



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:26 am BST

PDB ID : 1I41  
Title : CYSTATHIONINE GAMMA-SYNTHASE IN COMPLEX WITH THE INHIBITOR APPA  
Authors : Steegborn, C.; Laber, B.; Messerschmidt, A.; Huber, R.; Clausen, T.  
Deposited on : 2001-02-19  
Resolution : 3.20 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.

---

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

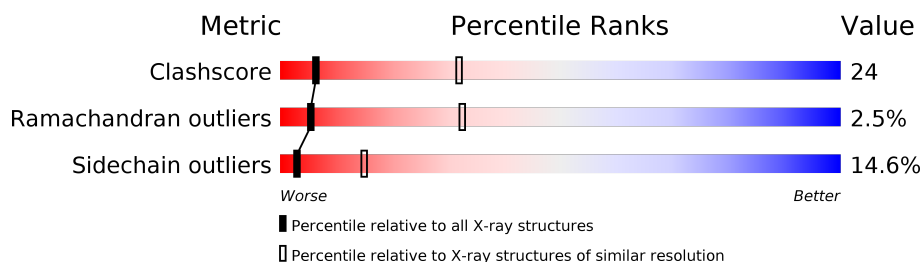
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)



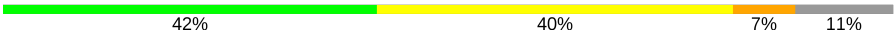
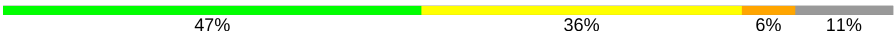
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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 style="width: 42%; background-color: green;"></div><div style="width: 40%; background-color: yellow;"></div><div style="width: 6%; background-color: orange;"></div><div style="width: 11%; background-color: grey;"></div></div>
1	B	445	<div><div style="width: 44%; background-color: green;"></div><div style="width: 39%; background-color: yellow;"></div><div style="width: 6%; background-color: orange;"></div><div style="width: 11%; background-color: grey;"></div></div>
1	C	445	<div><div style="width: 44%; background-color: green;"></div><div style="width: 38%; background-color: yellow;"></div><div style="width: 7%; background-color: orange;"></div><div style="width: 11%; background-color: grey;"></div></div>
1	D	445	<div><div style="width: 42%; background-color: green;"></div><div style="width: 40%; background-color: yellow;"></div><div style="width: 7%; background-color: orange;"></div><div style="width: 11%; background-color: grey;"></div></div>
1	E	445	<div><div style="width: 43%; background-color: green;"></div><div style="width: 39%; background-color: yellow;"></div><div style="width: 7%; background-color: orange;"></div><div style="width: 11%; background-color: grey;"></div></div>
1	F	445	<div><div style="width: 44%; background-color: green;"></div><div style="width: 38%; background-color: yellow;"></div><div style="width: 8%; background-color: orange;"></div><div style="width: 11%; background-color: grey;"></div></div>
1	G	445	<div><div style="width: 44%; background-color: green;"></div><div style="width: 39%; background-color: yellow;"></div><div style="width: 6%; background-color: orange;"></div><div style="width: 11%; background-color: grey;"></div></div>
1	H	445	<div><div style="width: 42%; background-color: green;"></div><div style="width: 41%; background-color: yellow;"></div><div style="width: 7%; background-color: orange;"></div><div style="width: 11%; background-color: grey;"></div></div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	I	445	 48% 36% 5% 11%
1	J	445	 43% 40% 6% 11%
1	K	445	 42% 40% 7% 11%
1	L	445	 47% 36% 6% 11%

## 2 Entry composition

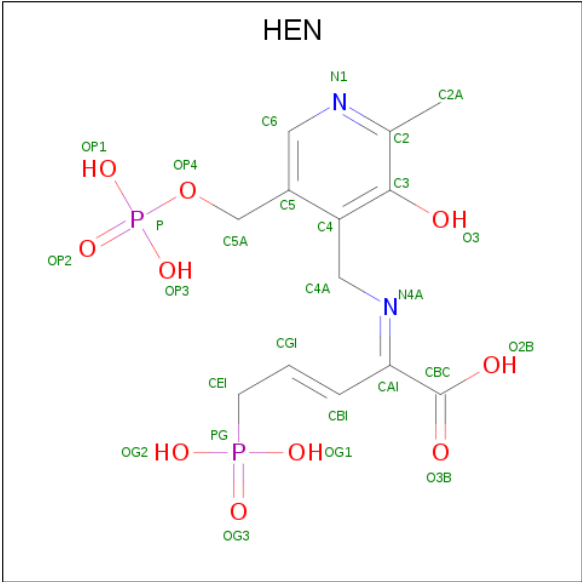
There are 2 unique types of molecules in this entry. The entry contains 36600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-IMINO]-5-PHOSPHONO-PENT-3-ENOIC ACID (three-letter code: HEN) (formula: C<sub>13</sub>H<sub>18</sub>N<sub>2</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	13	2	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	13	2	10	2		

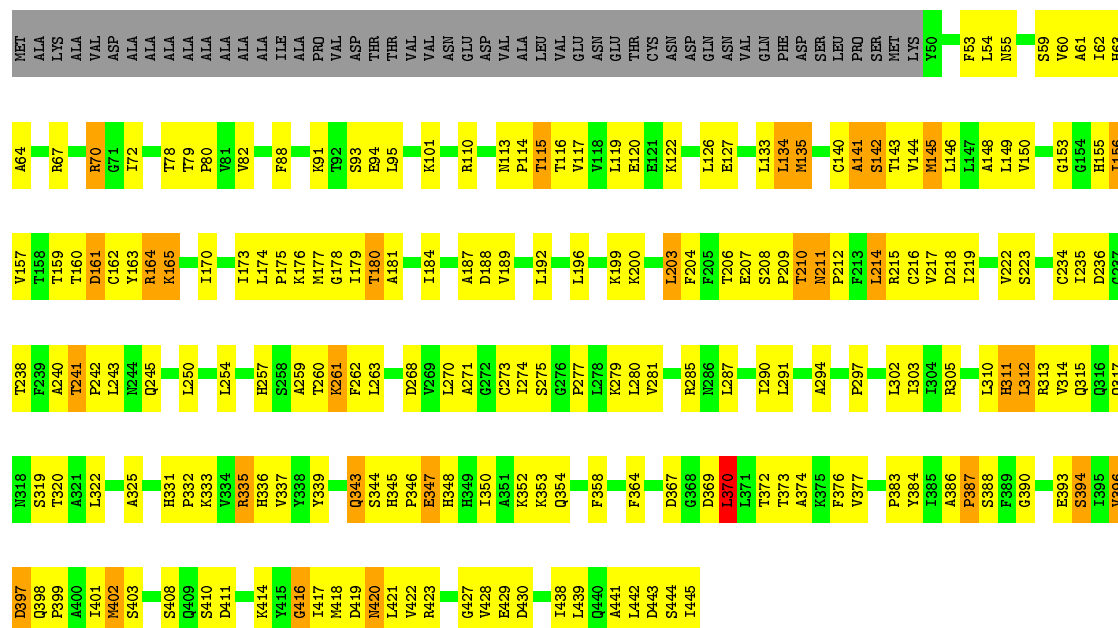






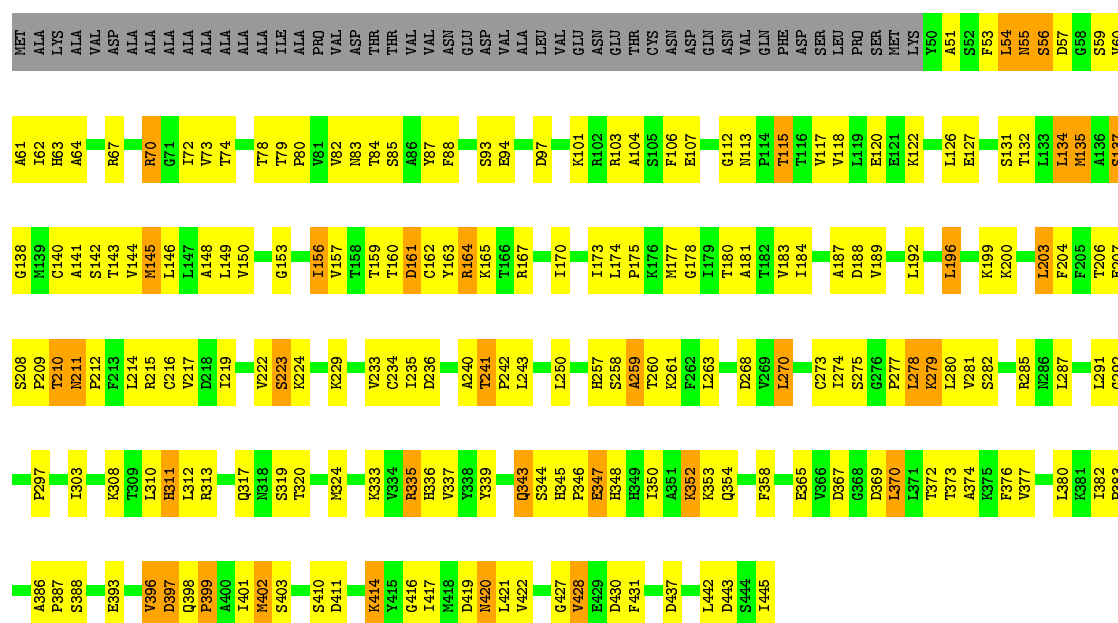
• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain E: 43% 39% 7% 11%



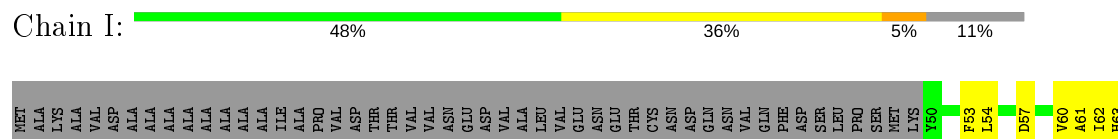
• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

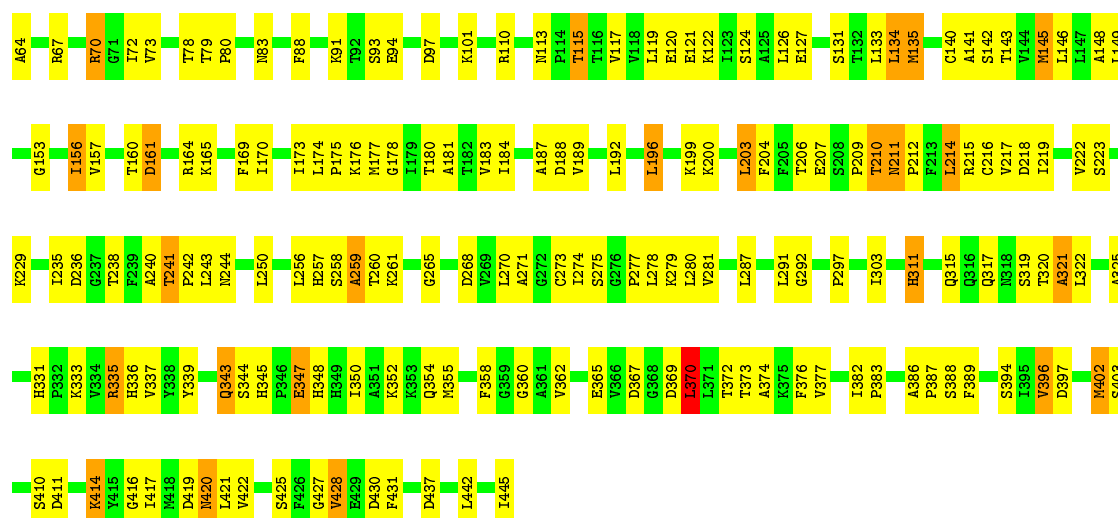
Chain F: 44% 38% 8% 11%



• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

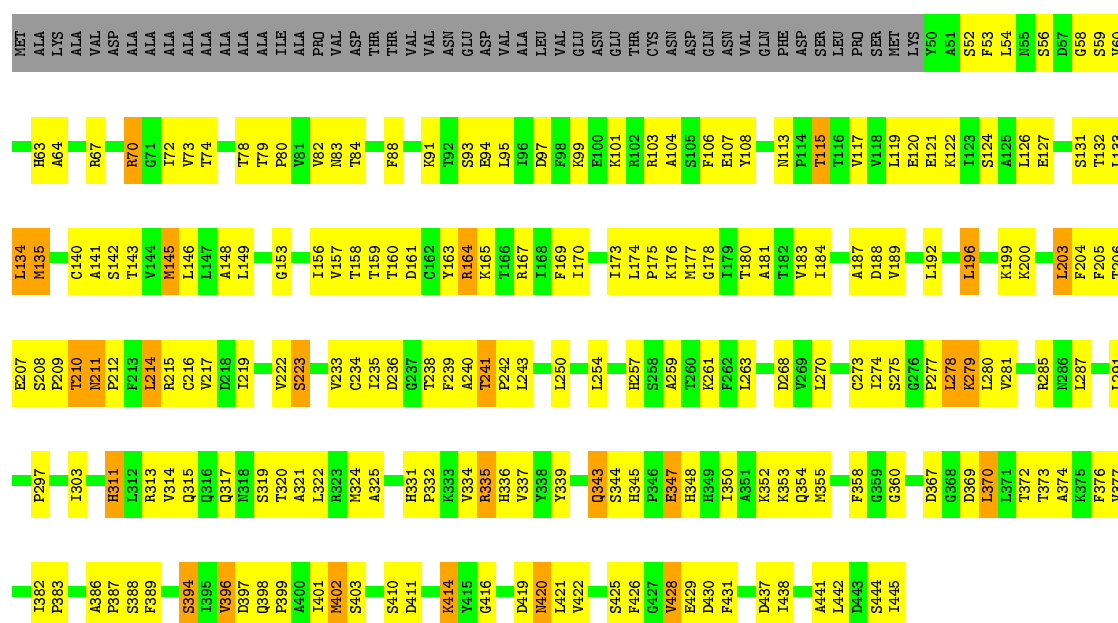






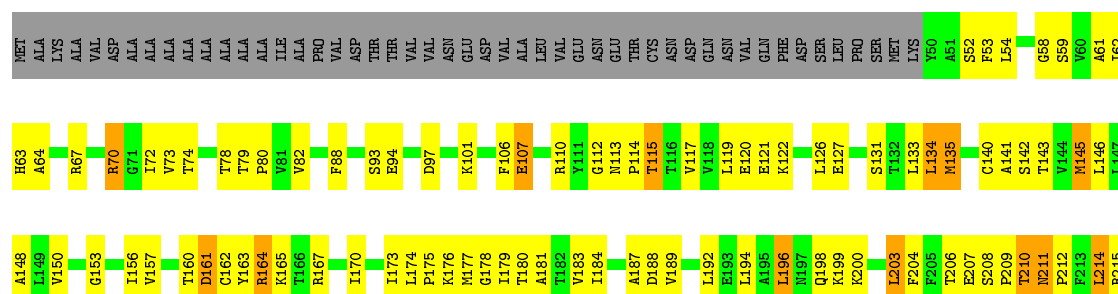
### • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

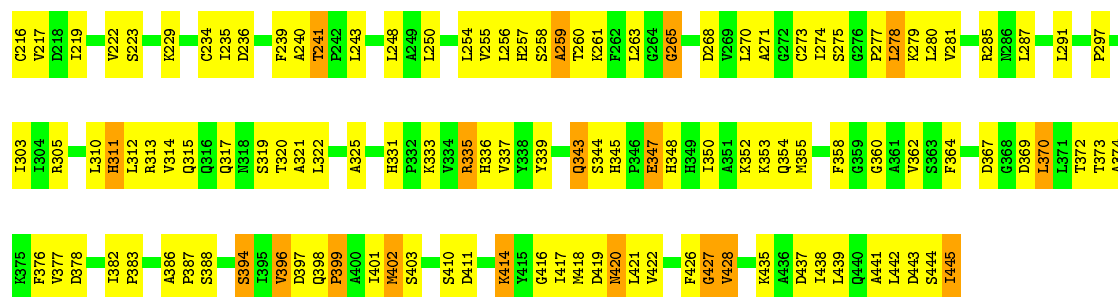
Chain J: 43% 40% 6% 11%



### • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

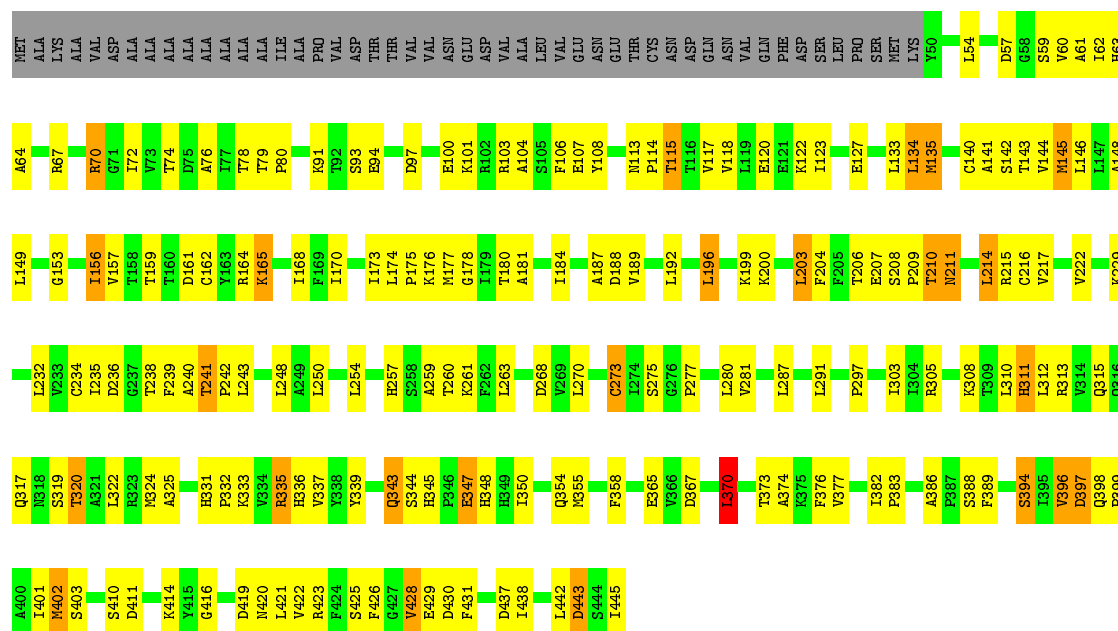
Chain K: 42% 40% 7% 11%





# Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain L:  47% 36% 6% 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, $\alpha$ , $\beta$ , $\gamma$	312.20Å 166.00Å 161.80Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.239 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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: HEN

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	0.33	0/3082	0.53	0/4179
1	B	0.31	0/3082	0.52	0/4179
1	C	0.32	0/3082	0.52	0/4179
1	D	0.32	0/3082	0.52	0/4179
1	E	0.33	0/3082	0.53	0/4179
1	F	0.32	0/3082	0.53	0/4179
1	G	0.33	0/3082	0.52	0/4179
1	H	0.33	0/3082	0.53	0/4179
1	I	0.32	0/3082	0.52	0/4179
1	J	0.31	0/3082	0.52	0/4179
1	K	0.31	0/3082	0.52	0/4179
1	L	0.31	0/3082	0.52	0/4179
All	All	0.32	0/36984	0.52	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	3054	164	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3023	0	3054	167	0
1	C	3023	0	3054	159	0
1	D	3023	0	3054	159	0
1	E	3023	0	3054	155	0
1	F	3023	0	3054	160	0
1	G	3023	0	3054	156	0
1	H	3023	0	3054	164	0
1	I	3023	0	3054	141	0
1	J	3023	0	3054	155	0
1	K	3023	0	3054	153	0
1	L	3023	0	3054	131	0
2	A	27	0	12	3	0
2	B	27	0	12	1	0
2	C	27	0	12	0	0
2	D	27	0	12	2	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	1	0
2	H	27	0	12	2	0
2	I	27	0	12	2	0
2	J	27	0	12	1	0
2	K	27	0	12	1	0
2	L	27	0	12	1	0
All	All	36600	0	36792	1765	0

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

All (1765) 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:F:64:ALA:HB3	1:F:122:LYS:HG3	1.44	0.98
1:L:54:LEU:HD22	1:L:59:SER:HB3	1.45	0.97
1:A:145:MET:HE1	1:A:146:LEU:HD23	1.47	0.96
1:A:383:PRO:HB2	1:A:396:VAL:HG22	1.49	0.93
1:H:241:THR:HG22	1:H:243:LEU:H	1.31	0.92
1:C:54:LEU:HD22	1:C:59:SER:HB3	1.49	0.92
1:B:78:THR:HG21	1:C:268:ASP:HB3	1.47	0.92
1:L:383:PRO:HB2	1:L:396:VAL:HG22	1.51	0.90
1:H:383:PRO:HB2	1:H:396:VAL:HG22	1.53	0.90
1:D:383:PRO:HB2	1:D:396:VAL:HG22	1.54	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:PHE:HB2	1:D:445:ILE:HD11	1.54	0.90
1:I:241:THR:HG22	1:I:243:LEU:H	1.36	0.89
1:D:64:ALA:HB3	1:D:122:LYS:HG3	1.53	0.89
1:D:241:THR:HG22	1:D:243:LEU:H	1.38	0.89
1:J:241:THR:HG22	1:J:243:LEU:H	1.35	0.88
1:J:383:PRO:HB2	1:J:396:VAL:HG22	1.54	0.88
1:K:438:ILE:O	1:K:441:ALA:HB3	1.73	0.87
1:G:383:PRO:HB2	1:G:396:VAL:HG22	1.56	0.87
1:F:383:PRO:HB2	1:F:396:VAL:HG22	1.56	0.86
1:K:241:THR:HG22	1:K:243:LEU:H	1.40	0.86
1:E:383:PRO:HB2	1:E:396:VAL:HG22	1.55	0.86
1:C:241:THR:HG22	1:C:243:LEU:H	1.39	0.86
1:J:207:GLU:HB3	1:J:236:ASP:HB3	1.58	0.86
1:I:383:PRO:HB2	1:I:396:VAL:HG22	1.57	0.85
1:G:210:THR:HG22	1:G:215:ARG:H	1.40	0.85
1:C:383:PRO:HB2	1:C:396:VAL:HG22	1.58	0.84
1:D:207:GLU:HB3	1:D:236:ASP:HB3	1.57	0.84
1:L:207:GLU:HB3	1:L:236:ASP:HB3	1.59	0.84
1:B:383:PRO:HB2	1:B:396:VAL:HG22	1.59	0.84
1:E:64:ALA:HB3	1:E:122:LYS:HG3	1.59	0.83
1:J:210:THR:HG22	1:J:215:ARG:H	1.41	0.83
1:A:64:ALA:HB3	1:A:122:LYS:HG3	1.59	0.82
1:I:207:GLU:HB3	1:I:236:ASP:HB3	1.59	0.82
1:B:207:GLU:HB3	1:B:236:ASP:HB3	1.61	0.82
1:L:115:THR:HG21	1:L:297:PRO:HB3	1.61	0.82
1:G:64:ALA:HB3	1:G:122:LYS:HG3	1.58	0.82
1:B:268:ASP:HB3	1:C:78:THR:HG21	1.61	0.82
1:J:170:ILE:HA	1:J:174:LEU:HD12	1.59	0.82
1:J:240:ALA:O	1:J:241:THR:HB	1.78	0.82
1:C:210:THR:HG22	1:C:215:ARG:H	1.44	0.82
1:F:442:LEU:HA	1:F:445:ILE:HD12	1.59	0.82
1:K:145:MET:HE1	1:K:146:LEU:HD23	1.60	0.82
1:I:64:ALA:HB3	1:I:122:LYS:HG3	1.61	0.81
1:K:210:THR:HG22	1:K:215:ARG:H	1.44	0.81
1:A:207:GLU:HB3	1:A:236:ASP:HB3	1.63	0.81
1:I:240:ALA:O	1:I:241:THR:HB	1.79	0.81
1:K:240:ALA:O	1:K:241:THR:HB	1.80	0.81
1:F:120:GLU:HG3	1:F:134:LEU:HD12	1.63	0.81
1:H:210:THR:HG22	1:H:215:ARG:H	1.43	0.81
1:K:207:GLU:HB3	1:K:236:ASP:HB3	1.63	0.81
1:B:240:ALA:O	1:B:241:THR:HB	1.80	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:GLU:HB3	1:H:236:ASP:HB3	1.63	0.80
1:E:145:MET:HE1	1:E:146:LEU:HD23	1.64	0.80
1:L:240:ALA:O	1:L:241:THR:HB	1.81	0.80
1:B:115:THR:HG21	1:B:297:PRO:HB3	1.63	0.80
1:C:64:ALA:HB3	1:C:122:LYS:HG3	1.62	0.79
1:F:241:THR:HG22	1:F:243:LEU:H	1.47	0.79
1:I:210:THR:HG22	1:I:215:ARG:H	1.47	0.79
1:B:210:THR:HG22	1:B:215:ARG:H	1.45	0.79
1:D:240:ALA:O	1:D:241:THR:HB	1.82	0.79
1:F:216:CYS:H	1:F:347:GLU:HG3	1.48	0.79
1:E:54:LEU:HD22	1:E:59:SER:HB3	1.65	0.79
1:E:210:THR:HG22	1:E:215:ARG:H	1.48	0.79
1:L:241:THR:HG22	1:L:243:LEU:H	1.49	0.78
1:H:240:ALA:O	1:H:241:THR:HB	1.83	0.78
1:C:207:GLU:HB3	1:C:236:ASP:HB3	1.66	0.78
1:C:170:ILE:HA	1:C:174:LEU:HD12	1.64	0.78
1:C:115:THR:HG21	1:C:297:PRO:HB3	1.66	0.77
1:D:135:MET:HE2	1:D:141:ALA:HA	1.65	0.77
1:I:261:LYS:NZ	1:I:388:SER:HA	1.99	0.77
1:C:240:ALA:O	1:C:241:THR:HB	1.82	0.77
1:L:210:THR:HG22	1:L:215:ARG:H	1.48	0.77
1:C:120:GLU:HG3	1:C:134:LEU:HD12	1.66	0.77
1:B:241:THR:HG22	1:B:243:LEU:H	1.48	0.77
1:E:207:GLU:HB3	1:E:236:ASP:HB3	1.67	0.77
1:E:216:CYS:H	1:E:347:GLU:HG3	1.47	0.77
1:F:261:LYS:HZ3	1:F:388:SER:HA	1.49	0.76
1:G:241:THR:HG22	1:G:243:LEU:H	1.49	0.76
1:A:240:ALA:O	1:A:241:THR:HB	1.84	0.76
1:B:53:PHE:HZ	1:B:68:LEU:HD21	1.50	0.76
1:G:207:GLU:HB3	1:G:236:ASP:HB3	1.67	0.75
1:G:135:MET:HE2	1:G:141:ALA:HA	1.68	0.75
1:K:383:PRO:HB2	1:K:396:VAL:HG22	1.69	0.75
1:B:216:CYS:H	1:B:347:GLU:HG3	1.51	0.75
1:G:120:GLU:HG3	1:G:134:LEU:HD12	1.69	0.75
1:D:210:THR:HG22	1:D:215:ARG:H	1.51	0.75
1:E:240:ALA:O	1:E:241:THR:HB	1.85	0.75
1:C:370:LEU:HD23	1:C:419:ASP:HB3	1.69	0.75
1:G:240:ALA:O	1:G:241:THR:HB	1.87	0.75
1:L:120:GLU:HG3	1:L:134:LEU:HD12	1.67	0.75
1:I:120:GLU:HG3	1:I:134:LEU:HD12	1.69	0.74
1:J:156:ILE:HG13	1:J:203:LEU:HD23	1.70	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:ASN:ND2	1:K:297:PRO:HG3	2.02	0.73
1:A:238:THR:HB	2:A:500:HEN:H2A2	1.70	0.73
1:A:210:THR:HG22	1:A:215:ARG:H	1.52	0.73
1:F:261:LYS:NZ	1:F:388:SER:HA	2.03	0.73
1:I:211:ASN:HD22	1:I:211:ASN:C	1.92	0.73
1:J:120:GLU:HG3	1:J:134:LEU:HD12	1.71	0.73
1:F:250:LEU:HD11	1:F:354:GLN:HB2	1.71	0.73
1:A:170:ILE:HA	1:A:174:LEU:HD12	1.70	0.72
1:E:241:THR:HG22	1:E:243:LEU:H	1.52	0.72
1:A:241:THR:HG22	1:A:243:LEU:H	1.54	0.72
1:L:64:ALA:HB3	1:L:122:LYS:HG3	1.71	0.72
1:G:170:ILE:HA	1:G:174:LEU:HD12	1.71	0.72
1:K:115:THR:HG21	1:K:297:PRO:HB3	1.70	0.72
1:D:120:GLU:HG3	1:D:134:LEU:HD12	1.70	0.72
1:A:211:ASN:HD22	1:A:211:ASN:C	1.93	0.72
1:A:261:LYS:NZ	1:A:388:SER:HA	2.05	0.72
1:E:261:LYS:NZ	1:E:388:SER:HA	2.05	0.72
1:G:145:MET:HE1	1:G:146:LEU:HD23	1.71	0.72
1:A:370:LEU:HD23	1:A:419:ASP:HB3	1.72	0.71
1:D:250:LEU:HD11	1:D:354:GLN:HB2	1.72	0.71
1:F:210:THR:HG22	1:F:215:ARG:H	1.55	0.71
1:G:370:LEU:HD23	1:G:419:ASP:HB3	1.70	0.71
1:K:170:ILE:HA	1:K:174:LEU:HD12	1.73	0.71
1:J:54:LEU:HD22	1:J:59:SER:HB3	1.71	0.71
1:K:313:ARG:O	1:K:317:GLN:HG3	1.90	0.71
1:B:335:ARG:HH21	1:B:367:ASP:HA	1.55	0.71
1:D:335:ARG:HH21	1:D:367:ASP:HA	1.55	0.70
1:J:216:CYS:H	1:J:347:GLU:HG3	1.56	0.70
1:G:216:CYS:H	1:G:347:GLU:HG3	1.54	0.70
1:J:64:ALA:HB3	1:J:122:LYS:HG3	1.73	0.70
1:F:240:ALA:O	1:F:241:THR:HB	1.91	0.70
1:L:347:GLU:HB3	1:L:350:ILE:HD12	1.72	0.70
1:L:216:CYS:H	1:L:347:GLU:HG3	1.57	0.70
1:H:64:ALA:HB3	1:H:122:LYS:HG3	1.73	0.70
1:E:250:LEU:HD11	1:E:354:GLN:HB2	1.72	0.70
1:E:261:LYS:HZ3	1:E:388:SER:HA	1.57	0.69
1:K:411:ASP:O	1:K:414:LYS:HB2	1.92	0.69
1:H:156:ILE:HG12	1:H:157:VAL:N	2.07	0.69
1:A:216:CYS:H	1:A:347:GLU:HG3	1.57	0.69
1:C:127:GLU:OE2	1:C:242:PRO:HB3	1.93	0.69
1:A:438:ILE:O	1:A:442:LEU:HD12	1.92	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:HD3	1:B:79:THR:OG1	1.90	0.69
1:A:259:ALA:HB3	1:A:271:ALA:HB3	1.73	0.69
1:E:78:THR:HG21	1:H:268:ASP:HB3	1.74	0.69
1:F:268:ASP:HB3	1:G:78:THR:HG21	1.73	0.69
1:K:64:ALA:HB3	1:K:122:LYS:HG3	1.75	0.69
1:K:343:GLN:HA	1:K:348:HIS:CD2	2.28	0.68
1:L:335:ARG:HH21	1:L:367:ASP:HA	1.59	0.68
1:B:64:ALA:HB3	1:B:122:LYS:HG3	1.74	0.68
1:D:343:GLN:HA	1:D:348:HIS:CD2	2.28	0.68
1:H:120:GLU:HG3	1:H:134:LEU:HD12	1.75	0.68
1:J:343:GLN:HA	1:J:348:HIS:CD2	2.28	0.68
1:K:277:PRO:HG2	1:K:280:LEU:HB2	1.74	0.68
1:E:140:CYS:O	1:E:144:VAL:HG23	1.93	0.67
1:H:170:ILE:HA	1:H:174:LEU:HD12	1.76	0.67
1:H:145:MET:HE3	1:H:149:LEU:HD12	1.74	0.67
1:K:211:ASN:C	1:K:211:ASN:HD22	1.97	0.67
1:G:211:ASN:HD22	1:G:211:ASN:C	1.97	0.67
1:L:145:MET:HE1	1:L:146:LEU:HD23	1.75	0.67
1:G:115:THR:HG21	1:G:297:PRO:HB3	1.75	0.67
1:K:370:LEU:HD23	1:K:419:ASP:HB3	1.76	0.67
1:C:211:ASN:HD22	1:C:211:ASN:C	1.98	0.67
1:E:268:ASP:HB3	1:H:78:THR:HG21	1.76	0.67
1:L:250:LEU:HD11	1:L:354:GLN:HB2	1.76	0.67
1:E:170:ILE:HA	1:E:174:LEU:HD12	1.77	0.67
1:E:291:LEU:HD22	1:G:143:THR:HG21	1.76	0.67
1:I:145:MET:HE1	1:I:146:LEU:HD23	1.77	0.67
1:J:78:THR:HG21	1:K:268:ASP:HB3	1.76	0.67
1:G:54:LEU:CD2	1:G:59:SER:HB3	2.25	0.66
1:B:133:LEU:HD23	1:B:135:MET:HE3	1.76	0.66
1:A:156:ILE:HG12	1:A:157:VAL:N	2.08	0.66
1:B:331:HIS:CD2	1:B:442:LEU:HD13	2.30	0.66
1:C:156:ILE:HG13	1:C:203:LEU:HD23	1.77	0.66
1:E:345:HIS:CE1	1:E:347:GLU:HG2	2.30	0.66
1:J:115:THR:HG21	1:J:297:PRO:HB3	1.78	0.66
1:J:347:GLU:HB3	1:J:350:ILE:HD12	1.78	0.66
1:G:54:LEU:HD22	1:G:59:SER:HB3	1.78	0.66
1:H:148:ALA:HB2	1:H:287:LEU:HD23	1.77	0.66
1:H:115:THR:HG21	1:H:297:PRO:HB3	1.77	0.66
1:I:115:THR:HG21	1:I:297:PRO:HB3	1.78	0.66
1:J:268:ASP:HB3	1:K:78:THR:HG21	1.78	0.66
1:K:216:CYS:H	1:K:347:GLU:HG3	1.61	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:156:ILE:HG12	1:L:157:VAL:N	2.11	0.65
1:E:115:THR:HG21	1:E:297:PRO:HB3	1.76	0.65
1:B:62:ILE:HD11	1:C:428:VAL:HG12	1.78	0.65
1:F:78:THR:HG21	1:G:268:ASP:HB3	1.78	0.65
1:L:113:ASN:ND2	1:L:297:PRO:HG3	2.12	0.65
1:I:261:LYS:HZ3	1:I:388:SER:HA	1.60	0.65
1:K:135:MET:HE2	1:K:141:ALA:HA	1.79	0.65
1:E:156:ILE:HG12	1:E:157:VAL:N	2.12	0.65
1:A:250:LEU:HD11	1:A:354:GLN:HB2	1.78	0.65
1:D:370:LEU:HD23	1:D:419:ASP:HB3	1.78	0.65
1:B:369:ASP:H	1:B:372:THR:HB	1.61	0.65
1:D:115:THR:HG21	1:D:297:PRO:HB3	1.78	0.65
1:H:335:ARG:HH21	1:H:367:ASP:HA	1.61	0.65
1:D:261:LYS:NZ	1:D:388:SER:HA	2.12	0.64
1:J:145:MET:HE1	1:J:146:LEU:HD23	1.79	0.64
1:C:148:ALA:HB2	1:C:287:LEU:HD23	1.79	0.64
1:A:78:THR:HG21	1:D:268:ASP:HB3	1.78	0.64
1:F:343:GLN:HA	1:F:348:HIS:CD2	2.33	0.64
1:I:156:ILE:HG12	1:I:157:VAL:N	2.11	0.64
1:I:421:LEU:HD12	1:I:422:VAL:N	2.13	0.64
1:G:148:ALA:HB2	1:G:287:LEU:HD23	1.79	0.64
1:H:343:GLN:HA	1:H:348:HIS:CD2	2.33	0.64
1:H:216:CYS:H	1:H:347:GLU:HG3	1.63	0.64
1:F:277:PRO:HG2	1:F:280:LEU:HB2	1.78	0.64
1:H:261:LYS:NZ	1:H:388:SER:HA	2.11	0.64
1:E:331:HIS:CE1	1:E:333:LYS:HB2	2.33	0.64
1:K:250:LEU:HD11	1:K:354:GLN:HB2	1.79	0.64
1:D:63:HIS:HB3	1:D:67:ARG:HB2	1.79	0.64
1:F:207:GLU:HB3	1:F:236:ASP:HB3	1.78	0.64
1:G:51:ALA:HB3	1:G:54:LEU:HB2	1.79	0.64
1:D:170:ILE:HA	1:D:174:LEU:HD12	1.78	0.63
1:A:113:ASN:ND2	1:A:297:PRO:HG3	2.14	0.63
1:H:54:LEU:HD23	1:H:59:SER:HB3	1.81	0.63
1:F:335:ARG:HH21	1:F:367:ASP:HA	1.64	0.63
1:G:345:HIS:CE1	1:G:347:GLU:HG2	2.34	0.63
1:E:370:LEU:HD23	1:E:419:ASP:HB3	1.78	0.63
1:F:170:ILE:HA	1:F:174:LEU:HD12	1.80	0.63
1:G:343:GLN:HA	1:G:348:HIS:CD2	2.34	0.63
1:I:216:CYS:H	1:I:347:GLU:HG3	1.62	0.63
1:C:153:GLY:HA2	1:C:178:GLY:O	1.98	0.63
1:D:148:ALA:HB2	1:D:287:LEU:HD23	1.81	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:HD23	1:B:419:ASP:HB3	1.80	0.63
1:G:156:ILE:HG12	1:G:157:VAL:N	2.14	0.63
1:L:343:GLN:HA	1:L:348:HIS:CD2	2.34	0.63
1:B:156:ILE:HG12	1:B:157:VAL:N	2.12	0.62
1:B:438:ILE:O	1:B:441:ALA:HB3	1.99	0.62
1:C:210:THR:HG23	1:C:211:ASN:N	2.13	0.62
1:A:115:THR:HG21	1:A:297:PRO:HB3	1.82	0.62
1:G:113:ASN:ND2	1:G:297:PRO:HG3	2.14	0.62
1:L:411:ASP:O	1:L:414:LYS:HB2	1.99	0.62
1:D:156:ILE:HG12	1:D:157:VAL:N	2.13	0.62
1:E:421:LEU:HD12	1:E:422:VAL:N	2.14	0.62
1:K:120:GLU:HG3	1:K:134:LEU:HD12	1.80	0.62
1:K:153:GLY:HA2	1:K:178:GLY:O	1.99	0.62
1:C:277:PRO:HG2	1:C:280:LEU:HB2	1.82	0.62
1:E:174:LEU:N	1:E:175:PRO:HD2	2.15	0.62
1:H:51:ALA:HB3	1:H:54:LEU:HD12	1.81	0.62
1:I:153:GLY:HA2	1:I:178:GLY:O	1.98	0.62
1:K:421:LEU:HD12	1:K:422:VAL:N	2.15	0.62
1:A:210:THR:HG23	1:A:211:ASN:N	2.15	0.62
1:H:397:ASP:HB2	1:H:402:MET:HG2	1.82	0.62
1:J:63:HIS:HB3	1:J:67:ARG:HB2	1.80	0.62
1:K:210:THR:HG23	1:K:211:ASN:N	2.15	0.61
1:E:120:GLU:HG3	1:E:134:LEU:HD12	1.82	0.61
1:A:261:LYS:HZ2	1:A:388:SER:HA	1.64	0.61
1:E:345:HIS:HE1	1:E:347:GLU:HG2	1.63	0.61
1:E:397:ASP:HB2	1:E:402:MET:HG2	1.83	0.61
1:A:277:PRO:HG2	1:A:280:LEU:HB2	1.80	0.61
1:A:335:ARG:HH21	1:A:367:ASP:HA	1.65	0.61
1:C:373:THR:O	1:C:376:PHE:HB3	2.01	0.61
1:K:369:ASP:H	1:K:372:THR:HB	1.64	0.61
1:D:53:PHE:CD1	1:D:54:LEU:HG	2.35	0.61
1:A:339:TYR:CZ	1:A:358:PHE:HB2	2.36	0.61
1:B:261:LYS:NZ	1:B:388:SER:HA	2.16	0.61
1:D:238:THR:HB	2:D:503:HEN:H2A2	1.83	0.61
1:D:421:LEU:HD12	1:D:422:VAL:N	2.16	0.61
1:B:120:GLU:HG3	1:B:134:LEU:HD12	1.82	0.61
1:E:335:ARG:HH21	1:E:367:ASP:HA	1.66	0.61
1:F:113:ASN:ND2	1:F:297:PRO:HG3	2.16	0.61
1:H:210:THR:HG23	1:H:211:ASN:N	2.15	0.61
1:B:127:GLU:OE2	1:B:242:PRO:HB3	2.01	0.61
1:H:347:GLU:HB3	1:H:350:ILE:HD12	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:ASN:HD22	1:I:212:PRO:N	1.99	0.61
1:I:343:GLN:HA	1:I:348:HIS:CD2	2.34	0.61
1:J:339:TYR:CZ	1:J:358:PHE:HB2	2.35	0.61
1:L:370:LEU:HD23	1:L:419:ASP:HB3	1.82	0.61
1:J:261:LYS:NZ	1:J:388:SER:HA	2.16	0.60
1:C:335:ARG:HH21	1:C:367:ASP:HA	1.66	0.60
1:E:333:LYS:HE2	1:E:445:ILE:HG22	1.82	0.60
1:F:211:ASN:C	1:F:211:ASN:HD22	2.04	0.60
1:I:268:ASP:HB3	1:L:78:THR:HG21	1.84	0.60
1:J:174:LEU:N	1:J:175:PRO:HD2	2.16	0.60
1:G:210:THR:HG23	1:G:211:ASN:N	2.16	0.60
1:J:250:LEU:HD11	1:J:354:GLN:HB2	1.83	0.60
1:C:216:CYS:H	1:C:347:GLU:HG3	1.66	0.60
1:H:250:LEU:HD11	1:H:354:GLN:HB2	1.83	0.60
1:G:173:ILE:C	1:G:175:PRO:HD2	2.22	0.60
1:B:143:THR:HG21	1:D:291:LEU:HD22	1.83	0.60
1:E:343:GLN:HA	1:E:348:HIS:CD2	2.36	0.60
1:E:53:PHE:CD1	1:E:54:LEU:HG	2.36	0.60
1:F:386:ALA:HB2	1:H:88:PHE:HA	1.83	0.60
1:I:148:ALA:HB2	1:I:287:LEU:HD23	1.84	0.60
1:K:347:GLU:HB3	1:K:350:ILE:HD12	1.82	0.60
1:F:204:PHE:CE2	1:F:222:VAL:HG11	2.36	0.60
1:B:113:ASN:ND2	1:B:297:PRO:HG3	2.15	0.60
1:B:331:HIS:CE1	1:B:333:LYS:HB2	2.37	0.60
1:I:210:THR:HG23	1:I:211:ASN:N	2.16	0.60
1:A:120:GLU:HG3	1:A:134:LEU:HD12	1.84	0.60
1:C:261:LYS:NZ	1:C:388:SER:HA	2.16	0.60
1:F:347:GLU:HB3	1:F:350:ILE:HD12	1.83	0.60
1:K:174:LEU:N	1:K:175:PRO:HD2	2.16	0.60
1:G:331:HIS:CE1	1:G:333:LYS:HB2	2.37	0.59
1:J:113:ASN:ND2	1:J:297:PRO:HG3	2.17	0.59
1:J:339:TYR:OH	1:J:358:PHE:HB2	2.02	0.59
1:C:80:PRO:HB3	1:D:82:VAL:HG22	1.84	0.59
1:H:369:ASP:H	1:H:372:THR:HB	1.67	0.59
1:C:442:LEU:HA	1:C:445:ILE:HD13	1.83	0.59
1:E:211:ASN:HD22	1:E:211:ASN:C	2.04	0.59
1:H:204:PHE:CE2	1:H:222:VAL:HG11	2.36	0.59
1:D:211:ASN:C	1:D:211:ASN:HD22	2.05	0.59
1:D:216:CYS:H	1:D:347:GLU:HG3	1.67	0.59
1:G:133:LEU:HD23	1:G:135:MET:HE1	1.85	0.59
1:K:70:ARG:HD3	1:K:79:THR:OG1	2.01	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LEU:N	1:D:175:PRO:HD2	2.18	0.59
1:G:156:ILE:HG13	1:G:203:LEU:HD23	1.83	0.59
1:L:421:LEU:HD12	1:L:422:VAL:N	2.17	0.59
1:H:127:GLU:OE2	1:H:242:PRO:HB3	2.03	0.59
1:J:421:LEU:HD12	1:J:422:VAL:N	2.18	0.59
1:C:156:ILE:HG12	1:C:157:VAL:N	2.16	0.59
1:D:156:ILE:HG13	1:D:203:LEU:HD23	1.84	0.59
1:H:370:LEU:HD23	1:H:419:ASP:HB3	1.83	0.59
1:A:343:GLN:HA	1:A:348:HIS:CD2	2.38	0.59
1:C:331:HIS:CE1	1:C:333:LYS:HB2	2.37	0.59
1:H:211:ASN:C	1:H:211:ASN:HD22	2.06	0.59
1:H:70:ARG:HD3	1:H:79:THR:OG1	2.03	0.59
1:E:113:ASN:ND2	1:E:297:PRO:HG3	2.17	0.59
1:H:210:THR:HG22	1:H:215:ARG:N	2.16	0.59
1:L:153:GLY:HA2	1:L:178:GLY:O	2.02	0.59
1:A:347:GLU:HB3	1:A:350:ILE:HD12	1.85	0.58
1:D:441:ALA:C	1:D:443:ASP:H	2.05	0.58
1:G:335:ARG:HH21	1:G:367:ASP:HA	1.68	0.58
1:G:204:PHE:N	1:G:232:LEU:O	2.32	0.58
1:I:277:PRO:HG2	1:I:280:LEU:HB2	1.84	0.58
1:A:373:THR:O	1:A:376:PHE:HB3	2.03	0.58
1:C:343:GLN:HA	1:C:348:HIS:CD2	2.37	0.58
1:D:204:PHE:CE2	1:D:222:VAL:HG11	2.39	0.58
1:D:261:LYS:HZ3	1:D:388:SER:HA	1.67	0.58
1:I:373:THR:O	1:I:376:PHE:HB3	2.02	0.58
1:J:153:GLY:HA2	1:J:178:GLY:O	2.03	0.58
1:C:277:PRO:O	1:C:281:VAL:HG12	2.03	0.58
1:J:211:ASN:C	1:J:211:ASN:HD22	2.06	0.58
1:K:335:ARG:HH21	1:K:367:ASP:HA	1.69	0.58
1:L:261:LYS:NZ	1:L:388:SER:HA	2.18	0.58
1:B:240:ALA:O	1:B:241:THR:CB	2.50	0.58
1:C:250:LEU:HD11	1:C:354:GLN:HB2	1.85	0.58
1:F:210:THR:HG23	1:F:211:ASN:N	2.17	0.58
1:L:373:THR:O	1:L:376:PHE:HB3	2.04	0.58
1:A:204:PHE:CE2	1:A:222:VAL:HG11	2.39	0.58
1:C:113:ASN:ND2	1:C:297:PRO:HG3	2.19	0.58
1:E:240:ALA:O	1:E:241:THR:CB	2.52	0.58
1:I:376:PHE:HB2	1:I:445:ILE:CD1	2.33	0.58
1:I:376:PHE:HB2	1:I:445:ILE:HD11	1.86	0.58
1:L:174:LEU:N	1:L:175:PRO:HD2	2.18	0.58
1:D:241:THR:HG23	1:D:242:PRO:HD2	1.84	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:ASP:H	1:E:372:THR:HB	1.67	0.58
1:I:156:ILE:HG13	1:I:203:LEU:HD23	1.85	0.58
1:K:54:LEU:CD2	1:K:59:SER:HB3	2.34	0.58
1:A:331:HIS:CG	1:A:332:PRO:HD2	2.38	0.58
1:F:215:ARG:HD2	1:F:347:GLU:OE2	2.03	0.58
1:J:173:ILE:C	1:J:175:PRO:HD2	2.24	0.58
1:B:343:GLN:HA	1:B:348:HIS:CD2	2.38	0.58
1:B:291:LEU:HD22	1:D:143:THR:HG21	1.84	0.58
1:D:369:ASP:H	1:D:372:THR:HB	1.69	0.58
1:G:261:LYS:NZ	1:G:388:SER:HA	2.19	0.58
1:F:156:ILE:HG13	1:F:203:LEU:HD23	1.84	0.58
1:G:170:ILE:HG23	1:G:174:LEU:HD12	1.85	0.58
1:I:174:LEU:N	1:I:175:PRO:HD2	2.18	0.58
1:I:113:ASN:ND2	1:I:297:PRO:HG3	2.17	0.58
1:A:397:ASP:HB2	1:A:402:MET:HG2	1.86	0.57
1:G:63:HIS:HB3	1:G:67:ARG:HB2	1.85	0.57
1:G:70:ARG:HD3	1:G:79:THR:OG1	2.04	0.57
1:K:119:LEU:HG	1:K:134:LEU:HD11	1.85	0.57
1:L:140:CYS:O	1:L:144:VAL:HG23	2.03	0.57
1:E:277:PRO:HG2	1:E:280:LEU:HB2	1.86	0.57
1:F:345:HIS:CE1	1:F:347:GLU:HG2	2.38	0.57
1:G:313:ARG:O	1:G:317:GLN:HG3	2.04	0.57
1:E:393:GLU:OE2	1:H:308:LYS:HD2	2.05	0.57
1:D:336:HIS:ND1	1:D:337:VAL:N	2.53	0.57
1:F:115:THR:HG21	1:F:297:PRO:HB3	1.85	0.57
1:L:211:ASN:C	1:L:211:ASN:HD22	2.07	0.57
1:B:210:THR:HG23	1:B:211:ASN:N	2.18	0.57
1:L:331:HIS:CE1	1:L:333:LYS:HB2	2.40	0.57
1:A:153:GLY:HA2	1:A:178:GLY:O	2.04	0.57
1:J:261:LYS:HZ3	1:J:388:SER:HA	1.69	0.57
1:B:148:ALA:HB2	1:B:287:LEU:HD23	1.87	0.57
1:B:347:GLU:HB3	1:B:350:ILE:HD12	1.86	0.57
1:H:438:ILE:O	1:H:442:LEU:HD12	2.04	0.57
1:I:335:ARG:HH21	1:I:367:ASP:HA	1.68	0.57
1:F:127:GLU:OE2	1:F:257:HIS:NE2	2.37	0.57
1:H:174:LEU:N	1:H:175:PRO:HD2	2.20	0.57
1:H:421:LEU:HD12	1:H:422:VAL:N	2.20	0.57
1:K:127:GLU:OE2	1:K:257:HIS:NE2	2.38	0.57
1:B:211:ASN:C	1:B:211:ASN:HD22	2.09	0.56
1:B:250:LEU:HD11	1:B:354:GLN:HB2	1.87	0.56
1:C:60:VAL:HG12	1:C:64:ALA:HB2	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:GLU:OE2	1:G:242:PRO:HB3	2.05	0.56
1:I:210:THR:O	1:I:214:LEU:HA	2.05	0.56
1:J:373:THR:O	1:J:376:PHE:HB3	2.05	0.56
1:B:386:ALA:HB2	1:D:88:PHE:HA	1.87	0.56
1:H:50:TYR:CE1	1:H:68:LEU:HD12	2.40	0.56
1:E:145:MET:HE2	1:E:149:LEU:HD12	1.86	0.56
1:L:313:ARG:O	1:L:317:GLN:HG3	2.05	0.56
1:C:438:ILE:O	1:C:441:ALA:HB3	2.06	0.56
1:G:174:LEU:N	1:G:175:PRO:HD2	2.21	0.56
1:J:156:ILE:HG12	1:J:157:VAL:N	2.21	0.56
1:A:135:MET:HE1	1:A:274:ILE:HD12	1.88	0.56
1:A:339:TYR:OH	1:A:358:PHE:HB2	2.06	0.56
1:G:240:ALA:O	1:G:244:ASN:HB2	2.04	0.56
1:E:386:ALA:HB2	1:G:88:PHE:HA	1.87	0.56
1:J:141:ALA:HB1	1:J:274:ILE:HD11	1.88	0.56
1:J:345:HIS:CE1	1:J:347:GLU:HG2	2.41	0.56
1:F:88:PHE:HA	1:H:386:ALA:HB2	1.88	0.56
1:I:369:ASP:H	1:I:372:THR:HB	1.70	0.56
1:B:140:CYS:O	1:B:144:VAL:HG23	2.05	0.56
1:G:161:ASP:HB3	1:G:210:THR:OG1	2.06	0.56
1:G:250:LEU:HD11	1:G:354:GLN:HB2	1.86	0.56
1:E:394:SER:OG	1:E:427:GLY:N	2.36	0.56
1:F:187:ALA:O	1:F:189:VAL:N	2.38	0.56
1:G:241:THR:HG23	1:G:242:PRO:HD2	1.87	0.56
1:A:211:ASN:ND2	1:A:211:ASN:C	2.59	0.56
1:A:369:ASP:H	1:A:372:THR:HB	1.70	0.56
1:C:63:HIS:HB3	1:C:67:ARG:HB2	1.88	0.56
1:D:347:GLU:HB3	1:D:350:ILE:HD12	1.87	0.56
1:G:143:THR:HG23	1:G:169:PHE:CE1	2.41	0.56
1:B:110:ARG:HH21	2:D:503:HEN:P	2.29	0.56
1:F:174:LEU:N	1:F:175:PRO:HD2	2.21	0.56
1:I:217:VAL:HG13	1:I:222:VAL:HG21	1.88	0.56
1:I:78:THR:HG21	1:L:268:ASP:HB3	1.87	0.56
1:F:140:CYS:O	1:F:143:THR:HB	2.05	0.55
1:F:336:HIS:ND1	1:F:337:VAL:N	2.54	0.55
1:G:310:LEU:HA	1:G:313:ARG:NH2	2.20	0.55
1:B:113:ASN:OD1	1:B:115:THR:HG22	2.06	0.55
1:J:321:ALA:HB2	1:J:360:GLY:HA2	1.89	0.55
1:J:335:ARG:HH21	1:J:367:ASP:HA	1.71	0.55
1:K:135:MET:CE	1:K:141:ALA:HA	2.36	0.55
1:L:170:ILE:HA	1:L:174:LEU:HD12	1.89	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:PRO:HB3	2:A:500:HEN:OG3	2.06	0.55
1:A:63:HIS:HB3	1:A:67:ARG:HB2	1.88	0.55
1:D:339:TYR:CZ	1:D:358:PHE:HB2	2.42	0.55
1:K:64:ALA:O	1:K:122:LYS:HE2	2.07	0.55
1:G:209:PRO:HG3	1:G:355:MET:HE1	1.89	0.55
1:I:170:ILE:HA	1:I:174:LEU:HD12	1.87	0.55
1:K:435:LYS:HG2	1:K:439:LEU:HD12	1.89	0.55
1:A:174:LEU:N	1:A:175:PRO:HD2	2.21	0.55
1:G:336:HIS:ND1	1:G:337:VAL:N	2.54	0.55
1:H:156:ILE:HG23	1:H:181:ALA:HB2	1.87	0.55
1:L:135:MET:HE1	1:L:141:ALA:HA	1.87	0.55
1:A:310:LEU:O	1:A:314:VAL:HG23	2.07	0.55
1:A:56:SER:HB3	1:D:433:ASP:OD2	2.07	0.55
1:D:133:LEU:HD23	1:D:135:MET:HE1	1.89	0.55
1:D:317:GLN:HG2	1:D:427:GLY:O	2.07	0.55
1:F:173:ILE:C	1:F:175:PRO:HD2	2.26	0.55
1:L:319:SER:O	1:L:320:THR:C	2.45	0.55
1:F:259:ALA:HA	1:F:263:LEU:HB2	1.89	0.55
1:G:82:VAL:HG22	1:H:80:PRO:HB3	1.89	0.55
1:I:250:LEU:HD11	1:I:354:GLN:HB2	1.89	0.55
1:L:115:THR:CG2	1:L:297:PRO:HB3	2.34	0.55
1:C:161:ASP:HB3	1:C:210:THR:OG1	2.07	0.55
1:E:259:ALA:HA	1:E:263:LEU:HB2	1.88	0.55
1:F:292:GLY:O	1:H:140:CYS:HB2	2.07	0.55
1:I:240:ALA:O	1:I:241:THR:CB	2.54	0.55
1:B:394:SER:OG	1:B:427:GLY:N	2.33	0.55
1:E:173:ILE:C	1:E:175:PRO:HD2	2.27	0.55
1:E:156:ILE:HG13	1:E:203:LEU:HD23	1.89	0.55
1:A:345:HIS:CE1	1:A:347:GLU:HG2	2.42	0.55
1:D:339:TYR:OH	1:D:358:PHE:HB2	2.07	0.55
1:E:155:HIS:HA	1:E:180:THR:O	2.07	0.55
1:L:240:ALA:O	1:L:241:THR:CB	2.54	0.55
1:B:345:HIS:CE1	1:B:347:GLU:HG2	2.43	0.54
1:K:206:THR:O	1:K:235:ILE:HA	2.07	0.54
1:L:70:ARG:HD3	1:L:79:THR:OG1	2.07	0.54
1:H:223:SER:HA	1:H:233:VAL:HG21	1.90	0.54
1:J:210:THR:O	1:J:214:LEU:HA	2.07	0.54
1:K:322:LEU:O	1:K:325:ALA:HB3	2.07	0.54
1:L:345:HIS:CE1	1:L:347:GLU:HG2	2.42	0.54
1:L:63:HIS:HB3	1:L:67:ARG:HB2	1.89	0.54
1:A:145:MET:HE1	1:A:146:LEU:CD2	2.30	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:GLU:OE2	1:F:242:PRO:HB3	2.07	0.54
1:G:259:ALA:HB3	1:G:271:ALA:HB3	1.88	0.54
1:I:321:ALA:HB2	1:I:360:GLY:HA2	1.88	0.54
1:J:243:LEU:HD12	1:J:314:VAL:HG21	1.89	0.54
1:J:374:ALA:O	1:J:377:VAL:HG22	2.07	0.54
1:L:127:GLU:OE2	1:L:257:HIS:NE2	2.40	0.54
1:E:339:TYR:CZ	1:E:358:PHE:HB2	2.43	0.54
1:I:217:VAL:O	1:I:219:ILE:N	2.41	0.54
1:L:72:ILE:HG23	1:L:72:ILE:O	2.08	0.54
1:G:210:THR:HG22	1:G:215:ARG:N	2.18	0.54
1:H:173:ILE:C	1:H:175:PRO:HD2	2.28	0.54
1:H:156:ILE:HG13	1:H:203:LEU:HD23	1.89	0.54
1:H:345:HIS:CE1	1:H:347:GLU:HG2	2.42	0.54
1:A:321:ALA:HB2	1:A:360:GLY:HA2	1.90	0.54
1:A:88:PHE:HA	1:C:386:ALA:HB2	1.90	0.54
1:B:94:GLU:O	1:B:97:ASP:HB2	2.08	0.54
1:C:174:LEU:N	1:C:175:PRO:HD2	2.23	0.54
1:B:83:ASN:O	1:D:268:ASP:HB2	2.07	0.54
1:E:238:THR:HB	2:E:504:HEN:H2A2	1.90	0.54
1:F:411:ASP:O	1:F:414:LYS:HB2	2.08	0.54
1:H:72:ILE:O	1:H:72:ILE:HG23	2.08	0.54
1:A:242:PRO:HD3	1:A:257:HIS:CE1	2.42	0.54
1:H:373:THR:O	1:H:376:PHE:HB3	2.07	0.54
1:I:331:HIS:CE1	1:I:333:LYS:HB2	2.42	0.54
1:I:70:ARG:HD3	1:I:79:THR:OG1	2.07	0.54
1:K:211:ASN:HB2	1:K:239:PHE:HE2	1.73	0.54
1:K:210:THR:CG2	1:K:215:ARG:H	2.17	0.54
1:J:88:PHE:HA	1:L:386:ALA:HB2	1.89	0.54
1:E:160:THR:HG23	1:E:184:ILE:O	2.07	0.54
1:F:55:ASN:HD22	1:F:55:ASN:N	2.06	0.54
1:G:369:ASP:H	1:G:372:THR:HB	1.72	0.54
1:H:153:GLY:HA2	1:H:178:GLY:O	2.07	0.54
1:I:319:SER:O	1:I:320:THR:C	2.46	0.54
1:I:370:LEU:HD23	1:I:419:ASP:HB3	1.89	0.54
1:L:277:PRO:O	1:L:281:VAL:HG12	2.07	0.54
1:A:140:CYS:O	1:A:144:VAL:HG23	2.08	0.54
1:B:174:LEU:N	1:B:175:PRO:HD2	2.23	0.54
1:D:277:PRO:O	1:D:281:VAL:HG12	2.08	0.54
1:E:63:HIS:HB3	1:E:67:ARG:HB2	1.90	0.54
1:G:311:HIS:ND1	1:G:311:HIS:N	2.56	0.54
1:K:156:ILE:HG13	1:K:203:LEU:HD23	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:398:GLN:HB3	1:K:401:ILE:HD12	1.90	0.54
1:L:60:VAL:HG12	1:L:64:ALA:HB2	1.88	0.54
1:C:313:ARG:O	1:C:317:GLN:HG3	2.07	0.53
1:C:421:LEU:HD12	1:C:422:VAL:N	2.23	0.53
1:C:445:ILE:HD12	1:C:445:ILE:N	2.23	0.53
1:D:155:HIS:HD1	1:D:180:THR:HG23	1.73	0.53
1:F:160:THR:HG23	1:F:184:ILE:O	2.08	0.53
1:H:277:PRO:O	1:H:281:VAL:HG12	2.08	0.53
1:J:210:THR:HG23	1:J:211:ASN:N	2.23	0.53
1:J:148:ALA:HB2	1:J:287:LEU:HD23	1.90	0.53
1:I:62:ILE:HD11	1:L:428:VAL:HG12	1.90	0.53
1:K:215:ARG:HD2	1:K:347:GLU:OE2	2.08	0.53
1:B:72:ILE:HG23	1:B:72:ILE:O	2.08	0.53
1:C:411:ASP:O	1:C:414:LYS:HB2	2.08	0.53
1:D:210:THR:HG23	1:D:211:ASN:N	2.24	0.53
1:E:277:PRO:O	1:E:281:VAL:HG12	2.08	0.53
1:H:140:CYS:O	1:H:144:VAL:HG23	2.08	0.53
1:J:70:ARG:HD3	1:J:79:THR:OG1	2.08	0.53
1:K:374:ALA:O	1:K:377:VAL:HG22	2.08	0.53
1:L:148:ALA:HB2	1:L:287:LEU:HD23	1.90	0.53
1:A:87:TYR:HA	1:B:75:ASP:O	2.09	0.53
1:B:63:HIS:HB3	1:B:67:ARG:HB2	1.91	0.53
1:D:145:MET:CE	1:D:146:LEU:HD23	2.39	0.53
1:G:215:ARG:HD2	1:G:347:GLU:OE2	2.09	0.53
1:I:211:ASN:ND2	1:I:211:ASN:C	2.61	0.53
1:K:133:LEU:HD23	1:K:135:MET:HE1	1.91	0.53
1:D:215:ARG:HD2	1:D:347:GLU:OE2	2.09	0.53
1:E:398:GLN:HB3	1:E:401:ILE:HD12	1.90	0.53
1:F:135:MET:HE1	1:F:274:ILE:HD12	1.90	0.53
1:I:145:MET:HE2	1:I:149:LEU:HD12	1.91	0.53
1:D:153:GLY:HA2	1:D:178:GLY:O	2.07	0.53
1:G:277:PRO:HG2	1:G:280:LEU:HB2	1.90	0.53
1:J:277:PRO:O	1:J:281:VAL:HG12	2.08	0.53
1:E:210:THR:HG23	1:E:211:ASN:N	2.23	0.53
1:G:160:THR:HG23	1:G:184:ILE:O	2.07	0.53
1:G:345:HIS:HE1	1:G:347:GLU:HG2	1.73	0.53
1:K:117:VAL:O	1:K:121:GLU:HG3	2.09	0.53
1:K:133:LEU:CD1	1:K:285:ARG:HD3	2.39	0.53
1:K:173:ILE:O	1:K:176:LYS:HB2	2.08	0.53
1:B:248:LEU:HG	1:B:255:VAL:HG12	1.91	0.53
1:E:153:GLY:HA2	1:E:178:GLY:O	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:MET:HE2	1:H:146:LEU:HD23	1.90	0.53
1:J:287:LEU:O	1:J:287:LEU:HD12	2.08	0.53
1:I:143:THR:HG21	1:K:291:LEU:HD22	1.90	0.53
1:A:70:ARG:HD3	1:A:79:THR:OG1	2.09	0.53
1:E:438:ILE:O	1:E:441:ALA:HB3	2.08	0.53
1:F:120:GLU:HG2	1:F:132:THR:O	2.09	0.53
1:F:370:LEU:HD23	1:F:419:ASP:HB3	1.91	0.53
1:G:210:THR:CG2	1:G:215:ARG:H	2.19	0.53
1:K:211:ASN:C	1:K:211:ASN:ND2	2.62	0.53
1:A:240:ALA:O	1:A:241:THR:CB	2.56	0.53
1:A:268:ASP:HB3	1:D:78:THR:HG21	1.91	0.53
1:B:397:ASP:HB2	1:B:402:MET:HG2	1.91	0.53
1:E:211:ASN:ND2	1:E:211:ASN:C	2.62	0.53
1:F:374:ALA:O	1:F:377:VAL:HG22	2.09	0.53
1:K:161:ASP:HB3	1:K:210:THR:OG1	2.09	0.53
1:C:261:LYS:HZ3	1:C:388:SER:HA	1.74	0.52
1:C:336:HIS:ND1	1:C:337:VAL:N	2.57	0.52
1:F:63:HIS:HB3	1:F:67:ARG:HB2	1.90	0.52
1:G:373:THR:O	1:G:376:PHE:HB3	2.09	0.52
1:H:117:VAL:O	1:H:121:GLU:HG3	2.09	0.52
1:H:374:ALA:O	1:H:377:VAL:HG22	2.08	0.52
1:A:240:ALA:O	1:A:244:ASN:HB2	2.10	0.52
1:A:270:LEU:N	1:A:270:LEU:HD23	2.25	0.52
1:C:319:SER:O	1:C:320:THR:C	2.48	0.52
1:H:399:PRO:HG2	1:H:421:LEU:HG	1.90	0.52
1:J:135:MET:HE1	1:J:274:ILE:HD12	1.92	0.52
1:J:210:THR:CG2	1:J:215:ARG:H	2.18	0.52
1:B:135:MET:HE1	1:B:141:ALA:HA	1.92	0.52
1:D:192:LEU:HD21	1:D:222:VAL:HG13	1.91	0.52
1:D:345:HIS:CE1	1:D:347:GLU:HG2	2.44	0.52
1:F:369:ASP:H	1:F:372:THR:HB	1.74	0.52
1:G:72:ILE:HD13	1:G:80:PRO:HG2	1.91	0.52
1:J:397:ASP:HB2	1:J:402:MET:HG2	1.90	0.52
1:J:426:PHE:HE1	1:J:438:ILE:HD11	1.75	0.52
1:L:210:THR:HG22	1:L:215:ARG:N	2.22	0.52
1:A:187:ALA:O	1:A:189:VAL:N	2.43	0.52
1:F:310:LEU:HA	1:F:313:ARG:NH2	2.25	0.52
1:G:321:ALA:HB2	1:G:360:GLY:HA2	1.91	0.52
1:H:211:ASN:HB2	1:H:239:PHE:HE2	1.74	0.52
1:A:207:GLU:CB	1:A:236:ASP:HB3	2.38	0.52
1:E:135:MET:CE	1:E:141:ALA:HA	2.40	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:THR:O	1:F:376:PHE:HB3	2.09	0.52
1:H:441:ALA:C	1:H:443:ASP:H	2.12	0.52
1:C:210:THR:CG2	1:C:215:ARG:H	2.17	0.52
1:C:60:VAL:CG1	1:C:64:ALA:HB2	2.39	0.52
1:D:173:ILE:C	1:D:175:PRO:HD2	2.30	0.52
1:F:291:LEU:HD22	1:H:143:THR:HG21	1.91	0.52
1:G:310:LEU:O	1:G:314:VAL:HG23	2.09	0.52
1:G:442:LEU:HA	1:G:445:ILE:HD12	1.92	0.52
1:L:133:LEU:HD23	1:L:135:MET:HE3	1.92	0.52
1:L:170:ILE:HG23	1:L:174:LEU:HD12	1.90	0.52
1:A:135:MET:HE2	1:A:141:ALA:HA	1.90	0.52
1:H:277:PRO:HG2	1:H:280:LEU:HB2	1.91	0.52
1:I:217:VAL:CG1	1:I:222:VAL:HG21	2.39	0.52
1:D:210:THR:O	1:D:214:LEU:HA	2.10	0.52
1:E:143:THR:HG21	1:G:291:LEU:HD22	1.92	0.52
1:K:160:THR:HG23	1:K:184:ILE:O	2.10	0.52
1:K:336:HIS:ND1	1:K:337:VAL:N	2.58	0.52
1:A:331:HIS:ND1	1:A:332:PRO:HD2	2.25	0.52
1:A:374:ALA:O	1:A:377:VAL:HG22	2.10	0.52
1:C:374:ALA:O	1:C:377:VAL:HG22	2.10	0.52
1:K:240:ALA:O	1:K:241:THR:CB	2.52	0.52
1:C:204:PHE:CE2	1:C:222:VAL:HG11	2.45	0.52
1:G:374:ALA:O	1:G:377:VAL:HG22	2.09	0.52
1:L:210:THR:HG23	1:L:211:ASN:N	2.24	0.52
1:A:421:LEU:HD12	1:A:422:VAL:N	2.25	0.51
1:C:70:ARG:HD3	1:C:79:THR:OG1	2.10	0.51
1:F:377:VAL:HA	1:F:380:LEU:HD12	1.91	0.51
1:I:261:LYS:HZ2	1:I:388:SER:HA	1.73	0.51
1:I:63:HIS:HB3	1:I:67:ARG:HB2	1.92	0.51
1:F:156:ILE:HG12	1:F:157:VAL:N	2.24	0.51
1:H:313:ARG:O	1:H:317:GLN:HG3	2.10	0.51
1:K:311:HIS:N	1:K:311:HIS:ND1	2.57	0.51
1:L:277:PRO:HG2	1:L:280:LEU:HB2	1.91	0.51
1:A:305:ARG:O	1:A:308:LYS:HB2	2.10	0.51
1:A:77:ILE:HD12	1:B:86:ALA:O	2.10	0.51
1:B:210:THR:CG2	1:B:215:ARG:H	2.21	0.51
1:A:80:PRO:HB3	1:B:82:VAL:HG22	1.92	0.51
1:B:384:TYR:CZ	1:C:67:ARG:HD2	2.45	0.51
1:D:145:MET:HE3	1:D:149:LEU:HD12	1.91	0.51
1:F:54:LEU:HD13	1:F:59:SER:HB3	1.93	0.51
1:I:133:LEU:HD23	1:I:135:MET:HE3	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:217:VAL:CG1	1:J:222:VAL:HG21	2.41	0.51
1:J:369:ASP:H	1:J:372:THR:HB	1.75	0.51
1:K:187:ALA:O	1:K:189:VAL:N	2.43	0.51
1:A:148:ALA:HB2	1:A:287:LEU:HD23	1.93	0.51
1:B:421:LEU:HD12	1:B:422:VAL:N	2.25	0.51
1:C:192:LEU:HD21	1:C:222:VAL:HG13	1.92	0.51
1:E:60:VAL:O	1:E:64:ALA:N	2.43	0.51
1:G:211:ASN:ND2	1:G:211:ASN:C	2.62	0.51
1:G:319:SER:O	1:G:320:THR:C	2.48	0.51
1:D:311:HIS:N	1:D:311:HIS:ND1	2.58	0.51
1:F:240:ALA:O	1:F:241:THR:CB	2.57	0.51
1:H:146:LEU:O	1:H:150:VAL:HG23	2.09	0.51
1:I:156:ILE:HG23	1:I:181:ALA:HB2	1.91	0.51
1:I:411:ASP:O	1:I:414:LYS:HB2	2.10	0.51
1:K:382:ILE:HD12	1:K:437:ASP:HB2	1.93	0.51
1:A:438:ILE:HG22	1:A:442:LEU:HD11	1.93	0.51
1:F:60:VAL:HG12	1:F:64:ALA:HB2	1.92	0.51
1:E:88:PHE:HA	1:G:386:ALA:HB2	1.93	0.51
1:G:411:ASP:O	1:G:414:LYS:HB2	2.10	0.51
1:K:156:ILE:HG12	1:K:157:VAL:N	2.25	0.51
1:K:319:SER:O	1:K:320:THR:C	2.48	0.51
1:L:261:LYS:HZ3	1:L:388:SER:HA	1.76	0.51
1:I:428:VAL:HG12	1:L:62:ILE:HD11	1.92	0.51
1:B:268:ASP:HB2	1:D:83:ASN:O	2.11	0.51
1:D:240:ALA:O	1:D:241:THR:CB	2.57	0.51
1:E:135:MET:HE1	1:E:274:ILE:HD12	1.92	0.51
1:E:240:ALA:HB1	1:E:245:GLN:HG2	1.93	0.51
1:E:339:TYR:OH	1:E:358:PHE:HB2	2.10	0.51
1:J:322:LEU:O	1:J:325:ALA:HB3	2.10	0.51
1:A:211:ASN:HD22	1:A:212:PRO:N	2.08	0.51
1:B:217:VAL:O	1:B:219:ILE:N	2.44	0.51
1:C:173:ILE:C	1:C:175:PRO:HD2	2.32	0.51
1:E:311:HIS:N	1:E:311:HIS:ND1	2.59	0.51
1:F:62:ILE:HD11	1:G:428:VAL:HG12	1.92	0.51
1:A:311:HIS:ND1	1:A:311:HIS:N	2.57	0.51
1:B:411:ASP:O	1:B:414:LYS:HB2	2.11	0.51
1:B:88:PHE:HA	1:D:386:ALA:HB2	1.91	0.51
1:E:140:CYS:HB2	1:G:292:GLY:O	2.11	0.51
1:E:163:TYR:CE2	1:E:165:LYS:HB2	2.46	0.51
1:L:311:HIS:N	1:L:311:HIS:ND1	2.59	0.51
1:B:350:ILE:O	1:B:354:GLN:HG2	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ALA:O	1:C:189:VAL:N	2.45	0.50
1:C:211:ASN:ND2	1:C:211:ASN:C	2.63	0.50
1:F:153:GLY:HA2	1:F:178:GLY:O	2.11	0.50
1:F:56:SER:OG	1:G:430:ASP:HB2	2.10	0.50
1:I:88:PHE:HA	1:K:386:ALA:HB2	1.92	0.50
1:K:82:VAL:HG22	1:L:80:PRO:HB3	1.93	0.50
1:F:170:ILE:HG23	1:F:174:LEU:HD12	1.92	0.50
1:G:53:PHE:CD1	1:G:54:LEU:HG	2.46	0.50
1:K:170:ILE:HG23	1:K:174:LEU:HD12	1.92	0.50
1:C:135:MET:CE	1:C:141:ALA:HA	2.41	0.50
1:C:135:MET:HE2	1:C:141:ALA:HA	1.93	0.50
1:E:70:ARG:HD3	1:E:79:THR:OG1	2.11	0.50
1:I:259:ALA:HB3	1:I:271:ALA:HB3	1.93	0.50
1:I:277:PRO:O	1:I:281:VAL:HG12	2.11	0.50
1:I:428:VAL:O	1:I:428:VAL:CG1	2.59	0.50
1:J:160:THR:HG22	1:J:183:VAL:HG12	1.92	0.50
1:J:209:PRO:HG3	1:J:355:MET:HE1	1.93	0.50
1:B:428:VAL:CG1	1:B:428:VAL:O	2.59	0.50
1:B:53:PHE:O	1:B:54:LEU:HD23	2.10	0.50
1:C:133:LEU:HD23	1:C:135:MET:HE1	1.92	0.50
1:F:319:SER:O	1:F:320:THR:C	2.50	0.50
1:F:55:ASN:N	1:F:55:ASN:ND2	2.59	0.50
1:H:324:MET:HG2	1:H:431:PHE:CE1	2.47	0.50
1:J:140:CYS:O	1:J:143:THR:HB	2.10	0.50
1:K:148:ALA:HB2	1:K:287:LEU:HD23	1.93	0.50
1:B:373:THR:O	1:B:376:PHE:HB3	2.11	0.50
1:D:210:THR:HG22	1:D:215:ARG:N	2.24	0.50
1:D:277:PRO:HG2	1:D:280:LEU:HB2	1.92	0.50
1:D:397:ASP:HB2	1:D:402:MET:HG2	1.92	0.50
1:F:215:ARG:NH1	1:F:347:GLU:OE2	2.42	0.50
1:F:421:LEU:HD12	1:F:422:VAL:N	2.26	0.50
1:H:336:HIS:ND1	1:H:337:VAL:N	2.60	0.50
1:H:324:MET:HG2	1:H:431:PHE:HE1	1.76	0.50
1:I:173:ILE:C	1:I:175:PRO:HD2	2.32	0.50
1:I:63:HIS:HD2	1:I:67:ARG:HD3	1.75	0.50
1:J:240:ALA:O	1:J:241:THR:CB	2.53	0.50
1:K:217:VAL:CG1	1:K:222:VAL:HG21	2.42	0.50
1:F:345:HIS:HE1	1:F:347:GLU:HG2	1.76	0.50
1:H:398:GLN:HB3	1:H:401:ILE:HD12	1.94	0.50
1:I:215:ARG:HD2	1:I:347:GLU:OE2	2.11	0.50
1:I:397:ASP:HB2	1:I:402:MET:HG2	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:347:GLU:CB	1:L:350:ILE:HD12	2.40	0.50
1:B:156:ILE:HG23	1:B:181:ALA:HB2	1.93	0.50
1:D:438:ILE:HG22	1:D:442:LEU:HD12	1.94	0.50
1:E:82:VAL:HG22	1:F:80:PRO:HB3	1.93	0.50
1:H:211:ASN:ND2	1:H:211:ASN:C	2.65	0.50
1:H:58:GLY:HA3	1:H:311:HIS:CD2	2.46	0.50
1:K:160:THR:HG22	1:K:183:VAL:HG12	1.93	0.50
1:A:394:SER:OG	1:A:427:GLY:N	2.39	0.50
1:A:72:ILE:HG23	1:A:72:ILE:O	2.12	0.50
1:C:127:GLU:CD	1:C:242:PRO:HB3	2.31	0.50
1:E:140:CYS:O	1:E:143:THR:HB	2.12	0.50
1:E:259:ALA:HB3	1:E:271:ALA:HB3	1.93	0.50
1:J:234:CYS:HA	1:J:254:LEU:O	2.12	0.50
1:J:320:THR:O	1:J:324:MET:HB2	2.11	0.50
1:K:397:ASP:HB2	1:K:402:MET:HG2	1.92	0.50
1:L:210:THR:O	1:L:214:LEU:HA	2.11	0.50
1:A:248:LEU:HG	1:A:255:VAL:HG12	1.92	0.50
1:A:411:ASP:O	1:A:414:LYS:HB2	2.12	0.50
1:C:87:TYR:CE1	1:C:106:PHE:HB2	2.46	0.50
1:D:373:THR:O	1:D:376:PHE:HB3	2.12	0.50
1:E:110:ARG:HH21	2:G:506:HEN:P	2.35	0.50
1:E:347:GLU:HB3	1:E:350:ILE:HD12	1.94	0.50
1:I:72:ILE:HG12	1:I:72:ILE:O	2.12	0.50
1:J:270:LEU:HD23	1:J:270:LEU:N	2.27	0.50
1:L:336:HIS:ND1	1:L:337:VAL:N	2.60	0.50
1:A:336:HIS:ND1	1:A:337:VAL:N	2.59	0.49
1:C:428:VAL:O	1:C:428:VAL:CG1	2.60	0.49
1:F:317:GLN:HG2	1:F:427:GLY:O	2.11	0.49
1:K:331:HIS:CE1	1:K:333:LYS:HB2	2.47	0.49
1:L:159:THR:HG23	1:L:206:THR:HB	1.94	0.49
1:C:103:ARG:HG2	1:C:104:ALA:N	2.26	0.49
1:C:311:HIS:N	1:C:311:HIS:ND1	2.60	0.49
1:D:113:ASN:ND2	1:D:297:PRO:HG3	2.27	0.49
1:H:187:ALA:O	1:H:189:VAL:N	2.45	0.49
1:E:331:HIS:HE1	1:E:333:LYS:HB2	1.76	0.49
1:F:277:PRO:O	1:F:281:VAL:HG12	2.12	0.49
1:C:310:LEU:HA	1:C:313:ARG:NH2	2.27	0.49
1:A:386:ALA:HB2	1:C:88:PHE:HA	1.94	0.49
1:E:319:SER:O	1:E:320:THR:C	2.50	0.49
1:F:192:LEU:HG	1:F:196:LEU:HD23	1.94	0.49
1:F:260:THR:HG23	1:F:270:LEU:HD22	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:215:ARG:NH1	1:J:347:GLU:OE2	2.42	0.49
1:L:215:ARG:HD2	1:L:347:GLU:OE2	2.13	0.49
1:A:438:ILE:O	1:A:441:ALA:HB3	2.12	0.49
1:E:127:GLU:OE2	1:E:257:HIS:NE2	2.45	0.49
1:F:211:ASN:C	1:F:211:ASN:ND2	2.65	0.49
1:G:240:ALA:O	1:G:241:THR:CB	2.59	0.49
1:I:206:THR:O	1:I:235:ILE:HA	2.12	0.49
1:K:204:PHE:CE2	1:K:222:VAL:HG11	2.48	0.49
1:D:145:MET:HE2	1:D:146:LEU:HA	1.94	0.49
1:D:319:SER:O	1:D:320:THR:C	2.51	0.49
1:E:217:VAL:O	1:E:219:ILE:N	2.46	0.49
1:F:397:ASP:HB2	1:F:402:MET:HG2	1.94	0.49
1:G:421:LEU:HD12	1:G:422:VAL:N	2.28	0.49
1:J:345:HIS:HE1	1:J:347:GLU:HG2	1.77	0.49
1:C:217:VAL:HG13	1:C:222:VAL:HG21	1.95	0.49
1:E:54:LEU:CD2	1:E:59:SER:HB3	2.38	0.49
1:F:250:LEU:CD1	1:F:354:GLN:HB2	2.40	0.49
1:G:428:VAL:CG1	1:G:428:VAL:O	2.61	0.49
1:H:63:HIS:HB3	1:H:67:ARG:HB2	1.93	0.49
1:B:215:ARG:HD2	1:B:347:GLU:OE2	2.12	0.49
1:E:331:HIS:CG	1:E:332:PRO:HD2	2.47	0.49
1:E:72:ILE:O	1:E:72:ILE:HG23	2.12	0.49
1:H:339:TYR:CZ	1:H:358:PHE:HB2	2.48	0.49
1:I:117:VAL:HA	1:I:120:GLU:HB2	1.95	0.49
1:I:210:THR:CG2	1:I:215:ARG:H	2.21	0.49
1:K:209:PRO:HG3	1:K:355:MET:HE1	1.95	0.49
1:B:428:VAL:HG12	1:C:62:ILE:HD11	1.94	0.49
1:D:72:ILE:O	1:D:72:ILE:HG23	2.13	0.49
1:G:114:PRO:O	1:G:117:VAL:HG22	2.13	0.49
1:I:215:ARG:NH1	1:I:347:GLU:OE2	2.38	0.49
1:L:145:MET:HE2	1:L:149:LEU:HD12	1.95	0.49
1:C:369:ASP:H	1:C:372:THR:HB	1.77	0.49
1:D:159:THR:HG23	1:D:206:THR:HB	1.95	0.49
1:F:145:MET:HG2	1:F:149:LEU:HD12	1.95	0.49
1:H:259:ALA:HB3	1:H:271:ALA:HB3	1.95	0.49
1:J:428:VAL:O	1:J:428:VAL:CG1	2.61	0.49
1:K:145:MET:CE	1:K:146:LEU:HD23	2.37	0.49
1:L:211:ASN:C	1:L:211:ASN:ND2	2.66	0.49
1:E:187:ALA:O	1:E:189:VAL:N	2.46	0.48
1:J:211:ASN:ND2	1:J:211:ASN:C	2.66	0.48
1:J:52:SER:C	1:J:54:LEU:H	2.16	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HA	1:A:313:ARG:NH2	2.28	0.48
1:B:146:LEU:O	1:B:150:VAL:HG23	2.13	0.48
1:B:60:VAL:HG12	1:B:64:ALA:HB2	1.96	0.48
1:H:113:ASN:ND2	1:H:297:PRO:HG3	2.28	0.48
1:H:161:ASP:HB3	1:H:210:THR:OG1	2.12	0.48
1:H:261:LYS:HZ3	1:H:388:SER:HA	1.75	0.48
1:I:322:LEU:O	1:I:325:ALA:HB3	2.14	0.48
1:J:156:ILE:CG2	1:J:181:ALA:HB2	2.44	0.48
1:D:127:GLU:OE2	1:D:242:PRO:HB3	2.13	0.48
1:D:374:ALA:O	1:D:377:VAL:HG22	2.13	0.48
1:D:73:VAL:O	1:D:74:THR:HG23	2.13	0.48
1:D:70:ARG:HD3	1:D:79:THR:OG1	2.12	0.48
1:E:336:HIS:ND1	1:E:337:VAL:N	2.61	0.48
1:F:51:ALA:HB1	1:F:53:PHE:CE2	2.48	0.48
1:G:166:THR:O	1:G:170:ILE:HG13	2.13	0.48
1:F:291:LEU:O	1:H:140:CYS:HA	2.12	0.48
1:J:370:LEU:HD23	1:J:419:ASP:HB3	1.95	0.48
1:J:438:ILE:HG22	1:J:442:LEU:HD11	1.94	0.48
1:A:145:MET:HE2	1:A:149:LEU:HD12	1.95	0.48
1:B:156:ILE:HG23	1:B:181:ALA:CB	2.44	0.48
1:D:206:THR:O	1:D:235:ILE:HA	2.13	0.48
1:E:127:GLU:OE2	1:E:242:PRO:HB3	2.14	0.48
1:E:80:PRO:HB3	1:F:82:VAL:HG22	1.94	0.48
1:H:54:LEU:CD2	1:H:59:SER:HB3	2.43	0.48
1:L:217:VAL:CG1	1:L:222:VAL:HG21	2.43	0.48
1:L:54:LEU:CD2	1:L:59:SER:HB3	2.32	0.48
1:D:411:ASP:O	1:D:414:LYS:HB2	2.12	0.48
1:F:145:MET:CE	1:F:146:LEU:HD23	2.43	0.48
1:H:435:LYS:HG2	1:H:439:LEU:HD12	1.96	0.48
1:I:53:PHE:O	1:I:54:LEU:HD23	2.14	0.48
1:K:173:ILE:C	1:K:175:PRO:HD2	2.34	0.48
1:K:196:LEU:HD12	1:K:229:LYS:HB2	1.96	0.48
1:L:135:MET:CE	1:L:141:ALA:HA	2.43	0.48
1:A:133:LEU:HD13	1:A:285:ARG:HD3	1.96	0.48
1:B:211:ASN:C	1:B:211:ASN:ND2	2.67	0.48
1:E:386:ALA:HB1	1:E:387:PRO:CD	2.44	0.48
1:F:223:SER:HA	1:F:233:VAL:HG21	1.95	0.48
1:J:64:ALA:O	1:J:122:LYS:HE2	2.14	0.48
1:B:321:ALA:HB2	1:B:360:GLY:HA2	1.96	0.48
1:C:219:ILE:HD12	1:C:250:LEU:HD12	1.95	0.48
1:C:339:TYR:CZ	1:C:358:PHE:HB2	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:THR:O	1:E:376:PHE:HB3	2.14	0.48
1:H:207:GLU:CB	1:H:236:ASP:HB3	2.40	0.48
1:J:210:THR:HG22	1:J:215:ARG:N	2.19	0.48
1:K:164:ARG:O	1:K:167:ARG:HB3	2.14	0.48
1:J:428:VAL:HG12	1:K:62:ILE:HD11	1.96	0.48
1:L:426:PHE:HE1	1:L:438:ILE:HD11	1.79	0.48
1:L:60:VAL:CG1	1:L:64:ALA:HB2	2.44	0.48
1:C:94:GLU:O	1:C:97:ASP:HB2	2.13	0.48
1:E:53:PHE:CE1	1:E:54:LEU:HG	2.49	0.48
1:F:382:ILE:HD12	1:F:437:ASP:HB2	1.95	0.48
1:H:270:LEU:HD23	1:H:270:LEU:N	2.28	0.48
1:H:428:VAL:CG1	1:H:428:VAL:O	2.62	0.48
1:K:277:PRO:O	1:K:281:VAL:HG12	2.13	0.48
1:K:345:HIS:CE1	1:K:347:GLU:HG2	2.49	0.48
1:A:370:LEU:HD23	1:A:419:ASP:CB	2.43	0.48
1:B:311:HIS:ND1	1:B:311:HIS:N	2.61	0.48
1:B:60:VAL:O	1:B:64:ALA:N	2.44	0.48
1:F:234:CYS:O	1:F:235:ILE:HD13	2.13	0.48
1:K:278:LEU:O	1:K:280:LEU:N	2.47	0.48
1:A:161:ASP:HB3	1:A:210:THR:OG1	2.13	0.48
1:B:277:PRO:O	1:B:281:VAL:HG12	2.13	0.48
1:E:216:CYS:N	1:E:347:GLU:HG3	2.25	0.48
1:E:374:ALA:O	1:E:377:VAL:HG22	2.13	0.48
1:E:317:GLN:HG2	1:E:427:GLY:O	2.14	0.48
1:H:240:ALA:O	1:H:241:THR:CB	2.56	0.48
1:H:442:LEU:HA	1:H:445:ILE:HD12	1.96	0.48
1:H:60:VAL:O	1:H:61:ALA:C	2.51	0.48
1:I:119:LEU:HG	1:I:134:LEU:HD11	1.96	0.48
1:D:428:VAL:CG1	1:D:428:VAL:O	2.61	0.47
1:F:148:ALA:HB2	1:F:287:LEU:HD23	1.96	0.47
1:H:135:MET:HE1	1:H:274:ILE:HD12	1.96	0.47
1:H:210:THR:O	1:H:214:LEU:HA	2.14	0.47
1:I:135:MET:CE	1:I:141:ALA:HA	2.44	0.47
1:I:209:PRO:HG3	1:I:355:MET:HE1	1.96	0.47
1:I:292:GLY:O	1:K:140:CYS:HB2	2.14	0.47
1:I:365:GLU:HB3	1:I:420:ASN:HB2	1.95	0.47
1:L:208:SER:HA	1:L:209:PRO:C	2.34	0.47
1:L:428:VAL:O	1:L:428:VAL:CG1	2.62	0.47
1:A:435:LYS:HG2	1:A:439:LEU:HD12	1.97	0.47
1:B:119:LEU:HG	1:B:134:LEU:HD11	1.95	0.47
1:C:64:ALA:O	1:C:122:LYS:HE2	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:THR:O	1:C:235:ILE:HA	2.14	0.47
1:D:123:ILE:HD13	1:D:273:CYS:SG	2.55	0.47
1:I:317:GLN:HG2	1:I:427:GLY:O	2.14	0.47
1:K:210:THR:O	1:K:214:LEU:HA	2.14	0.47
1:L:173:ILE:C	1:L:175:PRO:HD2	2.34	0.47
1:C:217:VAL:O	1:C:219:ILE:N	2.48	0.47
1:C:73:VAL:O	1:C:74:THR:HG23	2.14	0.47
1:E:215:ARG:NH1	1:E:347:GLU:OE2	2.42	0.47
1:G:187:ALA:O	1:G:189:VAL:N	2.47	0.47
1:I:120:GLU:CG	1:I:134:LEU:HD12	2.43	0.47
1:I:173:ILE:O	1:I:176:LYS:HB2	2.13	0.47
1:I:311:HIS:ND1	1:I:311:HIS:N	2.62	0.47
1:J:127:GLU:OE2	1:J:257:HIS:NE2	2.46	0.47
1:B:336:HIS:ND1	1:B:337:VAL:N	2.61	0.47
1:E:156:ILE:HG23	1:E:181:ALA:HB2	1.96	0.47
1:E:260:THR:HG23	1:E:270:LEU:HD22	1.97	0.47
1:E:428:VAL:O	1:E:428:VAL:CG1	2.62	0.47
1:I:127:GLU:OE2	1:I:257:HIS:NE2	2.48	0.47
1:K:261:LYS:NZ	1:K:388:SER:HA	2.29	0.47
1:A:261:LYS:HZ3	1:A:388:SER:HA	1.78	0.47
1:B:196:LEU:HD12	1:B:229:LYS:HB2	1.96	0.47
1:B:260:THR:HG23	1:B:270:LEU:HD22	1.95	0.47
1:B:322:LEU:O	1:B:325:ALA:HB3	2.14	0.47
1:C:426:PHE:HE1	1:C:438:ILE:HD11	1.78	0.47
1:E:217:VAL:CG1	1:E:222:VAL:HG21	2.44	0.47
1:G:127:GLU:OE2	1:G:257:HIS:NE2	2.47	0.47
1:J:208:SER:HA	1:J:209:PRO:C	2.33	0.47
1:J:336:HIS:ND1	1:J:337:VAL:N	2.62	0.47
1:L:60:VAL:O	1:L:61:ALA:C	2.53	0.47
1:A:322:LEU:O	1:A:325:ALA:HB3	2.13	0.47
1:B:210:THR:O	1:B:214:LEU:HA	2.14	0.47
1:B:335:ARG:HB2	1:B:335:ARG:HE	1.57	0.47
1:C:211:ASN:HD22	1:C:212:PRO:N	2.13	0.47
1:D:382:ILE:HD12	1:D:437:ASP:HB2	1.96	0.47
1:G:339:TYR:CZ	1:G:358:PHE:HB2	2.49	0.47
1:H:103:ARG:HG2	1:H:104:ALA:N	2.30	0.47
1:H:438:ILE:HG22	1:H:442:LEU:CD1	2.45	0.47
1:I:57:ASP:HB3	1:I:243:LEU:CD2	2.45	0.47
1:I:60:VAL:CG1	1:I:64:ALA:HB2	2.45	0.47
1:J:146:LEU:HD13	1:J:174:LEU:HD11	1.95	0.47
1:J:207:GLU:CB	1:J:236:ASP:HB3	2.38	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:313:ARG:O	1:J:317:GLN:HG3	2.13	0.47
1:K:339:TYR:CZ	1:K:358:PHE:HB2	2.49	0.47
1:L:339:TYR:CZ	1:L:358:PHE:HB2	2.48	0.47
1:A:173:ILE:C	1:A:175:PRO:HD2	2.34	0.47
1:A:217:VAL:O	1:A:219:ILE:N	2.47	0.47
1:B:204:PHE:CE2	1:B:222:VAL:HG11	2.50	0.47
1:B:331:HIS:ND1	1:B:332:PRO:HD2	2.30	0.47
1:B:140:CYS:HA	1:D:291:LEU:O	2.15	0.47
1:D:335:ARG:HB2	1:D:335:ARG:HE	1.64	0.47
1:D:438:ILE:HG22	1:D:442:LEU:CD1	2.45	0.47
1:E:373:THR:OG1	1:E:420:ASN:HA	2.14	0.47
1:F:145:MET:HE2	1:F:146:LEU:HA	1.96	0.47
1:F:339:TYR:CZ	1:F:358:PHE:HB2	2.50	0.47
1:H:135:MET:HE2	1:H:141:ALA:HA	1.97	0.47
1:K:248:LEU:HG	1:K:255:VAL:HG12	1.97	0.47
1:K:347:GLU:CB	1:K:350:ILE:HD12	2.44	0.47
1:K:373:THR:OG1	1:K:420:ASN:HA	2.15	0.47
1:L:127:GLU:OE2	1:L:242:PRO:HB3	2.15	0.47
1:L:310:LEU:HA	1:L:313:ARG:NH2	2.30	0.47
1:A:217:VAL:HG13	1:A:222:VAL:HG21	1.97	0.47
1:B:72:ILE:HD13	1:B:80:PRO:HG2	1.96	0.47
1:C:270:LEU:O	1:C:271:ALA:HB2	2.14	0.47
1:F:217:VAL:CG1	1:F:222:VAL:HG21	2.45	0.47
1:G:153:GLY:HA2	1:G:178:GLY:O	2.12	0.47
1:H:331:HIS:CG	1:H:332:PRO:HD2	2.49	0.47
1:H:373:THR:OG1	1:H:420:ASN:HA	2.15	0.47
1:I:216:CYS:SG	1:I:355:MET:HE1	2.54	0.47
1:I:345:HIS:CE1	1:I:347:GLU:HG2	2.50	0.47
1:J:217:VAL:O	1:J:219:ILE:N	2.46	0.47
1:K:420:ASN:O	1:K:422:VAL:HG23	2.15	0.47
1:A:217:VAL:CG1	1:A:222:VAL:HG21	2.44	0.47
1:B:140:CYS:HB2	1:D:292:GLY:O	2.15	0.47
1:B:159:THR:HG23	1:B:206:THR:HB	1.96	0.47
1:B:58:GLY:HA3	1:B:311:HIS:CD2	2.50	0.47
1:C:217:VAL:CG1	1:C:222:VAL:HG21	2.44	0.47
1:C:226:CYS:HB3	1:C:231:ALA:HB3	1.97	0.47
1:D:211:ASN:C	1:D:211:ASN:ND2	2.67	0.47
1:F:135:MET:CE	1:F:141:ALA:HA	2.45	0.47
1:G:217:VAL:CG1	1:G:222:VAL:HG21	2.44	0.47
1:I:140:CYS:O	1:I:143:THR:HB	2.14	0.47
1:K:73:VAL:O	1:K:74:THR:HG23	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:CG2	1:B:297:PRO:HB3	2.41	0.47
1:E:163:TYR:O	1:E:164:ARG:C	2.54	0.47
1:F:106:PHE:CD1	1:F:112:GLY:HA3	2.50	0.47
1:F:53:PHE:O	1:F:54:LEU:HD23	2.15	0.47
1:G:163:TYR:O	1:G:164:ARG:C	2.53	0.47
1:G:234:CYS:SG	1:G:256:LEU:HD23	2.54	0.47
1:E:140:CYS:HA	1:G:291:LEU:O	2.14	0.47
1:G:72:ILE:HG12	1:G:72:ILE:O	2.15	0.47
1:H:87:TYR:CE1	1:H:106:PHE:HB2	2.50	0.47
1:I:204:PHE:CE2	1:I:222:VAL:HG11	2.50	0.47
1:J:94:GLU:O	1:J:97:ASP:HB2	2.15	0.47
1:K:115:THR:CG2	1:K:297:PRO:HB3	2.43	0.47
1:K:428:VAL:O	1:K:428:VAL:CG1	2.62	0.47
1:K:442:LEU:HA	1:K:445:ILE:CD1	2.45	0.47
1:K:63:HIS:HB3	1:K:67:ARG:HB2	1.96	0.47
1:B:443:ASP:O	1:B:445:ILE:N	2.47	0.47
1:C:441:ALA:C	1:C:443:ASP:N	2.68	0.47
1:E:429:GLU:OE2	1:H:63:HIS:HE1	1.98	0.47
1:F:159:THR:HG23	1:F:206:THR:HB	1.96	0.47
1:F:313:ARG:O	1:F:317:GLN:HG3	2.14	0.47
1:H:73:VAL:O	1:H:74:THR:HG23	2.15	0.47
1:I:113:ASN:O	1:I:117:VAL:HG13	2.15	0.47
1:J:442:LEU:C	1:J:444:SER:H	2.17	0.47
1:A:428:VAL:O	1:A:428:VAL:CG1	2.62	0.46
1:B:320:THR:O	1:B:324:MET:HB2	2.14	0.46
1:B:63:HIS:HE1	1:C:429:GLU:OE2	1.99	0.46
1:H:319:SER:O	1:H:320:THR:C	2.52	0.46
1:K:94:GLU:O	1:K:97:ASP:HB2	2.15	0.46
1:A:145:MET:HG2	1:A:149:LEU:CD1	2.46	0.46
1:B:160:THR:HG22	1:B:183:VAL:HG12	1.96	0.46
1:D:173:ILE:O	1:D:176:LYS:HB2	2.14	0.46
1:D:260:THR:HG23	1:D:270:LEU:HD22	1.98	0.46
1:D:312:LEU:HD23	1:D:312:LEU:N	2.30	0.46
1:E:250:LEU:CD1	1:E:354:GLN:HB2	2.41	0.46
1:G:219:ILE:HG21	1:G:250:LEU:HB2	1.97	0.46
1:G:259:ALA:HA	1:G:263:LEU:HB2	1.98	0.46
1:J:311:HIS:N	1:J:311:HIS:ND1	2.62	0.46
1:K:310:LEU:HA	1:K:313:ARG:NH2	2.29	0.46
1:L:443:ASP:C	1:L:445:ILE:H	2.17	0.46
1:B:343:GLN:HB3	1:B:343:GLN:HE21	1.56	0.46
1:D:170:ILE:HG23	1:D:174:LEU:HD12	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:TYR:O	1:D:395:ILE:HG23	2.16	0.46
1:G:443:ASP:C	1:G:445:ILE:H	2.18	0.46
1:C:241:THR:HG23	1:C:242:PRO:HD2	1.98	0.46
1:C:322:LEU:O	1:C:325:ALA:HB3	2.16	0.46
1:E:313:ARG:O	1:E:317:GLN:HG3	2.15	0.46
1:F:311:HIS:N	1:F:311:HIS:ND1	2.63	0.46
1:G:420:ASN:O	1:G:422:VAL:HG23	2.15	0.46
1:G:64:ALA:O	1:G:122:LYS:HE2	2.15	0.46
1:H:156:ILE:HG23	1:H:181:ALA:CB	2.46	0.46
1:I:60:VAL:O	1:I:62:ILE:N	2.49	0.46
1:I:63:HIS:CD2	1:I:67:ARG:HD3	2.50	0.46
1:L:209:PRO:HG3	1:L:355:MET:HE1	1.97	0.46
1:L:397:ASP:HB2	1:L:402:MET:HG2	1.98	0.46
1:C:211:ASN:HB2	1:C:239:PHE:HE2	1.79	0.46
1:C:234:CYS:HA	1:C:254:LEU:O	2.15	0.46
1:G:135:MET:CE	1:G:141:ALA:HA	2.42	0.46
1:G:80:PRO:HB3	1:H:82:VAL:HG22	1.97	0.46
1:H:133:LEU:CD1	1:H:285:ARG:HD3	2.46	0.46
1:F:140:CYS:HA	1:H:291:LEU:O	2.14	0.46
1:A:127:GLU:OE2	1:A:257:HIS:NE2	2.48	0.46
1:C:208:SER:HA	1:C:209:PRO:C	2.36	0.46
1:I:336:HIS:ND1	1:I:337:VAL:N	2.63	0.46
1:J:133:LEU:HD23	1:J:135:MET:HE3	1.98	0.46
1:K:426:PHE:HE1	1:K:438:ILE:HD11	1.81	0.46
1:A:185:ASP:OD1	1:A:215:ARG:NH2	2.48	0.46
1:A:259:ALA:HA	1:A:263:LEU:HD12	1.98	0.46
1:E:135:MET:HB3	1:E:140:CYS:HB3	1.98	0.46
1:H:443:ASP:C	1:H:445:ILE:H	2.18	0.46
1:L:207:GLU:CB	1:L:236:ASP:HB3	2.39	0.46
1:C:135:MET:HE2	1:C:274:ILE:HD12	1.97	0.46
1:C:192:LEU:CD2	1:C:222:VAL:HG13	2.45	0.46
1:D:145:MET:HE2	1:D:146:LEU:HD23	1.98	0.46
1:D:94:GLU:O	1:D:97:ASP:HB2	2.16	0.46
1:E:234:CYS:HA	1:E:254:LEU:O	2.15	0.46
1:F:87:TYR:CE1	1:F:106:PHE:HB2	2.51	0.46
1:F:72:ILE:HG23	1:F:72:ILE:O	2.16	0.46
1:H:375:LYS:HD3	1:H:445:ILE:HG23	1.97	0.46
1:K:339:TYR:OH	1:K:358:PHE:HB2	2.16	0.46
1:A:343:GLN:HE21	1:A:343:GLN:HB3	1.56	0.46
1:B:160:THR:HG23	1:B:184:ILE:O	2.16	0.46
1:C:441:ALA:O	1:C:443:ASP:N	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ARG:HG2	1:D:104:ALA:N	2.31	0.46
1:D:331:HIS:CE1	1:D:333:LYS:HB2	2.51	0.46
1:E:173:ILE:O	1:E:176:LYS:HB2	2.16	0.46
1:F:398:GLN:O	1:F:401:ILE:N	2.48	0.46
1:G:160:THR:HG22	1:G:183:VAL:HG12	1.97	0.46
1:G:343:GLN:HB3	1:G:343:GLN:HE21	1.55	0.46
1:G:261:LYS:HZ3	1:G:388:SER:HA	1.79	0.46
1:H:312:LEU:HD23	1:H:312:LEU:N	2.30	0.46
1:H:382:ILE:HB	1:H:383:PRO:CD	2.46	0.46
1:I:211:ASN:ND2	1:I:212:PRO:N	2.64	0.46
1:I:260:THR:CG2	1:I:270:LEU:HD22	2.46	0.46
1:J:145:MET:CE	1:J:149:LEU:HD12	2.46	0.46
1:K:260:THR:HG23	1:K:270:LEU:HD22	1.98	0.46
1:L:113:ASN:O	1:L:117:VAL:HG13	2.16	0.46
1:L:192:LEU:HG	1:L:196:LEU:HD23	1.98	0.46
1:A:82:VAL:HG22	1:B:80:PRO:HB3	1.98	0.46
1:B:83:ASN:O	1:D:268:ASP:CB	2.63	0.46
1:D:164:ARG:O	1:D:167:ARG:HB3	2.16	0.46
1:F:157:VAL:O	1:F:204:PHE:CD1	2.69	0.46
1:G:208:SER:HA	1:G:209:PRO:C	2.35	0.46
1:G:350:ILE:O	1:G:354:GLN:HG2	2.17	0.46
1:H:269:VAL:C	1:H:270:LEU:HD23	2.37	0.46
1:H:311:HIS:N	1:H:311:HIS:ND1	2.64	0.46
1:I:121:GLU:O	1:I:124:SER:HB2	2.16	0.46
1:I:196:LEU:HD12	1:I:229:LYS:HB2	1.98	0.46
1:K:126:LEU:HD23	1:K:126:LEU:HA	1.82	0.46
1:K:259:ALA:HA	1:K:263:LEU:HB2	1.98	0.46
1:A:319:SER:O	1:A:320:THR:C	2.54	0.45
1:B:319:SER:O	1:B:320:THR:C	2.55	0.45
1:A:308:LYS:HD2	1:D:393:GLU:OE2	2.17	0.45
1:E:439:LEU:HA	1:E:442:LEU:HD12	1.98	0.45
1:G:270:LEU:N	1:G:270:LEU:HD23	2.30	0.45
1:G:384:TYR:O	1:G:395:ILE:HG23	2.16	0.45
1:G:53:PHE:HD1	1:G:54:LEU:HG	1.81	0.45
1:I:143:THR:HG23	1:I:169:PHE:CE1	2.50	0.45
1:I:260:THR:HG23	1:I:270:LEU:HD22	1.96	0.45
1:J:444:SER:C	1:J:445:ILE:HG13	2.36	0.45
1:L:159:THR:HA	1:L:184:ILE:O	2.16	0.45
1:B:113:ASN:OD1	1:B:115:THR:N	2.40	0.45
1:B:156:ILE:CG2	1:B:181:ALA:HB2	2.47	0.45
1:B:127:GLU:CD	1:B:242:PRO:HB3	2.36	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ALA:HA	1:B:263:LEU:HB2	1.97	0.45
1:B:50:TYR:CD2	1:B:54:LEU:HD12	2.52	0.45
1:E:210:THR:O	1:E:214:LEU:HA	2.16	0.45
1:H:438:ILE:HG22	1:H:442:LEU:HD11	1.97	0.45
1:J:382:ILE:HD12	1:J:437:ASP:HB2	1.98	0.45
1:A:60:VAL:CG1	1:A:64:ALA:HB2	2.46	0.45
1:B:145:MET:HE3	1:B:149:LEU:HD12	1.98	0.45
1:D:58:GLY:HA3	1:D:311:HIS:CD2	2.51	0.45
1:E:126:LEU:HA	1:E:126:LEU:HD23	1.77	0.45
1:H:217:VAL:O	1:H:219:ILE:N	2.48	0.45
1:H:345:HIS:HE1	1:H:347:GLU:HG2	1.81	0.45
1:I:192:LEU:HG	1:I:196:LEU:HD23	1.97	0.45
1:K:156:ILE:HG23	1:K:181:ALA:HB2	1.98	0.45
1:K:211:ASN:HD22	1:K:212:PRO:N	2.15	0.45
1:B:287:LEU:HD12	1:B:287:LEU:O	2.17	0.45
1:A:83:ASN:O	1:C:268:ASP:HB2	2.16	0.45
1:D:398:GLN:HB3	1:D:401:ILE:HD12	1.98	0.45
1:D:441:ALA:C	1:D:443:ASP:N	2.68	0.45
1:E:397:ASP:O	1:E:399:PRO:HD3	2.16	0.45
1:F:324:MET:HG2	1:F:431:PHE:HE1	1.81	0.45
1:J:103:ARG:HG2	1:J:104:ALA:N	2.31	0.45
1:K:192:LEU:HG	1:K:196:LEU:HD23	1.99	0.45
1:A:211:ASN:HB2	1:A:239:PHE:HE2	1.81	0.45
1:A:398:GLN:O	1:A:401:ILE:N	2.49	0.45
1:C:75:ASP:O	1:D:87:TYR:HA	2.17	0.45
1:D:57:ASP:HB3	1:D:243:LEU:CD2	2.47	0.45
1:D:441:ALA:O	1:D:443:ASP:N	2.50	0.45
1:F:243:LEU:CD1	1:F:311:HIS:HA	2.47	0.45
1:F:324:MET:HG2	1:F:431:PHE:CE1	2.52	0.45
1:A:60:VAL:O	1:A:64:ALA:N	2.44	0.45
1:B:339:TYR:CZ	1:B:358:PHE:HB2	2.51	0.45
1:C:373:THR:OG1	1:C:420:ASN:HA	2.16	0.45
1:D:208:SER:HA	1:D:209:PRO:C	2.37	0.45
1:F:386:ALA:HA	1:F:402:MET:CE	2.47	0.45
1:J:121:GLU:O	1:J:124:SER:HB2	2.17	0.45
1:K:54:LEU:HD23	1:K:59:SER:HB3	1.97	0.45
1:K:54:LEU:HD22	1:K:59:SER:HB3	1.97	0.45
1:B:261:LYS:HZ3	1:B:388:SER:HA	1.80	0.45
1:B:52:SER:C	1:B:54:LEU:H	2.20	0.45
1:F:140:CYS:O	1:F:144:VAL:HG23	2.17	0.45
1:F:442:LEU:CA	1:F:445:ILE:HD12	2.40	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:ARG:NH1	1:H:347:GLU:OE2	2.43	0.45
1:H:420:ASN:O	1:H:422:VAL:HG23	2.17	0.45
1:I:64:ALA:O	1:I:122:LYS:HE2	2.16	0.45
1:I:386:ALA:HB1	1:I:387:PRO:CD	2.47	0.45
1:J:133:LEU:CD1	1:J:285:ARG:HD3	2.46	0.45
1:J:389:PHE:HB2	1:J:425:SER:OG	2.17	0.45
1:K:312:LEU:N	1:K:312:LEU:HD23	2.31	0.45
1:A:210:THR:CG2	1:A:215:ARG:H	2.25	0.45
1:B:196:LEU:HD13	1:B:196:LEU:HA	1.82	0.45
1:C:196:LEU:HD12	1:C:229:LYS:HB2	1.99	0.45
1:D:143:THR:HG23	1:D:169:PHE:CE1	2.52	0.45
1:F:398:GLN:O	1:F:399:PRO:C	2.55	0.45
1:G:339:TYR:CD1	1:G:362:VAL:HG22	2.52	0.45
1:H:265:GLY:HA3	1:H:313:ARG:NH1	2.32	0.45
1:I:347:GLU:HB3	1:I:350:ILE:HD12	1.98	0.45
1:I:80:PRO:HB3	1:J:82:VAL:HG22	1.99	0.45
1:L:114:PRO:O	1:L:117:VAL:HG22	2.16	0.45
1:A:215:ARG:HD2	1:A:347:GLU:OE2	2.17	0.45
1:B:153:GLY:HA2	1:B:178:GLY:O	2.16	0.45
1:B:163:TYR:CE2	1:B:165:LYS:HB2	2.52	0.45
1:C:115:THR:CG2	1:C:297:PRO:HB3	2.42	0.45
1:C:335:ARG:HB2	1:C:335:ARG:HE	1.67	0.45
1:D:160:THR:HG23	1:D:184:ILE:O	2.17	0.45
1:E:312:LEU:N	1:E:312:LEU:HD23	2.32	0.45
1:F:206:THR:O	1:F:235:ILE:HA	2.16	0.45
1:G:206:THR:OG1	1:G:207:GLU:N	2.48	0.45
1:G:217:VAL:HG13	1:G:222:VAL:HG21	1.98	0.45
1:G:324:MET:HG2	1:G:431:PHE:HE1	1.82	0.45
1:I:339:TYR:CZ	1:I:358:PHE:HB2	2.52	0.45
1:J:441:ALA:O	1:J:444:SER:HB2	2.17	0.45
1:I:386:ALA:HB2	1:K:88:PHE:HA	1.98	0.45
1:B:277:PRO:HG2	1:B:280:LEU:HB2	1.99	0.45
1:B:84:THR:HA	1:D:268:ASP:HA	1.99	0.45
1:H:382:ILE:HB	1:H:383:PRO:HD3	1.98	0.45
1:H:261:LYS:HZ2	1:H:388:SER:HA	1.78	0.45
1:J:398:GLN:O	1:J:401:ILE:N	2.49	0.45
1:L:156:ILE:HG23	1:L:181:ALA:HB2	1.98	0.45
1:L:398:GLN:O	1:L:401:ILE:N	2.50	0.45
1:A:196:LEU:HD13	1:A:196:LEU:HA	1.79	0.44
1:B:53:PHE:CZ	1:B:68:LEU:HD21	2.41	0.44
1:C:278:LEU:O	1:C:280:LEU:N	2.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ASP:HB2	1:C:402:MET:HG2	1.99	0.44
1:E:242:PRO:HD3	1:E:257:HIS:CE1	2.53	0.44
1:E:148:ALA:HB2	1:E:287:LEU:HD23	2.00	0.44
1:F:217:VAL:HG13	1:F:222:VAL:HG21	1.99	0.44
1:G:215:ARG:NH1	1:G:347:GLU:OE2	2.49	0.44
1:J:204:PHE:CE2	1:J:222:VAL:HG11	2.52	0.44
1:J:63:HIS:HB3	1:J:67:ARG:CB	2.47	0.44
1:K:373:THR:O	1:K:376:PHE:HB3	2.17	0.44
1:B:258:SER:C	1:B:260:THR:N	2.71	0.44
1:C:339:TYR:OH	1:C:358:PHE:HB2	2.17	0.44
1:B:384:TYR:OH	1:C:67:ARG:HA	2.17	0.44
1:C:72:ILE:HG12	1:C:72:ILE:O	2.18	0.44
1:E:243:LEU:CD1	1:E:311:HIS:HA	2.47	0.44
1:F:442:LEU:HA	1:F:445:ILE:CD1	2.39	0.44
1:F:70:ARG:HD3	1:F:79:THR:OG1	2.17	0.44
1:G:377:VAL:CG2	1:G:378:ASP:N	2.80	0.44
1:G:324:MET:HG2	1:G:431:PHE:CE1	2.52	0.44
2:F:505:HEN:P	1:H:110:ARG:HH21	2.40	0.44
1:I:127:GLU:OE2	1:I:242:PRO:HB3	2.17	0.44
1:J:319:SER:O	1:J:320:THR:C	2.55	0.44
1:J:383:PRO:HA	1:J:394:SER:O	2.17	0.44
1:J:72:ILE:HG23	1:J:72:ILE:O	2.17	0.44
1:K:106:PHE:CD1	1:K:112:GLY:HA3	2.53	0.44
1:L:331:HIS:CG	1:L:332:PRO:HD2	2.52	0.44
1:A:133:LEU:HD23	1:A:135:MET:CE	2.48	0.44
1:A:256:LEU:HB2	1:A:274:ILE:HG12	1.98	0.44
1:B:260:THR:CG2	1:B:270:LEU:HD22	2.48	0.44
1:B:292:GLY:O	1:D:140:CYS:HB2	2.17	0.44
1:F:260:THR:CG2	1:F:270:LEU:HD22	2.47	0.44
1:G:63:HIS:HD2	1:G:67:ARG:HD3	1.81	0.44
1:H:321:ALA:HB2	1:H:360:GLY:HA2	1.98	0.44
1:J:119:LEU:HG	1:J:134:LEU:HD11	1.98	0.44
1:J:132:THR:HG22	1:J:133:LEU:N	2.33	0.44
1:K:394:SER:OG	1:K:427:GLY:N	2.36	0.44
1:A:386:ALA:HB1	1:A:387:PRO:CD	2.48	0.44
1:A:94:GLU:O	1:A:97:ASP:HB2	2.18	0.44
1:B:261:LYS:HZ2	1:B:388:SER:HA	1.83	0.44
1:C:60:VAL:O	1:C:62:ILE:N	2.50	0.44
1:D:106:PHE:O	1:D:108:TYR:N	2.50	0.44
1:D:373:THR:OG1	1:D:420:ASN:HA	2.17	0.44
1:F:167:ARG:HG2	1:F:167:ARG:HH11	1.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:LEU:HD23	1:F:280:LEU:HA	1.80	0.44
1:H:322:LEU:O	1:H:325:ALA:HB3	2.18	0.44
1:I:291:LEU:HD22	1:K:143:THR:HG21	1.99	0.44
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.84	0.44
1:B:258:SER:O	1:B:260:THR:N	2.51	0.44
1:C:103:ARG:HG2	1:C:104:ALA:H	1.80	0.44
1:C:60:VAL:O	1:C:61:ALA:C	2.55	0.44
1:D:163:TYR:O	1:D:164:ARG:C	2.55	0.44
1:F:127:GLU:CD	1:F:242:PRO:HB3	2.37	0.44
1:F:164:ARG:O	1:F:167:ARG:HB3	2.17	0.44
1:F:167:ARG:HG2	1:F:167:ARG:NH1	2.32	0.44
1:G:335:ARG:HB2	1:G:335:ARG:HE	1.66	0.44
1:G:398:GLN:HB3	1:G:401:ILE:HD12	1.98	0.44
1:J:223:SER:HA	1:J:233:VAL:HG21	1.98	0.44
1:L:259:ALA:HA	1:L:263:LEU:HB2	2.00	0.44
1:J:83:ASN:O	1:L:268:ASP:HB2	2.18	0.44
1:A:145:MET:HG2	1:A:149:LEU:HD12	1.98	0.44
1:A:393:GLU:OE2	1:D:308:LYS:HD2	2.17	0.44
1:B:106:PHE:O	1:B:108:TYR:N	2.51	0.44
1:B:208:SER:HA	1:B:209:PRO:C	2.38	0.44
1:D:217:VAL:CG1	1:D:222:VAL:HG21	2.47	0.44
1:F:159:THR:HA	1:F:184:ILE:O	2.17	0.44
1:F:308:LYS:HD2	1:G:393:GLU:OE2	2.17	0.44
1:J:159:THR:HA	1:J:184:ILE:O	2.17	0.44
1:K:72:ILE:HG23	1:K:72:ILE:O	2.17	0.44
1:A:106:PHE:O	1:A:107:GLU:HB3	2.18	0.44
1:A:127:GLU:OE2	1:A:242:PRO:HB3	2.18	0.44
1:A:133:LEU:HD23	1:A:135:MET:HE3	1.99	0.44
1:B:145:MET:HE1	1:B:146:LEU:HD23	2.00	0.44
1:B:258:SER:C	1:B:260:THR:H	2.21	0.44
1:B:215:ARG:NH1	1:B:347:GLU:OE2	2.46	0.44
1:C:113:ASN:O	1:C:117:VAL:HG13	2.18	0.44
1:D:250:LEU:CD1	1:D:354:GLN:HB2	2.46	0.44
1:F:241:THR:HG23	1:F:242:PRO:HD2	1.98	0.44
1:F:428:VAL:CG1	1:F:428:VAL:O	2.65	0.44
1:H:234:CYS:HA	1:H:254:LEU:O	2.18	0.44
1:J:135:MET:CE	1:J:141:ALA:HA	2.48	0.44
1:L:113:ASN:OD1	1:L:115:THR:N	2.49	0.44
1:A:345:HIS:HE1	1:A:347:GLU:HG2	1.83	0.44
1:B:393:GLU:OE2	1:C:308:LYS:HD2	2.17	0.44
1:D:217:VAL:O	1:D:219:ILE:N	2.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:VAL:O	1:D:64:ALA:N	2.50	0.44
1:F:160:THR:HG22	1:F:183:VAL:HG12	1.99	0.44
1:G:167:ARG:HG2	1:G:167:ARG:HH11	1.83	0.44
1:J:259:ALA:HA	1:J:263:LEU:HB2	1.98	0.44
1:K:217:VAL:HG13	1:K:222:VAL:HG21	1.99	0.44
1:K:343:GLN:HE21	1:K:343:GLN:HB3	1.61	0.44
1:B:209:PRO:HG3	1:B:355:MET:HE1	1.99	0.44
1:C:347:GLU:HB3	1:C:350:ILE:HD12	2.00	0.44
1:D:320:THR:O	1:D:324:MET:HB2	2.18	0.44
1:E:208:SER:HA	1:E:209:PRO:C	2.38	0.44
1:E:94:GLU:O	1:E:95:LEU:C	2.55	0.44
1:F:333:LYS:HE2	1:F:445:ILE:C	2.38	0.44
1:G:206:THR:O	1:G:235:ILE:HA	2.18	0.44
1:H:217:VAL:CG1	1:H:222:VAL:HG21	2.48	0.44
1:F:83:ASN:O	1:H:268:ASP:HB2	2.18	0.44
1:L:374:ALA:O	1:L:377:VAL:HG22	2.17	0.44
1:L:333:LYS:HE2	1:L:445:ILE:HG22	2.00	0.44
1:A:331:HIS:CE1	1:A:333:LYS:HB2	2.52	0.43
1:C:114:PRO:O	1:C:117:VAL:HG22	2.18	0.43
1:D:117:VAL:HA	1:D:120:GLU:HB2	2.00	0.43
1:E:291:LEU:O	1:G:140:CYS:HA	2.17	0.43
1:F:278:LEU:O	1:F:280:LEU:N	2.51	0.43
1:G:386:ALA:HB1	1:G:387:PRO:CD	2.48	0.43
1:H:244:ASN:O	1:H:245:GLN:HB3	2.18	0.43
1:H:93:SER:O	1:H:96:ILE:HB	2.18	0.43
1:I:343:GLN:HB3	1:I:343:GLN:HE21	1.62	0.43
1:B:64:ALA:O	1:B:122:LYS:HE2	2.18	0.43
1:C:317:GLN:HG2	1:C:427:GLY:O	2.18	0.43
1:E:116:THR:O	1:E:119:LEU:N	2.51	0.43
1:F:217:VAL:O	1:F:219:ILE:N	2.51	0.43
1:H:115:THR:CG2	1:H:297:PRO:HB3	2.48	0.43
1:H:411:ASP:O	1:H:414:LYS:HB2	2.18	0.43
1:I:258:SER:O	1:I:260:THR:N	2.51	0.43
1:J:215:ARG:HD2	1:J:347:GLU:OE2	2.18	0.43
1:J:386:ALA:HB1	1:J:387:PRO:CD	2.48	0.43
1:J:73:VAL:O	1:J:74:THR:HG23	2.18	0.43
1:B:192:LEU:HD21	1:B:222:VAL:HG13	2.01	0.43
1:D:141:ALA:HB1	1:D:274:ILE:HD11	2.00	0.43
1:D:122:LYS:NZ	1:D:308:LYS:HE2	2.33	0.43
1:D:94:GLU:O	1:D:95:LEU:C	2.56	0.43
1:E:161:ASP:HB3	1:E:210:THR:OG1	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:LEU:HD12	1:E:422:VAL:H	1.83	0.43
1:F:73:VAL:O	1:F:74:THR:HG23	2.19	0.43
1:G:287:LEU:O	1:G:287:LEU:HD12	2.19	0.43
1:G:370:LEU:HD23	1:G:419:ASP:CB	2.45	0.43
1:H:260:THR:HG23	1:H:270:LEU:HD22	2.00	0.43
1:H:423:ARG:NH2	2:H:507:HEN:O2B	2.51	0.43
1:L:113:ASN:OD1	1:L:115:THR:HG22	2.17	0.43
1:A:234:CYS:HA	1:A:254:LEU:O	2.17	0.43
1:A:325:ALA:O	1:A:328:LEU:HB2	2.18	0.43
1:C:428:VAL:O	1:C:428:VAL:HG13	2.18	0.43
1:H:320:THR:O	1:H:324:MET:HB2	2.17	0.43
1:H:331:HIS:ND1	1:H:332:PRO:HD2	2.33	0.43
1:I:161:ASP:HB3	1:I:210:THR:OG1	2.17	0.43
1:I:243:LEU:CD1	1:I:311:HIS:HA	2.48	0.43
1:K:270:LEU:O	1:K:271:ALA:HB2	2.18	0.43
1:L:241:THR:HG23	1:L:242:PRO:HD2	1.98	0.43
1:A:192:LEU:HG	1:A:196:LEU:HD23	2.00	0.43
1:C:210:THR:HG22	1:C:215:ARG:N	2.24	0.43
1:C:345:HIS:CE1	1:C:347:GLU:HG2	2.53	0.43
1:C:439:LEU:C	1:C:441:ALA:N	2.71	0.43
1:E:133:LEU:CD1	1:E:285:ARG:HD3	2.48	0.43
1:E:333:LYS:HE2	1:E:445:ILE:CG2	2.48	0.43
1:G:260:THR:CG2	1:G:270:LEU:HD22	2.48	0.43
1:H:117:VAL:HA	1:H:120:GLU:HB2	2.00	0.43
1:H:192:LEU:HG	1:H:196:LEU:HD23	2.01	0.43
1:H:240:ALA:O	1:H:244:ASN:HB2	2.19	0.43
1:H:94:GLU:O	1:H:95:LEU:C	2.57	0.43
1:I:156:ILE:HG23	1:I:181:ALA:CB	2.47	0.43
1:I:216:CYS:SG	1:I:355:MET:CE	3.07	0.43
1:J:241:THR:HG23	1:J:242:PRO:HD2	2.00	0.43
1:C:260:THR:CG2	1:C:270:LEU:HD22	2.49	0.43
1:C:323:ARG:O	1:C:327:ILE:HG13	2.19	0.43
1:D:127:GLU:OE2	1:D:257:HIS:NE2	2.52	0.43
1:D:135:MET:CE	1:D:141:ALA:HA	2.43	0.43
1:G:129:ALA:HB2	1:G:248:LEU:CD1	2.47	0.43
1:H:64:ALA:O	1:H:122:LYS:HE2	2.19	0.43
1:H:156:ILE:CG2	1:H:181:ALA:HB2	2.48	0.43
1:H:196:LEU:HD13	1:H:196:LEU:HA	1.82	0.43
1:I:339:TYR:CD1	1:I:362:VAL:HG22	2.54	0.43
1:J:143:THR:HG23	1:J:169:PHE:CE1	2.53	0.43
1:J:219:ILE:HG21	1:J:250:LEU:HB2	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:324:MET:HG2	1:J:431:PHE:CE1	2.53	0.43
1:L:117:VAL:HG23	1:L:118:VAL:N	2.34	0.43
1:L:203:LEU:HB2	1:L:232:LEU:HB2	2.01	0.43
1:L:421:LEU:HD12	1:L:422:VAL:H	1.82	0.43
1:A:159:THR:HA	1:A:184:ILE:O	2.19	0.43
1:A:209:PRO:HG3	1:A:355:MET:HE1	2.00	0.43
1:B:150:VAL:HB	1:B:179:ILE:HD13	2.01	0.43
1:B:244:ASN:O	1:B:245:GLN:HB3	2.19	0.43
1:B:373:THR:OG1	1:B:420:ASN:HA	2.18	0.43
1:C:211:ASN:HA	1:C:212:PRO:HA	1.87	0.43
1:C:240:ALA:O	1:C:241:THR:CB	2.56	0.43
1:D:113:ASN:O	1:D:117:VAL:HG13	2.19	0.43
1:D:209:PRO:HG3	1:D:355:MET:HE1	2.01	0.43
1:E:146:LEU:O	1:E:150:VAL:HG23	2.18	0.43
1:F:156:ILE:CG2	1:F:181:ALA:HB2	2.48	0.43
1:F:270:LEU:HD23	1:F:270:LEU:N	2.34	0.43
1:F:87:TYR:OH	1:F:113:ASN:HA	2.18	0.43
1:G:261:LYS:O	1:G:265:GLY:HA2	2.19	0.43
1:G:389:PHE:HB2	1:G:425:SER:OG	2.18	0.43
1:I:187:ALA:O	1:I:189:VAL:N	2.51	0.43
1:J:320:THR:HG23	1:J:431:PHE:HD1	1.84	0.43
1:L:204:PHE:CE2	1:L:222:VAL:HG11	2.53	0.43
1:L:322:LEU:O	1:L:325:ALA:HB3	2.19	0.43
1:A:58:GLY:HA3	1:A:311:HIS:CD2	2.54	0.43
1:E:119:LEU:HG	1:E:134:LEU:HD11	2.00	0.43
1:F:82:VAL:HG12	1:F:84:THR:HG22	2.01	0.43
1:G:103:ARG:HG2	1:G:104:ALA:N	2.34	0.43
1:G:121:GLU:O	1:G:124:SER:HB2	2.19	0.43
1:G:376:PHE:CE1	1:G:442:LEU:HG	2.54	0.43
1:G:426:PHE:HE1	1:G:438:ILE:HD11	1.84	0.43
1:I:258:SER:C	1:I:260:THR:N	2.72	0.43
1:I:256:LEU:HB2	1:I:274:ILE:HG12	2.00	0.43
1:J:343:GLN:HB3	1:J:343:GLN:HE21	1.56	0.43
1:L:103:ARG:HG2	1:L:104:ALA:N	2.34	0.43
1:L:74:THR:C	1:L:76:ALA:H	2.22	0.43
1:A:269:VAL:C	1:A:270:LEU:HD23	2.39	0.43
1:A:336:HIS:HB3	1:A:365:GLU:HG3	2.00	0.43
1:A:79:THR:HA	1:A:80:PRO:HD3	1.90	0.43
1:B:103:ARG:HG2	1:B:104:ALA:N	2.34	0.43
1:C:156:ILE:CG2	1:C:181:ALA:HB2	2.49	0.43
1:D:260:THR:CG2	1:D:270:LEU:HD22	2.49	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:MET:HB3	1:D:290:ILE:O	2.19	0.43
1:E:159:THR:HA	1:E:184:ILE:O	2.19	0.43
1:E:209:PRO:HD3	1:E:240:ALA:HB2	2.00	0.43
1:E:311:HIS:CD2	1:E:312:LEU:HD23	2.54	0.43
1:F:196:LEU:HD12	1:F:229:LYS:HB2	2.00	0.43
1:G:167:ARG:NH1	1:G:167:ARG:HG2	2.33	0.43
1:J:211:ASN:HA	1:J:212:PRO:HA	1.88	0.43
1:L:196:LEU:HD12	1:L:229:LYS:HB2	2.01	0.43
1:L:248:LEU:HA	1:L:248:LEU:HD23	1.87	0.43
1:L:443:ASP:C	1:L:445:ILE:N	2.72	0.43
1:L:94:GLU:O	1:L:97:ASP:HB2	2.18	0.43
1:B:217:VAL:CG1	1:B:222:VAL:HG21	2.49	0.43
1:C:160:THR:HG23	1:C:184:ILE:O	2.19	0.43
1:D:259:ALA:HB3	1:D:271:ALA:HB3	2.00	0.43
1:C:87:TYR:HA	1:D:75:ASP:O	2.18	0.43
1:E:192:LEU:HD21	1:E:222:VAL:HG13	2.01	0.43
1:E:310:LEU:O	1:E:314:VAL:HG23	2.18	0.43
1:E:370:LEU:HD23	1:E:419:ASP:CB	2.46	0.43
1:F:258:SER:O	1:F:260:THR:N	2.52	0.43
1:F:312:LEU:HD23	1:F:312:LEU:N	2.34	0.43
1:F:386:ALA:HB1	1:F:387:PRO:CD	2.49	0.43
1:G:204:PHE:CE2	1:G:222:VAL:HG11	2.54	0.43
1:G:234:CYS:HA	1:G:254:LEU:O	2.19	0.43
1:E:384:TYR:CZ	1:H:67:ARG:HD2	2.53	0.43
1:J:243:LEU:CD1	1:J:311:HIS:HA	2.49	0.43
1:A:320:THR:O	1:A:324:MET:HB2	2.17	0.42
1:C:262:PHE:CE1	1:C:390:GLY:HA2	2.54	0.42
1:C:164:ARG:HD3	1:C:404:TYR:CE2	2.54	0.42
1:D:138:GLY:O	1:D:141:ALA:HB3	2.19	0.42
1:D:270:LEU:N	1:D:270:LEU:HD23	2.33	0.42
1:E:187:ALA:O	1:E:189:VAL:HG23	2.19	0.42
1:G:211:ASN:HB2	1:G:239:PHE:HE2	1.83	0.42
1:G:373:THR:OG1	1:G:420:ASN:HA	2.19	0.42
1:J:187:ALA:O	1:J:189:VAL:N	2.52	0.42
1:K:265:GLY:HA3	1:K:313:ARG:NH1	2.34	0.42
1:K:416:GLY:O	1:K:418:MET:HG2	2.19	0.42
1:L:206:THR:O	1:L:235:ILE:HA	2.19	0.42
1:A:160:THR:HG23	1:A:184:ILE:O	2.19	0.42
1:A:439:LEU:HA	1:A:442:LEU:HD12	2.01	0.42
1:B:161:ASP:HB3	1:B:210:THR:OG1	2.19	0.42
1:B:60:VAL:CG1	1:B:64:ALA:HB2	2.49	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:HD22	1:C:143:THR:HG21	2.01	0.42
1:C:140:CYS:O	1:C:144:VAL:HG23	2.19	0.42
1:C:185:ASP:OD1	1:C:215:ARG:NH2	2.52	0.42
1:D:158:THR:HA	1:D:205:PHE:O	2.19	0.42
1:G:260:THR:HG23	1:G:270:LEU:HD22	2.01	0.42
1:H:243:LEU:CD1	1:H:311:HIS:HA	2.50	0.42
1:K:211:ASN:HB2	1:K:239:PHE:CE2	2.54	0.42
1:K:243:LEU:CD1	1:K:311:HIS:HA	2.50	0.42
1:J:291:LEU:HD22	1:L:143:THR:HG21	2.00	0.42
1:A:117:VAL:O	1:A:121:GLU:HG3	2.19	0.42
1:A:398:GLN:O	1:A:399:PRO:C	2.58	0.42
1:A:50:TYR:OH	1:A:68:LEU:HB2	2.19	0.42
1:C:87:TYR:OH	1:C:113:ASN:HA	2.19	0.42
1:D:64:ALA:O	1:D:122:LYS:HE2	2.19	0.42
1:D:60:VAL:HG12	1:D:64:ALA:HB2	2.01	0.42
1:E:206:THR:O	1:E:235:ILE:HA	2.19	0.42
1:H:215:ARG:HD2	1:H:347:GLU:OE2	2.19	0.42
1:I:160:THR:HG23	1:I:184:ILE:O	2.19	0.42
1:J:106:PHE:O	1:J:108:TYR:N	2.52	0.42
1:J:164:ARG:O	1:J:167:ARG:HB3	2.19	0.42
1:J:174:LEU:N	1:J:175:PRO:CD	2.83	0.42
1:J:211:ASN:HB2	1:J:239:PHE:HE2	1.83	0.42
1:J:95:LEU:O	1:J:95:LEU:HD12	2.18	0.42
1:K:398:GLN:O	1:K:401:ILE:N	2.51	0.42
1:L:165:LYS:HA	1:L:168:ILE:HD12	2.01	0.42
1:L:238:THR:HB	2:L:511:HEN:H2A2	2.00	0.42
1:B:345:HIS:HE1	1:B:347:GLU:HG2	1.83	0.42
1:C:243:LEU:CD1	1:C:311:HIS:HA	2.49	0.42
1:C:63:HIS:CD2	1:C:67:ARG:HD3	2.54	0.42
1:F:117:VAL:HG23	1:F:118:VAL:N	2.35	0.42
1:H:110:ARG:HD3	1:H:292:GLY:CA	2.50	0.42
1:H:259:ALA:HA	1:H:263:LEU:HB2	2.01	0.42
1:I:135:MET:HE1	1:I:141:ALA:HA	2.01	0.42
1:I:135:MET:HE1	1:I:274:ILE:HD12	2.02	0.42
1:K:58:GLY:HA3	1:K:311:HIS:CD2	2.55	0.42
1:K:377:VAL:HG23	1:K:378:ASP:N	2.34	0.42
1:K:72:ILE:O	1:K:72:ILE:HG12	2.18	0.42
1:B:163:TYR:O	1:B:164:ARG:C	2.58	0.42
1:B:217:VAL:HG13	1:B:222:VAL:HG21	2.02	0.42
1:D:331:HIS:CG	1:D:332:PRO:HD2	2.54	0.42
1:F:126:LEU:HD23	1:F:126:LEU:HA	1.82	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:TYR:O	1:F:164:ARG:C	2.58	0.42
1:I:238:THR:HB	2:I:508:HEN:H2A2	2.01	0.42
1:J:126:LEU:HA	1:J:126:LEU:HD23	1.80	0.42
1:J:173:ILE:O	1:J:176:LYS:HB2	2.18	0.42
1:J:428:VAL:HG13	1:J:428:VAL:O	2.20	0.42
1:K:150:VAL:HB	1:K:179:ILE:HD13	2.01	0.42
1:L:234:CYS:HA	1:L:254:LEU:O	2.19	0.42
1:A:211:ASN:ND2	1:A:212:PRO:N	2.67	0.42
1:B:313:ARG:O	1:B:317:GLN:HG3	2.20	0.42
1:C:250:LEU:CD1	1:C:354:GLN:HB2	2.50	0.42
1:D:322:LEU:O	1:D:325:ALA:HB3	2.20	0.42
1:I:389:PHE:HB2	1:I:425:SER:HB2	2.02	0.42
1:K:321:ALA:HB2	1:K:360:GLY:HA2	2.01	0.42
1:L:123:ILE:HD13	1:L:273:CYS:SG	2.60	0.42
1:L:242:PRO:HD3	1:L:257:HIS:CE1	2.54	0.42
1:A:209:PRO:HD3	1:A:240:ALA:HB2	2.02	0.42
1:A:313:ARG:O	1:A:317:GLN:HG3	2.19	0.42
1:A:373:THR:OG1	1:A:420:ASN:HA	2.19	0.42
1:B:173:ILE:O	1:B:176:LYS:HB2	2.20	0.42
1:D:394:SER:C	1:D:395:ILE:HG13	2.38	0.42
1:E:346:PRO:HB2	1:E:347:GLU:OE2	2.20	0.42
1:G:146:LEU:O	1:G:150:VAL:HG23	2.20	0.42
1:G:192:LEU:HG	1:G:196:LEU:HD23	2.02	0.42
1:H:163:TYR:O	1:H:164:ARG:C	2.58	0.42
1:J:331:HIS:HB3	1:J:334:VAL:HG23	2.01	0.42
1:J:72:ILE:O	1:J:72:ILE:HG12	2.20	0.42
1:J:82:VAL:HG12	1:J:84:THR:HG22	2.00	0.42
1:K:106:PHE:O	1:K:107:GLU:HB3	2.19	0.42
1:K:63:HIS:HD2	1:K:67:ARG:HD3	1.83	0.42
1:A:223:SER:HA	1:A:233:VAL:HG21	2.01	0.42
1:A:133:LEU:CD1	1:A:285:ARG:HD3	2.50	0.42
1:B:173:ILE:C	1:B:175:PRO:HD2	2.39	0.42
1:E:141:ALA:O	1:E:142:SER:C	2.58	0.42
1:E:150:VAL:CG1	1:E:179:ILE:HD13	2.49	0.42
1:E:156:ILE:HG23	1:E:181:ALA:CB	2.50	0.42
1:E:438:ILE:O	1:E:442:LEU:HD12	2.20	0.42
1:G:269:VAL:C	1:G:270:LEU:HD23	2.40	0.42
1:G:63:HIS:CD2	1:G:67:ARG:HD3	2.55	0.42
1:I:141:ALA:HB1	1:I:274:ILE:HD11	2.02	0.42
1:J:277:PRO:HG2	1:J:280:LEU:HB2	2.01	0.42
1:J:394:SER:HB2	1:J:429:GLU:OE2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:TYR:CD1	1:D:362:VAL:HG22	2.55	0.42
1:E:174:LEU:N	1:E:175:PRO:CD	2.80	0.42
1:E:211:ASN:HA	1:E:212:PRO:HA	1.82	0.42
1:E:60:VAL:O	1:E:61:ALA:C	2.57	0.42
1:G:72:ILE:HG23	1:G:72:ILE:O	2.20	0.42
1:H:172:THR:O	1:H:175:PRO:HG2	2.20	0.42
1:I:242:PRO:HD3	1:I:257:HIS:CE1	2.55	0.42
1:I:60:VAL:HG13	1:I:64:ALA:HB2	2.01	0.42
1:K:156:ILE:CG2	1:K:181:ALA:HB2	2.50	0.42
1:K:156:ILE:HG23	1:K:181:ALA:CB	2.50	0.42
1:K:156:ILE:O	1:K:181:ALA:HA	2.20	0.42
1:L:345:HIS:HE1	1:L:347:GLU:HG2	1.82	0.42
1:A:156:ILE:HG13	1:A:203:LEU:HD23	2.00	0.42
1:A:83:ASN:O	1:B:78:THR:OG1	2.33	0.42
1:B:243:LEU:CD1	1:B:311:HIS:HA	2.50	0.42
1:C:60:VAL:O	1:C:64:ALA:N	2.51	0.42
1:D:145:MET:HE1	1:D:146:LEU:HD23	2.01	0.42
1:D:196:LEU:HD12	1:D:229:LYS:HB2	2.02	0.42
1:E:60:VAL:CG1	1:E:64:ALA:HB2	2.50	0.42
1:F:146:LEU:O	1:F:150:VAL:HG23	2.19	0.42
1:G:94:GLU:O	1:G:97:ASP:HB2	2.20	0.42
1:I:126:LEU:HD23	1:I:126:LEU:HA	1.78	0.42
1:I:374:ALA:O	1:I:377:VAL:HG22	2.20	0.42
1:J:60:VAL:CG1	1:J:64:ALA:HB2	2.50	0.42
1:K:234:CYS:HA	1:K:254:LEU:O	2.20	0.42
1:L:217:VAL:HG13	1:L:222:VAL:HG21	2.02	0.42
1:B:242:PRO:HD3	1:B:257:HIS:CE1	2.54	0.41
1:F:196:LEU:HD13	1:F:196:LEU:HA	1.81	0.41
1:G:205:PHE:HE1	1:G:256:LEU:HD21	1.85	0.41
1:H:110:ARG:HD3	1:H:292:GLY:HA2	2.01	0.41
1:J:192:LEU:HG	1:J:196:LEU:HD23	2.02	0.41
1:J:206:THR:O	1:J:235:ILE:HA	2.20	0.41
1:J:421:LEU:HD12	1:J:422:VAL:H	1.85	0.41
1:K:398:GLN:O	1:K:399:PRO:C	2.58	0.41
1:K:52:SER:OG	1:K:53:PHE:N	2.53	0.41
1:L:324:MET:HG2	1:L:431:PHE:CE1	2.55	0.41
1:A:208:SER:HA	1:A:209:PRO:C	2.39	0.41
1:A:339:TYR:CD1	1:A:362:VAL:HG22	2.55	0.41
1:A:398:GLN:O	1:A:400:ALA:N	2.53	0.41
1:B:331:HIS:CG	1:B:332:PRO:HD2	2.55	0.41
1:C:383:PRO:HA	1:C:394:SER:O	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ALA:O	1:D:189:VAL:N	2.53	0.41
1:A:428:VAL:HG12	1:D:62:ILE:HD11	2.03	0.41
1:E:280:LEU:HA	1:E:280:LEU:HD23	1.91	0.41
1:F:161:ASP:HB3	1:F:210:THR:OG1	2.20	0.41
1:F:268:ASP:HB2	1:H:83:ASN:O	2.20	0.41
1:F:60:VAL:O	1:F:61:ALA:C	2.57	0.41
1:F:60:VAL:O	1:F:62:ILE:N	2.54	0.41
1:G:366:VAL:O	1:G:420:ASN:HB3	2.21	0.41
1:G:428:VAL:HG13	1:G:428:VAL:O	2.20	0.41
1:H:207:GLU:OE1	2:H:507:HEN:H2A3	2.19	0.41
1:J:238:THR:HB	2:J:509:HEN:H2A2	2.02	0.41
1:J:442:LEU:C	1:J:444:SER:N	2.74	0.41
1:K:270:LEU:N	1:K:270:LEU:HD23	2.34	0.41
1:A:73:VAL:O	1:A:74:THR:HG23	2.20	0.41
1:B:369:ASP:O	1:B:370:LEU:C	2.59	0.41
1:C:72:ILE:O	1:C:72:ILE:HG23	2.20	0.41
1:D:209:PRO:HA	1:D:215:ARG:O	2.20	0.41
1:D:211:ASN:HB2	1:D:239:PHE:HE2	1.85	0.41
1:D:278:LEU:O	1:D:280:LEU:N	2.53	0.41
1:E:159:THR:HG23	1:E:206:THR:HB	2.01	0.41
1:F:219:ILE:HB	1:F:250:LEU:HD12	2.01	0.41
1:G:207:GLU:CB	1:G:236:ASP:HB3	2.45	0.41
1:L:196:LEU:HA	1:L:196:LEU:HD13	1.82	0.41
1:A:121:GLU:O	1:A:124:SER:HB2	2.20	0.41
1:A:335:ARG:HE	1:A:335:ARG:HB2	1.71	0.41
1:B:238:THR:HB	2:B:501:HEN:H2A2	2.00	0.41
1:C:145:MET:HG2	1:C:149:LEU:HD12	2.02	0.41
1:C:170:ILE:HG23	1:C:174:LEU:HD12	2.01	0.41
1:E:336:HIS:O	1:E:364:PHE:HB2	2.20	0.41
1:F:208:SER:HA	1:F:209:PRO:C	2.39	0.41
1:F:393:GLU:OE2	1:G:308:LYS:HD2	2.21	0.41
1:H:196:LEU:HD12	1:H:229:LYS:HB2	2.01	0.41
1:H:89:PHE:CD2	1:H:95:LEU:HA	2.55	0.41
1:I:145:MET:HG2	1:I:149:LEU:HD12	2.03	0.41
1:I:383:PRO:HB3	1:I:394:SER:HB3	2.03	0.41
1:K:208:SER:HA	1:K:209:PRO:C	2.41	0.41
1:K:260:THR:CG2	1:K:270:LEU:HD22	2.51	0.41
1:K:79:THR:HA	1:K:80:PRO:HD3	1.89	0.41
1:L:428:VAL:HG13	1:L:428:VAL:O	2.20	0.41
1:A:420:ASN:O	1:A:422:VAL:HG23	2.21	0.41
1:A:60:VAL:O	1:A:61:ALA:C	2.58	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:THR:HG22	1:B:215:ARG:N	2.24	0.41
1:C:331:HIS:CG	1:C:332:PRO:HD2	2.56	0.41
1:C:82:VAL:HG22	1:D:80:PRO:HB3	2.02	0.41
1:D:210:THR:CG2	1:D:215:ARG:H	2.29	0.41
1:D:82:VAL:HG12	1:D:84:THR:HG22	2.01	0.41
1:E:290:ILE:O	1:G:139:MET:HB3	2.20	0.41
1:H:260:THR:CG2	1:H:270:LEU:HD22	2.49	0.41
1:H:296:ASN:OD1	1:H:298:ASN:HB2	2.21	0.41
1:H:347:GLU:CB	1:H:350:ILE:HD12	2.50	0.41
1:H:94:GLU:O	1:H:97:ASP:HB2	2.20	0.41
1:J:158:THR:HA	1:J:205:PHE:O	2.20	0.41
1:K:114:PRO:O	1:K:117:VAL:HG22	2.20	0.41
1:I:83:ASN:O	1:K:268:ASP:HB2	2.20	0.41
1:A:60:VAL:HG12	1:A:64:ALA:HB2	2.02	0.41
1:B:187:ALA:O	1:B:189:VAL:N	2.54	0.41
1:D:262:PHE:CE1	1:D:390:GLY:HA2	2.55	0.41
1:E:343:GLN:HB3	1:E:343:GLN:HE21	1.63	0.41
1:F:141:ALA:HB1	1:F:274:ILE:HD11	2.01	0.41
1:F:60:VAL:CG1	1:F:64:ALA:HB2	2.50	0.41
1:F:94:GLU:O	1:F:97:ASP:HB2	2.21	0.41
1:F:140:CYS:HB2	1:H:292:GLY:O	2.20	0.41
1:I:345:HIS:HE1	1:I:347:GLU:HG2	1.85	0.41
1:J:163:TYR:O	1:J:164:ARG:C	2.59	0.41
1:J:373:THR:OG1	1:J:420:ASN:HA	2.20	0.41
1:J:382:ILE:HB	1:J:383:PRO:HD3	2.03	0.41
1:J:58:GLY:HA3	1:J:311:HIS:CD2	2.55	0.41
1:K:135:MET:HE2	1:K:274:ILE:HD12	2.01	0.41
1:K:163:TYR:O	1:K:164:ARG:C	2.59	0.41
1:K:243:LEU:HD12	1:K:314:VAL:HG21	2.02	0.41
1:L:106:PHE:O	1:L:108:TYR:N	2.54	0.41
1:L:336:HIS:HB3	1:L:365:GLU:HG3	2.01	0.41
1:L:394:SER:HB2	1:L:429:GLU:OE2	2.19	0.41
1:A:64:ALA:O	1:A:122:LYS:HE2	2.21	0.41
1:A:57:ASP:HB3	1:A:243:LEU:CD2	2.51	0.41
1:A:259:ALA:HA	1:A:263:LEU:HB2	2.02	0.41
1:C:141:ALA:HB1	1:C:274:ILE:HD11	2.02	0.41
1:C:140:CYS:O	1:C:143:THR:HB	2.21	0.41
1:C:331:HIS:ND1	1:C:332:PRO:HD2	2.35	0.41
1:C:343:GLN:HE21	1:C:343:GLN:HB3	1.57	0.41
1:D:50:TYR:HB3	1:D:51:ALA:H	1.68	0.41
1:E:243:LEU:HD12	1:E:314:VAL:HG21	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:MET:HE2	1:F:141:ALA:HA	2.02	0.41
1:G:156:ILE:CG2	1:G:181:ALA:HB2	2.51	0.41
1:G:60:VAL:O	1:G:64:ALA:N	2.46	0.41
1:H:159:THR:HG23	1:H:206:THR:HB	2.02	0.41
1:F:85:SER:OG	1:H:267:ASN:HA	2.21	0.41
1:H:119:LEU:HD21	1:H:303:ILE:HG21	2.01	0.41
1:H:345:HIS:HA	1:H:346:PRO:HD3	1.95	0.41
1:I:376:PHE:HB2	1:I:445:ILE:HD12	2.03	0.41
1:J:170:ILE:HA	1:J:174:LEU:CD1	2.40	0.41
1:J:63:HIS:CD2	1:J:67:ARG:HD3	2.56	0.41
1:K:174:LEU:N	1:K:175:PRO:CD	2.82	0.41
1:K:217:VAL:O	1:K:219:ILE:N	2.52	0.41
1:L:57:ASP:HB3	1:L:243:LEU:CD2	2.50	0.41
1:L:305:ARG:O	1:L:308:LYS:HB2	2.21	0.41
1:A:383:PRO:HB2	1:A:396:VAL:CG2	2.35	0.41
1:B:206:THR:OG1	1:B:207:GLU:N	2.54	0.41
1:B:389:PHE:HB2	1:B:425:SER:HB2	2.03	0.41
1:C:143:THR:HG23	1:C:169:PHE:CE1	2.56	0.41
1:F:348:HIS:O	1:F:352:LYS:HB2	2.20	0.41
1:G:106:PHE:O	1:G:107:GLU:HB3	2.21	0.41
1:G:158:THR:HA	1:G:205:PHE:O	2.21	0.41
1:G:261:LYS:HB2	1:G:262:PHE:H	1.70	0.41
1:H:138:GLY:O	1:H:141:ALA:HB3	2.20	0.41
1:I:258:SER:C	1:I:260:THR:H	2.23	0.41
1:I:320:THR:HG23	1:I:431:PHE:HD1	1.85	0.41
1:I:72:ILE:HG23	1:I:72:ILE:O	2.20	0.41
1:J:331:HIS:CG	1:J:332:PRO:HD2	2.55	0.41
1:J:438:ILE:O	1:J:441:ALA:HB3	2.21	0.41
2:I:508:HEN:P	1:K:110:ARG:HH21	2.43	0.41
1:K:194:LEU:O	1:K:198:GLN:HG3	2.21	0.41
1:K:258:SER:C	1:K:260:THR:N	2.74	0.41
1:L:260:THR:CG2	1:L:270:LEU:HD22	2.50	0.41
1:A:397:ASP:OD1	1:A:399:PRO:HD3	2.21	0.41
1:B:103:ARG:HG2	1:B:104:ALA:H	1.85	0.41
1:B:143:THR:HG23	1:B:169:PHE:CE1	2.56	0.41
1:C:192:LEU:HG	1:C:196:LEU:HD23	2.03	0.41
1:D:174:LEU:N	1:D:175:PRO:CD	2.84	0.41
1:E:114:PRO:O	1:E:117:VAL:HG22	2.21	0.41
1:E:155:HIS:ND1	1:E:180:THR:O	2.54	0.41
1:E:204:PHE:CE2	1:E:222:VAL:HG11	2.56	0.41
1:E:302:LEU:HA	1:E:302:LEU:HD23	1.94	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:VAL:HG13	1:F:282:SER:N	2.35	0.41
1:H:208:SER:HA	1:H:209:PRO:C	2.41	0.41
1:J:382:ILE:HB	1:J:383:PRO:CD	2.51	0.41
1:J:261:LYS:HB3	1:J:389:PHE:O	2.21	0.41
1:K:248:LEU:HD23	1:K:248:LEU:HA	1.92	0.41
1:A:187:ALA:O	1:A:189:VAL:HG23	2.21	0.41
1:B:135:MET:CE	1:B:141:ALA:HA	2.51	0.41
1:B:211:ASN:HA	1:B:212:PRO:HA	1.84	0.41
1:B:443:ASP:C	1:B:445:ILE:N	2.74	0.41
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.74	0.41
1:B:67:ARG:HD2	1:C:384:TYR:CZ	2.56	0.41
1:D:240:ALA:O	1:D:244:ASN:HB2	2.20	0.41
1:F:145:MET:HE1	1:F:146:LEU:HD23	2.02	0.41
1:F:343:GLN:HB3	1:F:343:GLN:HE21	1.60	0.41
1:F:365:GLU:HB3	1:F:420:ASN:HB2	2.02	0.41
1:F:420:ASN:O	1:F:422:VAL:HG23	2.21	0.41
1:G:211:ASN:HD22	1:G:212:PRO:N	2.19	0.41
1:H:343:GLN:HE21	1:H:343:GLN:HB3	1.54	0.41
1:I:110:ARG:HH21	2:K:510:HEN:P	2.43	0.41
1:I:291:LEU:O	1:K:140:CYS:HA	2.21	0.41
1:K:145:MET:HE2	1:K:146:LEU:HA	2.01	0.41
1:K:211:ASN:HA	1:K:212:PRO:HA	1.89	0.41
1:L:156:ILE:HG23	1:L:181:ALA:CB	2.51	0.41
1:L:173:ILE:O	1:L:176:LYS:HB2	2.21	0.41
1:L:280:LEU:HD23	1:L:280:LEU:HA	1.95	0.41
1:J:143:THR:HG21	1:L:291:LEU:HD22	2.03	0.41
1:A:243:LEU:HD12	1:A:314:VAL:HG21	2.03	0.41
1:A:383:PRO:HA	1:A:394:SER:O	2.21	0.41
1:A:62:ILE:O	1:A:122:LYS:NZ	2.54	0.41
1:B:270:LEU:HD23	1:B:270:LEU:N	2.36	0.41
1:F:103:ARG:HG2	1:F:104:ALA:N	2.36	0.41
1:G:442:LEU:HD23	1:G:445:ILE:HD12	2.03	0.41
1:H:106:PHE:O	1:H:108:TYR:N	2.54	0.41
1:I:160:THR:HG22	1:I:183:VAL:HG12	2.03	0.41
1:J:113:ASN:OD1	1:J:115:THR:HG22	2.21	0.41
1:J:278:LEU:O	1:J:280:LEU:N	2.54	0.41
1:L:312:LEU:HD23	1:L:312:LEU:N	2.36	0.41
1:L:389:PHE:HB2	1:L:425:SER:OG	2.21	0.41
1:A:211:ASN:HA	1:A:212:PRO:HA	1.83	0.40
1:A:56:SER:OG	1:D:430:ASP:HB2	2.20	0.40
1:B:223:SER:HA	1:B:233:VAL:HG21	2.02	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:HA	1:C:196:LEU:HD13	1.85	0.40
1:C:280:LEU:HA	1:C:280:LEU:HD23	1.87	0.40
1:A:92:THR:OG1	1:C:378:ASP:OD1	2.36	0.40
1:C:420:ASN:O	1:C:422:VAL:HG23	2.21	0.40
1:D:376:PHE:HB2	1:D:445:ILE:CD1	2.38	0.40
1:B:268:ASP:CB	1:D:83:ASN:O	2.68	0.40
1:F:137:SER:O	1:F:138:GLY:C	2.60	0.40
1:H:331:HIS:CE1	1:H:333:LYS:HB2	2.56	0.40
1:H:335:ARG:HB2	1:H:335:ARG:HE	1.58	0.40
1:H:386:ALA:HB1	1:H:387:PRO:CD	2.51	0.40
1:I:350:ILE:O	1:I:354:GLN:HG2	2.21	0.40
1:J:113:ASN:O	1:J:117:VAL:HG13	2.21	0.40
1:J:127:GLU:OE2	1:J:242:PRO:HB3	2.21	0.40
1:J:411:ASP:O	1:J:414:LYS:HB2	2.21	0.40
1:K:377:VAL:CG2	1:K:378:ASP:N	2.84	0.40
1:L:287:LEU:HD12	1:L:287:LEU:O	2.20	0.40
1:B:117:VAL:O	1:B:121:GLU:HG3	2.21	0.40
1:C:258:SER:C	1:C:260:THR:N	2.74	0.40
1:E:322:LEU:O	1:E:325:ALA:HB3	2.21	0.40
1:F:57:ASP:HB3	1:F:243:LEU:CD2	2.51	0.40
1:G:87:TYR:CE1	1:G:106:PHE:HB2	2.56	0.40
1:F:83:ASN:O	1:H:268:ASP:CB	2.70	0.40
1:I:170:ILE:HG23	1:I:174:LEU:HD12	2.02	0.40
1:I:240:ALA:O	1:I:244:ASN:HB2	2.21	0.40
1:I:382:ILE:HD12	1:I:437:ASP:HB2	2.03	0.40
1:J:160:THR:HG23	1:J:184:ILE:O	2.21	0.40
1:J:72:ILE:HD13	1:J:80:PRO:HG2	2.03	0.40
1:K:119:LEU:HD12	1:K:119:LEU:O	2.21	0.40
1:K:339:TYR:CD1	1:K:362:VAL:HG22	2.55	0.40
1:L:211:ASN:HB2	1:L:239:PHE:HE2	1.85	0.40
1:A:277:PRO:O	1:A:281:VAL:HG12	2.21	0.40
1:B:139:MET:HG2	1:D:110:ARG:NH2	2.37	0.40
1:B:377:VAL:CG2	1:B:378:ASP:N	2.84	0.40
1:B:73:VAL:O	1:B:74:THR:HG23	2.21	0.40
2:A:500:HEN:OG2	1:C:111:TYR:HE2	2.03	0.40
1:C:336:HIS:HB3	1:C:365:GLU:HG3	2.04	0.40
1:C:72:ILE:HD13	1:C:80:PRO:HG2	2.02	0.40
1:D:132:THR:HG22	1:D:133:LEU:N	2.36	0.40
1:D:60:VAL:O	1:D:61:ALA:C	2.60	0.40
1:E:141:ALA:HB1	1:E:274:ILE:HD11	2.02	0.40
1:E:260:THR:CG2	1:E:270:LEU:HD22	2.50	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:ASN:HA	1:F:212:PRO:HA	1.87	0.40
1:F:345:HIS:HA	1:F:346:PRO:HD3	1.93	0.40
1:I:94:GLU:O	1:I:97:ASP:HB2	2.22	0.40
1:J:398:GLN:O	1:J:399:PRO:C	2.59	0.40
1:J:99:LYS:HD3	1:J:99:LYS:HA	1.90	0.40
1:K:364:PHE:CD2	1:K:364:PHE:O	2.74	0.40
1:L:187:ALA:O	1:L:189:VAL:N	2.55	0.40
1:A:163:TYR:O	1:A:164:ARG:C	2.60	0.40
1:A:320:THR:HG23	1:A:431:PHE:HD1	1.86	0.40
1:C:160:THR:HG22	1:C:183:VAL:HG12	2.03	0.40
1:C:377:VAL:HG23	1:C:378:ASP:N	2.37	0.40
1:C:79:THR:HA	1:C:80:PRO:HD3	1.93	0.40
1:C:91:LYS:HG3	1:C:94:GLU:HG3	2.03	0.40
1:E:262:PHE:CE1	1:E:390:GLY:HA2	2.56	0.40
1:E:408:SER:OG	1:E:411:ASP:HB2	2.21	0.40
1:E:439:LEU:C	1:E:441:ALA:N	2.74	0.40
1:E:62:ILE:HD11	1:H:428:VAL:HG12	2.03	0.40
1:G:203:LEU:HB2	1:G:232:LEU:HB2	2.02	0.40
1:H:160:THR:HG22	1:H:183:VAL:HG12	2.03	0.40
1:H:439:LEU:C	1:H:441:ALA:N	2.75	0.40
1:I:376:PHE:CE1	1:I:442:LEU:HG	2.56	0.40
1:L:156:ILE:HG13	1:L:203:LEU:HD23	2.02	0.40
1:A:82:VAL:HG21	1:A:114:PRO:HG2	2.02	0.40
1:B:117:VAL:HA	1:B:120:GLU:HB2	2.03	0.40
1:C:258:SER:C	1:C:260:THR:H	2.25	0.40
1:C:259:ALA:HA	1:C:263:LEU:HB2	2.04	0.40
1:D:160:THR:HG22	1:D:183:VAL:HG12	2.03	0.40
1:D:262:PHE:O	1:D:263:LEU:C	2.60	0.40
1:E:416:GLY:O	1:E:418:MET:HG2	2.20	0.40
1:G:305:ARG:O	1:G:308:LYS:HB2	2.21	0.40
1:G:377:VAL:HG23	1:G:378:ASP:N	2.37	0.40
1:I:287:LEU:O	1:I:287:LEU:HD12	2.22	0.40
1:L:382:ILE:HD12	1:L:437:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/445 (88%)	322 (82%)	64 (16%)	8 (2%)	7	38
1	B	394/445 (88%)	320 (81%)	63 (16%)	11 (3%)	5	29
1	C	394/445 (88%)	324 (82%)	56 (14%)	14 (4%)	3	23
1	D	394/445 (88%)	331 (84%)	55 (14%)	8 (2%)	7	38
1	E	394/445 (88%)	327 (83%)	56 (14%)	11 (3%)	5	29
1	F	394/445 (88%)	316 (80%)	69 (18%)	9 (2%)	6	34
1	G	394/445 (88%)	332 (84%)	54 (14%)	8 (2%)	7	38
1	H	394/445 (88%)	327 (83%)	61 (16%)	6 (2%)	10	44
1	I	394/445 (88%)	329 (84%)	52 (13%)	13 (3%)	4	25
1	J	394/445 (88%)	328 (83%)	59 (15%)	7 (2%)	8	41
1	K	394/445 (88%)	325 (82%)	57 (14%)	12 (3%)	4	28
1	L	394/445 (88%)	325 (82%)	60 (15%)	9 (2%)	6	34
All	All	4728/5340 (88%)	3906 (83%)	706 (15%)	116 (2%)	5	32

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	ASP
1	B	188	ASP
1	C	188	ASP
1	D	164	ARG
1	D	188	ASP
1	E	188	ASP
1	F	188	ASP
1	G	188	ASP
1	H	188	ASP
1	I	188	ASP
1	J	188	ASP
1	K	188	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	188	ASP
1	A	164	ARG
1	B	164	ARG
1	B	444	SER
1	C	164	ARG
1	C	265	GLY
1	D	279	LYS
1	D	442	LEU
1	E	164	ARG
1	E	370	LEU
1	F	164	ARG
1	G	164	ARG
1	H	164	ARG
1	I	164	ARG
1	J	164	ARG
1	K	164	ARG
1	K	265	GLY
1	K	279	LYS
1	L	164	ARG
1	C	61	ALA
1	C	279	LYS
1	E	261	LYS
1	F	279	LYS
1	G	265	GLY
1	G	444	SER
1	H	259	ALA
1	I	61	ALA
1	J	279	LYS
1	A	279	LYS
1	B	53	PHE
1	B	241	THR
1	B	259	ALA
1	B	416	GLY
1	C	320	THR
1	C	442	LEU
1	D	107	GLU
1	E	141	ALA
1	E	218	ASP
1	E	294	ALA
1	E	416	GLY
1	E	417	ILE
1	F	107	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	241	THR
1	F	259	ALA
1	H	442	LEU
1	I	218	ASP
1	I	259	ALA
1	I	321	ALA
1	J	107	GLU
1	K	61	ALA
1	K	241	THR
1	L	107	GLU
1	L	370	LEU
1	A	218	ASP
1	A	241	THR
1	A	370	LEU
1	A	399	PRO
1	B	107	GLU
1	B	279	LYS
1	B	370	LEU
1	C	107	GLU
1	C	198	GLN
1	C	241	THR
1	C	319	SER
1	C	370	LEU
1	D	370	LEU
1	E	241	THR
1	H	241	THR
1	I	241	THR
1	I	279	LYS
1	I	370	LEU
1	J	53	PHE
1	J	241	THR
1	K	107	GLU
1	K	259	ALA
1	L	241	THR
1	L	320	THR
1	L	442	LEU
1	A	416	GLY
1	D	241	THR
1	D	416	GLY
1	G	321	ALA
1	G	370	LEU
1	I	265	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	416	GLY
1	K	387	PRO
1	L	399	PRO
1	F	399	PRO
1	G	241	THR
1	L	416	GLY
1	G	219	ILE
1	H	399	PRO
1	I	417	ILE
1	K	417	ILE
1	F	416	GLY
1	I	416	GLY
1	K	399	PRO
1	K	427	GLY
1	B	399	PRO
1	C	399	PRO
1	C	416	GLY
1	E	387	PRO
1	F	417	ILE
1	I	73	VAL

### 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%)	278 (85%)	49 (15%)	3	14
1	B	327/364 (90%)	283 (86%)	44 (14%)	4	18
1	C	327/364 (90%)	275 (84%)	52 (16%)	2	12
1	D	327/364 (90%)	279 (85%)	48 (15%)	3	14
1	E	327/364 (90%)	276 (84%)	51 (16%)	2	12
1	F	327/364 (90%)	274 (84%)	53 (16%)	2	11
1	G	327/364 (90%)	282 (86%)	45 (14%)	3	16
1	H	327/364 (90%)	279 (85%)	48 (15%)	3	14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	327/364 (90%)	284 (87%)	43 (13%)	4	19
1	J	327/364 (90%)	281 (86%)	46 (14%)	3	16
1	K	327/364 (90%)	279 (85%)	48 (15%)	3	14
1	L	327/364 (90%)	283 (86%)	44 (14%)	4	18
All	All	3924/4368 (90%)	3353 (85%)	571 (15%)	3	15

All (571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	56	SER
1	A	70	ARG
1	A	91	LYS
1	A	93	SER
1	A	101	LYS
1	A	115	THR
1	A	134	LEU
1	A	135	MET
1	A	142	SER
1	A	145	MET
1	A	156	ILE
1	A	161	ASP
1	A	162	CYS
1	A	165	LYS
1	A	177	MET
1	A	180	THR
1	A	196	LEU
1	A	199	LYS
1	A	200	LYS
1	A	203	LEU
1	A	210	THR
1	A	211	ASN
1	A	214	LEU
1	A	273	CYS
1	A	275	SER
1	A	278	LEU
1	A	303	ILE
1	A	311	HIS
1	A	315	GLN
1	A	335	ARG
1	A	343	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	344	SER
1	A	347	GLU
1	A	352	LYS
1	A	370	LEU
1	A	394	SER
1	A	396	VAL
1	A	397	ASP
1	A	402	MET
1	A	403	SER
1	A	410	SER
1	A	414	LYS
1	A	420	ASN
1	A	423	ARG
1	A	428	VAL
1	A	430	ASP
1	A	443	ASP
1	A	445	ILE
1	B	52	SER
1	B	56	SER
1	B	70	ARG
1	B	79	THR
1	B	93	SER
1	B	101	LYS
1	B	115	THR
1	B	134	LEU
1	B	135	MET
1	B	142	SER
1	B	145	MET
1	B	156	ILE
1	B	161	ASP
1	B	165	LYS
1	B	177	MET
1	B	180	THR
1	B	196	LEU
1	B	199	LYS
1	B	200	LYS
1	B	203	LEU
1	B	210	THR
1	B	211	ASN
1	B	214	LEU
1	B	273	CYS
1	B	275	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	279	LYS
1	B	303	ILE
1	B	311	HIS
1	B	315	GLN
1	B	335	ARG
1	B	343	GLN
1	B	344	SER
1	B	347	GLU
1	B	352	LYS
1	B	353	LYS
1	B	370	LEU
1	B	396	VAL
1	B	402	MET
1	B	403	SER
1	B	410	SER
1	B	414	LYS
1	B	420	ASN
1	B	430	ASP
1	B	444	SER
1	C	56	SER
1	C	70	ARG
1	C	91	LYS
1	C	93	SER
1	C	100	GLU
1	C	101	LYS
1	C	115	THR
1	C	131	SER
1	C	134	LEU
1	C	135	MET
1	C	142	SER
1	C	145	MET
1	C	156	ILE
1	C	161	ASP
1	C	165	LYS
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	210	THR
1	C	211	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	214	LEU
1	C	223	SER
1	C	224	LYS
1	C	273	CYS
1	C	275	SER
1	C	278	LEU
1	C	279	LYS
1	C	303	ILE
1	C	311	HIS
1	C	315	GLN
1	C	335	ARG
1	C	343	GLN
1	C	344	SER
1	C	347	GLU
1	C	352	LYS
1	C	353	LYS
1	C	370	LEU
1	C	394	SER
1	C	396	VAL
1	C	397	ASP
1	C	402	MET
1	C	403	SER
1	C	410	SER
1	C	414	LYS
1	C	420	ASN
1	C	423	ARG
1	C	428	VAL
1	C	442	LEU
1	C	444	SER
1	D	70	ARG
1	D	91	LYS
1	D	93	SER
1	D	101	LYS
1	D	115	THR
1	D	134	LEU
1	D	135	MET
1	D	137	SER
1	D	142	SER
1	D	145	MET
1	D	156	ILE
1	D	161	ASP
1	D	165	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	177	MET
1	D	180	THR
1	D	196	LEU
1	D	199	LYS
1	D	200	LYS
1	D	203	LEU
1	D	210	THR
1	D	211	ASN
1	D	214	LEU
1	D	223	SER
1	D	273	CYS
1	D	275	SER
1	D	278	LEU
1	D	279	LYS
1	D	303	ILE
1	D	311	HIS
1	D	315	GLN
1	D	335	ARG
1	D	343	GLN
1	D	344	SER
1	D	347	GLU
1	D	352	LYS
1	D	353	LYS
1	D	370	LEU
1	D	394	SER
1	D	396	VAL
1	D	397	ASP
1	D	402	MET
1	D	403	SER
1	D	410	SER
1	D	414	LYS
1	D	420	ASN
1	D	423	ARG
1	D	428	VAL
1	D	430	ASP
1	E	55	ASN
1	E	70	ARG
1	E	91	LYS
1	E	93	SER
1	E	101	LYS
1	E	115	THR
1	E	134	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	135	MET
1	E	142	SER
1	E	145	MET
1	E	156	ILE
1	E	161	ASP
1	E	162	CYS
1	E	165	LYS
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	210	THR
1	E	211	ASN
1	E	214	LEU
1	E	223	SER
1	E	273	CYS
1	E	275	SER
1	E	279	LYS
1	E	303	ILE
1	E	305	ARG
1	E	311	HIS
1	E	312	LEU
1	E	315	GLN
1	E	335	ARG
1	E	343	GLN
1	E	344	SER
1	E	347	GLU
1	E	352	LYS
1	E	353	LYS
1	E	370	LEU
1	E	394	SER
1	E	396	VAL
1	E	397	ASP
1	E	402	MET
1	E	403	SER
1	E	410	SER
1	E	414	LYS
1	E	420	ASN
1	E	423	ARG
1	E	430	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	443	ASP
1	E	444	SER
1	F	54	LEU
1	F	55	ASN
1	F	56	SER
1	F	70	ARG
1	F	93	SER
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	145	MET
1	F	156	ILE
1	F	161	ASP
1	F	162	CYS
1	F	165	LYS
1	F	177	MET
1	F	180	THR
1	F	196	LEU
1	F	199	LYS
1	F	200	LYS
1	F	203	LEU
1	F	210	THR
1	F	211	ASN
1	F	214	LEU
1	F	223	SER
1	F	224	LYS
1	F	270	LEU
1	F	273	CYS
1	F	275	SER
1	F	278	LEU
1	F	279	LYS
1	F	285	ARG
1	F	303	ILE
1	F	311	HIS
1	F	335	ARG
1	F	343	GLN
1	F	344	SER
1	F	347	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	352	LYS
1	F	353	LYS
1	F	370	LEU
1	F	396	VAL
1	F	397	ASP
1	F	402	MET
1	F	403	SER
1	F	410	SER
1	F	414	LYS
1	F	420	ASN
1	F	428	VAL
1	F	430	ASP
1	F	443	ASP
1	G	56	SER
1	G	70	ARG
1	G	93	SER
1	G	101	LYS
1	G	115	THR
1	G	131	SER
1	G	134	LEU
1	G	142	SER
1	G	145	MET
1	G	150	VAL
1	G	161	ASP
1	G	162	CYS
1	G	165	LYS
1	G	177	MET
1	G	180	THR
1	G	196	LEU
1	G	199	LYS
1	G	200	LYS
1	G	203	LEU
1	G	210	THR
1	G	211	ASN
1	G	214	LEU
1	G	223	SER
1	G	273	CYS
1	G	275	SER
1	G	278	LEU
1	G	303	ILE
1	G	311	HIS
1	G	315	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	335	ARG
1	G	343	GLN
1	G	344	SER
1	G	347	GLU
1	G	352	LYS
1	G	353	LYS
1	G	370	LEU
1	G	396	VAL
1	G	402	MET
1	G	403	SER
1	G	410	SER
1	G	420	ASN
1	G	428	VAL
1	G	430	ASP
1	G	443	ASP
1	G	444	SER
1	H	56	SER
1	H	70	ARG
1	H	74	THR
1	H	91	LYS
1	H	93	SER
1	H	101	LYS
1	H	115	THR
1	H	134	LEU
1	H	135	MET
1	H	142	SER
1	H	156	ILE
1	H	161	ASP
1	H	162	CYS
1	H	165	LYS
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	210	THR
1	H	211	ASN
1	H	214	LEU
1	H	224	LYS
1	H	273	CYS
1	H	275	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	278	LEU
1	H	279	LYS
1	H	303	ILE
1	H	311	HIS
1	H	315	GLN
1	H	335	ARG
1	H	343	GLN
1	H	344	SER
1	H	347	GLU
1	H	352	LYS
1	H	353	LYS
1	H	394	SER
1	H	396	VAL
1	H	402	MET
1	H	403	SER
1	H	410	SER
1	H	414	LYS
1	H	420	ASN
1	H	423	ARG
1	H	430	ASP
1	H	443	ASP
1	H	445	ILE
1	I	70	ARG
1	I	91	LYS
1	I	93	SER
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	145	MET
1	I	156	ILE
1	I	161	ASP
1	I	165	LYS
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	211	ASN
1	I	214	LEU
1	I	223	SER
1	I	273	CYS
1	I	275	SER
1	I	278	LEU
1	I	303	ILE
1	I	311	HIS
1	I	315	GLN
1	I	335	ARG
1	I	343	GLN
1	I	344	SER
1	I	347	GLU
1	I	352	LYS
1	I	370	LEU
1	I	396	VAL
1	I	402	MET
1	I	403	SER
1	I	410	SER
1	I	414	LYS
1	I	420	ASN
1	I	428	VAL
1	I	430	ASP
1	J	56	SER
1	J	70	ARG
1	J	91	LYS
1	J	93	SER
1	J	101	LYS
1	J	115	THR
1	J	131	SER
1	J	134	LEU
1	J	135	MET
1	J	142	SER
1	J	145	MET
1	J	161	ASP
1	J	165	LYS
1	J	177	MET
1	J	180	THR
1	J	196	LEU
1	J	199	LYS
1	J	200	LYS
1	J	203	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	J	210	THR
1	J	211	ASN
1	J	214	LEU
1	J	223	SER
1	J	273	CYS
1	J	275	SER
1	J	278	LEU
1	J	279	LYS
1	J	303	ILE
1	J	311	HIS
1	J	315	GLN
1	J	335	ARG
1	J	343	GLN
1	J	344	SER
1	J	347	GLU
1	J	352	LYS
1	J	353	LYS
1	J	370	LEU
1	J	394	SER
1	J	396	VAL
1	J	402	MET
1	J	403	SER
1	J	410	SER
1	J	414	LYS
1	J	420	ASN
1	J	428	VAL
1	J	430	ASP
1	K	70	ARG
1	K	93	SER
1	K	101	LYS
1	K	115	THR
1	K	131	SER
1	K	134	LEU
1	K	135	MET
1	K	142	SER
1	K	145	MET
1	K	161	ASP
1	K	162	CYS
1	K	165	LYS
1	K	177	MET
1	K	180	THR
1	K	196	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	199	LYS
1	K	200	LYS
1	K	203	LEU
1	K	210	THR
1	K	211	ASN
1	K	214	LEU
1	K	223	SER
1	K	256	LEU
1	K	273	CYS
1	K	275	SER
1	K	278	LEU
1	K	303	ILE
1	K	305	ARG
1	K	311	HIS
1	K	315	GLN
1	K	335	ARG
1	K	343	GLN
1	K	344	SER
1	K	347	GLU
1	K	352	LYS
1	K	353	LYS
1	K	370	LEU
1	K	394	SER
1	K	396	VAL
1	K	402	MET
1	K	403	SER
1	K	410	SER
1	K	414	LYS
1	K	420	ASN
1	K	428	VAL
1	K	443	ASP
1	K	444	SER
1	K	445	ILE
1	L	70	ARG
1	L	91	LYS
1	L	93	SER
1	L	100	GLU
1	L	101	LYS
1	L	115	THR
1	L	134	LEU
1	L	135	MET
1	L	142	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	145	MET
1	L	156	ILE
1	L	161	ASP
1	L	162	CYS
1	L	165	LYS
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	210	THR
1	L	211	ASN
1	L	214	LEU
1	L	273	CYS
1	L	275	SER
1	L	303	ILE
1	L	311	HIS
1	L	315	GLN
1	L	335	ARG
1	L	343	GLN
1	L	344	SER
1	L	347	GLU
1	L	370	LEU
1	L	394	SER
1	L	396	VAL
1	L	397	ASP
1	L	402	MET
1	L	403	SER
1	L	410	SER
1	L	420	ASN
1	L	423	ARG
1	L	428	VAL
1	L	430	ASP
1	L	443	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	63	HIS
1	A	211	ASN

*Continued on next page...*

*Continued from previous page...*

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

### 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 ⓘ

12 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	$\# Z  > 2$
2	HEN	L	511	-	24,27,27	2.95	11 (45%)	29,39,39	2.17	10 (34%)
2	HEN	A	500	-	24,27,27	3.01	12 (50%)	29,39,39	2.36	10 (34%)
2	HEN	K	510	-	24,27,27	3.02	12 (50%)	29,39,39	2.10	11 (37%)
2	HEN	H	507	-	24,27,27	2.99	12 (50%)	29,39,39	2.15	10 (34%)
2	HEN	G	506	-	24,27,27	2.86	12 (50%)	29,39,39	2.08	10 (34%)
2	HEN	D	503	-	24,27,27	3.04	11 (45%)	29,39,39	2.16	11 (37%)
2	HEN	B	501	-	24,27,27	2.89	12 (50%)	29,39,39	2.07	10 (34%)
2	HEN	I	508	-	24,27,27	2.87	12 (50%)	29,39,39	2.21	12 (41%)
2	HEN	C	502	-	24,27,27	2.88	11 (45%)	29,39,39	2.20	11 (37%)
2	HEN	E	504	-	24,27,27	3.36	13 (54%)	29,39,39	2.28	11 (37%)
2	HEN	J	509	-	24,27,27	3.17	12 (50%)	29,39,39	2.20	10 (34%)
2	HEN	F	505	-	24,27,27	2.91	12 (50%)	29,39,39	2.15	11 (37%)

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
2	HEN	L	511	-	-	6/17/22/22	0/1/1/1
2	HEN	A	500	-	-	5/17/22/22	0/1/1/1
2	HEN	K	510	-	-	5/17/22/22	0/1/1/1
2	HEN	H	507	-	-	8/17/22/22	0/1/1/1
2	HEN	G	506	-	-	7/17/22/22	0/1/1/1
2	HEN	D	503	-	-	6/17/22/22	0/1/1/1
2	HEN	B	501	-	-	9/17/22/22	0/1/1/1
2	HEN	I	508	-	-	6/17/22/22	0/1/1/1
2	HEN	C	502	-	-	7/17/22/22	0/1/1/1
2	HEN	E	504	-	-	8/17/22/22	0/1/1/1
2	HEN	J	509	-	-	6/17/22/22	0/1/1/1
2	HEN	F	505	-	-	9/17/22/22	0/1/1/1

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	508	HEN	C5-C4	6.87	1.50	1.40
2	E	504	HEN	PG-CEI	6.78	1.90	1.79
2	E	504	HEN	C5-C4	6.73	1.49	1.40
2	L	511	HEN	C5-C4	6.70	1.49	1.40
2	K	510	HEN	C5-C4	6.69	1.49	1.40
2	J	509	HEN	PG-CEI	6.61	1.90	1.79
2	A	500	HEN	C5-C4	6.53	1.49	1.40
2	C	502	HEN	C5-C4	6.50	1.49	1.40
2	D	503	HEN	C5-C4	6.44	1.49	1.40
2	E	504	HEN	C3-C4	6.36	1.49	1.40
2	H	507	HEN	PG-CEI	6.34	1.89	1.79
2	B	501	HEN	C5-C4	6.30	1.49	1.40
2	F	505	HEN	C5-C4	6.26	1.49	1.40
2	K	510	HEN	PG-CEI	6.19	1.89	1.79
2	H	507	HEN	C5-C4	6.14	1.49	1.40
2	J	509	HEN	C5-C4	6.13	1.49	1.40
2	G	506	HEN	C5-C4	6.04	1.49	1.40
2	B	501	HEN	PG-CEI	5.79	1.88	1.79
2	F	505	HEN	PG-CEI	5.79	1.88	1.79
2	D	503	HEN	C4A-N4A	-5.66	1.38	1.46
2	J	509	HEN	C3-C4	5.64	1.48	1.40
2	G	506	HEN	PG-CEI	5.62	1.88	1.79
2	A	500	HEN	C3-C4	5.49	1.48	1.40
2	L	511	HEN	PG-CEI	5.42	1.88	1.79
2	A	500	HEN	C4A-N4A	-5.27	1.38	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	HEN	CAI-N4A	-5.26	1.21	1.30
2	D	503	HEN	PG-CEI	5.25	1.88	1.79
2	F	505	HEN	C4A-N4A	-5.16	1.38	1.46
2	C	502	HEN	PG-CEI	5.07	1.87	1.79
2	I	508	HEN	C3-C4	5.01	1.47	1.40
2	F	505	HEN	CAI-N4A	-4.87	1.22	1.30
2	L	511	HEN	C4A-N4A	-4.85	1.39	1.46
2	E	504	HEN	C3-C2	4.83	1.45	1.40
2	K	510	HEN	C3-C4	4.83	1.47	1.40
2	A	500	HEN	CAI-N4A	-4.81	1.22	1.30
2	G	506	HEN	C4A-N4A	-4.76	1.39	1.46
2	I	508	HEN	PG-CEI	4.73	1.87	1.79
2	L	511	HEN	CAI-N4A	-4.70	1.22	1.30
2	D	503	HEN	C3-C4	4.63	1.47	1.40
2	H	507	HEN	C3-C4	4.59	1.47	1.40
2	H	507	HEN	C4A-N4A	-4.58	1.39	1.46
2	B	501	HEN	C3-C4	4.55	1.47	1.40
2	J	509	HEN	C4A-N4A	-4.54	1.39	1.46
2	C	502	HEN	C3-C4	4.51	1.47	1.40
2	C	502	HEN	CAI-N4A	-4.47	1.23	1.30
2	A	500	HEN	PG-CEI	4.41	1.86	1.79
2	C	502	HEN	C4A-N4A	-4.35	1.40	1.46
2	B	501	HEN	C4A-N4A	-4.35	1.40	1.46
2	L	511	HEN	C3-C4	4.33	1.46	1.40
2	I	508	HEN	C4A-N4A	-4.25	1.40	1.46
2	G	506	HEN	CAI-N4A	-4.24	1.23	1.30
2	B	501	HEN	CAI-N4A	-4.20	1.23	1.30
2	D	503	HEN	C2-N1	4.13	1.41	1.33
2	H	507	HEN	CAI-N4A	-4.11	1.23	1.30
2	C	502	HEN	C2-N1	4.10	1.41	1.33
2	E	504	HEN	C4A-N4A	-4.09	1.40	1.46
2	J	509	HEN	CAI-N4A	-4.06	1.23	1.30
2	G	506	HEN	C3-C4	4.03	1.46	1.40
2	H	507	HEN	C2-N1	4.03	1.41	1.33
2	I	508	HEN	C2-N1	4.03	1.41	1.33
2	K	510	HEN	CAI-N4A	-4.01	1.23	1.30
2	G	506	HEN	C2-N1	3.99	1.41	1.33
2	K	510	HEN	CBI-CAI	3.98	1.53	1.46
2	B	501	HEN	C2-N1	3.98	1.41	1.33
2	L	511	HEN	C2-N1	3.96	1.41	1.33
2	K	510	HEN	C4A-N4A	-3.94	1.40	1.46
2	F	505	HEN	C3-C4	3.94	1.46	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	505	HEN	C2-N1	3.93	1.41	1.33
2	K	510	HEN	C2-N1	3.91	1.41	1.33
2	E	504	HEN	CBI-CAI	3.90	1.52	1.46
2	J	509	HEN	CBI-CAI	3.79	1.52	1.46
2	A	500	HEN	C2-N1	3.76	1.40	1.33
2	E	504	HEN	C2-N1	3.76	1.40	1.33
2	I	508	HEN	CAI-N4A	-3.68	1.24	1.30
2	J	509	HEN	C2-N1	3.64	1.40	1.33
2	B	501	HEN	CBI-CAI	3.53	1.52	1.46
2	E	504	HEN	PG-OG1	3.51	1.63	1.54
2	E	504	HEN	CAI-N4A	-3.50	1.24	1.30
2	J	509	HEN	CBC-CAI	3.39	1.57	1.52
2	L	511	HEN	CBI-CAI	3.27	1.51	1.46
2	C	502	HEN	CBC-CAI	3.26	1.57	1.52
2	G	506	HEN	CBI-CAI	3.25	1.51	1.46
2	E	504	HEN	CBC-CAI	3.23	1.56	1.52
2	J	509	HEN	PG-OG1	3.22	1.62	1.54
2	H	507	HEN	PG-OG1	3.20	1.62	1.54
2	E	504	HEN	PG-OG2	-3.16	1.47	1.54
2	A	500	HEN	PG-OG1	3.13	1.62	1.54
2	H	507	HEN	CBI-CAI	3.11	1.51	1.46
2	J	509	HEN	PG-OG2	-3.05	1.47	1.54
2	D	503	HEN	CBI-CAI	3.04	1.51	1.46
2	I	508	HEN	C3-C2	2.97	1.43	1.40
2	K	510	HEN	CBC-CAI	2.96	1.56	1.52
2	D	503	HEN	PG-OG1	2.95	1.61	1.54
2	G	506	HEN	PG-OG1	2.92	1.61	1.54
2	A	500	HEN	C3-C2	2.92	1.43	1.40
2	I	508	HEN	PG-OG1	2.91	1.61	1.54
2	F	505	HEN	CBI-CAI	2.88	1.51	1.46
2	L	511	HEN	PG-OG1	2.86	1.61	1.54
2	C	502	HEN	CBI-CAI	2.85	1.51	1.46
2	F	505	HEN	PG-OG1	2.84	1.61	1.54
2	K	510	HEN	PG-OG1	2.82	1.61	1.54
2	I	508	HEN	CBI-CAI	2.81	1.51	1.46
2	C	502	HEN	PG-OG1	2.81	1.61	1.54
2	J	509	HEN	C3-C2	2.76	1.43	1.40
2	H	507	HEN	O3-C3	-2.74	1.30	1.37
2	H	507	HEN	CBC-CAI	2.73	1.56	1.52
2	D	503	HEN	CBC-CAI	2.69	1.56	1.52
2	A	500	HEN	CBI-CAI	2.68	1.50	1.46
2	H	507	HEN	PG-OG2	-2.66	1.48	1.54

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEN	PG-OG2	-2.66	1.48	1.54
2	B	501	HEN	CBC-CAI	2.64	1.56	1.52
2	J	509	HEN	O3-C3	-2.62	1.30	1.37
2	L	511	HEN	CBC-CAI	2.60	1.56	1.52
2	D	503	HEN	O3-C3	-2.57	1.31	1.37
2	I	508	HEN	PG-OG2	-2.54	1.49	1.54
2	B	501	HEN	PG-OG1	2.52	1.60	1.54
2	C	502	HEN	O3-C3	-2.51	1.31	1.37
2	G	506	HEN	PG-OG2	-2.51	1.49	1.54
2	F	505	HEN	PG-OG2	-2.50	1.49	1.54
2	K	510	HEN	PG-OG2	-2.50	1.49	1.54
2	G	506	HEN	O3-C3	-2.48	1.31	1.37
2	L	511	HEN	O3-C3	-2.47	1.31	1.37
2	A	500	HEN	CBC-CAI	2.44	1.55	1.52
2	B	501	HEN	O3-C3	-2.44	1.31	1.37
2	D	503	HEN	PG-OG2	-2.39	1.49	1.54
2	I	508	HEN	CBC-CAI	2.32	1.55	1.52
2	K	510	HEN	C3-C2	2.31	1.43	1.40
2	L	511	HEN	PG-OG2	-2.31	1.49	1.54
2	A	500	HEN	O3-C3	-2.25	1.31	1.37
2	I	508	HEN	O3-C3	-2.25	1.31	1.37
2	C	502	HEN	PG-OG2	-2.25	1.49	1.54
2	K	510	HEN	O3-C3	-2.24	1.31	1.37
2	G	506	HEN	CBC-CAI	2.24	1.55	1.52
2	F	505	HEN	O3-C3	-2.24	1.31	1.37
2	F	505	HEN	CBC-CAI	2.22	1.55	1.52
2	G	506	HEN	C3-C2	2.13	1.43	1.40
2	B	501	HEN	PG-OG2	-2.13	1.50	1.54
2	F	505	HEN	C3-C2	2.12	1.43	1.40
2	H	507	HEN	C3-C2	2.11	1.43	1.40
2	E	504	HEN	O3-C3	-2.08	1.32	1.37
2	B	501	HEN	C3-C2	2.05	1.43	1.40
2	E	504	HEN	C4A-C4	2.01	1.56	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	504	HEN	C2A-C2-C3	5.72	127.95	120.89
2	J	509	HEN	C2A-C2-C3	5.51	127.69	120.89
2	A	500	HEN	C2A-C2-C3	5.49	127.67	120.89
2	A	500	HEN	PG-CEI-CGI	-5.45	102.84	114.02
2	I	508	HEN	C2A-C2-C3	5.44	127.61	120.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	505	HEN	C2A-C2-C3	5.28	127.42	120.89
2	G	506	HEN	C2A-C2-C3	5.25	127.38	120.89
2	K	510	HEN	C2A-C2-C3	5.21	127.32	120.89
2	B	501	HEN	C2A-C2-C3	5.16	127.27	120.89
2	L	511	HEN	C2A-C2-C3	5.11	127.20	120.89
2	C	502	HEN	C2A-C2-C3	5.06	127.14	120.89
2	H	507	HEN	C2A-C2-C3	5.05	127.13	120.89
2	D	503	HEN	C2A-C2-C3	4.95	127.01	120.89
2	A	500	HEN	C6-N1-C2	4.21	126.96	119.17
2	H	507	HEN	CGI-CBI-CAI	-4.19	116.23	124.90
2	I	508	HEN	C6-N1-C2	4.15	126.85	119.17
2	K	510	HEN	C6-N1-C2	4.13	126.82	119.17
2	J	509	HEN	C6-N1-C2	4.13	126.81	119.17
2	F	505	HEN	C6-N1-C2	4.12	126.80	119.17
2	D	503	HEN	PG-CEI-CGI	-4.12	105.58	114.02
2	B	501	HEN	C6-N1-C2	4.12	126.79	119.17
2	D	503	HEN	C6-N1-C2	4.11	126.79	119.17
2	L	511	HEN	C6-N1-C2	4.10	126.75	119.17
2	L	511	HEN	CGI-CBI-CAI	-4.08	116.46	124.90
2	C	502	HEN	C6-N1-C2	4.08	126.72	119.17
2	E	504	HEN	C6-N1-C2	4.04	126.66	119.17
2	G	506	HEN	C6-N1-C2	4.04	126.64	119.17
2	C	502	HEN	CGI-CBI-CAI	-4.04	116.56	124.90
2	H	507	HEN	C6-N1-C2	3.99	126.56	119.17
2	I	508	HEN	PG-CEI-CGI	-3.96	105.91	114.02
2	A	500	HEN	CGI-CBI-CAI	-3.76	117.14	124.90
2	D	503	HEN	CGI-CBI-CAI	-3.69	117.27	124.90
2	F	505	HEN	CGI-CBI-CAI	-3.69	117.28	124.90
2	L	511	HEN	PG-CEI-CGI	-3.66	106.52	114.02
2	C	502	HEN	PG-CEI-CGI	-3.57	106.69	114.02
2	E	504	HEN	C6-C5-C4	3.56	120.64	118.12
2	C	502	HEN	C5-C6-N1	-3.43	118.11	123.82
2	E	504	HEN	C4-C4A-N4A	3.37	130.02	113.81
2	B	501	HEN	C5-C6-N1	-3.37	118.21	123.82
2	J	509	HEN	PG-CEI-CGI	-3.36	107.13	114.02
2	G	506	HEN	C5-C6-N1	-3.36	118.23	123.82
2	F	505	HEN	C5-C6-N1	-3.35	118.24	123.82
2	K	510	HEN	C5-C6-N1	-3.34	118.25	123.82
2	J	509	HEN	CGI-CBI-CAI	-3.33	118.02	124.90
2	L	511	HEN	C5-C6-N1	-3.29	118.33	123.82
2	I	508	HEN	C5-C6-N1	-3.28	118.36	123.82
2	J	509	HEN	C5-C6-N1	-3.27	118.37	123.82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	HEN	C5-C6-N1	-3.26	118.38	123.82
2	H	507	HEN	C5-C6-N1	-3.23	118.43	123.82
2	A	500	HEN	C5-C6-N1	-3.20	118.48	123.82
2	J	509	HEN	C6-C5-C4	3.20	120.38	118.12
2	E	504	HEN	CGI-CBI-CAI	-3.17	118.35	124.90
2	E	504	HEN	OG1-PG-CEI	3.15	114.26	106.92
2	I	508	HEN	C4-C4A-N4A	3.12	128.79	113.81
2	A	500	HEN	C4-C4A-N4A	3.10	128.72	113.81
2	I	508	HEN	CGI-CBI-CAI	-3.09	118.51	124.90
2	E	504	HEN	C5-C6-N1	-3.08	118.68	123.82
2	H	507	HEN	PG-CEI-CGI	-3.07	107.72	114.02
2	K	510	HEN	C6-C5-C4	3.03	120.26	118.12
2	G	506	HEN	PG-CEI-CGI	-3.00	107.86	114.02
2	E	504	HEN	PG-CEI-CGI	-2.98	107.91	114.02
2	I	508	HEN	C6-C5-C4	2.96	120.21	118.12
2	K	510	HEN	C4-C4A-N4A	2.92	127.87	113.81
2	C	502	HEN	C6-C5-C4	2.91	120.17	118.12
2	B	501	HEN	C6-C5-C4	2.85	120.13	118.12
2	F	505	HEN	PG-CEI-CGI	-2.84	108.19	114.02
2	J	509	HEN	C4-C4A-N4A	2.81	127.34	113.81
2	H	507	HEN	C4-C4A-N4A	2.80	127.30	113.81
2	A	500	HEN	C6-C5-C4	2.80	120.10	118.12
2	G	506	HEN	C4-C4A-N4A	2.78	127.20	113.81
2	B	501	HEN	C4-C4A-N4A	2.77	127.15	113.81
2	C	502	HEN	C4-C4A-N4A	2.74	127.00	113.81
2	G	506	HEN	C6-C5-C4	2.72	120.04	118.12
2	G	506	HEN	CGI-CBI-CAI	-2.70	119.32	124.90
2	K	510	HEN	PG-CEI-CGI	-2.69	108.50	114.02
2	A	500	HEN	OG3-PG-CEI	-2.65	105.13	111.13
2	H	507	HEN	OG1-PG-CEI	2.62	113.03	106.92
2	F	505	HEN	C4-C4A-N4A	2.58	126.21	113.81
2	J	509	HEN	OG1-PG-CEI	2.56	112.89	106.92
2	B	501	HEN	CGI-CBI-CAI	-2.51	119.71	124.90
2	E	504	HEN	OG1-PG-OG3	-2.51	105.74	112.39
2	L	511	HEN	C6-C5-C4	2.49	119.88	118.12
2	H	507	HEN	C6-C5-C4	2.48	119.87	118.12
2	K	510	HEN	CGI-CBI-CAI	-2.48	119.78	124.90
2	F	505	HEN	C6-C5-C4	2.46	119.86	118.12
2	H	507	HEN	OG1-PG-OG3	-2.45	105.92	112.39
2	J	509	HEN	OG1-PG-OG3	-2.39	106.06	112.39
2	H	507	HEN	C3-C2-N1	-2.39	117.68	120.77
2	B	501	HEN	PG-CEI-CGI	-2.38	109.13	114.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	511	HEN	C4-C4A-N4A	2.38	125.26	113.81
2	L	511	HEN	C4A-C4-C5	2.38	122.60	119.73
2	D	503	HEN	OG3-PG-CEI	-2.38	105.75	111.13
2	D	503	HEN	C4-C4A-N4A	2.36	125.15	113.81
2	C	502	HEN	OG3-PG-CEI	-2.35	105.81	111.13
2	F	505	HEN	C3-C2-N1	-2.35	117.74	120.77
2	G	506	HEN	C3-C2-N1	-2.32	117.77	120.77
2	D	503	HEN	C3-C2-N1	-2.30	117.80	120.77
2	L	511	HEN	C3-C2-N1	-2.30	117.80	120.77
2	F	505	HEN	OG1-PG-OG3	-2.28	106.37	112.39
2	B	501	HEN	C3-C2-N1	-2.28	117.83	120.77
2	B	501	HEN	OG3-PG-CEI	-2.27	106.00	111.13
2	C	502	HEN	C3-C2-N1	-2.26	117.84	120.77
2	K	510	HEN	OG1-PG-OG3	-2.25	106.44	112.39
2	L	511	HEN	OG3-PG-CEI	-2.24	106.06	111.13
2	J	509	HEN	C3-C2-N1	-2.23	117.89	120.77
2	A	500	HEN	C3-C2-N1	-2.19	117.93	120.77
2	A	500	HEN	OG2-PG-OG3	2.18	118.16	112.39
2	I	508	HEN	C3-C2-N1	-2.17	117.96	120.77
2	K	510	HEN	C3-C2-N1	-2.15	118.00	120.77
2	D	503	HEN	C6-C5-C4	2.14	119.63	118.12
2	D	503	HEN	OG1-PG-OG3	-2.13	106.76	112.39
2	I	508	HEN	OP3-P-OP1	2.13	115.77	107.64
2	E	504	HEN	OP3-P-OP1	2.12	115.76	107.64
2	I	508	HEN	OG1-PG-OG3	-2.12	106.79	112.39
2	C	502	HEN	OP3-P-OP1	2.11	115.71	107.64
2	K	510	HEN	OP3-P-OP1	2.10	115.67	107.64
2	I	508	HEN	OG3-PG-CEI	-2.09	106.39	111.13
2	E	504	HEN	O3-C3-C4	2.09	124.26	118.13
2	F	505	HEN	OP3-P-OP1	2.06	115.51	107.64
2	F	505	HEN	OG1-PG-CEI	2.05	111.69	106.92
2	G	506	HEN	OP3-P-OP1	2.04	115.42	107.64
2	D	503	HEN	OP3-P-OP1	2.04	115.42	107.64
2	B	501	HEN	OP3-P-OP1	2.03	115.39	107.64
2	K	510	HEN	OG1-PG-CEI	2.02	111.63	106.92
2	G	506	HEN	OG1-PG-OG3	-2.02	107.05	112.39
2	C	502	HEN	OG1-PG-OG3	-2.02	107.06	112.39
2	I	508	HEN	OG2-PG-OG3	2.01	117.70	112.39

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	511	HEN	C3-C4-C4A-N4A
2	L	511	HEN	C5-C4-C4A-N4A
2	L	511	HEN	N4A-CAI-CBI-CGI
2	L	511	HEN	CBC-CAI-CBI-CGI
2	L	511	HEN	CGI-CEI-PG-OG3
2	A	500	HEN	C3-C4-C4A-N4A
2	A	500	HEN	C5-C4-C4A-N4A
2	A	500	HEN	N4A-CAI-CBI-CGI
2	A	500	HEN	CBC-CAI-CBI-CGI
2	K	510	HEN	C3-C4-C4A-N4A
2	K	510	HEN	C5-C4-C4A-N4A
2	K	510	HEN	PG-CEI-CGI-CBI
2	K	510	HEN	CGI-CEI-PG-OG3
2	H	507	HEN	C3-C4-C4A-N4A
2	H	507	HEN	C5-C4-C4A-N4A
2	H	507	HEN	N4A-CAI-CBI-CGI
2	H	507	HEN	CBC-CAI-CBI-CGI
2	H	507	HEN	PG-CEI-CGI-CBI
2	H	507	HEN	CGI-CEI-PG-OG3
2	I	508	HEN	C3-C4-C4A-N4A
2	I	508	HEN	C5-C4-C4A-N4A
2	I	508	HEN	N4A-CAI-CBI-CGI
2	I	508	HEN	CBC-CAI-CBI-CGI
2	I	508	HEN	PG-CEI-CGI-CBI
2	G	506	HEN	C3-C4-C4A-N4A
2	G	506	HEN	C5-C4-C4A-N4A
2	G	506	HEN	N4A-CAI-CBI-CGI
2	G	506	HEN	CBC-CAI-CBI-CGI
2	G	506	HEN	PG-CEI-CGI-CBI
2	D	503	HEN	C3-C4-C4A-N4A
2	D	503	HEN	C5-C4-C4A-N4A
2	D	503	HEN	C5A-OP4-P-OP1
2	D	503	HEN	N4A-CAI-CBI-CGI
2	D	503	HEN	CBC-CAI-CBI-CGI
2	D	503	HEN	PG-CEI-CGI-CBI
2	E	504	HEN	C3-C4-C4A-N4A
2	E	504	HEN	C5-C4-C4A-N4A
2	E	504	HEN	PG-CEI-CGI-CBI
2	E	504	HEN	CGI-CEI-PG-OG1
2	E	504	HEN	CGI-CEI-PG-OG3
2	C	502	HEN	C3-C4-C4A-N4A
2	C	502	HEN	C5-C4-C4A-N4A
2	C	502	HEN	C4-C5-C5A-OP4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	502	HEN	N4A-CAI-CBI-CGI
2	C	502	HEN	CBC-CAI-CBI-CGI
2	C	502	HEN	PG-CEI-CGI-CBI
2	B	501	HEN	C3-C4-C4A-N4A
2	B	501	HEN	C5-C4-C4A-N4A
2	B	501	HEN	N4A-CAI-CBI-CGI
2	B	501	HEN	CBC-CAI-CBI-CGI
2	B	501	HEN	PG-CEI-CGI-CBI
2	B	501	HEN	CGI-CEI-PG-OG1
2	B	501	HEN	CGI-CEI-PG-OG2
2	B	501	HEN	CGI-CEI-PG-OG3
2	J	509	HEN	C3-C4-C4A-N4A
2	J	509	HEN	C5-C4-C4A-N4A
2	J	509	HEN	C4-C5-C5A-OP4
2	J	509	HEN	PG-CEI-CGI-CBI
2	J	509	HEN	CGI-CEI-PG-OG3
2	F	505	HEN	C3-C4-C4A-N4A
2	F	505	HEN	C5-C4-C4A-N4A
2	F	505	HEN	N4A-CAI-CBI-CGI
2	F	505	HEN	CBC-CAI-CBI-CGI
2	F	505	HEN	PG-CEI-CGI-CBI
2	F	505	HEN	CGI-CEI-PG-OG3
2	E	504	HEN	CGI-CEI-PG-OG2
2	F	505	HEN	CGI-CEI-PG-OG1
2	C	502	HEN	C6-C5-C5A-OP4
2	J	509	HEN	C6-C5-C5A-OP4
2	I	508	HEN	C5A-OP4-P-OP1
2	F	505	HEN	C5A-OP4-P-OP1
2	G	506	HEN	C4-C5-C5A-OP4
2	A	500	HEN	PG-CEI-CGI-CBI
2	K	510	HEN	CGI-CEI-PG-OG1
2	H	507	HEN	CGI-CEI-PG-OG1
2	F	505	HEN	CGI-CEI-PG-OG2
2	L	511	HEN	CGI-CEI-PG-OG1
2	H	507	HEN	CGI-CEI-PG-OG2
2	G	506	HEN	C6-C5-C5A-OP4
2	E	504	HEN	N4A-CAI-CBI-CGI
2	E	504	HEN	CBC-CAI-CBI-CGI
2	B	501	HEN	C4-C5-C5A-OP4

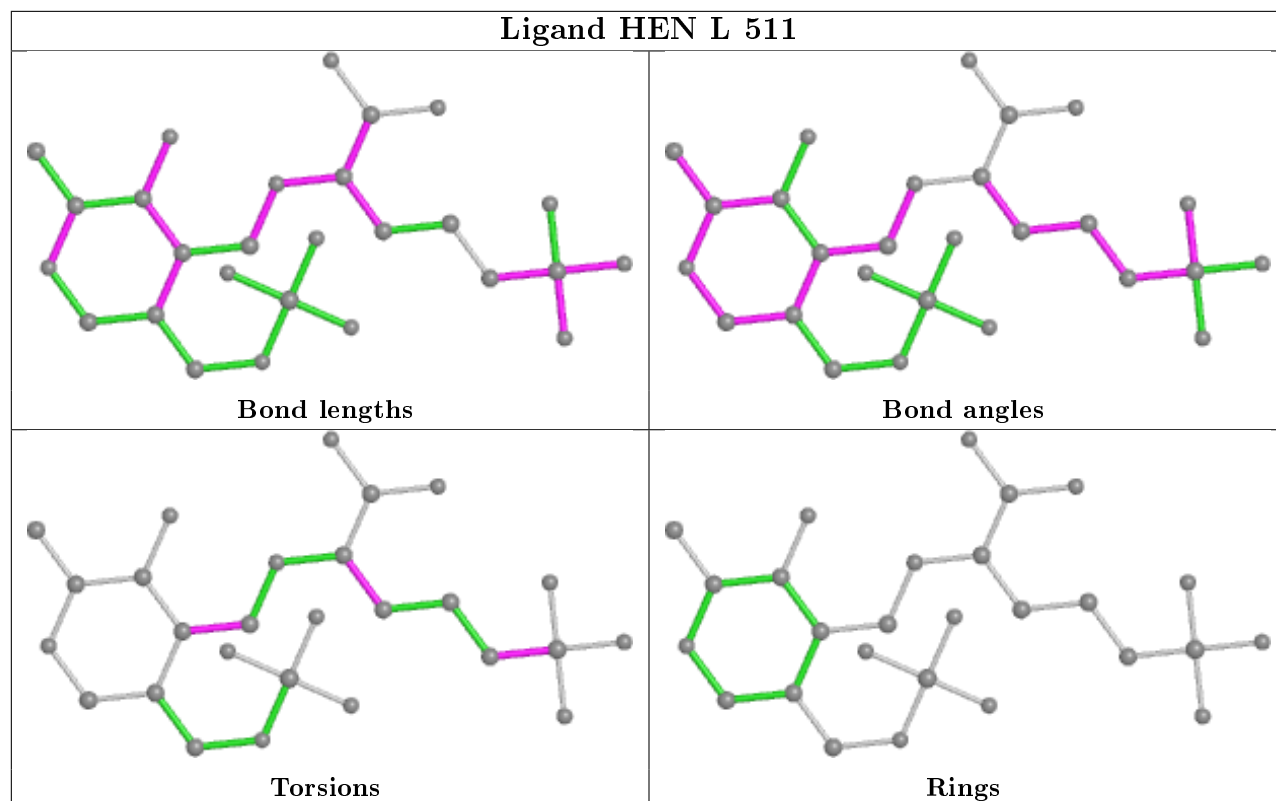
There are no ring outliers.

11 monomers are involved in 16 short contacts:

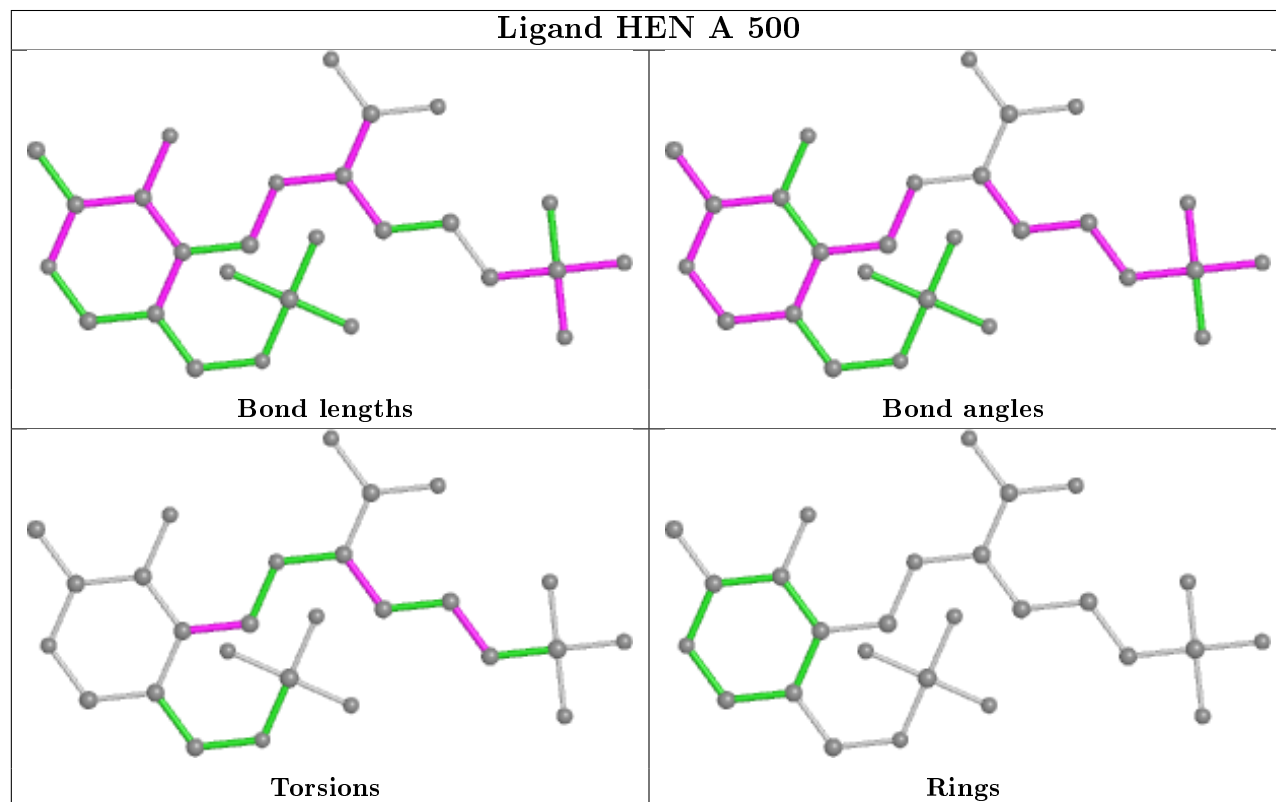
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	511	HEN	1	0
2	A	500	HEN	3	0
2	K	510	HEN	1	0
2	H	507	HEN	2	0
2	G	506	HEN	1	0
2	D	503	HEN	2	0
2	B	501	HEN	1	0
2	I	508	HEN	2	0
2	E	504	HEN	1	0
2	J	509	HEN	1	0
2	F	505	HEN	1	0

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.

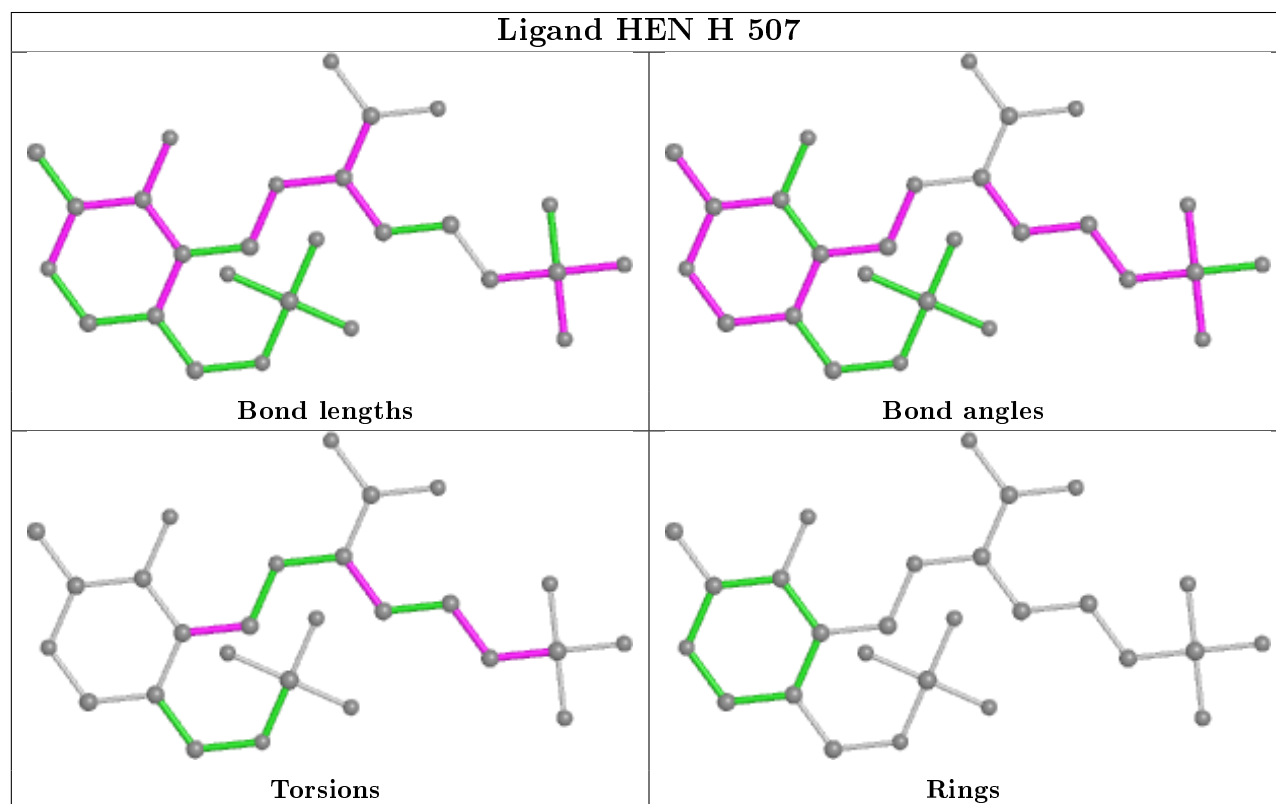
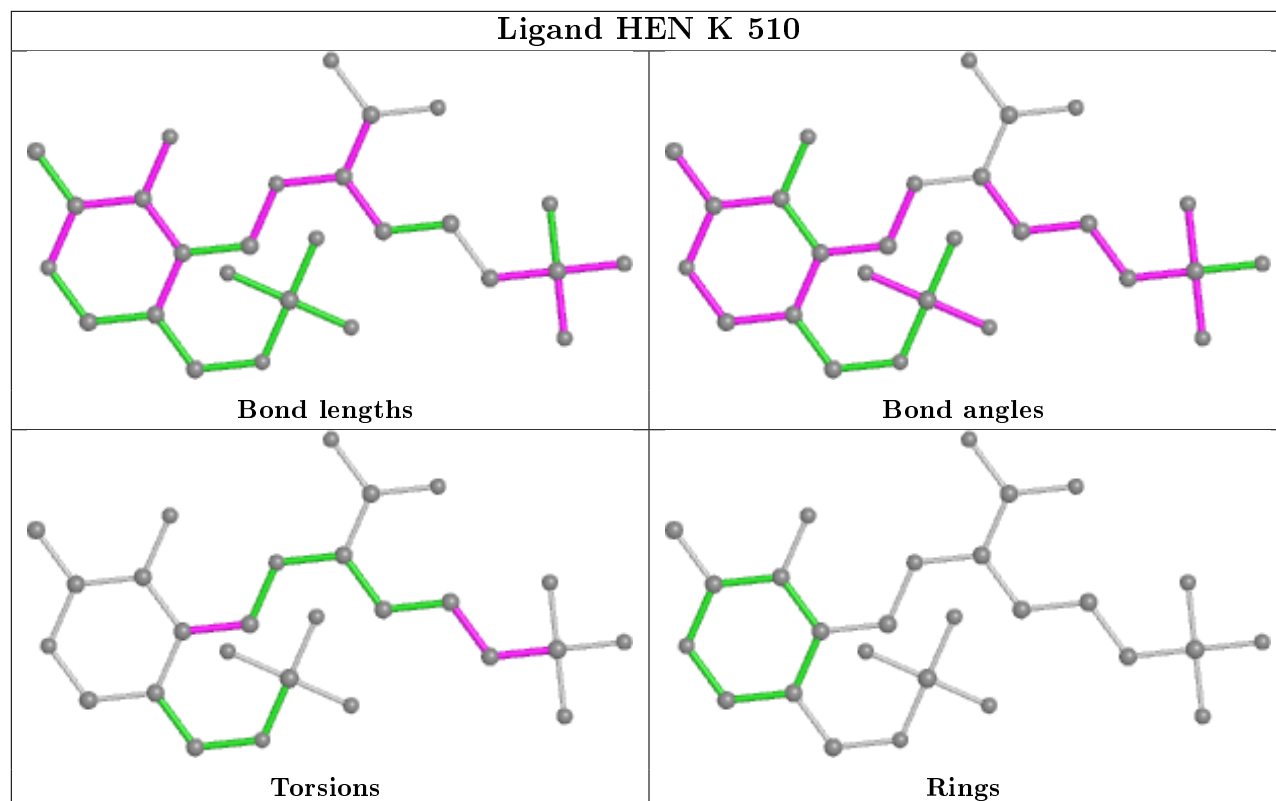
## Ligand HEN L 511

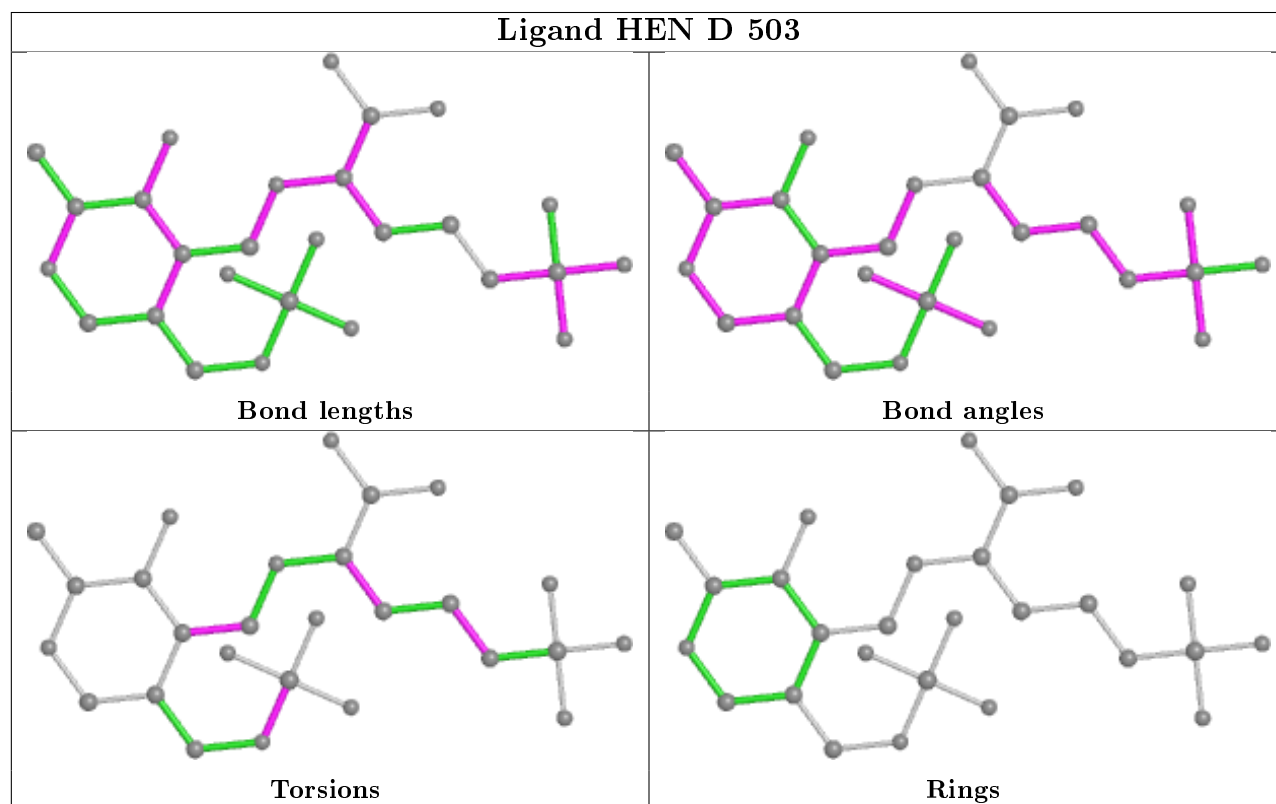
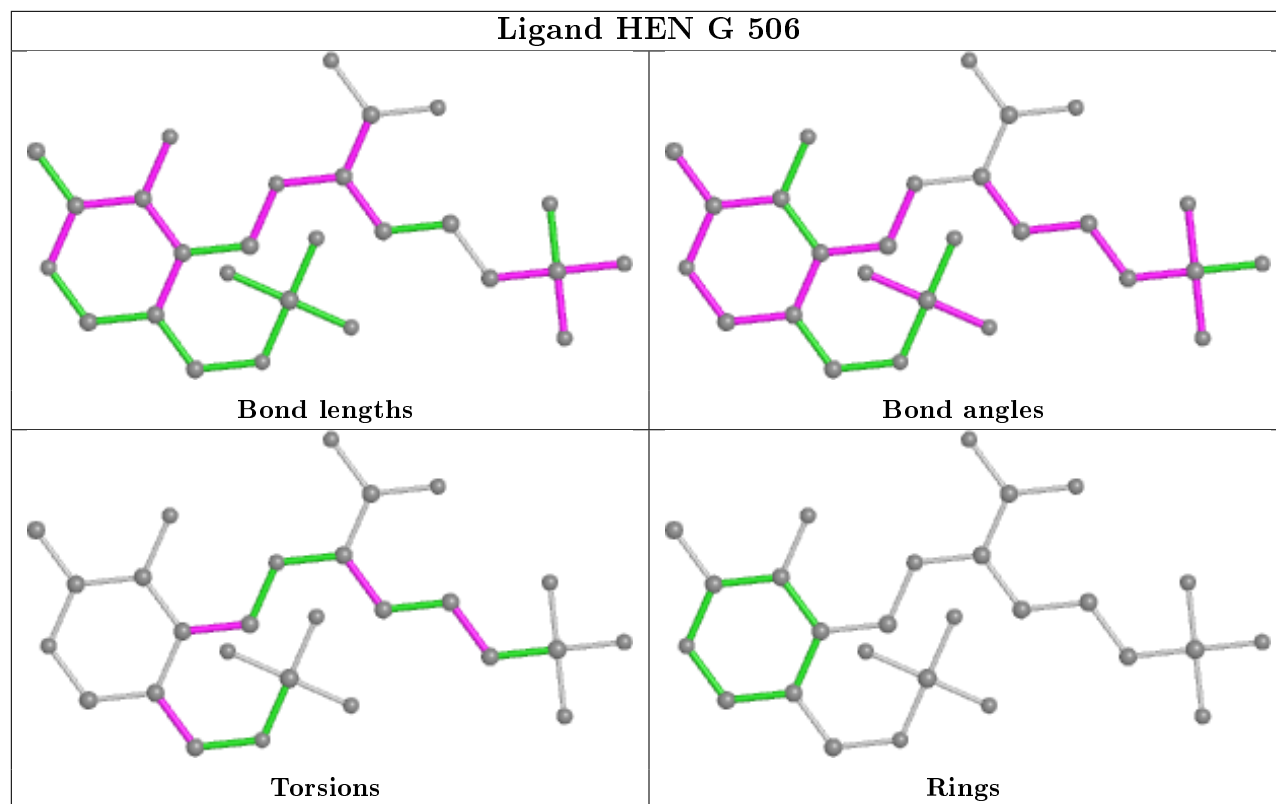


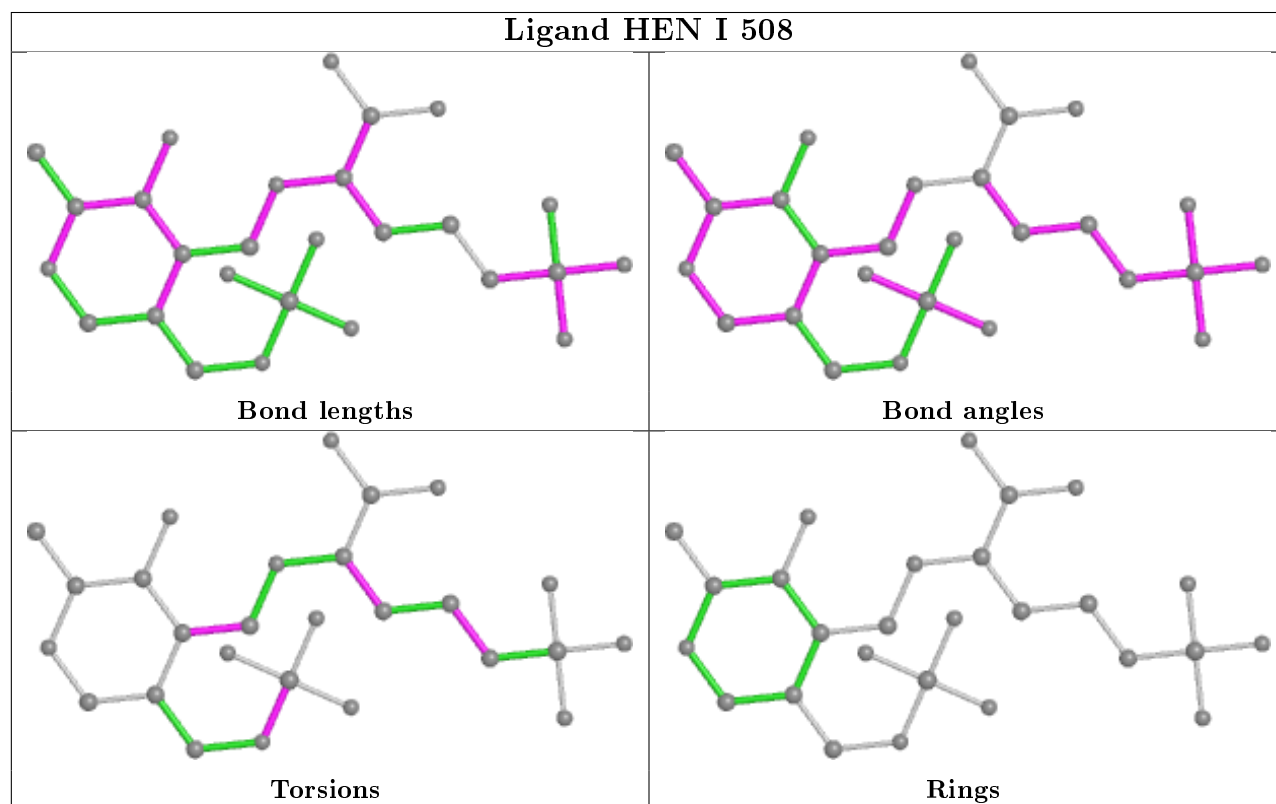
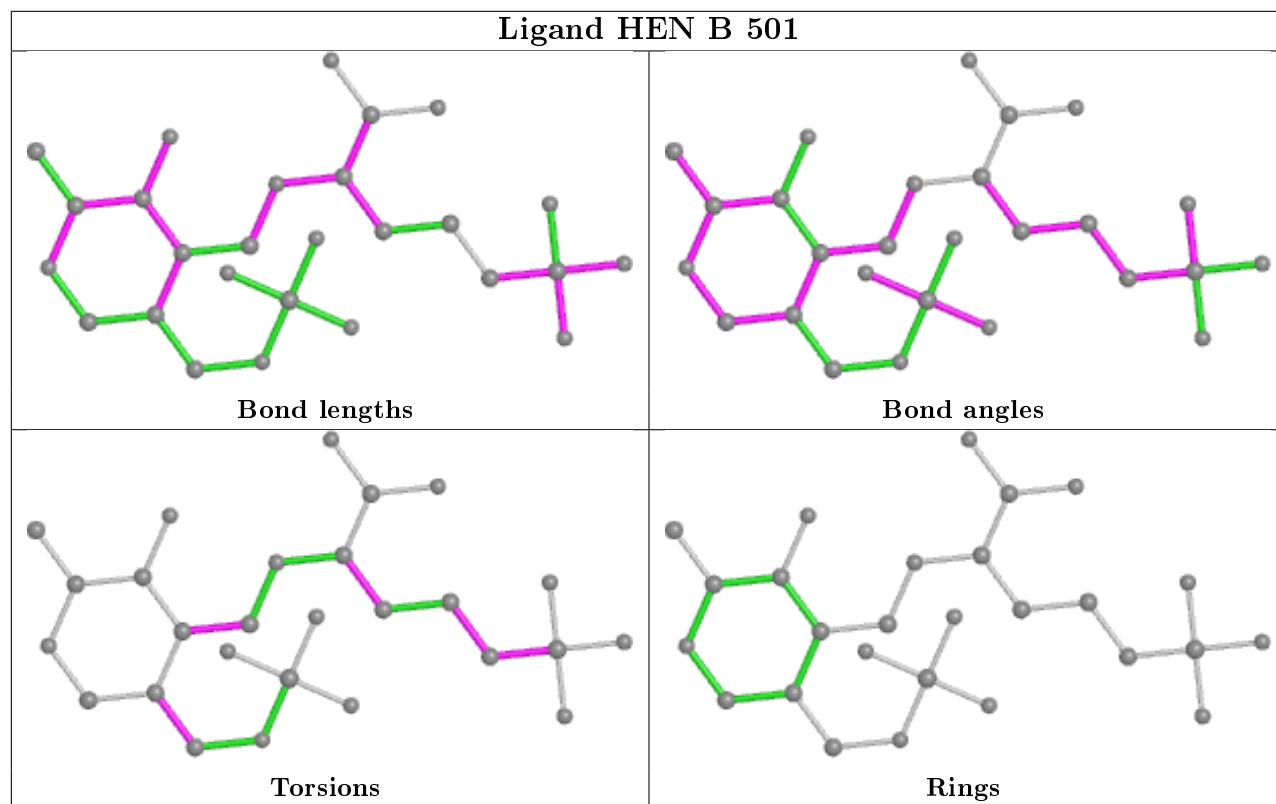
## Ligand HEN A 500

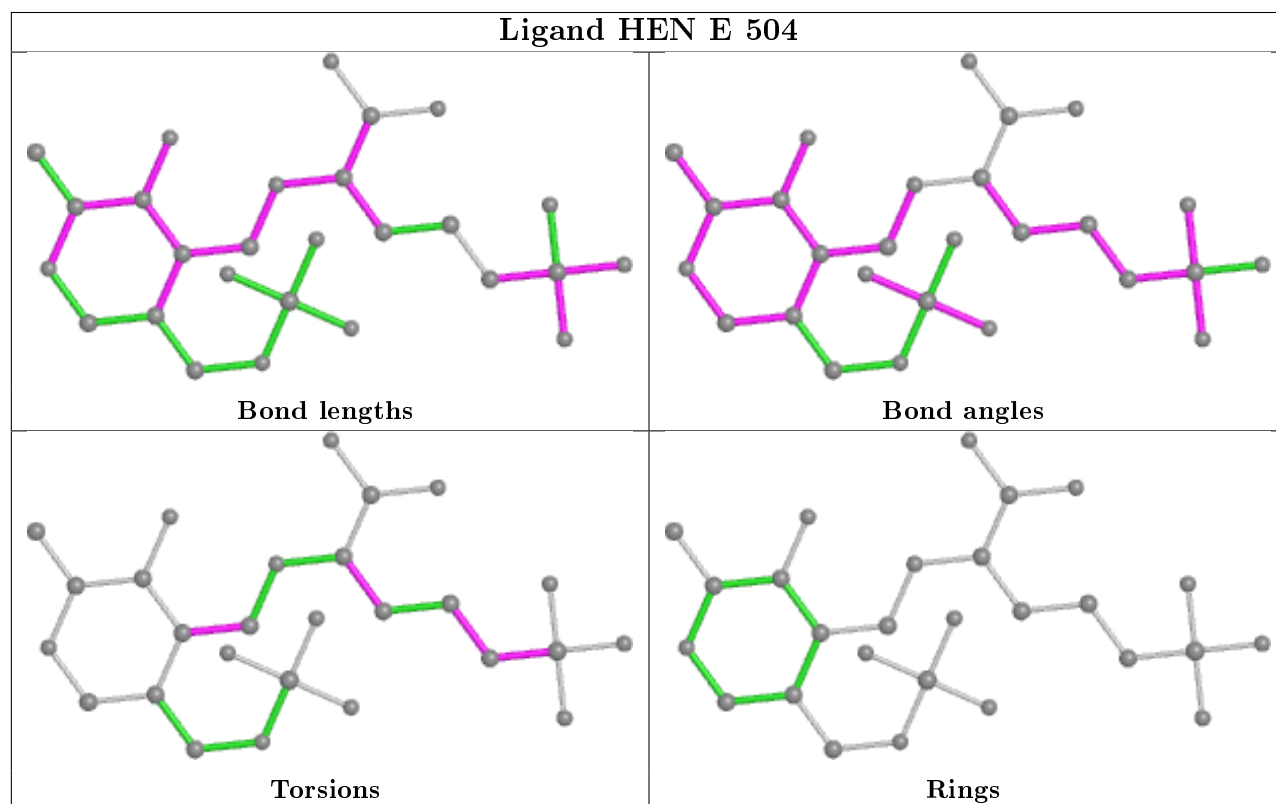
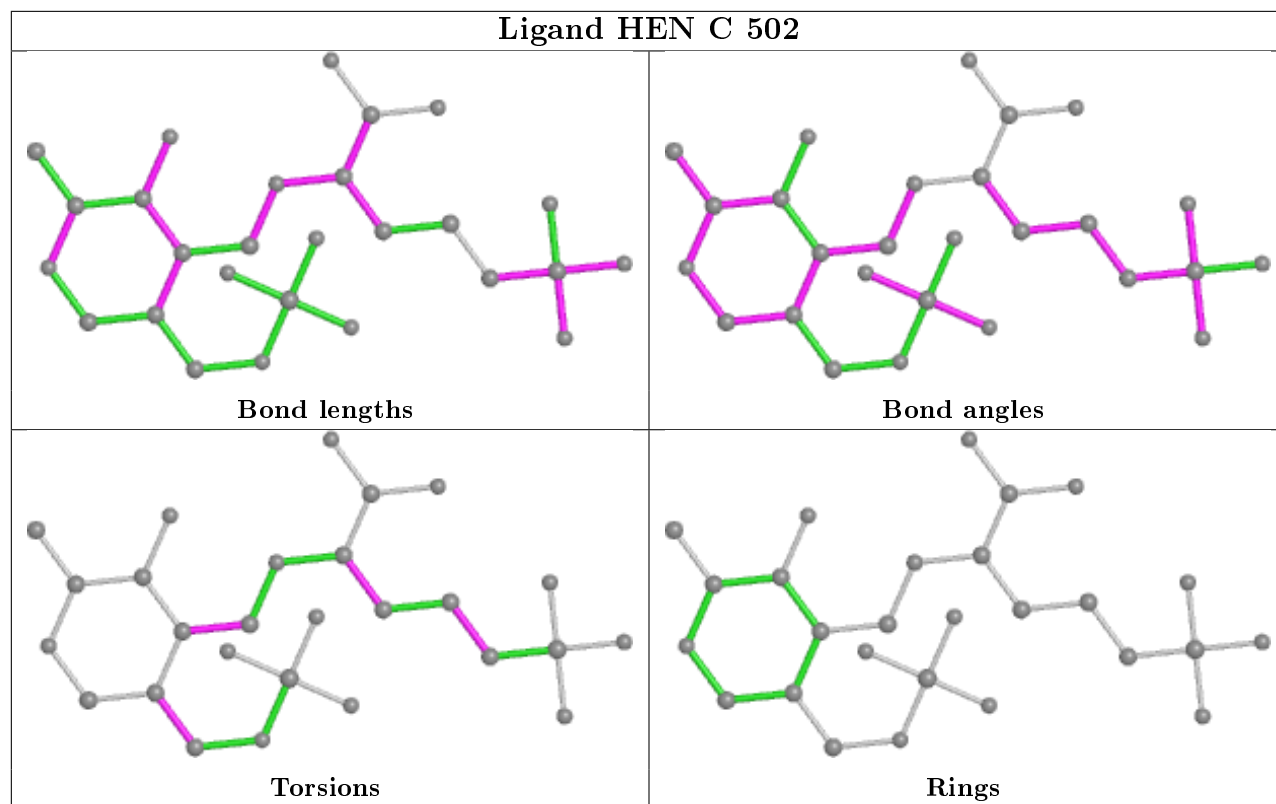


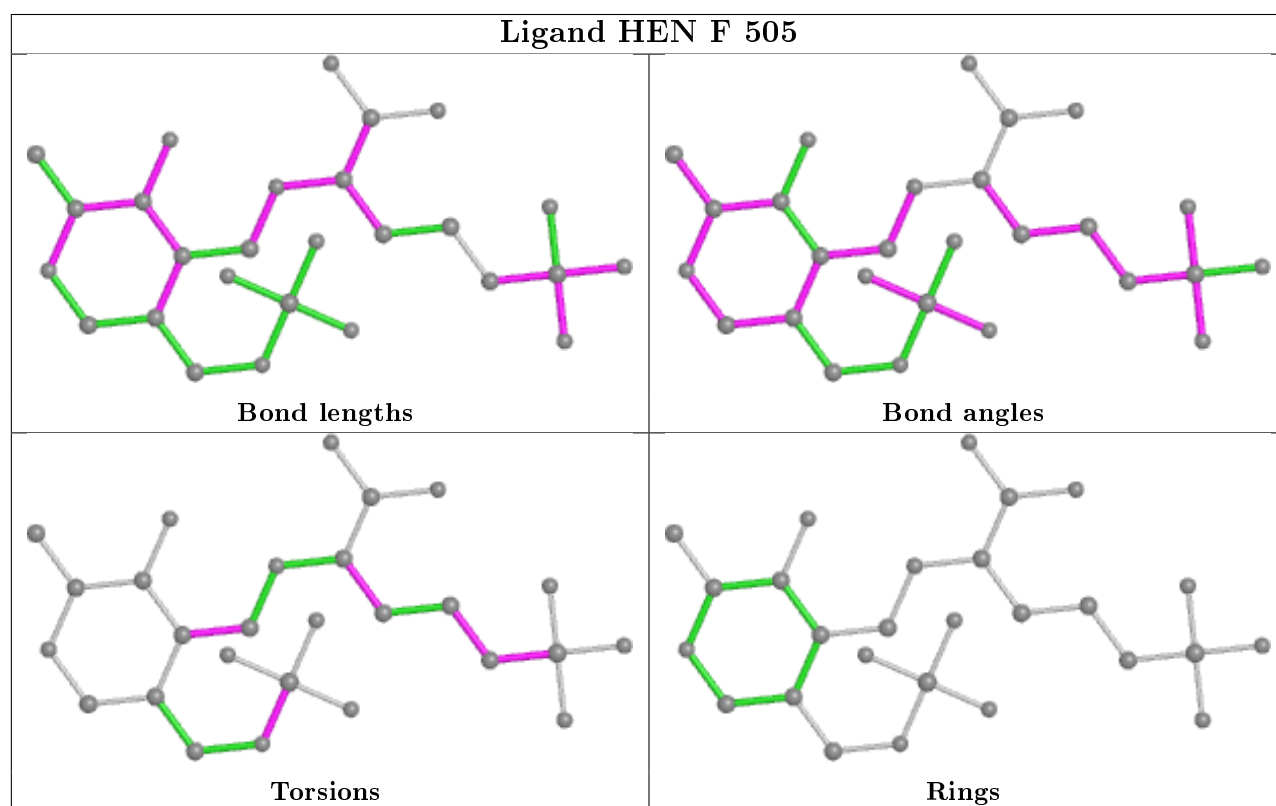
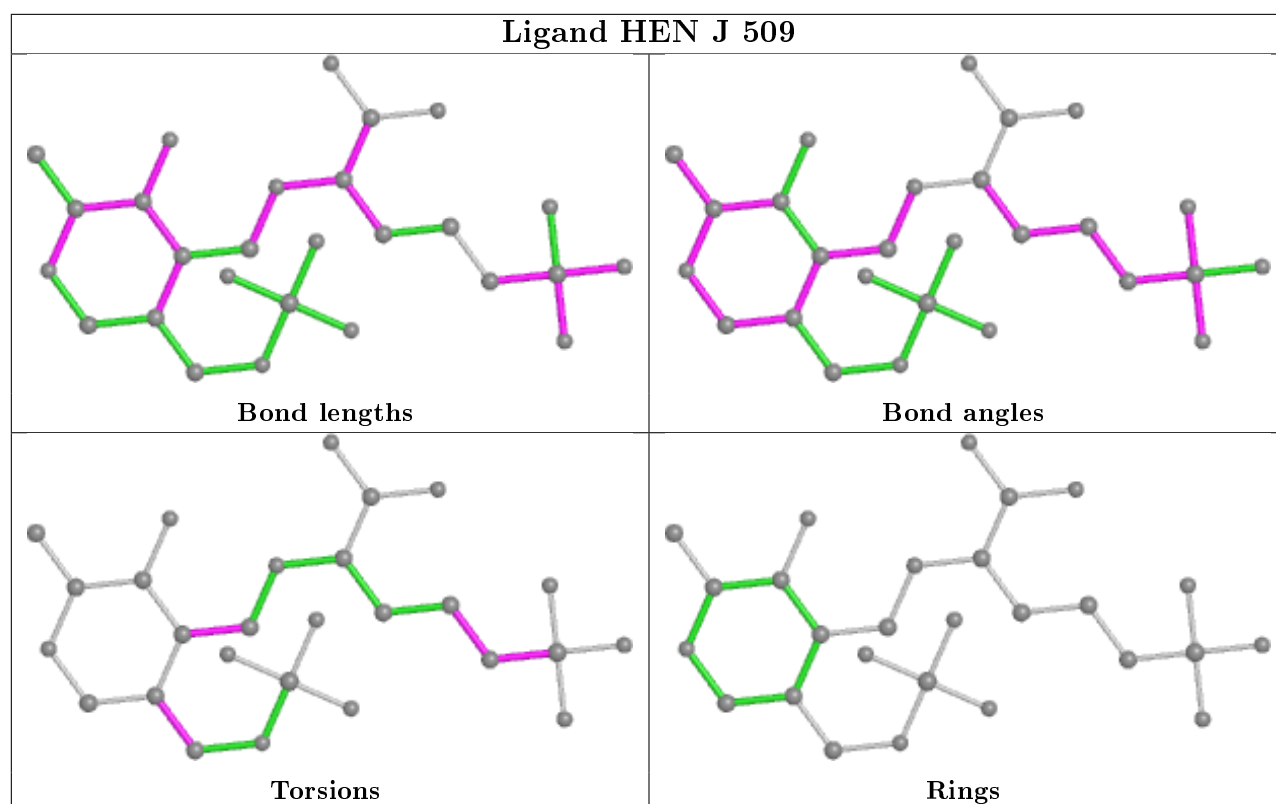












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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.