



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 06:33 pm BST

PDB ID : 1JRO
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 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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

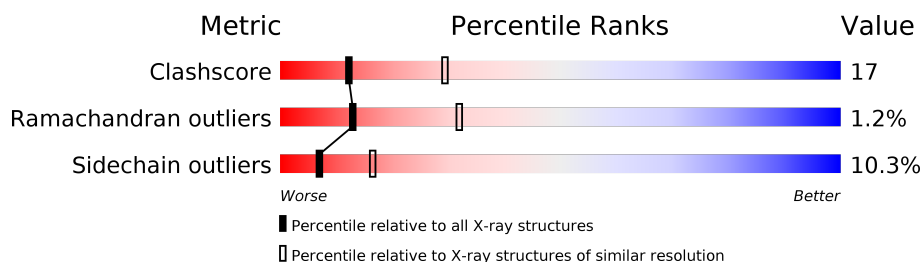
1 Overall quality at a glance

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 on 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	
1	C	462	
1	E	462	
1	G	462	
2	B	777	
2	D	777	
2	F	777	
2	H	777	

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 (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	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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

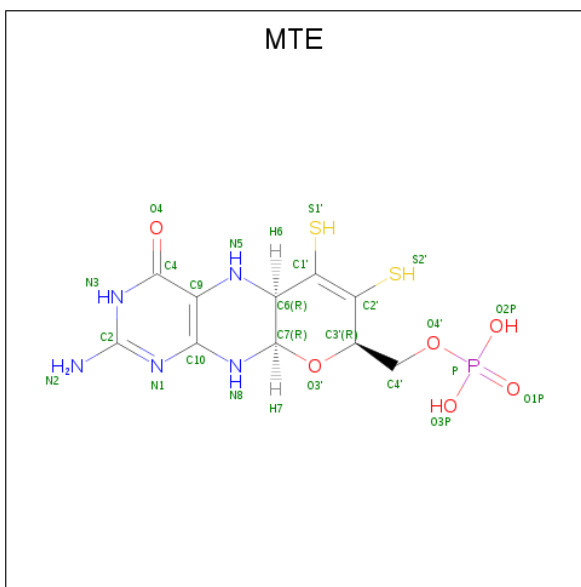


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

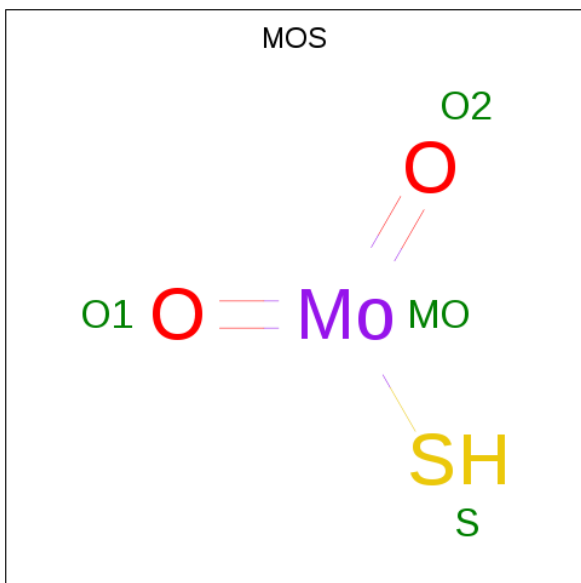
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

- 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 (three-letter code: 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 (three-letter code: 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.

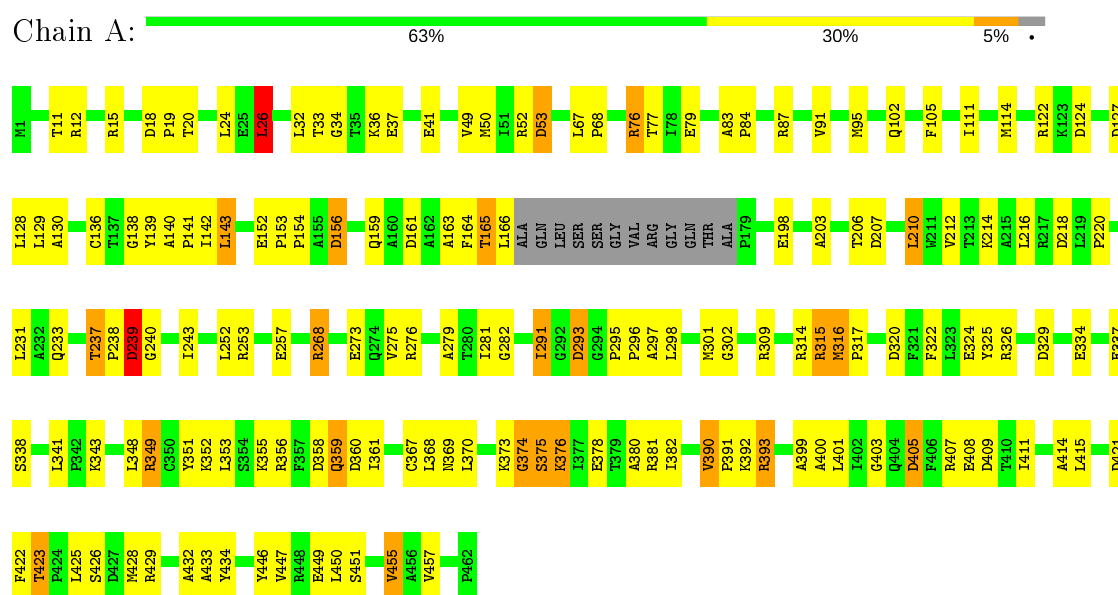
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total 11	O 11	0	0
8	B	26	Total 26	O 26	0	0
8	C	7	Total 7	O 7	0	0
8	D	25	Total 25	O 25	0	0
8	E	7	Total 7	O 7	0	0
8	F	20	Total 20	O 20	0	0
8	G	6	Total 6	O 6	0	0
8	H	21	Total 21	O 21	0	0

3 Residue-property plots

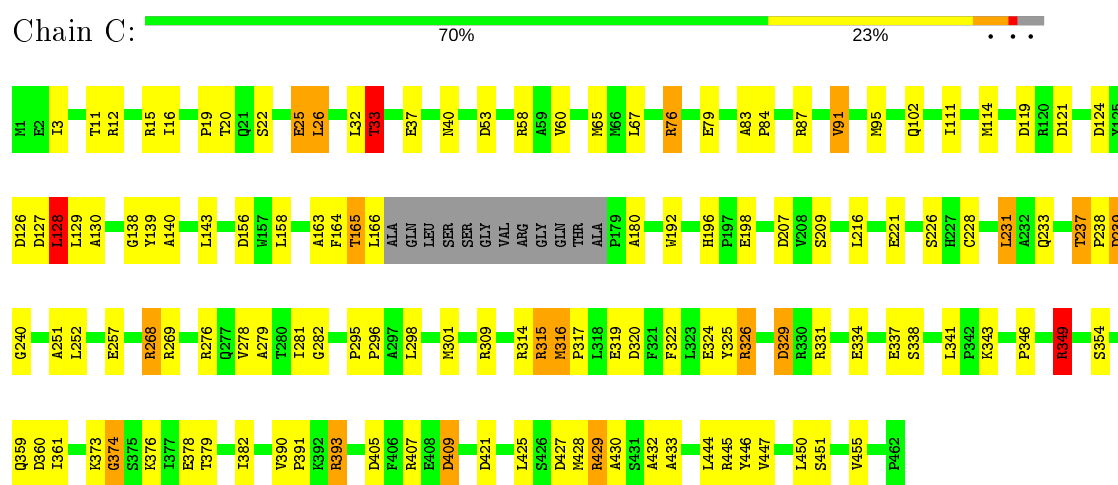
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

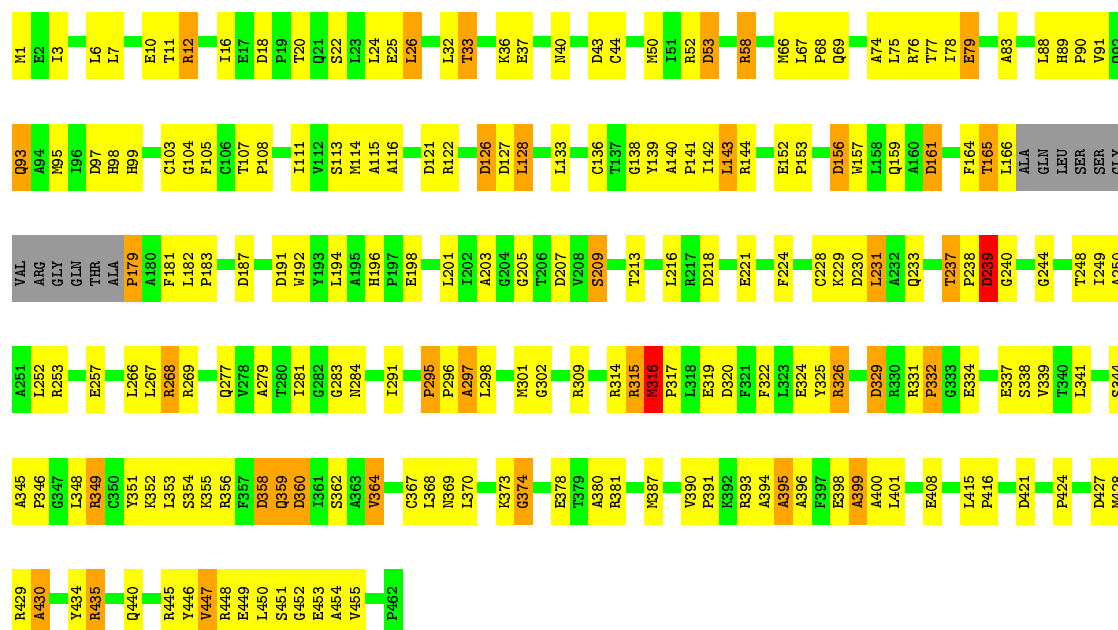


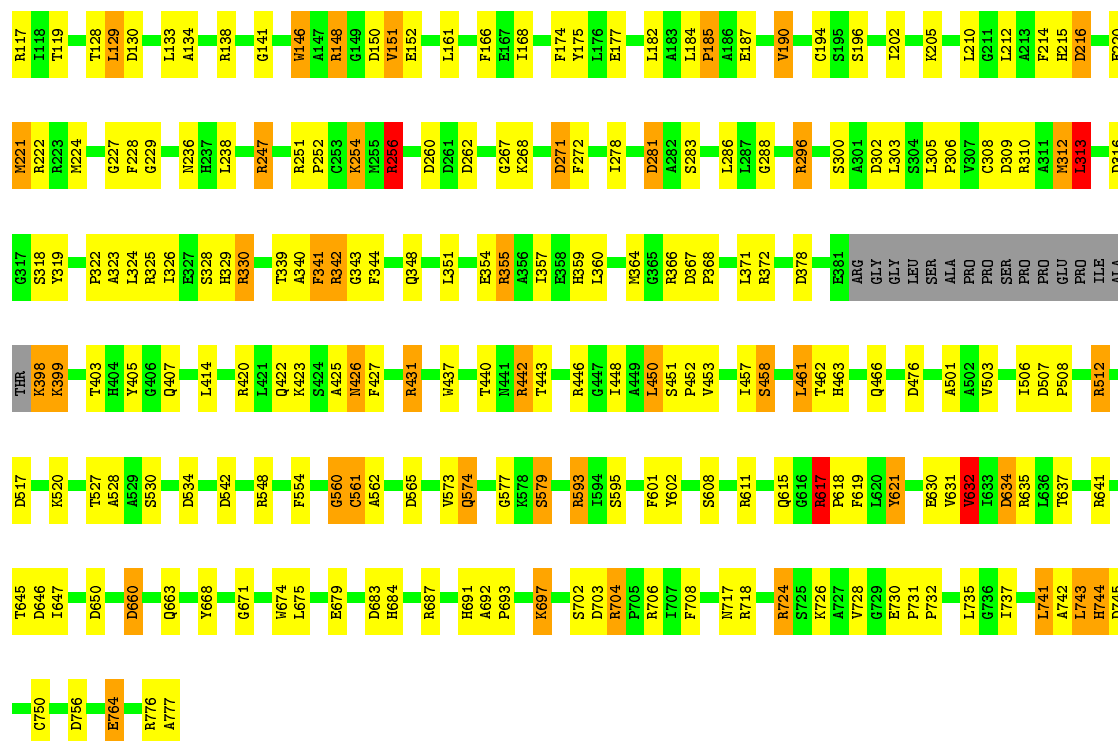
- Molecule 1: xanthine dehydrogenase, chain A



- Molecule 1: xanthine dehydrogenase, chain A

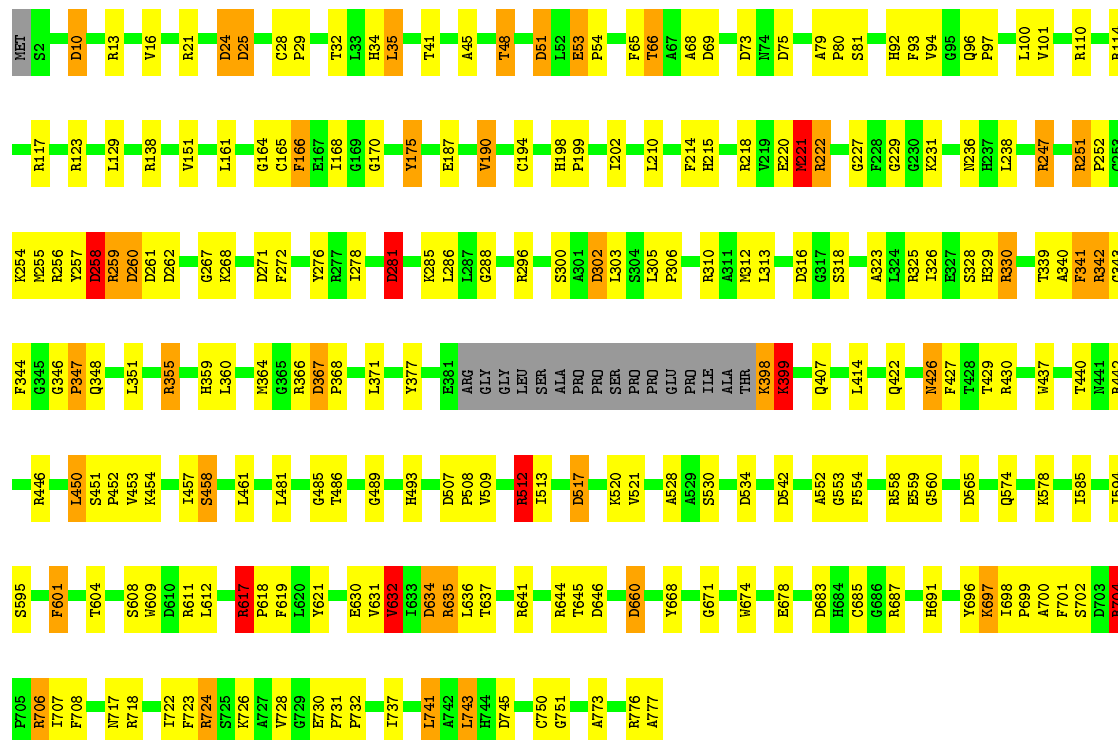
Chain E: 





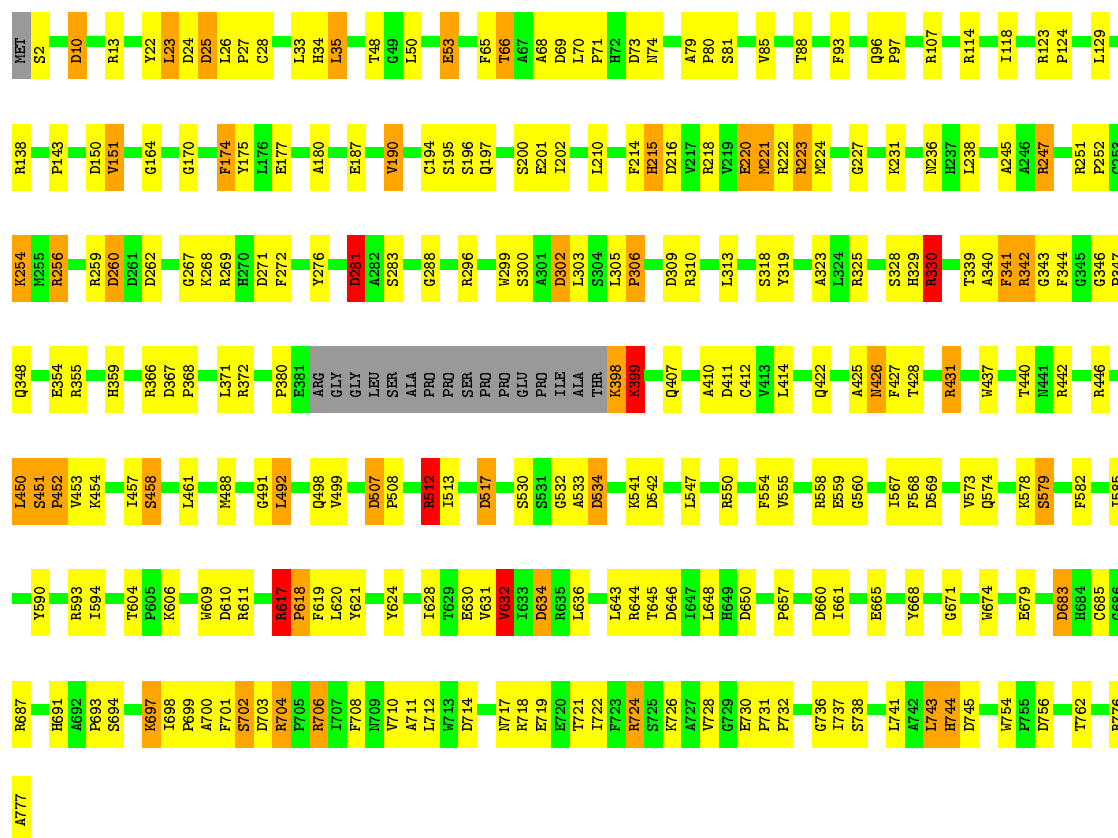
• Molecule 2: xanthine dehydrogenase, chain B

Chain D: 68% 24% 5% ..



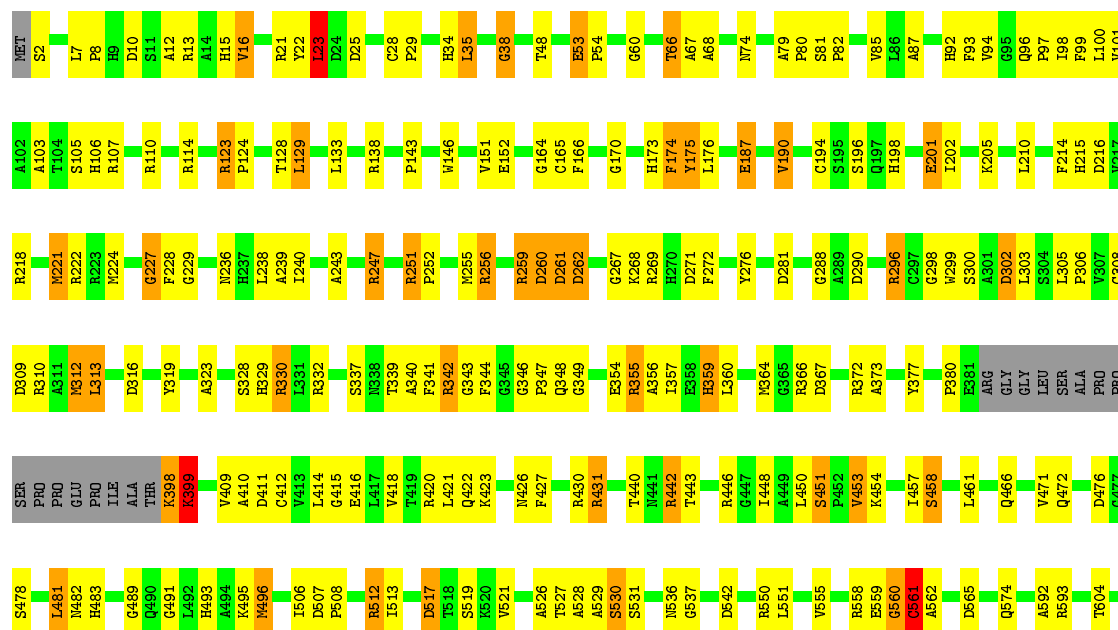
• Molecule 2: xanthine dehydrogenase, chain B

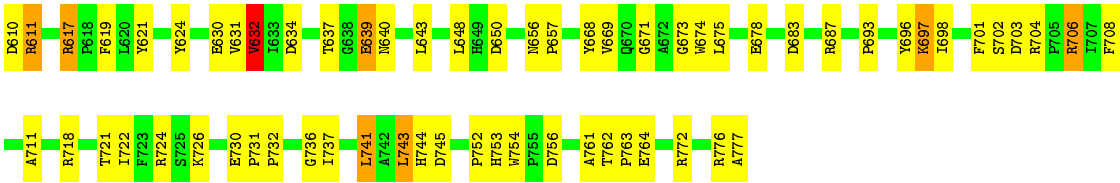
Chain F:  65% 27% 6% ..



• Molecule 2: xanthine dehydrogenase, chain B

Chain H:  61% 30% 6% ..





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, CA, FES, FAD, 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	0.94	1/3431 (0.0%)	1.11	17/4647 (0.4%)
1	C	1.17	4/3431 (0.1%)	1.25	23/4647 (0.5%)
1	E	0.99	1/3431 (0.0%)	1.17	20/4647 (0.4%)
1	G	0.98	7/3431 (0.2%)	1.18	26/4647 (0.6%)
2	B	1.16	6/5845 (0.1%)	1.25	49/7942 (0.6%)
2	D	1.26	9/5845 (0.2%)	1.29	47/7942 (0.6%)
2	F	1.17	4/5845 (0.1%)	1.26	43/7942 (0.5%)
2	H	1.14	7/5845 (0.1%)	1.23	38/7942 (0.5%)
All	All	1.13	39/37104 (0.1%)	1.23	263/50356 (0.5%)

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	258	ASP	CB-CG	-9.22	1.32	1.51
2	H	521	VAL	CA-CB	-8.89	1.36	1.54
1	G	325	TYR	CD1-CE1	-7.39	1.28	1.39
1	G	325	TYR	CB-CG	-7.20	1.40	1.51
1	G	325	TYR	CD2-CE2	-6.99	1.28	1.39

The worst 5 of 263 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	258	ASP	CB-CG-OD1	-13.50	106.15	118.30
1	C	349	ARG	NE-CZ-NH1	13.32	126.96	120.30
2	D	258	ASP	CB-CG-OD2	13.19	130.17	118.30
1	C	429	ARG	NE-CZ-NH2	-12.01	114.30	120.30
2	D	660	ASP	CB-CG-OD2	11.32	128.49	118.30

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	125	0
1	C	3370	0	3368	82	0
1	E	3370	0	3368	177	0
1	G	3370	0	3370	189	0
2	B	5717	0	5630	162	0
2	D	5717	0	5631	153	0
2	F	5717	0	5631	181	0
2	H	5717	0	5630	214	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	1239	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 17.

The worst 5 of 1239 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%)	17	40
1	C	446/462 (96%)	415 (93%)	27 (6%)	4 (1%)	17	40
1	E	446/462 (96%)	383 (86%)	53 (12%)	10 (2%)	6	17
1	G	446/462 (96%)	395 (89%)	44 (10%)	7 (2%)	9	24
2	B	756/777 (97%)	708 (94%)	40 (5%)	8 (1%)	14	34
2	D	756/777 (97%)	718 (95%)	31 (4%)	7 (1%)	17	40
2	F	756/777 (97%)	709 (94%)	39 (5%)	8 (1%)	14	34
2	H	756/777 (97%)	700 (93%)	47 (6%)	9 (1%)	13	32
All	All	4808/4956 (97%)	4429 (92%)	322 (7%)	57 (1%)	13	32

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	399	LYS

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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%)	302 (89%)	37 (11%)	6	14
1	C	339/347 (98%)	302 (89%)	37 (11%)	6	14
1	E	339/347 (98%)	301 (89%)	38 (11%)	6	13
1	G	339/347 (98%)	302 (89%)	37 (11%)	6	14
2	B	571/584 (98%)	515 (90%)	56 (10%)	8	18
2	D	571/584 (98%)	514 (90%)	57 (10%)	7	18
2	F	571/584 (98%)	513 (90%)	58 (10%)	7	17
2	H	571/584 (98%)	516 (90%)	55 (10%)	8	19
All	All	3640/3724 (98%)	3265 (90%)	375 (10%)	7	16

5 of 375 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	534	ASP
1	E	231	LEU
2	H	330	ARG
2	D	611	ARG
1	E	26	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	426	ASN

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Mol	Chain	Res	Type
1	E	196	HIS
2	H	236	ASN
2	D	691	HIS
2	D	744	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	FAD	C	3005	-	51,58,58	2.03	14 (27%)	60,89,89	3.10	30 (50%)
3	FES	A	3001	1	0,4,4	0.00	-	-		
4	FAD	A	3005	-	51,58,58	1.59	10 (19%)	60,89,89	2.93	20 (33%)
3	FES	E	3001	1	0,4,4	0.00	-	-		
3	FES	C	3002	1	0,4,4	0.00	-	-		
6	MTE	B	3003	7	21,26,26	5.38	10 (47%)	21,40,40	3.09	7 (33%)
6	MTE	F	3003	7	21,26,26	5.35	10 (47%)	21,40,40	4.71	9 (42%)
6	MTE	D	3003	7	21,26,26	4.61	12 (57%)	21,40,40	5.62	10 (47%)
3	FES	C	3001	1	0,4,4	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FES	E	3002	1	0,4,4	0.00	-	-		
7	MOS	F	3004	6	0,3,3	0.00	-	-		
7	MOS	H	3004	6	0,3,3	0.00	-	-		
3	FES	A	3002	1	0,4,4	0.00	-	-		
7	MOS	D	3004	6	0,3,3	0.00	-	-		
6	MTE	H	3003	7	21,26,26	5.27	11 (52%)	21,40,40	5.05	9 (42%)
7	MOS	B	3004	6	0,3,3	0.00	-	-		
4	FAD	G	3005	-	51,58,58	1.58	14 (27%)	60,89,89	2.49	24 (40%)
3	FES	G	3002	1	0,4,4	0.00	-	-		
4	FAD	E	3005	-	51,58,58	1.52	9 (17%)	60,89,89	2.57	26 (43%)
3	FES	G	3001	1	0,4,4	0.00	-	-		

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	FAD	C	3005	-	-	14/30/50/50	0/6/6/6
3	FES	A	3001	1	-	-	0/1/1/1
4	FAD	A	3005	-	-	16/30/50/50	0/6/6/6
3	FES	E	3001	1	-	-	0/1/1/1
3	FES	C	3002	1	-	-	0/1/1/1
6	MTE	B	3003	7	-	0/6/34/34	0/3/3/3
3	FES	E	3002	1	-	-	0/1/1/1
6	MTE	D	3003	7	-	2/6/34/34	0/3/3/3
3	FES	C	3001	1	-	-	0/1/1/1
6	MTE	F	3003	7	-	4/6/34/34	0/3/3/3
6	MTE	H	3003	7	-	1/6/34/34	0/3/3/3
3	FES	A	3002	1	-	-	0/1/1/1
4	FAD	G	3005	-	-	11/30/50/50	0/6/6/6
3	FES	G	3002	1	-	-	0/1/1/1
4	FAD	E	3005	-	-	12/30/50/50	0/6/6/6
3	FES	G	3001	1	-	-	0/1/1/1

The worst 5 of 90 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	3003	MTE	C7-C6	12.73	1.63	1.53
6	D	3003	MTE	C7-C6	10.22	1.61	1.53
6	F	3003	MTE	C9-C10	9.79	1.59	1.41

The worst 5 of 135 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	D	3003	MTE	C4-C9-N5	9.89	127.42	119.12
4	A	3005	FAD	C1'-N10-C9A	9.36	125.66	118.29

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3005	FAD	C5B-O5B-PA-O1A
4	C	3005	FAD	C2'-C1'-N10-C9A
4	C	3005	FAD	C2'-C1'-N10-C10
4	C	3005	FAD	N10-C1'-C2'-O2'
4	C	3005	FAD	N10-C1'-C2'-C3'

There are no ring outliers.

16 monomers are involved in 50 short contacts:

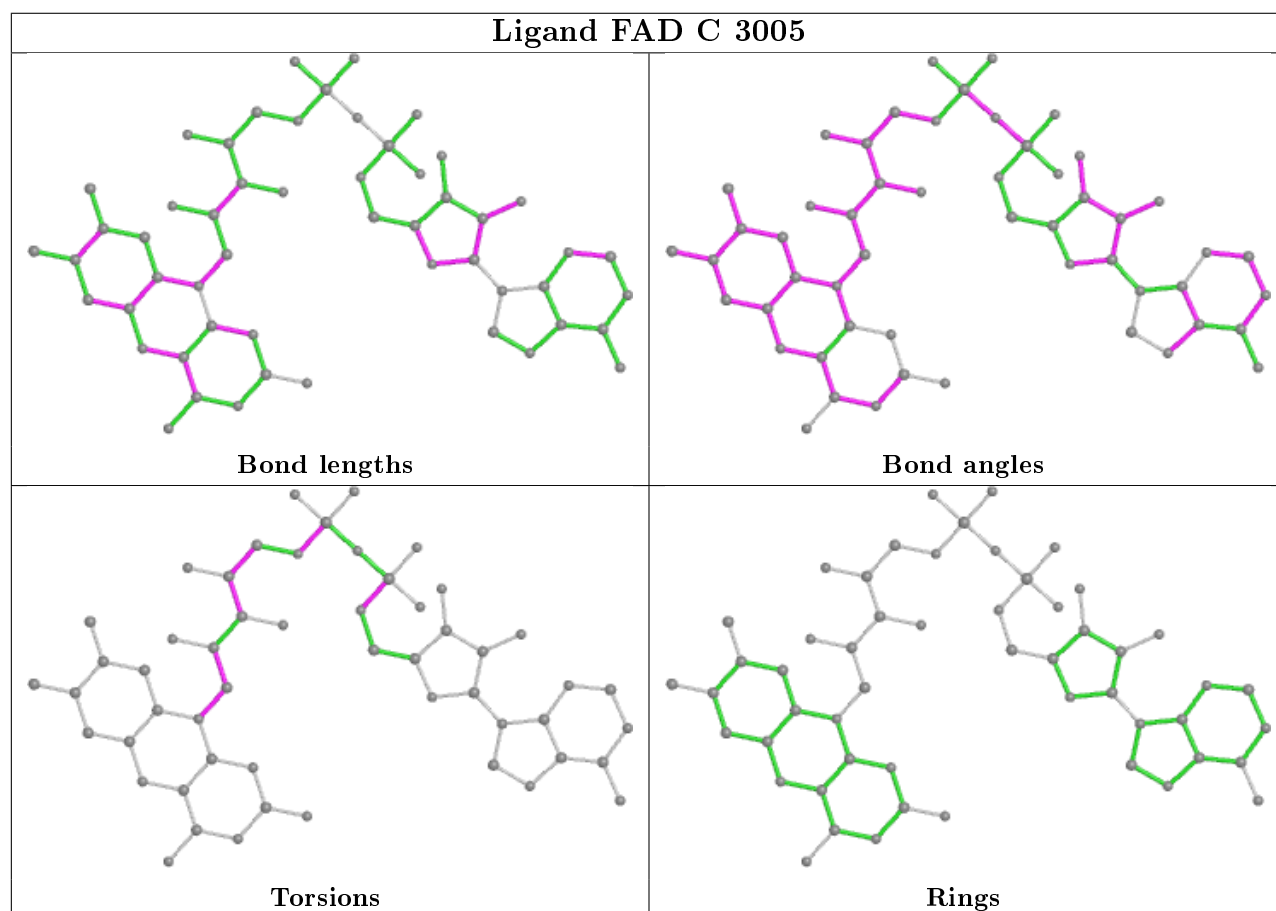
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3005	FAD	3	0
4	A	3005	FAD	6	0
3	E	3001	FES	1	0
6	B	3003	MTE	1	0
6	F	3003	MTE	1	0
6	D	3003	MTE	2	0
3	E	3002	FES	1	0
7	F	3004	MOS	2	0
7	H	3004	MOS	5	0
7	D	3004	MOS	5	0
6	H	3003	MTE	2	0
7	B	3004	MOS	5	0
4	G	3005	FAD	11	0
3	G	3002	FES	1	0

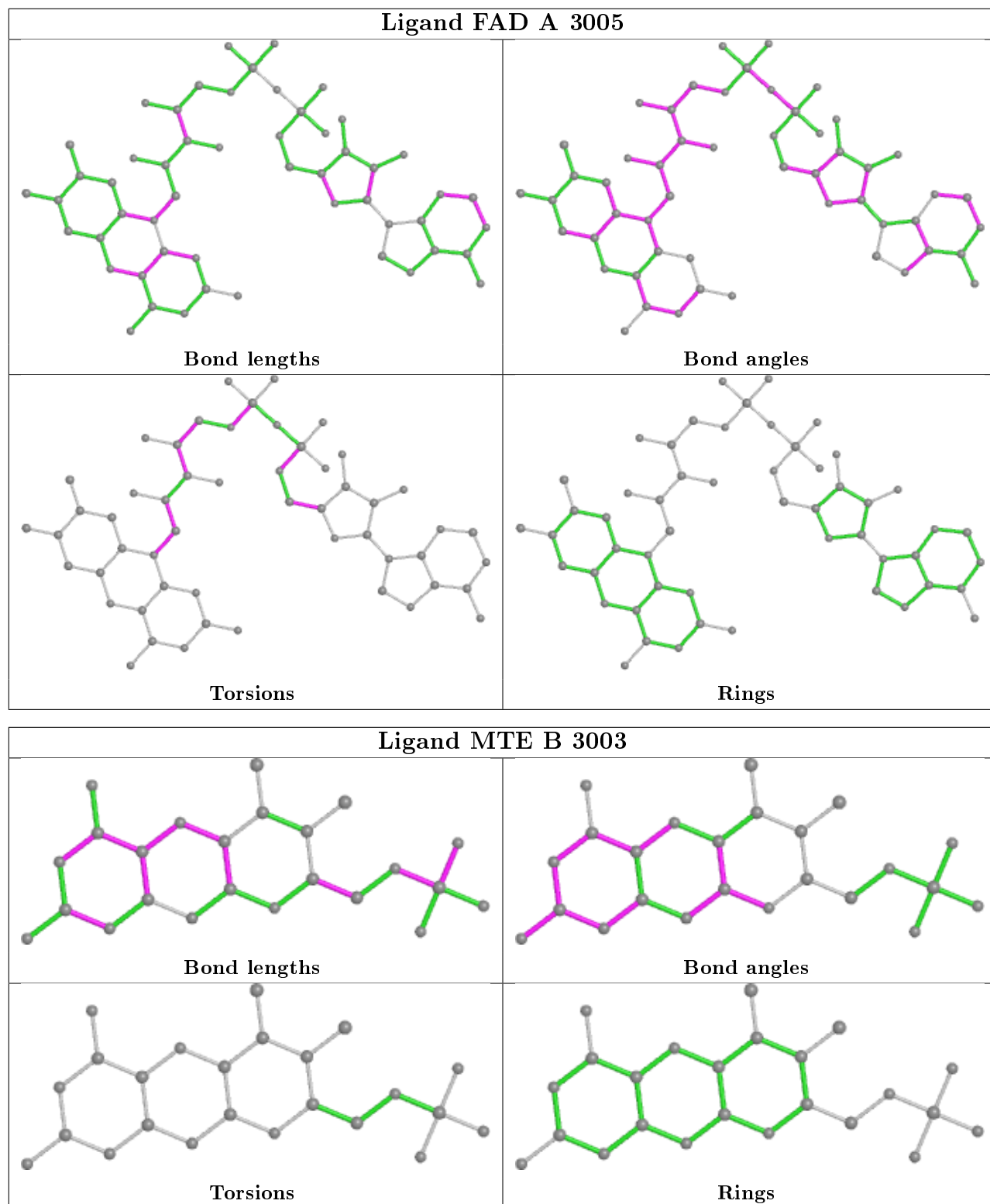
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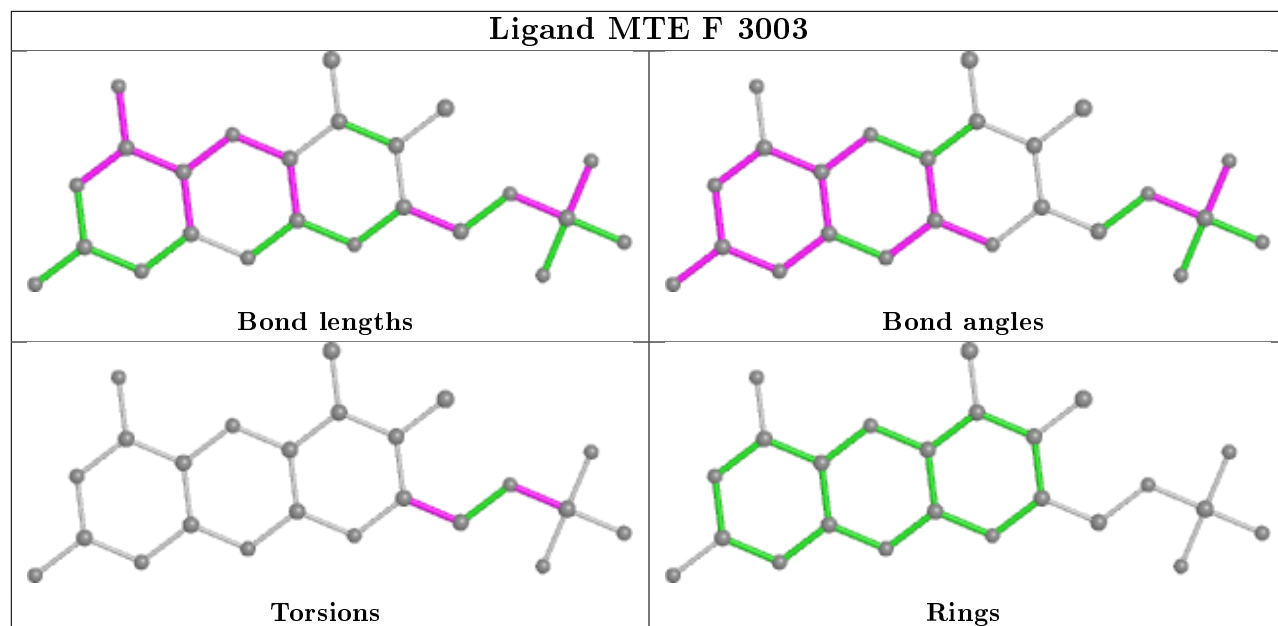
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	3005	FAD	6	0
3	G	3001	FES	2	0

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.

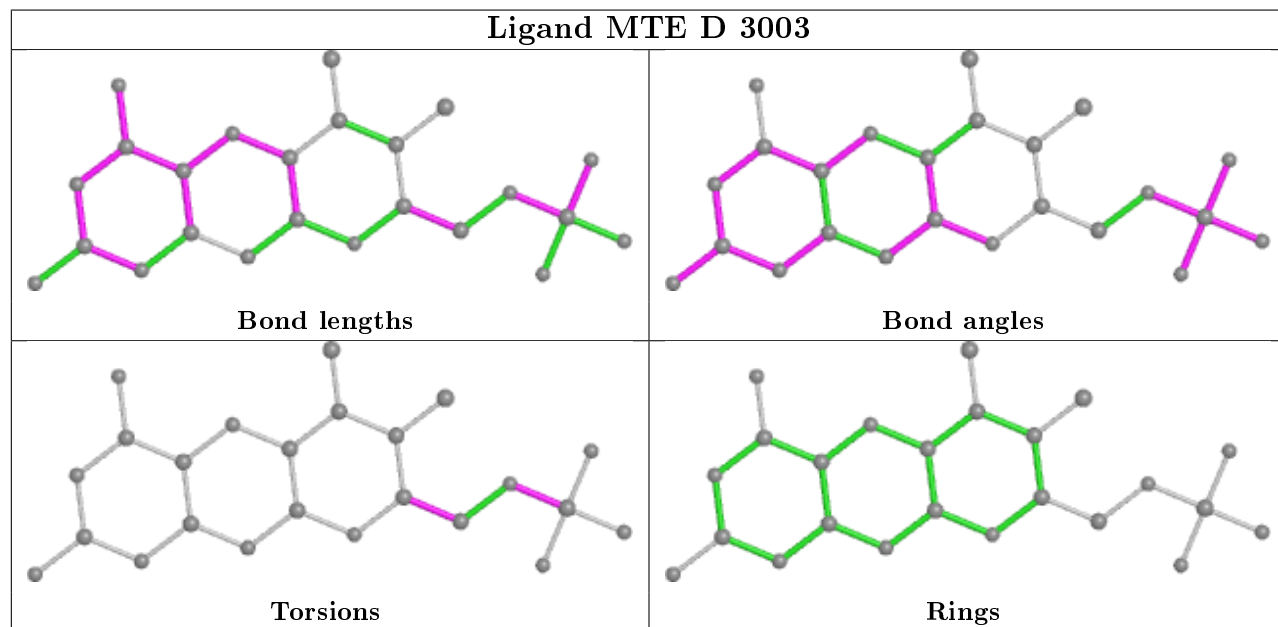




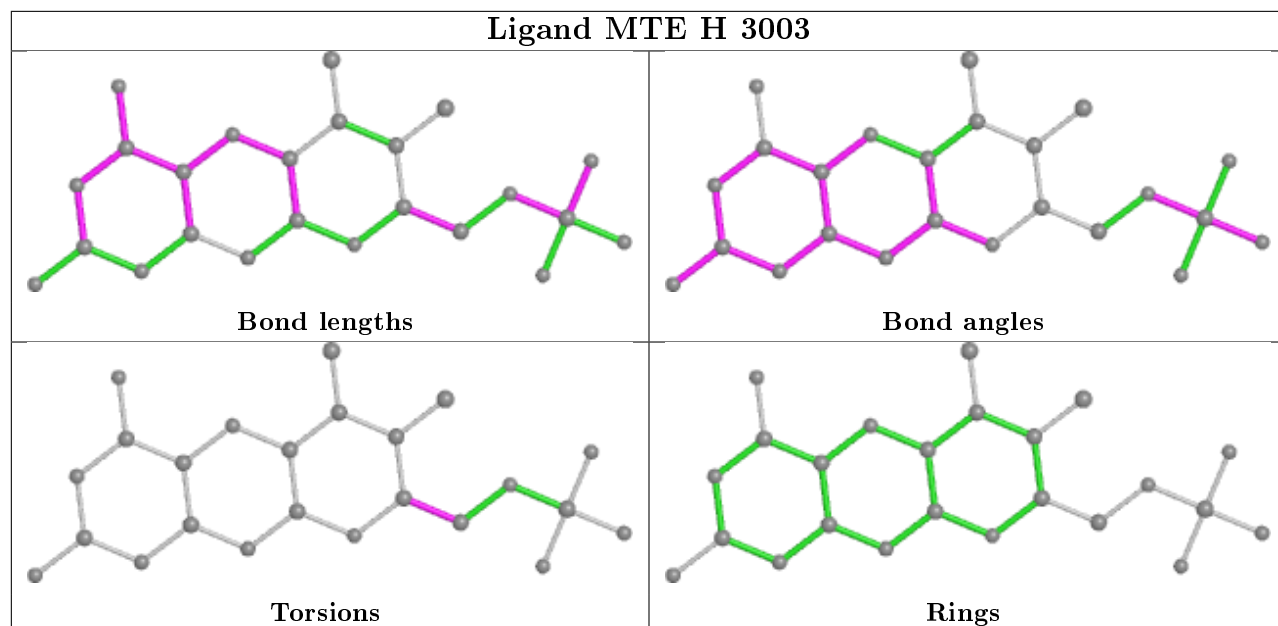
Ligand MTE F 3003



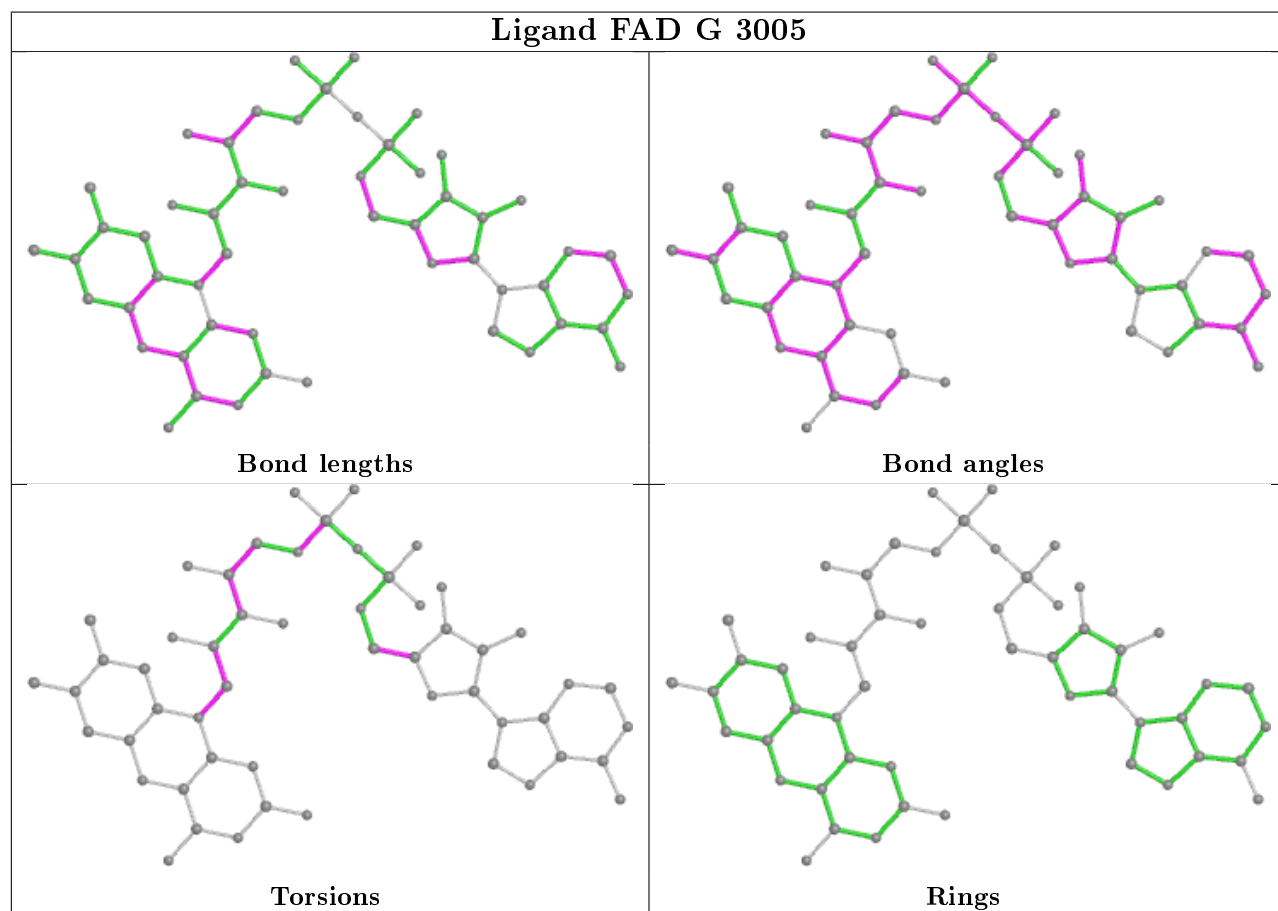
Ligand MTE D 3003

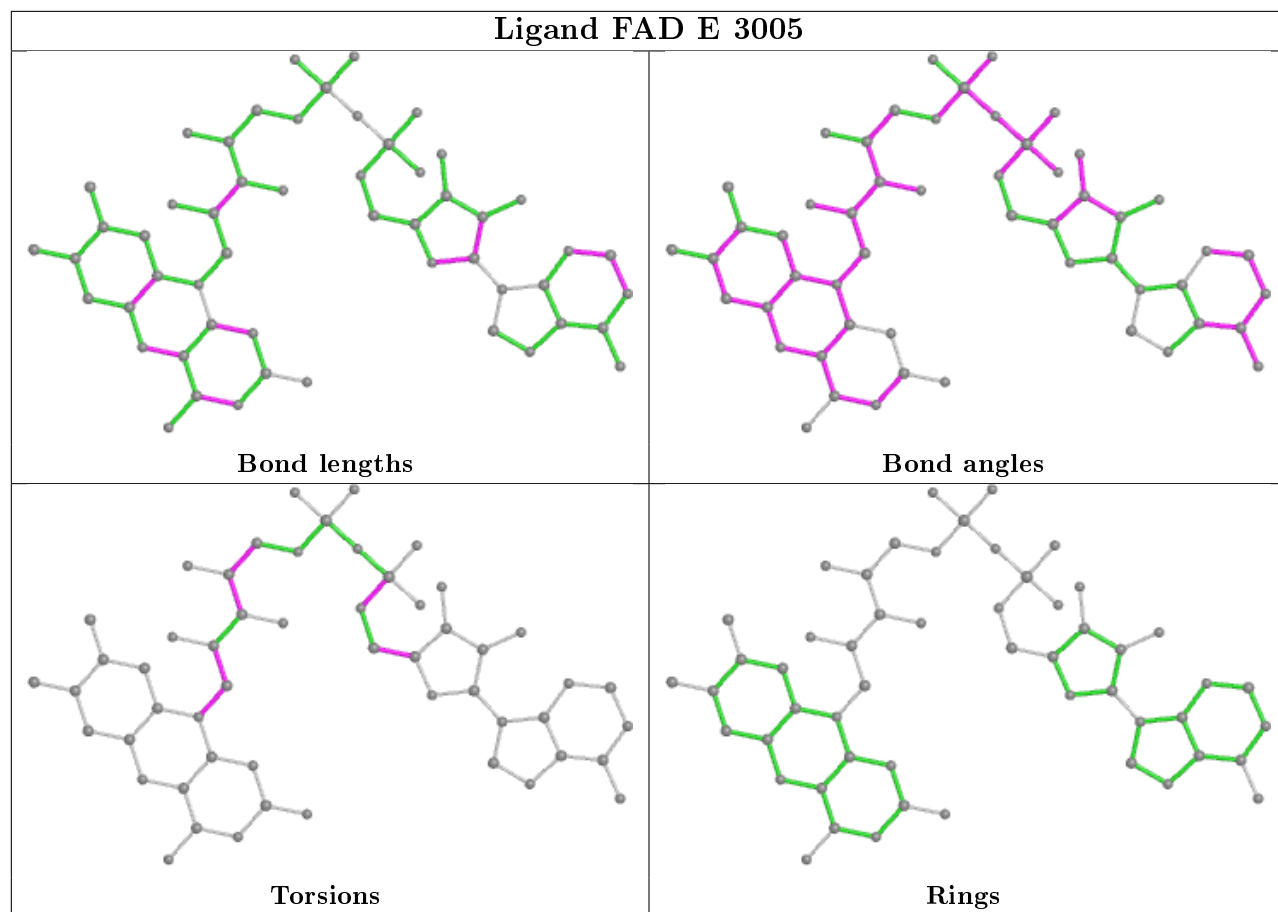


Ligand MTE H 3003



Ligand FAD G 3005





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.