



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:22 am BST

PDB ID : 1XC1
Title : Oxo Zirconium(IV) Cluster in the Ferric Binding Protein (FBP)
Authors : Zhong, W.; Alexeev, D.; Harvey, I.; Guo, M.; Hunter, D.J.B.; Zhu, H.; Campiano, D.J.; Sadler, P.J.
Deposited on : 2004-08-31
Resolution : 1.51 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

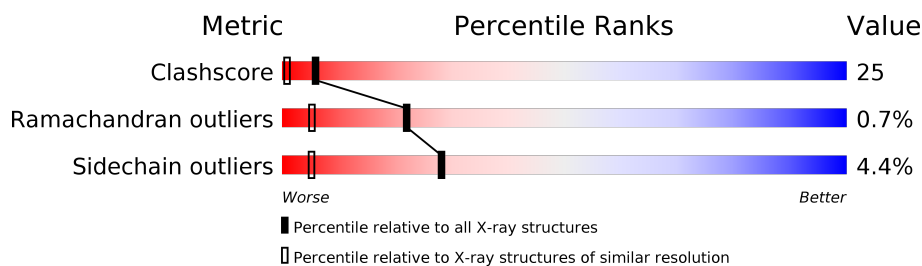
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	309	
1	B	309	
1	C	309	
1	D	309	
1	E	309	
1	F	309	
1	G	309	
1	H	309	

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Mol	Chain	Length	Quality of chain
1	I	309	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment on the left labeled '58%', a yellow segment in the middle labeled '39%', and a small orange segment on the right. A small black dot is located at the end of the orange segment.

2 Entry composition

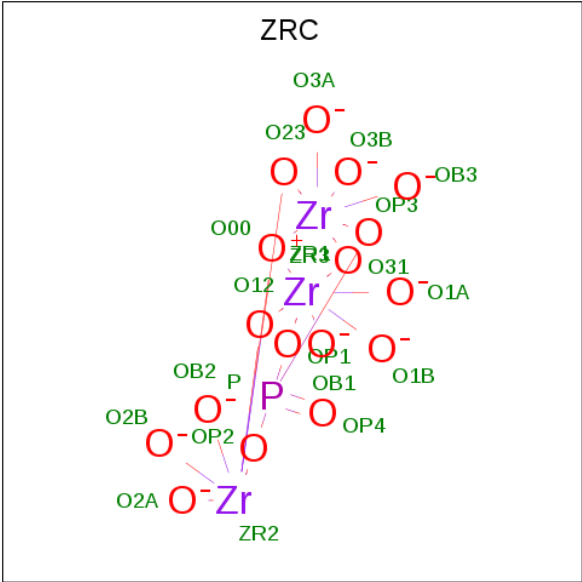
There are 3 unique types of molecules in this entry. The entry contains 22547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 periplasmic iron-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	B	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	C	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	D	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	E	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	F	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	G	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	H	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			
1	I	309	Total	C	N	O	S	0	0	0
			2378	1508	423	446	1			

- Molecule 2 is OXO ZIRCONIUM(IV) CLUSTER (three-letter code: ZRC) (formula: O₁₇PZr₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	P	Zr	0	0
			19	15	1	3		
2	B	1	Total	O	P	Zr	0	0
			19	15	1	3		
2	C	1	Total	O	P	Zr	0	0
			19	15	1	3		
2	D	1	Total	O	P	Zr	0	0
			19	15	1	3		
2	E	1	Total	O	P	Zr	0	0
			19	15	1	3		
2	F	1	Total	O	P	Zr	0	0
			19	15	1	3		
2	G	1	Total	O	P	Zr	0	0
			19	15	1	3		
2	H	1	Total	O	P	Zr	0	0
			19	15	1	3		
2	I	1	Total	O	P	Zr	0	0
			19	15	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	103	Total	O	0	0
			103	103		
3	C	111	Total	O	0	0
			111	111		

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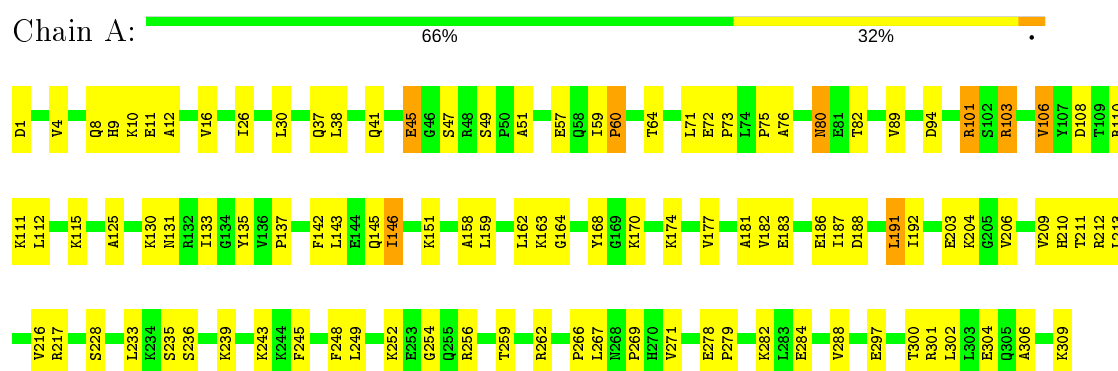
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	113	Total 113	O 113	0	0
3	E	136	Total 136	O 136	0	0
3	F	124	Total 124	O 124	0	0
3	G	79	Total 79	O 79	0	0
3	H	81	Total 81	O 81	0	0
3	I	85	Total 85	O 85	0	0

3 Residue-property plots

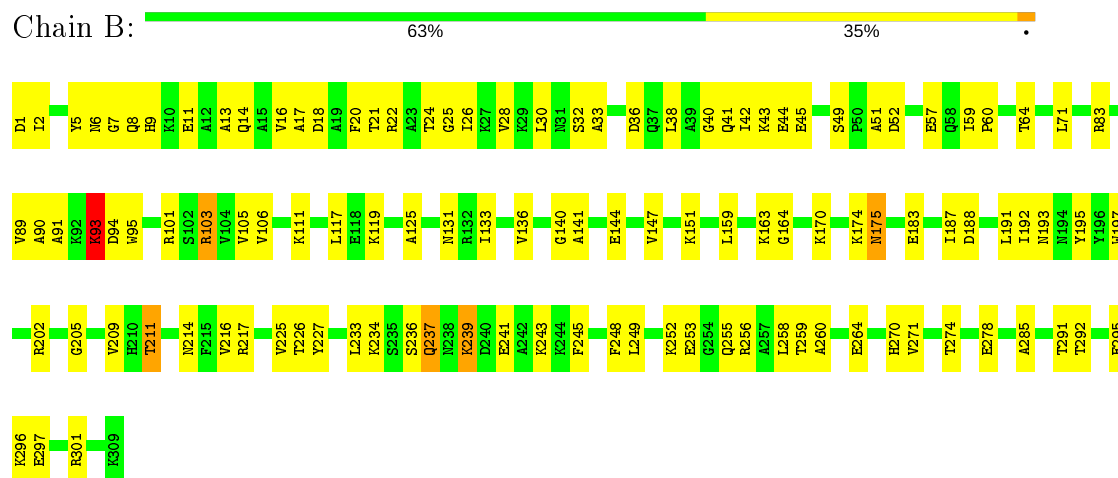
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

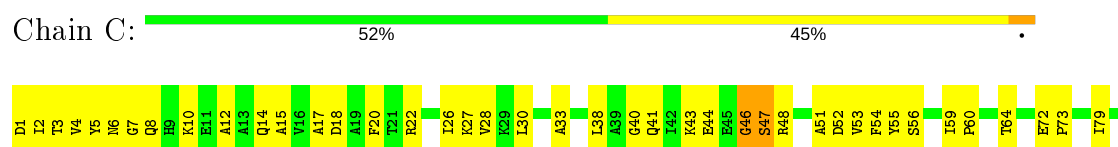
- Molecule 1: periplasmic iron-binding protein

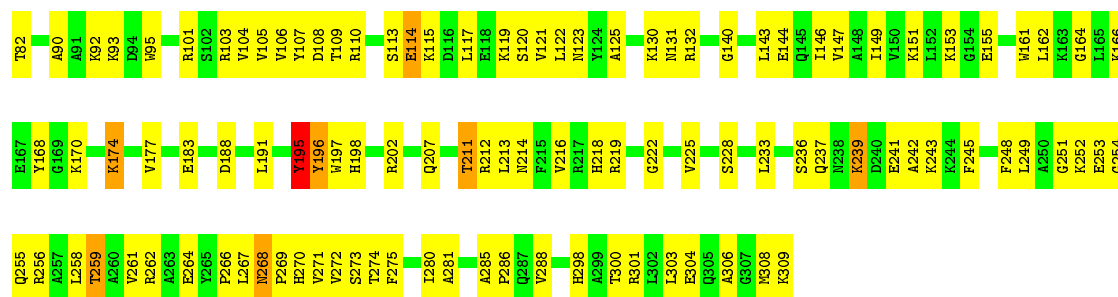


- Molecule 1: periplasmic iron-binding protein

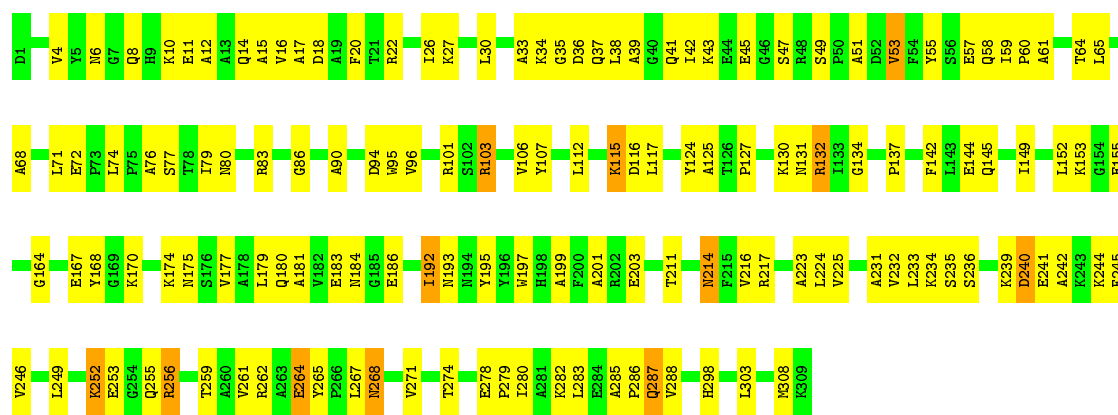


- Molecule 1: periplasmic iron-binding protein

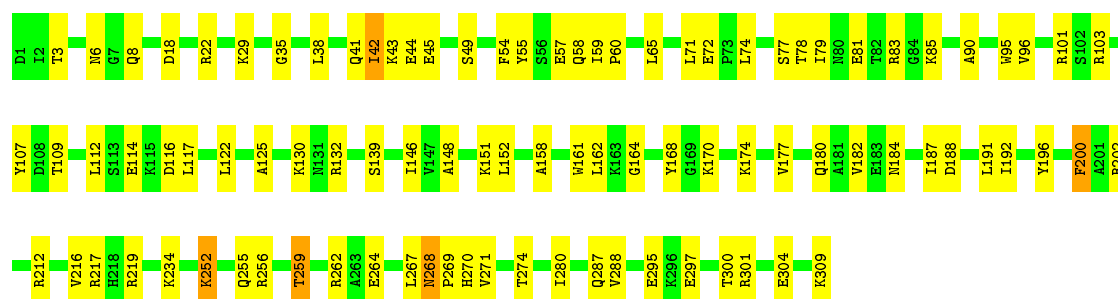




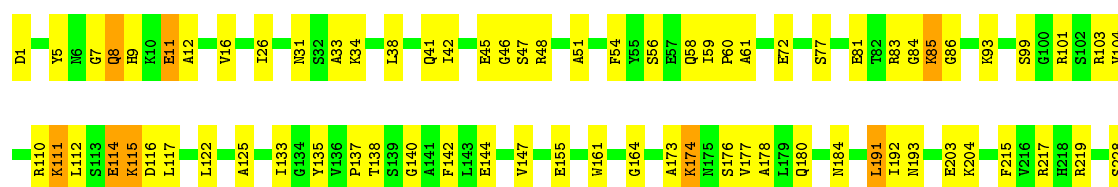
- Molecule 1: periplasmic iron-binding protein



- Molecule 1: periplasmic iron-binding protein



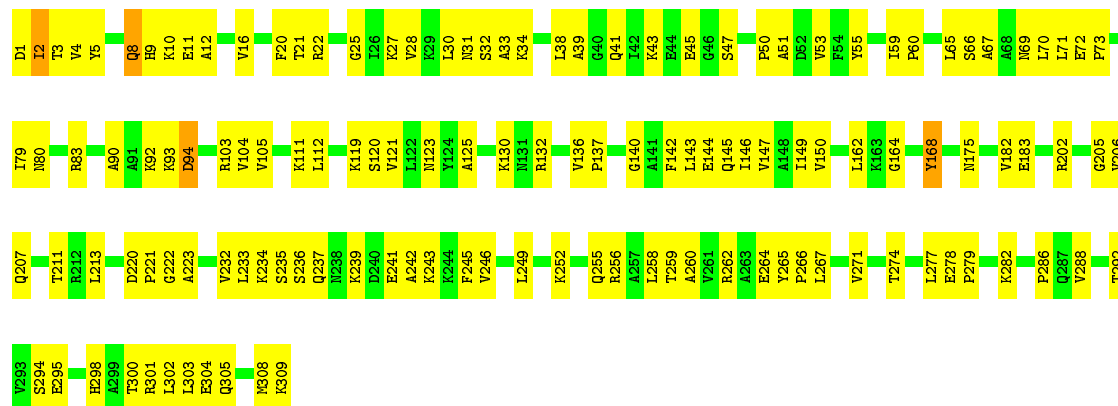
- Molecule 1: periplasmic iron-binding protein





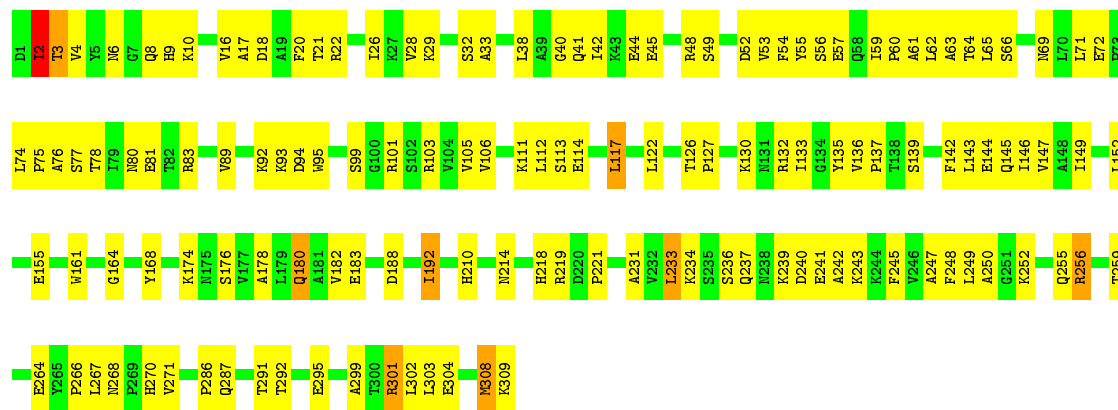
- Molecule 1: periplasmic iron-binding protein

Chain G: 57% 41%



- Molecule 1: periplasmic iron-binding protein

Chain H: 55% 42%



- Molecule 1: periplasmic iron-binding protein

Chain I: 58% 39%





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	146.20 Å 146.20 Å 113.56 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.51	Depositor
% Data completeness (in resolution range)	97.3 (20.00-1.51)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.191 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22547	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: ZRC

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	0.39	0/2423	0.63	0/3280
1	B	0.36	0/2423	0.63	1/3280 (0.0%)
1	C	0.41	0/2423	0.65	2/3280 (0.1%)
1	D	0.37	0/2423	0.59	0/3280
1	E	0.38	0/2423	0.63	0/3280
1	F	0.37	0/2423	0.63	0/3280
1	G	0.34	0/2423	0.60	0/3280
1	H	0.35	0/2423	0.60	0/3280
1	I	0.36	0/2423	0.61	0/3280
All	All	0.37	0/21807	0.62	3/29520 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	TYR	CB-CG-CD1	5.81	124.49	121.00
1	B	205	GLY	N-CA-C	-5.34	99.75	113.10
1	C	196	TYR	CB-CG-CD2	5.22	124.13	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2378	0	2424	98	0
1	B	2378	0	2424	102	0
1	C	2378	0	2424	149	0
1	D	2378	0	2424	147	0
1	E	2378	0	2424	93	0
1	F	2378	0	2424	95	0
1	G	2378	0	2424	140	0
1	H	2378	0	2424	139	0
1	I	2378	0	2424	127	0
2	A	19	0	0	0	0
2	B	19	0	0	1	0
2	C	19	0	0	1	0
2	D	19	0	0	2	0
2	E	19	0	0	0	0
2	F	19	0	0	0	0
2	G	19	0	0	0	0
2	H	19	0	0	1	0
2	I	19	0	0	1	0
3	A	142	0	0	3	0
3	B	103	0	0	4	0
3	C	111	0	0	11	0
3	D	113	0	0	10	0
3	E	136	0	0	5	0
3	F	124	0	0	8	0
3	G	79	0	0	5	0
3	H	81	0	0	6	0
3	I	85	0	0	3	0
All	All	22547	0	21816	1086	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 1086 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:THR:HG21	1:A:266:PRO:HG3	1.24	1.17
1:F:259:THR:HG21	1:F:266:PRO:HG3	1.14	1.11
1:H:80:ASN:HA	1:H:83:ARG:HG2	1.27	1.10
1:H:259:THR:HG21	1:H:266:PRO:HG3	1.35	1.07
1:G:259:THR:HG21	1:G:266:PRO:HG3	1.35	1.06

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/309 (99%)	288 (94%)	19 (6%)	0	100	100
1	B	307/309 (99%)	288 (94%)	17 (6%)	2 (1%)	22	5
1	C	307/309 (99%)	283 (92%)	20 (6%)	4 (1%)	12	1
1	D	307/309 (99%)	291 (95%)	14 (5%)	2 (1%)	22	5
1	E	307/309 (99%)	291 (95%)	12 (4%)	4 (1%)	12	1
1	F	307/309 (99%)	292 (95%)	13 (4%)	2 (1%)	22	5
1	G	307/309 (99%)	281 (92%)	23 (8%)	3 (1%)	15	3
1	H	307/309 (99%)	287 (94%)	18 (6%)	2 (1%)	22	5
1	I	307/309 (99%)	291 (95%)	15 (5%)	1 (0%)	41	18
All	All	2763/2781 (99%)	2592 (94%)	151 (6%)	20 (1%)	22	5

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	195	TYR
1	F	85	LYS
1	C	46	GLY
1	D	252	LYS
1	F	47	SER

5.3.2 Protein sidechains [i](#)

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	245/245 (100%)	233 (95%)	12 (5%)	25	3
1	B	245/245 (100%)	233 (95%)	12 (5%)	25	3
1	C	245/245 (100%)	234 (96%)	11 (4%)	27	5
1	D	245/245 (100%)	233 (95%)	12 (5%)	25	3
1	E	245/245 (100%)	236 (96%)	9 (4%)	34	8
1	F	245/245 (100%)	235 (96%)	10 (4%)	30	6
1	G	245/245 (100%)	238 (97%)	7 (3%)	42	13
1	H	245/245 (100%)	235 (96%)	10 (4%)	30	6
1	I	245/245 (100%)	232 (95%)	13 (5%)	22	3
All	All	2205/2205 (100%)	2109 (96%)	96 (4%)	28	5

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	256	ARG
1	E	259	THR
1	I	80	ASN
1	D	264	GLU
1	E	139	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	255	GLN
1	F	298	HIS
1	I	175	ASN
1	E	298	HIS
1	F	184	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ZRC	G	400	1	6,23,25	3.33	5 (83%)	3,66,78	0.23	0
2	ZRC	H	400	1	6,23,25	3.13	5 (83%)	3,66,78	0.21	0
2	ZRC	I	400	1	6,23,25	3.05	5 (83%)	3,66,78	0.19	0
2	ZRC	C	400	1	6,23,25	3.03	5 (83%)	3,66,78	0.23	0
2	ZRC	D	400	1	6,23,25	3.37	5 (83%)	3,66,78	0.27	0
2	ZRC	E	400	1	6,23,25	3.69	5 (83%)	3,66,78	0.31	0
2	ZRC	F	400	1	6,23,25	4.87	5 (83%)	3,66,78	0.29	0
2	ZRC	A	400	1	6,23,25	2.87	5 (83%)	3,66,78	0.25	0
2	ZRC	B	400	1	6,23,25	2.96	5 (83%)	3,66,78	0.23	0

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	ZRC	ZR2-OP2	7.74	2.43	2.11
2	F	400	ZRC	ZR2-O00	7.19	2.28	2.10
2	E	400	ZRC	ZR2-OP2	5.81	2.35	2.11
2	D	400	ZRC	ZR2-OP2	5.29	2.33	2.11
2	G	400	ZRC	ZR2-OP2	4.78	2.31	2.11

There are no bond angle outliers.

There are no chirality outliers.

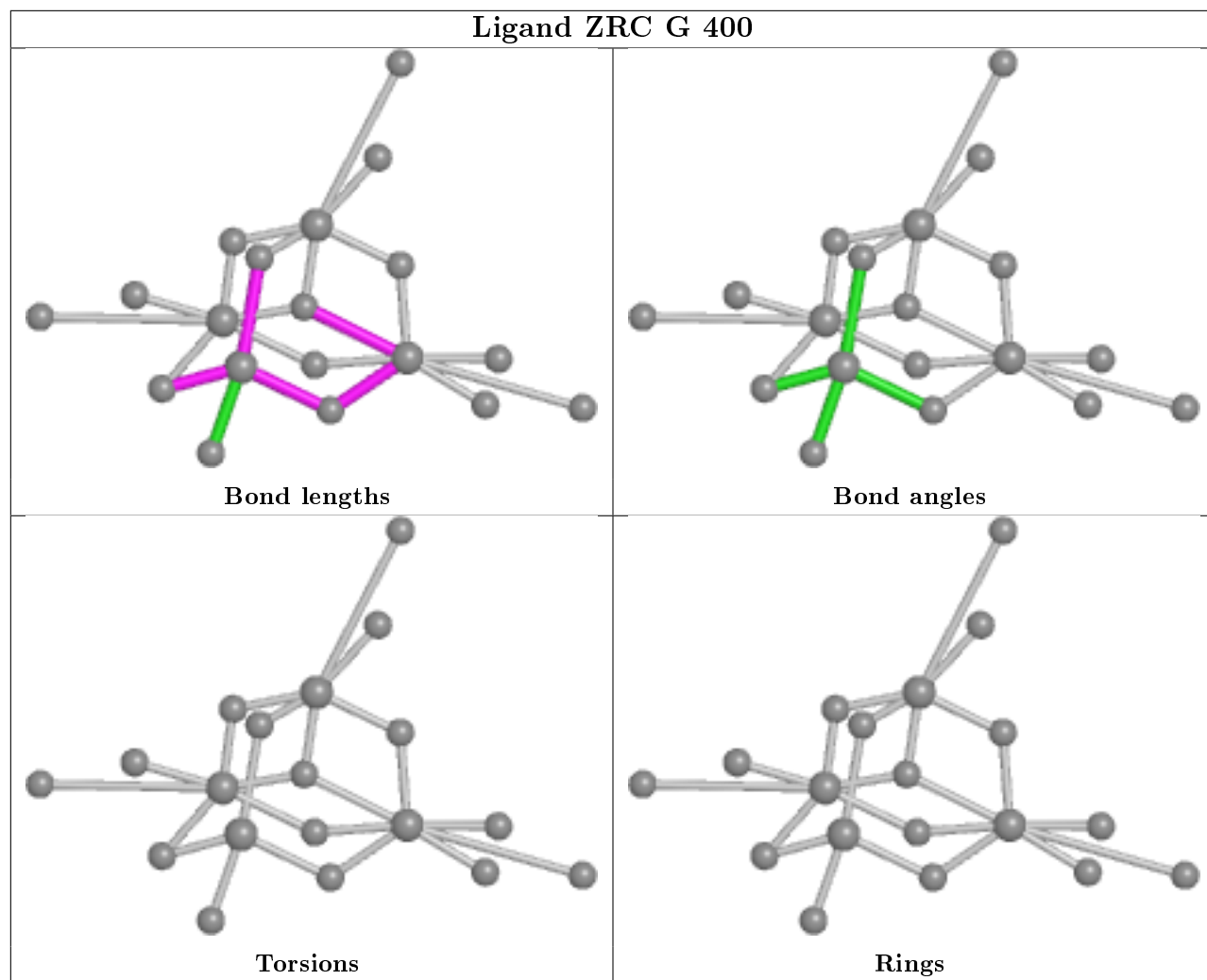
There are no torsion outliers.

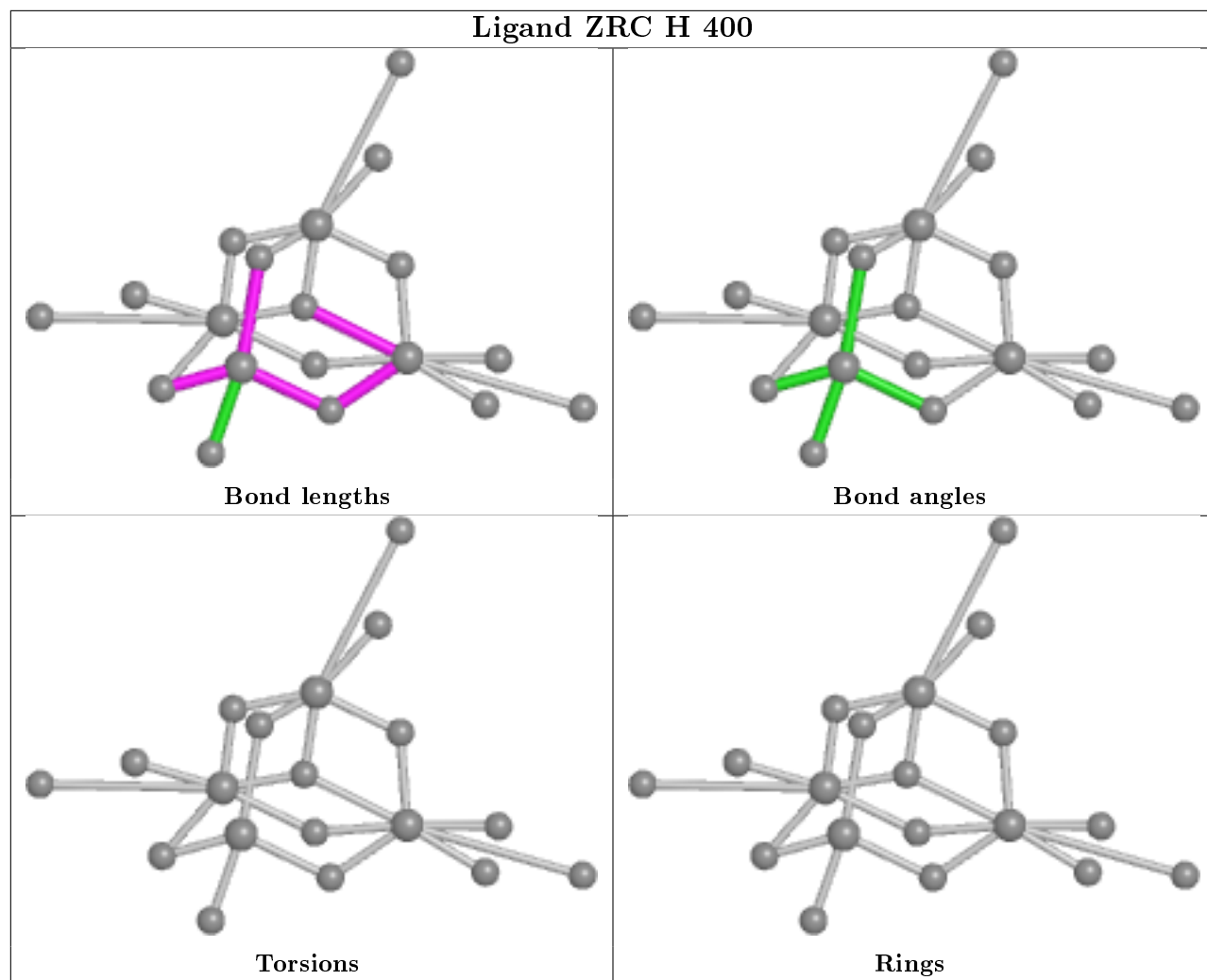
There are no ring outliers.

5 monomers are involved in 6 short contacts:

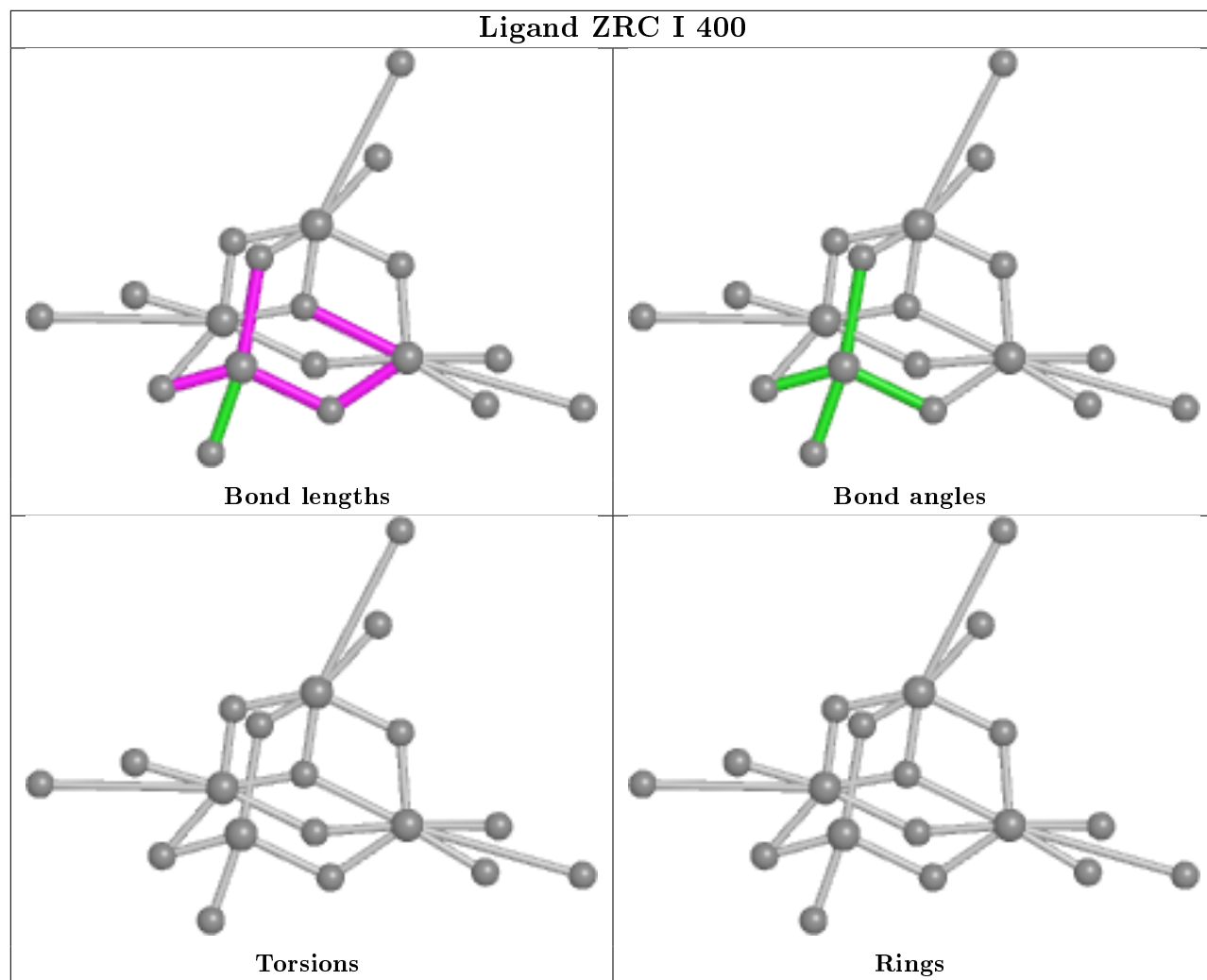
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	400	ZRC	1	0
2	I	400	ZRC	1	0
2	C	400	ZRC	1	0
2	D	400	ZRC	2	0
2	B	400	ZRC	1	0

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.

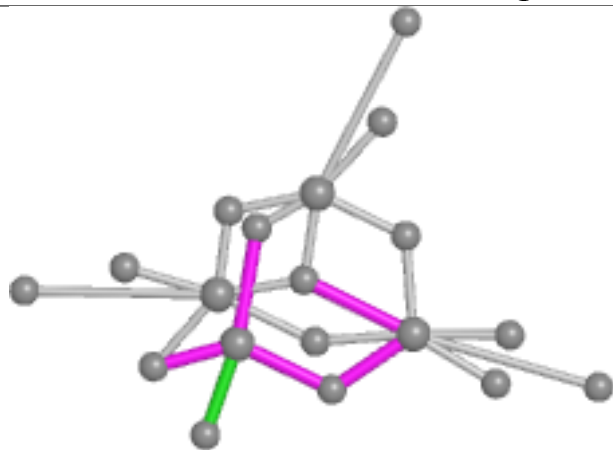




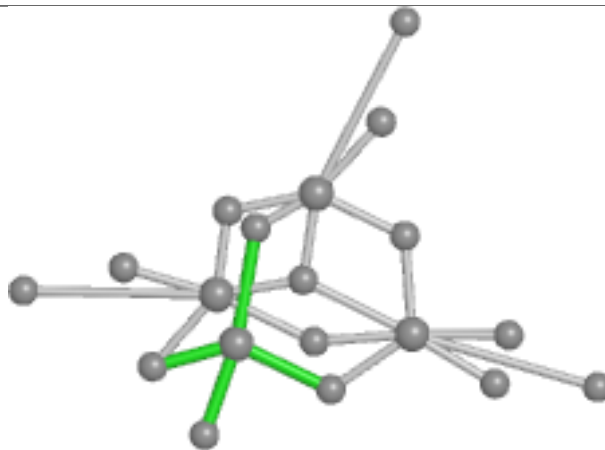
Ligand ZRC I 400



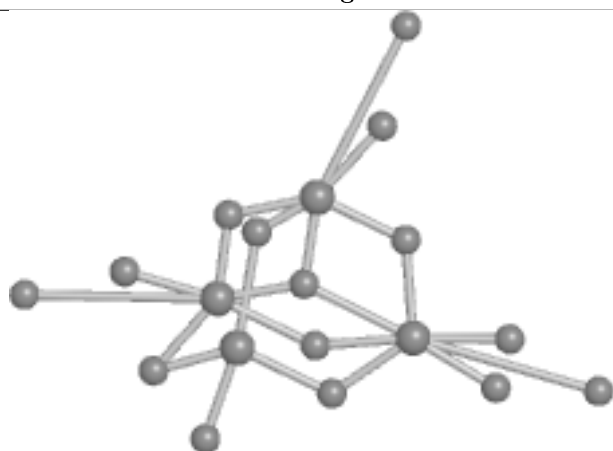
Ligand ZRC C 400



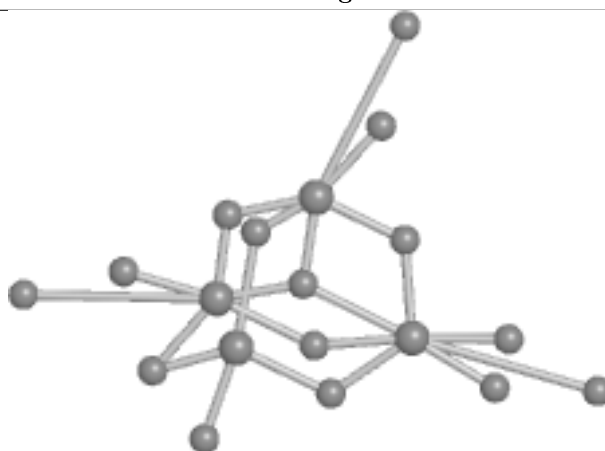
Bond lengths



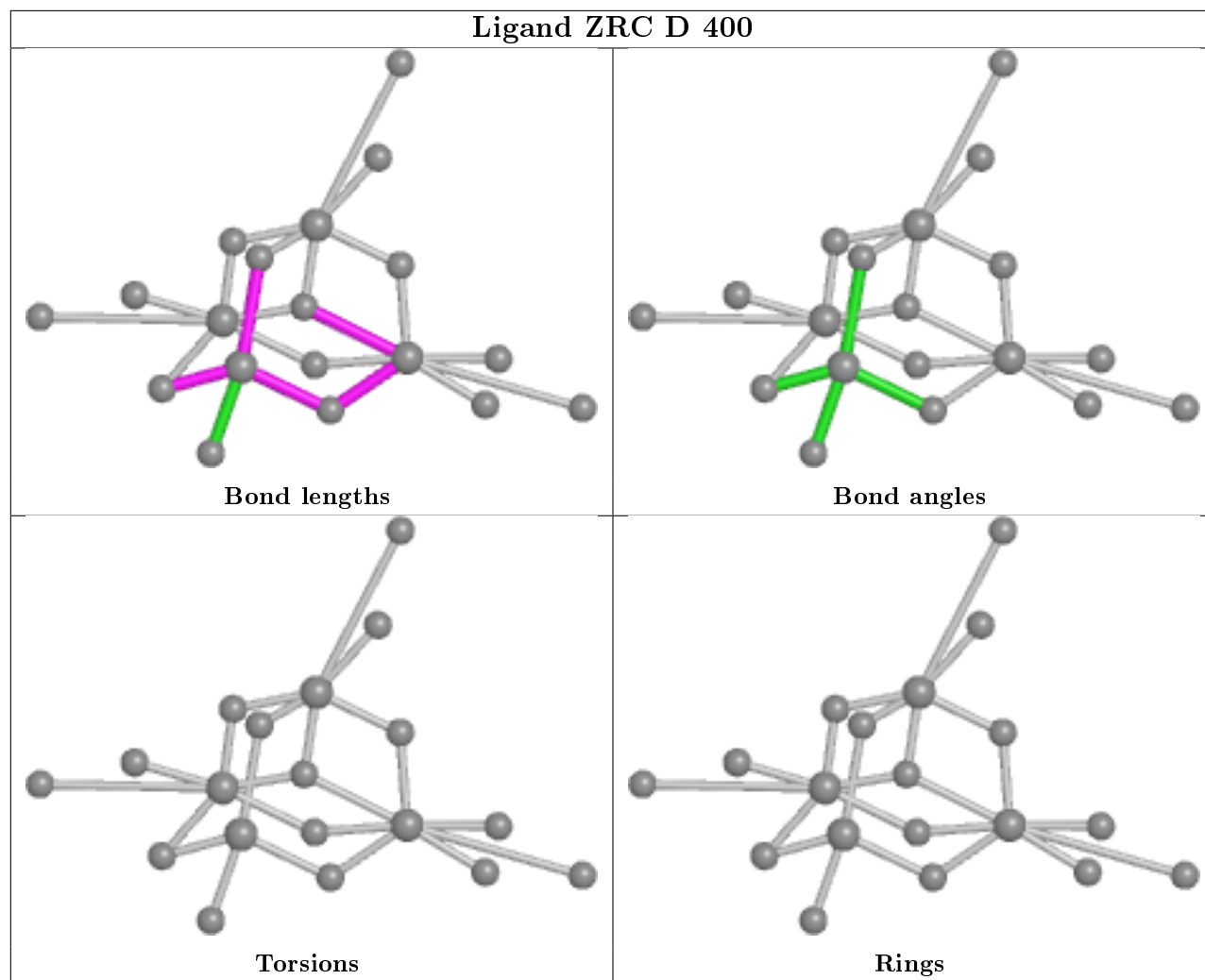
Bond angles



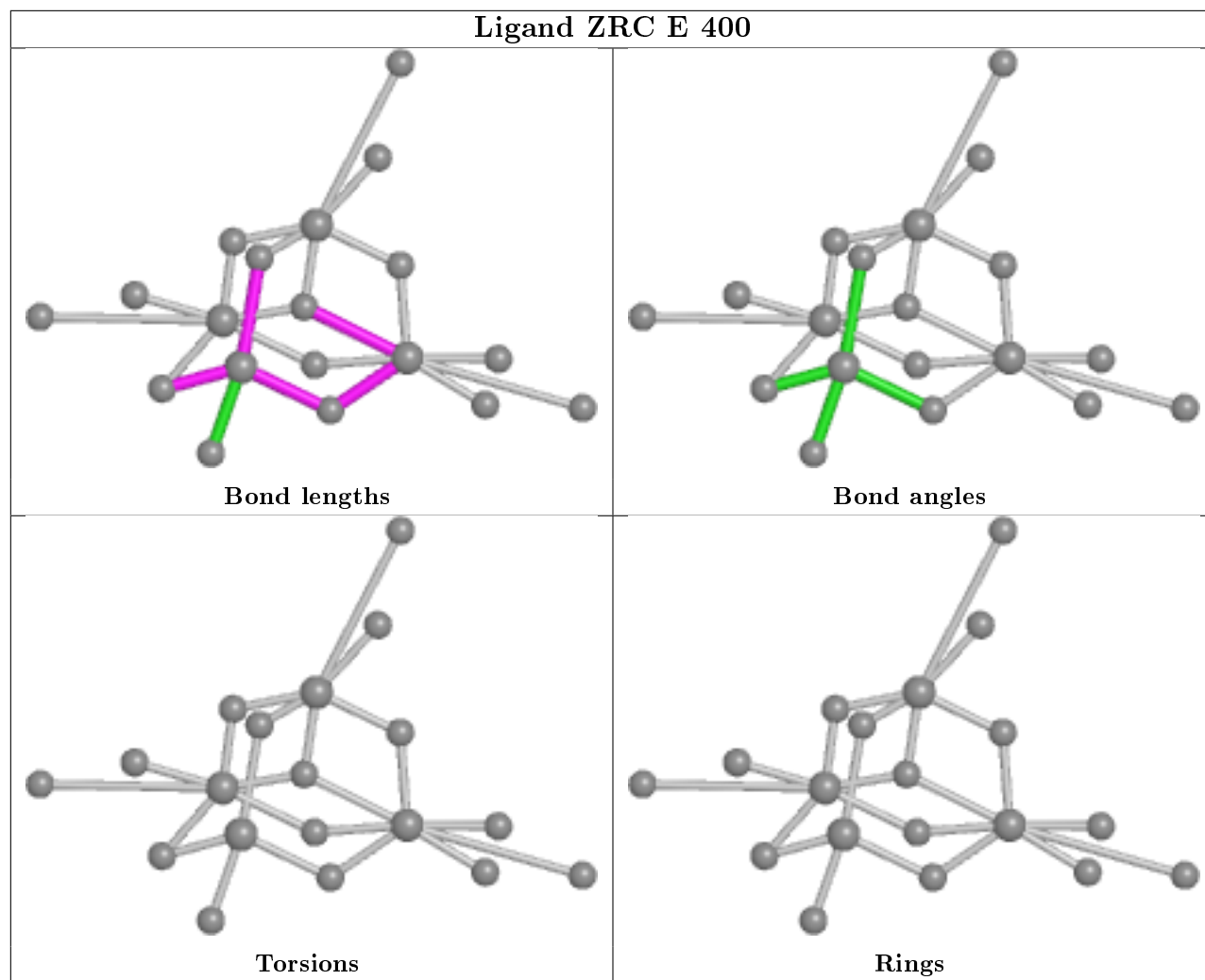
Torsions



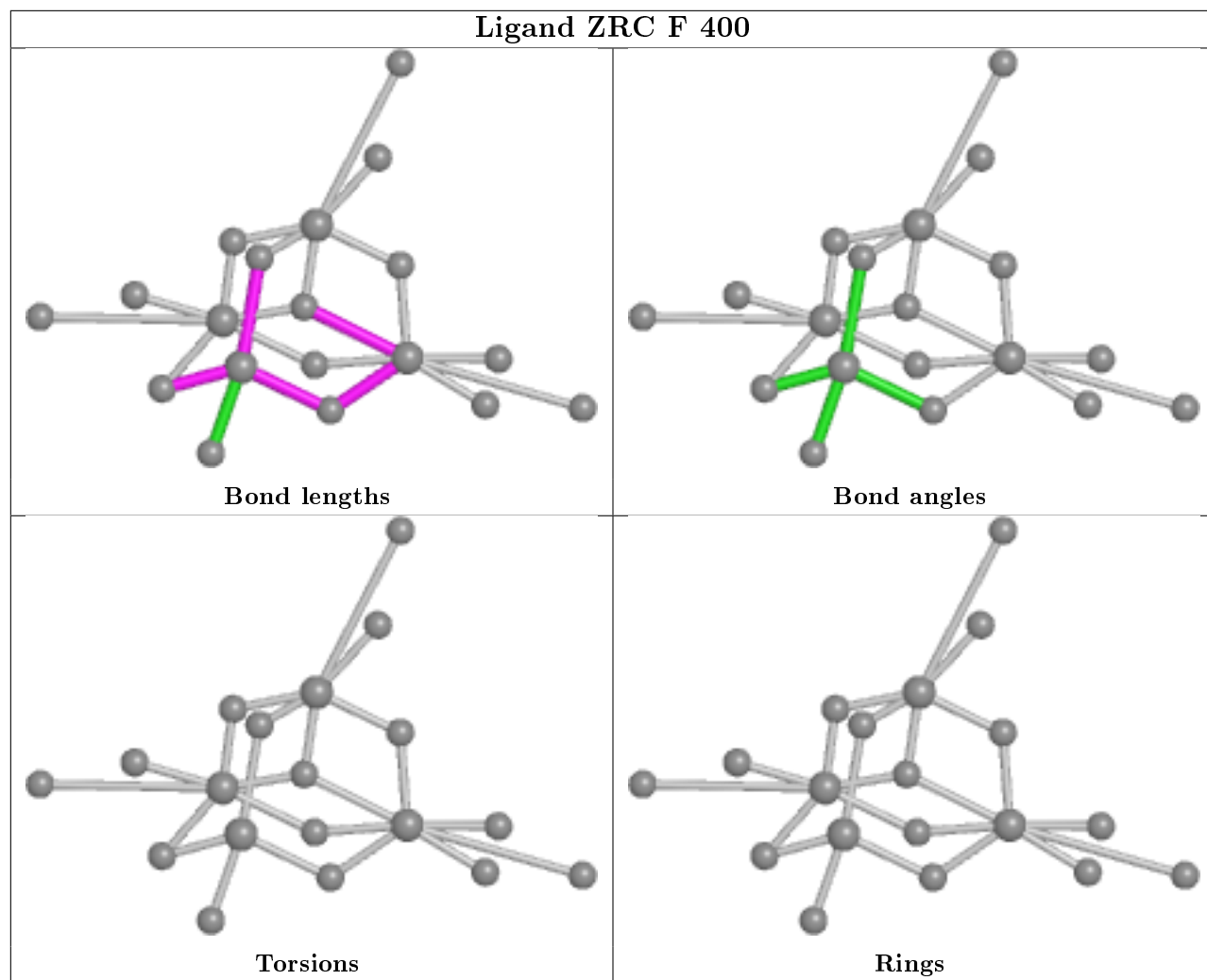
Rings



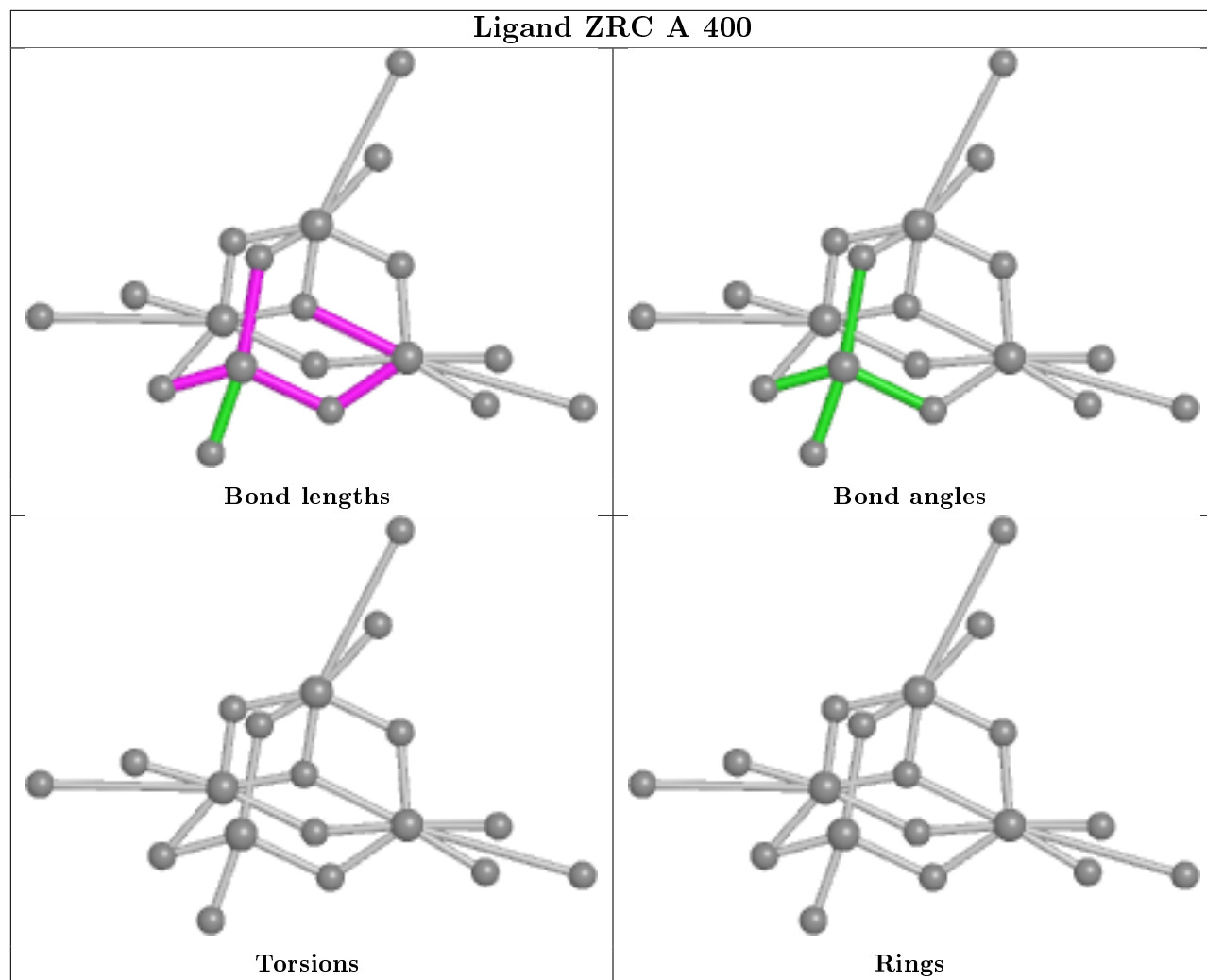
Ligand ZRC E 400

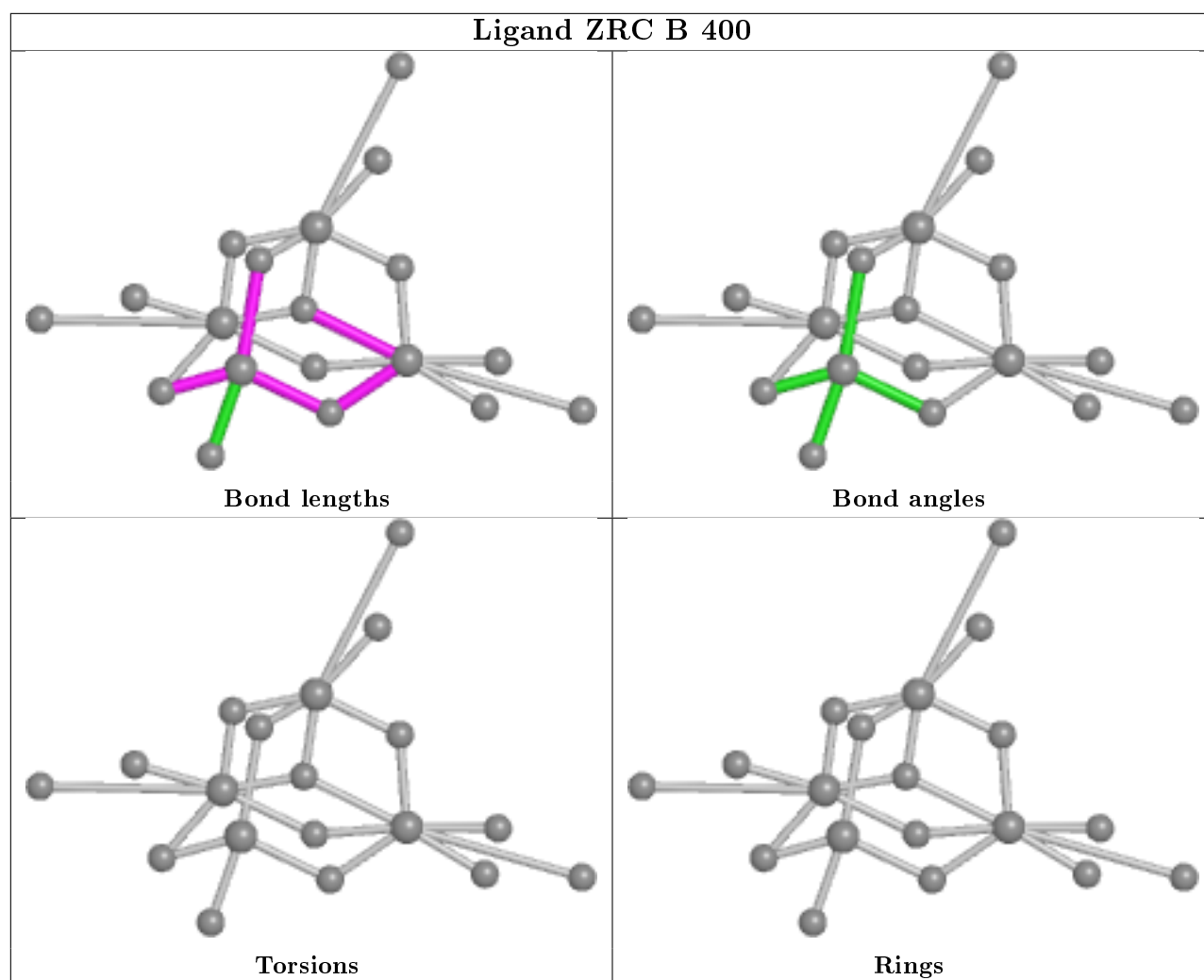


Ligand ZRC F 400



Ligand ZRC A 400





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.