



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:12 AM UTC

PDB ID : 1JRO / pdb_00001jro
Title : Crystal Structure of Xanthine Dehydrogenase from Rhodobacter capsulatus
Authors : Truglio, J.J.; Theis, K.; Leimkuhler, S.; Rappa, R.; Rajagopalan, K.V.; Kisker, C.
Deposited on : 2001-08-14
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

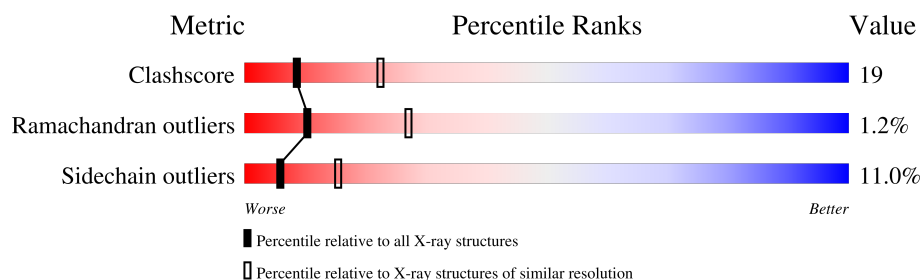
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	462	61% 29% 7% .
1	C	462	64% 26% 6% .
1	E	462	48% 38% 11% ..
1	G	462	47% 40% 9% ..
2	B	777	60% 31% 7% .
2	D	777	61% 30% 6% ..
2	F	777	56% 34% 7% ..
2	H	777	54% 34% 8% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	G	3001	-	-	X	-
7	MOS	B	3004	-	-	X	-
7	MOS	D	3004	-	-	X	-
7	MOS	F	3004	-	-	X	-
7	MOS	H	3004	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36831 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, chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	C	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	E	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	G	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			

- Molecule 2 is a protein called xanthine dehydrogenase, chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	D	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	F	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	H	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	conflict	EMBL 13397863
D	772	ARG	GLY	conflict	EMBL 13397863
F	772	ARG	GLY	conflict	EMBL 13397863
H	772	ARG	GLY	conflict	EMBL 13397863

- 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	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

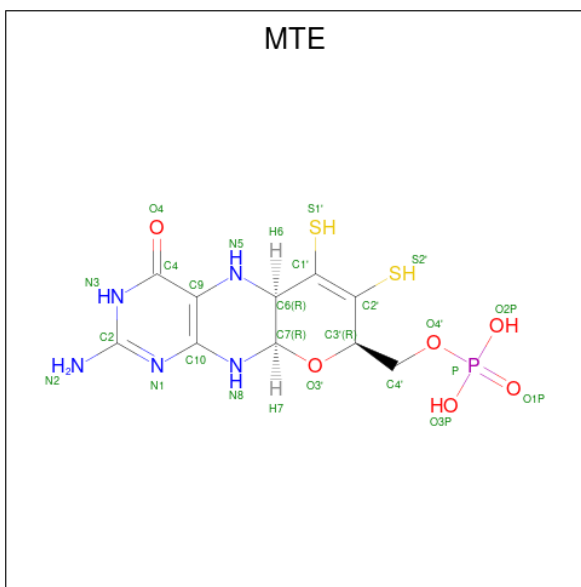


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

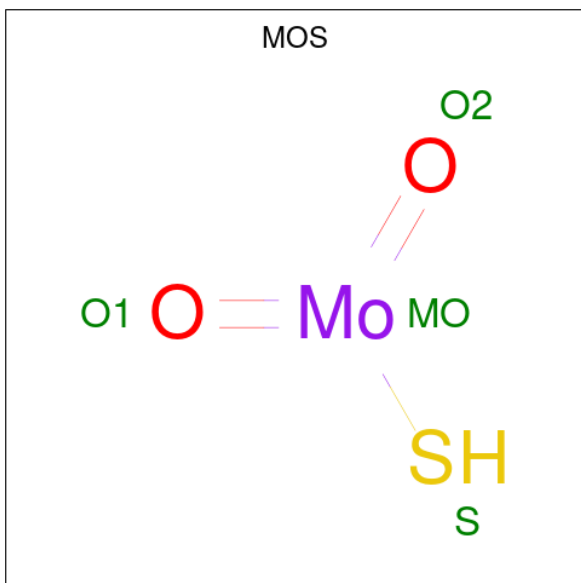
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		

- Molecule 6 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: C₁₀H₁₄N₅O₆PS₂).



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

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO_2S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total 4	Mo 1	O 2	S 1	0	0
7	D	1	Total 4	Mo 1	O 2	S 1	0	0
7	F	1	Total 4	Mo 1	O 2	S 1	0	0
7	H	1	Total 4	Mo 1	O 2	S 1	0	0

- Molecule 8 is water.

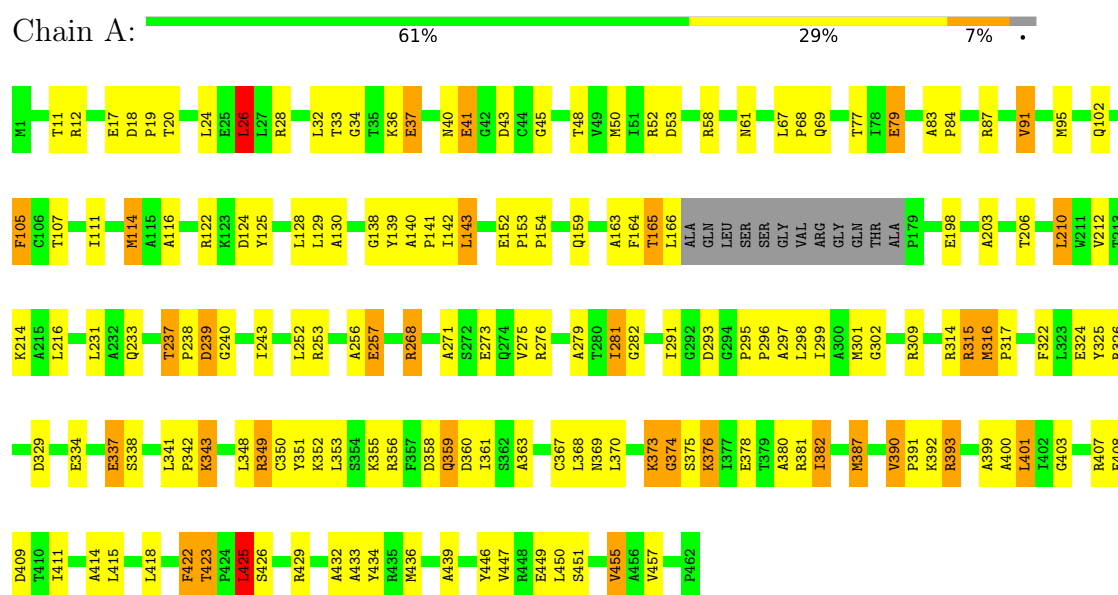
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total 11	O 11	0	0
8	B	26	Total 26	O 26	0	0
8	C	7	Total 7	O 7	0	0
8	D	25	Total 25	O 25	0	0
8	E	7	Total 7	O 7	0	0
8	F	20	Total 20	O 20	0	0
8	G	6	Total 6	O 6	0	0
8	H	21	Total 21	O 21	0	0

3 Residue-property plots

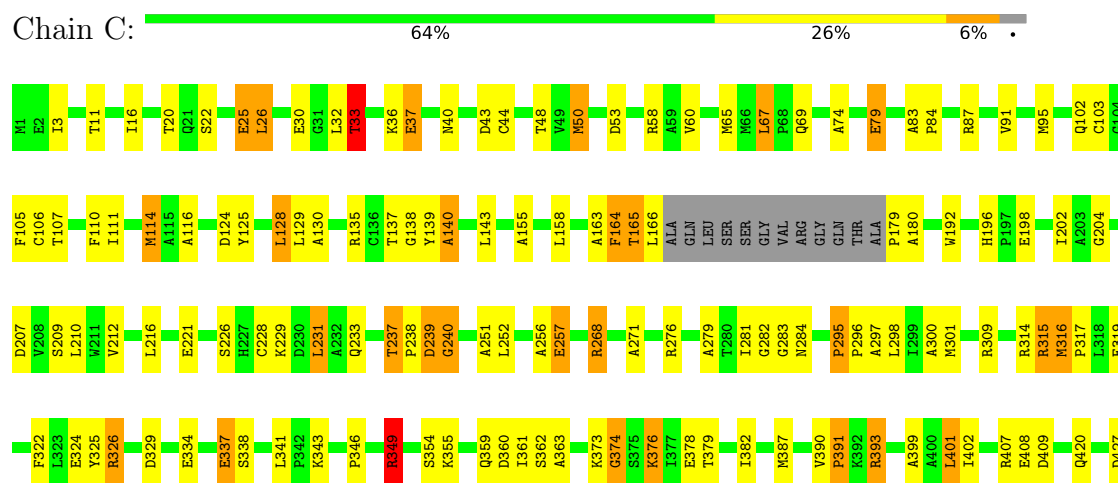
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

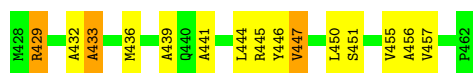
Note EDS was not executed.

• Molecule 1: xanthine dehydrogenase, chain A



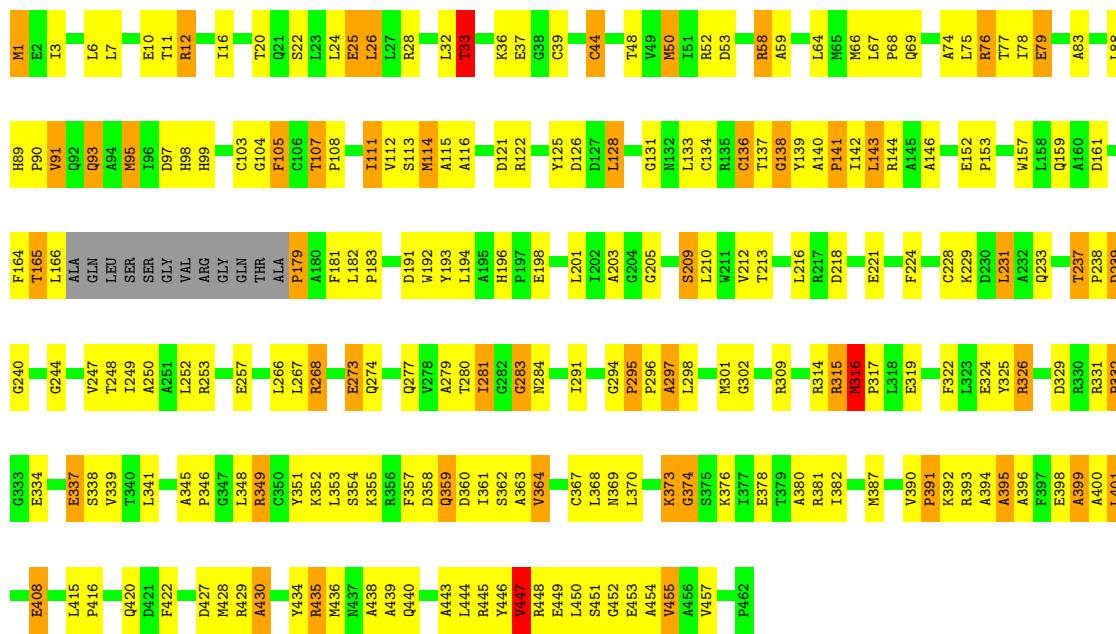
• Molecule 1: xanthine dehydrogenase, chain A





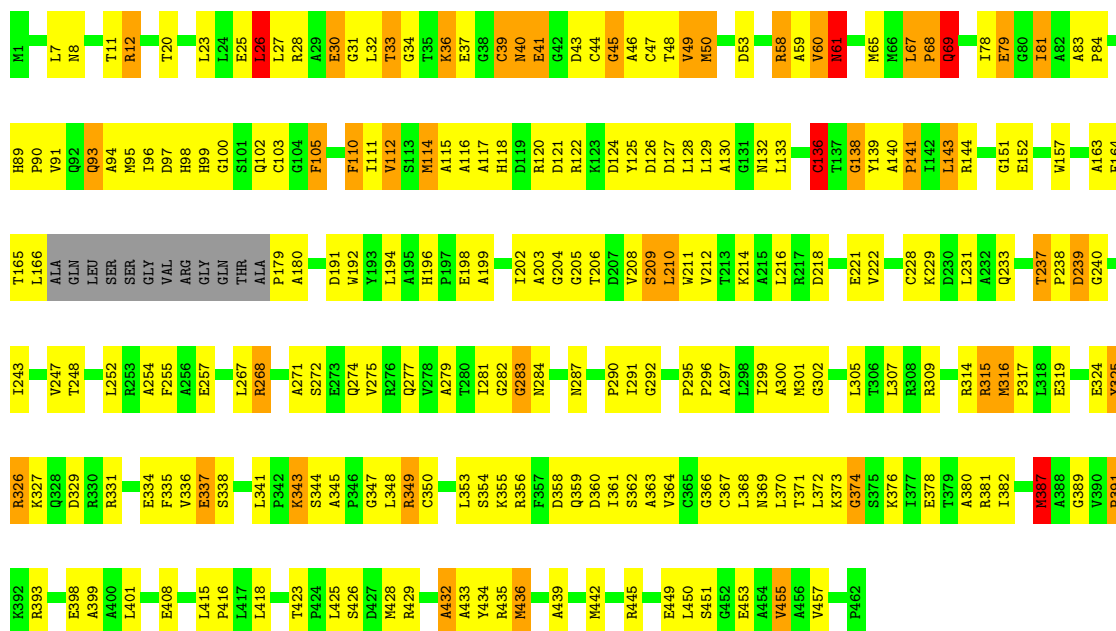
• Molecule 1: xanthine dehydrogenase, chain A

Chain E: 48% 38% 11% ..



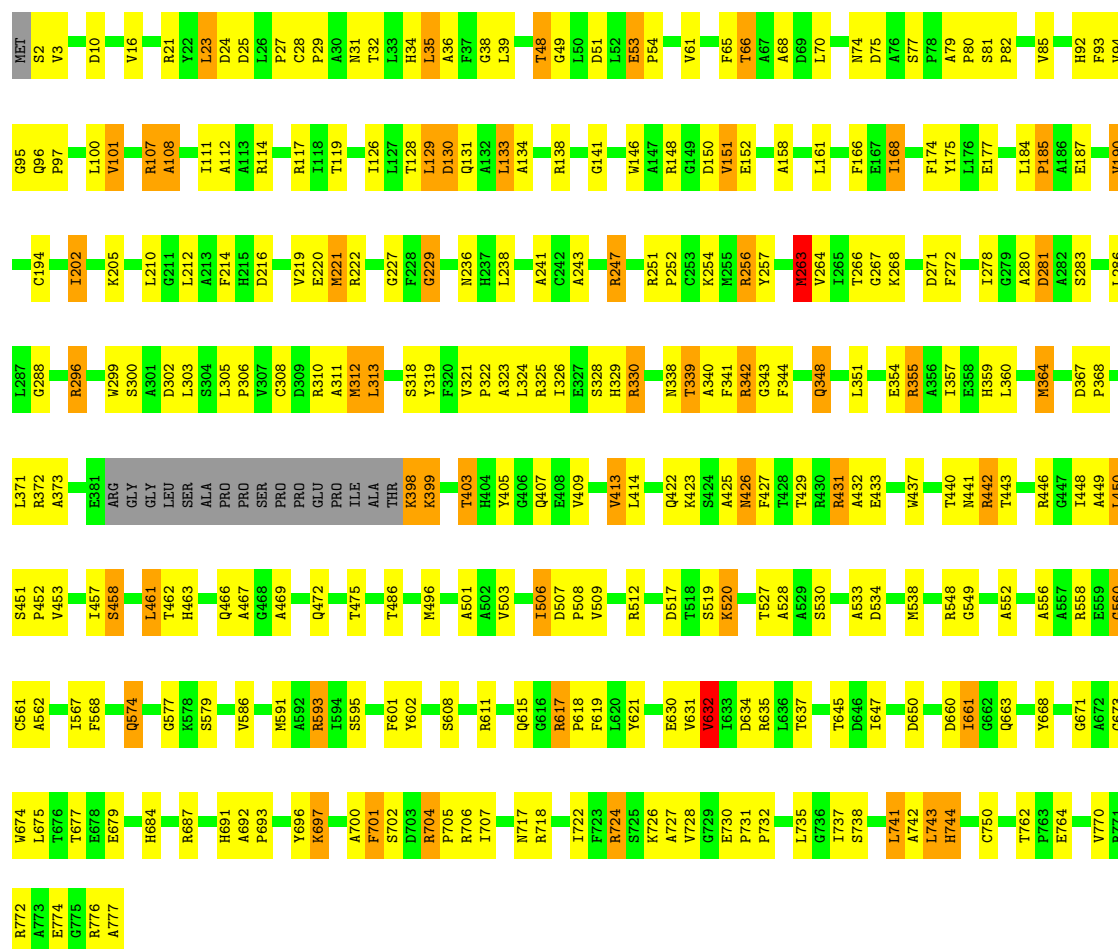
• Molecule 1: xanthine dehydrogenase, chain A

Chain G: 47% 40% 9% ..



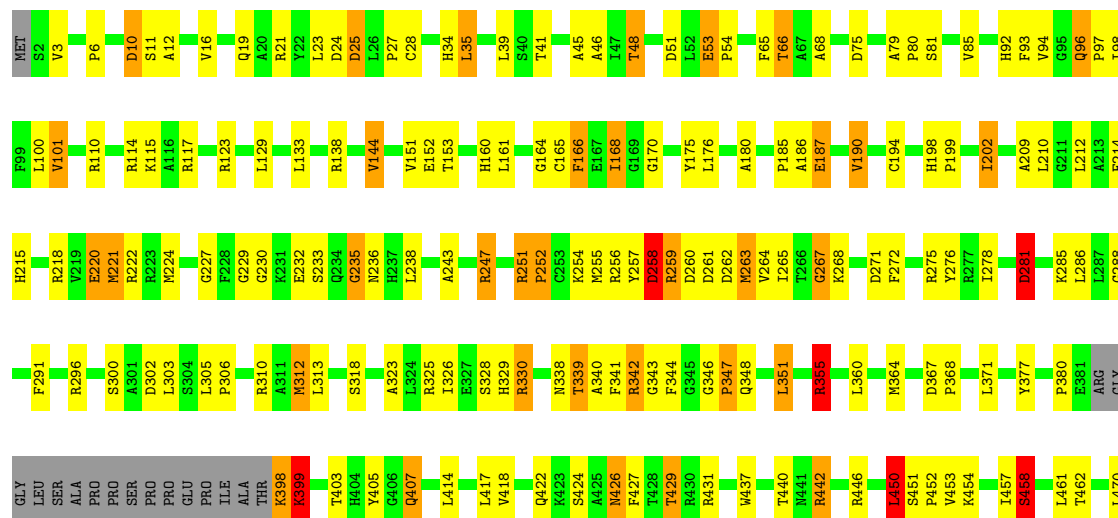
• Molecule 2: xanthine dehydrogenase, chain B

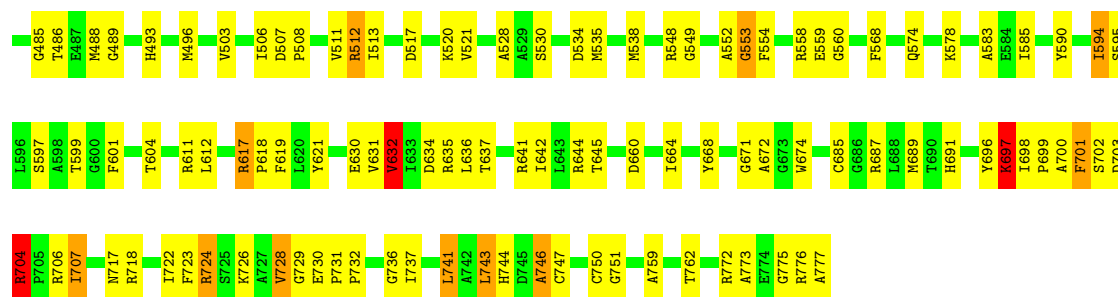
Chain B:



- Molecule 2: xanthine dehydrogenase, chain B

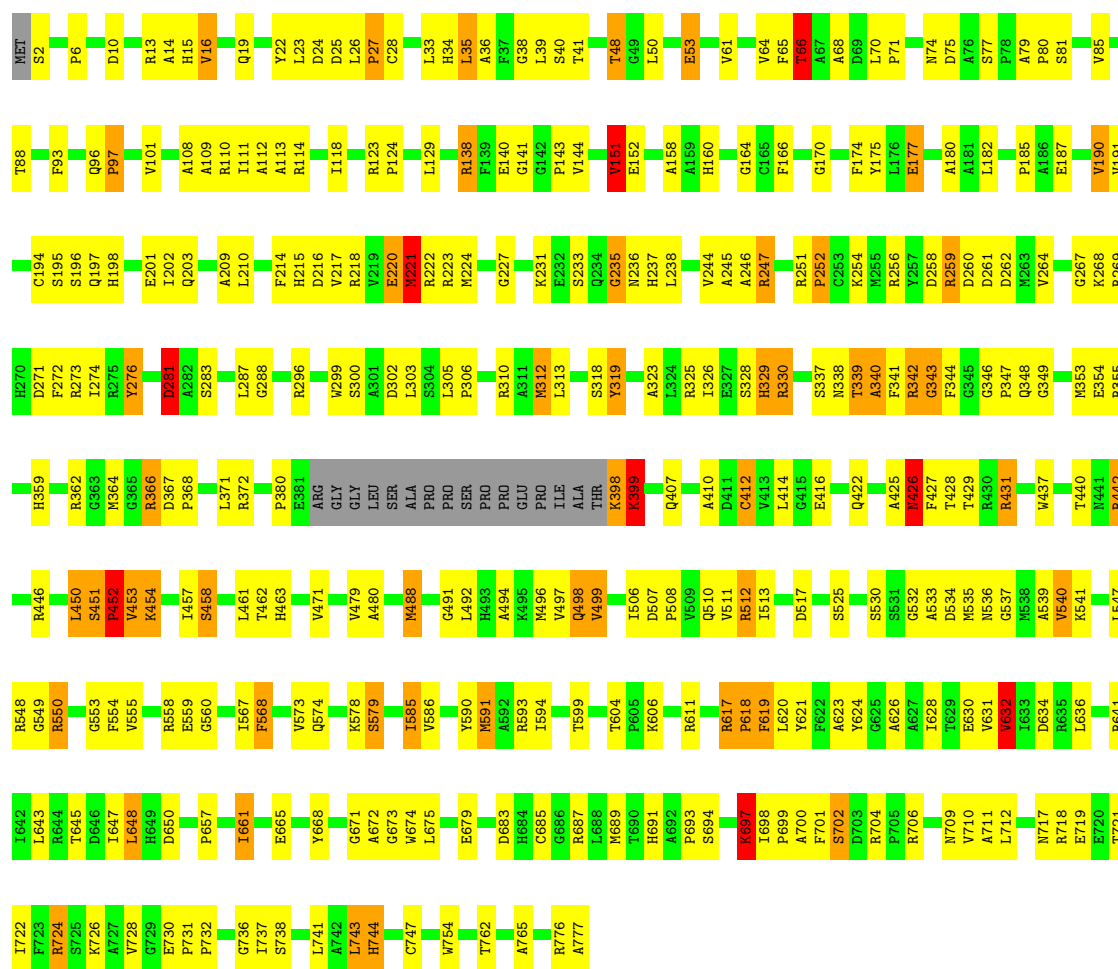
Chain D:





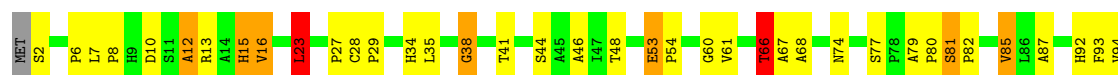
• Molecule 2: xanthine dehydrogenase, chain B

Chain F: 56% 34% 7% ..



• Molecule 2: xanthine dehydrogenase, chain B

Chain H: 54% 34% 8% ..



R724	D634	D517	F427	Q348	D262	A186	Q95
S725	G638	T518	T428	G349	M263	Q96	Q96
A726	E639	S519	T429	E354	V264	P97	P97
A727	N640	K520	R431	R355	T265	I98	I98
G729	L643	V521	T440	A356	G266	F99	F99
E730	L648	A526	M441	I357	K267	L100	L100
F731	L653	T527	T442	E358	K268	V101	V101
F732	A653	A528	T443	H359	R269	A102	A102
F733	L655	A529	R446	L360	D271	A103	A103
G736	L656	S530	G447	M364	F272	S105	S105
I737	M657	S531	I448	G365	Y276	H106	H106
S738	P657	G537	A449	R366	A280	R107	R107
L741	A658	L551	L450	D367	D281	A108	A108
A742	L659	K541	S451	P368	E201	A112	A112
L743	D660	R548	V453	R372	L202	A113	A113
H744	G662	G549	K454	A373	K205	R114	R114
B745	Q663	R550	L457	Y377	L210	R123	R123
A746	T664	L551	S458	P380	A213	P124	P124
C747	E665	V555	L461	E381	F214	A125	A125
F752	Y668	R588	T462	ARG	H215	I126	I126
H753	V669	E559	H463	GLY	D216	L127	L127
W754	Q670	G560	Q466	GLY	V217	T128	T128
A761	A672	C561	Q471	LEU	R218	L129	L129
T762	G673	A562	Q472	SER	V219	D130	D130
F763	W674	A563	T475	ALA	E220	Q131	Q131
E764	L675	R564	D476	PRO	M221	A132	A132
V770	E678	D565	S478	PRO	R222	L133	L133
R771	D683	Q574	Q477	PRO	R223	R138	R138
R772	R687	M591	V479	SER	M224	F139	F139
G776	P693	A592	A480	PRO	G227	E140	E140
R776	Y696	R593	L481	PRO	F228	G141	G141
A777	K697	T599	H483	GLU	G229	G142	G142
	I698	T604	T486	ILE	G230	P143	P143
	A700	G616	Q489	ALA	G235	V144	V144
	F701	G617	Q490	THR	N236	I145	I145
	S702	R618	L491	K398	H237	W146	W146
	B703	F619	L492	K399	L238	V151	V151
	R704	L620	H493		A239	E152	E152
	R705	Y621	A494		L240	A158	A158
	R706	Y624	M496		A243	L161	L161
	A711	Y624	I506		R247	G164	G164
	L712	E630	D507		R251	C165	C165
	W713	V631	P508		P252	F166	F166
	T721	V632	R512		C253	G170	G170
	I722	F633	I513		K254	M255	M255
	F723				F341	R256	R256
					R342	Y257	Y257
					F344	F174	F174
					G345	X175	X175
					D260	L176	L176
					P347	P185	P185

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.88Å 141.05Å 158.11Å 109.53° 105.83° 101.33°	Depositor
Resolution (Å)	50.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.2 (50.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.213 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36831	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: MOS, FAD, CA, FES, MTE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.25	10/3431 (0.3%)	1.39	19/4647 (0.4%)
1	C	1.58	27/3431 (0.8%)	1.49	34/4647 (0.7%)
1	E	1.31	17/3431 (0.5%)	1.49	35/4647 (0.8%)
1	G	1.23	10/3431 (0.3%)	1.49	32/4647 (0.7%)
2	B	1.52	38/5845 (0.7%)	1.54	46/7942 (0.6%)
2	D	1.67	52/5845 (0.9%)	1.57	52/7942 (0.7%)
2	F	1.55	45/5845 (0.8%)	1.58	70/7942 (0.9%)
2	H	1.46	30/5845 (0.5%)	1.55	63/7942 (0.8%)
All	All	1.48	229/37104 (0.6%)	1.53	351/50356 (0.7%)

The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	312	MET	SD-CE	-14.76	1.42	1.79
2	H	521	VAL	CA-CB	-14.02	1.36	1.54
2	B	312	MET	SD-CE	-12.82	1.47	1.79
1	C	114	MET	SD-CE	-11.94	1.49	1.79
2	D	521	VAL	CA-CB	-11.90	1.43	1.54

The worst 5 of 351 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	VAL	CB-CA-C	-10.65	92.29	110.30
2	D	632	VAL	CB-CA-C	-10.21	92.43	110.71
2	F	632	VAL	CB-CA-C	-10.08	94.97	110.50
1	C	125	TYR	N-CA-C	9.66	121.41	111.07
2	B	185	PRO	CB-CA-C	-9.56	99.42	111.56

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	3370	0	3368	134	0
1	C	3370	0	3368	90	0
1	E	3370	0	3368	187	0
1	G	3370	0	3370	210	0
2	B	5717	0	5630	179	0
2	D	5717	0	5631	173	0
2	F	5717	0	5631	206	0
2	H	5717	0	5630	239	0
3	A	8	0	0	0	0
3	C	8	0	0	0	0
3	E	8	0	0	2	0
3	G	8	0	0	3	0
4	A	53	0	31	6	0
4	C	53	0	30	3	0
4	E	53	0	31	6	0
4	G	53	0	31	11	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	B	24	0	10	1	0
6	D	24	0	10	2	0
6	F	24	0	10	1	0
6	H	24	0	10	2	0
7	B	4	0	0	5	0
7	D	4	0	0	5	0
7	F	4	0	0	2	0
7	H	4	0	0	5	0
8	A	11	0	0	1	0
8	B	26	0	0	1	0
8	C	7	0	0	0	0
8	D	25	0	0	1	0
8	E	7	0	0	0	0
8	F	20	0	0	0	0
8	G	6	0	0	6	0
8	H	21	0	0	4	0
All	All	36831	0	36159	1370	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 19.

The worst 5 of 1370 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:E:316:MET:SD	1:E:316:MET:CE	2.07	1.42
1:G:325:TYR:CE1	1:G:326:ARG:HG2	1.64	1.33
1:E:325:TYR:O	1:E:326:ARG:HB2	1.41	1.18
2:F:621:TYR:CE1	2:F:726:LYS:HG2	1.84	1.11
1:G:325:TYR:CD1	1:G:326:ARG:HG2	1.85	1.11

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	446/462 (96%)	401 (90%)	41 (9%)	4 (1%)	14	35
1	C	446/462 (96%)	415 (93%)	27 (6%)	4 (1%)	14	35
1	E	446/462 (96%)	383 (86%)	53 (12%)	10 (2%)	5	14
1	G	446/462 (96%)	395 (89%)	44 (10%)	7 (2%)	7	20
2	B	756/777 (97%)	708 (94%)	40 (5%)	8 (1%)	11	29
2	D	756/777 (97%)	718 (95%)	31 (4%)	7 (1%)	14	35
2	F	756/777 (97%)	709 (94%)	39 (5%)	8 (1%)	11	29
2	H	756/777 (97%)	700 (93%)	47 (6%)	9 (1%)	10	27
All	All	4808/4956 (97%)	4429 (92%)	322 (7%)	57 (1%)	10	27

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	399	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	458	SER
1	C	180	ALA
1	C	374	GLY
2	D	281	ASP

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	339/347 (98%)	301 (89%)	38 (11%)	6	15
1	C	339/347 (98%)	302 (89%)	37 (11%)	6	16
1	E	339/347 (98%)	295 (87%)	44 (13%)	4	10
1	G	339/347 (98%)	290 (86%)	49 (14%)	3	8
2	B	571/584 (98%)	515 (90%)	56 (10%)	7	19
2	D	571/584 (98%)	518 (91%)	53 (9%)	8	21
2	F	571/584 (98%)	512 (90%)	59 (10%)	7	18
2	H	571/584 (98%)	508 (89%)	63 (11%)	6	15
All	All	3640/3724 (98%)	3241 (89%)	399 (11%)	6	15

5 of 399 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	35	LEU
2	F	744	HIS
2	F	175	TYR
2	F	450	LEU
1	G	69	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	536	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	463	HIS
2	F	208	HIS
2	H	359	HIS
2	H	15	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 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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$
6	MTE	F	3003	7	21,26,26	5.61	10 (47%)	19,40,40	5.23	12 (63%)
7	MOS	D	3004	6	0,3,3	-	-	-		
3	FES	C	3002	1	0,4,4	-	-	-		
3	FES	G	3001	1	0,4,4	-	-	-		
3	FES	C	3001	1	0,4,4	-	-	-		
6	MTE	B	3003	7	21,26,26	5.53	10 (47%)	19,40,40	3.59	11 (57%)
7	MOS	B	3004	6	0,3,3	-	-	-		
4	FAD	C	3005	-	58,58,58	1.66	9 (15%)	85,89,89	2.54	38 (44%)
6	MTE	H	3003	7	21,26,26	5.58	10 (47%)	19,40,40	5.08	12 (63%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MOS	F	3004	6	0,3,3	-	-	-		
6	MTE	D	3003	7	21,26,26	4.79	11 (52%)	19,40,40	5.57	11 (57%)
4	FAD	E	3005	-	58,58,58	1.62	9 (15%)	85,89,89	2.10	29 (34%)
3	FES	E	3001	1	0,4,4	-	-	-		
4	FAD	G	3005	-	58,58,58	1.32	8 (13%)	85,89,89	2.23	34 (40%)
3	FES	A	3002	1	0,4,4	-	-	-		
3	FES	G	3002	1	0,4,4	-	-	-		
3	FES	A	3001	1	0,4,4	-	-	-		
3	FES	E	3002	1	0,4,4	-	-	-		
4	FAD	A	3005	-	58,58,58	1.34	8 (13%)	85,89,89	2.14	31 (36%)
7	MOS	H	3004	6	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MTE	F	3003	7	-	4/6/34/34	0/3/3/3
3	FES	C	3002	1	-	-	0/1/1/1
6	MTE	D	3003	7	-	3/6/34/34	0/3/3/3
3	FES	A	3002	1	-	-	0/1/1/1
3	FES	G	3002	1	-	-	0/1/1/1
4	FAD	E	3005	-	-	12/34/50/50	0/6/6/6
3	FES	C	3001	1	-	-	0/1/1/1
3	FES	E	3001	1	-	-	0/1/1/1
3	FES	E	3002	1	-	-	0/1/1/1
3	FES	G	3001	1	-	-	0/1/1/1
6	MTE	B	3003	7	-	0/6/34/34	0/3/3/3
4	FAD	A	3005	-	-	14/34/50/50	0/6/6/6
4	FAD	G	3005	-	-	9/34/50/50	0/6/6/6
4	FAD	C	3005	-	-	10/34/50/50	0/6/6/6
6	MTE	H	3003	7	-	1/6/34/34	0/3/3/3
3	FES	A	3001	1	-	-	0/1/1/1

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3003	MTE	C7-C6	14.92	1.65	1.53
6	B	3003	MTE	C7-C6	14.34	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	3003	MTE	C7-C6	12.73	1.63	1.53
6	F	3003	MTE	C9-C10	12.48	1.59	1.38
6	H	3003	MTE	C9-C10	12.43	1.59	1.38

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3003	MTE	O3'-C7-C6	-19.89	95.70	108.96
6	F	3003	MTE	O3'-C7-C6	-16.03	98.27	108.96
6	H	3003	MTE	O3'-C7-C6	-15.63	98.54	108.96
6	F	3003	MTE	C2-N1-C10	8.72	128.76	113.36
6	D	3003	MTE	C2-N1-C10	8.53	128.42	113.36

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3005	FAD	C5B-O5B-PA-O2A
4	A	3005	FAD	C5B-O5B-PA-O3P
4	A	3005	FAD	C2'-C1'-N10-C10
4	A	3005	FAD	N10-C1'-C2'-O2'
4	A	3005	FAD	N10-C1'-C2'-C3'

There are no ring outliers.

16 monomers are involved in 50 short contacts:

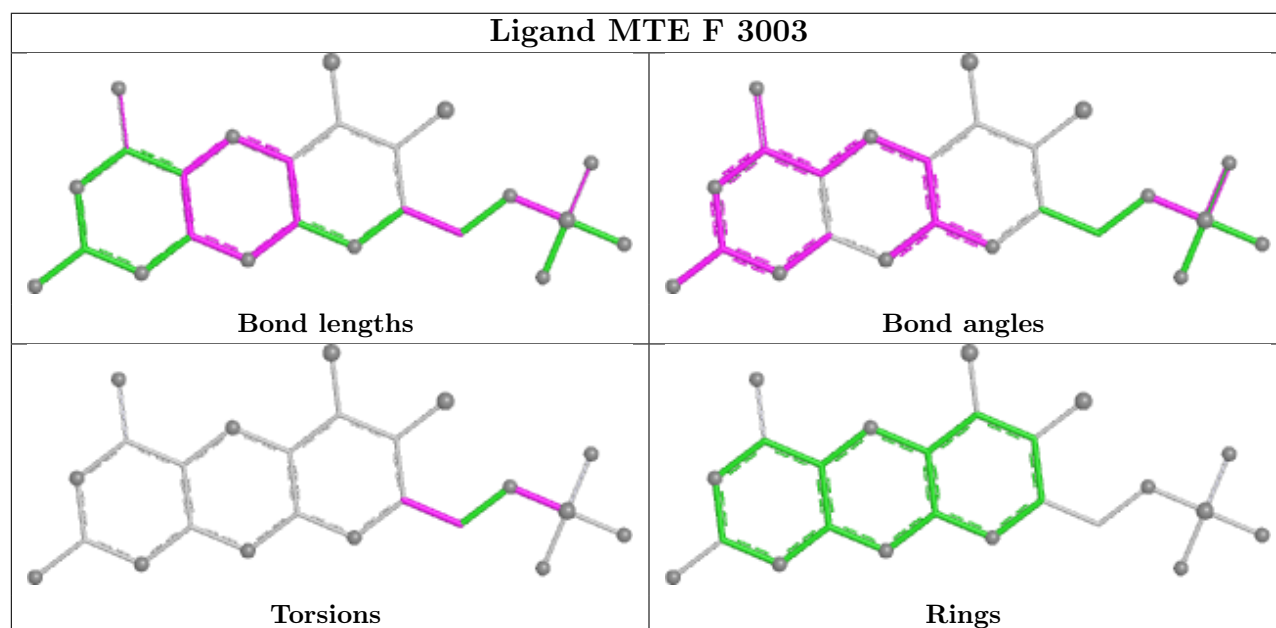
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	3003	MTE	1	0
7	D	3004	MOS	5	0
3	G	3001	FES	2	0
6	B	3003	MTE	1	0
7	B	3004	MOS	5	0
4	C	3005	FAD	3	0
6	H	3003	MTE	2	0
7	F	3004	MOS	2	0
6	D	3003	MTE	2	0
4	E	3005	FAD	6	0
3	E	3001	FES	1	0
4	G	3005	FAD	11	0
3	G	3002	FES	1	0
3	E	3002	FES	1	0

Continued on next page...

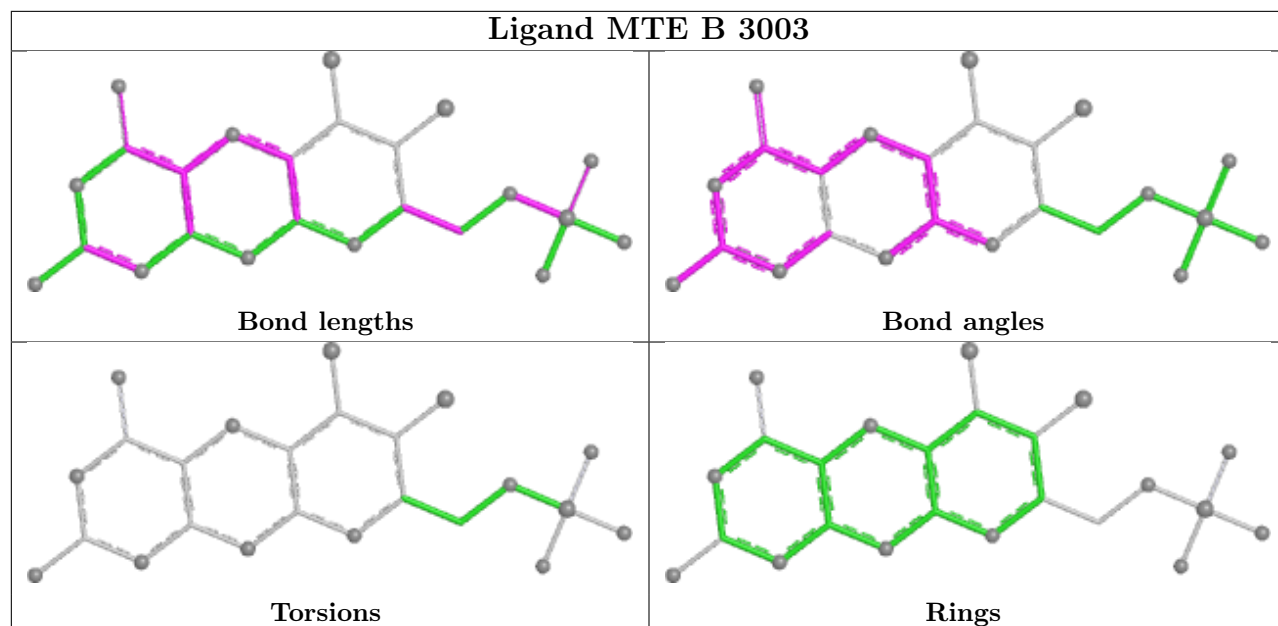
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3005	FAD	6	0
7	H	3004	MOS	5	0

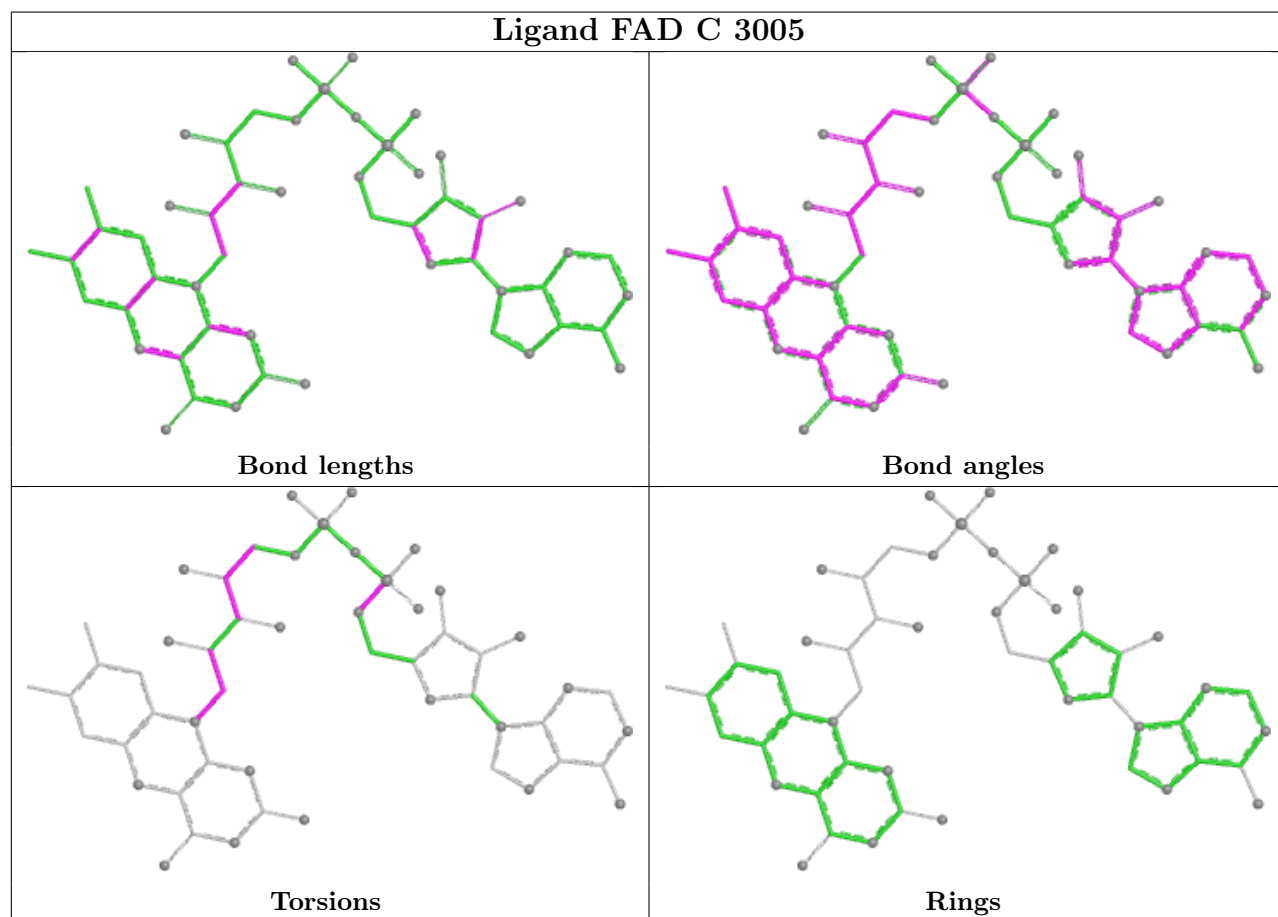
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



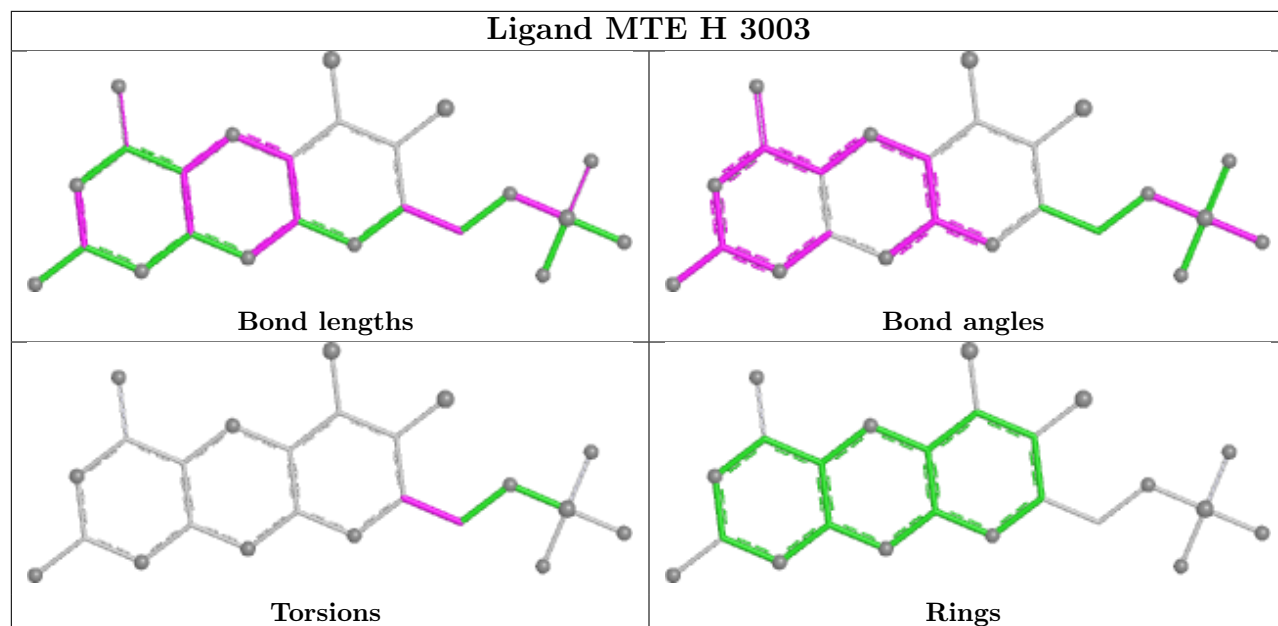
Ligand MTE B 3003



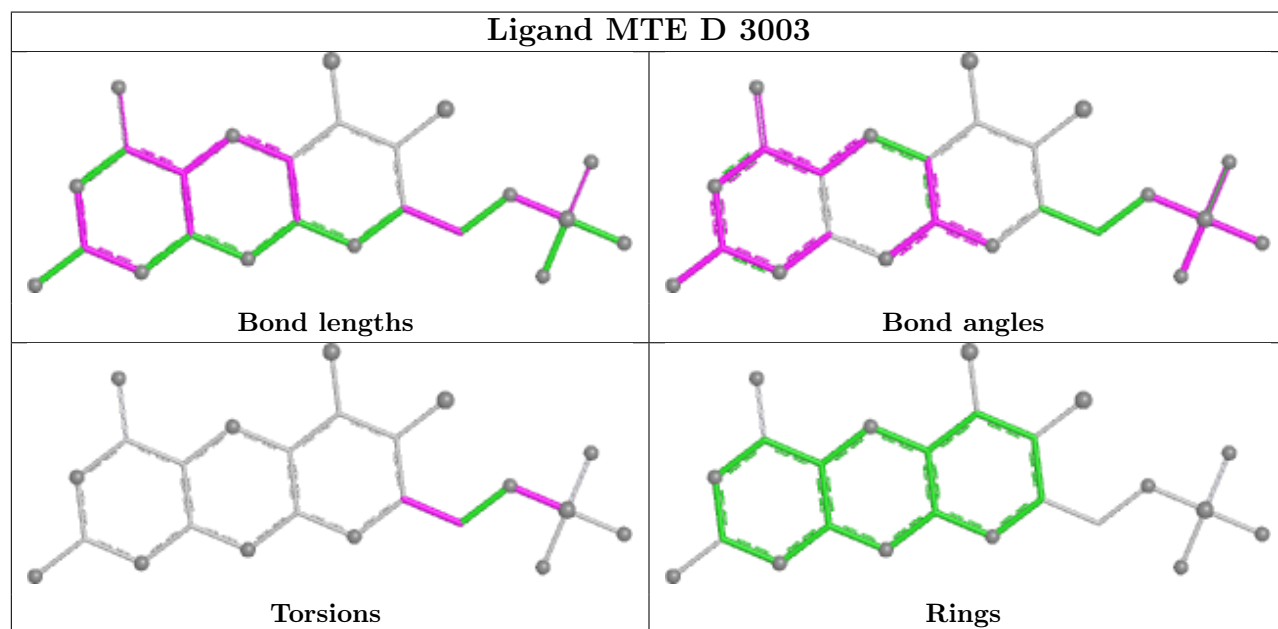
Ligand FAD C 3005

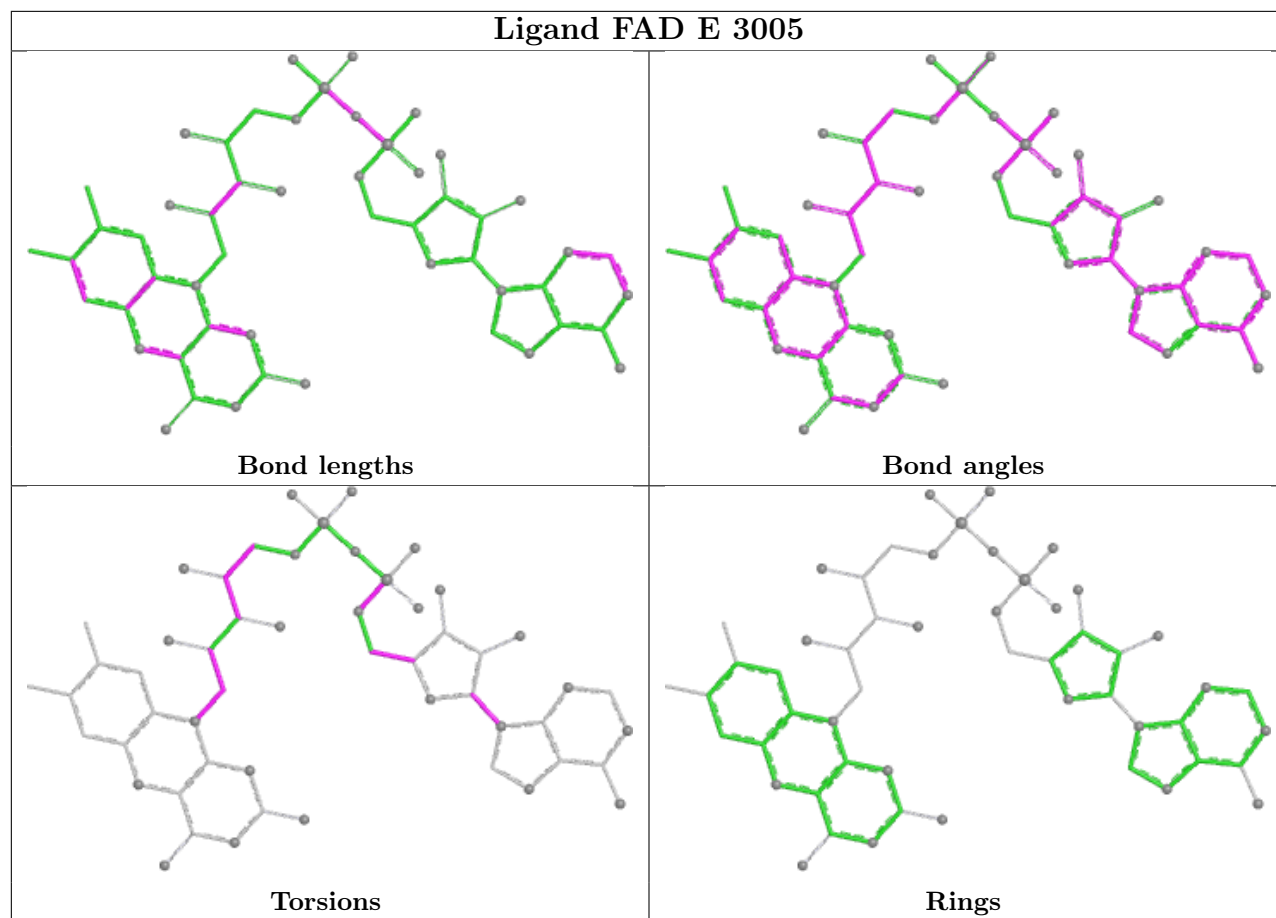


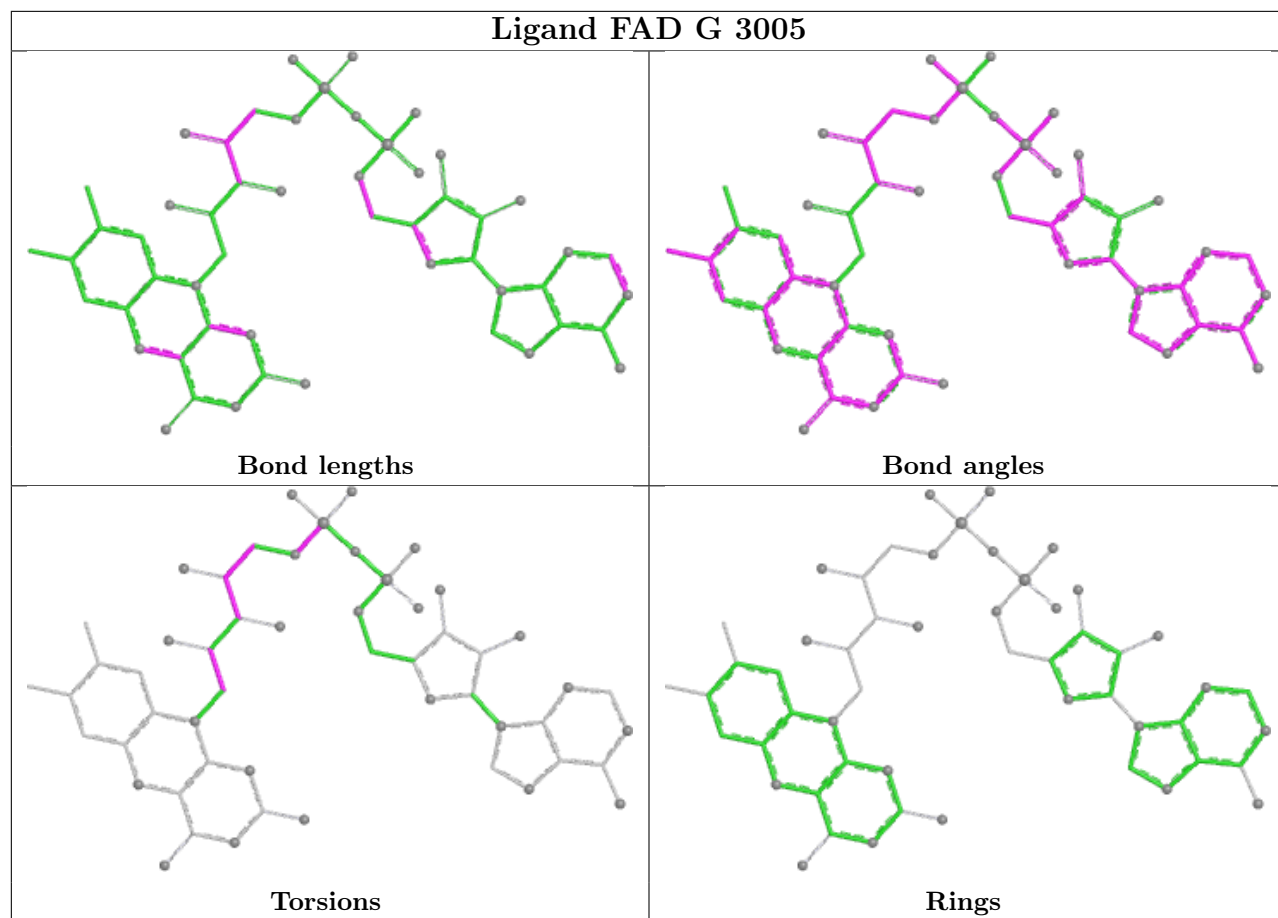
Ligand MTE H 3003

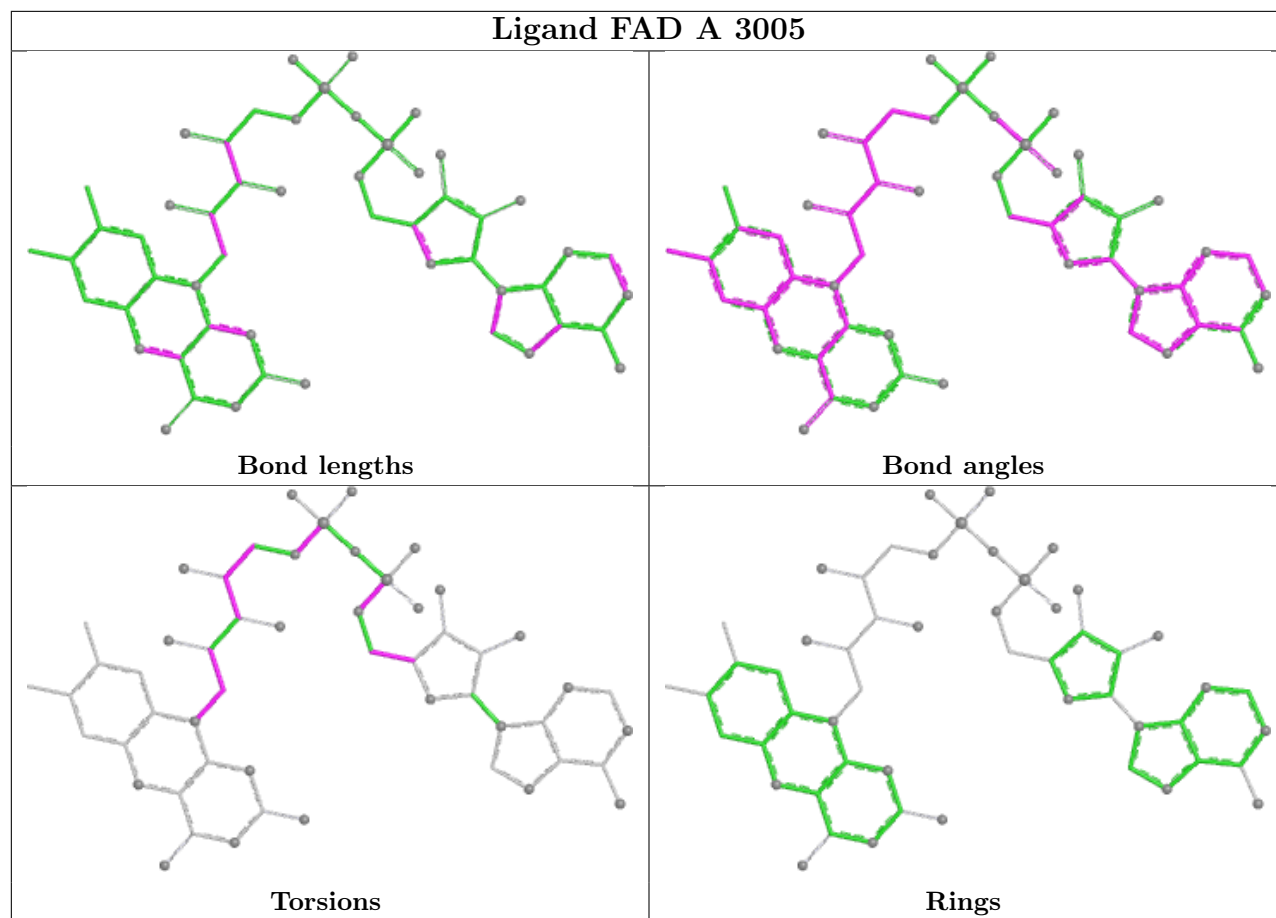


Ligand MTE D 3003









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.