



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:48 AM UTC

PDB ID : 1XI2 / pdb_00001xi2
Title : Quinone Reductase 2 in Complex with Cancer Prodrug CB1954
Authors : Fu, Y.; Buryanovskyy, L.; Zhang, Z.
Deposited on : 2004-09-21
Resolution : 1.50 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 ⓘ 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) : 2.49

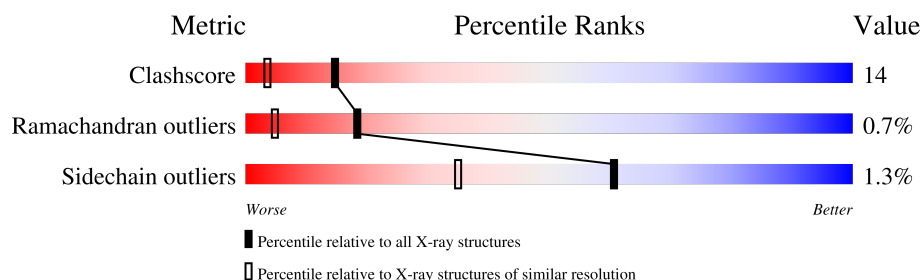
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)

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	230	 74% 23% •
1	B	230	 80% 18% •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4155 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.

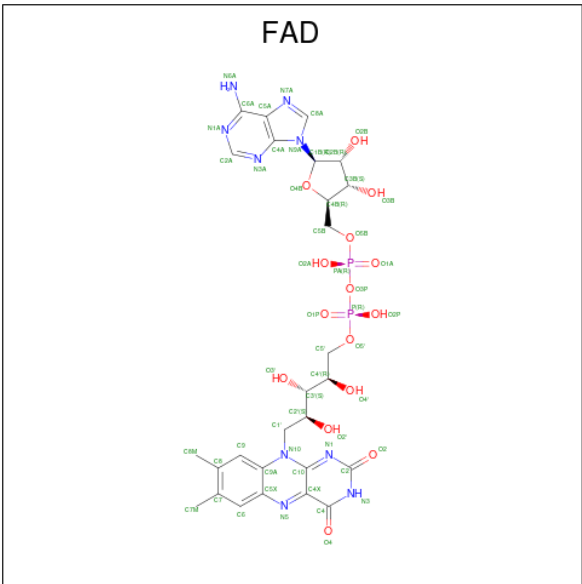
- Molecule 1 is a protein called NRH dehydrogenase [quinone] 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1824	1174	304	338	8			
1	B	230	Total	C	N	O	S	0	0	0
			1824	1174	304	338	8			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

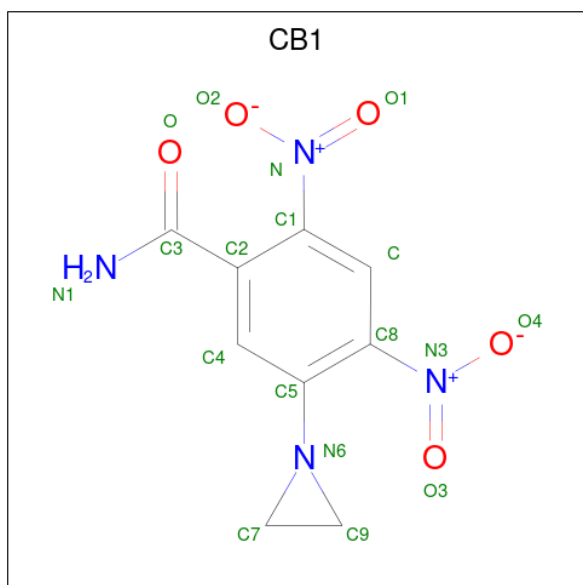
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 5-(AZIRIDIN-1-YL)-2,4-DINITROBENZAMIDE (CCD ID: CB1) (formula: $C_9H_8N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	9	4	5		
4	B	1	Total	C	N	O	0	0
			18	9	4	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total	O	0	0
			156	156		
5	B	206	Total	O	0	0
			206	206		

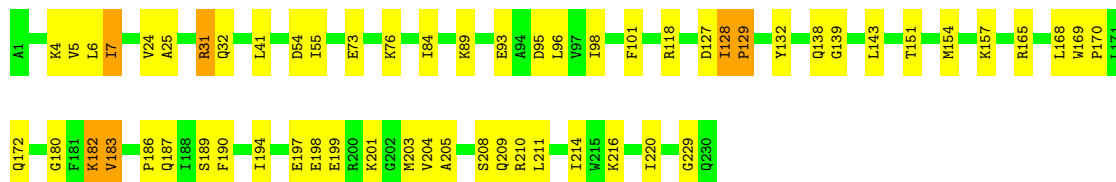
3 Residue-property plots

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.

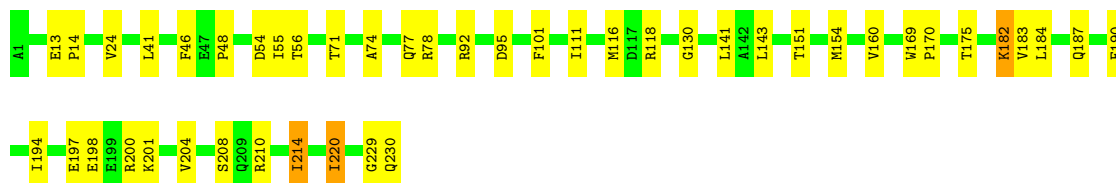
• Molecule 1: NRH dehydrogenase [quinone] 2

Chain A: 



• Molecule 1: NRH dehydrogenase [quinone] 2

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.47Å 106.45Å 56.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.20 – 1.50	Depositor
% Data completeness (in resolution range)	(Not available) (35.20-1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4155	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: ZN, FAD, CB1

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	0.32	0/1874	0.87	5/2542 (0.2%)
1	B	0.34	0/1874	0.88	5/2542 (0.2%)
All	All	0.33	0/3748	0.88	10/5084 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	LYS	N-CA-C	-8.62	95.63	109.76
1	A	101	PHE	N-CA-C	8.26	115.66	108.22
1	B	101	PHE	N-CA-C	8.16	115.57	108.22
1	A	182	LYS	N-CA-C	-6.87	98.06	109.46
1	A	41	LEU	N-CA-C	5.89	118.18	111.11
1	A	183	VAL	N-CA-C	5.83	116.50	107.99
1	B	95	ASP	N-CA-C	-5.71	106.44	113.41
1	A	95	ASP	N-CA-C	-5.61	106.56	113.41
1	B	41	LEU	N-CA-C	5.58	117.81	111.11
1	B	190	PHE	N-CA-C	5.02	118.13	110.20

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	1824	0	1779	58	0
1	B	1824	0	1779	40	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	1	0
4	A	18	0	8	3	0
4	B	18	0	8	3	0
5	A	156	0	0	1	0
5	B	206	0	0	4	0
All	All	4155	0	3636	103	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 14.

All (103) 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:128:ILE:HG23	1:A:129:PRO:HD3	1.30	1.11
1:A:31:ARG:HH11	1:A:31:ARG:HB3	1.16	1.10
1:B:151:THR:H	1:B:154:MET:HE3	1.22	1.04
1:A:211:LEU:HA	1:A:214:ILE:HG23	1.52	0.90
1:B:116:MET:HE2	1:B:175:THR:HG21	1.53	0.88
1:B:48:PRO:HG3	1:B:111:ILE:HD12	1.66	0.78
1:A:128:ILE:CG2	1:A:129:PRO:HD3	2.14	0.74
1:A:187:GLN:HE21	1:A:210:ARG:HH11	1.37	0.73
1:A:31:ARG:HB3	1:A:31:ARG:NH1	2.00	0.73
1:B:187:GLN:HE21	1:B:210:ARG:HH11	1.35	0.72
1:B:48:PRO:HG3	1:B:111:ILE:CD1	2.20	0.71
1:A:211:LEU:HA	1:A:214:ILE:CG2	2.19	0.70
1:B:46:PHE:O	1:B:111:ILE:HD11	1.91	0.70
1:A:151:THR:H	1:A:154:MET:HE3	1.57	0.70
4:A:501:CB1:H91	5:B:1395:HOH:O	1.92	0.69
1:A:31:ARG:HH11	1:A:31:ARG:CB	2.01	0.68
1:B:151:THR:N	1:B:154:MET:HE3	2.05	0.68
1:B:214:ILE:HD13	1:B:214:ILE:O	1.93	0.66
1:A:96:LEU:HG	1:A:98:ILE:CD1	2.26	0.66
1:A:169:TRP:HB3	1:A:170:PRO:HD3	1.79	0.65
1:A:199:GLU:O	1:A:203:MET:HG3	1.97	0.65
1:A:211:LEU:HD23	1:A:214:ILE:HG21	1.80	0.64
1:B:24:VAL:CG1	1:B:208:SER:HB3	2.27	0.64
1:B:184:LEU:CD1	1:B:214:ILE:HD11	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ILE:HD12	1:B:74:ALA:CB	2.30	0.62
1:A:7:ILE:HD12	1:A:7:ILE:N	2.15	0.61
1:A:139:GLY:H	1:A:182:LYS:HZ2	1.50	0.60
1:A:84:ILE:HD11	1:A:118:ARG:HB3	1.83	0.59
1:A:96:LEU:HG	1:A:98:ILE:HD11	1.84	0.59
1:A:139:GLY:H	1:A:182:LYS:NZ	2.01	0.58
1:A:194:ILE:HG12	5:A:1312:HOH:O	2.04	0.58
3:B:1233:FAD:C9A	4:B:502:CB1:H92	2.34	0.58
1:B:24:VAL:HG21	1:B:204:VAL:CG1	2.34	0.57
1:A:76:LYS:HB2	1:A:76:LYS:HZ2	1.69	0.56
1:A:98:ILE:HD12	1:A:98:ILE:N	2.21	0.56
1:A:190:PHE:N	1:A:203:MET:HE1	2.21	0.55
1:A:187:GLN:NE2	1:A:210:ARG:HH11	2.03	0.55
1:B:187:GLN:NE2	1:B:210:ARG:HH11	2.03	0.54
1:A:151:THR:HG23	1:A:154:MET:HE3	1.89	0.54
1:A:54:ASP:OD2	1:A:118:ARG:HD2	2.08	0.54
1:B:169:TRP:HB3	1:B:170:PRO:HD3	1.90	0.53
1:B:55:ILE:HD12	1:B:74:ALA:HB2	1.91	0.53
1:A:132:TYR:CE2	1:B:160:VAL:HG22	2.45	0.52
1:B:141:LEU:HD23	1:B:182:LYS:HB2	1.91	0.52
1:A:76:LYS:HB2	1:A:76:LYS:NZ	2.24	0.51
1:B:214:ILE:HD13	1:B:214:ILE:C	2.34	0.51
1:A:96:LEU:HG	1:A:98:ILE:HD12	1.92	0.51
1:A:96:LEU:CD2	1:A:98:ILE:HD11	2.40	0.51
1:A:197:GLU:O	1:A:201:LYS:HG2	2.11	0.51
1:A:198:GLU:CD	1:A:198:GLU:H	2.19	0.51
1:B:229:GLY:O	1:B:230:GLN:HB3	2.10	0.50
1:B:182:LYS:HE3	5:B:1382:HOH:O	2.11	0.50
1:B:24:VAL:HG11	1:B:208:SER:HB3	1.93	0.50
1:A:31:ARG:HH12	1:A:32:GLN:HG3	1.76	0.49
1:A:165:ARG:HA	1:A:168:LEU:HD12	1.94	0.49
1:B:54:ASP:OD2	1:B:118:ARG:HD2	2.12	0.49
1:B:56:THR:HG23	5:B:1425:HOH:O	2.12	0.49
1:A:157:LYS:NZ	1:A:157:LYS:HB3	2.27	0.49
1:A:172:GLN:HE22	1:A:186:PRO:HD3	1.78	0.49
1:A:127:ASP:HB3	1:A:129:PRO:HD2	1.95	0.49
1:A:84:ILE:CD1	1:A:118:ARG:HB3	2.43	0.49
1:B:143:LEU:C	1:B:143:LEU:HD23	2.38	0.48
1:B:24:VAL:HG13	1:B:208:SER:HB3	1.96	0.48
1:B:46:PHE:O	1:B:111:ILE:CD1	2.59	0.48
1:B:197:GLU:HA	1:B:200:ARG:HH21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ILE:HD11	1:B:71:THR:HG22	1.94	0.48
1:A:216:LYS:N	1:A:216:LYS:HD2	2.29	0.47
1:A:25:ALA:HA	1:A:211:LEU:CD1	2.45	0.47
1:A:96:LEU:CG	1:A:98:ILE:HD11	2.45	0.47
1:A:24:VAL:HG11	1:A:208:SER:HB3	1.97	0.47
1:A:189:SER:HA	1:A:203:MET:HE2	1.97	0.47
1:A:24:VAL:CG1	1:A:208:SER:HB3	2.45	0.46
1:B:194:ILE:HG12	5:B:1287:HOH:O	2.14	0.46
4:B:502:CB1:C3	4:B:502:CB1:O2	2.63	0.46
1:B:198:GLU:H	1:B:198:GLU:CD	2.24	0.46
1:A:25:ALA:HA	1:A:211:LEU:HD13	1.97	0.46
4:A:501:CB1:O2	4:A:501:CB1:C3	2.63	0.46
1:B:151:THR:H	1:B:154:MET:CE	2.10	0.46
1:A:5:VAL:CG1	1:A:98:ILE:HD13	2.45	0.46
1:A:151:THR:OG1	1:A:154:MET:HE3	2.16	0.45
1:B:151:THR:HG23	1:B:154:MET:CE	2.48	0.44
1:A:201:LYS:O	1:A:204:VAL:HG22	2.18	0.43
1:A:138:GLN:HA	1:A:180:GLY:O	2.19	0.43
1:B:197:GLU:HG3	1:B:201:LYS:HE3	2.01	0.43
4:B:502:CB1:O3	4:B:502:CB1:C9	2.67	0.43
1:B:77:GLN:O	1:B:78:ARG:HB2	2.19	0.42
1:B:197:GLU:HA	1:B:200:ARG:HE	1.85	0.42
1:A:73:GLU:HA	1:A:76:LYS:HZ2	1.84	0.42
1:A:6:LEU:C	1:A:7:ILE:HD12	2.45	0.42
1:A:143:LEU:HD23	1:A:143:LEU:C	2.43	0.42
1:A:55:ILE:HD12	1:A:55:ILE:N	2.34	0.42
4:A:501:CB1:C9	4:A:501:CB1:O3	2.67	0.42
1:A:205:ALA:O	1:A:209:GLN:HG3	2.19	0.42
1:A:7:ILE:N	1:A:7:ILE:CD1	2.83	0.42
1:B:198:GLU:CD	1:B:198:GLU:N	2.78	0.42
1:A:183:VAL:O	1:A:220:ILE:HG12	2.20	0.41
1:A:89:LYS:O	1:A:93:GLU:HG3	2.20	0.41
1:A:204:VAL:HG23	1:A:205:ALA:N	2.34	0.41
1:A:4:LYS:HD2	1:A:93:GLU:O	2.20	0.41
1:B:151:THR:HG23	1:B:154:MET:HE3	2.02	0.41
1:B:13:GLU:HA	1:B:14:PRO:HD3	1.94	0.41
1:B:92:ARG:HG3	1:B:92:ARG:HH11	1.86	0.41
1:B:183:VAL:HB	1:B:220:ILE:CD1	2.52	0.40

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	228/230 (99%)	215 (94%)	11 (5%)	2 (1%)	14	3
1	B	228/230 (99%)	218 (96%)	9 (4%)	1 (0%)	30	12
All	All	456/460 (99%)	433 (95%)	20 (4%)	3 (1%)	18	5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	PRO
1	A	229	GLY
1	B	130	GLY

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	194/194 (100%)	191 (98%)	3 (2%)	57	31
1	B	194/194 (100%)	192 (99%)	2 (1%)	68	45
All	All	388/388 (100%)	383 (99%)	5 (1%)	61	35

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	31	ARG
1	A	128	ILE

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Mol	Chain	Res	Type
1	B	214	ILE
1	B	220	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	100	GLN
1	A	172	GLN
1	A	187	GLN
1	A	212	GLN
1	B	100	GLN
1	B	138	GLN
1	B	161	ASN
1	B	187	GLN
1	B	230	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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
4	CB1	B	502	-	19,19,19	3.13	9 (47%)	16,28,28	5.91	9 (56%)
4	CB1	A	501	-	19,19,19	3.13	9 (47%)	16,28,28	5.91	9 (56%)
3	FAD	B	1233	-	58,58,58	1.70	7 (12%)	85,89,89	1.98	14 (16%)
3	FAD	A	1234	-	58,58,58	1.61	9 (15%)	85,89,89	1.98	15 (17%)

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
4	CB1	B	502	-	-	5/12/18/18	0/2/2/2
4	CB1	A	501	-	-	5/12/18/18	0/2/2/2
3	FAD	B	1233	-	-	6/34/50/50	0/6/6/6
3	FAD	A	1234	-	-	9/34/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1233	FAD	PA-O3P	6.95	1.67	1.59
4	A	501	CB1	C8-N3	-6.65	1.33	1.45
4	B	502	CB1	C1-N	-6.64	1.33	1.45
4	A	501	CB1	C1-N	-6.63	1.33	1.45
4	B	502	CB1	C8-N3	-6.62	1.33	1.45
3	B	1233	FAD	P-O3P	6.07	1.66	1.59
3	A	1234	FAD	PA-O3P	6.02	1.66	1.59
3	A	1234	FAD	P-O3P	5.27	1.65	1.59
4	B	502	CB1	O3-N3	-5.16	1.13	1.22
4	A	501	CB1	O3-N3	-5.15	1.13	1.22
4	B	502	CB1	O1-N	-4.87	1.14	1.22
4	A	501	CB1	O1-N	-4.87	1.14	1.22
3	A	1234	FAD	C4X-N5	4.16	1.39	1.30
3	B	1233	FAD	C4X-N5	4.08	1.39	1.30
4	A	501	CB1	C5-N6	-3.66	1.33	1.41
4	B	502	CB1	C5-N6	-3.65	1.33	1.41
4	B	502	CB1	O2-N	-3.29	1.13	1.35
4	A	501	CB1	O2-N	-3.28	1.13	1.35
3	A	1234	FAD	C9A-C5X	2.78	1.45	1.41
4	A	501	CB1	O4-N3	-2.76	1.16	1.35
3	B	1233	FAD	C9A-C5X	2.75	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	CB1	O4-N3	-2.75	1.16	1.35
3	A	1234	FAD	C9A-N10	2.68	1.45	1.41
3	B	1233	FAD	C9A-N10	2.62	1.45	1.41
3	A	1234	FAD	C2A-N1A	2.61	1.38	1.33
4	A	501	CB1	C2-C3	2.58	1.53	1.50
3	B	1233	FAD	C2A-N1A	2.53	1.38	1.33
4	B	502	CB1	C2-C3	2.51	1.53	1.50
3	A	1234	FAD	C10-N1	2.43	1.38	1.33
3	A	1234	FAD	C9-C9A	2.41	1.43	1.39
3	B	1233	FAD	C10-N1	2.35	1.38	1.33
4	B	502	CB1	C9-C7	2.26	1.52	1.47
4	A	501	CB1	C9-C7	2.25	1.52	1.47
3	A	1234	FAD	C9-C8	2.12	1.42	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CB1	O-C3-C2	-16.87	100.35	120.24
4	B	502	CB1	O-C3-C2	-16.87	100.35	120.24
4	A	501	CB1	O-C3-N1	13.94	142.76	122.62
4	B	502	CB1	O-C3-N1	13.94	142.75	122.62
3	A	1234	FAD	O3P-P-O1P	-9.00	83.63	110.70
3	B	1233	FAD	O3P-P-O1P	-8.98	83.69	110.70
3	B	1233	FAD	O2P-P-O3P	-7.28	87.59	107.27
3	A	1234	FAD	O2P-P-O3P	-7.24	87.71	107.27
3	B	1233	FAD	O2A-PA-O3P	-6.25	90.38	107.27
3	A	1234	FAD	O2A-PA-O3P	-6.25	90.38	107.27
3	A	1234	FAD	O3P-PA-O1A	-6.05	92.49	110.70
3	B	1233	FAD	O3P-PA-O1A	-6.03	92.57	110.70
4	B	502	CB1	O1-N-C1	4.72	127.11	119.03
4	A	501	CB1	O1-N-C1	4.70	127.08	119.03
3	A	1234	FAD	O5'-P-O1P	4.34	126.14	108.94
4	A	501	CB1	C9-N6-C7	4.32	62.39	60.60
4	B	502	CB1	C9-N6-C7	4.29	62.38	60.60
3	B	1233	FAD	O5'-P-O1P	4.24	125.74	108.94
4	A	501	CB1	C4-C5-N6	-3.11	118.06	122.59
4	B	502	CB1	C4-C5-N6	-3.10	118.08	122.59
3	B	1233	FAD	O2A-PA-O5B	2.97	121.03	107.57
3	A	1234	FAD	O2A-PA-O5B	2.95	120.94	107.57
4	A	501	CB1	C7-C9-N6	-2.95	58.77	59.70
4	B	502	CB1	C7-C9-N6	-2.94	58.77	59.70
3	A	1234	FAD	O2A-PA-O1A	2.79	125.43	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1233	FAD	O2A-PA-O1A	2.74	125.17	112.44
4	A	501	CB1	C9-C7-N6	-2.73	58.84	59.70
4	B	502	CB1	C9-C7-N6	-2.70	58.85	59.70
3	A	1234	FAD	C4X-C10-N10	2.44	119.97	116.48
3	B	1233	FAD	C4X-C10-N10	2.42	119.94	116.48
3	B	1233	FAD	C1'-N10-C9A	2.41	125.32	120.63
3	A	1234	FAD	O4B-C1B-C2B	-2.40	101.49	106.62
3	A	1234	FAD	C1'-N10-C9A	2.36	125.22	120.63
3	B	1233	FAD	O4B-C1B-C2B	-2.35	101.58	106.62
3	B	1233	FAD	C9A-C5X-N5	-2.31	120.00	122.45
4	A	501	CB1	C2-C3-N1	-2.27	114.76	118.29
4	B	502	CB1	C2-C3-N1	-2.27	114.77	118.29
3	B	1233	FAD	O3'-C3'-C4'	-2.25	103.81	108.93
3	B	1233	FAD	N3A-C2A-N1A	-2.25	125.18	128.58
3	A	1234	FAD	N3A-C2A-N1A	-2.25	125.18	128.58
3	A	1234	FAD	C4-C4X-N5	2.24	121.31	118.21
4	A	501	CB1	O3-N3-C8	2.20	122.80	119.03
4	B	502	CB1	O3-N3-C8	2.20	122.79	119.03
3	A	1234	FAD	O3'-C3'-C4'	-2.13	104.08	108.93
3	B	1233	FAD	C4-C4X-N5	2.13	121.15	118.21
3	A	1234	FAD	C9A-C5X-N5	-2.09	120.24	122.45
3	A	1234	FAD	C10-C4X-N5	-2.01	120.70	124.81

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1234	FAD	C5B-O5B-PA-O1A
3	A	1234	FAD	C5B-O5B-PA-O3P
3	B	1233	FAD	C5B-O5B-PA-O3P
3	B	1233	FAD	C5'-O5'-P-O1P
4	A	501	CB1	C-C1-N-O1
4	A	501	CB1	C4-C5-N6-C7
4	A	501	CB1	C8-C5-N6-C7
4	A	501	CB1	C8-C5-N6-C9
4	B	502	CB1	C-C1-N-O1
4	B	502	CB1	C4-C5-N6-C7
4	B	502	CB1	C8-C5-N6-C7
4	B	502	CB1	C8-C5-N6-C9
3	A	1234	FAD	C4'-C5'-O5'-P
3	B	1233	FAD	C4'-C5'-O5'-P
4	A	501	CB1	C1-C2-C3-O

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Mol	Chain	Res	Type	Atoms
4	B	502	CB1	C1-C2-C3-O
3	A	1234	FAD	C2B-C1B-N9A-C8A
3	A	1234	FAD	C2'-C1'-N10-C10
3	A	1234	FAD	C5'-O5'-P-O3P
3	B	1233	FAD	C2'-C1'-N10-C10
3	A	1234	FAD	C4B-C5B-O5B-PA
3	B	1233	FAD	C4B-C5B-O5B-PA
3	A	1234	FAD	O4B-C1B-N9A-C8A
3	B	1233	FAD	C2B-C1B-N9A-C8A
3	A	1234	FAD	C2B-C1B-N9A-C4A

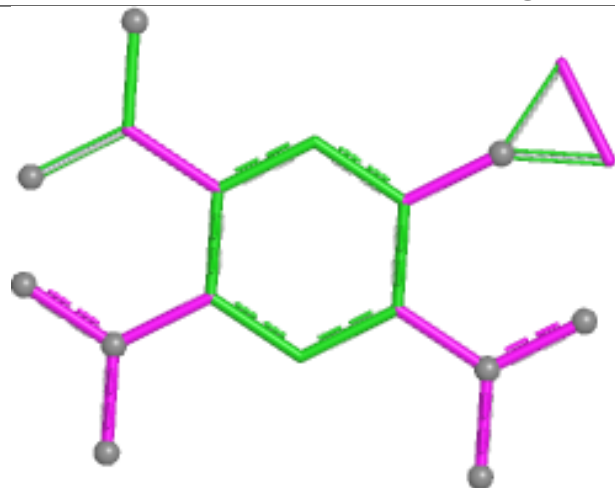
There are no ring outliers.

3 monomers are involved in 6 short contacts:

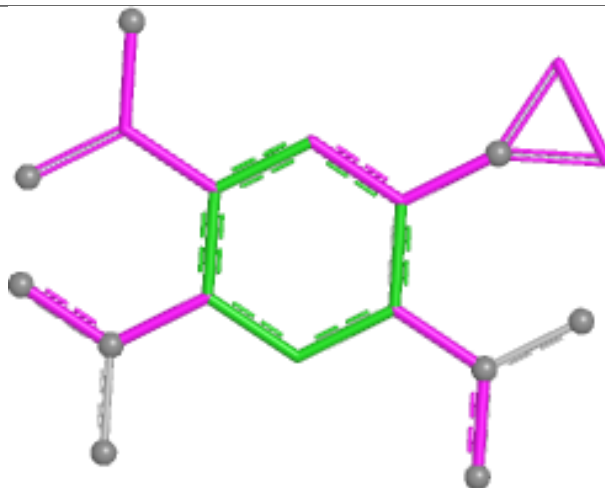
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	CB1	3	0
4	A	501	CB1	3	0
3	B	1233	FAD	1	0

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.

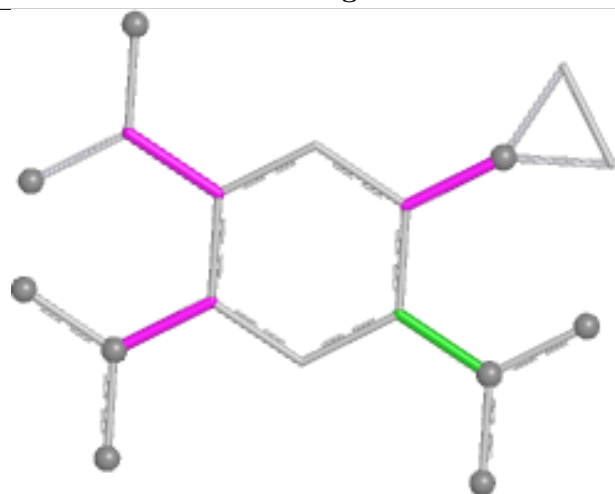
Ligand CB1 B 502



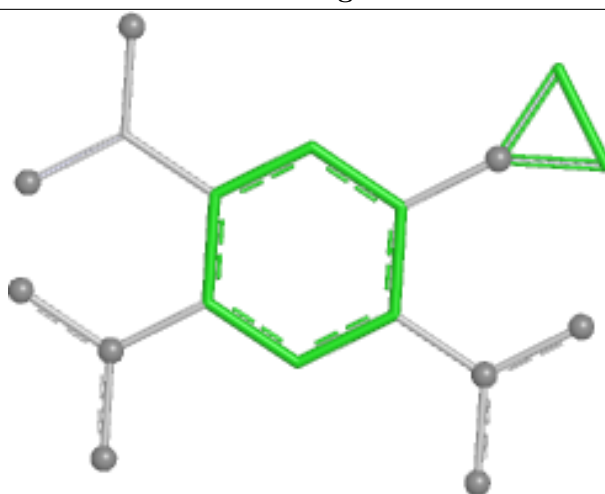
Bond lengths



Bond angles

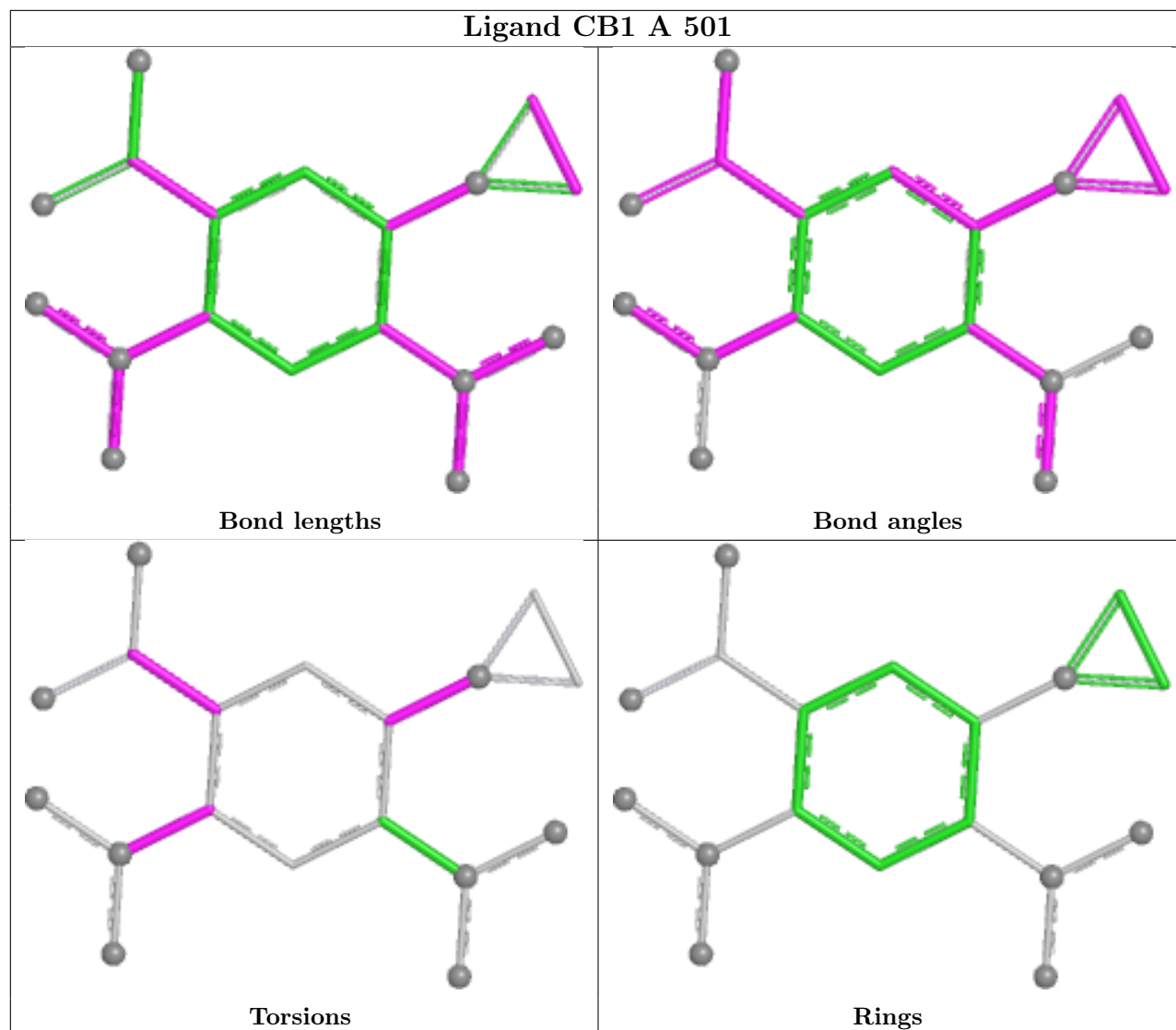


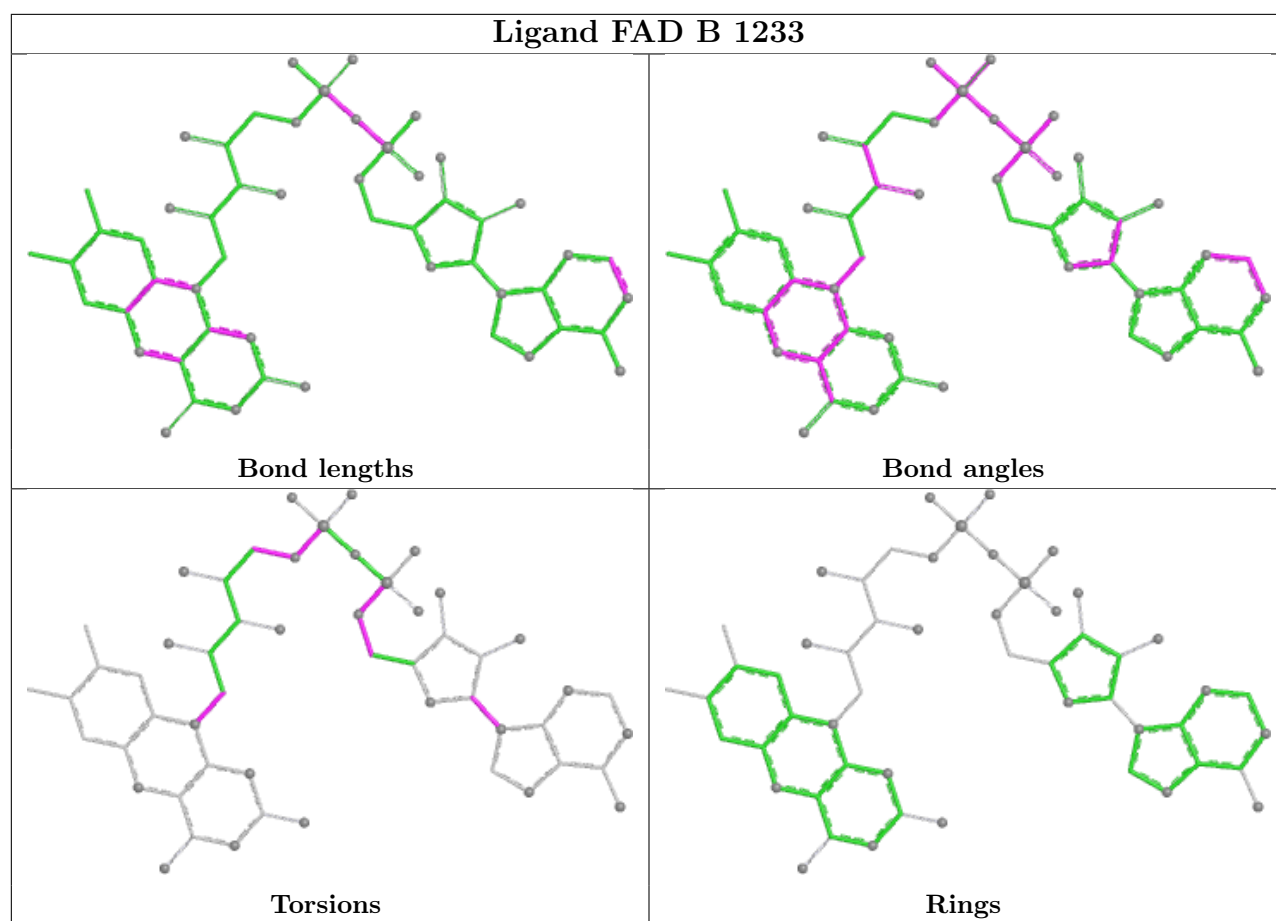
Torsions

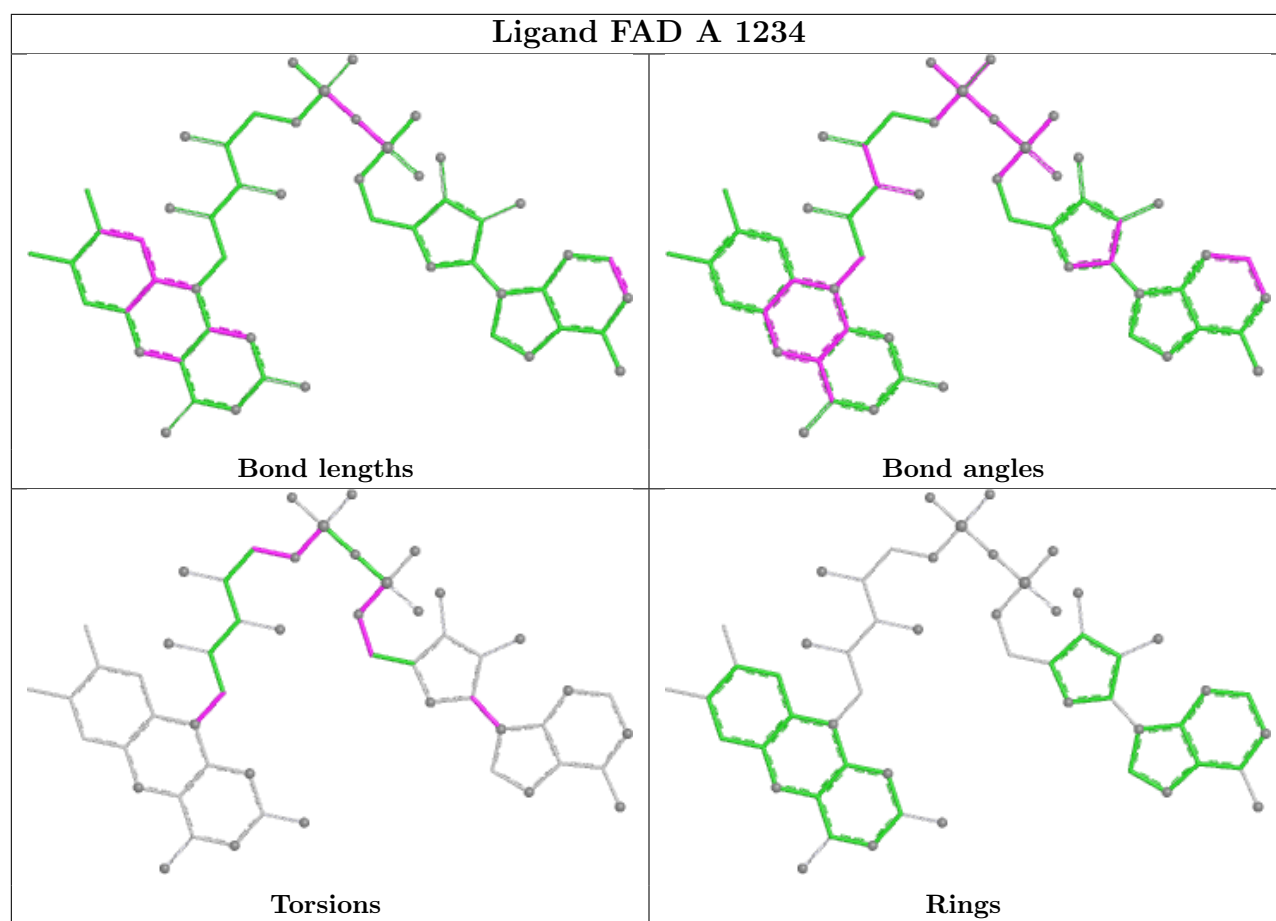


Rings

Ligand CB1 A 501







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.