



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 20, 2023 – 06:59 AM EST

PDB ID : 1VDV
Title : Bovine Milk Xanthine Dehydrogenase Y-700 Bound Form
Authors : Fukunari, A.; Okamoto, K.; Nishino, T.; Eger, B.T.; Pai, E.F.; Kamezawa, M.; Yamada, I.; Kato, N.
Deposited on : 2004-03-25
Resolution : 1.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

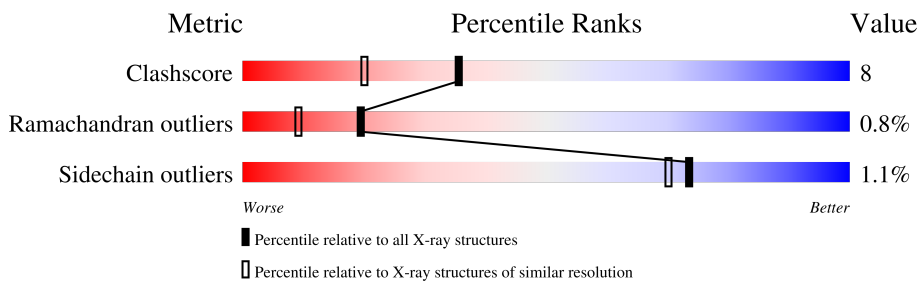
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)

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	1332	81% 15% ..
1	B	1332	83% 13% ..

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
5	MOS	B	4004	-	-	X	-
9	ACY	A	5201	-	-	X	-
9	ACY	B	5202	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22610 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 Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1299	10077	6404	1728	1884	61	0	0	0
1	B	1296	10054	6391	1724	1878	61	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P80457
B	1	MET	-	initiating methionine	UNP P80457

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

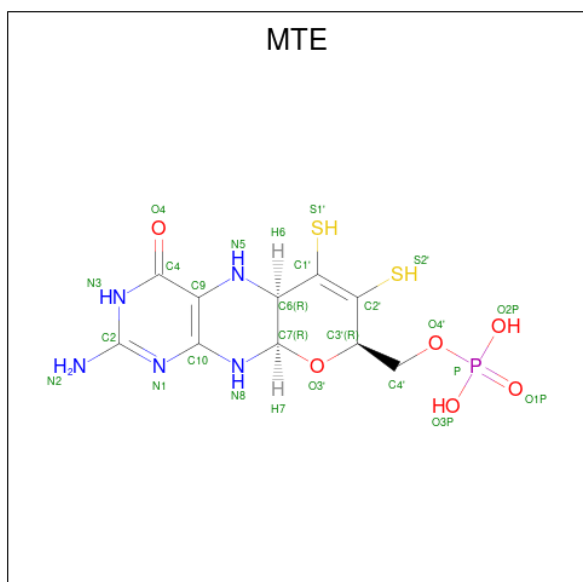
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



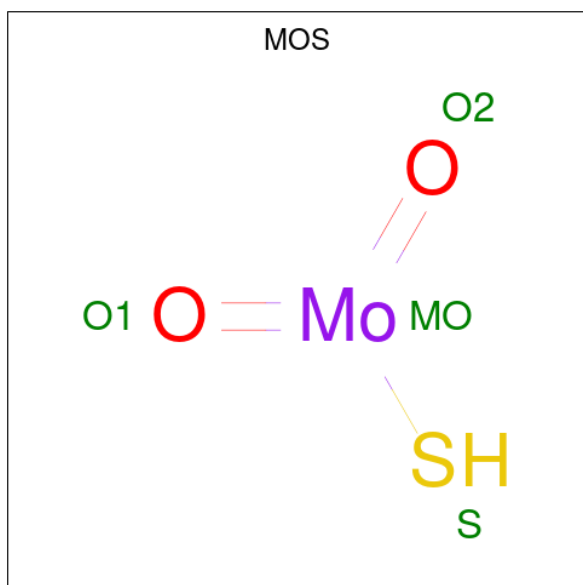
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



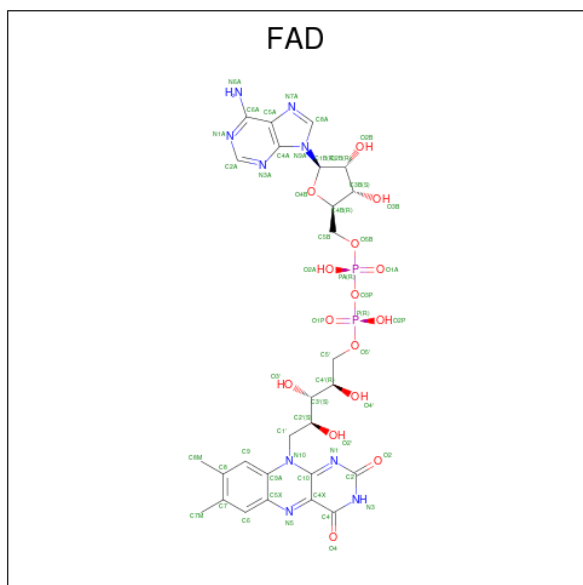
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
4	A	1	24	10	5	6	1	2	0	0
4	B	1	24	10	5	6	1	2	0	0

- Molecule 5 is DIOXOTHIO MOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO_2S).



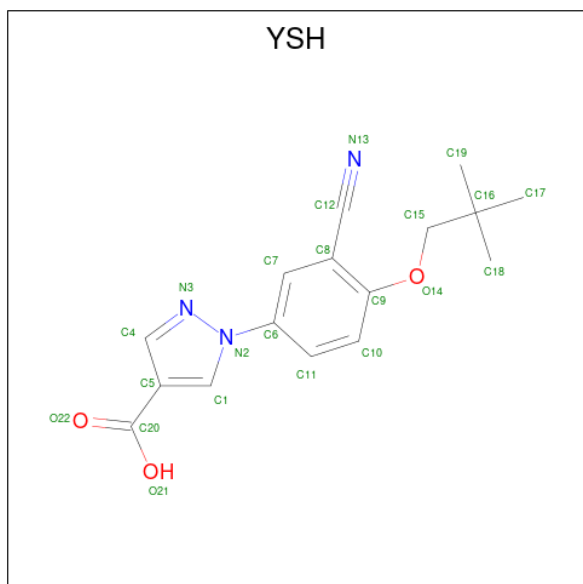
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Mo	O	S		
5	A	1	4	1	2	1	0	0
5	B	1	4	1	2	1	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 7 is 1-[3-CYANO-4-(NEOPENTYLOXY)PHENYL]-1H-PYRAZOLE-4-CARBOXYLIC ACID (three-letter code: YSH) (formula: C₁₆H₁₇N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	22	16	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
7	B	1	22	16	3	3	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



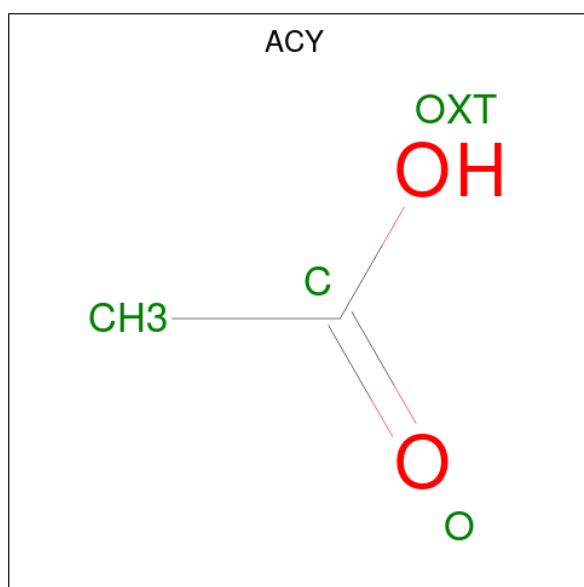
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0
8	A	1	6	3	3	0	0
8	A	1	6	3	3	0	0
8	A	1	6	3	3	0	0
8	A	1	6	3	3	0	0
8	A	1	6	3	3	0	0
8	A	1	6	3	3	0	0
8	A	1	6	3	3	0	0
8	A	1	6	3	3	0	0
8	A	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

- Molecule 10 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1086	Total O 1086 1086	0	0
10	B	1033	Total O 1033 1033	0	0

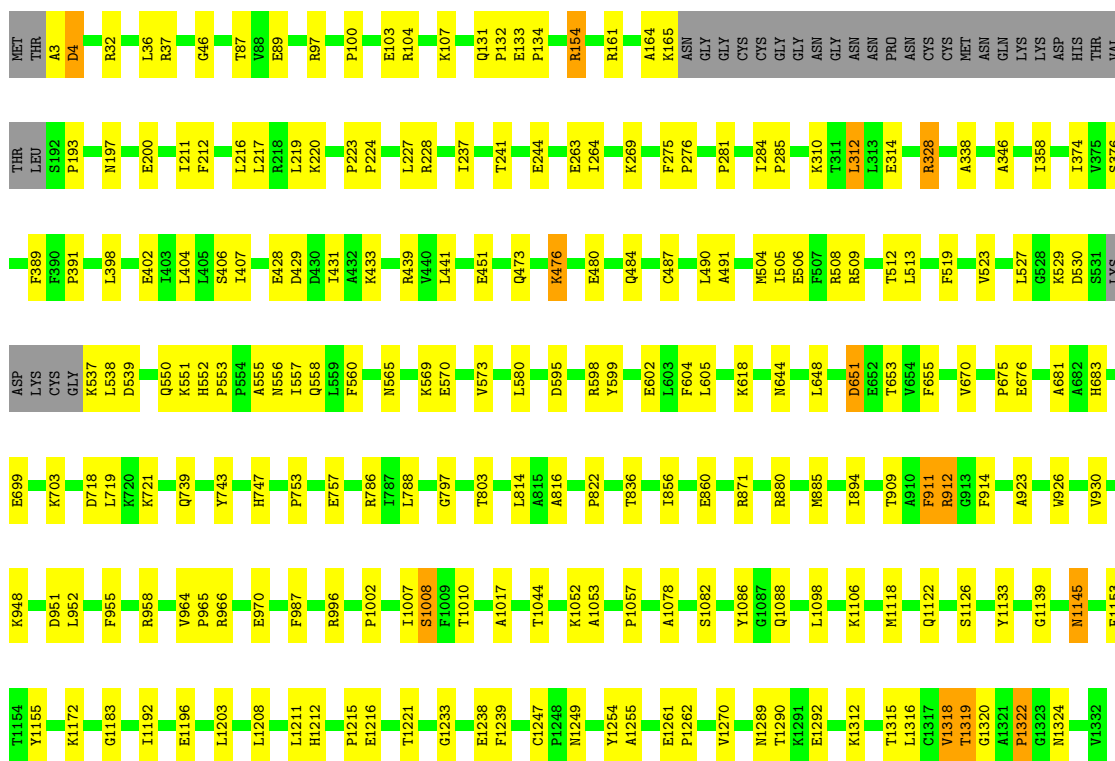
3 Residue-property plots [i](#)

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.

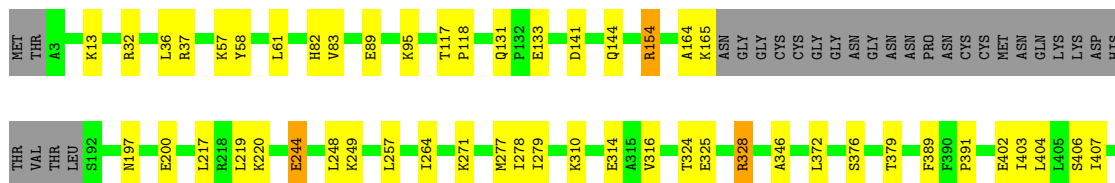
- Molecule 1: Xanthine dehydrogenase/oxidase

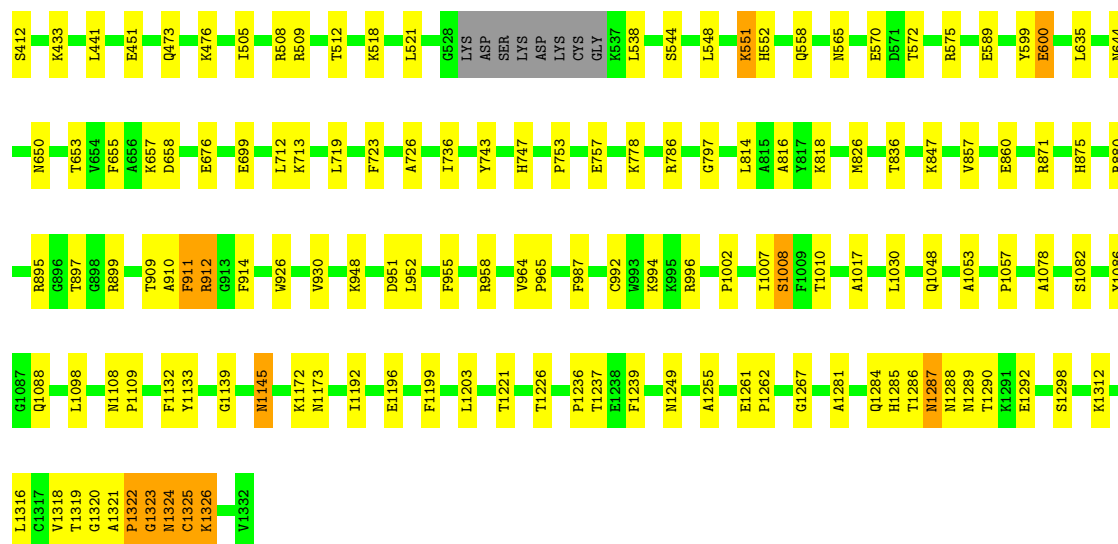
Chain A: 



- Molecule 1: Xanthine dehydrogenase/oxidase

Chain B: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.82Å 123.94Å 148.89Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	20.00 – 1.98	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.98)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.178 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	22610	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: FAD, GOL, ACY, MTE, MOS, YSH, FES, CA

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	0/10298	0.60	0/13939
1	B	0.31	0/10275	0.60	0/13909
All	All	0.32	0/20573	0.60	0/27848

There are no bond length outliers.

There are no bond angle outliers.

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	10077	0	10076	172	0
1	B	10054	0	10053	155	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	0	0
4	A	24	0	10	1	0
4	B	24	0	10	1	0
5	A	4	0	0	1	0
5	B	4	0	0	2	0
6	A	53	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	53	0	31	3	0
7	A	22	0	16	3	0
7	B	22	0	16	3	0
8	A	66	0	88	8	0
8	B	60	0	80	8	0
9	A	4	0	3	4	0
9	B	4	0	3	4	0
10	A	1086	0	0	9	0
10	B	1033	0	0	7	0
All	All	22610	0	20417	331	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 8.

The worst 5 of 331 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)
7:B:5102:YSH:N2	7:B:5102:YSH:C1	1.70	1.52
7:A:5101:YSH:N2	7:A:5101:YSH:C1	1.68	1.51
1:A:3:ALA:HB1	1:A:228:ARG:H	1.20	1.06
1:A:537:LYS:HG2	1:A:538:LEU:H	1.28	0.98
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.30	0.97

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	1293/1332 (97%)	1244 (96%)	41 (3%)	8 (1%)	25 14
1	B	1290/1332 (97%)	1234 (96%)	44 (3%)	12 (1%)	17 8
All	All	2583/2664 (97%)	2478 (96%)	85 (3%)	20 (1%)	19 9

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	B	1008	SER
1	B	1287	ASN
1	B	1324	ASN

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	1101/1128 (98%)	1086 (99%)	15 (1%)	67	62
1	B	1098/1128 (97%)	1088 (99%)	10 (1%)	78	77
All	All	2199/2256 (98%)	2174 (99%)	25 (1%)	73	70

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1239	PHE
1	B	551	LYS
1	B	1239	PHE
1	B	328	ARG
1	B	565	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1289	ASN
1	B	1145	ASN
1	B	146	ASN
1	B	1287	ASN
1	B	650	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](#)

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](#)

Of 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 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
8	GOL	B	5022	-	5,5,5	0.23	0	5,5,5	0.36	0
9	ACY	B	5202	-	3,3,3	1.13	0	3,3,3	1.73	1 (33%)
8	GOL	A	5019	-	5,5,5	0.32	0	5,5,5	0.29	0
3	FES	B	4001	1	0,4,4	-	-	-	-	-
8	GOL	B	5021	-	5,5,5	0.27	0	5,5,5	0.39	0
7	YSH	B	5102	-	19,23,23	6.75	10 (52%)	26,33,33	3.53	7 (26%)
6	FAD	B	4005	-	53,58,58	2.44	22 (41%)	68,89,89	2.02	25 (36%)
5	MOS	A	3004	4	0,3,3	-	-	-	-	-
8	GOL	A	5004	-	5,5,5	0.28	0	5,5,5	0.32	0
3	FES	B	4002	1	0,4,4	-	-	-	-	-
8	GOL	A	5011	-	5,5,5	0.21	0	5,5,5	0.36	0
3	FES	A	3001	1	0,4,4	-	-	-	-	-
8	GOL	A	5006	-	5,5,5	0.24	0	5,5,5	0.41	0
3	FES	A	3002	1	0,4,4	-	-	-	-	-
8	GOL	B	5012	-	5,5,5	0.22	0	5,5,5	0.42	0
8	GOL	A	5018	-	5,5,5	0.34	0	5,5,5	0.27	0
4	MTE	B	4003	5	21,26,26	6.02	13 (61%)	21,40,40	4.41	9 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FAD	A	3005	-	53,58,58	2.33	19 (35%)	68,89,89	2.03	24 (35%)
8	GOL	A	5002	-	5,5,5	0.22	0	5,5,5	0.36	0
8	GOL	A	5016	-	5,5,5	0.27	0	5,5,5	0.48	0
8	GOL	B	5007	-	5,5,5	0.28	0	5,5,5	0.32	0
8	GOL	B	5013	-	5,5,5	0.23	0	5,5,5	0.29	0
4	MTE	A	3003	5	21,26,26	6.25	13 (61%)	21,40,40	4.02	8 (38%)
8	GOL	A	5003	-	5,5,5	0.31	0	5,5,5	0.32	0
8	GOL	B	5015	-	5,5,5	0.26	0	5,5,5	0.30	0
8	GOL	B	5008	-	5,5,5	0.26	0	5,5,5	0.39	0
8	GOL	A	5017	-	5,5,5	0.28	0	5,5,5	0.31	0
8	GOL	B	5020	-	5,5,5	0.25	0	5,5,5	0.34	0
8	GOL	B	5014	-	5,5,5	0.21	0	5,5,5	0.38	0
8	GOL	A	5001	-	5,5,5	0.31	0	5,5,5	0.39	0
9	ACY	A	5201	-	3,3,3	1.03	0	3,3,3	1.80	1 (33%)
7	YSH	A	5101	-	19,23,23	6.67	10 (52%)	26,33,33	3.50	7 (26%)
8	GOL	B	5009	-	5,5,5	0.31	0	5,5,5	0.29	0
8	GOL	A	5005	-	5,5,5	0.31	0	5,5,5	0.34	0
5	MOS	B	4004	4	0,3,3	-	-	-	-	-

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	5022	-	-	0/4/4/4	-
8	GOL	A	5019	-	-	0/4/4/4	-
3	FES	B	4001	1	-	-	0/1/1/1
8	GOL	B	5021	-	-	0/4/4/4	-
7	YSH	B	5102	-	-	1/10/16/16	0/2/2/2
6	FAD	B	4005	-	-	2/30/50/50	0/6/6/6
8	GOL	A	5004	-	-	0/4/4/4	-
3	FES	B	4002	1	-	-	0/1/1/1
8	GOL	A	5011	-	-	0/4/4/4	-
3	FES	A	3001	1	-	-	0/1/1/1
8	GOL	A	5006	-	-	0/4/4/4	-
3	FES	A	3002	1	-	-	0/1/1/1
8	GOL	B	5012	-	-	0/4/4/4	-
8	GOL	A	5018	-	-	0/4/4/4	-
4	MTE	B	4003	5	-	6/6/34/34	0/3/3/3
6	FAD	A	3005	-	-	4/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	5002	-	-	0/4/4/4	-
8	GOL	A	5016	-	-	0/4/4/4	-
8	GOL	B	5007	-	-	0/4/4/4	-
8	GOL	B	5013	-	-	0/4/4/4	-
4	MTE	A	3003	5	-	4/6/34/34	0/3/3/3
8	GOL	A	5003	-	-	0/4/4/4	-
8	GOL	B	5015	-	-	0/4/4/4	-
8	GOL	B	5008	-	-	0/4/4/4	-
8	GOL	A	5017	-	-	0/4/4/4	-
8	GOL	B	5020	-	-	0/4/4/4	-
8	GOL	B	5014	-	-	0/4/4/4	-
8	GOL	A	5001	-	-	0/4/4/4	-
7	YSH	A	5101	-	-	1/10/16/16	0/2/2/2
8	GOL	B	5009	-	-	0/4/4/4	-
8	GOL	A	5005	-	-	0/4/4/4	-

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3003	MTE	C7-C6	19.00	1.68	1.53
4	B	4003	MTE	C7-C6	18.55	1.68	1.53
7	B	5102	YSH	C1-C5	18.40	1.71	1.39
7	A	5101	YSH	C1-C5	18.13	1.71	1.39
7	B	5102	YSH	C11-C6	17.98	1.62	1.41

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	5102	YSH	C4-N3-N2	14.75	114.44	103.70
7	A	5101	YSH	C4-N3-N2	14.27	114.09	103.70
4	A	3003	MTE	C4-C9-N5	13.22	130.22	119.12
4	B	4003	MTE	C4-C9-N5	12.89	129.94	119.12
4	B	4003	MTE	P-O4'-C4'	11.08	148.82	118.30

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3003	MTE	C4'-O4'-P-O2P
4	A	3003	MTE	C4'-O4'-P-O3P
4	B	4003	MTE	C2'-C3'-C4'-O4'

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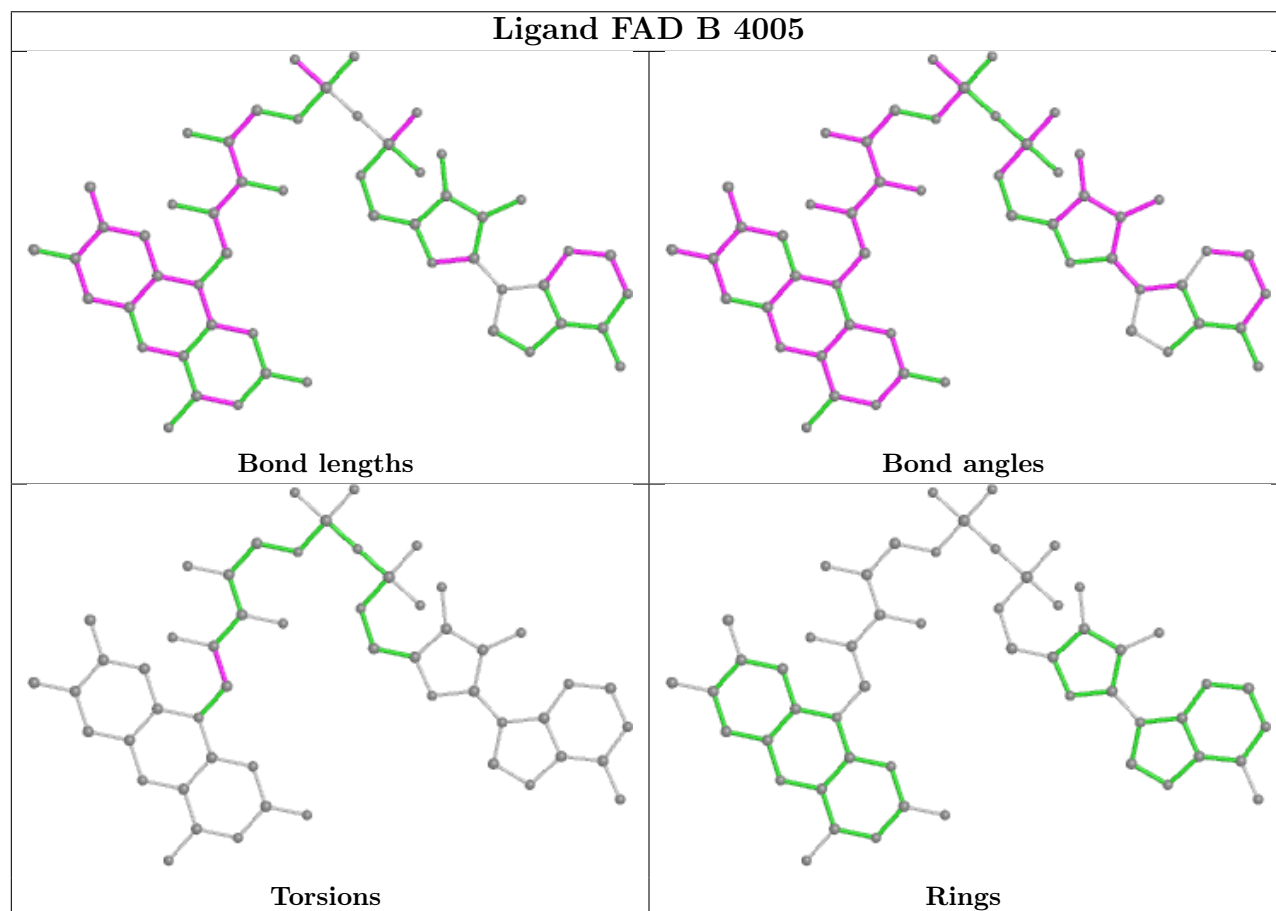
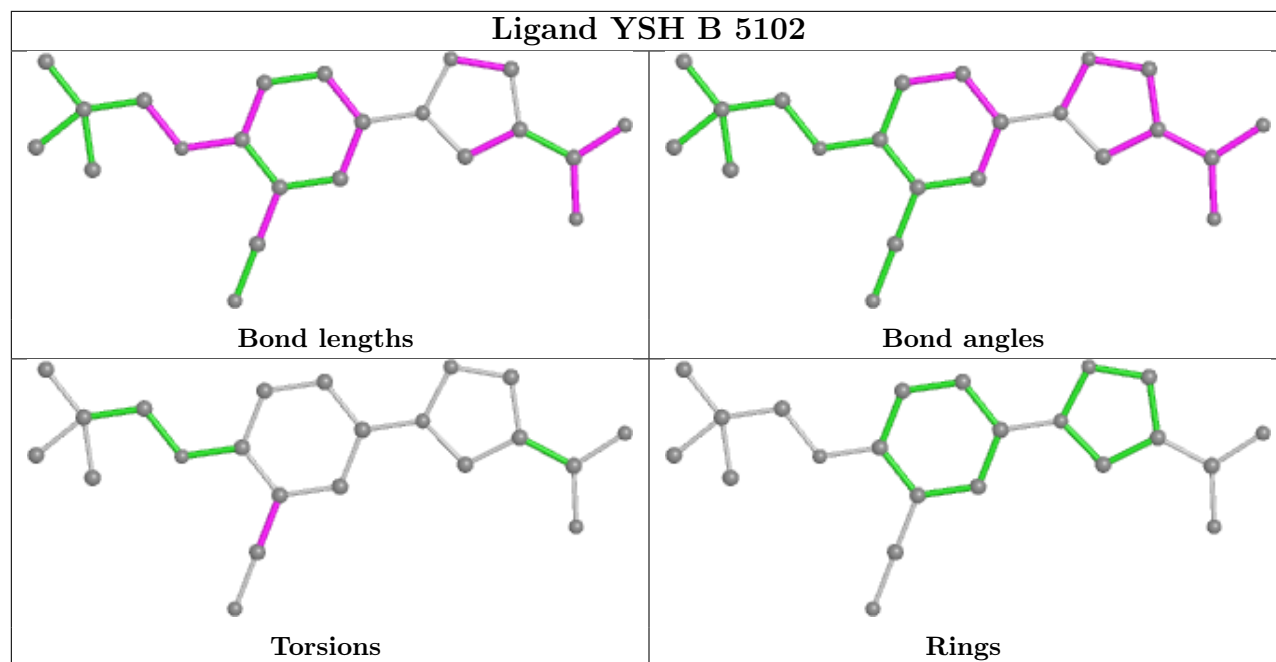
Mol	Chain	Res	Type	Atoms
4	B	4003	MTE	O3'-C3'-C4'-O4'
4	B	4003	MTE	C3'-C4'-O4'-P

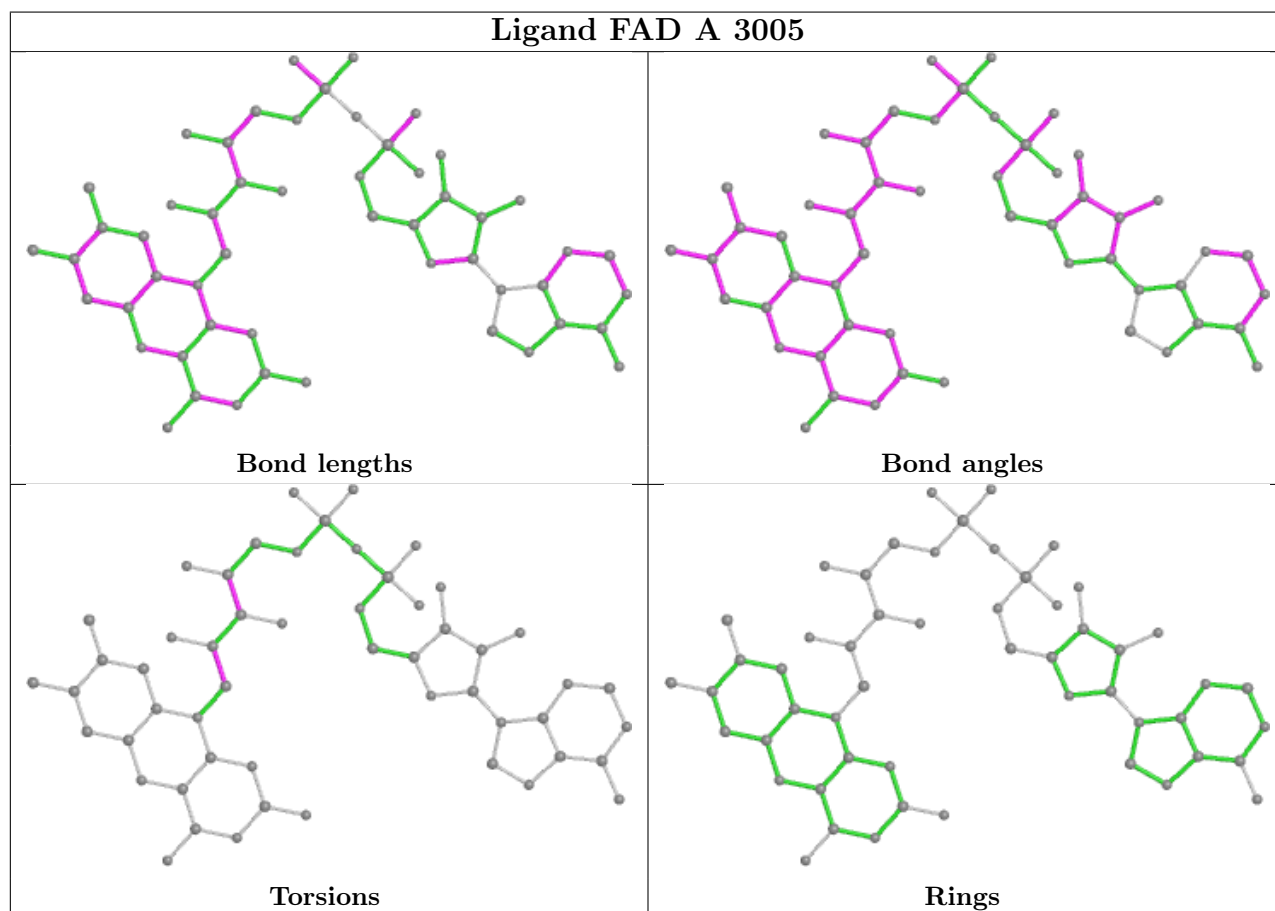
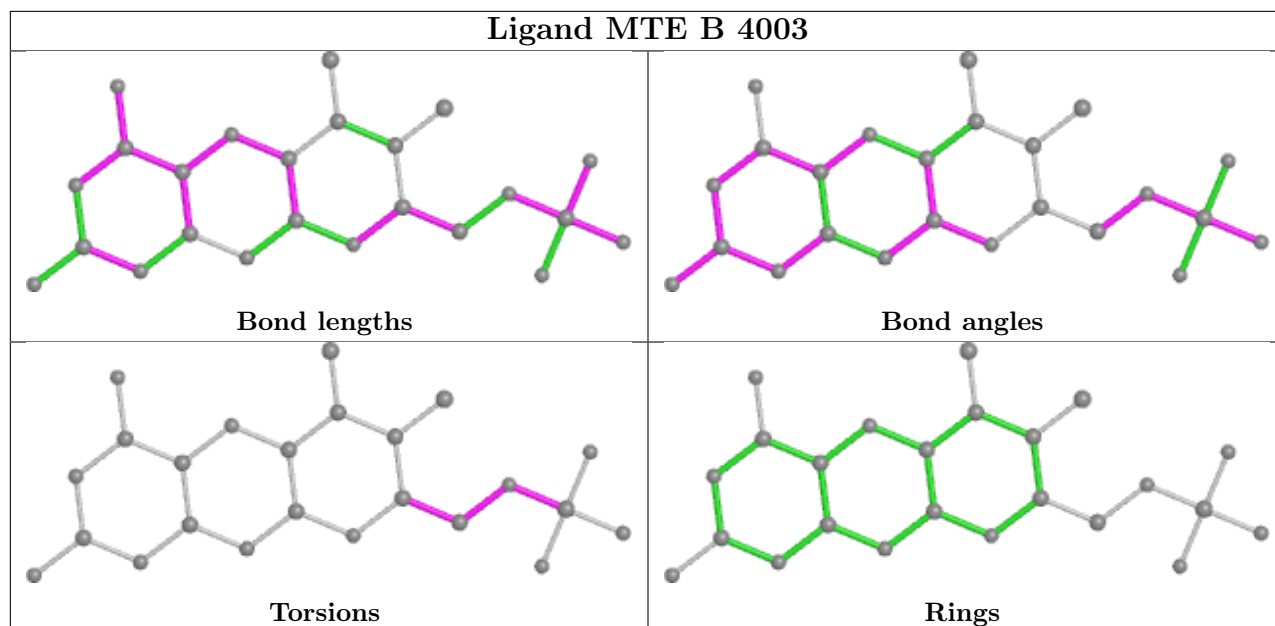
There are no ring outliers.

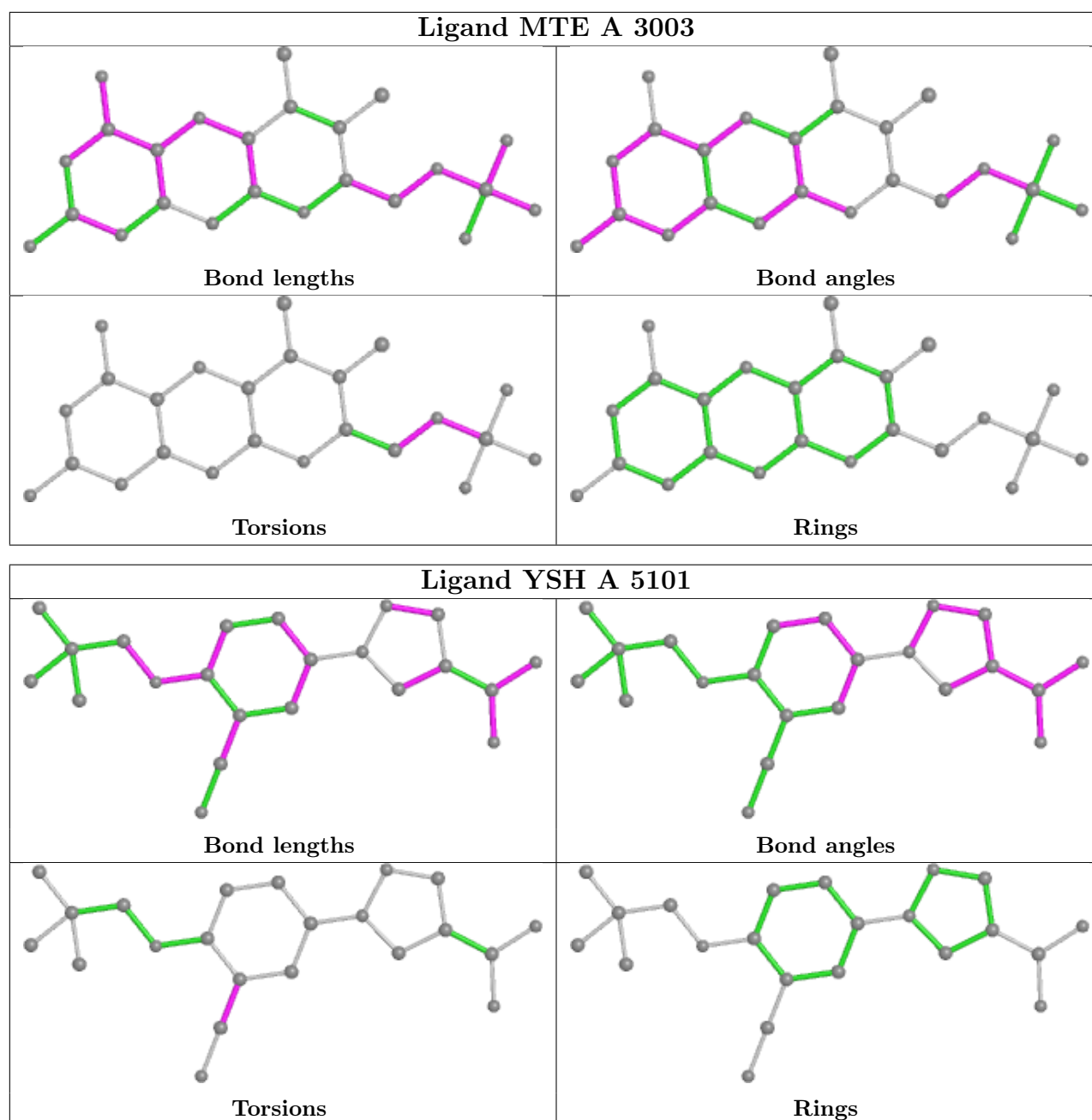
21 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	5022	GOL	2	0
9	B	5202	ACY	4	0
8	A	5019	GOL	1	0
7	B	5102	YSH	3	0
6	B	4005	FAD	3	0
5	A	3004	MOS	1	0
8	A	5011	GOL	2	0
8	A	5006	GOL	2	0
3	A	3002	FES	1	0
4	B	4003	MTE	1	0
6	A	3005	FAD	4	0
8	A	5002	GOL	2	0
8	B	5013	GOL	1	0
4	A	3003	MTE	1	0
8	B	5008	GOL	2	0
8	B	5020	GOL	1	0
8	B	5014	GOL	2	0
8	A	5001	GOL	1	0
9	A	5201	ACY	4	0
7	A	5101	YSH	3	0
5	B	4004	MOS	2	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.