



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 12:39 AM EDT

PDB ID : 1JRP / pdb_00001jrp
Title : Crystal Structure of Xanthine Dehydrogenase inhibited by alloxanthine from Rhodobacter capsulatus
Authors : Truglio, J.J.; Theis, K.; Leimkuhler, S.; Rappa, R.; Rajagopalan, K.V.; Kisker, C.
Deposited on : 2001-08-14
Resolution : 3.00 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (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)	:	2.50

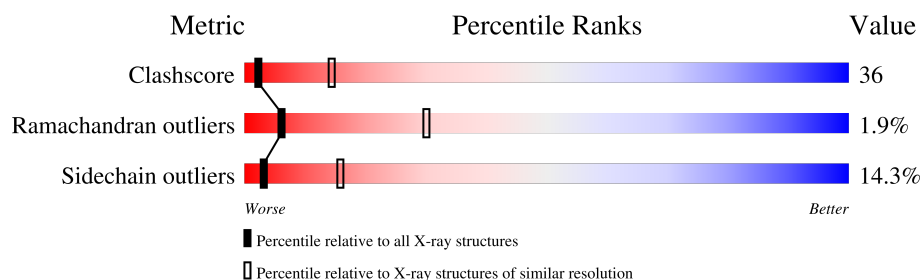
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	37% 42% 18% ..
1	C	462	42% 40% 14% ..
1	E	462	32% 45% 18% ..
1	G	462	32% 43% 19% ..
2	B	777	37% 43% 15% ..
2	D	777	37% 42% 16% ..
2	F	777	33% 45% 17% ..
2	H	777	33% 48% 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
3	FES	E	3002	-	-	X	-
3	FES	G	3001	-	-	X	-
6	MTE	F	3003	-	-	X	-
6	MTE	H	3003	-	-	X	-
7	MOS	B	3004	-	-	X	-
7	MOS	D	3004	-	-	X	-
7	MOS	F	3004	-	-	X	-
7	MOS	H	3004	-	-	X	-
8	141	B	4000	-	-	X	-
8	141	D	4000	-	-	X	-
8	141	F	4000	-	-	X	-
8	141	H	4000	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36748 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			

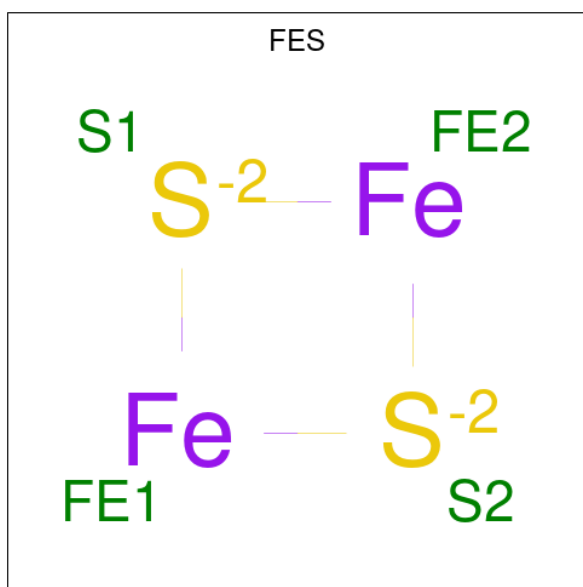
- Molecule 2 is a protein called xanthine dehydrogenase, chain B.

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:

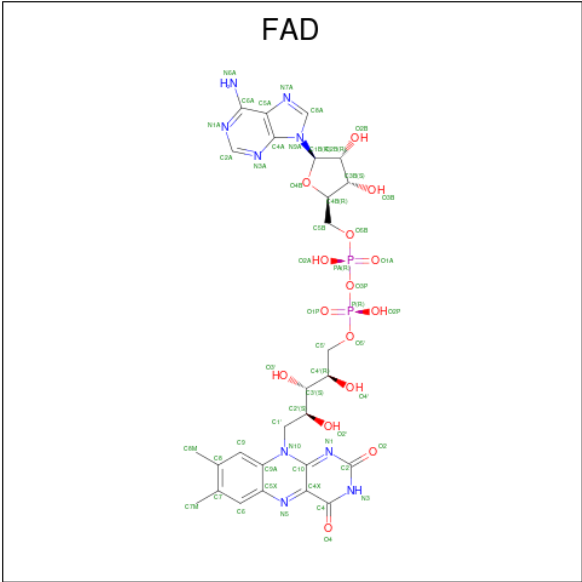
Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	conflict	EMBL 13397863
D	772	ARG	GLY	conflict	EMBL 13397863
F	772	ARG	GLY	conflict	EMBL 13397863
H	772	ARG	GLY	conflict	EMBL 13397863

- 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: $C_{27}H_{33}N_9O_{15}P_2$).

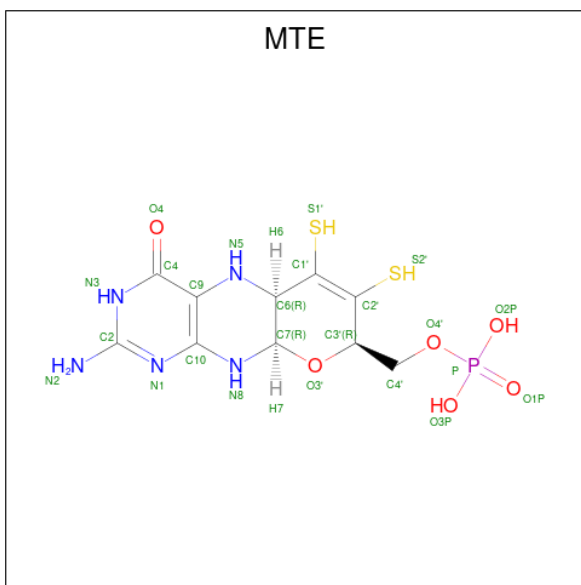


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

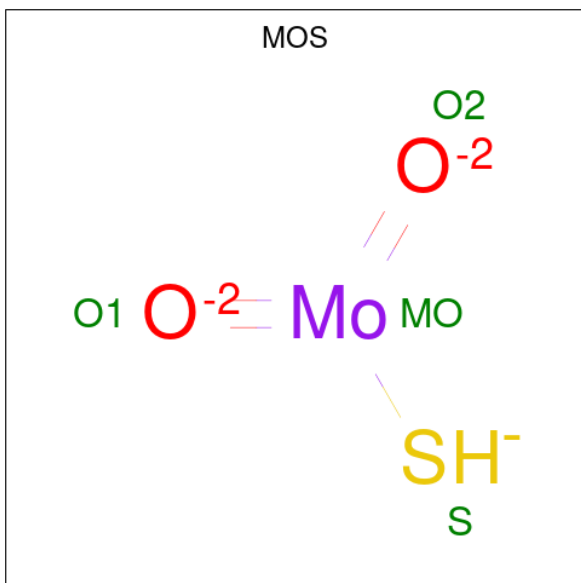
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		

- 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).



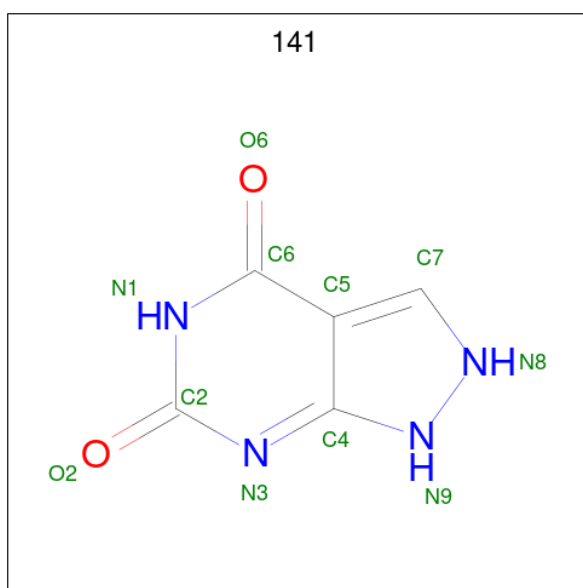
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	D	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	F	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	H	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	Mo	O	S	0	0
			3	1	1	1		
7	D	1	Total	Mo	O	S	0	0
			3	1	1	1		
7	F	1	Total	Mo	O	S	0	0
			3	1	1	1		
7	H	1	Total	Mo	O	S	0	0
			3	1	1	1		

- Molecule 8 is Oxypurinol (CCD ID: 141) (formula: $C_5H_4N_4O_2$).



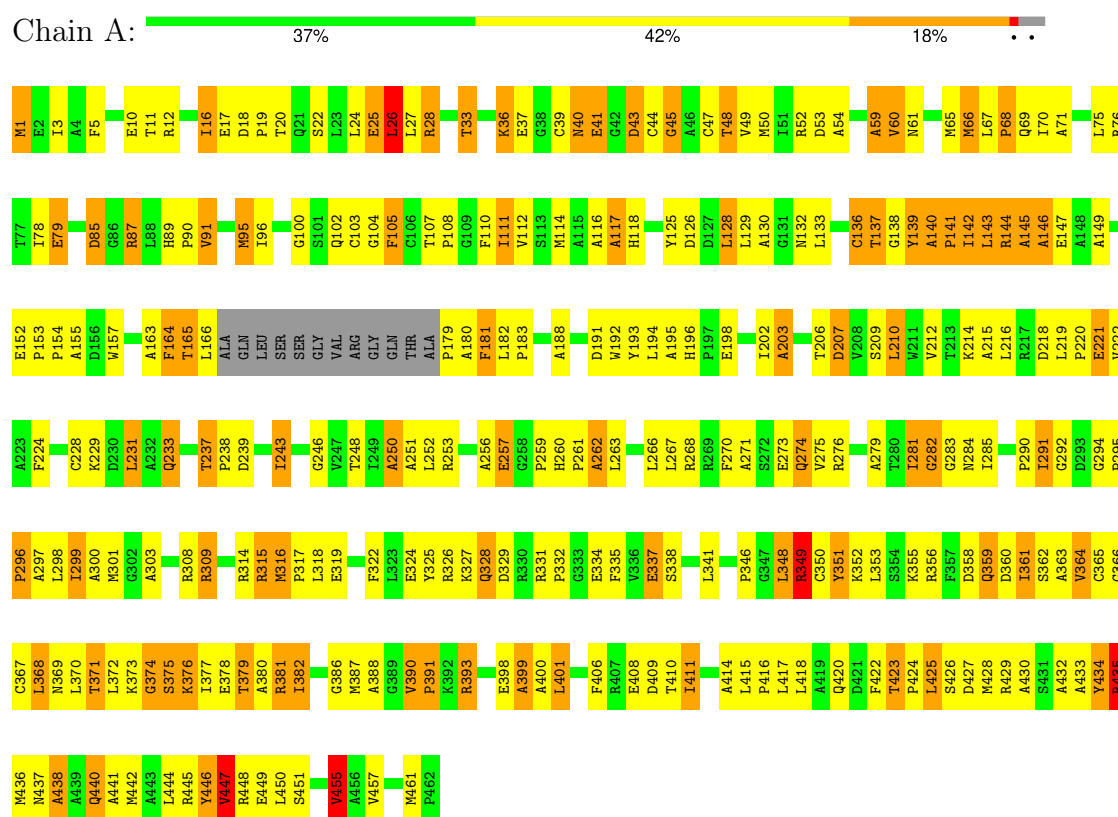
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			11	5	4	2		
8	D	1	Total	C	N	O	0	0
			11	5	4	2		
8	F	1	Total	C	N	O	0	0
			11	5	4	2		
8	H	1	Total	C	N	O	0	0
			11	5	4	2		

3 Residue-property plots

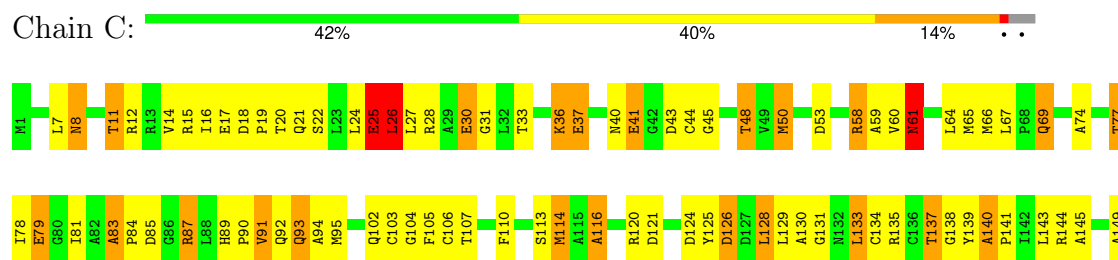
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

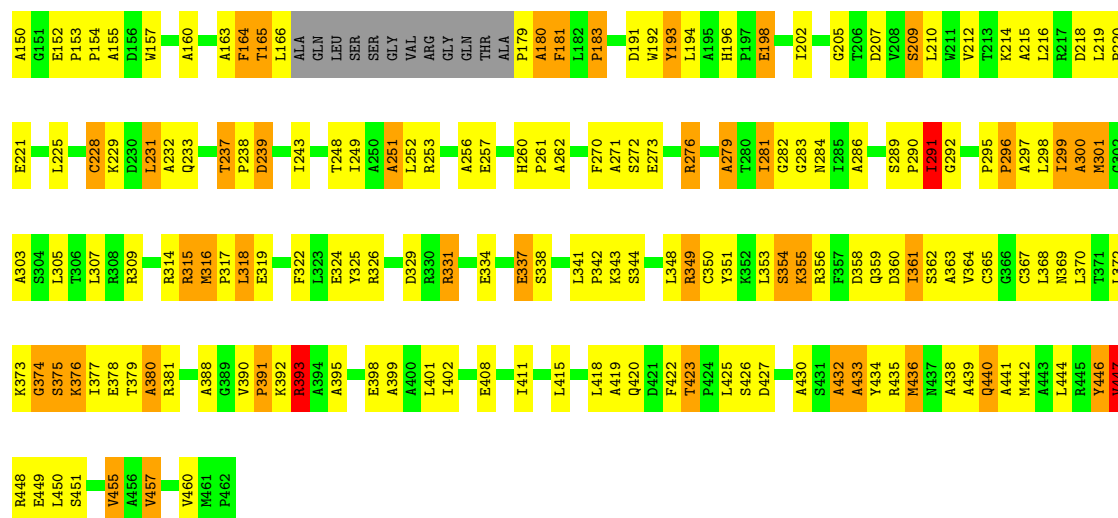
Note EDS was not executed.

• Molecule 1: xanthine dehydrogenase, chain A



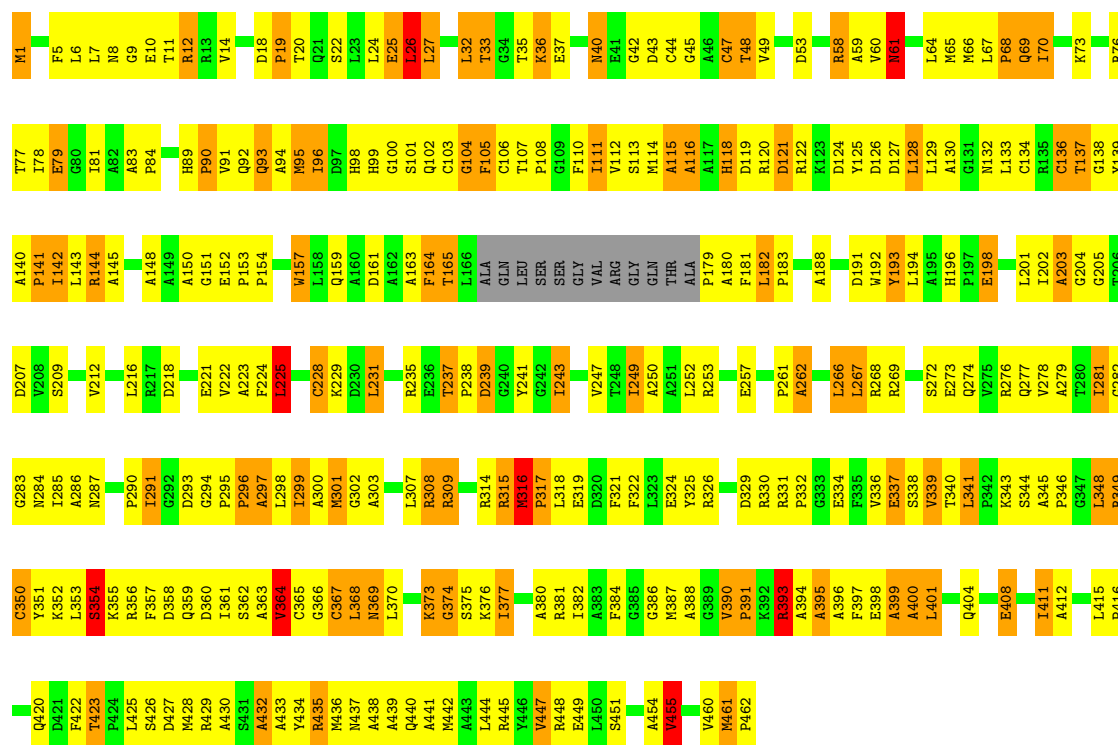
• Molecule 1: xanthine dehydrogenase, chain A





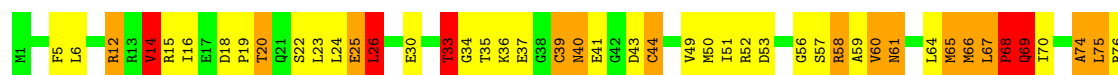
• Molecule 1: xanthine dehydrogenase, chain A

Chain E: 32% 45% 18%

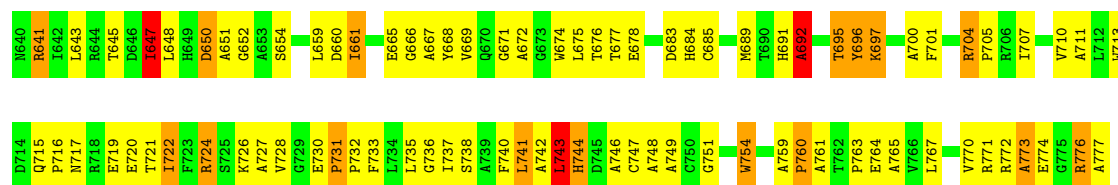


• Molecule 1: xanthine dehydrogenase, chain A

Chain G: 32% 43% 19%

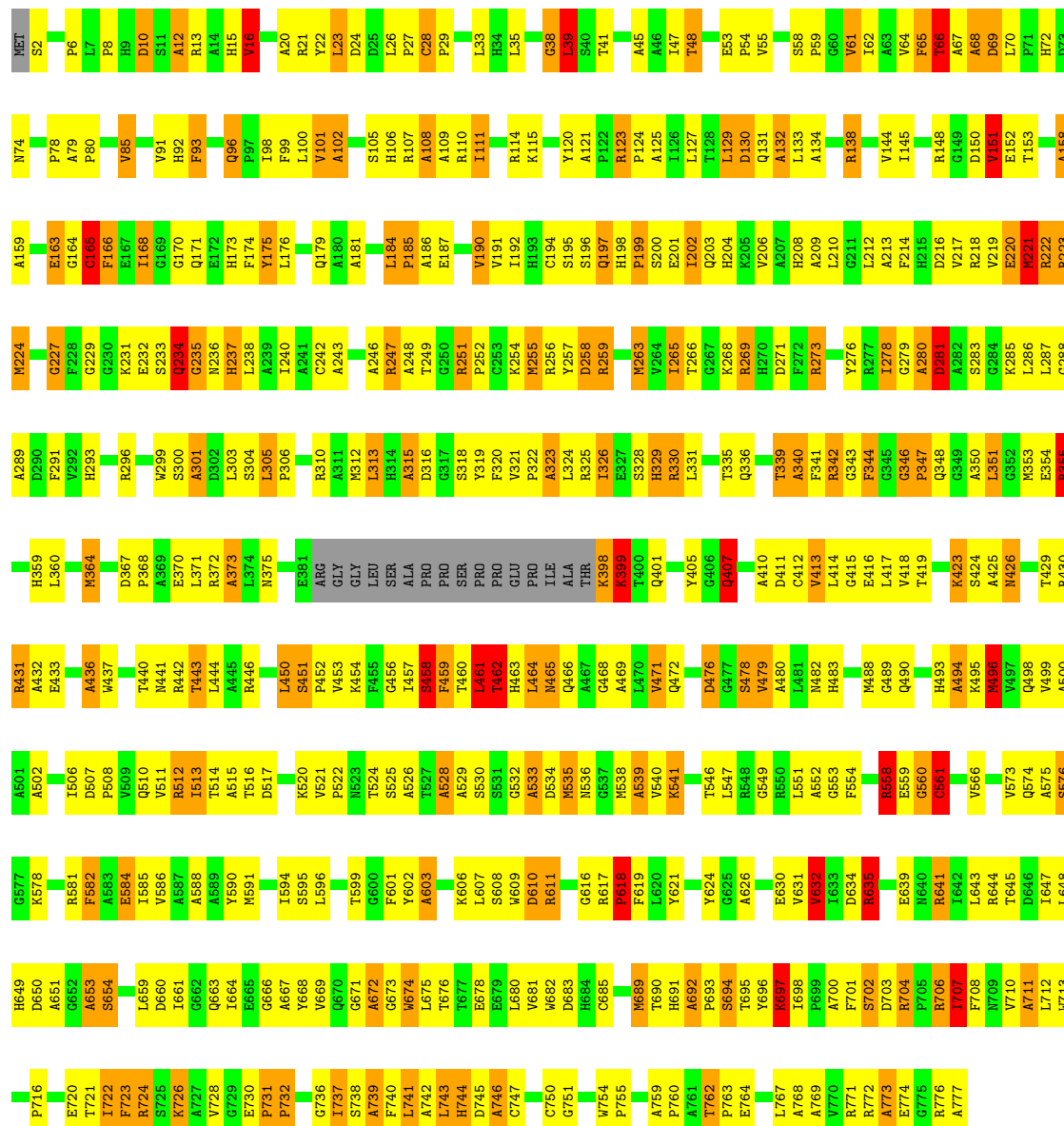






• Molecule 2: xanthine dehydrogenase, chain B

Chain D: 37% 42% 16%



• Molecule 2: xanthine dehydrogenase, chain B

Chain F: 33% 45% 17%



Chain H:  33% 48% 15% ..



A761	A762	A763	E764	A765	A766	L767	A768	A769	R770	R771	R772	A773	R776	A777	T695	Y696	R697	T698	P699	A700	F701	S702	D703	R704	P705	R706	L707	A711	L712	W713	N717	R718	E719	E720	T721	I722	F723	R724	S725	K726	A727	V728	G729	E730	F731	F732	F733	L734	L735	G736	I737	S738	A739	F740	L741	A742	L743	D745	H744	A746	C747	C750	H753	W754	P755	D756	L757	Q758	A759	P760	L551	A552	F553	F554	V555	A556	A557	R558	E559	G560	G561	A562	A563	R564	D565	I567	F568	Q572	V573	Q574	F582	A583	E584	I585	V586	A587	A588	A589	Y590	M591	Q592	R593	I594	S595	L596	T599	G600	F601	Y602	A603	T604	S608	W609	D610	R611	R617	P618	F619	L620	Y621	Y624	A627	I628	T629	E630	V631	F632	T633	D634	R635	L636	T637	G638	E639	N640	R641	I642	L643	R644	T645	L648	R649	D650	A651	G652	A653	S654	L655	N656	P657	A658	L659	D660	T661	Q662	G663	I664	A667	Y668	V669	Q670	G671	A672	G673	W674	L675	T676	T677	E678	E679	L680	V681	V682	D683	T690	H691	A692	P693	S694	E487	M488	G489	Q490	Q491	L492	H493	A494	K495	M496	V497	Q498	V499	A500	V503	L504	G505	I506	D507	P508	V511	R512	I513	T514	A515	T516	D517	T518	S519	A520	F521	P522	N523	A526	T527	A528	A529	S530	S531	G532	A533	D534	M535	N536	G537	M538	A539	V540	K541	E545	T546	L547	R548	R550	E487	M488	G489	Q490	Q491	L492	H493	A494	K495	M496	V497	Q498	V499	A500	V503	L504	G505	I506	D507	P508	V511	R512	I513	T514	A515	T516	D517	T518	S519	A520	F521	P522	N523	A526	T527	A528	A529	S530	S531	G532	A533	D534	M535	N536	G537	M538	A539	V540	K541	E545	T546	L547	R548	R550	T419	R420	L421	Q422	K423	S424	A425	M426	P427	T428	L429	L360	H359	E358	I357	A356	R355	L286	G288	A289	D290	F291	V292	R296	C297	G298	W299	A301	S300	D302	L303	S304	L305	P306	V307	C308	D309	R310	A311	M312	L313	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	G349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q348	R420	L421	Q422	K423	S424	A425	M426	P427	T428	L429	L360	H359	E358	I357	A356	R355	L286	G288	A289	D290	F291	V292	R296	C297	G298	W299	A301	S300	D302	L303	S304	L305	P306	V307	C308	D309	R310	A311	M312	L313	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336	T339	A340	F341	R342	G343	F344	G345	L416	L417	V418	Q349	A350	L351	R355	A356	I357	E358	H359	L360	A361	R362	G363	M364	D367	P368	A369	E370	L371	R372	A373	L374	N375	F376	P380	E381	ARG	GLY	LEU	SER	ALA	I457	PRO	SER	PRO	R325	I326	GLU	E327	S328	H329	R330	L331	R332	T333	N334	T335	Q336</
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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	92.62Å 140.73Å 157.66Å 109.59° 105.84° 101.25°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.1 (30.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.193 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36748	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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, 141, MTE, CA, FAD, FES

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	1.60	43/3431 (1.3%)	1.72	64/4647 (1.4%)
1	C	1.98	74/3431 (2.2%)	1.72	67/4647 (1.4%)
1	E	1.64	40/3431 (1.2%)	1.77	62/4647 (1.3%)
1	G	1.50	31/3431 (0.9%)	1.76	73/4647 (1.6%)
2	B	1.88	115/5845 (2.0%)	1.87	146/7942 (1.8%)
2	D	2.02	159/5845 (2.7%)	1.87	124/7942 (1.6%)
2	F	1.85	111/5845 (1.9%)	1.88	145/7942 (1.8%)
2	H	1.75	82/5845 (1.4%)	1.85	146/7942 (1.8%)
All	All	1.81	655/37104 (1.8%)	1.82	827/50356 (1.6%)

The worst 5 of 655 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	521	VAL	CA-CB	-14.39	1.41	1.54
2	D	759	ALA	CA-CB	-12.55	1.36	1.53
2	B	16	VAL	CA-CB	-12.25	1.40	1.54
2	D	669	VAL	CA-CB	-11.86	1.41	1.54
2	B	321	VAL	CA-CB	-11.71	1.45	1.54

The worst 5 of 827 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	632	VAL	CB-CA-C	-11.48	92.82	110.50
2	B	151	VAL	N-CA-C	11.00	121.91	110.36
2	D	521	VAL	CB-CA-C	-10.89	98.44	110.52
1	E	136	CYS	N-CA-C	10.53	122.51	111.14
2	B	462	THR	N-CA-C	10.41	123.60	111.11

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	272	0
1	C	3370	0	3368	184	0
1	E	3370	0	3370	319	1
1	G	3370	0	3370	323	1
2	B	5717	0	5630	362	0
2	D	5717	0	5631	343	0
2	F	5717	0	5631	422	0
2	H	5717	0	5630	454	0
3	A	8	0	0	1	0
3	C	8	0	0	0	0
3	E	8	0	0	6	0
3	G	8	0	0	3	0
4	A	53	0	31	10	0
4	C	53	0	30	3	0
4	E	53	0	30	10	0
4	G	53	0	31	9	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	4	0
6	D	24	0	10	4	0
6	F	24	0	11	7	0
6	H	24	0	10	7	0
7	B	3	0	0	4	0
7	D	3	0	0	7	0
7	F	3	0	0	8	0
7	H	3	0	0	5	0
8	B	11	0	3	9	0
8	D	11	0	3	5	0
8	F	11	0	3	5	0
8	H	11	0	3	4	0
All	All	36748	0	36173	2615	1

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 36.

The worst 5 of 2615 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)
2:D:689:MET:CE	2:D:689:MET:SD	2.04	1.46
1:E:95:MET:SD	1:E:114:MET:HE1	1.62	1.36
1:E:381:ARG:HH21	1:E:393:ARG:NH2	1.30	1.28
1:A:425:LEU:CD1	2:F:579:SER:HB3	1.62	1.27
2:D:496:MET:HE2	2:D:496:MET:CA	1.68	1.20

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ARG:CD	1:G:152:GLU:OE2[1_655]	2.08	0.12

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%)	385 (86%)	53 (12%)	8 (2%)	6	31
1	C	446/462 (96%)	408 (92%)	31 (7%)	7 (2%)	7	34
1	E	446/462 (96%)	370 (83%)	63 (14%)	13 (3%)	3	20
1	G	446/462 (96%)	375 (84%)	58 (13%)	13 (3%)	3	20
2	B	756/777 (97%)	696 (92%)	47 (6%)	13 (2%)	7	32
2	D	756/777 (97%)	697 (92%)	46 (6%)	13 (2%)	7	32
2	F	756/777 (97%)	688 (91%)	57 (8%)	11 (2%)	8	35
2	H	756/777 (97%)	678 (90%)	67 (9%)	11 (2%)	8	35
All	All	4808/4956 (97%)	4297 (89%)	422 (9%)	89 (2%)	6	30

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ALA
2	B	281	ASP
2	B	399	LYS
2	B	458	SER
2	B	561	CYS

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%)	284 (84%)	55 (16%)	2	12
1	C	339/347 (98%)	290 (86%)	49 (14%)	3	15
1	E	339/347 (98%)	277 (82%)	62 (18%)	2	9
1	G	339/347 (98%)	276 (81%)	63 (19%)	1	9
2	B	571/584 (98%)	491 (86%)	80 (14%)	3	16
2	D	571/584 (98%)	498 (87%)	73 (13%)	4	19
2	F	571/584 (98%)	500 (88%)	71 (12%)	4	20
2	H	571/584 (98%)	502 (88%)	69 (12%)	5	21
All	All	3640/3724 (98%)	3118 (86%)	522 (14%)	3	16

5 of 522 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	129	LEU
2	H	260	ASP
2	H	105	SER
2	H	744	HIS
2	D	163	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	498	GLN

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Mol	Chain	Res	Type
2	H	293	HIS
1	E	118	HIS
2	H	236	ASN
2	H	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\# Z > 2$
3	FES	C	3001	1	0,4,4	-	-	-		
6	MTE	H	3003	7	21,26,26	6.13	11 (52%)	19,40,40	6.07	10 (52%)
4	FAD	A	3005	-	58,58,58	1.53	10 (17%)	85,89,89	2.48	36 (42%)
3	FES	E	3001	1	0,4,4	-	-	-		
6	MTE	B	3003	7	21,26,26	5.21	12 (57%)	19,40,40	6.11	13 (68%)
4	FAD	E	3005	-	58,58,58	1.62	13 (22%)	85,89,89	2.59	41 (48%)
4	FAD	C	3005	-	58,58,58	1.68	13 (22%)	85,89,89	2.66	39 (45%)
3	FES	G	3002	1	0,4,4	-	-	-		
3	FES	G	3001	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	141	F	4000	7	11,12,12	3.57	5 (45%)	11,17,17	1.96	4 (36%)
7	MOS	B	3004	6,8	0,2,3	-	-	-	-	-
8	141	D	4000	7	11,12,12	3.25	4 (36%)	11,17,17	1.69	3 (27%)
7	MOS	H	3004	6,8	0,2,3	-	-	-	-	-
8	141	B	4000	7	11,12,12	3.23	6 (54%)	11,17,17	2.10	4 (36%)
3	FES	A	3001	1	0,4,4	-	-	-	-	-
8	141	H	4000	7	11,12,12	3.16	5 (45%)	11,17,17	2.34	7 (63%)
3	FES	E	3002	1	0,4,4	-	-	-	-	-
3	FES	C	3002	1	0,4,4	-	-	-	-	-
7	MOS	F	3004	6,8,2	0,2,3	-	-	-	-	-
4	FAD	G	3005	-	58,58,58	1.38	6 (10%)	85,89,89	2.30	35 (41%)
7	MOS	D	3004	6,8,2	0,2,3	-	-	-	-	-
6	MTE	F	3003	7	21,26,26	5.55	13 (61%)	19,40,40	6.72	13 (68%)
3	FES	A	3002	1	0,4,4	-	-	-	-	-
6	MTE	D	3003	7	21,26,26	5.56	13 (61%)	19,40,40	7.43	12 (63%)

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
3	FES	C	3001	1	-	-	0/1/1/1
6	MTE	H	3003	7	-	2/6/34/34	0/3/3/3
4	FAD	A	3005	-	-	14/34/50/50	0/6/6/6
3	FES	E	3001	1	-	-	0/1/1/1
6	MTE	B	3003	7	-	0/6/34/34	0/3/3/3
4	FAD	E	3005	-	-	15/34/50/50	0/6/6/6
4	FAD	C	3005	-	-	14/34/50/50	0/6/6/6
3	FES	G	3002	1	-	-	0/1/1/1
3	FES	G	3001	1	-	-	0/1/1/1
8	141	F	4000	7	-	-	0/2/2/2
8	141	D	4000	7	-	-	0/2/2/2
8	141	B	4000	7	-	-	0/2/2/2
3	FES	A	3001	1	-	-	0/1/1/1
8	141	H	4000	7	-	-	0/2/2/2
3	FES	E	3002	1	-	-	0/1/1/1
3	FES	C	3002	1	-	-	0/1/1/1
4	FAD	G	3005	-	-	17/34/50/50	0/6/6/6
6	MTE	F	3003	7	-	0/6/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	3002	1	-	-	0/1/1/1
6	MTE	D	3003	7	-	5/6/34/34	0/3/3/3

The worst 5 of 111 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	3003	MTE	C7-C6	15.71	1.66	1.53
6	B	3003	MTE	C7-C6	13.70	1.64	1.53
6	H	3003	MTE	C9-C10	13.39	1.61	1.38
6	D	3003	MTE	C9-C10	13.19	1.61	1.38
6	F	3003	MTE	C7-C6	12.95	1.63	1.53

The worst 5 of 217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3003	MTE	O3'-C7-C6	-29.62	89.21	108.96
6	F	3003	MTE	O3'-C7-C6	-24.82	92.41	108.96
6	H	3003	MTE	O3'-C7-C6	-23.00	93.63	108.96
6	B	3003	MTE	O3'-C7-C6	-20.63	95.20	108.96
6	F	3003	MTE	C2-N1-C10	9.94	130.91	113.36

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3005	FAD	C2'-C1'-N10-C10
4	A	3005	FAD	N10-C1'-C2'-O2'
4	A	3005	FAD	N10-C1'-C2'-C3'
4	A	3005	FAD	C2'-C3'-C4'-O4'
4	A	3005	FAD	O3'-C3'-C4'-O4'

There are no ring outliers.

21 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	3003	MTE	7	0
4	A	3005	FAD	10	0
3	E	3001	FES	1	0
6	B	3003	MTE	4	0
4	E	3005	FAD	10	0
4	C	3005	FAD	3	0

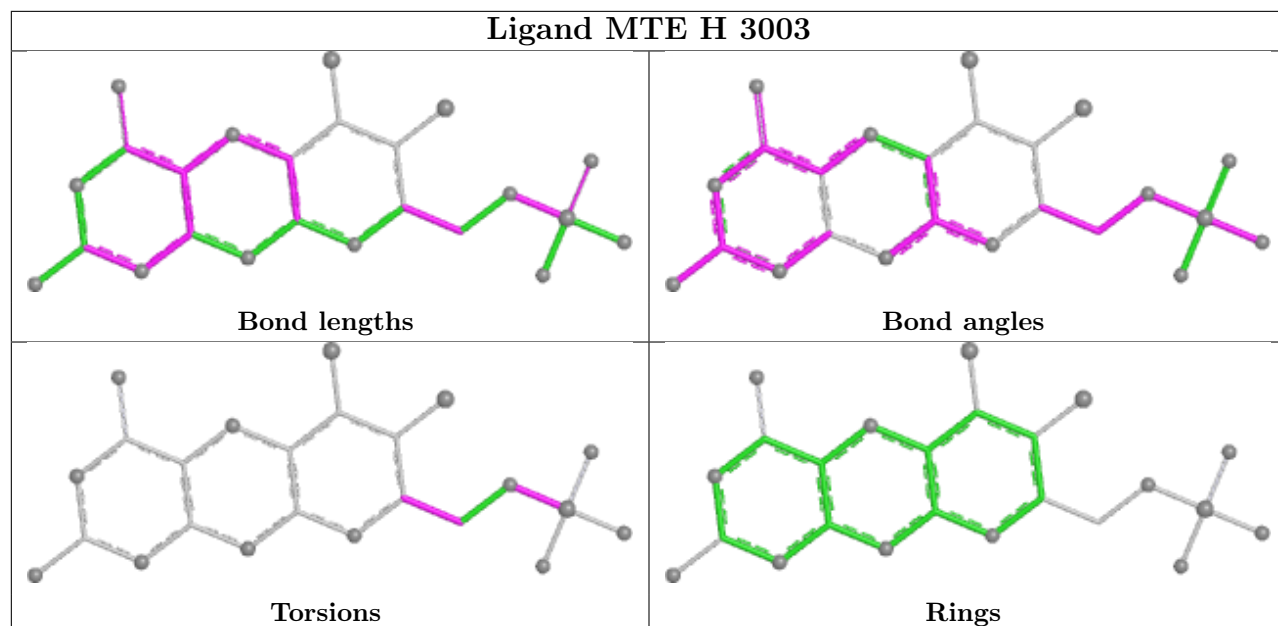
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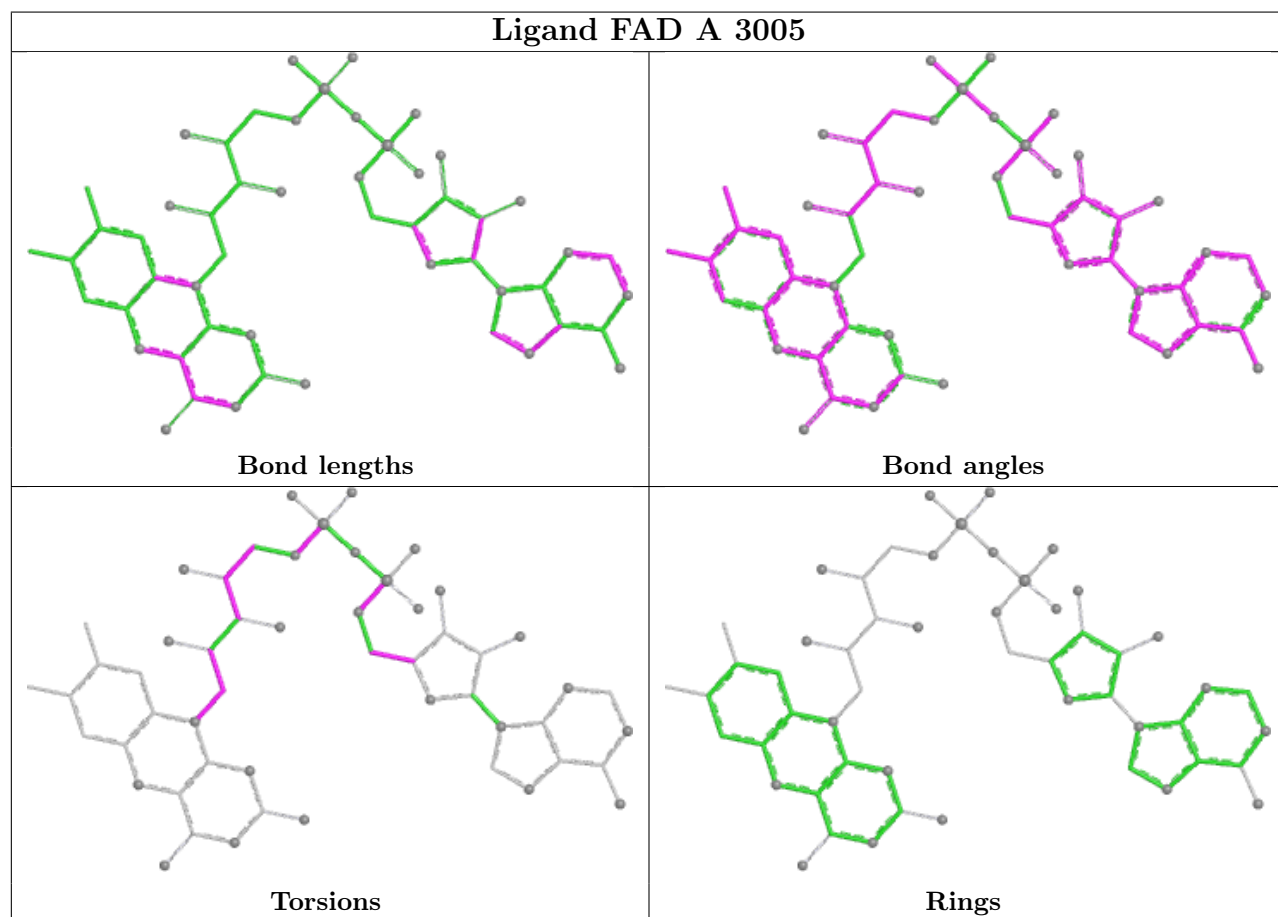
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3002	FES	1	0
3	G	3001	FES	2	0
8	F	4000	141	5	0
7	B	3004	MOS	4	0
8	D	4000	141	5	0
7	H	3004	MOS	5	0
8	B	4000	141	9	0
8	H	4000	141	4	0
3	E	3002	FES	5	0
7	F	3004	MOS	8	0
4	G	3005	FAD	9	0
7	D	3004	MOS	7	0
6	F	3003	MTE	7	0
3	A	3002	FES	1	0
6	D	3003	MTE	4	0

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.

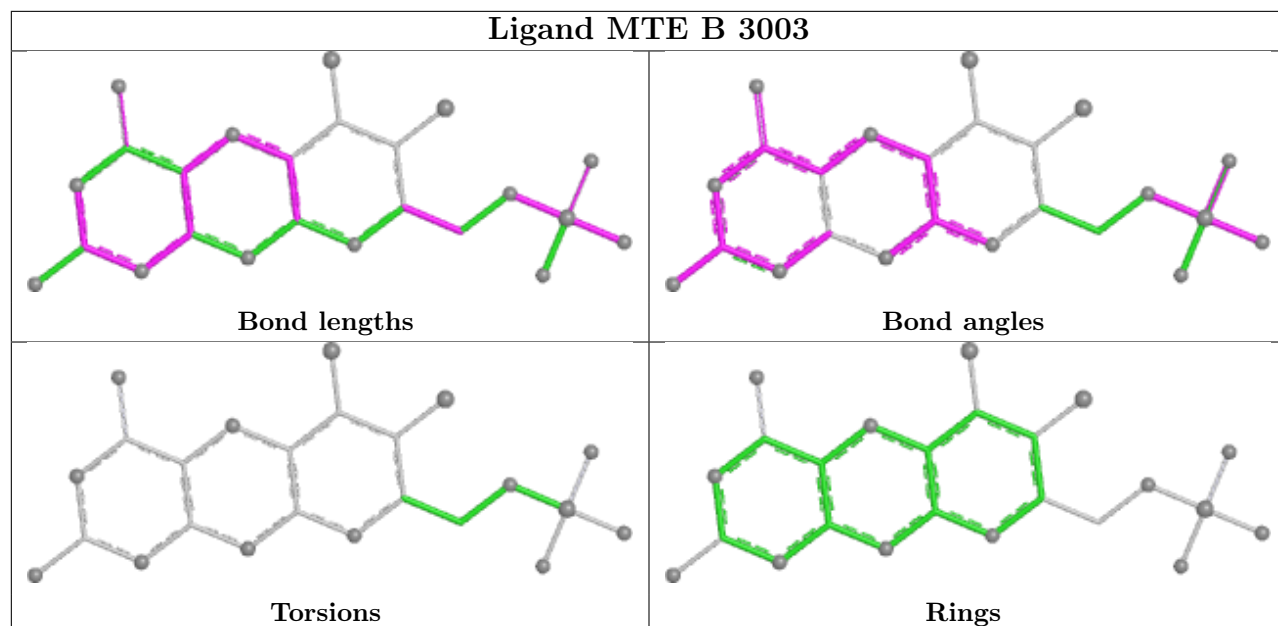
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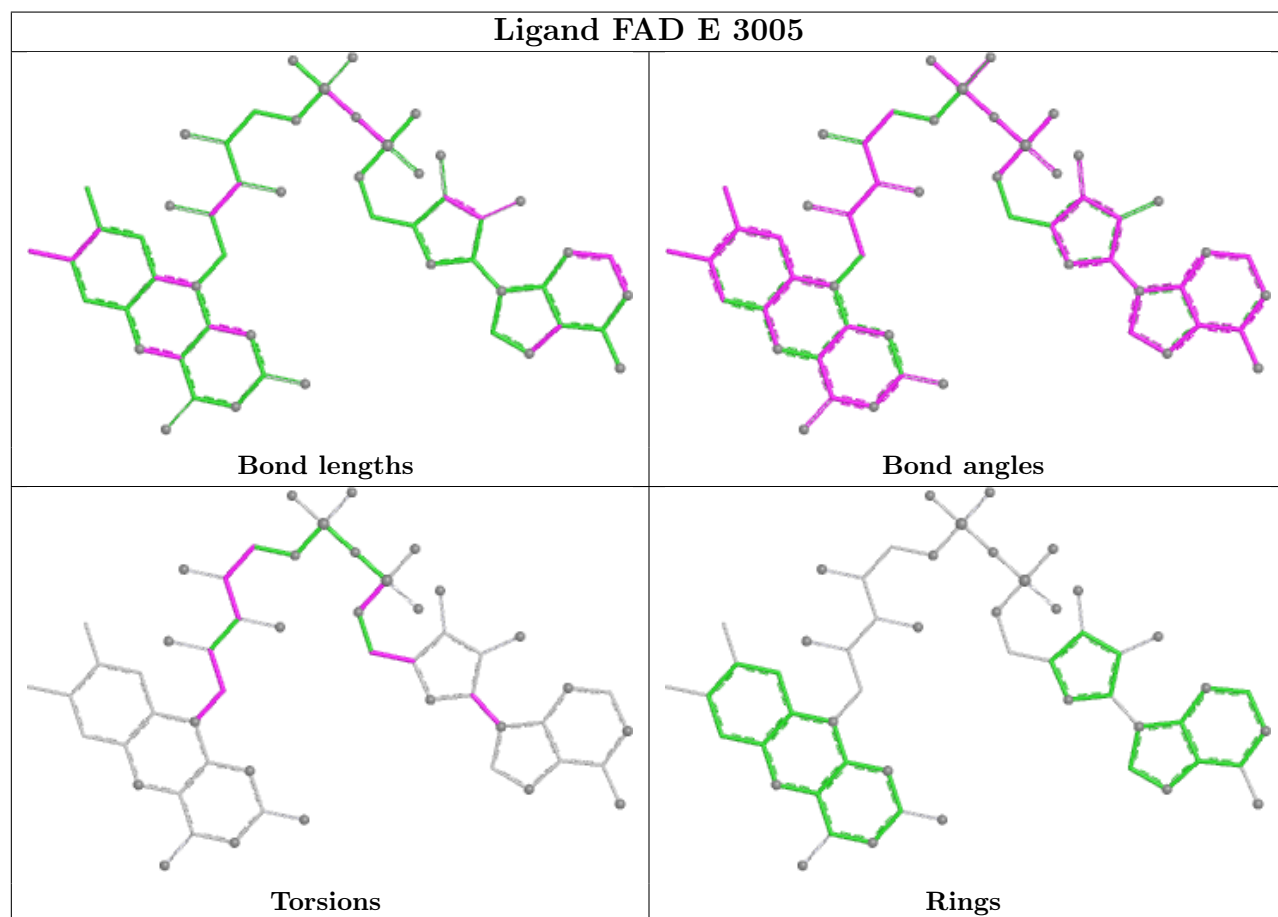
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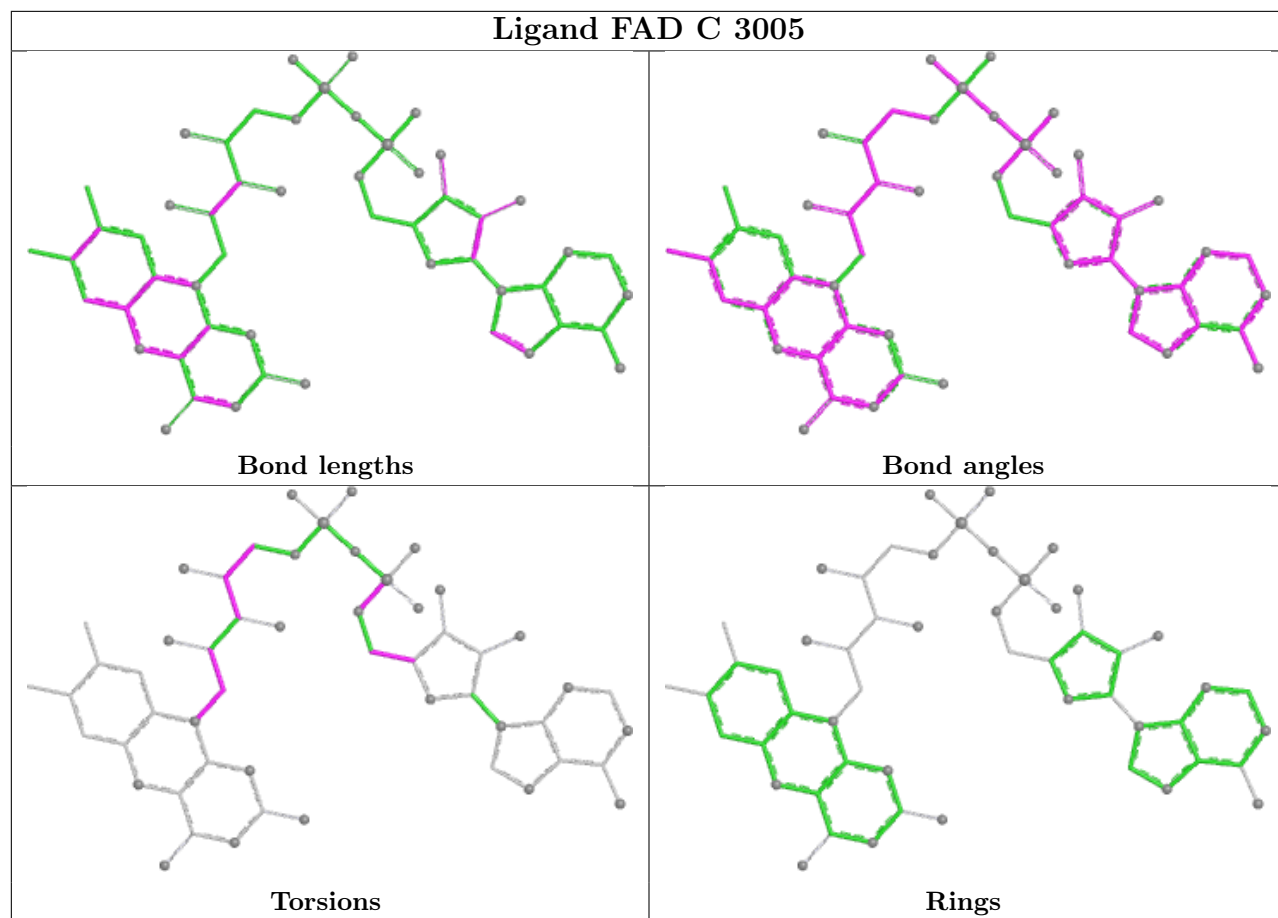


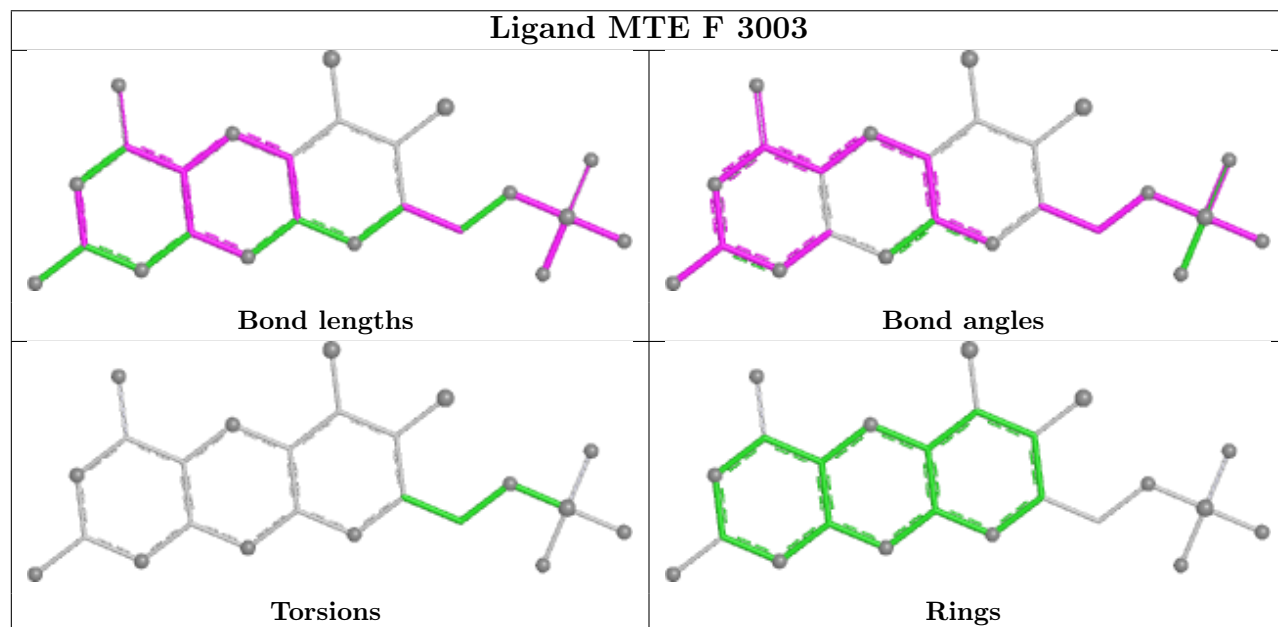
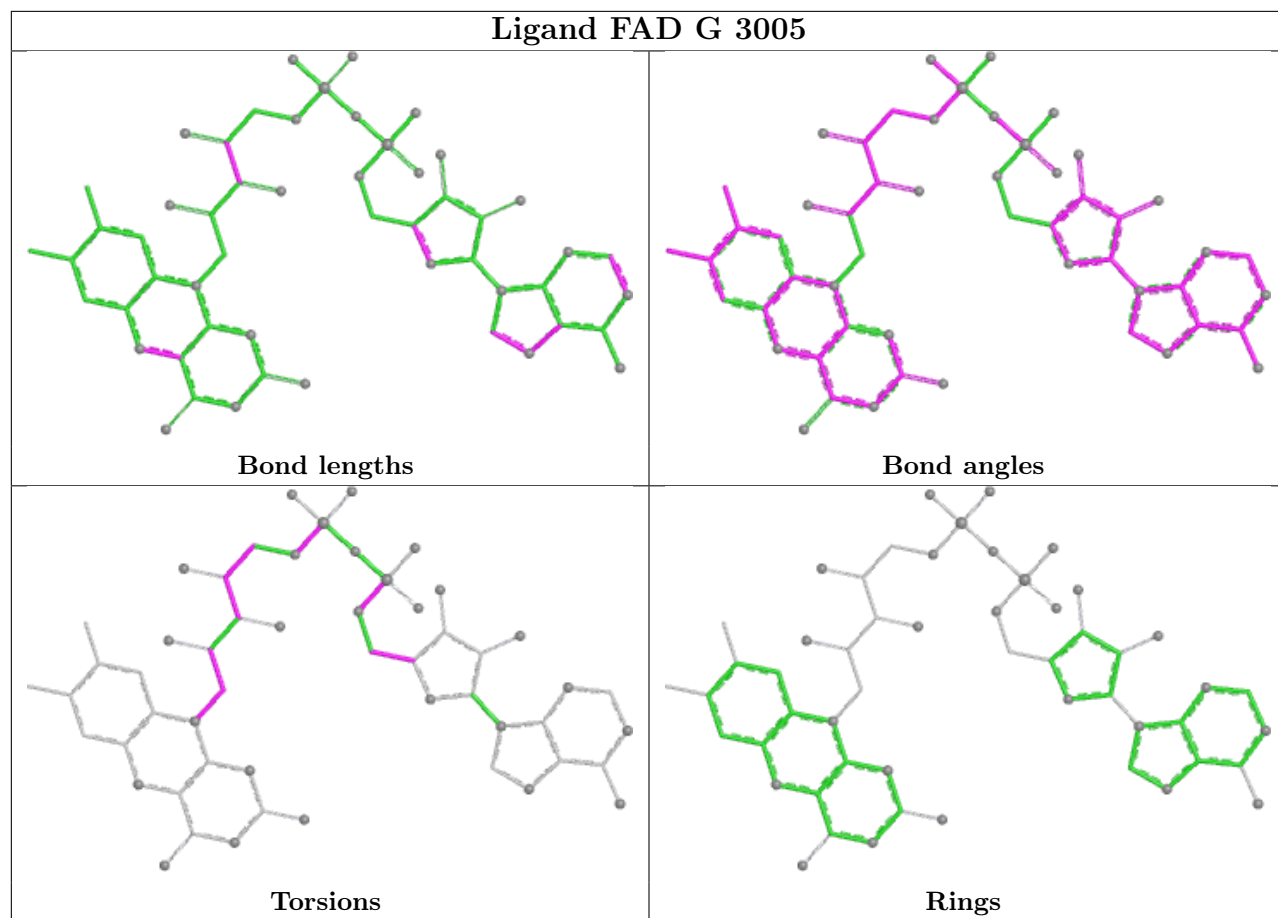
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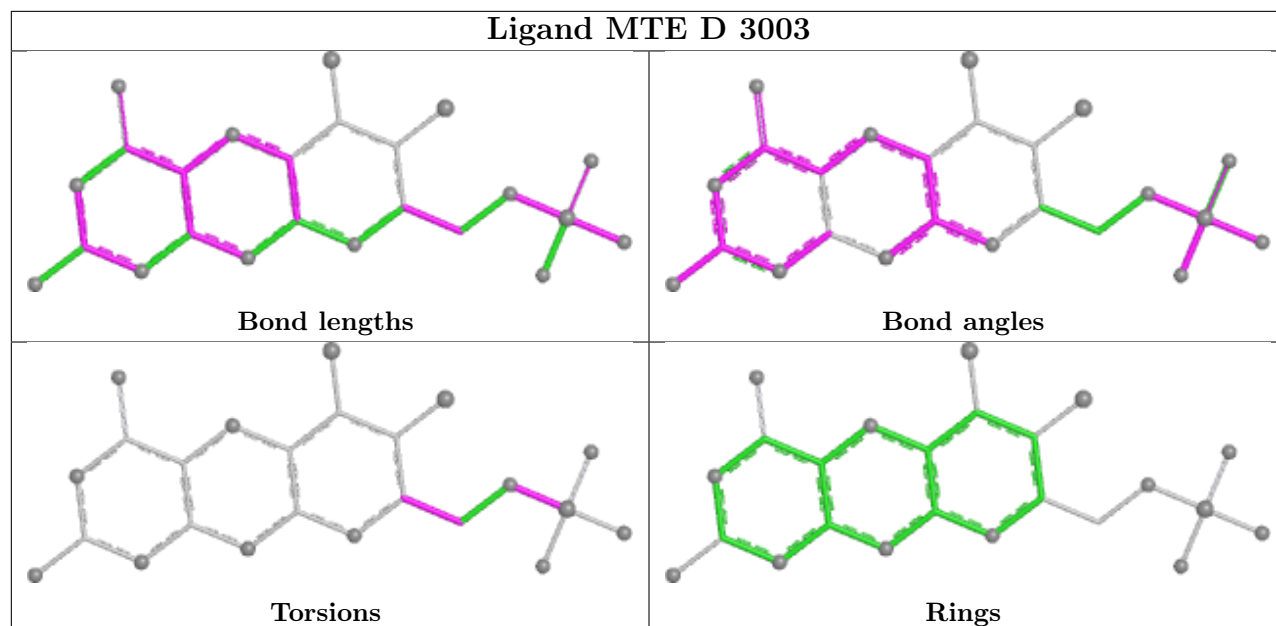


Ligand FAD E 3005









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.