Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 05:40 PM EDT

PDB ID	:	2AOU
Title	:	Histamine Methyltransferase Complexed with the Antimalarial Drug Amodiaquine
Authors	:	Horton, J.R.; Sawada, K.; Nishibori, M.; Cheng, X.
Deposited on	:	2005-08-14
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (1)) were used in the production of this report:

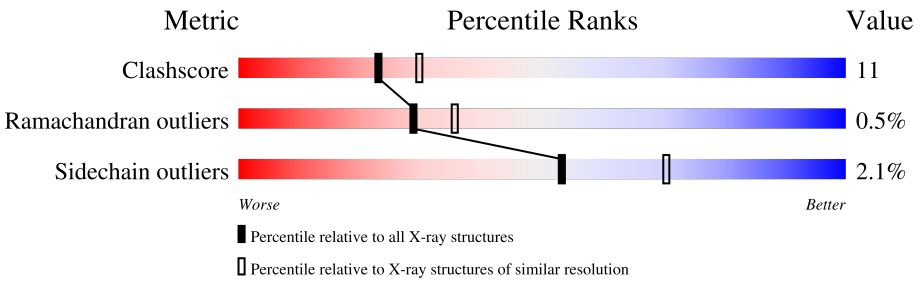
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	292	74% 22% • •
2	B	292	80% 18% • •

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
1	DCY	A	248	X	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4917 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 Histamine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2245	1435	363	432	15	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	CYS	CYS	modified residue	UNP P50135
A	217	CSO	CYS	modified residue	UNP P50135
A	248	DCY	CYS	modified residue	UNP P50135

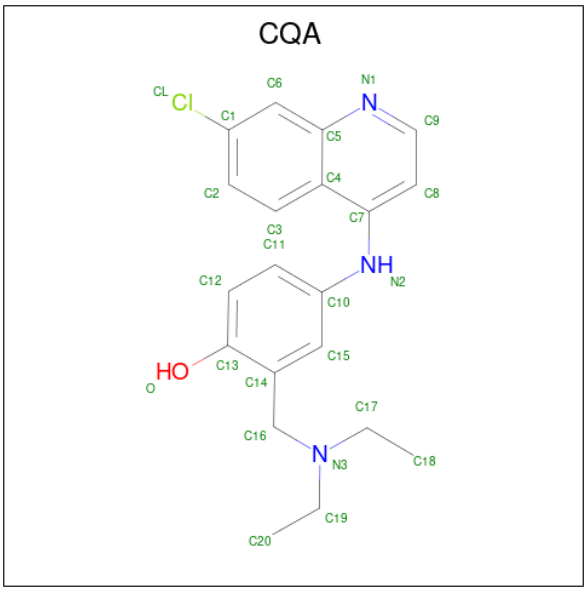
- Molecule 2 is a protein called Histamine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	289	2270	1445	368	441	16	0	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	CSO	CYS	modified residue	UNP P50135
B	217	CYS	CYS	modified residue	UNP P50135
B	248	CYS	CYS	modified residue	UNP P50135

- Molecule 3 is 4-[(7-CHLOROQUINOLIN-4-YL)AMINO]-2-[(DIETHYLAMINO)METHYL] PHENOL (three-letter code: CQA) (formula: $C_{20}H_{22}ClN_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			25	20	1	3	1		
3	A	1	Total	C	Cl	N	O	0	0
			23	18	1	3	1		
3	B	1	Total	C	Cl	N	O	0	1
			27	22	1	3	1		
3	B	1	Total	C	Cl	N	O	0	0
			21	16	1	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total	O	0	0
			147	147		
4	B	159	Total	O	0	0
			159	159		

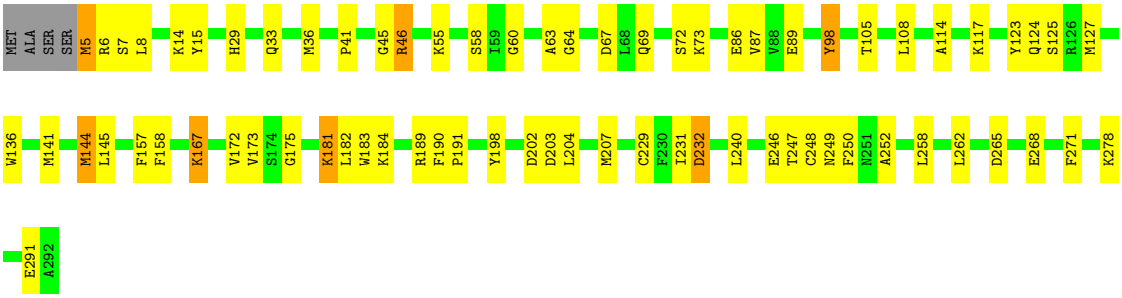
3 Residue-property plots (i)

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.

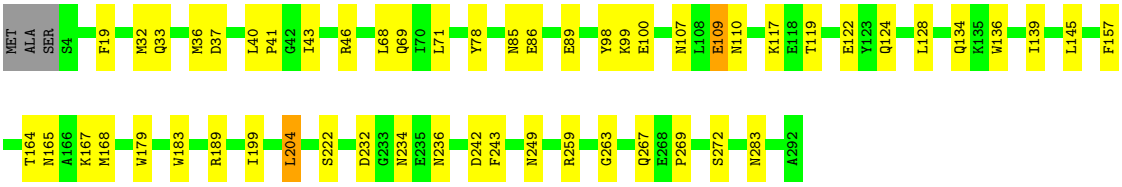
• Molecule 1: Histamine N-methyltransferase

Chain A:



• Molecule 2: Histamine N-methyltransferase

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	130.89Å 130.89Å 63.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30	Depositor
% Data completeness (in resolution range)	97.4 (30.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4917	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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: DCY, CQA, CSO

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	0/2278	0.55	0/3080
2	B	0.35	0/2303	0.56	0/3114
All	All	0.34	0/4581	0.55	0/6194

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
2	B	0	1
All	All	1	1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	248	DCY	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	109[B]	GLU	Mainchain

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	2245	0	2131	60	0
2	B	2270	0	2153	40	0
3	A	48	0	39	7	0
3	B	48	0	27	7	0
4	A	147	0	0	5	0
4	B	159	0	0	3	0
All	All	4917	0	4350	102	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.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:GLU:HG3	2:B:136:TRP:HH2	1.27	0.97
2:B:86:GLU:HG3	2:B:136:TRP:CH2	2.01	0.96
1:A:265:ASP:HA	1:A:268:GLU:HG2	1.62	0.81
1:A:183:TRP:HB3	3:A:403:CQA:H161	1.62	0.80
1:A:33:GLN:OE1	1:A:69:GLN:HG2	1.85	0.76
1:A:5:MET:CE	1:A:247:THR:HG21	2.16	0.75
1:A:141:MET:HB3	1:A:144:MET:CE	2.17	0.74
1:A:86:GLU:HG2	1:A:114:ALA:HB3	1.69	0.72
1:A:144:MET:HE3	1:A:145:LEU:N	2.05	0.72
2:B:107:ASN:HA	2:B:109[B]:GLU:OE2	1.90	0.71
2:B:134:GLN:HG3	4:B:455:HOH:O	1.91	0.71
2:B:68:LEU:HD23	2:B:71:LEU:HD12	1.74	0.70
1:A:5:MET:HE3	1:A:247:THR:HG21	1.75	0.68
2:B:189[B]:ARG:HH11	2:B:189[B]:ARG:HB3	1.62	0.64
1:A:189:ARG:HD2	1:A:258:LEU:HD13	1.79	0.64
2:B:43:ILE:HG23	2:B:167:LYS:HD3	1.81	0.62
1:A:144:MET:CE	1:A:145:LEU:HG	2.29	0.62
1:A:14:LYS:HZ2	1:A:248:DCY:HB2	1.64	0.62
2:B:222:SER:HB3	2:B:283:ASN:O	1.99	0.62
1:A:141:MET:HB3	1:A:144:MET:HE1	1.82	0.62
1:A:14:LYS:NZ	1:A:248:DCY:HB2	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:MET:HE2	1:A:247:THR:HG21	1.84	0.60
2:B:243:PHE:CE1	3:B:400[C]:CQA:H182	2.37	0.60
1:A:69:GLN:HE21	1:A:73:LYS:HE2	1.67	0.59
1:A:183:TRP:CZ2	3:A:402:CQA:H183	2.37	0.58
1:A:175:GLY:HA3	1:A:202:ASP:OD2	2.06	0.56
1:A:144:MET:HE3	1:A:145:LEU:CA	2.36	0.56
1:A:89:GLU:O	1:A:117:LYS:HA	2.06	0.55
1:A:144:MET:HE3	1:A:145:LEU:HG	1.87	0.55
1:A:63:ALA:HB3	4:A:427:HOH:O	2.07	0.55
2:B:269:PRO:HA	2:B:272:SER:O	2.06	0.55
3:A:402:CQA:H172	3:A:402:CQA:O	2.06	0.54
2:B:43:ILE:O	2:B:167:LYS:HD2	2.08	0.53
1:A:6:ARG:O	1:A:248:DCY:SG	2.62	0.53
2:B:119:THR:OG1	2:B:122:GLU:HG3	2.09	0.53
2:B:145:LEU:HD13	2:B:204:LEU:HD21	1.92	0.52
2:B:134:GLN:NE2	4:B:501:HOH:O	2.43	0.51
1:A:184:LYS:HG3	3:A:403:CQA:H202	1.92	0.51
1:A:202:ASP:OD1	2:B:99:LYS:HE3	2.11	0.51
1:A:125:SER:HA	4:A:533:HOH:O	2.10	0.50
2:B:124:GLN:O	2:B:128:LEU:HG	2.11	0.50
2:B:234:ASN:OD1	2:B:236:ASN:HB3	2.10	0.50
1:A:141:MET:HB3	1:A:144:MET:HE2	1.94	0.50
1:A:36:MET:O	1:A:41:PRO:HD3	2.11	0.50
1:A:183:TRP:HB2	3:A:403:CQA:H203	1.93	0.49
1:A:14:LYS:HE3	1:A:248:DCY:HB2	1.95	0.49
2:B:183:TRP:HB3	3:B:401:CQA:H12	1.95	0.49
1:A:203:ASP:O	1:A:207:MET:HG3	2.13	0.49
1:A:45:GLY:HA3	1:A:46:ARG:NH2	2.27	0.49
1:A:69:GLN:O	1:A:72:SER:HB3	2.13	0.48
1:A:167:LYS:HD2	1:A:291:GLU:OE2	2.12	0.48
2:B:242:ASP:OD2	2:B:249:ASN:N	2.35	0.48
1:A:14:LYS:CE	1:A:248:DCY:HB2	2.44	0.47
1:A:60:GLY:HA2	4:A:454:HOH:O	2.13	0.47
1:A:144:MET:HE3	1:A:145:LEU:CG	2.44	0.47
2:B:189[B]:ARG:HB3	2:B:189[B]:ARG:NH1	2.29	0.47
2:B:89:GLU:O	2:B:117:LYS:HA	2.16	0.46
2:B:179:TRP:CD2	3:B:400[A]:CQA:H181	2.50	0.46
1:A:181:LYS:N	1:A:181:LYS:HE3	2.31	0.46
1:A:123:TYR:O	1:A:127:MET:HG2	2.16	0.46
1:A:64:GLY:O	1:A:67:ASP:HB2	2.15	0.46
1:A:58:SER:HB3	1:A:87:VAL:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ASN:CA	2:B:109[B]:GLU:OE2	2.63	0.45
2:B:33:GLN:HE21	2:B:37:ASP:CG	2.21	0.45
4:A:517:HOH:O	2:B:100:GLU:HG2	2.17	0.45
2:B:36:MET:O	2:B:41:PRO:HD3	2.17	0.44
1:A:14:LYS:NZ	1:A:249:ASN:ND2	2.64	0.44
1:A:246:GLU:OE1	3:A:402:CQA:H203	2.17	0.44
2:B:46:ARG:HA	2:B:78:TYR:OH	2.17	0.44
2:B:183:TRP:HB3	3:B:401:CQA:C12	2.48	0.44
1:A:7:SER:O	1:A:248:DCY:SG	2.76	0.44
2:B:71:LEU:HD21	2:B:85:ASN:OD1	2.18	0.44
1:A:63:ALA:O	1:A:98:TYR:HA	2.18	0.44
2:B:164:THR:HG22	2:B:165:ASN:ND2	2.33	0.44
2:B:124:GLN:HG3	2:B:157:PHE:CG	2.53	0.43
1:A:198:TYR:CD1	1:A:198:TYR:N	2.84	0.43
2:B:183:TRP:CZ2	3:B:400[A]:CQA:H183	2.54	0.43
3:B:401:CQA:H9	4:B:483:HOH:O	2.18	0.43
1:A:249:ASN:HB3	1:A:252:ALA:HB3	2.01	0.43
1:A:250:PHE:HZ	1:A:262:LEU:HD12	1.83	0.43
2:B:263:GLY:O	2:B:267:GLN:NE2	2.50	0.43
1:A:189:ARG:CD	1:A:258:LEU:HD13	2.47	0.43
1:A:182:LEU:HA	1:A:271:PHE:HE2	1.83	0.43
1:A:105:THR:HB	1:A:108:LEU:CD1	2.49	0.42
1:A:141:MET:CE	1:A:158:PHE:CD2	3.01	0.42
2:B:69:GLN:HA	2:B:69:GLN:OE1	2.19	0.42
2:B:36:MET:HA	2:B:40:LEU:HB2	2.01	0.42
1:A:173:VAL:HG11	3:A:402:CQA:H181	2.01	0.42
2:B:124:GLN:HG3	2:B:157:PHE:CD2	2.54	0.42
1:A:231:ILE:O	1:A:232:ASP:C	2.58	0.42
1:A:8:LEU:HG	1:A:15:TYR:HD1	1.85	0.42
1:A:229:CYS:SG	1:A:240:LEU:HB2	2.60	0.42
1:A:55:LYS:HB3	1:A:136:TRP:CE3	2.56	0.41
1:A:190:PHE:HA	1:A:191:PRO:HD3	1.87	0.41
1:A:172:VAL:HG21	1:A:204:LEU:HD22	2.01	0.41
1:A:124:GLN:HG3	1:A:157:PHE:CD2	2.56	0.41
2:B:139:ILE:O	2:B:168:MET:HA	2.20	0.41
1:A:278:LYS:HG3	4:A:529:HOH:O	2.20	0.41
2:B:199:ILE:HD12	2:B:204:LEU:HD23	2.03	0.40
2:B:32:MET:O	2:B:36:MET:HG2	2.22	0.40

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	285/292 (98%)	267 (94%)	17 (6%)	1 (0%)	34	42
2	B	288/292 (99%)	279 (97%)	7 (2%)	2 (1%)	22	26
All	All	573/584 (98%)	546 (95%)	24 (4%)	3 (0%)	29	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	110	ASN
2	B	232	ASP
1	A	232	ASP

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	235/258 (91%)	227 (97%)	8 (3%)	37	51
2	B	241/259 (93%)	238 (99%)	3 (1%)	71	84
All	All	476/517 (92%)	465 (98%)	11 (2%)	53	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	29[A]	HIS
1	A	29[B]	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	46	ARG
1	A	98	TYR
1	A	144	MET
1	A	167	LYS
1	A	181	LYS
2	B	98	TYR
2	B	204	LEU
2	B	259	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	165	ASN
1	A	236	ASN
1	A	249	ASN
2	B	77	GLN
2	B	165	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	CSO	B	82[B]	2	4,5,7	0.67	0	1,5,8	0.32	0
2	CSO	B	82[A]	2	3,6,7	0.73	0	0,6,8	-	-
1	CSO	A	217	1	3,6,7	0.68	0	0,6,8	-	-

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	CSO	B	82[B]	2	-	0/1/4/7	-
2	CSO	B	82[A]	2	-	0/1/5/7	-
1	DCY	A	248	1	1/1/1/2	-	-
1	CSO	A	217	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	248	DCY	CA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	217	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	248	DCY	6	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	CQA	A	402	-	27,27,27	3.02	15 (55%)	37,37,37	3.84	10 (27%)
3	CQA	B	400[C]	-	25,25,27	3.05	15 (60%)	33,34,37	2.80	8 (24%)
3	CQA	B	400[B]	-	25,25,27	3.05	15 (60%)	33,34,37	2.78	8 (24%)
3	CQA	B	400[A]	-	25,25,27	3.05	15 (60%)	33,34,37	2.75	7 (21%)
3	CQA	A	403	-	25,25,27	3.19	17 (68%)	33,34,37	1.00	3 (9%)
3	CQA	B	401	-	23,23,27	3.30	16 (69%)	32,32,37	1.01	2 (6%)

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	CQA	A	402	-	-	5/12/12/12	0/3/3/3
3	CQA	B	400[C]	-	-	4/8/8/12	0/3/3/3
3	CQA	B	400[B]	-	-	3/8/8/12	0/3/3/3
3	CQA	B	400[A]	-	-	4/8/8/12	0/3/3/3
3	CQA	A	403	-	-	1/8/8/12	0/3/3/3
3	CQA	B	401	-	-	1/6/6/12	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	CQA	O-C13	8.24	1.53	1.36
3	B	401	CQA	O-C13	8.00	1.52	1.36
3	A	402	CQA	O-C13	7.98	1.52	1.36
3	B	400[A]	CQA	O-C13	7.81	1.52	1.36
3	B	400[B]	CQA	O-C13	7.81	1.52	1.36
3	B	400[C]	CQA	O-C13	7.81	1.52	1.36
3	A	402	CQA	C13-C14	4.94	1.47	1.40
3	B	400[A]	CQA	C13-C14	4.76	1.47	1.40
3	B	400[B]	CQA	C13-C14	4.76	1.47	1.40
3	B	400[C]	CQA	C13-C14	4.76	1.47	1.40
3	A	403	CQA	C6-C1	4.31	1.45	1.36
3	B	400[A]	CQA	C3-C2	4.30	1.45	1.36
3	B	400[B]	CQA	C3-C2	4.30	1.45	1.36
3	B	400[C]	CQA	C3-C2	4.30	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	CQA	C6-C1	4.19	1.44	1.36
3	B	401	CQA	C3-C2	4.18	1.45	1.36
3	B	401	CQA	C13-C14	4.16	1.46	1.40
3	A	403	CQA	C3-C2	4.10	1.45	1.36
3	A	402	CQA	C3-C2	4.09	1.45	1.36
3	A	403	CQA	C13-C14	4.00	1.45	1.40
3	A	402	CQA	C6-C1	3.93	1.44	1.36
3	B	401	CQA	C7-N2	3.91	1.49	1.38
3	A	403	CQA	C15-C10	3.88	1.45	1.39
3	B	400[A]	CQA	C2-C1	3.86	1.45	1.38
3	B	400[B]	CQA	C2-C1	3.86	1.45	1.38
3	B	400[C]	CQA	C2-C1	3.86	1.45	1.38
3	A	402	CQA	C7-N2	3.84	1.49	1.38
3	A	402	CQA	C8-C7	3.83	1.46	1.38
3	B	400[A]	CQA	C8-C7	3.76	1.46	1.38
3	B	400[B]	CQA	C8-C7	3.76	1.46	1.38
3	B	400[C]	CQA	C8-C7	3.76	1.46	1.38
3	B	401	CQA	C2-C1	3.76	1.45	1.38
3	A	402	CQA	C2-C1	3.75	1.45	1.38
3	A	403	CQA	C7-N2	3.66	1.48	1.38
3	B	401	CQA	C10-N2	3.65	1.48	1.40
3	B	400[A]	CQA	C7-N2	3.57	1.48	1.38
3	B	400[B]	CQA	C7-N2	3.57	1.48	1.38
3	B	400[C]	CQA	C7-N2	3.57	1.48	1.38
3	B	400[A]	CQA	C6-C1	3.48	1.43	1.36
3	B	400[B]	CQA	C6-C1	3.48	1.43	1.36
3	B	400[C]	CQA	C6-C1	3.48	1.43	1.36
3	A	403	CQA	C2-C1	3.47	1.44	1.38
3	B	401	CQA	C15-C14	3.44	1.45	1.39
3	A	403	CQA	C15-C14	3.41	1.45	1.39
3	B	400[A]	CQA	C12-C13	3.37	1.45	1.39
3	B	400[B]	CQA	C12-C13	3.37	1.45	1.39
3	B	400[C]	CQA	C12-C13	3.37	1.45	1.39
3	B	401	CQA	C8-C7	3.36	1.45	1.38
3	B	401	CQA	C15-C10	3.32	1.44	1.39
3	B	401	CQA	C11-C10	3.28	1.44	1.39
3	A	403	CQA	C12-C13	3.27	1.45	1.39
3	A	403	CQA	C8-C7	3.27	1.45	1.38
3	A	403	CQA	C10-N2	3.27	1.48	1.40
3	B	400[A]	CQA	C10-N2	3.25	1.48	1.40
3	B	400[B]	CQA	C10-N2	3.25	1.48	1.40
3	B	400[C]	CQA	C10-N2	3.25	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400[A]	CQA	C12-C11	3.24	1.44	1.38
3	B	400[B]	CQA	C12-C11	3.24	1.44	1.38
3	B	400[C]	CQA	C12-C11	3.24	1.44	1.38
3	A	403	CQA	C12-C11	3.19	1.44	1.38
3	A	402	CQA	C12-C13	3.16	1.45	1.39
3	A	402	CQA	C10-N2	3.14	1.47	1.40
3	A	402	CQA	C12-C11	3.14	1.44	1.38
3	A	403	CQA	C11-C10	3.07	1.44	1.39
3	A	402	CQA	C9-N1	3.05	1.38	1.32
3	A	403	CQA	C9-N1	3.02	1.38	1.32
3	B	401	CQA	C12-C11	2.98	1.44	1.38
3	B	401	CQA	C9-N1	2.96	1.38	1.32
3	A	402	CQA	C11-C10	2.93	1.44	1.39
3	B	400[A]	CQA	C11-C10	2.87	1.44	1.39
3	B	400[B]	CQA	C11-C10	2.87	1.44	1.39
3	B	400[C]	CQA	C11-C10	2.87	1.44	1.39
3	B	400[A]	CQA	C9-N1	2.77	1.38	1.32
3	B	400[B]	CQA	C9-N1	2.77	1.38	1.32
3	B	400[C]	CQA	C9-N1	2.77	1.38	1.32
3	A	402	CQA	C15-C10	2.72	1.43	1.39
3	B	401	CQA	C8-C9	2.67	1.44	1.38
3	A	403	CQA	C8-C9	2.62	1.43	1.38
3	B	401	CQA	C12-C13	2.60	1.44	1.39
3	A	402	CQA	C4-C5	2.59	1.46	1.42
3	B	401	CQA	C4-C5	2.52	1.46	1.42
3	B	400[A]	CQA	C15-C10	2.51	1.43	1.39
3	B	400[B]	CQA	C15-C10	2.51	1.43	1.39
3	B	400[C]	CQA	C15-C10	2.51	1.43	1.39
3	A	403	CQA	C4-C5	2.40	1.46	1.42
3	A	402	CQA	C8-C9	2.21	1.43	1.38
3	B	400[A]	CQA	C8-C9	2.15	1.42	1.38
3	B	400[B]	CQA	C8-C9	2.15	1.42	1.38
3	B	400[C]	CQA	C8-C9	2.15	1.42	1.38
3	B	400[A]	CQA	C4-C5	2.15	1.46	1.42
3	B	400[B]	CQA	C4-C5	2.15	1.46	1.42
3	B	400[C]	CQA	C4-C5	2.15	1.46	1.42
3	A	403	CQA	C6-C5	2.06	1.45	1.41

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	CQA	C16-C14-C13	-15.01	105.49	120.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400[A]	CQA	C16-C14-C13	-11.04	105.35	120.00
3	B	400[B]	CQA	C16-C14-C13	-11.04	105.35	120.00
3	B	400[C]	CQA	C16-C14-C13	-11.04	105.35	120.00
3	A	402	CQA	C14-C16-N3	10.63	131.35	112.75
3	A	402	CQA	C16-C14-C15	8.60	135.70	120.38
3	B	400[A]	CQA	C16-C14-C15	7.72	135.28	120.41
3	B	400[B]	CQA	C16-C14-C15	7.72	135.28	120.41
3	B	400[C]	CQA	C16-C14-C15	7.72	135.28	120.41
3	A	402	CQA	C20-C19-N3	6.06	156.27	114.37
3	A	402	CQA	C16-N3-C17	-5.13	94.58	111.57
3	A	402	CQA	C18-C17-N3	4.63	146.40	114.37
3	B	400[A]	CQA	C14-C16-N3	3.98	134.95	114.41
3	B	400[B]	CQA	C14-C16-N3	3.98	134.95	114.41
3	B	400[C]	CQA	C14-C16-N3	3.98	134.95	114.41
3	B	400[C]	CQA	C18-C17-N3	3.59	164.47	115.79
3	B	400[B]	CQA	C18-C17-N3	3.08	157.66	115.79
3	A	402	CQA	C16-N3-C19	-2.93	101.87	111.57
3	B	400[A]	CQA	C10-N2-C7	-2.77	119.84	126.71
3	B	400[B]	CQA	C10-N2-C7	-2.77	119.84	126.71
3	B	400[C]	CQA	C10-N2-C7	-2.77	119.84	126.71
3	A	402	CQA	C10-N2-C7	-2.61	120.23	126.71
3	A	403	CQA	C14-C16-N3	2.37	126.65	114.41
3	B	400[A]	CQA	C9-N1-C5	2.19	120.32	116.93
3	B	400[B]	CQA	C9-N1-C5	2.19	120.32	116.93
3	B	400[C]	CQA	C9-N1-C5	2.19	120.32	116.93
3	B	401	CQA	C7-C4-C5	2.18	119.44	118.06
3	B	400[A]	CQA	C6-C1-CL	-2.10	117.01	119.64
3	B	400[B]	CQA	C6-C1-CL	-2.10	117.01	119.64
3	B	400[C]	CQA	C6-C1-CL	-2.10	117.01	119.64
3	A	403	CQA	C9-C8-C7	-2.09	118.56	119.60
3	A	402	CQA	O-C13-C14	2.07	124.21	118.89
3	B	401	CQA	C9-C8-C7	-2.05	118.58	119.60
3	A	403	CQA	C7-C4-C5	2.03	119.34	118.06
3	B	400[A]	CQA	O-C13-C14	2.02	124.07	118.89
3	B	400[B]	CQA	O-C13-C14	2.02	124.07	118.89
3	B	400[C]	CQA	O-C13-C14	2.02	124.07	118.89
3	A	402	CQA	C9-N1-C5	2.02	120.06	116.93

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	400[C]	CQA	C18-C17-N3-C16
3	B	401	CQA	C13-C14-C16-N3
3	B	400[B]	CQA	C14-C16-N3-C17
3	A	402	CQA	C14-C16-N3-C17
3	B	400[C]	CQA	C14-C16-N3-C17
3	B	400[A]	CQA	C14-C16-N3-C17
3	A	402	CQA	C14-C16-N3-C19
3	A	402	CQA	C18-C17-N3-C19
3	A	402	CQA	C11-C10-N2-C7
3	A	403	CQA	C20-C19-N3-C16
3	B	400[A]	CQA	C18-C17-N3-C16
3	A	402	CQA	C15-C10-N2-C7
3	B	400[A]	CQA	C15-C10-N2-C7
3	B	400[B]	CQA	C15-C10-N2-C7
3	B	400[C]	CQA	C15-C10-N2-C7
3	B	400[A]	CQA	C11-C10-N2-C7
3	B	400[B]	CQA	C11-C10-N2-C7
3	B	400[C]	CQA	C11-C10-N2-C7

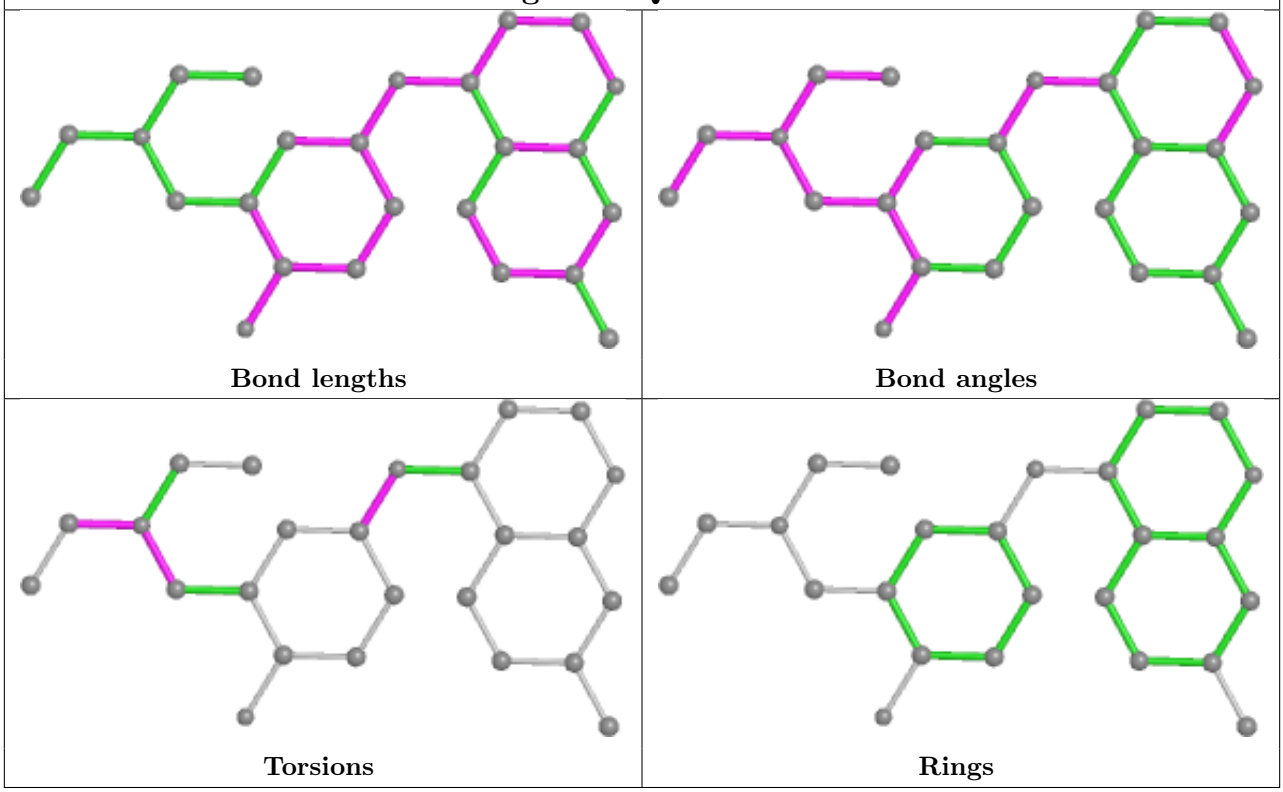
There are no ring outliers.

5 monomers are involved in 14 short contacts:

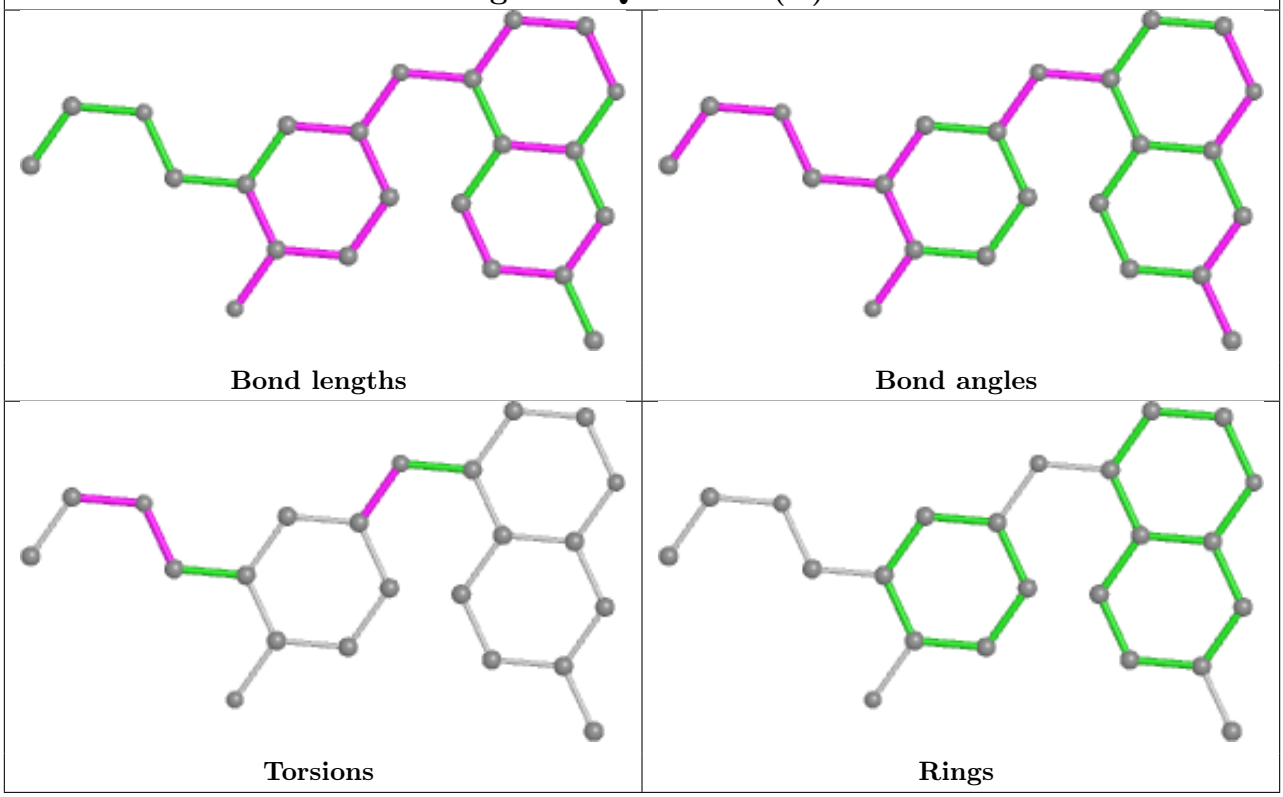
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	CQA	4	0
3	B	400[C]	CQA	1	0
3	B	400[A]	CQA	3	0
3	A	403	CQA	3	0
3	B	401	CQA	3	0

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.

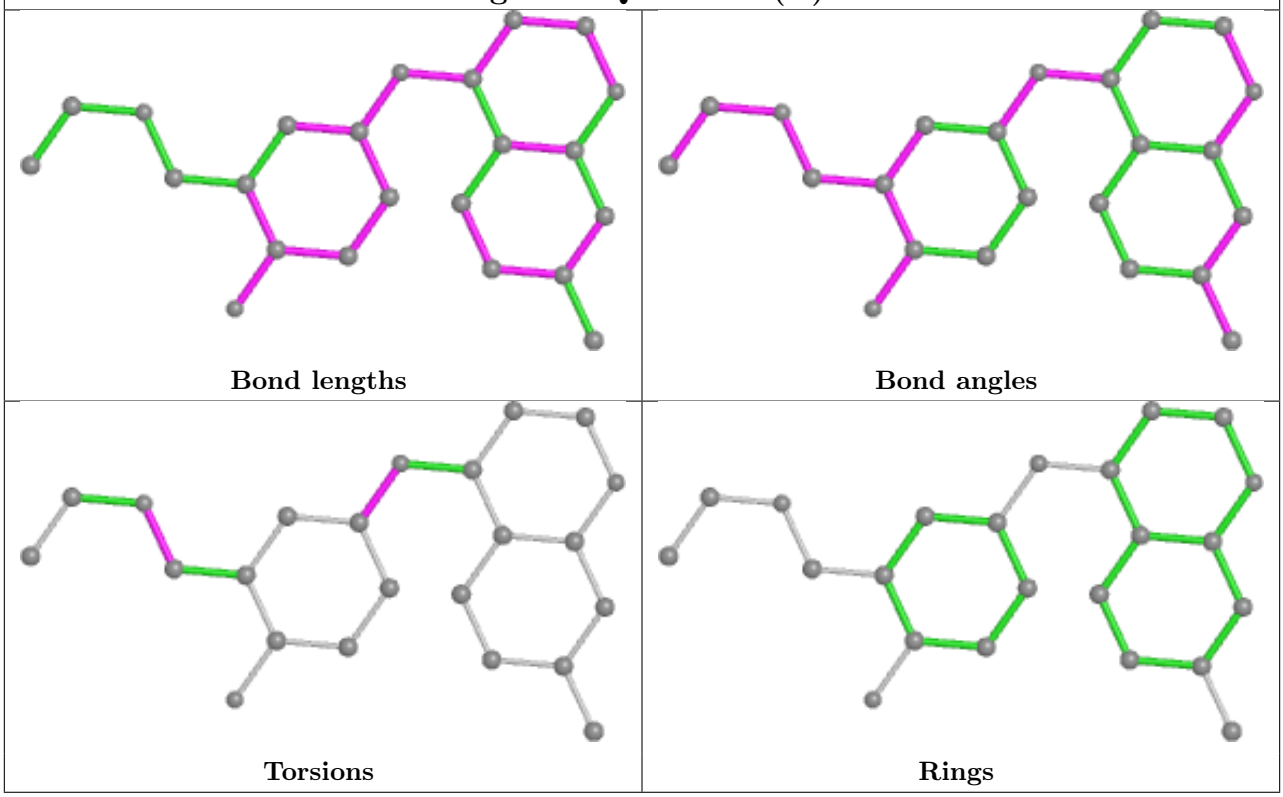
Ligand CQA A 402



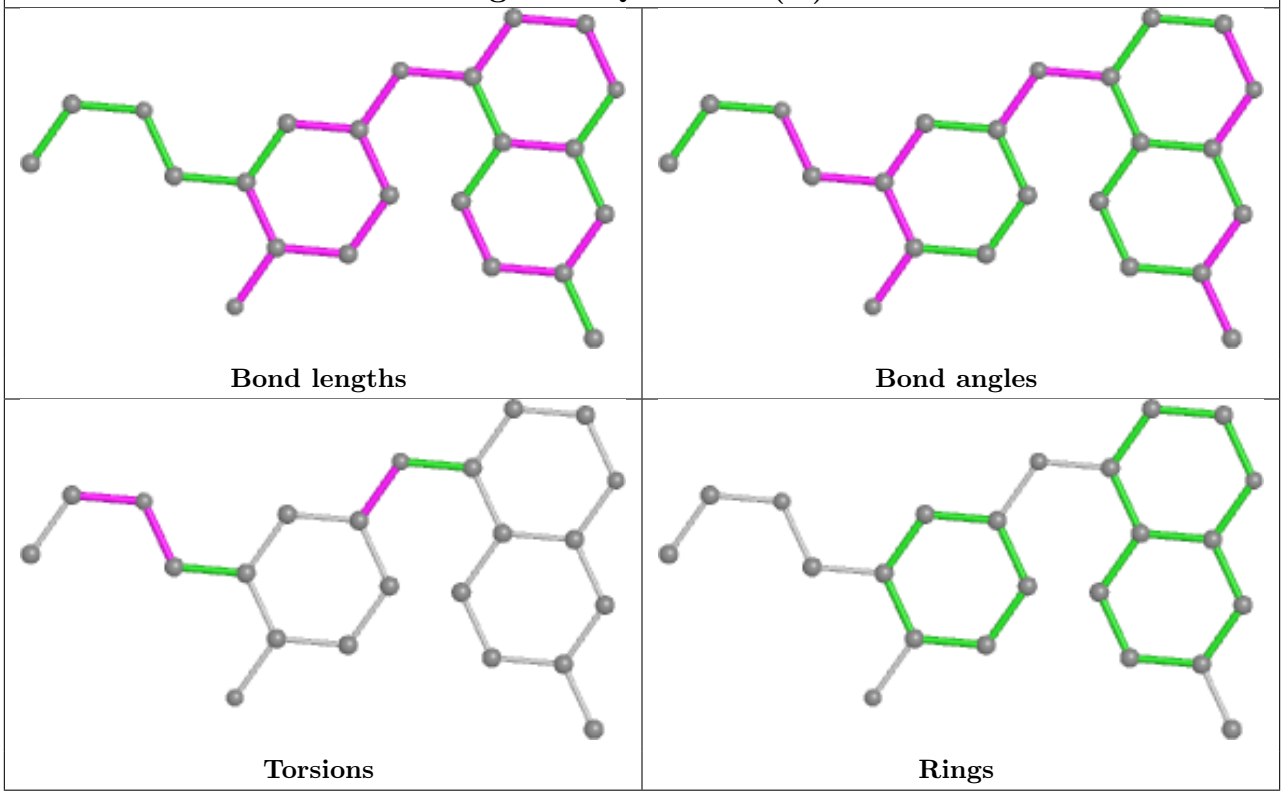
Ligand CQA B 400 (C)



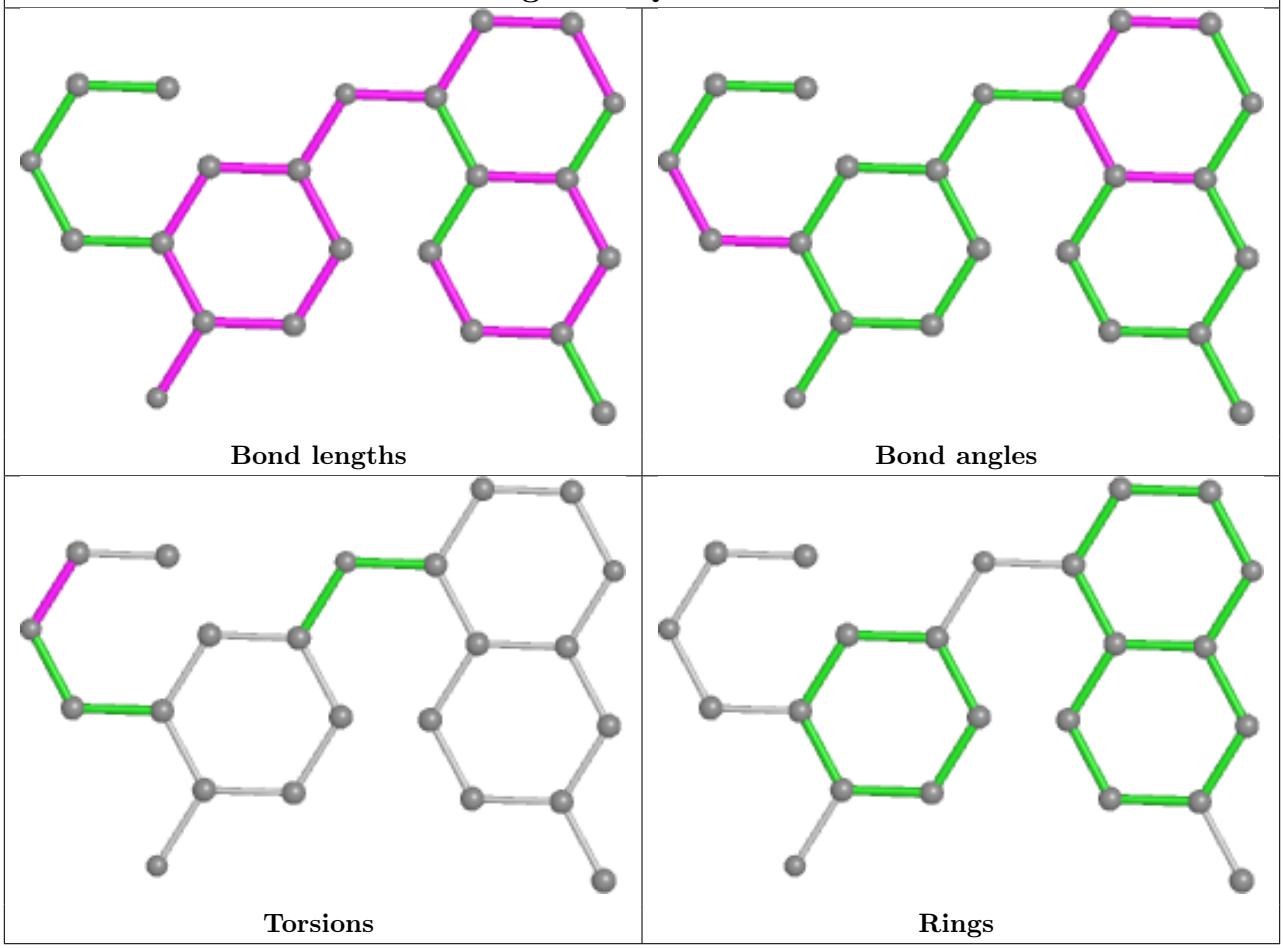
Ligand CQA B 400 (B)



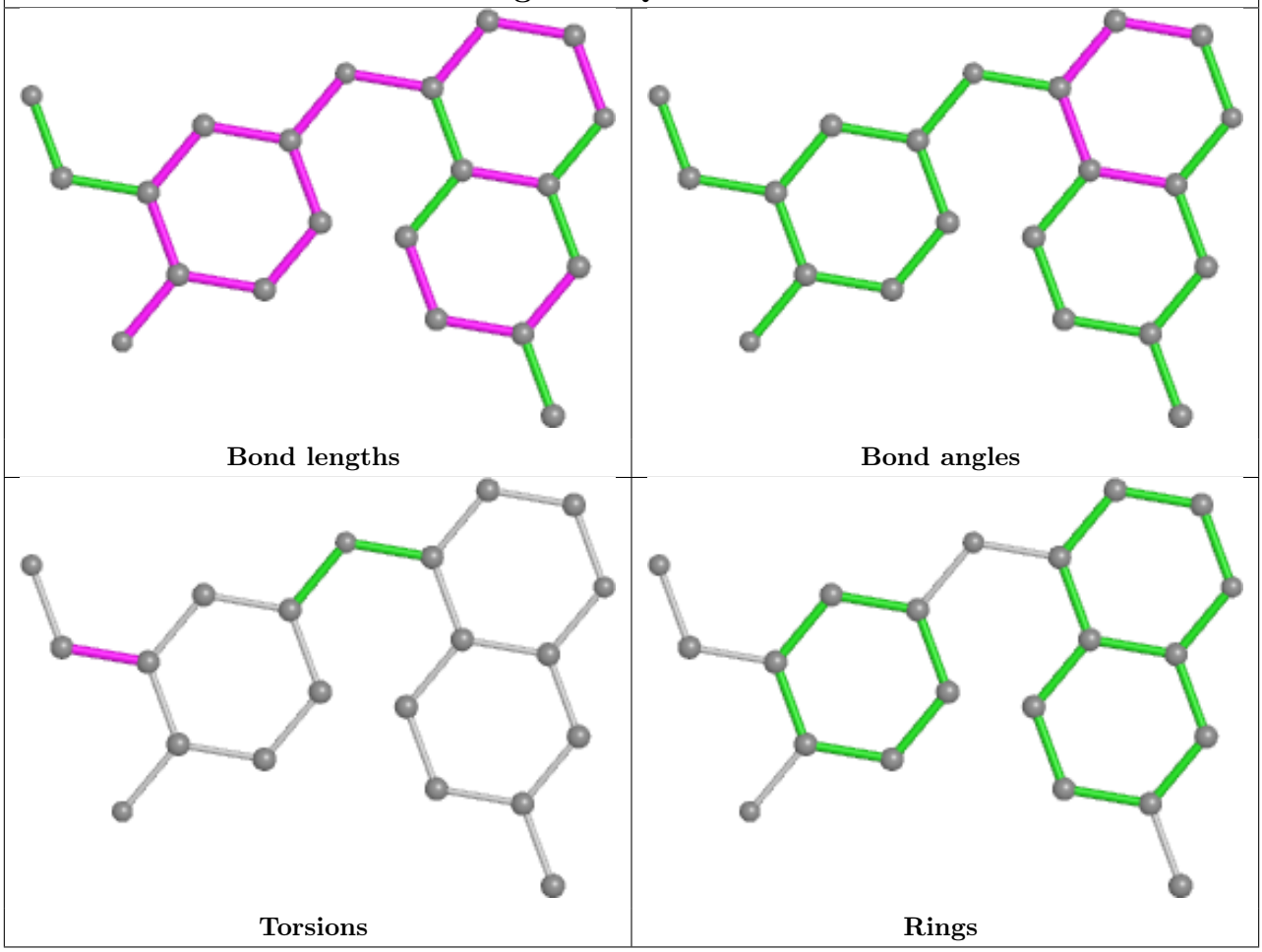
Ligand CQA B 400 (A)



Ligand CQA A 403



Ligand CQA B 401



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.