



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2020 – 05:21 am BST

PDB ID : 1I48  
Title : CYSTATHIONINE GAMMA-SYNTHASE IN COMPLEX WITH THE INHIBITOR CTCPO  
Authors : Steegborn, C.; Laber, B.; Messerschmidt, A.; Huber, R.; Clausen, T.  
Deposited on : 2001-02-20  
Resolution : 3.25 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

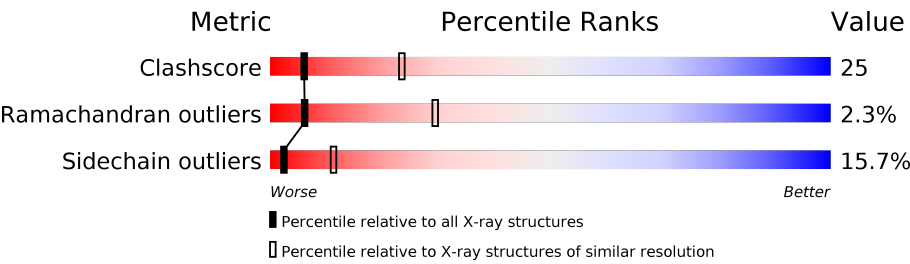
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)


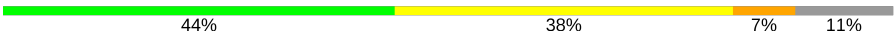
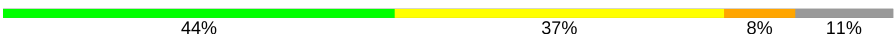

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	<div><div>46%</div><div>36%</div><div>7%</div><div>11%</div></div>
1	B	445	<div><div>45%</div><div>37%</div><div>7%</div><div>11%</div></div>
1	C	445	<div><div>44%</div><div>39%</div><div>6%</div><div>11%</div></div>
1	D	445	<div><div>44%</div><div>37%</div><div>8%</div><div>11%</div></div>
1	E	445	<div><div>45%</div><div>37%</div><div>7%</div><div>11%</div></div>
1	F	445	<div><div>44%</div><div>38%</div><div>7%</div><div>11%</div></div>
1	G	445	<div><div>43%</div><div>38%</div><div>8%</div><div>11%</div></div>
1	H	445	<div><div>43%</div><div>38%</div><div>8%</div><div>11%</div></div>

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Mol	Chain	Length	Quality of chain
1	I	445	 45% 38% 6% 11%
1	J	445	 44% 38% 7% 11%
1	K	445	 44% 37% 8% 11%
1	L	445	 45% 36% 7% 11%

## 2 Entry composition

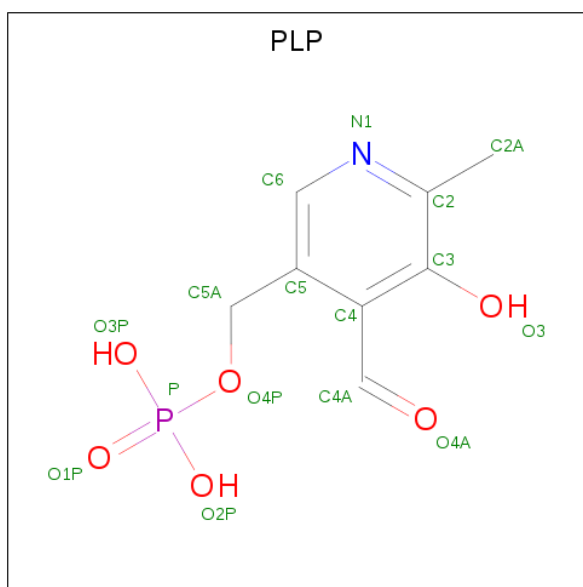
There are 3 unique types of molecules in this entry. The entry contains 36660 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYSTATHIONINE GAMMA-SYNTHASE.

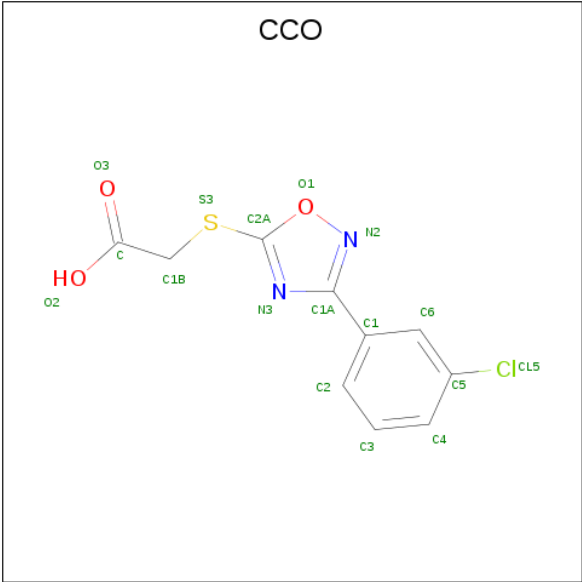
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	B	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	C	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	D	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	E	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	F	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	G	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	H	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	I	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	J	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	K	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	L	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



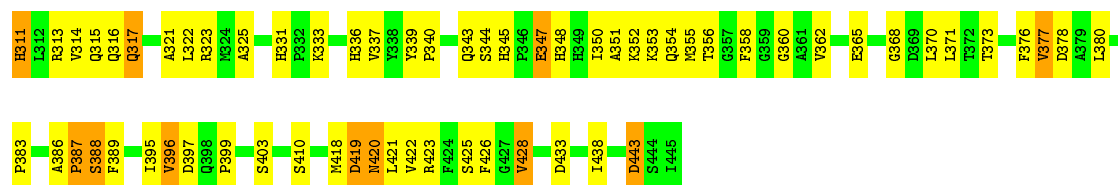
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	L	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is CARBOXYMETHYLTHIO-3-(3-CHLOROPHENYL)-1,2,4-OXADIAZOL (three-letter code: CCO) (formula: C<sub>10</sub>H<sub>7</sub>ClN<sub>2</sub>O<sub>3</sub>S).



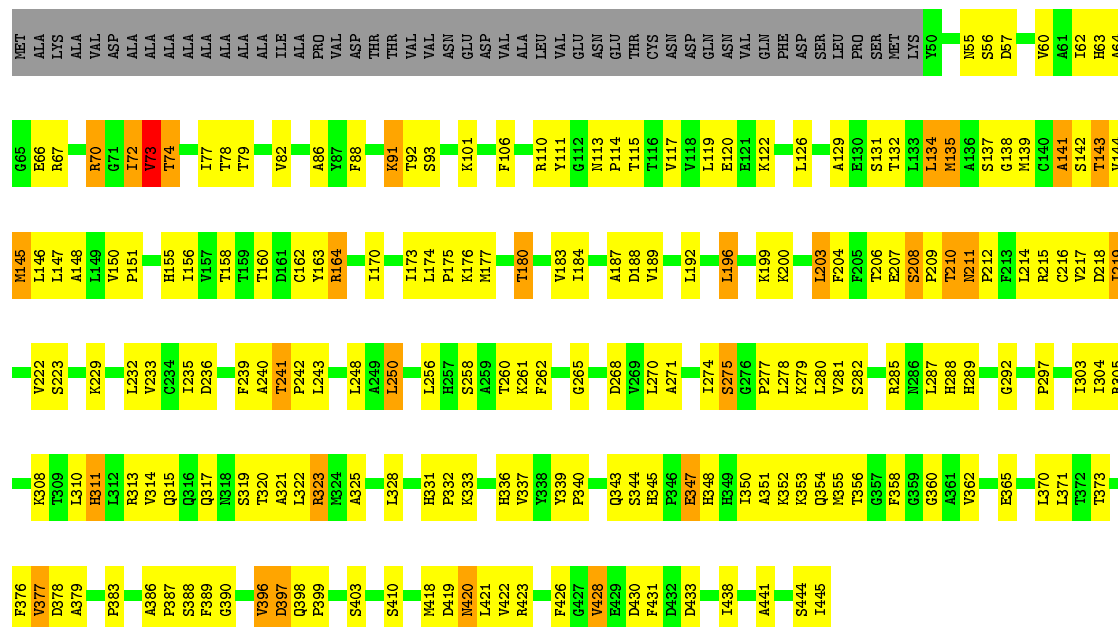
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	C	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	E	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	F	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	G	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	H	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	I	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	J	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	K	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	L	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		





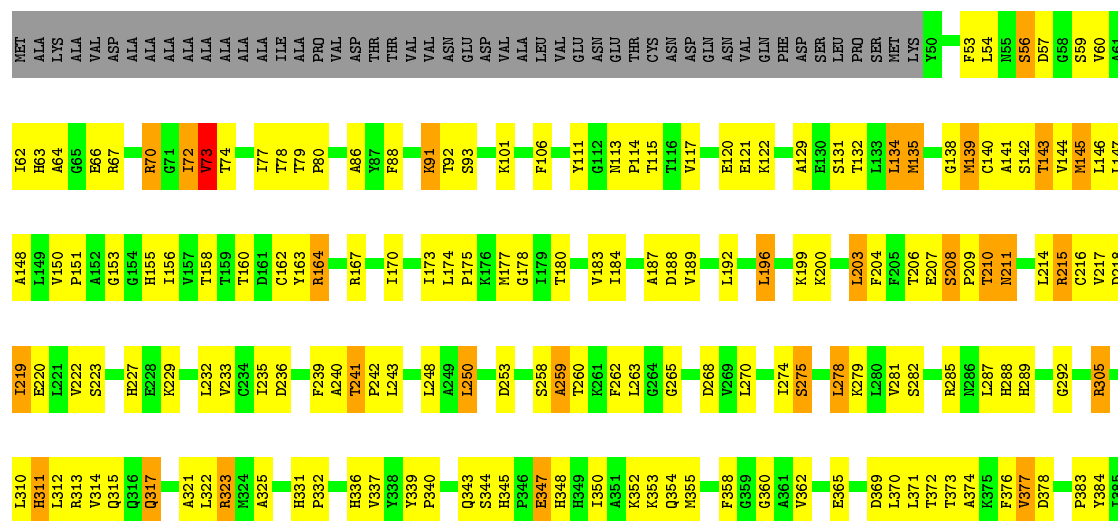
• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain C: 44% 39% 6% 11%



• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain D: 44% 37% 8% 11%

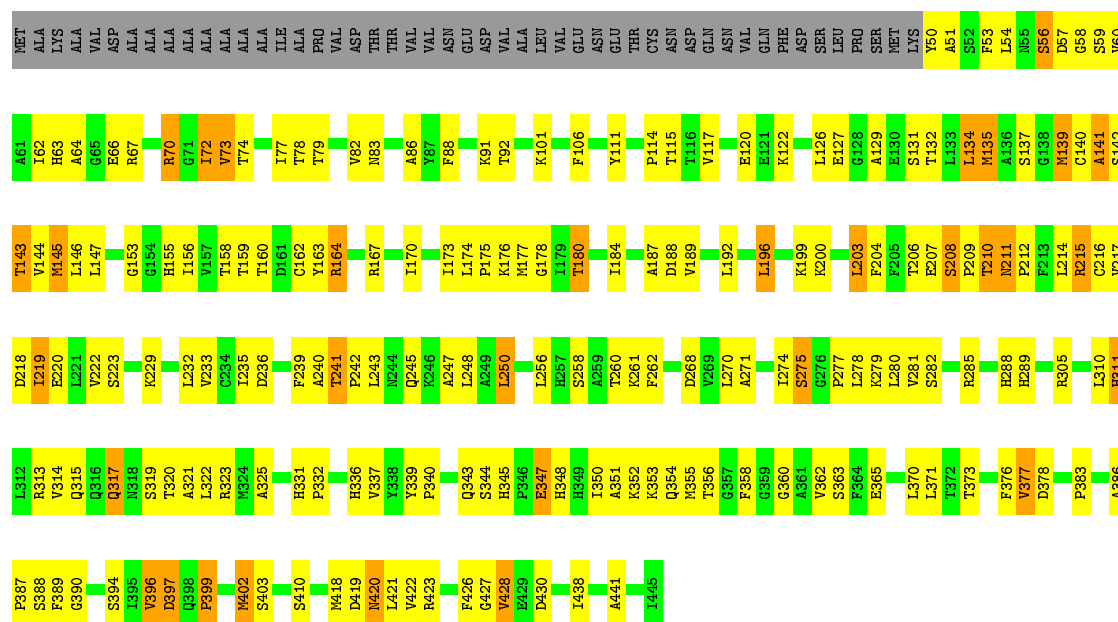






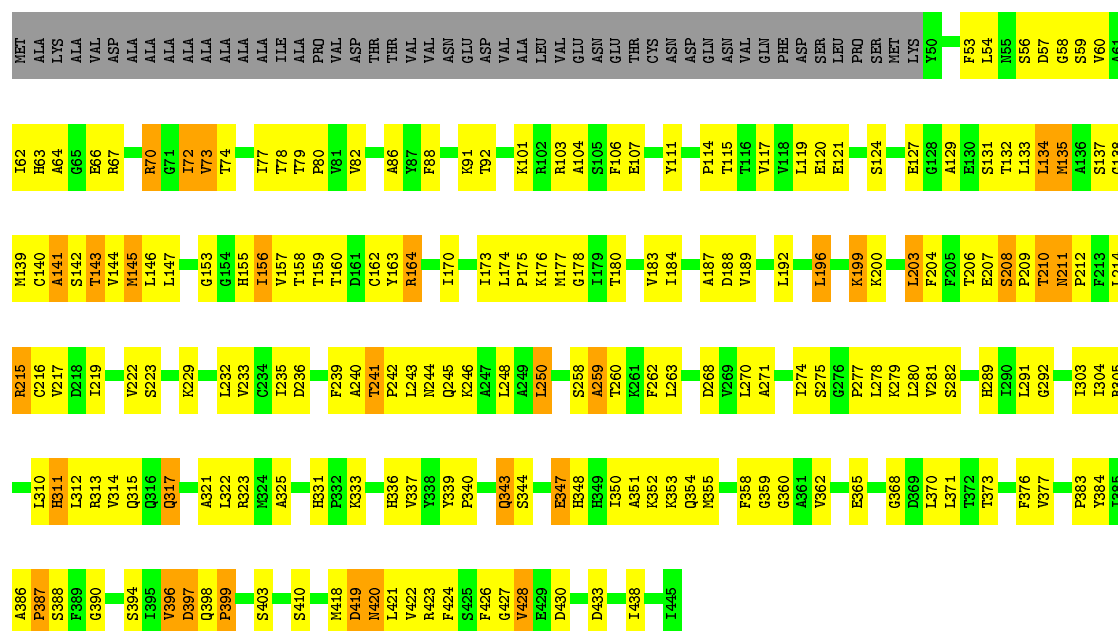
# • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain E: 45% 37% 7% 11%



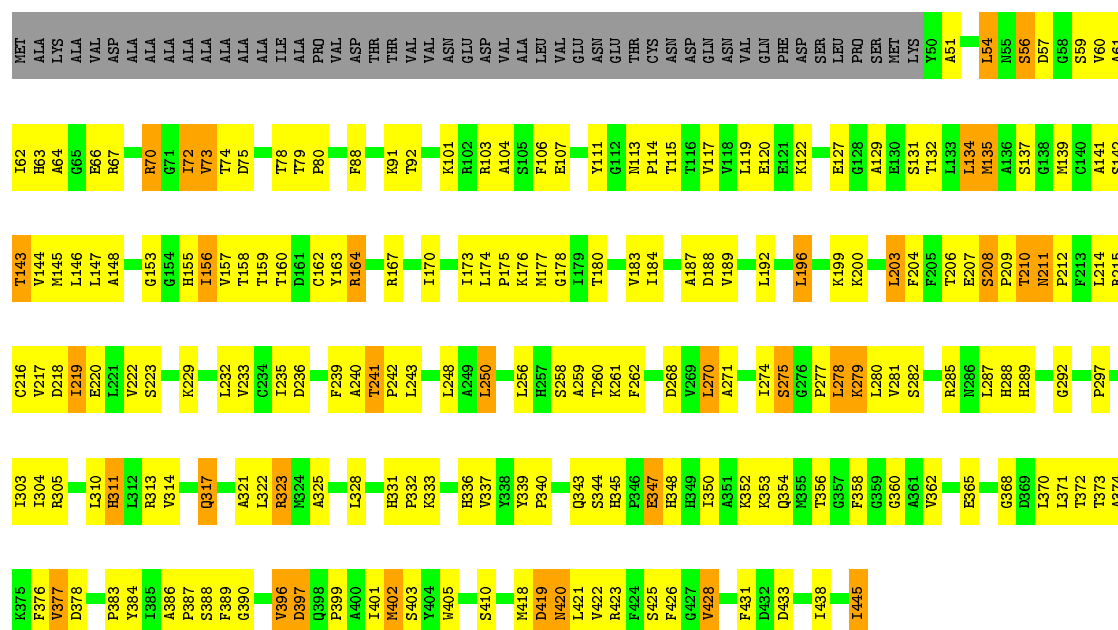
# • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain F: 44% 38% 7% 11%



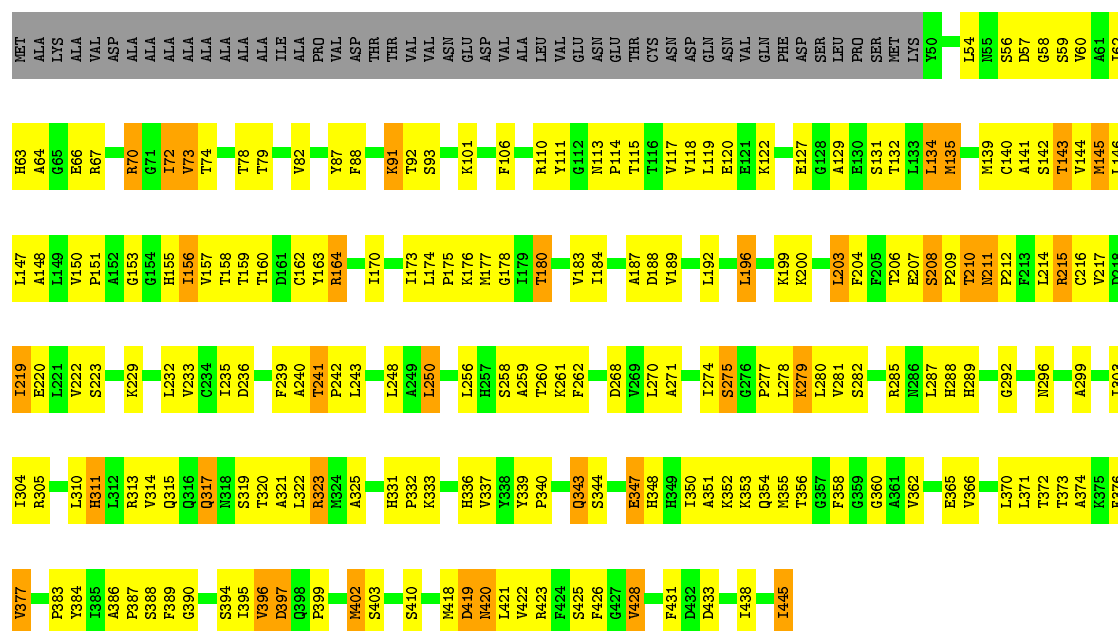
# • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain G:



- Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

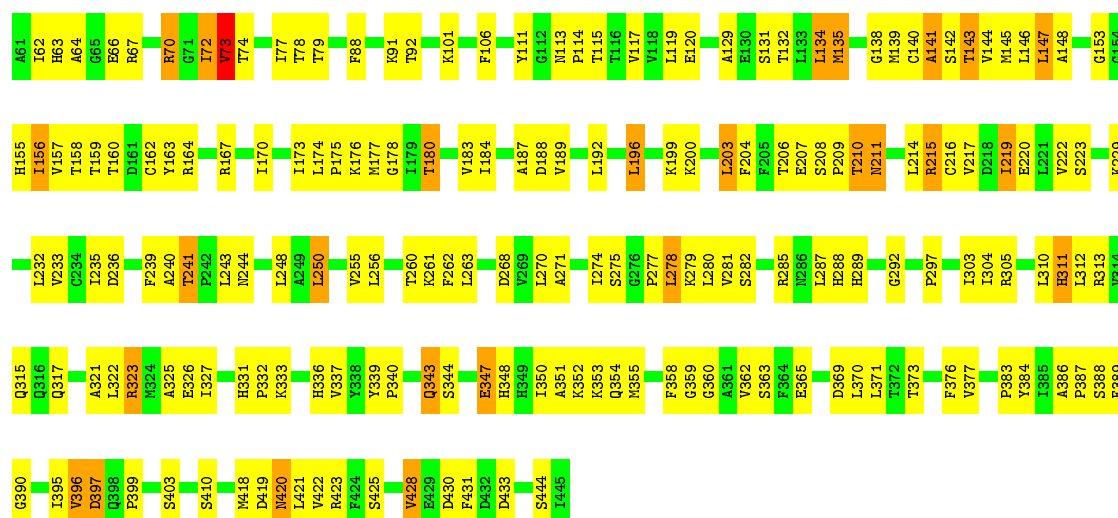
Chain H:



- Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

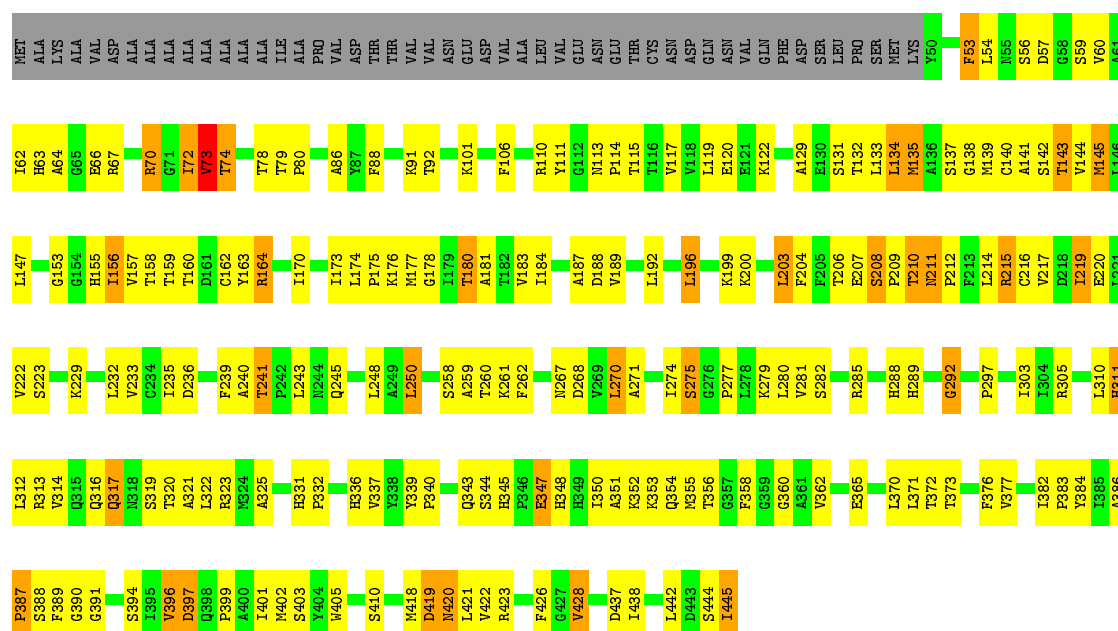
Chain I:





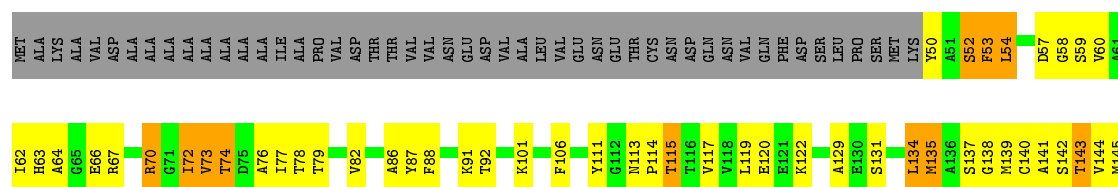
### • Molecule 1: CYSTATHIONINE GAMMA-SYNTASE

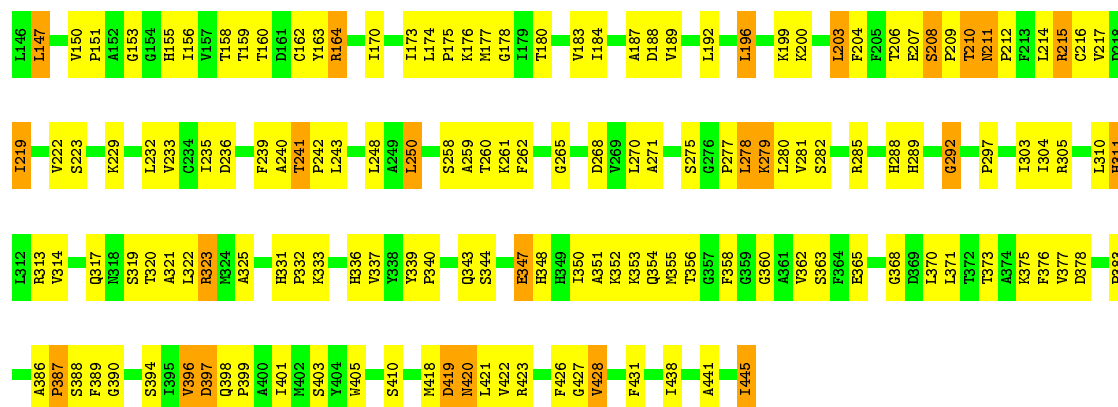
Chain J: 44% 38% 7% 11%



### • Molecule 1: CYSTATHIONINE GAMMA-SYNTASE

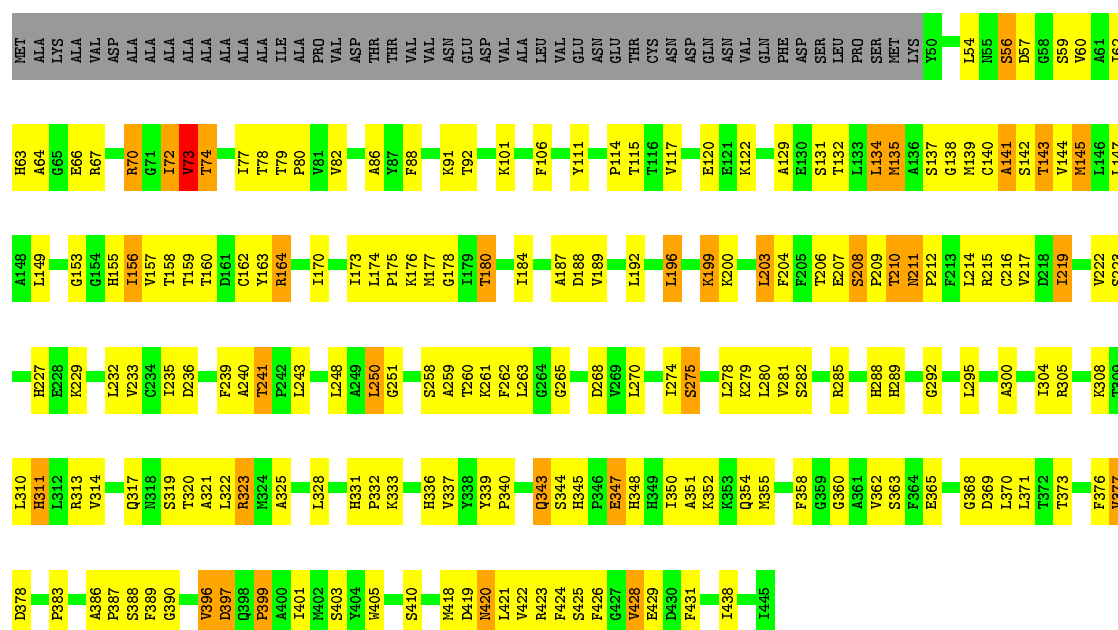
Chain K: 44% 37% 8% 11%





• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain L: 45% 36% 7% 11%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	312.40Å 165.60Å 162.20Å 90.00° 89.80° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.25)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.226 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CCO, PLP

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	0.30	0/3082	0.49	0/4179
1	B	0.30	0/3082	0.50	0/4179
1	C	0.29	0/3082	0.49	0/4179
1	D	0.30	0/3082	0.49	0/4179
1	E	0.30	0/3082	0.49	0/4179
1	F	0.29	0/3082	0.49	0/4179
1	G	0.29	0/3082	0.48	0/4179
1	H	0.29	0/3082	0.49	0/4179
1	I	0.29	0/3082	0.49	0/4179
1	J	0.29	0/3082	0.48	0/4179
1	K	0.29	0/3082	0.48	0/4179
1	L	0.29	0/3082	0.49	0/4179
All	All	0.29	0/36984	0.49	0/50148

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3023	0	3052	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3023	0	3052	157	0
1	C	3023	0	3052	160	0
1	D	3023	0	3052	155	0
1	E	3023	0	3052	155	0
1	F	3023	0	3052	165	0
1	G	3023	0	3052	172	0
1	H	3023	0	3052	160	0
1	I	3023	0	3052	151	0
1	J	3023	0	3052	163	0
1	K	3023	0	3052	165	0
1	L	3023	0	3052	156	0
2	A	15	0	6	2	0
2	B	15	0	6	0	0
2	C	15	0	6	2	0
2	D	15	0	6	0	0
2	E	15	0	6	0	0
2	F	15	0	6	1	0
2	G	15	0	6	1	0
2	H	15	0	6	0	0
2	I	15	0	6	1	0
2	J	15	0	6	1	0
2	K	15	0	6	1	0
2	L	15	0	6	1	0
3	A	17	0	6	1	0
3	B	17	0	6	1	0
3	C	17	0	6	1	0
3	D	17	0	6	1	0
3	E	17	0	6	1	0
3	F	17	0	6	2	0
3	G	17	0	6	1	0
3	H	17	0	6	2	0
3	I	17	0	6	1	0
3	J	17	0	6	2	0
3	K	17	0	6	2	0
3	L	17	0	6	1	0
All	All	36660	0	36768	1810	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 25.

All (1810) 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:H:241:THR:HG22	1:H:243:LEU:H	1.33	0.94
1:E:370:LEU:HD23	1:E:419:ASP:HB3	1.49	0.92
1:G:241:THR:HG22	1:G:243:LEU:H	1.33	0.92
1:A:241:THR:HG22	1:A:243:LEU:H	1.34	0.92
1:A:370:LEU:HD23	1:A:419:ASP:HB3	1.50	0.91
1:C:210:THR:HG22	1:C:215:ARG:H	1.36	0.90
1:F:210:THR:HG22	1:F:215:ARG:H	1.35	0.89
1:D:241:THR:HG22	1:D:243:LEU:H	1.36	0.88
1:B:210:THR:HG22	1:B:215:ARG:H	1.36	0.88
1:I:241:THR:HG22	1:I:243:LEU:H	1.37	0.88
1:C:241:THR:HG22	1:C:243:LEU:H	1.39	0.88
1:D:370:LEU:HD23	1:D:419:ASP:HB3	1.54	0.88
1:B:241:THR:HG22	1:B:243:LEU:H	1.39	0.88
1:G:210:THR:HG22	1:G:215:ARG:H	1.38	0.87
1:J:370:LEU:HD23	1:J:419:ASP:HB3	1.56	0.87
1:H:370:LEU:HD23	1:H:419:ASP:HB3	1.57	0.87
1:F:241:THR:HG22	1:F:243:LEU:H	1.38	0.87
1:K:370:LEU:HD23	1:K:419:ASP:HB3	1.56	0.87
1:K:210:THR:HG22	1:K:215:ARG:H	1.37	0.87
1:K:241:THR:HG22	1:K:243:LEU:H	1.37	0.87
1:L:370:LEU:HD23	1:L:419:ASP:HB3	1.56	0.87
1:B:383:PRO:HB2	1:B:396:VAL:HG22	1.57	0.86
1:B:120:GLU:HG3	1:B:134:LEU:HD12	1.57	0.86
1:G:383:PRO:HB2	1:G:396:VAL:HG22	1.58	0.86
1:H:210:THR:HG22	1:H:215:ARG:H	1.40	0.86
1:J:241:THR:HG22	1:J:243:LEU:H	1.38	0.86
1:G:51:ALA:HB3	1:G:54:LEU:HB2	1.56	0.86
1:G:370:LEU:HD23	1:G:419:ASP:HB3	1.57	0.85
1:G:240:ALA:O	1:G:241:THR:HB	1.76	0.85
1:C:383:PRO:HB2	1:C:396:VAL:HG22	1.58	0.85
1:E:120:GLU:HG3	1:E:134:LEU:HD12	1.59	0.84
1:F:199:LYS:HD2	1:L:153:GLY:HA2	1.59	0.84
1:A:210:THR:HG22	1:A:215:ARG:H	1.44	0.83
1:D:210:THR:HG22	1:D:215:ARG:H	1.42	0.83
1:A:383:PRO:HB2	1:A:396:VAL:HG22	1.60	0.83
1:I:240:ALA:O	1:I:241:THR:HB	1.77	0.83
1:L:383:PRO:HB2	1:L:396:VAL:HG22	1.61	0.83
1:E:241:THR:HG22	1:E:243:LEU:H	1.43	0.82
1:L:210:THR:HG22	1:L:215:ARG:H	1.42	0.82
1:J:240:ALA:O	1:J:241:THR:HB	1.77	0.81
1:D:120:GLU:HG3	1:D:134:LEU:HD12	1.62	0.81
1:I:370:LEU:HD23	1:I:419:ASP:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:PHE:HA	1:D:386:ALA:HB2	1.62	0.81
1:J:210:THR:HG22	1:J:215:ARG:H	1.46	0.81
1:I:210:THR:HG22	1:I:215:ARG:H	1.45	0.81
1:D:383:PRO:HB2	1:D:396:VAL:HG22	1.62	0.80
1:J:88:PHE:HA	1:L:386:ALA:HB2	1.64	0.80
1:C:240:ALA:O	1:C:241:THR:HB	1.79	0.80
1:B:370:LEU:HD23	1:B:419:ASP:HB3	1.62	0.80
1:I:120:GLU:HG3	1:I:134:LEU:HD12	1.64	0.80
1:E:210:THR:HG22	1:E:215:ARG:H	1.46	0.79
1:K:240:ALA:O	1:K:241:THR:HB	1.80	0.79
1:C:370:LEU:HD23	1:C:419:ASP:HB3	1.63	0.79
1:F:370:LEU:HD23	1:F:419:ASP:HB3	1.63	0.79
1:A:240:ALA:O	1:A:241:THR:HB	1.82	0.78
1:A:216:CYS:H	1:A:347:GLU:HG3	1.49	0.78
1:B:216:CYS:H	1:B:347:GLU:HG3	1.48	0.78
1:F:383:PRO:HB2	1:F:396:VAL:HG22	1.66	0.78
1:B:240:ALA:O	1:B:241:THR:HB	1.82	0.78
1:H:240:ALA:O	1:H:241:THR:HB	1.82	0.77
1:L:240:ALA:O	1:L:241:THR:HB	1.83	0.77
1:G:120:GLU:HG3	1:G:134:LEU:HD12	1.65	0.77
1:L:241:THR:HG22	1:L:243:LEU:H	1.49	0.77
1:K:383:PRO:HB2	1:K:396:VAL:HG22	1.67	0.77
1:I:321:ALA:HB2	1:I:360:GLY:HA2	1.67	0.76
1:G:216:CYS:H	1:G:347:GLU:HG3	1.50	0.76
1:H:383:PRO:HB2	1:H:396:VAL:HG22	1.66	0.76
1:L:120:GLU:HG3	1:L:134:LEU:HD12	1.67	0.76
1:H:216:CYS:H	1:H:347:GLU:HG3	1.49	0.76
1:K:387:PRO:HA	3:K:610:CCO:HC2	1.67	0.75
1:E:240:ALA:O	1:E:241:THR:HB	1.84	0.75
1:D:240:ALA:O	1:D:241:THR:HB	1.86	0.75
1:J:120:GLU:HG3	1:J:134:LEU:HD12	1.68	0.75
1:L:421:LEU:HD12	1:L:422:VAL:H	1.51	0.75
1:L:216:CYS:H	1:L:347:GLU:HG3	1.51	0.75
1:J:216:CYS:H	1:J:347:GLU:HG3	1.52	0.75
1:E:383:PRO:HB2	1:E:396:VAL:HG22	1.69	0.74
1:E:216:CYS:H	1:E:347:GLU:HG3	1.51	0.74
1:F:240:ALA:O	1:F:241:THR:HB	1.86	0.74
1:F:120:GLU:HG3	1:F:134:LEU:HD12	1.70	0.74
1:F:139:MET:O	1:F:143:THR:HB	1.87	0.74
1:I:383:PRO:HB2	1:I:396:VAL:HG22	1.69	0.74
1:K:207:GLU:HB3	1:K:236:ASP:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:CYS:H	1:F:347:GLU:HG3	1.52	0.73
1:E:268:ASP:HB3	1:H:78:THR:HG21	1.70	0.73
1:K:216:CYS:H	1:K:347:GLU:HG3	1.52	0.73
1:E:421:LEU:HD12	1:E:422:VAL:H	1.53	0.73
1:C:216:CYS:H	1:C:347:GLU:HG3	1.53	0.73
1:G:139:MET:O	1:G:143:THR:HB	1.88	0.73
1:H:421:LEU:HD12	1:H:422:VAL:H	1.51	0.73
1:C:63:HIS:HB3	1:C:67:ARG:HB2	1.71	0.73
1:D:216:CYS:H	1:D:347:GLU:HG3	1.53	0.72
1:I:139:MET:O	1:I:143:THR:HB	1.89	0.72
1:H:139:MET:O	1:H:143:THR:HB	1.89	0.72
1:J:207:GLU:HB3	1:J:236:ASP:HB3	1.71	0.72
1:G:250:LEU:HD11	1:G:354:GLN:HB2	1.72	0.72
1:F:63:HIS:HB3	1:F:67:ARG:HB2	1.72	0.72
1:I:216:CYS:H	1:I:347:GLU:HG3	1.53	0.72
1:B:433:ASP:OD2	1:C:56:SER:HB3	1.90	0.72
1:A:139:MET:O	1:A:143:THR:HB	1.90	0.71
1:B:63:HIS:HB3	1:B:67:ARG:HB2	1.72	0.71
1:I:62:ILE:HD11	1:L:428:VAL:HG12	1.72	0.71
1:B:399:PRO:HG3	1:B:423:ARG:NE	2.04	0.71
1:J:383:PRO:HB2	1:J:396:VAL:HG22	1.71	0.71
1:K:120:GLU:HG3	1:K:134:LEU:HD12	1.71	0.71
1:L:139:MET:O	1:L:143:THR:HB	1.91	0.71
1:H:120:GLU:HG3	1:H:134:LEU:HD12	1.71	0.71
1:K:170:ILE:HG23	1:K:174:LEU:HD12	1.71	0.71
1:D:421:LEU:HD12	1:D:422:VAL:H	1.55	0.71
1:F:210:THR:O	1:F:214:LEU:HA	1.91	0.70
1:H:372:THR:HG23	1:H:445:ILE:HG21	1.73	0.70
1:A:207:GLU:HB3	1:A:236:ASP:HB3	1.71	0.70
1:I:63:HIS:HB3	1:I:67:ARG:HB2	1.73	0.70
1:B:207:GLU:HB3	1:B:236:ASP:HB3	1.71	0.70
1:D:207:GLU:HB3	1:D:236:ASP:HB3	1.72	0.70
1:J:78:THR:HG21	1:K:268:ASP:HB3	1.73	0.70
1:K:63:HIS:HB3	1:K:67:ARG:HB2	1.74	0.70
1:L:397:ASP:OD1	1:L:423:ARG:HB2	1.91	0.70
1:F:268:ASP:HB3	1:G:78:THR:HG21	1.72	0.70
1:J:399:PRO:HG3	1:J:423:ARG:NE	2.07	0.70
1:J:421:LEU:HD12	1:J:422:VAL:H	1.57	0.70
1:A:397:ASP:OD1	1:A:423:ARG:HB2	1.92	0.69
1:B:421:LEU:HD12	1:B:422:VAL:H	1.55	0.69
1:E:170:ILE:HG23	1:E:174:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:GLU:HB3	1:G:236:ASP:HB3	1.74	0.69
1:J:223:SER:HA	1:J:233:VAL:HG21	1.74	0.69
1:B:386:ALA:HB2	1:D:88:PHE:HA	1.74	0.69
1:F:347:GLU:HB3	1:F:350:ILE:HD12	1.75	0.69
1:D:139:MET:O	1:D:143:THR:HB	1.92	0.69
1:A:174:LEU:N	1:A:175:PRO:HD2	2.08	0.69
1:D:223:SER:HA	1:D:233:VAL:HG21	1.75	0.69
1:K:421:LEU:HD12	1:K:422:VAL:H	1.56	0.69
1:E:88:PHE:HA	1:G:386:ALA:HB2	1.75	0.69
1:J:54:LEU:HD22	1:J:59:SER:HB3	1.73	0.69
1:B:250:LEU:HD11	1:B:354:GLN:HB2	1.75	0.69
1:B:397:ASP:OD1	1:B:423:ARG:HB2	1.93	0.69
1:K:348:HIS:NE2	1:K:352:LYS:HD2	2.07	0.68
1:I:78:THR:HG21	1:L:268:ASP:HB3	1.74	0.68
1:H:207:GLU:HB3	1:H:236:ASP:HB3	1.75	0.68
1:E:54:LEU:HD22	1:E:59:SER:HB3	1.76	0.68
1:E:386:ALA:HB2	1:G:88:PHE:HA	1.75	0.68
1:K:399:PRO:HG3	1:K:423:ARG:NE	2.08	0.68
1:L:207:GLU:HB3	1:L:236:ASP:HB3	1.75	0.68
1:F:174:LEU:N	1:F:175:PRO:HD2	2.09	0.68
1:I:250:LEU:HD11	1:I:354:GLN:HB2	1.76	0.68
1:E:399:PRO:HG3	1:E:423:ARG:NE	2.08	0.68
1:I:421:LEU:HD12	1:I:422:VAL:H	1.58	0.68
1:L:348:HIS:NE2	1:L:352:LYS:HD2	2.09	0.68
1:E:207:GLU:HB3	1:E:236:ASP:HB3	1.76	0.68
1:J:268:ASP:HB3	1:K:78:THR:HG21	1.75	0.68
1:J:321:ALA:HB2	1:J:360:GLY:HA2	1.76	0.68
1:D:153:GLY:HA2	1:D:178:GLY:O	1.94	0.68
1:C:120:GLU:HG3	1:C:134:LEU:HD12	1.76	0.67
1:I:347:GLU:HB3	1:I:350:ILE:HD12	1.77	0.67
1:L:174:LEU:N	1:L:175:PRO:HD2	2.10	0.67
1:C:174:LEU:N	1:C:175:PRO:HD2	2.10	0.67
1:G:170:ILE:HG23	1:G:174:LEU:HD12	1.75	0.67
1:K:243:LEU:HD12	1:K:314:VAL:HG21	1.76	0.67
1:F:78:THR:HG21	1:G:268:ASP:HB3	1.76	0.67
1:F:88:PHE:HA	1:H:386:ALA:HB2	1.74	0.67
1:E:64:ALA:O	1:E:122:LYS:HG3	1.94	0.67
1:F:207:GLU:HB3	1:F:236:ASP:HB3	1.75	0.67
1:A:120:GLU:HG3	1:A:134:LEU:HD12	1.75	0.67
1:A:386:ALA:HB2	1:C:88:PHE:HA	1.77	0.67
1:E:56:SER:HB3	1:H:433:ASP:OD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:LEU:HD22	1:H:59:SER:HB3	1.76	0.67
1:E:397:ASP:OD1	1:E:423:ARG:HB2	1.95	0.66
1:J:250:LEU:HD11	1:J:354:GLN:HB2	1.77	0.66
1:C:207:GLU:HB3	1:C:236:ASP:HB3	1.76	0.66
1:E:347:GLU:HB3	1:E:350:ILE:HD12	1.78	0.66
1:E:78:THR:HG21	1:H:268:ASP:HB3	1.77	0.66
1:I:88:PHE:HA	1:K:386:ALA:HB2	1.76	0.66
1:D:340:PRO:HB2	1:D:358:PHE:HD1	1.59	0.66
1:H:174:LEU:N	1:H:175:PRO:HD2	2.11	0.66
1:K:174:LEU:N	1:K:175:PRO:HD2	2.10	0.66
1:I:397:ASP:OD1	1:I:423:ARG:HB2	1.96	0.66
1:L:210:THR:HG22	1:L:215:ARG:N	2.11	0.66
1:A:250:LEU:HD11	1:A:354:GLN:HB2	1.77	0.66
1:F:210:THR:HG22	1:F:215:ARG:N	2.10	0.66
1:L:399:PRO:HG3	1:L:423:ARG:NE	2.11	0.66
1:A:63:HIS:HB3	1:A:67:ARG:HB2	1.78	0.66
1:J:174:LEU:N	1:J:175:PRO:HD2	2.11	0.66
1:B:51:ALA:HB3	1:B:54:LEU:HD12	1.77	0.65
1:I:223:SER:HA	1:I:233:VAL:HG21	1.78	0.65
1:J:135:MET:CE	1:J:141:ALA:HA	2.26	0.65
1:J:340:PRO:HB2	1:J:358:PHE:HD1	1.61	0.65
1:H:347:GLU:HB3	1:H:350:ILE:HD12	1.78	0.65
1:J:135:MET:HE1	1:J:141:ALA:HA	1.78	0.65
1:D:155:HIS:ND1	1:D:180:THR:HG23	2.11	0.65
1:E:174:LEU:N	1:E:175:PRO:HD2	2.11	0.65
1:B:421:LEU:HD12	1:B:422:VAL:N	2.12	0.65
1:C:139:MET:O	1:C:143:THR:HB	1.97	0.65
1:F:350:ILE:O	1:F:354:GLN:HG2	1.97	0.65
1:K:340:PRO:HB2	1:K:358:PHE:HD1	1.62	0.65
1:B:70:ARG:HD3	1:B:79:THR:OG1	1.96	0.65
1:B:340:PRO:HB2	1:B:358:PHE:HD1	1.61	0.65
1:D:210:THR:HG22	1:D:215:ARG:N	2.12	0.65
1:K:139:MET:O	1:K:143:THR:HB	1.96	0.65
1:L:223:SER:HA	1:L:233:VAL:HG21	1.78	0.65
1:J:386:ALA:HB2	1:L:88:PHE:HA	1.78	0.65
1:I:204:PHE:CE2	1:I:222:VAL:HG11	2.32	0.65
1:J:170:ILE:HG23	1:J:174:LEU:HD12	1.77	0.65
1:B:174:LEU:N	1:B:175:PRO:HD2	2.12	0.65
1:G:211:ASN:HB2	1:G:239:PHE:HE2	1.62	0.65
1:J:387:PRO:HA	3:J:609:CCO:HC2	1.78	0.65
1:B:310:LEU:HA	1:B:313:ARG:NH2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:428:VAL:HG12	1:L:62:ILE:HD11	1.79	0.64
1:I:174:LEU:N	1:I:175:PRO:HD2	2.12	0.64
1:F:143:THR:HG22	1:F:144:VAL:N	2.13	0.64
1:B:223:SER:HA	1:B:233:VAL:HG21	1.80	0.64
1:H:170:ILE:HG23	1:H:174:LEU:HD12	1.79	0.64
1:J:347:GLU:HB3	1:J:350:ILE:HD12	1.80	0.64
1:L:170:ILE:HG23	1:L:174:LEU:HD12	1.78	0.64
1:E:421:LEU:HD12	1:E:422:VAL:N	2.12	0.64
1:F:399:PRO:HG3	1:F:423:ARG:NE	2.13	0.64
1:A:155:HIS:ND1	1:A:180:THR:HG23	2.12	0.64
1:F:170:ILE:HG23	1:F:174:LEU:HD12	1.80	0.64
1:H:348:HIS:NE2	1:H:352:LYS:HD2	2.12	0.64
1:E:139:MET:O	1:E:143:THR:HB	1.97	0.64
1:F:178:GLY:O	1:L:199:LYS:HD2	1.98	0.64
1:F:66:GLU:HG2	1:F:70:ARG:NH1	2.13	0.64
1:K:210:THR:HG22	1:K:215:ARG:N	2.11	0.64
1:G:153:GLY:HA2	1:G:178:GLY:O	1.97	0.64
1:I:143:THR:HG22	1:I:144:VAL:N	2.13	0.64
1:H:421:LEU:HD12	1:H:422:VAL:N	2.12	0.64
1:K:66:GLU:HG2	1:K:70:ARG:NH1	2.13	0.64
1:F:386:ALA:HB2	1:H:88:PHE:HA	1.79	0.64
1:K:250:LEU:HD11	1:K:354:GLN:HB2	1.80	0.64
1:H:143:THR:HG22	1:H:144:VAL:N	2.13	0.63
1:H:196:LEU:HG	1:H:229:LYS:HG3	1.80	0.63
1:J:143:THR:HG22	1:J:144:VAL:N	2.12	0.63
1:L:153:GLY:HA2	1:L:178:GLY:O	1.98	0.63
1:C:376:PHE:HB2	1:C:445:ILE:HD11	1.80	0.63
1:C:399:PRO:HG3	1:C:423:ARG:NE	2.13	0.63
1:D:63:HIS:HB3	1:D:67:ARG:HB2	1.80	0.63
1:E:70:ARG:HD3	1:E:79:THR:OG1	1.98	0.63
1:B:78:THR:HG21	1:C:268:ASP:HB3	1.81	0.63
1:K:207:GLU:CB	1:K:236:ASP:HB3	2.28	0.63
1:L:421:LEU:HD12	1:L:422:VAL:N	2.12	0.63
1:D:347:GLU:HB3	1:D:350:ILE:HD12	1.81	0.63
1:H:210:THR:HG22	1:H:215:ARG:N	2.14	0.63
1:B:53:PHE:HD1	1:B:54:LEU:HG	1.63	0.63
1:C:260:THR:HG23	1:C:270:LEU:HD22	1.80	0.63
1:D:70:ARG:HD3	1:D:79:THR:OG1	1.99	0.63
1:G:63:HIS:HB3	1:G:67:ARG:HB2	1.80	0.63
1:J:63:HIS:HB3	1:J:67:ARG:HB2	1.79	0.63
1:B:321:ALA:HB2	1:B:360:GLY:HA2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:LEU:N	1:G:175:PRO:HD2	2.13	0.63
1:K:135:MET:CE	1:K:141:ALA:HA	2.29	0.63
1:E:196:LEU:HG	1:E:229:LYS:HG3	1.81	0.63
1:H:250:LEU:HD11	1:H:354:GLN:HB2	1.81	0.63
1:K:196:LEU:HG	1:K:229:LYS:HG3	1.81	0.63
1:B:170:ILE:HG23	1:B:174:LEU:HD12	1.81	0.62
1:C:348:HIS:NE2	1:C:352:LYS:HD2	2.14	0.62
1:F:250:LEU:HD11	1:F:354:GLN:HB2	1.80	0.62
1:K:155:HIS:ND1	1:K:180:THR:HG23	2.13	0.62
1:A:143:THR:HG22	1:A:144:VAL:N	2.13	0.62
1:E:428:VAL:HG12	1:H:62:ILE:HD11	1.81	0.62
1:J:210:THR:O	1:J:214:LEU:HA	1.98	0.62
1:L:347:GLU:HB3	1:L:350:ILE:HD12	1.80	0.62
1:C:135:MET:CE	1:C:141:ALA:HA	2.29	0.62
1:E:143:THR:HG22	1:E:144:VAL:N	2.14	0.62
1:F:223:SER:HA	1:F:233:VAL:HG21	1.80	0.62
1:L:143:THR:HG22	1:L:144:VAL:N	2.13	0.62
1:C:310:LEU:HA	1:C:313:ARG:NH2	2.15	0.62
1:E:340:PRO:HB2	1:E:358:PHE:HD1	1.64	0.62
1:E:373:THR:O	1:E:376:PHE:HB3	1.99	0.62
1:G:210:THR:HG22	1:G:215:ARG:N	2.10	0.62
1:J:207:GLU:CB	1:J:236:ASP:HB3	2.28	0.62
1:D:170:ILE:HA	1:D:174:LEU:HD12	1.82	0.62
1:H:155:HIS:ND1	1:H:180:THR:HG23	2.14	0.62
1:H:340:PRO:HB2	1:H:358:PHE:HD1	1.64	0.62
1:B:418:MET:C	1:B:420:ASN:H	2.03	0.62
1:J:348:HIS:NE2	1:J:352:LYS:HD2	2.15	0.62
1:I:386:ALA:HB2	1:K:88:PHE:HA	1.81	0.62
1:E:250:LEU:HD11	1:E:354:GLN:HB2	1.82	0.62
1:H:207:GLU:CB	1:H:236:ASP:HB3	2.30	0.62
1:L:54:LEU:HD22	1:L:59:SER:HB3	1.82	0.62
1:F:348:HIS:NE2	1:F:352:LYS:HD2	2.14	0.61
1:F:421:LEU:HD12	1:F:422:VAL:H	1.63	0.61
1:A:268:ASP:HB3	1:D:78:THR:HG21	1.82	0.61
1:D:207:GLU:CB	1:D:236:ASP:HB3	2.30	0.61
1:D:210:THR:HG23	1:D:211:ASN:N	2.14	0.61
1:I:207:GLU:HB3	1:I:236:ASP:HB3	1.81	0.61
1:K:153:GLY:HA2	1:K:178:GLY:O	2.00	0.61
1:J:397:ASP:OD1	1:J:423:ARG:HB2	2.01	0.61
1:B:139:MET:O	1:B:143:THR:HB	1.99	0.61
1:A:78:THR:HG21	1:D:268:ASP:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:339:TYR:CD1	1:K:362:VAL:HG22	2.36	0.61
1:D:174:LEU:N	1:D:175:PRO:HD2	2.15	0.61
1:I:170:ILE:HG23	1:I:174:LEU:HD12	1.83	0.61
1:C:207:GLU:CB	1:C:236:ASP:HB3	2.31	0.61
1:D:143:THR:HG22	1:D:144:VAL:N	2.14	0.61
1:H:204:PHE:CE2	1:H:222:VAL:HG11	2.36	0.61
1:B:135:MET:CE	1:B:141:ALA:HA	2.31	0.61
1:A:88:PHE:HA	1:C:386:ALA:HB2	1.82	0.60
1:B:292:GLY:O	1:D:140:CYS:HB2	2.00	0.60
1:D:243:LEU:HD11	1:D:310:LEU:HG	1.82	0.60
1:G:143:THR:HG22	1:G:144:VAL:N	2.15	0.60
1:G:397:ASP:OD1	1:G:423:ARG:HB2	2.01	0.60
1:H:63:HIS:HB3	1:H:67:ARG:HB2	1.83	0.60
1:B:215:ARG:HD2	1:B:347:GLU:OE2	2.01	0.60
1:B:204:PHE:CE2	1:B:222:VAL:HG11	2.36	0.60
1:D:397:ASP:OD1	1:D:423:ARG:HB2	2.01	0.60
1:A:207:GLU:CB	1:A:236:ASP:HB3	2.31	0.60
1:A:260:THR:HG23	1:A:270:LEU:HD22	1.84	0.60
1:A:421:LEU:HD12	1:A:422:VAL:H	1.65	0.60
1:C:340:PRO:HB2	1:C:358:PHE:HD1	1.65	0.60
1:G:339:TYR:CD1	1:G:362:VAL:HG22	2.36	0.60
1:J:421:LEU:HD12	1:J:422:VAL:N	2.15	0.60
1:L:135:MET:HE1	1:L:141:ALA:HA	1.83	0.60
1:C:210:THR:O	1:C:214:LEU:HA	2.02	0.60
1:D:114:PRO:O	1:D:117:VAL:HG22	2.01	0.60
1:F:340:PRO:HB2	1:F:358:PHE:HD1	1.67	0.60
1:F:163:TYR:CE1	3:F:605:CCO:H1B1	2.36	0.60
1:G:210:THR:HG23	1:G:211:ASN:N	2.15	0.60
1:F:428:VAL:HG12	1:G:62:ILE:HD11	1.83	0.60
1:J:210:THR:HG23	1:J:211:ASN:N	2.15	0.60
1:D:211:ASN:HB2	1:D:239:PHE:HE2	1.67	0.60
1:F:373:THR:O	1:F:376:PHE:HB3	2.02	0.60
1:I:348:HIS:NE2	1:I:352:LYS:HD2	2.16	0.60
1:B:373:THR:O	1:B:376:PHE:HB3	2.01	0.60
1:E:339:TYR:CD1	1:E:362:VAL:HG22	2.37	0.59
1:F:348:HIS:O	1:F:352:LYS:HG3	2.02	0.59
1:H:135:MET:CE	1:H:141:ALA:HA	2.32	0.59
1:D:204:PHE:CE2	1:D:222:VAL:HG11	2.37	0.59
1:G:421:LEU:HD12	1:G:422:VAL:H	1.67	0.59
1:K:322:LEU:O	1:K:325:ALA:HB3	2.02	0.59
1:B:155:HIS:ND1	1:B:180:THR:HG23	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASN:HB2	1:C:239:PHE:HE2	1.68	0.59
1:D:321:ALA:HB2	1:D:360:GLY:HA2	1.83	0.59
1:I:277:PRO:HG2	1:I:280:LEU:HB2	1.85	0.59
1:L:163:TYR:CE1	3:L:611:CCO:H1B1	2.38	0.59
1:F:199:LYS:HD2	1:L:153:GLY:CA	2.32	0.59
1:I:62:ILE:CD1	1:L:428:VAL:HG12	2.31	0.59
1:K:210:THR:HG23	1:K:211:ASN:N	2.16	0.59
1:B:268:ASP:HB3	1:C:78:THR:HG21	1.84	0.59
1:F:321:ALA:HB2	1:F:360:GLY:HA2	1.84	0.59
1:K:348:HIS:O	1:K:352:LYS:HG3	2.03	0.59
1:B:210:THR:HG23	1:B:211:ASN:N	2.17	0.59
1:J:243:LEU:HD12	1:J:314:VAL:HG21	1.84	0.59
1:L:135:MET:CE	1:L:141:ALA:HA	2.32	0.59
1:A:373:THR:O	1:A:376:PHE:HB3	2.03	0.59
1:C:223:SER:HA	1:C:233:VAL:HG21	1.85	0.59
1:D:310:LEU:HA	1:D:313:ARG:NH2	2.17	0.59
1:E:243:LEU:HD12	1:E:314:VAL:HG21	1.83	0.59
1:F:70:ARG:HD3	1:F:79:THR:OG1	2.02	0.59
1:G:155:HIS:ND1	1:G:180:THR:HG23	2.18	0.59
1:B:348:HIS:NE2	1:B:352:LYS:HD2	2.18	0.59
1:I:153:GLY:HA2	1:I:178:GLY:O	2.03	0.59
1:I:268:ASP:HB3	1:L:78:THR:HG21	1.85	0.59
1:B:196:LEU:HG	1:B:229:LYS:HG3	1.84	0.59
1:C:210:THR:HG22	1:C:215:ARG:N	2.14	0.59
1:J:66:GLU:HG2	1:J:70:ARG:NH1	2.17	0.59
1:C:170:ILE:HG23	1:C:174:LEU:HD12	1.85	0.58
1:C:421:LEU:HD12	1:C:422:VAL:H	1.68	0.58
1:H:111:TYR:HA	1:H:289:HIS:NE2	2.18	0.58
1:B:66:GLU:HG2	1:B:70:ARG:NH1	2.18	0.58
1:I:240:ALA:O	1:I:241:THR:CB	2.50	0.58
1:K:57:ASP:HB3	1:K:243:LEU:HD22	1.85	0.58
1:D:418:MET:C	1:D:420:ASN:H	2.05	0.58
1:I:292:GLY:O	1:K:140:CYS:HB2	2.03	0.58
1:I:340:PRO:HB2	1:I:358:PHE:HD1	1.68	0.58
1:K:260:THR:HG23	1:K:270:LEU:HD22	1.85	0.58
1:B:53:PHE:CD1	1:B:54:LEU:HG	2.37	0.58
1:E:204:PHE:CE2	1:E:222:VAL:HG11	2.39	0.58
1:G:240:ALA:O	1:G:241:THR:CB	2.51	0.58
1:H:210:THR:O	1:H:214:LEU:HA	2.03	0.58
1:I:210:THR:O	1:I:214:LEU:HA	2.03	0.58
1:K:262:PHE:CE1	1:K:390:GLY:HA2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:CYS:HB2	1:D:292:GLY:O	2.03	0.58
1:F:207:GLU:CB	1:F:236:ASP:HB3	2.34	0.58
1:A:348:HIS:NE2	1:A:352:LYS:HD2	2.18	0.58
1:B:339:TYR:CD1	1:B:362:VAL:HG22	2.39	0.58
1:D:438:ILE:O	1:D:441:ALA:HB3	2.02	0.58
1:G:347:GLU:HB3	1:G:350:ILE:HD12	1.85	0.58
1:G:348:HIS:O	1:G:352:LYS:HG3	2.04	0.58
1:J:285:ARG:O	1:J:288:HIS:HB3	2.02	0.58
1:A:135:MET:CE	1:A:141:ALA:HA	2.34	0.58
1:G:207:GLU:CB	1:G:236:ASP:HB3	2.32	0.58
1:I:155:HIS:ND1	1:I:180:THR:HG23	2.19	0.58
1:K:223:SER:HA	1:K:233:VAL:HG21	1.84	0.58
1:C:66:GLU:HG2	1:C:70:ARG:NH1	2.19	0.58
1:G:173:ILE:O	1:G:176:LYS:HB2	2.04	0.58
1:A:170:ILE:HG23	1:A:174:LEU:HD12	1.84	0.58
1:C:347:GLU:HB3	1:C:350:ILE:HD12	1.86	0.58
1:F:311:HIS:CE1	1:F:312:LEU:HD23	2.39	0.58
1:G:135:MET:CE	1:G:141:ALA:HA	2.33	0.58
1:G:211:ASN:HD22	1:G:211:ASN:C	2.07	0.58
1:G:373:THR:O	1:G:376:PHE:HB3	2.03	0.58
1:J:372:THR:HG23	1:J:445:ILE:HG21	1.86	0.58
1:K:114:PRO:O	1:K:117:VAL:HG22	2.03	0.58
1:D:421:LEU:HD12	1:D:422:VAL:N	2.19	0.57
1:H:428:VAL:HG13	1:H:428:VAL:O	2.04	0.57
1:I:163:TYR:CE1	3:I:608:CCO:H1B1	2.39	0.57
1:J:62:ILE:HD11	1:K:428:VAL:HG12	1.86	0.57
1:L:129:ALA:HB2	1:L:248:LEU:CD1	2.34	0.57
1:E:331:HIS:CG	1:E:332:PRO:HD2	2.40	0.57
1:J:418:MET:C	1:J:420:ASN:H	2.07	0.57
1:F:62:ILE:HD11	1:G:428:VAL:HG12	1.86	0.57
1:K:204:PHE:CE2	1:K:222:VAL:HG11	2.39	0.57
1:A:129:ALA:HB2	1:A:248:LEU:CD1	2.35	0.57
1:A:66:GLU:HG2	1:A:70:ARG:NH1	2.19	0.57
1:E:212:PRO:HB3	1:E:423:ARG:HD3	1.86	0.57
1:K:321:ALA:HB2	1:K:360:GLY:HA2	1.86	0.57
1:C:250:LEU:HD11	1:C:354:GLN:HB2	1.87	0.57
1:E:63:HIS:HB3	1:E:67:ARG:HB2	1.85	0.57
1:G:243:LEU:HD12	1:G:314:VAL:HG21	1.86	0.57
1:H:277:PRO:HG2	1:H:280:LEU:HB2	1.86	0.57
1:H:397:ASP:OD1	1:H:423:ARG:HB2	2.04	0.57
1:A:310:LEU:HA	1:A:313:ARG:NH2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ALA:HB3	1:A:54:LEU:HD12	1.86	0.57
1:G:70:ARG:HD3	1:G:79:THR:OG1	2.04	0.57
1:I:433:ASP:OD2	1:L:56:SER:HB3	2.05	0.57
1:K:135:MET:HE1	1:K:141:ALA:HA	1.87	0.57
1:C:143:THR:HG22	1:C:144:VAL:N	2.20	0.57
1:F:211:ASN:HB2	1:F:239:PHE:HE2	1.69	0.57
1:K:240:ALA:O	1:K:241:THR:CB	2.49	0.57
1:L:211:ASN:HB2	1:L:239:PHE:HE2	1.69	0.57
1:A:223:SER:HA	1:A:233:VAL:HG21	1.86	0.57
1:C:209:PRO:HG3	1:C:355:MET:HE1	1.87	0.57
1:D:70:ARG:HB3	1:D:72:ILE:HG22	1.86	0.57
1:L:57:ASP:HB3	1:L:243:LEU:CD2	2.35	0.57
1:L:340:PRO:HB2	1:L:358:PHE:HD1	1.70	0.57
1:E:57:ASP:HB3	1:E:243:LEU:HD22	1.87	0.56
1:I:135:MET:CE	1:I:141:ALA:HA	2.35	0.56
1:K:143:THR:HG22	1:K:144:VAL:N	2.19	0.56
1:B:207:GLU:CB	1:B:236:ASP:HB3	2.36	0.56
1:K:54:LEU:HD23	1:K:59:SER:HB3	1.87	0.56
1:D:373:THR:O	1:D:376:PHE:HB3	2.05	0.56
1:G:223:SER:HA	1:G:233:VAL:HG21	1.86	0.56
1:C:210:THR:HG23	1:C:211:ASN:N	2.19	0.56
1:D:209:PRO:HG3	1:D:355:MET:HE1	1.87	0.56
1:F:428:VAL:HG13	1:F:428:VAL:O	2.04	0.56
1:I:421:LEU:HD12	1:I:422:VAL:N	2.21	0.56
1:B:187:ALA:O	1:B:189:VAL:N	2.38	0.56
1:I:428:VAL:O	1:I:428:VAL:HG13	2.05	0.56
1:L:339:TYR:CD1	1:L:362:VAL:HG22	2.41	0.56
1:A:196:LEU:HG	1:A:229:LYS:HG3	1.88	0.56
1:A:240:ALA:O	1:A:241:THR:CB	2.54	0.56
1:B:106:PHE:O	1:B:111:TYR:HB2	2.06	0.56
1:C:145:MET:HB2	1:C:274:ILE:CD1	2.35	0.56
1:G:348:HIS:NE2	1:G:352:LYS:HD2	2.21	0.56
1:J:373:THR:O	1:J:376:PHE:HB3	2.06	0.56
1:F:187:ALA:O	1:F:189:VAL:N	2.39	0.56
1:G:340:PRO:HB2	1:G:358:PHE:HD1	1.71	0.56
1:G:60:VAL:CG1	1:G:64:ALA:HB2	2.35	0.56
1:K:351:ALA:O	1:K:355:MET:HB2	2.05	0.56
1:C:240:ALA:O	1:C:241:THR:CB	2.54	0.56
1:C:285:ARG:O	1:C:288:HIS:HB3	2.06	0.56
1:E:207:GLU:CB	1:E:236:ASP:HB3	2.35	0.56
1:G:260:THR:HG23	1:G:270:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:348:HIS:O	1:H:352:LYS:HG3	2.06	0.56
1:J:170:ILE:HA	1:J:174:LEU:HD12	1.87	0.56
1:B:51:ALA:CB	1:B:54:LEU:HD12	2.36	0.56
1:E:210:THR:HG23	1:E:211:ASN:N	2.19	0.56
1:E:86:ALA:O	1:F:77:ILE:HD12	2.06	0.56
1:F:433:ASP:OD2	1:G:56:SER:HB3	2.06	0.56
1:J:153:GLY:HA2	1:J:178:GLY:O	2.06	0.56
1:B:173:ILE:O	1:B:176:LYS:HB2	2.06	0.56
1:G:210:THR:O	1:G:214:LEU:HA	2.06	0.56
1:I:217:VAL:CG1	1:I:222:VAL:HG21	2.36	0.56
1:J:210:THR:HG22	1:J:215:ARG:N	2.17	0.56
1:J:53:PHE:CD1	1:J:54:LEU:HG	2.41	0.56
1:K:170:ILE:HA	1:K:174:LEU:HD12	1.88	0.56
1:K:336:HIS:HB3	1:K:365:GLU:HG3	1.87	0.56
1:K:421:LEU:HD12	1:K:422:VAL:N	2.20	0.56
1:C:148:ALA:HB2	1:C:287:LEU:HD23	1.87	0.55
1:E:336:HIS:ND1	1:E:337:VAL:N	2.53	0.55
1:K:211:ASN:C	1:K:211:ASN:HD22	2.09	0.55
1:F:336:HIS:ND1	1:F:337:VAL:N	2.54	0.55
1:H:203:LEU:HB2	1:H:232:LEU:HB2	1.87	0.55
1:J:204:PHE:CE2	1:J:222:VAL:HG11	2.41	0.55
1:J:217:VAL:CG1	1:J:222:VAL:HG21	2.36	0.55
1:L:196:LEU:HG	1:L:229:LYS:HG3	1.88	0.55
1:C:336:HIS:ND1	1:C:337:VAL:N	2.54	0.55
1:D:196:LEU:HG	1:D:229:LYS:HG3	1.87	0.55
1:E:155:HIS:ND1	1:E:180:THR:HG23	2.22	0.55
1:E:60:VAL:CG1	1:E:64:ALA:HB2	2.36	0.55
1:G:418:MET:C	1:G:420:ASN:H	2.07	0.55
1:J:348:HIS:O	1:J:352:LYS:HG3	2.07	0.55
1:F:153:GLY:HA2	1:F:178:GLY:O	2.07	0.55
1:G:260:THR:CG2	1:G:270:LEU:HD22	2.37	0.55
1:A:210:THR:HG22	1:A:215:ARG:N	2.18	0.55
1:A:140:CYS:HB2	1:C:292:GLY:O	2.06	0.55
1:E:428:VAL:HG13	1:E:428:VAL:O	2.05	0.55
1:J:196:LEU:HG	1:J:229:LYS:HG3	1.88	0.55
1:B:135:MET:HE1	1:B:141:ALA:HA	1.87	0.55
1:B:143:THR:HG22	1:B:144:VAL:N	2.22	0.55
1:C:250:LEU:HD11	1:C:354:GLN:CB	2.37	0.55
1:D:215:ARG:HD2	1:D:347:GLU:OE2	2.06	0.55
1:E:348:HIS:NE2	1:E:352:LYS:HD2	2.22	0.55
1:A:350:ILE:O	1:A:354:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:ASP:OD1	1:F:423:ARG:HB2	2.07	0.55
1:G:187:ALA:O	1:G:189:VAL:N	2.39	0.55
1:E:348:HIS:O	1:E:352:LYS:HG3	2.07	0.55
1:F:62:ILE:CD1	1:G:428:VAL:HG12	2.37	0.55
1:H:217:VAL:CG1	1:H:222:VAL:HG21	2.37	0.55
1:B:163:TYR:CE1	3:B:601:CCO:H1B1	2.42	0.55
1:E:210:THR:HG22	1:E:215:ARG:N	2.18	0.55
1:E:211:ASN:HD22	1:E:211:ASN:C	2.11	0.55
1:E:397:ASP:OD1	1:E:399:PRO:HD3	2.07	0.55
1:H:418:MET:C	1:H:420:ASN:H	2.11	0.55
1:I:373:THR:O	1:I:376:PHE:HB3	2.06	0.55
1:A:210:THR:HG23	1:A:211:ASN:N	2.21	0.54
1:B:62:ILE:HD11	1:C:428:VAL:HG12	1.89	0.54
1:D:243:LEU:HD12	1:D:314:VAL:HG21	1.88	0.54
1:D:250:LEU:HD11	1:D:354:GLN:HB2	1.88	0.54
1:E:211:ASN:HB2	1:E:239:PHE:HE2	1.72	0.54
1:L:210:THR:O	1:L:214:LEU:HA	2.08	0.54
1:A:321:ALA:HB2	1:A:360:GLY:HA2	1.89	0.54
1:G:196:LEU:HG	1:G:229:LYS:HG3	1.88	0.54
1:G:127:GLU:OE2	1:G:242:PRO:HB3	2.07	0.54
1:C:260:THR:CG2	1:C:270:LEU:HD22	2.36	0.54
1:E:187:ALA:O	1:E:189:VAL:N	2.41	0.54
1:E:215:ARG:HD2	1:E:347:GLU:OE2	2.07	0.54
1:L:204:PHE:CE2	1:L:222:VAL:HG11	2.43	0.54
1:L:240:ALA:O	1:L:241:THR:CB	2.56	0.54
1:B:64:ALA:O	1:B:122:LYS:HG3	2.07	0.54
1:E:418:MET:C	1:E:420:ASN:H	2.09	0.54
1:F:243:LEU:HD12	1:F:314:VAL:HG21	1.88	0.54
1:H:223:SER:HA	1:H:233:VAL:HG21	1.89	0.54
1:E:163:TYR:CE1	3:E:604:CCO:H1B1	2.43	0.54
1:H:129:ALA:HB2	1:H:248:LEU:CD1	2.38	0.54
1:I:210:THR:HG23	1:I:211:ASN:N	2.21	0.54
1:L:336:HIS:ND1	1:L:337:VAL:N	2.56	0.54
1:A:208:SER:HA	1:A:209:PRO:C	2.27	0.54
1:B:418:MET:C	1:B:420:ASN:N	2.61	0.54
1:D:348:HIS:NE2	1:D:352:LYS:HD2	2.23	0.54
1:E:262:PHE:CE1	1:E:390:GLY:HA2	2.42	0.54
1:H:63:HIS:CD2	1:H:67:ARG:HD3	2.42	0.54
1:I:389:PHE:HB2	1:I:425:SER:HB2	1.89	0.54
1:L:207:GLU:CB	1:L:236:ASP:HB3	2.35	0.54
1:C:114:PRO:O	1:C:117:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:PHE:CE2	1:C:222:VAL:HG11	2.41	0.54
1:G:256:LEU:HB3	1:G:274:ILE:HG12	1.89	0.54
1:I:70:ARG:HD3	1:I:79:THR:OG1	2.08	0.54
1:J:64:ALA:O	1:J:122:LYS:HG3	2.07	0.54
1:K:310:LEU:HA	1:K:313:ARG:NH2	2.23	0.54
1:L:106:PHE:O	1:L:111:TYR:HB2	2.07	0.54
1:B:285:ARG:O	1:B:288:HIS:HB3	2.07	0.54
1:F:63:HIS:CD2	1:F:67:ARG:HD3	2.42	0.54
1:I:310:LEU:HA	1:I:313:ARG:NH2	2.23	0.54
1:K:260:THR:CG2	1:K:270:LEU:HD22	2.37	0.54
1:K:418:MET:C	1:K:420:ASN:H	2.10	0.54
1:K:426:PHE:HE1	1:K:438:ILE:HD11	1.73	0.54
1:A:399:PRO:HG3	1:A:423:ARG:NE	2.22	0.54
1:F:135:MET:CE	1:F:141:ALA:HA	2.38	0.54
1:H:240:ALA:O	1:H:241:THR:CB	2.53	0.54
1:J:292:GLY:O	1:L:140:CYS:HB2	2.07	0.54
1:L:397:ASP:OD1	1:L:399:PRO:HD3	2.08	0.54
1:B:210:THR:HG22	1:B:215:ARG:N	2.12	0.54
1:B:347:GLU:HB3	1:B:350:ILE:HD12	1.89	0.54
1:B:348:HIS:O	1:B:352:LYS:HG3	2.07	0.54
1:C:348:HIS:O	1:C:352:LYS:HG3	2.08	0.54
1:F:196:LEU:HG	1:F:229:LYS:HG3	1.89	0.54
1:G:111:TYR:HA	1:G:289:HIS:NE2	2.23	0.54
1:I:196:LEU:HG	1:I:229:LYS:HG3	1.89	0.54
1:J:428:VAL:HG13	1:J:428:VAL:O	2.07	0.54
1:L:170:ILE:HA	1:L:174:LEU:HD12	1.89	0.54
1:L:348:HIS:O	1:L:352:LYS:HG3	2.08	0.54
1:B:217:VAL:CG1	1:B:222:VAL:HG21	2.38	0.53
1:E:256:LEU:HB3	1:E:274:ILE:HG12	1.90	0.53
1:G:217:VAL:CG1	1:G:222:VAL:HG21	2.38	0.53
1:H:70:ARG:HD3	1:H:79:THR:OG1	2.08	0.53
1:I:348:HIS:O	1:I:352:LYS:HG3	2.08	0.53
1:J:209:PRO:HG3	1:J:355:MET:HE1	1.90	0.53
1:L:321:ALA:HB2	1:L:360:GLY:HA2	1.89	0.53
1:C:187:ALA:O	1:C:189:VAL:N	2.41	0.53
1:D:170:ILE:HG23	1:D:174:LEU:HD12	1.89	0.53
1:F:292:GLY:O	1:H:140:CYS:HB2	2.09	0.53
1:F:418:MET:C	1:F:420:ASN:H	2.10	0.53
1:G:204:PHE:CE2	1:G:222:VAL:HG11	2.43	0.53
1:G:203:LEU:HB2	1:G:232:LEU:HB2	1.90	0.53
1:G:399:PRO:HG3	1:G:423:ARG:NE	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:339:TYR:CD1	1:I:362:VAL:HG22	2.43	0.53
1:J:111:TYR:HA	1:J:289:HIS:NE2	2.24	0.53
1:A:260:THR:CG2	1:A:270:LEU:HD22	2.37	0.53
1:C:170:ILE:HA	1:C:174:LEU:HD12	1.89	0.53
1:C:64:ALA:HB3	1:C:122:LYS:HG3	1.91	0.53
1:D:336:HIS:HB3	1:D:365:GLU:HG3	1.89	0.53
1:D:418:MET:C	1:D:420:ASN:N	2.61	0.53
1:J:211:ASN:HB2	1:J:239:PHE:HE2	1.72	0.53
1:A:442:LEU:C	1:A:444:SER:H	2.10	0.53
1:B:173:ILE:C	1:B:175:PRO:HD2	2.29	0.53
1:F:210:THR:HG23	1:F:211:ASN:N	2.23	0.53
1:I:350:ILE:O	1:I:354:GLN:HG2	2.09	0.53
1:K:82:VAL:HG22	1:L:80:PRO:HB3	1.90	0.53
1:C:271:ALA:HB3	1:C:303:ILE:HD11	1.91	0.53
1:I:418:MET:C	1:I:420:ASN:H	2.11	0.53
1:K:243:LEU:HD11	1:K:310:LEU:HG	1.89	0.53
1:A:210:THR:O	1:A:214:LEU:HA	2.09	0.53
1:A:277:PRO:HG2	1:A:280:LEU:HB2	1.90	0.53
1:B:203:LEU:HB2	1:B:232:LEU:HB2	1.90	0.53
1:E:51:ALA:HB1	1:E:53:PHE:CE2	2.43	0.53
1:H:373:THR:O	1:H:376:PHE:HB3	2.09	0.53
1:J:212:PRO:HB3	1:J:423:ARG:HD3	1.91	0.53
1:K:50:TYR:CE2	1:K:64:ALA:HA	2.44	0.53
1:L:373:THR:O	1:L:376:PHE:HB3	2.08	0.53
1:C:217:VAL:CG1	1:C:222:VAL:HG21	2.39	0.53
1:D:54:LEU:CD2	1:D:59:SER:HB3	2.39	0.53
1:E:173:ILE:C	1:E:175:PRO:HD2	2.29	0.53
1:F:260:THR:HG23	1:F:270:LEU:HD22	1.90	0.53
1:H:350:ILE:O	1:H:354:GLN:HG2	2.09	0.53
1:J:132:THR:OG1	1:J:275:SER:HB3	2.09	0.53
1:K:428:VAL:HG13	1:K:428:VAL:O	2.08	0.53
1:K:70:ARG:HD3	1:K:79:THR:OG1	2.09	0.53
1:L:210:THR:HG23	1:L:211:ASN:N	2.22	0.53
1:L:70:ARG:HD3	1:L:79:THR:OG1	2.08	0.53
1:B:426:PHE:HE1	1:B:438:ILE:HD11	1.74	0.53
1:A:106:PHE:O	1:A:111:TYR:HB2	2.09	0.53
1:B:260:THR:HG23	1:B:270:LEU:HD22	1.90	0.53
1:B:339:TYR:CZ	1:B:358:PHE:HB2	2.44	0.53
1:D:350:ILE:O	1:D:354:GLN:HG2	2.09	0.53
1:H:111:TYR:HA	1:H:289:HIS:CD2	2.44	0.53
1:L:217:VAL:CG1	1:L:222:VAL:HG21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LEU:HB2	1:D:232:LEU:HB2	1.91	0.53
1:D:53:PHE:HD2	1:D:53:PHE:H	1.57	0.53
1:E:153:GLY:HA2	1:E:178:GLY:O	2.09	0.53
1:G:214:LEU:HD12	1:G:214:LEU:N	2.23	0.53
1:K:210:THR:O	1:K:214:LEU:HA	2.08	0.53
1:K:58:GLY:HA3	1:K:311:HIS:CD2	2.44	0.53
1:A:418:MET:C	1:A:420:ASN:H	2.12	0.52
1:D:260:THR:CG2	1:D:270:LEU:HD22	2.40	0.52
1:D:339:TYR:CD1	1:D:362:VAL:HG22	2.44	0.52
1:F:211:ASN:C	1:F:211:ASN:HD22	2.11	0.52
1:H:114:PRO:O	1:H:117:VAL:HG22	2.08	0.52
1:H:70:ARG:HB3	1:H:72:ILE:HG22	1.90	0.52
1:I:260:THR:CG2	1:I:270:LEU:HD22	2.38	0.52
1:J:418:MET:C	1:J:420:ASN:N	2.62	0.52
1:A:336:HIS:HB3	1:A:365:GLU:HG3	1.90	0.52
1:F:145:MET:HE2	1:F:146:LEU:HG	1.90	0.52
1:F:421:LEU:HD12	1:F:422:VAL:N	2.24	0.52
1:G:66:GLU:HG2	1:G:70:ARG:NH1	2.24	0.52
1:I:129:ALA:HB2	1:I:248:LEU:CD1	2.39	0.52
1:J:208:SER:HA	1:J:209:PRO:C	2.29	0.52
1:K:173:ILE:C	1:K:175:PRO:HD2	2.30	0.52
1:C:196:LEU:HG	1:C:229:LYS:HG3	1.92	0.52
1:C:428:VAL:O	1:C:428:VAL:HG13	2.09	0.52
1:D:214:LEU:HD12	1:D:214:LEU:N	2.24	0.52
1:E:223:SER:HA	1:E:233:VAL:HG21	1.89	0.52
1:G:321:ALA:HB2	1:G:360:GLY:HA2	1.91	0.52
1:C:321:ALA:HB2	1:C:360:GLY:HA2	1.91	0.52
1:E:111:TYR:HA	1:E:289:HIS:CD2	2.44	0.52
1:E:217:VAL:CG1	1:E:222:VAL:HG21	2.39	0.52
1:F:204:PHE:CE2	1:F:222:VAL:HG11	2.44	0.52
1:G:111:TYR:HA	1:G:289:HIS:CD2	2.43	0.52
1:F:428:VAL:HG12	1:G:62:ILE:CD1	2.39	0.52
1:I:57:ASP:HB3	1:I:243:LEU:CD2	2.39	0.52
1:K:160:THR:HG22	1:K:183:VAL:HG12	1.91	0.52
1:L:428:VAL:HG13	1:L:428:VAL:O	2.08	0.52
1:L:63:HIS:HB3	1:L:67:ARG:HB2	1.91	0.52
1:A:192:LEU:CD2	1:A:222:VAL:HG13	2.39	0.52
1:E:418:MET:C	1:E:420:ASN:N	2.63	0.52
1:F:106:PHE:O	1:F:111:TYR:HB2	2.09	0.52
1:G:155:HIS:HA	1:G:180:THR:O	2.09	0.52
1:G:310:LEU:HA	1:G:313:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:339:TYR:CD1	1:H:362:VAL:HG22	2.45	0.52
1:J:219:ILE:HB	1:J:250:LEU:HD12	1.91	0.52
1:L:350:ILE:O	1:L:354:GLN:HG2	2.10	0.52
1:A:170:ILE:HA	1:A:174:LEU:HD12	1.90	0.52
1:D:348:HIS:O	1:D:352:LYS:HG3	2.10	0.52
1:F:173:ILE:O	1:F:176:LYS:HB2	2.10	0.52
1:H:148:ALA:HB2	1:H:287:LEU:HD23	1.92	0.52
1:H:351:ALA:O	1:H:355:MET:HB2	2.10	0.52
1:E:428:VAL:HG12	1:H:62:ILE:CD1	2.40	0.52
1:J:155:HIS:ND1	1:J:180:THR:HG23	2.25	0.52
1:J:260:THR:HG23	1:J:270:LEU:HD22	1.91	0.52
1:I:428:VAL:HG12	1:L:62:ILE:CD1	2.40	0.52
1:A:119:LEU:HG	1:A:134:LEU:HD11	1.92	0.52
1:A:397:ASP:OD1	1:A:399:PRO:HD3	2.10	0.52
1:B:219:ILE:HB	1:B:250:LEU:HD12	1.92	0.52
1:C:106:PHE:O	1:C:111:TYR:HB2	2.09	0.52
1:D:260:THR:HG23	1:D:270:LEU:HD22	1.92	0.52
1:E:143:THR:CG2	1:E:144:VAL:N	2.72	0.52
1:G:170:ILE:HA	1:G:174:LEU:HD12	1.90	0.52
1:H:54:LEU:CD2	1:H:59:SER:HB3	2.40	0.52
1:K:203:LEU:HB2	1:K:232:LEU:HB2	1.92	0.52
1:I:211:ASN:HD22	1:I:211:ASN:C	2.13	0.52
1:I:211:ASN:HB2	1:I:239:PHE:HE2	1.75	0.52
1:I:72:ILE:HD13	1:I:72:ILE:O	2.10	0.52
1:K:311:HIS:N	1:K:311:HIS:ND1	2.58	0.52
1:B:111:TYR:HA	1:B:289:HIS:CD2	2.45	0.52
1:C:111:TYR:HA	1:C:289:HIS:NE2	2.25	0.52
1:H:336:HIS:HB3	1:H:365:GLU:HG3	1.91	0.52
1:K:209:PRO:HG3	1:K:355:MET:HE1	1.90	0.52
1:C:243:LEU:HD12	1:C:314:VAL:HG21	1.91	0.52
1:E:77:ILE:HD12	1:F:86:ALA:O	2.09	0.52
1:F:322:LEU:O	1:F:325:ALA:HB3	2.10	0.52
1:J:70:ARG:HD3	1:J:79:THR:OG1	2.09	0.52
1:B:336:HIS:ND1	1:B:337:VAL:N	2.57	0.51
1:B:70:ARG:HB3	1:B:72:ILE:HG22	1.92	0.51
1:D:217:VAL:CG1	1:D:222:VAL:HG21	2.41	0.51
1:E:210:THR:O	1:E:214:LEU:HA	2.10	0.51
1:I:77:ILE:HD12	1:J:86:ALA:O	2.10	0.51
1:J:173:ILE:C	1:J:175:PRO:HD2	2.30	0.51
1:J:203:LEU:HB2	1:J:232:LEU:HB2	1.92	0.51
1:L:389:PHE:HB2	1:L:425:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:ALA:HB2	1:F:248:LEU:CD1	2.40	0.51
1:F:155:HIS:ND1	1:F:180:THR:HG23	2.24	0.51
1:G:63:HIS:CD2	1:G:67:ARG:HD3	2.45	0.51
1:G:70:ARG:HB3	1:G:72:ILE:HG22	1.92	0.51
1:H:208:SER:HA	1:H:209:PRO:C	2.31	0.51
1:H:210:THR:HG23	1:H:211:ASN:N	2.25	0.51
1:K:187:ALA:O	1:K:189:VAL:N	2.44	0.51
1:A:80:PRO:HB3	1:B:82:VAL:HG22	1.92	0.51
1:D:258:SER:O	1:D:260:THR:N	2.43	0.51
1:I:250:LEU:HD11	1:I:354:GLN:CB	2.39	0.51
1:C:211:ASN:HD22	1:C:211:ASN:C	2.14	0.51
1:C:397:ASP:OD1	1:C:423:ARG:HB2	2.10	0.51
1:I:322:LEU:O	1:I:325:ALA:HB3	2.11	0.51
1:K:250:LEU:HD11	1:K:354:GLN:CB	2.40	0.51
1:K:347:GLU:HB3	1:K:350:ILE:HD12	1.92	0.51
1:L:208:SER:HA	1:L:209:PRO:C	2.30	0.51
1:D:285:ARG:O	1:D:288:HIS:HB3	2.11	0.51
1:D:399:PRO:HG3	1:D:423:ARG:NE	2.25	0.51
1:E:322:LEU:O	1:E:325:ALA:HB3	2.11	0.51
1:F:212:PRO:HB3	1:F:423:ARG:HD3	1.92	0.51
1:J:63:HIS:CD2	1:J:67:ARG:HD3	2.46	0.51
1:K:106:PHE:O	1:K:111:TYR:HB2	2.10	0.51
1:L:418:MET:C	1:L:420:ASN:H	2.12	0.51
1:A:348:HIS:O	1:A:352:LYS:HG3	2.09	0.51
1:B:351:ALA:O	1:B:355:MET:HB2	2.11	0.51
1:B:377:VAL:HA	1:B:380:LEU:HD12	1.91	0.51
1:C:373:THR:O	1:C:376:PHE:HB3	2.10	0.51
1:E:214:LEU:HD12	1:E:214:LEU:N	2.25	0.51
1:H:260:THR:CG2	1:H:270:LEU:HD22	2.40	0.51
1:I:140:CYS:O	1:I:144:VAL:HG23	2.11	0.51
1:J:114:PRO:O	1:J:117:VAL:HG22	2.10	0.51
1:F:418:MET:C	1:F:420:ASN:N	2.62	0.51
1:I:351:ALA:O	1:I:355:MET:HB2	2.10	0.51
1:C:155:HIS:ND1	1:C:180:THR:HG23	2.26	0.51
1:D:215:ARG:NH1	1:D:347:GLU:OE2	2.44	0.51
1:H:243:LEU:HD12	1:H:314:VAL:HG21	1.91	0.51
1:I:60:VAL:HG13	1:I:64:ALA:HB2	1.92	0.51
1:K:217:VAL:CG1	1:K:222:VAL:HG21	2.41	0.51
1:K:394:SER:OG	1:K:427:GLY:N	2.35	0.51
1:K:397:ASP:OD1	1:K:399:PRO:HD3	2.11	0.51
1:L:331:HIS:CG	1:L:332:PRO:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:VAL:CG1	1:L:64:ALA:HB2	2.41	0.51
1:C:311:HIS:N	1:C:311:HIS:ND1	2.59	0.51
1:D:129:ALA:HB2	1:D:248:LEU:CD1	2.41	0.51
1:G:64:ALA:O	1:G:122:LYS:HG3	2.11	0.51
1:G:418:MET:C	1:G:420:ASN:N	2.64	0.51
1:H:211:ASN:HB2	1:H:239:PHE:HE2	1.76	0.51
1:J:419:ASP:OD1	1:J:419:ASP:N	2.44	0.51
1:L:111:TYR:HA	1:L:289:HIS:NE2	2.25	0.51
1:A:173:ILE:C	1:A:175:PRO:HD2	2.32	0.51
1:C:261:LYS:HD2	1:C:389:PHE:CE2	2.46	0.51
1:C:421:LEU:HD12	1:C:422:VAL:N	2.26	0.51
1:D:173:ILE:C	1:D:175:PRO:HD2	2.31	0.51
1:D:187:ALA:O	1:D:189:VAL:N	2.44	0.51
1:D:208:SER:HA	1:D:209:PRO:C	2.31	0.51
1:D:339:TYR:CZ	1:D:358:PHE:HB2	2.46	0.51
1:F:114:PRO:O	1:F:117:VAL:HG22	2.10	0.51
1:G:114:PRO:O	1:G:117:VAL:HG22	2.10	0.51
1:H:66:GLU:HG2	1:H:70:ARG:NH1	2.26	0.51
1:K:160:THR:HG23	1:K:184:ILE:O	2.11	0.51
1:D:336:HIS:ND1	1:D:337:VAL:N	2.59	0.50
1:E:57:ASP:HB3	1:E:243:LEU:CD2	2.40	0.50
1:H:250:LEU:HD11	1:H:354:GLN:CB	2.41	0.50
1:H:397:ASP:HB2	1:H:402:MET:HG2	1.93	0.50
1:J:139:MET:O	1:J:143:THR:HB	2.10	0.50
1:J:240:ALA:O	1:J:241:THR:CB	2.53	0.50
1:K:336:HIS:ND1	1:K:337:VAL:N	2.58	0.50
1:L:243:LEU:HD12	1:L:314:VAL:HG21	1.93	0.50
1:L:310:LEU:HA	1:L:313:ARG:NH2	2.26	0.50
1:I:430:ASP:HB2	1:L:56:SER:OG	2.12	0.50
1:E:311:HIS:N	1:E:311:HIS:ND1	2.58	0.50
1:F:240:ALA:O	1:F:241:THR:CB	2.57	0.50
1:G:106:PHE:O	1:G:111:TYR:HB2	2.11	0.50
1:I:336:HIS:ND1	1:I:337:VAL:N	2.60	0.50
1:J:173:ILE:O	1:J:176:LYS:HB2	2.11	0.50
1:J:339:TYR:CZ	1:J:358:PHE:HB2	2.46	0.50
1:E:351:ALA:O	1:E:355:MET:HB2	2.11	0.50
1:G:192:LEU:CD2	1:G:222:VAL:HG13	2.41	0.50
1:G:336:HIS:ND1	1:G:337:VAL:N	2.59	0.50
1:G:54:LEU:HD22	1:G:59:SER:HB3	1.93	0.50
1:H:170:ILE:HA	1:H:174:LEU:HD12	1.93	0.50
1:J:426:PHE:HE1	1:J:438:ILE:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:MET:CE	1:E:141:ALA:HA	2.40	0.50
1:K:208:SER:HA	1:K:209:PRO:C	2.32	0.50
1:K:277:PRO:HG2	1:K:280:LEU:HB2	1.93	0.50
1:L:140:CYS:O	1:L:144:VAL:HG23	2.10	0.50
1:A:442:LEU:C	1:A:444:SER:N	2.65	0.50
1:E:394:SER:OG	1:E:427:GLY:N	2.36	0.50
1:G:143:THR:CG2	1:G:144:VAL:N	2.74	0.50
1:G:241:THR:HG22	1:G:243:LEU:N	2.14	0.50
1:H:106:PHE:O	1:H:111:TYR:HB2	2.12	0.50
1:I:207:GLU:CB	1:I:236:ASP:HB3	2.41	0.50
1:J:163:TYR:O	1:J:164:ARG:C	2.49	0.50
1:J:243:LEU:HD11	1:J:310:LEU:HG	1.94	0.50
1:L:111:TYR:HA	1:L:289:HIS:CD2	2.47	0.50
1:B:240:ALA:O	1:B:241:THR:CB	2.57	0.50
1:C:278:LEU:HA	1:C:281:VAL:HG12	1.93	0.50
1:D:207:GLU:HB2	1:D:236:ASP:O	2.12	0.50
1:D:340:PRO:HB2	1:D:358:PHE:CD1	2.45	0.50
1:H:258:SER:O	1:H:260:THR:N	2.45	0.50
1:H:64:ALA:HB3	1:H:122:LYS:HG3	1.92	0.50
1:J:143:THR:CG2	1:J:144:VAL:N	2.74	0.50
1:J:261:LYS:HD2	1:J:389:PHE:CE2	2.47	0.50
1:K:373:THR:O	1:K:376:PHE:HB3	2.11	0.50
1:L:418:MET:C	1:L:420:ASN:N	2.65	0.50
1:A:347:GLU:HB3	1:A:350:ILE:HD12	1.93	0.50
1:B:143:THR:O	1:B:147:LEU:HD12	2.12	0.50
1:E:331:HIS:ND1	1:E:332:PRO:HD2	2.26	0.50
1:F:127:GLU:OE2	1:F:242:PRO:HB3	2.10	0.50
1:F:208:SER:HA	1:F:209:PRO:C	2.32	0.50
1:G:113:ASN:ND2	1:G:297:PRO:HG3	2.27	0.50
1:H:187:ALA:O	1:H:189:VAL:N	2.45	0.50
1:H:211:ASN:C	1:H:211:ASN:HD22	2.15	0.50
1:H:271:ALA:HB3	1:H:303:ILE:HD11	1.92	0.50
1:I:138:GLY:N	2:I:500:PLP:O3P	2.44	0.50
1:D:72:ILE:O	1:D:72:ILE:HD13	2.12	0.50
1:H:260:THR:HG23	1:H:270:LEU:HD22	1.92	0.50
1:I:281:VAL:HG13	1:I:282:SER:N	2.26	0.50
1:J:111:TYR:HA	1:J:289:HIS:CD2	2.46	0.50
1:K:211:ASN:HB2	1:K:239:PHE:HE2	1.76	0.50
1:A:421:LEU:HD12	1:A:422:VAL:N	2.26	0.50
1:C:203:LEU:HB2	1:C:232:LEU:HB2	1.94	0.50
1:B:111:TYR:HA	1:B:289:HIS:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:HIS:N	1:B:311:HIS:ND1	2.59	0.49
1:C:111:TYR:HA	1:C:289:HIS:CD2	2.47	0.49
1:D:160:THR:HG23	1:D:184:ILE:O	2.12	0.49
1:D:210:THR:O	1:D:214:LEU:HA	2.11	0.49
1:D:322:LEU:O	1:D:325:ALA:HB3	2.12	0.49
1:G:236:ASP:OD2	2:G:500:PLP:H2A2	2.12	0.49
1:I:145:MET:HE2	1:I:146:LEU:HG	1.94	0.49
1:J:62:ILE:CD1	1:K:428:VAL:HG12	2.41	0.49
1:L:187:ALA:O	1:L:189:VAL:N	2.45	0.49
1:A:418:MET:C	1:A:420:ASN:N	2.66	0.49
1:D:240:ALA:O	1:D:241:THR:CB	2.59	0.49
1:E:170:ILE:HA	1:E:174:LEU:HD12	1.93	0.49
1:H:127:GLU:OE2	1:H:242:PRO:HB3	2.12	0.49
1:H:310:LEU:HA	1:H:313:ARG:NH2	2.27	0.49
1:I:106:PHE:O	1:I:111:TYR:HB2	2.11	0.49
1:A:271:ALA:HB3	1:A:303:ILE:HD11	1.94	0.49
1:E:219:ILE:HB	1:E:250:LEU:HD12	1.93	0.49
1:F:163:TYR:O	1:F:164:ARG:C	2.51	0.49
1:F:339:TYR:CD1	1:F:362:VAL:HG22	2.47	0.49
1:G:278:LEU:HA	1:G:281:VAL:HG12	1.93	0.49
1:G:428:VAL:HG13	1:G:428:VAL:O	2.12	0.49
1:H:212:PRO:HB3	1:H:423:ARG:HD3	1.94	0.49
1:H:72:ILE:O	1:H:72:ILE:HG23	2.12	0.49
1:I:62:ILE:HD11	1:L:428:VAL:CG1	2.40	0.49
1:J:160:THR:HG22	1:J:183:VAL:HG12	1.93	0.49
1:L:285:ARG:O	1:L:288:HIS:HB3	2.12	0.49
1:A:70:ARG:HB3	1:A:72:ILE:HG22	1.93	0.49
1:D:155:HIS:HA	1:D:180:THR:O	2.13	0.49
1:E:66:GLU:HG2	1:E:70:ARG:NH1	2.27	0.49
1:G:145:MET:HB2	1:G:274:ILE:CD1	2.42	0.49
1:G:163:TYR:CE1	3:G:606:CCO:H1B1	2.46	0.49
1:I:187:ALA:O	1:I:189:VAL:N	2.45	0.49
1:J:339:TYR:CD1	1:J:362:VAL:HG22	2.47	0.49
1:K:60:VAL:CG1	1:K:64:ALA:HB2	2.43	0.49
1:L:250:LEU:HD11	1:L:354:GLN:HB2	1.93	0.49
1:A:428:VAL:O	1:A:428:VAL:HG13	2.13	0.49
1:B:56:SER:OG	1:C:430:ASP:HB2	2.12	0.49
1:F:138:GLY:N	2:F:500:PLP:O3P	2.45	0.49
1:L:173:ILE:O	1:L:176:LYS:HB2	2.12	0.49
1:C:397:ASP:OD1	1:C:399:PRO:HD3	2.12	0.49
1:D:345:HIS:CE1	1:D:347:GLU:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LEU:HD22	1:D:59:SER:HB3	1.95	0.49
1:G:57:ASP:HB3	1:G:243:LEU:CD2	2.43	0.49
1:H:173:ILE:C	1:H:175:PRO:HD2	2.32	0.49
1:H:336:HIS:ND1	1:H:337:VAL:N	2.60	0.49
1:K:206:THR:O	1:K:235:ILE:HA	2.13	0.49
1:K:397:ASP:OD1	1:K:423:ARG:HB2	2.13	0.49
1:A:250:LEU:HD11	1:A:354:GLN:CB	2.40	0.49
1:E:321:ALA:HB2	1:E:360:GLY:HA2	1.94	0.49
1:F:310:LEU:HA	1:F:313:ARG:NH2	2.28	0.49
1:G:331:HIS:CG	1:G:332:PRO:HD2	2.47	0.49
1:G:60:VAL:O	1:G:62:ILE:N	2.45	0.49
1:H:143:THR:CG2	1:H:144:VAL:N	2.76	0.49
1:K:285:ARG:O	1:K:288:HIS:HB3	2.12	0.49
1:A:262:PHE:CE1	1:A:390:GLY:HA2	2.48	0.49
1:A:60:VAL:CG1	1:A:64:ALA:HB2	2.42	0.49
1:C:418:MET:C	1:C:420:ASN:H	2.15	0.49
1:E:114:PRO:O	1:E:117:VAL:HG22	2.13	0.49
1:I:111:TYR:HA	1:I:289:HIS:NE2	2.28	0.49
1:I:260:THR:HG23	1:I:270:LEU:HD22	1.95	0.49
1:A:140:CYS:O	1:A:144:VAL:HG23	2.12	0.49
1:B:260:THR:CG2	1:B:270:LEU:HD22	2.43	0.49
1:D:60:VAL:CG1	1:D:64:ALA:HB2	2.43	0.49
1:I:143:THR:CG2	1:I:144:VAL:N	2.76	0.49
1:I:210:THR:HG22	1:I:215:ARG:N	2.20	0.49
1:K:331:HIS:CG	1:K:332:PRO:HD2	2.47	0.49
1:L:203:LEU:HB2	1:L:232:LEU:HB2	1.93	0.49
1:A:62:ILE:HD11	1:D:428:VAL:HG12	1.94	0.49
1:B:322:LEU:O	1:B:325:ALA:HB3	2.12	0.49
1:D:428:VAL:HG13	1:D:428:VAL:O	2.12	0.49
1:H:163:TYR:O	1:H:164:ARG:C	2.51	0.49
1:J:442:LEU:O	1:J:445:ILE:HG13	2.13	0.49
1:K:339:TYR:CZ	1:K:358:PHE:HB2	2.48	0.49
1:K:52:SER:OG	1:K:53:PHE:N	2.46	0.49
1:H:119:LEU:HB2	1:H:304:ILE:CG1	2.42	0.48
1:I:156:ILE:HG12	1:I:157:VAL:N	2.20	0.48
1:J:187:ALA:O	1:J:189:VAL:N	2.46	0.48
1:J:277:PRO:HG2	1:J:280:LEU:HB2	1.94	0.48
1:L:163:TYR:O	1:L:164:ARG:C	2.51	0.48
1:C:208:SER:HA	1:C:209:PRO:C	2.33	0.48
1:D:278:LEU:HA	1:D:281:VAL:HG12	1.95	0.48
1:E:111:TYR:HA	1:E:289:HIS:NE2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:LEU:HA	1:E:313:ARG:NH2	2.29	0.48
1:G:336:HIS:HB3	1:G:365:GLU:HG3	1.95	0.48
1:H:423:ARG:HH12	3:H:607:CCO:C	2.26	0.48
1:J:106:PHE:O	1:J:111:TYR:HB2	2.13	0.48
1:J:336:HIS:ND1	1:J:337:VAL:N	2.61	0.48
1:A:143:THR:CG2	1:A:144:VAL:N	2.76	0.48
1:A:311:HIS:N	1:A:311:HIS:ND1	2.61	0.48
1:C:350:ILE:O	1:C:354:GLN:HG2	2.13	0.48
1:G:206:THR:O	1:G:235:ILE:HA	2.13	0.48
1:G:331:HIS:CE1	1:G:333:LYS:HB2	2.48	0.48
1:I:208:SER:HA	1:I:209:PRO:C	2.33	0.48
1:I:278:LEU:HA	1:I:281:VAL:HG12	1.95	0.48
1:J:211:ASN:C	1:J:211:ASN:HD22	2.16	0.48
1:B:163:TYR:O	1:B:164:ARG:C	2.52	0.48
1:B:211:ASN:HB2	1:B:239:PHE:HE2	1.77	0.48
1:B:214:LEU:HD12	1:B:214:LEU:N	2.28	0.48
1:C:163:TYR:O	1:C:164:ARG:C	2.50	0.48
1:C:331:HIS:CE1	1:C:333:LYS:HB2	2.49	0.48
1:D:258:SER:C	1:D:260:THR:N	2.66	0.48
1:F:143:THR:CG2	1:F:144:VAL:N	2.77	0.48
1:F:203:LEU:HB2	1:F:232:LEU:HB2	1.96	0.48
1:G:421:LEU:HD12	1:G:422:VAL:N	2.26	0.48
1:H:258:SER:C	1:H:260:THR:N	2.66	0.48
1:L:156:ILE:HG12	1:L:157:VAL:N	2.24	0.48
1:A:62:ILE:CD1	1:D:428:VAL:HG12	2.43	0.48
1:E:261:LYS:HD2	1:E:389:PHE:CE2	2.49	0.48
1:F:57:ASP:HB3	1:F:243:LEU:CD2	2.43	0.48
1:H:214:LEU:N	1:H:214:LEU:HD12	2.28	0.48
1:J:250:LEU:HD11	1:J:354:GLN:CB	2.43	0.48
1:A:153:GLY:HA2	1:A:178:GLY:O	2.12	0.48
1:C:350:ILE:O	1:C:353:LYS:HG2	2.12	0.48
1:D:243:LEU:CD1	1:D:310:LEU:HG	2.42	0.48
1:E:140:CYS:HB2	1:G:292:GLY:O	2.13	0.48
1:E:60:VAL:HG13	1:E:64:ALA:HB2	1.95	0.48
1:F:174:LEU:N	1:F:175:PRO:CD	2.76	0.48
1:G:60:VAL:HG12	1:G:64:ALA:HB2	1.95	0.48
1:J:145:MET:HB2	1:J:274:ILE:CD1	2.44	0.48
1:K:119:LEU:HG	1:K:134:LEU:HD11	1.94	0.48
1:K:418:MET:C	1:K:420:ASN:N	2.66	0.48
1:L:215:ARG:HD2	1:L:347:GLU:OE2	2.14	0.48
1:B:159:THR:HA	1:B:184:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:THR:HG23	1:D:242:PRO:HD2	1.96	0.48
1:D:60:VAL:HG13	1:D:64:ALA:HB2	1.95	0.48
1:G:163:TYR:O	1:G:164:ARG:C	2.51	0.48
1:G:212:PRO:HB3	1:G:423:ARG:HD3	1.96	0.48
1:H:58:GLY:HA3	1:H:311:HIS:CD2	2.49	0.48
1:J:70:ARG:HB3	1:J:72:ILE:HG22	1.95	0.48
1:K:163:TYR:O	1:K:164:ARG:C	2.52	0.48
1:K:212:PRO:HB3	1:K:423:ARG:HD3	1.95	0.48
1:L:265:GLY:HA3	1:L:313:ARG:NH1	2.29	0.48
1:C:143:THR:CG2	1:C:144:VAL:N	2.76	0.48
1:E:370:LEU:CD2	1:E:419:ASP:HB3	2.34	0.48
1:E:62:ILE:HD11	1:H:428:VAL:HG12	1.96	0.48
1:F:351:ALA:O	1:F:355:MET:HB2	2.13	0.48
1:G:250:LEU:HD11	1:G:354:GLN:CB	2.41	0.48
1:H:155:HIS:HA	1:H:180:THR:O	2.14	0.48
1:K:140:CYS:O	1:K:144:VAL:HG23	2.14	0.48
1:B:250:LEU:HD11	1:B:354:GLN:CB	2.43	0.48
1:E:72:ILE:O	1:E:72:ILE:HD13	2.14	0.48
1:G:311:HIS:ND1	1:G:311:HIS:N	2.62	0.48
1:K:52:SER:C	1:K:54:LEU:H	2.16	0.48
1:E:127:GLU:OE2	1:E:242:PRO:HB3	2.13	0.48
1:E:397:ASP:HB2	1:E:402:MET:HG2	1.95	0.48
1:F:260:THR:CG2	1:F:270:LEU:HD22	2.44	0.48
1:F:145:MET:HB2	1:F:274:ILE:CD1	2.44	0.48
1:F:311:HIS:N	1:F:311:HIS:ND1	2.62	0.48
1:H:322:LEU:O	1:H:325:ALA:HB3	2.13	0.48
1:H:331:HIS:CG	1:H:332:PRO:HD2	2.49	0.48
1:I:261:LYS:HD2	1:I:389:PHE:CE2	2.49	0.48
1:I:53:PHE:HD2	1:I:53:PHE:H	1.57	0.48
1:J:311:HIS:N	1:J:311:HIS:ND1	2.61	0.48
1:J:383:PRO:HB3	1:J:394:SER:HB3	1.95	0.48
1:A:217:VAL:CG1	1:A:222:VAL:HG21	2.43	0.47
1:B:210:THR:O	1:B:214:LEU:HA	2.13	0.47
1:B:256:LEU:HB3	1:B:274:ILE:HG12	1.96	0.47
1:D:211:ASN:C	1:D:211:ASN:HD22	2.17	0.47
1:F:160:THR:HG22	1:F:183:VAL:HG12	1.96	0.47
1:H:418:MET:C	1:H:420:ASN:N	2.65	0.47
1:I:418:MET:C	1:I:420:ASN:N	2.66	0.47
1:I:54:LEU:HD22	1:I:59:SER:HB3	1.96	0.47
1:K:143:THR:CG2	1:K:144:VAL:N	2.77	0.47
1:L:155:HIS:HA	1:L:180:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:PRO:HB2	1:A:358:PHE:HD1	1.78	0.47
1:C:145:MET:HE2	1:C:146:LEU:HG	1.95	0.47
1:I:311:HIS:ND1	1:I:311:HIS:N	2.62	0.47
1:E:240:ALA:O	1:E:241:THR:CB	2.57	0.47
1:E:339:TYR:CZ	1:E:358:PHE:HB2	2.49	0.47
1:G:339:TYR:CZ	1:G:358:PHE:HB2	2.50	0.47
1:H:311:HIS:ND1	1:H:311:HIS:N	2.61	0.47
1:H:321:ALA:HB2	1:H:360:GLY:HA2	1.95	0.47
1:I:143:THR:O	1:I:147:LEU:HD12	2.14	0.47
1:K:173:ILE:O	1:K:176:LYS:HB2	2.15	0.47
1:L:214:LEU:N	1:L:214:LEU:HD12	2.29	0.47
1:A:277:PRO:O	1:A:281:VAL:HG12	2.14	0.47
1:B:72:ILE:O	1:B:72:ILE:HD13	2.14	0.47
1:C:322:LEU:O	1:C:325:ALA:HB3	2.13	0.47
1:C:70:ARG:HB3	1:C:72:ILE:HG22	1.94	0.47
1:D:331:HIS:CG	1:D:332:PRO:HD2	2.50	0.47
1:E:261:LYS:HB3	1:E:389:PHE:O	2.14	0.47
1:E:63:HIS:CD2	1:E:67:ARG:HD3	2.50	0.47
1:H:163:TYR:CE1	3:H:607:CCO:H1B1	2.48	0.47
1:I:397:ASP:OD1	1:I:399:PRO:HD3	2.15	0.47
1:J:155:HIS:HA	1:J:180:THR:O	2.14	0.47
1:B:153:GLY:HA2	1:B:178:GLY:O	2.14	0.47
1:C:173:ILE:O	1:C:176:LYS:HB2	2.15	0.47
1:D:143:THR:CG2	1:D:144:VAL:N	2.77	0.47
1:E:208:SER:HA	1:E:209:PRO:C	2.34	0.47
1:G:218:ASP:O	1:G:222:VAL:HG23	2.15	0.47
1:H:310:LEU:O	1:H:314:VAL:HG23	2.15	0.47
1:J:313:ARG:O	1:J:317:GLN:HG3	2.14	0.47
1:A:211:ASN:HB2	1:A:239:PHE:HE2	1.78	0.47
1:A:111:TYR:HA	1:A:289:HIS:CD2	2.50	0.47
1:A:426:PHE:HE1	1:A:438:ILE:HD11	1.78	0.47
1:B:117:VAL:HA	1:B:120:GLU:HB2	1.96	0.47
1:B:336:HIS:HB3	1:B:365:GLU:HG3	1.95	0.47
1:B:428:VAL:HG13	1:B:428:VAL:O	2.13	0.47
1:F:250:LEU:HD11	1:F:354:GLN:CB	2.43	0.47
1:J:350:ILE:O	1:J:353:LYS:HG2	2.15	0.47
1:I:140:CYS:HB2	1:K:292:GLY:O	2.14	0.47
1:K:64:ALA:O	1:K:122:LYS:HG3	2.15	0.47
1:A:70:ARG:HD3	1:A:79:THR:OG1	2.15	0.47
1:C:214:LEU:N	1:C:214:LEU:HD12	2.30	0.47
1:C:256:LEU:HB3	1:C:274:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:VAL:HG22	1:D:80:PRO:HB3	1.97	0.47
1:E:438:ILE:O	1:E:441:ALA:HB3	2.14	0.47
1:G:160:THR:HG22	1:G:183:VAL:HG12	1.95	0.47
1:I:111:TYR:HA	1:I:289:HIS:CD2	2.49	0.47
1:J:310:LEU:HA	1:J:313:ARG:NH2	2.30	0.47
1:J:140:CYS:HB2	1:L:292:GLY:O	2.14	0.47
1:C:236:ASP:OD2	2:C:500:PLP:H2A2	2.15	0.47
1:D:372:THR:HG23	1:D:445:ILE:HG21	1.96	0.47
1:F:217:VAL:CG1	1:F:222:VAL:HG21	2.45	0.47
1:L:260:THR:HG23	1:L:270:LEU:HD22	1.97	0.47
1:A:187:ALA:O	1:A:189:VAL:N	2.48	0.47
1:A:261:LYS:HD2	1:A:389:PHE:CE2	2.50	0.47
1:C:323:ARG:HB2	1:C:431:PHE:CE2	2.50	0.47
1:H:350:ILE:O	1:H:353:LYS:HG2	2.15	0.47
1:I:209:PRO:HG3	1:I:355:MET:HE1	1.97	0.47
1:A:50:TYR:CE2	1:A:64:ALA:HA	2.50	0.47
1:B:419:ASP:OD1	1:B:419:ASP:N	2.48	0.47
1:G:132:THR:OG1	1:G:275:SER:HB3	2.15	0.47
1:G:208:SER:HA	1:G:209:PRO:C	2.33	0.47
1:H:383:PRO:HB3	1:H:394:SER:HB3	1.97	0.47
1:I:173:ILE:O	1:I:176:LYS:HB2	2.15	0.47
1:K:113:ASN:ND2	1:K:297:PRO:HG3	2.30	0.47
1:J:428:VAL:HG12	1:K:62:ILE:HD11	1.97	0.47
1:L:143:THR:CG2	1:L:144:VAL:N	2.77	0.47
1:L:212:PRO:HB3	1:L:423:ARG:HD3	1.97	0.47
1:D:111:TYR:HA	1:D:289:HIS:CD2	2.50	0.47
1:D:66:GLU:HG2	1:D:70:ARG:NH1	2.30	0.47
1:I:203:LEU:HB2	1:I:232:LEU:HB2	1.96	0.47
1:J:145:MET:HB2	1:J:274:ILE:HD13	1.96	0.47
1:A:114:PRO:O	1:A:117:VAL:HG22	2.15	0.46
1:A:207:GLU:HB2	1:A:236:ASP:O	2.15	0.46
1:A:343:GLN:HE21	1:A:343:GLN:HB3	1.54	0.46
1:A:72:ILE:HG23	1:A:72:ILE:O	2.15	0.46
1:C:426:PHE:HE1	1:C:438:ILE:HD11	1.79	0.46
1:A:428:VAL:HG12	1:D:62:ILE:CD1	2.45	0.46
1:F:258:SER:C	1:F:260:THR:N	2.68	0.46
1:H:132:THR:OG1	1:H:275:SER:HB3	2.15	0.46
1:J:260:THR:CG2	1:J:270:LEU:HD22	2.44	0.46
1:J:336:HIS:HB3	1:J:365:GLU:HG3	1.97	0.46
1:K:77:ILE:HD12	1:L:86:ALA:O	2.14	0.46
1:B:243:LEU:HD12	1:B:314:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ILE:C	1:C:175:PRO:HD2	2.35	0.46
1:D:259:ALA:HB2	1:D:263:LEU:HD12	1.97	0.46
1:E:278:LEU:HA	1:E:281:VAL:HG12	1.96	0.46
1:F:259:ALA:HA	1:F:263:LEU:HB2	1.96	0.46
1:G:60:VAL:HG13	1:G:64:ALA:HB2	1.96	0.46
1:I:206:THR:O	1:I:235:ILE:HA	2.15	0.46
1:L:70:ARG:HB3	1:L:72:ILE:HG22	1.97	0.46
1:A:174:LEU:N	1:A:175:PRO:CD	2.76	0.46
1:B:174:LEU:N	1:B:175:PRO:CD	2.78	0.46
1:B:313:ARG:O	1:B:317:GLN:HG3	2.16	0.46
1:D:219:ILE:HB	1:D:250:LEU:HD12	1.98	0.46
1:H:145:MET:HE2	1:H:146:LEU:HG	1.97	0.46
1:J:262:PHE:CE1	1:J:390:GLY:HA2	2.51	0.46
1:K:155:HIS:HA	1:K:180:THR:O	2.16	0.46
1:L:322:LEU:O	1:L:325:ALA:HB3	2.16	0.46
1:D:311:HIS:N	1:D:311:HIS:ND1	2.63	0.46
1:F:140:CYS:O	1:F:144:VAL:HG23	2.15	0.46
1:H:174:LEU:N	1:H:175:PRO:CD	2.78	0.46
1:H:206:THR:O	1:H:235:ILE:HA	2.15	0.46
1:H:63:HIS:CD2	1:H:67:ARG:HB2	2.51	0.46
1:L:145:MET:HB2	1:L:274:ILE:HD13	1.98	0.46
1:L:211:ASN:C	1:L:211:ASN:HD22	2.18	0.46
1:L:243:LEU:CD1	1:L:311:HIS:HA	2.45	0.46
1:A:206:THR:O	1:A:235:ILE:HA	2.16	0.46
1:A:322:LEU:O	1:A:325:ALA:HB3	2.16	0.46
1:C:117:VAL:HA	1:C:120:GLU:HB2	1.98	0.46
1:D:135:MET:CE	1:D:141:ALA:HA	2.46	0.46
1:D:387:PRO:HA	3:D:603:CCO:HC2	1.97	0.46
1:F:214:LEU:HD12	1:F:214:LEU:N	2.29	0.46
1:G:145:MET:HE2	1:G:146:LEU:HG	1.97	0.46
1:G:419:ASP:OD1	1:G:419:ASP:N	2.46	0.46
1:I:285:ARG:O	1:I:288:HIS:HB3	2.16	0.46
1:I:53:PHE:N	1:I:53:PHE:CD2	2.82	0.46
1:B:91:LYS:HD2	1:B:93:SER:OG	2.15	0.46
1:C:174:LEU:N	1:C:175:PRO:CD	2.78	0.46
1:D:419:ASP:OD1	1:D:419:ASP:N	2.48	0.46
1:E:160:THR:HG23	1:E:184:ILE:O	2.15	0.46
1:F:277:PRO:O	1:F:281:VAL:HG12	2.16	0.46
1:F:56:SER:HB3	1:G:433:ASP:OD2	2.15	0.46
1:G:160:THR:HG23	1:G:184:ILE:O	2.16	0.46
1:G:258:SER:C	1:G:260:THR:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:317:GLN:NE2	1:G:426:PHE:O	2.49	0.46
1:H:258:SER:C	1:H:260:THR:H	2.19	0.46
1:H:399:PRO:HG3	1:H:423:ARG:NE	2.30	0.46
1:I:243:LEU:CD1	1:I:311:HIS:HA	2.45	0.46
1:B:63:HIS:CD2	1:B:67:ARG:HD3	2.50	0.46
1:C:160:THR:HG23	1:C:184:ILE:O	2.16	0.46
1:C:365:GLU:HB3	1:C:420:ASN:HB3	1.97	0.46
1:D:145:MET:HB2	1:D:274:ILE:CD1	2.45	0.46
1:D:206:THR:O	1:D:235:ILE:HA	2.15	0.46
1:D:397:ASP:HB2	1:D:402:MET:HG2	1.96	0.46
1:J:119:LEU:HG	1:J:134:LEU:HD11	1.98	0.46
1:K:350:ILE:O	1:K:354:GLN:HG2	2.16	0.46
1:K:438:ILE:O	1:K:441:ALA:HB3	2.15	0.46
1:L:60:VAL:HG12	1:L:64:ALA:HB2	1.98	0.46
1:A:163:TYR:O	1:A:164:ARG:C	2.52	0.46
1:C:418:MET:C	1:C:420:ASN:N	2.69	0.46
1:D:111:TYR:HA	1:D:289:HIS:NE2	2.31	0.46
1:E:60:VAL:HG12	1:E:64:ALA:HB2	1.98	0.46
1:G:60:VAL:C	1:G:62:ILE:N	2.69	0.46
1:J:322:LEU:O	1:J:325:ALA:HB3	2.16	0.46
1:J:350:ILE:O	1:J:354:GLN:HG2	2.15	0.46
1:L:207:GLU:HB2	1:L:236:ASP:O	2.16	0.46
1:L:219:ILE:HB	1:L:250:LEU:HD12	1.98	0.46
1:L:259:ALA:HA	1:L:263:LEU:HB2	1.98	0.46
1:A:215:ARG:HD2	1:A:347:GLU:OE2	2.15	0.46
1:A:261:LYS:HB3	1:A:389:PHE:O	2.16	0.46
1:A:163:TYR:CE1	3:A:600:CCO:H1B1	2.51	0.46
1:C:331:HIS:CG	1:C:332:PRO:HD2	2.51	0.46
1:E:192:LEU:CD2	1:E:222:VAL:HG13	2.45	0.46
1:F:135:MET:HE1	1:F:141:ALA:HA	1.98	0.46
1:F:394:SER:OG	1:F:427:GLY:N	2.38	0.46
1:F:60:VAL:CG1	1:F:64:ALA:HB2	2.46	0.46
1:G:174:LEU:N	1:G:175:PRO:CD	2.79	0.46
1:G:211:ASN:ND2	1:G:211:ASN:C	2.69	0.46
1:G:277:PRO:HG2	1:G:280:LEU:HB2	1.96	0.46
1:G:148:ALA:HB2	1:G:287:LEU:HD23	1.98	0.46
1:G:262:PHE:CE1	1:G:390:GLY:HA2	2.51	0.46
1:F:384:TYR:CZ	1:G:67:ARG:HD2	2.50	0.46
1:H:281:VAL:HG13	1:H:282:SER:N	2.30	0.46
1:J:174:LEU:N	1:J:175:PRO:CD	2.78	0.46
1:J:351:ALA:O	1:J:355:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:129:ALA:HB2	1:K:248:LEU:CD1	2.46	0.46
1:A:135:MET:HE1	1:A:141:ALA:HA	1.97	0.46
1:A:192:LEU:HD21	1:A:222:VAL:HG13	1.97	0.46
1:B:209:PRO:HG3	1:B:355:MET:HE1	1.98	0.46
1:B:291:LEU:O	1:D:140:CYS:HA	2.16	0.46
1:C:277:PRO:HG2	1:C:280:LEU:HB2	1.98	0.46
1:C:281:VAL:HG13	1:C:282:SER:N	2.31	0.46
1:C:351:ALA:O	1:C:355:MET:HB2	2.15	0.46
1:D:106:PHE:O	1:D:111:TYR:HB2	2.16	0.46
1:D:227:HIS:HE2	1:D:253:ASP:CG	2.19	0.46
1:E:67:ARG:HD2	1:H:384:TYR:CZ	2.51	0.46
1:H:159:THR:HA	1:H:184:ILE:O	2.15	0.46
1:H:72:ILE:O	1:H:72:ILE:HD13	2.17	0.46
1:I:145:MET:HB2	1:I:274:ILE:CD1	2.46	0.46
1:I:63:HIS:CD2	1:I:67:ARG:HD3	2.51	0.46
1:J:138:GLY:N	2:J:500:PLP:O3P	2.48	0.46
1:J:261:LYS:HB3	1:J:389:PHE:O	2.15	0.46
1:L:174:LEU:N	1:L:175:PRO:CD	2.78	0.46
1:A:243:LEU:CD1	1:A:311:HIS:HA	2.45	0.45
1:B:62:ILE:CD1	1:C:428:VAL:HG12	2.46	0.45
1:G:350:ILE:O	1:G:353:LYS:HG2	2.16	0.45
1:H:119:LEU:HG	1:H:134:LEU:HD11	1.97	0.45
1:I:148:ALA:HB2	1:I:287:LEU:HD23	1.97	0.45
1:I:60:VAL:CG1	1:I:64:ALA:HB2	2.46	0.45
1:K:375:LYS:HD2	1:K:445:ILE:CG2	2.45	0.45
1:L:260:THR:CG2	1:L:270:LEU:HD22	2.46	0.45
1:L:336:HIS:HB3	1:L:365:GLU:HG3	1.98	0.45
1:L:262:PHE:CE1	1:L:390:GLY:HA2	2.51	0.45
1:C:86:ALA:O	1:D:77:ILE:HD12	2.17	0.45
1:F:419:ASP:N	1:F:419:ASP:OD1	2.48	0.45
1:J:129:ALA:HB2	1:J:248:LEU:CD1	2.46	0.45
1:J:156:ILE:HG12	1:J:157:VAL:N	2.21	0.45
1:J:382:ILE:HD12	1:J:437:ASP:HB2	1.98	0.45
1:L:66:GLU:HG2	1:L:70:ARG:NH1	2.31	0.45
1:F:206:THR:O	1:F:235:ILE:HA	2.15	0.45
1:G:72:ILE:HD13	1:G:72:ILE:O	2.16	0.45
1:K:214:LEU:N	1:K:214:LEU:HD12	2.32	0.45
1:A:351:ALA:O	1:A:355:MET:HB2	2.16	0.45
1:B:210:THR:HB	1:B:215:ARG:O	2.16	0.45
1:B:277:PRO:HG2	1:B:280:LEU:HB2	1.98	0.45
1:B:345:HIS:CE1	1:B:347:GLU:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:PHE:HB2	1:D:425:SER:HB2	1.99	0.45
1:D:442:LEU:C	1:D:444:SER:H	2.19	0.45
1:E:155:HIS:HA	1:E:180:THR:O	2.15	0.45
1:E:260:THR:HG23	1:E:270:LEU:HD22	1.98	0.45
1:F:428:VAL:CG1	1:G:62:ILE:HD11	2.45	0.45
1:H:110:ARG:HD3	1:H:292:GLY:CA	2.45	0.45
1:H:60:VAL:C	1:H:62:ILE:N	2.69	0.45
1:I:113:ASN:ND2	1:I:297:PRO:HG3	2.31	0.45
1:K:72:ILE:HD13	1:K:72:ILE:O	2.16	0.45
1:A:63:HIS:CD2	1:A:67:ARG:HD3	2.51	0.45
1:C:72:ILE:HD13	1:C:72:ILE:O	2.16	0.45
1:D:163:TYR:O	1:D:164:ARG:C	2.55	0.45
1:D:281:VAL:HG13	1:D:282:SER:N	2.32	0.45
1:E:145:MET:HE2	1:E:146:LEU:HG	1.98	0.45
1:G:258:SER:O	1:G:260:THR:N	2.50	0.45
1:H:173:ILE:O	1:H:176:LYS:HB2	2.16	0.45
1:H:160:THR:HG22	1:H:183:VAL:HG12	1.99	0.45
1:K:419:ASP:OD1	1:K:419:ASP:N	2.49	0.45
1:L:64:ALA:O	1:L:122:LYS:HG3	2.17	0.45
1:A:145:MET:HE2	1:A:146:LEU:HG	1.98	0.45
1:A:155:HIS:HA	1:A:180:THR:O	2.16	0.45
1:A:173:ILE:O	1:A:176:LYS:HB2	2.17	0.45
1:B:208:SER:HA	1:B:209:PRO:C	2.37	0.45
1:B:64:ALA:HB3	1:B:122:LYS:HG3	1.99	0.45
1:H:135:MET:HE1	1:H:141:ALA:HA	1.97	0.45
1:J:401:ILE:HA	1:J:405:TRP:HB2	1.99	0.45
1:K:211:ASN:C	1:K:211:ASN:ND2	2.70	0.45
1:K:319:SER:O	1:K:320:THR:C	2.54	0.45
1:L:159:THR:HA	1:L:184:ILE:O	2.17	0.45
1:L:206:THR:O	1:L:235:ILE:HA	2.16	0.45
1:L:426:PHE:HE1	1:L:438:ILE:HD11	1.82	0.45
1:A:53:PHE:CD1	1:A:54:LEU:HG	2.52	0.45
1:A:63:HIS:CD2	1:A:67:ARG:HB2	2.52	0.45
1:A:72:ILE:HD13	1:A:72:ILE:O	2.16	0.45
1:B:211:ASN:HD22	1:B:211:ASN:C	2.20	0.45
1:D:394:SER:OG	1:D:427:GLY:N	2.39	0.45
1:E:174:LEU:N	1:E:175:PRO:CD	2.78	0.45
1:H:153:GLY:HA2	1:H:178:GLY:O	2.17	0.45
1:H:397:ASP:OD1	1:H:399:PRO:HD3	2.17	0.45
1:I:159:THR:HA	1:I:184:ILE:O	2.17	0.45
1:I:331:HIS:CG	1:I:332:PRO:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:192:LEU:O	1:K:196:LEU:HB2	2.17	0.45
1:C:319:SER:O	1:C:320:THR:C	2.55	0.45
1:C:70:ARG:HD3	1:C:79:THR:OG1	2.16	0.45
1:C:77:ILE:HD12	1:D:86:ALA:O	2.17	0.45
1:E:173:ILE:O	1:E:176:LYS:HB2	2.16	0.45
1:F:82:VAL:HG21	1:F:114:PRO:HG2	1.98	0.45
1:F:365:GLU:HB3	1:F:420:ASN:HB3	1.99	0.45
1:F:63:HIS:HB3	1:F:67:ARG:CB	2.45	0.45
1:G:397:ASP:OD1	1:G:399:PRO:HD3	2.17	0.45
1:G:426:PHE:HE1	1:G:438:ILE:HD11	1.81	0.45
1:H:145:MET:HB2	1:H:274:ILE:CD1	2.47	0.45
1:H:57:ASP:HB3	1:H:243:LEU:CD2	2.47	0.45
1:L:114:PRO:O	1:L:117:VAL:HG22	2.16	0.45
1:A:401:ILE:HA	1:A:405:TRP:HB2	1.99	0.45
1:C:135:MET:HE1	1:C:141:ALA:HA	1.99	0.45
1:C:345:HIS:CE1	1:C:347:GLU:HG2	2.51	0.45
1:C:57:ASP:HB3	1:C:243:LEU:HD22	1.98	0.45
1:F:160:THR:HG23	1:F:184:ILE:O	2.17	0.45
1:G:117:VAL:HA	1:G:120:GLU:HB2	1.98	0.45
1:H:339:TYR:CZ	1:H:358:PHE:HB2	2.51	0.45
1:J:192:LEU:O	1:J:196:LEU:HB2	2.17	0.45
1:J:215:ARG:HD2	1:J:347:GLU:OE2	2.17	0.45
1:J:207:GLU:HB2	1:J:236:ASP:O	2.16	0.45
1:J:317:GLN:NE2	1:J:426:PHE:O	2.50	0.45
1:L:311:HIS:N	1:L:311:HIS:ND1	2.64	0.45
1:A:132:THR:OG1	1:A:275:SER:HB3	2.17	0.45
1:B:192:LEU:CD2	1:B:222:VAL:HG13	2.47	0.45
1:E:270:LEU:O	1:E:271:ALA:HB2	2.17	0.45
1:E:285:ARG:O	1:E:288:HIS:HB3	2.16	0.45
1:F:210:THR:CG2	1:F:215:ARG:H	2.18	0.45
1:G:281:VAL:HG13	1:G:282:SER:N	2.31	0.45
1:H:323:ARG:HB2	1:H:431:PHE:CE2	2.52	0.45
1:I:117:VAL:HA	1:I:120:GLU:HB2	1.98	0.45
1:L:261:LYS:HD2	1:L:389:PHE:CE2	2.52	0.45
1:L:278:LEU:HA	1:L:281:VAL:HG12	1.99	0.45
1:A:211:ASN:HD22	1:A:211:ASN:C	2.20	0.44
1:A:219:ILE:HB	1:A:250:LEU:HD12	1.99	0.44
1:C:212:PRO:HB3	1:C:423:ARG:HD3	1.98	0.44
1:C:163:TYR:CE1	3:C:602:CCO:H1B1	2.52	0.44
1:F:281:VAL:HG13	1:F:282:SER:N	2.32	0.44
1:F:430:ASP:HB2	1:G:56:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:ILE:HD11	1:G:428:VAL:CG1	2.45	0.44
1:I:120:GLU:HG2	1:I:132:THR:O	2.16	0.44
1:I:173:ILE:C	1:I:175:PRO:HD2	2.36	0.44
1:K:271:ALA:HB3	1:K:303:ILE:HD11	1.99	0.44
1:L:57:ASP:HB3	1:L:243:LEU:HD22	1.99	0.44
1:A:236:ASP:OD2	2:A:500:PLP:H2A2	2.17	0.44
1:C:215:ARG:HD2	1:C:347:GLU:OE2	2.18	0.44
1:E:280:LEU:HA	1:E:280:LEU:HD23	1.85	0.44
1:E:350:ILE:O	1:E:354:GLN:HG2	2.16	0.44
1:F:173:ILE:C	1:F:175:PRO:HD2	2.37	0.44
1:F:426:PHE:HE1	1:F:438:ILE:HD11	1.81	0.44
1:J:60:VAL:CG1	1:J:64:ALA:HB2	2.47	0.44
1:K:278:LEU:HA	1:K:281:VAL:HG12	2.00	0.44
1:D:160:THR:HG22	1:D:183:VAL:HG12	1.98	0.44
1:E:159:THR:HA	1:E:184:ILE:O	2.17	0.44
1:F:53:PHE:CD1	1:F:54:LEU:HG	2.52	0.44
1:G:72:ILE:HG23	1:G:72:ILE:O	2.17	0.44
1:K:368:GLY:O	1:K:420:ASN:ND2	2.51	0.44
1:L:339:TYR:CZ	1:L:358:PHE:HB2	2.52	0.44
1:D:210:THR:HB	1:D:215:ARG:O	2.17	0.44
1:D:369:ASP:H	1:D:372:THR:HB	1.83	0.44
1:E:340:PRO:HB2	1:E:358:PHE:CD1	2.49	0.44
1:E:82:VAL:HG21	1:E:114:PRO:HG2	1.99	0.44
1:H:319:SER:O	1:H:320:THR:C	2.56	0.44
1:H:384:TYR:O	1:H:395:ILE:HG23	2.17	0.44
1:I:370:LEU:CD2	1:I:419:ASP:HB3	2.41	0.44
1:I:70:ARG:HB3	1:I:72:ILE:HG22	1.99	0.44
1:J:280:LEU:HA	1:J:280:LEU:HD23	1.87	0.44
1:A:148:ALA:HB2	1:A:287:LEU:HD23	1.99	0.44
1:A:160:THR:HG23	1:A:184:ILE:O	2.17	0.44
1:A:281:VAL:HG13	1:A:282:SER:N	2.32	0.44
1:A:302:LEU:HB3	1:D:305:ARG:NH2	2.32	0.44
1:A:73:VAL:O	1:A:74:THR:HG23	2.18	0.44
1:B:143:THR:CG2	1:B:144:VAL:N	2.80	0.44
1:B:243:LEU:CD1	1:B:311:HIS:HA	2.47	0.44
1:B:365:GLU:HB3	1:B:420:ASN:HB3	1.99	0.44
1:F:121:GLU:O	1:F:124:SER:HB2	2.17	0.44
1:F:387:PRO:HA	3:F:605:CCO:HC2	2.00	0.44
1:G:261:LYS:HD2	1:G:389:PHE:CE2	2.53	0.44
1:I:271:ALA:HB3	1:I:303:ILE:HD11	2.00	0.44
1:J:160:THR:HG23	1:J:184:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:397:ASP:HB2	1:J:402:MET:HG2	2.00	0.44
1:L:173:ILE:C	1:L:175:PRO:HD2	2.36	0.44
1:A:336:HIS:ND1	1:A:337:VAL:N	2.64	0.44
1:B:192:LEU:O	1:B:196:LEU:HB2	2.17	0.44
1:B:206:THR:O	1:B:235:ILE:HA	2.17	0.44
1:B:399:PRO:HG3	1:B:423:ARG:HE	1.78	0.44
1:C:192:LEU:CD2	1:C:222:VAL:HG13	2.47	0.44
1:C:206:THR:O	1:C:235:ILE:HA	2.18	0.44
1:D:219:ILE:O	1:D:220:GLU:C	2.55	0.44
1:D:374:ALA:O	1:D:377:VAL:HG22	2.17	0.44
1:E:129:ALA:HB2	1:E:248:LEU:CD1	2.47	0.44
1:F:280:LEU:HD23	1:F:280:LEU:HA	1.87	0.44
1:H:278:LEU:HA	1:H:281:VAL:HG12	2.00	0.44
1:L:351:ALA:O	1:L:355:MET:HB2	2.17	0.44
1:L:72:ILE:HD12	1:L:80:PRO:HG2	2.00	0.44
1:B:212:PRO:HB3	1:B:423:ARG:HD3	1.99	0.44
1:F:156:ILE:HG12	1:F:157:VAL:N	2.24	0.44
1:F:210:THR:HB	1:F:215:ARG:O	2.18	0.44
1:G:322:LEU:O	1:G:325:ALA:HB3	2.18	0.44
1:G:350:ILE:O	1:G:354:GLN:HG2	2.17	0.44
1:I:119:LEU:HB2	1:I:304:ILE:CG1	2.47	0.44
1:K:280:LEU:HD23	1:K:280:LEU:HA	1.85	0.44
1:D:310:LEU:HA	1:D:313:ARG:HH21	1.81	0.44
1:E:209:PRO:HG3	1:E:355:MET:HE1	1.99	0.44
1:G:270:LEU:O	1:G:271:ALA:HB2	2.18	0.44
1:G:75:ASP:O	1:H:87:TYR:HA	2.18	0.44
1:I:163:TYR:O	1:I:164:ARG:C	2.55	0.44
1:I:215:ARG:HD2	1:I:347:GLU:OE2	2.17	0.44
1:J:60:VAL:HG13	1:J:64:ALA:HB2	2.00	0.44
1:E:203:LEU:HB2	1:E:232:LEU:HB2	2.00	0.44
1:I:365:GLU:HB3	1:I:420:ASN:HB3	2.00	0.44
1:K:60:VAL:C	1:K:62:ILE:H	2.21	0.44
1:L:261:LYS:HD2	1:L:389:PHE:CZ	2.53	0.44
1:A:419:ASP:N	1:A:419:ASP:OD1	2.51	0.43
1:B:62:ILE:O	1:B:308:LYS:HE2	2.18	0.43
1:B:54:LEU:HD22	1:B:59:SER:HB3	2.00	0.43
1:F:397:ASP:OD1	1:F:399:PRO:HD3	2.17	0.43
1:G:211:ASN:HD22	1:G:212:PRO:N	2.16	0.43
1:H:280:LEU:HD23	1:H:280:LEU:HA	1.83	0.43
1:E:428:VAL:CG1	1:H:62:ILE:HD11	2.46	0.43
1:J:311:HIS:CE1	1:J:312:LEU:HD23	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:ASN:OD1	1:K:115:THR:N	2.50	0.43
1:K:207:GLU:HB2	1:K:236:ASP:O	2.18	0.43
1:K:401:ILE:HA	1:K:405:TRP:HB2	2.00	0.43
1:L:331:HIS:CE1	1:L:333:LYS:HB2	2.52	0.43
1:B:278:LEU:HA	1:B:281:VAL:HG12	2.00	0.43
1:D:384:TYR:O	1:D:395:ILE:HG23	2.17	0.43
1:E:126:LEU:HA	1:E:126:LEU:HD23	1.88	0.43
1:E:277:PRO:HG2	1:E:280:LEU:HB2	1.99	0.43
1:F:350:ILE:O	1:F:353:LYS:HG2	2.18	0.43
1:I:331:HIS:CE1	1:I:333:LYS:HB2	2.52	0.43
1:K:144:VAL:HA	1:K:147:LEU:HD12	1.99	0.43
1:K:163:TYR:CE1	3:K:610:CCO:H1B1	2.53	0.43
1:A:258:SER:C	1:A:260:THR:N	2.71	0.43
1:C:339:TYR:CD1	1:C:362:VAL:HG22	2.53	0.43
1:E:163:TYR:O	1:E:164:ARG:C	2.56	0.43
1:H:140:CYS:O	1:H:144:VAL:HG23	2.18	0.43
1:J:397:ASP:OD1	1:J:399:PRO:HD3	2.18	0.43
1:K:211:ASN:HD22	1:K:212:PRO:N	2.16	0.43
1:K:310:LEU:O	1:K:314:VAL:HG23	2.19	0.43
1:K:60:VAL:C	1:K:62:ILE:N	2.72	0.43
1:K:70:ARG:HB3	1:K:72:ILE:HG22	2.00	0.43
1:L:145:MET:HB2	1:L:274:ILE:CD1	2.48	0.43
1:B:219:ILE:O	1:B:220:GLU:C	2.56	0.43
1:B:241:THR:HG23	1:B:242:PRO:HD2	2.00	0.43
1:B:271:ALA:HB3	1:B:303:ILE:HD11	2.00	0.43
1:B:340:PRO:HB2	1:B:358:PHE:CD1	2.47	0.43
1:B:389:PHE:HB2	1:B:425:SER:HB2	2.00	0.43
1:C:57:ASP:HB3	1:C:243:LEU:CD2	2.48	0.43
1:C:129:ALA:HB2	1:C:248:LEU:CD1	2.48	0.43
1:D:377:VAL:CG2	1:D:378:ASP:N	2.82	0.43
1:F:211:ASN:HD22	1:F:212:PRO:N	2.16	0.43
1:G:135:MET:HE2	1:G:141:ALA:HA	2.01	0.43
1:G:192:LEU:O	1:G:196:LEU:HB2	2.18	0.43
1:H:219:ILE:O	1:H:220:GLU:C	2.56	0.43
1:I:114:PRO:O	1:I:117:VAL:HG22	2.18	0.43
1:I:399:PRO:HG3	1:I:423:ARG:NE	2.34	0.43
1:L:155:HIS:ND1	1:L:180:THR:HG23	2.32	0.43
1:A:214:LEU:N	1:A:214:LEU:HD12	2.33	0.43
1:A:331:HIS:CE1	1:A:333:LYS:HB2	2.53	0.43
1:C:113:ASN:ND2	1:C:297:PRO:HG3	2.33	0.43
1:C:110:ARG:HD3	1:C:292:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:PRO:HB2	1:C:358:PHE:CD1	2.49	0.43
1:C:379:ALA:HB3	1:C:441:ALA:HB1	2.00	0.43
1:C:62:ILE:O	1:C:308:LYS:HE2	2.18	0.43
1:D:138:GLY:O	1:D:141:ALA:HB3	2.18	0.43
1:E:345:HIS:CE1	1:E:347:GLU:HG2	2.53	0.43
1:H:376:PHE:HB2	1:H:445:ILE:HD11	2.00	0.43
1:I:174:LEU:N	1:I:175:PRO:CD	2.79	0.43
1:K:111:TYR:HA	1:K:289:HIS:CD2	2.53	0.43
1:K:375:LYS:HD2	1:K:445:ILE:HG23	1.99	0.43
1:K:377:VAL:CG2	1:K:378:ASP:N	2.80	0.43
1:F:271:ALA:HB3	1:F:303:ILE:HD11	2.00	0.43
1:G:119:LEU:HB2	1:G:304:ILE:CG1	2.48	0.43
1:I:160:THR:HG22	1:I:183:VAL:HG12	2.01	0.43
1:I:207:GLU:HG2	1:I:207:GLU:O	2.18	0.43
1:J:214:LEU:N	1:J:214:LEU:HD12	2.34	0.43
1:J:316:GLN:HG2	1:J:428:VAL:HG22	2.00	0.43
1:K:174:LEU:N	1:K:175:PRO:CD	2.78	0.43
1:L:300:ALA:O	1:L:304:ILE:HG13	2.18	0.43
1:C:207:GLU:HG2	1:C:207:GLU:O	2.19	0.43
1:C:132:THR:OG1	1:C:275:SER:HB3	2.19	0.43
1:D:397:ASP:OD1	1:D:399:PRO:HD3	2.18	0.43
1:D:426:PHE:HE1	1:D:438:ILE:HD11	1.83	0.43
1:E:377:VAL:CG2	1:E:378:ASP:N	2.82	0.43
1:F:211:ASN:C	1:F:211:ASN:ND2	2.72	0.43
1:F:278:LEU:HA	1:F:281:VAL:HG12	2.01	0.43
1:G:258:SER:C	1:G:260:THR:H	2.20	0.43
1:G:285:ARG:O	1:G:288:HIS:HB3	2.18	0.43
1:G:60:VAL:C	1:G:62:ILE:H	2.22	0.43
1:H:192:LEU:O	1:H:196:LEU:HB2	2.17	0.43
1:F:140:CYS:HB2	1:H:292:GLY:O	2.19	0.43
1:H:91:LYS:HD2	1:H:93:SER:OG	2.18	0.43
1:I:160:THR:HG23	1:I:184:ILE:O	2.19	0.43
1:L:132:THR:OG1	1:L:275:SER:HB3	2.18	0.43
1:A:111:TYR:HA	1:A:289:HIS:NE2	2.34	0.43
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.82	0.43
1:B:56:SER:HB3	1:C:433:ASP:OD2	2.18	0.43
1:E:140:CYS:O	1:E:144:VAL:HG23	2.17	0.43
1:E:319:SER:O	1:E:320:THR:C	2.57	0.43
1:F:111:TYR:HA	1:F:289:HIS:NE2	2.34	0.43
1:F:258:SER:O	1:F:260:THR:N	2.51	0.43
1:F:340:PRO:HB2	1:F:358:PHE:CD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:HIS:CD2	1:F:67:ARG:HB2	2.54	0.43
1:J:261:LYS:HD2	1:J:389:PHE:CZ	2.54	0.43
1:K:57:ASP:HB3	1:K:243:LEU:CD2	2.48	0.43
1:K:243:LEU:CD1	1:K:311:HIS:HA	2.49	0.43
1:K:350:ILE:O	1:K:353:LYS:HG2	2.18	0.43
1:A:60:VAL:HG13	1:A:64:ALA:HB2	2.00	0.43
1:B:119:LEU:HG	1:B:134:LEU:HD11	1.99	0.43
1:B:350:ILE:O	1:B:353:LYS:HG2	2.19	0.43
1:C:339:TYR:CZ	1:C:358:PHE:HB2	2.53	0.43
1:D:218:ASP:O	1:D:222:VAL:HG23	2.18	0.43
1:A:428:VAL:HG12	1:D:62:ILE:HD11	2.00	0.43
1:I:350:ILE:O	1:I:353:LYS:HG2	2.19	0.43
1:L:328:LEU:HD23	1:L:328:LEU:HA	1.86	0.43
1:L:401:ILE:HA	1:L:405:TRP:HB2	2.01	0.43
1:L:62:ILE:O	1:L:308:LYS:HE2	2.18	0.43
1:A:296:ASN:O	1:A:299:ALA:HB3	2.19	0.43
1:C:207:GLU:HB2	1:C:236:ASP:O	2.19	0.43
1:C:336:HIS:HB3	1:C:365:GLU:HG3	2.00	0.43
1:D:64:ALA:O	1:D:122:LYS:HG3	2.19	0.43
1:D:258:SER:C	1:D:260:THR:H	2.21	0.43
1:E:211:ASN:ND2	1:E:211:ASN:C	2.72	0.43
1:E:250:LEU:HD11	1:E:354:GLN:CB	2.46	0.43
1:E:60:VAL:C	1:E:62:ILE:N	2.72	0.43
1:F:207:GLU:HB2	1:F:236:ASP:O	2.19	0.43
1:G:103:ARG:HG2	1:G:104:ALA:N	2.34	0.43
1:G:261:LYS:HB3	1:G:389:PHE:O	2.19	0.43
1:H:331:HIS:CE1	1:H:333:LYS:HB2	2.53	0.43
1:H:209:PRO:HG3	1:H:355:MET:HE1	2.00	0.43
1:I:119:LEU:HB2	1:I:304:ILE:HG13	2.01	0.43
1:I:363:SER:HB3	1:I:421:LEU:HD11	2.01	0.43
1:J:192:LEU:CD2	1:J:222:VAL:HG13	2.48	0.43
1:J:60:VAL:C	1:J:62:ILE:N	2.72	0.43
1:K:138:GLY:N	2:K:500:PLP:O3P	2.50	0.43
1:L:280:LEU:HD23	1:L:280:LEU:HA	1.88	0.43
1:B:58:GLY:HA3	1:B:311:HIS:CD2	2.54	0.42
1:C:150:VAL:HA	1:C:151:PRO:HD3	1.87	0.42
1:D:148:ALA:HB2	1:D:287:LEU:HD23	2.01	0.42
1:E:132:THR:OG1	1:E:275:SER:HB3	2.19	0.42
1:F:192:LEU:CD2	1:F:222:VAL:HG13	2.49	0.42
1:F:244:ASN:ND2	1:F:359:GLY:H	2.18	0.42
1:F:72:ILE:O	1:F:72:ILE:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:369:ASP:O	1:I:370:LEU:C	2.57	0.42
1:J:117:VAL:HA	1:J:120:GLU:HB2	2.01	0.42
1:K:87:TYR:CE1	1:K:106:PHE:HB2	2.54	0.42
1:K:261:LYS:HD2	1:K:389:PHE:CE2	2.54	0.42
1:L:345:HIS:CE1	1:L:347:GLU:HG2	2.54	0.42
1:I:63:HIS:HE1	1:L:429:GLU:OE2	2.02	0.42
1:A:345:HIS:CE1	1:A:347:GLU:HG2	2.54	0.42
1:A:339:TYR:CD1	1:A:362:VAL:HG22	2.54	0.42
1:B:387:PRO:O	1:B:388:SER:O	2.36	0.42
1:C:211:ASN:ND2	1:C:211:ASN:C	2.72	0.42
1:D:150:VAL:HA	1:D:151:PRO:HD3	1.90	0.42
1:D:398:GLN:O	1:D:401:ILE:N	2.45	0.42
1:F:170:ILE:HA	1:F:174:LEU:HD12	2.01	0.42
1:F:70:ARG:HB3	1:F:72:ILE:HG22	2.00	0.42
1:H:113:ASN:O	1:H:117:VAL:HG13	2.19	0.42
1:J:163:TYR:CE1	3:J:609:CCO:H1B1	2.54	0.42
1:J:345:HIS:CE1	1:J:347:GLU:HG2	2.54	0.42
1:K:331:HIS:CE1	1:K:333:LYS:HB2	2.54	0.42
1:B:106:PHE:HD1	1:B:112:GLY:HA3	1.83	0.42
1:E:241:THR:HG23	1:E:242:PRO:HD2	2.01	0.42
1:E:58:GLY:HA3	1:E:311:HIS:CD2	2.54	0.42
1:F:58:GLY:HA3	1:F:311:HIS:CD2	2.53	0.42
1:G:159:THR:HA	1:G:184:ILE:O	2.19	0.42
1:H:317:GLN:NE2	1:H:426:PHE:O	2.52	0.42
1:I:52:SER:C	1:I:54:LEU:H	2.23	0.42
1:J:113:ASN:ND2	1:J:297:PRO:HG3	2.33	0.42
1:J:57:ASP:HB3	1:J:243:LEU:CD2	2.49	0.42
1:A:331:HIS:CG	1:A:332:PRO:HD2	2.54	0.42
1:A:77:ILE:HD12	1:B:86:ALA:O	2.19	0.42
1:C:64:ALA:HB3	1:C:122:LYS:CG	2.49	0.42
1:D:117:VAL:O	1:D:121:GLU:HG3	2.19	0.42
1:D:174:LEU:N	1:D:175:PRO:CD	2.82	0.42
1:I:119:LEU:HG	1:I:134:LEU:HD11	2.01	0.42
1:J:159:THR:HA	1:J:184:ILE:O	2.19	0.42
1:K:340:PRO:HB2	1:K:358:PHE:CD1	2.48	0.42
1:L:56:SER:O	1:L:60:VAL:HG23	2.20	0.42
1:B:331:HIS:CE1	1:B:333:LYS:HB2	2.54	0.42
1:B:60:VAL:HG13	1:B:64:ALA:HB2	2.01	0.42
1:D:311:HIS:CE1	1:D:312:LEU:HD23	2.54	0.42
1:E:106:PHE:O	1:E:111:TYR:HB2	2.19	0.42
1:E:219:ILE:O	1:E:220:GLU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:VAL:HG13	1:E:282:SER:N	2.34	0.42
1:F:262:PHE:CE1	1:F:390:GLY:HA2	2.55	0.42
1:G:173:ILE:C	1:G:175:PRO:HD2	2.40	0.42
1:G:192:LEU:HD21	1:G:222:VAL:HG13	2.00	0.42
1:G:323:ARG:HB2	1:G:431:PHE:CE2	2.55	0.42
1:F:291:LEU:O	1:H:140:CYS:HA	2.20	0.42
1:I:241:THR:HG22	1:I:243:LEU:N	2.19	0.42
1:I:322:LEU:O	1:I:323:ARG:C	2.58	0.42
1:K:398:GLN:O	1:K:399:PRO:C	2.58	0.42
1:L:129:ALA:HB2	1:L:248:LEU:HD11	2.01	0.42
1:B:145:MET:HB2	1:B:274:ILE:CD1	2.50	0.42
1:B:119:LEU:HB2	1:B:304:ILE:CG1	2.49	0.42
1:B:215:ARG:NH1	1:B:347:GLU:OE2	2.53	0.42
1:D:350:ILE:O	1:D:353:LYS:HG2	2.19	0.42
1:F:398:GLN:O	1:F:399:PRO:C	2.58	0.42
1:F:67:ARG:HA	1:G:384:TYR:OH	2.19	0.42
1:G:192:LEU:HG	1:G:196:LEU:CD2	2.50	0.42
1:G:215:ARG:HD2	1:G:347:GLU:OE2	2.19	0.42
1:J:271:ALA:HB3	1:J:303:ILE:HD11	2.02	0.42
1:J:384:TYR:CZ	1:K:67:ARG:HD2	2.54	0.42
1:L:145:MET:HG2	1:L:149:LEU:CD1	2.49	0.42
1:A:160:THR:HG22	1:A:183:VAL:HG12	2.01	0.42
1:B:339:TYR:OH	1:B:358:PHE:HB2	2.19	0.42
1:E:206:THR:O	1:E:235:ILE:HA	2.20	0.42
1:E:350:ILE:O	1:E:353:LYS:HG2	2.19	0.42
1:F:368:GLY:O	1:F:420:ASN:ND2	2.52	0.42
1:G:278:LEU:HA	1:G:281:VAL:CG1	2.49	0.42
1:G:345:HIS:CE1	1:G:347:GLU:HG2	2.55	0.42
1:H:156:ILE:HG12	1:H:157:VAL:N	2.27	0.42
1:I:243:LEU:HD11	1:I:310:LEU:HG	2.00	0.42
1:I:326:GLU:O	1:I:327:ILE:C	2.58	0.42
1:I:244:ASN:ND2	1:I:359:GLY:H	2.18	0.42
1:I:384:TYR:O	1:I:395:ILE:HG23	2.20	0.42
1:K:258:SER:C	1:K:260:THR:N	2.72	0.42
1:L:319:SER:O	1:L:320:THR:C	2.56	0.42
1:B:377:VAL:CG2	1:B:378:ASP:N	2.82	0.42
1:C:243:LEU:HD11	1:C:310:LEU:HG	2.01	0.42
1:E:336:HIS:HB3	1:E:365:GLU:HG3	2.02	0.42
1:F:119:LEU:HB2	1:F:304:ILE:CG1	2.50	0.42
1:F:72:ILE:HD13	1:F:72:ILE:O	2.20	0.42
1:G:271:ALA:HB3	1:G:303:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:262:PHE:CE1	1:I:390:GLY:HA2	2.55	0.42
1:J:207:GLU:HG2	1:J:207:GLU:O	2.19	0.42
1:K:281:VAL:HG13	1:K:282:SER:N	2.35	0.42
1:L:419:ASP:OD1	1:L:419:ASP:N	2.53	0.42
1:B:145:MET:HB2	1:B:274:ILE:HD13	2.01	0.42
1:B:192:LEU:HG	1:B:196:LEU:CD2	2.49	0.42
1:C:258:SER:C	1:C:260:THR:N	2.73	0.42
1:D:72:ILE:O	1:D:73:VAL:O	2.37	0.42
1:E:317:GLN:NE2	1:E:426:PHE:O	2.52	0.42
1:F:111:TYR:HA	1:F:289:HIS:CD2	2.55	0.42
1:H:261:LYS:HB3	1:H:389:PHE:O	2.20	0.42
1:J:138:GLY:O	1:J:139:MET:C	2.58	0.42
1:J:211:ASN:C	1:J:211:ASN:ND2	2.73	0.42
1:J:258:SER:C	1:J:260:THR:N	2.72	0.42
1:J:331:HIS:CG	1:J:332:PRO:HD2	2.54	0.42
1:K:241:THR:HG23	1:K:242:PRO:HD2	2.01	0.42
1:A:145:MET:HB2	1:A:274:ILE:CD1	2.49	0.42
1:C:210:THR:HB	1:C:215:ARG:O	2.20	0.42
1:C:110:ARG:HD3	1:C:292:GLY:HA3	2.02	0.42
1:E:117:VAL:HA	1:E:120:GLU:HB2	2.02	0.42
1:E:218:ASP:O	1:E:222:VAL:HG23	2.20	0.42
1:F:57:ASP:HB3	1:F:243:LEU:HD22	2.01	0.42
1:F:54:LEU:HD22	1:F:59:SER:HB3	2.02	0.42
1:H:117:VAL:HA	1:H:120:GLU:HB2	2.02	0.42
1:J:319:SER:O	1:J:320:THR:C	2.58	0.42
1:K:150:VAL:HA	1:K:151:PRO:HD3	1.90	0.42
1:K:211:ASN:ND2	1:K:212:PRO:N	2.68	0.42
1:A:159:THR:HA	1:A:184:ILE:O	2.20	0.41
1:A:248:LEU:HA	1:A:248:LEU:HD23	1.92	0.41
1:A:389:PHE:HB2	1:A:425:SER:HB2	2.01	0.41
1:B:113:ASN:ND2	1:B:297:PRO:HG3	2.35	0.41
1:B:443:ASP:OD1	1:B:443:ASP:N	2.52	0.41
1:D:113:ASN:O	1:D:117:VAL:HG13	2.20	0.41
1:F:103:ARG:HG2	1:F:104:ALA:N	2.35	0.41
1:F:132:THR:HG22	1:F:133:LEU:N	2.35	0.41
1:H:256:LEU:HB3	1:H:274:ILE:HG12	2.02	0.41
1:I:339:TYR:CZ	1:I:358:PHE:HB2	2.55	0.41
1:C:138:GLY:O	1:C:141:ALA:HB3	2.20	0.41
1:C:145:MET:HB2	1:C:274:ILE:HD13	2.02	0.41
1:C:218:ASP:O	1:C:222:VAL:HG23	2.19	0.41
1:D:345:HIS:HE1	1:D:347:GLU:HG2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:THR:HA	1:F:184:ILE:O	2.20	0.41
1:F:343:GLN:HB3	1:F:343:GLN:HE21	1.55	0.41
1:G:156:ILE:HG12	1:G:157:VAL:N	2.25	0.41
1:K:331:HIS:ND1	1:K:332:PRO:HD2	2.35	0.41
1:L:227:HIS:HE1	1:L:251:GLY:O	2.03	0.41
1:L:281:VAL:HG13	1:L:282:SER:N	2.34	0.41
1:L:368:GLY:O	1:L:420:ASN:ND2	2.53	0.41
1:A:243:LEU:HD12	1:A:314:VAL:HG21	2.01	0.41
1:B:60:VAL:CG1	1:B:64:ALA:HB2	2.51	0.41
1:C:72:ILE:O	1:C:73:VAL:O	2.38	0.41
1:D:132:THR:OG1	1:D:275:SER:HB3	2.21	0.41
1:D:323:ARG:HB2	1:D:431:PHE:CE2	2.55	0.41
1:G:129:ALA:HB2	1:G:248:LEU:CD1	2.51	0.41
1:H:285:ARG:O	1:H:288:HIS:HB3	2.21	0.41
1:H:60:VAL:C	1:H:62:ILE:H	2.24	0.41
1:I:256:LEU:HB3	1:I:274:ILE:HG12	2.01	0.41
1:K:215:ARG:HD2	1:K:347:GLU:OE2	2.20	0.41
1:K:339:TYR:OH	1:K:358:PHE:HB2	2.21	0.41
1:A:259:ALA:HA	1:A:263:LEU:HB2	2.00	0.41
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.87	0.41
1:C:217:VAL:HG13	1:C:222:VAL:HG21	2.02	0.41
1:D:323:ARG:H	1:D:323:ARG:HG2	1.57	0.41
1:E:278:LEU:HA	1:E:281:VAL:CG1	2.50	0.41
1:E:365:GLU:HB3	1:E:420:ASN:HB3	2.01	0.41
1:F:311:HIS:NE2	1:F:312:LEU:HD23	2.35	0.41
1:I:214:LEU:N	1:I:214:LEU:HD12	2.36	0.41
1:I:311:HIS:CE1	1:I:312:LEU:HD23	2.55	0.41
1:K:217:VAL:O	1:K:219:ILE:N	2.53	0.41
1:K:370:LEU:CD2	1:K:419:ASP:HB3	2.40	0.41
1:L:73:VAL:O	1:L:74:THR:HG23	2.20	0.41
1:A:433:ASP:OD2	1:D:56:SER:HB3	2.20	0.41
1:A:438:ILE:O	1:A:441:ALA:HB3	2.20	0.41
1:A:91:LYS:HD2	1:A:93:SER:OG	2.20	0.41
1:B:129:ALA:HB2	1:B:248:LEU:CD1	2.49	0.41
1:C:192:LEU:O	1:C:196:LEU:HB2	2.20	0.41
1:D:91:LYS:HD2	1:D:93:SER:OG	2.21	0.41
1:E:243:LEU:CD1	1:E:311:HIS:HA	2.50	0.41
1:E:258:SER:C	1:E:260:THR:N	2.74	0.41
1:F:339:TYR:CZ	1:F:358:PHE:HB2	2.56	0.41
1:J:339:TYR:OH	1:J:358:PHE:HB2	2.21	0.41
1:J:60:VAL:C	1:J:62:ILE:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:258:SER:C	1:K:260:THR:H	2.24	0.41
1:L:369:ASP:O	1:L:370:LEU:C	2.59	0.41
1:L:72:ILE:HD13	1:L:72:ILE:O	2.21	0.41
1:B:397:ASP:OD1	1:B:399:PRO:HD3	2.21	0.41
1:B:54:LEU:CD2	1:B:59:SER:HB3	2.51	0.41
1:C:119:LEU:HB2	1:C:304:ILE:CG1	2.51	0.41
1:C:187:ALA:O	1:C:189:VAL:HG23	2.21	0.41
1:E:192:LEU:HD21	1:E:222:VAL:HG13	2.02	0.41
1:F:155:HIS:HA	1:F:180:THR:O	2.20	0.41
1:G:243:LEU:CD1	1:G:311:HIS:HA	2.50	0.41
1:G:377:VAL:CG2	1:G:378:ASP:N	2.83	0.41
1:I:260:THR:HG21	1:I:270:LEU:HD22	2.03	0.41
1:J:243:LEU:CD1	1:J:310:LEU:HG	2.50	0.41
1:J:62:ILE:HD11	1:K:428:VAL:CG1	2.50	0.41
1:L:343:GLN:HB3	1:L:343:GLN:HE21	1.54	0.41
1:B:65:GLY:O	1:B:118:VAL:HG13	2.21	0.41
1:B:127:GLU:OE2	1:B:257:HIS:NE2	2.53	0.41
1:B:155:HIS:HA	1:B:180:THR:O	2.20	0.41
1:E:145:MET:HB2	1:E:274:ILE:CD1	2.50	0.41
1:F:331:HIS:CE1	1:F:333:LYS:HB2	2.55	0.41
1:G:219:ILE:O	1:G:220:GLU:C	2.59	0.41
1:E:83:ASN:O	1:G:268:ASP:HB2	2.21	0.41
1:G:372:THR:HG23	1:G:445:ILE:HG21	2.02	0.41
1:G:389:PHE:HB2	1:G:425:SER:HB2	2.02	0.41
1:G:80:PRO:HB3	1:H:82:VAL:HG22	2.03	0.41
1:H:150:VAL:HA	1:H:151:PRO:HD3	1.91	0.41
1:H:419:ASP:N	1:H:419:ASP:OD1	2.52	0.41
1:K:74:THR:C	1:K:76:ALA:H	2.24	0.41
1:L:323:ARG:HB2	1:L:431:PHE:CE2	2.56	0.41
1:K:86:ALA:O	1:L:77:ILE:HD12	2.21	0.41
1:A:218:ASP:O	1:A:222:VAL:HG23	2.21	0.41
1:C:119:LEU:HB2	1:C:304:ILE:HG13	2.03	0.41
1:C:323:ARG:H	1:C:323:ARG:HG2	1.61	0.41
1:C:138:GLY:N	2:C:500:PLP:O3P	2.51	0.41
1:E:50:TYR:CG	1:E:51:ALA:N	2.88	0.41
1:E:70:ARG:HB3	1:E:72:ILE:HG22	2.03	0.41
1:F:243:LEU:CD1	1:F:311:HIS:HA	2.51	0.41
1:F:215:ARG:HD2	1:F:347:GLU:OE2	2.21	0.41
1:G:445:ILE:HG13	1:G:445:ILE:H	1.75	0.41
1:G:57:ASP:HB3	1:G:243:LEU:HD22	2.03	0.41
1:H:343:GLN:HE21	1:H:343:GLN:HB3	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:323:ARG:HB2	1:I:431:PHE:CE2	2.56	0.41
1:J:267:ASN:ND2	1:J:391:GLY:HA3	2.36	0.41
1:L:192:LEU:HG	1:L:196:LEU:CD2	2.51	0.41
1:A:62:ILE:HD11	1:D:428:VAL:CG1	2.50	0.41
1:C:278:LEU:HA	1:C:281:VAL:CG1	2.51	0.41
1:C:377:VAL:CG2	1:C:378:ASP:N	2.83	0.41
1:F:241:THR:HG23	1:F:242:PRO:HD2	2.03	0.41
1:G:401:ILE:HA	1:G:405:TRP:HB2	2.03	0.41
1:G:397:ASP:HB2	1:G:402:MET:HG2	2.03	0.41
1:H:217:VAL:HG13	1:H:222:VAL:HG21	2.03	0.41
1:J:210:THR:CG2	1:J:211:ASN:N	2.84	0.41
1:J:281:VAL:HG13	1:J:282:SER:N	2.35	0.41
1:K:258:SER:O	1:K:260:THR:N	2.53	0.41
1:L:160:THR:HG23	1:L:184:ILE:O	2.21	0.41
1:A:156:ILE:HG12	1:A:157:VAL:N	2.27	0.41
1:B:277:PRO:O	1:B:281:VAL:HG12	2.21	0.41
1:C:398:GLN:O	1:C:399:PRO:C	2.59	0.41
1:C:73:VAL:O	1:C:74:THR:HG23	2.21	0.41
1:E:82:VAL:HG22	1:F:80:PRO:HB3	2.03	0.41
1:G:106:PHE:O	1:G:107:GLU:HB3	2.20	0.41
1:H:114:PRO:O	1:H:118:VAL:HG23	2.21	0.41
1:H:145:MET:HB2	1:H:274:ILE:HD13	2.03	0.41
1:H:296:ASN:O	1:H:299:ALA:HB3	2.21	0.41
1:J:206:THR:O	1:J:235:ILE:HA	2.20	0.41
1:J:72:ILE:HG23	1:J:72:ILE:O	2.21	0.41
1:K:243:LEU:CD1	1:K:310:LEU:HG	2.50	0.41
1:K:60:VAL:HG12	1:K:64:ALA:HB2	2.02	0.41
1:L:82:VAL:HG21	1:L:114:PRO:HG2	2.03	0.41
1:L:135:MET:O	1:L:295:LEU:HB2	2.21	0.41
1:L:365:GLU:HB3	1:L:420:ASN:HB3	2.02	0.41
1:L:60:VAL:C	1:L:62:ILE:N	2.75	0.41
1:A:311:HIS:O	1:A:312:LEU:C	2.60	0.41
1:B:114:PRO:O	1:B:117:VAL:HG22	2.21	0.41
1:C:160:THR:HG22	1:C:183:VAL:HG12	2.02	0.41
1:C:280:LEU:HA	1:C:280:LEU:HD23	1.87	0.41
1:C:91:LYS:HD2	1:C:93:SER:OG	2.21	0.41
1:F:211:ASN:ND2	1:F:212:PRO:N	2.69	0.41
1:G:383:PRO:CB	1:G:396:VAL:HG22	2.41	0.41
1:H:262:PHE:CE1	1:H:390:GLY:HA2	2.55	0.41
1:H:366:VAL:O	1:H:420:ASN:ND2	2.54	0.41
1:I:343:GLN:HE21	1:I:343:GLN:HB3	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:GLU:HG2	1:I:70:ARG:NH1	2.36	0.41
1:J:132:THR:HG22	1:J:133:LEU:N	2.36	0.41
1:J:57:ASP:O	1:J:60:VAL:HB	2.21	0.41
1:K:196:LEU:HD13	1:K:196:LEU:HA	1.96	0.41
1:L:261:LYS:HB3	1:L:389:PHE:O	2.21	0.41
1:A:138:GLY:N	2:A:500:PLP:O3P	2.43	0.40
1:B:278:LEU:HA	1:B:281:VAL:CG1	2.51	0.40
1:C:217:VAL:O	1:C:219:ILE:N	2.54	0.40
1:C:63:HIS:CD2	1:C:67:ARG:HD3	2.57	0.40
1:D:192:LEU:HG	1:D:196:LEU:CD2	2.51	0.40
1:E:232:LEU:HA	1:E:232:LEU:HD23	1.93	0.40
1:E:310:LEU:O	1:E:314:VAL:HG23	2.22	0.40
1:F:242:PRO:O	1:F:246:LYS:HD3	2.22	0.40
1:F:397:ASP:OD2	1:F:423:ARG:NH2	2.51	0.40
1:G:328:LEU:HA	1:G:328:LEU:HD23	1.92	0.40
1:G:215:ARG:NH1	1:G:347:GLU:OE2	2.54	0.40
1:J:160:THR:HA	1:J:183:VAL:CG1	2.52	0.40
1:J:156:ILE:HD13	1:J:181:ALA:HB2	2.03	0.40
1:J:73:VAL:O	1:J:74:THR:HG23	2.21	0.40
1:K:119:LEU:HB2	1:K:304:ILE:CG1	2.51	0.40
1:K:261:LYS:HB3	1:K:389:PHE:O	2.21	0.40
1:A:113:ASN:OD1	1:A:115:THR:N	2.50	0.40
1:B:281:VAL:HG13	1:B:282:SER:N	2.36	0.40
1:B:368:GLY:O	1:B:420:ASN:ND2	2.55	0.40
1:C:60:VAL:C	1:C:62:ILE:N	2.75	0.40
1:G:243:LEU:HD11	1:G:310:LEU:HG	2.03	0.40
1:H:389:PHE:HB2	1:H:425:SER:HB2	2.03	0.40
1:I:155:HIS:HA	1:I:180:THR:O	2.22	0.40
1:I:196:LEU:HA	1:I:196:LEU:HD13	1.93	0.40
1:J:196:LEU:HA	1:J:196:LEU:HD13	1.91	0.40
1:J:243:LEU:CD1	1:J:311:HIS:HA	2.52	0.40
1:J:383:PRO:HA	1:J:394:SER:O	2.21	0.40
1:J:72:ILE:HD12	1:J:80:PRO:CG	2.51	0.40
1:L:138:GLY:N	2:L:500:PLP:O3P	2.53	0.40
1:A:370:LEU:CD2	1:A:419:ASP:HB3	2.36	0.40
1:B:258:SER:C	1:B:260:THR:N	2.75	0.40
1:B:60:VAL:C	1:B:62:ILE:N	2.73	0.40
1:C:241:THR:HG23	1:C:242:PRO:HD2	2.03	0.40
1:D:262:PHE:CE1	1:D:390:GLY:HA2	2.56	0.40
1:D:394:SER:HG	1:D:429:GLU:CD	2.25	0.40
1:D:57:ASP:O	1:D:60:VAL:HB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:ALA:O	1:E:250:LEU:HB2	2.21	0.40
1:G:368:GLY:O	1:G:420:ASN:ND2	2.54	0.40
1:G:54:LEU:CD2	1:G:59:SER:HB3	2.52	0.40
1:H:243:LEU:CD1	1:H:311:HIS:HA	2.52	0.40
1:H:426:PHE:HE1	1:H:438:ILE:HD11	1.85	0.40
1:E:430:ASP:HB2	1:H:56:SER:HB3	2.02	0.40
1:I:389:PHE:HB2	1:I:425:SER:CB	2.50	0.40
1:I:72:ILE:O	1:I:73:VAL:O	2.39	0.40
1:J:110:ARG:HD3	1:J:292:GLY:CA	2.52	0.40
1:K:323:ARG:HB2	1:K:431:PHE:CE2	2.57	0.40
1:L:207:GLU:O	1:L:207:GLU:HG2	2.21	0.40
1:A:398:GLN:O	1:A:399:PRO:C	2.60	0.40
1:B:280:LEU:HA	1:B:280:LEU:HD23	1.84	0.40
1:C:145:MET:HB2	1:C:274:ILE:HD11	2.03	0.40
1:C:262:PHE:CE1	1:C:390:GLY:HA2	2.56	0.40
1:D:145:MET:HE2	1:D:146:LEU:HG	2.02	0.40
1:E:215:ARG:NH1	1:E:347:GLU:OE2	2.54	0.40
1:E:426:PHE:HE1	1:E:438:ILE:HD11	1.86	0.40
1:F:106:PHE:O	1:F:107:GLU:HB3	2.21	0.40
1:F:243:LEU:HD11	1:F:310:LEU:HG	2.02	0.40
1:F:60:VAL:C	1:F:62:ILE:N	2.74	0.40
1:H:374:ALA:O	1:H:377:VAL:HG22	2.21	0.40
1:I:192:LEU:CD2	1:I:222:VAL:HG13	2.51	0.40
1:L:258:SER:C	1:L:260:THR:N	2.73	0.40
1:A:203:LEU:HB2	1:A:232:LEU:HB2	2.04	0.40
1:A:350:ILE:O	1:A:353:LYS:HG2	2.21	0.40
1:A:80:PRO:O	1:A:115:THR:OG1	2.39	0.40
1:B:140:CYS:O	1:B:144:VAL:HG23	2.21	0.40
1:B:316:GLN:HG2	1:B:428:VAL:HG22	2.03	0.40
1:B:389:PHE:HA	1:B:395:ILE:HD12	2.03	0.40
1:C:328:LEU:HD23	1:C:328:LEU:HA	1.90	0.40
1:C:60:VAL:HG12	1:C:64:ALA:HB2	2.02	0.40
1:D:317:GLN:NE2	1:D:426:PHE:O	2.55	0.40
1:F:317:GLN:NE2	1:F:426:PHE:O	2.55	0.40
1:G:144:VAL:O	1:G:145:MET:C	2.60	0.40
1:G:374:ALA:O	1:G:377:VAL:HG22	2.22	0.40
1:I:135:MET:HE1	1:I:141:ALA:HA	2.03	0.40
1:I:219:ILE:O	1:I:220:GLU:C	2.59	0.40
1:I:235:ILE:O	1:I:255:VAL:HA	2.22	0.40
1:I:263:LEU:HA	1:I:263:LEU:HD23	1.94	0.40
1:J:219:ILE:O	1:J:220:GLU:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:159:THR:HA	1:K:184:ILE:O	2.21	0.40
1:K:363:SER:HB3	1:K:421:LEU:HD11	2.04	0.40
1:K:72:ILE:HG23	1:K:72:ILE:O	2.20	0.40
1:L:313:ARG:O	1:L:314:VAL:C	2.59	0.40
1:L:377:VAL:CG2	1:L:378:ASP:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/445 (88%)	324 (82%)	62 (16%)	8 (2%)	7	33
1	B	394/445 (88%)	327 (83%)	61 (16%)	6 (2%)	10	39
1	C	394/445 (88%)	320 (81%)	65 (16%)	9 (2%)	6	29
1	D	394/445 (88%)	312 (79%)	73 (18%)	9 (2%)	6	29
1	E	394/445 (88%)	310 (79%)	75 (19%)	9 (2%)	6	29
1	F	394/445 (88%)	319 (81%)	65 (16%)	10 (2%)	5	28
1	G	394/445 (88%)	319 (81%)	65 (16%)	10 (2%)	5	28
1	H	394/445 (88%)	316 (80%)	69 (18%)	9 (2%)	6	29
1	I	394/445 (88%)	316 (80%)	71 (18%)	7 (2%)	8	35
1	J	394/445 (88%)	316 (80%)	68 (17%)	10 (2%)	5	28
1	K	394/445 (88%)	312 (79%)	70 (18%)	12 (3%)	4	24
1	L	394/445 (88%)	318 (81%)	67 (17%)	9 (2%)	6	29
All	All	4728/5340 (88%)	3809 (81%)	811 (17%)	108 (2%)	6	29

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
1	A	188	ASP
1	B	73	VAL
1	B	188	ASP
1	C	73	VAL
1	C	188	ASP
1	D	73	VAL
1	D	188	ASP
1	E	73	VAL
1	E	188	ASP
1	F	73	VAL
1	F	188	ASP
1	G	73	VAL
1	G	188	ASP
1	H	73	VAL
1	H	188	ASP
1	I	73	VAL
1	I	188	ASP
1	J	73	VAL
1	J	188	ASP
1	K	73	VAL
1	K	188	ASP
1	L	73	VAL
1	L	188	ASP
1	A	388	SER
1	B	219	ILE
1	B	388	SER
1	D	259	ALA
1	H	388	SER
1	B	387	PRO
1	C	265	GLY
1	C	388	SER
1	D	219	ILE
1	F	387	PRO
1	F	388	SER
1	G	61	ALA
1	G	219	ILE
1	H	259	ALA
1	J	53	PHE
1	K	53	PHE
1	L	388	SER
1	A	241	THR
1	A	387	PRO

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Mol	Chain	Res	Type
1	C	164	ARG
1	C	241	THR
1	C	387	PRO
1	D	241	THR
1	D	387	PRO
1	D	388	SER
1	E	241	THR
1	E	388	SER
1	F	141	ALA
1	F	164	ARG
1	F	241	THR
1	F	259	ALA
1	G	164	ARG
1	G	241	THR
1	G	259	ALA
1	G	387	PRO
1	G	388	SER
1	H	164	ARG
1	H	241	THR
1	H	387	PRO
1	I	241	THR
1	J	164	ARG
1	J	241	THR
1	J	387	PRO
1	J	388	SER
1	K	241	THR
1	K	259	ALA
1	K	387	PRO
1	L	241	THR
1	L	387	PRO
1	A	164	ARG
1	A	219	ILE
1	B	241	THR
1	C	141	ALA
1	C	219	ILE
1	E	141	ALA
1	E	219	ILE
1	E	387	PRO
1	H	219	ILE
1	I	141	ALA
1	I	219	ILE
1	I	387	PRO

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Mol	Chain	Res	Type
1	I	388	SER
1	J	219	ILE
1	K	164	ARG
1	K	388	SER
1	L	141	ALA
1	L	164	ARG
1	A	322	LEU
1	D	164	ARG
1	E	164	ARG
1	F	399	PRO
1	G	279	LYS
1	H	279	LYS
1	J	259	ALA
1	K	219	ILE
1	K	279	LYS
1	D	265	GLY
1	F	219	ILE
1	K	265	GLY
1	K	292	GLY
1	E	399	PRO
1	L	219	ILE
1	J	292	GLY
1	L	399	PRO

### 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	327/364 (90%)	280 (86%)	47 (14%)	3	14
1	B	327/364 (90%)	275 (84%)	52 (16%)	2	11
1	C	327/364 (90%)	277 (85%)	50 (15%)	2	12
1	D	327/364 (90%)	273 (84%)	54 (16%)	2	10
1	E	327/364 (90%)	272 (83%)	55 (17%)	2	9
1	F	327/364 (90%)	277 (85%)	50 (15%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	327/364 (90%)	274 (84%)	53 (16%)	2	10
1	H	327/364 (90%)	276 (84%)	51 (16%)	2	11
1	I	327/364 (90%)	277 (85%)	50 (15%)	2	12
1	J	327/364 (90%)	273 (84%)	54 (16%)	2	10
1	K	327/364 (90%)	276 (84%)	51 (16%)	2	11
1	L	327/364 (90%)	278 (85%)	49 (15%)	3	12
All	All	3924/4368 (90%)	3308 (84%)	616 (16%)	2	11

All (616) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	70	ARG
1	A	72	ILE
1	A	73	VAL
1	A	74	THR
1	A	91	LYS
1	A	92	THR
1	A	101	LYS
1	A	115	THR
1	A	131	SER
1	A	134	LEU
1	A	135	MET
1	A	142	SER
1	A	143	THR
1	A	145	MET
1	A	147	LEU
1	A	156	ILE
1	A	158	THR
1	A	162	CYS
1	A	177	MET
1	A	196	LEU
1	A	199	LYS
1	A	203	LEU
1	A	208	SER
1	A	210	THR
1	A	211	ASN
1	A	215	ARG
1	A	250	LEU
1	A	275	SER

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Mol	Chain	Res	Type
1	A	279	LYS
1	A	305	ARG
1	A	311	HIS
1	A	315	GLN
1	A	317	GLN
1	A	323	ARG
1	A	343	GLN
1	A	344	SER
1	A	347	GLU
1	A	356	THR
1	A	371	LEU
1	A	377	VAL
1	A	396	VAL
1	A	397	ASP
1	A	403	SER
1	A	410	SER
1	A	420	ASN
1	A	428	VAL
1	B	55	ASN
1	B	56	SER
1	B	70	ARG
1	B	72	ILE
1	B	73	VAL
1	B	74	THR
1	B	91	LYS
1	B	92	THR
1	B	101	LYS
1	B	115	THR
1	B	131	SER
1	B	134	LEU
1	B	135	MET
1	B	137	SER
1	B	142	SER
1	B	143	THR
1	B	145	MET
1	B	147	LEU
1	B	156	ILE
1	B	158	THR
1	B	162	CYS
1	B	177	MET
1	B	180	THR
1	B	196	LEU

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Mol	Chain	Res	Type
1	B	199	LYS
1	B	200	LYS
1	B	203	LEU
1	B	208	SER
1	B	210	THR
1	B	211	ASN
1	B	250	LEU
1	B	275	SER
1	B	279	LYS
1	B	305	ARG
1	B	307	MET
1	B	311	HIS
1	B	315	GLN
1	B	317	GLN
1	B	323	ARG
1	B	343	GLN
1	B	344	SER
1	B	347	GLU
1	B	356	THR
1	B	371	LEU
1	B	377	VAL
1	B	396	VAL
1	B	403	SER
1	B	410	SER
1	B	419	ASP
1	B	420	ASN
1	B	428	VAL
1	B	443	ASP
1	C	55	ASN
1	C	70	ARG
1	C	72	ILE
1	C	73	VAL
1	C	74	THR
1	C	91	LYS
1	C	92	THR
1	C	101	LYS
1	C	115	THR
1	C	131	SER
1	C	134	LEU
1	C	135	MET
1	C	137	SER
1	C	142	SER

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Mol	Chain	Res	Type
1	C	143	THR
1	C	145	MET
1	C	147	LEU
1	C	156	ILE
1	C	158	THR
1	C	162	CYS
1	C	177	MET
1	C	180	THR
1	C	196	LEU
1	C	199	LYS
1	C	200	LYS
1	C	203	LEU
1	C	208	SER
1	C	210	THR
1	C	211	ASN
1	C	250	LEU
1	C	275	SER
1	C	279	LYS
1	C	305	ARG
1	C	311	HIS
1	C	315	GLN
1	C	317	GLN
1	C	323	ARG
1	C	343	GLN
1	C	344	SER
1	C	347	GLU
1	C	356	THR
1	C	371	LEU
1	C	377	VAL
1	C	396	VAL
1	C	397	ASP
1	C	403	SER
1	C	410	SER
1	C	420	ASN
1	C	428	VAL
1	C	444	SER
1	D	56	SER
1	D	70	ARG
1	D	72	ILE
1	D	73	VAL
1	D	74	THR
1	D	91	LYS

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Mol	Chain	Res	Type
1	D	92	THR
1	D	101	LYS
1	D	115	THR
1	D	131	SER
1	D	134	LEU
1	D	135	MET
1	D	139	MET
1	D	142	SER
1	D	143	THR
1	D	145	MET
1	D	147	LEU
1	D	156	ILE
1	D	158	THR
1	D	162	CYS
1	D	167	ARG
1	D	177	MET
1	D	196	LEU
1	D	199	LYS
1	D	200	LYS
1	D	203	LEU
1	D	208	SER
1	D	210	THR
1	D	211	ASN
1	D	215	ARG
1	D	250	LEU
1	D	275	SER
1	D	278	LEU
1	D	279	LYS
1	D	305	ARG
1	D	311	HIS
1	D	315	GLN
1	D	317	GLN
1	D	323	ARG
1	D	343	GLN
1	D	344	SER
1	D	347	GLU
1	D	371	LEU
1	D	377	VAL
1	D	396	VAL
1	D	397	ASP
1	D	402	MET
1	D	403	SER

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Mol	Chain	Res	Type
1	D	410	SER
1	D	419	ASP
1	D	420	ASN
1	D	428	VAL
1	D	444	SER
1	D	445	ILE
1	E	56	SER
1	E	70	ARG
1	E	72	ILE
1	E	73	VAL
1	E	74	THR
1	E	91	LYS
1	E	92	THR
1	E	101	LYS
1	E	115	THR
1	E	131	SER
1	E	134	LEU
1	E	135	MET
1	E	137	SER
1	E	139	MET
1	E	142	SER
1	E	143	THR
1	E	145	MET
1	E	147	LEU
1	E	156	ILE
1	E	158	THR
1	E	162	CYS
1	E	167	ARG
1	E	177	MET
1	E	180	THR
1	E	196	LEU
1	E	199	LYS
1	E	200	LYS
1	E	203	LEU
1	E	208	SER
1	E	210	THR
1	E	211	ASN
1	E	215	ARG
1	E	245	GLN
1	E	250	LEU
1	E	275	SER
1	E	279	LYS

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Mol	Chain	Res	Type
1	E	305	ARG
1	E	311	HIS
1	E	315	GLN
1	E	317	GLN
1	E	323	ARG
1	E	343	GLN
1	E	344	SER
1	E	347	GLU
1	E	356	THR
1	E	363	SER
1	E	371	LEU
1	E	377	VAL
1	E	396	VAL
1	E	397	ASP
1	E	402	MET
1	E	403	SER
1	E	410	SER
1	E	420	ASN
1	E	428	VAL
1	F	70	ARG
1	F	72	ILE
1	F	73	VAL
1	F	74	THR
1	F	91	LYS
1	F	92	THR
1	F	101	LYS
1	F	115	THR
1	F	131	SER
1	F	134	LEU
1	F	135	MET
1	F	137	SER
1	F	142	SER
1	F	143	THR
1	F	145	MET
1	F	147	LEU
1	F	156	ILE
1	F	158	THR
1	F	162	CYS
1	F	177	MET
1	F	196	LEU
1	F	199	LYS
1	F	200	LYS

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Mol	Chain	Res	Type
1	F	203	LEU
1	F	208	SER
1	F	210	THR
1	F	211	ASN
1	F	215	ARG
1	F	245	GLN
1	F	250	LEU
1	F	275	SER
1	F	279	LYS
1	F	305	ARG
1	F	311	HIS
1	F	315	GLN
1	F	317	GLN
1	F	323	ARG
1	F	343	GLN
1	F	344	SER
1	F	347	GLU
1	F	371	LEU
1	F	377	VAL
1	F	396	VAL
1	F	397	ASP
1	F	403	SER
1	F	410	SER
1	F	419	ASP
1	F	420	ASN
1	F	424	PHE
1	F	428	VAL
1	G	54	LEU
1	G	56	SER
1	G	70	ARG
1	G	72	ILE
1	G	73	VAL
1	G	74	THR
1	G	91	LYS
1	G	92	THR
1	G	101	LYS
1	G	115	THR
1	G	131	SER
1	G	134	LEU
1	G	135	MET
1	G	137	SER
1	G	142	SER

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Mol	Chain	Res	Type
1	G	143	THR
1	G	147	LEU
1	G	156	ILE
1	G	158	THR
1	G	162	CYS
1	G	167	ARG
1	G	177	MET
1	G	196	LEU
1	G	199	LYS
1	G	200	LYS
1	G	203	LEU
1	G	208	SER
1	G	210	THR
1	G	211	ASN
1	G	250	LEU
1	G	270	LEU
1	G	275	SER
1	G	278	LEU
1	G	279	LYS
1	G	305	ARG
1	G	311	HIS
1	G	317	GLN
1	G	323	ARG
1	G	343	GLN
1	G	344	SER
1	G	347	GLU
1	G	356	THR
1	G	371	LEU
1	G	377	VAL
1	G	396	VAL
1	G	397	ASP
1	G	402	MET
1	G	403	SER
1	G	410	SER
1	G	419	ASP
1	G	420	ASN
1	G	428	VAL
1	G	445	ILE
1	H	70	ARG
1	H	72	ILE
1	H	73	VAL
1	H	74	THR

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Mol	Chain	Res	Type
1	H	91	LYS
1	H	92	THR
1	H	101	LYS
1	H	115	THR
1	H	131	SER
1	H	134	LEU
1	H	135	MET
1	H	142	SER
1	H	143	THR
1	H	145	MET
1	H	147	LEU
1	H	156	ILE
1	H	158	THR
1	H	162	CYS
1	H	177	MET
1	H	180	THR
1	H	196	LEU
1	H	199	LYS
1	H	200	LYS
1	H	203	LEU
1	H	208	SER
1	H	210	THR
1	H	211	ASN
1	H	215	ARG
1	H	250	LEU
1	H	275	SER
1	H	279	LYS
1	H	305	ARG
1	H	311	HIS
1	H	315	GLN
1	H	317	GLN
1	H	323	ARG
1	H	343	GLN
1	H	344	SER
1	H	347	GLU
1	H	356	THR
1	H	371	LEU
1	H	377	VAL
1	H	396	VAL
1	H	397	ASP
1	H	402	MET
1	H	403	SER

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Mol	Chain	Res	Type
1	H	410	SER
1	H	419	ASP
1	H	420	ASN
1	H	428	VAL
1	H	445	ILE
1	I	52	SER
1	I	56	SER
1	I	70	ARG
1	I	72	ILE
1	I	73	VAL
1	I	74	THR
1	I	91	LYS
1	I	92	THR
1	I	101	LYS
1	I	115	THR
1	I	131	SER
1	I	134	LEU
1	I	135	MET
1	I	142	SER
1	I	143	THR
1	I	147	LEU
1	I	156	ILE
1	I	158	THR
1	I	162	CYS
1	I	167	ARG
1	I	177	MET
1	I	180	THR
1	I	196	LEU
1	I	199	LYS
1	I	200	LYS
1	I	203	LEU
1	I	210	THR
1	I	211	ASN
1	I	215	ARG
1	I	250	LEU
1	I	275	SER
1	I	278	LEU
1	I	279	LYS
1	I	305	ARG
1	I	311	HIS
1	I	315	GLN
1	I	317	GLN

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Mol	Chain	Res	Type
1	I	323	ARG
1	I	343	GLN
1	I	344	SER
1	I	347	GLU
1	I	371	LEU
1	I	377	VAL
1	I	396	VAL
1	I	397	ASP
1	I	403	SER
1	I	410	SER
1	I	420	ASN
1	I	428	VAL
1	I	444	SER
1	J	56	SER
1	J	70	ARG
1	J	72	ILE
1	J	73	VAL
1	J	74	THR
1	J	91	LYS
1	J	92	THR
1	J	101	LYS
1	J	115	THR
1	J	131	SER
1	J	134	LEU
1	J	135	MET
1	J	137	SER
1	J	142	SER
1	J	143	THR
1	J	145	MET
1	J	147	LEU
1	J	156	ILE
1	J	158	THR
1	J	162	CYS
1	J	177	MET
1	J	180	THR
1	J	196	LEU
1	J	199	LYS
1	J	200	LYS
1	J	203	LEU
1	J	208	SER
1	J	210	THR
1	J	211	ASN

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Mol	Chain	Res	Type
1	J	215	ARG
1	J	245	GLN
1	J	250	LEU
1	J	270	LEU
1	J	275	SER
1	J	279	LYS
1	J	305	ARG
1	J	311	HIS
1	J	317	GLN
1	J	323	ARG
1	J	343	GLN
1	J	344	SER
1	J	347	GLU
1	J	356	THR
1	J	371	LEU
1	J	377	VAL
1	J	396	VAL
1	J	397	ASP
1	J	403	SER
1	J	410	SER
1	J	419	ASP
1	J	420	ASN
1	J	428	VAL
1	J	444	SER
1	J	445	ILE
1	K	52	SER
1	K	54	LEU
1	K	70	ARG
1	K	72	ILE
1	K	73	VAL
1	K	74	THR
1	K	91	LYS
1	K	92	THR
1	K	101	LYS
1	K	115	THR
1	K	131	SER
1	K	134	LEU
1	K	135	MET
1	K	137	SER
1	K	142	SER
1	K	143	THR
1	K	145	MET

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Mol	Chain	Res	Type
1	K	147	LEU
1	K	156	ILE
1	K	158	THR
1	K	162	CYS
1	K	177	MET
1	K	196	LEU
1	K	199	LYS
1	K	200	LYS
1	K	203	LEU
1	K	208	SER
1	K	210	THR
1	K	211	ASN
1	K	215	ARG
1	K	250	LEU
1	K	275	SER
1	K	278	LEU
1	K	279	LYS
1	K	305	ARG
1	K	311	HIS
1	K	317	GLN
1	K	323	ARG
1	K	343	GLN
1	K	344	SER
1	K	347	GLU
1	K	356	THR
1	K	371	LEU
1	K	396	VAL
1	K	397	ASP
1	K	403	SER
1	K	410	SER
1	K	419	ASP
1	K	420	ASN
1	K	428	VAL
1	K	445	ILE
1	L	56	SER
1	L	70	ARG
1	L	72	ILE
1	L	73	VAL
1	L	74	THR
1	L	91	LYS
1	L	92	THR
1	L	101	LYS

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Mol	Chain	Res	Type
1	L	115	THR
1	L	131	SER
1	L	134	LEU
1	L	135	MET
1	L	137	SER
1	L	142	SER
1	L	143	THR
1	L	145	MET
1	L	147	LEU
1	L	156	ILE
1	L	158	THR
1	L	162	CYS
1	L	177	MET
1	L	180	THR
1	L	196	LEU
1	L	199	LYS
1	L	200	LYS
1	L	203	LEU
1	L	208	SER
1	L	210	THR
1	L	211	ASN
1	L	250	LEU
1	L	275	SER
1	L	279	LYS
1	L	305	ARG
1	L	311	HIS
1	L	317	GLN
1	L	323	ARG
1	L	343	GLN
1	L	344	SER
1	L	347	GLU
1	L	363	SER
1	L	371	LEU
1	L	377	VAL
1	L	396	VAL
1	L	397	ASP
1	L	403	SER
1	L	410	SER
1	L	420	ASN
1	L	424	PHE
1	L	428	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	211	ASN
1	A	317	GLN
1	A	343	GLN
1	A	420	ASN
1	B	63	HIS
1	B	211	ASN
1	B	317	GLN
1	B	343	GLN
1	B	420	ASN
1	C	63	HIS
1	C	211	ASN
1	C	317	GLN
1	C	343	GLN
1	C	420	ASN
1	D	63	HIS
1	D	211	ASN
1	D	317	GLN
1	D	343	GLN
1	D	420	ASN
1	E	55	ASN
1	E	63	HIS
1	E	211	ASN
1	E	317	GLN
1	E	343	GLN
1	E	420	ASN
1	F	63	HIS
1	F	211	ASN
1	F	317	GLN
1	F	343	GLN
1	F	420	ASN
1	G	63	HIS
1	G	211	ASN
1	G	317	GLN
1	G	343	GLN
1	G	420	ASN
1	H	63	HIS
1	H	211	ASN
1	H	317	GLN
1	H	343	GLN
1	H	420	ASN
1	I	63	HIS

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Mol	Chain	Res	Type
1	I	211	ASN
1	I	317	GLN
1	I	343	GLN
1	I	420	ASN
1	J	63	HIS
1	J	211	ASN
1	J	317	GLN
1	J	343	GLN
1	J	420	ASN
1	K	63	HIS
1	K	211	ASN
1	K	317	GLN
1	K	343	GLN
1	K	420	ASN
1	L	63	HIS
1	L	211	ASN
1	L	317	GLN
1	L	343	GLN
1	L	420	ASN

### 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 ⓘ

24 ligands are modelled in this entry.

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	CCO	K	610	-	11,18,18	1.54	2 (18%)	14,24,24	1.84	3 (21%)
3	CCO	B	601	-	11,18,18	1.59	2 (18%)	14,24,24	1.81	2 (14%)
2	PLP	I	500	1	15,15,16	3.51	6 (40%)	20,22,23	2.36	9 (45%)
3	CCO	J	609	-	11,18,18	1.65	2 (18%)	14,24,24	1.89	1 (7%)
2	PLP	J	500	1	15,15,16	3.60	5 (33%)	20,22,23	2.33	8 (40%)
3	CCO	E	604	-	11,18,18	1.63	2 (18%)	14,24,24	1.87	2 (14%)
2	PLP	L	500	1	15,15,16	3.45	5 (33%)	20,22,23	2.35	8 (40%)
2	PLP	B	500	1	15,15,16	3.29	6 (40%)	20,22,23	2.38	8 (40%)
3	CCO	F	605	-	11,18,18	1.61	2 (18%)	14,24,24	1.82	2 (14%)
3	CCO	C	602	-	11,18,18	1.66	2 (18%)	14,24,24	1.90	2 (14%)
2	PLP	K	500	1	15,15,16	3.69	6 (40%)	20,22,23	2.42	10 (50%)
2	PLP	H	500	1	15,15,16	3.49	5 (33%)	20,22,23	2.41	9 (45%)
3	CCO	I	608	-	11,18,18	1.59	2 (18%)	14,24,24	1.89	3 (21%)
2	PLP	C	500	1	15,15,16	3.51	5 (33%)	20,22,23	2.44	9 (45%)
3	CCO	G	606	-	11,18,18	1.64	2 (18%)	14,24,24	1.81	3 (21%)
3	CCO	D	603	-	11,18,18	1.64	2 (18%)	14,24,24	1.91	3 (21%)
2	PLP	E	500	1	15,15,16	3.66	5 (33%)	20,22,23	2.41	8 (40%)
3	CCO	L	611	-	11,18,18	1.66	2 (18%)	14,24,24	1.89	2 (14%)
2	PLP	F	500	1	15,15,16	3.52	6 (40%)	20,22,23	2.38	8 (40%)
2	PLP	D	500	1	15,15,16	3.59	6 (40%)	20,22,23	2.39	9 (45%)
2	PLP	A	500	1	15,15,16	3.81	4 (26%)	20,22,23	2.41	10 (50%)
2	PLP	G	500	1	15,15,16	3.55	6 (40%)	20,22,23	2.44	10 (50%)
3	CCO	H	607	-	11,18,18	1.57	2 (18%)	14,24,24	1.79	2 (14%)
3	CCO	A	600	-	11,18,18	1.64	2 (18%)	14,24,24	1.79	3 (21%)

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	CCO	K	610	-	-	4/5/9/9	0/2/2/2
3	CCO	B	601	-	-	4/5/9/9	0/2/2/2
2	PLP	I	500	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CCO	J	609	-	-	4/5/9/9	0/2/2/2
2	PLP	J	500	1	-	0/6/6/8	0/1/1/1
3	CCO	E	604	-	-	4/5/9/9	0/2/2/2
2	PLP	L	500	1	-	0/6/6/8	0/1/1/1
2	PLP	B	500	1	-	0/6/6/8	0/1/1/1
3	CCO	F	605	-	-	0/5/9/9	0/2/2/2
3	CCO	C	602	-	-	0/5/9/9	0/2/2/2
2	PLP	K	500	1	-	0/6/6/8	0/1/1/1
2	PLP	H	500	1	-	0/6/6/8	0/1/1/1
3	CCO	I	608	-	-	4/5/9/9	0/2/2/2
2	PLP	C	500	1	-	0/6/6/8	0/1/1/1
3	CCO	G	606	-	-	4/5/9/9	0/2/2/2
3	CCO	D	603	-	-	4/5/9/9	0/2/2/2
2	PLP	E	500	1	-	0/6/6/8	0/1/1/1
3	CCO	L	611	-	-	4/5/9/9	0/2/2/2
2	PLP	F	500	1	-	0/6/6/8	0/1/1/1
2	PLP	D	500	1	-	0/6/6/8	0/1/1/1
2	PLP	A	500	1	-	0/6/6/8	0/1/1/1
2	PLP	G	500	1	-	0/6/6/8	0/1/1/1
3	CCO	H	607	-	-	2/5/9/9	0/2/2/2
3	CCO	A	600	-	-	0/5/9/9	0/2/2/2

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PLP	C5-C4	10.96	1.52	1.40
2	E	500	PLP	C5-C4	10.61	1.52	1.40
2	K	500	PLP	C5-C4	10.53	1.52	1.40
2	D	500	PLP	C5-C4	10.44	1.52	1.40
2	J	500	PLP	C5-C4	10.33	1.51	1.40
2	G	500	PLP	C5-C4	10.23	1.51	1.40
2	I	500	PLP	C5-C4	10.22	1.51	1.40
2	F	500	PLP	C5-C4	10.10	1.51	1.40
2	L	500	PLP	C5-C4	10.08	1.51	1.40
2	C	500	PLP	C5-C4	9.90	1.51	1.40
2	H	500	PLP	C5-C4	9.79	1.51	1.40
2	B	500	PLP	C5-C4	9.21	1.50	1.40
2	A	500	PLP	C3-C2	7.94	1.48	1.40
2	K	500	PLP	C3-C2	7.57	1.48	1.40
2	C	500	PLP	C3-C2	7.48	1.48	1.40
2	G	500	PLP	C3-C2	7.17	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500	PLP	C3-C2	7.00	1.47	1.40
2	E	500	PLP	C3-C2	6.96	1.47	1.40
2	F	500	PLP	C3-C2	6.86	1.47	1.40
2	J	500	PLP	C3-C2	6.79	1.47	1.40
2	B	500	PLP	C3-C2	6.54	1.47	1.40
2	I	500	PLP	C3-C2	6.50	1.47	1.40
2	L	500	PLP	C3-C2	6.48	1.47	1.40
2	D	500	PLP	C3-C2	6.47	1.47	1.40
2	D	500	PLP	C2-N1	3.91	1.41	1.33
2	J	500	PLP	C2-N1	3.91	1.41	1.33
2	A	500	PLP	C2-N1	3.81	1.41	1.33
2	E	500	PLP	C2-N1	3.73	1.40	1.33
2	H	500	PLP	C2-N1	3.69	1.40	1.33
2	K	500	PLP	C2-N1	3.67	1.40	1.33
2	G	500	PLP	C2-N1	3.65	1.40	1.33
2	I	500	PLP	C2-N1	3.50	1.40	1.33
2	F	500	PLP	C2-N1	3.41	1.40	1.33
2	C	500	PLP	C2-N1	3.36	1.40	1.33
2	B	500	PLP	C2-N1	3.32	1.40	1.33
2	L	500	PLP	C2-N1	3.27	1.40	1.33
2	B	500	PLP	C4A-C4	-2.86	1.45	1.51
3	J	609	CCO	C6-C5	2.86	1.43	1.38
3	E	604	CCO	C6-C5	2.78	1.42	1.38
2	I	500	PLP	C4A-C4	-2.74	1.45	1.51
3	D	603	CCO	C4-C5	2.71	1.43	1.38
3	L	611	CCO	C6-C5	2.66	1.42	1.38
3	F	605	CCO	C4-C5	2.66	1.43	1.38
3	I	608	CCO	C6-C5	2.63	1.42	1.38
3	G	606	CCO	C6-C5	2.63	1.42	1.38
3	A	600	CCO	C4-C5	2.63	1.43	1.38
3	H	607	CCO	C4-C5	2.62	1.43	1.38
3	L	611	CCO	C4-C5	2.62	1.43	1.38
2	J	500	PLP	C4A-C4	-2.62	1.46	1.51
3	C	602	CCO	C6-C5	2.62	1.42	1.38
3	B	601	CCO	C6-C5	2.61	1.42	1.38
2	H	500	PLP	C4A-C4	-2.61	1.46	1.51
3	C	602	CCO	C4-C5	2.60	1.43	1.38
3	K	610	CCO	C4-C5	2.57	1.42	1.38
3	B	601	CCO	C4-C5	2.57	1.42	1.38
2	L	500	PLP	C4A-C4	-2.54	1.46	1.51
2	D	500	PLP	C4A-C4	-2.52	1.46	1.51
3	D	603	CCO	C6-C5	2.52	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	PLP	C4A-C4	-2.50	1.46	1.51
3	J	609	CCO	C4-C5	2.50	1.42	1.38
3	K	610	CCO	C6-C5	2.47	1.42	1.38
2	F	500	PLP	C4A-C4	-2.46	1.46	1.51
3	F	605	CCO	C6-C5	2.46	1.42	1.38
3	G	606	CCO	C4-C5	2.45	1.42	1.38
3	E	604	CCO	C4-C5	2.41	1.42	1.38
3	A	600	CCO	C6-C5	2.36	1.42	1.38
3	I	608	CCO	C4-C5	2.30	1.42	1.38
2	B	500	PLP	P-O3P	-2.26	1.46	1.54
2	F	500	PLP	P-O3P	-2.25	1.46	1.54
2	G	500	PLP	P-O3P	-2.18	1.46	1.54
3	H	607	CCO	C6-C5	2.18	1.41	1.38
2	A	500	PLP	P-O3P	-2.17	1.46	1.54
2	C	500	PLP	P-O3P	-2.16	1.46	1.54
2	K	500	PLP	C4A-C4	-2.14	1.47	1.51
2	I	500	PLP	P-O2P	-2.10	1.46	1.54
2	I	500	PLP	P-O3P	-2.10	1.46	1.54
2	E	500	PLP	P-O3P	-2.10	1.46	1.54
2	G	500	PLP	C4A-C4	-2.10	1.47	1.51
2	L	500	PLP	P-O3P	-2.08	1.46	1.54
2	F	500	PLP	P-O2P	-2.08	1.46	1.54
2	J	500	PLP	P-O3P	-2.08	1.46	1.54
2	K	500	PLP	P-O3P	-2.08	1.46	1.54
2	H	500	PLP	P-O3P	-2.08	1.46	1.54
2	B	500	PLP	P-O2P	-2.05	1.47	1.54
2	K	500	PLP	P-O2P	-2.04	1.47	1.54
2	D	500	PLP	P-O2P	-2.03	1.47	1.54
2	G	500	PLP	P-O2P	-2.02	1.47	1.54
2	C	500	PLP	P-O2P	-2.01	1.47	1.54
2	D	500	PLP	P-O3P	-2.00	1.47	1.54

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	PLP	C2A-C2-C3	6.35	128.74	120.89
2	H	500	PLP	C2A-C2-C3	6.14	128.47	120.89
2	K	500	PLP	C2A-C2-C3	6.14	128.47	120.89
2	G	500	PLP	C2A-C2-C3	6.13	128.46	120.89
2	L	500	PLP	C2A-C2-C3	6.12	128.45	120.89
2	E	500	PLP	C2A-C2-C3	6.11	128.44	120.89
2	B	500	PLP	C2A-C2-C3	6.10	128.43	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	PLP	C2A-C2-C3	6.10	128.42	120.89
3	L	611	CCO	C1-C1A-N2	6.09	127.04	119.12
3	J	609	CCO	C1-C1A-N2	6.03	126.97	119.12
3	C	602	CCO	C1-C1A-N2	6.02	126.95	119.12
2	I	500	PLP	C2A-C2-C3	6.01	128.31	120.89
2	A	500	PLP	C2A-C2-C3	6.01	128.31	120.89
3	E	604	CCO	C1-C1A-N2	5.95	126.86	119.12
3	I	608	CCO	C1-C1A-N2	5.88	126.78	119.12
3	D	603	CCO	C1-C1A-N2	5.87	126.75	119.12
2	J	500	PLP	C2A-C2-C3	5.84	128.10	120.89
3	G	606	CCO	C1-C1A-N2	5.80	126.67	119.12
2	D	500	PLP	C2A-C2-C3	5.78	128.03	120.89
3	B	601	CCO	C1-C1A-N2	5.76	126.61	119.12
3	F	605	CCO	C1-C1A-N2	5.62	126.44	119.12
3	A	600	CCO	C1-C1A-N2	5.50	126.27	119.12
3	K	610	CCO	C1-C1A-N2	5.49	126.26	119.12
3	H	607	CCO	C1-C1A-N2	5.44	126.20	119.12
2	E	500	PLP	C6-N1-C2	3.91	126.41	119.17
2	D	500	PLP	C6-N1-C2	3.82	126.25	119.17
2	I	500	PLP	C6-N1-C2	3.78	126.18	119.17
2	J	500	PLP	C6-N1-C2	3.78	126.18	119.17
2	L	500	PLP	C6-N1-C2	3.77	126.15	119.17
2	C	500	PLP	C6-N1-C2	3.75	126.11	119.17
2	F	500	PLP	C6-N1-C2	3.75	126.11	119.17
2	H	500	PLP	C6-N1-C2	3.73	126.08	119.17
2	K	500	PLP	C6-N1-C2	3.73	126.08	119.17
2	G	500	PLP	C6-N1-C2	3.73	126.07	119.17
2	B	500	PLP	C6-N1-C2	3.71	126.05	119.17
2	I	500	PLP	O3-C3-C4	3.69	127.83	118.10
2	A	500	PLP	C6-N1-C2	3.67	125.97	119.17
2	E	500	PLP	O3-C3-C4	3.66	127.73	118.10
2	D	500	PLP	O3-C3-C4	3.63	127.67	118.10
2	J	500	PLP	O3-C3-C4	3.59	127.56	118.10
2	H	500	PLP	O3-C3-C4	3.57	127.51	118.10
2	B	500	PLP	O3-C3-C4	3.57	127.50	118.10
2	G	500	PLP	O3-C3-C4	3.54	127.44	118.10
2	F	500	PLP	O3-C3-C4	3.54	127.42	118.10
2	L	500	PLP	O3-C3-C4	3.54	127.41	118.10
2	C	500	PLP	O3-C3-C4	3.53	127.41	118.10
2	K	500	PLP	O3-C3-C4	3.52	127.37	118.10
2	A	500	PLP	O3-C3-C4	3.44	127.16	118.10
2	G	500	PLP	C6-C5-C4	3.43	120.86	118.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	PLP	C3-C2-N1	-3.42	116.35	120.77
2	C	500	PLP	C6-C5-C4	3.41	120.84	118.16
2	H	500	PLP	C3-C2-N1	-3.38	116.40	120.77
2	B	500	PLP	C3-C2-N1	-3.35	116.44	120.77
2	A	500	PLP	C6-C5-C4	3.33	120.78	118.16
2	E	500	PLP	C3-C2-N1	-3.33	116.47	120.77
2	J	500	PLP	C3-C2-N1	-3.31	116.49	120.77
2	G	500	PLP	C3-C2-N1	-3.30	116.50	120.77
2	C	500	PLP	C3-C2-N1	-3.29	116.51	120.77
2	L	500	PLP	C3-C2-N1	-3.29	116.52	120.77
2	F	500	PLP	C3-C2-N1	-3.29	116.52	120.77
2	K	500	PLP	C3-C2-N1	-3.26	116.56	120.77
2	I	500	PLP	C3-C2-N1	-3.23	116.59	120.77
2	D	500	PLP	O4P-C5A-C5	3.16	115.37	109.35
2	E	500	PLP	O4P-C5A-C5	3.10	115.27	109.35
2	K	500	PLP	C6-C5-C4	3.02	120.53	118.16
2	A	500	PLP	C3-C2-N1	-3.02	116.87	120.77
2	G	500	PLP	C5-C6-N1	-3.01	118.80	123.82
2	A	500	PLP	C5-C6-N1	-3.01	118.81	123.82
2	B	500	PLP	C5-C6-N1	-2.98	118.85	123.82
2	B	500	PLP	C6-C5-C4	2.97	120.50	118.16
2	H	500	PLP	C6-C5-C4	2.96	120.49	118.16
2	H	500	PLP	C5-C6-N1	-2.95	118.91	123.82
2	J	500	PLP	C5-C6-N1	-2.93	118.94	123.82
2	D	500	PLP	C5-C6-N1	-2.92	118.95	123.82
2	K	500	PLP	C5-C6-N1	-2.91	118.98	123.82
2	E	500	PLP	C5-C6-N1	-2.90	118.98	123.82
2	F	500	PLP	C5-C6-N1	-2.90	118.98	123.82
2	C	500	PLP	C5-C6-N1	-2.89	119.01	123.82
2	I	500	PLP	C5-C6-N1	-2.89	119.01	123.82
2	L	500	PLP	C5-C6-N1	-2.83	119.11	123.82
3	K	610	CCO	C1B-S3-C2A	-2.76	98.84	101.20
2	F	500	PLP	C6-C5-C4	2.69	120.28	118.16
2	J	500	PLP	C6-C5-C4	2.66	120.25	118.16
2	I	500	PLP	O4P-C5A-C5	2.66	114.42	109.35
2	K	500	PLP	O4P-C5A-C5	2.63	114.37	109.35
2	J	500	PLP	O4P-C5A-C5	2.63	114.37	109.35
2	F	500	PLP	O4P-C5A-C5	2.61	114.33	109.35
2	A	500	PLP	O4P-C5A-C5	2.55	114.20	109.35
2	L	500	PLP	O4P-C5A-C5	2.54	114.19	109.35
3	D	603	CCO	C1B-S3-C2A	-2.53	99.04	101.20
2	E	500	PLP	C6-C5-C4	2.52	120.14	118.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	500	PLP	C6-C5-C4	2.44	120.08	118.16
2	H	500	PLP	O4P-C5A-C5	2.42	113.97	109.35
3	H	607	CCO	C1-C1A-N3	2.39	126.70	123.71
2	I	500	PLP	O3-C3-C2	-2.37	112.33	117.49
2	D	500	PLP	O3-C3-C2	-2.36	112.35	117.49
3	B	601	CCO	C1-C1A-N3	2.35	126.64	123.71
2	L	500	PLP	C6-C5-C4	2.35	120.00	118.16
2	A	500	PLP	C4A-C4-C5	2.33	123.34	120.94
3	A	600	CCO	C1-C1A-N3	2.33	126.62	123.71
2	D	500	PLP	C6-C5-C4	2.32	119.98	118.16
2	G	500	PLP	O3-C3-C2	-2.29	112.51	117.49
2	G	500	PLP	O4P-C5A-C5	2.28	113.70	109.35
3	F	605	CCO	C1-C1A-N3	2.28	126.56	123.71
2	B	500	PLP	O4P-C5A-C5	2.27	113.69	109.35
3	I	608	CCO	C-C1B-S3	2.27	114.05	109.54
2	H	500	PLP	O3-C3-C2	-2.27	112.54	117.49
2	L	500	PLP	O3-C3-C2	-2.27	112.55	117.49
2	H	500	PLP	O3P-P-O2P	2.27	116.31	107.64
3	K	610	CCO	C1-C1A-N3	2.26	126.53	123.71
2	K	500	PLP	O3-C3-C2	-2.24	112.62	117.49
2	J	500	PLP	O3-C3-C2	-2.22	112.65	117.49
2	B	500	PLP	O3-C3-C2	-2.21	112.67	117.49
2	F	500	PLP	O3-C3-C2	-2.21	112.67	117.49
2	E	500	PLP	O3-C3-C2	-2.21	112.67	117.49
3	E	604	CCO	C1-C1A-N3	2.21	126.47	123.71
2	C	500	PLP	O3-C3-C2	-2.19	112.72	117.49
3	G	606	CCO	C1-C1A-N3	2.19	126.45	123.71
2	D	500	PLP	O3P-P-O2P	2.17	115.94	107.64
2	G	500	PLP	C4A-C4-C5	2.16	123.16	120.94
3	I	608	CCO	C1-C1A-N3	2.15	126.40	123.71
2	A	500	PLP	O3P-P-O2P	2.14	115.81	107.64
2	C	500	PLP	O3P-P-O2P	2.12	115.72	107.64
2	C	500	PLP	C4A-C4-C5	2.11	123.11	120.94
2	G	500	PLP	O3P-P-O2P	2.09	115.62	107.64
3	C	602	CCO	C-C1B-S3	2.06	113.63	109.54
2	K	500	PLP	O3P-P-O2P	2.06	115.52	107.64
3	L	611	CCO	C-C1B-S3	2.05	113.61	109.54
3	G	606	CCO	C-C1B-S3	2.05	113.60	109.54
2	A	500	PLP	O3-C3-C2	-2.04	113.04	117.49
3	D	603	CCO	C-C1B-S3	2.04	113.58	109.54
2	K	500	PLP	C4A-C4-C5	2.02	123.02	120.94
3	A	600	CCO	C-C1B-S3	2.02	113.54	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	500	PLP	O3P-P-O2P	2.00	115.28	107.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	610	CCO	C2-C1-C1A-N3
3	K	610	CCO	C2-C1-C1A-N2
3	K	610	CCO	C6-C1-C1A-N3
3	K	610	CCO	C6-C1-C1A-N2
3	J	609	CCO	C2-C1-C1A-N2
3	J	609	CCO	C6-C1-C1A-N2
3	E	604	CCO	C2-C1-C1A-N3
3	E	604	CCO	C2-C1-C1A-N2
3	E	604	CCO	C6-C1-C1A-N2
3	I	608	CCO	C2-C1-C1A-N2
3	L	611	CCO	C2-C1-C1A-N2
3	L	611	CCO	C6-C1-C1A-N2
3	I	608	CCO	C6-C1-C1A-N2
3	D	603	CCO	C2-C1-C1A-N2
3	D	603	CCO	C6-C1-C1A-N2
3	E	604	CCO	C6-C1-C1A-N3
3	B	601	CCO	C2-C1-C1A-N2
3	B	601	CCO	C6-C1-C1A-N2
3	G	606	CCO	C2-C1-C1A-N2
3	G	606	CCO	C6-C1-C1A-N2
3	J	609	CCO	C6-C1-C1A-N3
3	L	611	CCO	C6-C1-C1A-N3
3	B	601	CCO	C6-C1-C1A-N3
3	J	609	CCO	C2-C1-C1A-N3
3	I	608	CCO	C6-C1-C1A-N3
3	G	606	CCO	C6-C1-C1A-N3
3	D	603	CCO	C6-C1-C1A-N3
3	L	611	CCO	C2-C1-C1A-N3
3	H	607	CCO	C2-C1-C1A-N2
3	B	601	CCO	C2-C1-C1A-N3
3	I	608	CCO	C2-C1-C1A-N3
3	G	606	CCO	C2-C1-C1A-N3
3	D	603	CCO	C2-C1-C1A-N3
3	H	607	CCO	C6-C1-C1A-N3

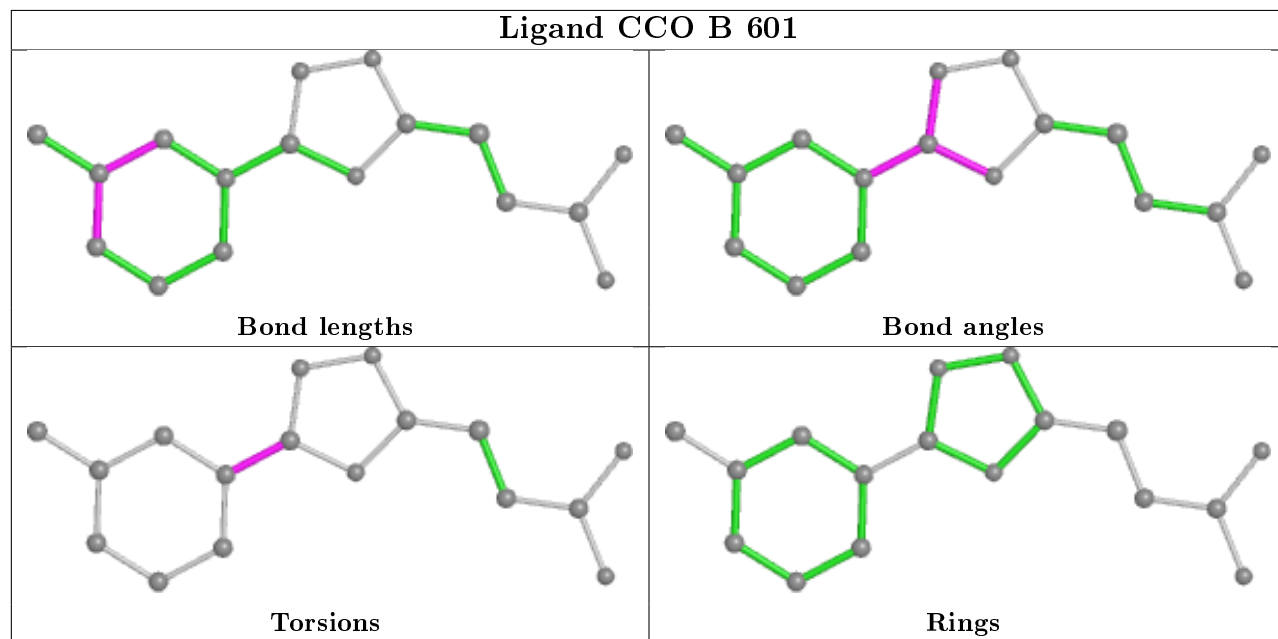
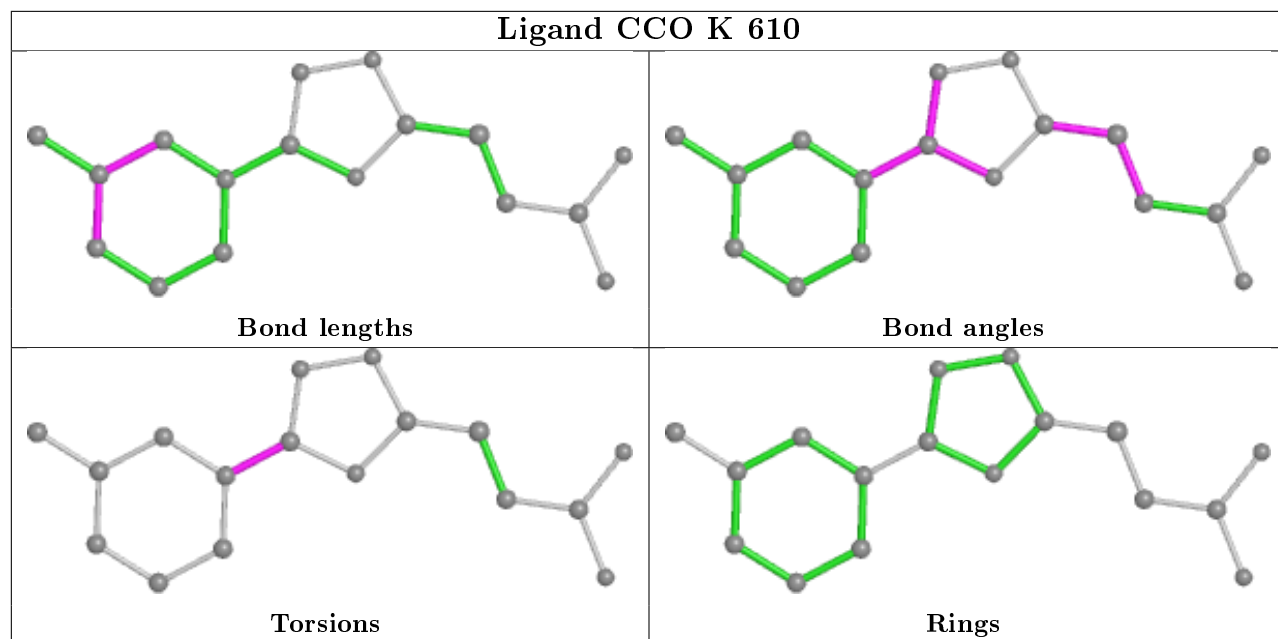
There are no ring outliers.



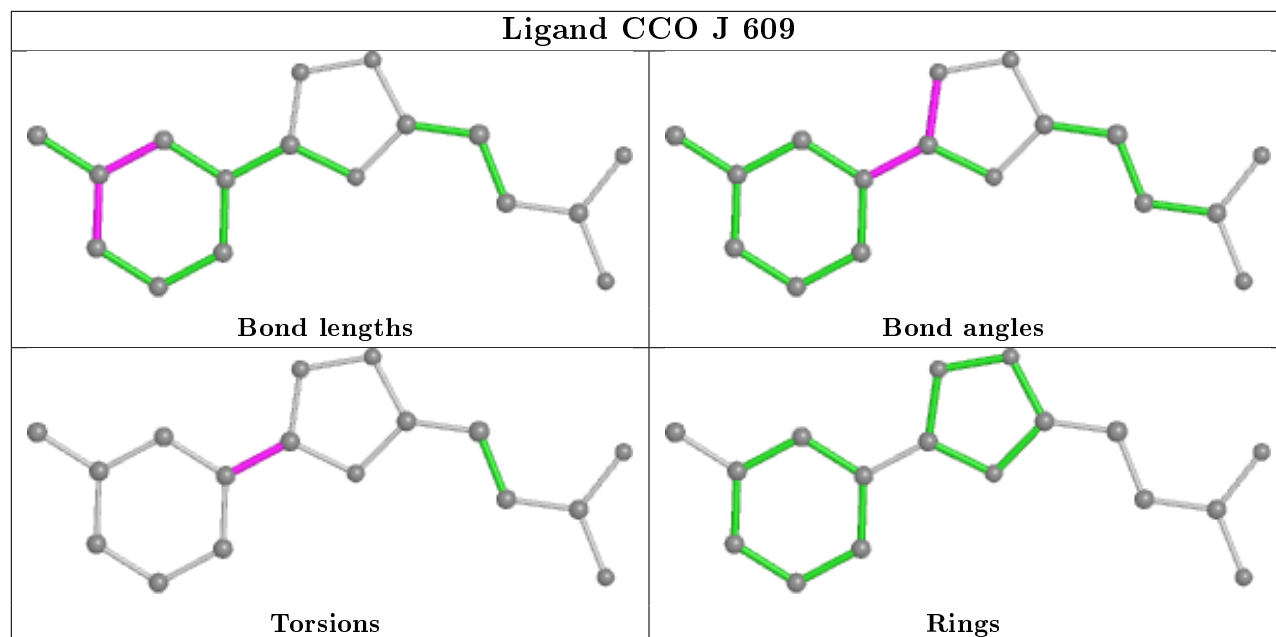
20 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	610	CCO	2	0
3	B	601	CCO	1	0
2	I	500	PLP	1	0
3	J	609	CCO	2	0
2	J	500	PLP	1	0
3	E	604	CCO	1	0
2	L	500	PLP	1	0
3	F	605	CCO	2	0
3	C	602	CCO	1	0
2	K	500	PLP	1	0
3	I	608	CCO	1	0
2	C	500	PLP	2	0
3	G	606	CCO	1	0
3	D	603	CCO	1	0
3	L	611	CCO	1	0
2	F	500	PLP	1	0
2	A	500	PLP	2	0
2	G	500	PLP	1	0
3	H	607	CCO	2	0
3	A	600	CCO	1	0

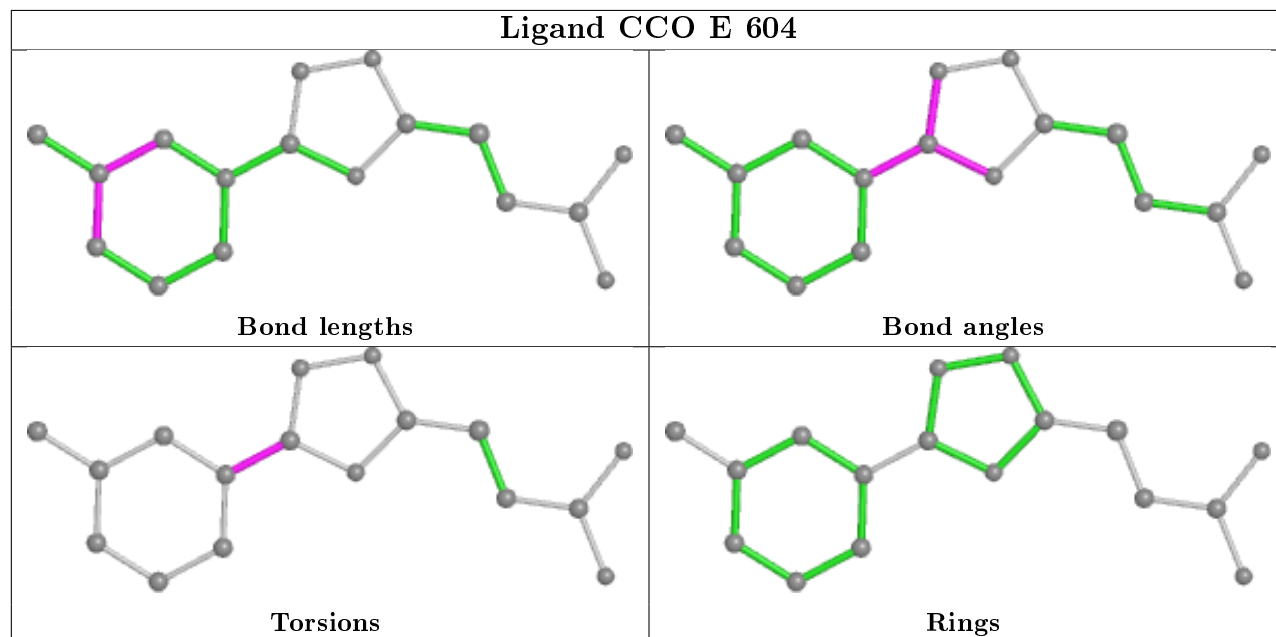
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



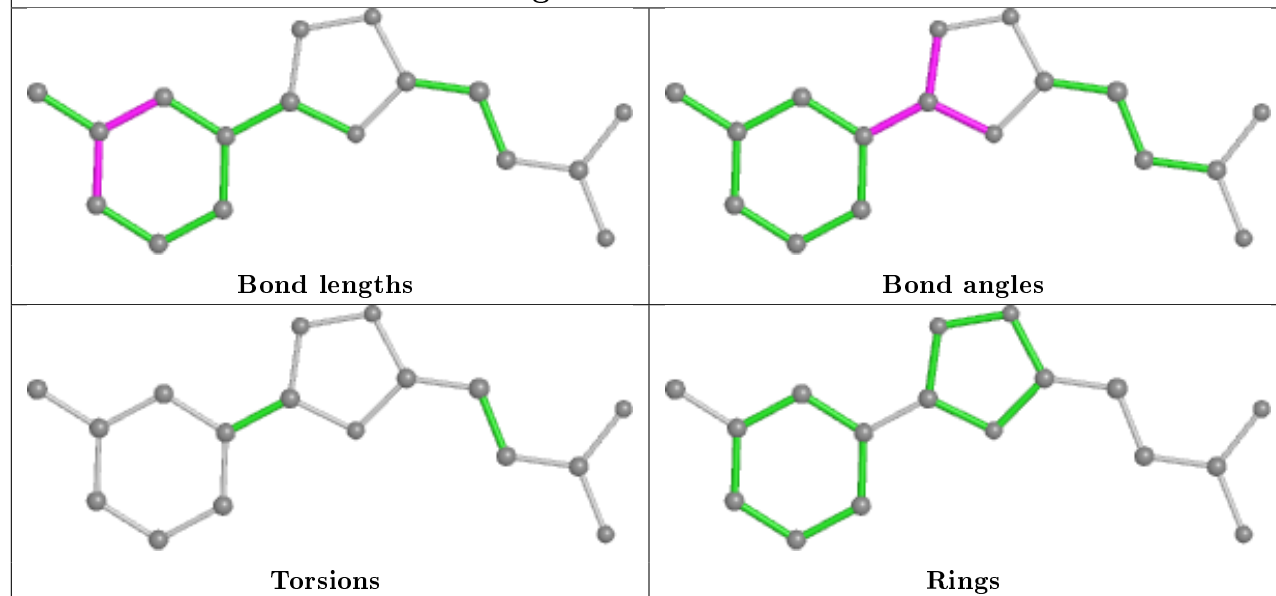
## Ligand CCO J 609



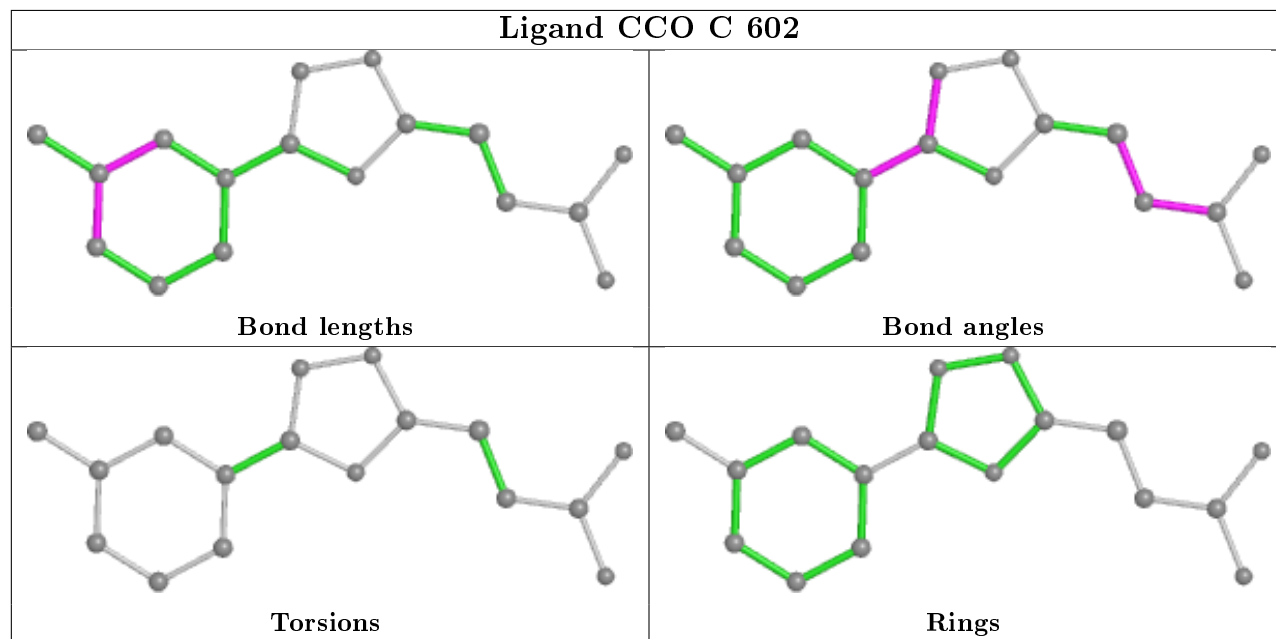
## Ligand CCO E 604



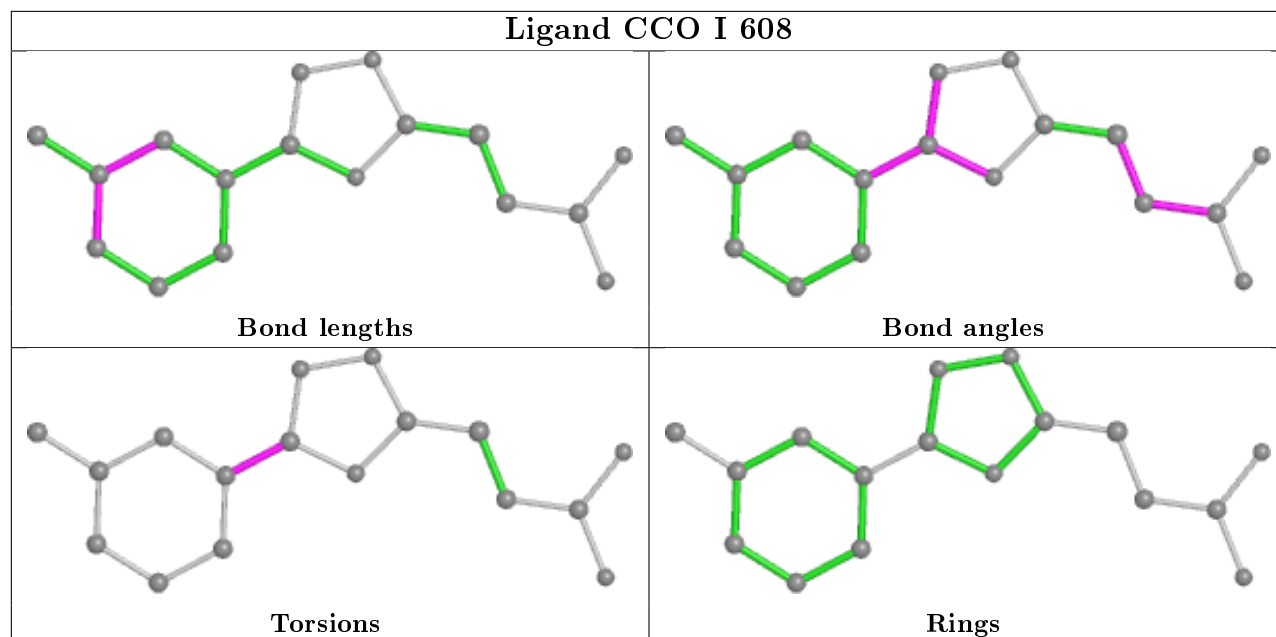
## Ligand CCO F 605



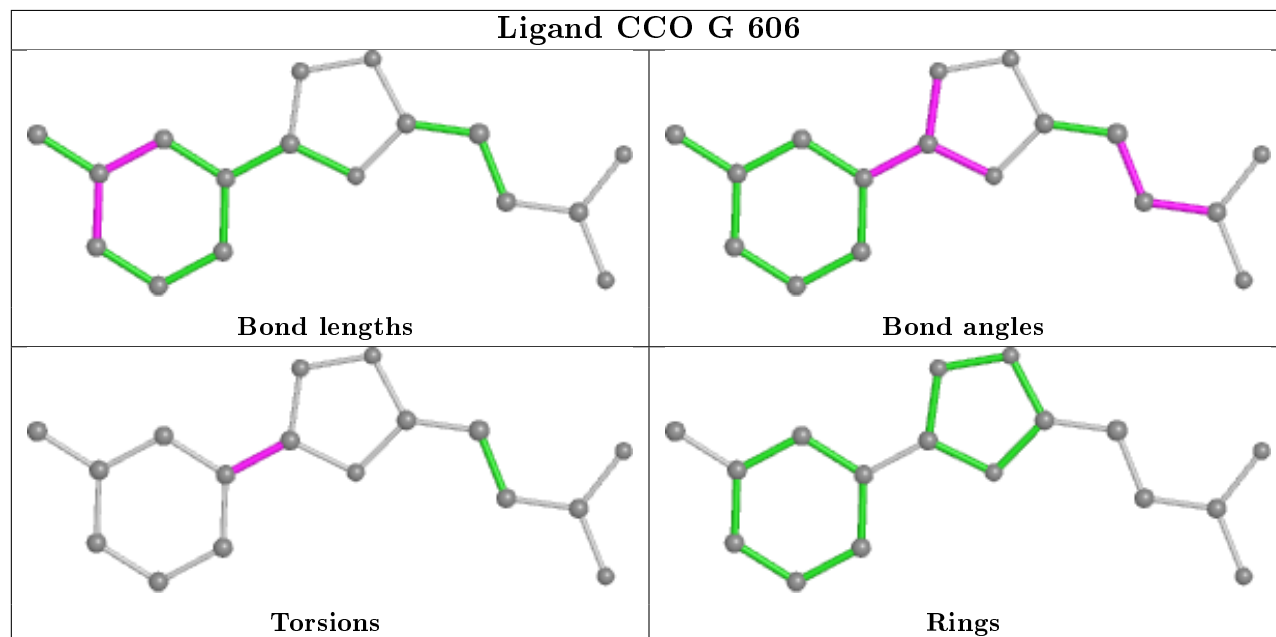
## Ligand CCO C 602

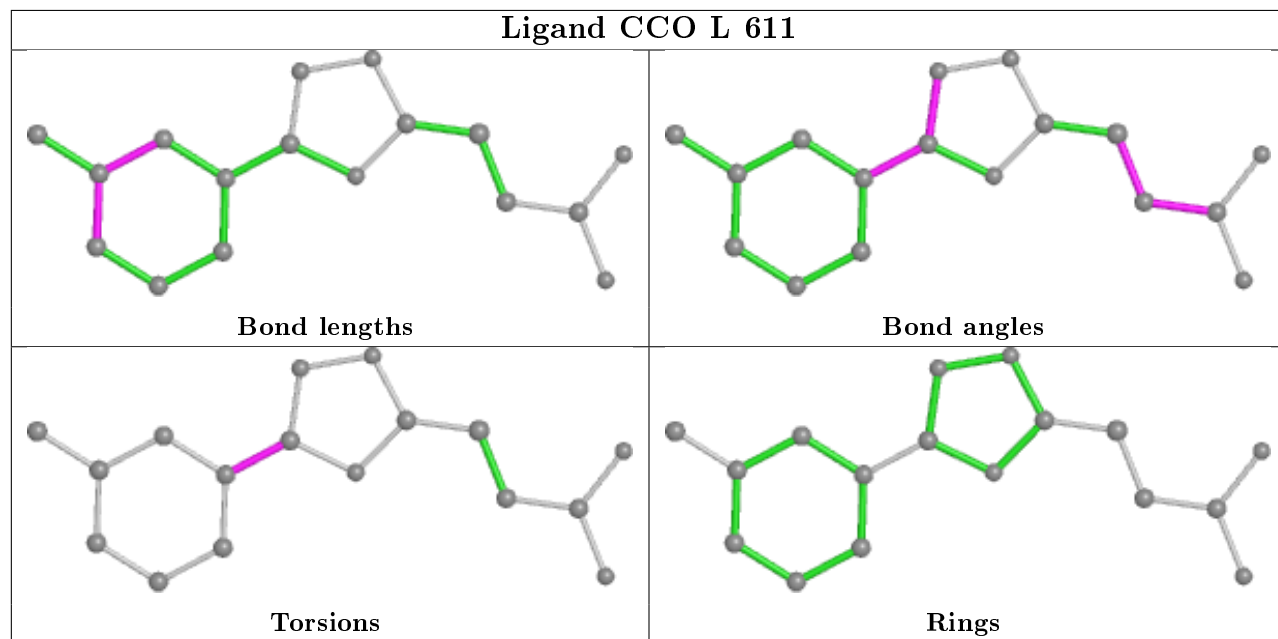
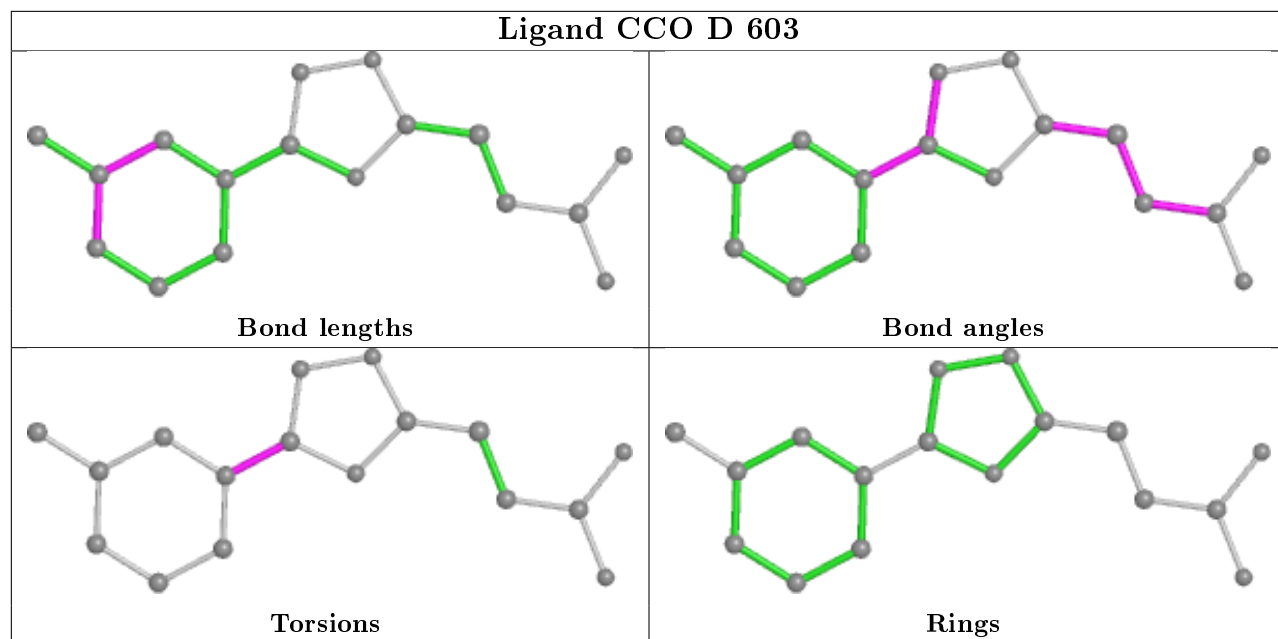


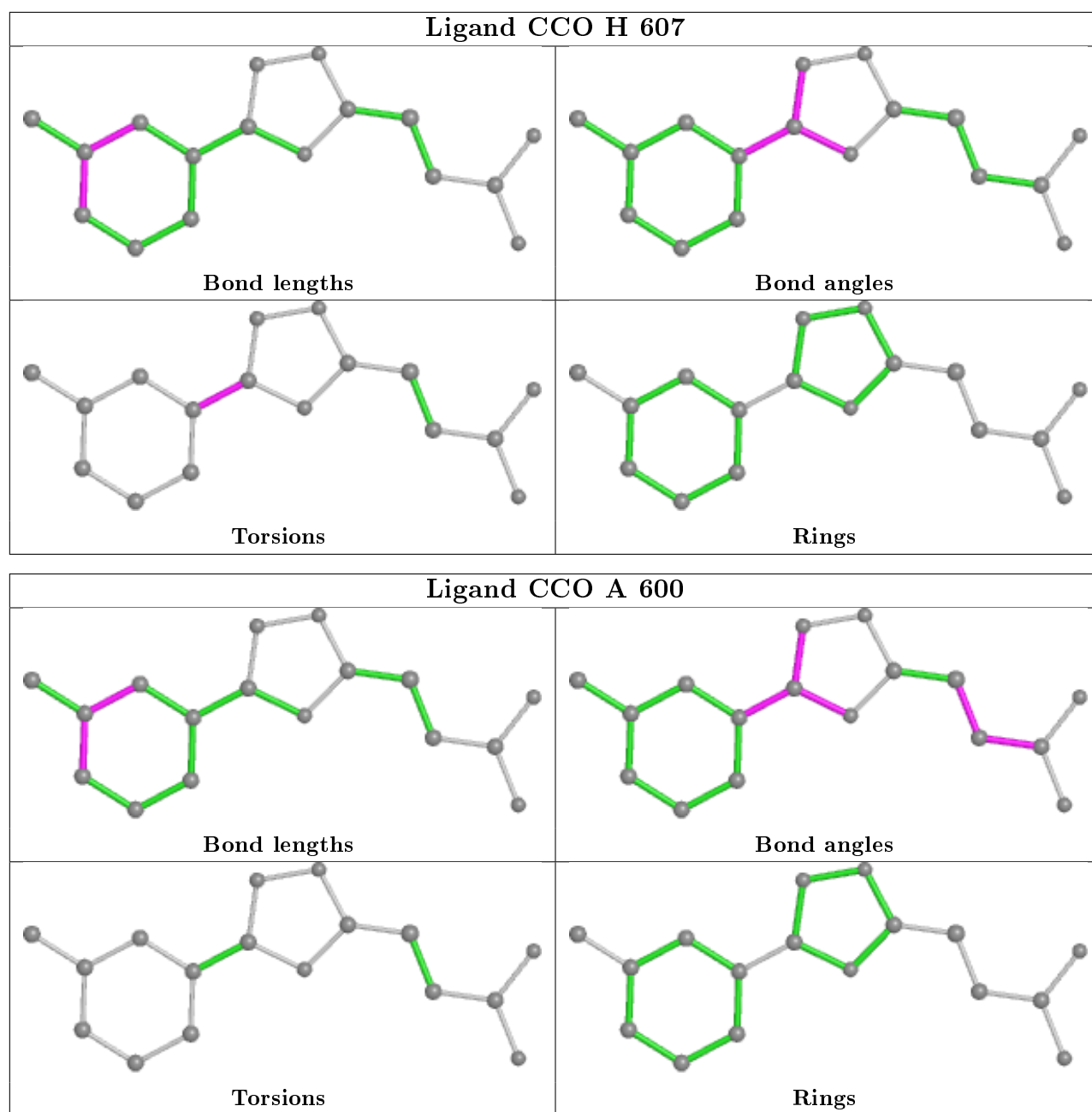
## Ligand CCO I 608



## Ligand CCO G 606







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.