



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:23 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

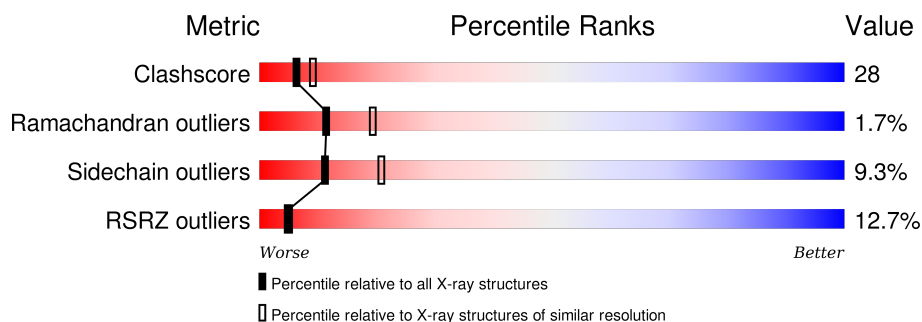
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 Å.

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



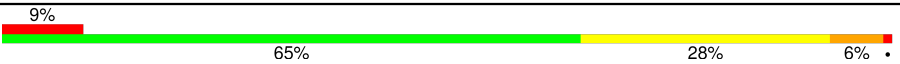

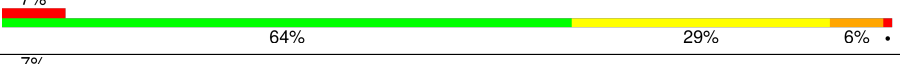
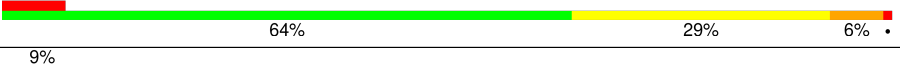
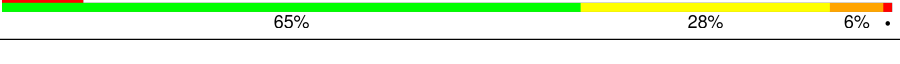
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	<div> <div>31%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
1	B	468	<div> <div>16%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
1	C	468	<div> <div>15%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
1	D	468	<div> <div>11%</div> <div>66%</div> <div>27%</div> <div>6%</div> </div>
1	E	468	<div> <div>17%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
1	F	468	<div> <div>12%</div> <div>63%</div> <div>29%</div> <div>6%</div> </div>
1	G	468	<div> <div>10%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>

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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	A	4471	-	-	-	X
3	ADP	B	4472	-	-	-	X
3	ADP	F	4476	-	-	-	X
3	ADP	G	4477	-	-	-	X
3	ADP	I	4479	-	-	-	X
3	ADP	J	4480	-	-	-	X
3	ADP	K	4481	-	-	-	X
3	ADP	L	4482	-	-	-	X
4	MPD	A	5472	-	-	X	X
4	MPD	A	5481	-	-	X	X
4	MPD	B	5471	-	-	X	X
4	MPD	B	5474	-	-	X	X
4	MPD	C	5473	-	-	X	X
4	MPD	C	5476	-	-	X	X
4	MPD	D	5475	-	-	X	X
4	MPD	D	5478	-	-	X	X
4	MPD	E	5477	-	-	X	X
4	MPD	E	5480	-	-	X	X
4	MPD	F	5479	-	-	X	X
4	MPD	F	5482	-	-	X	X
4	MPD	G	5484	-	-	X	X
4	MPD	G	5485	-	-	X	X
4	MPD	H	5486	-	-	X	X
4	MPD	H	5487	-	-	X	X
4	MPD	I	5488	-	-	X	X
4	MPD	I	5489	-	-	X	X
4	MPD	J	5490	-	-	X	X
4	MPD	J	5491	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	K	5492	-	-	X	X
4	MPD	K	5493	-	-	X	X
4	MPD	L	5483	-	-	X	X
4	MPD	L	5494	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	B	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	C	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	D	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	E	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	F	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	G	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	H	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	I	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	J	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	K	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	L	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			

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

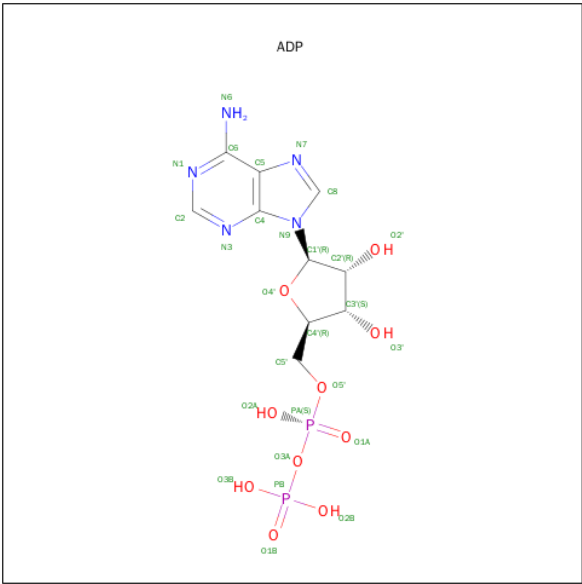
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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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).



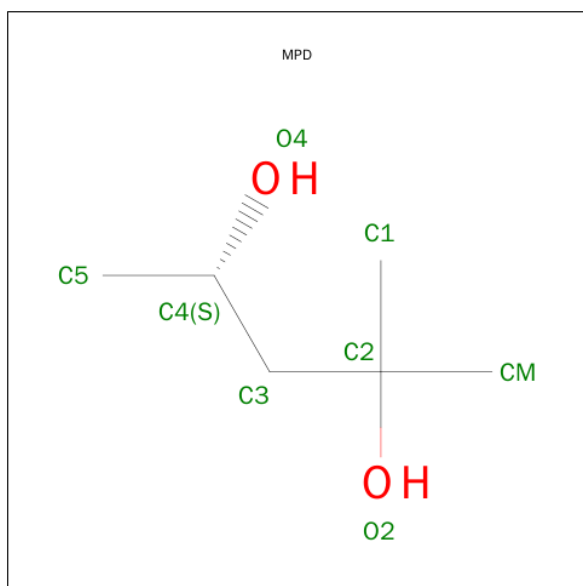
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O P	0	0
			27	10	5	10 2		

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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

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

- Molecule 5 is water.

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

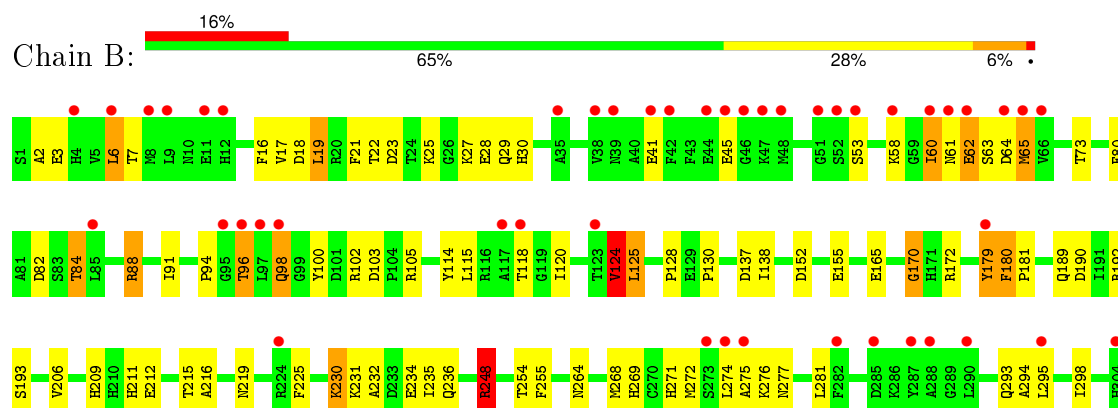
3 Residue-property plots

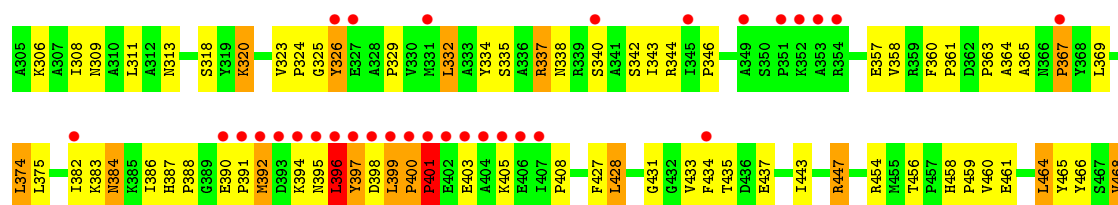
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: GLUTAMINE SYNTHETASE

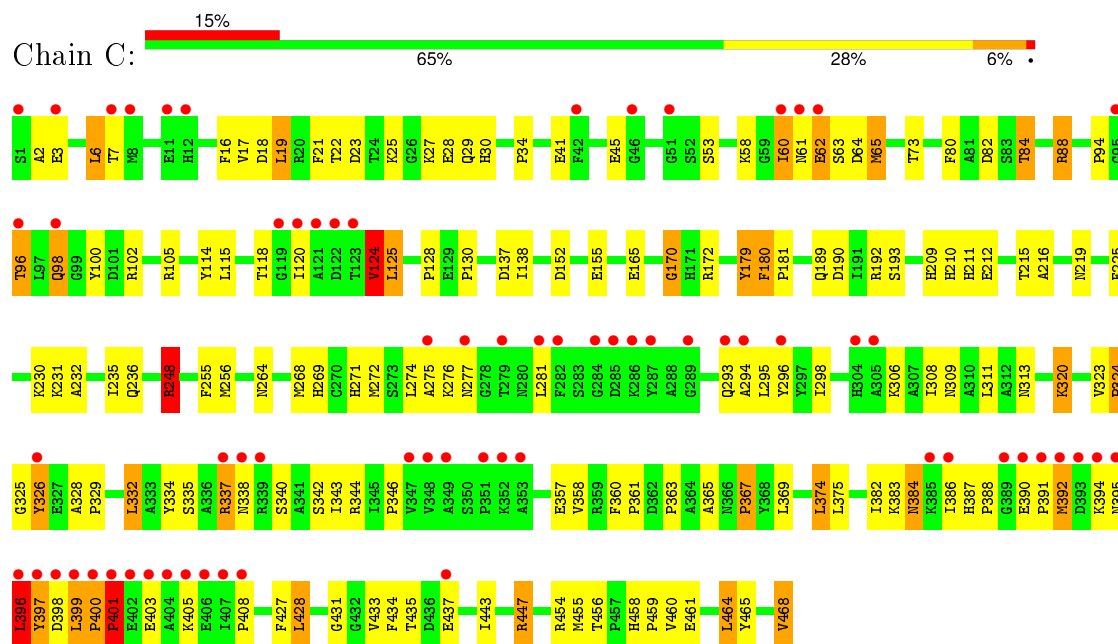


• Molecule 1: GLUTAMINE SYNTHETASE

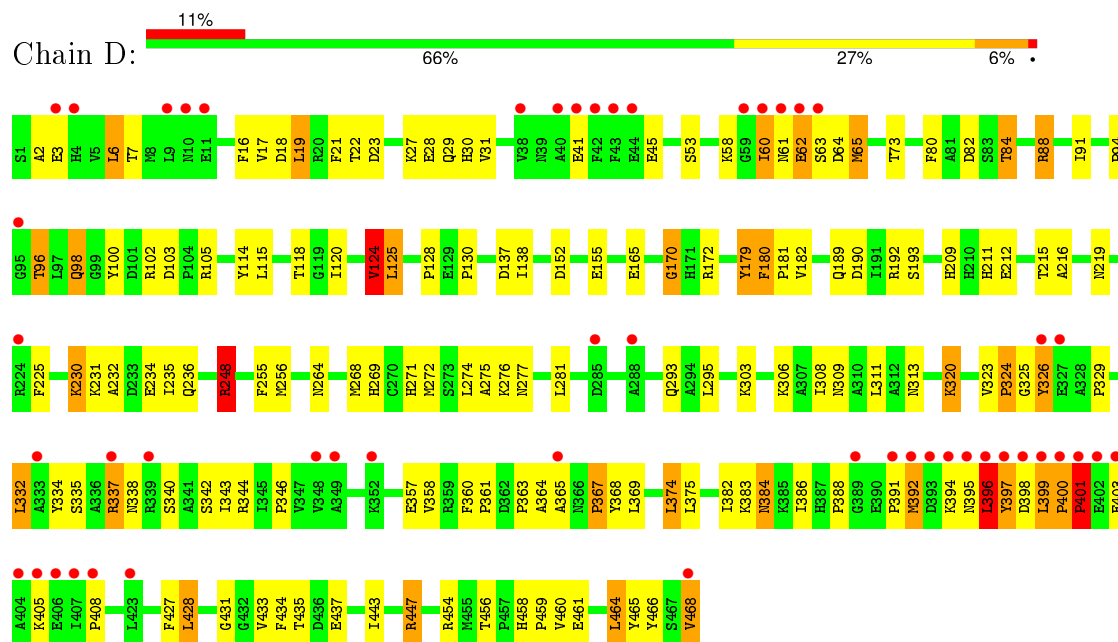




• Molecule 1: GLUTAMINE SYNTHETASE



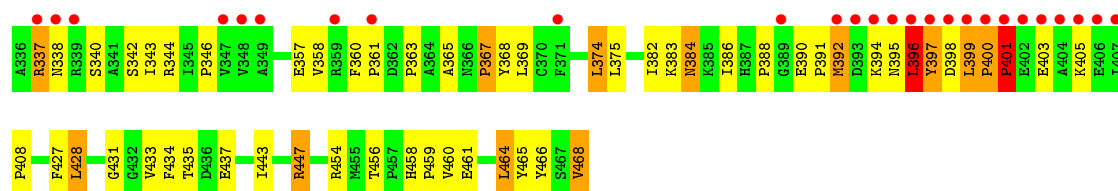
• Molecule 1: GLUTAMINE SYNTHETASE



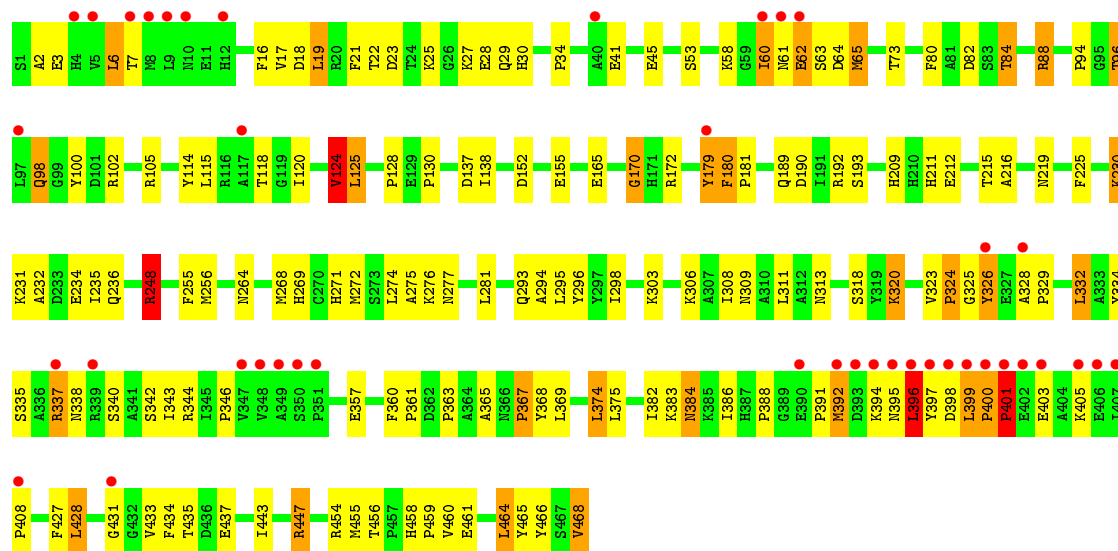
• Molecule 1: GLUTAMINE SYNTHETASE



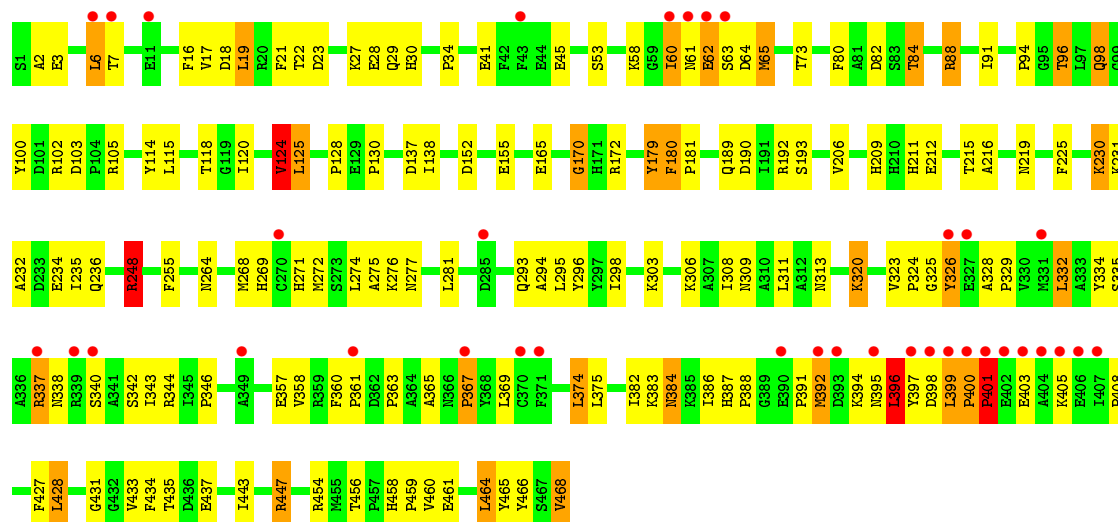




• Molecule 1: GLUTAMINE SYNTHETASE

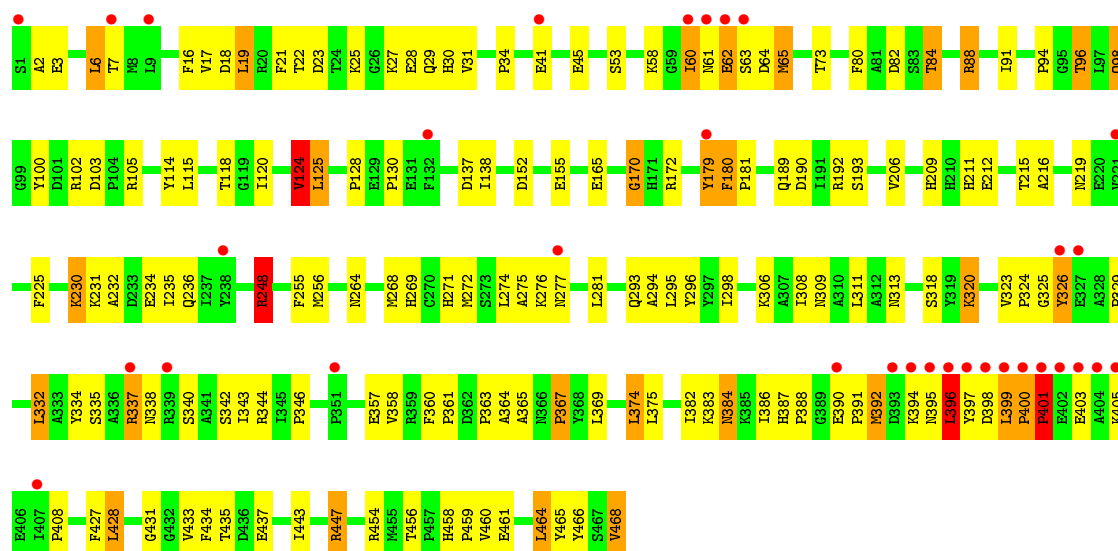


• Molecule 1: GLUTAMINE SYNTHETASE

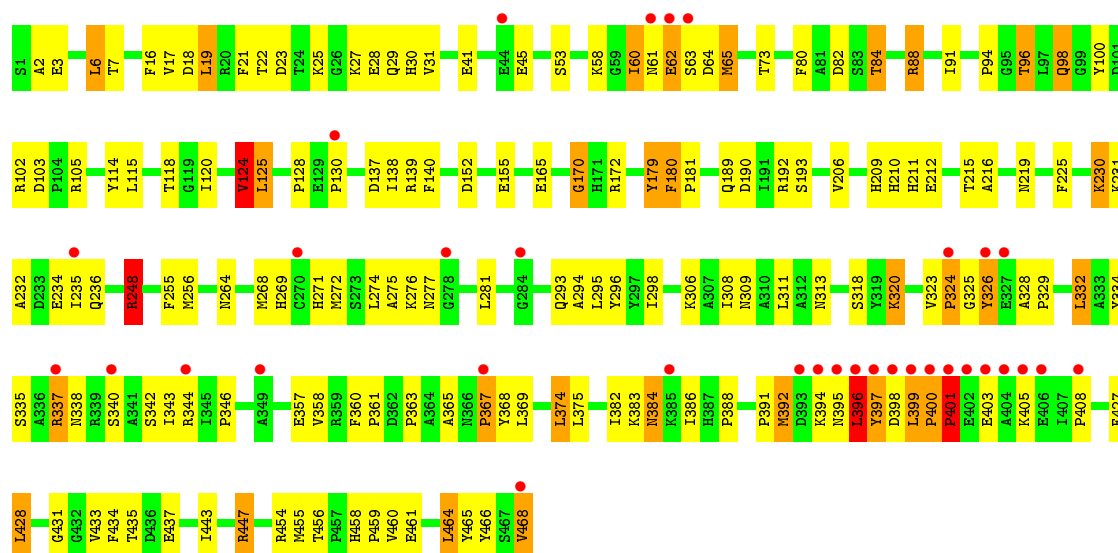


• Molecule 1: GLUTAMINE SYNTHETASE

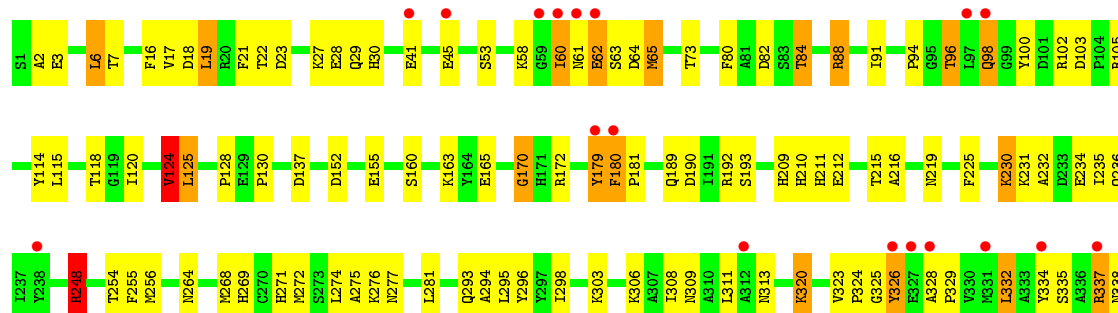


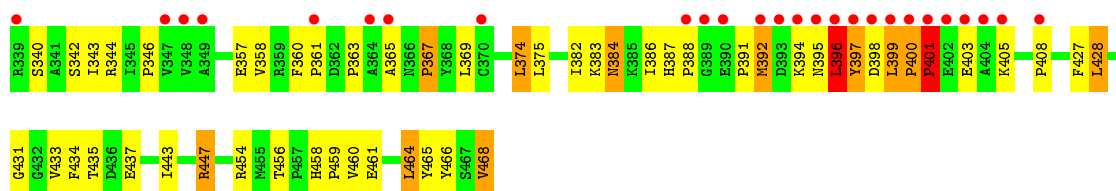


- Molecule 1: GLUTAMINE SYNTHETASE



- Molecule 1: GLUTAMINE SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	230.60 Å 132.50 Å 195.90 Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	34.90 – 2.49 34.90 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.90-2.49) 97.9 (34.90-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.67 (at 2.48 Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.243 , 0.257 0.261 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.6	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 196561 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47688	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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, 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	0.53	0/3724	0.85	4/5043 (0.1%)
1	B	0.53	0/3724	0.85	4/5043 (0.1%)
1	C	0.53	0/3724	0.85	4/5043 (0.1%)
1	D	0.53	0/3724	0.85	4/5043 (0.1%)
1	E	0.53	0/3724	0.85	4/5043 (0.1%)
1	F	0.53	0/3724	0.85	4/5043 (0.1%)
1	G	0.53	0/3724	0.85	4/5043 (0.1%)
1	H	0.53	0/3724	0.85	4/5043 (0.1%)
1	I	0.53	0/3724	0.85	4/5043 (0.1%)
1	J	0.53	0/3724	0.85	4/5043 (0.1%)
1	K	0.53	0/3724	0.85	4/5043 (0.1%)
1	L	0.53	0/3724	0.85	4/5043 (0.1%)
All	All	0.53	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	E	401	PRO	CA-N-CD	-6.91	101.83	111.50
1	J	401	PRO	CA-N-CD	-6.90	101.84	111.50
1	I	401	PRO	CA-N-CD	-6.89	101.86	111.50
1	L	401	PRO	CA-N-CD	-6.89	101.86	111.50
1	F	401	PRO	CA-N-CD	-6.88	101.86	111.50
1	H	401	PRO	CA-N-CD	-6.88	101.87	111.50
1	A	401	PRO	CA-N-CD	-6.88	101.87	111.50
1	G	401	PRO	CA-N-CD	-6.88	101.88	111.50
1	D	401	PRO	CA-N-CD	-6.87	101.89	111.50
1	C	401	PRO	CA-N-CD	-6.87	101.89	111.50
1	B	401	PRO	CA-N-CD	-6.85	101.92	111.50
1	K	401	PRO	CA-N-CD	-6.84	101.92	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	F	248	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	J	248	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	K	248	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	D	248	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	A	248	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	E	248	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	I	248	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	H	248	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	G	248	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	L	248	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	L	367	PRO	O-C-N	5.37	131.29	122.70
1	C	248	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	D	367	PRO	O-C-N	5.36	131.28	122.70
1	K	367	PRO	O-C-N	5.34	131.25	122.70
1	A	367	PRO	O-C-N	5.33	131.23	122.70
1	I	367	PRO	O-C-N	5.33	131.23	122.70
1	C	367	PRO	O-C-N	5.32	131.22	122.70
1	G	367	PRO	O-C-N	5.32	131.21	122.70
1	B	367	PRO	O-C-N	5.32	131.21	122.70
1	H	367	PRO	O-C-N	5.31	131.20	122.70
1	E	367	PRO	O-C-N	5.30	131.18	122.70
1	J	367	PRO	O-C-N	5.30	131.18	122.70
1	F	367	PRO	O-C-N	5.30	131.18	122.70
1	L	124	VAL	CB-CA-C	-5.28	101.37	111.40
1	G	124	VAL	CB-CA-C	-5.28	101.38	111.40
1	C	124	VAL	CB-CA-C	-5.27	101.39	111.40
1	E	124	VAL	CB-CA-C	-5.27	101.39	111.40
1	B	124	VAL	CB-CA-C	-5.27	101.39	111.40
1	H	124	VAL	CB-CA-C	-5.26	101.40	111.40
1	A	124	VAL	CB-CA-C	-5.26	101.40	111.40
1	D	124	VAL	CB-CA-C	-5.25	101.42	111.40
1	I	124	VAL	CB-CA-C	-5.25	101.43	111.40
1	F	124	VAL	CB-CA-C	-5.24	101.44	111.40
1	K	124	VAL	CB-CA-C	-5.24	101.44	111.40
1	J	124	VAL	CB-CA-C	-5.23	101.45	111.40

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	3544	210	0
1	B	3637	0	3544	204	0
1	C	3637	0	3544	207	0
1	D	3637	0	3544	205	0
1	E	3637	0	3544	199	0
1	F	3637	0	3544	218	0
1	G	3637	0	3544	205	0
1	H	3637	0	3544	213	0
1	I	3637	0	3544	211	0
1	J	3637	0	3544	221	0
1	K	3637	0	3544	220	0
1	L	3637	0	3544	216	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	27	0	10	1	0
3	B	27	0	10	1	0
3	C	27	0	10	1	0
3	D	27	0	10	1	0
3	E	27	0	10	1	0
3	F	27	0	10	1	0
3	G	27	0	10	1	0
3	H	27	0	10	1	0
3	I	27	0	10	1	0
3	J	27	0	10	1	0
3	K	27	0	10	1	0
3	L	27	0	10	1	0
4	A	16	0	27	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	27	60	0
4	C	16	0	27	62	0
4	D	16	0	27	61	0
4	E	16	0	27	54	0
4	F	16	0	27	62	0
4	G	16	0	27	60	0
4	H	16	0	27	65	0
4	I	16	0	27	62	0
4	J	16	0	27	68	0
4	K	16	0	27	66	0
4	L	16	0	27	65	0
5	A	294	0	0	6	0
5	B	297	0	0	7	0
5	C	293	0	0	8	0
5	D	295	0	0	7	0
5	E	294	0	0	8	0
5	F	293	0	0	8	0
5	G	288	0	0	8	0
5	H	288	0	0	7	0
5	I	295	0	0	7	0
5	J	287	0	0	8	0
5	K	288	0	0	7	0
5	L	292	0	0	7	0
All	All	47688	0	42972	2421	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 28.

All (2421) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:84:THR:HG21	4:J:5491:MPD:C5	1.53	1.36
1:J:84:THR:CG2	4:J:5491:MPD:H52	1.60	1.32
1:F:84:THR:HG21	4:F:5479:MPD:C5	1.57	1.32
1:L:84:THR:HG21	4:L:5483:MPD:C5	1.60	1.31
1:I:61:ASN:O	1:J:337:ARG:HB2	1.29	1.29
1:H:80:PHE:CB	4:H:5487:MPD:H12	1.63	1.28
1:F:84:THR:CG2	4:F:5479:MPD:H52	1.63	1.28
1:B:84:THR:HG21	4:B:5471:MPD:C5	1.63	1.27
1:G:84:THR:HG21	4:G:5485:MPD:C5	1.65	1.27
1:I:84:THR:HG21	4:I:5489:MPD:C5	1.64	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:PHE:CB	4:L:5483:MPD:H12	1.65	1.25
1:G:61:ASN:O	1:H:337:ARG:HB2	1.35	1.25
1:K:84:THR:HG21	4:K:5493:MPD:C5	1.65	1.25
1:E:84:THR:HG21	4:E:5477:MPD:C5	1.66	1.24
1:J:80:PHE:CB	4:J:5491:MPD:H12	1.66	1.24
1:D:84:THR:HG21	4:D:5475:MPD:C5	1.66	1.23
1:E:84:THR:CG2	4:E:5477:MPD:H52	1.68	1.23
1:L:84:THR:CG2	4:L:5483:MPD:H52	1.66	1.22
1:C:337:ARG:HB2	1:D:61:ASN:O	1.37	1.22
1:A:337:ARG:HB2	1:B:61:ASN:O	1.36	1.22
1:F:80:PHE:CB	4:F:5479:MPD:H12	1.69	1.22
1:C:84:THR:HG21	4:C:5473:MPD:C5	1.68	1.22
1:B:84:THR:CG2	4:B:5471:MPD:H52	1.68	1.22
1:H:84:THR:HG21	4:H:5487:MPD:C5	1.69	1.21
1:G:84:THR:CG2	4:G:5485:MPD:H52	1.69	1.21
1:D:84:THR:CG2	4:D:5475:MPD:H52	1.70	1.20
1:K:84:THR:CG2	4:K:5493:MPD:H52	1.70	1.20
1:A:84:THR:HG21	4:A:5481:MPD:C5	1.70	1.20
1:I:84:THR:CG2	4:I:5489:MPD:H52	1.70	1.19
1:C:80:PHE:CB	4:C:5473:MPD:H12	1.71	1.19
1:K:80:PHE:CB	4:K:5493:MPD:H12	1.71	1.19
1:C:190:ASP:HA	4:D:5475:MPD:HM3	1.19	1.19
1:A:84:THR:CG2	4:A:5481:MPD:H52	1.72	1.19
4:K:5493:MPD:HM1	1:L:193:SER:HB2	1.25	1.18
1:J:61:ASN:O	1:K:337:ARG:HB2	1.41	1.18
1:C:84:THR:CG2	4:C:5473:MPD:H52	1.74	1.18
1:A:60:ILE:H	1:A:60:ILE:HD13	1.08	1.18
1:L:80:PHE:HB3	4:L:5483:MPD:C1	1.74	1.17
1:J:60:ILE:H	1:J:60:ILE:HD13	1.08	1.17
4:G:5485:MPD:HM1	1:H:193:SER:HB2	1.25	1.16
1:I:80:PHE:CB	4:I:5489:MPD:H12	1.73	1.16
1:G:360:PHE:CD2	1:G:361:PRO:HD3	1.81	1.16
1:B:360:PHE:CD2	1:B:361:PRO:HD3	1.81	1.16
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.81	1.16
1:K:360:PHE:CD2	1:K:361:PRO:HD3	1.81	1.16
1:J:360:PHE:CD2	1:J:361:PRO:HD3	1.81	1.16
1:J:80:PHE:HB3	4:J:5491:MPD:C1	1.73	1.15
1:E:193:SER:HB2	4:F:5479:MPD:HM1	1.25	1.15
1:H:84:THR:CG2	4:H:5487:MPD:H52	1.76	1.15
1:G:337:ARG:HB2	1:L:61:ASN:O	1.46	1.15
4:A:5481:MPD:HM1	1:F:193:SER:HB2	1.25	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.81	1.15
1:B:80:PHE:CB	4:B:5471:MPD:H12	1.77	1.15
1:F:360:PHE:CD2	1:F:361:PRO:HD3	1.81	1.14
1:I:360:PHE:CD2	1:I:361:PRO:HD3	1.81	1.14
1:F:80:PHE:HB3	4:F:5479:MPD:C1	1.77	1.14
1:C:193:SER:HB2	4:D:5475:MPD:HM1	1.25	1.14
1:B:193:SER:HB2	4:C:5473:MPD:HM1	1.25	1.14
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.81	1.14
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.81	1.14
4:I:5489:MPD:HM1	1:J:193:SER:HB2	1.25	1.14
1:L:360:PHE:CD2	1:L:361:PRO:HD3	1.81	1.14
4:G:5485:MPD:HM3	1:H:190:ASP:HA	1.19	1.13
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.81	1.13
1:A:193:SER:HB2	4:B:5471:MPD:HM1	1.25	1.13
4:H:5487:MPD:HM3	1:I:190:ASP:HA	1.19	1.13
1:B:60:ILE:H	1:B:60:ILE:HD13	1.08	1.13
1:J:399:LEU:N	1:J:401:PRO:HG2	1.64	1.13
1:H:399:LEU:N	1:H:401:PRO:HG2	1.64	1.13
1:D:193:SER:HB2	4:E:5477:MPD:HM1	1.25	1.13
4:I:5489:MPD:HM3	1:J:190:ASP:HA	1.19	1.12
1:C:399:LEU:N	1:C:401:PRO:HG2	1.64	1.12
1:E:60:ILE:HD13	1:E:60:ILE:H	1.08	1.12
1:E:190:ASP:HA	4:F:5479:MPD:HM3	1.19	1.12
1:G:193:SER:HB2	4:L:5483:MPD:HM1	1.25	1.12
1:L:399:LEU:N	1:L:401:PRO:HG2	1.64	1.12
1:A:190:ASP:HA	4:B:5471:MPD:HM3	1.19	1.12
1:H:60:ILE:H	1:H:60:ILE:HD13	1.08	1.12
1:K:60:ILE:HD13	1:K:60:ILE:H	1.08	1.12
4:J:5491:MPD:HM3	1:K:190:ASP:HA	1.19	1.12
1:H:80:PHE:HB3	4:H:5487:MPD:C1	1.77	1.12
4:K:5493:MPD:HM3	1:L:190:ASP:HA	1.19	1.12
1:F:60:ILE:HD13	1:F:60:ILE:H	1.08	1.12
1:E:399:LEU:N	1:E:401:PRO:HG2	1.64	1.12
1:G:399:LEU:N	1:G:401:PRO:HG2	1.64	1.12
1:F:399:LEU:H	1:F:401:PRO:HG2	0.95	1.11
1:F:399:LEU:N	1:F:401:PRO:HG2	1.64	1.11
1:I:399:LEU:N	1:I:401:PRO:HG2	1.64	1.11
1:B:399:LEU:N	1:B:401:PRO:HG2	1.64	1.11
1:G:60:ILE:H	1:G:60:ILE:HD13	1.08	1.11
4:A:5481:MPD:HM3	1:F:190:ASP:HA	1.19	1.11
1:A:399:LEU:N	1:A:401:PRO:HG2	1.64	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:PHE:CB	4:D:5475:MPD:H12	1.79	1.11
1:E:399:LEU:H	1:E:401:PRO:HG2	0.95	1.11
1:D:399:LEU:N	1:D:401:PRO:HG2	1.64	1.11
1:K:80:PHE:HB3	4:K:5493:MPD:C1	1.81	1.10
4:J:5491:MPD:HM1	1:K:193:SER:HB2	1.25	1.10
1:A:399:LEU:H	1:A:401:PRO:HG2	0.95	1.10
1:K:399:LEU:N	1:K:401:PRO:HG2	1.64	1.10
1:G:190:ASP:HA	4:L:5483:MPD:HM3	1.19	1.09
1:C:400:PRO:HB3	1:C:405:LYS:HE3	1.34	1.09
1:G:22:THR:N	4:G:5484:MPD:H52	1.67	1.09
1:B:190:ASP:HA	4:C:5473:MPD:HM3	1.19	1.09
1:C:60:ILE:HD13	1:C:60:ILE:H	1.08	1.09
1:L:60:ILE:HD13	1:L:60:ILE:H	1.08	1.09
4:H:5487:MPD:HM1	1:I:193:SER:HB2	1.25	1.09
1:A:400:PRO:HB3	1:A:405:LYS:HE3	1.35	1.09
1:E:22:THR:N	4:E:5480:MPD:H52	1.67	1.09
1:D:190:ASP:HA	4:E:5477:MPD:HM3	1.19	1.09
1:E:400:PRO:HB3	1:E:405:LYS:HE3	1.35	1.09
1:K:400:PRO:HB3	1:K:405:LYS:HE3	1.35	1.09
1:I:22:THR:N	4:I:5488:MPD:H52	1.67	1.09
1:F:22:THR:N	4:F:5482:MPD:H52	1.67	1.09
1:B:22:THR:N	4:B:5474:MPD:H52	1.67	1.09
1:D:22:THR:N	4:D:5478:MPD:H52	1.67	1.09
1:K:22:THR:N	4:K:5492:MPD:H52	1.67	1.09
1:G:400:PRO:HB3	1:G:405:LYS:HE3	1.35	1.08
1:J:22:THR:N	4:J:5490:MPD:H52	1.67	1.08
1:I:60:ILE:H	1:I:60:ILE:HD13	1.08	1.08
1:C:399:LEU:H	1:C:401:PRO:HG2	0.95	1.08
1:J:399:LEU:H	1:J:401:PRO:HG2	0.95	1.08
1:C:22:THR:N	4:C:5476:MPD:H52	1.67	1.08
1:H:22:THR:N	4:H:5486:MPD:H52	1.67	1.08
1:I:400:PRO:HB3	1:I:405:LYS:HE3	1.35	1.08
1:D:60:ILE:HD13	1:D:60:ILE:H	1.08	1.08
1:L:399:LEU:H	1:L:401:PRO:HG2	0.95	1.07
1:G:399:LEU:H	1:G:401:PRO:HG2	0.95	1.07
1:J:400:PRO:HB3	1:J:405:LYS:HE3	1.35	1.07
1:A:22:THR:N	4:A:5472:MPD:H52	1.67	1.07
1:A:61:ASN:O	1:F:337:ARG:HB2	1.54	1.07
1:H:400:PRO:HB3	1:H:405:LYS:HE3	1.35	1.07
1:I:399:LEU:H	1:I:401:PRO:HG2	0.95	1.07
1:L:22:THR:N	4:L:5494:MPD:H52	1.67	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:PHE:HB3	4:I:5489:MPD:C1	1.84	1.06
1:C:80:PHE:HB3	4:C:5473:MPD:C1	1.84	1.06
1:F:400:PRO:HB3	1:F:405:LYS:HE3	1.35	1.06
1:B:400:PRO:HB3	1:B:405:LYS:HE3	1.35	1.06
1:H:399:LEU:H	1:H:401:PRO:HG2	0.95	1.06
1:D:399:LEU:H	1:D:401:PRO:HG2	0.95	1.06
1:D:21:PHE:HB2	4:D:5478:MPD:H53	1.38	1.06
1:H:21:PHE:HB2	4:H:5486:MPD:H53	1.38	1.06
1:A:21:PHE:HB2	4:A:5472:MPD:H53	1.38	1.06
1:K:21:PHE:HB2	4:K:5492:MPD:H53	1.38	1.06
1:B:399:LEU:H	1:B:401:PRO:HG2	0.95	1.06
1:H:22:THR:OG1	4:H:5486:MPD:H13	1.56	1.06
1:K:399:LEU:H	1:K:401:PRO:HG2	0.95	1.05
1:G:80:PHE:CB	4:G:5485:MPD:H12	1.85	1.05
1:E:22:THR:OG1	4:E:5480:MPD:H13	1.56	1.05
1:B:21:PHE:HB2	4:B:5474:MPD:H53	1.38	1.05
1:L:400:PRO:HB3	1:L:405:LYS:HE3	1.35	1.05
1:L:21:PHE:HB2	4:L:5494:MPD:H53	1.38	1.05
1:B:80:PHE:HB3	4:B:5471:MPD:C1	1.86	1.05
1:E:21:PHE:HB2	4:E:5480:MPD:H53	1.38	1.05
1:I:21:PHE:HB2	4:I:5488:MPD:H53	1.38	1.05
1:A:22:THR:OG1	4:A:5472:MPD:H13	1.56	1.05
1:A:80:PHE:CB	4:A:5481:MPD:H12	1.86	1.05
1:C:22:THR:OG1	4:C:5476:MPD:H13	1.56	1.05
1:F:22:THR:OG1	4:F:5482:MPD:H13	1.56	1.04
1:D:80:PHE:HB3	4:D:5475:MPD:C1	1.88	1.04
1:F:21:PHE:HB2	4:F:5482:MPD:H53	1.38	1.04
1:K:22:THR:OG1	4:K:5492:MPD:H13	1.56	1.04
1:G:80:PHE:HB3	4:G:5485:MPD:H12	1.05	1.04
1:D:22:THR:OG1	4:D:5478:MPD:H13	1.56	1.04
1:A:22:THR:H	4:A:5472:MPD:C5	1.71	1.04
1:I:22:THR:H	4:I:5488:MPD:C5	1.71	1.03
1:B:22:THR:H	4:B:5474:MPD:C5	1.71	1.03
1:K:22:THR:H	4:K:5492:MPD:C5	1.71	1.03
1:J:21:PHE:HB2	4:J:5490:MPD:H53	1.38	1.03
1:J:22:THR:OG1	4:J:5490:MPD:H13	1.56	1.03
1:G:22:THR:H	4:G:5484:MPD:C5	1.71	1.03
1:L:22:THR:OG1	4:L:5494:MPD:H13	1.56	1.03
1:D:400:PRO:HB3	1:D:405:LYS:HE3	1.35	1.03
1:E:22:THR:H	4:E:5480:MPD:C5	1.71	1.03
1:I:22:THR:OG1	4:I:5488:MPD:H13	1.56	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:PHE:HB2	4:C:5476:MPD:H53	1.38	1.03
1:L:22:THR:H	4:L:5494:MPD:C5	1.71	1.03
1:C:22:THR:H	4:C:5476:MPD:C5	1.71	1.02
1:B:22:THR:OG1	4:B:5474:MPD:H13	1.56	1.02
1:D:22:THR:H	4:D:5478:MPD:C5	1.71	1.02
1:J:22:THR:H	4:J:5490:MPD:C5	1.71	1.02
1:G:21:PHE:HB2	4:G:5484:MPD:H53	1.38	1.02
1:B:337:ARG:HB2	1:C:61:ASN:O	1.60	1.02
1:H:22:THR:H	4:H:5486:MPD:C5	1.71	1.02
1:G:22:THR:OG1	4:G:5484:MPD:H13	1.56	1.01
1:E:80:PHE:CB	4:E:5477:MPD:H12	1.89	1.01
1:E:80:PHE:HB3	4:E:5477:MPD:H12	1.04	1.01
1:F:22:THR:H	4:F:5482:MPD:C5	1.71	1.01
1:I:22:THR:HG1	4:I:5488:MPD:H13	1.23	1.01
1:K:61:ASN:O	1:L:337:ARG:HB2	1.61	1.01
1:H:61:ASN:O	1:I:337:ARG:HB2	1.61	1.00
1:D:337:ARG:HB2	1:E:61:ASN:O	1.60	1.00
1:A:80:PHE:HB3	4:A:5481:MPD:C1	1.93	0.99
1:A:80:PHE:HB3	4:A:5481:MPD:H12	1.00	0.99
1:G:80:PHE:HB3	4:G:5485:MPD:C1	1.93	0.98
1:C:22:THR:H	4:C:5476:MPD:H52	0.82	0.98
1:L:22:THR:H	4:L:5494:MPD:H52	0.81	0.98
1:E:80:PHE:HB3	4:E:5477:MPD:C1	1.94	0.97
1:E:337:ARG:HB2	1:F:61:ASN:O	1.61	0.97
1:A:22:THR:H	4:A:5472:MPD:H52	0.82	0.97
1:B:80:PHE:HB3	4:B:5471:MPD:H12	0.97	0.97
1:D:22:THR:H	4:D:5478:MPD:H52	0.82	0.97
1:E:22:THR:H	4:E:5480:MPD:H52	0.82	0.97
1:K:22:THR:H	4:K:5492:MPD:H52	0.82	0.97
1:B:22:THR:H	4:B:5474:MPD:H52	0.81	0.96
1:F:22:THR:H	4:F:5482:MPD:H52	0.81	0.96
1:D:80:PHE:HB3	4:D:5475:MPD:H12	0.97	0.96
1:J:22:THR:H	4:J:5490:MPD:H52	0.81	0.96
1:C:80:PHE:HB3	4:C:5473:MPD:H12	0.96	0.95
1:H:22:THR:H	4:H:5486:MPD:H52	0.82	0.95
1:I:80:PHE:HB3	4:I:5489:MPD:H12	0.97	0.95
1:I:22:THR:H	4:I:5488:MPD:H52	0.81	0.95
1:G:22:THR:H	4:G:5484:MPD:H52	0.82	0.95
1:C:235:ILE:HG21	1:C:367:PRO:HG3	1.49	0.95
1:K:235:ILE:HG21	1:K:367:PRO:HG3	1.49	0.94
1:B:235:ILE:HG21	1:B:367:PRO:HG3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:235:ILE:HG21	1:I:367:PRO:HG3	1.49	0.94
1:H:80:PHE:CD1	4:H:5487:MPD:C5	2.51	0.94
1:J:235:ILE:HG21	1:J:367:PRO:HG3	1.49	0.94
1:G:190:ASP:OD2	4:L:5483:MPD:H13	1.68	0.94
1:C:190:ASP:OD2	4:D:5475:MPD:H13	1.68	0.94
4:A:5481:MPD:H13	1:F:190:ASP:OD2	1.68	0.94
1:F:235:ILE:HG21	1:F:367:PRO:HG3	1.49	0.93
1:L:235:ILE:HG21	1:L:367:PRO:HG3	1.49	0.93
1:G:235:ILE:HG21	1:G:367:PRO:HG3	1.49	0.93
1:H:84:THR:HG21	4:H:5487:MPD:H52	0.93	0.93
1:J:60:ILE:H	1:J:60:ILE:CD1	1.82	0.93
1:E:190:ASP:OD2	4:F:5479:MPD:H13	1.68	0.92
4:I:5489:MPD:H13	1:J:190:ASP:OD2	1.68	0.92
4:K:5493:MPD:H13	1:L:190:ASP:OD2	1.68	0.92
1:A:235:ILE:HG21	1:A:367:PRO:HG3	1.49	0.92
1:G:60:ILE:CD1	1:G:60:ILE:H	1.82	0.92
1:B:190:ASP:OD2	4:C:5473:MPD:H13	1.68	0.92
1:H:80:PHE:CD1	4:H:5487:MPD:H53	2.05	0.92
4:H:5487:MPD:H13	1:I:190:ASP:OD2	1.68	0.92
1:A:190:ASP:OD2	4:B:5471:MPD:H13	1.68	0.92
1:H:235:ILE:HG21	1:H:367:PRO:HG3	1.49	0.92
1:D:235:ILE:HG21	1:D:367:PRO:HG3	1.49	0.92
1:E:235:ILE:HG21	1:E:367:PRO:HG3	1.49	0.91
4:G:5485:MPD:H13	1:H:190:ASP:OD2	1.68	0.91
1:H:60:ILE:H	1:H:60:ILE:CD1	1.82	0.91
1:C:60:ILE:CD1	1:C:60:ILE:H	1.82	0.91
4:J:5491:MPD:H13	1:K:190:ASP:OD2	1.68	0.91
1:K:60:ILE:H	1:K:60:ILE:CD1	1.82	0.91
1:D:190:ASP:OD2	4:E:5477:MPD:H13	1.68	0.91
1:B:395:ASN:HB3	1:B:400:PRO:HD2	1.54	0.90
1:K:60:ILE:HD13	1:K:60:ILE:N	1.87	0.90
1:G:60:ILE:N	1:G:60:ILE:HD13	1.87	0.90
1:I:60:ILE:HD13	1:I:60:ILE:N	1.87	0.90
4:K:5493:MPD:HM1	1:L:193:SER:CB	2.02	0.90
1:J:395:ASN:HB3	1:J:400:PRO:HD2	1.54	0.90
1:E:60:ILE:HD13	1:E:60:ILE:N	1.87	0.90
1:H:60:ILE:N	1:H:60:ILE:HD13	1.87	0.90
1:I:395:ASN:HB3	1:I:400:PRO:HD2	1.54	0.90
1:D:60:ILE:HD13	1:D:60:ILE:N	1.87	0.90
1:K:395:ASN:HB3	1:K:400:PRO:HD2	1.54	0.89
1:D:395:ASN:HB3	1:D:400:PRO:HD2	1.54	0.89

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ASP:O	1:D:399:LEU:C	2.11	0.87
1:F:21:PHE:HA	4:F:5482:MPD:H31	1.56	0.87
1:L:21:PHE:HA	4:L:5494:MPD:H31	1.56	0.87
1:J:84:THR:HG21	4:J:5491:MPD:C4	2.05	0.87
1:H:80:PHE:HB3	4:H:5487:MPD:H12	0.87	0.87
1:H:398:ASP:O	1:H:399:LEU:C	2.11	0.87
1:C:21:PHE:HA	4:C:5476:MPD:H31	1.57	0.87
1:E:395:ASN:HB3	1:E:400:PRO:HD2	1.54	0.87
1:B:398:ASP:O	1:B:399:LEU:C	2.11	0.87
1:J:82:ASP:HB2	4:J:5491:MPD:H31	1.55	0.86
1:K:21:PHE:CA	4:K:5492:MPD:HM2	2.06	0.86
1:K:80:PHE:HB3	4:K:5493:MPD:H12	0.90	0.86
1:G:22:THR:OG1	4:G:5484:MPD:C1	2.24	0.86
1:G:21:PHE:CA	4:G:5484:MPD:HM2	2.05	0.86
1:E:22:THR:OG1	4:E:5480:MPD:C1	2.24	0.86
1:B:21:PHE:HA	4:B:5474:MPD:H31	1.56	0.86
1:L:22:THR:N	4:L:5494:MPD:H11	1.91	0.86
1:E:22:THR:N	4:E:5480:MPD:H11	1.91	0.86
1:E:21:PHE:CA	4:E:5480:MPD:HM2	2.05	0.86
1:B:21:PHE:CA	4:B:5474:MPD:HM2	2.05	0.86
1:K:22:THR:OG1	4:K:5492:MPD:C1	2.24	0.86
1:K:22:THR:N	4:K:5492:MPD:H11	1.91	0.86
1:C:22:THR:OG1	4:C:5476:MPD:C1	2.24	0.86
1:H:21:PHE:CA	4:H:5486:MPD:HM2	2.05	0.86
1:A:21:PHE:HA	4:A:5472:MPD:H31	1.56	0.86
1:D:21:PHE:HA	4:D:5478:MPD:H31	1.56	0.86
1:H:22:THR:N	4:H:5486:MPD:H11	1.91	0.86
1:E:82:ASP:O	1:E:84:THR:HG22	1.76	0.86
1:C:82:ASP:O	1:C:84:THR:HG22	1.76	0.86
1:J:22:THR:OG1	4:J:5490:MPD:C1	2.24	0.86
1:C:22:THR:N	4:C:5476:MPD:H11	1.91	0.86
1:A:22:THR:N	4:A:5472:MPD:H11	1.91	0.86
1:G:82:ASP:O	1:G:84:THR:HG22	1.76	0.85
1:I:21:PHE:CA	4:I:5488:MPD:HM2	2.05	0.85
1:I:22:THR:N	4:I:5488:MPD:H11	1.91	0.85
1:F:22:THR:N	4:F:5482:MPD:H11	1.91	0.85
1:C:21:PHE:CA	4:C:5476:MPD:HM2	2.06	0.85
1:H:22:THR:OG1	4:H:5486:MPD:C1	2.24	0.85
1:H:82:ASP:O	1:H:84:THR:HG22	1.76	0.85
1:I:80:PHE:CD1	4:I:5489:MPD:H53	2.12	0.85
1:G:21:PHE:HA	4:G:5484:MPD:H31	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:OG1	4:B:5474:MPD:C1	2.24	0.85
1:F:82:ASP:O	1:F:84:THR:HG22	1.76	0.85
1:B:82:ASP:O	1:B:84:THR:HG22	1.76	0.85
1:J:82:ASP:O	1:J:84:THR:HG22	1.76	0.85
1:C:80:PHE:CD1	4:C:5473:MPD:H53	2.12	0.85
1:D:21:PHE:CA	4:D:5478:MPD:HM2	2.06	0.85
1:K:21:PHE:HA	4:K:5492:MPD:H31	1.57	0.85
1:J:22:THR:N	4:J:5490:MPD:H11	1.91	0.85
1:L:21:PHE:CA	4:L:5494:MPD:HM2	2.05	0.85
1:A:22:THR:OG1	4:A:5472:MPD:C1	2.24	0.85
1:K:82:ASP:O	1:K:84:THR:HG22	1.76	0.85
1:F:22:THR:OG1	4:F:5482:MPD:C1	2.24	0.85
1:I:82:ASP:O	1:I:84:THR:HG22	1.76	0.85
1:G:22:THR:N	4:G:5484:MPD:H11	1.91	0.85
1:I:21:PHE:HA	4:I:5488:MPD:H31	1.56	0.85
1:A:458:HIS:HD2	1:A:460:VAL:H	1.25	0.85
1:D:458:HIS:HD2	1:D:460:VAL:H	1.25	0.85
1:E:21:PHE:HA	4:E:5480:MPD:H31	1.57	0.85
1:A:82:ASP:O	1:A:84:THR:HG22	1.76	0.85
1:K:398:ASP:O	1:K:399:LEU:C	2.11	0.85
1:F:21:PHE:CA	4:F:5482:MPD:HM2	2.05	0.85
1:D:22:THR:OG1	4:D:5478:MPD:C1	2.24	0.85
1:D:82:ASP:O	1:D:84:THR:HG22	1.76	0.84
1:I:22:THR:OG1	4:I:5488:MPD:C1	2.24	0.84
1:A:21:PHE:CA	4:A:5472:MPD:HM2	2.05	0.84
1:J:80:PHE:HB3	4:J:5491:MPD:H12	0.86	0.84
1:B:22:THR:N	4:B:5474:MPD:H11	1.91	0.84
1:D:22:THR:N	4:D:5478:MPD:H11	1.91	0.84
1:L:22:THR:OG1	4:L:5494:MPD:C1	2.24	0.84
1:J:21:PHE:CA	4:J:5490:MPD:HM2	2.05	0.84
1:J:398:ASP:O	1:J:399:LEU:C	2.11	0.84
1:H:21:PHE:HA	4:H:5486:MPD:H31	1.57	0.84
1:F:80:PHE:CD1	4:F:5479:MPD:C5	2.61	0.84
1:C:84:THR:HG21	4:C:5473:MPD:H52	0.87	0.84
1:H:458:HIS:HD2	1:H:460:VAL:H	1.25	0.84
1:I:458:HIS:HD2	1:I:460:VAL:H	1.25	0.84
1:L:458:HIS:HD2	1:L:460:VAL:H	1.25	0.84
1:F:398:ASP:O	1:F:399:LEU:C	2.11	0.83
1:I:22:THR:CB	4:I:5488:MPD:H11	2.09	0.83
1:B:22:THR:CB	4:B:5474:MPD:H11	2.09	0.83
1:K:458:HIS:HD2	1:K:460:VAL:H	1.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:82:ASP:O	1:L:84:THR:HG22	1.76	0.83
1:E:22:THR:CB	4:E:5480:MPD:H11	2.09	0.83
1:C:22:THR:CB	4:C:5476:MPD:H11	2.09	0.83
1:L:22:THR:CB	4:L:5494:MPD:H11	2.09	0.83
1:I:61:ASN:O	1:J:337:ARG:CB	2.21	0.83
1:E:60:ILE:H	1:E:60:ILE:CD1	1.82	0.83
1:A:22:THR:CB	4:A:5472:MPD:H11	2.09	0.83
1:G:22:THR:CB	4:G:5484:MPD:H11	2.09	0.82
1:F:22:THR:CB	4:F:5482:MPD:H11	2.09	0.82
1:D:22:THR:CB	4:D:5478:MPD:H11	2.09	0.82
1:H:22:THR:CB	4:H:5486:MPD:H11	2.09	0.82
1:B:458:HIS:HD2	1:B:460:VAL:H	1.25	0.82
1:F:80:PHE:CD1	4:F:5479:MPD:H53	2.14	0.82
1:K:80:PHE:CD1	4:K:5493:MPD:C5	2.63	0.82
1:K:22:THR:CB	4:K:5492:MPD:H11	2.09	0.82
1:E:82:ASP:HB2	4:E:5477:MPD:H31	1.61	0.82
1:J:22:THR:CB	4:J:5490:MPD:H11	2.09	0.82
1:C:458:HIS:HD2	1:C:460:VAL:H	1.25	0.82
1:F:105:ARG:HB2	4:F:5482:MPD:H4	1.62	0.82
1:K:80:PHE:CD1	4:K:5493:MPD:H53	2.15	0.81
1:K:22:THR:CB	4:K:5492:MPD:C1	2.58	0.81
1:E:458:HIS:HD2	1:E:460:VAL:H	1.25	0.81
1:L:84:THR:HG21	4:L:5483:MPD:C4	2.08	0.81
1:D:21:PHE:HA	4:D:5478:MPD:HM2	1.62	0.81
1:J:22:THR:CB	4:J:5490:MPD:C1	2.58	0.81
1:I:105:ARG:HB2	4:I:5488:MPD:H4	1.62	0.81
1:F:22:THR:CB	4:F:5482:MPD:C1	2.58	0.81
1:C:22:THR:CB	4:C:5476:MPD:C1	2.58	0.81
1:A:22:THR:CB	4:A:5472:MPD:C1	2.58	0.81
1:G:458:HIS:HD2	1:G:460:VAL:H	1.25	0.81
1:B:21:PHE:HA	4:B:5474:MPD:HM2	1.62	0.81
1:H:84:THR:HG21	4:H:5487:MPD:C4	2.11	0.81
1:G:21:PHE:HA	4:G:5484:MPD:HM2	1.62	0.81
1:I:21:PHE:HA	4:I:5488:MPD:HM2	1.62	0.81
1:B:80:PHE:CD1	4:B:5471:MPD:C5	2.63	0.81
1:J:458:HIS:HD2	1:J:460:VAL:H	1.25	0.81
1:G:22:THR:CB	4:G:5484:MPD:C1	2.58	0.81
1:D:105:ARG:HB2	4:D:5478:MPD:H4	1.62	0.81
1:J:21:PHE:HA	4:J:5490:MPD:HM2	1.62	0.81
1:F:458:HIS:HD2	1:F:460:VAL:H	1.25	0.81
1:J:398:ASP:O	1:J:399:LEU:O	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:ARG:HB2	4:G:5484:MPD:H4	1.62	0.81
1:L:22:THR:CB	4:L:5494:MPD:C1	2.58	0.81
1:I:84:THR:HG21	4:I:5489:MPD:H52	0.83	0.81
1:C:398:ASP:O	1:C:399:LEU:C	2.11	0.81
1:F:21:PHE:HA	4:F:5482:MPD:HM2	1.62	0.81
1:B:105:ARG:HB2	4:B:5474:MPD:H4	1.62	0.81
1:D:22:THR:CB	4:D:5478:MPD:C1	2.58	0.81
1:C:21:PHE:HA	4:C:5476:MPD:HM2	1.62	0.81
1:L:84:THR:HG21	4:L:5483:MPD:H52	0.82	0.80
1:K:84:THR:HG21	4:K:5493:MPD:H52	0.85	0.80
1:E:398:ASP:O	1:E:399:LEU:O	1.99	0.80
1:G:82:ASP:HB2	4:G:5485:MPD:H31	1.62	0.80
1:L:82:ASP:HB2	4:L:5483:MPD:H31	1.62	0.80
1:K:105:ARG:HB2	4:K:5492:MPD:H4	1.62	0.80
1:A:84:THR:HG21	4:A:5481:MPD:H52	0.84	0.80
1:G:398:ASP:O	1:G:399:LEU:O	1.99	0.80
1:E:22:THR:CB	4:E:5480:MPD:C1	2.58	0.80
1:B:22:THR:CB	4:B:5474:MPD:C1	2.58	0.80
1:L:105:ARG:HB2	4:L:5494:MPD:H4	1.62	0.80
1:L:398:ASP:O	1:L:399:LEU:O	1.99	0.80
1:L:21:PHE:HA	4:L:5494:MPD:HM2	1.62	0.80
1:C:398:ASP:O	1:C:399:LEU:O	1.99	0.80
1:H:398:ASP:O	1:H:399:LEU:O	1.99	0.80
1:B:398:ASP:O	1:B:399:LEU:O	1.99	0.80
1:I:22:THR:CB	4:I:5488:MPD:C1	2.58	0.80
1:I:82:ASP:HB2	4:I:5489:MPD:H31	1.64	0.80
1:A:398:ASP:O	1:A:399:LEU:O	1.99	0.80
1:B:82:ASP:HB2	4:B:5471:MPD:H31	1.61	0.80
1:E:21:PHE:HA	4:E:5480:MPD:HM2	1.62	0.80
1:H:105:ARG:HB2	4:H:5486:MPD:H4	1.62	0.80
1:H:21:PHE:HA	4:H:5486:MPD:HM2	1.62	0.80
1:H:22:THR:CB	4:H:5486:MPD:C1	2.58	0.80
1:G:398:ASP:O	1:G:399:LEU:C	2.11	0.80
1:K:21:PHE:HA	4:K:5492:MPD:HM2	1.62	0.80
1:K:398:ASP:O	1:K:399:LEU:O	1.99	0.79
1:L:80:PHE:HB3	4:L:5483:MPD:H12	0.84	0.79
1:A:105:ARG:HB2	4:A:5472:MPD:H4	1.62	0.79
1:A:21:PHE:HA	4:A:5472:MPD:HM2	1.62	0.79
1:C:105:ARG:HB2	4:C:5476:MPD:H4	1.62	0.79
1:F:84:THR:HG21	4:F:5479:MPD:C4	2.11	0.79
1:J:105:ARG:HB2	4:J:5490:MPD:H4	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ILE:CD1	1:D:60:ILE:H	1.82	0.79
1:C:337:ARG:CB	1:D:61:ASN:O	2.27	0.79
1:F:398:ASP:O	1:F:399:LEU:O	1.99	0.78
1:I:398:ASP:O	1:I:399:LEU:O	1.99	0.78
1:E:105:ARG:HB2	4:E:5480:MPD:H4	1.62	0.78
1:A:337:ARG:CB	1:B:61:ASN:O	2.26	0.78
1:C:21:PHE:C	4:C:5476:MPD:HM2	2.04	0.78
1:D:84:THR:HG21	4:D:5475:MPD:H52	0.83	0.78
1:L:21:PHE:C	4:L:5494:MPD:HM2	2.04	0.78
1:A:193:SER:HB2	4:B:5471:MPD:CM	2.11	0.78
1:D:193:SER:HB2	4:E:5477:MPD:CM	2.11	0.78
1:D:398:ASP:O	1:D:399:LEU:O	1.99	0.78
4:H:5487:MPD:CM	1:I:193:SER:HB2	2.11	0.78
1:K:82:ASP:HB2	4:K:5493:MPD:H31	1.66	0.78
1:B:21:PHE:C	4:B:5474:MPD:HM2	2.04	0.78
1:J:21:PHE:C	4:J:5490:MPD:HM2	2.04	0.78
1:B:80:PHE:CD1	4:B:5471:MPD:H53	2.18	0.78
1:F:21:PHE:C	4:F:5482:MPD:HM2	2.04	0.78
1:D:21:PHE:C	4:D:5478:MPD:HM2	2.04	0.78
1:H:21:PHE:C	4:H:5486:MPD:HM2	2.04	0.78
1:G:193:SER:HB2	4:L:5483:MPD:CM	2.11	0.77
1:I:21:PHE:C	4:I:5488:MPD:HM2	2.04	0.77
1:C:82:ASP:HB2	4:C:5473:MPD:H31	1.66	0.77
1:K:21:PHE:C	4:K:5492:MPD:HM2	2.04	0.77
1:G:21:PHE:C	4:G:5484:MPD:HM2	2.04	0.77
1:B:58:LYS:HD2	1:B:62:GLU:HB2	1.67	0.77
1:E:21:PHE:C	4:E:5480:MPD:HM2	2.04	0.77
1:A:21:PHE:C	4:A:5472:MPD:HM2	2.04	0.77
1:I:84:THR:HG21	4:I:5489:MPD:C4	2.15	0.77
1:G:61:ASN:O	1:H:337:ARG:CB	2.28	0.77
1:G:399:LEU:HA	1:G:400:PRO:C	2.06	0.77
1:J:58:LYS:HD2	1:J:62:GLU:HB2	1.67	0.77
1:D:58:LYS:HD2	1:D:62:GLU:HB2	1.67	0.77
1:L:58:LYS:HD2	1:L:62:GLU:HB2	1.67	0.77
1:F:58:LYS:HD2	1:F:62:GLU:HB2	1.67	0.77
1:I:58:LYS:HD2	1:I:62:GLU:HB2	1.67	0.76
4:G:5485:MPD:CM	1:H:193:SER:HB2	2.11	0.76
1:C:193:SER:HB2	4:D:5475:MPD:CM	2.11	0.76
1:I:399:LEU:HA	1:I:400:PRO:C	2.06	0.76
1:A:399:LEU:HA	1:A:400:PRO:C	2.06	0.76
1:C:58:LYS:HD2	1:C:62:GLU:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:LYS:HD2	1:H:62:GLU:HB2	1.67	0.76
1:F:399:LEU:HA	1:F:400:PRO:C	2.06	0.76
1:I:395:ASN:HB3	1:I:400:PRO:CD	2.16	0.76
1:D:399:LEU:HA	1:D:400:PRO:C	2.06	0.76
1:G:58:LYS:HD2	1:G:62:GLU:HB2	1.67	0.76
1:D:82:ASP:HB2	4:D:5475:MPD:H31	1.68	0.76
1:E:395:ASN:HB3	1:E:400:PRO:CD	2.16	0.76
1:G:395:ASN:HB3	1:G:400:PRO:CD	2.16	0.76
1:G:80:PHE:CD1	4:G:5485:MPD:C5	2.68	0.76
1:D:80:PHE:CD1	4:D:5475:MPD:C5	2.68	0.76
1:D:80:PHE:CD1	4:D:5475:MPD:H53	2.21	0.76
1:H:399:LEU:HA	1:H:400:PRO:C	2.06	0.76
1:K:395:ASN:HB3	1:K:400:PRO:CD	2.16	0.76
4:I:5489:MPD:CM	1:J:193:SER:HB2	2.11	0.76
1:C:399:LEU:HA	1:C:400:PRO:C	2.06	0.76
1:L:395:ASN:HB3	1:L:400:PRO:CD	2.16	0.76
1:K:399:LEU:HA	1:K:400:PRO:C	2.06	0.76
1:A:395:ASN:HB3	1:A:400:PRO:CD	2.16	0.76
1:J:399:LEU:HA	1:J:400:PRO:C	2.06	0.75
1:L:399:LEU:HA	1:L:400:PRO:C	2.06	0.75
1:B:395:ASN:HB3	1:B:400:PRO:CD	2.16	0.75
1:D:395:ASN:HB3	1:D:400:PRO:CD	2.16	0.75
1:C:84:THR:HG21	4:C:5473:MPD:C4	2.16	0.75
1:K:58:LYS:HD2	1:K:62:GLU:HB2	1.67	0.75
1:A:58:LYS:HD2	1:A:62:GLU:HB2	1.67	0.75
4:K:5493:MPD:CM	1:L:193:SER:HB2	2.11	0.75
1:J:395:ASN:HB3	1:J:400:PRO:CD	2.16	0.75
1:C:395:ASN:HB3	1:C:400:PRO:CD	2.16	0.75
1:G:190:ASP:CA	4:L:5483:MPD:HM3	2.11	0.75
1:K:84:THR:HG21	4:K:5493:MPD:C4	2.16	0.75
1:A:27:LYS:HA	5:A:5743:HOH:O	1.87	0.75
1:E:193:SER:HB2	4:F:5479:MPD:CM	2.11	0.75
1:B:399:LEU:HA	1:B:400:PRO:C	2.06	0.75
1:G:27:LYS:HA	5:G:5754:HOH:O	1.87	0.75
1:I:27:LYS:HA	5:I:5769:HOH:O	1.87	0.75
1:J:248:ARG:HH21	1:J:248:ARG:CG	2.00	0.75
1:E:399:LEU:HA	1:E:400:PRO:C	2.06	0.75
1:I:248:ARG:CG	1:I:248:ARG:HH21	2.00	0.75
4:I:5489:MPD:HM3	1:J:190:ASP:CA	2.11	0.74
1:E:27:LYS:HA	5:E:1454:HOH:O	1.87	0.74
1:E:58:LYS:HD2	1:E:62:GLU:HB2	1.67	0.74

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:ARG:HE	4:H:5486:MPD:CM	2.02	0.72
1:F:192:ARG:HH21	1:F:219:ASN:ND2	1.86	0.72
1:C:190:ASP:CA	4:D:5475:MPD:HM3	2.11	0.72
1:H:192:ARG:HH21	1:H:219:ASN:ND2	1.86	0.72
1:L:192:ARG:HH21	1:L:219:ASN:ND2	1.86	0.72
4:J:5491:MPD:CM	1:K:193:SER:HB2	2.11	0.72
1:H:82:ASP:HB2	4:H:5487:MPD:H31	1.71	0.72
1:A:82:ASP:HB2	4:A:5481:MPD:H31	1.70	0.72
1:I:88:ARG:HE	4:I:5488:MPD:CM	2.02	0.72
4:I:5489:MPD:O4	4:I:5489:MPD:HM2	1.90	0.72
1:B:88:ARG:HE	4:B:5474:MPD:CM	2.02	0.72
1:A:88:ARG:HE	4:A:5472:MPD:CM	2.02	0.72
1:E:88:ARG:HE	4:E:5480:MPD:CM	2.02	0.72
1:A:96:THR:OG1	1:A:98:GLN:HB2	1.90	0.72
1:G:88:ARG:HE	4:G:5484:MPD:CM	2.02	0.72
1:E:96:THR:OG1	1:E:98:GLN:HB2	1.90	0.72
4:C:5473:MPD:HM2	4:C:5473:MPD:O4	1.90	0.71
4:L:5483:MPD:O4	4:L:5483:MPD:HM2	1.90	0.71
4:D:5475:MPD:HM2	4:D:5475:MPD:O4	1.90	0.71
1:K:88:ARG:HE	4:K:5492:MPD:CM	2.02	0.71
1:J:96:THR:OG1	1:J:98:GLN:HB2	1.90	0.71
1:G:96:THR:OG1	1:G:98:GLN:HB2	1.90	0.71
1:C:96:THR:OG1	1:C:98:GLN:HB2	1.90	0.71
1:L:96:THR:OG1	1:L:98:GLN:HB2	1.90	0.71
1:G:80:PHE:CD1	4:G:5485:MPD:H53	2.24	0.71
1:F:96:THR:OG1	1:F:98:GLN:HB2	1.90	0.71
1:K:96:THR:OG1	1:K:98:GLN:HB2	1.90	0.71
1:F:22:THR:HB	4:F:5482:MPD:C1	2.21	0.71
1:D:96:THR:OG1	1:D:98:GLN:HB2	1.90	0.71
4:J:5491:MPD:HM2	4:J:5491:MPD:O4	1.90	0.71
1:F:84:THR:HG21	4:F:5479:MPD:H52	0.76	0.71
4:H:5487:MPD:HM2	4:H:5487:MPD:O4	1.90	0.71
1:H:22:THR:HB	4:H:5486:MPD:C1	2.21	0.71
4:G:5485:MPD:HM2	4:G:5485:MPD:O4	1.90	0.71
4:E:5477:MPD:O4	4:E:5477:MPD:HM2	1.90	0.71
4:B:5471:MPD:O4	4:B:5471:MPD:HM2	1.90	0.71
1:I:96:THR:OG1	1:I:98:GLN:HB2	1.90	0.71
1:E:190:ASP:CA	4:F:5479:MPD:HM3	2.11	0.70
1:B:22:THR:HB	4:B:5474:MPD:C1	2.21	0.70
1:J:84:THR:HG21	4:J:5491:MPD:H52	0.75	0.70
1:L:22:THR:HB	4:L:5494:MPD:C1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:384:ASN:HD22	1:K:384:ASN:N	1.89	0.70
4:A:5481:MPD:HM2	4:A:5481:MPD:O4	1.90	0.70
1:A:22:THR:HB	4:A:5472:MPD:C1	2.21	0.70
4:F:5479:MPD:HM2	4:F:5479:MPD:O4	1.90	0.70
1:L:399:LEU:H	1:L:401:PRO:CG	1.90	0.70
1:D:22:THR:HB	4:D:5478:MPD:C1	2.21	0.70
1:F:82:ASP:HB2	4:F:5479:MPD:C3	2.21	0.70
4:K:5493:MPD:HM2	4:K:5493:MPD:O4	1.90	0.70
1:I:22:THR:HB	4:I:5488:MPD:C1	2.21	0.70
1:H:384:ASN:HD22	1:H:384:ASN:N	1.89	0.70
1:E:22:THR:HB	4:E:5480:MPD:C1	2.21	0.70
1:J:22:THR:HB	4:J:5490:MPD:C1	2.21	0.70
1:E:384:ASN:HD22	1:E:384:ASN:N	1.89	0.70
1:A:384:ASN:HD22	1:A:384:ASN:N	1.89	0.70
1:H:96:THR:OG1	1:H:98:GLN:HB2	1.90	0.70
1:L:384:ASN:HD22	1:L:384:ASN:N	1.89	0.70
1:E:21:PHE:HA	4:E:5480:MPD:CM	2.22	0.70
1:K:22:THR:HB	4:K:5492:MPD:C1	2.21	0.70
1:C:384:ASN:N	1:C:384:ASN:HD22	1.89	0.70
4:G:5485:MPD:HM3	1:H:190:ASP:CA	2.11	0.69
1:G:82:ASP:HB2	4:G:5485:MPD:C3	2.22	0.69
1:G:22:THR:HB	4:G:5484:MPD:C1	2.21	0.69
1:H:21:PHE:HA	4:H:5486:MPD:CM	2.22	0.69
1:G:21:PHE:HA	4:G:5484:MPD:CM	2.22	0.69
1:K:21:PHE:HA	4:K:5492:MPD:CM	2.22	0.69
1:B:96:THR:OG1	1:B:98:GLN:HB2	1.90	0.69
1:I:384:ASN:HD22	1:I:384:ASN:N	1.89	0.69
1:G:84:THR:HG21	4:G:5485:MPD:H52	0.78	0.69
1:G:337:ARG:CB	1:L:61:ASN:O	2.34	0.69
1:G:384:ASN:N	1:G:384:ASN:HD22	1.89	0.69
1:A:190:ASP:CA	4:B:5471:MPD:HM3	2.11	0.69
1:E:399:LEU:H	1:E:401:PRO:CG	1.90	0.69
1:C:22:THR:HB	4:C:5476:MPD:C1	2.21	0.69
1:C:21:PHE:HA	4:C:5476:MPD:CM	2.22	0.69
1:C:22:THR:HB	4:C:5476:MPD:H11	1.75	0.69
1:L:22:THR:HB	4:L:5494:MPD:H11	1.75	0.69
1:L:21:PHE:HA	4:L:5494:MPD:CM	2.22	0.69
1:J:384:ASN:N	1:J:384:ASN:HD22	1.89	0.69
1:I:22:THR:HB	4:I:5488:MPD:H11	1.75	0.69
1:A:21:PHE:HA	4:A:5472:MPD:CM	2.22	0.69
1:J:82:ASP:HB2	4:J:5491:MPD:C3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:THR:HB	4:D:5478:MPD:H11	1.75	0.69
1:I:21:PHE:HA	4:I:5488:MPD:CM	2.22	0.68
1:E:22:THR:HB	4:E:5480:MPD:H11	1.75	0.68
1:F:21:PHE:HA	4:F:5482:MPD:CM	2.22	0.68
1:H:22:THR:HB	4:H:5486:MPD:H11	1.75	0.68
1:D:399:LEU:HA	1:D:400:PRO:O	1.94	0.68
1:H:399:LEU:HA	1:H:400:PRO:O	1.94	0.68
1:B:21:PHE:HA	4:B:5474:MPD:CM	2.22	0.68
1:D:21:PHE:HA	4:D:5478:MPD:CM	2.22	0.68
4:H:5487:MPD:HM3	1:I:190:ASP:CA	2.11	0.68
1:D:84:THR:HG21	4:D:5475:MPD:C4	2.22	0.68
1:B:190:ASP:CA	4:C:5473:MPD:HM3	2.10	0.68
1:E:399:LEU:HA	1:E:400:PRO:O	1.94	0.68
1:A:399:LEU:HA	1:A:400:PRO:O	1.94	0.68
1:K:399:LEU:HA	1:K:400:PRO:O	1.94	0.68
4:J:5491:MPD:HM3	1:K:190:ASP:CA	2.11	0.68
1:B:399:LEU:HA	1:B:400:PRO:O	1.94	0.68
1:E:461:GLU:OE1	1:K:320:LYS:NZ	2.27	0.68
1:I:88:ARG:HE	4:I:5488:MPD:HM1	1.60	0.68
1:L:88:ARG:HE	4:L:5494:MPD:HM1	1.59	0.68
1:D:384:ASN:N	1:D:384:ASN:HD22	1.89	0.68
1:F:384:ASN:N	1:F:384:ASN:HD22	1.89	0.68
1:B:384:ASN:N	1:B:384:ASN:HD22	1.89	0.68
1:G:84:THR:HG21	4:G:5485:MPD:C4	2.24	0.67
4:C:5473:MPD:H11	4:C:5473:MPD:H53	1.77	0.67
1:I:399:LEU:HA	1:I:400:PRO:O	1.94	0.67
1:A:22:THR:HB	4:A:5472:MPD:H11	1.75	0.67
4:L:5483:MPD:H53	4:L:5483:MPD:H11	1.76	0.67
1:C:399:LEU:HA	1:C:400:PRO:O	1.94	0.67
1:J:399:LEU:HA	1:J:400:PRO:O	1.94	0.67
1:L:399:LEU:HA	1:L:400:PRO:O	1.94	0.67
1:A:399:LEU:N	1:A:401:PRO:CG	2.52	0.67
1:J:21:PHE:HA	4:J:5490:MPD:CM	2.22	0.67
1:A:88:ARG:HE	4:A:5472:MPD:HM1	1.60	0.67
1:E:458:HIS:CD2	1:E:460:VAL:H	2.11	0.67
4:I:5489:MPD:H53	4:I:5489:MPD:H11	1.76	0.67
1:C:399:LEU:N	1:C:401:PRO:CG	2.52	0.67
1:G:399:LEU:HA	1:G:400:PRO:O	1.94	0.67
1:K:22:THR:HB	4:K:5492:MPD:H11	1.75	0.67
1:G:295:LEU:O	1:G:388:PRO:CG	2.43	0.67
1:L:399:LEU:N	1:L:401:PRO:CG	2.52	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:LEU:O	1:D:388:PRO:CG	2.43	0.67
4:A:5481:MPD:H11	4:A:5481:MPD:H53	1.77	0.67
4:D:5478:MPD:H11	4:D:5478:MPD:H52	1.77	0.67
4:K:5492:MPD:H52	4:K:5492:MPD:H11	1.77	0.67
1:K:295:LEU:O	1:K:388:PRO:CG	2.43	0.67
4:E:5477:MPD:H53	4:E:5477:MPD:H11	1.77	0.67
1:F:88:ARG:HE	4:F:5482:MPD:HM1	1.60	0.67
4:H:5486:MPD:H11	4:H:5486:MPD:H52	1.77	0.67
1:C:295:LEU:O	1:C:388:PRO:CG	2.43	0.67
1:L:80:PHE:CB	4:L:5483:MPD:C1	2.53	0.67
1:H:399:LEU:N	1:H:401:PRO:CG	2.52	0.67
1:J:88:ARG:HE	4:J:5490:MPD:HM1	1.60	0.67
1:H:88:ARG:HE	4:H:5486:MPD:HM1	1.60	0.67
1:I:458:HIS:CD2	1:I:460:VAL:H	2.12	0.67
1:H:295:LEU:O	1:H:388:PRO:CG	2.43	0.67
1:B:399:LEU:N	1:B:401:PRO:CG	2.52	0.67
4:B:5474:MPD:H11	4:B:5474:MPD:H52	1.77	0.67
1:F:295:LEU:O	1:F:388:PRO:CG	2.43	0.67
1:B:295:LEU:O	1:B:388:PRO:CG	2.43	0.67
4:J:5491:MPD:H53	4:J:5491:MPD:H11	1.76	0.67
1:D:190:ASP:CA	4:E:5477:MPD:HM3	2.11	0.67
1:D:461:GLU:OE1	1:J:320:LYS:NZ	2.26	0.67
1:A:295:LEU:O	1:A:388:PRO:CG	2.43	0.67
1:J:30:HIS:H	1:K:180:PHE:HB3	1.58	0.67
1:J:80:PHE:HD1	4:J:5491:MPD:C5	2.09	0.66
1:H:80:PHE:CB	4:H:5487:MPD:C1	2.53	0.66
1:G:88:ARG:HE	4:G:5484:MPD:HM1	1.59	0.66
1:G:458:HIS:CD2	1:G:460:VAL:H	2.11	0.66
1:E:295:LEU:O	1:E:388:PRO:CG	2.43	0.66
1:D:88:ARG:HE	4:D:5478:MPD:HM1	1.59	0.66
1:I:295:LEU:O	1:I:388:PRO:CG	2.43	0.66
1:L:295:LEU:O	1:L:388:PRO:CG	2.43	0.66
1:A:80:PHE:CD1	4:A:5481:MPD:H53	2.30	0.66
1:D:399:LEU:H	1:D:401:PRO:CG	1.90	0.66
4:F:5482:MPD:H52	4:F:5482:MPD:H11	1.77	0.66
1:C:105:ARG:HB2	4:C:5476:MPD:C4	2.26	0.66
4:A:5472:MPD:H11	4:A:5472:MPD:H52	1.77	0.66
1:A:53:SER:HB2	1:F:179:TYR:CD2	2.30	0.66
4:K:5493:MPD:H53	4:K:5493:MPD:H11	1.76	0.66
1:F:399:LEU:HA	1:F:400:PRO:O	1.94	0.66
1:J:295:LEU:O	1:J:388:PRO:CG	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:80:PHE:CB	4:J:5491:MPD:C1	2.53	0.66
4:B:5471:MPD:H53	4:B:5471:MPD:H11	1.76	0.66
1:B:82:ASP:HB2	4:B:5471:MPD:C3	2.24	0.66
1:C:88:ARG:HE	4:C:5476:MPD:HM1	1.59	0.66
4:H:5487:MPD:H53	4:H:5487:MPD:H11	1.77	0.66
4:G:5485:MPD:H11	4:G:5485:MPD:H53	1.77	0.66
1:I:399:LEU:N	1:I:401:PRO:CG	2.52	0.66
1:G:22:THR:HB	4:G:5484:MPD:H11	1.75	0.66
1:A:29:GLN:OE1	1:F:181:PRO:HD3	1.96	0.66
1:A:82:ASP:HB2	4:A:5481:MPD:C3	2.25	0.66
1:G:105:ARG:HB2	4:G:5484:MPD:C4	2.26	0.66
1:J:22:THR:HB	4:J:5490:MPD:H11	1.75	0.66
4:J:5490:MPD:H52	4:J:5490:MPD:H11	1.77	0.66
4:F:5479:MPD:H11	4:F:5479:MPD:H53	1.77	0.66
1:J:105:ARG:HB2	4:J:5490:MPD:C4	2.26	0.66
1:L:365:ALA:O	1:L:367:PRO:HD3	1.96	0.66
1:A:365:ALA:O	1:A:367:PRO:HD3	1.96	0.66
4:G:5484:MPD:H52	4:G:5484:MPD:H11	1.77	0.66
1:B:105:ARG:HB2	4:B:5474:MPD:C4	2.26	0.66
1:J:458:HIS:CD2	1:J:460:VAL:H	2.11	0.66
1:E:88:ARG:HE	4:E:5480:MPD:HM1	1.60	0.65
1:D:105:ARG:HB2	4:D:5478:MPD:C4	2.26	0.65
1:H:105:ARG:HB2	4:H:5486:MPD:C4	2.26	0.65
1:F:320:LYS:NZ	1:L:461:GLU:OE1	2.27	0.65
1:G:30:HIS:H	1:H:180:PHE:HB3	1.61	0.65
4:D:5475:MPD:H53	4:D:5475:MPD:H11	1.76	0.65
4:E:5480:MPD:H52	4:E:5480:MPD:H11	1.77	0.65
4:I:5488:MPD:H52	4:I:5488:MPD:H11	1.77	0.65
4:L:5494:MPD:H11	4:L:5494:MPD:H52	1.77	0.65
1:I:365:ALA:O	1:I:367:PRO:HD3	1.96	0.65
1:I:30:HIS:H	1:J:180:PHE:HB3	1.62	0.65
1:I:105:ARG:HB2	4:I:5488:MPD:C4	2.26	0.65
1:B:88:ARG:HE	4:B:5474:MPD:HM1	1.59	0.65
1:D:365:ALA:O	1:D:367:PRO:HD3	1.96	0.65
1:K:88:ARG:HE	4:K:5492:MPD:HM1	1.59	0.65
4:C:5476:MPD:H52	4:C:5476:MPD:H11	1.77	0.65
1:L:458:HIS:CD2	1:L:460:VAL:H	2.11	0.65
1:H:80:PHE:HD1	4:H:5487:MPD:H52	1.61	0.65
1:F:105:ARG:HB2	4:F:5482:MPD:C4	2.26	0.65
1:C:365:ALA:O	1:C:367:PRO:HD3	1.96	0.65
1:H:365:ALA:O	1:H:367:PRO:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:NZ	1:G:461:GLU:OE1	2.24	0.65
1:D:320:LYS:NZ	1:J:461:GLU:OE1	2.28	0.65
1:F:22:THR:HB	4:F:5482:MPD:H11	1.75	0.65
1:H:53:SER:HB2	1:I:179:TYR:CD2	2.32	0.65
1:A:80:PHE:CD1	4:A:5481:MPD:C5	2.80	0.65
1:C:399:LEU:H	1:C:401:PRO:CG	1.90	0.65
1:K:105:ARG:HB2	4:K:5492:MPD:C4	2.26	0.65
1:L:105:ARG:HB2	4:L:5494:MPD:C4	2.26	0.65
1:B:22:THR:HB	4:B:5474:MPD:H11	1.75	0.65
1:A:105:ARG:HB2	4:A:5472:MPD:C4	2.26	0.65
1:E:105:ARG:HB2	4:E:5480:MPD:C4	2.26	0.65
1:G:399:LEU:N	1:G:401:PRO:CG	2.52	0.64
1:C:179:TYR:CD2	1:D:53:SER:HB2	2.32	0.64
1:F:365:ALA:O	1:F:367:PRO:HD3	1.96	0.64
1:K:458:HIS:CD2	1:K:460:VAL:H	2.11	0.64
1:J:80:PHE:CA	4:J:5491:MPD:H12	2.28	0.64
1:I:170:GLY:HA2	1:I:172:ARG:NH2	2.13	0.64
1:E:399:LEU:N	1:E:401:PRO:CG	2.52	0.64
1:D:458:HIS:CD2	1:D:460:VAL:H	2.11	0.64
1:D:82:ASP:HB2	4:D:5475:MPD:C3	2.28	0.64
1:K:365:ALA:O	1:K:367:PRO:HD3	1.96	0.64
1:G:211:HIS:HD2	1:G:212:GLU:O	1.81	0.64
1:I:211:HIS:HD2	1:I:212:GLU:O	1.81	0.64
1:J:170:GLY:HA2	1:J:172:ARG:NH2	2.13	0.64
1:J:399:LEU:N	1:J:401:PRO:CG	2.52	0.64
1:F:399:LEU:N	1:F:401:PRO:CG	2.52	0.64
1:K:170:GLY:HA2	1:K:172:ARG:NH2	2.13	0.64
1:F:170:GLY:HA2	1:F:172:ARG:NH2	2.13	0.64
1:L:211:HIS:HD2	1:L:212:GLU:O	1.81	0.64
1:G:399:LEU:H	1:G:401:PRO:CG	1.90	0.64
1:D:170:GLY:HA2	1:D:172:ARG:NH2	2.13	0.64
1:A:170:GLY:HA2	1:A:172:ARG:NH2	2.13	0.64
1:J:211:HIS:HD2	1:J:212:GLU:O	1.81	0.64
1:E:80:PHE:CD1	4:E:5477:MPD:C5	2.81	0.64
1:B:365:ALA:O	1:B:367:PRO:HD3	1.96	0.64
1:J:365:ALA:O	1:J:367:PRO:HD3	1.96	0.64
1:G:365:ALA:O	1:G:367:PRO:HD3	1.96	0.64
1:E:80:PHE:CD1	4:E:5477:MPD:H53	2.34	0.63
1:E:365:ALA:O	1:E:367:PRO:HD3	1.96	0.63
1:F:211:HIS:HD2	1:F:212:GLU:O	1.81	0.63
1:K:399:LEU:N	1:K:401:PRO:CG	2.52	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:HIS:CD2	1:C:460:VAL:H	2.11	0.63
1:H:211:HIS:HD2	1:H:212:GLU:O	1.81	0.63
1:H:170:GLY:HA2	1:H:172:ARG:NH2	2.13	0.63
1:B:170:GLY:HA2	1:B:172:ARG:NH2	2.13	0.63
1:H:80:PHE:CA	4:H:5487:MPD:H12	2.29	0.63
1:H:458:HIS:CD2	1:H:460:VAL:H	2.11	0.63
1:L:386:ILE:O	1:L:388:PRO:HD3	1.99	0.63
1:C:211:HIS:HD2	1:C:212:GLU:O	1.81	0.63
1:K:211:HIS:HD2	1:K:212:GLU:O	1.81	0.63
1:B:386:ILE:O	1:B:388:PRO:HD3	1.99	0.63
1:G:170:GLY:HA2	1:G:172:ARG:NH2	2.13	0.63
1:E:386:ILE:O	1:E:388:PRO:HD3	1.99	0.63
1:C:170:GLY:HA2	1:C:172:ARG:NH2	2.13	0.63
1:A:461:GLU:OE1	1:G:320:LYS:NZ	2.25	0.63
1:L:170:GLY:HA2	1:L:172:ARG:NH2	2.13	0.63
1:A:211:HIS:HD2	1:A:212:GLU:O	1.81	0.63
1:E:211:HIS:HD2	1:E:212:GLU:O	1.81	0.63
1:F:396:LEU:HD12	1:F:398:ASP:H	1.64	0.63
1:B:399:LEU:H	1:B:401:PRO:CG	1.90	0.63
1:G:386:ILE:O	1:G:388:PRO:HD3	1.99	0.63
1:L:82:ASP:HB2	4:L:5483:MPD:C3	2.28	0.62
1:I:82:ASP:HB2	4:I:5489:MPD:C3	2.29	0.62
1:H:386:ILE:O	1:H:388:PRO:HD3	1.99	0.62
1:F:386:ILE:O	1:F:388:PRO:HD3	1.99	0.62
1:I:386:ILE:O	1:I:388:PRO:HD3	1.99	0.62
1:E:170:GLY:HA2	1:E:172:ARG:NH2	2.13	0.62
1:F:437:GLU:HG3	5:F:5724:HOH:O	1.99	0.62
1:D:211:HIS:HD2	1:D:212:GLU:O	1.81	0.62
1:A:396:LEU:HD12	1:A:398:ASP:H	1.64	0.62
1:D:386:ILE:O	1:D:388:PRO:HD3	1.99	0.62
1:C:386:ILE:O	1:C:388:PRO:HD3	1.99	0.62
1:J:386:ILE:O	1:J:388:PRO:HD3	1.99	0.62
1:B:211:HIS:HD2	1:B:212:GLU:O	1.81	0.62
1:L:396:LEU:HD12	1:L:398:ASP:H	1.64	0.62
1:I:396:LEU:HD12	1:I:398:ASP:H	1.64	0.62
1:D:399:LEU:N	1:D:401:PRO:CG	2.52	0.62
1:A:458:HIS:CD2	1:A:460:VAL:H	2.11	0.62
1:J:437:GLU:HG3	5:J:2881:HOH:O	1.99	0.62
1:F:80:PHE:CA	4:F:5479:MPD:H12	2.29	0.62
1:I:80:PHE:HD1	4:I:5489:MPD:C5	2.12	0.62
1:C:396:LEU:HD12	1:C:398:ASP:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:ILE:CG2	1:H:367:PRO:HG3	2.28	0.62
1:A:386:ILE:O	1:A:388:PRO:HD3	1.99	0.62
1:E:84:THR:HG21	4:E:5477:MPD:H52	0.77	0.62
1:J:396:LEU:HD12	1:J:398:ASP:H	1.64	0.62
1:F:458:HIS:CD2	1:F:460:VAL:H	2.11	0.62
1:L:437:GLU:HG3	5:L:3465:HOH:O	1.99	0.62
1:K:396:LEU:HD12	1:K:398:ASP:H	1.64	0.62
1:J:235:ILE:CG2	1:J:367:PRO:HG3	2.28	0.62
1:K:386:ILE:O	1:K:388:PRO:HD3	1.99	0.62
1:C:437:GLU:HG3	5:C:5712:HOH:O	1.99	0.62
1:H:396:LEU:HD12	1:H:398:ASP:H	1.64	0.62
1:E:396:LEU:HD12	1:E:398:ASP:H	1.64	0.62
1:A:155:GLU:OE1	1:A:211:HIS:HE1	1.83	0.62
1:K:82:ASP:HB2	4:K:5493:MPD:C3	2.30	0.62
1:G:437:GLU:HG3	5:G:5723:HOH:O	1.99	0.62
1:H:399:LEU:H	1:H:401:PRO:CG	1.90	0.62
1:D:235:ILE:CG2	1:D:367:PRO:HG3	2.28	0.62
1:B:437:GLU:HG3	5:B:5712:HOH:O	1.99	0.62
1:G:396:LEU:HD12	1:G:398:ASP:H	1.64	0.62
1:D:155:GLU:OE1	1:D:211:HIS:HE1	1.83	0.62
1:I:437:GLU:HG3	5:I:5738:HOH:O	1.99	0.62
1:B:360:PHE:CG	1:B:361:PRO:HD3	2.35	0.61
1:I:235:ILE:CG2	1:I:367:PRO:HG3	2.27	0.61
1:B:155:GLU:OE1	1:B:211:HIS:HE1	1.83	0.61
1:A:180:PHE:HB3	1:B:30:HIS:H	1.65	0.61
1:A:84:THR:HG21	4:A:5481:MPD:C4	2.30	0.61
1:D:360:PHE:CG	1:D:361:PRO:HD3	2.35	0.61
1:B:248:ARG:HG2	1:B:248:ARG:HH21	1.66	0.61
1:L:155:GLU:OE1	1:L:211:HIS:HE1	1.83	0.61
1:A:437:GLU:HG3	5:A:5711:HOH:O	1.99	0.61
1:B:427:PHE:CE1	1:B:428:LEU:HD13	2.36	0.61
1:H:437:GLU:HG3	5:H:5731:HOH:O	1.99	0.61
1:C:427:PHE:CE1	1:C:428:LEU:HD13	2.36	0.61
1:D:437:GLU:HG3	5:D:1129:HOH:O	1.99	0.61
1:J:248:ARG:HH21	1:J:248:ARG:HG2	1.65	0.61
1:K:155:GLU:OE1	1:K:211:HIS:HE1	1.83	0.61
1:E:155:GLU:OE1	1:E:211:HIS:HE1	1.83	0.61
1:K:53:SER:HB2	1:L:179:TYR:CD2	2.35	0.61
1:K:437:GLU:HG3	5:K:3173:HOH:O	1.99	0.61
1:J:427:PHE:CE1	1:J:428:LEU:HD13	2.36	0.61
1:D:396:LEU:HD12	1:D:398:ASP:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ARG:HH21	1:C:248:ARG:HG2	1.66	0.61
1:I:427:PHE:CE1	1:I:428:LEU:HD13	2.35	0.61
1:B:396:LEU:HD12	1:B:398:ASP:H	1.64	0.61
1:J:155:GLU:OE1	1:J:211:HIS:HE1	1.83	0.61
1:H:155:GLU:OE1	1:H:211:HIS:HE1	1.83	0.61
1:A:427:PHE:CE1	1:A:428:LEU:HD13	2.36	0.61
1:E:437:GLU:HG3	5:E:1421:HOH:O	1.99	0.61
1:H:248:ARG:HG2	1:H:248:ARG:HH21	1.66	0.61
1:F:155:GLU:OE1	1:F:211:HIS:HE1	1.83	0.61
1:E:22:THR:H	4:E:5480:MPD:H11	1.66	0.61
1:I:248:ARG:HH21	1:I:248:ARG:HG2	1.66	0.61
1:G:248:ARG:HG2	1:G:248:ARG:HH21	1.66	0.61
1:G:155:GLU:OE1	1:G:211:HIS:HE1	1.83	0.61
1:I:155:GLU:OE1	1:I:211:HIS:HE1	1.83	0.61
1:D:427:PHE:CE1	1:D:428:LEU:HD13	2.36	0.61
1:E:427:PHE:CE1	1:E:428:LEU:HD13	2.36	0.61
1:I:80:PHE:CA	4:I:5489:MPD:H12	2.30	0.61
1:C:80:PHE:CA	4:C:5473:MPD:H12	2.30	0.61
1:G:427:PHE:CE1	1:G:428:LEU:HD13	2.36	0.61
1:K:427:PHE:CE1	1:K:428:LEU:HD13	2.35	0.61
1:G:22:THR:H	4:G:5484:MPD:H11	1.66	0.60
1:C:235:ILE:CG2	1:C:367:PRO:HG3	2.28	0.60
1:F:235:ILE:CG2	1:F:367:PRO:HG3	2.28	0.60
1:B:458:HIS:CD2	1:B:460:VAL:H	2.11	0.60
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.36	0.60
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.36	0.60
1:L:427:PHE:CE1	1:L:428:LEU:HD13	2.36	0.60
1:F:248:ARG:HG2	1:F:248:ARG:HH21	1.66	0.60
1:G:21:PHE:HB2	4:G:5484:MPD:C5	2.25	0.60
1:C:155:GLU:OE1	1:C:211:HIS:HE1	1.83	0.60
1:F:427:PHE:CE1	1:F:428:LEU:HD13	2.35	0.60
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.36	0.60
1:J:360:PHE:CG	1:J:361:PRO:HD3	2.35	0.60
1:H:427:PHE:CE1	1:H:428:LEU:HD13	2.36	0.60
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.36	0.60
1:K:22:THR:H	4:K:5492:MPD:H11	1.66	0.60
1:A:235:ILE:CG2	1:A:367:PRO:HG3	2.28	0.60
1:E:248:ARG:HG2	1:E:248:ARG:HH21	1.65	0.60
1:B:323:VAL:O	1:B:325:GLY:N	2.35	0.60
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.36	0.60
1:C:360:PHE:CG	1:C:361:PRO:HD3	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:399:LEU:H	1:I:401:PRO:CG	1.90	0.60
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.36	0.60
1:E:323:VAL:O	1:E:325:GLY:N	2.35	0.60
1:E:320:LYS:NZ	1:K:461:GLU:OE1	2.27	0.60
1:L:80:PHE:CA	4:L:5483:MPD:H12	2.30	0.60
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.36	0.60
1:K:248:ARG:HH21	1:K:248:ARG:HG2	1.65	0.60
1:K:29:GLN:OE1	1:L:181:PRO:HD3	2.01	0.60
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.36	0.60
1:F:323:VAL:O	1:F:325:GLY:N	2.35	0.60
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.35	0.60
1:A:360:PHE:CG	1:A:361:PRO:HD3	2.35	0.60
1:A:248:ARG:HH21	1:A:248:ARG:HG2	1.66	0.60
1:H:323:VAL:O	1:H:325:GLY:N	2.35	0.60
1:D:323:VAL:O	1:D:325:GLY:N	2.35	0.60
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.36	0.60
1:K:323:VAL:O	1:K:325:GLY:N	2.35	0.60
1:C:80:PHE:HD1	4:C:5473:MPD:H52	1.67	0.59
1:L:323:VAL:O	1:L:325:GLY:N	2.35	0.59
1:J:323:VAL:O	1:J:325:GLY:N	2.35	0.59
1:A:399:LEU:H	1:A:401:PRO:CG	1.90	0.59
1:A:22:THR:H	4:A:5472:MPD:H11	1.66	0.59
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.36	0.59
1:F:80:PHE:HD1	4:F:5479:MPD:C5	2.14	0.59
1:E:84:THR:HG21	4:E:5477:MPD:C4	2.30	0.59
1:A:323:VAL:O	1:A:325:GLY:N	2.35	0.59
1:I:323:VAL:O	1:I:325:GLY:N	2.35	0.59
1:L:80:PHE:HD1	4:L:5483:MPD:C5	2.10	0.59
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.36	0.59
1:K:332:LEU:HB2	1:K:408:PRO:HB2	1.85	0.59
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.36	0.59
1:C:320:LYS:NZ	1:I:461:GLU:OE1	2.30	0.59
1:C:80:PHE:CB	4:C:5473:MPD:C1	2.60	0.59
1:F:22:THR:H	4:F:5482:MPD:H11	1.66	0.59
1:A:332:LEU:HB2	1:A:408:PRO:HB2	1.85	0.59
1:B:332:LEU:HB2	1:B:408:PRO:HB2	1.85	0.59
1:D:181:PRO:HD3	1:E:29:GLN:OE1	2.03	0.59
1:L:80:PHE:HD1	4:L:5483:MPD:H52	1.68	0.59
1:D:248:ARG:HH21	1:D:248:ARG:HG2	1.65	0.59
1:G:323:VAL:O	1:G:325:GLY:N	2.35	0.59
1:I:332:LEU:HB2	1:I:408:PRO:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:PRO:HD3	1:D:29:GLN:OE1	2.01	0.59
1:E:360:PHE:CG	1:E:361:PRO:HD3	2.35	0.59
1:C:360:PHE:CE2	1:C:361:PRO:HD3	2.36	0.59
1:J:399:LEU:H	1:J:401:PRO:CG	1.90	0.59
1:K:235:ILE:CG2	1:K:367:PRO:HG3	2.28	0.59
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.36	0.59
1:E:180:PHE:HB3	1:F:30:HIS:H	1.66	0.59
5:H:5633:HOH:O	1:I:181:PRO:HG3	2.01	0.59
1:I:80:PHE:HD1	4:I:5489:MPD:H52	1.68	0.59
1:I:21:PHE:HB2	4:I:5488:MPD:C5	2.25	0.59
1:C:21:PHE:HB2	4:C:5476:MPD:C5	2.25	0.59
1:E:235:ILE:CG2	1:E:367:PRO:HG3	2.28	0.59
1:L:248:ARG:HG2	1:L:248:ARG:HH21	1.66	0.59
1:K:18:ASP:OD2	1:K:30:HIS:HD2	1.86	0.59
1:H:18:ASP:OD2	1:H:30:HIS:HD2	1.86	0.59
1:C:332:LEU:HB2	1:C:408:PRO:HB2	1.85	0.59
1:L:22:THR:H	4:L:5494:MPD:H11	1.66	0.58
1:G:235:ILE:CG2	1:G:367:PRO:HG3	2.28	0.58
1:C:180:PHE:HB3	1:D:30:HIS:H	1.66	0.58
1:D:332:LEU:HB2	1:D:408:PRO:HB2	1.85	0.58
1:C:80:PHE:CD1	4:C:5473:MPD:H52	2.38	0.58
1:I:22:THR:H	4:I:5488:MPD:H11	1.66	0.58
1:B:22:THR:H	4:B:5474:MPD:H11	1.66	0.58
1:B:18:ASP:OD2	1:B:30:HIS:HD2	1.86	0.58
1:E:18:ASP:OD2	1:E:30:HIS:HD2	1.86	0.58
1:H:118:THR:OG1	1:H:120:ILE:HG13	2.04	0.58
1:C:82:ASP:HB2	4:C:5473:MPD:C3	2.33	0.58
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.36	0.58
1:A:18:ASP:OD2	1:A:30:HIS:HD2	1.86	0.58
1:L:18:ASP:OD2	1:L:30:HIS:HD2	1.86	0.58
1:L:332:LEU:HB2	1:L:408:PRO:HB2	1.85	0.58
1:F:80:PHE:CB	4:F:5479:MPD:C1	2.56	0.58
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.36	0.58
1:H:360:PHE:CG	1:H:361:PRO:HD3	2.35	0.58
1:G:332:LEU:HB2	1:G:408:PRO:HB2	1.85	0.58
1:C:323:VAL:O	1:C:325:GLY:N	2.35	0.58
1:B:179:TYR:CD2	1:C:53:SER:HB2	2.38	0.58
1:G:360:PHE:CE2	1:G:361:PRO:HD3	2.36	0.58
1:D:22:THR:H	4:D:5478:MPD:H11	1.66	0.58
1:J:21:PHE:HB2	4:J:5490:MPD:C5	2.25	0.58
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:SER:HB2	1:J:179:TYR:CD2	2.38	0.58
1:L:360:PHE:CG	1:L:361:PRO:HD3	2.35	0.58
1:L:235:ILE:CG2	1:L:367:PRO:HG3	2.28	0.58
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.03	0.58
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.03	0.58
1:H:332:LEU:HB2	1:H:408:PRO:HB2	1.85	0.58
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.04	0.58
1:C:18:ASP:OD2	1:C:30:HIS:HD2	1.86	0.58
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.36	0.58
1:B:21:PHE:HB2	4:B:5474:MPD:C5	2.25	0.58
1:C:22:THR:H	4:C:5476:MPD:H11	1.66	0.58
1:I:18:ASP:OD2	1:I:30:HIS:HD2	1.86	0.58
1:K:308:ILE:HG21	1:K:374:LEU:HD13	1.86	0.58
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.86	0.58
1:G:443:ILE:O	1:G:447:ARG:HG3	2.04	0.58
1:J:332:LEU:HB2	1:J:408:PRO:HB2	1.85	0.58
1:J:443:ILE:O	1:J:447:ARG:HG3	2.04	0.58
1:J:82:ASP:O	1:J:84:THR:CG2	2.51	0.58
1:J:22:THR:H	4:J:5490:MPD:H11	1.66	0.58
1:A:21:PHE:HB2	4:A:5472:MPD:C5	2.25	0.58
1:F:443:ILE:O	1:F:447:ARG:HG3	2.04	0.58
1:A:118:THR:OG1	1:A:120:ILE:HG13	2.03	0.58
1:D:18:ASP:OD2	1:D:30:HIS:HD2	1.86	0.58
1:L:118:THR:OG1	1:L:120:ILE:HG13	2.03	0.58
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.86	0.58
1:D:443:ILE:O	1:D:447:ARG:HG3	2.04	0.58
1:E:82:ASP:O	1:E:84:THR:CG2	2.51	0.57
1:J:18:ASP:OD2	1:J:30:HIS:HD2	1.86	0.57
1:F:332:LEU:HB2	1:F:408:PRO:HB2	1.85	0.57
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.04	0.57
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.04	0.57
1:K:360:PHE:CG	1:K:361:PRO:HD3	2.35	0.57
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.35	0.57
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.86	0.57
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.04	0.57
1:K:443:ILE:O	1:K:447:ARG:HG3	2.04	0.57
1:B:443:ILE:O	1:B:447:ARG:HG3	2.04	0.57
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.36	0.57
1:C:443:ILE:O	1:C:447:ARG:HG3	2.04	0.57
1:E:332:LEU:HB2	1:E:408:PRO:HB2	1.85	0.57
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:21:PHE:HB2	4:K:5492:MPD:C5	2.25	0.57
1:B:383:LYS:C	1:B:384:ASN:HD22	2.08	0.57
1:A:332:LEU:CB	1:A:408:PRO:HB2	2.35	0.57
1:F:435:THR:HG23	5:F:5531:HOH:O	2.05	0.57
1:H:443:ILE:O	1:H:447:ARG:HG3	2.04	0.57
1:J:383:LYS:C	1:J:384:ASN:HD22	2.08	0.57
1:G:435:THR:HG23	5:G:5529:HOH:O	2.05	0.57
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.04	0.57
1:I:82:ASP:O	1:I:84:THR:CG2	2.51	0.57
1:G:383:LYS:C	1:G:384:ASN:HD22	2.08	0.57
1:K:332:LEU:CB	1:K:408:PRO:HB2	2.35	0.57
1:G:180:PHE:HB3	1:L:30:HIS:H	1.68	0.57
1:G:332:LEU:CB	1:G:408:PRO:HB2	2.35	0.57
1:I:120:ILE:HD13	1:I:382:ILE:HG21	1.87	0.57
1:L:435:THR:HG23	5:L:3254:HOH:O	2.05	0.57
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.04	0.57
1:F:120:ILE:HD13	1:F:382:ILE:HG21	1.87	0.57
1:C:435:THR:HG23	5:C:5518:HOH:O	2.05	0.57
1:E:435:THR:HG23	5:E:1210:HOH:O	2.05	0.57
1:G:82:ASP:O	1:G:84:THR:CG2	2.51	0.57
1:I:80:PHE:CD1	4:I:5489:MPD:H52	2.39	0.57
1:H:192:ARG:HH21	1:H:219:ASN:HD22	1.52	0.57
1:B:332:LEU:CB	1:B:408:PRO:HB2	2.35	0.57
1:G:120:ILE:HD13	1:G:382:ILE:HG21	1.87	0.57
1:G:53:SER:HB2	1:H:179:TYR:CD2	2.40	0.57
4:K:5493:MPD:H11	1:L:189:GLN:HG3	1.87	0.57
1:I:360:PHE:CG	1:I:361:PRO:HD3	2.35	0.57
1:K:399:LEU:H	1:K:401:PRO:CG	1.90	0.57
1:B:235:ILE:CG2	1:B:367:PRO:HG3	2.28	0.57
1:F:192:ARG:HH21	1:F:219:ASN:HD22	1.52	0.57
1:H:383:LYS:C	1:H:384:ASN:HD22	2.08	0.57
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.86	0.57
1:A:443:ILE:O	1:A:447:ARG:HG3	2.04	0.57
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.86	0.57
1:F:21:PHE:HB2	4:F:5482:MPD:C5	2.25	0.57
1:H:22:THR:H	4:H:5486:MPD:H11	1.66	0.57
1:D:192:ARG:HH21	1:D:219:ASN:HD22	1.52	0.57
1:C:192:ARG:HH21	1:C:219:ASN:HD22	1.52	0.57
1:E:383:LYS:C	1:E:384:ASN:HD22	2.08	0.57
1:D:180:PHE:HB3	1:E:30:HIS:H	1.70	0.57
1:C:180:PHE:O	1:D:29:GLN:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:332:LEU:CB	1:L:408:PRO:HB2	2.35	0.57
1:D:120:ILE:HD13	1:D:382:ILE:HG21	1.87	0.57
1:E:443:ILE:O	1:E:447:ARG:HG3	2.04	0.57
1:A:179:TYR:CD2	1:B:53:SER:HB2	2.40	0.57
1:C:189:GLN:HG3	4:D:5475:MPD:H11	1.87	0.56
1:J:326:TYR:HA	1:J:396:LEU:HD13	1.87	0.56
1:D:383:LYS:C	1:D:384:ASN:HD22	2.08	0.56
1:C:120:ILE:HD13	1:C:382:ILE:HG21	1.87	0.56
1:K:120:ILE:HD13	1:K:382:ILE:HG21	1.87	0.56
1:A:189:GLN:HG3	4:B:5471:MPD:H11	1.87	0.56
1:K:80:PHE:CB	4:K:5493:MPD:C1	2.60	0.56
1:G:460:VAL:HG12	1:G:464:LEU:HD22	1.88	0.56
1:L:443:ILE:O	1:L:447:ARG:HG3	2.04	0.56
1:H:435:THR:HG23	5:H:5540:HOH:O	2.05	0.56
1:I:435:THR:HG23	5:I:5542:HOH:O	2.05	0.56
4:H:5487:MPD:H11	1:I:189:GLN:HG3	1.87	0.56
1:B:80:PHE:HD1	4:B:5471:MPD:C5	2.18	0.56
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.36	0.56
1:C:340:SER:HB3	1:C:396:LEU:HA	1.88	0.56
1:F:326:TYR:HA	1:F:396:LEU:HD13	1.87	0.56
1:G:18:ASP:OD2	1:G:30:HIS:HD2	1.86	0.56
1:F:18:ASP:OD2	1:F:30:HIS:HD2	1.86	0.56
1:D:332:LEU:CB	1:D:408:PRO:HB2	2.35	0.56
1:L:120:ILE:HD13	1:L:382:ILE:HG21	1.87	0.56
1:B:120:ILE:HD13	1:B:382:ILE:HG21	1.87	0.56
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.86	0.56
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.86	0.56
1:C:460:VAL:HG12	1:C:464:LEU:HD22	1.88	0.56
1:F:460:VAL:HG12	1:F:464:LEU:HD22	1.88	0.56
1:A:383:LYS:C	1:A:384:ASN:HD22	2.08	0.56
1:L:383:LYS:C	1:L:384:ASN:HD22	2.08	0.56
1:F:383:LYS:C	1:F:384:ASN:HD22	2.08	0.56
1:B:435:THR:HG23	5:B:5518:HOH:O	2.05	0.56
4:I:5489:MPD:H11	1:J:189:GLN:HG3	1.87	0.56
1:K:80:PHE:HD1	4:K:5493:MPD:C5	2.17	0.56
1:J:340:SER:HB3	1:J:396:LEU:HA	1.87	0.56
1:L:326:TYR:HA	1:L:396:LEU:HD13	1.87	0.56
1:G:340:SER:HB3	1:G:396:LEU:HA	1.88	0.56
1:K:192:ARG:HH21	1:K:219:ASN:HD22	1.52	0.56
1:H:332:LEU:CB	1:H:408:PRO:HB2	2.35	0.56
1:E:332:LEU:CB	1:E:408:PRO:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:TYR:CD2	1:E:53:SER:HB2	2.41	0.56
1:K:435:THR:HG23	5:K:2962:HOH:O	2.05	0.56
1:L:82:ASP:O	1:L:84:THR:CG2	2.51	0.56
1:E:192:ARG:HH21	1:E:219:ASN:HD22	1.52	0.56
1:A:120:ILE:HD13	1:A:382:ILE:HG21	1.87	0.56
1:D:130:PRO:HB3	1:D:268:MET:HE3	1.88	0.56
1:E:189:GLN:HG3	4:F:5479:MPD:H11	1.87	0.56
1:B:82:ASP:O	1:B:84:THR:CG2	2.51	0.56
1:G:326:TYR:HA	1:G:396:LEU:HD13	1.87	0.56
1:B:326:TYR:HA	1:B:396:LEU:HD13	1.88	0.56
1:I:460:VAL:HG12	1:I:464:LEU:HD22	1.88	0.56
1:F:248:ARG:CG	1:F:248:ARG:NH2	2.67	0.56
1:L:192:ARG:HH21	1:L:219:ASN:HD22	1.52	0.56
1:J:120:ILE:HD13	1:J:382:ILE:HG21	1.87	0.56
1:F:332:LEU:CB	1:F:408:PRO:HB2	2.35	0.56
1:I:443:ILE:O	1:I:447:ARG:HG3	2.04	0.56
1:J:435:THR:HG23	5:J:2670:HOH:O	2.05	0.56
1:K:82:ASP:O	1:K:84:THR:CG2	2.51	0.56
1:H:398:ASP:O	1:H:399:LEU:HG	2.06	0.56
1:C:326:TYR:HA	1:C:396:LEU:HD13	1.87	0.56
1:E:340:SER:HB3	1:E:396:LEU:HA	1.88	0.56
1:D:398:ASP:O	1:D:399:LEU:HG	2.06	0.56
1:I:332:LEU:CB	1:I:408:PRO:HB2	2.35	0.56
1:A:435:THR:HG23	5:A:5515:HOH:O	2.05	0.56
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.86	0.56
1:J:61:ASN:O	1:K:337:ARG:CB	2.34	0.56
1:A:326:TYR:HA	1:A:396:LEU:HD13	1.87	0.56
1:D:21:PHE:HB2	4:D:5478:MPD:C5	2.25	0.56
1:K:383:LYS:C	1:K:384:ASN:HD22	2.08	0.56
1:C:332:LEU:CB	1:C:408:PRO:HB2	2.35	0.56
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.86	0.56
4:J:5491:MPD:H11	1:K:189:GLN:HG3	1.87	0.56
1:K:398:ASP:O	1:K:399:LEU:HG	2.06	0.56
1:G:192:ARG:HH21	1:G:219:ASN:HD22	1.52	0.56
1:G:179:TYR:CD2	1:L:53:SER:HB2	2.40	0.56
1:B:189:GLN:HG3	4:C:5473:MPD:H11	1.87	0.55
1:H:340:SER:HB3	1:H:396:LEU:HA	1.88	0.55
1:I:340:SER:HB3	1:I:396:LEU:HA	1.87	0.55
1:B:398:ASP:O	1:B:399:LEU:HG	2.06	0.55
1:K:326:TYR:HA	1:K:396:LEU:HD13	1.87	0.55
1:I:383:LYS:C	1:I:384:ASN:HD22	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ILE:HD13	1:E:382:ILE:HG21	1.87	0.55
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.41	0.55
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.41	0.55
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.74	0.55
1:F:340:SER:HB3	1:F:396:LEU:HA	1.88	0.55
1:E:460:VAL:HG12	1:E:464:LEU:HD22	1.88	0.55
1:J:460:VAL:HG12	1:J:464:LEU:HD22	1.88	0.55
1:H:114:TYR:CD2	1:H:431:GLY:HA3	2.41	0.55
1:J:332:LEU:CB	1:J:408:PRO:HB2	2.35	0.55
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.41	0.55
4:A:5481:MPD:H11	1:F:189:GLN:HG3	1.87	0.55
1:B:360:PHE:CD2	1:B:361:PRO:CD	2.74	0.55
1:H:326:TYR:HA	1:H:396:LEU:HD13	1.87	0.55
1:E:326:TYR:HA	1:E:396:LEU:HD13	1.87	0.55
1:J:192:ARG:HH21	1:J:219:ASN:HD22	1.52	0.55
1:B:181:PRO:HG3	5:C:5611:HOH:O	2.07	0.55
1:C:82:ASP:O	1:C:84:THR:CG2	2.51	0.55
1:J:398:ASP:O	1:J:399:LEU:HG	2.06	0.55
1:L:340:SER:HB3	1:L:396:LEU:HA	1.88	0.55
1:A:340:SER:HB3	1:A:396:LEU:HA	1.88	0.55
1:A:460:VAL:HG12	1:A:464:LEU:HD22	1.88	0.55
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.41	0.55
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.86	0.55
1:J:80:PHE:HD1	4:J:5491:MPD:H52	1.69	0.55
1:G:189:GLN:HG3	4:L:5483:MPD:H11	1.87	0.55
1:H:120:ILE:HD13	1:H:382:ILE:HG21	1.87	0.55
1:F:461:GLU:OE1	1:L:320:LYS:NZ	2.30	0.55
1:D:435:THR:HG23	5:D:918:HOH:O	2.05	0.55
1:D:189:GLN:HG3	4:E:5477:MPD:H11	1.87	0.55
1:L:398:ASP:O	1:L:399:LEU:HG	2.06	0.55
1:D:340:SER:HB3	1:D:396:LEU:HA	1.88	0.55
1:C:383:LYS:C	1:C:384:ASN:HD22	2.08	0.55
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.86	0.55
1:D:82:ASP:O	1:D:84:THR:CG2	2.51	0.55
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.74	0.55
1:I:398:ASP:O	1:I:399:LEU:HG	2.06	0.55
1:A:398:ASP:O	1:A:399:LEU:HG	2.06	0.55
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.41	0.55
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.41	0.55
1:H:84:THR:CG2	4:H:5487:MPD:H32	2.37	0.55
1:B:80:PHE:CA	4:B:5471:MPD:H12	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:5485:MPD:H11	1:H:189:GLN:HG3	1.87	0.55
1:E:21:PHE:HB2	4:E:5480:MPD:C5	2.25	0.55
1:H:460:VAL:HG12	1:H:464:LEU:HD22	1.88	0.55
1:I:29:GLN:HA	1:J:180:PHE:O	2.06	0.55
1:B:340:SER:HB3	1:B:396:LEU:HA	1.88	0.55
1:D:326:TYR:HA	1:D:396:LEU:HD13	1.87	0.55
1:K:460:VAL:HG12	1:K:464:LEU:HD22	1.87	0.55
1:B:460:VAL:HG12	1:B:464:LEU:HD22	1.88	0.55
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.41	0.55
1:A:82:ASP:O	1:A:84:THR:CG2	2.51	0.55
1:D:460:VAL:HG12	1:D:464:LEU:HD22	1.88	0.55
1:L:128:PRO:HD2	1:L:231:LYS:HE2	1.89	0.55
1:C:398:ASP:O	1:C:399:LEU:HG	2.06	0.54
1:G:398:ASP:O	1:G:399:LEU:HG	2.06	0.54
1:K:340:SER:HB3	1:K:396:LEU:HA	1.88	0.54
1:H:248:ARG:NH2	1:H:248:ARG:CG	2.67	0.54
1:G:29:GLN:OE1	1:H:181:PRO:HD3	2.07	0.54
1:I:114:TYR:CD2	1:I:431:GLY:HA3	2.41	0.54
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.74	0.54
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.37	0.54
1:E:398:ASP:O	1:E:399:LEU:HG	2.06	0.54
1:I:22:THR:HG1	4:I:5488:MPD:C1	2.08	0.54
1:J:105:ARG:HD2	4:J:5490:MPD:H32	1.90	0.54
1:L:460:VAL:HG12	1:L:464:LEU:HD22	1.88	0.54
1:J:248:ARG:NH2	1:J:248:ARG:HG2	2.23	0.54
1:B:192:ARG:HH21	1:B:219:ASN:HD22	1.52	0.54
1:I:192:ARG:HH21	1:I:219:ASN:HD22	1.52	0.54
1:J:29:GLN:HA	1:K:180:PHE:O	2.07	0.54
1:C:181:PRO:HG3	5:D:1020:HOH:O	2.07	0.54
1:J:128:PRO:HD2	1:J:231:LYS:HE2	1.89	0.54
1:L:21:PHE:HB2	4:L:5494:MPD:C5	2.25	0.54
1:E:248:ARG:HG2	1:E:248:ARG:NH2	2.23	0.54
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.41	0.54
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.41	0.54
1:K:114:TYR:CD2	1:K:431:GLY:HA3	2.41	0.54
1:B:128:PRO:HD2	1:B:231:LYS:HE2	1.89	0.54
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.36	0.54
1:F:398:ASP:O	1:F:399:LEU:HG	2.06	0.54
1:K:30:HIS:H	1:L:180:PHE:HB3	1.73	0.54
1:K:29:GLN:HA	1:L:180:PHE:O	2.08	0.54
1:H:128:PRO:HD2	1:H:231:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:PRO:HD2	1:F:231:LYS:HE2	1.89	0.54
1:L:84:THR:CG2	4:L:5483:MPD:H32	2.37	0.54
1:B:456:THR:O	1:H:458:HIS:HE1	1.91	0.54
1:H:248:ARG:HG2	1:H:248:ARG:NH2	2.23	0.54
1:G:248:ARG:HG2	1:G:248:ARG:NH2	2.23	0.54
1:D:128:PRO:HD2	1:D:231:LYS:HE2	1.89	0.54
1:H:82:ASP:O	1:H:84:THR:CG2	2.51	0.54
1:C:248:ARG:NH2	1:C:248:ARG:HG2	2.23	0.54
1:B:320:LYS:NZ	1:H:461:GLU:OE1	2.35	0.54
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.36	0.54
1:H:21:PHE:HB2	4:H:5486:MPD:C5	2.25	0.54
1:A:61:ASN:O	1:F:337:ARG:CB	2.44	0.54
1:C:105:ARG:HD2	4:C:5476:MPD:H32	1.90	0.54
1:L:248:ARG:HG2	1:L:248:ARG:NH2	2.23	0.54
1:J:29:GLN:OE1	1:K:181:PRO:HD3	2.08	0.54
1:K:80:PHE:HD1	4:K:5493:MPD:H52	1.73	0.54
1:I:326:TYR:HA	1:I:396:LEU:HD13	1.88	0.54
1:B:105:ARG:HD2	4:B:5474:MPD:H32	1.90	0.54
1:B:180:PHE:HB3	1:C:30:HIS:H	1.73	0.54
5:K:3064:HOH:O	1:L:181:PRO:HG3	2.07	0.54
1:E:128:PRO:HD2	1:E:231:LYS:HE2	1.89	0.54
1:H:105:ARG:HD2	4:H:5486:MPD:H32	1.90	0.53
1:L:105:ARG:HD2	4:L:5494:MPD:H32	1.90	0.53
1:H:80:PHE:CG	4:H:5487:MPD:H12	2.37	0.53
1:D:105:ARG:HD2	4:D:5478:MPD:H32	1.90	0.53
1:A:192:ARG:HH21	1:A:219:ASN:HD22	1.52	0.53
1:C:461:GLU:OE1	1:I:320:LYS:NZ	2.33	0.53
1:A:128:PRO:HD2	1:A:231:LYS:HE2	1.89	0.53
1:H:80:PHE:CG	4:H:5487:MPD:C1	2.92	0.53
1:B:248:ARG:NH2	1:B:248:ARG:HG2	2.23	0.53
5:I:5635:HOH:O	1:J:181:PRO:HG3	2.07	0.53
1:D:248:ARG:HG2	1:D:248:ARG:NH2	2.23	0.53
1:H:80:PHE:CD1	4:H:5487:MPD:H52	2.33	0.53
1:K:105:ARG:HD2	4:K:5492:MPD:H32	1.90	0.53
1:I:80:PHE:CB	4:I:5489:MPD:C1	2.61	0.53
1:E:105:ARG:HD2	4:E:5480:MPD:H32	1.90	0.53
1:A:105:ARG:HD2	4:A:5472:MPD:H32	1.90	0.53
1:I:128:PRO:HD2	1:I:231:LYS:HE2	1.89	0.53
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.74	0.53
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.74	0.53
1:A:29:GLN:HA	1:F:180:PHE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:PRO:HD2	1:C:231:LYS:HE2	1.89	0.53
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.74	0.53
1:F:399:LEU:H	1:F:401:PRO:CG	1.90	0.53
1:F:105:ARG:HD2	4:F:5482:MPD:H32	1.90	0.53
1:K:128:PRO:HD2	1:K:231:LYS:HE2	1.89	0.53
1:B:461:GLU:OE1	1:H:320:LYS:NZ	2.33	0.53
1:F:82:ASP:O	1:F:84:THR:CG2	2.51	0.53
1:G:105:ARG:HD2	4:G:5484:MPD:H32	1.90	0.53
1:B:295:LEU:O	1:B:388:PRO:HG3	2.09	0.53
1:H:29:GLN:HA	1:I:180:PHE:O	2.09	0.53
1:D:295:LEU:O	1:D:388:PRO:HG3	2.09	0.52
1:F:80:PHE:HD1	4:F:5479:MPD:H52	1.74	0.52
1:F:256:MET:HG3	1:L:466:TYR:HA	1.91	0.52
1:H:360:PHE:CD2	1:H:361:PRO:CD	2.74	0.52
1:G:21:PHE:HA	4:G:5484:MPD:C3	2.36	0.52
1:K:248:ARG:NH2	1:K:248:ARG:HG2	2.23	0.52
1:A:248:ARG:HH21	1:A:248:ARG:HG3	1.75	0.52
1:K:295:LEU:O	1:K:388:PRO:HG3	2.09	0.52
1:G:128:PRO:HD2	1:G:231:LYS:HE2	1.89	0.52
1:J:16:PHE:HB2	1:J:84:THR:HB	1.92	0.52
1:B:80:PHE:HD1	4:B:5471:MPD:H52	1.75	0.52
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.74	0.52
1:I:105:ARG:HD2	4:I:5488:MPD:H32	1.90	0.52
1:I:29:GLN:HB3	1:J:180:PHE:HB2	1.91	0.52
1:H:16:PHE:HB2	1:H:84:THR:HB	1.92	0.52
1:B:16:PHE:HB2	1:B:84:THR:HB	1.92	0.52
1:A:88:ARG:HH11	4:A:5472:MPD:HM3	1.75	0.52
1:H:295:LEU:O	1:H:388:PRO:HG3	2.09	0.52
1:L:295:LEU:O	1:L:388:PRO:HG3	2.09	0.52
1:J:295:LEU:O	1:J:388:PRO:HG3	2.09	0.52
1:K:80:PHE:CA	4:K:5493:MPD:H12	2.38	0.52
1:J:88:ARG:HH11	4:J:5490:MPD:HM3	1.75	0.52
1:C:88:ARG:HH11	4:C:5476:MPD:HM3	1.75	0.52
1:A:248:ARG:NH2	1:A:248:ARG:HG2	2.23	0.52
1:A:30:HIS:H	1:F:180:PHE:HB3	1.73	0.52
1:I:29:GLN:HB3	1:J:180:PHE:CB	2.40	0.52
1:D:80:PHE:HD1	4:D:5475:MPD:C5	2.23	0.52
1:F:88:ARG:HH11	4:F:5482:MPD:HM3	1.75	0.52
1:I:295:LEU:O	1:I:388:PRO:HG3	2.09	0.52
1:A:256:MET:HG3	1:G:466:TYR:HA	1.91	0.52
1:E:16:PHE:HB2	1:E:84:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:THR:O	1:J:458:HIS:HE1	1.93	0.52
1:B:248:ARG:HH21	1:B:248:ARG:HG3	1.75	0.52
1:J:29:GLN:HB3	1:K:180:PHE:HB2	1.92	0.52
1:D:16:PHE:HB2	1:D:84:THR:HB	1.92	0.52
1:B:88:ARG:HH11	4:B:5474:MPD:HM3	1.75	0.52
1:H:88:ARG:HH11	4:H:5486:MPD:HM3	1.75	0.52
1:I:248:ARG:HG3	1:I:248:ARG:HH21	1.75	0.52
1:B:181:PRO:HD3	1:C:29:GLN:OE1	2.10	0.52
1:C:16:PHE:HB2	1:C:84:THR:HB	1.92	0.51
1:I:311:LEU:HD22	1:I:369:LEU:HB3	1.93	0.51
1:L:399:LEU:CA	1:L:400:PRO:C	2.78	0.51
1:I:88:ARG:HH11	4:I:5488:MPD:HM3	1.75	0.51
1:F:248:ARG:HG2	1:F:248:ARG:NH2	2.23	0.51
1:L:311:LEU:HD22	1:L:369:LEU:HB3	1.93	0.51
1:B:399:LEU:CA	1:B:400:PRO:C	2.78	0.51
1:I:21:PHE:HA	4:I:5488:MPD:C3	2.36	0.51
1:A:295:LEU:O	1:A:388:PRO:HG3	2.09	0.51
1:E:295:LEU:O	1:E:388:PRO:HG3	2.09	0.51
5:A:5609:HOH:O	1:F:181:PRO:HG3	2.10	0.51
1:I:29:GLN:OE1	1:J:181:PRO:HD3	2.10	0.51
1:H:84:THR:HG21	4:H:5487:MPD:H32	1.92	0.51
1:D:88:ARG:HH11	4:D:5478:MPD:HM3	1.75	0.51
1:I:248:ARG:NH2	1:I:248:ARG:HG2	2.23	0.51
1:B:311:LEU:HD22	1:B:369:LEU:HB3	1.93	0.51
1:E:311:LEU:HD22	1:E:369:LEU:HB3	1.93	0.51
1:A:311:LEU:HD22	1:A:369:LEU:HB3	1.93	0.51
1:F:399:LEU:CA	1:F:400:PRO:C	2.78	0.51
1:I:399:LEU:CA	1:I:400:PRO:C	2.78	0.51
1:C:295:LEU:O	1:C:388:PRO:HG3	2.09	0.51
1:I:16:PHE:HB2	1:I:84:THR:HB	1.92	0.51
1:K:399:LEU:CA	1:K:400:PRO:C	2.78	0.51
1:D:458:HIS:HE1	1:J:456:THR:O	1.94	0.51
1:C:180:PHE:CB	1:D:29:GLN:HB3	2.41	0.51
1:J:84:THR:CG2	4:J:5491:MPD:H32	2.40	0.51
1:F:16:PHE:HB2	1:F:84:THR:HB	1.92	0.51
1:G:29:GLN:HA	1:H:180:PHE:O	2.11	0.51
1:K:311:LEU:HD22	1:K:369:LEU:HB3	1.93	0.51
1:K:403:GLU:C	1:K:405:LYS:H	2.14	0.51
1:B:458:HIS:HE1	1:H:456:THR:O	1.93	0.51
1:G:295:LEU:O	1:G:388:PRO:HG3	2.09	0.51
1:F:295:LEU:O	1:F:388:PRO:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:LEU:O	1:G:400:PRO:HG2	2.11	0.51
1:G:403:GLU:C	1:G:405:LYS:H	2.14	0.51
1:K:88:ARG:HH11	4:K:5492:MPD:HM3	1.75	0.51
1:A:248:ARG:CG	1:A:248:ARG:NH2	2.67	0.51
1:H:29:GLN:OE1	1:I:181:PRO:HD3	2.10	0.51
1:C:311:LEU:HD22	1:C:369:LEU:HB3	1.93	0.51
1:F:311:LEU:HD22	1:F:369:LEU:HB3	1.93	0.51
1:K:16:PHE:HB2	1:K:84:THR:HB	1.92	0.51
1:L:88:ARG:HH11	4:L:5494:MPD:HM3	1.75	0.51
1:J:248:ARG:HH21	1:J:248:ARG:HG3	1.75	0.51
1:G:248:ARG:HG3	1:G:248:ARG:HH21	1.75	0.51
1:G:16:PHE:HB2	1:G:84:THR:HB	1.92	0.50
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.74	0.50
1:C:248:ARG:HG3	1:C:248:ARG:HH21	1.75	0.50
1:G:180:PHE:O	1:L:29:GLN:HA	2.10	0.50
1:D:130:PRO:HB3	1:D:268:MET:CE	2.41	0.50
1:J:53:SER:HB2	1:K:179:TYR:CD2	2.46	0.50
1:L:130:PRO:HB3	1:L:268:MET:CE	2.41	0.50
1:F:403:GLU:C	1:F:405:LYS:H	2.14	0.50
1:J:82:ASP:N	4:J:5491:MPD:O2	2.39	0.50
1:J:403:GLU:C	1:J:405:LYS:H	2.14	0.50
1:B:403:GLU:C	1:B:405:LYS:H	2.14	0.50
1:G:88:ARG:HH11	4:G:5484:MPD:HM3	1.75	0.50
1:C:21:PHE:CB	4:C:5476:MPD:H53	2.27	0.50
1:J:130:PRO:HB3	1:J:268:MET:CE	2.41	0.50
1:A:399:LEU:CA	1:A:400:PRO:C	2.78	0.50
1:B:124:VAL:HG13	1:B:274:LEU:HD21	1.94	0.50
1:E:124:VAL:HG13	1:E:274:LEU:HD21	1.94	0.50
1:F:335:SER:HB2	1:F:392:MET:O	2.12	0.50
1:L:16:PHE:HB2	1:L:84:THR:HB	1.92	0.50
1:C:396:LEU:O	1:C:400:PRO:HG2	2.11	0.50
1:E:396:LEU:O	1:E:400:PRO:HG2	2.11	0.50
1:I:403:GLU:C	1:I:405:LYS:H	2.14	0.50
1:E:88:ARG:HH11	4:E:5480:MPD:HM3	1.75	0.50
1:I:28:GLU:OE1	1:I:88:ARG:NH1	2.45	0.50
1:H:192:ARG:HD3	1:H:219:ASN:HD22	1.77	0.50
1:D:124:VAL:HG13	1:D:274:LEU:HD21	1.94	0.50
1:D:335:SER:HB2	1:D:392:MET:O	2.12	0.50
1:L:124:VAL:HG13	1:L:274:LEU:HD21	1.94	0.50
1:I:124:VAL:HG13	1:I:274:LEU:HD21	1.94	0.50
1:A:16:PHE:HB2	1:A:84:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LEU:O	1:B:400:PRO:HG2	2.12	0.50
1:C:458:HIS:HE1	1:I:456:THR:O	1.95	0.50
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.77	0.50
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.77	0.50
1:C:180:PHE:HB2	1:D:29:GLN:HB3	1.92	0.50
1:A:130:PRO:HB3	1:A:268:MET:CE	2.41	0.50
1:H:124:VAL:HG13	1:H:274:LEU:HD21	1.94	0.50
1:J:335:SER:HB2	1:J:392:MET:O	2.12	0.50
1:K:124:VAL:HG13	1:K:274:LEU:HD21	1.94	0.50
1:A:124:VAL:HG13	1:A:274:LEU:HD21	1.94	0.50
1:D:255:PHE:HB3	1:D:363:PRO:HB2	1.94	0.50
1:D:311:LEU:HD22	1:D:369:LEU:HB3	1.93	0.50
1:L:335:SER:HB2	1:L:392:MET:O	2.12	0.50
1:F:82:ASP:N	4:F:5479:MPD:O2	2.40	0.50
1:C:403:GLU:C	1:C:405:LYS:H	2.14	0.50
1:E:399:LEU:CA	1:E:400:PRO:C	2.78	0.50
1:D:399:LEU:CA	1:D:400:PRO:C	2.78	0.50
1:F:22:THR:CA	4:F:5482:MPD:H11	2.42	0.50
1:G:29:GLN:HB3	1:H:180:PHE:HB2	1.94	0.50
1:A:255:PHE:HB3	1:A:363:PRO:HB2	1.94	0.50
1:H:255:PHE:HB3	1:H:363:PRO:HB2	1.94	0.50
1:K:84:THR:CG2	4:K:5493:MPD:H32	2.42	0.50
1:J:396:LEU:O	1:J:400:PRO:HG2	2.12	0.50
1:D:396:LEU:O	1:D:400:PRO:HG2	2.12	0.50
1:B:22:THR:CA	4:B:5474:MPD:H11	2.42	0.50
1:L:22:THR:CA	4:L:5494:MPD:H11	2.42	0.50
1:H:248:ARG:HG3	1:H:248:ARG:HH21	1.75	0.50
1:E:256:MET:HG3	1:K:466:TYR:HA	1.94	0.50
1:K:255:PHE:HB3	1:K:363:PRO:HB2	1.94	0.50
1:H:311:LEU:HD22	1:H:369:LEU:HB3	1.93	0.50
1:G:335:SER:HB2	1:G:392:MET:O	2.12	0.50
4:F:5479:MPD:O4	4:F:5479:MPD:CM	2.60	0.50
4:K:5493:MPD:CM	4:K:5493:MPD:O4	2.60	0.50
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.77	0.50
1:H:130:PRO:HB3	1:H:268:MET:CE	2.41	0.50
1:H:335:SER:HB2	1:H:392:MET:O	2.12	0.50
1:B:255:PHE:HB3	1:B:363:PRO:HB2	1.94	0.50
1:J:311:LEU:HD22	1:J:369:LEU:HB3	1.93	0.50
1:G:399:LEU:CA	1:G:400:PRO:C	2.78	0.49
1:I:396:LEU:O	1:I:400:PRO:HG2	2.11	0.49
1:F:21:PHE:HA	4:F:5482:MPD:C3	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ARG:HH21	1:D:248:ARG:HG3	1.75	0.49
1:L:255:PHE:HB3	1:L:363:PRO:HB2	1.94	0.49
1:F:255:PHE:HB3	1:F:363:PRO:HB2	1.94	0.49
1:B:335:SER:HB2	1:B:392:MET:O	2.12	0.49
1:F:80:PHE:CD1	4:F:5479:MPD:H52	2.46	0.49
1:G:80:PHE:HD1	4:G:5485:MPD:C5	2.25	0.49
1:C:80:PHE:HD1	4:C:5473:MPD:C5	2.13	0.49
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.74	0.49
1:H:396:LEU:O	1:H:400:PRO:HG2	2.11	0.49
1:E:22:THR:CA	4:E:5480:MPD:H11	2.42	0.49
1:I:22:THR:CA	4:I:5488:MPD:H11	2.42	0.49
1:D:28:GLU:OE1	1:D:88:ARG:NH1	2.45	0.49
1:C:21:PHE:HA	4:C:5476:MPD:C3	2.36	0.49
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.77	0.49
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.77	0.49
1:A:335:SER:HB2	1:A:392:MET:O	2.12	0.49
1:J:124:VAL:HG13	1:J:274:LEU:HD21	1.94	0.49
1:G:130:PRO:HB3	1:G:268:MET:CE	2.42	0.49
1:L:84:THR:CB	4:L:5483:MPD:H52	2.38	0.49
1:H:84:THR:HG21	4:H:5487:MPD:C3	2.41	0.49
1:B:80:PHE:CD1	4:B:5471:MPD:H52	2.46	0.49
4:D:5475:MPD:CM	4:D:5475:MPD:O4	2.60	0.49
1:C:399:LEU:CA	1:C:400:PRO:C	2.78	0.49
1:F:396:LEU:O	1:F:400:PRO:HG2	2.11	0.49
1:K:28:GLU:OE1	1:K:88:ARG:NH1	2.45	0.49
1:C:130:PRO:HB3	1:C:268:MET:CE	2.41	0.49
1:G:124:VAL:HG13	1:G:274:LEU:HD21	1.94	0.49
1:G:311:LEU:HD22	1:G:369:LEU:HB3	1.93	0.49
1:I:255:PHE:HB3	1:I:363:PRO:HB2	1.94	0.49
1:J:255:PHE:HB3	1:J:363:PRO:HB2	1.94	0.49
1:E:255:PHE:HB3	1:E:363:PRO:HB2	1.94	0.49
4:B:5471:MPD:O4	4:B:5471:MPD:CM	2.60	0.49
1:A:84:THR:CB	4:A:5481:MPD:H52	2.38	0.49
1:A:403:GLU:C	1:A:405:LYS:H	2.14	0.49
1:D:403:GLU:C	1:D:405:LYS:H	2.14	0.49
1:K:396:LEU:O	1:K:400:PRO:HG2	2.11	0.49
1:E:88:ARG:HD2	5:E:1252:HOH:O	2.13	0.49
1:J:21:PHE:HA	4:J:5490:MPD:C3	2.36	0.49
1:G:384:ASN:ND2	1:G:384:ASN:N	2.60	0.49
1:B:180:PHE:O	1:C:29:GLN:HA	2.13	0.49
1:F:130:PRO:HB3	1:F:268:MET:CE	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:PRO:HB3	1:I:268:MET:CE	2.41	0.49
1:I:335:SER:HB2	1:I:392:MET:O	2.12	0.49
1:B:130:PRO:HB3	1:B:268:MET:CE	2.41	0.49
1:K:130:PRO:HB3	1:K:268:MET:CE	2.42	0.49
1:K:84:THR:CB	4:K:5493:MPD:H52	2.40	0.49
1:L:403:GLU:C	1:L:405:LYS:H	2.14	0.49
1:E:403:GLU:C	1:E:405:LYS:H	2.14	0.49
1:A:88:ARG:HD2	5:A:5553:HOH:O	2.13	0.49
1:I:248:ARG:CG	1:I:248:ARG:NH2	2.67	0.49
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.77	0.49
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.77	0.49
1:C:454:ARG:O	1:I:320:LYS:HG3	2.11	0.49
1:K:335:SER:HB2	1:K:392:MET:O	2.12	0.49
1:C:335:SER:HB2	1:C:392:MET:O	2.12	0.49
1:E:130:PRO:HB3	1:E:268:MET:CE	2.42	0.49
1:H:403:GLU:C	1:H:405:LYS:H	2.14	0.49
1:A:396:LEU:O	1:A:400:PRO:HG2	2.11	0.49
1:A:22:THR:CA	4:A:5472:MPD:H11	2.42	0.49
1:L:28:GLU:OE1	1:L:88:ARG:NH1	2.45	0.49
1:H:399:LEU:CA	1:H:400:PRO:C	2.78	0.49
1:G:88:ARG:HD2	5:G:5566:HOH:O	2.13	0.49
1:K:22:THR:CA	4:K:5492:MPD:H11	2.42	0.49
1:H:22:THR:CA	4:H:5486:MPD:H11	2.42	0.49
1:F:456:THR:O	1:L:458:HIS:HE1	1.96	0.49
1:H:82:ASP:HB2	4:H:5487:MPD:C3	2.39	0.49
1:L:396:LEU:O	1:L:400:PRO:HG2	2.11	0.49
1:C:22:THR:CA	4:C:5476:MPD:H11	2.42	0.49
1:H:21:PHE:HA	4:H:5486:MPD:C3	2.36	0.49
1:L:88:ARG:HD2	5:L:3296:HOH:O	2.13	0.49
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.77	0.49
1:E:181:PRO:HD3	1:F:29:GLN:OE1	2.12	0.49
1:G:181:PRO:HD3	1:L:29:GLN:OE1	2.13	0.49
1:F:364:ALA:HA	1:L:468:VAL:HG13	1.95	0.49
1:E:335:SER:HB2	1:E:392:MET:O	2.12	0.49
1:F:124:VAL:HG13	1:F:274:LEU:HD21	1.94	0.49
1:D:22:THR:CA	4:D:5478:MPD:H11	2.42	0.49
1:G:181:PRO:HG3	5:L:3356:HOH:O	2.11	0.49
1:I:88:ARG:HD2	5:I:5579:HOH:O	2.13	0.49
1:F:88:ARG:HD2	5:F:5568:HOH:O	2.13	0.49
1:E:248:ARG:HH21	1:E:248:ARG:HG3	1.75	0.49
1:I:384:ASN:N	1:I:384:ASN:ND2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ARG:O	1:G:320:LYS:HG3	2.12	0.49
1:C:124:VAL:HG13	1:C:274:LEU:HD21	1.94	0.49
1:E:466:TYR:HA	1:K:256:MET:HG3	1.94	0.49
1:G:22:THR:CA	4:G:5484:MPD:H11	2.42	0.48
1:K:88:ARG:HD2	5:K:3004:HOH:O	2.13	0.48
1:L:248:ARG:HH21	1:L:248:ARG:HG3	1.75	0.48
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.77	0.48
1:A:384:ASN:N	1:A:384:ASN:ND2	2.60	0.48
1:C:387:HIS:HA	1:C:388:PRO:HD2	1.73	0.48
1:B:396:LEU:HB2	1:B:397:TYR:H	1.36	0.48
1:K:21:PHE:CB	4:K:5492:MPD:H53	2.27	0.48
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.77	0.48
1:C:384:ASN:ND2	1:C:384:ASN:N	2.60	0.48
1:B:306:LYS:HE2	5:B:5572:HOH:O	2.13	0.48
1:J:306:LYS:HE2	5:J:2729:HOH:O	2.13	0.48
1:D:396:LEU:HB2	1:D:397:TYR:H	1.36	0.48
1:D:21:PHE:HA	4:D:5478:MPD:C3	2.36	0.48
1:D:22:THR:HG22	1:D:23:ASP:O	2.14	0.48
1:J:22:THR:CA	4:J:5490:MPD:H11	2.42	0.48
1:J:88:ARG:HD2	5:J:2712:HOH:O	2.13	0.48
1:H:88:ARG:HD2	5:H:5577:HOH:O	2.13	0.48
1:J:384:ASN:ND2	1:J:384:ASN:N	2.60	0.48
1:G:306:LYS:HE2	5:G:5583:HOH:O	2.13	0.48
1:C:255:PHE:HB3	1:C:363:PRO:HB2	1.94	0.48
1:L:84:THR:HG21	4:L:5483:MPD:H32	1.96	0.48
4:K:5493:MPD:CM	1:L:193:SER:CB	2.84	0.48
1:D:84:THR:CB	4:D:5475:MPD:H52	2.41	0.48
1:J:399:LEU:CA	1:J:400:PRO:C	2.78	0.48
1:G:22:THR:HG22	1:G:23:ASP:O	2.14	0.48
1:E:22:THR:HG22	1:E:23:ASP:O	2.14	0.48
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.77	0.48
1:J:398:ASP:OD1	1:J:399:LEU:HD23	2.14	0.48
1:G:21:PHE:CB	4:G:5484:MPD:H53	2.27	0.48
1:I:96:THR:HG1	1:I:98:GLN:HB2	1.76	0.48
1:E:179:TYR:CD2	1:F:53:SER:HB2	2.49	0.48
1:K:329:PRO:O	1:K:342:SER:HB3	2.14	0.48
4:I:5489:MPD:CM	4:I:5489:MPD:O4	2.60	0.48
1:I:22:THR:HG22	1:I:23:ASP:O	2.14	0.48
1:G:255:PHE:HB3	1:G:363:PRO:HB2	1.94	0.48
4:G:5485:MPD:CM	1:H:193:SER:CB	2.84	0.48
1:L:398:ASP:OD1	1:L:399:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:ASP:OD1	1:E:399:LEU:HD23	2.14	0.48
1:K:22:THR:HG22	1:K:23:ASP:O	2.14	0.48
1:C:22:THR:HG22	1:C:23:ASP:O	2.14	0.48
1:F:458:HIS:HE1	1:L:456:THR:O	1.96	0.48
1:B:329:PRO:O	1:B:342:SER:HB3	2.14	0.48
1:E:306:LYS:HE2	5:E:1269:HOH:O	2.13	0.48
1:C:329:PRO:O	1:C:342:SER:HB3	2.14	0.48
1:J:329:PRO:O	1:J:342:SER:HB3	2.14	0.48
1:B:22:THR:HG22	1:B:23:ASP:O	2.14	0.48
1:H:22:THR:HG22	1:H:23:ASP:O	2.14	0.48
1:A:28:GLU:OE1	1:A:88:ARG:NH1	2.45	0.48
1:J:29:GLN:HB3	1:K:180:PHE:CB	2.44	0.48
1:A:329:PRO:O	1:A:342:SER:HB3	2.14	0.48
1:A:398:ASP:OD1	1:A:399:LEU:HD23	2.14	0.48
1:A:180:PHE:O	1:B:29:GLN:HA	2.13	0.48
1:H:30:HIS:H	1:I:180:PHE:HB3	1.78	0.48
1:F:364:ALA:HA	1:L:468:VAL:CG1	2.44	0.48
1:H:329:PRO:O	1:H:342:SER:HB3	2.14	0.48
1:L:329:PRO:O	1:L:342:SER:HB3	2.14	0.48
1:F:329:PRO:O	1:F:342:SER:HB3	2.14	0.48
1:D:329:PRO:O	1:D:342:SER:HB3	2.14	0.48
1:J:84:THR:CB	4:J:5491:MPD:H52	2.37	0.48
4:L:5483:MPD:CM	4:L:5483:MPD:O4	2.60	0.48
1:L:84:THR:HG21	4:L:5483:MPD:C3	2.43	0.48
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.74	0.48
1:C:398:ASP:OD1	1:C:399:LEU:HD23	2.14	0.48
1:A:22:THR:HG22	1:A:23:ASP:O	2.14	0.48
4:K:5493:MPD:O4	1:L:193:SER:OG	2.28	0.47
1:B:396:LEU:H	1:B:396:LEU:HG	1.46	0.47
1:F:22:THR:HG22	1:F:23:ASP:O	2.14	0.47
1:C:88:ARG:HD2	5:C:5555:HOH:O	2.13	0.47
1:A:181:PRO:HD3	1:B:29:GLN:OE1	2.14	0.47
1:K:130:PRO:HB3	1:K:268:MET:HE3	1.96	0.47
1:K:328:ALA:HA	1:K:329:PRO:HD3	1.73	0.47
1:L:306:LYS:HE2	5:L:3313:HOH:O	2.13	0.47
1:G:398:ASP:OD1	1:G:399:LEU:HD23	2.14	0.47
1:D:88:ARG:HD2	5:D:960:HOH:O	2.13	0.47
1:E:384:ASN:N	1:E:384:ASN:ND2	2.60	0.47
1:J:124:VAL:HG13	1:J:274:LEU:CD2	2.45	0.47
1:F:306:LYS:HE2	5:F:5585:HOH:O	2.13	0.47
1:J:82:ASP:O	4:J:5491:MPD:H32	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ASP:OD1	1:B:399:LEU:HD23	2.14	0.47
1:E:232:ALA:HB1	1:E:367:PRO:HB2	1.97	0.47
1:D:384:ASN:N	1:D:384:ASN:ND2	2.60	0.47
1:D:124:VAL:HG13	1:D:274:LEU:CD2	2.45	0.47
1:G:124:VAL:HG13	1:G:274:LEU:CD2	2.45	0.47
1:K:271:HIS:CD2	1:K:357:GLU:HG3	2.50	0.47
1:K:306:LYS:HE2	5:K:3021:HOH:O	2.14	0.47
1:E:329:PRO:O	1:E:342:SER:HB3	2.14	0.47
1:B:21:PHE:HA	4:B:5474:MPD:C3	2.36	0.47
1:J:22:THR:HG22	1:J:23:ASP:O	2.13	0.47
1:I:124:VAL:HG13	1:I:274:LEU:CD2	2.45	0.47
1:F:124:VAL:HG13	1:F:274:LEU:CD2	2.45	0.47
1:G:329:PRO:O	1:G:342:SER:HB3	2.14	0.47
1:D:100:TYR:CE2	1:D:102:ARG:HB2	2.50	0.47
1:G:271:HIS:CD2	1:G:357:GLU:HG3	2.50	0.47
1:I:271:HIS:CD2	1:I:357:GLU:HG3	2.50	0.47
1:E:193:SER:CB	4:F:5479:MPD:CM	2.84	0.47
1:C:396:LEU:HB2	1:C:397:TYR:H	1.36	0.47
1:L:21:PHE:CB	4:L:5494:MPD:H53	2.27	0.47
1:G:232:ALA:HB1	1:G:367:PRO:HB2	1.97	0.47
1:E:320:LYS:HG3	1:K:454:ARG:O	2.13	0.47
1:C:320:LYS:HG3	1:I:454:ARG:O	2.15	0.47
1:E:271:HIS:CD2	1:E:357:GLU:HG3	2.50	0.47
1:K:465:TYR:O	1:K:468:VAL:HB	2.15	0.47
1:C:465:TYR:O	1:C:468:VAL:HB	2.15	0.47
1:F:21:PHE:CB	4:F:5482:MPD:H53	2.27	0.47
1:H:28:GLU:OE1	1:H:88:ARG:NH1	2.45	0.47
1:J:232:ALA:HB1	1:J:367:PRO:HB2	1.97	0.47
1:K:124:VAL:HG13	1:K:274:LEU:CD2	2.45	0.47
1:A:124:VAL:HG13	1:A:274:LEU:CD2	2.45	0.47
1:H:306:LYS:HE2	5:H:5594:HOH:O	2.13	0.47
1:A:271:HIS:CD2	1:A:357:GLU:HG3	2.50	0.47
1:B:271:HIS:CD2	1:B:357:GLU:HG3	2.50	0.47
1:L:80:PHE:CG	4:L:5483:MPD:C1	2.97	0.47
1:A:21:PHE:CB	4:A:5472:MPD:H53	2.27	0.47
1:L:22:THR:HG22	1:L:23:ASP:O	2.14	0.47
1:B:232:ALA:HB1	1:B:367:PRO:HB2	1.97	0.47
1:H:232:ALA:HB1	1:H:367:PRO:HB2	1.97	0.47
1:D:232:ALA:HB1	1:D:367:PRO:HB2	1.97	0.47
1:C:456:THR:O	1:I:458:HIS:HE1	1.98	0.47
1:J:248:ARG:NH2	1:J:248:ARG:CG	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:ARG:HG3	1:F:248:ARG:HH21	1.75	0.47
1:E:454:ARG:O	1:K:320:LYS:HG3	2.13	0.47
1:C:124:VAL:HG13	1:C:274:LEU:CD2	2.45	0.47
1:D:465:TYR:O	1:D:468:VAL:HB	2.15	0.47
1:D:306:LYS:HE2	5:D:977:HOH:O	2.14	0.47
1:J:272:MET:HE1	1:J:358:VAL:HG21	1.97	0.47
1:C:100:TYR:CE2	1:C:102:ARG:HB2	2.50	0.47
1:A:100:TYR:CE2	1:A:102:ARG:HB2	2.50	0.47
1:A:193:SER:CB	4:B:5471:MPD:CM	2.84	0.47
1:G:80:PHE:CA	4:G:5485:MPD:H12	2.42	0.47
1:H:398:ASP:OD1	1:H:399:LEU:HD23	2.14	0.47
1:B:28:GLU:OE1	1:B:88:ARG:NH1	2.45	0.47
1:L:21:PHE:HA	4:L:5494:MPD:C3	2.36	0.47
1:C:232:ALA:HB1	1:C:367:PRO:HB2	1.97	0.47
1:F:232:ALA:HB1	1:F:367:PRO:HB2	1.97	0.47
1:C:455:MET:HG2	1:I:323:VAL:HG11	1.97	0.47
1:A:306:LYS:HE2	5:A:5570:HOH:O	2.13	0.47
1:L:100:TYR:CE2	1:L:102:ARG:HB2	2.50	0.47
1:H:465:TYR:O	1:H:468:VAL:HB	2.15	0.47
1:L:272:MET:HE1	1:L:358:VAL:HG21	1.97	0.47
1:F:398:ASP:OD1	1:F:399:LEU:HD23	2.14	0.47
1:G:28:GLU:OE1	1:G:88:ARG:NH1	2.45	0.47
1:E:21:PHE:CB	4:E:5480:MPD:H53	2.27	0.47
1:B:88:ARG:HD2	5:B:5555:HOH:O	2.13	0.47
1:K:295:LEU:O	1:K:388:PRO:HG2	2.15	0.47
1:E:124:VAL:HG13	1:E:274:LEU:CD2	2.45	0.47
1:H:328:ALA:HA	1:H:329:PRO:HD3	1.73	0.47
1:L:271:HIS:CD2	1:L:357:GLU:HG3	2.50	0.47
1:I:306:LYS:HE2	5:I:5596:HOH:O	2.13	0.47
1:F:100:TYR:CE2	1:F:102:ARG:HB2	2.50	0.47
1:G:465:TYR:O	1:G:468:VAL:HB	2.15	0.47
1:I:329:PRO:O	1:I:342:SER:HB3	2.14	0.47
1:G:100:TYR:CE2	1:G:102:ARG:HB2	2.50	0.47
1:J:84:THR:HG21	4:J:5491:MPD:C3	2.45	0.47
1:C:193:SER:OG	4:D:5475:MPD:O4	2.28	0.47
1:I:398:ASP:OD1	1:I:399:LEU:HD23	2.14	0.47
1:E:28:GLU:OE1	1:E:88:ARG:NH1	2.45	0.47
1:K:368:TYR:OH	4:K:5492:MPD:O2	2.27	0.47
1:J:28:GLU:OE1	1:J:88:ARG:NH1	2.45	0.47
1:A:320:LYS:HG3	1:G:454:ARG:O	2.15	0.47
1:L:465:TYR:O	1:L:468:VAL:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:TYR:CE2	1:B:102:ARG:HB2	2.50	0.47
1:A:31:VAL:HG23	1:F:210:HIS:HB3	1.97	0.47
1:C:256:MET:HG3	1:I:466:TYR:HA	1.97	0.47
1:D:80:PHE:HD1	4:D:5475:MPD:H52	1.80	0.46
1:D:398:ASP:OD1	1:D:399:LEU:HD23	2.14	0.46
1:K:398:ASP:OD1	1:K:399:LEU:HD23	2.14	0.46
1:L:384:ASN:ND2	1:L:384:ASN:N	2.60	0.46
1:K:41:GLU:OE2	1:K:45:GLU:OE2	2.34	0.46
1:C:306:LYS:HE2	5:C:5572:HOH:O	2.13	0.46
1:F:271:HIS:CD2	1:F:357:GLU:HG3	2.50	0.46
1:A:465:TYR:O	1:A:468:VAL:HB	2.15	0.46
1:A:41:GLU:OE2	1:A:45:GLU:OE2	2.34	0.46
1:D:466:TYR:HA	1:J:256:MET:HG3	1.97	0.46
1:J:80:PHE:CG	4:J:5491:MPD:H53	2.50	0.46
1:K:232:ALA:HB1	1:K:367:PRO:HB2	1.97	0.46
5:G:5622:HOH:O	1:H:181:PRO:HG3	2.13	0.46
1:A:181:PRO:HG3	5:B:5611:HOH:O	2.14	0.46
1:H:130:PRO:HB3	1:H:268:MET:HE3	1.96	0.46
1:J:100:TYR:CE2	1:J:102:ARG:HB2	2.50	0.46
1:E:100:TYR:CE2	1:E:102:ARG:HB2	2.50	0.46
1:L:41:GLU:OE2	1:L:45:GLU:OE2	2.34	0.46
1:K:80:PHE:CD1	4:K:5493:MPD:H52	2.46	0.46
1:G:368:TYR:OH	4:G:5484:MPD:O2	2.26	0.46
1:K:248:ARG:HG3	1:K:248:ARG:HH21	1.75	0.46
1:F:465:TYR:O	1:F:468:VAL:HB	2.15	0.46
1:A:272:MET:HE1	1:A:358:VAL:HG21	1.98	0.46
1:I:465:TYR:O	1:I:468:VAL:HB	2.15	0.46
4:I:5489:MPD:CM	1:J:193:SER:CB	2.84	0.46
1:E:396:LEU:H	1:E:396:LEU:HG	1.46	0.46
1:H:295:LEU:O	1:H:388:PRO:HG2	2.15	0.46
1:B:295:LEU:O	1:B:388:PRO:HG2	2.15	0.46
1:L:328:ALA:HA	1:L:329:PRO:HD3	1.73	0.46
1:J:465:TYR:O	1:J:468:VAL:HB	2.15	0.46
1:D:41:GLU:OE2	1:D:45:GLU:OE2	2.34	0.46
1:E:41:GLU:OE2	1:E:45:GLU:OE2	2.34	0.46
1:I:41:GLU:OE2	1:I:45:GLU:OE2	2.34	0.46
1:H:271:HIS:CD2	1:H:357:GLU:HG3	2.50	0.46
1:H:41:GLU:OE2	1:H:45:GLU:OE2	2.34	0.46
1:B:465:TYR:O	1:B:468:VAL:HB	2.15	0.46
1:B:41:GLU:OE2	1:B:45:GLU:OE2	2.34	0.46
1:C:271:HIS:CD2	1:C:357:GLU:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:271:HIS:CD2	1:J:357:GLU:HG3	2.50	0.46
1:A:21:PHE:HA	4:A:5472:MPD:C3	2.36	0.46
1:L:232:ALA:HB1	1:L:367:PRO:HB2	1.97	0.46
1:B:130:PRO:HB3	1:B:268:MET:HE3	1.98	0.46
1:I:3:GLU:O	1:I:7:THR:HG23	2.16	0.46
1:E:128:PRO:HA	1:E:269:HIS:O	2.16	0.46
1:B:124:VAL:HG13	1:B:274:LEU:CD2	2.44	0.46
1:E:465:TYR:O	1:E:468:VAL:HB	2.15	0.46
1:H:100:TYR:CE2	1:H:102:ARG:HB2	2.50	0.46
1:G:41:GLU:OE2	1:G:45:GLU:OE2	2.34	0.46
1:D:272:MET:HE1	1:D:358:VAL:HG21	1.97	0.46
1:C:88:ARG:NE	4:C:5476:MPD:HM1	2.30	0.46
1:A:387:HIS:HA	1:A:388:PRO:HD2	1.73	0.46
1:F:454:ARG:O	1:L:320:LYS:HG3	2.16	0.46
1:A:128:PRO:HA	1:A:269:HIS:O	2.16	0.46
1:I:100:TYR:CE2	1:I:102:ARG:HB2	2.50	0.46
1:J:41:GLU:OE2	1:J:45:GLU:OE2	2.34	0.46
1:G:3:GLU:O	1:G:7:THR:HG23	2.16	0.46
1:D:271:HIS:CD2	1:D:357:GLU:HG3	2.50	0.46
1:I:21:PHE:CB	4:I:5488:MPD:H53	2.27	0.46
1:A:232:ALA:HB1	1:A:367:PRO:HB2	1.97	0.46
1:J:295:LEU:O	1:J:388:PRO:HG2	2.15	0.46
1:B:320:LYS:HG3	1:H:454:ARG:O	2.16	0.46
1:H:128:PRO:HA	1:H:269:HIS:O	2.16	0.46
1:H:124:VAL:HG13	1:H:274:LEU:CD2	2.45	0.46
1:F:328:ALA:HA	1:F:329:PRO:HD3	1.73	0.46
1:F:272:MET:HE1	1:F:358:VAL:HG21	1.98	0.46
1:J:84:THR:CG2	4:J:5491:MPD:C5	2.48	0.46
1:B:88:ARG:NE	4:B:5474:MPD:HM1	2.30	0.46
1:F:384:ASN:N	1:F:384:ASN:ND2	2.60	0.46
1:E:295:LEU:O	1:E:388:PRO:HG2	2.15	0.46
1:F:254:THR:HB	1:L:466:TYR:CE1	2.51	0.46
1:D:3:GLU:O	1:D:7:THR:HG23	2.16	0.46
1:K:100:TYR:CE2	1:K:102:ARG:HB2	2.50	0.46
1:B:80:PHE:CB	4:B:5471:MPD:C1	2.65	0.46
1:G:396:LEU:HB2	1:G:397:TYR:H	1.36	0.46
1:I:232:ALA:HB1	1:I:367:PRO:HB2	1.97	0.46
1:J:128:PRO:HA	1:J:269:HIS:O	2.16	0.46
1:C:128:PRO:HA	1:C:269:HIS:O	2.16	0.46
1:G:128:PRO:HA	1:G:269:HIS:O	2.16	0.46
1:L:3:GLU:O	1:L:7:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:GLU:O	1:F:7:THR:HG23	2.16	0.46
1:G:80:PHE:HD1	4:G:5485:MPD:H52	1.81	0.45
4:A:5481:MPD:CM	4:A:5481:MPD:O4	2.60	0.45
1:B:313:ASN:HD21	1:B:360:PHE:HD2	1.65	0.45
5:J:2772:HOH:O	1:K:181:PRO:HG3	2.15	0.45
1:L:124:VAL:HG13	1:L:274:LEU:CD2	2.45	0.45
1:J:3:GLU:O	1:J:7:THR:HG23	2.16	0.45
1:A:3:GLU:O	1:A:7:THR:HG23	2.16	0.45
1:F:84:THR:CG2	4:F:5479:MPD:H32	2.46	0.45
1:D:80:PHE:CA	4:D:5475:MPD:H12	2.45	0.45
1:G:313:ASN:HD21	1:G:360:PHE:HD2	1.65	0.45
1:F:313:ASN:HD21	1:F:360:PHE:HD2	1.65	0.45
1:A:396:LEU:HG	1:A:396:LEU:H	1.46	0.45
1:E:3:GLU:O	1:E:7:THR:HG23	2.16	0.45
1:C:41:GLU:OE2	1:C:45:GLU:OE2	2.34	0.45
1:A:466:TYR:HA	1:G:256:MET:HG3	1.97	0.45
1:J:84:THR:CG2	4:J:5491:MPD:C4	2.88	0.45
1:J:21:PHE:CB	4:J:5490:MPD:H53	2.27	0.45
1:G:29:GLN:HB3	1:H:180:PHE:CB	2.46	0.45
1:D:180:PHE:O	1:E:29:GLN:HA	2.16	0.45
1:B:128:PRO:HA	1:B:269:HIS:O	2.16	0.45
1:K:128:PRO:HA	1:K:269:HIS:O	2.16	0.45
1:K:231:LYS:HD2	1:K:231:LYS:HA	1.74	0.45
1:F:41:GLU:OE2	1:F:45:GLU:OE2	2.34	0.45
1:C:210:HIS:HB3	1:D:31:VAL:HG23	1.99	0.45
1:G:80:PHE:CD1	4:G:5485:MPD:H52	2.51	0.45
1:J:313:ASN:HD21	1:J:360:PHE:HD2	1.65	0.45
1:C:28:GLU:OE1	1:C:88:ARG:NH1	2.45	0.45
1:E:180:PHE:O	1:F:29:GLN:HA	2.16	0.45
1:C:3:GLU:O	1:C:7:THR:HG23	2.16	0.45
1:K:313:ASN:HD21	1:K:360:PHE:HD2	1.65	0.45
1:K:248:ARG:NH2	1:K:248:ARG:CG	2.66	0.45
1:D:128:PRO:HA	1:D:269:HIS:O	2.16	0.45
1:I:128:PRO:HA	1:I:269:HIS:O	2.16	0.45
1:I:328:ALA:HA	1:I:329:PRO:HD3	1.73	0.45
1:L:295:LEU:O	1:L:388:PRO:HG2	2.15	0.45
1:H:170:GLY:HA2	1:H:172:ARG:HH22	1.81	0.45
1:B:323:VAL:HG11	1:H:455:MET:HG2	1.98	0.45
1:H:3:GLU:O	1:H:7:THR:HG23	2.16	0.45
1:I:80:PHE:CG	4:I:5489:MPD:H53	2.50	0.45
1:L:180:PHE:O	1:L:181:PRO:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:GLU:O	1:K:7:THR:HG23	2.16	0.45
1:C:80:PHE:CG	4:C:5473:MPD:H12	2.48	0.45
1:H:21:PHE:CB	4:H:5486:MPD:H53	2.27	0.45
1:J:31:VAL:HG23	1:K:210:HIS:HB3	1.98	0.45
1:J:34:PRO:HG2	1:K:206:VAL:O	2.17	0.45
1:H:84:THR:CB	4:H:5487:MPD:H52	2.45	0.45
1:E:84:THR:CB	4:E:5477:MPD:H52	2.41	0.45
1:C:340:SER:HB3	1:C:396:LEU:HB3	1.99	0.45
1:K:340:SER:HB3	1:K:396:LEU:HB3	1.99	0.45
1:F:28:GLU:OE1	1:F:88:ARG:NH1	2.45	0.45
1:K:21:PHE:HA	4:K:5492:MPD:C3	2.36	0.45
1:A:235:ILE:HA	1:A:235:ILE:HD13	1.82	0.45
1:A:458:HIS:CD2	1:A:459:PRO:HD2	2.52	0.45
1:B:387:HIS:HA	1:B:388:PRO:HD2	1.73	0.45
1:I:170:GLY:HA2	1:I:172:ARG:HH22	1.81	0.45
1:A:180:PHE:HB2	1:B:29:GLN:HB3	1.99	0.45
1:F:128:PRO:HA	1:F:269:HIS:O	2.16	0.45
1:B:454:ARG:O	1:H:320:LYS:HG3	2.17	0.45
1:K:84:THR:HG21	4:K:5493:MPD:H32	1.99	0.45
1:E:340:SER:HB3	1:E:396:LEU:HB3	1.99	0.45
1:G:340:SER:HB3	1:G:396:LEU:HB3	1.99	0.45
1:I:340:SER:HB3	1:I:396:LEU:HB3	1.99	0.45
1:B:340:SER:HB3	1:B:396:LEU:HB3	1.99	0.45
1:K:458:HIS:CD2	1:K:459:PRO:HD2	2.52	0.45
1:L:128:PRO:HA	1:L:269:HIS:O	2.16	0.45
1:D:65:MET:HA	1:D:94:PRO:HG3	1.99	0.45
1:I:276:LYS:HG2	1:I:277:ASN:ND2	2.33	0.45
1:A:340:SER:HB3	1:A:396:LEU:HB3	1.99	0.44
1:D:88:ARG:NE	4:D:5478:MPD:HM1	2.30	0.44
1:A:295:LEU:O	1:A:388:PRO:HG2	2.15	0.44
1:E:180:PHE:O	1:E:181:PRO:C	2.54	0.44
1:E:181:PRO:HG3	5:F:5624:HOH:O	2.18	0.44
1:F:25:LYS:NZ	5:F:5746:HOH:O	2.44	0.44
1:L:276:LYS:HG2	1:L:277:ASN:ND2	2.32	0.44
1:A:276:LYS:HG2	1:A:277:ASN:ND2	2.33	0.44
1:D:276:LYS:HG2	1:D:277:ASN:ND2	2.33	0.44
1:L:313:ASN:HD21	1:L:360:PHE:HD2	1.65	0.44
1:E:458:HIS:CD2	1:E:459:PRO:HD2	2.52	0.44
1:D:180:PHE:O	1:D:181:PRO:C	2.54	0.44
1:C:328:ALA:HA	1:C:329:PRO:HD3	1.73	0.44
1:G:276:LYS:HG2	1:G:277:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:O	1:B:7:THR:HG23	2.16	0.44
1:E:313:ASN:HD21	1:E:360:PHE:HD2	1.65	0.44
1:J:340:SER:HB3	1:J:396:LEU:HB3	1.99	0.44
1:J:88:ARG:NE	4:J:5490:MPD:HM1	2.30	0.44
1:D:458:HIS:CD2	1:D:459:PRO:HD2	2.52	0.44
1:D:295:LEU:O	1:D:388:PRO:HG2	2.15	0.44
1:D:320:LYS:HG3	1:J:454:ARG:O	2.18	0.44
1:A:65:MET:HA	1:A:94:PRO:HG3	2.00	0.44
1:C:80:PHE:CG	4:C:5473:MPD:H53	2.51	0.44
1:I:295:LEU:O	1:I:388:PRO:HG2	2.15	0.44
1:G:180:PHE:O	1:G:181:PRO:C	2.54	0.44
1:A:328:ALA:HA	1:A:329:PRO:HD3	1.73	0.44
1:E:215:THR:O	1:E:216:ALA:HB3	2.18	0.44
1:K:65:MET:HA	1:K:94:PRO:HG3	2.00	0.44
1:A:313:ASN:HD21	1:A:360:PHE:HD2	1.65	0.44
1:F:88:ARG:NE	4:F:5482:MPD:HM1	2.30	0.44
1:H:458:HIS:CD2	1:H:459:PRO:HD2	2.52	0.44
1:B:458:HIS:CD2	1:B:459:PRO:HD2	2.52	0.44
1:B:170:GLY:HA2	1:B:172:ARG:HH22	1.81	0.44
1:A:215:THR:O	1:A:216:ALA:HB3	2.18	0.44
1:C:17:VAL:HG12	1:C:19:LEU:HD13	2.00	0.44
1:B:276:LYS:HG2	1:B:277:ASN:ND2	2.33	0.44
1:L:215:THR:O	1:L:216:ALA:HB3	2.18	0.44
1:J:80:PHE:CG	4:J:5491:MPD:C1	3.00	0.44
1:I:309:ASN:HD22	1:I:313:ASN:HD22	1.66	0.44
1:C:313:ASN:HD21	1:C:360:PHE:HD2	1.64	0.44
1:A:396:LEU:HB2	1:A:397:TYR:H	1.36	0.44
1:E:21:PHE:HA	4:E:5480:MPD:C3	2.36	0.44
1:J:73:THR:HG21	1:J:88:ARG:HB3	2.00	0.44
1:H:88:ARG:NE	4:H:5486:MPD:HM1	2.30	0.44
1:H:61:ASN:O	1:I:337:ARG:CB	2.50	0.44
1:F:295:LEU:O	1:F:388:PRO:HG2	2.15	0.44
1:G:130:PRO:HB3	1:G:268:MET:HE3	1.99	0.44
1:E:130:PRO:HB3	1:E:268:MET:HE3	1.98	0.44
1:E:272:MET:HE1	1:E:358:VAL:HG21	1.99	0.44
1:A:17:VAL:HG12	1:A:19:LEU:HD13	2.00	0.44
4:G:5485:MPD:O4	1:H:193:SER:OG	2.28	0.44
1:D:193:SER:CB	4:E:5477:MPD:CM	2.84	0.44
1:D:84:THR:CG2	4:D:5475:MPD:H32	2.48	0.44
1:F:340:SER:HB3	1:F:396:LEU:HB3	1.99	0.44
1:L:458:HIS:CD2	1:L:459:PRO:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:458:HIS:CD2	1:G:459:PRO:HD2	2.52	0.44
1:F:180:PHE:O	1:F:181:PRO:C	2.54	0.44
1:C:180:PHE:O	1:C:181:PRO:C	2.54	0.44
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.74	0.44
1:I:231:LYS:HA	1:I:231:LYS:HD2	1.74	0.44
1:I:275:ALA:HA	1:I:281:LEU:HD13	2.00	0.44
1:H:215:THR:O	1:H:216:ALA:HB3	2.18	0.44
1:I:65:MET:HA	1:I:94:PRO:HG3	2.00	0.44
1:K:276:LYS:HG2	1:K:277:ASN:ND2	2.32	0.44
1:F:275:ALA:HA	1:F:281:LEU:HD13	2.00	0.44
1:G:275:ALA:HA	1:G:281:LEU:HD13	2.00	0.44
1:K:17:VAL:HG12	1:K:19:LEU:HD13	2.00	0.44
1:C:275:ALA:HA	1:C:281:LEU:HD13	2.00	0.44
1:G:309:ASN:HD22	1:G:313:ASN:HD22	1.66	0.44
1:B:73:THR:HG21	1:B:88:ARG:HB3	2.00	0.44
1:C:458:HIS:CD2	1:C:459:PRO:HD2	2.53	0.44
1:G:180:PHE:CB	1:L:29:GLN:HB3	2.48	0.44
1:F:231:LYS:HA	1:F:231:LYS:HD2	1.74	0.44
1:A:130:PRO:HB3	1:A:268:MET:HE3	1.99	0.44
1:E:276:LYS:HG2	1:E:277:ASN:ND2	2.33	0.44
1:G:17:VAL:HG12	1:G:19:LEU:HD13	2.00	0.44
1:K:215:THR:O	1:K:216:ALA:HB3	2.18	0.44
1:C:272:MET:HE1	1:C:358:VAL:HG21	2.00	0.44
1:E:309:ASN:HD22	1:E:313:ASN:HD22	1.66	0.44
1:I:313:ASN:HD21	1:I:360:PHE:HD2	1.64	0.44
1:D:309:ASN:HD22	1:D:313:ASN:HD22	1.66	0.44
1:H:340:SER:HB3	1:H:396:LEU:HB3	1.99	0.44
1:C:295:LEU:O	1:C:388:PRO:HG2	2.15	0.44
1:B:231:LYS:HA	1:B:231:LYS:HD2	1.74	0.44
1:A:139:ARG:HD3	1:F:163:LYS:HG2	1.99	0.44
1:I:215:THR:O	1:I:216:ALA:HB3	2.18	0.44
1:E:17:VAL:HG12	1:E:19:LEU:HD13	2.00	0.44
1:F:82:ASP:O	4:F:5479:MPD:H32	2.18	0.43
1:H:313:ASN:HD21	1:H:360:PHE:HD2	1.65	0.43
1:I:458:HIS:CD2	1:I:459:PRO:HD2	2.52	0.43
1:F:458:HIS:CD2	1:F:459:PRO:HD2	2.52	0.43
1:D:468:VAL:HG13	1:J:364:ALA:HA	1.99	0.43
1:F:125:LEU:O	1:F:272:MET:HA	2.18	0.43
1:G:65:MET:HA	1:G:94:PRO:HG3	2.00	0.43
1:D:215:THR:O	1:D:216:ALA:HB3	2.18	0.43
1:H:65:MET:HA	1:H:94:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LYS:HG2	1:C:277:ASN:ND2	2.32	0.43
4:G:5485:MPD:H11	1:H:189:GLN:CG	2.48	0.43
4:E:5477:MPD:O4	4:E:5477:MPD:CM	2.60	0.43
1:F:396:LEU:HB2	1:F:397:TYR:H	1.36	0.43
1:F:73:THR:HG21	1:F:88:ARG:HB3	2.00	0.43
1:K:235:ILE:HA	1:K:235:ILE:HD13	1.82	0.43
1:J:458:HIS:CD2	1:J:459:PRO:HD2	2.52	0.43
1:J:170:GLY:HA2	1:J:172:ARG:HH22	1.81	0.43
1:H:137:ASP:HB3	1:H:152:ASP:HB3	2.01	0.43
1:C:215:THR:O	1:C:216:ALA:HB3	2.18	0.43
1:J:215:THR:O	1:J:216:ALA:HB3	2.18	0.43
1:B:344:ARG:NH1	1:B:346:PRO:HA	2.34	0.43
1:H:17:VAL:HG12	1:H:19:LEU:HD13	2.00	0.43
1:B:125:LEU:O	1:B:272:MET:HA	2.19	0.43
1:E:344:ARG:NH1	1:E:346:PRO:HA	2.34	0.43
1:L:236:GLN:HA	1:L:236:GLN:OE1	2.19	0.43
1:A:189:GLN:CG	4:B:5471:MPD:H11	2.48	0.43
1:D:189:GLN:CG	4:E:5477:MPD:H11	2.48	0.43
1:I:88:ARG:NE	4:I:5488:MPD:HM1	2.30	0.43
1:B:21:PHE:CB	4:B:5474:MPD:H53	2.27	0.43
1:C:235:ILE:HA	1:C:235:ILE:HD13	1.82	0.43
1:F:256:MET:CG	1:L:466:TYR:HA	2.49	0.43
1:D:468:VAL:CG1	1:J:364:ALA:HA	2.49	0.43
1:J:125:LEU:O	1:J:272:MET:HA	2.19	0.43
1:A:125:LEU:O	1:A:272:MET:HA	2.19	0.43
1:B:272:MET:HE1	1:B:358:VAL:HG21	2.00	0.43
1:F:17:VAL:HG12	1:F:19:LEU:HD13	2.00	0.43
1:A:344:ARG:NH1	1:A:346:PRO:HA	2.34	0.43
1:G:272:MET:HE1	1:G:358:VAL:HG21	2.00	0.43
1:H:344:ARG:NH1	1:H:346:PRO:HA	2.34	0.43
1:F:215:THR:O	1:F:216:ALA:HB3	2.18	0.43
1:J:17:VAL:HG12	1:J:19:LEU:HD13	2.00	0.43
1:F:236:GLN:OE1	1:F:236:GLN:HA	2.19	0.43
1:J:276:LYS:HG2	1:J:277:ASN:ND2	2.33	0.43
1:G:236:GLN:OE1	1:G:236:GLN:HA	2.19	0.43
1:K:236:GLN:OE1	1:K:236:GLN:HA	2.19	0.43
4:J:5491:MPD:H11	1:K:189:GLN:CG	2.48	0.43
4:L:5483:MPD:H53	4:L:5483:MPD:C1	2.48	0.43
1:H:309:ASN:HD22	1:H:313:ASN:HD22	1.66	0.43
1:D:313:ASN:HD21	1:D:360:PHE:HD2	1.65	0.43
1:L:396:LEU:HB2	1:L:397:TYR:H	1.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:O	1:C:272:MET:HA	2.19	0.43
1:L:344:ARG:NH1	1:L:346:PRO:HA	2.34	0.43
1:K:275:ALA:HA	1:K:281:LEU:HD13	2.00	0.43
1:B:65:MET:HA	1:B:94:PRO:HG3	2.00	0.43
1:F:276:LYS:HG2	1:F:277:ASN:ND2	2.33	0.43
1:C:65:MET:HA	1:C:94:PRO:HG3	2.00	0.43
1:L:65:MET:HA	1:L:94:PRO:HG3	2.00	0.43
1:I:344:ARG:NH1	1:I:346:PRO:HA	2.34	0.43
1:H:276:LYS:HG2	1:H:277:ASN:ND2	2.33	0.43
1:D:344:ARG:NH1	1:D:346:PRO:HA	2.34	0.43
1:H:236:GLN:HA	1:H:236:GLN:OE1	2.19	0.43
1:J:236:GLN:OE1	1:J:236:GLN:HA	2.19	0.43
4:K:5493:MPD:H11	1:L:189:GLN:CG	2.48	0.43
1:B:309:ASN:HD22	1:B:313:ASN:HD22	1.66	0.43
1:K:309:ASN:HD22	1:K:313:ASN:HD22	1.66	0.43
1:A:309:ASN:HD22	1:A:313:ASN:HD22	1.66	0.43
1:D:73:THR:HG21	1:D:88:ARG:HB3	2.00	0.43
1:J:387:HIS:HA	1:J:388:PRO:HD2	1.73	0.43
1:D:170:GLY:HA2	1:D:172:ARG:HH22	1.81	0.43
1:A:180:PHE:CB	1:B:29:GLN:HB3	2.49	0.43
1:B:215:THR:O	1:B:216:ALA:HB3	2.18	0.43
1:D:275:ALA:HA	1:D:281:LEU:HD13	2.00	0.43
1:C:236:GLN:HA	1:C:236:GLN:OE1	2.19	0.43
1:I:73:THR:HG21	1:I:88:ARG:HB3	2.00	0.43
1:G:231:LYS:HA	1:G:231:LYS:HD2	1.74	0.43
1:L:125:LEU:O	1:L:272:MET:HA	2.19	0.43
1:D:125:LEU:O	1:D:272:MET:HA	2.19	0.43
1:E:125:LEU:O	1:E:272:MET:HA	2.19	0.43
1:D:137:ASP:HB3	1:D:152:ASP:HB3	2.01	0.43
1:J:80:PHE:CD1	4:J:5491:MPD:H52	2.44	0.43
4:H:5487:MPD:O4	4:H:5487:MPD:CM	2.60	0.43
4:I:5489:MPD:H11	1:J:189:GLN:CG	2.48	0.43
1:A:80:PHE:CB	4:A:5481:MPD:C1	2.75	0.43
1:F:309:ASN:HD22	1:F:313:ASN:HD22	1.66	0.43
1:H:396:LEU:H	1:H:396:LEU:HG	1.46	0.43
1:D:368:TYR:OH	4:D:5478:MPD:O2	2.27	0.43
1:A:29:GLN:HB3	1:F:180:PHE:HB2	2.00	0.43
1:B:320:LYS:HG2	1:H:455:MET:O	2.19	0.43
1:E:231:LYS:HD2	1:E:231:LYS:HA	1.74	0.43
1:K:25:LYS:NZ	5:K:3196:HOH:O	2.44	0.43
1:F:65:MET:HA	1:F:94:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ALA:HA	1:E:281:LEU:HD13	2.00	0.43
1:J:65:MET:HA	1:J:94:PRO:HG3	1.99	0.43
1:A:236:GLN:HA	1:A:236:GLN:OE1	2.19	0.43
4:H:5487:MPD:CM	1:I:193:SER:CB	2.84	0.43
4:A:5481:MPD:CM	1:F:193:SER:CB	2.84	0.43
1:D:340:SER:HB3	1:D:396:LEU:HB3	1.99	0.43
1:G:73:THR:HG21	1:G:88:ARG:HB3	2.00	0.43
1:L:88:ARG:NE	4:L:5494:MPD:HM1	2.30	0.43
1:H:180:PHE:O	1:H:181:PRO:C	2.54	0.43
1:L:334:TYR:HA	1:L:343:ILE:O	2.19	0.43
1:H:29:GLN:HB3	1:I:180:PHE:CB	2.49	0.43
1:I:130:PRO:HB3	1:I:268:MET:HE3	2.01	0.43
1:F:137:ASP:HB3	1:F:152:ASP:HB3	2.01	0.43
1:J:275:ALA:HA	1:J:281:LEU:HD13	2.00	0.43
1:G:344:ARG:NH1	1:G:346:PRO:HA	2.34	0.43
1:L:275:ALA:HA	1:L:281:LEU:HD13	2.00	0.43
1:L:2:ALA:O	1:L:6:LEU:HD12	2.19	0.43
1:I:17:VAL:HG12	1:I:19:LEU:HD13	2.00	0.43
1:J:25:LYS:NZ	5:J:2904:HOH:O	2.44	0.43
1:E:137:ASP:HB3	1:E:152:ASP:HB3	2.01	0.43
1:B:236:GLN:HA	1:B:236:GLN:OE1	2.19	0.43
1:L:137:ASP:HB3	1:L:152:ASP:HB3	2.01	0.43
1:C:189:GLN:CG	4:D:5475:MPD:H11	2.48	0.43
4:C:5473:MPD:CM	4:C:5473:MPD:O4	2.60	0.43
1:L:340:SER:HB3	1:L:396:LEU:HB3	1.99	0.43
1:K:396:LEU:HG	1:K:396:LEU:H	1.46	0.43
1:D:21:PHE:CB	4:D:5478:MPD:H53	2.27	0.43
1:L:73:THR:HG21	1:L:88:ARG:HB3	2.00	0.43
1:C:231:LYS:HA	1:C:231:LYS:HD2	1.74	0.43
1:D:2:ALA:O	1:D:6:LEU:HD12	2.19	0.43
1:A:275:ALA:HA	1:A:281:LEU:HD13	2.00	0.43
1:B:275:ALA:HA	1:B:281:LEU:HD13	2.00	0.43
1:I:236:GLN:HA	1:I:236:GLN:OE1	2.19	0.43
1:G:189:GLN:CG	4:L:5483:MPD:H11	2.48	0.43
1:K:80:PHE:CG	4:K:5493:MPD:H12	2.48	0.43
1:C:309:ASN:HD22	1:C:313:ASN:HD22	1.66	0.43
1:G:88:ARG:NE	4:G:5484:MPD:HM1	2.29	0.43
1:C:73:THR:HG21	1:C:88:ARG:HB3	2.00	0.43
1:H:334:TYR:HA	1:H:343:ILE:O	2.19	0.43
1:F:130:PRO:HB3	1:F:268:MET:HE3	2.01	0.43
1:G:125:LEU:O	1:G:272:MET:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ALA:O	1:C:6:LEU:HD12	2.19	0.43
1:K:139:ARG:HD3	1:L:163:LYS:HG2	2.01	0.43
1:K:125:LEU:O	1:K:272:MET:HA	2.19	0.43
1:F:466:TYR:HA	1:L:256:MET:HG3	2.01	0.43
1:F:2:ALA:O	1:F:6:LEU:HD12	2.19	0.43
1:H:2:ALA:O	1:H:6:LEU:HD12	2.19	0.43
1:I:2:ALA:O	1:I:6:LEU:HD12	2.19	0.43
1:J:84:THR:HG21	4:J:5491:MPD:H32	2.01	0.42
1:D:80:PHE:CB	4:D:5475:MPD:C1	2.68	0.42
1:D:80:PHE:CD1	4:D:5475:MPD:H52	2.51	0.42
1:C:80:PHE:CG	4:C:5473:MPD:C1	3.01	0.42
1:I:387:HIS:HA	1:I:388:PRO:HD2	1.73	0.42
1:F:170:GLY:HA2	1:F:172:ARG:HH22	1.81	0.42
1:E:334:TYR:HA	1:E:343:ILE:O	2.19	0.42
1:K:29:GLN:HB3	1:L:180:PHE:CB	2.49	0.42
1:J:390:GLU:HA	1:J:391:PRO:HD3	1.89	0.42
1:C:334:TYR:HA	1:C:343:ILE:O	2.19	0.42
1:I:272:MET:HE1	1:I:358:VAL:HG21	2.01	0.42
1:G:215:THR:O	1:G:216:ALA:HB3	2.18	0.42
1:E:2:ALA:O	1:E:6:LEU:HD12	2.19	0.42
1:K:344:ARG:NH1	1:K:346:PRO:HA	2.34	0.42
1:A:2:ALA:O	1:A:6:LEU:HD12	2.19	0.42
1:K:31:VAL:HG23	1:L:210:HIS:HB3	2.01	0.42
1:B:466:TYR:HA	1:H:256:MET:HG3	2.02	0.42
1:K:396:LEU:HB2	1:K:397:TYR:H	1.36	0.42
1:K:73:THR:HG21	1:K:88:ARG:HB3	2.00	0.42
1:A:73:THR:HG21	1:A:88:ARG:HB3	2.00	0.42
1:A:29:GLN:HB3	1:F:180:PHE:CB	2.49	0.42
1:A:30:HIS:HB3	1:F:182:VAL:HG12	2.01	0.42
1:C:170:GLY:HA2	1:C:172:ARG:HH22	1.81	0.42
1:B:390:GLU:HA	1:B:391:PRO:HD3	1.89	0.42
1:J:334:TYR:HA	1:J:343:ILE:O	2.19	0.42
1:H:125:LEU:O	1:H:272:MET:HA	2.19	0.42
1:E:65:MET:HA	1:E:94:PRO:HG3	2.00	0.42
1:J:344:ARG:NH1	1:J:346:PRO:HA	2.33	0.42
4:A:5481:MPD:H11	1:F:189:GLN:CG	2.49	0.42
1:H:73:THR:HG21	1:H:88:ARG:HB3	2.00	0.42
1:A:88:ARG:NE	4:A:5472:MPD:HM1	2.30	0.42
1:E:458:HIS:HE1	1:K:456:THR:O	2.03	0.42
1:D:334:TYR:HA	1:D:343:ILE:O	2.19	0.42
1:I:332:LEU:HB2	1:I:408:PRO:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:LYS:NZ	5:E:1444:HOH:O	2.44	0.42
1:J:2:ALA:O	1:J:6:LEU:HD12	2.19	0.42
1:K:2:ALA:O	1:K:6:LEU:HD12	2.19	0.42
1:J:137:ASP:HB3	1:J:152:ASP:HB3	2.01	0.42
1:I:137:ASP:HB3	1:I:152:ASP:HB3	2.01	0.42
1:H:275:ALA:HA	1:H:281:LEU:HD13	2.00	0.42
1:G:193:SER:CB	4:L:5483:MPD:CM	2.84	0.42
1:K:80:PHE:CG	4:K:5493:MPD:C1	3.01	0.42
4:C:5473:MPD:H53	4:C:5473:MPD:C1	2.48	0.42
4:A:5481:MPD:H53	4:A:5481:MPD:C1	2.48	0.42
1:E:88:ARG:NE	4:E:5480:MPD:HM1	2.30	0.42
1:J:180:PHE:O	1:J:181:PRO:C	2.54	0.42
1:G:334:TYR:HA	1:G:343:ILE:O	2.19	0.42
1:F:334:TYR:HA	1:F:343:ILE:O	2.19	0.42
1:I:180:PHE:O	1:I:181:PRO:C	2.54	0.42
1:J:130:PRO:HB3	1:J:268:MET:HE2	2.02	0.42
1:I:125:LEU:O	1:I:272:MET:HA	2.19	0.42
1:L:17:VAL:HG12	1:L:19:LEU:HD13	2.00	0.42
1:G:138:ILE:O	1:G:138:ILE:HG23	2.20	0.42
1:A:138:ILE:O	1:A:138:ILE:HG23	2.20	0.42
1:L:309:ASN:HD22	1:L:313:ASN:HD22	1.66	0.42
1:F:396:LEU:HG	1:F:396:LEU:H	1.46	0.42
1:B:384:ASN:N	1:B:384:ASN:ND2	2.60	0.42
1:K:170:GLY:HA2	1:K:172:ARG:HH22	1.81	0.42
1:K:29:GLN:HB3	1:L:180:PHE:HB2	2.01	0.42
1:B:332:LEU:HB2	1:B:408:PRO:CB	2.50	0.42
1:F:332:LEU:HB2	1:F:408:PRO:CB	2.50	0.42
1:A:364:ALA:HA	1:G:468:VAL:HG13	2.01	0.42
1:C:344:ARG:NH1	1:C:346:PRO:HA	2.34	0.42
1:K:138:ILE:O	1:K:138:ILE:HG23	2.20	0.42
1:B:334:TYR:HA	1:B:343:ILE:O	2.19	0.42
1:I:334:TYR:HA	1:I:343:ILE:O	2.19	0.42
1:C:281:LEU:HB3	1:C:293:GLN:OE1	2.20	0.42
1:F:344:ARG:NH1	1:F:346:PRO:HA	2.34	0.42
1:B:17:VAL:HG12	1:B:19:LEU:HD13	2.00	0.42
1:C:137:ASP:HB3	1:C:152:ASP:HB3	2.01	0.42
1:B:25:LYS:NZ	5:B:5734:HOH:O	2.44	0.42
1:K:137:ASP:HB3	1:K:152:ASP:HB3	2.01	0.42
1:I:138:ILE:HG23	1:I:138:ILE:O	2.20	0.42
1:E:138:ILE:HG23	1:E:138:ILE:O	2.20	0.42
1:E:236:GLN:OE1	1:E:236:GLN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:PHE:CG	4:L:5483:MPD:H53	2.53	0.42
1:K:84:THR:HG21	4:K:5493:MPD:C3	2.48	0.42
1:J:309:ASN:HD22	1:J:313:ASN:HD22	1.66	0.42
1:D:192:ARG:NH2	1:D:219:ASN:ND2	2.63	0.42
1:D:454:ARG:O	1:J:320:LYS:HG3	2.20	0.42
1:G:170:GLY:HA2	1:G:172:ARG:HH22	1.81	0.42
1:A:256:MET:CG	1:G:466:TYR:HA	2.49	0.42
1:L:130:PRO:HB3	1:L:268:MET:HE3	2.01	0.42
1:B:281:LEU:HB3	1:B:293:GLN:OE1	2.20	0.42
1:A:137:ASP:HB3	1:A:152:ASP:HB3	2.01	0.42
1:B:189:GLN:CG	4:C:5473:MPD:H11	2.49	0.42
1:E:456:THR:O	1:K:458:HIS:HE1	2.02	0.42
1:A:53:SER:CB	1:F:179:TYR:CD2	3.01	0.42
1:A:170:GLY:HA2	1:A:172:ARG:HH22	1.81	0.42
1:L:170:GLY:HA2	1:L:172:ARG:HH22	1.81	0.42
1:D:332:LEU:HB2	1:D:408:PRO:CB	2.50	0.42
1:G:180:PHE:HB2	1:L:29:GLN:HB3	2.00	0.42
1:I:281:LEU:HB3	1:I:293:GLN:OE1	2.20	0.42
1:E:281:LEU:HB3	1:E:293:GLN:OE1	2.20	0.42
1:A:281:LEU:HB3	1:A:293:GLN:OE1	2.20	0.42
1:H:281:LEU:HB3	1:H:293:GLN:OE1	2.20	0.42
1:B:137:ASP:HB3	1:B:152:ASP:HB3	2.01	0.42
1:D:17:VAL:HG12	1:D:19:LEU:HD13	2.00	0.42
1:G:137:ASP:HB3	1:G:152:ASP:HB3	2.01	0.42
1:G:295:LEU:O	1:G:388:PRO:HG2	2.15	0.42
1:L:387:HIS:HA	1:L:388:PRO:HD2	1.73	0.42
1:D:181:PRO:HG3	5:E:1312:HOH:O	2.19	0.42
1:L:332:LEU:HA	1:L:332:LEU:HD12	1.90	0.42
1:L:231:LYS:HA	1:L:231:LYS:HD2	1.74	0.42
1:L:281:LEU:HB3	1:L:293:GLN:OE1	2.20	0.42
1:D:256:MET:HG3	1:J:466:TYR:HA	2.02	0.42
1:J:138:ILE:O	1:J:138:ILE:HG23	2.20	0.42
1:C:84:THR:CG2	4:C:5473:MPD:H32	2.49	0.42
1:A:84:THR:CG2	4:A:5481:MPD:H32	2.50	0.42
1:C:396:LEU:H	1:C:396:LEU:HG	1.46	0.42
1:E:73:THR:HG21	1:E:88:ARG:HB3	2.00	0.42
4:B:5474:MPD:H12	4:B:5474:MPD:H4	1.82	0.42
1:F:192:ARG:NH2	1:F:219:ASN:ND2	2.63	0.42
1:H:332:LEU:HB2	1:H:408:PRO:CB	2.50	0.42
1:E:272:MET:HE1	1:E:358:VAL:CG2	2.50	0.42
1:B:138:ILE:HG23	1:B:138:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:GLY:HA2	1:E:172:ARG:HH22	1.81	0.41
1:K:334:TYR:HA	1:K:343:ILE:O	2.19	0.41
1:C:332:LEU:HB2	1:C:408:PRO:CB	2.50	0.41
1:J:332:LEU:HA	1:J:332:LEU:HD12	1.90	0.41
1:K:281:LEU:HB3	1:K:293:GLN:OE1	2.20	0.41
1:D:281:LEU:HB3	1:D:293:GLN:OE1	2.20	0.41
1:C:225:PHE:HD1	3:C:4473:ADP:O2'	2.03	0.41
1:G:68:MET:HA	1:G:69:PRO:HD2	1.95	0.41
4:J:5491:MPD:CM	1:K:193:SER:CB	2.84	0.41
1:I:84:THR:CG2	4:I:5489:MPD:H32	2.50	0.41
1:A:456:THR:O	1:G:458:HIS:HE1	2.02	0.41
1:K:192:ARG:NH2	1:K:219:ASN:ND2	2.63	0.41
1:K:180:PHE:O	1:K:181:PRO:C	2.54	0.41
1:A:334:TYR:HA	1:A:343:ILE:O	2.19	0.41
1:A:296:TYR:HB3	1:A:382:ILE:HA	2.03	0.41
1:A:364:ALA:HA	1:G:468:VAL:CG1	2.50	0.41
1:G:91:ILE:HB	1:G:103:ASP:HB2	2.02	0.41
1:L:433:VAL:HG12	1:L:434:PHE:CD2	2.55	0.41
1:L:230:LYS:O	1:L:234:GLU:HG3	2.20	0.41
1:B:91:ILE:HB	1:B:103:ASP:HB2	2.02	0.41
1:C:433:VAL:HG12	1:C:434:PHE:CD2	2.55	0.41
1:D:138:ILE:O	1:D:138:ILE:HG23	2.20	0.41
4:H:5487:MPD:H11	1:I:189:GLN:CG	2.48	0.41
1:K:88:ARG:NE	4:K:5492:MPD:HM1	2.30	0.41
1:A:180:PHE:O	1:A:181:PRO:C	2.54	0.41
1:E:296:TYR:HB3	1:E:382:ILE:HA	2.03	0.41
1:G:281:LEU:HB3	1:G:293:GLN:OE1	2.20	0.41
1:F:433:VAL:HG12	1:F:434:PHE:CD2	2.55	0.41
1:G:433:VAL:HG12	1:G:434:PHE:CD2	2.56	0.41
1:L:225:PHE:HD1	3:L:4482:ADP:O2'	2.03	0.41
1:H:138:ILE:O	1:H:138:ILE:HG23	2.20	0.41
1:F:138:ILE:HG23	1:F:138:ILE:O	2.20	0.41
1:H:80:PHE:CG	4:H:5487:MPD:H53	2.50	0.41
1:C:296:TYR:HB3	1:C:382:ILE:HA	2.03	0.41
1:H:25:LYS:NZ	5:H:5752:HOH:O	2.44	0.41
1:G:2:ALA:O	1:G:6:LEU:HD12	2.19	0.41
1:K:332:LEU:HB2	1:K:408:PRO:CB	2.50	0.41
1:H:433:VAL:HG12	1:H:434:PHE:CD2	2.55	0.41
1:F:230:LYS:O	1:F:234:GLU:HG3	2.21	0.41
1:F:91:ILE:HB	1:F:103:ASP:HB2	2.03	0.41
1:K:225:PHE:HD1	3:K:4481:ADP:O2'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:GLU:C	1:C:405:LYS:N	2.74	0.41
1:I:396:LEU:H	1:I:396:LEU:HG	1.46	0.41
1:A:403:GLU:C	1:A:405:LYS:N	2.74	0.41
1:C:390:GLU:HA	1:C:391:PRO:HD3	1.89	0.41
1:L:332:LEU:HB2	1:L:408:PRO:CB	2.50	0.41
1:I:231:LYS:HE2	5:I:5517:HOH:O	2.21	0.41
1:G:231:LYS:HE2	5:G:5504:HOH:O	2.21	0.41
1:F:281:LEU:HB3	1:F:293:GLN:OE1	2.20	0.41
1:F:318:SER:OG	1:F:362:ASP:OD2	2.27	0.41
1:B:254:THR:HB	1:H:466:TYR:CE1	2.56	0.41
1:I:433:VAL:HG12	1:I:434:PHE:CD2	2.55	0.41
1:K:91:ILE:HB	1:K:103:ASP:HB2	2.03	0.41
1:A:225:PHE:HD1	3:A:4471:ADP:O2'	2.03	0.41
1:C:138:ILE:O	1:C:138:ILE:HG23	2.20	0.41
1:D:236:GLN:OE1	1:D:236:GLN:HA	2.19	0.41
1:E:80:PHE:CB	4:E:5477:MPD:C1	2.76	0.41
1:J:396:LEU:HG	1:J:396:LEU:H	1.46	0.41
1:A:458:HIS:HE1	1:G:456:THR:O	2.03	0.41
1:H:384:ASN:N	1:H:384:ASN:ND2	2.60	0.41
1:F:320:LYS:HG3	1:L:454:ARG:O	2.21	0.41
1:I:296:TYR:HB3	1:I:382:ILE:HA	2.03	0.41
1:F:296:TYR:HB3	1:F:382:ILE:HA	2.03	0.41
1:J:281:LEU:HB3	1:J:293:GLN:OE1	2.20	0.41
1:K:272:MET:HE1	1:K:358:VAL:HG21	2.01	0.41
1:H:230:LYS:O	1:H:234:GLU:HG3	2.20	0.41
1:E:225:PHE:HD1	3:E:4475:ADP:O2'	2.03	0.41
1:J:91:ILE:HB	1:J:103:ASP:HB2	2.03	0.41
1:J:230:LYS:O	1:J:234:GLU:HG3	2.21	0.41
1:J:433:VAL:HG12	1:J:434:PHE:CD2	2.55	0.41
1:L:91:ILE:HB	1:L:103:ASP:HB2	2.02	0.41
4:J:5491:MPD:C1	4:J:5491:MPD:H53	2.48	0.41
1:K:403:GLU:C	1:K:405:LYS:N	2.74	0.41
1:H:114:TYR:O	1:H:118:THR:HG23	2.21	0.41
1:H:296:TYR:HB3	1:H:382:ILE:HA	2.03	0.41
1:J:296:TYR:HB3	1:J:382:ILE:HA	2.03	0.41
1:G:296:TYR:HB3	1:G:382:ILE:HA	2.03	0.41
1:J:231:LYS:HE2	5:J:2640:HOH:O	2.21	0.41
1:C:231:LYS:HE2	5:C:5493:HOH:O	2.21	0.41
1:C:130:PRO:HB3	1:C:268:MET:HE3	2.02	0.41
1:B:230:LYS:O	1:B:234:GLU:HG3	2.20	0.41
1:I:225:PHE:HD1	3:I:4479:ADP:O2'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:433:VAL:HG12	1:K:434:PHE:CD2	2.55	0.41
1:D:225:PHE:HD1	3:D:4474:ADP:O2'	2.03	0.41
1:B:206:VAL:O	1:C:34:PRO:HG2	2.20	0.41
4:J:5491:MPD:CM	4:J:5491:MPD:O4	2.60	0.41
1:C:193:SER:CB	4:D:5475:MPD:CM	2.84	0.41
1:B:313:ASN:HB3	1:B:318:SER:HB3	2.03	0.41
1:I:403:GLU:C	1:I:405:LYS:N	2.74	0.41
4:G:5484:MPD:C5	4:G:5484:MPD:H11	2.45	0.41
1:H:368:TYR:OH	4:H:5486:MPD:O2	2.27	0.41
1:E:390:GLU:HA	1:E:391:PRO:HD3	1.89	0.41
1:B:320:LYS:HG2	1:H:455:MET:C	2.42	0.41
1:E:323:VAL:HG11	1:K:455:MET:HG2	2.03	0.41
1:D:332:LEU:HA	1:D:332:LEU:HD12	1.90	0.41
1:D:114:TYR:O	1:D:118:THR:HG23	2.21	0.41
1:L:296:TYR:HB3	1:L:382:ILE:HA	2.03	0.41
1:L:114:TYR:O	1:L:118:THR:HG23	2.21	0.41
1:G:114:TYR:O	1:G:118:THR:HG23	2.21	0.41
1:E:231:LYS:HE2	5:E:1180:HOH:O	2.21	0.41
1:A:272:MET:HE1	1:A:358:VAL:CG2	2.51	0.41
1:D:364:ALA:HA	1:J:468:VAL:HG13	2.03	0.41
1:G:230:LYS:O	1:G:234:GLU:HG3	2.21	0.41
1:A:230:LYS:O	1:A:234:GLU:HG3	2.21	0.41
1:I:34:PRO:HG2	1:J:206:VAL:O	2.20	0.41
1:G:25:LYS:NZ	5:G:5744:HOH:O	2.44	0.41
1:C:294:ALA:O	1:C:298:ILE:HG13	2.21	0.41
1:D:91:ILE:HB	1:D:103:ASP:HB2	2.03	0.41
1:A:433:VAL:HG12	1:A:434:PHE:CD2	2.55	0.41
1:E:206:VAL:O	1:F:34:PRO:HG2	2.20	0.41
1:E:433:VAL:HG12	1:E:434:PHE:CD2	2.56	0.41
1:E:230:LYS:O	1:E:234:GLU:HG3	2.21	0.41
1:B:2:ALA:O	1:B:6:LEU:HD12	2.19	0.41
4:K:5493:MPD:H53	4:K:5493:MPD:C1	2.48	0.41
1:D:303:LYS:HD2	1:D:386:ILE:HD13	2.04	0.41
1:I:114:TYR:O	1:I:118:THR:HG23	2.21	0.41
1:B:114:TYR:O	1:B:118:THR:HG23	2.21	0.41
1:K:114:TYR:O	1:K:118:THR:HG23	2.21	0.41
1:L:231:LYS:HE2	5:L:3224:HOH:O	2.21	0.41
1:D:231:LYS:HE2	5:D:888:HOH:O	2.21	0.41
1:E:254:THR:HB	1:K:466:TYR:CE1	2.56	0.41
1:A:91:ILE:HB	1:A:103:ASP:HB2	2.03	0.41
1:F:294:ALA:O	1:F:298:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:HD1	3:B:4472:ADP:O2'	2.03	0.41
1:K:140:PHE:CE1	1:L:160:SER:HB2	2.56	0.41
1:H:294:ALA:O	1:H:298:ILE:HG13	2.21	0.41
1:F:80:PHE:CG	4:F:5479:MPD:C1	3.04	0.40
1:L:82:ASP:O	4:L:5483:MPD:H32	2.20	0.40
1:B:84:THR:CG2	4:B:5471:MPD:H32	2.51	0.40
1:I:80:PHE:CG	4:I:5489:MPD:C1	3.04	0.40
1:G:313:ASN:HB3	1:G:318:SER:HB3	2.03	0.40
1:E:313:ASN:HB3	1:E:318:SER:HB3	2.03	0.40
1:J:313:ASN:HB3	1:J:318:SER:HB3	2.03	0.40
1:L:248:ARG:NH2	1:L:248:ARG:CG	2.67	0.40
1:H:303:LYS:HD2	1:H:386:ILE:HD13	2.03	0.40
1:G:332:LEU:HA	1:G:332:LEU:HD12	1.90	0.40
1:J:114:TYR:O	1:J:118:THR:HG23	2.21	0.40
1:A:114:TYR:O	1:A:118:THR:HG23	2.21	0.40
1:K:296:TYR:HB3	1:K:382:ILE:HA	2.03	0.40
1:F:466:TYR:CE1	1:L:254:THR:HB	2.56	0.40
1:K:294:ALA:O	1:K:298:ILE:HG13	2.22	0.40
1:E:294:ALA:O	1:E:298:ILE:HG13	2.21	0.40
1:L:294:ALA:O	1:L:298:ILE:HG13	2.21	0.40
1:G:294:ALA:O	1:G:298:ILE:HG13	2.21	0.40
1:D:433:VAL:HG12	1:D:434:PHE:CD2	2.55	0.40
1:F:225:PHE:HD1	3:F:4476:ADP:O2'	2.03	0.40
1:E:189:GLN:CG	4:F:5479:MPD:H11	2.48	0.40
4:H:5487:MPD:H53	4:H:5487:MPD:C1	2.48	0.40
1:K:105:ARG:HH21	1:K:105:ARG:HD3	1.76	0.40
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.82	0.40
1:J:235:ILE:HD13	1:J:235:ILE:HA	1.82	0.40
1:G:390:GLU:HA	1:G:391:PRO:HD3	1.89	0.40
1:F:332:LEU:HA	1:F:332:LEU:HD12	1.90	0.40
1:F:231:LYS:HE2	5:F:5506:HOH:O	2.21	0.40
1:I:230:LYS:O	1:I:234:GLU:HG3	2.21	0.40
1:J:225:PHE:HD1	3:J:4480:ADP:O2'	2.03	0.40
1:D:230:LYS:O	1:D:234:GLU:HG3	2.21	0.40
1:H:34:PRO:HG2	1:I:206:VAL:O	2.21	0.40
1:A:294:ALA:O	1:A:298:ILE:HG13	2.21	0.40
1:C:25:LYS:NZ	5:C:5734:HOH:O	2.44	0.40
1:B:294:ALA:O	1:B:298:ILE:HG13	2.21	0.40
4:B:5471:MPD:C1	4:B:5471:MPD:H53	2.48	0.40
1:K:313:ASN:HB3	1:K:318:SER:HB3	2.03	0.40
1:D:403:GLU:C	1:D:405:LYS:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:THR:HG1	4:C:5476:MPD:C1	2.33	0.40
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.82	0.40
1:L:303:LYS:HD2	1:L:386:ILE:HD13	2.04	0.40
1:D:182:VAL:HG12	1:E:30:HIS:HB3	2.03	0.40
1:E:114:TYR:O	1:E:118:THR:HG23	2.21	0.40
1:B:180:PHE:O	1:B:181:PRO:C	2.54	0.40
1:E:328:ALA:HA	1:E:329:PRO:HD3	1.73	0.40
1:E:364:ALA:HA	1:K:468:VAL:HG13	2.03	0.40
1:B:364:ALA:HA	1:H:468:VAL:CG1	2.51	0.40
1:I:91:ILE:HB	1:I:103:ASP:HB2	2.02	0.40
1:A:140:PHE:CE1	1:F:160:SER:HB2	2.56	0.40
1:B:433:VAL:HG12	1:B:434:PHE:CD2	2.55	0.40
1:K:230:LYS:O	1:K:234:GLU:HG3	2.21	0.40
1:G:225:PHE:HD1	3:G:4477:ADP:O2'	2.03	0.40
1:H:403:GLU:C	1:H:405:LYS:N	2.74	0.40
1:F:403:GLU:C	1:F:405:LYS:N	2.74	0.40
1:E:303:LYS:HD2	1:E:386:ILE:HD13	2.03	0.40
1:I:303:LYS:HD2	1:I:386:ILE:HD13	2.04	0.40
1:A:332:LEU:HA	1:A:332:LEU:HD12	1.90	0.40
1:I:332:LEU:HD12	1:I:332:LEU:HA	1.90	0.40
1:J:332:LEU:HB2	1:J:408:PRO:CB	2.50	0.40
1:I:294:ALA:O	1:I:298:ILE:HG13	2.22	0.40
1:E:193:SER:OG	4:F:5479:MPD:O4	2.28	0.40
4:G:5485:MPD:CM	4:G:5485:MPD:O4	2.60	0.40
1:H:313:ASN:HB3	1:H:318:SER:HB3	2.03	0.40
4:G:5484:MPD:H12	4:G:5484:MPD:H4	1.82	0.40
4:L:5494:MPD:C5	4:L:5494:MPD:H11	2.45	0.40
1:K:384:ASN:ND2	1:K:384:ASN:N	2.60	0.40
1:F:303:LYS:HD2	1:F:386:ILE:HD13	2.04	0.40
1:A:332:LEU:HB3	1:A:408:PRO:HB2	2.04	0.40
1:J:125:LEU:HD12	1:J:125:LEU:HA	1.91	0.40
1:J:294:ALA:O	1:J:298:ILE:HG13	2.21	0.40
1:H:225:PHE:HD1	3:H:4478:ADP:O2'	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
1	B	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
1	C	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
1	D	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
1	E	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
1	F	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
1	G	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
1	H	466/468 (100%)	427 (92%)	31 (7%)	8 (2%)	11	19
1	I	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
1	J	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
1	K	466/468 (100%)	427 (92%)	31 (7%)	8 (2%)	11	19
1	L	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	11	19
All	All	5592/5616 (100%)	5114 (92%)	382 (7%)	96 (2%)	11	19

All (96) Ramachandran outliers are listed below:

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

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/384 (100%)	348 (91%)	36 (9%)	11	20
1	B	384/384 (100%)	349 (91%)	35 (9%)	12	22
1	C	384/384 (100%)	348 (91%)	36 (9%)	11	20
1	D	384/384 (100%)	348 (91%)	36 (9%)	11	20
1	E	384/384 (100%)	348 (91%)	36 (9%)	11	20
1	F	384/384 (100%)	349 (91%)	35 (9%)	12	22
1	G	384/384 (100%)	348 (91%)	36 (9%)	11	20
1	H	384/384 (100%)	348 (91%)	36 (9%)	11	20
1	I	384/384 (100%)	349 (91%)	35 (9%)	12	22
1	J	384/384 (100%)	349 (91%)	35 (9%)	12	22
1	K	384/384 (100%)	348 (91%)	36 (9%)	11	20
1	L	384/384 (100%)	349 (91%)	35 (9%)	12	22
All	All	4608/4608 (100%)	4181 (91%)	427 (9%)	11	21

All (427) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	19	LEU
1	A	60	ILE
1	A	62	GLU
1	A	63	SER
1	A	64	ASP
1	A	65	MET
1	A	84	THR
1	A	88	ARG
1	A	96	THR
1	A	98	GLN
1	A	115	LEU
1	A	124	VAL
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	165	GLU
1	A	179	TYR
1	A	209	HIS
1	A	230	LYS
1	A	248	ARG
1	A	264	ASN
1	A	320	LYS
1	A	324	PRO
1	A	326	TYR
1	A	332	LEU
1	A	337	ARG
1	A	374	LEU
1	A	375	LEU
1	A	384	ASN
1	A	392	MET
1	A	396	LEU
1	A	397	TYR
1	A	399	LEU
1	A	428	LEU
1	A	447	ARG
1	A	464	LEU
1	A	468	VAL
1	B	6	LEU
1	B	19	LEU
1	B	60	ILE
1	B	62	GLU
1	B	63	SER
1	B	64	ASP
1	B	65	MET
1	B	84	THR
1	B	88	ARG
1	B	96	THR
1	B	98	GLN
1	B	115	LEU
1	B	124	VAL
1	B	125	LEU
1	B	165	GLU
1	B	179	TYR
1	B	209	HIS
1	B	230	LYS
1	B	248	ARG
1	B	264	ASN

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Mol	Chain	Res	Type
1	B	320	LYS
1	B	326	TYR
1	B	332	LEU
1	B	337	ARG
1	B	374	LEU
1	B	375	LEU
1	B	384	ASN
1	B	392	MET
1	B	396	LEU
1	B	397	TYR
1	B	399	LEU
1	B	428	LEU
1	B	447	ARG
1	B	464	LEU
1	B	468	VAL
1	C	6	LEU
1	C	19	LEU
1	C	60	ILE
1	C	62	GLU
1	C	63	SER
1	C	64	ASP
1	C	65	MET
1	C	84	THR
1	C	88	ARG
1	C	96	THR
1	C	98	GLN
1	C	115	LEU
1	C	124	VAL
1	C	125	LEU
1	C	165	GLU
1	C	179	TYR
1	C	209	HIS
1	C	230	LYS
1	C	248	ARG
1	C	264	ASN
1	C	320	LYS
1	C	324	PRO
1	C	326	TYR
1	C	332	LEU
1	C	337	ARG
1	C	374	LEU
1	C	375	LEU

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Mol	Chain	Res	Type
1	C	384	ASN
1	C	392	MET
1	C	396	LEU
1	C	397	TYR
1	C	399	LEU
1	C	428	LEU
1	C	447	ARG
1	C	464	LEU
1	C	468	VAL
1	D	6	LEU
1	D	19	LEU
1	D	60	ILE
1	D	62	GLU
1	D	63	SER
1	D	64	ASP
1	D	65	MET
1	D	84	THR
1	D	88	ARG
1	D	96	THR
1	D	98	GLN
1	D	115	LEU
1	D	124	VAL
1	D	125	LEU
1	D	165	GLU
1	D	179	TYR
1	D	209	HIS
1	D	230	LYS
1	D	248	ARG
1	D	264	ASN
1	D	320	LYS
1	D	324	PRO
1	D	326	TYR
1	D	332	LEU
1	D	337	ARG
1	D	374	LEU
1	D	375	LEU
1	D	384	ASN
1	D	392	MET
1	D	396	LEU
1	D	397	TYR
1	D	399	LEU
1	D	428	LEU

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Mol	Chain	Res	Type
1	D	447	ARG
1	D	464	LEU
1	D	468	VAL
1	E	6	LEU
1	E	19	LEU
1	E	60	ILE
1	E	62	GLU
1	E	63	SER
1	E	64	ASP
1	E	65	MET
1	E	84	THR
1	E	88	ARG
1	E	96	THR
1	E	98	GLN
1	E	115	LEU
1	E	124	VAL
1	E	125	LEU
1	E	165	GLU
1	E	179	TYR
1	E	209	HIS
1	E	230	LYS
1	E	248	ARG
1	E	264	ASN
1	E	320	LYS
1	E	324	PRO
1	E	326	TYR
1	E	332	LEU
1	E	337	ARG
1	E	374	LEU
1	E	375	LEU
1	E	384	ASN
1	E	392	MET
1	E	396	LEU
1	E	397	TYR
1	E	399	LEU
1	E	428	LEU
1	E	447	ARG
1	E	464	LEU
1	E	468	VAL
1	F	6	LEU
1	F	19	LEU
1	F	60	ILE

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Mol	Chain	Res	Type
1	F	62	GLU
1	F	63	SER
1	F	64	ASP
1	F	65	MET
1	F	84	THR
1	F	88	ARG
1	F	96	THR
1	F	98	GLN
1	F	115	LEU
1	F	124	VAL
1	F	125	LEU
1	F	165	GLU
1	F	179	TYR
1	F	209	HIS
1	F	230	LYS
1	F	248	ARG
1	F	264	ASN
1	F	320	LYS
1	F	326	TYR
1	F	332	LEU
1	F	337	ARG
1	F	374	LEU
1	F	375	LEU
1	F	384	ASN
1	F	392	MET
1	F	396	LEU
1	F	397	TYR
1	F	399	LEU
1	F	428	LEU
1	F	447	ARG
1	F	464	LEU
1	F	468	VAL
1	G	6	LEU
1	G	19	LEU
1	G	60	ILE
1	G	62	GLU
1	G	63	SER
1	G	64	ASP
1	G	65	MET
1	G	84	THR
1	G	88	ARG
1	G	96	THR

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Mol	Chain	Res	Type
1	G	98	GLN
1	G	115	LEU
1	G	124	VAL
1	G	125	LEU
1	G	165	GLU
1	G	179	TYR
1	G	209	HIS
1	G	230	LYS
1	G	248	ARG
1	G	264	ASN
1	G	320	LYS
1	G	324	PRO
1	G	326	TYR
1	G	332	LEU
1	G	337	ARG
1	G	374	LEU
1	G	375	LEU
1	G	384	ASN
1	G	392	MET
1	G	396	LEU
1	G	397	TYR
1	G	399	LEU
1	G	428	LEU
1	G	447	ARG
1	G	464	LEU
1	G	468	VAL
1	H	6	LEU
1	H	19	LEU
1	H	60	ILE
1	H	62	GLU
1	H	63	SER
1	H	64	ASP
1	H	65	MET
1	H	84	THR
1	H	88	ARG
1	H	96	THR
1	H	98	GLN
1	H	115	LEU
1	H	124	VAL
1	H	125	LEU
1	H	165	GLU
1	H	179	TYR

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Mol	Chain	Res	Type
1	H	209	HIS
1	H	230	LYS
1	H	248	ARG
1	H	264	ASN
1	H	320	LYS
1	H	324	PRO
1	H	326	TYR
1	H	332	LEU
1	H	337	ARG
1	H	374	LEU
1	H	375	LEU
1	H	384	ASN
1	H	392	MET
1	H	396	LEU
1	H	397	TYR
1	H	399	LEU
1	H	428	LEU
1	H	447	ARG
1	H	464	LEU
1	H	468	VAL
1	I	6	LEU
1	I	19	LEU
1	I	60	ILE
1	I	62	GLU
1	I	63	SER
1	I	64	ASP
1	I	65	MET
1	I	84	THR
1	I	88	ARG
1	I	96	THR
1	I	98	GLN
1	I	115	LEU
1	I	124	VAL
1	I	125	LEU
1	I	165	GLU
1	I	179	TYR
1	I	209	HIS
1	I	230	LYS
1	I	248	ARG
1	I	264	ASN
1	I	320	LYS
1	I	326	TYR

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Mol	Chain	Res	Type
1	I	332	LEU
1	I	337	ARG
1	I	374	LEU
1	I	375	LEU
1	I	384	ASN
1	I	392	MET
1	I	396	LEU
1	I	397	TYR
1	I	399	LEU
1	I	428	LEU
1	I	447	ARG
1	I	464	LEU
1	I	468	VAL
1	J	6	LEU
1	J	19	LEU
1	J	60	ILE
1	J	62	GLU
1	J	63	SER
1	J	64	ASP
1	J	65	MET
1	J	84	THR
1	J	88	ARG
1	J	96	THR
1	J	98	GLN
1	J	115	LEU
1	J	124	VAL
1	J	125	LEU
1	J	165	GLU
1	J	179	TYR
1	J	209	HIS
1	J	230	LYS
1	J	248	ARG
1	J	264	ASN
1	J	320	LYS
1	J	326	TYR
1	J	332	LEU
1	J	337	ARG
1	J	374	LEU
1	J	375	LEU
1	J	384	ASN
1	J	392	MET
1	J	396	LEU

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Mol	Chain	Res	Type
1	J	397	TYR
1	J	399	LEU
1	J	428	LEU
1	J	447	ARG
1	J	464	LEU
1	J	468	VAL
1	K	6	LEU
1	K	19	LEU
1	K	60	ILE
1	K	62	GLU
1	K	63	SER
1	K	64	ASP
1	K	65	MET
1	K	84	THR
1	K	88	ARG
1	K	96	THR
1	K	98	GLN
1	K	115	LEU
1	K	124	VAL
1	K	125	LEU
1	K	165	GLU
1	K	179	TYR
1	K	209	HIS
1	K	230	LYS
1	K	248	ARG
1	K	264	ASN
1	K	320	LYS
1	K	324	PRO
1	K	326	TYR
1	K	332	LEU
1	K	337	ARG
1	K	374	LEU
1	K	375	LEU
1	K	384	ASN
1	K	392	MET
1	K	396	LEU
1	K	397	TYR
1	K	399	LEU
1	K	428	LEU
1	K	447	ARG
1	K	464	LEU
1	K	468	VAL

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Mol	Chain	Res	Type
1	L	6	LEU
1	L	19	LEU
1	L	60	ILE
1	L	62	GLU
1	L	63	SER
1	L	64	ASP
1	L	65	MET
1	L	84	THR
1	L	88	ARG
1	L	96	THR
1	L	98	GLN
1	L	115	LEU
1	L	124	VAL
1	L	125	LEU
1	L	165	GLU
1	L	179	TYR
1	L	209	HIS
1	L	230	LYS
1	L	248	ARG
1	L	264	ASN
1	L	320	LYS
1	L	326	TYR
1	L	332	LEU
1	L	337	ARG
1	L	374	LEU
1	L	375	LEU
1	L	384	ASN
1	L	392	MET
1	L	396	LEU
1	L	397	TYR
1	L	399	LEU
1	L	428	LEU
1	L	447	ARG
1	L	464	LEU
1	L	468	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	211	HIS
1	A	218	GLN

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Continued from previous page...

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

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 60 ligands modelled in this entry, 24 are monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ADP	A	4471	2	22,29,29	3.09	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	A	5472	-	6,7,7	3.15	2 (33%)	7,10,10	1.42	1 (14%)
4	MPD	A	5481	-	6,7,7	1.54	1 (16%)	7,10,10	0.95	0
3	ADP	B	4472	2	22,29,29	3.07	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	B	5471	-	6,7,7	1.54	1 (16%)	7,10,10	0.95	0
4	MPD	B	5474	-	6,7,7	3.15	2 (33%)	7,10,10	1.42	1 (14%)
3	ADP	C	4473	2	22,29,29	3.08	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	C	5473	-	6,7,7	1.53	1 (16%)	7,10,10	0.95	0
4	MPD	C	5476	-	6,7,7	3.14	2 (33%)	7,10,10	1.42	1 (14%)
3	ADP	D	4474	2	22,29,29	3.09	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	D	5475	-	6,7,7	1.54	1 (16%)	7,10,10	0.95	0
4	MPD	D	5478	-	6,7,7	3.14	2 (33%)	7,10,10	1.42	1 (14%)
3	ADP	E	4475	2	22,29,29	3.09	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	E	5477	-	6,7,7	1.54	1 (16%)	7,10,10	0.95	0
4	MPD	E	5480	-	6,7,7	3.15	2 (33%)	7,10,10	1.42	1 (14%)
3	ADP	F	4476	2	22,29,29	3.09	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	F	5479	-	6,7,7	1.54	1 (16%)	7,10,10	0.96	0
4	MPD	F	5482	-	6,7,7	3.14	2 (33%)	7,10,10	1.42	1 (14%)
3	ADP	G	4477	2	22,29,29	3.08	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	G	5484	-	6,7,7	3.14	2 (33%)	7,10,10	1.42	1 (14%)
4	MPD	G	5485	-	6,7,7	1.54	1 (16%)	7,10,10	0.95	0
3	ADP	H	4478	2	22,29,29	3.09	8 (36%)	27,45,45	3.49	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	H	5486	-	6,7,7	3.14	2 (33%)	7,10,10	1.42	1 (14%)
4	MPD	H	5487	-	6,7,7	1.54	1 (16%)	7,10,10	0.95	0
3	ADP	I	4479	2	22,29,29	3.09	8 (36%)	27,45,45	3.49	10 (37%)
4	MPD	I	5488	-	6,7,7	3.14	2 (33%)	7,10,10	1.42	1 (14%)
4	MPD	I	5489	-	6,7,7	1.55	1 (16%)	7,10,10	0.95	0
3	ADP	J	4480	2	22,29,29	3.09	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	J	5490	-	6,7,7	3.14	2 (33%)	7,10,10	1.42	1 (14%)
4	MPD	J	5491	-	6,7,7	1.54	1 (16%)	7,10,10	0.95	0
3	ADP	K	4481	2	22,29,29	3.09	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	K	5492	-	6,7,7	3.14	2 (33%)	7,10,10	1.42	1 (14%)
4	MPD	K	5493	-	6,7,7	1.54	1 (16%)	7,10,10	0.95	0
3	ADP	L	4482	2	22,29,29	3.09	8 (36%)	27,45,45	3.48	10 (37%)
4	MPD	L	5483	-	6,7,7	1.54	1 (16%)	7,10,10	0.96	0
4	MPD	L	5494	-	6,7,7	3.16	2 (33%)	7,10,10	1.42	1 (14%)

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	4471	2	-	0/12/32/32	0/3/3/3
4	MPD	A	5472	-	-	0/5/5/5	0/0/0/0
4	MPD	A	5481	-	-	0/5/5/5	0/0/0/0
3	ADP	B	4472	2	-	0/12/32/32	0/3/3/3
4	MPD	B	5471	-	-	0/5/5/5	0/0/0/0
4	MPD	B	5474	-	-	0/5/5/5	0/0/0/0
3	ADP	C	4473	2	-	0/12/32/32	0/3/3/3
4	MPD	C	5473	-	-	0/5/5/5	0/0/0/0
4	MPD	C	5476	-	-	0/5/5/5	0/0/0/0
3	ADP	D	4474	2	-	0/12/32/32	0/3/3/3
4	MPD	D	5475	-	-	0/5/5/5	0/0/0/0
4	MPD	D	5478	-	-	0/5/5/5	0/0/0/0
3	ADP	E	4475	2	-	0/12/32/32	0/3/3/3
4	MPD	E	5477	-	-	0/5/5/5	0/0/0/0
4	MPD	E	5480	-	-	0/5/5/5	0/0/0/0
3	ADP	F	4476	2	-	0/12/32/32	0/3/3/3
4	MPD	F	5479	-	-	0/5/5/5	0/0/0/0
4	MPD	F	5482	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	G	4477	2	-	0/12/32/32	0/3/3/3
4	MPD	G	5484	-	-	0/5/5/5	0/0/0/0
4	MPD	G	5485	-	-	0/5/5/5	0/0/0/0
3	ADP	H	4478	2	-	0/12/32/32	0/3/3/3
4	MPD	H	5486	-	-	0/5/5/5	0/0/0/0
4	MPD	H	5487	-	-	0/5/5/5	0/0/0/0
3	ADP	I	4479	2	-	0/12/32/32	0/3/3/3
4	MPD	I	5488	-	-	0/5/5/5	0/0/0/0
4	MPD	I	5489	-	-	0/5/5/5	0/0/0/0
3	ADP	J	4480	2	-	0/12/32/32	0/3/3/3
4	MPD	J	5490	-	-	0/5/5/5	0/0/0/0
4	MPD	J	5491	-	-	0/5/5/5	0/0/0/0
3	ADP	K	4481	2	-	0/12/32/32	0/3/3/3
4	MPD	K	5492	-	-	0/5/5/5	0/0/0/0
4	MPD	K	5493	-	-	0/5/5/5	0/0/0/0
3	ADP	L	4482	2	-	0/12/32/32	0/3/3/3
4	MPD	L	5483	-	-	0/5/5/5	0/0/0/0
4	MPD	L	5494	-	-	0/5/5/5	0/0/0/0

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	5494	MPD	C1-C2	-6.20	1.31	1.52
4	E	5480	MPD	C1-C2	-6.18	1.31	1.52
4	C	5476	MPD	C1-C2	-6.18	1.31	1.52
4	B	5474	MPD	C1-C2	-6.18	1.31	1.52
4	A	5472	MPD	C1-C2	-6.17	1.31	1.52
4	K	5492	MPD	C1-C2	-6.17	1.31	1.52
4	D	5478	MPD	C1-C2	-6.16	1.31	1.52
4	I	5488	MPD	C1-C2	-6.16	1.31	1.52
4	G	5484	MPD	C1-C2	-6.16	1.31	1.52
4	H	5486	MPD	C1-C2	-6.16	1.31	1.52
4	J	5490	MPD	C1-C2	-6.15	1.31	1.52
4	F	5482	MPD	C1-C2	-6.15	1.31	1.52
3	B	4472	ADP	C6-N6	-4.11	1.22	1.34
3	D	4474	ADP	C6-N6	-4.10	1.22	1.34
3	I	4479	ADP	C6-N6	-4.10	1.22	1.34
3	J	4480	ADP	C6-N6	-4.09	1.22	1.34
3	A	4471	ADP	C6-N6	-4.09	1.22	1.34
3	F	4476	ADP	C6-N6	-4.09	1.22	1.34
3	H	4478	ADP	C6-N6	-4.08	1.22	1.34
3	K	4481	ADP	C6-N6	-4.08	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	4482	ADP	C6-N6	-4.08	1.22	1.34
3	C	4473	ADP	C6-N6	-4.08	1.22	1.34
3	E	4475	ADP	C6-N6	-4.08	1.22	1.34
3	G	4477	ADP	C6-N6	-4.07	1.22	1.34
4	B	5474	MPD	O2-C2	-4.06	1.33	1.44
4	F	5482	MPD	O2-C2	-4.06	1.33	1.44
4	A	5472	MPD	O2-C2	-4.05	1.33	1.44
4	J	5490	MPD	O2-C2	-4.05	1.33	1.44
4	L	5494	MPD	O2-C2	-4.05	1.33	1.44
4	K	5492	MPD	O2-C2	-4.05	1.33	1.44
4	I	5488	MPD	O2-C2	-4.05	1.33	1.44
4	H	5486	MPD	O2-C2	-4.05	1.33	1.44
4	E	5480	MPD	O2-C2	-4.04	1.33	1.44
4	G	5484	MPD	O2-C2	-4.04	1.33	1.44
4	C	5476	MPD	O2-C2	-4.04	1.33	1.44
4	D	5478	MPD	O2-C2	-4.03	1.33	1.44
4	H	5487	MPD	CM-C2	-2.77	1.43	1.52
4	E	5477	MPD	CM-C2	-2.77	1.43	1.52
4	F	5479	MPD	CM-C2	-2.77	1.43	1.52
4	L	5483	MPD	CM-C2	-2.76	1.43	1.52
4	I	5489	MPD	CM-C2	-2.76	1.43	1.52
4	G	5485	MPD	CM-C2	-2.76	1.43	1.52
4	B	5471	MPD	CM-C2	-2.75	1.43	1.52
4	K	5493	MPD	CM-C2	-2.75	1.43	1.52
4	A	5481	MPD	CM-C2	-2.75	1.43	1.52
4	C	5473	MPD	CM-C2	-2.74	1.43	1.52
4	J	5491	MPD	CM-C2	-2.74	1.43	1.52
4	D	5475	MPD	CM-C2	-2.73	1.43	1.52
3	F	4476	ADP	C3'-C4'	-2.37	1.46	1.53
3	J	4480	ADP	C3'-C4'	-2.36	1.46	1.53
3	I	4479	ADP	C3'-C4'	-2.35	1.46	1.53
3	D	4474	ADP	C3'-C4'	-2.35	1.46	1.53
3	L	4482	ADP	C3'-C4'	-2.35	1.46	1.53
3	C	4473	ADP	C3'-C4'	-2.35	1.46	1.53
3	A	4471	ADP	C3'-C4'	-2.35	1.46	1.53
3	E	4475	ADP	C3'-C4'	-2.34	1.46	1.53
3	H	4478	ADP	C3'-C4'	-2.34	1.46	1.53
3	B	4472	ADP	C3'-C4'	-2.33	1.46	1.53
3	K	4481	ADP	C3'-C4'	-2.33	1.46	1.53
3	G	4477	ADP	C3'-C4'	-2.33	1.46	1.53
3	H	4478	ADP	C5-C4	2.43	1.46	1.40
3	B	4472	ADP	C5-C4	2.44	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	4482	ADP	C5-C4	2.45	1.46	1.40
3	C	4473	ADP	C5-C4	2.46	1.46	1.40
3	I	4479	ADP	C5-C4	2.46	1.46	1.40
3	F	4476	ADP	C5-C4	2.46	1.46	1.40
3	A	4471	ADP	C5-C4	2.47	1.46	1.40
3	J	4480	ADP	C5-C4	2.47	1.46	1.40
3	K	4481	ADP	C5-C4	2.47	1.46	1.40
3	D	4474	ADP	C5-C4	2.48	1.46	1.40
3	G	4477	ADP	C5-C4	2.48	1.46	1.40
3	E	4475	ADP	C5-C4	2.49	1.46	1.40
3	L	4482	ADP	C2-N3	3.44	1.38	1.32
3	F	4476	ADP	C2-N3	3.46	1.38	1.32
3	E	4475	ADP	C2-N3	3.47	1.38	1.32
3	B	4472	ADP	C2-N3	3.47	1.38	1.32
3	D	4474	ADP	C2-N3	3.48	1.38	1.32
3	H	4478	ADP	C2-N3	3.48	1.38	1.32
3	A	4471	ADP	C2-N3	3.49	1.38	1.32
3	C	4473	ADP	C2-N3	3.49	1.38	1.32
3	G	4477	ADP	C2-N3	3.50	1.38	1.32
3	I	4479	ADP	C2-N3	3.50	1.38	1.32
3	J	4480	ADP	C2-N3	3.50	1.38	1.32
3	K	4481	ADP	C2-N3	3.51	1.38	1.32
3	F	4476	ADP	PB-O3B	3.58	1.67	1.54
3	K	4481	ADP	PB-O3B	3.59	1.67	1.54
3	J	4480	ADP	PB-O3B	3.59	1.67	1.54
3	B	4472	ADP	PB-O3B	3.60	1.67	1.54
3	C	4473	ADP	PB-O3B	3.60	1.67	1.54
3	E	4475	ADP	PB-O3B	3.60	1.67	1.54
3	L	4482	ADP	PB-O3B	3.60	1.67	1.54
3	G	4477	ADP	PB-O3B	3.60	1.67	1.54
3	A	4471	ADP	PB-O3B	3.61	1.67	1.54
3	I	4479	ADP	PB-O3B	3.61	1.67	1.54
3	H	4478	ADP	PB-O3B	3.61	1.67	1.54
3	D	4474	ADP	PB-O3B	3.61	1.67	1.54
3	I	4479	ADP	C4-N3	4.64	1.42	1.35
3	B	4472	ADP	C4-N3	4.64	1.42	1.35
3	E	4475	ADP	C4-N3	4.65	1.42	1.35
3	K	4481	ADP	C4-N3	4.65	1.42	1.35
3	C	4473	ADP	C4-N3	4.65	1.42	1.35
3	J	4480	ADP	C4-N3	4.66	1.42	1.35
3	A	4471	ADP	C4-N3	4.66	1.42	1.35
3	G	4477	ADP	C4-N3	4.66	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4474	ADP	C4-N3	4.67	1.42	1.35
3	F	4476	ADP	C4-N3	4.70	1.42	1.35
3	H	4478	ADP	C4-N3	4.70	1.42	1.35
3	L	4482	ADP	C4-N3	4.71	1.42	1.35
3	H	4478	ADP	O4'-C4'	5.51	1.57	1.45
3	C	4473	ADP	O4'-C4'	5.51	1.57	1.45
3	K	4481	ADP	O4'-C4'	5.52	1.57	1.45
3	B	4472	ADP	O4'-C4'	5.52	1.57	1.45
3	L	4482	ADP	O4'-C4'	5.52	1.57	1.45
3	G	4477	ADP	O4'-C4'	5.53	1.57	1.45
3	A	4471	ADP	O4'-C4'	5.54	1.57	1.45
3	J	4480	ADP	O4'-C4'	5.54	1.57	1.45
3	F	4476	ADP	O4'-C4'	5.55	1.57	1.45
3	D	4474	ADP	O4'-C4'	5.55	1.57	1.45
3	I	4479	ADP	O4'-C4'	5.55	1.57	1.45
3	E	4475	ADP	O4'-C4'	5.58	1.57	1.45
3	B	4472	ADP	O4'-C1'	9.56	1.53	1.41
3	I	4479	ADP	O4'-C1'	9.59	1.53	1.41
3	E	4475	ADP	O4'-C1'	9.59	1.53	1.41
3	G	4477	ADP	O4'-C1'	9.60	1.53	1.41
3	J	4480	ADP	O4'-C1'	9.60	1.53	1.41
3	A	4471	ADP	O4'-C1'	9.61	1.53	1.41
3	H	4478	ADP	O4'-C1'	9.61	1.53	1.41
3	D	4474	ADP	O4'-C1'	9.62	1.53	1.41
3	C	4473	ADP	O4'-C1'	9.62	1.53	1.41
3	F	4476	ADP	O4'-C1'	9.64	1.53	1.41
3	L	4482	ADP	O4'-C1'	9.66	1.53	1.41
3	K	4481	ADP	O4'-C1'	9.67	1.53	1.41

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	4480	ADP	C4'-O4'-C1'	-9.92	98.82	109.72
3	F	4476	ADP	C4'-O4'-C1'	-9.92	98.82	109.72
3	D	4474	ADP	C4'-O4'-C1'	-9.92	98.82	109.72
3	C	4473	ADP	C4'-O4'-C1'	-9.91	98.83	109.72
3	I	4479	ADP	C4'-O4'-C1'	-9.91	98.83	109.72
3	E	4475	ADP	C4'-O4'-C1'	-9.90	98.85	109.72
3	H	4478	ADP	C4'-O4'-C1'	-9.89	98.86	109.72
3	A	4471	ADP	C4'-O4'-C1'	-9.89	98.86	109.72
3	K	4481	ADP	C4'-O4'-C1'	-9.88	98.86	109.72
3	G	4477	ADP	C4'-O4'-C1'	-9.88	98.86	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	4482	ADP	C4'-O4'-C1'	-9.88	98.87	109.72
3	B	4472	ADP	C4'-O4'-C1'	-9.86	98.88	109.72
3	G	4477	ADP	C5'-C4'-C3'	-3.91	99.71	115.21
3	D	4474	ADP	C5'-C4'-C3'	-3.90	99.71	115.21
3	B	4472	ADP	C5'-C4'-C3'	-3.90	99.72	115.21
3	C	4473	ADP	C5'-C4'-C3'	-3.90	99.74	115.21
3	L	4482	ADP	C5'-C4'-C3'	-3.90	99.74	115.21
3	K	4481	ADP	C5'-C4'-C3'	-3.90	99.74	115.21
3	A	4471	ADP	C5'-C4'-C3'	-3.90	99.75	115.21
3	H	4478	ADP	C5'-C4'-C3'	-3.89	99.76	115.21
3	F	4476	ADP	C5'-C4'-C3'	-3.89	99.77	115.21
3	J	4480	ADP	C5'-C4'-C3'	-3.89	99.77	115.21
3	E	4475	ADP	C5'-C4'-C3'	-3.89	99.78	115.21
3	I	4479	ADP	C5'-C4'-C3'	-3.89	99.78	115.21
4	J	5490	MPD	O2-C2-C1	-3.05	96.93	108.09
4	I	5488	MPD	O2-C2-C1	-3.04	96.93	108.09
4	E	5480	MPD	O2-C2-C1	-3.04	96.94	108.09
4	F	5482	MPD	O2-C2-C1	-3.04	96.96	108.09
4	C	5476	MPD	O2-C2-C1	-3.04	96.96	108.09
4	A	5472	MPD	O2-C2-C1	-3.03	96.97	108.09
4	G	5484	MPD	O2-C2-C1	-3.03	96.97	108.09
4	H	5486	MPD	O2-C2-C1	-3.03	96.97	108.09
4	D	5478	MPD	O2-C2-C1	-3.03	96.98	108.09
4	B	5474	MPD	O2-C2-C1	-3.03	96.99	108.09
4	L	5494	MPD	O2-C2-C1	-3.03	96.99	108.09
4	K	5492	MPD	O2-C2-C1	-3.03	97.00	108.09
3	F	4476	ADP	PA-O3A-PB	2.00	139.37	132.67
3	J	4480	ADP	PA-O3A-PB	2.00	139.38	132.67
3	I	4479	ADP	PA-O3A-PB	2.01	139.40	132.67
3	C	4473	ADP	PA-O3A-PB	2.01	139.40	132.67
3	D	4474	ADP	PA-O3A-PB	2.01	139.40	132.67
3	A	4471	ADP	PA-O3A-PB	2.01	139.41	132.67
3	L	4482	ADP	PA-O3A-PB	2.01	139.41	132.67
3	B	4472	ADP	PA-O3A-PB	2.01	139.41	132.67
3	K	4481	ADP	PA-O3A-PB	2.02	139.42	132.67
3	H	4478	ADP	PA-O3A-PB	2.02	139.43	132.67
3	G	4477	ADP	PA-O3A-PB	2.02	139.43	132.67
3	E	4475	ADP	PA-O3A-PB	2.02	139.45	132.67
3	L	4482	ADP	O3'-C3'-C2'	2.24	119.13	111.83
3	D	4474	ADP	O3'-C3'-C2'	2.25	119.16	111.83
3	F	4476	ADP	O3'-C3'-C2'	2.26	119.16	111.83
3	C	4473	ADP	O3'-C3'-C2'	2.26	119.17	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4477	ADP	O3'-C3'-C2'	2.26	119.18	111.83
3	K	4481	ADP	O3'-C3'-C2'	2.26	119.18	111.83
3	A	4471	ADP	O3'-C3'-C2'	2.26	119.19	111.83
3	J	4480	ADP	O3'-C3'-C2'	2.26	119.19	111.83
3	E	4475	ADP	O3'-C3'-C2'	2.27	119.20	111.83
3	B	4472	ADP	O3'-C3'-C2'	2.27	119.21	111.83
3	H	4478	ADP	O3'-C3'-C2'	2.27	119.22	111.83
3	I	4479	ADP	O3'-C3'-C2'	2.27	119.22	111.83
3	I	4479	ADP	O4'-C4'-C5'	3.17	120.64	109.32
3	C	4473	ADP	O4'-C4'-C5'	3.17	120.64	109.32
3	F	4476	ADP	O4'-C4'-C5'	3.17	120.65	109.32
3	E	4475	ADP	O4'-C4'-C5'	3.17	120.66	109.32
3	G	4477	ADP	O4'-C4'-C5'	3.17	120.66	109.32
3	D	4474	ADP	O4'-C4'-C5'	3.17	120.66	109.32
3	A	4471	ADP	O4'-C4'-C5'	3.17	120.67	109.32
3	H	4478	ADP	O4'-C4'-C5'	3.18	120.68	109.32
3	L	4482	ADP	O4'-C4'-C5'	3.18	120.68	109.32
3	K	4481	ADP	O4'-C4'-C5'	3.18	120.68	109.32
3	J	4480	ADP	O4'-C4'-C5'	3.18	120.68	109.32
3	B	4472	ADP	O4'-C4'-C5'	3.19	120.71	109.32
3	F	4476	ADP	O3A-PA-O5'	3.58	112.42	102.94
3	I	4479	ADP	O3A-PA-O5'	3.59	112.45	102.94
3	D	4474	ADP	O3A-PA-O5'	3.59	112.46	102.94
3	C	4473	ADP	O3A-PA-O5'	3.59	112.47	102.94
3	J	4480	ADP	O3A-PA-O5'	3.60	112.48	102.94
3	A	4471	ADP	O3A-PA-O5'	3.60	112.48	102.94
3	L	4482	ADP	O3A-PA-O5'	3.60	112.48	102.94
3	B	4472	ADP	O3A-PA-O5'	3.60	112.48	102.94
3	K	4481	ADP	O3A-PA-O5'	3.60	112.49	102.94
3	G	4477	ADP	O3A-PA-O5'	3.60	112.49	102.94
3	H	4478	ADP	O3A-PA-O5'	3.60	112.50	102.94
3	E	4475	ADP	O3A-PA-O5'	3.61	112.51	102.94
3	D	4474	ADP	C4-C5-N7	5.31	114.36	109.48
3	G	4477	ADP	C4-C5-N7	5.33	114.38	109.48
3	K	4481	ADP	C4-C5-N7	5.33	114.38	109.48
3	F	4476	ADP	C4-C5-N7	5.33	114.39	109.48
3	J	4480	ADP	C4-C5-N7	5.34	114.39	109.48
3	C	4473	ADP	C4-C5-N7	5.35	114.40	109.48
3	A	4471	ADP	C4-C5-N7	5.35	114.40	109.48
3	L	4482	ADP	C4-C5-N7	5.36	114.41	109.48
3	H	4478	ADP	C4-C5-N7	5.36	114.41	109.48
3	I	4479	ADP	C4-C5-N7	5.37	114.42	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4475	ADP	C4-C5-N7	5.39	114.43	109.48
3	B	4472	ADP	C4-C5-N7	5.42	114.46	109.48
3	B	4472	ADP	C1'-N9-C4	5.70	135.54	126.94
3	G	4477	ADP	C1'-N9-C4	5.70	135.54	126.94
3	F	4476	ADP	C1'-N9-C4	5.71	135.55	126.94
3	D	4474	ADP	C1'-N9-C4	5.71	135.55	126.94
3	E	4475	ADP	C1'-N9-C4	5.71	135.56	126.94
3	K	4481	ADP	C1'-N9-C4	5.72	135.57	126.94
3	A	4471	ADP	C1'-N9-C4	5.73	135.58	126.94
3	C	4473	ADP	C1'-N9-C4	5.73	135.59	126.94
3	I	4479	ADP	C1'-N9-C4	5.73	135.59	126.94
3	J	4480	ADP	C1'-N9-C4	5.74	135.59	126.94
3	L	4482	ADP	C1'-N9-C4	5.74	135.60	126.94
3	H	4478	ADP	C1'-N9-C4	5.75	135.61	126.94
3	E	4475	ADP	O4'-C1'-N9	6.27	121.23	108.10
3	J	4480	ADP	O4'-C1'-N9	6.28	121.23	108.10
3	D	4474	ADP	O4'-C1'-N9	6.28	121.24	108.10
3	G	4477	ADP	O4'-C1'-N9	6.28	121.25	108.10
3	I	4479	ADP	O4'-C1'-N9	6.28	121.25	108.10
3	A	4471	ADP	O4'-C1'-N9	6.29	121.26	108.10
3	K	4481	ADP	O4'-C1'-N9	6.29	121.26	108.10
3	H	4478	ADP	O4'-C1'-N9	6.29	121.26	108.10
3	F	4476	ADP	O4'-C1'-N9	6.29	121.26	108.10
3	L	4482	ADP	O4'-C1'-N9	6.30	121.29	108.10
3	C	4473	ADP	O4'-C1'-N9	6.30	121.29	108.10
3	B	4472	ADP	O4'-C1'-N9	6.31	121.30	108.10
3	B	4472	ADP	O5'-C5'-C4'	7.74	137.64	109.12
3	G	4477	ADP	O5'-C5'-C4'	7.74	137.66	109.12
3	K	4481	ADP	O5'-C5'-C4'	7.74	137.66	109.12
3	A	4471	ADP	O5'-C5'-C4'	7.75	137.68	109.12
3	H	4478	ADP	O5'-C5'-C4'	7.75	137.69	109.12
3	E	4475	ADP	O5'-C5'-C4'	7.75	137.69	109.12
3	C	4473	ADP	O5'-C5'-C4'	7.75	137.69	109.12
3	D	4474	ADP	O5'-C5'-C4'	7.75	137.69	109.12
3	F	4476	ADP	O5'-C5'-C4'	7.75	137.70	109.12
3	I	4479	ADP	O5'-C5'-C4'	7.76	137.71	109.12
3	J	4480	ADP	O5'-C5'-C4'	7.76	137.73	109.12
3	L	4482	ADP	O5'-C5'-C4'	7.76	137.73	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

36 monomers are involved in 753 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4471	ADP	1	0
4	A	5472	MPD	29	0
4	A	5481	MPD	27	0
3	B	4472	ADP	1	0
4	B	5471	MPD	30	0
4	B	5474	MPD	30	0
3	C	4473	ADP	1	0
4	C	5473	MPD	32	0
4	C	5476	MPD	30	0
3	D	4474	ADP	1	0
4	D	5475	MPD	31	0
4	D	5478	MPD	30	0
3	E	4475	ADP	1	0
4	E	5477	MPD	25	0
4	E	5480	MPD	29	0
3	F	4476	ADP	1	0
4	F	5479	MPD	33	0
4	F	5482	MPD	29	0
3	G	4477	ADP	1	0
4	G	5484	MPD	32	0
4	G	5485	MPD	28	0
3	H	4478	ADP	1	0
4	H	5486	MPD	30	0
4	H	5487	MPD	35	0
3	I	4479	ADP	1	0
4	I	5488	MPD	31	0
4	I	5489	MPD	31	0
3	J	4480	ADP	1	0
4	J	5490	MPD	29	0
4	J	5491	MPD	39	0
3	K	4481	ADP	1	0
4	K	5492	MPD	30	0
4	K	5493	MPD	36	0
3	L	4482	ADP	1	0
4	L	5483	MPD	35	0
4	L	5494	MPD	30	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	468/468 (100%)	1.56	147 (31%) 1 0	28, 48, 96, 100	19 (4%)
1	B	468/468 (100%)	0.93	77 (16%) 2 2	28, 48, 96, 100	19 (4%)
1	C	468/468 (100%)	0.84	68 (14%) 3 3	28, 48, 96, 100	19 (4%)
1	D	468/468 (100%)	0.50	50 (10%) 8 8	28, 48, 96, 100	19 (4%)
1	E	468/468 (100%)	0.85	79 (16%) 2 2	28, 48, 96, 100	19 (4%)
1	F	468/468 (100%)	0.86	56 (11%) 6 6	28, 48, 96, 100	19 (4%)
1	G	468/468 (100%)	0.60	48 (10%) 9 9	28, 48, 96, 100	19 (4%)
1	H	468/468 (100%)	0.59	41 (8%) 12 13	28, 48, 96, 100	19 (4%)
1	I	468/468 (100%)	0.54	36 (7%) 16 18	28, 48, 96, 100	19 (4%)
1	J	468/468 (100%)	0.55	33 (7%) 19 21	28, 48, 96, 100	19 (4%)
1	K	468/468 (100%)	0.47	34 (7%) 18 20	28, 48, 96, 100	19 (4%)
1	L	468/468 (100%)	0.71	44 (9%) 11 11	28, 48, 96, 100	19 (4%)
All	All	5616/5616 (100%)	0.75	713 (12%) 5 5	28, 48, 96, 100	228 (4%)

All (713) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	397	TYR	14.8
1	J	397	TYR	13.4
1	G	397	TYR	12.7
1	B	397	TYR	12.7
1	A	397	TYR	12.6
1	F	398	ASP	12.5
1	C	398	ASP	12.5
1	F	397	TYR	12.4
1	A	398	ASP	12.4
1	I	397	TYR	12.1
1	C	399	LEU	11.5

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Mol	Chain	Res	Type	RSRZ
1	L	397	TYR	11.2
1	E	395	ASN	11.2
1	F	404	ALA	10.8
1	E	397	TYR	10.6
1	G	399	LEU	10.4
1	A	277	ASN	10.2
1	E	399	LEU	10.1
1	C	404	ALA	10.1
1	D	326	TYR	9.9
1	A	351	PRO	9.9
1	E	404	ALA	9.9
1	D	399	LEU	9.8
1	K	397	TYR	9.7
1	A	395	ASN	9.5
1	B	399	LEU	9.5
1	I	398	ASP	9.5
1	A	326	TYR	9.4
1	L	399	LEU	9.3
1	B	398	ASP	9.1
1	A	334	TYR	9.0
1	E	400	PRO	8.9
1	K	399	LEU	8.9
1	F	399	LEU	8.7
1	A	285	ASP	8.6
1	H	395	ASN	8.6
1	D	400	PRO	8.5
1	I	399	LEU	8.4
1	B	394	LYS	8.3
1	H	398	ASP	8.2
1	D	397	TYR	8.2
1	B	401	PRO	8.1
1	B	61	ASN	8.1
1	H	402	GLU	8.1
1	F	326	TYR	8.0
1	H	399	LEU	7.9
1	B	404	ALA	7.7
1	C	396	LEU	7.7
1	F	401	PRO	7.6
1	B	326	TYR	7.6
1	E	396	LEU	7.6
1	F	395	ASN	7.6
1	A	337	ARG	7.6

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Mol	Chain	Res	Type	RSRZ
1	K	398	ASP	7.6
1	I	404	ALA	7.4
1	A	296	TYR	7.4
1	G	398	ASP	7.4
1	H	403	GLU	7.3
1	J	398	ASP	7.3
1	B	395	ASN	7.3
1	B	396	LEU	7.3
1	A	345	ILE	7.2
1	A	116	ARG	7.2
1	A	404	ALA	7.2
1	I	405	LYS	7.0
1	D	394	LYS	7.0
1	E	394	LYS	7.0
1	K	326	TYR	6.9
1	A	396	LEU	6.9
1	F	394	LYS	6.9
1	C	394	LYS	6.9
1	L	61	ASN	6.9
1	D	395	ASN	6.9
1	A	347	VAL	6.8
1	C	400	PRO	6.8
1	H	397	TYR	6.7
1	E	349	ALA	6.7
1	A	348	VAL	6.7
1	L	405	LYS	6.6
1	F	400	PRO	6.6
1	F	62	GLU	6.5
1	F	60	ILE	6.5
1	F	337	ARG	6.4
1	G	403	GLU	6.3
1	L	326	TYR	6.3
1	A	278	GLY	6.3
1	A	399	LEU	6.3
1	F	402	GLU	6.2
1	E	326	TYR	6.1
1	H	61	ASN	6.1
1	C	401	PRO	6.1
1	A	333	ALA	6.0
1	E	402	GLU	6.0
1	F	396	LEU	6.0
1	E	398	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	1	SER	5.9
1	J	326	TYR	5.9
1	I	61	ASN	5.9
1	D	403	GLU	5.8
1	G	404	ALA	5.8
1	K	395	ASN	5.8
1	B	392	MET	5.7
1	A	288	ALA	5.7
1	C	395	ASN	5.7
1	G	61	ASN	5.7
1	I	326	TYR	5.7
1	A	354	ARG	5.7
1	D	60	ILE	5.6
1	E	12	HIS	5.6
1	A	292	GLU	5.6
1	A	61	ASN	5.6
1	C	326	TYR	5.5
1	A	338	ASN	5.5
1	C	402	GLU	5.5
1	A	287	TYR	5.4
1	F	406	GLU	5.4
1	I	402	GLU	5.4
1	A	392	MET	5.3
1	L	398	ASP	5.3
1	H	326	TYR	5.3
1	L	62	GLU	5.3
1	A	123	THR	5.3
1	B	95	GLY	5.3
1	A	91	ILE	5.2
1	G	400	PRO	5.2
1	A	286	LYS	5.2
1	D	398	ASP	5.2
1	F	405	LYS	5.2
1	L	400	PRO	5.2
1	G	62	GLU	5.1
1	B	60	ILE	5.1
1	F	403	GLU	5.1
1	C	61	ASN	5.1
1	G	402	GLU	5.1
1	B	402	GLU	5.1
1	E	348	VAL	5.1
1	A	401	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	J	399	LEU	5.0
1	C	287	TYR	5.0
1	C	337	ARG	5.0
1	I	337	ARG	5.0
1	D	401	PRO	5.0
1	A	60	ILE	5.0
1	L	395	ASN	5.0
1	L	401	PRO	5.0
1	A	391	PRO	5.0
1	K	403	GLU	4.9
1	E	61	ASN	4.9
1	A	294	ALA	4.9
1	H	405	LYS	4.9
1	C	403	GLU	4.9
1	A	382	ILE	4.9
1	B	400	PRO	4.9
1	G	406	GLU	4.9
1	C	405	LYS	4.8
1	B	351	PRO	4.8
1	K	402	GLU	4.8
1	E	401	PRO	4.8
1	A	352	LYS	4.8
1	A	274	LEU	4.8
1	L	396	LEU	4.8
1	A	402	GLU	4.8
1	A	299	GLY	4.7
1	H	337	ARG	4.7
1	G	405	LYS	4.7
1	H	400	PRO	4.7
1	E	7	THR	4.7
1	H	60	ILE	4.7
1	L	60	ILE	4.7
1	E	4	HIS	4.7
1	H	12	HIS	4.7
1	F	61	ASN	4.7
1	C	62	GLU	4.7
1	I	62	GLU	4.6
1	B	406	GLU	4.6
1	I	403	GLU	4.6
1	F	349	ALA	4.6
1	A	344	ARG	4.6
1	A	275	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	407	ILE	4.6
1	J	60	ILE	4.6
1	G	395	ASN	4.6
1	F	98	GLN	4.5
1	I	401	PRO	4.4
1	E	337	ARG	4.4
1	B	393	ASP	4.4
1	G	326	TYR	4.4
1	E	283	SER	4.4
1	D	402	GLU	4.4
1	L	394	LYS	4.4
1	G	63	SER	4.3
1	G	396	LEU	4.2
1	F	351	PRO	4.2
1	J	400	PRO	4.2
1	I	400	PRO	4.2
1	A	3	GLU	4.2
1	A	118	THR	4.2
1	A	121	ALA	4.2
1	F	353	ALA	4.2
1	H	7	THR	4.2
1	A	405	LYS	4.2
1	E	62	GLU	4.2
1	E	277	ASN	4.2
1	K	396	LEU	4.2
1	C	406	GLU	4.2
1	A	280	ASN	4.2
1	G	401	PRO	4.2
1	E	405	LYS	4.1
1	A	390	GLU	4.1
1	B	327	GLU	4.1
1	H	62	GLU	4.1
1	B	405	LYS	4.1
1	J	337	ARG	4.1
1	A	380	ASP	4.1
1	E	60	ILE	4.1
1	A	117	ALA	4.1
1	D	405	LYS	4.0
1	J	395	ASN	4.0
1	A	124	VAL	4.0
1	B	403	GLU	4.0
1	C	282	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	394	LYS	4.0
1	E	279	THR	4.0
1	A	335	SER	3.9
1	D	348	VAL	3.9
1	E	392	MET	3.9
1	L	404	ALA	3.9
1	G	339	ARG	3.9
1	A	273	SER	3.9
1	C	296	TYR	3.9
1	A	122	ASP	3.9
1	C	60	ILE	3.9
1	A	293	GLN	3.9
1	B	117	ALA	3.9
1	A	2	ALA	3.8
1	A	340	SER	3.8
1	J	405	LYS	3.8
1	E	339	ARG	3.8
1	G	1	SER	3.8
1	A	387	HIS	3.8
1	C	348	VAL	3.8
1	A	276	LYS	3.8
1	E	42	PHE	3.8
1	A	179	TYR	3.7
1	G	337	ARG	3.7
1	D	393	ASP	3.7
1	E	282	PHE	3.7
1	A	328	ALA	3.7
1	L	402	GLU	3.7
1	D	396	LEU	3.7
1	E	285	ASP	3.7
1	B	62	GLU	3.7
1	K	394	LYS	3.7
1	C	285	ASP	3.7
1	D	391	PRO	3.7
1	K	404	ALA	3.6
1	A	290	LEU	3.6
1	E	278	GLY	3.6
1	A	224	ARG	3.6
1	K	327	GLU	3.6
1	F	296	TYR	3.6
1	J	401	PRO	3.6
1	B	12	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	42	PHE	3.6
1	G	349	ALA	3.6
1	K	385	LYS	3.6
1	F	333	ALA	3.5
1	B	65	MET	3.5
1	H	8	MET	3.5
1	C	293	GLN	3.5
1	L	339	ARG	3.5
1	F	407	ILE	3.5
1	A	379	LEU	3.5
1	F	327	GLU	3.5
1	A	355	ARG	3.5
1	A	126	PHE	3.5
1	G	44	GLU	3.5
1	H	394	LYS	3.5
1	J	403	GLU	3.5
1	A	51	GLY	3.4
1	A	356	ILE	3.4
1	D	352	LYS	3.4
1	A	62	GLU	3.4
1	F	348	VAL	3.4
1	C	392	MET	3.4
1	G	60	ILE	3.4
1	A	330	VAL	3.4
1	J	7	THR	3.4
1	B	391	PRO	3.4
1	K	401	PRO	3.4
1	L	59	GLY	3.4
1	K	405	LYS	3.4
1	A	279	THR	3.4
1	A	353	ALA	3.4
1	J	404	ALA	3.4
1	A	327	GLU	3.3
1	L	403	GLU	3.3
1	A	38	VAL	3.3
1	B	331	MET	3.3
1	H	339	ARG	3.3
1	E	354	ARG	3.3
1	K	337	ARG	3.3
1	B	123	THR	3.3
1	C	281	LEU	3.3
1	C	386	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	351	PRO	3.3
1	B	51	GLY	3.3
1	A	5	VAL	3.3
1	A	400	PRO	3.3
1	A	108	ALA	3.3
1	F	390	GLU	3.2
1	K	400	PRO	3.2
1	A	349	ALA	3.2
1	E	353	ALA	3.2
1	C	389	GLY	3.2
1	J	393	ASP	3.2
1	I	285	ASP	3.2
1	I	393	ASP	3.2
1	A	339	ARG	3.2
1	A	343	ILE	3.2
1	E	347	VAL	3.2
1	D	9	LEU	3.2
1	D	40	ALA	3.2
1	J	394	LYS	3.2
1	E	351	PRO	3.2
1	H	5	VAL	3.2
1	H	4	HIS	3.2
1	A	7	THR	3.2
1	A	375	LEU	3.1
1	C	407	ILE	3.1
1	J	402	GLU	3.1
1	C	275	ALA	3.1
1	G	393	ASP	3.1
1	C	408	PRO	3.1
1	A	431	GLY	3.1
1	C	349	ALA	3.1
1	D	4	HIS	3.1
1	G	179	TYR	3.1
1	A	403	GLU	3.1
1	H	10	ASN	3.1
1	K	62	GLU	3.1
1	A	324	PRO	3.1
1	C	96	THR	3.1
1	A	406	GLU	3.1
1	C	437	GLU	3.1
1	L	349	ALA	3.1
1	A	52	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	354	ARG	3.1
1	D	404	ALA	3.1
1	A	63	SER	3.1
1	F	352	LYS	3.1
1	I	60	ILE	3.1
1	K	349	ALA	3.1
1	J	62	GLU	3.1
1	J	339	ARG	3.1
1	H	407	ILE	3.0
1	E	393	ASP	3.0
1	G	2	ALA	3.0
1	A	383	LYS	3.0
1	A	94	PRO	3.0
1	L	408	PRO	3.0
1	A	282	PHE	3.0
1	E	423	LEU	3.0
1	A	10	ASN	3.0
1	I	407	ILE	3.0
1	A	289	GLY	3.0
1	H	408	PRO	3.0
1	C	7	THR	3.0
1	B	35	ALA	3.0
1	C	347	VAL	3.0
1	A	11	GLU	3.0
1	J	407	ILE	3.0
1	H	401	PRO	3.0
1	L	388	PRO	3.0
1	A	284	GLY	3.0
1	D	349	ALA	3.0
1	A	332	LEU	2.9
1	C	279	THR	2.9
1	B	275	ALA	2.9
1	F	277	ASN	2.9
1	A	323	VAL	2.9
1	H	350	SER	2.9
1	C	121	ALA	2.9
1	C	120	ILE	2.9
1	J	179	TYR	2.9
1	A	346	PRO	2.9
1	E	293	GLN	2.9
1	A	423	LEU	2.9
1	G	96	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	61	ASN	2.9
1	A	408	PRO	2.9
1	I	406	GLU	2.9
1	A	381	GLY	2.9
1	C	393	ASP	2.9
1	A	291	SER	2.9
1	G	348	VAL	2.9
1	E	428	LEU	2.9
1	I	395	ASN	2.9
1	H	179	TYR	2.9
1	E	323	VAL	2.9
1	E	403	GLU	2.9
1	C	98	GLN	2.9
1	A	40	ALA	2.9
1	D	285	ASP	2.9
1	A	342	SER	2.8
1	A	272	MET	2.8
1	L	393	ASP	2.8
1	I	349	ALA	2.8
1	J	61	ASN	2.8
1	F	282	PHE	2.8
1	J	390	GLU	2.8
1	A	46	GLY	2.8
1	B	58	LYS	2.8
1	E	327	GLU	2.8
1	D	42	PHE	2.8
1	F	116	ARG	2.8
1	A	100	TYR	2.8
1	E	430	ALA	2.8
1	B	11	GLU	2.8
1	E	292	GLU	2.8
1	C	122	ASP	2.8
1	A	115	LEU	2.8
1	A	125	LEU	2.8
1	I	6	LEU	2.8
1	D	392	MET	2.8
1	F	331	MET	2.8
1	F	392	MET	2.8
1	F	2	ALA	2.8
1	D	224	ARG	2.8
1	A	120	ILE	2.8
1	D	95	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	331	MET	2.8
1	G	407	ILE	2.7
1	E	9	LEU	2.7
1	D	339	ARG	2.7
1	I	63	SER	2.7
1	B	98	GLN	2.7
1	B	6	LEU	2.7
1	C	339	ARG	2.7
1	G	165	GLU	2.7
1	A	336	ALA	2.7
1	C	277	ASN	2.7
1	A	45	GLU	2.7
1	B	8	MET	2.7
1	J	327	GLU	2.7
1	L	327	GLU	2.7
1	B	4	HIS	2.7
1	A	203	GLY	2.7
1	A	389	GLY	2.7
1	C	284	GLY	2.7
1	C	51	GLY	2.7
1	H	406	GLU	2.7
1	C	338	ASN	2.7
1	D	38	VAL	2.7
1	L	179	TYR	2.7
1	D	423	LEU	2.7
1	A	283	SER	2.7
1	E	123	THR	2.7
1	B	39	ASN	2.7
1	F	44	GLU	2.6
1	A	281	LEU	2.6
1	F	324	PRO	2.6
1	C	353	ALA	2.6
1	L	390	GLU	2.6
1	C	351	PRO	2.6
1	A	112	GLU	2.6
1	D	288	ALA	2.6
1	B	345	ILE	2.6
1	E	290	LEU	2.6
1	C	46	GLY	2.6
1	I	390	GLU	2.6
1	A	6	LEU	2.6
1	A	407	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	426	GLU	2.6
1	C	289	GLY	2.6
1	A	48	MET	2.6
1	B	304	HIS	2.6
1	E	44	GLU	2.6
1	L	98	GLN	2.6
1	E	350	SER	2.6
1	B	290	LEU	2.6
1	K	393	ASP	2.6
1	A	331	MET	2.6
1	A	371	PHE	2.6
1	C	42	PHE	2.6
1	F	165	GLU	2.6
1	C	119	GLY	2.6
1	H	392	MET	2.6
1	G	328	ALA	2.6
1	K	367	PRO	2.5
1	K	408	PRO	2.5
1	A	86	ILE	2.5
1	E	386	ILE	2.5
1	E	43	PHE	2.5
1	B	64	ASP	2.5
1	E	41	GLU	2.5
1	A	386	ILE	2.5
1	D	333	ALA	2.5
1	E	434	PHE	2.5
1	C	286	LYS	2.5
1	J	396	LEU	2.5
1	C	123	THR	2.5
1	J	238	TYR	2.5
1	K	235	ILE	2.5
1	D	62	GLU	2.5
1	H	117	ALA	2.5
1	B	285	ASP	2.5
1	A	44	GLU	2.5
1	B	41	GLU	2.5
1	D	41	GLU	2.5
1	B	85	LEU	2.5
1	B	352	LYS	2.5
1	C	12	HIS	2.5
1	B	48	MET	2.5
1	F	59	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	349	ALA	2.5
1	L	328	ALA	2.5
1	D	43	PHE	2.5
1	K	63	SER	2.5
1	C	385	LYS	2.5
1	A	376	MET	2.5
1	K	278	GLY	2.5
1	A	303	LYS	2.4
1	J	221	VAL	2.4
1	J	277	ASN	2.4
1	K	61	ASN	2.4
1	A	1	SER	2.4
1	B	288	ALA	2.4
1	I	361	PRO	2.4
1	A	394	LYS	2.4
1	E	284	GLY	2.4
1	I	331	MET	2.4
1	B	282	PHE	2.4
1	I	43	PHE	2.4
1	G	267	GLY	2.4
1	B	96	THR	2.4
1	E	13	GLU	2.4
1	E	340	SER	2.4
1	A	434	PHE	2.4
1	B	367	PRO	2.4
1	E	388	PRO	2.4
1	A	99	GLY	2.4
1	A	432	GLY	2.4
1	D	10	ASN	2.4
1	H	347	VAL	2.4
1	B	9	LEU	2.4
1	J	1	SER	2.4
1	K	340	SER	2.4
1	E	286	LYS	2.4
1	A	166	GLY	2.4
1	E	280	ASN	2.4
1	F	278	GLY	2.4
1	A	53	SER	2.4
1	F	1	SER	2.4
1	C	8	MET	2.4
1	D	44	GLU	2.4
1	C	95	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	58	LYS	2.4
1	G	6	LEU	2.4
1	G	97	LEU	2.4
1	B	118	THR	2.4
1	B	382	ILE	2.4
1	H	328	ALA	2.4
1	D	408	PRO	2.3
1	E	295	LEU	2.3
1	B	52	SER	2.3
1	A	230	LYS	2.3
1	A	180	PHE	2.3
1	B	179	TYR	2.3
1	E	296	TYR	2.3
1	E	276	LYS	2.3
1	C	390	GLU	2.3
1	F	92	LEU	2.3
1	C	11	GLU	2.3
1	E	3	GLU	2.3
1	E	40	ALA	2.3
1	L	364	ALA	2.3
1	B	38	VAL	2.3
1	J	41	GLU	2.3
1	I	270	CYS	2.3
1	D	365	ALA	2.3
1	L	361	PRO	2.3
1	I	339	ARG	2.3
1	K	44	GLU	2.3
1	C	304	HIS	2.3
1	A	388	PRO	2.3
1	H	97	LEU	2.3
1	E	289	GLY	2.3
1	H	431	GLY	2.3
1	H	348	VAL	2.3
1	E	8	MET	2.2
1	E	341	ALA	2.2
1	L	45	GLU	2.2
1	C	352	LYS	2.2
1	B	434	PHE	2.2
1	I	371	PHE	2.2
1	J	63	SER	2.2
1	D	389	GLY	2.2
1	A	205	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	301	VAL	2.2
1	D	11	GLU	2.2
1	E	124	VAL	2.2
1	K	324	PRO	2.2
1	B	349	ALA	2.2
1	B	353	ALA	2.2
1	G	371	PHE	2.2
1	H	393	ASP	2.2
1	B	46	GLY	2.2
1	C	3	GLU	2.2
1	D	3	GLU	2.2
1	I	370	CYS	2.2
1	F	123	THR	2.2
1	F	5	VAL	2.2
1	F	179	TYR	2.2
1	D	407	ILE	2.2
1	B	273	SER	2.2
1	E	1	SER	2.2
1	E	387	HIS	2.2
1	I	11	GLU	2.2
1	F	325	GLY	2.2
1	H	396	LEU	2.2
1	A	435	THR	2.2
1	I	7	THR	2.2
1	G	270	CYS	2.2
1	F	334	TYR	2.2
1	I	367	PRO	2.2
1	L	41	GLU	2.2
1	L	97	LEU	2.2
1	E	408	PRO	2.2
1	A	468	VAL	2.2
1	F	66	VAL	2.2
1	F	114	TYR	2.2
1	L	348	VAL	2.2
1	F	393	ASP	2.2
1	L	370	CYS	2.2
1	G	392	MET	2.2
1	J	132	PHE	2.2
1	B	274	LEU	2.2
1	E	346	PRO	2.2
1	E	391	PRO	2.2
1	E	336	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	296	TYR	2.2
1	B	53	SER	2.2
1	B	340	SER	2.2
1	E	11	GLU	2.2
1	F	93	GLU	2.2
1	K	130	PRO	2.2
1	A	433	VAL	2.1
1	L	347	VAL	2.1
1	E	275	ALA	2.1
1	E	406	GLU	2.1
1	F	290	LEU	2.1
1	J	9	LEU	2.1
1	G	338	ASN	2.1
1	A	4	HIS	2.1
1	K	406	GLU	2.1
1	A	42	PHE	2.1
1	F	285	ASP	2.1
1	L	180	PHE	2.1
1	H	390	GLU	2.1
1	A	55	GLY	2.1
1	I	340	SER	2.1
1	B	287	TYR	2.1
1	L	392	MET	2.1
1	E	383	LYS	2.1
1	F	47	LYS	2.1
1	D	59	GLY	2.1
1	C	294	ALA	2.1
1	C	305	ALA	2.1
1	K	468	VAL	2.1
1	L	365	ALA	2.1
1	B	390	GLU	2.1
1	H	9	LEU	2.1
1	K	344	ARG	2.1
1	D	63	SER	2.1
1	B	45	GLU	2.1
1	D	406	GLU	2.1
1	D	468	VAL	2.1
1	K	270	CYS	2.1
1	L	238	TYR	2.1
1	A	49	PHE	2.1
1	A	427	PHE	2.1
1	G	51	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	389	GLY	2.1
1	L	389	GLY	2.1
1	I	327	GLU	2.1
1	G	117	ALA	2.1
1	H	40	ALA	2.1
1	E	98	GLN	2.1
1	G	347	VAL	2.1
1	F	65	MET	2.1
1	G	359	ARG	2.1
1	D	327	GLU	2.1
1	L	334	TYR	2.1
1	C	391	PRO	2.1
1	G	361	PRO	2.1
1	D	337	ARG	2.0
1	L	312	ALA	2.0
1	B	66	VAL	2.0
1	G	268	MET	2.0
1	I	392	MET	2.0
1	E	343	ILE	2.0
1	B	97	LEU	2.0
1	B	44	GLU	2.0
1	F	121	ALA	2.0
1	B	47	LYS	2.0
1	B	295	LEU	2.0
1	A	350	SER	2.0
1	B	224	ARG	2.0
1	L	337	ARG	2.0
1	K	284	GLY	2.0
1	J	351	PRO	2.0
1	G	53	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MPD	J	5491	8/8	0.92	0.43	17.92	37,50,65,66	8
4	MPD	H	5487	8/8	0.87	0.45	14.49	37,50,65,66	8
4	MPD	B	5474	8/8	0.58	0.47	13.25	63,68,75,98	8
4	MPD	B	5471	8/8	0.74	0.46	13.03	37,50,65,66	8
4	MPD	L	5483	8/8	0.89	0.42	12.87	37,50,65,66	8
4	MPD	F	5479	8/8	0.83	0.43	12.82	37,50,65,66	8
4	MPD	D	5478	8/8	0.77	0.50	12.61	63,68,75,98	8
4	MPD	I	5489	8/8	0.88	0.40	12.48	37,50,65,66	8
4	MPD	G	5485	8/8	0.88	0.45	12.10	37,50,65,66	8
4	MPD	H	5486	8/8	0.65	0.53	11.75	63,68,75,98	8
4	MPD	L	5494	8/8	0.82	0.52	11.37	63,68,75,98	8
4	MPD	E	5477	8/8	0.87	0.40	10.97	37,50,65,66	8
4	MPD	J	5490	8/8	0.75	0.49	10.81	63,68,75,98	8
4	MPD	I	5488	8/8	0.75	0.56	10.69	63,68,75,98	8
4	MPD	C	5473	8/8	0.89	0.39	9.97	37,50,65,66	8
4	MPD	G	5484	8/8	0.75	0.51	9.38	63,68,75,98	8
4	MPD	E	5480	8/8	0.77	0.46	9.10	63,68,75,98	8
4	MPD	K	5493	8/8	0.93	0.44	9.06	37,50,65,66	8
4	MPD	K	5492	8/8	0.80	0.50	9.05	63,68,75,98	8
4	MPD	D	5475	8/8	0.82	0.37	8.31	37,50,65,66	8
4	MPD	F	5482	8/8	0.77	0.38	8.25	63,68,75,98	8
4	MPD	C	5476	8/8	0.58	0.46	7.76	63,68,75,98	8
4	MPD	A	5481	8/8	0.83	0.37	6.80	37,50,65,66	8
3	ADP	I	4479	27/27	0.73	0.41	4.41	38,77,100,100	27
3	ADP	L	4482	27/27	0.70	0.44	3.73	38,77,100,100	27
4	MPD	A	5472	8/8	0.63	0.49	3.54	63,68,75,98	8
3	ADP	K	4481	27/27	0.72	0.41	3.51	38,77,100,100	27
3	ADP	J	4480	27/27	0.81	0.39	3.20	38,77,100,100	27
3	ADP	B	4472	27/27	0.64	0.45	3.13	38,77,100,100	27
3	ADP	F	4476	27/27	0.69	0.43	2.74	38,77,100,100	27
3	ADP	G	4477	27/27	0.75	0.39	2.20	38,77,100,100	27
3	ADP	C	4473	27/27	0.76	0.34	1.84	38,77,100,100	27
3	ADP	H	4478	27/27	0.80	0.33	1.79	38,77,100,100	27
3	ADP	A	4471	27/27	0.53	0.53	1.58	38,77,100,100	27

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ADP	D	4474	27/27	0.74	0.34	1.46	38,77,100,100	27
3	ADP	E	4475	27/27	0.70	0.36	1.42	38,77,100,100	27
2	MN	A	470	1/1	0.88	0.07	-1.81	46,46,46,46	0
2	MN	D	470	1/1	0.92	0.05	-1.93	46,46,46,46	0
2	MN	J	470	1/1	0.98	0.10	-2.31	46,46,46,46	0
2	MN	K	470	1/1	0.99	0.12	-2.37	46,46,46,46	0
2	MN	H	470	1/1	0.96	0.08	-3.06	46,46,46,46	0
2	MN	E	470	1/1	0.94	0.06	-3.17	46,46,46,46	0
2	MN	G	470	1/1	0.97	0.10	-3.18	46,46,46,46	0
2	MN	F	470	1/1	0.98	0.04	-3.22	46,46,46,46	0
2	MN	C	470	1/1	0.97	0.04	-3.32	46,46,46,46	0
2	MN	L	470	1/1	0.98	0.13	-3.78	46,46,46,46	0
2	MN	B	470	1/1	0.94	0.07	-3.95	46,46,46,46	0
2	MN	I	470	1/1	0.97	0.08	-4.55	46,46,46,46	0
2	MN	H	469	1/1	0.96	0.15	-	47,47,47,47	0
2	MN	B	469	1/1	0.96	0.06	-	47,47,47,47	0
2	MN	A	469	1/1	0.91	0.07	-	47,47,47,47	0
2	MN	I	469	1/1	0.97	0.11	-	47,47,47,47	0
2	MN	C	469	1/1	0.93	0.08	-	47,47,47,47	0
2	MN	K	469	1/1	0.97	0.15	-	47,47,47,47	0
2	MN	L	469	1/1	0.92	0.17	-	47,47,47,47	0
2	MN	J	469	1/1	0.97	0.15	-	47,47,47,47	0
2	MN	D	469	1/1	0.98	0.09	-	47,47,47,47	0
2	MN	E	469	1/1	0.97	0.04	-	47,47,47,47	0
2	MN	F	469	1/1	0.95	0.07	-	47,47,47,47	0
2	MN	G	469	1/1	0.99	0.09	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.