



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 01:39 PM EDT

PDB ID : 1XC1 / pdb_00001xc1
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

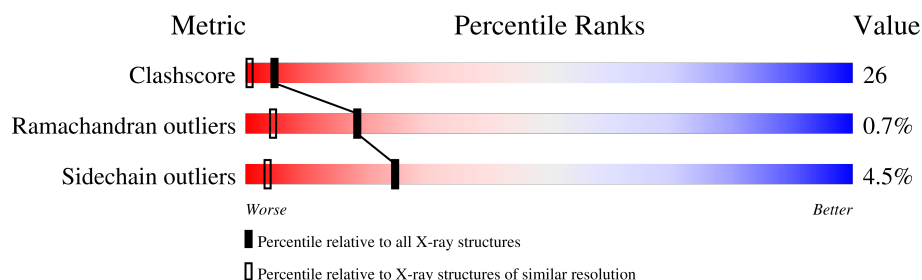
1 Overall quality at a glance

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	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (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 of 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	63% 33% .
1	B	309	61% 36% ..
1	C	309	52% 41% 6%
1	D	309	53% 42% 5%
1	E	309	68% 30% .
1	F	309	63% 33% .
1	G	309	54% 43% .
1	H	309	53% 42% .

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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: green (57%), yellow (38%), and orange (5%). The percentages are labeled below the segments.

2 Entry composition

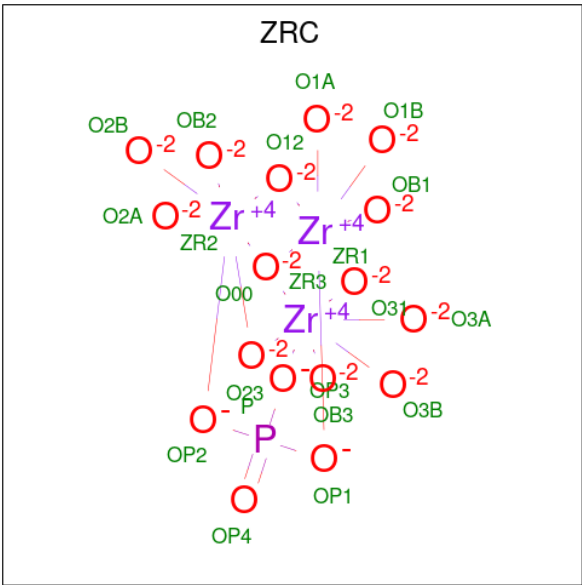
There are 3 unique types of molecules in this entry. The entry contains 22547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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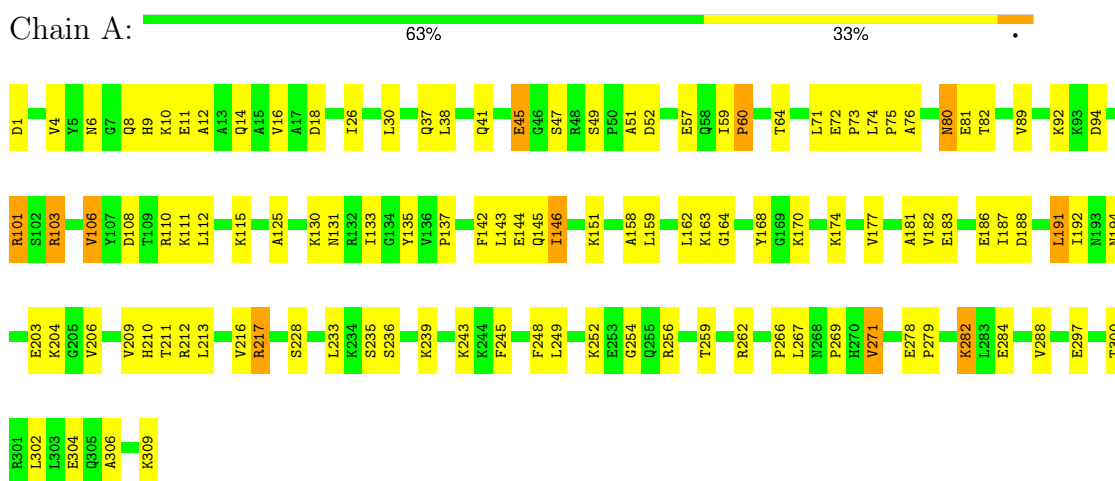
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	113	Total 113	O 113	0	0
3	E	136	Total 136	O 136	0	0
3	F	124	Total 124	O 124	0	0
3	G	79	Total 79	O 79	0	0
3	H	81	Total 81	O 81	0	0
3	I	85	Total 85	O 85	0	0

3 Residue-property plots

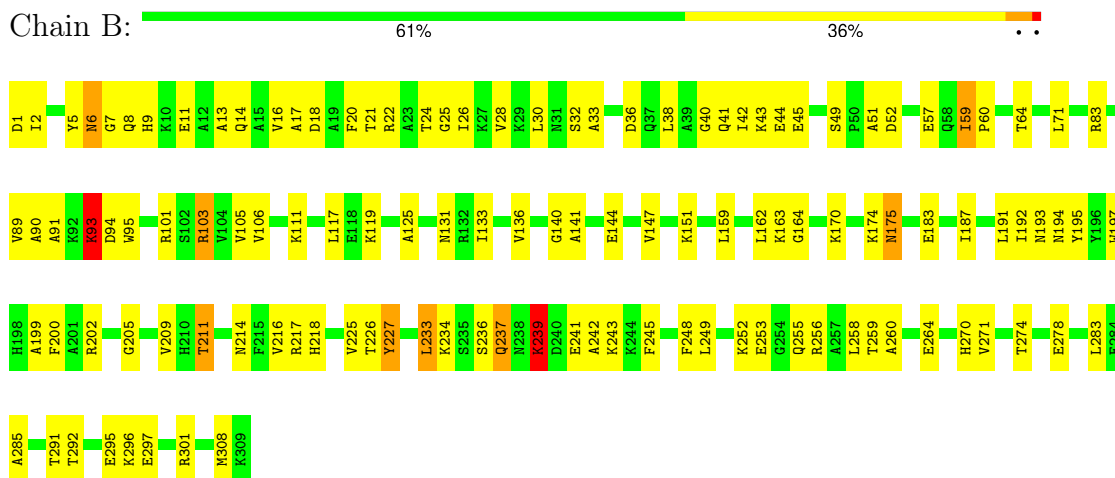
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: periplasmic iron-binding protein

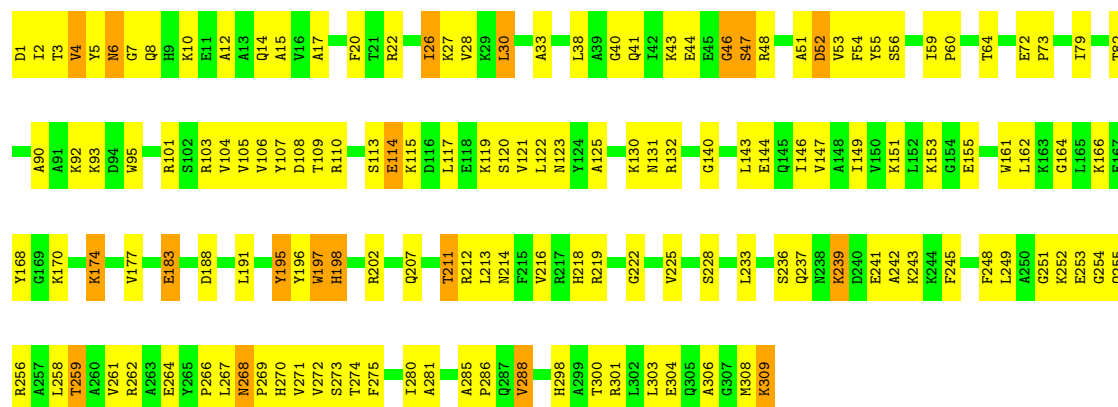


- Molecule 1: periplasmic iron-binding protein



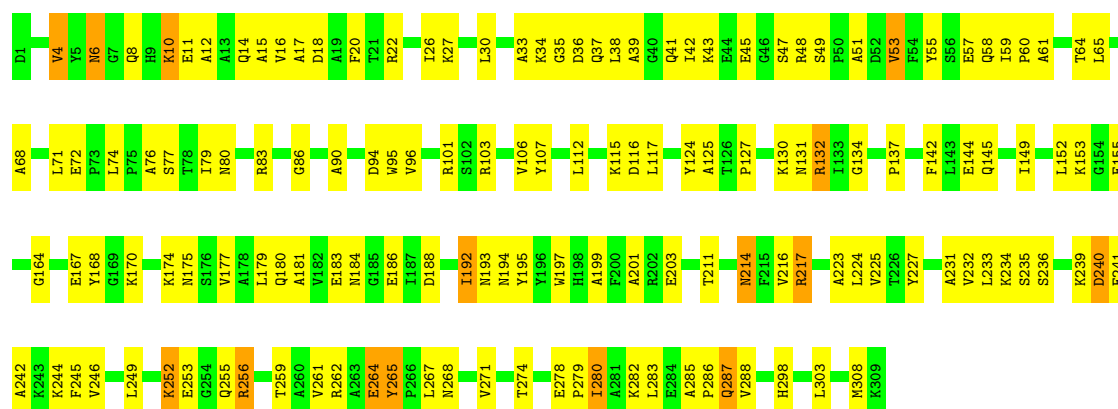
- Molecule 1: periplasmic iron-binding protein





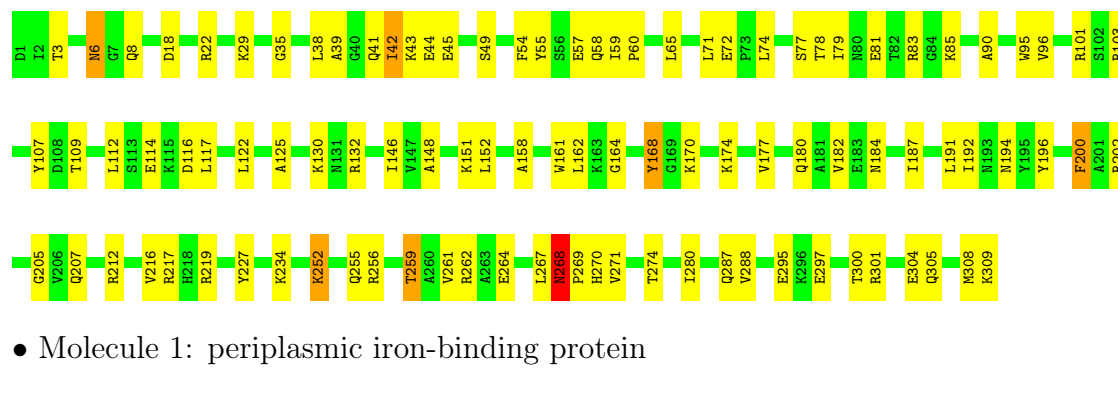
- Molecule 1: periplasmic iron-binding protein

Chain D: 53% 42% 5%



- Molecule 1: periplasmic iron-binding protein

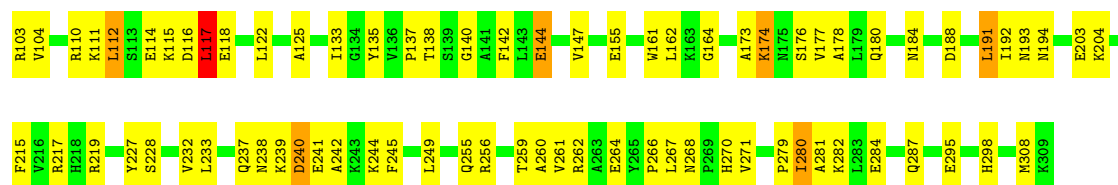
Chain E: 68% 30% 2%



- Molecule 1: periplasmic iron-binding protein

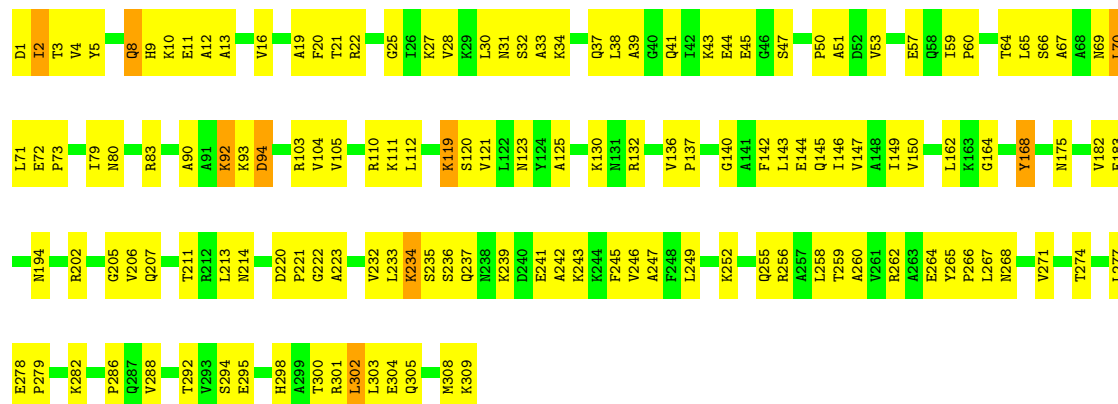
Chain F: 63% 33% 4%





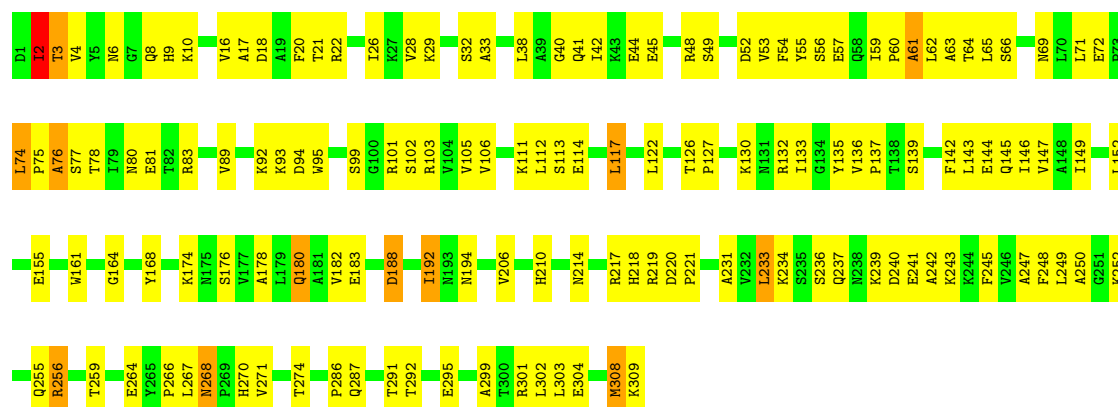
- Molecule 1: periplasmic iron-binding protein

Chain G: 54% 43% .



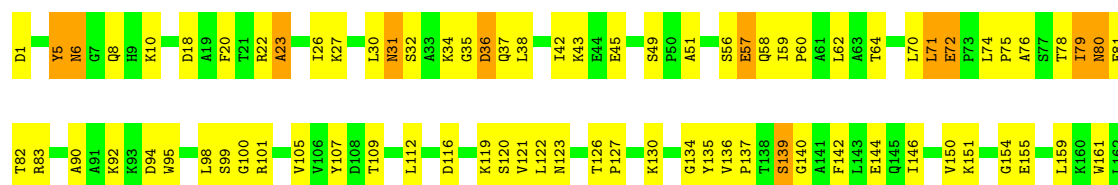
- Molecule 1: periplasmic iron-binding protein

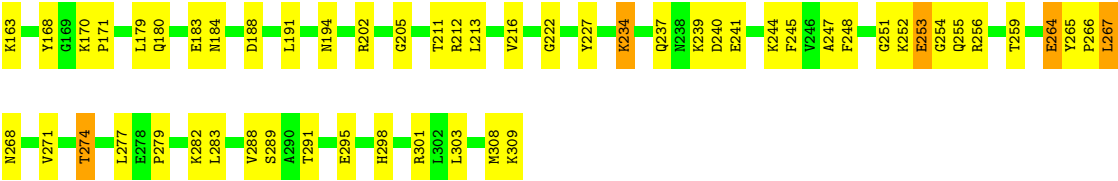
Chain H: 53% 42% .



- Molecule 1: periplasmic iron-binding protein

Chain I: 57% 38% 5%





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	0.47	0/2423	0.98	7/3280 (0.2%)
1	B	0.44	0/2423	1.00	9/3280 (0.3%)
1	C	0.52	2/2423 (0.1%)	0.99	5/3280 (0.2%)
1	D	0.43	0/2423	0.95	8/3280 (0.2%)
1	E	0.47	0/2423	0.97	10/3280 (0.3%)
1	F	0.47	0/2423	0.98	9/3280 (0.3%)
1	G	0.40	0/2423	1.00	13/3280 (0.4%)
1	H	0.42	0/2423	1.00	12/3280 (0.4%)
1	I	0.43	0/2423	0.99	11/3280 (0.3%)
All	All	0.45	2/21807 (0.0%)	0.98	84/29520 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	HIS	N-CA	-7.61	1.37	1.46
1	C	197	TRP	C-N	-5.23	1.27	1.33

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	ASN	N-CA-C	8.82	120.51	111.07
1	I	194	ASN	N-CA-C	8.38	120.11	110.97
1	D	265	TYR	N-CA-C	7.30	119.11	109.83
1	H	194	ASN	N-CA-C	7.30	118.88	111.07
1	B	283	LEU	N-CA-C	-7.28	104.38	113.18

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	101	0
1	B	2378	0	2424	105	0
1	C	2378	0	2424	152	0
1	D	2378	0	2424	149	0
1	E	2378	0	2424	94	0
1	F	2378	0	2424	101	0
1	G	2378	0	2424	141	0
1	H	2378	0	2424	143	0
1	I	2378	0	2424	130	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	1111	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 26.

The worst 5 of 1111 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

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	307/309 (99%)	288 (94%)	19 (6%)	0	100	100
1	B	307/309 (99%)	288 (94%)	17 (6%)	2 (1%)	18	4
1	C	307/309 (99%)	283 (92%)	20 (6%)	4 (1%)	9	1
1	D	307/309 (99%)	291 (95%)	14 (5%)	2 (1%)	18	4
1	E	307/309 (99%)	291 (95%)	12 (4%)	4 (1%)	9	1
1	F	307/309 (99%)	292 (95%)	13 (4%)	2 (1%)	18	4
1	G	307/309 (99%)	281 (92%)	23 (8%)	3 (1%)	12	2
1	H	307/309 (99%)	287 (94%)	18 (6%)	2 (1%)	18	4
1	I	307/309 (99%)	291 (95%)	15 (5%)	1 (0%)	36	18
All	All	2763/2781 (99%)	2592 (94%)	151 (6%)	20 (1%)	18	4

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 ⓘ

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%)	232 (95%)	13 (5%)	20	2
1	B	245/245 (100%)	233 (95%)	12 (5%)	22	3
1	C	245/245 (100%)	232 (95%)	13 (5%)	20	2
1	D	245/245 (100%)	234 (96%)	11 (4%)	24	3
1	E	245/245 (100%)	237 (97%)	8 (3%)	33	7
1	F	245/245 (100%)	234 (96%)	11 (4%)	24	3
1	G	245/245 (100%)	236 (96%)	9 (4%)	30	6
1	H	245/245 (100%)	236 (96%)	9 (4%)	30	6
1	I	245/245 (100%)	231 (94%)	14 (6%)	18	2
All	All	2205/2205 (100%)	2105 (96%)	100 (4%)	24	3

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	8	GLN
1	G	168	TYR
1	I	301	ARG
1	F	60	PRO
1	F	240	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	37	GLN
1	H	9	HIS
1	G	69	ASN
1	G	237	GLN
1	H	41	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	I	400	1	13,23,25	3.51	8 (61%)	3,66,78	0.19	0
2	ZRC	B	400	1	13,23,25	3.14	9 (69%)	3,66,78	0.23	0
2	ZRC	F	400	1	13,23,25	4.58	9 (69%)	3,66,78	0.29	0
2	ZRC	E	400	1	13,23,25	3.25	8 (61%)	3,66,78	0.31	0
2	ZRC	G	400	1	13,23,25	3.83	7 (53%)	3,66,78	0.23	0
2	ZRC	A	400	1	13,23,25	3.29	9 (69%)	3,66,78	0.25	0
2	ZRC	H	400	1	13,23,25	3.62	8 (61%)	3,66,78	0.21	0
2	ZRC	D	400	1	13,23,25	3.82	9 (69%)	3,66,78	0.27	0
2	ZRC	C	400	1	13,23,25	3.84	11 (84%)	3,66,78	0.23	0

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	ZRC	ZR2-O23	8.79	2.37	2.11
2	H	400	ZRC	ZR2-O12	8.65	2.36	2.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	400	ZRC	ZR2-O12	8.33	2.35	2.11
2	D	400	ZRC	ZR2-O23	8.02	2.34	2.11
2	F	400	ZRC	ZR2-OP2	7.96	2.43	2.10

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

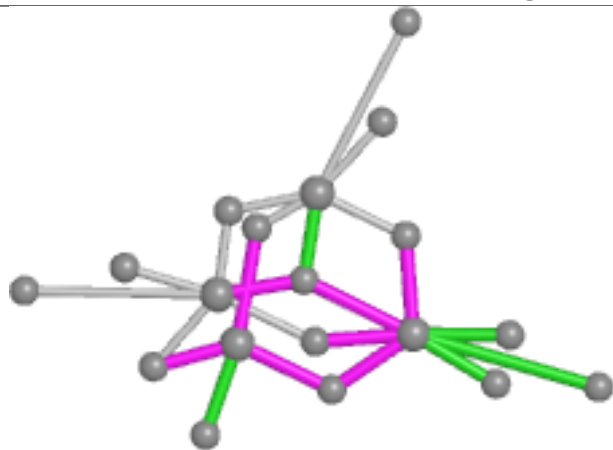
There are no ring outliers.

5 monomers are involved in 6 short contacts:

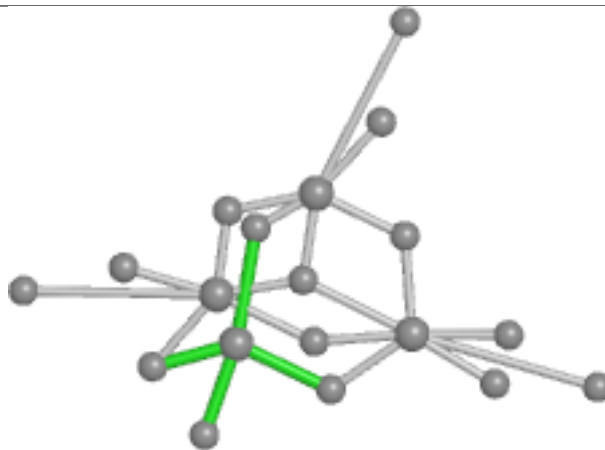
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	400	ZRC	1	0
2	B	400	ZRC	1	0
2	H	400	ZRC	1	0
2	D	400	ZRC	2	0
2	C	400	ZRC	1	0

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.

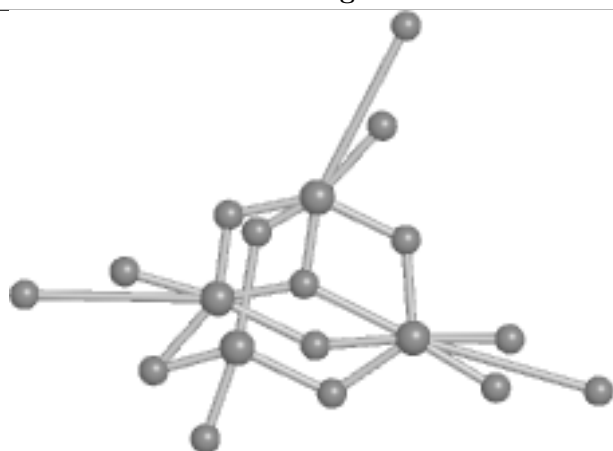
Ligand ZRC I 400



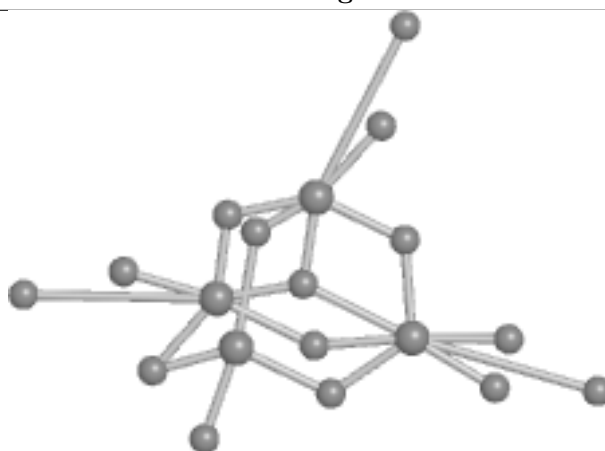
Bond lengths



Bond angles

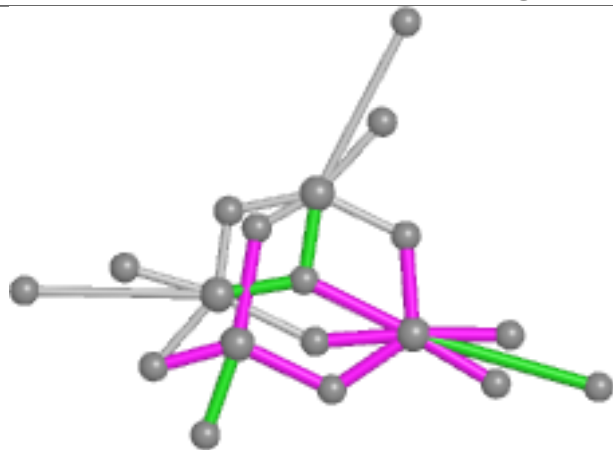


Torsions

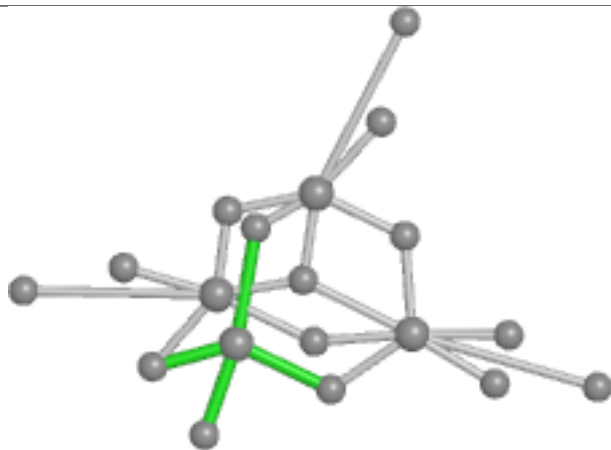


Rings

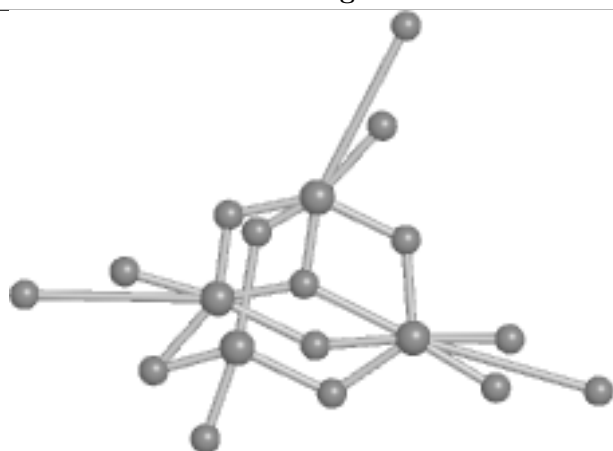
Ligand ZRC B 400



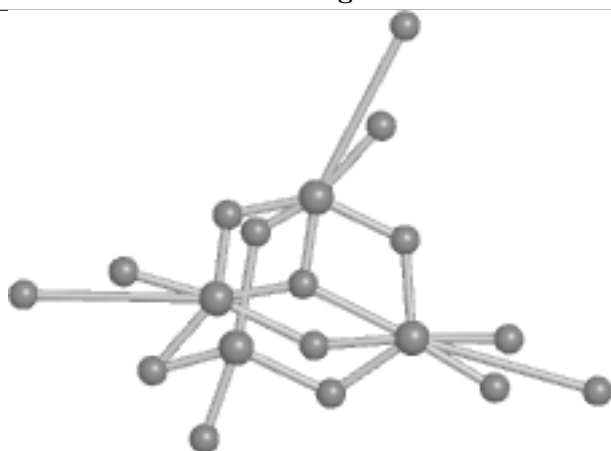
Bond lengths



Bond angles

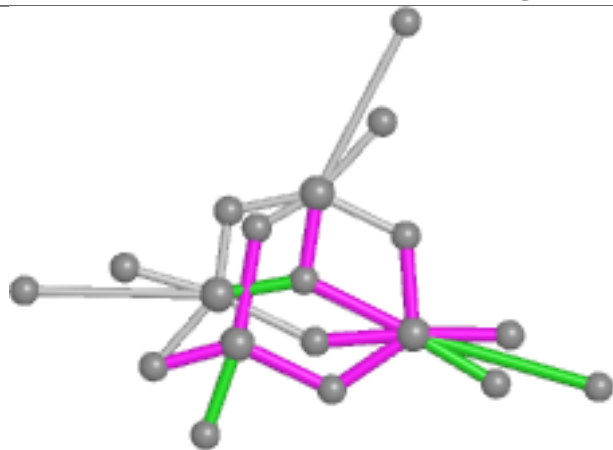


Torsions

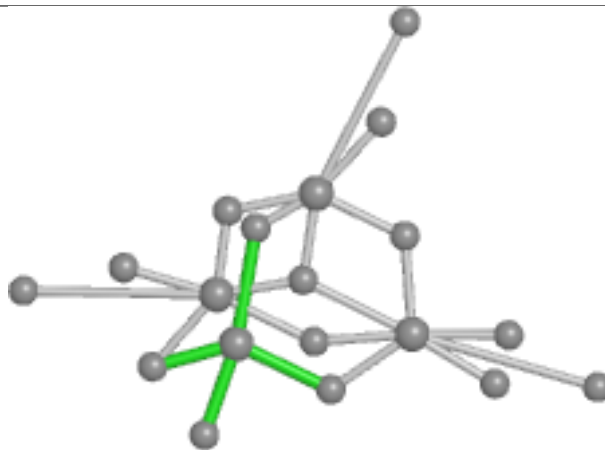


Rings

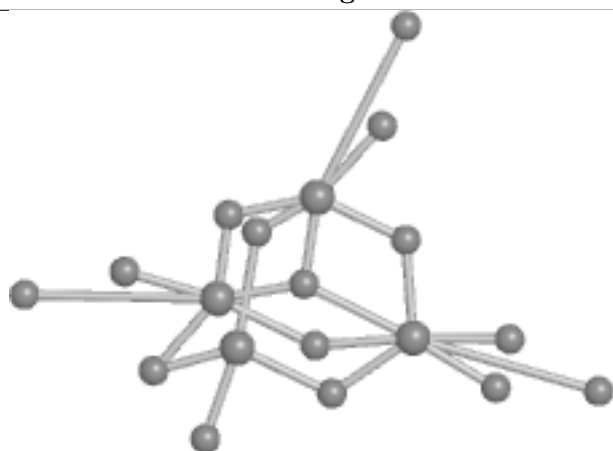
Ligand ZRC F 400



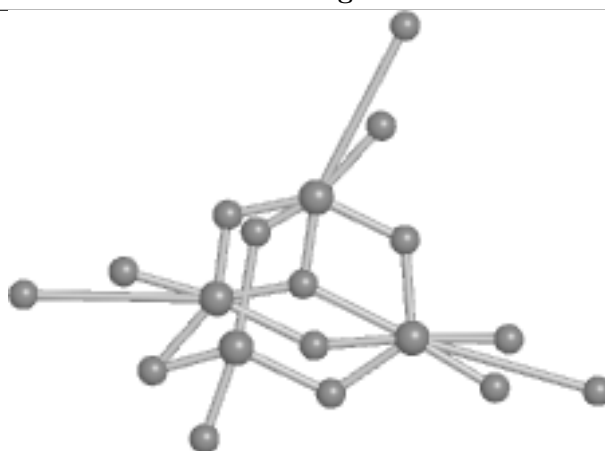
Bond lengths



Bond angles

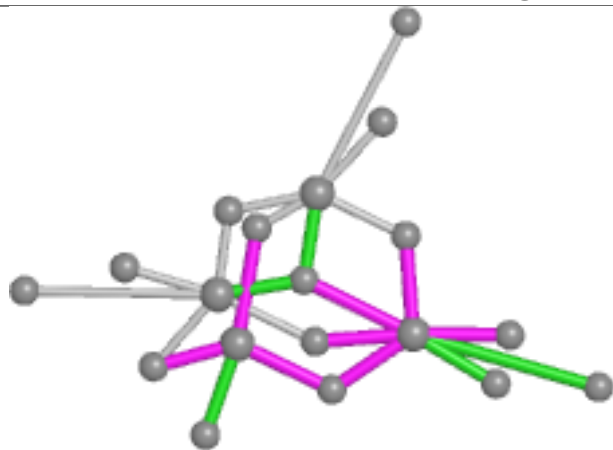


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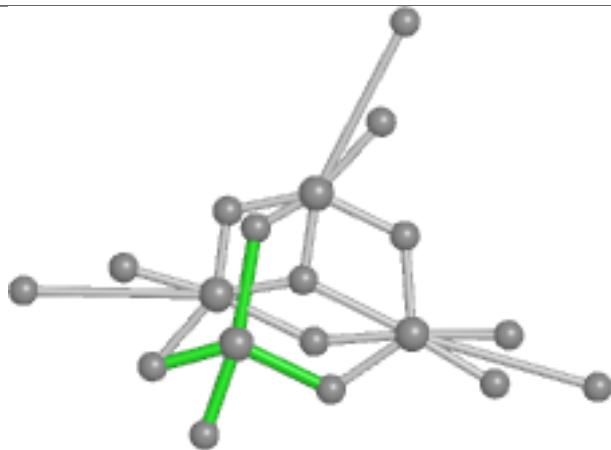


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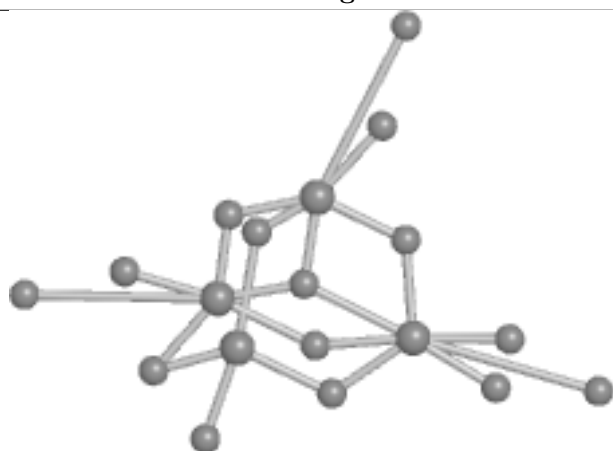
Ligand ZRC E 400



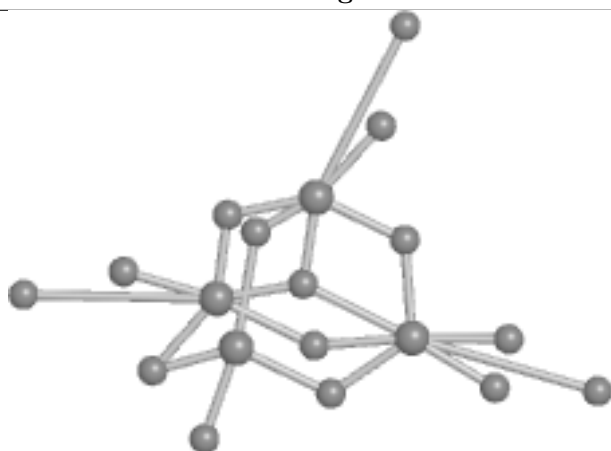
Bond lengths



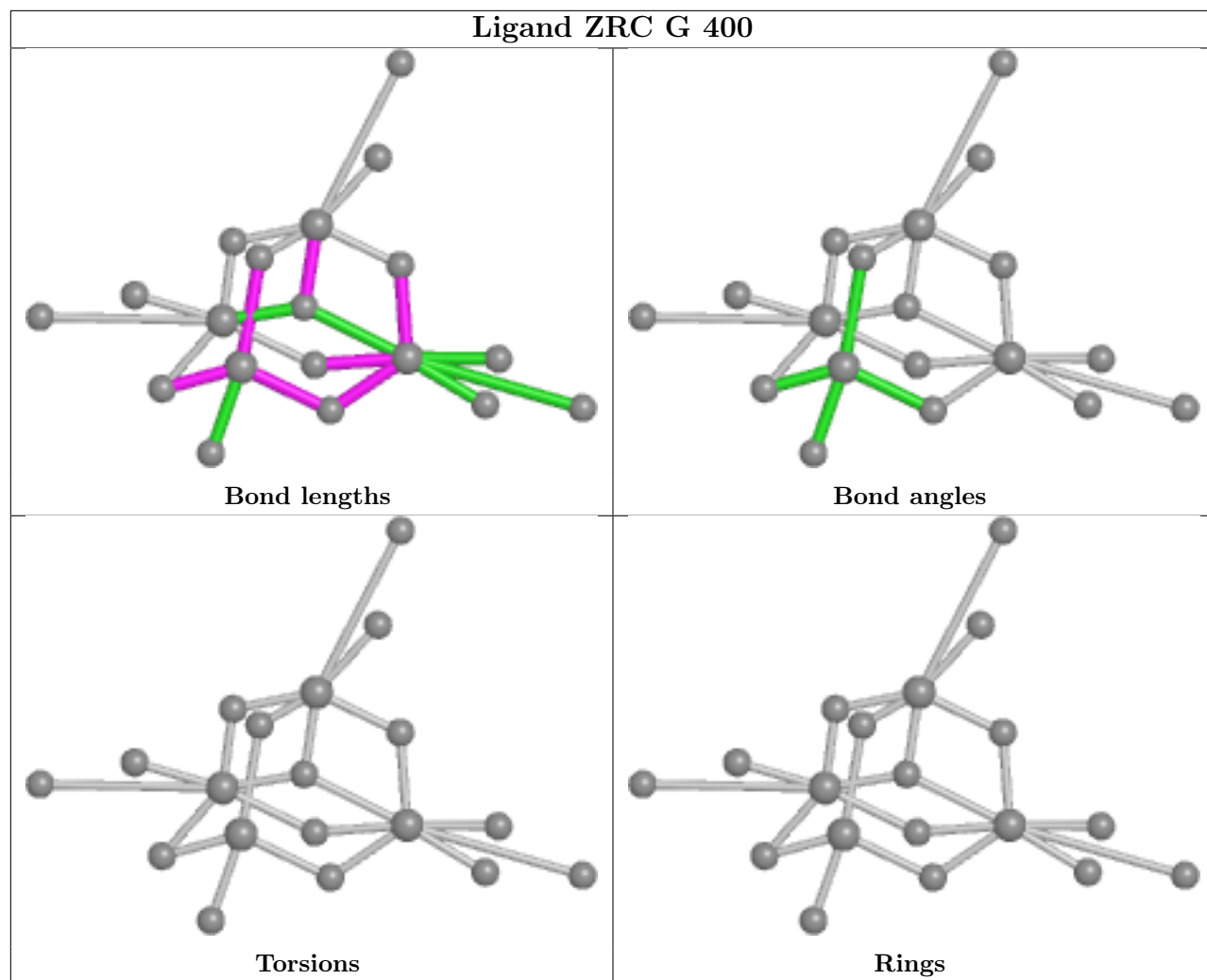
Bond angles



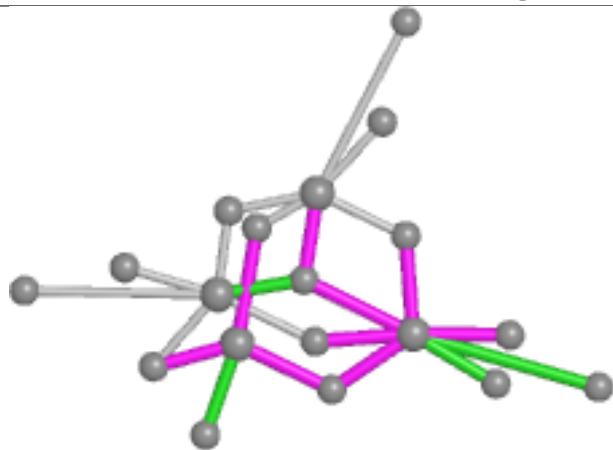
Torsions



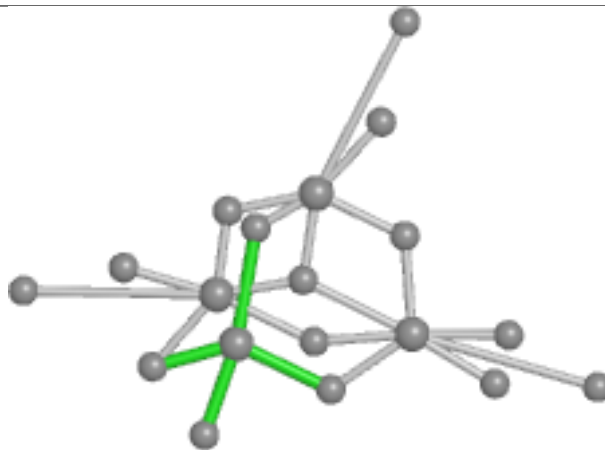
Rings



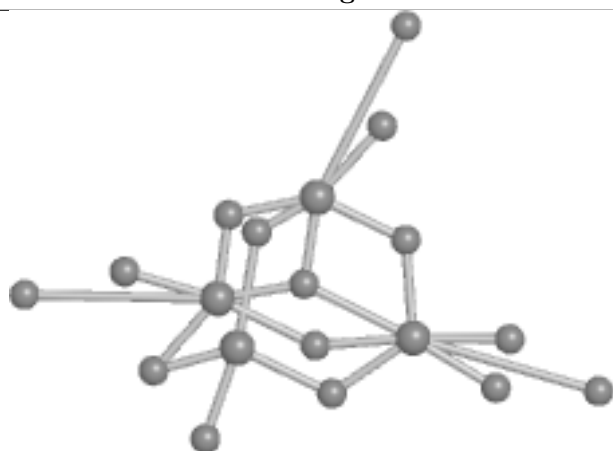
Ligand ZRC A 400



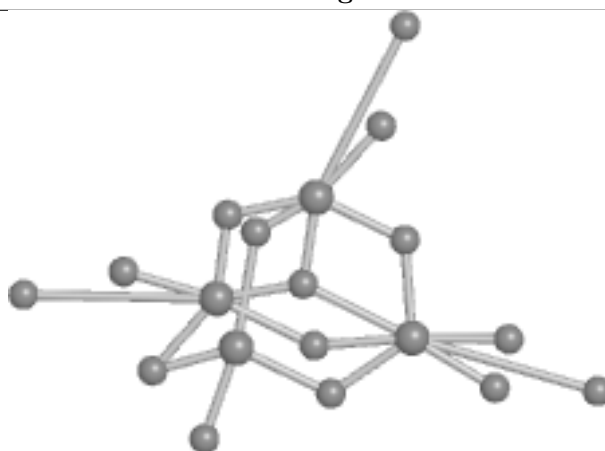
Bond lengths



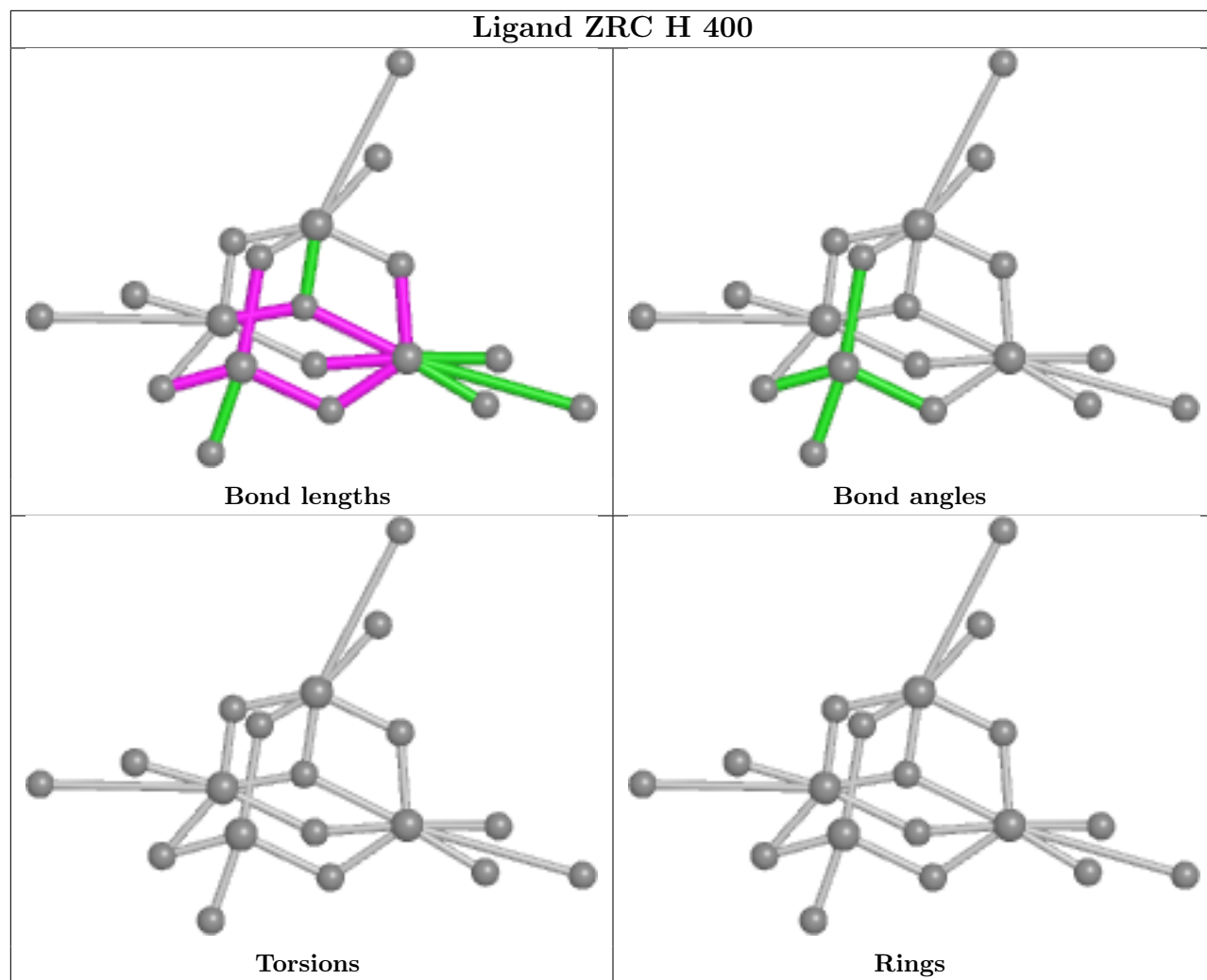
Bond angles

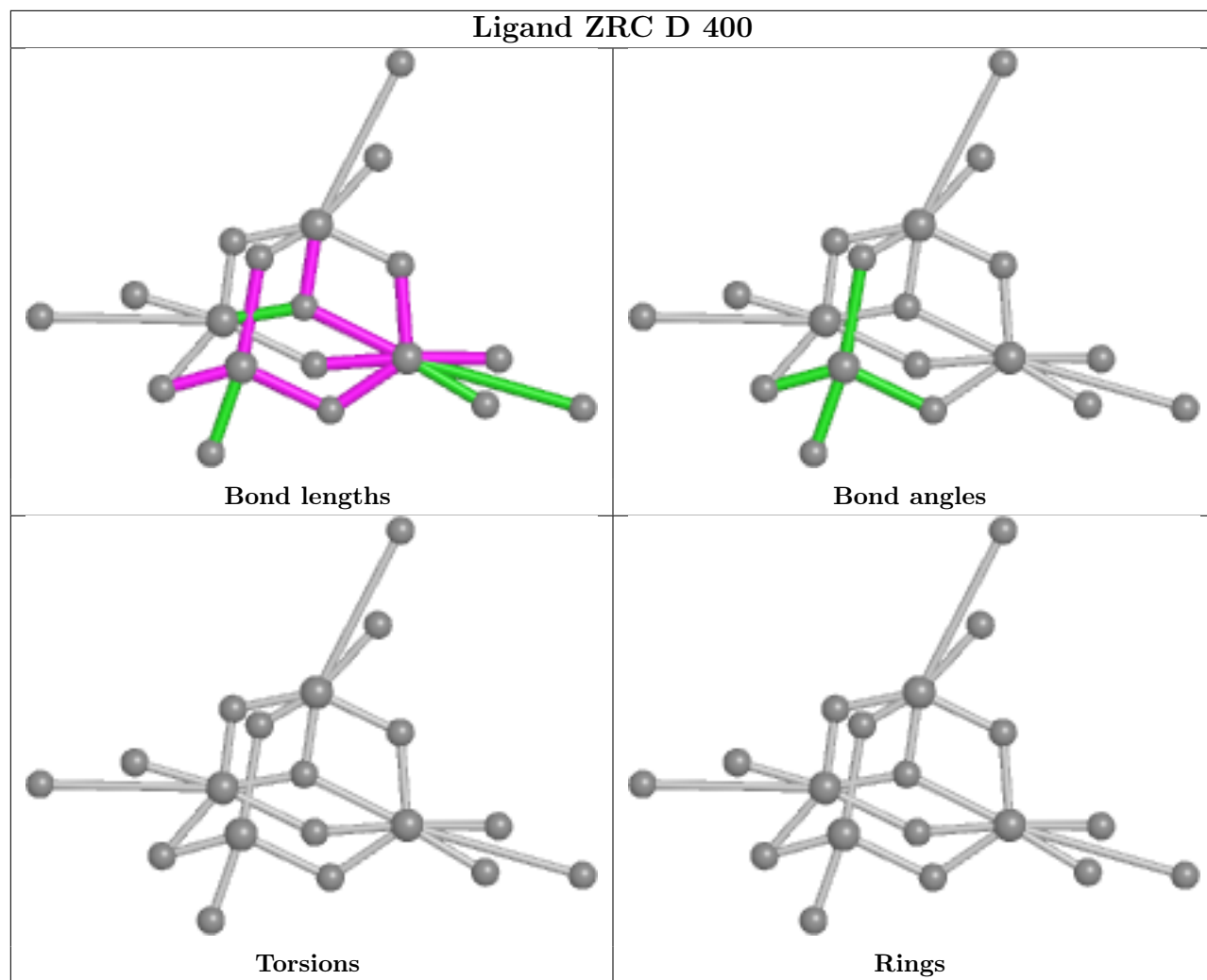


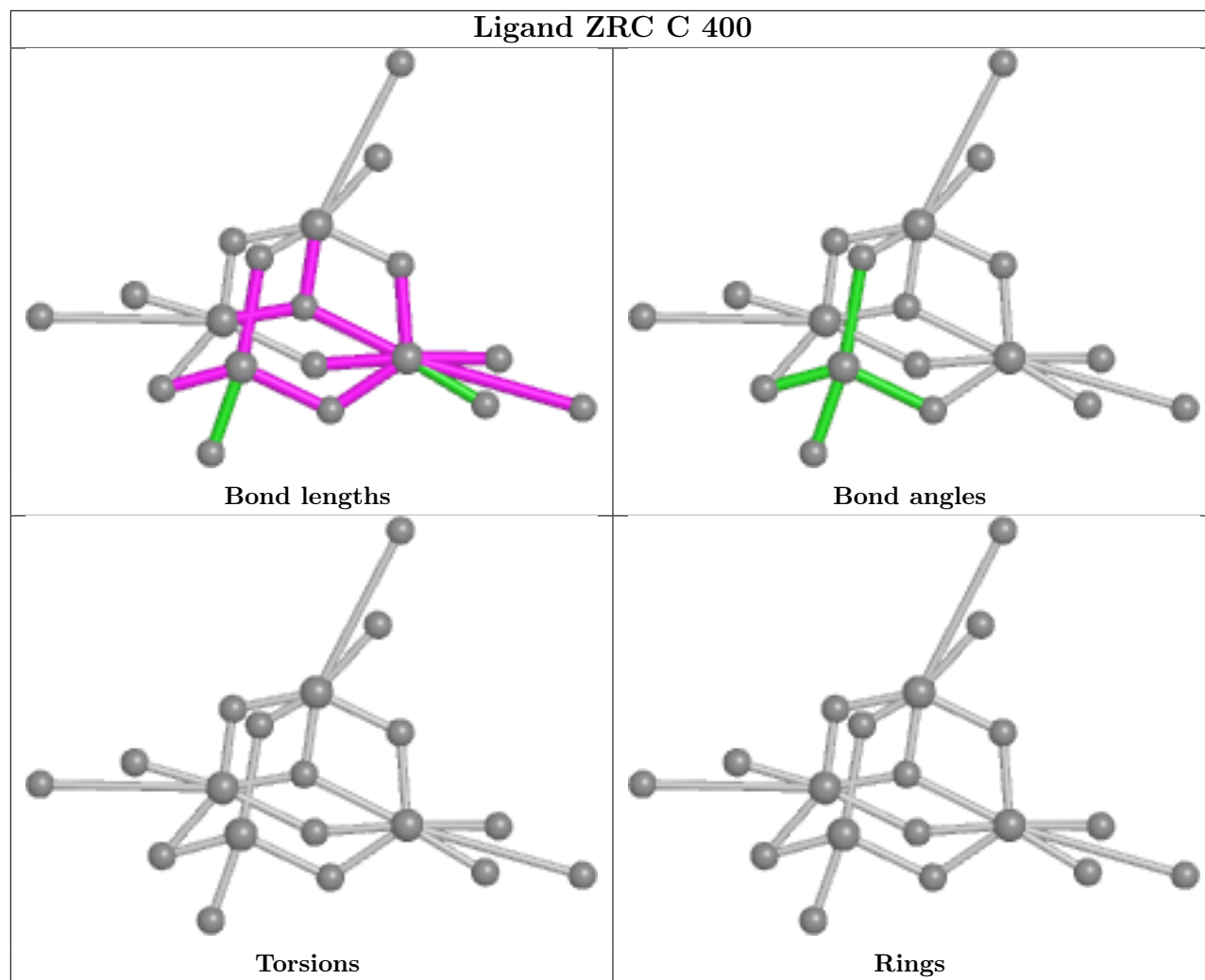
Torsions



Rings







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.