wwPDB X-ray Structure Validation Summary Report (i)

Dec 4, 2023 – 01:36 am GMT

PDB ID	:	2BT4
Title	:	Type II Dehydroquinase inhibitor complex
Authors	:	Toscano, M.D.; Stewart, K.A.; Coggins, J.R.; Lapthorn, A.J.; Abell, C.
Deposited on	:	2005-05-26
Resolution	:	1.70 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 (i) 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 (i)) were used in the production of this report:

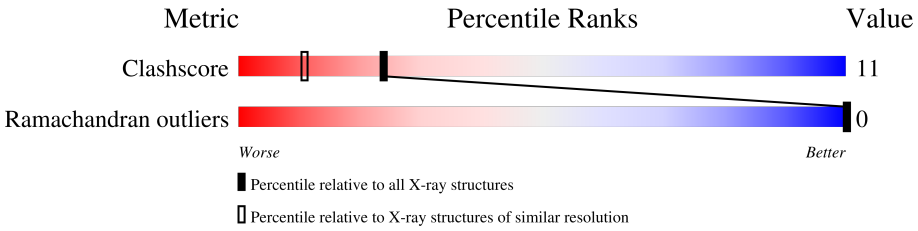
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	157	84% 11% 5%
1	B	157	87% 7% • 5%
1	C	157	87% 8% 5%
1	D	157	83% 12% 5%
1	E	157	81% 12% • 5%
1	F	157	81% 13% • 5%
1	G	157	87% 8% • 5%
1	H	157	85% 10% 5%
1	I	157	82% 13% 5%

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Mol	Chain	Length	Quality of chain
1	J	157	82% 13% 5%
1	K	157	83% 12% 5%
1	L	157	83% 11% 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
3	PO4	A	2401	-	-	X	-
5	GOL	B	2414	-	-	X	-
5	GOL	C	2415	-	-	X	-
5	GOL	D	2416	-	-	X	-
5	GOL	E	2419	-	-	X	-
5	GOL	E	2422	-	-	X	-
5	GOL	F	2418	-	-	X	-
5	GOL	G	2417	-	-	X	-
5	GOL	H	2411	-	-	X	-
5	GOL	I	2420	-	-	X	-
5	GOL	J	2412	-	-	X	-
5	GOL	K	2421	-	-	X	-

2 Entry composition (i)

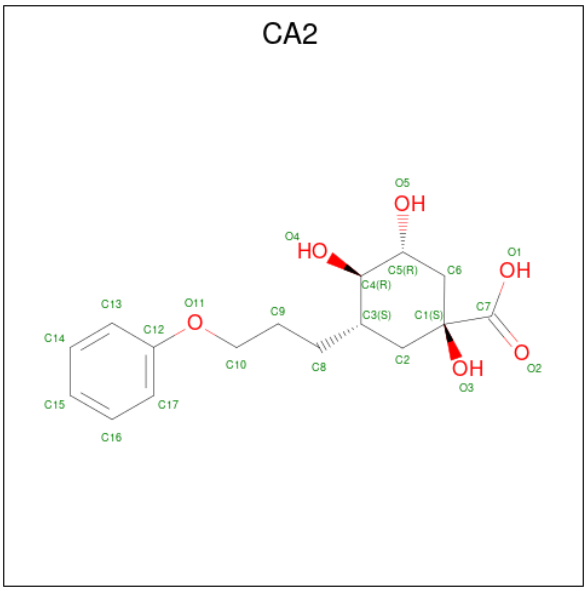
There are 6 unique types of molecules in this entry. The entry contains 15641 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-DEHYDROQUINATE DEHYDRATASE.

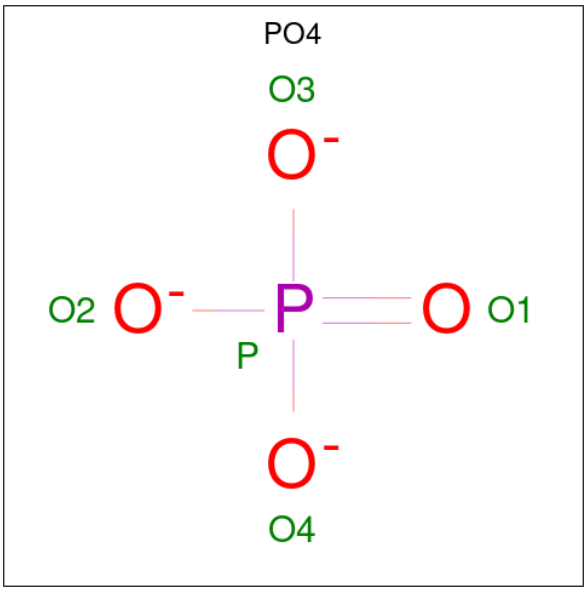
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	B	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	C	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	D	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	E	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	F	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	G	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	H	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	I	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	J	149	Total	C	N	O	S	0	2	0
			1132	704	213	210	5			
1	K	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	L	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			

- Molecule 2 is (1S,3R,4R,5S)-1,3,4-TRIHYDROXY-5-(3-PHENOXYPROPYL)CYCLOHEXANECARBOXYLIC ACID (three-letter code: CA2) (formula: $C_{16}H_{22}O_6$).



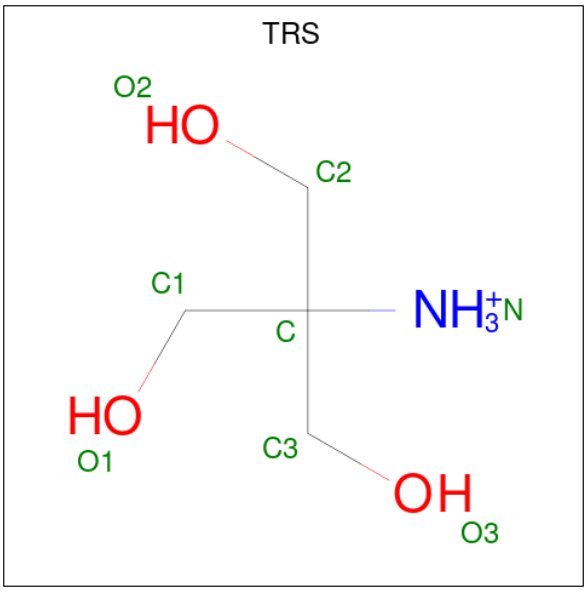
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 22 16 6	0	0
2	B	1	Total C O 22 16 6	0	0
2	C	1	Total C O 22 16 6	0	0
2	D	1	Total C O 22 16 6	0	0
2	E	1	Total C O 22 16 6	0	0
2	F	1	Total C O 22 16 6	0	0
2	G	1	Total C O 22 16 6	0	0
2	H	1	Total C O 22 16 6	0	0
2	I	1	Total C O 22 16 6	0	0
2	J	1	Total C O 22 16 6	0	0
2	K	1	Total C O 22 16 6	0	0
2	L	1	Total C O 22 16 6	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



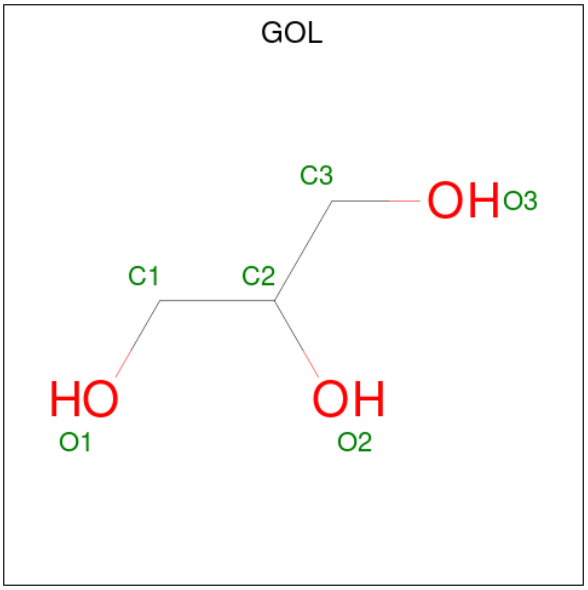
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	I	1	Total O P 5 4 1	0	0
3	L	1	Total O P 5 4 1	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	F	1	Total C N O 8 4 1 3	0	0
4	H	1	Total C N O 8 4 1 3	0	0
4	L	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	135	Total O 135 135	0	0
6	B	152	Total O 152 152	0	0
6	C	146	Total O 146 146	0	0
6	D	146	Total O 146 146	0	0
6	E	186	Total O 186 186	0	0
6	F	146	Total O 146 146	0	0
6	G	148	Total O 148 148	0	0
6	H	124	Total O 124 124	0	0
6	I	156	Total O 156 156	0	0
6	J	120	Total O 120 120	0	0
6	K	123	Total O 123 123	0	0
6	L	149	Total O 149 149	0	0

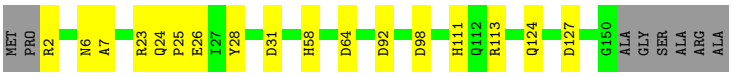
3 Residue-property plots (i)

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 was not executed.

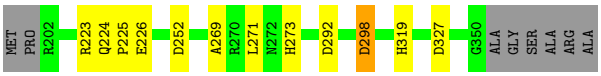
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain A:



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain B:

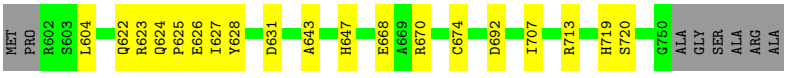


• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain C:

• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain D:

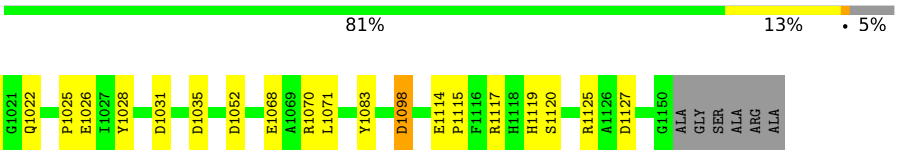


• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain E:

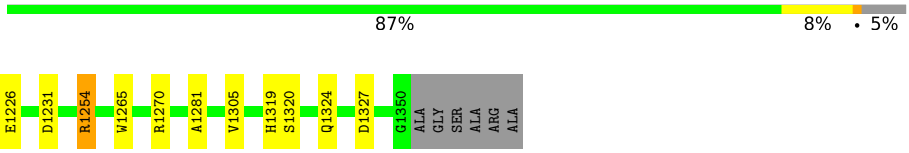
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain F:



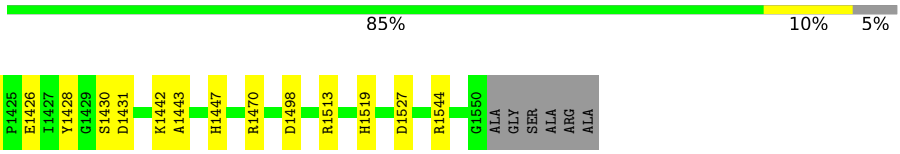
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain G:



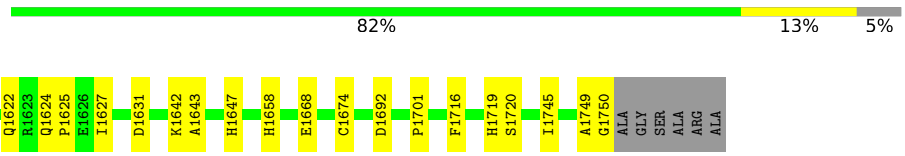
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain H:



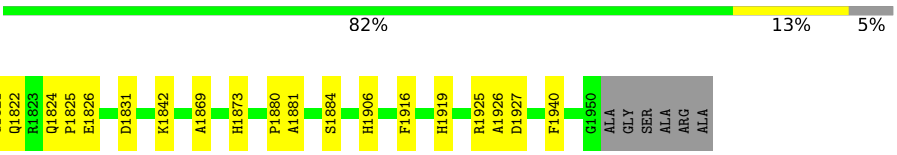
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain I:



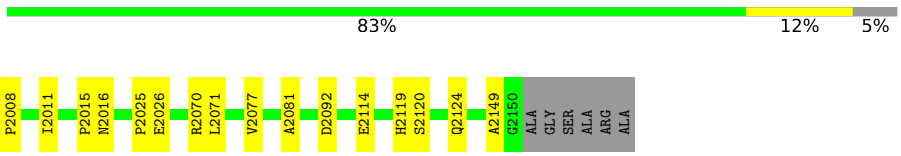
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain J:



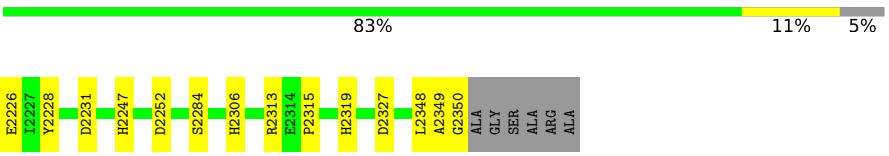
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain K:



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain L:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	196.62Å 196.49Å 240.63Å 65.91° 65.91° 90.01°	Depositor
Resolution (Å)	27.00 – 1.70	Depositor
% Data completeness (in resolution range)	75.8 (27.00-1.70)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15641	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, PO4, CA2, GOL

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	1.02	0/1161	1.04	4/1582 (0.3%)
1	B	1.05	0/1155	0.99	4/1574 (0.3%)
1	C	1.01	0/1155	0.95	3/1574 (0.2%)
1	D	1.05	0/1161	0.95	2/1582 (0.1%)
1	E	1.01	2/1155 (0.2%)	0.94	3/1574 (0.2%)
1	F	1.06	1/1155 (0.1%)	1.02	6/1574 (0.4%)
1	G	1.03	1/1161 (0.1%)	1.01	3/1582 (0.2%)
1	H	1.04	0/1155	1.02	2/1574 (0.1%)
1	I	1.00	0/1155	0.96	2/1574 (0.1%)
1	J	1.02	1/1166 (0.1%)	0.98	3/1588 (0.2%)
1	K	1.00	0/1155	0.93	0/1574
1	L	1.02	0/1161	0.98	3/1582 (0.2%)
All	All	1.03	5/13895 (0.0%)	0.98	35/18934 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1083	TYR	CD1-CE1	6.32	1.48	1.39
1	G	1305	VAL	CB-CG2	-5.66	1.41	1.52
1	E	828	TYR	CD2-CE2	-5.37	1.31	1.39
1	E	939	VAL	CB-CG1	-5.24	1.41	1.52
1	J	1940	PHE	CD2-CE2	5.09	1.49	1.39

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	1527	ASP	CB-CG-OD2	13.19	130.17	118.30
1	G	1327	ASP	CB-CG-OD2	8.20	125.68	118.30
1	C	527	ASP	CB-CG-OD2	7.63	125.17	118.30
1	B	252	ASP	CB-CG-OD1	7.24	124.82	118.30
1	D	631	ASP	CB-CG-OD2	7.06	124.65	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1127	0	1093	20	0
1	B	1126	0	1092	14	0
1	C	1126	0	1092	17	0
1	D	1127	0	1093	18	0
1	E	1126	0	1092	38	0
1	F	1126	0	1092	36	0
1	G	1127	0	1093	16	0
1	H	1126	0	1092	27	0
1	I	1126	0	1092	41	0
1	J	1132	0	1102	19	0
1	K	1126	0	1092	20	0
1	L	1127	0	1093	22	0
2	A	22	0	21	1	0
2	B	22	0	21	2	0
2	C	22	0	21	0	0
2	D	22	0	21	0	0
2	E	22	0	21	2	0
2	F	22	0	21	2	0
2	G	22	0	21	1	0
2	H	22	0	21	1	0
2	I	22	0	21	0	0
2	J	22	0	21	1	0
2	K	22	0	21	0	0
2	L	22	0	21	0	0
3	A	5	0	0	2	0
3	D	5	0	0	1	0
3	I	5	0	0	1	0
3	L	5	0	0	0	0
4	A	8	0	12	0	0
4	F	8	0	12	0	0
4	H	8	0	12	0	0
4	L	8	0	12	0	0
5	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	8	6	0
5	C	6	0	8	9	0
5	D	6	0	8	9	0
5	E	12	0	16	15	0
5	F	6	0	8	13	0
5	G	6	0	8	7	0
5	H	6	0	8	7	0
5	I	6	0	8	21	0
5	J	6	0	8	4	0
5	K	6	0	8	12	0
6	A	135	0	0	10	0
6	B	152	0	0	8	0
6	C	146	0	0	10	0
6	D	146	0	0	5	0
6	E	186	0	0	17	0
6	F	146	0	0	10	0
6	G	148	0	0	0	0
6	H	124	0	0	18	0
6	I	156	0	0	22	0
6	J	120	0	0	13	0
6	K	123	0	0	2	0
6	L	149	0	0	13	0
All	All	15641	0	13514	305	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 11.

The worst 5 of 305 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:I:1719[A]:HIS:CD2	5:I:2420:GOL:H11	1.62	1.33
1:F:1098:ASP:CB	6:F:2109:HOH:O	1.68	1.31
1:H:1519[A]:HIS:CD2	5:H:2411:GOL:H12	1.72	1.25
5:B:2414:GOL:C1	6:B:2150:HOH:O	1.88	1.22
1:I:1602:ARG:N	6:I:2022:HOH:O	1.76	1.18

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	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
1	B	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	C	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	D	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
1	E	148/157 (94%)	144 (97%)	4 (3%)	0	100	100
1	F	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	G	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
1	H	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	I	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	J	148/157 (94%)	144 (97%)	4 (3%)	0	100	100
1	K	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	L	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
All	All	1780/1884 (94%)	1740 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

32 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	CA2	B	360	-	23,23,23	1.00	2 (8%)	28,32,32	2.74	10 (35%)
4	TRS	F	2406	-	7,7,7	0.62	0	9,9,9	0.69	0
2	CA2	L	2360	-	23,23,23	1.30	1 (4%)	28,32,32	1.91	6 (21%)
2	CA2	G	1360	-	23,23,23	1.79	4 (17%)	28,32,32	2.71	9 (32%)
5	GOL	E	2422	-	5,5,5	0.92	0	5,5,5	0.43	0
5	GOL	I	2420	-	5,5,5	0.55	0	5,5,5	0.77	0
2	CA2	E	960	-	23,23,23	1.08	1 (4%)	28,32,32	2.50	8 (28%)
5	GOL	C	2415	-	5,5,5	0.77	0	5,5,5	0.80	0
5	GOL	J	2412	-	5,5,5	0.51	0	5,5,5	1.01	0
2	CA2	K	2160	-	23,23,23	0.84	1 (4%)	28,32,32	2.22	8 (28%)
5	GOL	F	2418	-	5,5,5	0.96	0	5,5,5	1.97	3 (60%)
2	CA2	H	1560	-	23,23,23	1.44	1 (4%)	28,32,32	1.96	9 (32%)
3	PO4	I	2403	-	4,4,4	1.40	1 (25%)	6,6,6	1.67	2 (33%)
2	CA2	F	1160	-	23,23,23	1.67	2 (8%)	28,32,32	2.11	8 (28%)
3	PO4	A	2401	-	4,4,4	1.62	1 (25%)	6,6,6	1.78	2 (33%)
5	GOL	H	2411	-	5,5,5	0.41	0	5,5,5	0.60	0
4	TRS	H	2407	-	7,7,7	0.91	0	9,9,9	0.83	0
3	PO4	L	2404	-	4,4,4	1.06	0	6,6,6	2.15	2 (33%)
5	GOL	G	2417	-	5,5,5	0.77	0	5,5,5	1.41	1 (20%)
2	CA2	D	760	-	23,23,23	1.01	2 (8%)	28,32,32	2.47	10 (35%)
4	TRS	L	2408	-	7,7,7	0.45	0	9,9,9	0.97	0
5	GOL	B	2414	-	5,5,5	0.53	0	5,5,5	0.49	0
5	GOL	K	2421	-	5,5,5	0.64	0	5,5,5	0.91	0
4	TRS	A	2405	-	7,7,7	0.68	0	9,9,9	1.47	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	E	2419	-	5,5,5	0.72	0	5,5,5	0.86	0
3	PO4	D	2402	-	4,4,4	1.50	1 (25%)	6,6,6	0.76	0
5	GOL	D	2416	-	5,5,5	0.56	0	5,5,5	0.55	0
2	CA2	J	1960	-	23,23,23	1.50	4 (17%)	28,32,32	1.96	8 (28%)
2	CA2	C	560	-	23,23,23	1.25	2 (8%)	28,32,32	1.72	8 (28%)
2	CA2	A	160	-	23,23,23	1.61	4 (17%)	28,32,32	2.15	8 (28%)
2	CA2	I	1760	-	23,23,23	1.29	2 (8%)	28,32,32	1.99	9 (32%)
5	GOL	A	2413	-	5,5,5	0.76	0	5,5,5	0.69	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	CA2	B	360	-	-	2/13/31/31	0/2/2/2
4	TRS	F	2406	-	-	0/9/9/9	-
2	CA2	L	2360	-	-	3/13/31/31	0/2/2/2
2	CA2	G	1360	-	-	1/13/31/31	0/2/2/2
5	GOL	E	2422	-	-	4/4/4/4	-
5	GOL	I	2420	-	-	3/4/4/4	-
2	CA2	E	960	-	-	1/13/31/31	0/2/2/2
5	GOL	C	2415	-	-	3/4/4/4	-
5	GOL	J	2412	-	-	4/4/4/4	-
2	CA2	K	2160	-	-	3/13/31/31	0/2/2/2
5	GOL	F	2418	-	-	0/4/4/4	-
2	CA2	H	1560	-	-	3/13/31/31	0/2/2/2
2	CA2	F	1160	-	-	2/13/31/31	0/2/2/2
5	GOL	H	2411	-	-	0/4/4/4	-
4	TRS	H	2407	-	-	0/9/9/9	-
5	GOL	G	2417	-	-	1/4/4/4	-
2	CA2	D	760	-	-	1/13/31/31	0/2/2/2
4	TRS	L	2408	-	-	0/9/9/9	-
5	GOL	B	2414	-	-	2/4/4/4	-
5	GOL	K	2421	-	-	2/4/4/4	-
4	TRS	A	2405	-	-	0/9/9/9	-
5	GOL	E	2419	-	-	2/4/4/4	-
5	GOL	D	2416	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CA2	J	1960	-	-	2/13/31/31	0/2/2/2
2	CA2	C	560	-	-	4/13/31/31	0/2/2/2
2	CA2	A	160	-	-	1/13/31/31	0/2/2/2
2	CA2	I	1760	-	-	2/13/31/31	0/2/2/2
5	GOL	A	2413	-	-	4/4/4/4	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1360	CA2	C1-C7	-6.45	1.46	1.53
2	F	1160	CA2	C1-C7	-6.40	1.46	1.53
2	H	1560	CA2	C1-C7	-5.35	1.47	1.53
2	L	2360	CA2	C1-C7	-4.84	1.48	1.53
2	A	160	CA2	C1-C7	-4.78	1.48	1.53

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	360	CA2	C6-C1-C2	8.22	115.99	110.72
2	G	1360	CA2	O2-C7-C1	-7.44	111.72	122.25
2	E	960	CA2	C6-C1-C2	-6.62	106.48	110.72
2	A	160	CA2	C2-C3-C4	6.46	117.40	109.20
2	H	1560	CA2	C2-C3-C4	6.01	116.83	109.20

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	2360	CA2	O3-C1-C7-O1
5	A	2413	GOL	C1-C2-C3-O3
5	B	2414	GOL	C1-C2-C3-O3
5	C	2415	GOL	C1-C2-C3-O3
5	E	2419	GOL	C1-C2-C3-O3

There are no ring outliers.

22 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	360	CA2	2	0
2	G	1360	CA2	1	0

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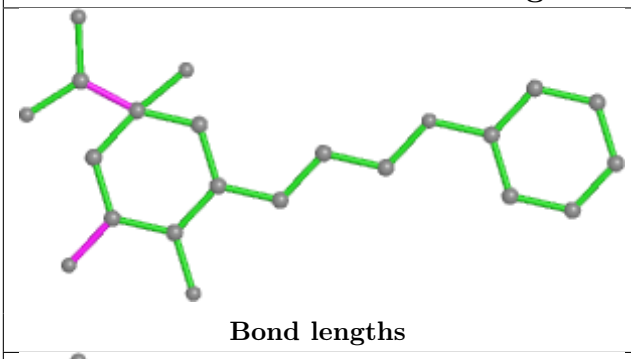
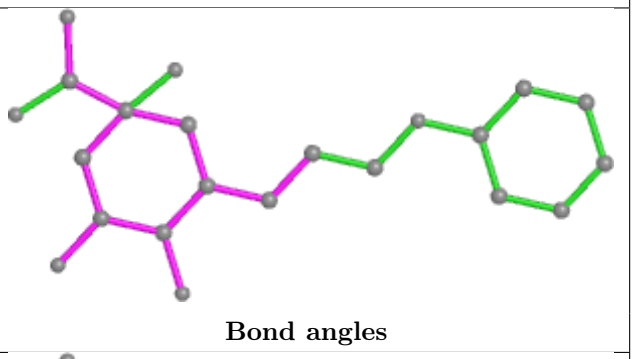
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2422	GOL	5	0
5	I	2420	GOL	21	0
2	E	960	CA2	2	0
5	C	2415	GOL	9	0
5	J	2412	GOL	4	0
5	F	2418	GOL	13	0
2	H	1560	CA2	1	0
3	I	2403	PO4	1	0
2	F	1160	CA2	2	0
3	A	2401	PO4	2	0
5	H	2411	GOL	7	0
5	G	2417	GOL	7	0
5	B	2414	GOL	6	0
5	K	2421	GOL	12	0
5	E	2419	GOL	10	0
3	D	2402	PO4	1	0
5	D	2416	GOL	9	0
2	J	1960	CA2	1	0
2	A	160	CA2	1	0
5	A	2413	GOL	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 then 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.

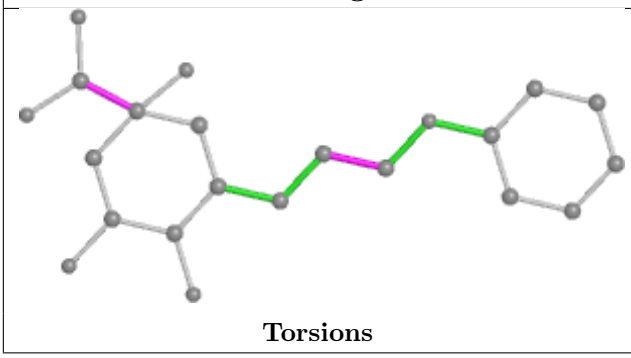
Ligand CA2 B 360



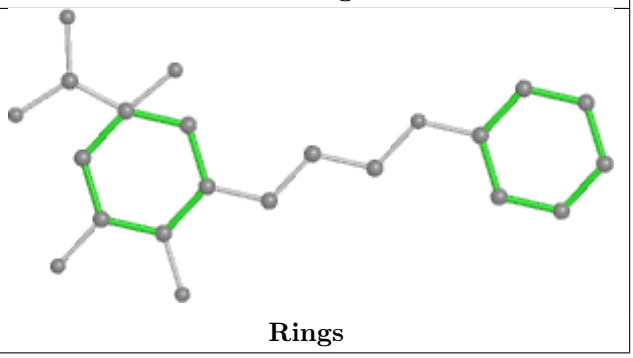
Bond lengths



Bond angles

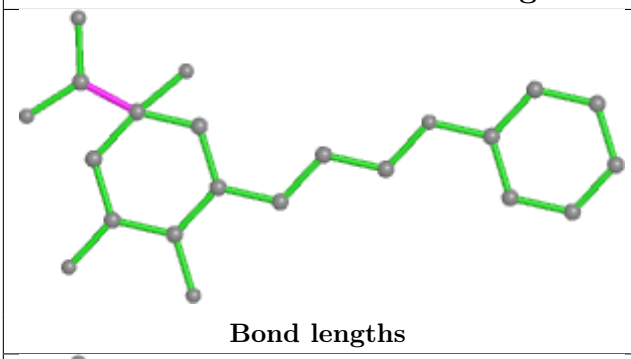


Torsions

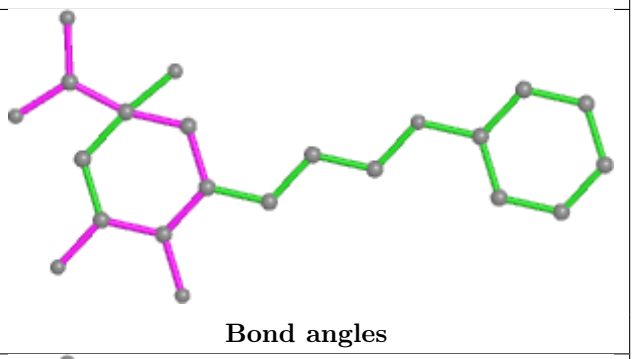


Rings

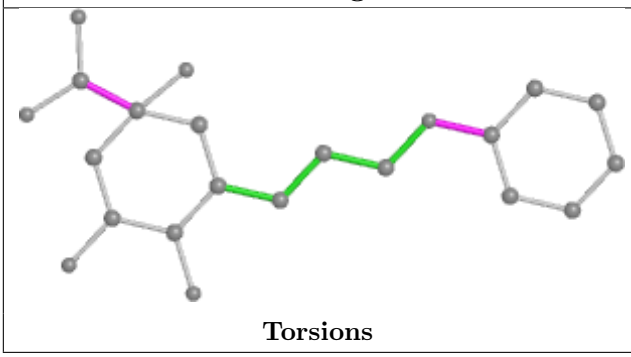
Ligand CA2 L 2360



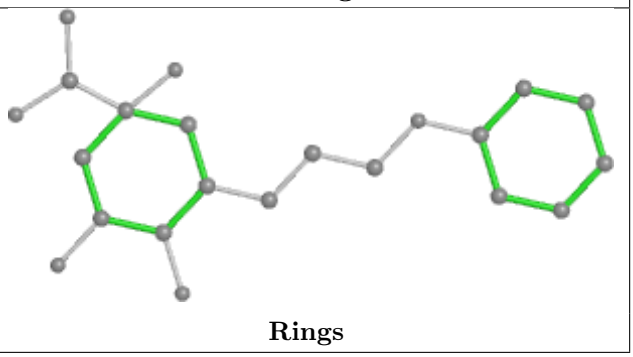
Bond lengths



Bond angles

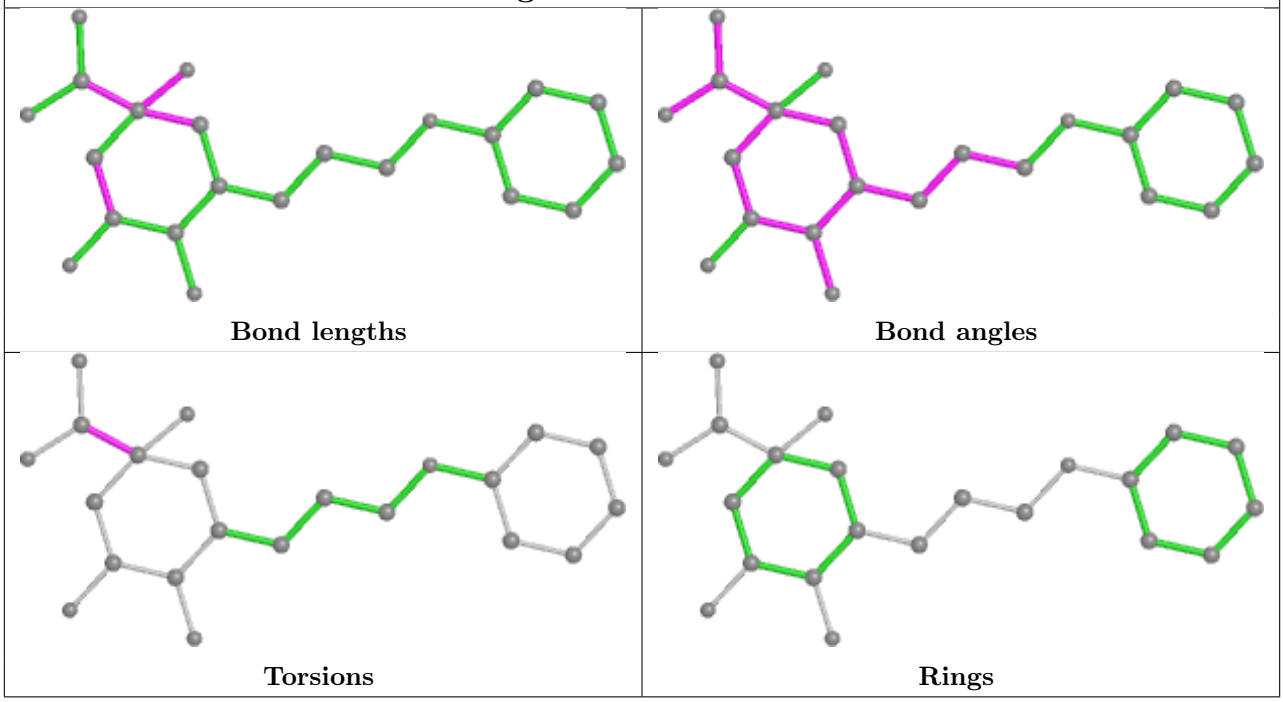


Torsions

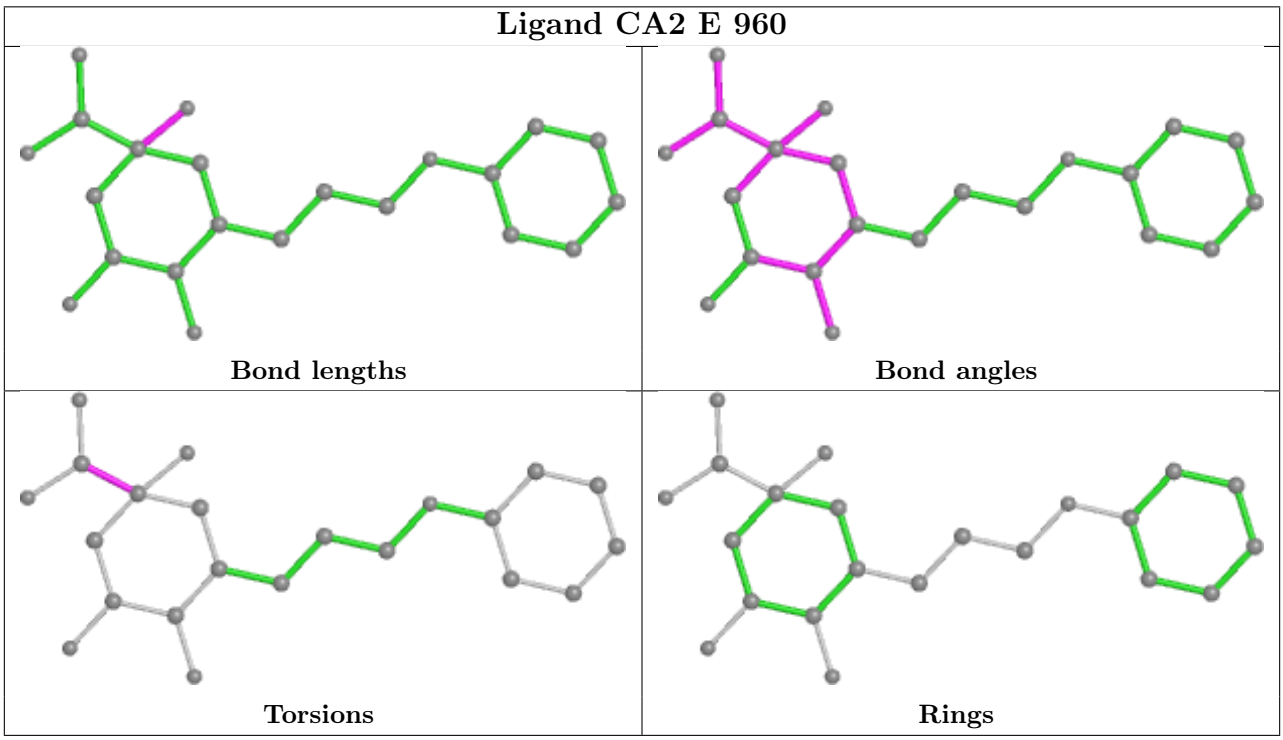


Rings

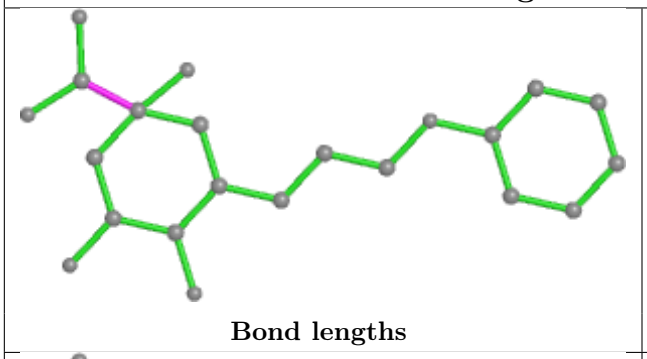
Ligand CA2 G 1360



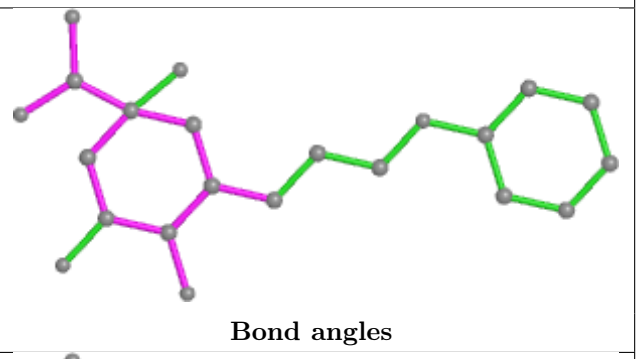
Ligand CA2 E 960



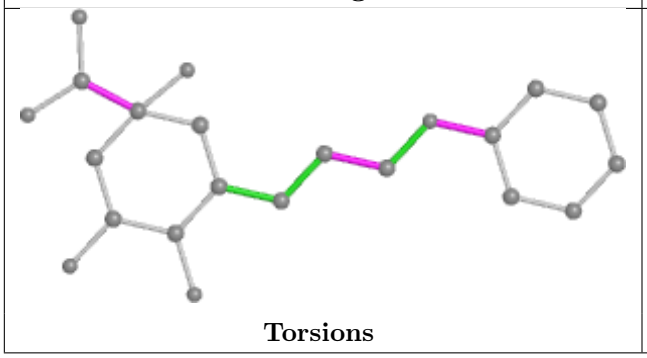
Ligand CA2 K 2160



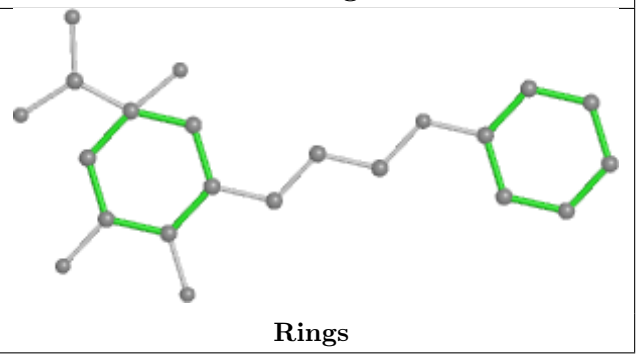
Bond lengths



Bond angles

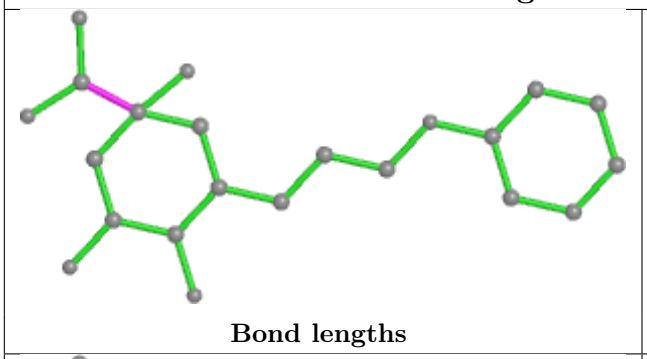


Torsions

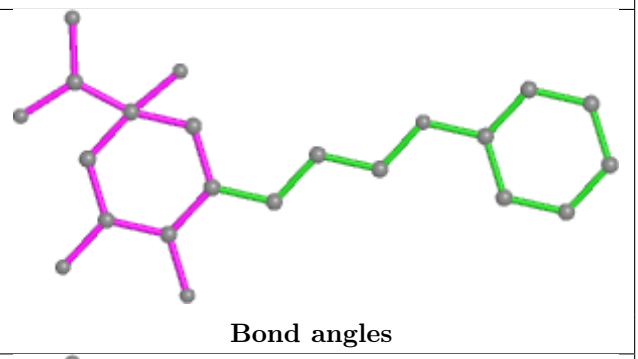


Rings

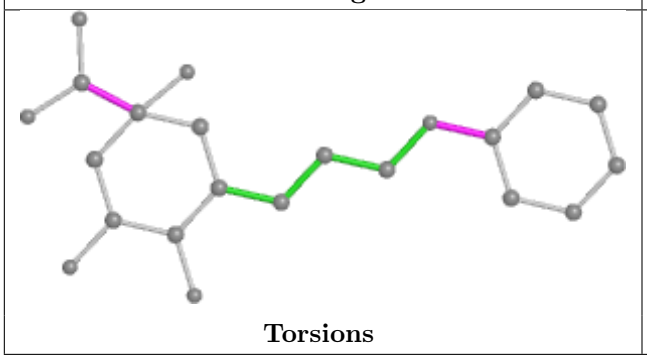
Ligand CA2 H 1560



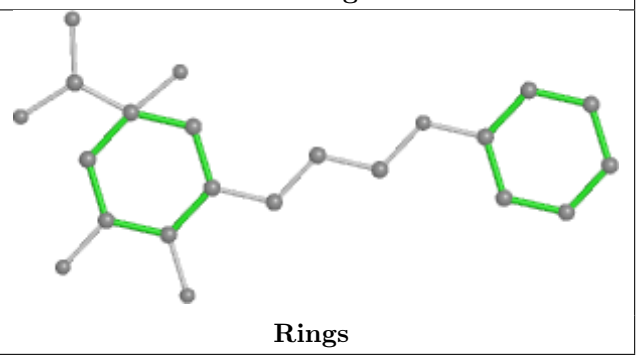
Bond lengths



Bond angles

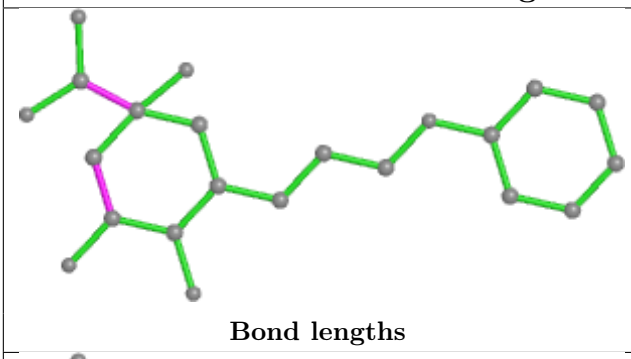


Torsions

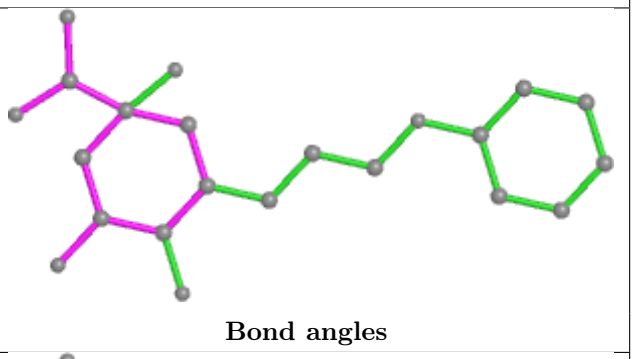


Rings

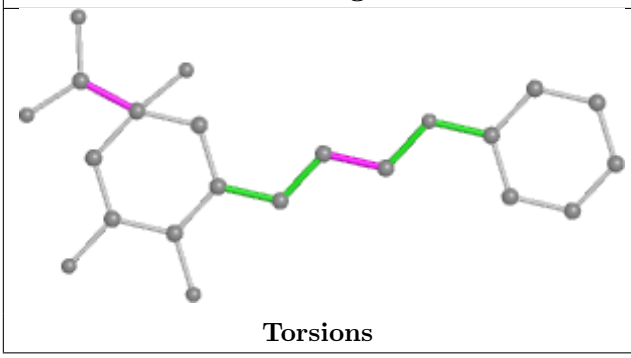
Ligand CA2 F 1160



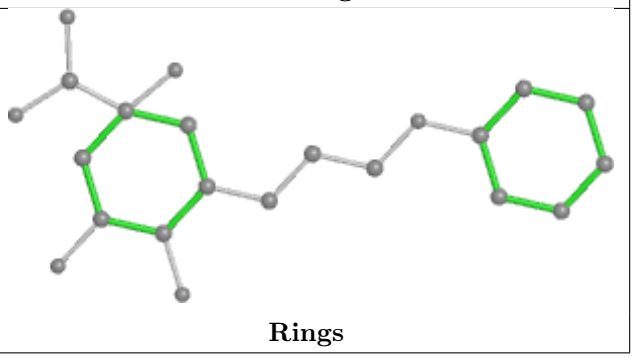
Bond lengths



Bond angles

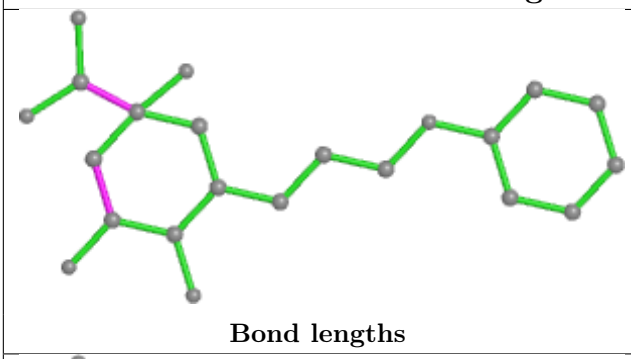


Torsions

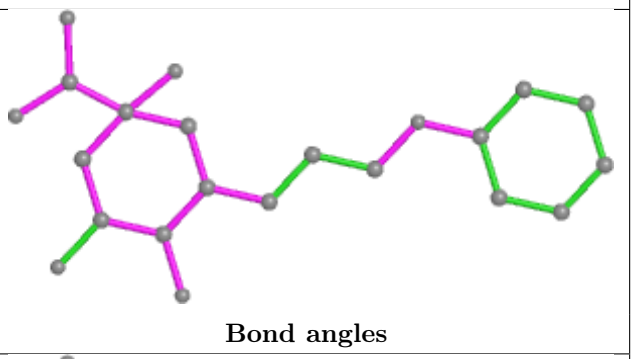


Rings

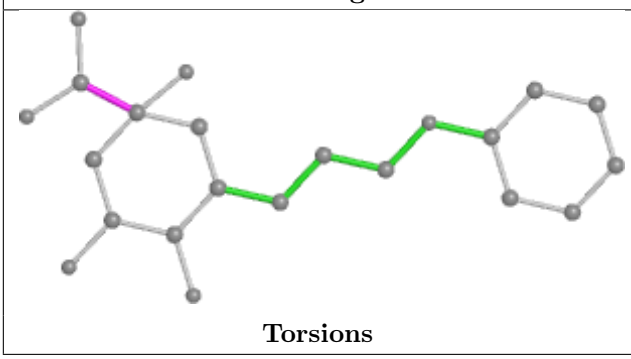
Ligand CA2 D 760



Bond lengths



Bond angles



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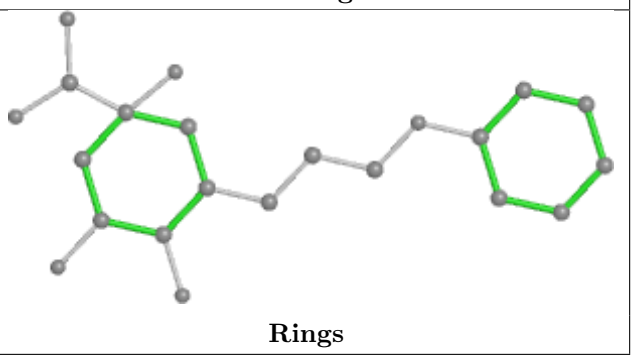
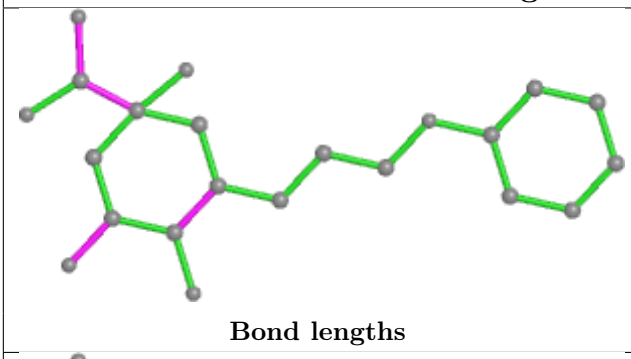
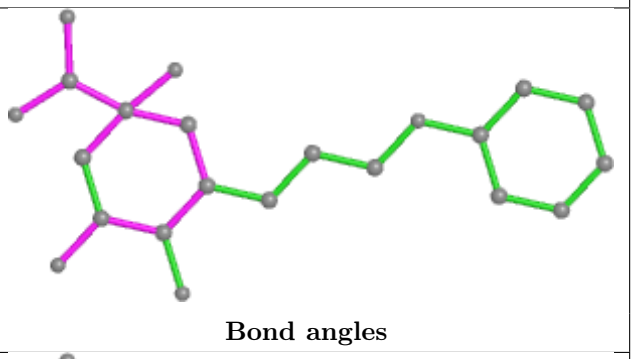


Rings

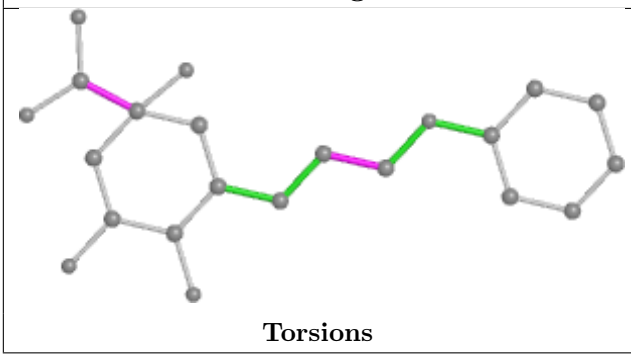
Ligand CA2 J 1960



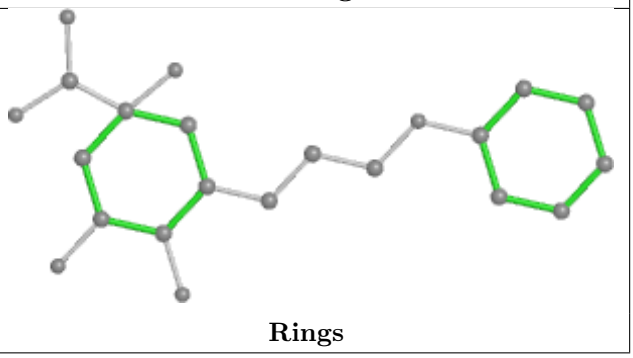
Bond lengths



Bond angles

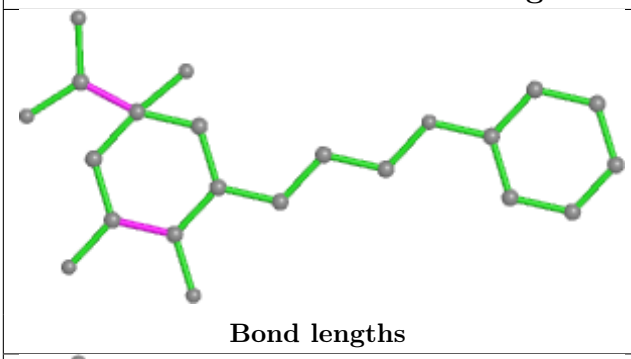


Torsions

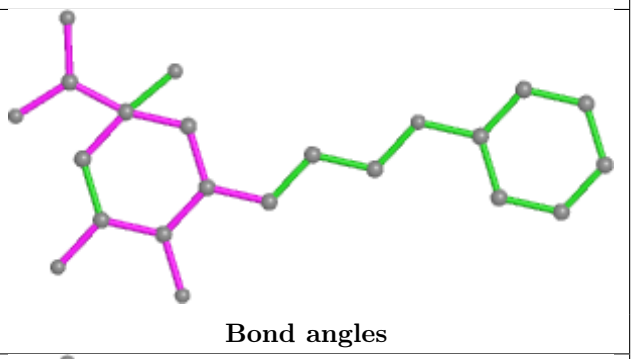


Rings

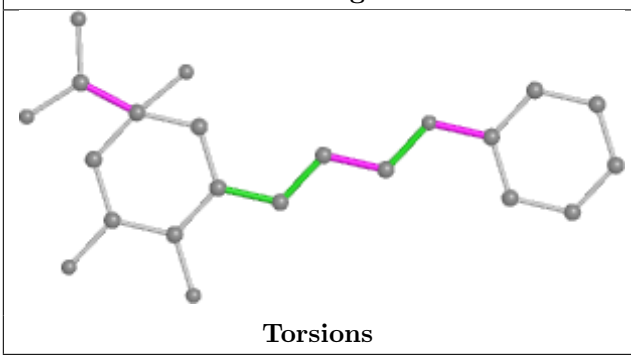
Ligand CA2 C 560



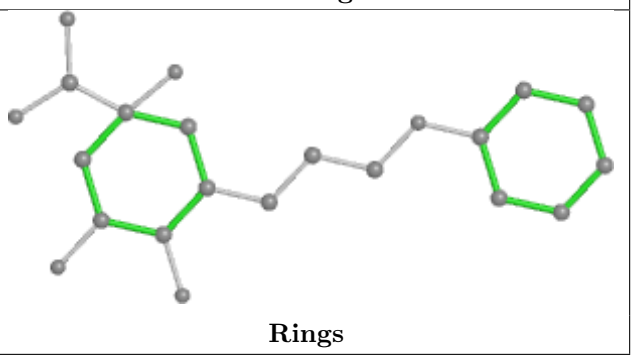
Bond lengths



Bond angles

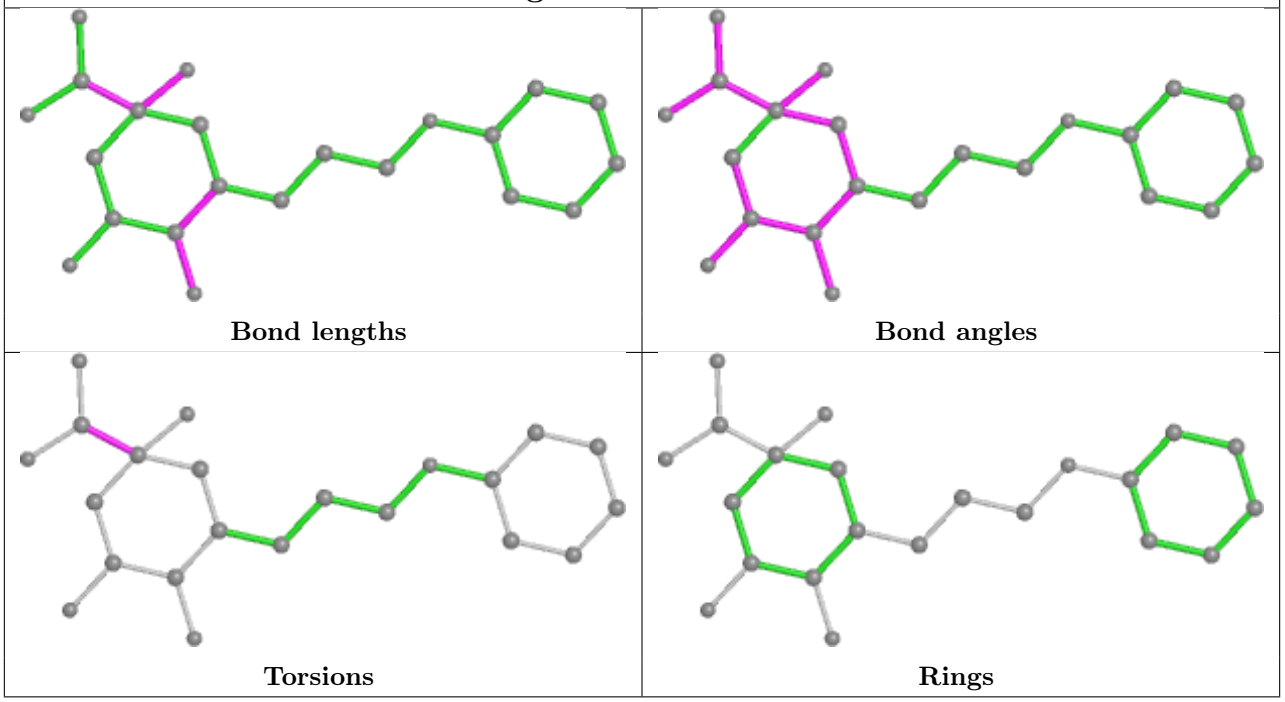


Torsions

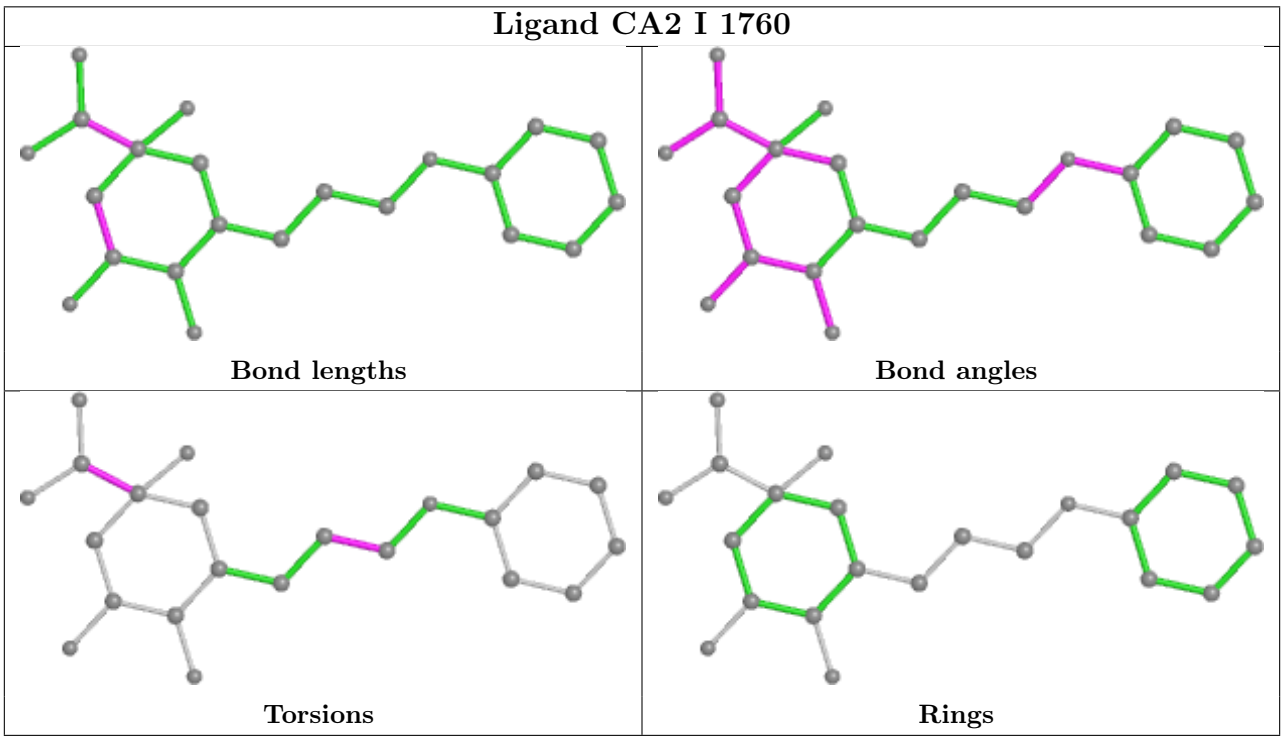


Rings

Ligand CA2 A 160



Ligand CA2 I 1760



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.