



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 01:42 am BST

PDB ID : 3PCI
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 3-iodo-4-HYDROXYBENZOATE
Authors : Orville, A.M.; Elango, N.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-07-02
Resolution : 2.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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

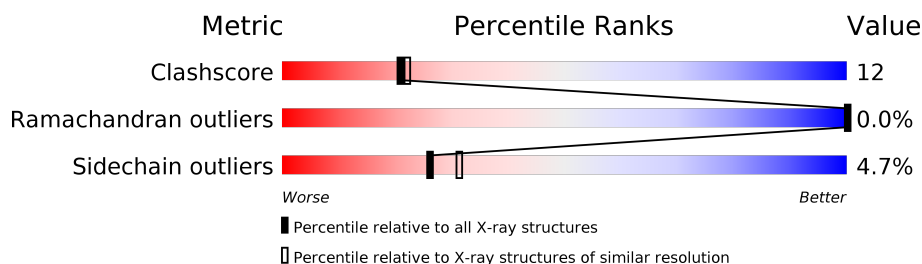
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)

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 ≥ 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	200	75% 21% 5%
1	B	200	70% 27% .
1	C	200	77% 20% ..
1	D	200	73% 22% 5% .
1	E	200	67% 30% .
1	F	200	67% 28% 5% .
2	M	238	72% 21% . . .
2	N	238	76% 18% . . .

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Mol	Chain	Length	Quality of chain
2	O	238	<div><div></div><div>76%19%<div><div></div><div></div><div></div></div></div></div>
2	P	238	<div><div></div><div>77%17%<div><div></div><div></div><div></div></div></div></div>
2	Q	238	<div><div></div><div>69%21%7%<div><div></div><div></div><div></div></div></div></div>
2	R	238	<div><div></div><div>68%24%5%<div><div></div><div></div><div></div></div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22104 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 PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	B	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	C	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	D	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	E	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	F	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			

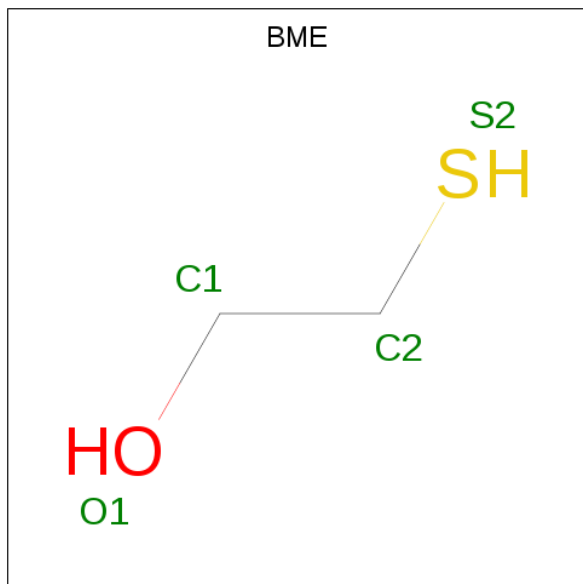
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	N	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	O	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	P	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	Q	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	R	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

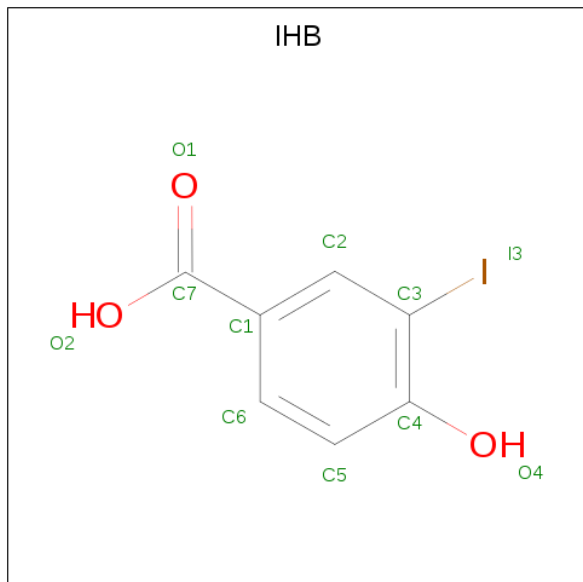
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0
3	M	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O S 4 2 1 1	0	0
4	N	1	Total C O S 4 2 1 1	0	0
4	O	1	Total C O S 4 2 1 1	0	0
4	P	1	Total C O S 4 2 1 1	0	0
4	Q	1	Total C O S 4 2 1 1	0	0
4	R	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is 3-iodo-4-hydroxybenzoic acid (three-letter code: IHB) (formula: $C_7H_5IO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	I	O	0	0
			11	7	1	3		
5	M	1	Total	C	I	O	0	0
			11	7	1	3		
5	N	1	Total	C	I	O	0	0
			11	7	1	3		
5	N	1	Total	C	I	O	0	0
			11	7	1	3		
5	O	1	Total	C	I	O	0	0
			11	7	1	3		
5	O	1	Total	C	I	O	0	0
			11	7	1	3		
5	P	1	Total	C	I	O	0	0
			11	7	1	3		
5	P	1	Total	C	I	O	0	0
			11	7	1	3		
5	Q	1	Total	C	I	O	0	0
			11	7	1	3		
5	Q	1	Total	C	I	O	0	0
			11	7	1	3		
5	R	1	Total	C	I	O	0	0
			11	7	1	3		
5	R	1	Total	C	I	O	0	0
			11	7	1	3		

- Molecule 6 is water.

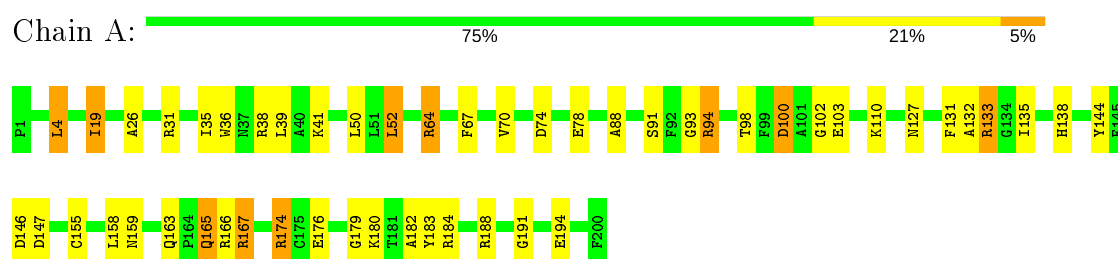
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	82	Total 82	O 82	0	0
6	M	163	Total 163	O 163	0	0
6	B	85	Total 85	O 85	0	0
6	N	167	Total 167	O 167	0	0
6	C	82	Total 82	O 82	0	0
6	O	162	Total 162	O 162	0	0
6	D	81	Total 81	O 81	0	0
6	P	157	Total 157	O 157	0	0
6	E	84	Total 84	O 84	0	0
6	Q	165	Total 165	O 165	0	0
6	F	81	Total 81	O 81	0	0
6	R	167	Total 167	O 167	0	0

3 Residue-property plots

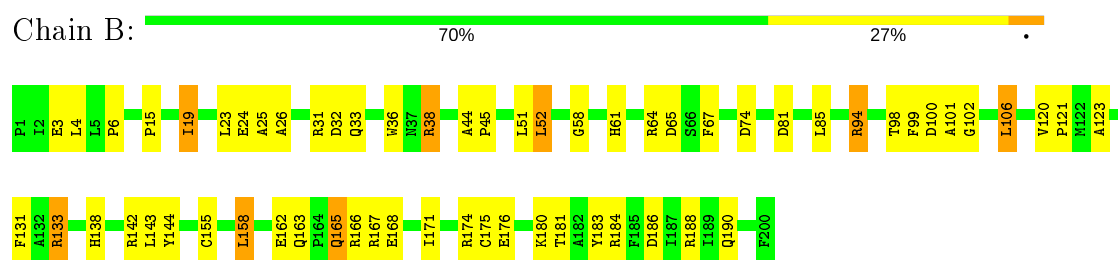
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 was not executed.

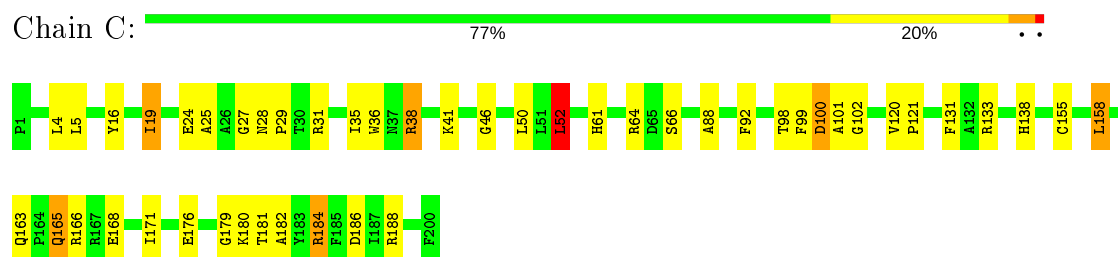
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



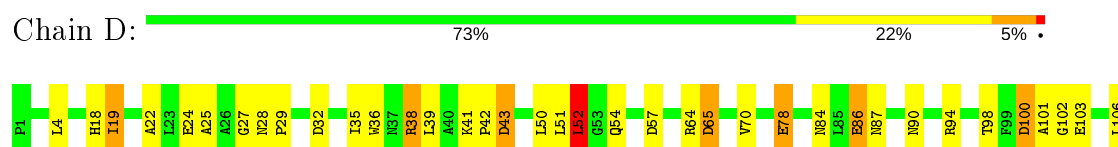
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

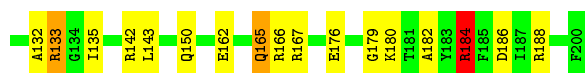


• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE





• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



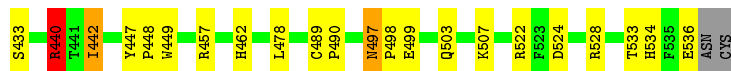
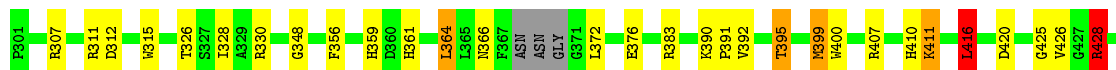
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



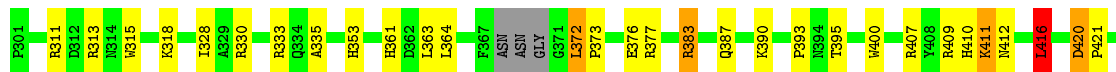
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

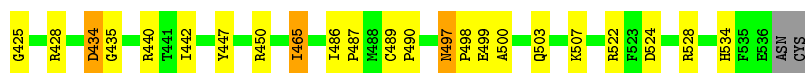


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



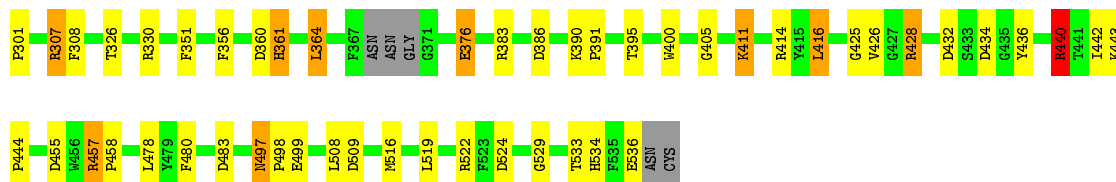
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE





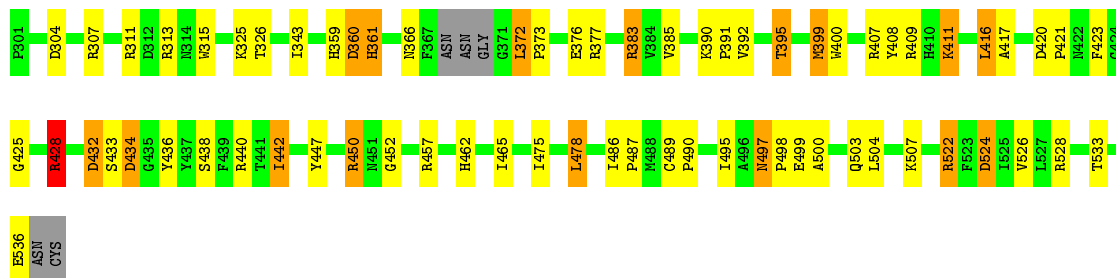
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 77% 17%



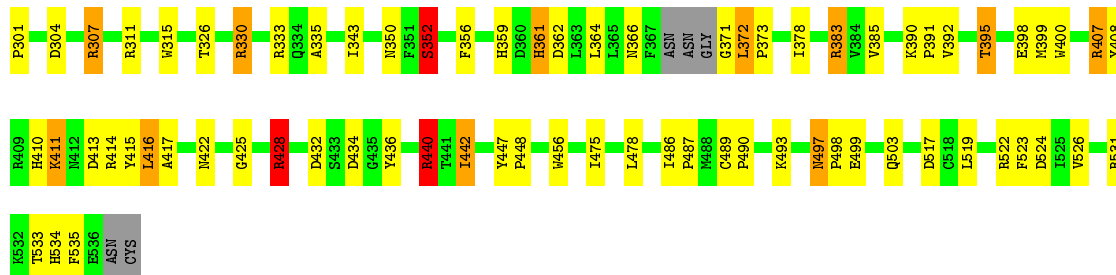
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 69% 21% 7%



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 68% 24% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.00Å 127.07Å 134.08Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	6.00 – 2.21	Depositor
% Data completeness (in resolution range)	83.0 (6.00-2.21)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22104	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHB, FE, BME

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	0.94	1/1611 (0.1%)	1.66	30/2195 (1.4%)
1	B	0.95	0/1611	1.66	33/2195 (1.5%)
1	C	0.95	1/1611 (0.1%)	1.50	14/2195 (0.6%)
1	D	0.92	0/1611	1.52	23/2195 (1.0%)
1	E	0.97	0/1611	1.52	23/2195 (1.0%)
1	F	0.98	0/1611	1.55	25/2195 (1.1%)
2	M	1.00	0/1895	1.54	25/2580 (1.0%)
2	N	0.98	0/1895	1.50	16/2580 (0.6%)
2	O	1.00	0/1895	1.55	24/2580 (0.9%)
2	P	0.97	0/1895	1.53	21/2580 (0.8%)
2	Q	1.02	1/1895 (0.1%)	1.54	24/2580 (0.9%)
2	R	1.00	1/1895 (0.1%)	1.56	24/2580 (0.9%)
All	All	0.98	4/21036 (0.0%)	1.55	282/28650 (1.0%)

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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-5.16	1.37	1.46
1	C	66	SER	CB-OG	-5.10	1.35	1.42
2	R	428	ARG	CD-NE	-5.07	1.37	1.46
2	Q	433	SER	CB-OG	5.05	1.48	1.42

The worst 5 of 282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	440	ARG	NE-CZ-NH2	-20.04	110.28	120.30
2	P	440	ARG	NE-CZ-NH2	-19.34	110.63	120.30
2	R	440	ARG	NE-CZ-NH2	-18.26	111.17	120.30
2	M	440	ARG	NE-CZ-NH2	-16.43	112.08	120.30
2	Q	440	ARG	NE-CZ-NH2	-15.94	112.33	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	184	ARG	Sidechain

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	1571	0	1499	37	0
1	B	1571	0	1499	40	0
1	C	1571	0	1499	29	1
1	D	1571	0	1499	35	1
1	E	1571	0	1499	47	0
1	F	1571	0	1499	66	0
2	M	1840	0	1792	57	0
2	N	1840	0	1792	39	0
2	O	1840	0	1792	36	0
2	P	1840	0	1792	41	0
2	Q	1840	0	1792	56	0
2	R	1840	0	1792	56	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	4	0	5	1	0
4	N	4	0	5	0	0
4	O	4	0	5	1	0
4	P	4	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	4	0	5	2	0
4	R	4	0	5	0	0
5	M	22	0	7	1	0
5	N	22	0	7	1	0
5	O	22	0	7	2	0
5	P	22	0	7	0	0
5	Q	22	0	7	2	0
5	R	22	0	7	3	0
6	A	82	0	0	0	0
6	B	85	0	0	0	0
6	C	82	0	0	0	0
6	D	81	0	0	0	0
6	E	84	0	0	2	0
6	F	81	0	0	2	0
6	M	163	0	0	7	0
6	N	167	0	0	3	0
6	O	162	0	0	6	0
6	P	157	0	0	4	0
6	Q	165	0	0	8	1
6	R	167	0	0	4	0
All	All	22104	0	19818	492	2

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 12.

The worst 5 of 492 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:M:364:LEU:HD22	2:M:440:ARG:HD3	1.25	1.16
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.22	1.12
1:D:64:ARG:NH1	1:D:100:ASP:O	1.81	1.12
1:B:165:GLN:NE2	1:B:165:GLN:H	1.49	1.10
1:F:165:GLN:NE2	1:F:165:GLN:H	1.50	1.09

All (2) 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:C:46:GLY:O	1:D:150:GLN:OE1[3_554]	1.84	0.36
6:Q:1200:HOH:O	6:Q:1200:HOH:O[2_555]	2.10	0.10

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	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	D	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	F	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
2	M	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	N	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	Q	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
2	R	229/238 (96%)	221 (96%)	7 (3%)	1 (0%)	34	37
All	All	2562/2628 (98%)	2475 (97%)	86 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	535	PHE

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	162/163 (99%)	156 (96%)	6 (4%)	34	42
1	B	162/163 (99%)	155 (96%)	7 (4%)	29	35
1	C	162/163 (99%)	155 (96%)	7 (4%)	29	35
1	D	162/163 (99%)	155 (96%)	7 (4%)	29	35
1	E	162/163 (99%)	155 (96%)	7 (4%)	29	35
1	F	162/163 (99%)	155 (96%)	7 (4%)	29	35
2	M	196/202 (97%)	188 (96%)	8 (4%)	30	37
2	N	196/202 (97%)	183 (93%)	13 (7%)	16	17
2	O	196/202 (97%)	186 (95%)	10 (5%)	24	27
2	P	196/202 (97%)	189 (96%)	7 (4%)	35	43
2	Q	196/202 (97%)	185 (94%)	11 (6%)	21	23
2	R	196/202 (97%)	185 (94%)	11 (6%)	21	23
All	All	2148/2190 (98%)	2047 (95%)	101 (5%)	26	31

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	416	LEU
1	D	52	LEU
2	R	399	MET
2	O	465	ILE
1	D	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	163	GLN
2	P	497	ASN
2	R	497	ASN
2	P	361	HIS
1	B	165	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	$\# Z > 2$
5	IHB	M	550	3	9,11,11	3.10	2 (22%)	12,15,15	0.63	0
4	BME	N	601	2	3,3,3	0.50	0	1,2,2	0.06	0
4	BME	O	601	2	3,3,3	0.66	0	1,2,2	0.15	0
5	IHB	P	551	-	9,11,11	2.82	2 (22%)	12,15,15	0.83	0
4	BME	P	601	2	3,3,3	0.56	0	1,2,2	0.74	0
4	BME	Q	601	2	3,3,3	0.36	0	1,2,2	0.18	0
5	IHB	O	550	3	9,11,11	3.14	2 (22%)	12,15,15	0.53	0
5	IHB	P	550	3	9,11,11	2.84	2 (22%)	12,15,15	0.60	0
5	IHB	Q	550	3	9,11,11	3.17	2 (22%)	12,15,15	0.53	0
5	IHB	R	550	3	9,11,11	2.75	2 (22%)	12,15,15	0.58	0
5	IHB	N	550	3	9,11,11	3.45	2 (22%)	12,15,15	0.99	1 (8%)
5	IHB	Q	551	-	9,11,11	2.54	2 (22%)	12,15,15	0.62	0
4	BME	R	601	2	3,3,3	0.53	0	1,2,2	0.48	0
5	IHB	R	551	-	9,11,11	2.49	2 (22%)	12,15,15	0.95	0
5	IHB	O	551	-	9,11,11	2.57	2 (22%)	12,15,15	0.89	1 (8%)
4	BME	M	601	2	3,3,3	0.55	0	1,2,2	0.16	0
5	IHB	N	551	-	9,11,11	2.85	2 (22%)	12,15,15	0.65	0
5	IHB	M	551	-	9,11,11	2.76	2 (22%)	12,15,15	0.58	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
5	IHB	M	550	3	-	0/0/4/4	0/1/1/1
4	BME	N	601	2	-	0/1/1/1	-
4	BME	O	601	2	-	0/1/1/1	-
5	IHB	P	551	-	-	0/0/4/4	0/1/1/1
4	BME	P	601	2	-	1/1/1/1	-
4	BME	Q	601	2	-	1/1/1/1	-
5	IHB	O	550	3	-	0/0/4/4	0/1/1/1
5	IHB	P	550	3	-	0/0/4/4	0/1/1/1
5	IHB	Q	550	3	-	0/0/4/4	0/1/1/1
5	IHB	R	550	3	-	0/0/4/4	0/1/1/1
5	IHB	N	550	3	-	0/0/4/4	0/1/1/1
5	IHB	Q	551	-	-	0/0/4/4	0/1/1/1
4	BME	R	601	2	-	0/1/1/1	-
5	IHB	R	551	-	-	0/0/4/4	0/1/1/1
5	IHB	O	551	-	-	0/0/4/4	0/1/1/1
4	BME	M	601	2	-	1/1/1/1	-
5	IHB	N	551	-	-	0/0/4/4	0/1/1/1
5	IHB	M	551	-	-	0/0/4/4	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	550	IHB	C1-C7	9.57	1.56	1.47
5	O	550	IHB	C1-C7	8.85	1.56	1.47
5	Q	550	IHB	C1-C7	8.74	1.55	1.47
5	M	550	IHB	C1-C7	8.23	1.55	1.47
5	N	551	IHB	C1-C7	7.99	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	550	IHB	C4-C3-I3	-2.24	117.59	119.81
5	O	551	IHB	C4-C3-I3	-2.10	117.72	119.81

There are no chirality outliers.

All (3) torsion outliers are listed below:

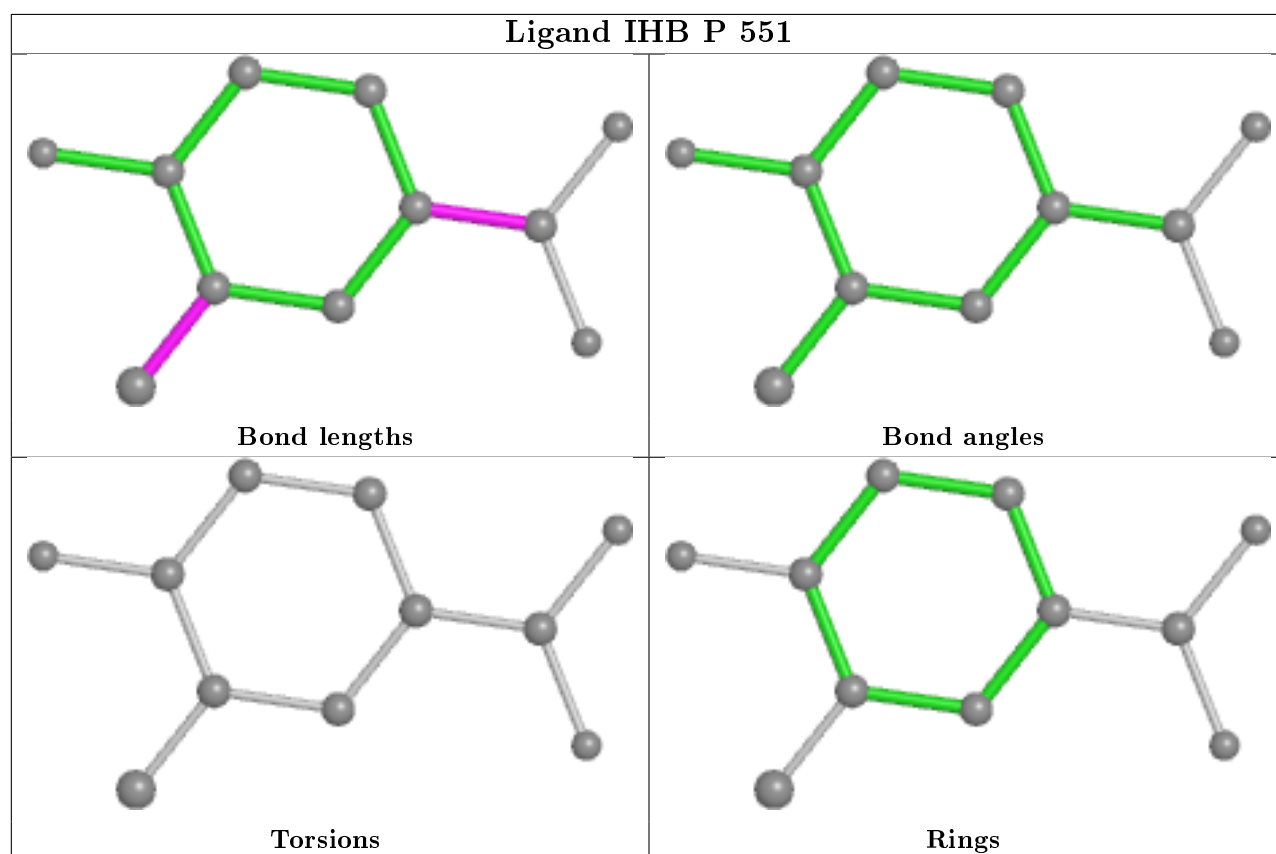
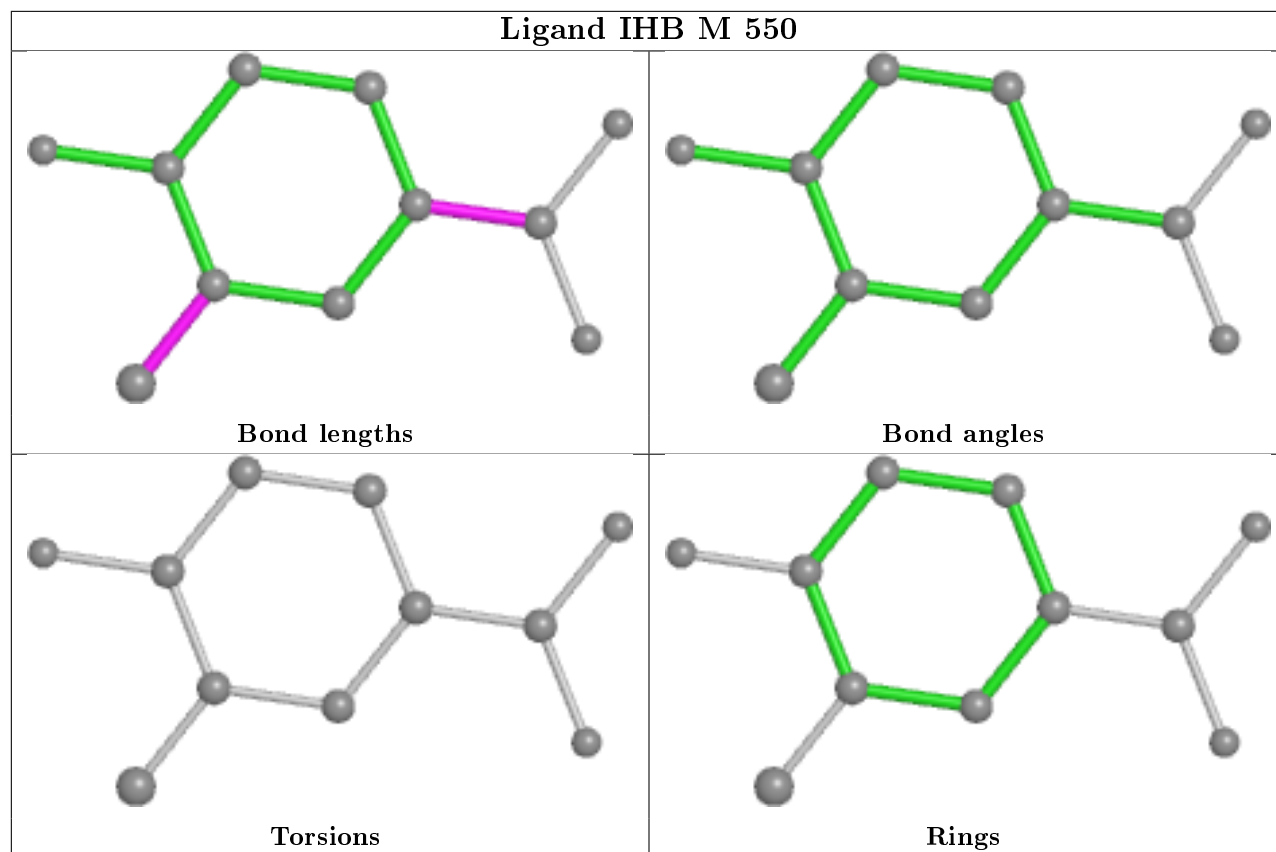
Mol	Chain	Res	Type	Atoms
4	P	601	BME	O1-C1-C2-S2
4	M	601	BME	O1-C1-C2-S2
4	Q	601	BME	O1-C1-C2-S2

There are no ring outliers.

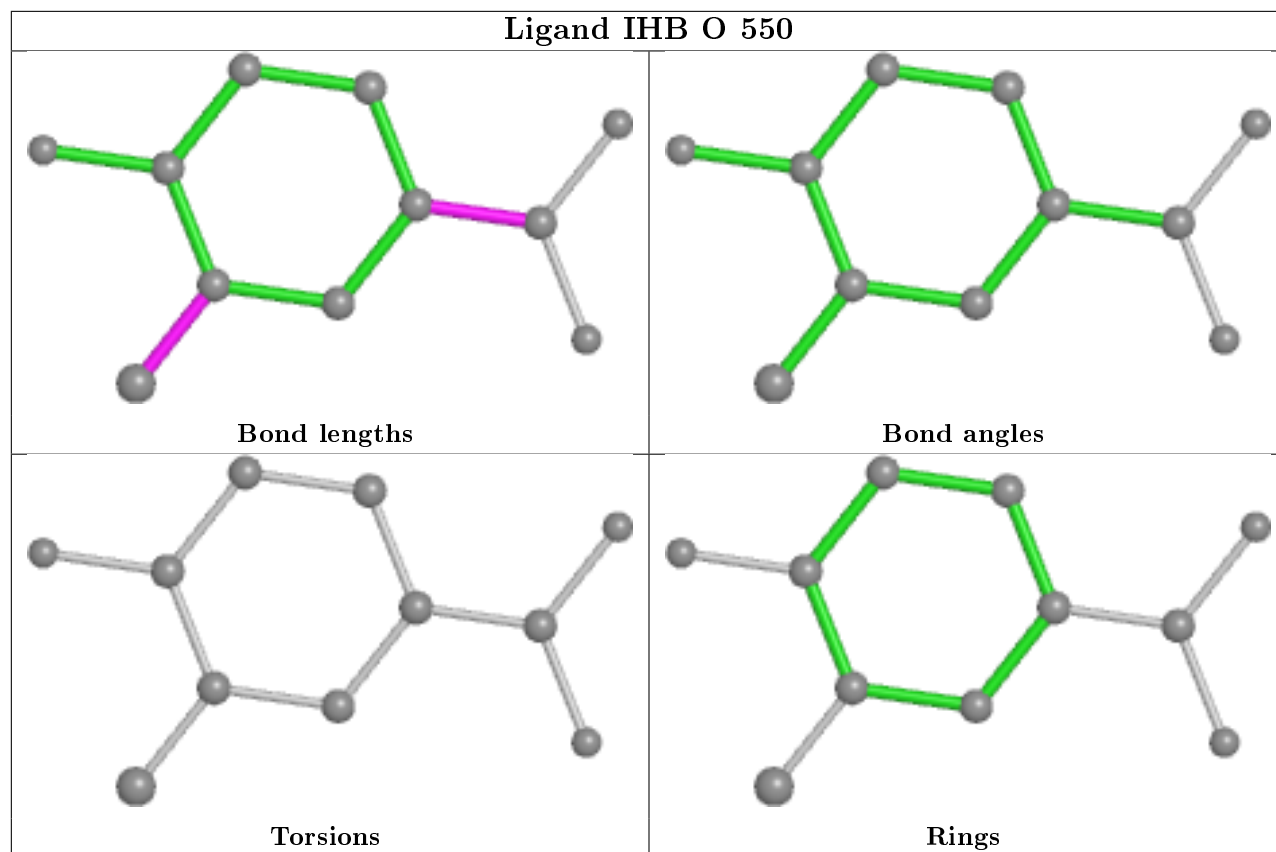
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	550	IHB	1	0
4	O	601	BME	1	0
4	Q	601	BME	2	0
5	O	550	IHB	2	0
5	Q	550	IHB	2	0
5	R	550	IHB	3	0
5	N	550	IHB	1	0
4	M	601	BME	1	0

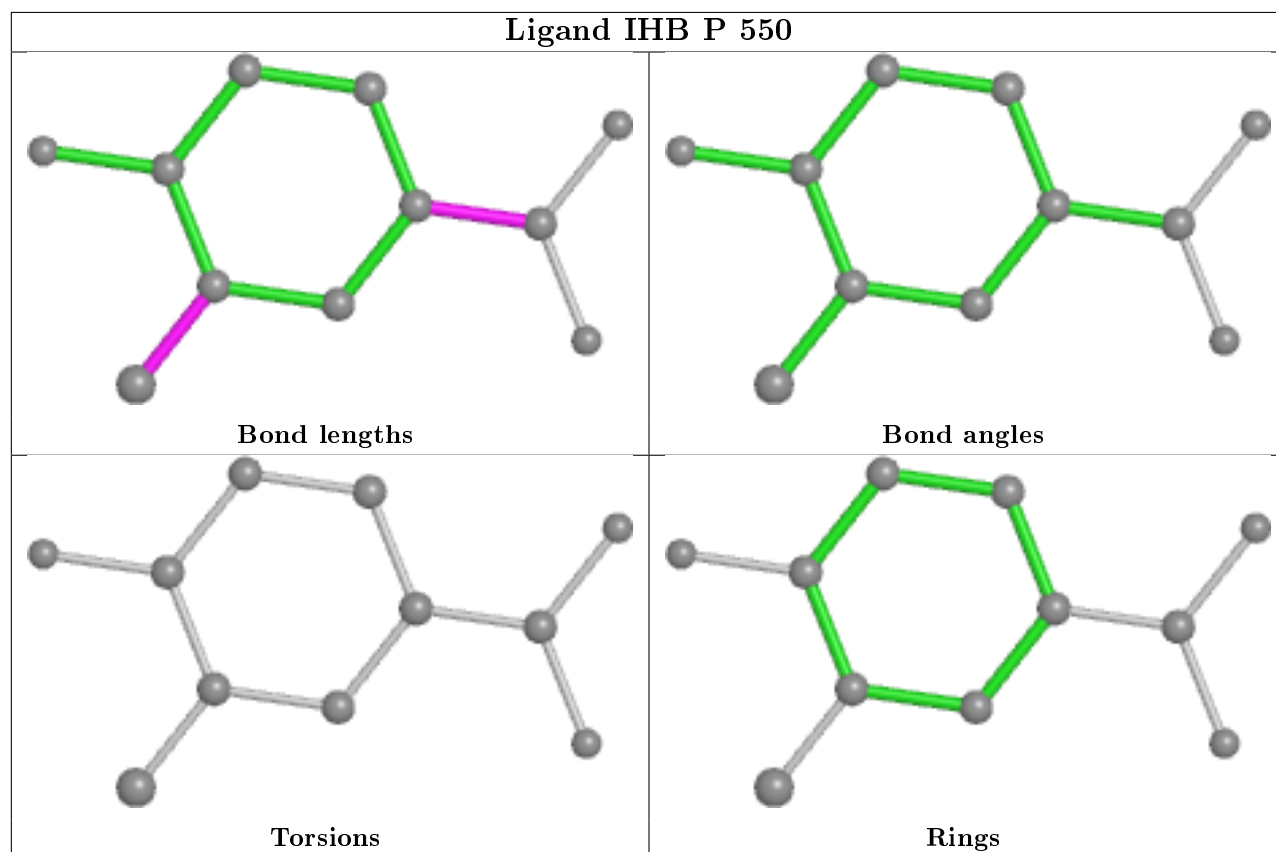
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

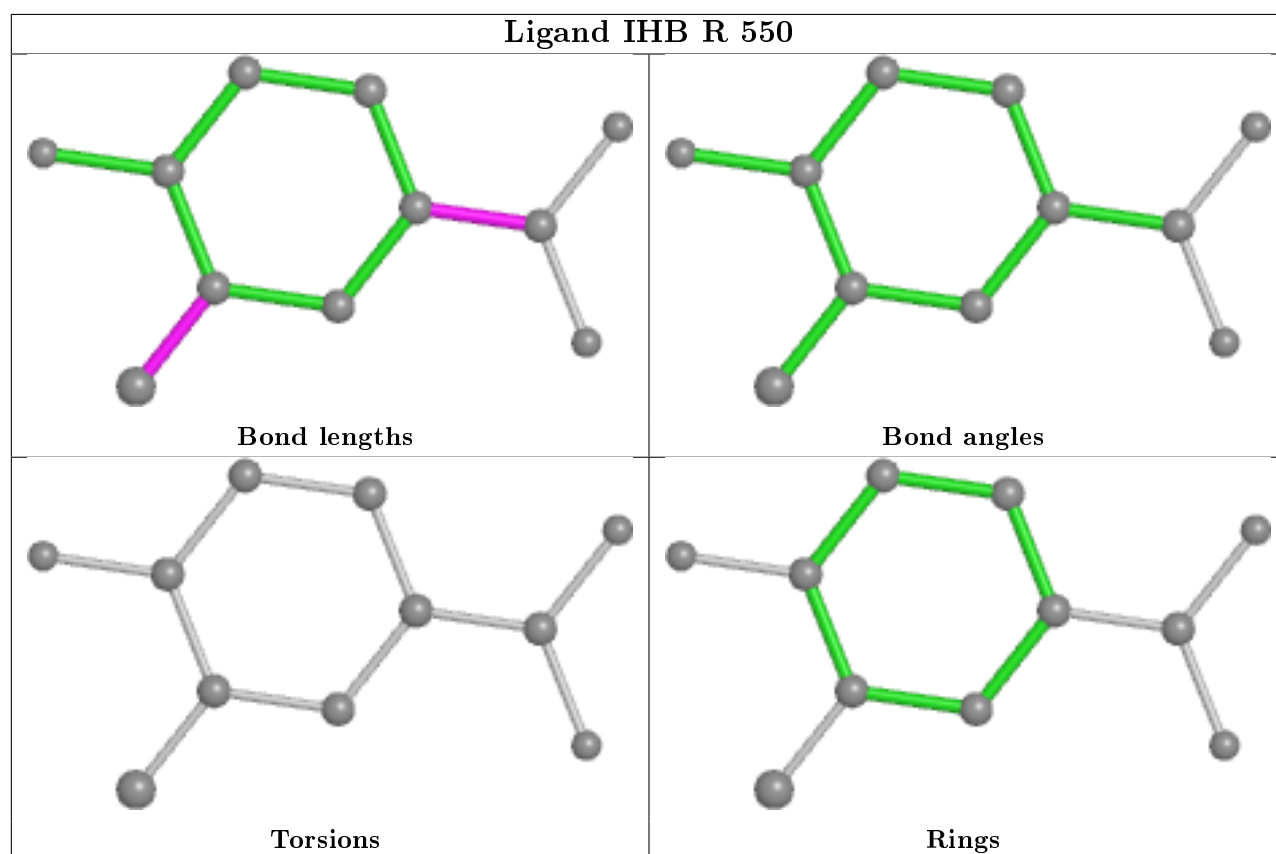
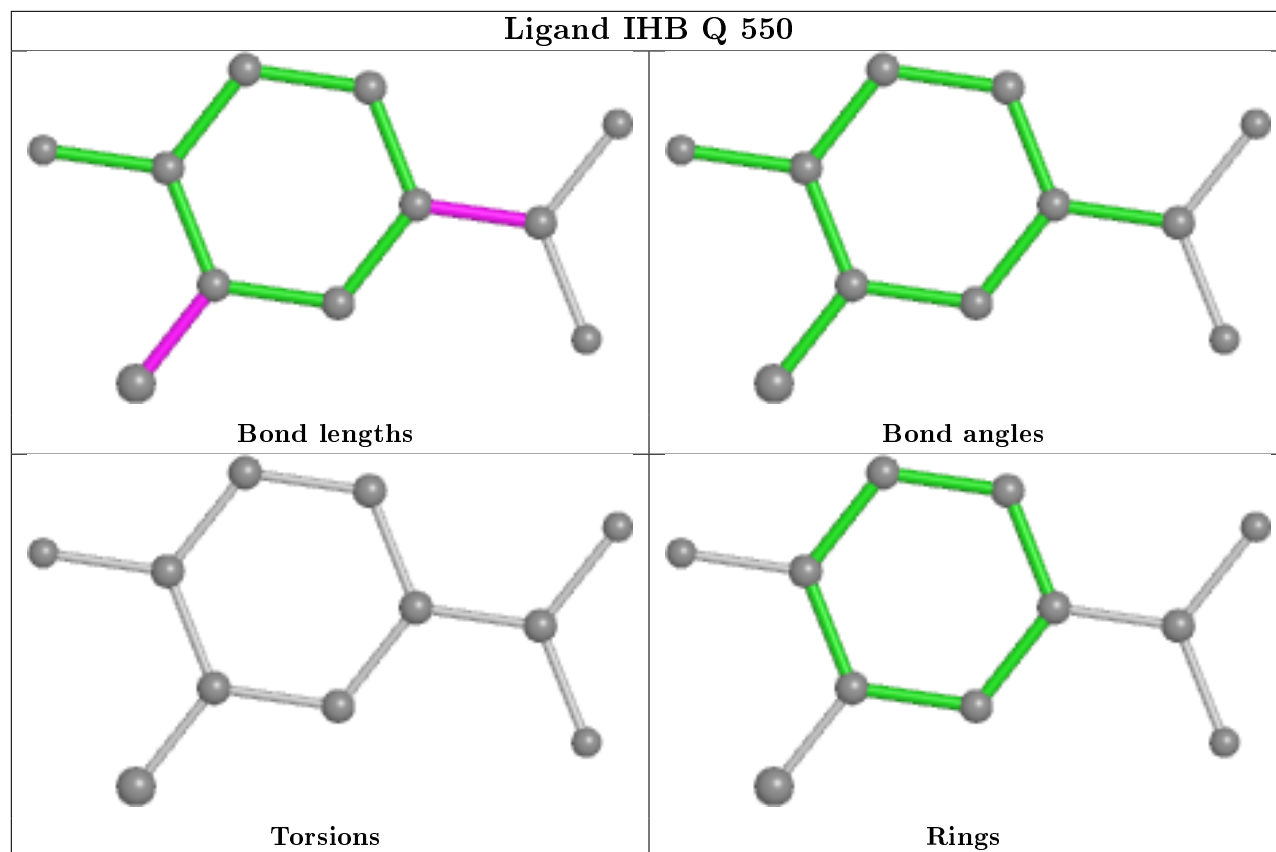


Ligand IHB O 550

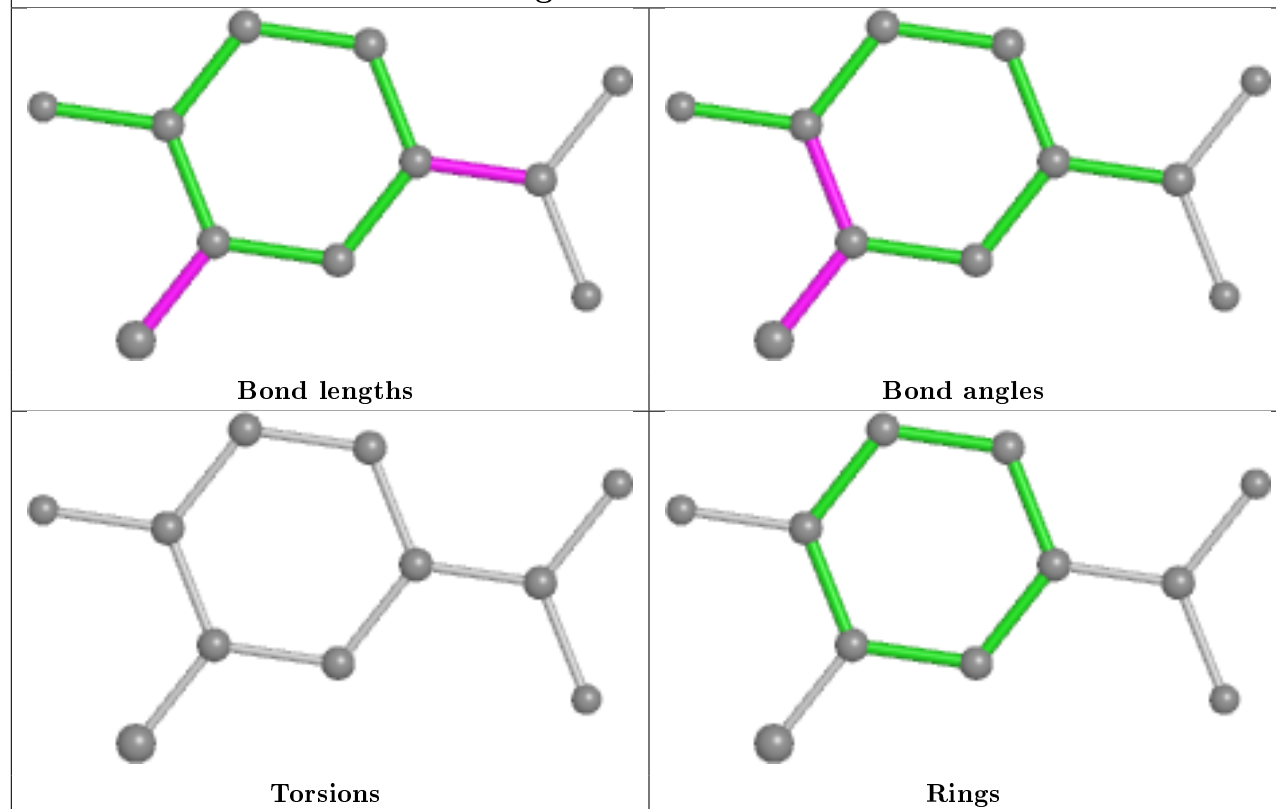


Ligand IHB P 550

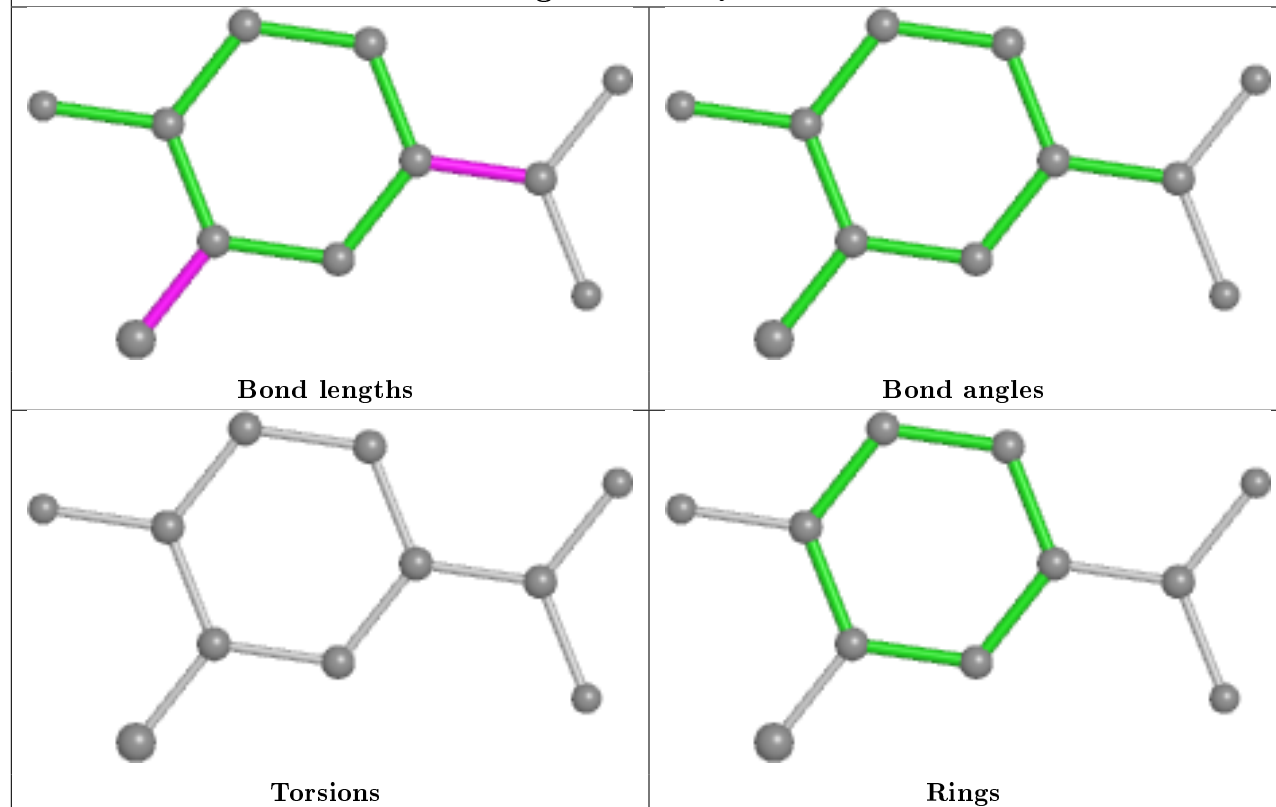




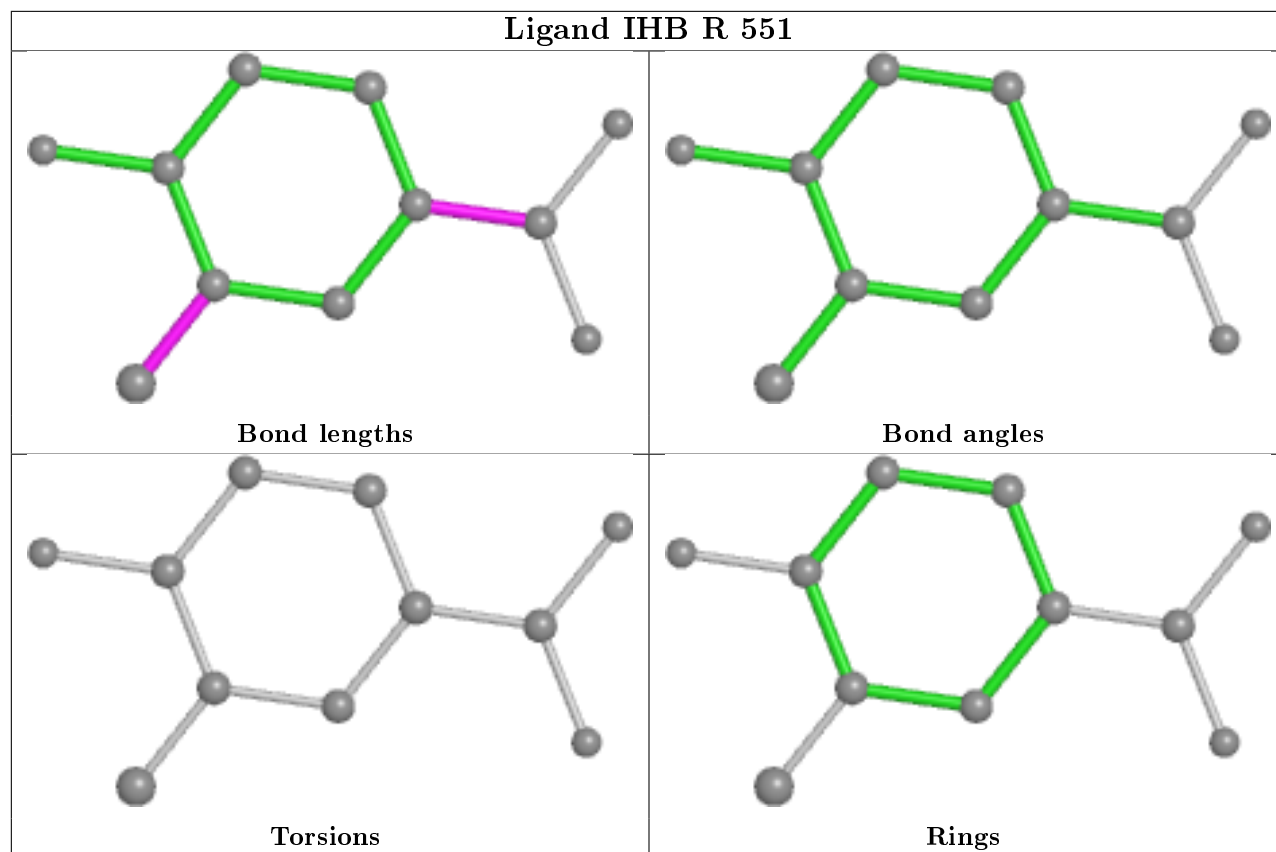
Ligand IHB N 550



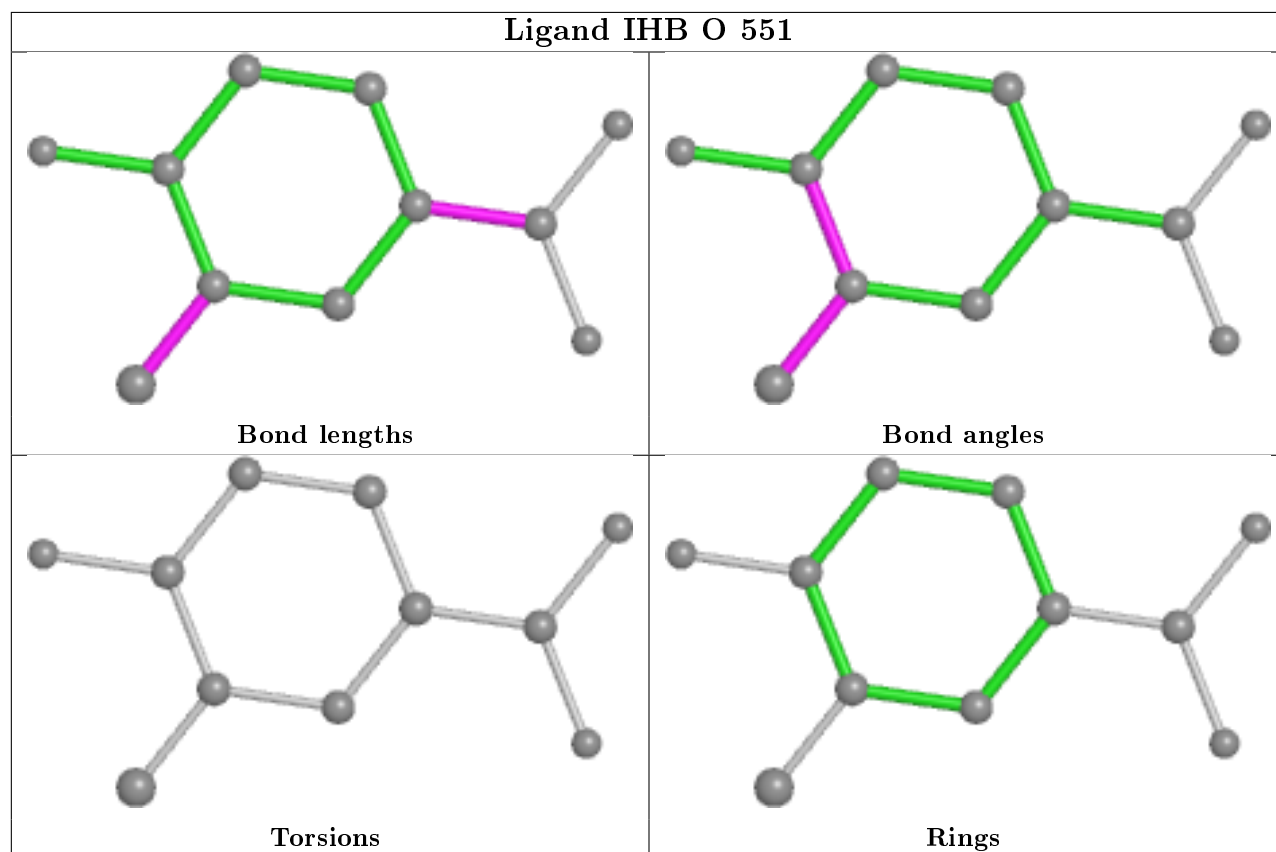
Ligand IHB Q 551



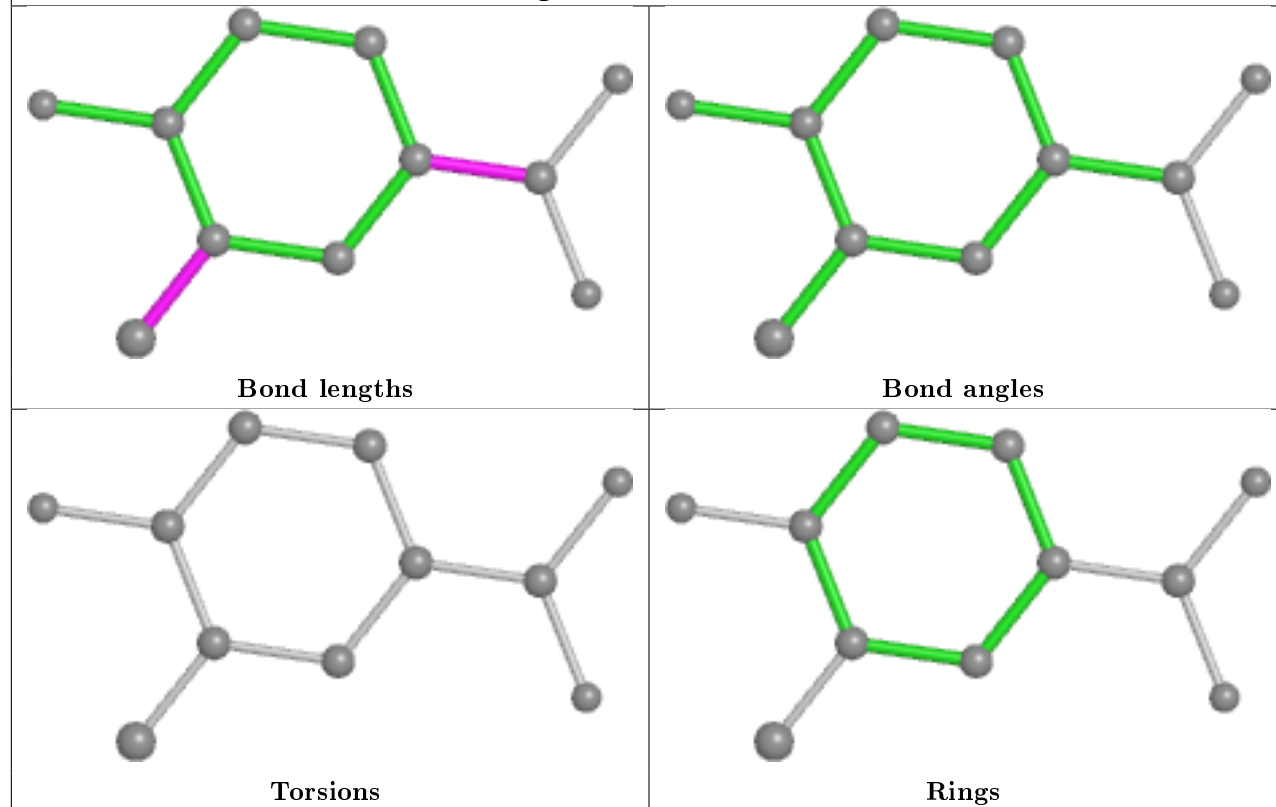
Ligand IHB R 551



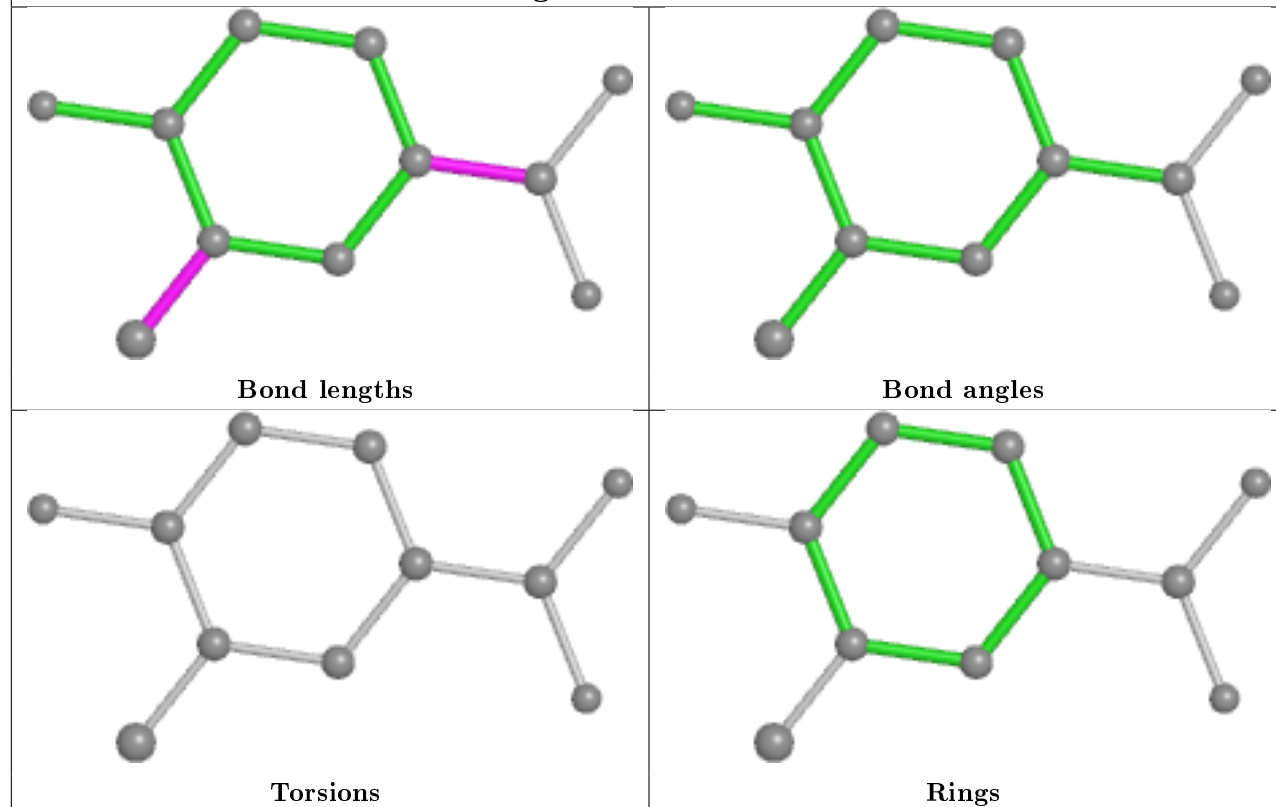
Ligand IHB O 551



Ligand IHB N 551



Ligand IHB M 551



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.