



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:39 PM UTC

PDB ID : 1VDV / pdb_00001vdv
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.

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

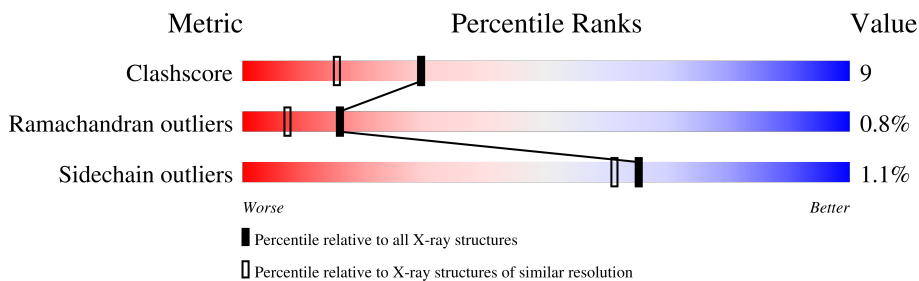
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (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	79% 17% ..
1	B	1332	80% 15% ..

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
1	A	1299	Total	C	N	O	S	0	0	0
			10077	6404	1728	1884	61			
1	B	1296	Total	C	N	O	S	0	0	0
			10054	6391	1724	1878	61			

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 (CCD ID: CA) (formula: Ca).

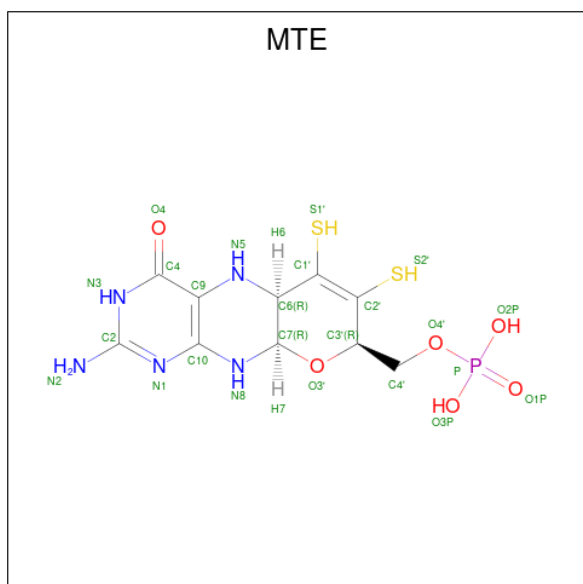
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



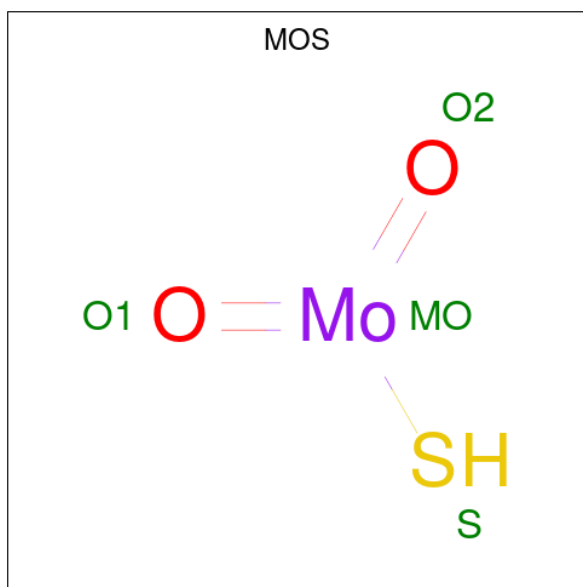
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- 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 (CCD ID: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



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

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO_2S).



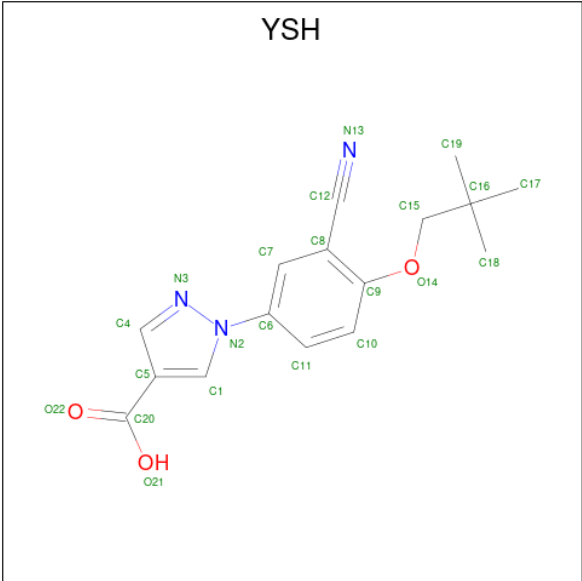
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S		
			4	1	2	1		
5	B	1	Total	Mo	O	S		
			4	1	2	1		

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



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

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



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

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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



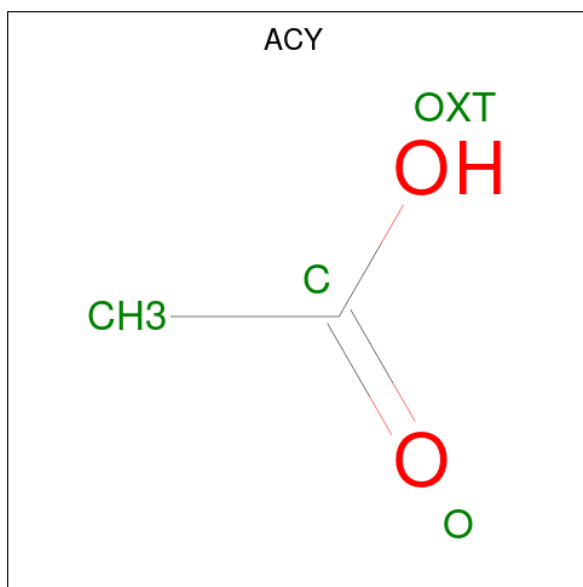
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

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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 (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 10 is water.

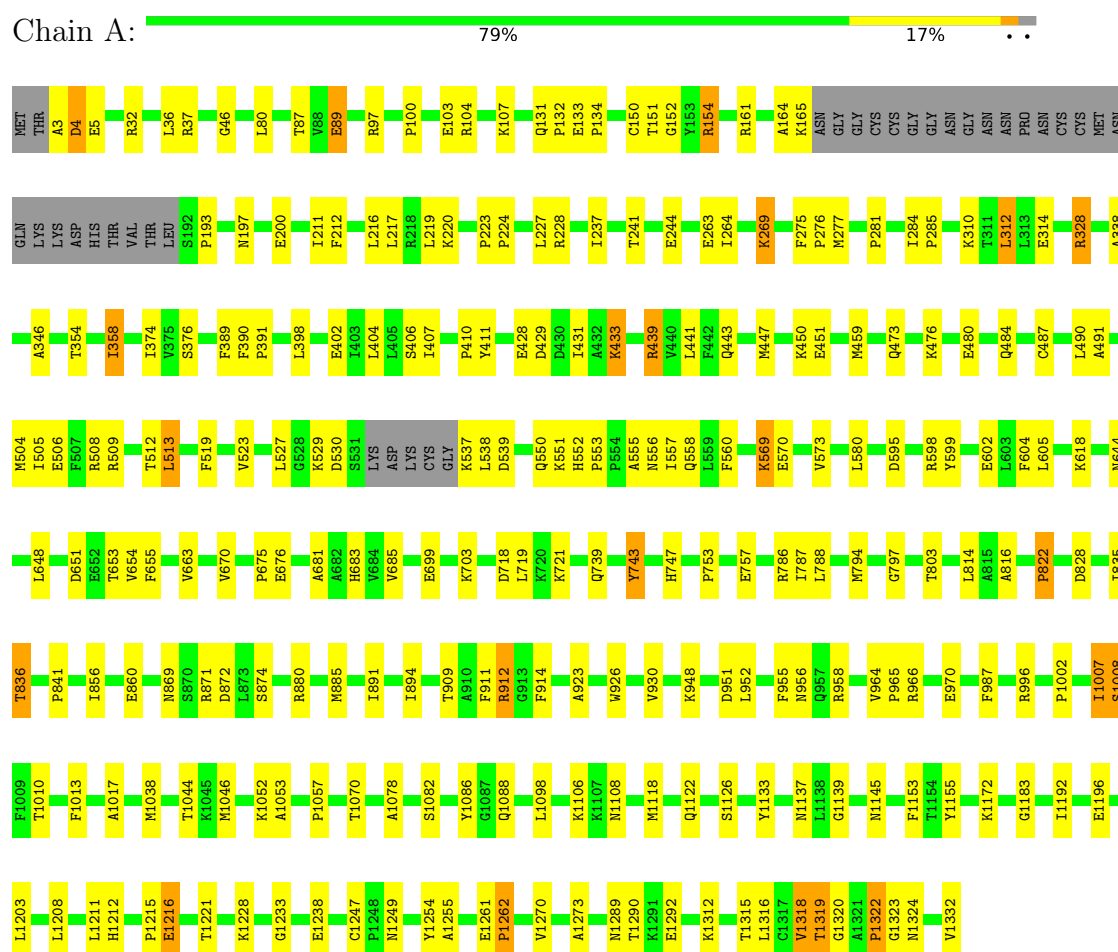
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1086	Total 1086	O 1086	0	0
10	B	1033	Total 1033	O 1033	0	0

3 Residue-property plots

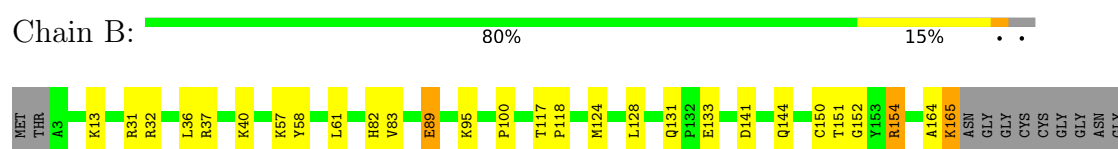
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase



ASN	ASN	L372	L538	H747	A910	N1108	K1312
	ASN	S376	T543	P753	R912	P1109	L1316
ASN	ASN	T379	S544	E757	G913	F1132	G1317
CYS	CYS		L548	V764	F914	Y1133	V1318
MET	MET	F389	K551	K778	W926	G1139	T1319
ASN	ASN	F390	H552		V930	N1145	G1320
GLN	LYS	P391			K948	K1172	A1321
LYS	LYS	E402	Q558	R786		N1173	P1322
LYS	ASP	I403		I787	D951	I1192	G1323
HIS	HIS	L404	E570	G797	L952	E1196	N1324
THR	THR	L405	D571		F955	F1199	G1325
VAL	VAL	S406	T572		R956	L1203	K1326
THR	THR	I407			Q957		V1332
LEU	LEU				R958		
S192	S192	P410	R575	L814	V964	L1207	
N197	N197	Y411	E589	A816	P965	L1208	
E200	E200	S412	Y599	K818		T1221	
E200	E200	D430	E600	H821	F987	T1226	
L217	L217	K433	L605	M826		K1228	
R218	R218			L827	C992	T1227	
L219	L219	C436	L635	D928	W993	T1227	
K220	K220	L441	N644	I835	K994	T1226	
L237	L237			T836	Y995	Y1227	
E244	E244	K450	N650		R996	K1228	
L248	L248	E451		P841	P1002	P1236	
K249	K249	M459	T653	K947	I1007	T1237	
E254	E254	Q473	V654	M851	S1008	N1249	
L257	L257	K476	K456		F1009	A1255	
			D558	V857	T1010		
				E860	A1017	E1261	
L264	L264	I505	V663		L1030	P1262	
K271	K271	R508	E676	N869		P1263	
M277	M277	R509		S870	M1046	L1264	
L278	L278	T512	T696	R871	G1267		
		L513	E699	H875	Q1048	A1273	
K310	K310	K518	L712	R880	A1053	A1281	
E314	E314	L521	K713	M885	P1057	Q1284	
A315	A315	L719		I891	A1078	H1285	
V316	V316	F723		I894	S1082	T1286	
ASP	ASP			R895		N1287	
T324	T324	SER	A726	G896	I1085	N1288	
E325	E325	LYS	D727	T897	Y1086	N1289	
L328	L328	ASP			G1291	T1290	
R328	R328	LYS	I736	G898	K1291	K1291	
CYS	CYS	CYS		R899	Q1088	E1292	
A346	A346	GLY	Y743	T900	L1093	S1298	

4 Data and refinement statistics

Xtriage (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.	Xtriage
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: ACY, YSH, MOS, FAD, MTE, GOL, 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	0.36	0/10298	0.91	41/13939 (0.3%)
1	B	0.36	0/10275	0.91	40/13909 (0.3%)
All	All	0.36	0/20573	0.91	81/27848 (0.3%)

There are no bond length outliers.

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	835	ILE	N-CA-C	10.79	123.01	111.58
1	A	835	ILE	N-CA-C	10.43	122.64	111.58
1	B	151	THR	N-CA-C	10.30	123.77	111.82
1	A	151	THR	N-CA-C	10.11	123.55	111.82
1	B	836	THR	N-CA-C	8.76	123.80	113.20

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	182	0
1	B	10054	0	10053	167	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
6	B	53	0	31	2	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	8	0
10	B	1033	0	0	6	0
All	All	22610	0	20417	351	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 9.

The worst 5 of 351 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%)	21	12
1	B	1290/1332 (97%)	1234 (96%)	44 (3%)	12 (1%)	14	6
All	All	2583/2664 (97%)	2478 (96%)	85 (3%)	20 (1%)	16	7

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 ⓘ

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%)	59	54
1	B	1098/1128 (97%)	1088 (99%)	10 (1%)	70	67
All	All	2199/2256 (98%)	2174 (99%)	25 (1%)	65	61

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

Mol	Chain	Res	Type
1	A	1332	VAL
1	B	154	ARG
1	B	1002	PRO
1	B	100	PRO
1	B	165	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	626	GLN
1	B	1145	ASN
1	B	650	ASN
1	B	869	ASN
1	B	1220	HIS

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 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	A	5016	-	5,5,5	0.28	0	5,5,5	0.51	0
3	FES	B	4001	1	0,4,4	-	-	-		
8	GOL	B	5020	-	5,5,5	0.26	0	5,5,5	0.36	0
8	GOL	A	5001	-	5,5,5	0.32	0	5,5,5	0.42	0
3	FES	B	4002	1	0,4,4	-	-	-		
3	FES	A	3001	1	0,4,4	-	-	-		
8	GOL	B	5022	-	5,5,5	0.23	0	5,5,5	0.39	0
8	GOL	B	5014	-	5,5,5	0.22	0	5,5,5	0.40	0
8	GOL	B	5021	-	5,5,5	0.28	0	5,5,5	0.42	0
8	GOL	B	5009	-	5,5,5	0.32	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MTE	B	4003	5	21,26,26	6.20	11 (52%)	19,40,40	3.22	11 (57%)
5	MOS	B	4004	4	0,3,3	-	-	-	-	-
7	YSH	B	5102	-	23,23,23	7.44	15 (65%)	33,33,33	4.14	11 (33%)
8	GOL	A	5006	-	5,5,5	0.25	0	5,5,5	0.44	0
9	ACY	B	5202	-	3,3,3	1.19	0	3,3,3	1.70	1 (33%)
9	ACY	A	5201	-	3,3,3	1.09	0	3,3,3	1.76	1 (33%)
8	GOL	A	5002	-	5,5,5	0.23	0	5,5,5	0.39	0
8	GOL	B	5008	-	5,5,5	0.27	0	5,5,5	0.42	0
3	FES	A	3002	1	0,4,4	-	-	-	-	-
5	MOS	A	3004	4	0,3,3	-	-	-	-	-
8	GOL	A	5017	-	5,5,5	0.28	0	5,5,5	0.34	0
8	GOL	B	5007	-	5,5,5	0.29	0	5,5,5	0.34	0
8	GOL	A	5011	-	5,5,5	0.21	0	5,5,5	0.40	0
8	GOL	A	5019	-	5,5,5	0.33	0	5,5,5	0.32	0
8	GOL	B	5012	-	5,5,5	0.23	0	5,5,5	0.45	0
7	YSH	A	5101	-	23,23,23	7.30	13 (56%)	33,33,33	4.20	12 (36%)
8	GOL	A	5018	-	5,5,5	0.35	0	5,5,5	0.29	0
8	GOL	B	5013	-	5,5,5	0.23	0	5,5,5	0.32	0
6	FAD	A	3005	-	58,58,58	2.27	19 (32%)	85,89,89	2.09	29 (34%)
8	GOL	A	5005	-	5,5,5	0.31	0	5,5,5	0.36	0
8	GOL	B	5015	-	5,5,5	0.26	0	5,5,5	0.33	0
8	GOL	A	5004	-	5,5,5	0.29	0	5,5,5	0.35	0
4	MTE	A	3003	5	21,26,26	6.54	12 (57%)	19,40,40	3.21	10 (52%)
8	GOL	A	5003	-	5,5,5	0.32	0	5,5,5	0.35	0
6	FAD	B	4005	-	58,58,58	2.37	24 (41%)	85,89,89	2.07	31 (36%)

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
8	GOL	A	5016	-	-	0/4/4/4	-
8	GOL	B	5020	-	-	0/4/4/4	-
3	FES	B	4001	1	-	-	0/1/1/1
8	GOL	A	5001	-	-	0/4/4/4	-
3	FES	A	3001	1	-	-	0/1/1/1
3	FES	B	4002	1	-	-	0/1/1/1
8	GOL	B	5022	-	-	0/4/4/4	-
8	GOL	B	5014	-	-	0/4/4/4	-
8	GOL	B	5021	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	5009	-	-	0/4/4/4	-
4	MTE	B	4003	5	-	6/6/34/34	0/3/3/3
7	YSH	B	5102	-	-	2/16/16/16	0/2/2/2
8	GOL	A	5006	-	-	0/4/4/4	-
8	GOL	A	5002	-	-	0/4/4/4	-
8	GOL	B	5008	-	-	0/4/4/4	-
8	GOL	B	5007	-	-	0/4/4/4	-
8	GOL	A	5017	-	-	0/4/4/4	-
3	FES	A	3002	1	-	-	0/1/1/1
8	GOL	A	5011	-	-	0/4/4/4	-
8	GOL	A	5019	-	-	0/4/4/4	-
8	GOL	B	5012	-	-	0/4/4/4	-
7	YSH	A	5101	-	-	0/16/16/16	0/2/2/2
8	GOL	A	5018	-	-	0/4/4/4	-
8	GOL	B	5013	-	-	0/4/4/4	-
6	FAD	A	3005	-	-	4/34/50/50	0/6/6/6
8	GOL	A	5005	-	-	0/4/4/4	-
8	GOL	B	5015	-	-	0/4/4/4	-
8	GOL	A	5004	-	-	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	-
6	FAD	B	4005	-	-	2/34/50/50	0/6/6/6

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	5102	YSH	C1-C5	21.19	1.71	1.38
7	A	5101	YSH	C1-C5	20.87	1.71	1.38
7	B	5102	YSH	C1-N2	19.56	1.70	1.35
4	A	3003	MTE	C7-C6	19.00	1.68	1.53
7	A	5101	YSH	C1-N2	18.95	1.68	1.35

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	5101	YSH	C5-C1-N2	-14.03	90.97	107.09
7	B	5102	YSH	C5-C1-N2	-13.97	91.05	107.09
7	B	5102	YSH	C4-N3-N2	12.88	114.44	104.19
7	A	5101	YSH	C4-N3-N2	12.44	114.09	104.19
7	A	5101	YSH	C1-C5-C4	9.21	112.35	104.22

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'
4	B	4003	MTE	O3'-C3'-C4'-O4'
4	B	4003	MTE	C3'-C4'-O4'-P

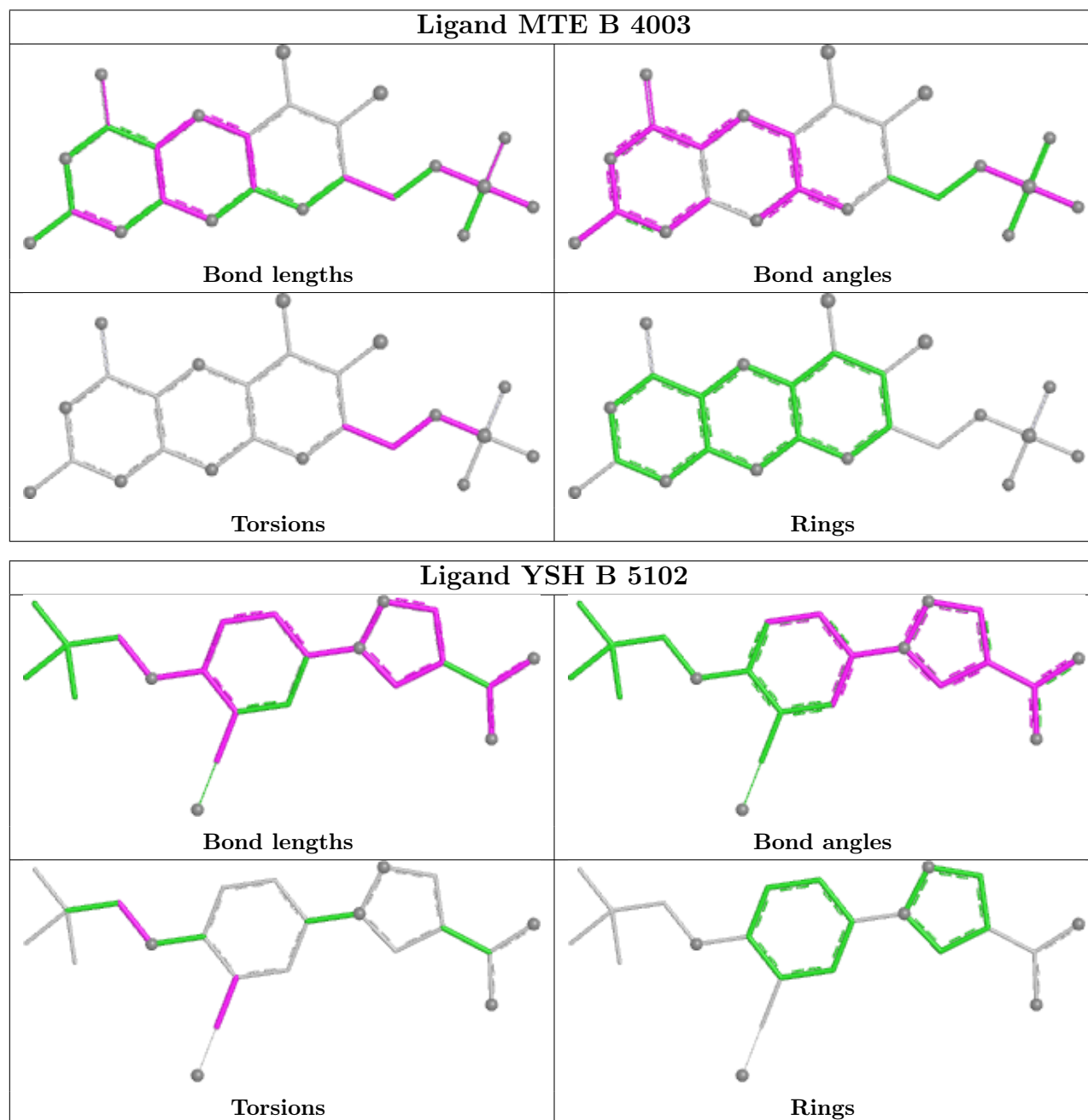
There are no ring outliers.

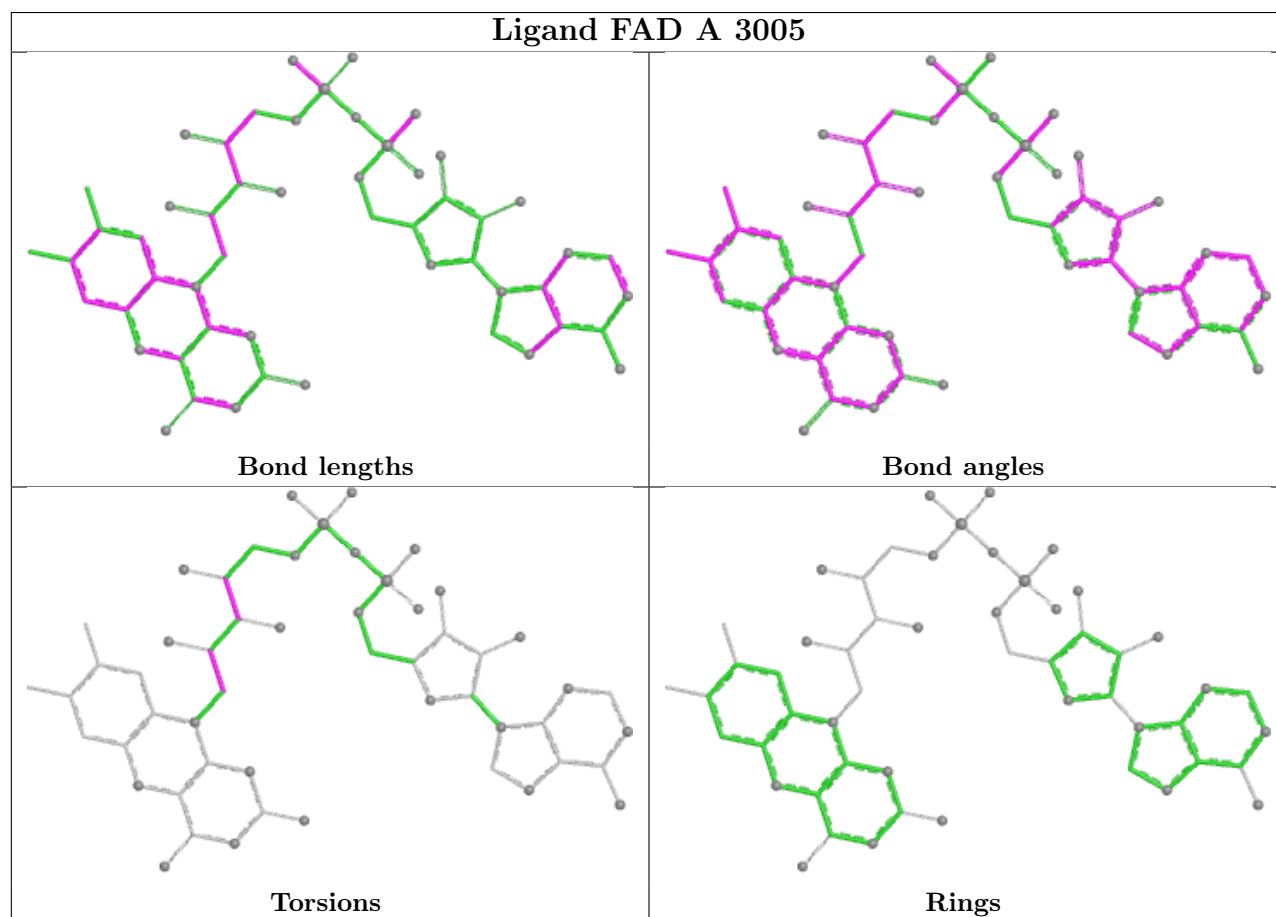
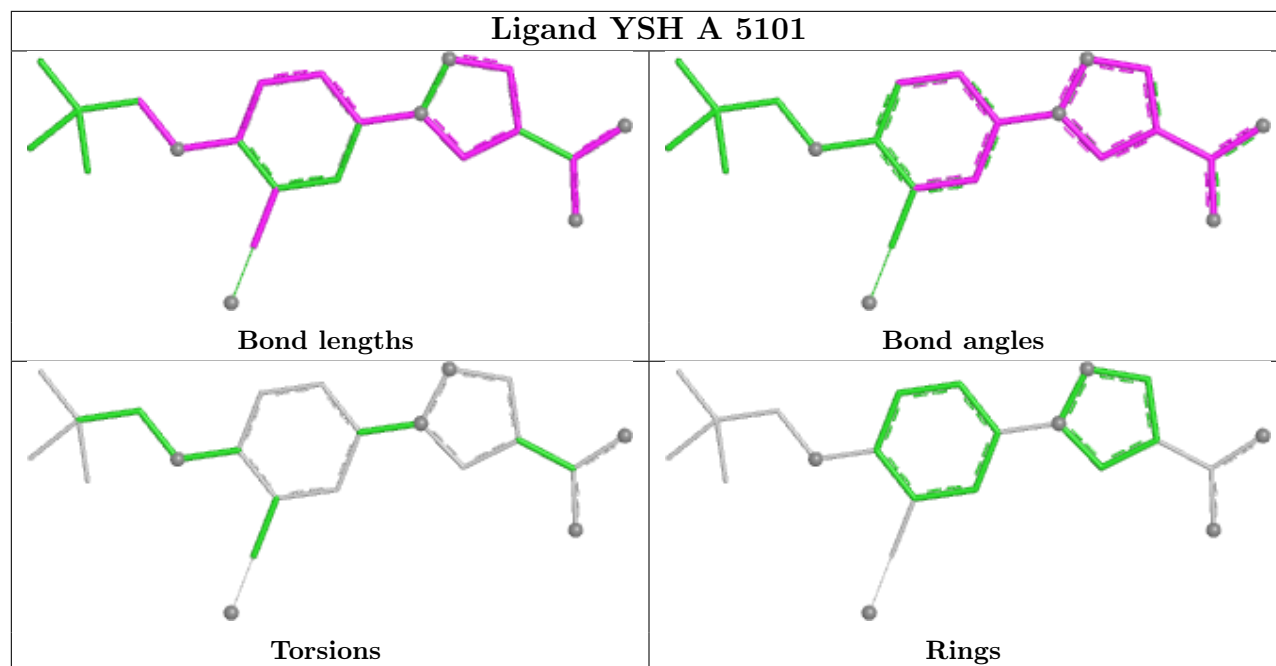
21 monomers are involved in 41 short contacts:

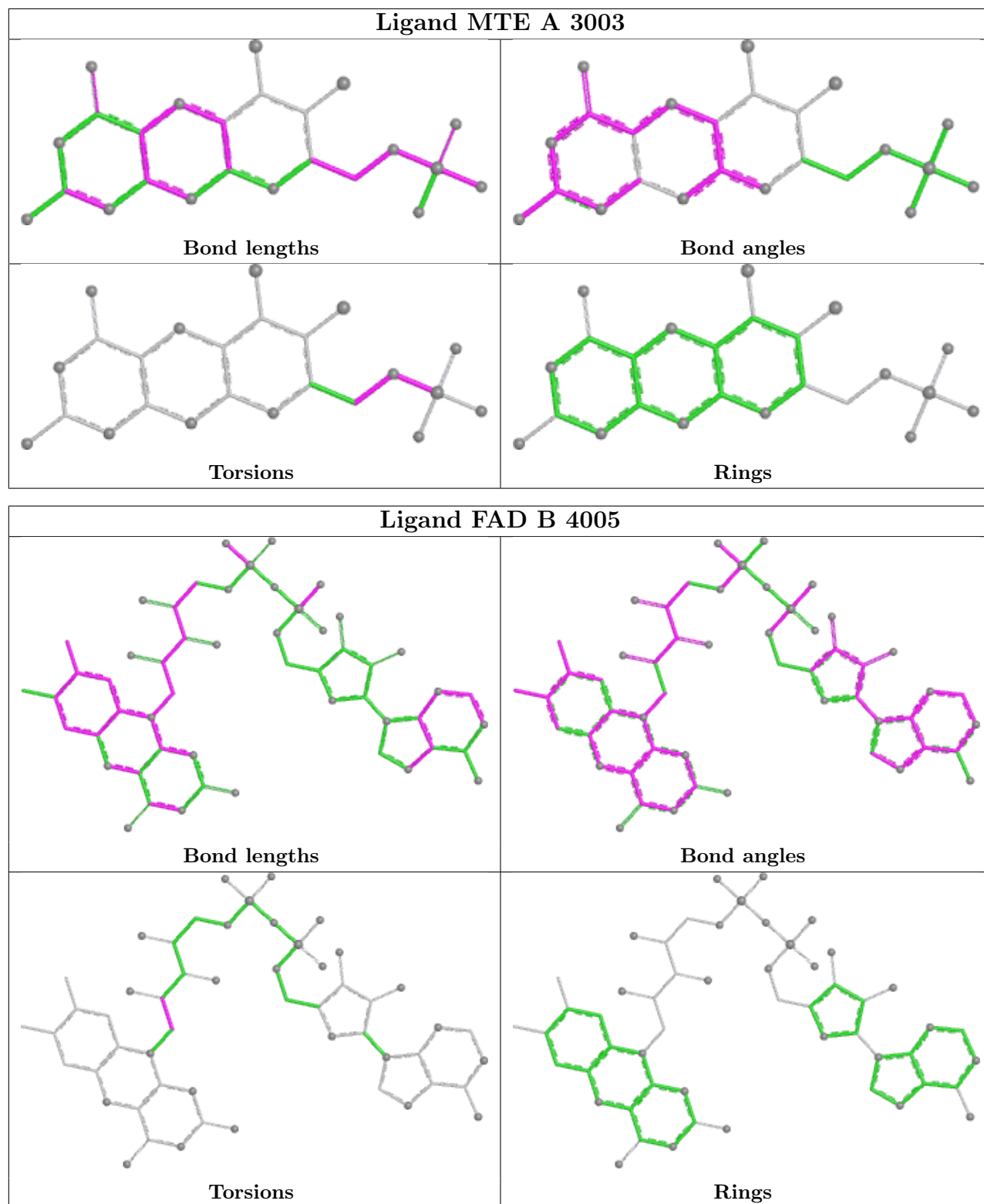
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	5020	GOL	1	0
8	A	5001	GOL	1	0
8	B	5022	GOL	2	0
8	B	5014	GOL	2	0
4	B	4003	MTE	1	0
5	B	4004	MOS	2	0
7	B	5102	YSH	3	0
8	A	5006	GOL	2	0
9	B	5202	ACY	4	0
9	A	5201	ACY	4	0
8	A	5002	GOL	2	0
8	B	5008	GOL	2	0
3	A	3002	FES	1	0
5	A	3004	MOS	1	0
8	A	5011	GOL	2	0
8	A	5019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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.