



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 06:36 AM BST

PDB ID : 5EC5  
Title : Crystal structure of lysenin pore  
Authors : Podobnik, M.; Savory, P.; Rojko, N.; Kisovec, M.; Bruce, M.; Jayasinghe, L.; Anderluh, G.  
Deposited on : 2015-10-20  
Resolution : 3.10 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) : 1.13  
EDS : **FAILED**  
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) : 2.13

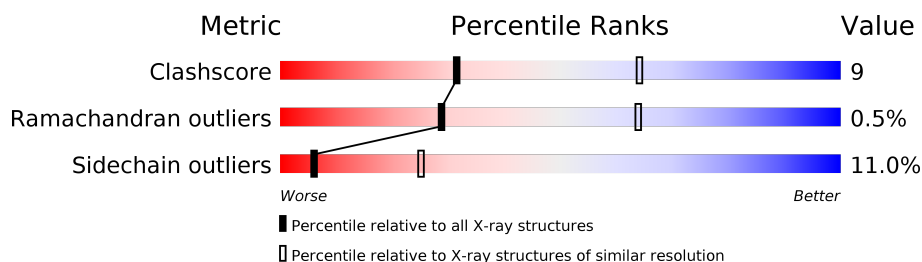
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)











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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	298	
1	B	298	
1	C	298	
1	D	298	
1	E	298	
1	F	298	
1	G	298	
1	H	298	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	I	298	 73% 19% 5%
1	J	298	 75% 20% 5%
1	K	298	 74% 20% 5%
1	L	298	 74% 18% 5%
1	M	298	 72% 22% 5%
1	N	298	 76% 18% 5%
1	O	298	 74% 21% 5%
1	P	298	 72% 24% 5%
1	R	298	 74% 18% 5%
1	S	298	 73% 20% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MBO	A	302	-	-	X	-
2	MBO	B	301	-	-	X	-
2	MBO	C	301	-	-	X	-
2	MBO	D	301	-	-	X	-
2	MBO	E	301	-	-	X	-
2	MBO	F	302	-	-	X	-
2	MBO	G	301	-	-	X	-
2	MBO	H	301	-	-	X	-
2	MBO	H	302	-	-	X	-
2	MBO	I	302	-	-	X	-
2	MBO	K	301	-	-	X	-
2	MBO	K	302	-	-	X	-
2	MBO	L	301	-	-	X	-
2	MBO	L	302	-	-	X	-
2	MBO	M	301	-	-	X	-
2	MBO	O	301	-	-	X	-
2	MBO	P	302	-	-	X	-
2	MBO	R	301	-	-	X	-
2	MBO	S	301	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 41248 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 Lysenin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2301	1459	390	444	8			
1	B	284	Total	C	N	O	S	0	0	0
			2260	1432	384	436	8			
1	C	286	Total	C	N	O	S	0	0	0
			2268	1436	386	438	8			
1	D	285	Total	C	N	O	S	0	0	0
			2265	1435	385	437	8			
1	E	283	Total	C	N	O	S	0	0	0
			2252	1428	383	433	8			
1	F	283	Total	C	N	O	S	0	0	0
			2252	1428	383	433	8			
1	G	290	Total	C	N	O	S	0	0	0
			2301	1459	390	444	8			
1	H	283	Total	C	N	O	S	0	0	0
			2252	1428	383	433	8			
1	I	282	Total	C	N	O	S	0	0	0
			2248	1426	382	432	8			
1	J	290	Total	C	N	O	S	0	0	0
			2301	1459	390	444	8			
1	K	290	Total	C	N	O	S	0	0	0
			2301	1459	390	444	8			
1	L	284	Total	C	N	O	S	0	0	0
			2260	1434	384	434	8			
1	M	289	Total	C	N	O	S	0	0	0
			2297	1457	389	443	8			
1	N	289	Total	C	N	O	S	0	0	0
			2297	1457	389	443	8			
1	O	289	Total	C	N	O	S	0	0	0
			2297	1457	389	443	8			
1	P	289	Total	C	N	O	S	0	0	0
			2297	1457	389	443	8			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	283	Total	C	N	O	S	0	0	0
			2252	1428	383	433	8			
1	S	283	Total	C	N	O	S	0	0	0
			2252	1428	383	433	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O18423
A	84	GLN	GLU	engineered mutation	UNP O18423
A	85	LYS	GLU	engineered mutation	UNP O18423
A	92	GLN	GLU	engineered mutation	UNP O18423
A	97	SER	GLU	engineered mutation	UNP O18423
A	126	GLY	ASP	engineered mutation	UNP O18423
B	0	GLY	-	expression tag	UNP O18423
B	84	GLN	GLU	engineered mutation	UNP O18423
B	85	LYS	GLU	engineered mutation	UNP O18423
B	92	GLN	GLU	engineered mutation	UNP O18423
B	97	SER	GLU	engineered mutation	UNP O18423
B	126	GLY	ASP	engineered mutation	UNP O18423
C	0	GLY	-	expression tag	UNP O18423
C	84	GLN	GLU	engineered mutation	UNP O18423
C	85	LYS	GLU	engineered mutation	UNP O18423
C	92	GLN	GLU	engineered mutation	UNP O18423
C	97	SER	GLU	engineered mutation	UNP O18423
C	126	GLY	ASP	engineered mutation	UNP O18423
D	0	GLY	-	expression tag	UNP O18423
D	84	GLN	GLU	engineered mutation	UNP O18423
D	85	LYS	GLU	engineered mutation	UNP O18423
D	92	GLN	GLU	engineered mutation	UNP O18423
D	97	SER	GLU	engineered mutation	UNP O18423
D	126	GLY	ASP	engineered mutation	UNP O18423
E	0	GLY	-	expression tag	UNP O18423
E	84	GLN	GLU	engineered mutation	UNP O18423
E	85	LYS	GLU	engineered mutation	UNP O18423
E	92	GLN	GLU	engineered mutation	UNP O18423
E	97	SER	GLU	engineered mutation	UNP O18423
E	126	GLY	ASP	engineered mutation	UNP O18423
F	0	GLY	-	expression tag	UNP O18423
F	84	GLN	GLU	engineered mutation	UNP O18423
F	85	LYS	GLU	engineered mutation	UNP O18423
F	92	GLN	GLU	engineered mutation	UNP O18423

*Continued on next page...*

*Continued from previous page...*

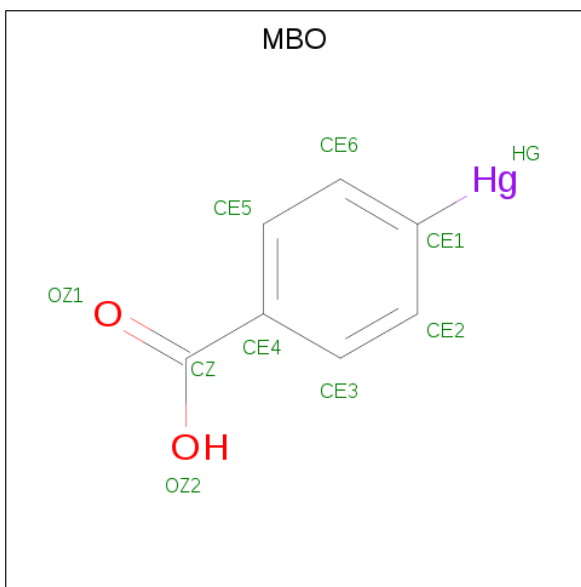
Chain	Residue	Modelled	Actual	Comment	Reference
F	97	SER	GLU	engineered mutation	UNP O18423
F	126	GLY	ASP	engineered mutation	UNP O18423
G	0	GLY	-	expression tag	UNP O18423
G	84	GLN	GLU	engineered mutation	UNP O18423
G	85	LYS	GLU	engineered mutation	UNP O18423
G	92	GLN	GLU	engineered mutation	UNP O18423
G	97	SER	GLU	engineered mutation	UNP O18423
G	126	GLY	ASP	engineered mutation	UNP O18423
H	0	GLY	-	expression tag	UNP O18423
H	84	GLN	GLU	engineered mutation	UNP O18423
H	85	LYS	GLU	engineered mutation	UNP O18423
H	92	GLN	GLU	engineered mutation	UNP O18423
H	97	SER	GLU	engineered mutation	UNP O18423
H	126	GLY	ASP	engineered mutation	UNP O18423
I	0	GLY	-	expression tag	UNP O18423
I	84	GLN	GLU	engineered mutation	UNP O18423
I	85	LYS	GLU	engineered mutation	UNP O18423
I	92	GLN	GLU	engineered mutation	UNP O18423
I	97	SER	GLU	engineered mutation	UNP O18423
I	126	GLY	ASP	engineered mutation	UNP O18423
J	0	GLY	-	expression tag	UNP O18423
J	84	GLN	GLU	engineered mutation	UNP O18423
J	85	LYS	GLU	engineered mutation	UNP O18423
J	92	GLN	GLU	engineered mutation	UNP O18423
J	97	SER	GLU	engineered mutation	UNP O18423
J	126	GLY	ASP	engineered mutation	UNP O18423
K	0	GLY	-	expression tag	UNP O18423
K	84	GLN	GLU	engineered mutation	UNP O18423
K	85	LYS	GLU	engineered mutation	UNP O18423
K	92	GLN	GLU	engineered mutation	UNP O18423
K	97	SER	GLU	engineered mutation	UNP O18423
K	126	GLY	ASP	engineered mutation	UNP O18423
L	0	GLY	-	expression tag	UNP O18423
L	84	GLN	GLU	engineered mutation	UNP O18423
L	85	LYS	GLU	engineered mutation	UNP O18423
L	92	GLN	GLU	engineered mutation	UNP O18423
L	97	SER	GLU	engineered mutation	UNP O18423
L	126	GLY	ASP	engineered mutation	UNP O18423
M	0	GLY	-	expression tag	UNP O18423
M	84	GLN	GLU	engineered mutation	UNP O18423
M	85	LYS	GLU	engineered mutation	UNP O18423
M	92	GLN	GLU	engineered mutation	UNP O18423

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	97	SER	GLU	engineered mutation	UNP O18423
M	126	GLY	ASP	engineered mutation	UNP O18423
N	0	GLY	-	expression tag	UNP O18423
N	84	GLN	GLU	engineered mutation	UNP O18423
N	85	LYS	GLU	engineered mutation	UNP O18423
N	92	GLN	GLU	engineered mutation	UNP O18423
N	97	SER	GLU	engineered mutation	UNP O18423
N	126	GLY	ASP	engineered mutation	UNP O18423
O	0	GLY	-	expression tag	UNP O18423
O	84	GLN	GLU	engineered mutation	UNP O18423
O	85	LYS	GLU	engineered mutation	UNP O18423
O	92	GLN	GLU	engineered mutation	UNP O18423
O	97	SER	GLU	engineered mutation	UNP O18423
O	126	GLY	ASP	engineered mutation	UNP O18423
P	0	GLY	-	expression tag	UNP O18423
P	84	GLN	GLU	engineered mutation	UNP O18423
P	85	LYS	GLU	engineered mutation	UNP O18423
P	92	GLN	GLU	engineered mutation	UNP O18423
P	97	SER	GLU	engineered mutation	UNP O18423
P	126	GLY	ASP	engineered mutation	UNP O18423
R	0	GLY	-	expression tag	UNP O18423
R	84	GLN	GLU	engineered mutation	UNP O18423
R	85	LYS	GLU	engineered mutation	UNP O18423
R	92	GLN	GLU	engineered mutation	UNP O18423
R	97	SER	GLU	engineered mutation	UNP O18423
R	126	GLY	ASP	engineered mutation	UNP O18423
S	0	GLY	-	expression tag	UNP O18423
S	84	GLN	GLU	engineered mutation	UNP O18423
S	85	LYS	GLU	engineered mutation	UNP O18423
S	92	GLN	GLU	engineered mutation	UNP O18423
S	97	SER	GLU	engineered mutation	UNP O18423
S	126	GLY	ASP	engineered mutation	UNP O18423

- Molecule 2 is MERCURIBENZOIC ACID (three-letter code: MBO) (formula: C<sub>7</sub>H<sub>5</sub>HgO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	A	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	B	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	B	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	C	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	D	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	E	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	F	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	G	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	H	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	H	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	I	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	K	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	K	1	Total	C	Hg	O	0	0
			10	7	1	2		

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	L	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	L	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	M	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	M	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	O	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	P	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	R	1	Total	C	Hg	O	0	0
			10	7	1	2		
2	S	1	Total	C	Hg	O	0	0
			10	7	1	2		

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Hg	0	0
			1	1		
3	G	1	Total	Hg	0	0
			1	1		
3	J	2	Total	Hg	0	0
			2	2		
3	D	1	Total	Hg	0	0
			1	1		
3	E	1	Total	Hg	0	0
			1	1		
3	I	1	Total	Hg	0	0
			1	1		
3	C	1	Total	Hg	0	0
			1	1		
3	N	2	Total	Hg	0	0
			2	2		
3	O	1	Total	Hg	0	0
			1	1		
3	R	1	Total	Hg	0	0
			1	1		
3	S	1	Total	Hg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Hg	0	0
			1	1		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	2	Total	O	0	0
			2	2		
4	C	2	Total	O	0	0
			2	2		
4	D	7	Total	O	0	0
			7	7		
4	E	5	Total	O	0	0
			5	5		
4	F	5	Total	O	0	0
			5	5		
4	G	2	Total	O	0	0
			2	2		
4	H	2	Total	O	0	0
			2	2		
4	I	4	Total	O	0	0
			4	4		
4	J	4	Total	O	0	0
			4	4		
4	K	8	Total	O	0	0
			8	8		
4	L	2	Total	O	0	0
			2	2		
4	M	2	Total	O	0	0
			2	2		
4	N	2	Total	O	0	0
			2	2		
4	O	2	Total	O	0	0
			2	2		
4	P	1	Total	O	0	0
			1	1		
4	R	3	Total	O	0	0
			3	3		
4	S	1	Total	O	0	0
			1	1		

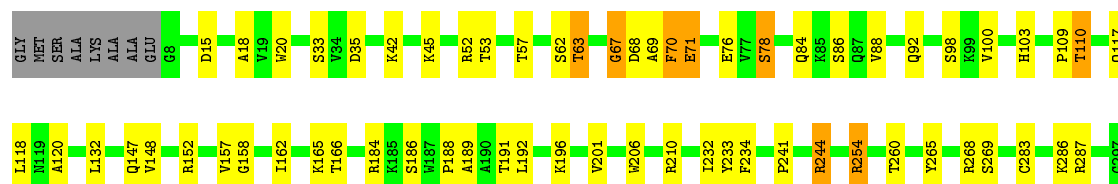
### 3 Residue-property plots [i](#)

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

Note EDS failed to run properly.

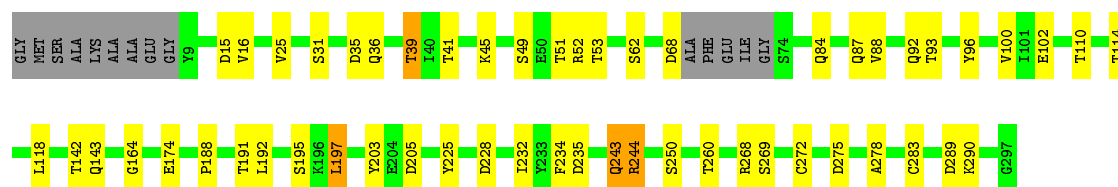
#### • Molecule 1: Lysenin

Chain A: 



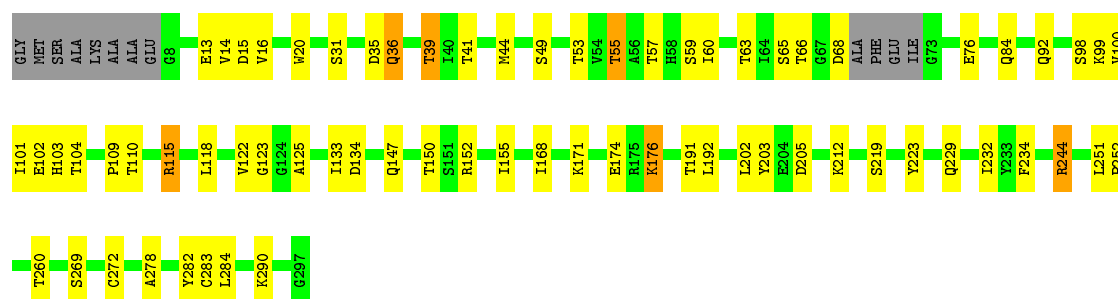
#### • Molecule 1: Lysenin

Chain B: 



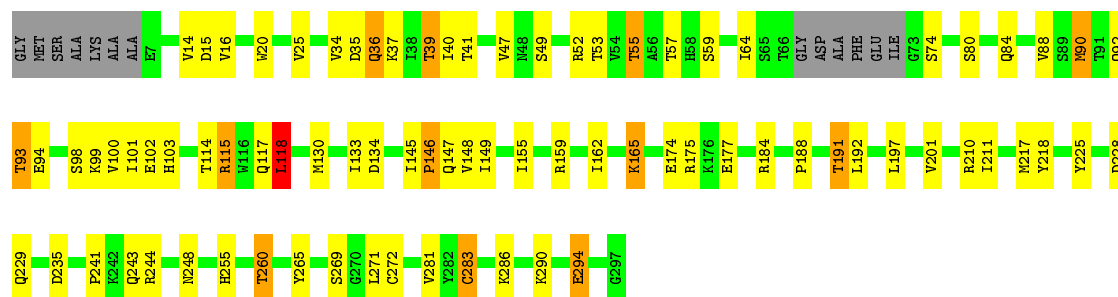
#### • Molecule 1: Lysenin

Chain C: 



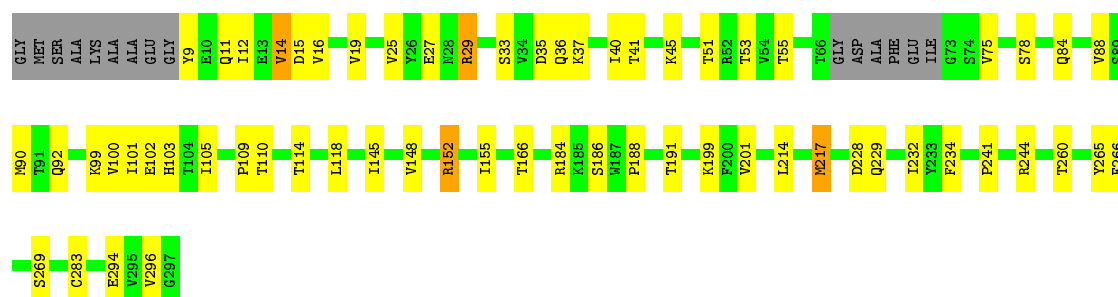
#### • Molecule 1: Lysenin

Chain D: 



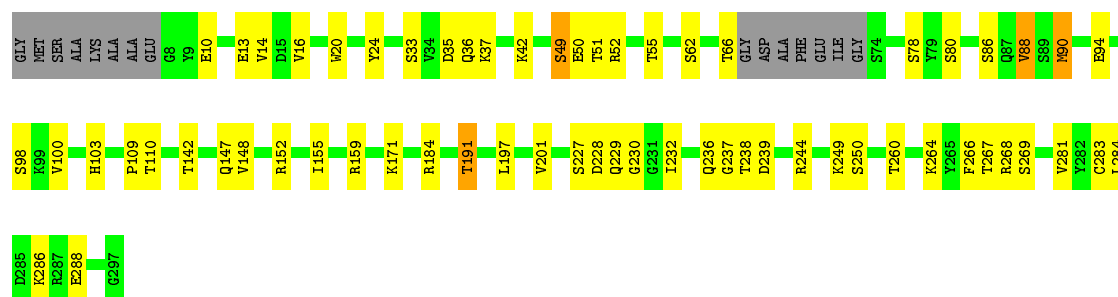
- Molecule 1: Lysenin

Chain E: 74% 19% 5%



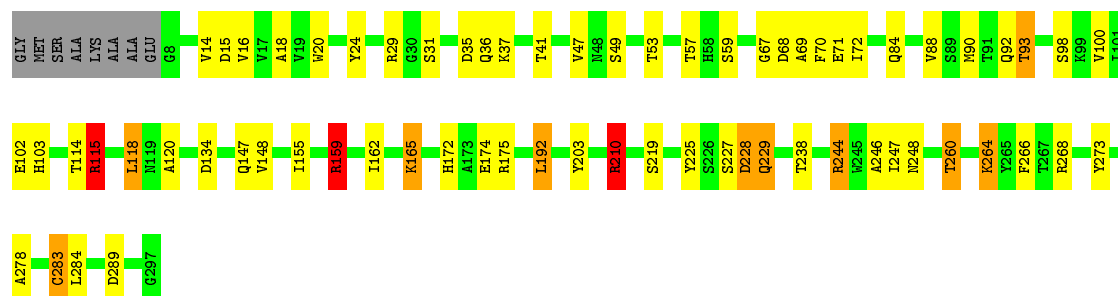
- Molecule 1: Lysenin

Chain F: 74% 20% 5%



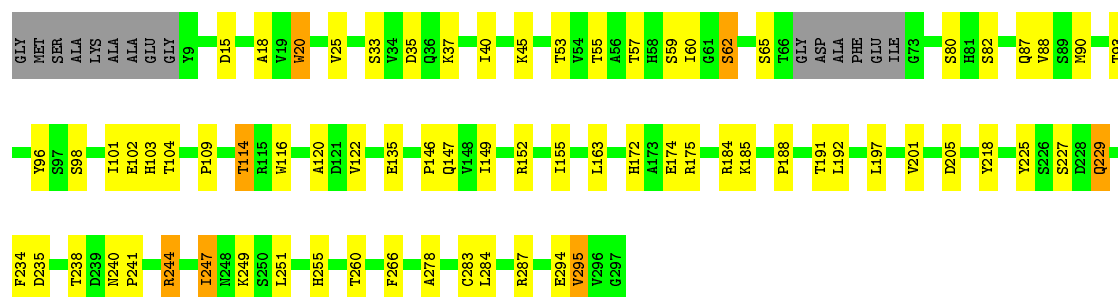
- Molecule 1: Lysenin

Chain G: 74% 18% 5%



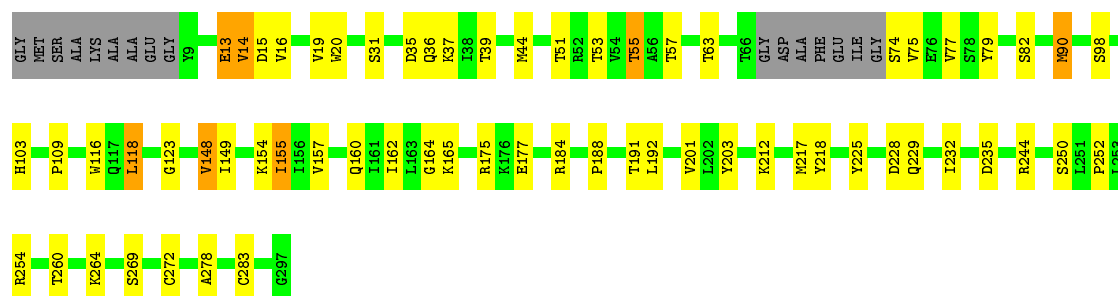
- Molecule 1: Lysenin

Chain H:  70% 22% • 5%



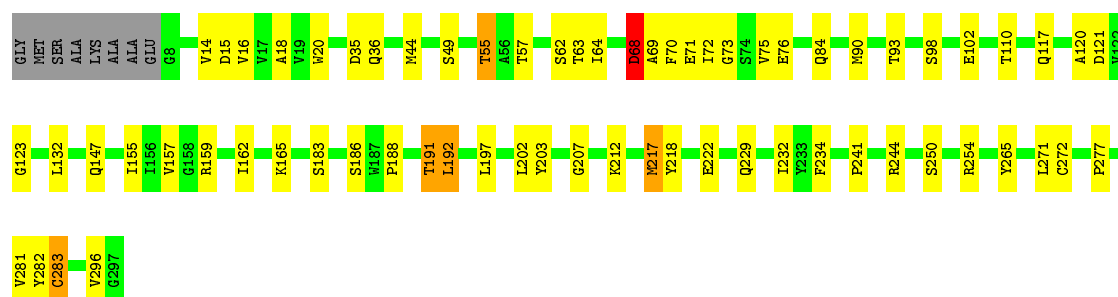
- Molecule 1: Lysenin

Chain I:  73% 19% • 5%



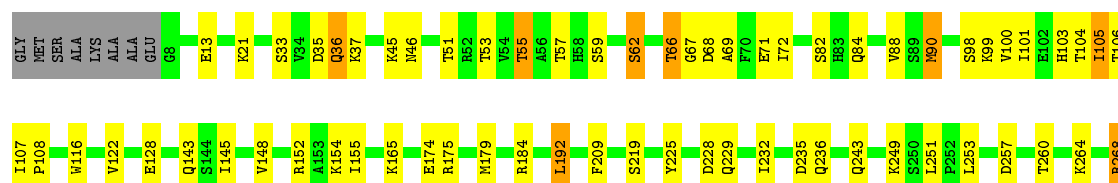
- Molecule 1: Lysenin

Chain J:  75% 20% . .



- Molecule 1: Lysenin

Chain K:  74% 20% .





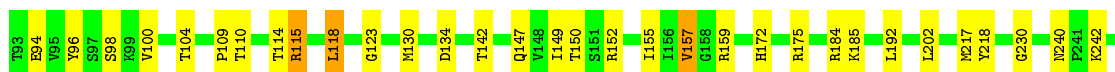
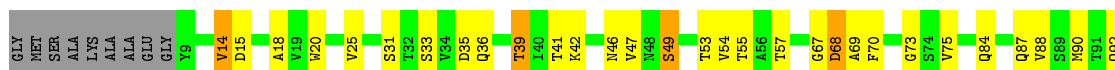
• Molecule 1: Lysenin

Chain L: 74% 18% 5%



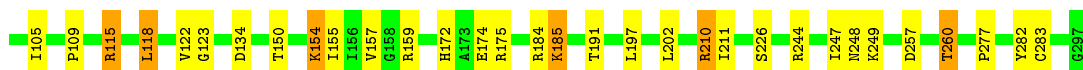
• Molecule 1: Lysenin

Chain M: 72% 22% 2%



• Molecule 1: Lysenin

Chain N: 76% 18% 2%



• Molecule 1: Lysenin

Chain O: 74% 21% 2%





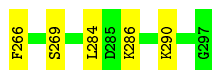
• Molecule 1: Lysenin

Chain P:  72% 24% • •



• Molecule 1: Lysenin

Chain R:  74% 18% 5% •



• Molecule 1: Lysenin

Chain S:  73% 20% 5% •



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.99Å 192.99Å 493.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 3.10	Depositor
% Data completeness (in resolution range)	99.9 (49.10-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.214 , 0.258	Depositor
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.541	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	41248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.49	0/2352	0.73	0/3186
1	B	0.48	0/2309	0.70	0/3127
1	C	0.49	0/2317	0.69	0/3137
1	D	0.49	0/2314	0.73	1/3133 (0.0%)
1	E	0.50	0/2301	0.73	0/3116
1	F	0.55	0/2301	0.77	0/3116
1	G	0.56	0/2352	0.81	4/3186 (0.1%)
1	H	0.51	0/2301	0.75	0/3116
1	I	0.50	0/2297	0.73	1/3111 (0.0%)
1	J	0.49	0/2352	0.69	0/3186
1	K	0.51	0/2352	0.75	0/3186
1	L	0.48	0/2309	0.71	1/3127 (0.0%)
1	M	0.49	0/2348	0.70	0/3181
1	N	0.50	0/2348	0.72	1/3181 (0.0%)
1	O	0.50	0/2348	0.72	0/3181
1	P	0.51	0/2348	0.72	0/3181
1	R	0.49	0/2301	0.72	0/3116
1	S	0.49	0/2301	0.71	1/3116 (0.0%)
All	All	0.50	0/41851	0.73	9/56683 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	S	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	LEU	CA-CB-CG	7.35	132.21	115.30
1	N	118	LEU	CA-CB-CG	6.95	131.29	115.30
1	G	115	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	G	210	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	G	118	LEU	CA-CB-CG	6.00	129.11	115.30
1	G	159	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	L	197	LEU	CA-CB-CG	5.60	128.18	115.30
1	I	118	LEU	CA-CB-CG	5.42	127.76	115.30
1	S	284	LEU	CA-CB-CG	5.18	127.23	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	GLY	Peptide
1	S	221	TYR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2301	0	2264	32	0
1	B	2260	0	2226	26	0
1	C	2268	0	2233	31	0
1	D	2265	0	2232	42	0
1	E	2252	0	2222	33	0
1	F	2252	0	2222	35	1
1	G	2301	0	2265	53	0
1	H	2252	0	2223	49	0
1	I	2248	0	2219	30	0
1	J	2301	0	2265	26	0
1	K	2301	0	2265	32	0
1	L	2260	0	2234	39	0
1	M	2297	0	2262	45	0
1	N	2297	0	2262	37	0
1	O	2297	0	2262	39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	2297	0	2261	36	0
1	R	2252	0	2222	35	1
1	S	2252	0	2223	33	0
2	A	20	0	8	9	0
2	B	20	0	8	16	0
2	C	10	0	4	9	0
2	D	10	0	4	17	0
2	E	10	0	4	5	0
2	F	10	0	4	19	0
2	G	10	0	4	13	0
2	H	20	0	8	29	0
2	I	10	0	4	6	0
2	K	20	0	8	29	0
2	L	20	0	8	25	0
2	M	20	0	8	18	0
2	O	10	0	4	12	0
2	P	10	0	4	20	0
2	R	10	0	4	7	0
2	S	10	0	4	15	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	N	2	0	0	0	0
3	O	1	0	0	1	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
4	A	7	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	7	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	8	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	1	0	0	0	0
4	R	3	0	0	0	0
4	S	1	0	0	0	0
All	All	41248	0	40450	735	1

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 9.

All (735) 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)
2:H:301:MBO:HE6	2:H:301:MBO:CE1	2.06	1.24
2:S:301:MBO:HE2	2:S:301:MBO:CE3	2.06	1.24
2:L:302:MBO:CE5	2:L:302:MBO:HE6	2.06	1.24
2:B:301:MBO:CE4	2:B:301:MBO:HE3	2.06	1.24
2:O:301:MBO:HE6	2:O:301:MBO:CE1	2.06	1.24
2:R:301:MBO:HE3	2:R:301:MBO:CE2	2.06	1.24
2:F:302:MBO:HE3	2:F:302:MBO:CE2	2.05	1.24
2:L:301:MBO:CE2	2:L:301:MBO:HE3	2.06	1.24
2:S:301:MBO:HE2	2:S:301:MBO:CE1	2.06	1.24
2:M:301:MBO:CE1	2:M:301:MBO:HE2	2.06	1.23
2:L:302:MBO:CE1	2:L:302:MBO:HE6	2.06	1.23
2:D:301:MBO:HE2	2:D:301:MBO:CE3	2.06	1.23
2:H:301:MBO:HE6	2:H:301:MBO:CE5	2.06	1.23
2:K:301:MBO:HE6	2:K:301:MBO:CE5	2.06	1.23
2:P:302:MBO:HE5	2:P:302:MBO:CE6	2.07	1.23
2:S:301:MBO:HE3	2:S:301:MBO:CE2	2.06	1.23
2:H:301:MBO:HE5	2:H:301:MBO:CE4	2.06	1.23
2:H:301:MBO:HE3	2:H:301:MBO:CE4	2.07	1.23
2:O:301:MBO:HE6	2:O:301:MBO:CE5	2.06	1.23
2:P:302:MBO:CE2	2:P:302:MBO:HE3	2.06	1.23
2:B:301:MBO:HE6	2:B:301:MBO:CE1	2.07	1.23
2:H:301:MBO:HE3	2:H:301:MBO:CE2	2.06	1.23
2:L:301:MBO:HE6	2:L:301:MBO:CE5	2.06	1.23
2:O:301:MBO:CE4	2:O:301:MBO:HE5	2.06	1.23
2:R:301:MBO:HE3	2:R:301:MBO:CE4	2.06	1.23
2:S:301:MBO:HE6	2:S:301:MBO:CE1	2.07	1.23

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:MBO:HE5	2:D:301:MBO:CE6	2.06	1.23
2:H:301:MBO:HE5	2:H:301:MBO:CE6	2.06	1.23
2:H:302:MBO:CE4	2:H:302:MBO:HE5	2.07	1.23
2:I:302:MBO:HE2	2:I:302:MBO:CE1	2.06	1.23
2:O:301:MBO:HE5	2:O:301:MBO:CE6	2.06	1.23
2:K:301:MBO:HE5	2:K:301:MBO:CE6	2.05	1.22
2:K:302:MBO:HE3	2:K:302:MBO:CE2	2.06	1.22
2:M:301:MBO:CE3	2:M:301:MBO:HE2	2.06	1.22
2:M:301:MBO:HE5	2:M:301:MBO:CE6	2.07	1.22
2:P:302:MBO:CE1	2:P:302:MBO:HE6	2.06	1.22
2:P:302:MBO:HE6	2:P:302:MBO:CE5	2.06	1.22
2:F:302:MBO:HE3	2:F:302:MBO:CE4	2.06	1.22
2:K:302:MBO:CE6	2:K:302:MBO:HE5	2.06	1.22
2:S:301:MBO:HE6	2:S:301:MBO:CE5	2.07	1.22
2:F:302:MBO:CE1	2:F:302:MBO:HE6	2.07	1.22
2:H:302:MBO:CE6	2:H:302:MBO:HE5	2.06	1.22
2:L:301:MBO:CE6	2:L:301:MBO:HE5	2.06	1.22
2:M:301:MBO:CE2	2:M:301:MBO:HE3	2.06	1.22
2:G:301:MBO:HE3	2:G:301:MBO:CE2	2.06	1.22
2:G:301:MBO:HE3	2:G:301:MBO:CE4	2.07	1.22
2:H:302:MBO:CE2	2:H:302:MBO:HE3	2.07	1.22
2:K:302:MBO:HE2	2:K:302:MBO:CE3	2.06	1.22
2:A:302:MBO:CE3	2:A:302:MBO:HE2	2.06	1.22
2:D:301:MBO:HE6	2:D:301:MBO:CE5	2.07	1.22
2:G:301:MBO:HE2	2:G:301:MBO:CE3	2.07	1.22
2:P:302:MBO:HE3	2:P:302:MBO:CE4	2.07	1.22
2:C:301:MBO:HE6	2:C:301:MBO:CE5	2.06	1.22
2:L:301:MBO:CE4	2:L:301:MBO:HE3	2.06	1.22
2:B:301:MBO:CE2	2:B:301:MBO:HE3	2.06	1.22
2:C:301:MBO:HE5	2:C:301:MBO:CE6	2.06	1.22
2:F:302:MBO:HE5	2:F:302:MBO:CE6	2.07	1.22
2:M:301:MBO:HE5	2:M:301:MBO:CE4	2.07	1.22
2:C:301:MBO:HE6	2:C:301:MBO:CE1	2.07	1.22
2:D:301:MBO:HE2	2:D:301:MBO:CE1	2.06	1.22
2:I:302:MBO:HE2	2:I:302:MBO:CE3	2.06	1.22
2:M:301:MBO:CE4	2:M:301:MBO:HE3	2.06	1.22
2:P:302:MBO:HE5	2:P:302:MBO:CE4	2.07	1.22
2:G:301:MBO:HE2	2:G:301:MBO:CE1	2.06	1.21
2:K:302:MBO:HE2	2:K:302:MBO:CE1	2.06	1.21
2:K:302:MBO:CE4	2:K:302:MBO:HE5	2.07	1.21
2:A:302:MBO:HE2	2:A:302:MBO:CE1	2.06	1.21

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:302:MBO:HE3	2:A:302:MBO:CE4	2.07	1.21
2:C:301:MBO:HE5	2:C:301:MBO:CE4	2.06	1.21
2:D:301:MBO:CE4	2:D:301:MBO:HE5	2.07	1.21
2:L:302:MBO:CE3	2:L:302:MBO:HE2	2.07	1.21
2:F:302:MBO:HE6	2:F:302:MBO:CE5	2.07	1.21
2:K:301:MBO:HE2	2:K:301:MBO:CE1	2.07	1.21
2:K:301:MBO:HE6	2:K:301:MBO:CE1	2.06	1.21
2:K:302:MBO:HE3	2:K:302:MBO:CE4	2.06	1.21
2:L:301:MBO:CE1	2:L:301:MBO:HE6	2.06	1.21
2:A:302:MBO:HE3	2:A:302:MBO:CE2	2.07	1.21
2:S:301:MBO:CE4	2:S:301:MBO:HE3	2.06	1.21
2:L:302:MBO:HE2	2:L:302:MBO:CE1	2.07	1.21
2:L:301:MBO:CE4	2:L:301:MBO:HE5	2.06	1.21
2:B:301:MBO:CE5	2:B:301:MBO:HE6	2.07	1.21
2:K:301:MBO:HE2	2:K:301:MBO:CE3	2.07	1.21
2:K:301:MBO:HE5	2:K:301:MBO:CE4	2.06	1.20
2:B:301:MBO:HE5	2:B:301:MBO:CE4	2.07	1.20
2:B:301:MBO:HE5	2:B:301:MBO:CE6	2.07	1.20
2:D:301:MBO:CE1	2:D:301:MBO:HE6	2.07	1.20
2:F:302:MBO:CE4	2:F:302:MBO:HE5	2.08	1.20
2:H:302:MBO:HE3	2:H:302:MBO:CE4	2.07	1.19
2:C:301:MBO:HE6	2:C:301:MBO:CE6	0.97	1.07
2:G:301:MBO:HE2	2:G:301:MBO:CE2	0.97	1.07
2:P:302:MBO:CE3	2:P:302:MBO:HE3	0.97	1.07
2:P:302:MBO:CE6	2:P:302:MBO:HE6	0.97	1.07
2:S:301:MBO:HE2	2:S:301:MBO:CE2	0.97	1.07
2:K:302:MBO:CE3	2:K:302:MBO:HE3	0.97	1.07
2:S:301:MBO:HE6	2:S:301:MBO:CE6	0.97	1.07
2:A:302:MBO:HE2	2:A:302:MBO:CE2	0.97	1.07
2:L:302:MBO:CE6	2:L:302:MBO:HE6	0.97	1.07
2:O:301:MBO:CE5	2:O:301:MBO:HE5	0.97	1.07
2:P:302:MBO:HE5	2:P:302:MBO:CE5	0.97	1.07
2:S:301:MBO:HE3	2:S:301:MBO:CE3	0.97	1.07
2:A:302:MBO:CE3	2:A:302:MBO:HE3	0.97	1.07
2:D:301:MBO:HE6	2:D:301:MBO:CE6	0.97	1.07
2:H:302:MBO:CE3	2:H:302:MBO:HE3	0.97	1.07
2:M:301:MBO:HE5	2:M:301:MBO:CE5	0.97	1.07
2:R:301:MBO:HE3	2:R:301:MBO:CE3	0.97	1.07
2:H:301:MBO:HE6	2:H:301:MBO:CE6	0.97	1.06
2:H:302:MBO:CE5	2:H:302:MBO:HE5	0.97	1.06
2:K:302:MBO:HE2	2:K:302:MBO:CE2	0.97	1.06

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:301:MBO:CE2	2:M:301:MBO:HE2	0.97	1.06
2:B:301:MBO:CE3	2:B:301:MBO:HE3	0.97	1.06
2:B:301:MBO:CE5	2:B:301:MBO:HE5	0.97	1.06
2:C:301:MBO:HE5	2:C:301:MBO:CE5	0.97	1.06
2:K:302:MBO:HE5	2:K:302:MBO:CE5	0.97	1.06
2:L:302:MBO:HE2	2:L:302:MBO:CE2	0.97	1.06
2:M:301:MBO:CE3	2:M:301:MBO:HE3	0.97	1.06
2:B:301:MBO:HE6	2:B:301:MBO:CE6	0.97	1.06
2:F:302:MBO:HE3	2:F:302:MBO:CE3	0.97	1.06
2:F:302:MBO:CE5	2:F:302:MBO:HE5	0.97	1.06
2:H:301:MBO:HE5	2:H:301:MBO:CE5	0.97	1.06
2:I:302:MBO:HE2	2:I:302:MBO:CE2	0.97	1.06
2:K:301:MBO:HE6	2:K:301:MBO:CE6	0.97	1.06
2:K:301:MBO:HE2	2:K:301:MBO:CE2	0.97	1.06
2:O:301:MBO:HE6	2:O:301:MBO:CE6	0.97	1.06
2:F:302:MBO:HE6	2:F:302:MBO:CE6	0.97	1.06
2:L:301:MBO:HE5	2:L:301:MBO:CE5	0.97	1.06
2:G:301:MBO:HE3	2:G:301:MBO:CE3	0.97	1.06
2:L:301:MBO:CE3	2:L:301:MBO:HE3	0.97	1.06
2:D:301:MBO:CE5	2:D:301:MBO:HE5	0.97	1.06
2:K:301:MBO:HE5	2:K:301:MBO:CE5	0.97	1.06
2:L:301:MBO:CE6	2:L:301:MBO:HE6	0.97	1.06
2:D:301:MBO:HE2	2:D:301:MBO:CE2	0.97	1.06
2:H:301:MBO:HE3	2:H:301:MBO:CE3	0.97	1.06
1:F:36:GLN:HE21	1:G:103:HIS:CE1	1.76	1.02
1:H:37:LYS:HG3	1:H:104:THR:HG22	1.45	0.99
1:F:229:GLN:HA	2:F:302:MBO:HE3	1.82	0.99
1:F:36:GLN:HE21	1:G:103:HIS:HE1	1.02	0.93
1:A:254:ARG:HG2	1:A:254:ARG:HH11	1.33	0.91
1:G:210:ARG:HG3	1:G:210:ARG:HH11	1.34	0.91
1:M:230:GLY:HA2	2:M:301:MBO:HE2	1.91	0.90
1:L:122:VAL:HG11	1:L:155:ILE:HD11	1.54	0.90
2:H:302:MBO:HE5	2:H:302:MBO:HE6	2.36	0.84
2:C:301:MBO:HE6	2:C:301:MBO:HE5	2.37	0.83
2:H:301:MBO:HE6	2:H:301:MBO:HE5	2.37	0.83
2:I:302:MBO:HE3	2:I:302:MBO:HE2	2.37	0.83
2:K:301:MBO:HE6	2:K:301:MBO:HE5	2.37	0.83
2:L:301:MBO:HE2	2:L:301:MBO:HE3	2.37	0.83
2:K:302:MBO:HE2	2:K:302:MBO:HE3	2.37	0.82
2:M:301:MBO:HE2	2:M:301:MBO:HE3	2.36	0.82
1:R:228:ASP:O	2:R:301:MBO:HE3	2.17	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:302:MBO:HE3	2:P:302:MBO:HE2	2.37	0.82
1:G:172:HIS:HD2	1:G:175:ARG:H	1.27	0.82
2:O:301:MBO:HE6	2:O:301:MBO:HE5	2.36	0.82
1:M:172:HIS:HD2	1:M:175:ARG:H	1.26	0.82
2:S:301:MBO:HE2	2:S:301:MBO:HE3	2.37	0.82
2:F:302:MBO:HE2	2:F:302:MBO:HE3	2.36	0.82
2:L:301:MBO:HE6	2:L:301:MBO:HE5	2.37	0.82
2:R:301:MBO:HE3	2:R:301:MBO:HE2	2.36	0.82
2:A:302:MBO:HE3	2:A:302:MBO:HE2	2.37	0.81
2:H:301:MBO:HE3	2:H:301:MBO:HE2	2.38	0.81
2:L:302:MBO:HE2	2:L:302:MBO:HE3	2.37	0.81
2:M:301:MBO:HE5	2:M:301:MBO:HE6	2.37	0.81
2:P:302:MBO:HE5	2:P:302:MBO:HE6	2.37	0.81
2:D:301:MBO:HE2	2:D:301:MBO:HE3	2.37	0.81
2:G:301:MBO:HE2	2:G:301:MBO:HE3	2.38	0.81
1:N:13:GLU:HG3	1:N:154:LYS:HE2	1.62	0.81
2:B:301:MBO:HE3	2:B:301:MBO:HE2	2.36	0.81
2:B:301:MBO:HE5	2:B:301:MBO:HE6	2.38	0.81
2:D:301:MBO:HE6	2:D:301:MBO:HE5	2.38	0.81
2:L:302:MBO:HE5	2:L:302:MBO:HE6	2.37	0.81
1:P:230:GLY:HA2	2:P:302:MBO:HE2	2.01	0.81
2:F:302:MBO:HE6	2:F:302:MBO:HE5	2.39	0.80
1:R:172:HIS:HD2	1:R:175:ARG:H	1.28	0.79
2:S:301:MBO:HE6	2:S:301:MBO:HE5	2.38	0.79
2:K:302:MBO:HE5	2:K:302:MBO:HE6	2.37	0.79
1:H:37:LYS:HG3	1:H:104:THR:CG2	2.14	0.77
2:H:302:MBO:HE2	2:H:302:MBO:HE3	2.39	0.77
1:M:90:MET:HB3	1:N:49:SER:HB2	1.66	0.77
2:K:301:MBO:HE3	2:K:301:MBO:HE2	2.39	0.76
1:N:115:ARG:HD2	1:N:134:ASP:OD2	1.84	0.76
1:E:228:ASP:O	2:E:301:MBO:HE3	2.23	0.76
1:G:115:ARG:HH11	1:G:115:ARG:HG3	1.48	0.76
1:B:25:VAL:HG22	1:B:114:THR:HG22	1.69	0.75
1:I:228:ASP:O	2:I:302:MBO:HE5	2.26	0.74
1:C:36:GLN:HG3	1:D:103:HIS:CE1	2.23	0.73
1:L:122:VAL:CG1	1:L:155:ILE:HD11	2.19	0.73
1:L:283:CYS:SG	2:L:301:MBO:HG	2.07	0.72
1:F:229:GLN:CA	2:F:302:MBO:HE3	2.56	0.72
1:K:67:GLY:O	1:K:69:ALA:N	2.22	0.72
1:M:230:GLY:CA	2:M:301:MBO:HE2	2.58	0.72
1:M:73:GLY:HA2	1:N:67:GLY:H	1.53	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:266:PHE:CD1	2:H:302:MBO:HE6	2.62	0.71
1:S:228:ASP:O	2:S:301:MBO:HE3	2.29	0.71
1:M:14:VAL:HG21	1:M:123:GLY:O	1.90	0.71
1:L:90:MET:HB3	1:M:49:SER:HB2	1.70	0.70
1:M:266:PHE:HB3	2:M:301:MBO:HE6	2.10	0.70
1:H:20:TRP:HZ3	1:H:116:TRP:CE3	2.10	0.70
1:S:192:LEU:HB2	1:S:280:ASN:HD21	1.56	0.70
1:S:283:CYS:SG	2:S:301:MBO:HG	2.10	0.69
1:G:29:ARG:HB2	1:H:135:GLU:HB3	1.76	0.68
1:P:230:GLY:CA	2:P:302:MBO:HE2	2.61	0.68
1:E:9:TYR:HE2	1:E:11:GLN:HE21	1.41	0.68
1:I:188:PRO:HD3	1:I:218:TYR:HD1	1.58	0.68
1:F:230:GLY:HA2	2:F:302:MBO:HE2	2.13	0.68
1:J:117:GLN:HG3	1:J:132:LEU:HD13	1.76	0.68
1:D:36:GLN:HG3	1:E:103:HIS:NE2	2.08	0.68
2:O:301:MBO:HE5	2:O:301:MBO:CZ	2.61	0.68
1:G:172:HIS:CD2	1:G:175:ARG:H	2.12	0.67
2:B:301:MBO:CZ	2:B:301:MBO:HE3	2.63	0.67
1:P:90:MET:HB3	1:R:49:SER:HB2	1.74	0.67
1:R:55:THR:HB	1:R:86:SER:HB2	1.75	0.67
2:H:302:MBO:CZ	2:H:302:MBO:HE5	2.63	0.67
2:R:301:MBO:HE3	2:R:301:MBO:CZ	2.63	0.67
2:F:302:MBO:CZ	2:F:302:MBO:HE3	2.62	0.66
1:J:76:GLU:O	1:K:62:SER:HB2	1.96	0.66
1:N:84:GLN:HB3	1:O:55:THR:HG23	1.77	0.66
1:J:155:ILE:HG22	1:K:145:ILE:HB	1.76	0.66
2:K:301:MBO:HE5	2:K:301:MBO:CZ	2.63	0.66
1:N:100:VAL:HB	1:O:39:THR:HG23	1.77	0.66
2:A:302:MBO:HE3	2:A:302:MBO:CZ	2.64	0.66
1:P:41:THR:HG23	1:P:100:VAL:HG22	1.76	0.66
1:D:115:ARG:HD2	1:D:134:ASP:OD2	1.95	0.66
1:L:282:TYR:HB3	1:L:284:LEU:CD2	2.26	0.66
2:M:301:MBO:CZ	2:M:301:MBO:HE3	2.64	0.66
1:M:41:THR:HG23	1:M:100:VAL:HG22	1.78	0.66
1:O:100:VAL:HB	1:P:39:THR:HG23	1.78	0.66
1:O:103:HIS:NE2	1:P:36:GLN:HG3	2.11	0.65
1:R:39:THR:HB	1:R:102:GLU:HG3	1.77	0.65
2:S:301:MBO:HE3	2:S:301:MBO:CZ	2.65	0.65
1:C:115:ARG:HD3	1:C:134:ASP:OD2	1.96	0.65
1:E:51:THR:HB	1:F:88:VAL:HG13	1.78	0.65
1:K:228:ASP:O	2:K:301:MBO:HE5	2.35	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:CYS:SG	2:D:301:MBO:HG	2.15	0.65
1:O:232:ILE:HD11	1:O:283:CYS:HB2	1.78	0.64
1:O:269:SER:HB3	2:O:301:MBO:HE6	2.17	0.64
1:G:248:ASN:HB3	1:G:260:THR:HG22	1.79	0.64
1:R:17:VAL:HG13	1:R:150:THR:HG22	1.78	0.64
1:J:64:ILE:HG13	1:S:75:VAL:HG22	1.79	0.64
1:R:115:ARG:HD3	1:R:134:ASP:OD2	1.97	0.64
2:H:301:MBO:CZ	2:H:301:MBO:HE5	2.65	0.64
1:P:84:GLN:HB3	1:R:55:THR:HG23	1.79	0.64
1:G:172:HIS:HE1	1:G:289:ASP:OD2	1.78	0.64
1:F:14:VAL:HG12	1:F:155:ILE:HD13	1.79	0.64
2:C:301:MBO:CZ	2:C:301:MBO:HE5	2.66	0.64
1:O:25:VAL:HG22	1:O:114:THR:HG22	1.80	0.64
1:G:67:GLY:O	1:G:69:ALA:N	2.31	0.63
1:B:53:THR:HG23	1:B:88:VAL:HG22	1.79	0.63
1:D:55:THR:HG23	1:E:84:GLN:HB3	1.78	0.63
1:F:36:GLN:NE2	1:G:103:HIS:HE1	1.85	0.63
1:O:272:CYS:SG	3:O:302:HG:HG	2.16	0.63
1:G:283:CYS:SG	2:G:301:MBO:HG	2.17	0.63
1:K:84:GLN:HB3	1:L:55:THR:HG23	1.80	0.63
2:K:302:MBO:HE5	2:K:302:MBO:CZ	2.67	0.63
1:N:14:VAL:HG21	1:N:123:GLY:O	1.98	0.63
1:B:269:SER:HB3	2:B:302:MBO:HE6	2.19	0.62
2:K:302:MBO:HE3	2:K:302:MBO:CZ	2.67	0.62
1:O:269:SER:CB	2:O:301:MBO:HE6	2.68	0.62
1:P:33:SER:HB3	1:P:109:PRO:HD3	1.81	0.62
1:C:49:SER:HB2	1:D:90:MET:HG2	1.81	0.62
1:K:103:HIS:NE2	1:L:36:GLN:HG3	2.15	0.62
1:C:39:THR:HG23	1:D:100:VAL:HB	1.82	0.61
1:D:228:ASP:O	2:D:301:MBO:HE3	2.38	0.61
1:H:266:PHE:CE1	2:H:302:MBO:HE6	2.73	0.61
1:H:20:TRP:CZ3	1:H:116:TRP:CE3	2.89	0.61
1:N:45:LYS:HG3	1:N:96:TYR:HB3	1.81	0.61
2:L:301:MBO:CZ	2:L:301:MBO:HE3	2.67	0.61
2:P:302:MBO:CZ	2:P:302:MBO:HE3	2.68	0.61
1:H:40:ILE:HG13	1:H:101:ILE:HG23	1.80	0.61
1:K:225:TYR:CD1	1:K:235:ASP:HB2	2.36	0.61
1:M:100:VAL:HB	1:N:39:THR:HG23	1.82	0.61
1:S:14:VAL:HG22	1:S:155:ILE:CD1	2.31	0.61
1:K:100:VAL:HB	1:L:39:THR:HG23	1.82	0.61
1:L:41:THR:HG23	1:L:100:VAL:HG22	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:269:SER:HB3	2:S:301:MBO:HE6	2.21	0.61
1:I:20:TRP:HZ3	1:I:116:TRP:CE3	2.19	0.60
1:R:90:MET:HG2	1:S:49:SER:HB3	1.81	0.60
1:M:287:ARG:HH11	2:M:302:MBO:HE6	2.05	0.60
1:P:34:VAL:HG23	1:P:107:ILE:HB	1.83	0.60
2:D:301:MBO:HE5	2:D:301:MBO:CZ	2.67	0.60
2:P:302:MBO:CZ	2:P:302:MBO:HE5	2.70	0.60
1:H:225:TYR:CD1	1:H:235:ASP:HB2	2.35	0.60
2:G:301:MBO:HE3	2:G:301:MBO:CZ	2.70	0.60
1:C:59:SER:HB2	1:D:80:SER:HB3	1.83	0.60
1:A:109:PRO:O	1:A:110:THR:HB	2.02	0.60
1:R:238:THR:O	1:R:244:ARG:NH2	2.35	0.60
1:L:53:THR:HG23	1:L:88:VAL:HG22	1.82	0.59
2:H:301:MBO:CZ	2:H:301:MBO:HE3	2.70	0.59
1:O:67:GLY:O	1:O:69:ALA:N	2.32	0.59
1:J:188:PRO:HD3	1:J:218:TYR:HD1	1.68	0.59
2:M:301:MBO:HE5	2:M:301:MBO:CZ	2.71	0.59
1:J:20:TRP:HB2	1:J:147:GLN:HA	1.85	0.59
2:L:301:MBO:CZ	2:L:301:MBO:HE5	2.69	0.59
1:R:172:HIS:CD2	1:R:175:ARG:H	2.15	0.59
1:M:75:VAL:HG22	1:N:64:ILE:HG12	1.85	0.58
1:R:84:GLN:HB3	1:S:55:THR:HG23	1.84	0.58
2:H:302:MBO:CZ	2:H:302:MBO:HE3	2.71	0.58
1:K:122:VAL:CG1	1:K:155:ILE:HD11	2.33	0.58
1:R:90:MET:HG2	1:S:49:SER:CB	2.34	0.58
1:M:25:VAL:HG22	1:M:114:THR:HG22	1.85	0.58
1:H:25:VAL:HG22	1:H:114:THR:HG22	1.84	0.58
1:O:269:SER:OG	2:O:301:MBO:HE6	2.41	0.58
1:E:53:THR:HB	1:F:86:SER:HB3	1.85	0.58
1:N:122:VAL:HG11	1:N:155:ILE:HD11	1.84	0.58
1:A:269:SER:HB3	2:A:301:MBO:HE6	2.24	0.57
1:L:282:TYR:HB3	1:L:284:LEU:HD22	1.85	0.57
1:P:230:GLY:N	2:P:302:MBO:HE2	2.57	0.57
1:B:268:ARG:HD2	1:C:278:ALA:HB1	1.85	0.57
1:H:284:LEU:CD1	2:H:301:MBO:HE6	2.72	0.57
1:K:53:THR:HG23	1:K:88:VAL:HG22	1.86	0.57
1:S:39:THR:HB	1:S:102:GLU:HG3	1.87	0.57
1:G:210:ARG:HG3	1:G:210:ARG:NH1	2.11	0.57
1:F:33:SER:HB3	1:F:109:PRO:HD3	1.86	0.57
1:O:41:THR:HG23	1:O:100:VAL:HG22	1.86	0.57
1:E:33:SER:HB3	1:E:109:PRO:HD3	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:HIS:HD2	1:H:175:ARG:H	1.52	0.56
1:M:115:ARG:HD3	1:M:134:ASP:OD2	2.06	0.56
1:D:49:SER:HB3	1:D:92:GLN:HG3	1.86	0.56
1:G:36:GLN:NE2	1:H:103:HIS:NE2	2.48	0.56
1:J:14:VAL:HG21	1:J:123:GLY:O	2.05	0.56
1:H:40:ILE:HG13	1:H:101:ILE:CG2	2.36	0.56
1:G:49:SER:HB2	1:H:90:MET:HB2	1.88	0.56
1:L:100:VAL:HB	1:M:39:THR:HG23	1.88	0.56
1:B:49:SER:HB3	1:B:92:GLN:HG3	1.88	0.56
2:F:302:MBO:CZ	2:F:302:MBO:HE5	2.73	0.56
1:H:255:HIS:HB2	1:H:295:VAL:CG2	2.36	0.56
1:M:47:VAL:HG22	1:M:94:GLU:HB3	1.88	0.56
1:S:14:VAL:HG22	1:S:155:ILE:HD11	1.88	0.56
1:F:266:PHE:HB2	1:F:269:SER:OG	2.06	0.56
1:I:157:VAL:HB	1:I:254:ARG:HD3	1.88	0.56
1:L:25:VAL:HG22	1:L:114:THR:HG22	1.86	0.56
1:E:188:PRO:HB2	1:E:234:PHE:HB2	1.87	0.55
1:I:13:GLU:HG2	1:I:154:LYS:HG3	1.87	0.55
1:N:53:THR:HG23	1:N:88:VAL:HG22	1.88	0.55
1:P:225:TYR:CD1	1:P:235:ASP:HB2	2.40	0.55
1:L:228:ASP:O	2:L:301:MBO:HE5	2.43	0.55
1:S:53:THR:HG23	1:S:88:VAL:HG22	1.87	0.55
1:K:236:GLN:O	1:K:243:GLN:NE2	2.39	0.55
1:L:195:SER:OG	1:L:197:LEU:HD12	2.06	0.55
1:C:99:LYS:HE3	1:C:101:ILE:HD11	1.87	0.55
1:P:266:PHE:HB3	2:P:302:MBO:HE6	2.26	0.55
1:E:145:ILE:HB	1:F:155:ILE:HG13	1.88	0.55
1:A:268:ARG:HD2	1:B:278:ALA:HB1	1.88	0.55
1:H:284:LEU:HA	2:H:302:MBO:HE2	2.27	0.55
1:J:162:ILE:HG23	1:J:165:LYS:HB3	1.87	0.55
1:L:73:GLY:HA2	1:M:67:GLY:H	1.71	0.55
1:N:48:ASN:HB2	1:N:93:THR:HG22	1.88	0.55
2:B:301:MBO:HE5	2:B:301:MBO:CZ	2.72	0.55
1:I:184:ARG:HD2	1:I:278:ALA:HB3	1.89	0.55
1:B:188:PRO:HB2	1:B:234:PHE:HB2	1.89	0.54
1:H:147:GLN:HB2	1:I:155:ILE:HD12	1.88	0.54
1:I:188:PRO:HD3	1:I:218:TYR:CD1	2.42	0.54
1:B:41:THR:HG23	1:B:100:VAL:HG22	1.88	0.54
1:B:39:THR:HG23	1:C:100:VAL:HB	1.89	0.54
1:G:248:ASN:HB3	1:G:260:THR:CG2	2.36	0.54
1:H:266:PHE:CG	2:H:302:MBO:HE6	2.80	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:116:TRP:HH2	1:K:143:GLN:NE2	2.04	0.54
1:K:269:SER:HB3	2:K:301:MBO:HE2	2.27	0.54
1:A:162:ILE:HG23	1:A:165:LYS:HB3	1.88	0.54
1:C:55:THR:HG23	1:D:84:GLN:HB3	1.88	0.54
1:S:115:ARG:HD3	1:S:134:ASP:OD2	2.07	0.54
1:A:254:ARG:HG2	1:A:254:ARG:NH1	2.11	0.54
1:C:282:TYR:HB3	1:C:284:LEU:HD23	1.88	0.54
1:M:14:VAL:HG11	1:M:155:ILE:HD11	1.89	0.54
1:A:20:TRP:HA	1:A:118:LEU:HG	1.90	0.54
1:A:84:GLN:HB3	1:I:55:THR:HG23	1.89	0.54
1:F:230:GLY:N	2:F:302:MBO:HE2	2.61	0.54
1:P:18:ALA:HB1	1:P:118:LEU:HD12	1.90	0.54
1:N:75:VAL:HG22	1:O:64:ILE:HD12	1.89	0.54
1:I:160:GLN:NE2	1:I:252:PRO:HB3	2.22	0.54
1:A:110:THR:CG2	1:A:110:THR:O	2.56	0.54
1:M:84:GLN:HB3	1:N:55:THR:HG23	1.90	0.54
1:A:33:SER:HB3	1:A:109:PRO:HD3	1.90	0.53
1:D:99:LYS:HE3	1:D:101:ILE:HD11	1.89	0.53
1:F:228:ASP:O	2:F:302:MBO:HE3	2.46	0.53
1:I:203:TYR:HE1	1:I:212:LYS:HD3	1.74	0.53
1:J:192:LEU:HD13	1:J:281:VAL:HG22	1.91	0.53
1:G:20:TRP:HB2	1:G:147:GLN:HA	1.89	0.53
1:O:20:TRP:HB2	1:O:147:GLN:HA	1.90	0.53
1:S:25:VAL:HG22	1:S:114:THR:HG22	1.89	0.53
1:G:14:VAL:HG22	1:G:155:ILE:HD11	1.90	0.53
1:K:99:LYS:HE3	1:K:101:ILE:HD11	1.90	0.53
1:B:205:ASP:OD1	1:B:244:ARG:NH1	2.41	0.53
1:C:260:THR:HG22	1:C:290:LYS:HA	1.90	0.53
1:L:99:LYS:HE2	1:L:101:ILE:HD11	1.91	0.53
1:M:266:PHE:CB	2:M:301:MBO:HE6	2.77	0.53
1:H:247:ILE:HG23	1:H:249:LYS:H	1.74	0.53
1:K:249:LYS:HE3	1:K:253:LEU:HD23	1.90	0.53
1:E:188:PRO:HA	1:E:217:MET:HE1	1.89	0.53
1:G:49:SER:HB2	1:H:90:MET:CB	2.39	0.53
1:R:19:VAL:HG22	1:R:148:VAL:HG22	1.89	0.53
1:L:115:ARG:HD2	1:L:132:LEU:HD22	1.91	0.53
1:M:94:GLU:HG3	1:N:45:LYS:HB3	1.91	0.53
1:D:146:PRO:CB	1:D:149:ILE:HD11	2.38	0.52
1:M:246:ALA:HB2	1:M:264:LYS:HE2	1.91	0.52
1:N:184:ARG:HG2	1:N:185:LYS:HD2	1.91	0.52
1:H:163:LEU:HD11	1:H:251:LEU:HD21	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:PRO:HG2	1:L:109:PRO:HG2	1.92	0.52
1:G:47:VAL:HA	1:G:93:THR:O	2.08	0.52
1:N:72:ILE:HG12	1:O:69:ALA:HB2	1.91	0.52
1:D:14:VAL:HG12	1:D:155:ILE:HD13	1.91	0.52
1:K:13:GLU:HG2	1:K:152:ARG:HH21	1.75	0.52
1:P:47:VAL:HG22	1:P:94:GLU:HG2	1.91	0.52
1:G:159:ARG:CB	1:G:159:ARG:HH11	2.22	0.52
1:L:47:VAL:HG22	1:L:94:GLU:HG3	1.92	0.52
1:H:25:VAL:HG22	1:H:114:THR:CG2	2.40	0.52
1:H:33:SER:HB3	1:H:109:PRO:HD3	1.92	0.52
1:F:230:GLY:CA	2:F:302:MBO:HE2	2.78	0.52
1:G:29:ARG:HB2	1:H:135:GLU:CB	2.39	0.51
1:I:20:TRP:CZ3	1:I:116:TRP:CE3	2.99	0.51
1:N:105:ILE:HB	1:O:34:VAL:HG12	1.91	0.51
1:N:172:HIS:HD2	1:N:175:ARG:H	1.57	0.51
1:A:20:TRP:HB2	1:A:147:GLN:HA	1.93	0.51
1:G:192:LEU:HD22	1:G:273:TYR:CD1	2.46	0.51
1:G:59:SER:HB2	1:H:80:SER:HB3	1.93	0.51
1:H:146:PRO:HB2	1:H:149:ILE:HD11	1.92	0.51
1:I:164:GLY:HA2	1:I:203:TYR:CE2	2.46	0.51
1:J:102:GLU:O	1:K:36:GLN:HA	2.10	0.51
1:N:122:VAL:CG1	1:N:155:ILE:HD11	2.41	0.51
1:O:14:VAL:HG21	1:O:123:GLY:O	2.11	0.51
1:A:86:SER:HB3	1:I:53:THR:HB	1.92	0.51
1:R:157:VAL:HB	1:R:254:ARG:HD3	1.92	0.51
1:S:190:ALA:HB3	1:S:232:ILE:HG22	1.93	0.51
1:B:232:ILE:HD11	1:B:283:CYS:HB2	1.92	0.51
1:M:184:ARG:HG2	1:M:185:LYS:HD2	1.93	0.51
1:M:31:SER:HA	1:M:109:PRO:HB3	1.93	0.51
1:S:41:THR:HG23	1:S:100:VAL:HG22	1.93	0.51
1:C:14:VAL:HG21	1:C:123:GLY:O	2.11	0.51
1:S:210:ARG:HG2	1:S:223:TYR:CD2	2.46	0.51
1:C:31:SER:HA	1:C:109:PRO:HB3	1.92	0.51
1:N:172:HIS:CD2	1:N:175:ARG:H	2.28	0.51
1:A:188:PRO:HG2	1:A:234:PHE:HB2	1.93	0.50
1:G:53:THR:HG23	1:G:88:VAL:HB	1.93	0.50
1:H:284:LEU:HD12	2:H:301:MBO:HE6	2.31	0.50
1:C:39:THR:HB	1:C:102:GLU:HG3	1.93	0.50
1:B:36:GLN:HG3	1:C:103:HIS:NE2	2.26	0.50
1:H:184:ARG:HD2	1:H:278:ALA:HB3	1.94	0.50
1:I:14:VAL:HG21	1:I:123:GLY:O	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:LYS:HE2	1:E:101:ILE:HD11	1.94	0.50
1:P:180:THR:HG23	1:P:198:PHE:CE1	2.46	0.50
1:P:86:SER:HB3	1:R:53:THR:HB	1.94	0.50
1:B:39:THR:HB	1:B:102:GLU:HG3	1.93	0.50
1:E:269:SER:HB3	2:E:301:MBO:HE6	2.32	0.50
1:I:225:TYR:CD1	1:I:235:ASP:HB2	2.47	0.50
1:O:260:THR:HG22	1:O:290:LYS:HA	1.94	0.50
1:K:45:LYS:O	1:K:46:ASN:ND2	2.41	0.50
1:D:210:ARG:HG2	1:D:243:GLN:O	2.12	0.50
1:D:248:ASN:HB3	1:D:260:THR:CG2	2.42	0.50
1:O:84:GLN:HB3	1:P:55:THR:HG23	1.94	0.50
1:D:269:SER:HB3	2:D:301:MBO:HE6	2.32	0.49
1:F:36:GLN:NE2	1:G:103:HIS:CE1	2.62	0.49
1:H:146:PRO:CB	1:H:149:ILE:HD11	2.43	0.49
1:P:75:VAL:HG22	1:R:64:ILE:HG12	1.95	0.49
1:D:175:ARG:NH1	1:D:177:GLU:OE1	2.45	0.49
1:L:57:THR:HG23	1:L:84:GLN:HB3	1.92	0.49
1:M:115:ARG:CD	1:M:134:ASP:OD2	2.60	0.49
1:O:17:VAL:HG22	1:O:150:THR:HG22	1.94	0.49
1:S:47:VAL:HG22	1:S:94:GLU:HG3	1.94	0.49
1:D:41:THR:HG23	1:D:100:VAL:HG22	1.93	0.49
1:O:39:THR:HB	1:O:102:GLU:HG3	1.93	0.49
1:J:84:GLN:HB3	1:K:55:THR:HG23	1.95	0.49
1:A:254:ARG:CG	1:A:254:ARG:HH11	2.15	0.49
1:N:76:GLU:O	1:O:62:SER:HB2	2.13	0.49
1:B:31:SER:O	1:R:109:PRO:HG2	2.13	0.49
1:S:164:GLY:HA2	1:S:203:TYR:CE2	2.48	0.49
1:D:37:LYS:HB3	1:E:102:GLU:HG2	1.94	0.48
1:M:20:TRP:HB2	1:M:147:GLN:HA	1.95	0.48
1:R:90:MET:CG	1:S:49:SER:HB3	2.43	0.48
1:O:17:VAL:HG13	1:O:150:THR:HG22	1.94	0.48
1:P:241:PRO:HB2	1:P:265:TYR:HB2	1.95	0.48
1:A:117:GLN:HG3	1:A:132:LEU:HD21	1.94	0.48
1:J:36:GLN:HG3	1:S:103:HIS:NE2	2.29	0.48
1:G:37:LYS:HB3	1:H:102:GLU:HG2	1.96	0.48
1:L:20:TRP:HB2	1:L:147:GLN:HA	1.95	0.48
1:M:260:THR:HG22	1:M:289:ASP:O	2.14	0.48
1:H:122:VAL:CG1	1:H:155:ILE:HD11	2.44	0.48
1:N:210:ARG:HE	1:N:244:ARG:HE	1.60	0.48
1:P:115:ARG:CD	1:P:134:ASP:OD2	2.61	0.48
1:A:286:LYS:HE3	1:B:275:ASP:OD1	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ASP:OD1	1:C:244:ARG:NH1	2.47	0.48
1:D:47:VAL:HG22	1:D:94:GLU:HG3	1.95	0.48
1:F:51:THR:HB	1:G:88:VAL:HG13	1.95	0.48
1:P:172:HIS:HD2	1:P:175:ARG:H	1.61	0.48
1:H:60:ILE:HG13	1:I:79:TYR:HD1	1.77	0.47
1:N:210:ARG:HH21	1:N:244:ARG:HH21	1.62	0.47
1:R:225:TYR:CE1	1:R:233:TYR:HB2	2.49	0.47
1:C:168:ILE:HD11	1:C:202:LEU:HD13	1.97	0.47
1:H:238:THR:O	1:H:244:ARG:NH2	2.47	0.47
1:D:146:PRO:HB3	1:D:149:ILE:HD11	1.97	0.47
1:G:246:ALA:HB2	1:G:264:LYS:HE3	1.96	0.47
1:L:33:SER:HB3	1:L:109:PRO:HD3	1.95	0.47
1:H:53:THR:HG23	1:H:88:VAL:HG22	1.97	0.47
1:J:191:THR:HA	1:J:281:VAL:HG23	1.96	0.47
1:M:42:LYS:HE3	1:M:130:MET:CE	2.44	0.47
1:C:41:THR:HG23	1:C:100:VAL:HG22	1.96	0.47
1:D:20:TRP:HA	1:D:118:LEU:HB3	1.97	0.47
1:E:14:VAL:HG12	1:E:155:ILE:CD1	2.44	0.47
1:G:238:THR:O	1:G:244:ARG:NH2	2.48	0.47
1:A:76:GLU:HB3	1:I:63:THR:OG1	2.14	0.47
1:L:84:GLN:HG3	1:M:55:THR:HG23	1.97	0.47
1:P:103:HIS:NE2	1:R:36:GLN:HG3	2.30	0.47
1:D:20:TRP:HB2	1:D:147:GLN:HA	1.96	0.46
1:G:24:TYR:CZ	1:H:101:ILE:HD11	2.50	0.46
1:N:249:LYS:HE2	1:N:257:ASP:OD2	2.14	0.46
1:O:162:ILE:HG23	1:O:165:LYS:HB3	1.97	0.46
1:H:240:ASN:HD22	1:H:241:PRO:HD2	1.80	0.46
1:D:118:LEU:HD21	1:D:133:ILE:HD12	1.98	0.46
1:G:115:ARG:NH1	1:G:115:ARG:HG3	2.21	0.46
1:S:31:SER:HA	1:S:109:PRO:HB3	1.98	0.46
1:J:203:TYR:HE1	1:J:212:LYS:HD3	1.79	0.46
1:S:20:TRP:HB2	1:S:147:GLN:HA	1.96	0.46
1:D:40:ILE:HG22	1:E:99:LYS:HG3	1.97	0.46
1:F:288:GLU:HG3	1:F:288:GLU:O	2.16	0.46
1:G:227:SER:C	1:G:229:GLN:H	2.17	0.46
1:L:72:ILE:HG23	1:L:73:GLY:H	1.81	0.46
1:A:241:PRO:HB2	1:A:265:TYR:HB2	1.98	0.46
1:C:125:ALA:HB2	1:C:155:ILE:HD13	1.98	0.46
1:E:109:PRO:O	1:E:110:THR:HG22	2.16	0.46
1:F:36:GLN:HG3	1:G:103:HIS:CE1	2.50	0.46
1:H:20:TRP:C	1:H:20:TRP:CD1	2.88	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:SER:O	1:I:74:SER:N	2.48	0.46
1:K:269:SER:CB	2:K:301:MBO:HE2	2.84	0.46
1:N:33:SER:HB3	1:N:109:PRO:HD3	1.96	0.46
1:E:188:PRO:HA	1:E:217:MET:CE	2.46	0.46
1:E:27:GLU:OE1	1:E:29:ARG:NH1	2.45	0.46
1:M:87:GLN:OE1	1:N:52:ARG:HB3	2.16	0.46
1:B:45:LYS:HG3	1:B:96:TYR:HB3	1.97	0.46
1:C:118:LEU:HD11	1:C:133:ILE:HD12	1.98	0.46
1:D:191:THR:HA	1:D:281:VAL:HG23	1.98	0.46
1:E:269:SER:CB	2:E:301:MBO:HE6	2.84	0.46
1:A:103:HIS:NE2	1:I:36:GLN:HG3	2.31	0.46
1:P:276:GLY:O	1:R:286:LYS:HE3	2.16	0.46
1:S:260:THR:HG22	1:S:290:LYS:HA	1.98	0.46
1:J:73:GLY:HA3	1:K:66:THR:HA	1.97	0.46
1:A:189:ALA:HA	1:A:233:TYR:HA	1.98	0.45
1:C:20:TRP:HB2	1:C:147:GLN:HA	1.98	0.45
1:E:266:PHE:HB3	2:E:301:MBO:HE6	2.36	0.45
1:H:45:LYS:HG3	1:H:96:TYR:HB3	1.98	0.45
1:A:67:GLY:C	1:A:69:ALA:H	2.18	0.45
1:C:65:SER:HB2	1:C:76:GLU:HG2	1.99	0.45
1:E:269:SER:OG	2:E:301:MBO:HE6	2.55	0.45
1:M:46:ASN:O	1:M:94:GLU:HA	2.16	0.45
1:R:47:VAL:HG22	1:R:94:GLU:HG3	1.98	0.45
1:A:210:ARG:HD3	1:A:244:ARG:HE	1.81	0.45
1:G:14:VAL:HG22	1:G:155:ILE:CD1	2.46	0.45
1:G:159:ARG:HB2	1:G:159:ARG:HH11	1.80	0.45
1:G:162:ILE:HG23	1:G:165:LYS:HB3	1.97	0.45
1:K:192:LEU:HD22	1:K:273:TYR:HD1	1.81	0.45
1:K:51:THR:HG23	1:K:90:MET:HB3	1.98	0.45
1:G:41:THR:HG23	1:G:100:VAL:HG22	1.97	0.45
1:G:228:ASP:O	2:G:301:MBO:HE3	2.54	0.45
1:L:108:PRO:O	1:L:111:SER:HB2	2.16	0.45
1:O:53:THR:HG23	1:O:88:VAL:HG22	1.97	0.45
1:B:195:SER:OG	1:B:197:LEU:HB2	2.16	0.45
1:D:117:GLN:HE21	1:D:130:MET:HG3	1.82	0.45
1:F:49:SER:HB2	1:G:90:MET:HE2	1.99	0.45
1:D:39:THR:HB	1:D:102:GLU:HG3	1.98	0.45
1:D:25:VAL:HG22	1:D:114:THR:HG22	1.99	0.45
1:K:209:PHE:HZ	1:K:251:LEU:HD11	1.82	0.45
1:G:31:SER:O	1:M:109:PRO:HD2	2.16	0.45
1:M:18:ALA:HB1	1:M:118:LEU:HB3	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:13:GLU:CG	1:N:154:LYS:HE2	2.39	0.45
1:S:273:TYR:HD1	1:S:280:ASN:HD22	1.62	0.45
1:E:53:THR:HG23	1:E:88:VAL:HG22	1.97	0.45
1:F:37:LYS:HB3	1:G:102:GLU:HG2	1.98	0.45
1:F:51:THR:HB	1:G:88:VAL:CG1	2.47	0.45
1:L:122:VAL:HG11	1:L:155:ILE:CD1	2.37	0.45
1:M:53:THR:HG23	1:M:88:VAL:HG22	1.98	0.45
1:O:45:LYS:HG3	1:O:96:TYR:HB3	1.98	0.45
1:P:53:THR:HG23	1:P:88:VAL:HG22	1.97	0.45
1:B:225:TYR:CD1	1:B:235:ASP:HB2	2.52	0.45
1:G:115:ARG:CG	1:G:115:ARG:HH11	2.24	0.45
1:M:217:MET:HG2	1:M:218:TYR:CE2	2.52	0.45
1:O:99:LYS:HE3	1:O:101:ILE:HD11	1.98	0.45
1:O:278:ALA:HB1	1:P:268:ARG:HD2	1.99	0.44
1:E:36:GLN:NE2	1:F:103:HIS:NE2	2.61	0.44
1:J:277:PRO:HD2	1:J:282:TYR:OH	2.17	0.44
1:A:232:ILE:HD11	1:A:283:CYS:HB2	1.98	0.44
1:C:232:ILE:HD11	1:C:283:CYS:HB2	1.99	0.44
1:O:203:TYR:HE1	1:O:212:LYS:HD3	1.83	0.44
1:L:34:VAL:HG23	1:L:107:ILE:HB	1.98	0.44
1:L:85:LYS:HG2	1:M:54:VAL:HG22	1.99	0.44
1:E:232:ILE:HD11	1:E:283:CYS:HB2	1.99	0.44
1:K:105:ILE:HB	1:L:34:VAL:HG12	1.99	0.44
1:N:31:SER:HA	1:N:109:PRO:HB3	1.98	0.44
1:D:225:TYR:CD1	1:D:235:ASP:HB2	2.53	0.44
1:D:269:SER:CB	2:D:301:MBO:HE6	2.86	0.44
1:G:192:LEU:HD22	1:G:273:TYR:HD1	1.83	0.44
1:H:188:PRO:HD3	1:H:218:TYR:HD1	1.82	0.44
1:K:268:ARG:HH11	1:K:268:ARG:HB2	1.82	0.44
1:D:255:HIS:CE1	1:D:294:GLU:HB3	2.53	0.44
1:G:268:ARG:HD2	1:H:278:ALA:HB1	2.00	0.44
1:K:249:LYS:HE2	1:K:257:ASP:OD2	2.18	0.44
1:L:238:THR:O	1:L:244:ARG:NH2	2.51	0.44
1:L:84:GLN:HB2	1:L:84:GLN:HE21	1.61	0.44
1:N:85:LYS:HG2	1:O:54:VAL:HG22	1.98	0.44
1:P:17:VAL:HG13	1:P:150:THR:HG22	1.99	0.44
1:A:52:ARG:HG2	1:B:87:GLN:OE1	2.17	0.44
1:C:171:LYS:HD3	1:C:176:LYS:HG2	2.00	0.44
1:F:20:TRP:HB2	1:F:147:GLN:HA	1.99	0.44
1:S:266:PHE:HB2	1:S:269:SER:OG	2.18	0.44
1:B:269:SER:CB	2:B:302:MBO:HE6	2.87	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:TRP:C	1:I:20:TRP:CD1	2.92	0.43
1:O:115:ARG:HD3	1:O:134:ASP:OD2	2.17	0.43
1:O:278:ALA:HB1	1:P:268:ARG:CD	2.48	0.43
1:E:199:LYS:HD3	1:E:296:VAL:HG11	1.99	0.43
1:F:50:GLU:O	1:F:90:MET:HA	2.18	0.43
1:I:162:ILE:HG13	1:I:165:LYS:HB3	2.00	0.43
1:J:18:ALA:HA	1:J:120:ALA:HA	2.00	0.43
1:N:99:LYS:HG3	1:O:40:ILE:HG22	1.99	0.43
1:R:103:HIS:NE2	1:S:36:GLN:HG3	2.33	0.43
1:D:34:VAL:HG12	1:E:105:ILE:HB	1.99	0.43
1:E:41:THR:HG23	1:E:100:VAL:HG22	2.01	0.43
1:L:188:PRO:HG2	1:L:234:PHE:HB2	2.00	0.43
1:G:115:ARG:HG3	1:G:134:ASP:OD2	2.18	0.43
1:H:122:VAL:HG11	1:H:155:ILE:HD11	2.01	0.43
1:G:203:TYR:HB2	1:G:210:ARG:HB2	1.99	0.43
1:H:62:SER:HB2	1:I:77:VAL:HG22	2.00	0.43
1:I:175:ARG:NH1	1:I:177:GLU:OE1	2.51	0.43
1:M:33:SER:HB3	1:M:109:PRO:HD3	2.00	0.43
1:M:240:ASN:HD21	1:M:242:LYS:HB2	1.83	0.43
1:M:268:ARG:NH1	1:M:285:ASP:OD2	2.52	0.43
1:N:249:LYS:HB3	1:N:249:LYS:HE3	1.71	0.43
1:S:225:TYR:HB3	1:S:243:GLN:HB3	1.99	0.43
1:P:115:ARG:HD3	1:P:134:ASP:OD2	2.19	0.43
1:B:228:ASP:O	2:B:302:MBO:HE3	2.57	0.43
1:F:191:THR:HA	1:F:281:VAL:HG23	2.00	0.43
1:F:236:GLN:O	1:F:238:THR:HG23	2.19	0.43
2:G:301:MBO:OZ2	2:G:301:MBO:HE5	2.51	0.43
1:L:103:HIS:NE2	1:M:36:GLN:HG3	2.33	0.43
1:G:18:ALA:HA	1:G:120:ALA:HA	2.01	0.43
1:I:232:ILE:HD11	1:I:283:CYS:HB2	2.01	0.43
1:C:16:VAL:HG12	1:C:122:VAL:HA	2.01	0.43
1:C:223:TYR:O	1:C:234:PHE:HA	2.19	0.42
2:G:301:MBO:HE3	2:G:301:MBO:OZ1	2.57	0.42
2:P:302:MBO:OZ2	2:P:302:MBO:HE3	2.56	0.42
1:B:142:THR:HG21	1:C:152:ARG:HB2	2.01	0.42
1:C:269:SER:HB3	2:C:301:MBO:HE6	2.38	0.42
1:F:55:THR:HG23	1:G:84:GLN:HB3	2.00	0.42
1:E:25:VAL:HG22	1:E:114:THR:HG22	2.00	0.42
1:I:31:SER:HA	1:I:109:PRO:HB3	2.01	0.42
1:D:162:ILE:HG23	1:D:165:LYS:HB3	2.02	0.42
1:D:188:PRO:HD3	1:D:218:TYR:HD1	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:ALA:HA	1:H:120:ALA:HA	2.01	0.42
1:H:205:ASP:OD2	1:H:244:ARG:NH1	2.51	0.42
1:A:158:GLY:N	1:I:148:VAL:HG13	2.35	0.42
1:J:55:THR:HG23	1:S:84:GLN:HB3	2.01	0.42
1:K:107:ILE:HA	1:K:108:PRO:HD3	1.90	0.42
1:L:245:TRP:CH2	1:L:271:LEU:HD13	2.55	0.42
2:L:301:MBO:OZ1	2:L:301:MBO:HE3	2.57	0.42
1:N:48:ASN:HB2	1:N:93:THR:CG2	2.48	0.42
1:P:115:ARG:HD2	1:P:134:ASP:OD2	2.19	0.42
1:P:162:ILE:HD12	1:P:166:THR:HG23	2.01	0.42
1:C:251:LEU:HB3	1:C:252:PRO:HA	2.02	0.42
1:D:146:PRO:HB2	1:D:149:ILE:CD1	2.49	0.42
1:H:188:PRO:HG2	1:H:234:PHE:HB2	2.01	0.42
1:J:232:ILE:HD11	1:J:283:CYS:HB2	2.00	0.42
1:L:205:ASP:OD2	1:L:244:ARG:NH1	2.53	0.42
1:O:225:TYR:CD1	1:O:235:ASP:HB2	2.54	0.42
1:P:188:PRO:HG2	1:P:234:PHE:HB2	2.01	0.42
1:R:175:ARG:NH1	1:R:177:GLU:OE1	2.53	0.42
1:R:225:TYR:CD1	1:R:235:ASP:HB2	2.55	0.42
1:E:152:ARG:HD3	1:E:152:ARG:HA	1.82	0.42
1:O:285:ASP:OD1	2:O:301:MBO:HE5	2.58	0.42
1:R:228:ASP:C	2:R:301:MBO:HE3	2.76	0.42
1:A:63:THR:HG23	1:A:78:SER:HB3	2.02	0.42
1:K:152:ARG:HB2	1:L:142:THR:HG21	2.02	0.42
1:K:260:THR:HG22	1:K:290:LYS:HA	2.01	0.42
1:M:157:VAL:HB	1:M:254:ARG:HD3	2.01	0.42
1:B:243:GLN:HE21	1:B:244:ARG:HE	1.68	0.42
1:C:65:SER:CB	1:C:76:GLU:HG2	2.50	0.42
1:N:248:ASN:HB3	1:N:260:THR:CG2	2.50	0.41
1:P:260:THR:HG22	1:P:290:LYS:HA	2.02	0.41
1:B:272:CYS:HA	1:B:289:ASP:HB2	2.02	0.41
1:E:45:LYS:HB3	1:F:94:GLU:HB2	2.02	0.41
1:A:92:GLN:HE21	1:A:92:GLN:HB2	1.62	0.41
1:F:14:VAL:CG1	1:F:155:ILE:HD13	2.47	0.41
1:S:210:ARG:HG2	1:S:223:TYR:HD2	1.85	0.41
1:D:269:SER:OG	2:D:301:MBO:HE6	2.58	0.41
1:L:115:ARG:HD3	1:L:134:ASP:OD2	2.20	0.41
1:M:96:TYR:CZ	1:N:43:GLY:HA3	2.55	0.41
2:P:302:MBO:OZ1	2:P:302:MBO:HE5	2.57	0.41
1:F:24:TYR:OH	1:F:36:GLN:NE2	2.53	0.41
1:J:183:SER:HB2	1:J:217:MET:HE1	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ALA:HA	1:A:120:ALA:HA	2.02	0.41
2:K:302:MBO:HE5	2:K:302:MBO:OZ2	2.58	0.41
1:L:248:ASN:HB3	1:L:260:THR:CG2	2.50	0.41
1:M:152:ARG:HA	1:M:152:ARG:HD2	1.88	0.41
1:O:22:GLU:HB3	1:O:117:GLN:HG2	2.01	0.41
1:A:110:THR:HG23	1:A:110:THR:O	2.20	0.41
1:J:207:GLY:HA3	1:J:244:ARG:HD3	2.01	0.41
1:J:188:PRO:HG2	1:J:234:PHE:HB2	2.03	0.41
1:R:260:THR:HG22	1:R:290:LYS:HA	2.01	0.41
1:B:243:GLN:HE22	1:B:244:ARG:HH21	1.67	0.41
1:P:152:ARG:HB2	1:R:142:THR:HG21	2.02	0.41
1:D:146:PRO:HB2	1:D:149:ILE:HD11	2.01	0.41
1:G:266:PHE:HB3	2:G:301:MBO:HE6	2.41	0.41
1:I:269:SER:HB3	2:I:302:MBO:HE2	2.41	0.41
1:J:157:VAL:HB	1:J:254:ARG:HD3	2.03	0.41
1:R:223:TYR:O	1:R:234:PHE:HA	2.21	0.41
1:C:203:TYR:HE1	1:C:212:LYS:HD3	1.86	0.41
1:E:201:VAL:HG12	1:E:214:LEU:HD21	2.03	0.41
1:E:241:PRO:HB2	1:E:265:TYR:HB2	2.03	0.41
1:D:64:ILE:HG12	1:E:75:VAL:HG23	2.03	0.41
1:J:241:PRO:HB2	1:J:265:TYR:HB2	2.02	0.41
1:K:45:LYS:HB3	1:K:45:LYS:HE2	1.91	0.41
2:L:301:MBO:HE5	2:L:301:MBO:OZ2	2.59	0.41
1:P:266:PHE:CB	2:P:302:MBO:HE6	2.89	0.41
1:R:80:SER:OG	1:S:59:SER:HB2	2.21	0.41
1:S:106:THR:O	1:S:108:PRO:HD3	2.21	0.41
1:A:117:GLN:HG3	1:A:132:LEU:CD2	2.51	0.40
1:D:47:VAL:HA	1:D:93:THR:O	2.22	0.40
1:O:164:GLY:HA2	1:O:203:TYR:CE2	2.56	0.40
1:O:90:MET:HB2	1:P:49:SER:HB2	2.02	0.40
1:A:53:THR:HG23	1:A:88:VAL:HG12	2.03	0.40
1:B:164:GLY:HA2	1:B:203:TYR:CE2	2.56	0.40
1:D:241:PRO:HB2	1:D:265:TYR:HB2	2.02	0.40
1:F:232:ILE:HD11	1:F:283:CYS:HB2	2.02	0.40
1:F:49:SER:HB3	1:G:90:MET:HB3	2.03	0.40
1:H:240:ASN:HA	1:H:241:PRO:HD2	1.88	0.40
1:N:277:PRO:HD2	1:N:282:TYR:OH	2.20	0.40
1:R:112:LYS:HB3	1:R:112:LYS:HE2	1.95	0.40
1:R:92:GLN:HB3	1:S:47:VAL:HB	2.04	0.40
1:I:37:LYS:HA	1:I:103:HIS:O	2.21	0.40
1:J:212:LYS:HA	1:J:222:GLU:O	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:172:HIS:CD2	1:M:175:ARG:HB2	2.56	0.40
1:P:68:ASP:C	1:P:70:PHE:H	2.25	0.40
1:R:266:PHE:HB3	1:R:269:SER:OG	2.20	0.40
1:A:286:LYS:HB2	1:A:286:LYS:HE2	1.87	0.40
1:J:68:ASP:C	1:J:70:PHE:H	2.25	0.40
1:K:36:GLN:HG2	1:K:107:ILE:CD1	2.52	0.40
1:O:157:VAL:HB	1:O:254:ARG:HD3	2.03	0.40
1:F:268:ARG:HD2	1:G:278:ALA:HB1	2.04	0.40
1:H:227:SER:C	1:H:229:GLN:H	2.25	0.40
1:I:51:THR:HG23	1:I:90:MET:HB3	2.03	0.40
1:M:67:GLY:O	1:M:69:ALA:N	2.54	0.40
1:R:33:SER:HB3	1:R:109:PRO:HD3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:ASP:OD2	1:R:236:GLN:OE1[7_556]	1.52	0.68

## 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	288/298 (97%)	273 (95%)	12 (4%)	3 (1%)	15	49
1	B	280/298 (94%)	269 (96%)	11 (4%)	0	100	100
1	C	282/298 (95%)	269 (95%)	13 (5%)	0	100	100
1	D	281/298 (94%)	272 (97%)	8 (3%)	1 (0%)	34	69
1	E	279/298 (94%)	267 (96%)	12 (4%)	0	100	100
1	F	279/298 (94%)	259 (93%)	18 (6%)	2 (1%)	22	57
1	G	288/298 (97%)	273 (95%)	11 (4%)	4 (1%)	11	40

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	279/298 (94%)	272 (98%)	7 (2%)	0	100	100
1	I	278/298 (93%)	269 (97%)	9 (3%)	0	100	100
1	J	288/298 (97%)	274 (95%)	11 (4%)	3 (1%)	15	49
1	K	288/298 (97%)	272 (94%)	13 (4%)	3 (1%)	15	49
1	L	280/298 (94%)	268 (96%)	12 (4%)	0	100	100
1	M	287/298 (96%)	265 (92%)	20 (7%)	2 (1%)	22	57
1	N	287/298 (96%)	270 (94%)	16 (6%)	1 (0%)	41	73
1	O	287/298 (96%)	274 (96%)	10 (4%)	3 (1%)	15	49
1	P	287/298 (96%)	270 (94%)	15 (5%)	2 (1%)	22	57
1	R	279/298 (94%)	270 (97%)	9 (3%)	0	100	100
1	S	279/298 (94%)	263 (94%)	15 (5%)	1 (0%)	34	69
All	All	5096/5364 (95%)	4849 (95%)	222 (4%)	25 (0%)	29	64

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	70	PHE
1	A	71	GLU
1	G	68	ASP
1	G	72	ILE
1	K	68	ASP
1	K	71	GLU
1	O	68	ASP
1	O	71	GLU
1	P	72	ILE
1	S	143	GLN
1	K	72	ILE
1	N	72	ILE
1	O	72	ILE
1	P	69	ALA
1	G	71	GLU
1	M	68	ASP
1	F	110	THR
1	J	71	GLU
1	M	70	PHE
1	F	237	GLY
1	G	228	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	68	ASP
1	J	69	ALA
1	D	146	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/257 (98%)	225 (89%)	28 (11%)	6	24
1	B	250/257 (97%)	228 (91%)	22 (9%)	10	36
1	C	250/257 (97%)	222 (89%)	28 (11%)	6	24
1	D	250/257 (97%)	212 (85%)	38 (15%)	3	12
1	E	249/257 (97%)	224 (90%)	25 (10%)	7	28
1	F	249/257 (97%)	216 (87%)	33 (13%)	4	16
1	G	253/257 (98%)	227 (90%)	26 (10%)	7	27
1	H	249/257 (97%)	222 (89%)	27 (11%)	6	25
1	I	249/257 (97%)	221 (89%)	28 (11%)	6	24
1	J	253/257 (98%)	223 (88%)	30 (12%)	5	20
1	K	253/257 (98%)	220 (87%)	33 (13%)	4	18
1	L	250/257 (97%)	227 (91%)	23 (9%)	9	33
1	M	253/257 (98%)	231 (91%)	22 (9%)	10	36
1	N	253/257 (98%)	226 (89%)	27 (11%)	6	26
1	O	253/257 (98%)	230 (91%)	23 (9%)	9	33
1	P	253/257 (98%)	222 (88%)	31 (12%)	4	19
1	R	249/257 (97%)	224 (90%)	25 (10%)	7	28
1	S	249/257 (97%)	223 (90%)	26 (10%)	7	27
All	All	4518/4626 (98%)	4023 (89%)	495 (11%)	6	25

All (495) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	15	ASP
1	A	35	ASP
1	A	42	LYS
1	A	45	LYS
1	A	57	THR
1	A	62	SER
1	A	63	THR
1	A	70	PHE
1	A	71	GLU
1	A	78	SER
1	A	98	SER
1	A	100	VAL
1	A	110	THR
1	A	148	VAL
1	A	152	ARG
1	A	157	VAL
1	A	166	THR
1	A	184	ARG
1	A	186	SER
1	A	191	THR
1	A	192	LEU
1	A	196	LYS
1	A	201	VAL
1	A	206	TRP
1	A	244	ARG
1	A	254	ARG
1	A	260	THR
1	A	287	ARG
1	B	15	ASP
1	B	16	VAL
1	B	35	ASP
1	B	39	THR
1	B	51	THR
1	B	52	ARG
1	B	62	SER
1	B	68	ASP
1	B	84	GLN
1	B	93	THR
1	B	110	THR
1	B	118	LEU
1	B	143	GLN
1	B	174	GLU
1	B	191	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	192	LEU
1	B	197	LEU
1	B	243	GLN
1	B	244	ARG
1	B	250	SER
1	B	260	THR
1	B	290	LYS
1	C	13	GLU
1	C	15	ASP
1	C	35	ASP
1	C	36	GLN
1	C	39	THR
1	C	44	MET
1	C	53	THR
1	C	55	THR
1	C	57	THR
1	C	60	ILE
1	C	63	THR
1	C	66	THR
1	C	68	ASP
1	C	84	GLN
1	C	92	GLN
1	C	98	SER
1	C	104	THR
1	C	110	THR
1	C	115	ARG
1	C	150	THR
1	C	174	GLU
1	C	176	LYS
1	C	191	THR
1	C	192	LEU
1	C	219	SER
1	C	229	GLN
1	C	244	ARG
1	C	272	CYS
1	D	15	ASP
1	D	16	VAL
1	D	35	ASP
1	D	36	GLN
1	D	39	THR
1	D	52	ARG
1	D	53	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	55	THR
1	D	57	THR
1	D	59	SER
1	D	74	SER
1	D	88	VAL
1	D	90	MET
1	D	93	THR
1	D	98	SER
1	D	115	ARG
1	D	118	LEU
1	D	145	ILE
1	D	148	VAL
1	D	159	ARG
1	D	165	LYS
1	D	174	GLU
1	D	184	ARG
1	D	191	THR
1	D	192	LEU
1	D	197	LEU
1	D	201	VAL
1	D	211	ILE
1	D	217	MET
1	D	229	GLN
1	D	244	ARG
1	D	260	THR
1	D	271	LEU
1	D	272	CYS
1	D	283	CYS
1	D	286	LYS
1	D	290	LYS
1	D	294	GLU
1	E	12	ILE
1	E	14	VAL
1	E	15	ASP
1	E	16	VAL
1	E	19	VAL
1	E	29	ARG
1	E	35	ASP
1	E	37	LYS
1	E	40	ILE
1	E	55	THR
1	E	78	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	90	MET
1	E	92	GLN
1	E	118	LEU
1	E	148	VAL
1	E	152	ARG
1	E	166	THR
1	E	184	ARG
1	E	186	SER
1	E	191	THR
1	E	217	MET
1	E	229	GLN
1	E	244	ARG
1	E	260	THR
1	E	294	GLU
1	F	10	GLU
1	F	13	GLU
1	F	16	VAL
1	F	35	ASP
1	F	42	LYS
1	F	49	SER
1	F	52	ARG
1	F	62	SER
1	F	66	THR
1	F	78	SER
1	F	80	SER
1	F	88	VAL
1	F	90	MET
1	F	98	SER
1	F	100	VAL
1	F	142	THR
1	F	148	VAL
1	F	152	ARG
1	F	159	ARG
1	F	171	LYS
1	F	184	ARG
1	F	191	THR
1	F	197	LEU
1	F	201	VAL
1	F	227	SER
1	F	244	ARG
1	F	249	LYS
1	F	250	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	260	THR
1	F	264	LYS
1	F	267	THR
1	F	284	LEU
1	F	286	LYS
1	G	15	ASP
1	G	16	VAL
1	G	35	ASP
1	G	57	THR
1	G	70	PHE
1	G	92	GLN
1	G	93	THR
1	G	98	SER
1	G	114	THR
1	G	115	ARG
1	G	118	LEU
1	G	148	VAL
1	G	159	ARG
1	G	165	LYS
1	G	174	GLU
1	G	192	LEU
1	G	210	ARG
1	G	219	SER
1	G	225	TYR
1	G	229	GLN
1	G	244	ARG
1	G	247	ILE
1	G	260	THR
1	G	264	LYS
1	G	283	CYS
1	G	284	LEU
1	H	15	ASP
1	H	20	TRP
1	H	35	ASP
1	H	55	THR
1	H	57	THR
1	H	59	SER
1	H	62	SER
1	H	82	SER
1	H	87	GLN
1	H	93	THR
1	H	98	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	114	THR
1	H	152	ARG
1	H	174	GLU
1	H	185	LYS
1	H	191	THR
1	H	192	LEU
1	H	197	LEU
1	H	201	VAL
1	H	229	GLN
1	H	244	ARG
1	H	247	ILE
1	H	260	THR
1	H	283	CYS
1	H	287	ARG
1	H	294	GLU
1	H	295	VAL
1	I	13	GLU
1	I	14	VAL
1	I	15	ASP
1	I	16	VAL
1	I	19	VAL
1	I	35	ASP
1	I	39	THR
1	I	44	MET
1	I	55	THR
1	I	57	THR
1	I	75	VAL
1	I	82	SER
1	I	90	MET
1	I	98	SER
1	I	118	LEU
1	I	148	VAL
1	I	149	ILE
1	I	155	ILE
1	I	191	THR
1	I	192	LEU
1	I	201	VAL
1	I	217	MET
1	I	229	GLN
1	I	244	ARG
1	I	250	SER
1	I	260	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	264	LYS
1	I	272	CYS
1	J	15	ASP
1	J	16	VAL
1	J	35	ASP
1	J	44	MET
1	J	49	SER
1	J	55	THR
1	J	57	THR
1	J	62	SER
1	J	63	THR
1	J	68	ASP
1	J	72	ILE
1	J	75	VAL
1	J	90	MET
1	J	93	THR
1	J	98	SER
1	J	110	THR
1	J	121	ASP
1	J	159	ARG
1	J	186	SER
1	J	191	THR
1	J	192	LEU
1	J	197	LEU
1	J	202	LEU
1	J	217	MET
1	J	229	GLN
1	J	250	SER
1	J	271	LEU
1	J	272	CYS
1	J	283	CYS
1	J	296	VAL
1	K	21	LYS
1	K	33	SER
1	K	35	ASP
1	K	36	GLN
1	K	37	LYS
1	K	55	THR
1	K	57	THR
1	K	59	SER
1	K	62	SER
1	K	66	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	82	SER
1	K	90	MET
1	K	98	SER
1	K	104	THR
1	K	105	ILE
1	K	106	THR
1	K	128	GLU
1	K	148	VAL
1	K	154	LYS
1	K	165	LYS
1	K	174	GLU
1	K	175	ARG
1	K	179	MET
1	K	184	ARG
1	K	192	LEU
1	K	219	SER
1	K	229	GLN
1	K	232	ILE
1	K	264	LYS
1	K	268	ARG
1	K	286	LYS
1	K	287	ARG
1	K	290	LYS
1	L	13	GLU
1	L	16	VAL
1	L	21	LYS
1	L	34	VAL
1	L	35	ASP
1	L	36	GLN
1	L	39	THR
1	L	45	LYS
1	L	84	GLN
1	L	98	SER
1	L	104	THR
1	L	110	THR
1	L	115	ARG
1	L	174	GLU
1	L	184	ARG
1	L	192	LEU
1	L	197	LEU
1	L	206	TRP
1	L	219	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	L	244	ARG
1	L	260	THR
1	L	283	CYS
1	L	286	LYS
1	M	14	VAL
1	M	15	ASP
1	M	35	ASP
1	M	39	THR
1	M	49	SER
1	M	57	THR
1	M	68	ASP
1	M	92	GLN
1	M	98	SER
1	M	104	THR
1	M	110	THR
1	M	115	ARG
1	M	118	LEU
1	M	142	THR
1	M	149	ILE
1	M	150	THR
1	M	157	VAL
1	M	159	ARG
1	M	192	LEU
1	M	202	LEU
1	M	283	CYS
1	M	294	GLU
1	N	13	GLU
1	N	15	ASP
1	N	16	VAL
1	N	34	VAL
1	N	35	ASP
1	N	39	THR
1	N	44	MET
1	N	52	ARG
1	N	57	THR
1	N	90	MET
1	N	115	ARG
1	N	118	LEU
1	N	150	THR
1	N	154	LYS
1	N	157	VAL
1	N	159	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	N	174	GLU
1	N	185	LYS
1	N	191	THR
1	N	197	LEU
1	N	202	LEU
1	N	210	ARG
1	N	211	ILE
1	N	226	SER
1	N	247	ILE
1	N	260	THR
1	N	283	CYS
1	O	13	GLU
1	O	15	ASP
1	O	32	THR
1	O	35	ASP
1	O	39	THR
1	O	55	THR
1	O	62	SER
1	O	70	PHE
1	O	90	MET
1	O	93	THR
1	O	104	THR
1	O	110	THR
1	O	115	ARG
1	O	117	GLN
1	O	186	SER
1	O	191	THR
1	O	214	LEU
1	O	217	MET
1	O	244	ARG
1	O	272	CYS
1	O	284	LEU
1	O	286	LYS
1	O	294	GLU
1	P	14	VAL
1	P	16	VAL
1	P	34	VAL
1	P	35	ASP
1	P	37	LYS
1	P	39	THR
1	P	54	VAL
1	P	57	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	P	62	SER
1	P	93	THR
1	P	98	SER
1	P	104	THR
1	P	115	ARG
1	P	118	LEU
1	P	142	THR
1	P	149	ILE
1	P	157	VAL
1	P	159	ARG
1	P	176	LYS
1	P	186	SER
1	P	191	THR
1	P	196	LYS
1	P	197	LEU
1	P	206	TRP
1	P	211	ILE
1	P	217	MET
1	P	229	GLN
1	P	244	ARG
1	P	272	CYS
1	P	286	LYS
1	P	292	ILE
1	R	14	VAL
1	R	15	ASP
1	R	29	ARG
1	R	35	ASP
1	R	37	LYS
1	R	39	THR
1	R	65	SER
1	R	86	SER
1	R	90	MET
1	R	98	SER
1	R	99	LYS
1	R	115	ARG
1	R	157	VAL
1	R	165	LYS
1	R	176	LYS
1	R	191	THR
1	R	196	LYS
1	R	197	LEU
1	R	211	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	R	212	LYS
1	R	217	MET
1	R	219	SER
1	R	225	TYR
1	R	244	ARG
1	R	284	LEU
1	S	15	ASP
1	S	16	VAL
1	S	17	VAL
1	S	35	ASP
1	S	37	LYS
1	S	39	THR
1	S	90	MET
1	S	98	SER
1	S	110	THR
1	S	115	ARG
1	S	118	LEU
1	S	149	ILE
1	S	150	THR
1	S	152	ARG
1	S	184	ARG
1	S	186	SER
1	S	191	THR
1	S	197	LEU
1	S	202	LEU
1	S	210	ARG
1	S	219	SER
1	S	225	TYR
1	S	264	LYS
1	S	283	CYS
1	S	284	LEU
1	S	290	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	58	HIS
1	A	92	GLN
1	B	243	GLN
1	C	84	GLN
1	C	92	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	194	HIS
1	D	117	GLN
1	D	236	GLN
1	E	11	GLN
1	E	36	GLN
1	E	92	GLN
1	E	229	GLN
1	F	36	GLN
1	F	92	GLN
1	F	117	GLN
1	F	147	GLN
1	G	36	GLN
1	G	103	HIS
1	G	172	HIS
1	G	194	HIS
1	H	36	GLN
1	H	58	HIS
1	H	172	HIS
1	H	194	HIS
1	I	11	GLN
1	I	92	GLN
1	I	160	GLN
1	I	229	GLN
1	J	28	ASN
1	K	58	HIS
1	K	84	GLN
1	K	143	GLN
1	L	28	ASN
1	L	58	HIS
1	L	84	GLN
1	L	119	ASN
1	L	147	GLN
1	L	160	GLN
1	M	92	GLN
1	M	172	HIS
1	N	117	GLN
1	N	119	ASN
1	N	172	HIS
1	O	58	HIS
1	P	58	HIS
1	P	117	GLN
1	P	172	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	P	229	GLN
1	R	92	GLN
1	R	172	HIS
1	S	11	GLN
1	S	58	HIS
1	S	236	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 14 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MBO	M	301	1	5,10,10	1.46	1 (20%)	8,13,13	1.06	0
2	MBO	P	302	1	5,10,10	1.84	1 (20%)	8,13,13	0.67	0
2	MBO	L	301	1	5,10,10	1.81	1 (20%)	8,13,13	0.85	0
2	MBO	A	301	1	5,10,10	1.75	1 (20%)	8,13,13	0.79	0
2	MBO	H	302	1	5,10,10	1.36	1 (20%)	8,13,13	1.34	1 (12%)
2	MBO	F	302	1	5,10,10	1.62	1 (20%)	8,13,13	1.28	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MBO	B	302	1	5,10,10	1.53	1 (20%)	8,13,13	0.91	0
2	MBO	E	301	1	5,10,10	1.44	1 (20%)	8,13,13	1.07	0
2	MBO	H	301	1	5,10,10	1.51	1 (20%)	8,13,13	1.06	0
2	MBO	D	301	1	5,10,10	1.33	1 (20%)	8,13,13	1.27	0
2	MBO	R	301	1	5,10,10	1.45	1 (20%)	8,13,13	1.10	0
2	MBO	S	301	1	5,10,10	1.40	1 (20%)	8,13,13	1.12	0
2	MBO	K	301	1	5,10,10	1.52	1 (20%)	8,13,13	1.38	0
2	MBO	G	301	1	5,10,10	1.69	1 (20%)	8,13,13	1.01	0
2	MBO	M	302	1	5,10,10	1.47	1 (20%)	8,13,13	1.79	2 (25%)
2	MBO	I	302	1	5,10,10	1.89	1 (20%)	8,13,13	0.93	0
2	MBO	O	301	1	5,10,10	1.51	1 (20%)	8,13,13	1.40	1 (12%)
2	MBO	K	302	1	5,10,10	1.50	1 (20%)	8,13,13	0.99	0
2	MBO	A	302	1	5,10,10	1.79	1 (20%)	8,13,13	1.12	0
2	MBO	L	302	1	5,10,10	1.75	1 (20%)	8,13,13	0.96	0
2	MBO	B	301	1	5,10,10	1.71	1 (20%)	8,13,13	1.22	1 (12%)
2	MBO	C	301	1	5,10,10	1.60	1 (20%)	8,13,13	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MBO	M	301	1	-	0/0/4/4	0/1/1/1
2	MBO	P	302	1	-	0/0/4/4	0/1/1/1
2	MBO	L	301	1	-	0/0/4/4	0/1/1/1
2	MBO	A	301	1	-	0/0/4/4	0/1/1/1
2	MBO	H	302	1	-	0/0/4/4	0/1/1/1
2	MBO	F	302	1	-	0/0/4/4	0/1/1/1
2	MBO	B	302	1	-	0/0/4/4	0/1/1/1
2	MBO	E	301	1	-	0/0/4/4	0/1/1/1
2	MBO	H	301	1	-	0/0/4/4	0/1/1/1
2	MBO	D	301	1	-	0/0/4/4	0/1/1/1
2	MBO	R	301	1	-	0/0/4/4	0/1/1/1
2	MBO	S	301	1	-	0/0/4/4	0/1/1/1
2	MBO	K	301	1	-	0/0/4/4	0/1/1/1
2	MBO	G	301	1	-	0/0/4/4	0/1/1/1
2	MBO	M	302	1	-	0/0/4/4	0/1/1/1
2	MBO	I	302	1	-	0/0/4/4	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MBO	O	301	1	-	0/0/4/4	0/1/1/1
2	MBO	K	302	1	-	0/0/4/4	0/1/1/1
2	MBO	A	302	1	-	0/0/4/4	0/1/1/1
2	MBO	L	302	1	-	0/0/4/4	0/1/1/1
2	MBO	B	301	1	-	0/0/4/4	0/1/1/1
2	MBO	C	301	1	-	0/0/4/4	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	302	MBO	CE4-CZ	3.96	1.51	1.47
2	L	301	MBO	CE4-CZ	3.85	1.51	1.47
2	P	302	MBO	CE4-CZ	3.77	1.51	1.47
2	L	302	MBO	CE4-CZ	3.60	1.50	1.47
2	A	301	MBO	CE4-CZ	3.58	1.50	1.47
2	G	301	MBO	CE4-CZ	3.52	1.50	1.47
2	A	302	MBO	CE4-CZ	3.51	1.50	1.47
2	B	301	MBO	CE4-CZ	3.50	1.50	1.47
2	C	301	MBO	CE4-CZ	3.21	1.50	1.47
2	F	302	MBO	CE4-CZ	3.19	1.50	1.47
2	K	302	MBO	CE4-CZ	3.14	1.50	1.47
2	B	302	MBO	CE4-CZ	3.07	1.50	1.47
2	H	301	MBO	CE4-CZ	3.06	1.50	1.47
2	O	301	MBO	CE4-CZ	3.01	1.50	1.47
2	E	301	MBO	CE4-CZ	3.00	1.50	1.47
2	K	301	MBO	CE4-CZ	2.98	1.50	1.47
2	M	301	MBO	CE4-CZ	2.98	1.50	1.47
2	M	302	MBO	CE4-CZ	2.94	1.50	1.47
2	R	301	MBO	CE4-CZ	2.94	1.50	1.47
2	S	301	MBO	CE4-CZ	2.91	1.50	1.47
2	D	301	MBO	CE4-CZ	2.74	1.50	1.47
2	H	302	MBO	CE4-CZ	2.66	1.50	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	302	MBO	CE5-CE4-CZ	-3.33	115.90	120.37
2	O	301	MBO	CE5-CE4-CZ	-2.44	117.09	120.37
2	H	302	MBO	CE5-CE4-CZ	-2.09	117.57	120.37
2	M	302	MBO	CE3-CE4-CZ	2.06	123.14	120.37
2	B	301	MBO	CE3-CE4-CZ	-2.01	117.67	120.37
2	F	302	MBO	CE3-CE4-CZ	-2.01	117.67	120.37



There are no chirality outliers.

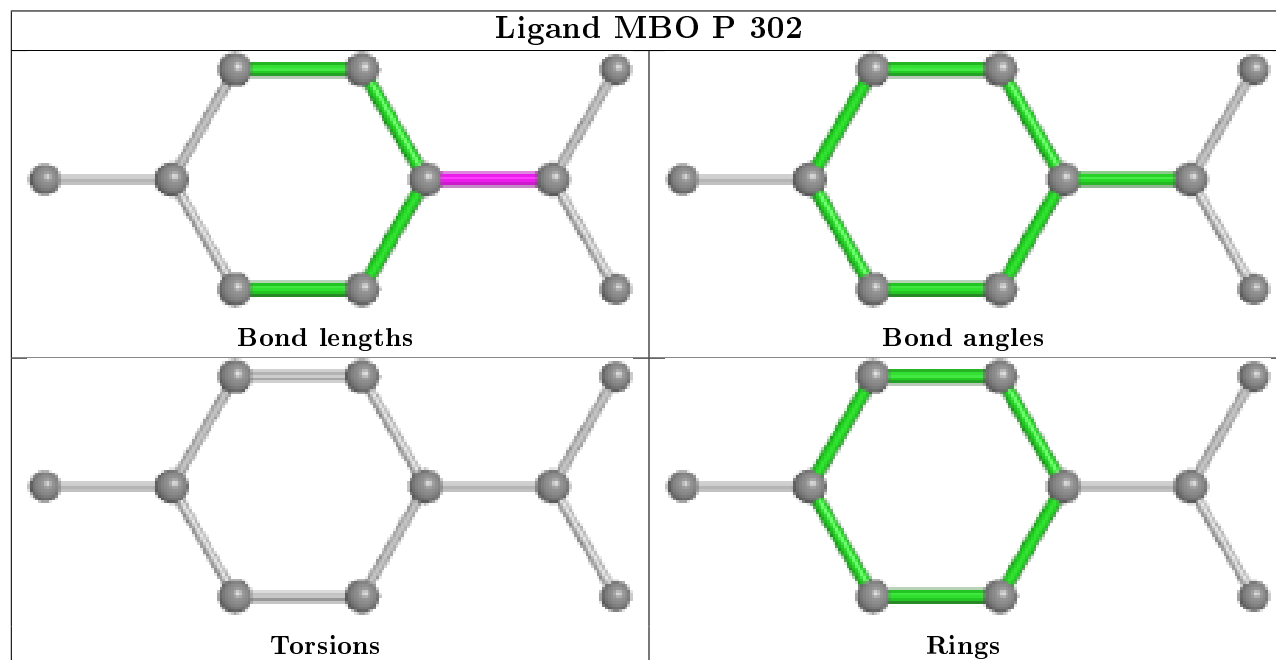
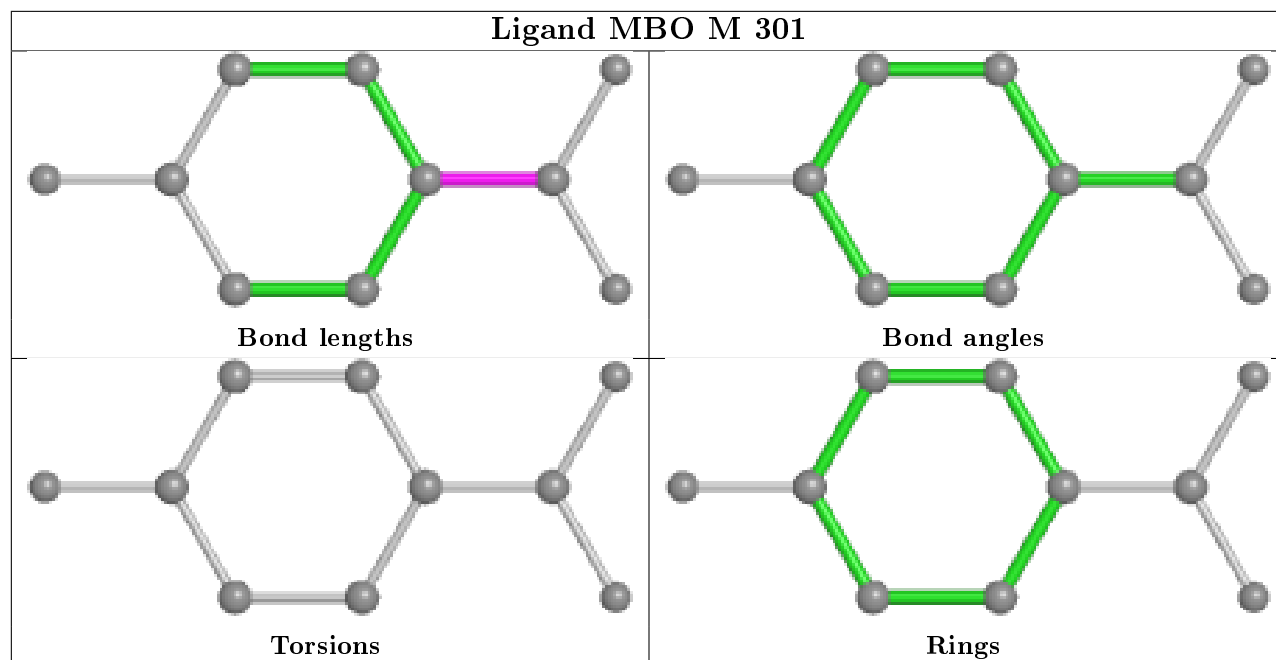
There are no torsion outliers.

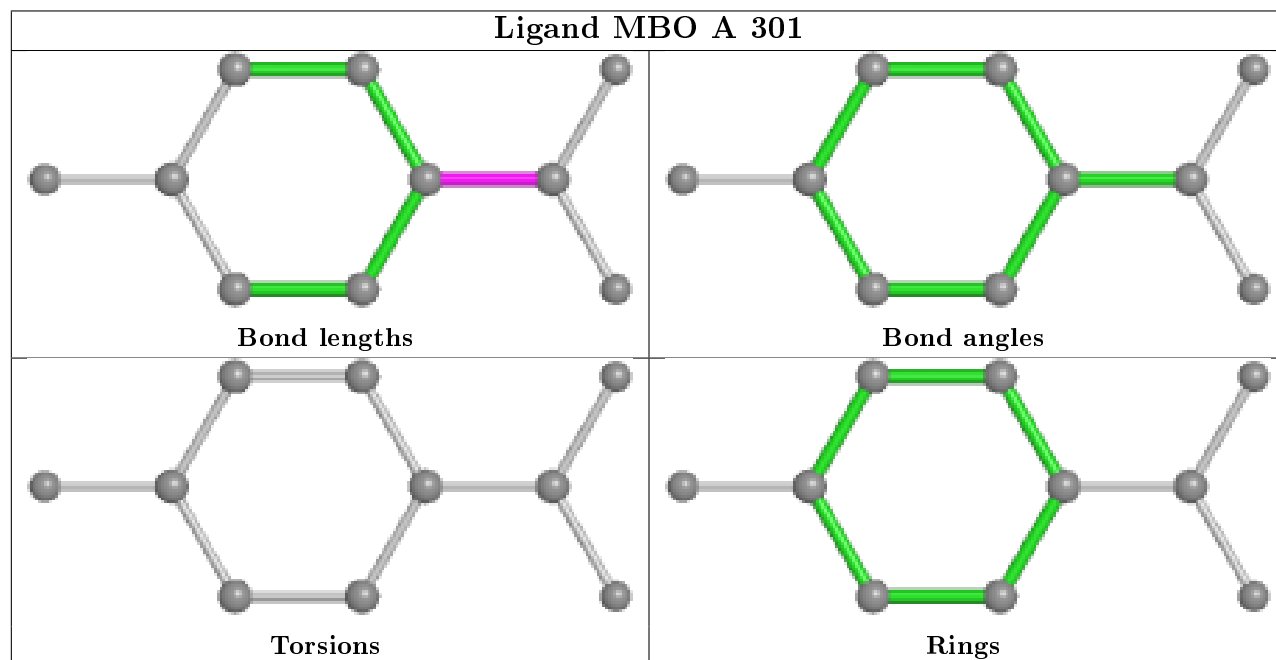
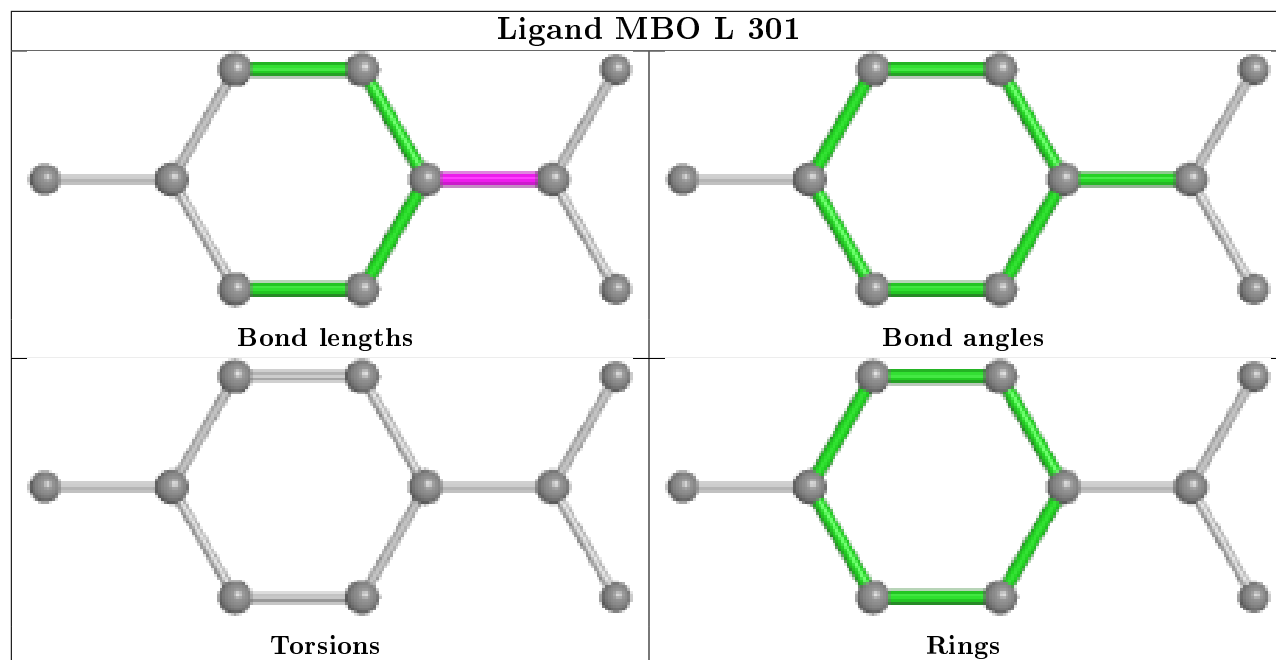
There are no ring outliers.

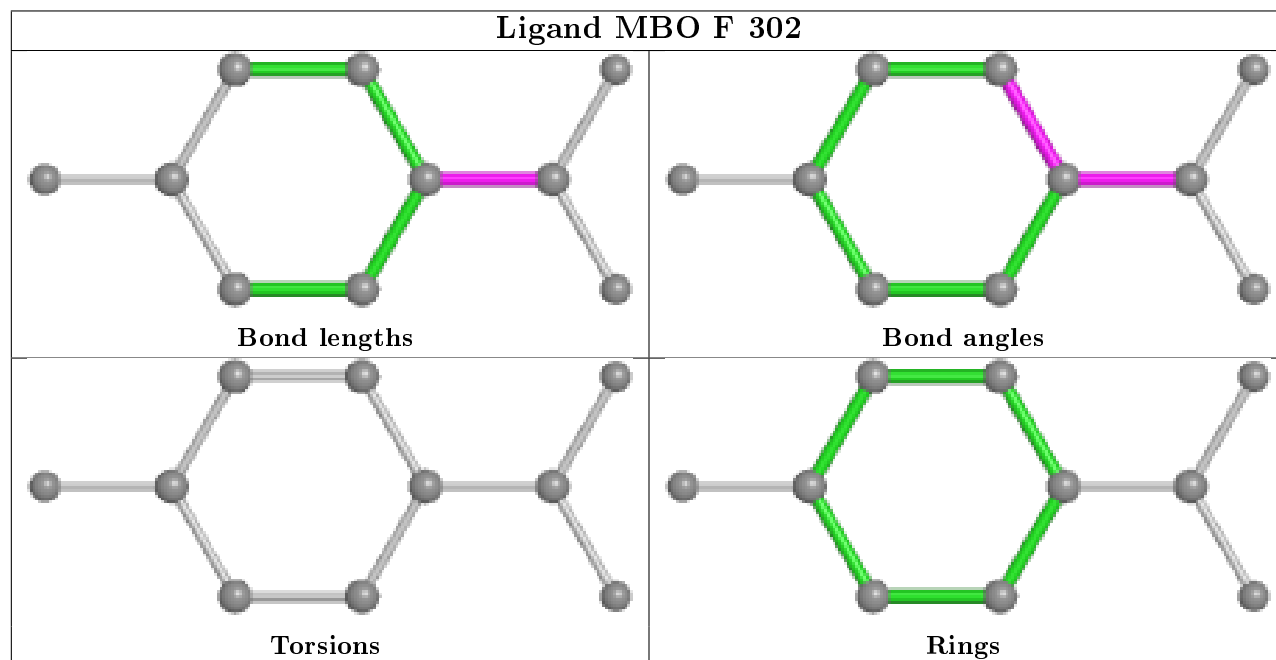
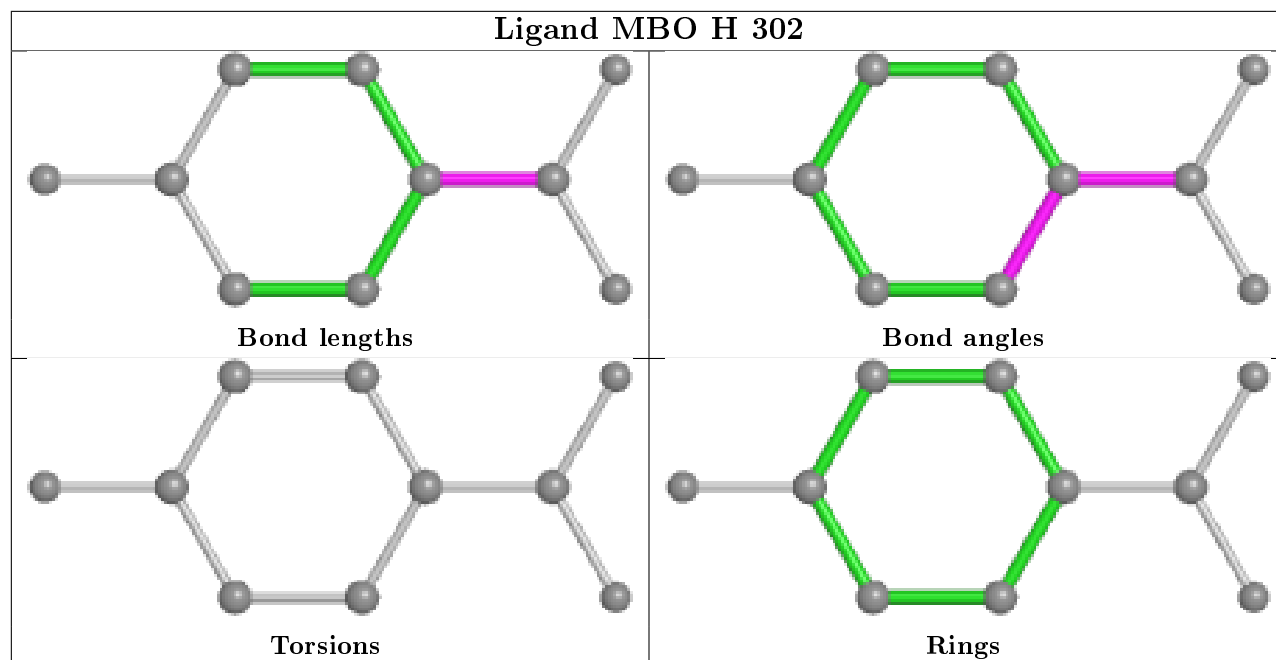
22 monomers are involved in 249 short contacts:

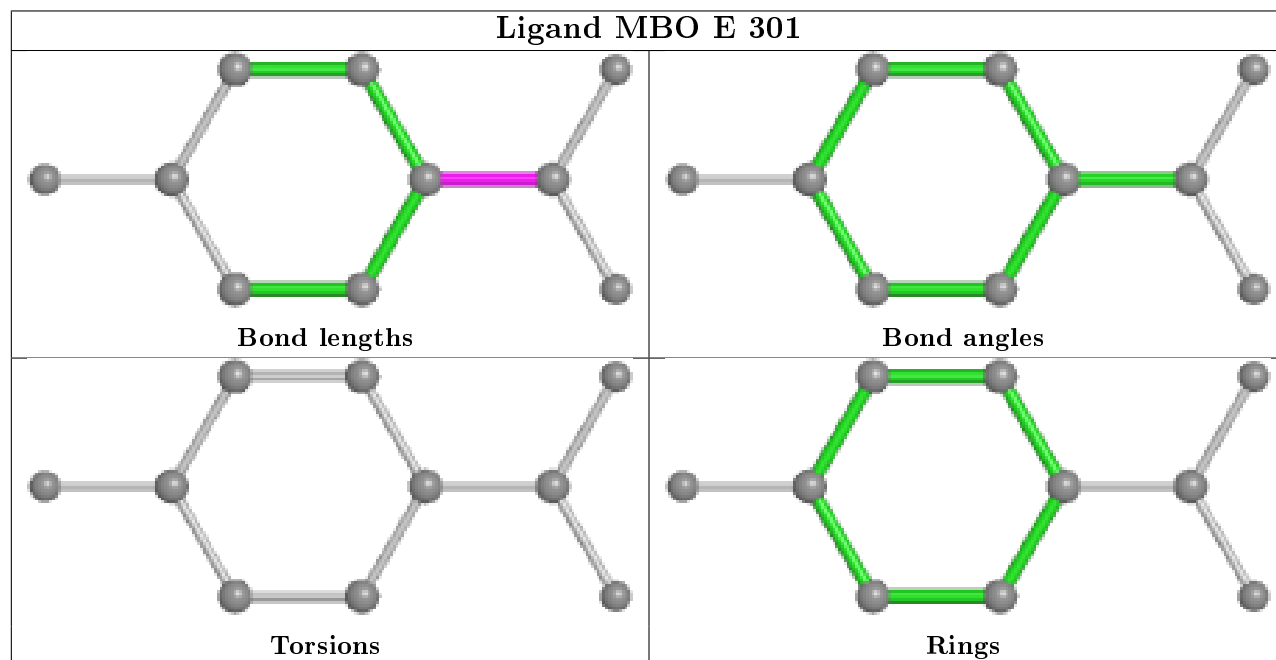
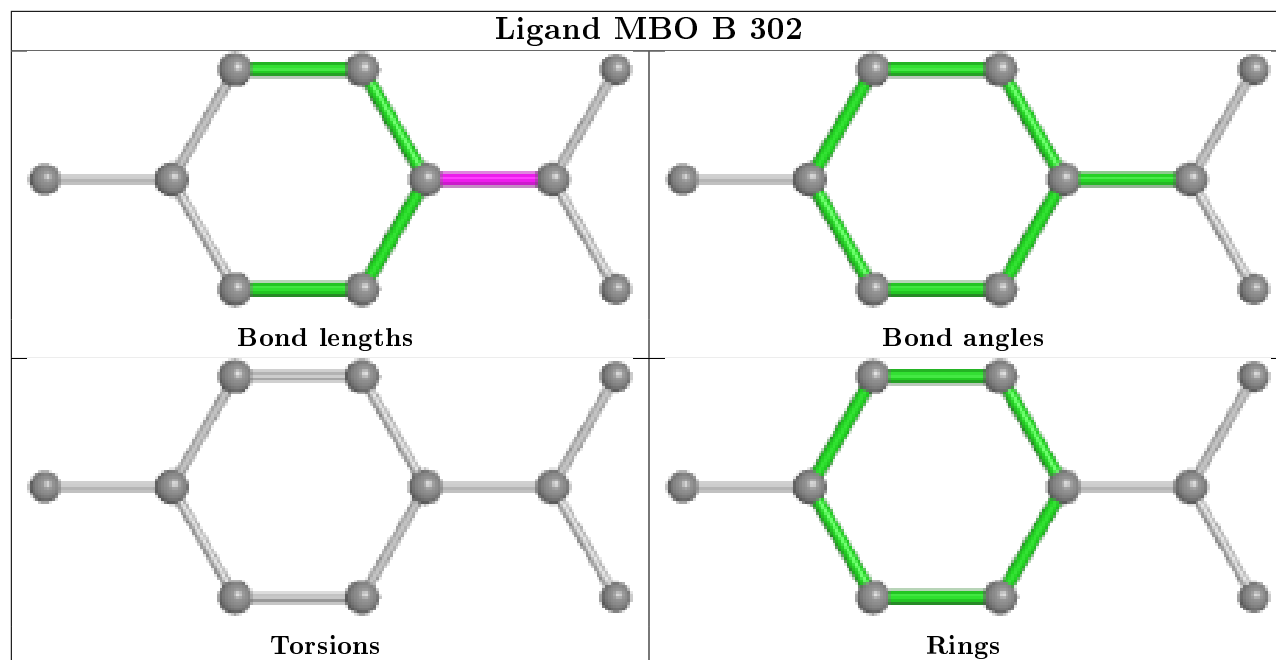
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	301	MBO	17	0
2	P	302	MBO	20	0
2	L	301	MBO	17	0
2	A	301	MBO	1	0
2	H	302	MBO	14	0
2	F	302	MBO	19	0
2	B	302	MBO	3	0
2	E	301	MBO	5	0
2	H	301	MBO	15	0
2	D	301	MBO	17	0
2	R	301	MBO	7	0
2	S	301	MBO	15	0
2	K	301	MBO	15	0
2	G	301	MBO	13	0
2	M	302	MBO	1	0
2	I	302	MBO	6	0
2	O	301	MBO	12	0
2	K	302	MBO	14	0
2	A	302	MBO	8	0
2	L	302	MBO	8	0
2	B	301	MBO	13	0
2	C	301	MBO	9	0

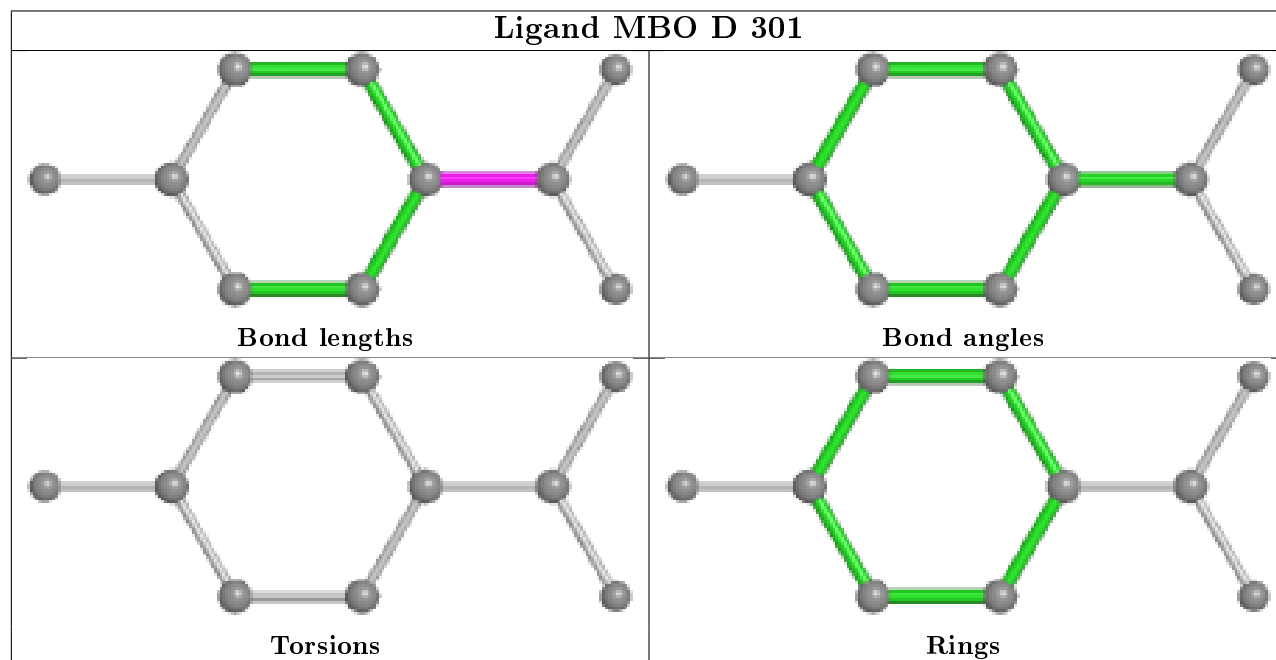
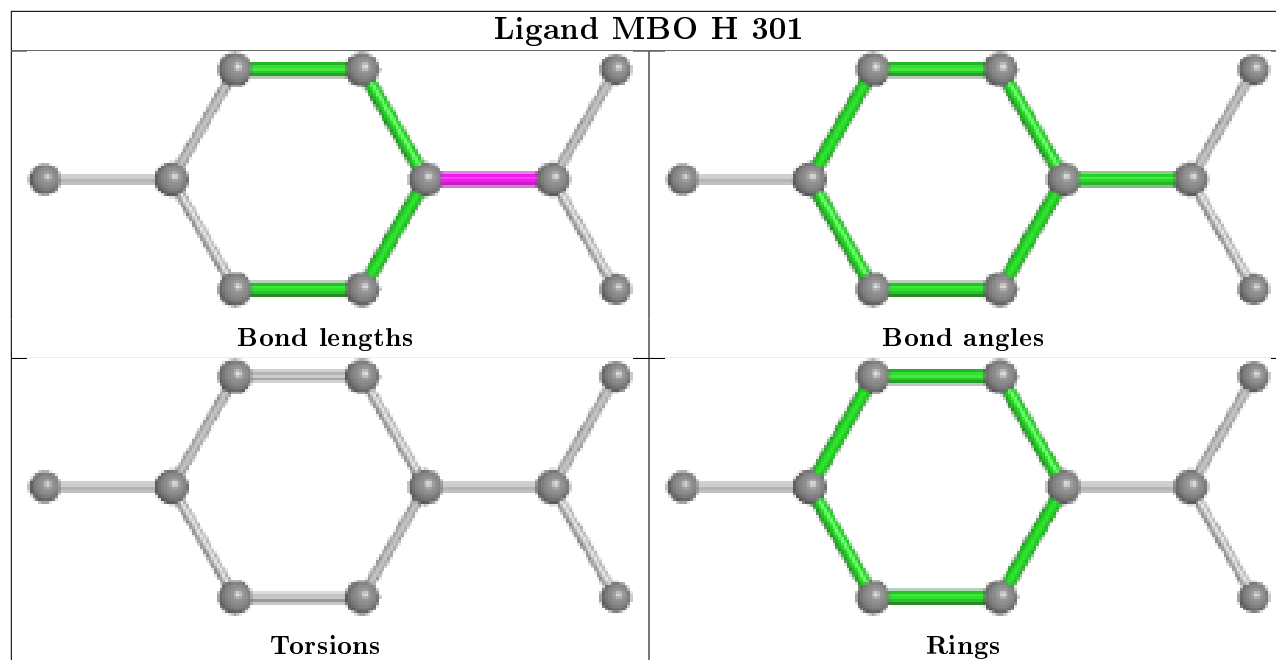
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

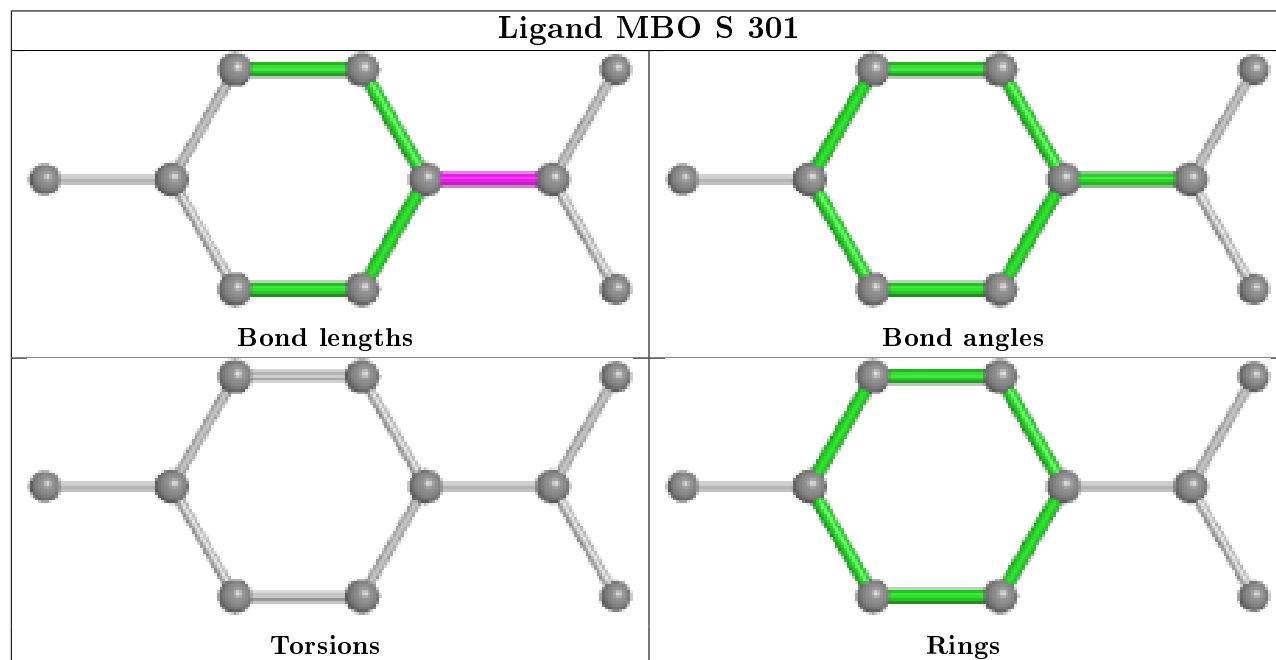
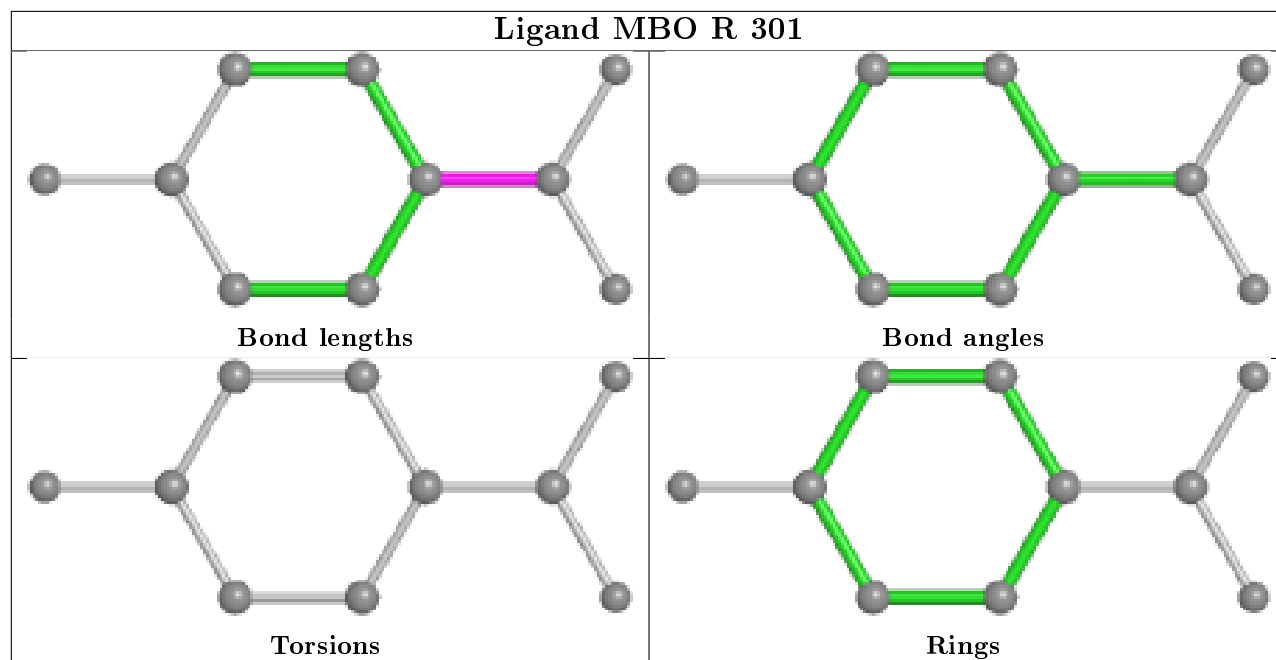


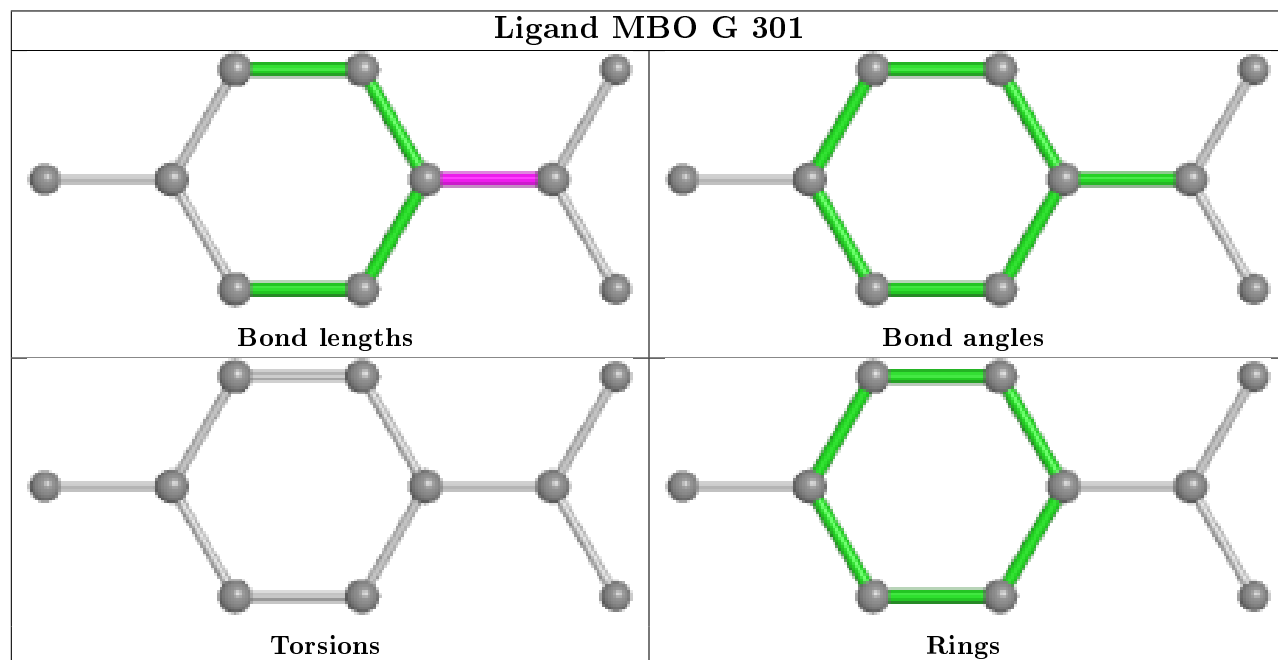
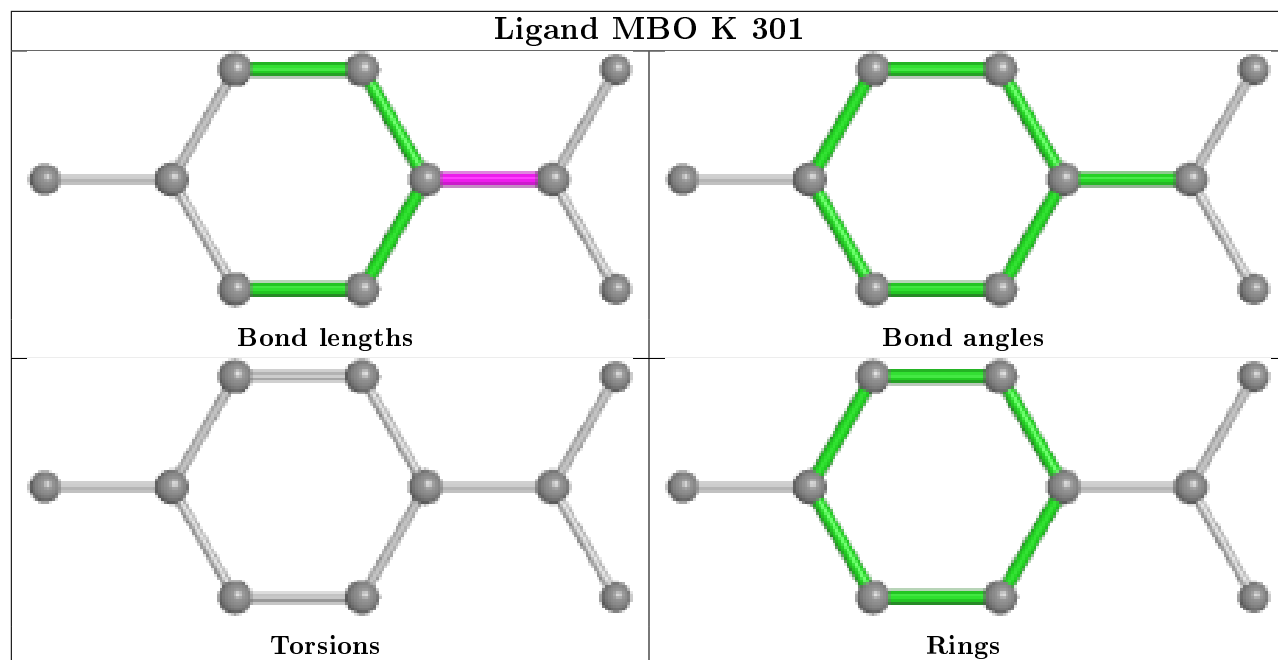




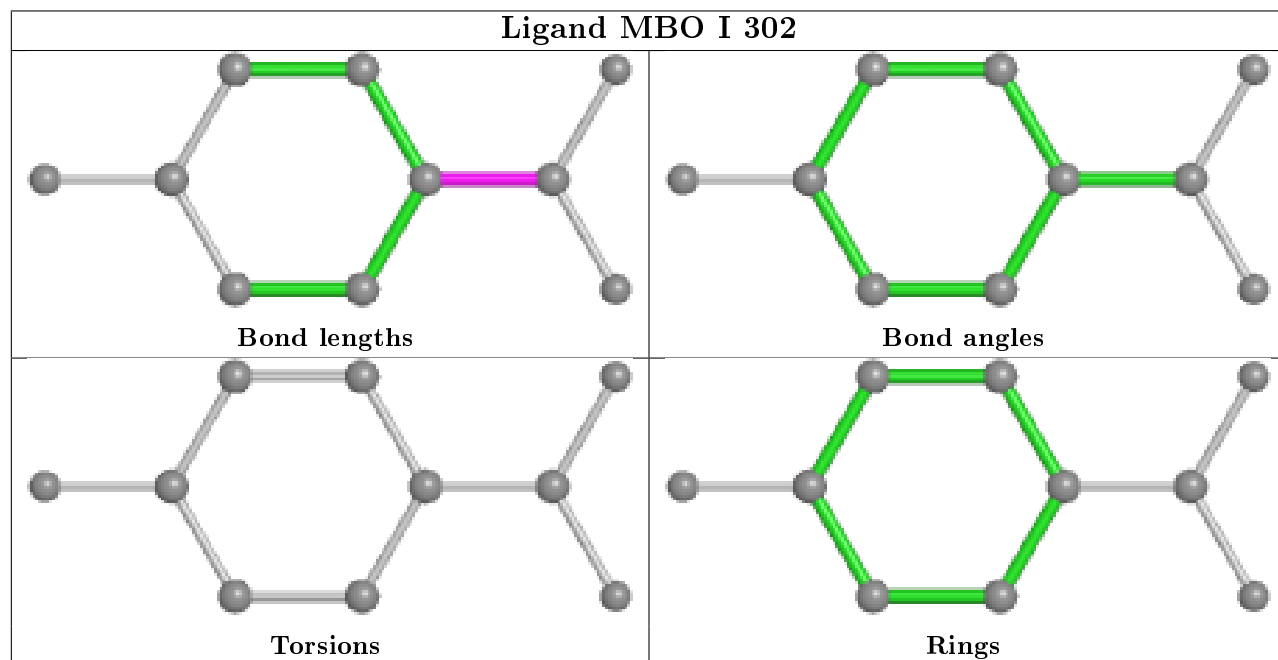
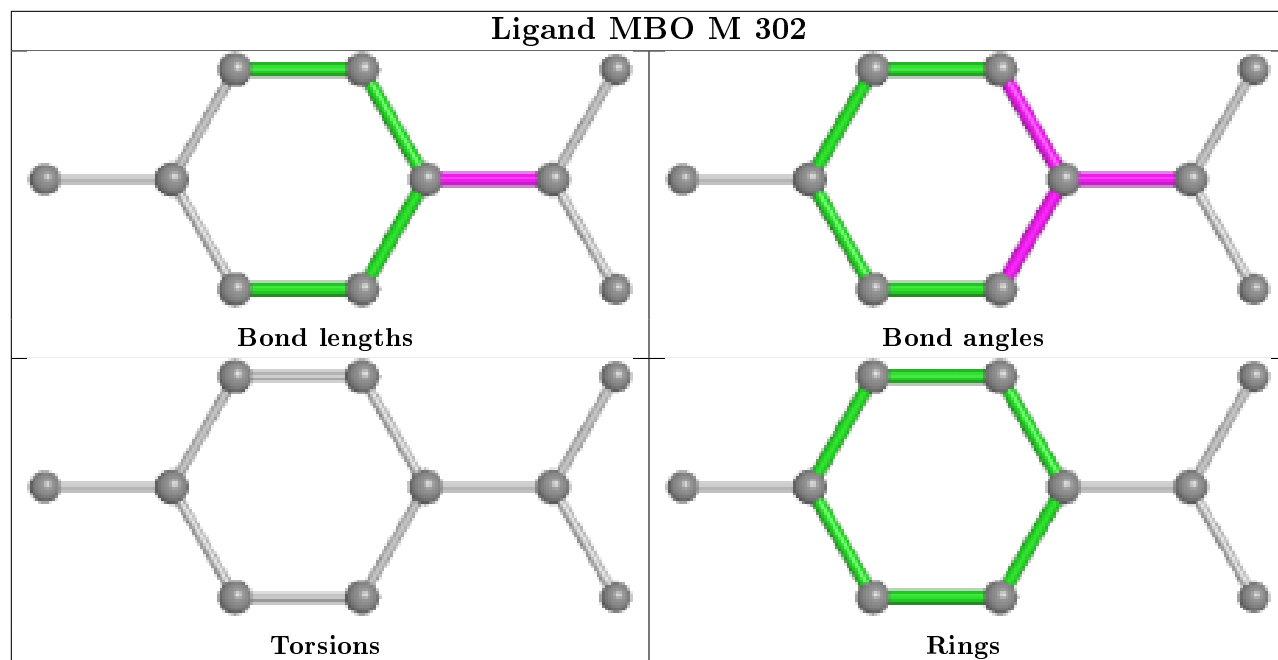


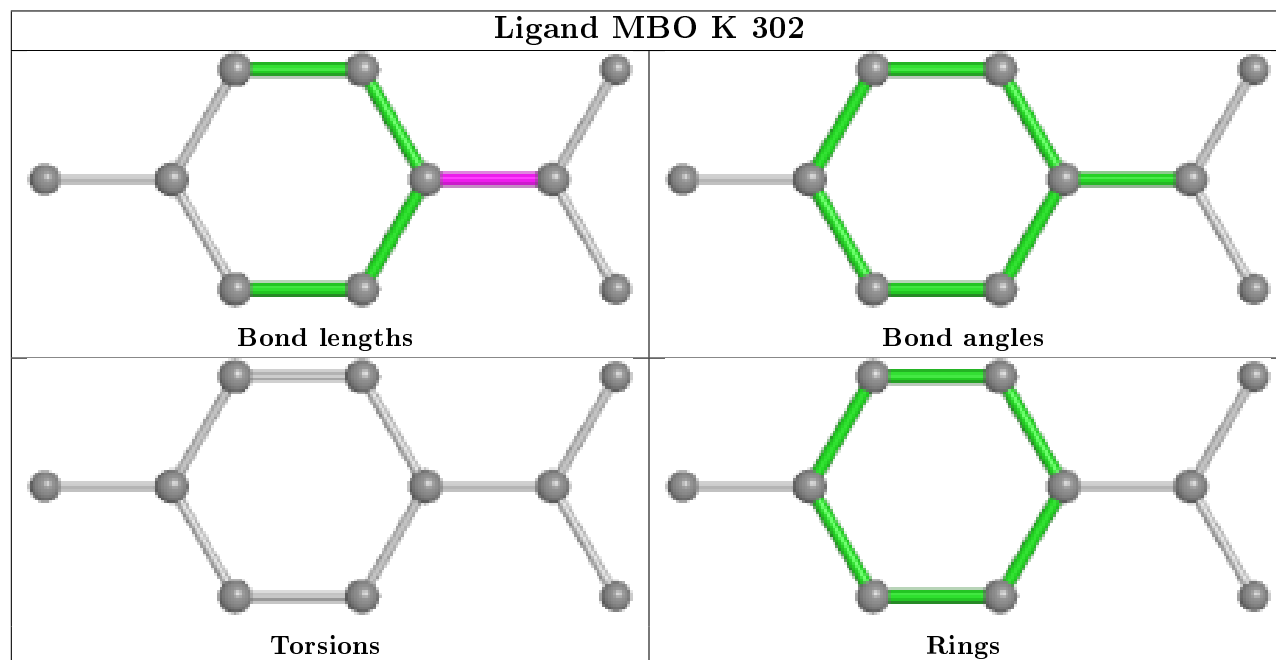
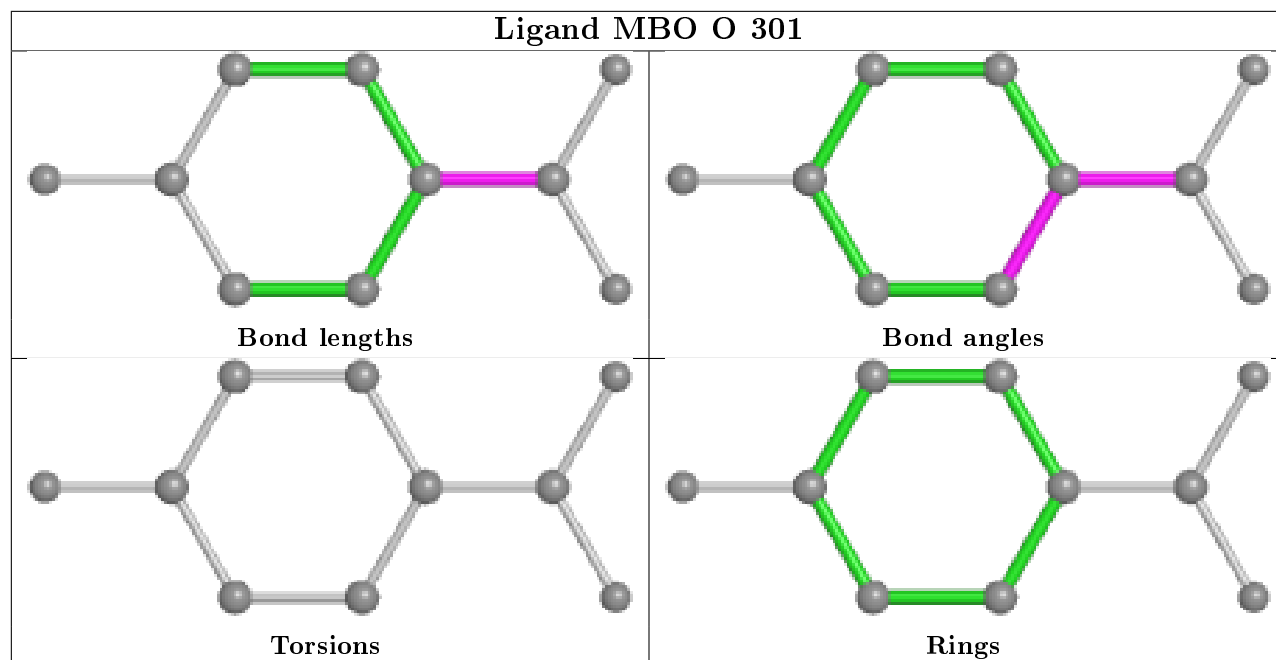


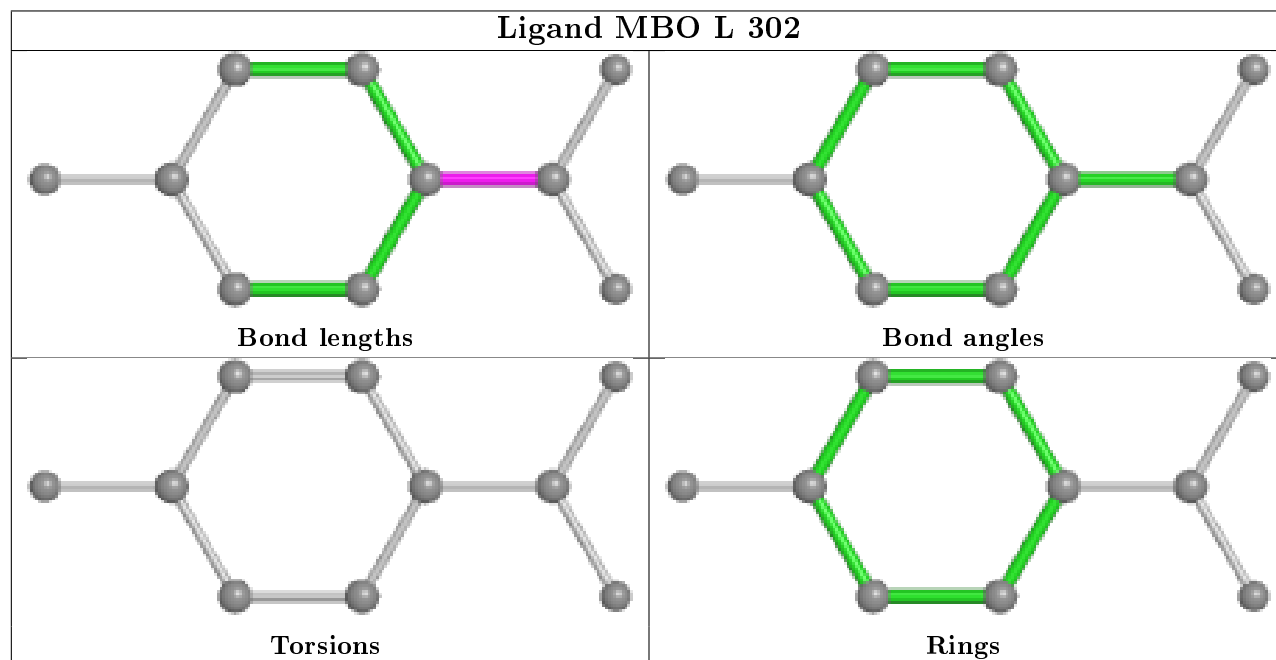
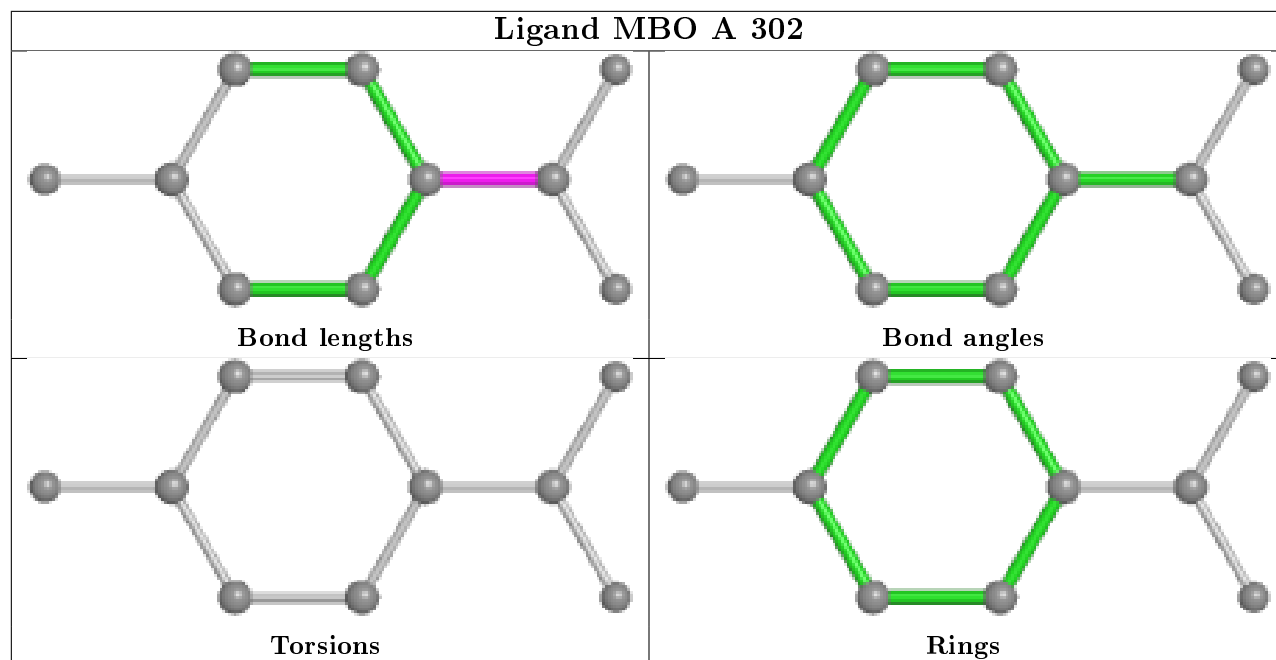


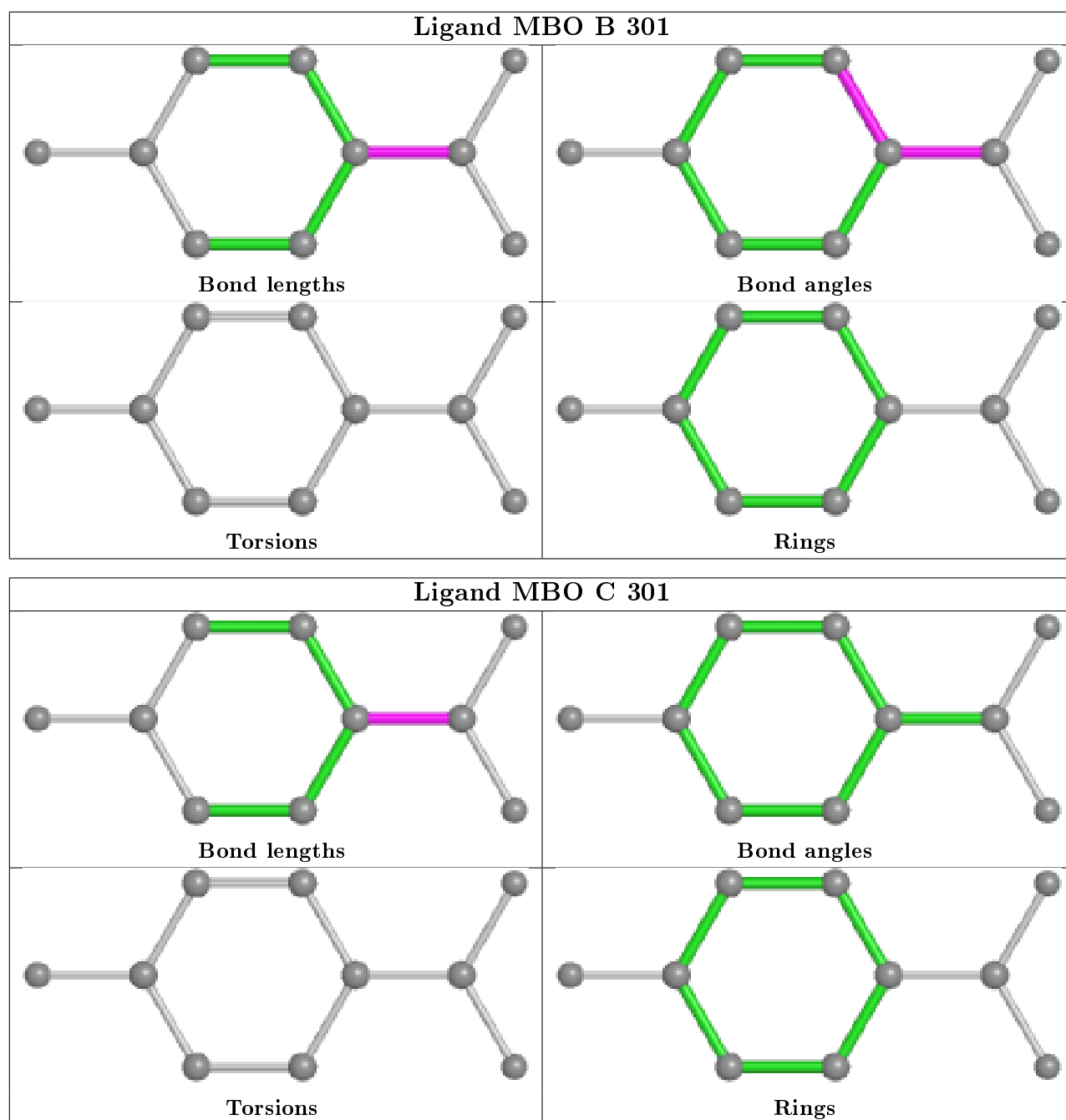












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.