



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 09:29 am BST

PDB ID : 1R1N
Title : Tri-nuclear oxo-iron clusters in the ferric binding protein from *N. gonorrhoeae*
Authors : Zhu, H.; Alexeev, D.; Hunter, D.J.; Campopiano, D.J.; Sadler, P.J.
Deposited on : 2003-09-24
Resolution : 1.74 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

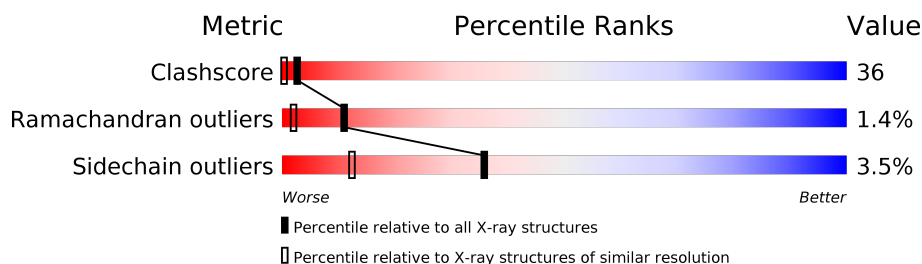
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)


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 chain 1. The bar is divided into two segments: a green segment on the left labeled '46%' and a yellow segment on the right labeled '53%'. A small red dot is at the far right end of the bar.

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
3	CN1	G	400	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24350 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.

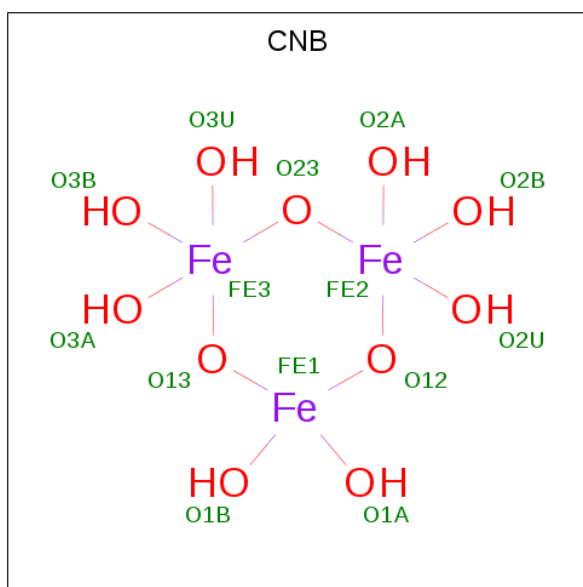
- Molecule 1 is a protein called Ferric-iron Binding Protein.

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			

There are 9 discrepancies between the modelled and reference sequences:

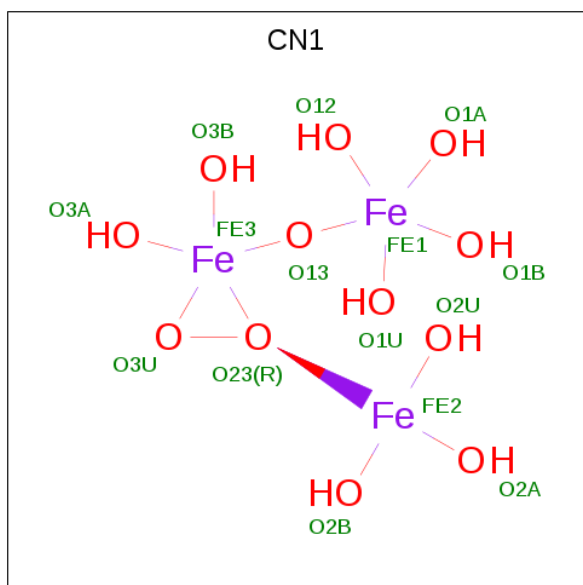
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	VAL	ILE	CONFLICT	UNP P17259
B	87	VAL	ILE	CONFLICT	UNP P17259
C	87	VAL	ILE	CONFLICT	UNP P17259
D	87	VAL	ILE	CONFLICT	UNP P17259
E	87	VAL	ILE	CONFLICT	UNP P17259
F	87	VAL	ILE	CONFLICT	UNP P17259
G	87	VAL	ILE	CONFLICT	UNP P17259
H	87	VAL	ILE	CONFLICT	UNP P17259
I	87	VAL	ILE	CONFLICT	UNP P17259

- Molecule 2 is OXO-IRON CLUSTER 1 (three-letter code: CNB) (formula: Fe₃H₈O₁₁).



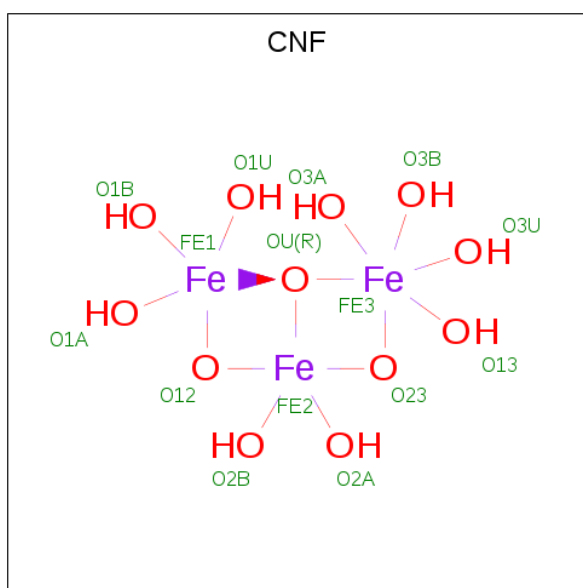
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	O	0	0
			14	3	11		
2	B	1	Total	Fe	O	0	0
			14	3	11		
2	D	1	Total	Fe	O	0	0
			14	3	11		
2	H	1	Total	Fe	O	0	0
			14	3	11		

- Molecule 3 is OXO-IRON CLUSTER 2 (three-letter code: CN1) (formula: $\text{Fe}_3\text{H}_9\text{O}_{12}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	Fe	O	0	0
			15	3	12		
3	E	1	Total	Fe	O	0	0
			15	3	12		
3	G	1	Total	Fe	O	0	0
			15	3	12		
3	I	1	Total	Fe	O	0	0
			15	3	12		

- Molecule 4 is OXO-IRON CLUSTER 3 (three-letter code: CNF) (formula: $\text{Fe}_3\text{H}_9\text{O}_{12}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	Fe	O	0	0
			15	3	12		

- Molecule 5 is water.

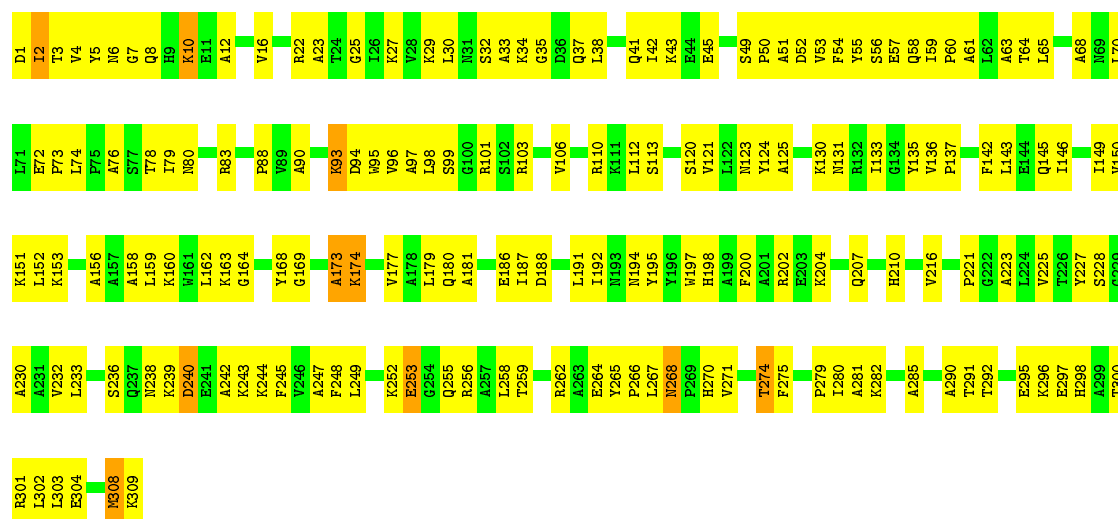
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	367	Total	O	0	0
			367	367		
5	B	323	Total	O	0	0
			323	323		
5	C	298	Total	O	0	0
			298	298		
5	D	291	Total	O	0	0
			291	291		
5	E	331	Total	O	0	0
			331	331		

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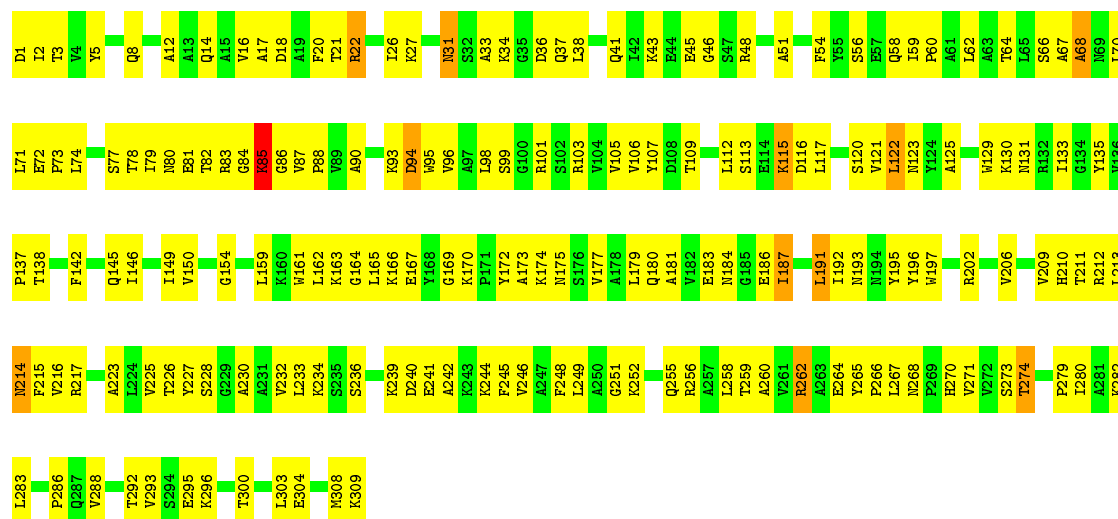
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	301	Total 301	O 301	0	0
5	G	340	Total 340	O 340	0	0
5	H	295	Total 295	O 295	0	0
5	I	271	Total 271	O 271	0	0

Chain C: 



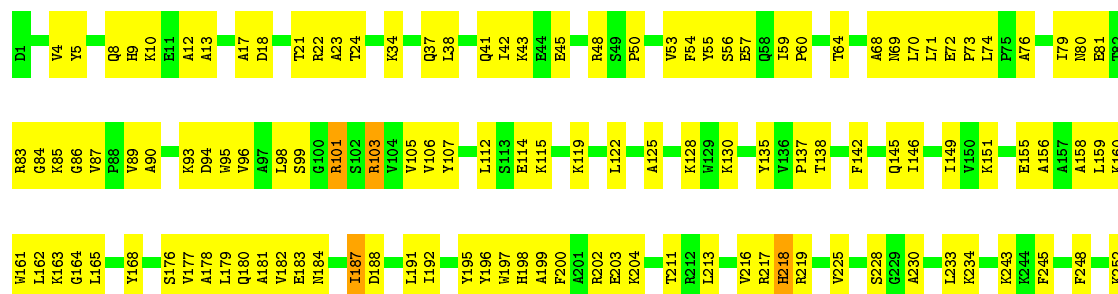
• Molecule 1: Ferric-iron Binding Protein

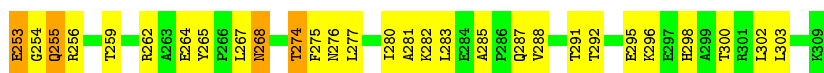
Chain D: 



• Molecule 1: Ferric-iron Binding Protein

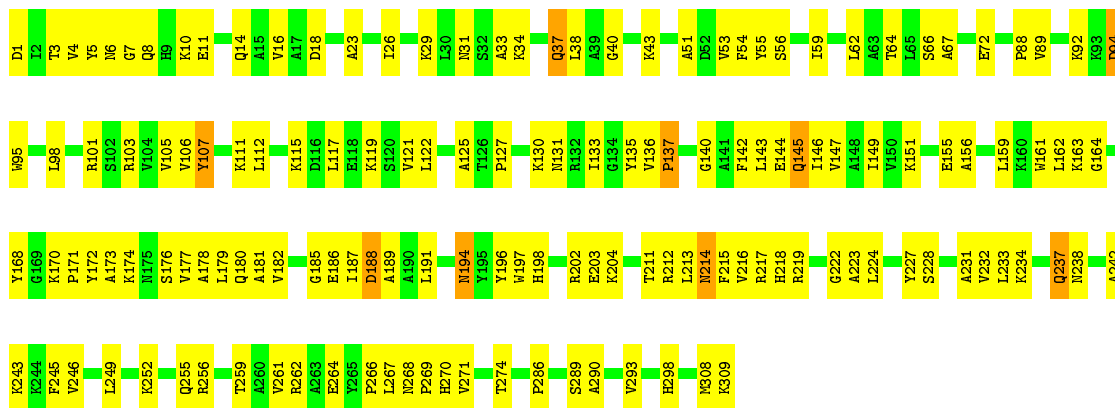
Chain E: 





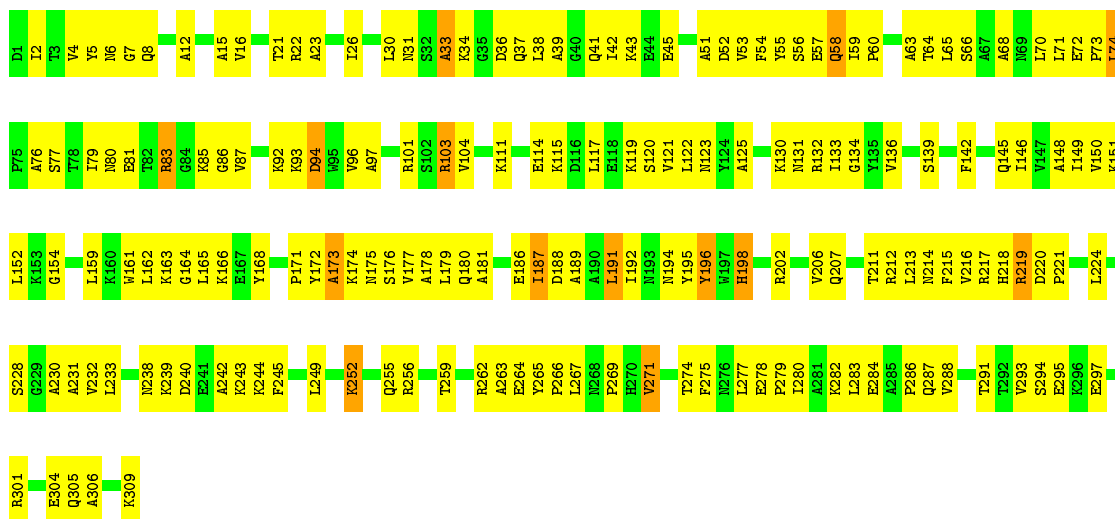
• Molecule 1: Ferric-iron Binding Protein

Chain F: 52% 45%



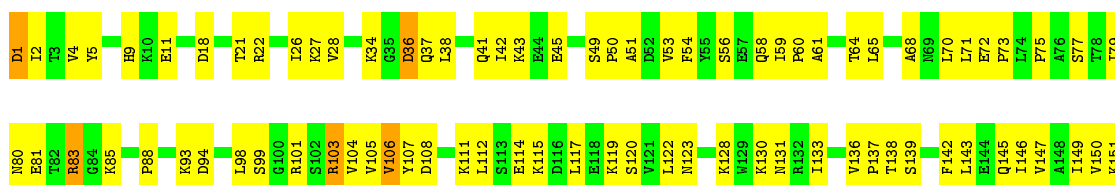
• Molecule 1: Ferric-iron Binding Protein

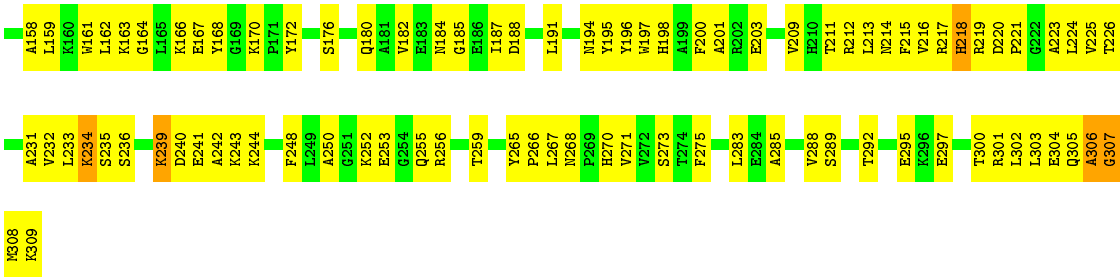
Chain G: 42% 53% 5%



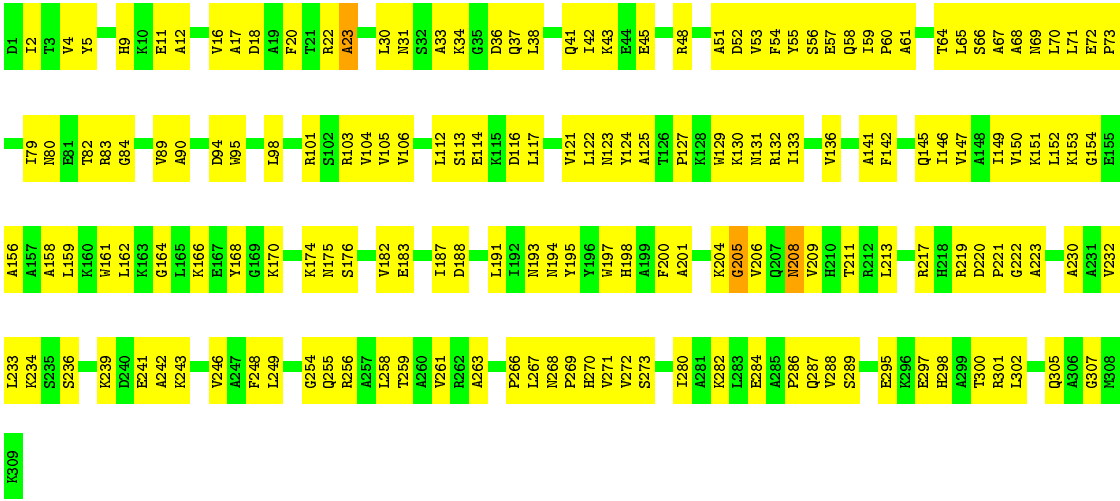
• Molecule 1: Ferric-iron Binding Protein

Chain H: 46% 51%





• Molecule 1: Ferric-iron Binding Protein



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	146.50 Å 146.50 Å 114.97 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.74	Depositor
% Data completeness (in resolution range)	99.0 (30.00-1.74)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.167 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24350	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: CNF, CNB, CN1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/2423	0.59	1/3280 (0.0%)
1	B	0.33	0/2423	0.61	0/3280
1	C	0.33	0/2423	0.56	0/3280
1	D	0.32	0/2423	0.58	0/3280
1	E	0.33	0/2423	0.60	0/3280
1	F	0.31	0/2423	0.58	0/3280
1	G	0.32	0/2423	0.58	1/3280 (0.0%)
1	H	0.32	0/2423	0.58	0/3280
1	I	0.34	0/2423	0.54	0/3280
All	All	0.33	0/21807	0.58	2/29520 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	196	TYR	CB-CG-CD1	6.02	124.61	121.00
1	A	196	TYR	CB-CG-CD1	5.42	124.25	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	123	0
1	B	2378	0	2424	195	0
1	C	2378	0	2425	197	0
1	D	2378	0	2424	216	0
1	E	2378	0	2425	149	0
1	F	2378	0	2425	160	0
1	G	2378	0	2425	197	0
1	H	2378	0	2423	177	0
1	I	2378	0	2425	157	0
2	A	14	0	0	2	0
2	B	14	0	0	2	0
2	D	14	0	0	1	0
2	H	14	0	0	0	0
3	C	15	0	0	2	0
3	E	15	0	0	0	0
3	G	15	0	0	7	0
3	I	15	0	0	2	0
4	F	15	0	0	0	0
5	A	367	0	0	37	0
5	B	323	0	0	43	0
5	C	298	0	0	41	0
5	D	291	0	0	34	0
5	E	331	0	0	40	0
5	F	301	0	0	33	0
5	G	340	0	0	34	0
5	H	295	0	0	36	0
5	I	271	0	0	19	0
All	All	24350	0	21820	1567	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 36.

The worst 5 of 1567 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:H:111:LYS:NZ	1:H:188:ASP:OD1	1.59	1.34
1:G:202:ARG:HH22	1:G:274:THR:HG22	1.08	1.09
1:G:80:ASN:HA	1:G:83:ARG:HG2	1.33	1.07
1:C:202:ARG:HH22	1:C:274:THR:HG23	1.17	1.06
1:F:259:THR:HG21	1:F:266:PRO:HG3	1.31	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%)	289 (94%)	16 (5%)	2 (1%)	22	8
1	B	307/309 (99%)	271 (88%)	31 (10%)	5 (2%)	9	1
1	C	307/309 (99%)	282 (92%)	20 (6%)	5 (2%)	9	1
1	D	307/309 (99%)	268 (87%)	35 (11%)	4 (1%)	12	2
1	E	307/309 (99%)	288 (94%)	18 (6%)	1 (0%)	41	23
1	F	307/309 (99%)	279 (91%)	26 (8%)	2 (1%)	22	8
1	G	307/309 (99%)	271 (88%)	28 (9%)	8 (3%)	5	0
1	H	307/309 (99%)	278 (91%)	23 (8%)	6 (2%)	7	1
1	I	307/309 (99%)	272 (89%)	28 (9%)	7 (2%)	6	1
All	All	2763/2781 (99%)	2498 (90%)	225 (8%)	40 (1%)	11	2

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	10	LYS
1	C	308	MET
1	F	186	GLU
1	H	239	LYS
1	I	23	ALA

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%)	238 (97%)	7 (3%)	42	18
1	B	245/245 (100%)	237 (97%)	8 (3%)	38	14
1	C	245/245 (100%)	236 (96%)	9 (4%)	34	11
1	D	245/245 (100%)	232 (95%)	13 (5%)	22	5
1	E	245/245 (100%)	235 (96%)	10 (4%)	30	9
1	F	245/245 (100%)	235 (96%)	10 (4%)	30	9
1	G	245/245 (100%)	235 (96%)	10 (4%)	30	9
1	H	245/245 (100%)	239 (98%)	6 (2%)	49	26
1	I	245/245 (100%)	240 (98%)	5 (2%)	55	33
All	All	2205/2205 (100%)	2127 (96%)	78 (4%)	36	12

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	262	ARG
1	E	253	GLU
1	H	234	LYS
1	D	274	THR
1	E	103	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	255	GLN
1	F	31	ASN
1	I	123	ASN
1	D	268	ASN
1	E	123	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
3	CN1	G	400	1	0,15,15	0.00	-	-		
3	CN1	C	400	1	0,15,15	0.00	-	-		
4	CNF	F	400	1	5,16,16	0.28	0	-		
3	CN1	I	400	1	0,15,15	0.00	-	-		
2	CNB	B	400	1	4,14,14	5.68	4 (100%)	-		
2	CNB	A	400	1	4,14,14	5.71	4 (100%)	-		
2	CNB	H	400	1	4,14,14	5.67	4 (100%)	-		
2	CNB	D	400	1	4,14,14	5.74	4 (100%)	-		
3	CN1	E	400	1	0,15,15	0.00	-	-		

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
3	CN1	G	400	1	-	-	0/1/1/1
3	CN1	C	400	1	-	-	0/1/1/1
4	CNF	F	400	1	-	-	0/2/2/2
3	CN1	I	400	1	-	-	0/1/1/1
2	CNB	B	400	1	-	-	0/0/1/1
2	CNB	A	400	1	-	-	0/0/1/1
2	CNB	H	400	1	-	-	0/0/1/1
2	CNB	D	400	1	-	-	0/0/1/1
3	CN1	E	400	1	-	-	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	CNB	O23-FE2	5.83	2.10	1.92
2	D	400	CNB	O23-FE3	5.83	2.10	1.92
2	A	400	CNB	O12-FE2	5.78	2.10	1.92
2	H	400	CNB	O12-FE2	5.77	2.10	1.92
2	A	400	CNB	O23-FE2	5.71	2.10	1.92

There are no bond angle outliers.

There are no chirality outliers.

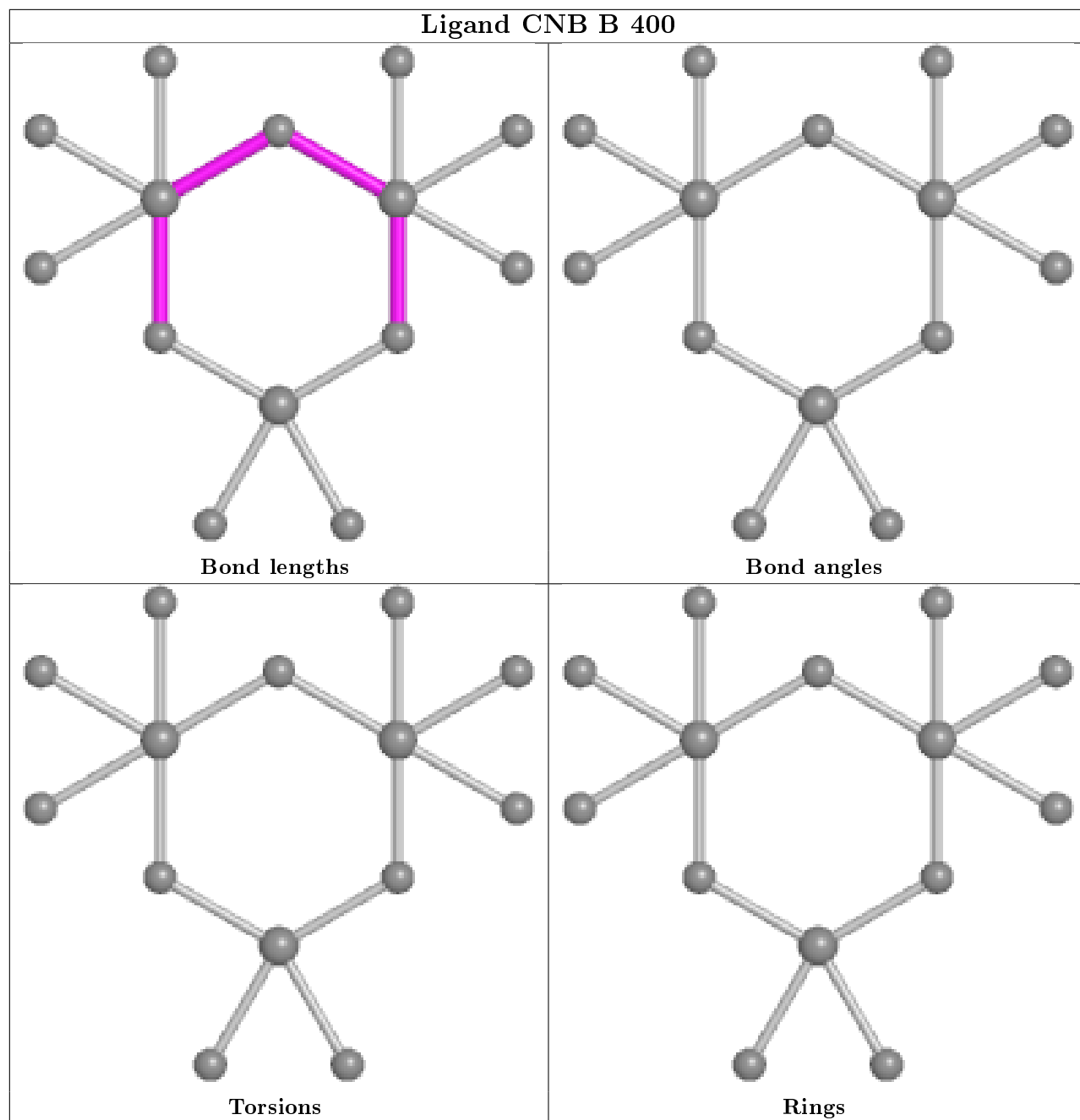
There are no torsion outliers.

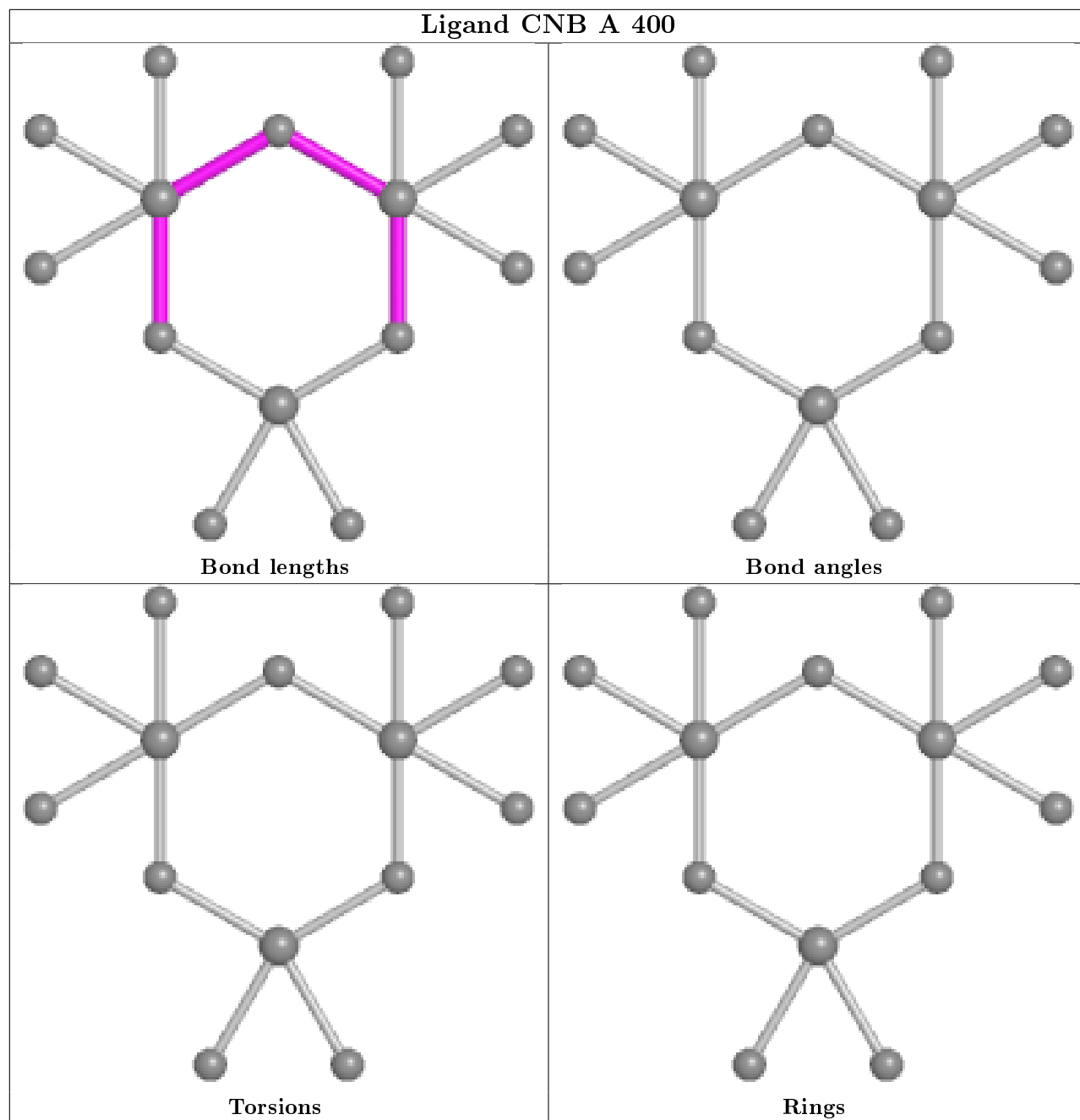
There are no ring outliers.

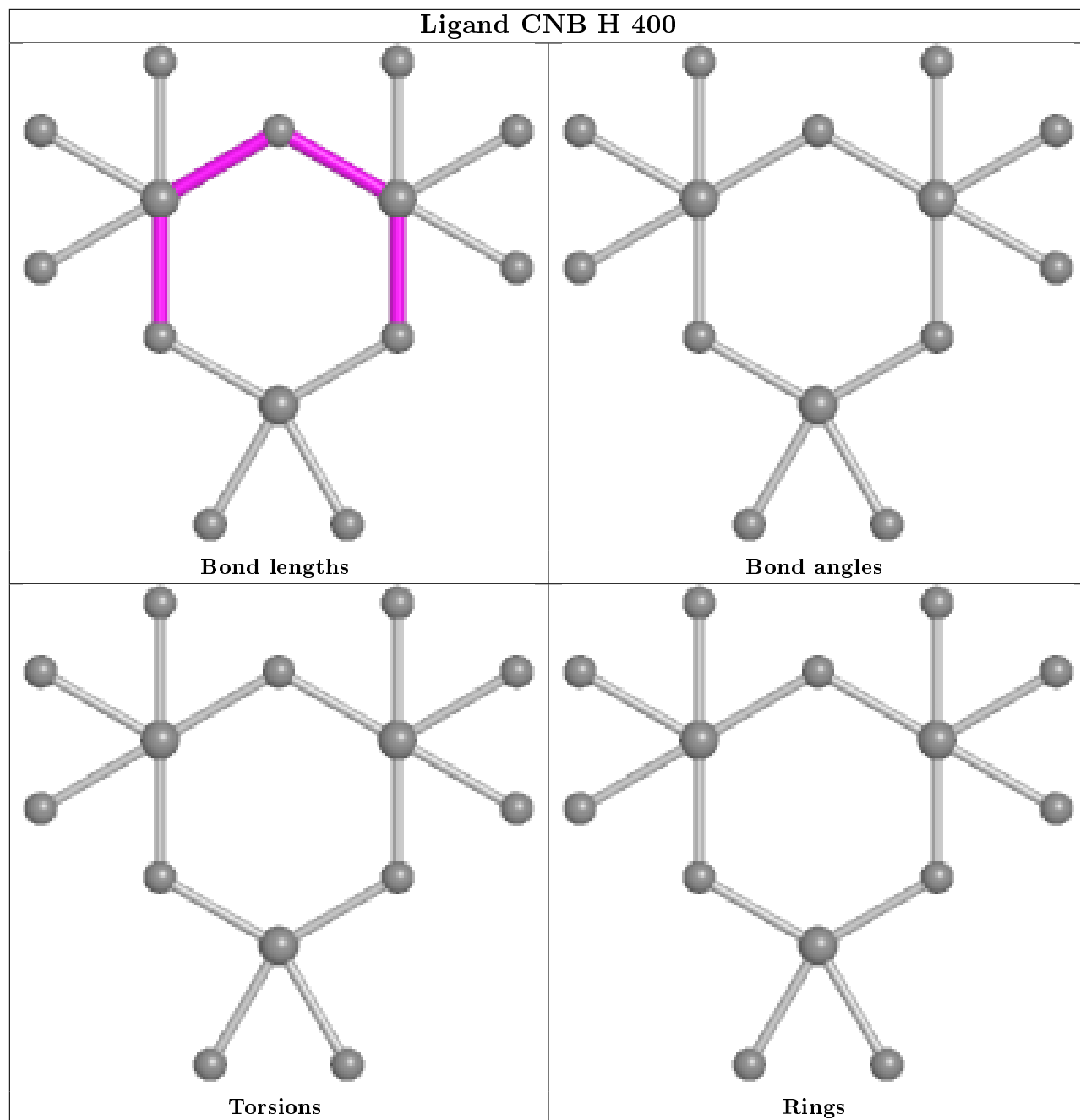
6 monomers are involved in 16 short contacts:

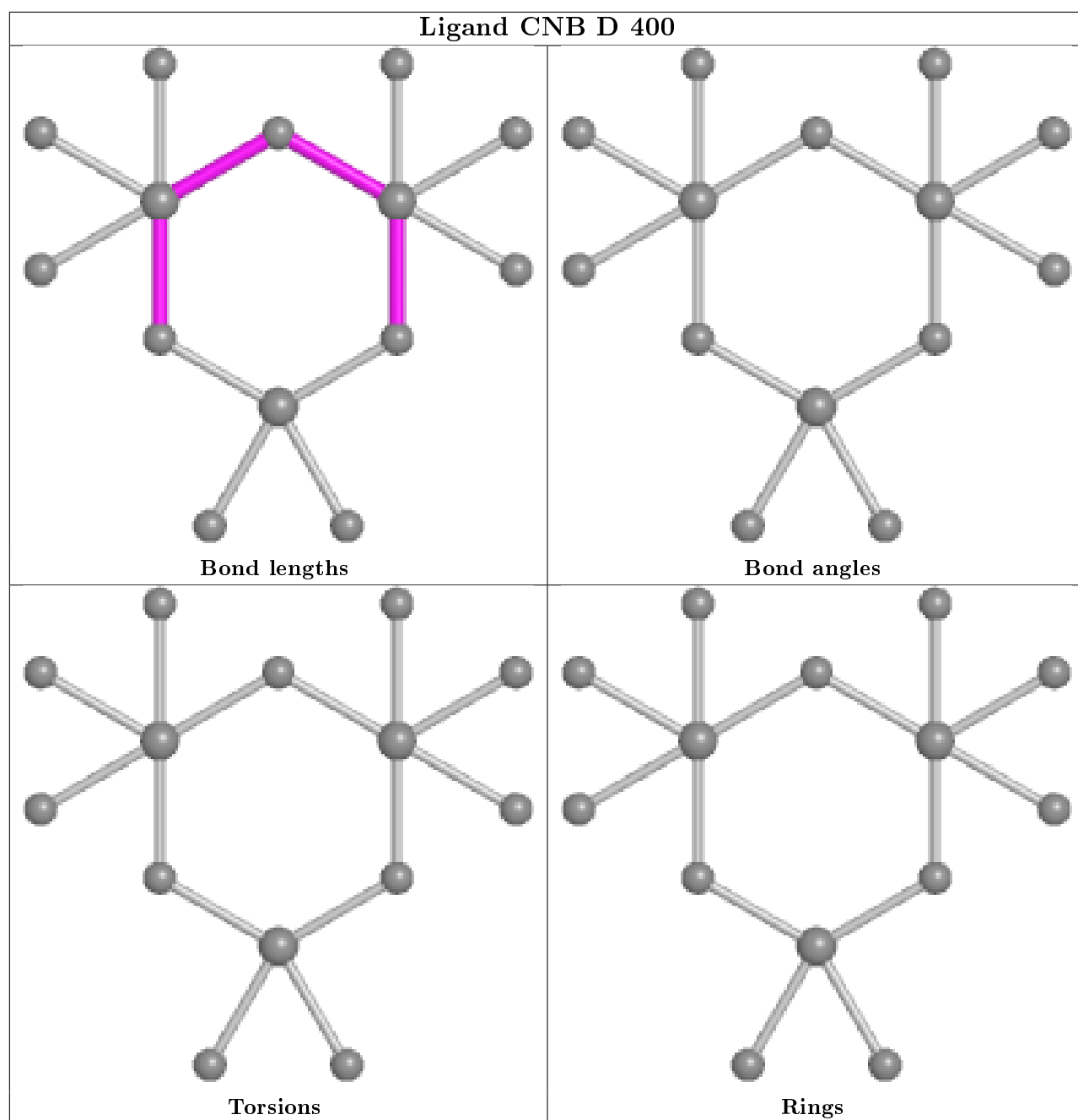
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	400	CN1	7	0
3	C	400	CN1	2	0
3	I	400	CN1	2	0
2	B	400	CNB	2	0
2	A	400	CNB	2	0
2	D	400	CNB	1	0

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.









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.