34,34,34,34	0
4	TL	A	473	1/1	0.90	0.19	-0.80	67,67,67,67	1
4	TL	I	474	1/1	0.96	0.13	-0.83	75,75,75,75	1
4	TL	H	473	1/1	0.95	0.19	-0.87	67,67,67,67	1
2	MN	G	469	1/1	0.98	0.07	-0.96	34,34,34,34	0
2	MN	J	469	1/1	0.96	0.12	-0.97	34,34,34,34	0
2	MN	H	470	1/1	0.95	0.09	-0.97	41,41,41,41	0
2	MN	J	470	1/1	0.99	0.10	-0.99	41,41,41,41	0
2	MN	I	469	1/1	0.99	0.07	-0.99	34,34,34,34	0
4	TL	C	473	1/1	0.96	0.16	-1.01	67,67,67,67	1
2	MN	L	469	1/1	0.98	0.12	-1.04	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	K	469	1/1	0.97	0.13	-1.05	34,34,34,34	0
2	MN	H	469	1/1	0.99	0.08	-1.06	34,34,34,34	0
2	MN	E	469	1/1	0.98	0.05	-1.09	34,34,34,34	0
2	MN	C	469	1/1	0.96	0.08	-1.19	34,34,34,34	0
2	MN	B	469	1/1	0.97	0.06	-1.21	34,34,34,34	0
4	TL	D	474	1/1	0.93	0.09	-1.26	75,75,75,75	1
2	MN	F	469	1/1	0.99	0.04	-1.28	34,34,34,34	0
4	TL	F	473	1/1	0.90	0.11	-1.28	67,67,67,67	1
4	TL	E	473	1/1	0.97	0.06	-1.29	67,67,67,67	1
4	TL	K	473	1/1	0.93	0.12	-1.30	67,67,67,67	1
4	TL	L	474	1/1	0.95	0.12	-1.34	75,75,75,75	1
4	TL	D	473	1/1	0.96	0.05	-1.37	67,67,67,67	1
4	TL	E	474	1/1	0.91	0.10	-1.42	75,75,75,75	1
2	MN	A	469	1/1	0.95	0.04	-1.54	34,34,34,34	0
4	TL	B	473	1/1	0.97	0.04	-1.58	67,67,67,67	1
2	MN	A	470	1/1	0.91	0.05	-1.61	41,41,41,41	0
4	TL	J	474	1/1	0.89	0.11	-1.79	75,75,75,75	1
2	MN	C	470	1/1	0.99	0.04	-2.02	41,41,41,41	0
4	TL	K	474	1/1	0.97	0.12	-2.60	75,75,75,75	1
4	TL	A	474	1/1	0.96	0.08	-2.67	75,75,75,75	1
4	TL	B	474	1/1	0.93	0.08	-3.40	75,75,75,75	1
4	TL	F	474	1/1	0.97	0.04	-3.98	75,75,75,75	1
4	TL	H	474	1/1	0.92	0.05	-4.84	75,75,75,75	1
4	TL	C	474	1/1	0.94	0.05	-6.10	75,75,75,75	1
2	MN	D	470	1/1	0.96	0.10	-	41,41,41,41	0
2	MN	F	470	1/1	0.96	0.06	-	41,41,41,41	0
2	MN	G	470	1/1	0.97	0.13	-	41,41,41,41	0
2	MN	L	470	1/1	0.97	0.18	-	41,41,41,41	0
2	MN	E	470	1/1	0.98	0.09	-	41,41,41,41	0
2	MN	B	470	1/1	0.94	0.04	-	41,41,41,41	0
2	MN	I	470	1/1	0.95	0.13	-	41,41,41,41	0
2	MN	K	470	1/1	0.99	0.16	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.