



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:15 am BST

PDB ID : 2CKJ
Title : Human milk xanthine oxidoreductase
Authors : Pearson, A.R.; Godber, B.L.J.; Eissenthal, R.; Taylor, G.L.; Harrison, R.
Deposited on : 2006-04-19
Resolution : 3.59 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

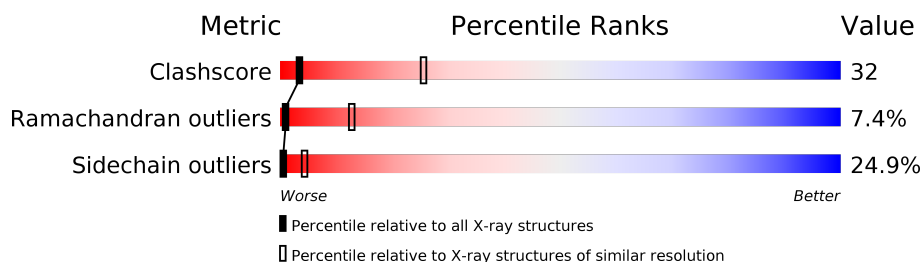
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)

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	1333	
1	B	1333	
1	C	1333	
1	D	1333	

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
2	FES	A	3002	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FES	B	3002	-	-	X	-
4	GOL	A	3007	-	-	X	-
4	GOL	B	3007	-	-	X	-
4	GOL	C	3007	-	-	X	-
4	GOL	D	3007	-	-	X	-

2 Entry composition [i](#)

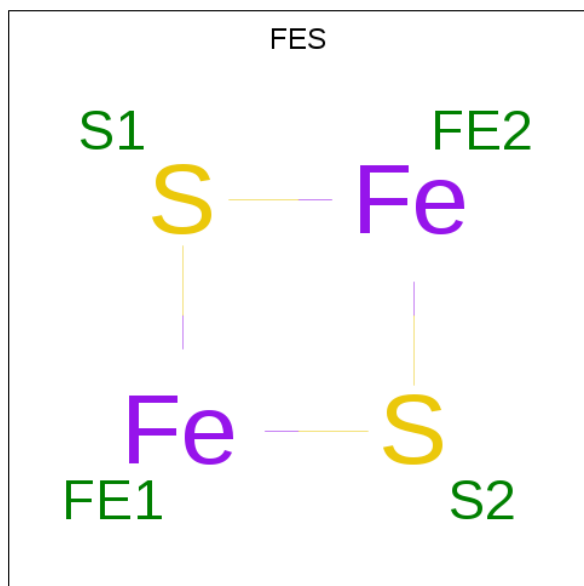
There are 6 unique types of molecules in this entry. The entry contains 39807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1264	Total	C	N	O	S	0	0	0
			9764	6195	1679	1826	64			
1	B	1289	Total	C	N	O	S	0	0	0
			9951	6307	1713	1865	66			
1	C	1283	Total	C	N	O	S	0	0	0
			9905	6280	1706	1854	65			
1	D	1283	Total	C	N	O	S	0	0	0
			9910	6281	1707	1856	66			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



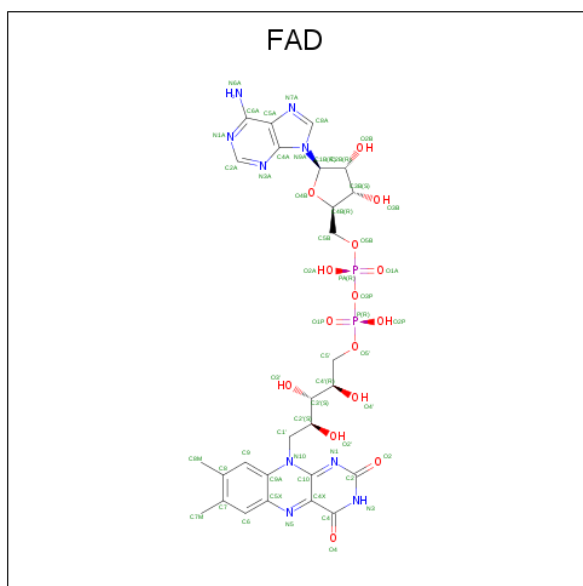
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 4	Fe 2	S 2	0	0
2	B	1	Total 4	Fe 2	S 2	0	0
2	C	1	Total 4	Fe 2	S 2	0	0
2	C	1	Total 4	Fe 2	S 2	0	0
2	D	1	Total 4	Fe 2	S 2	0	0
2	D	1	Total 4	Fe 2	S 2	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



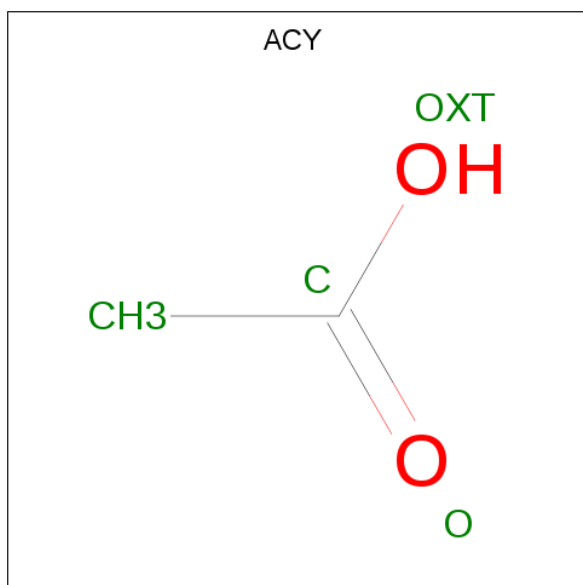
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



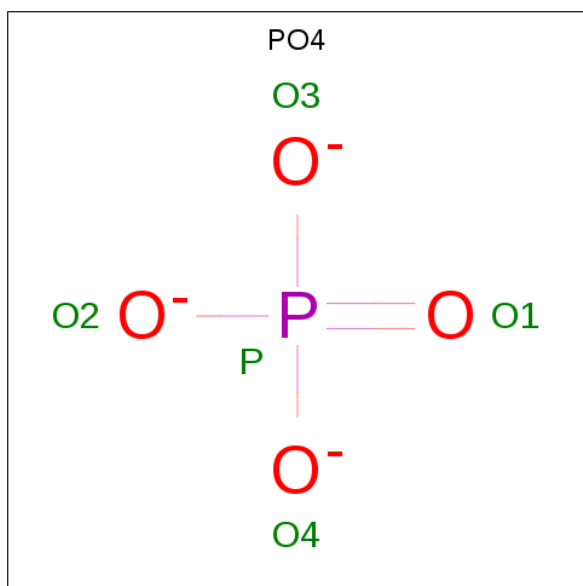
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



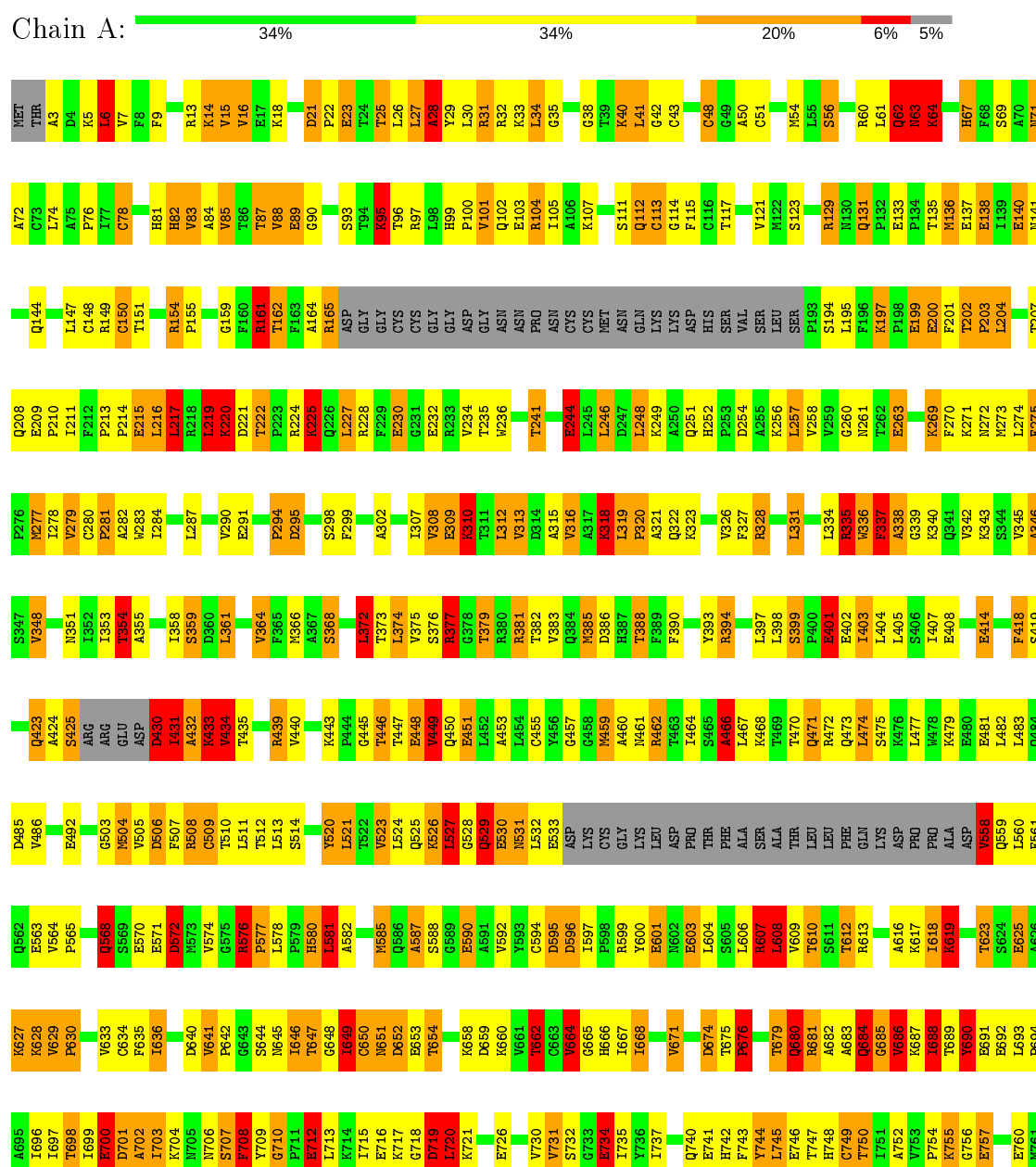
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			5	4	1		

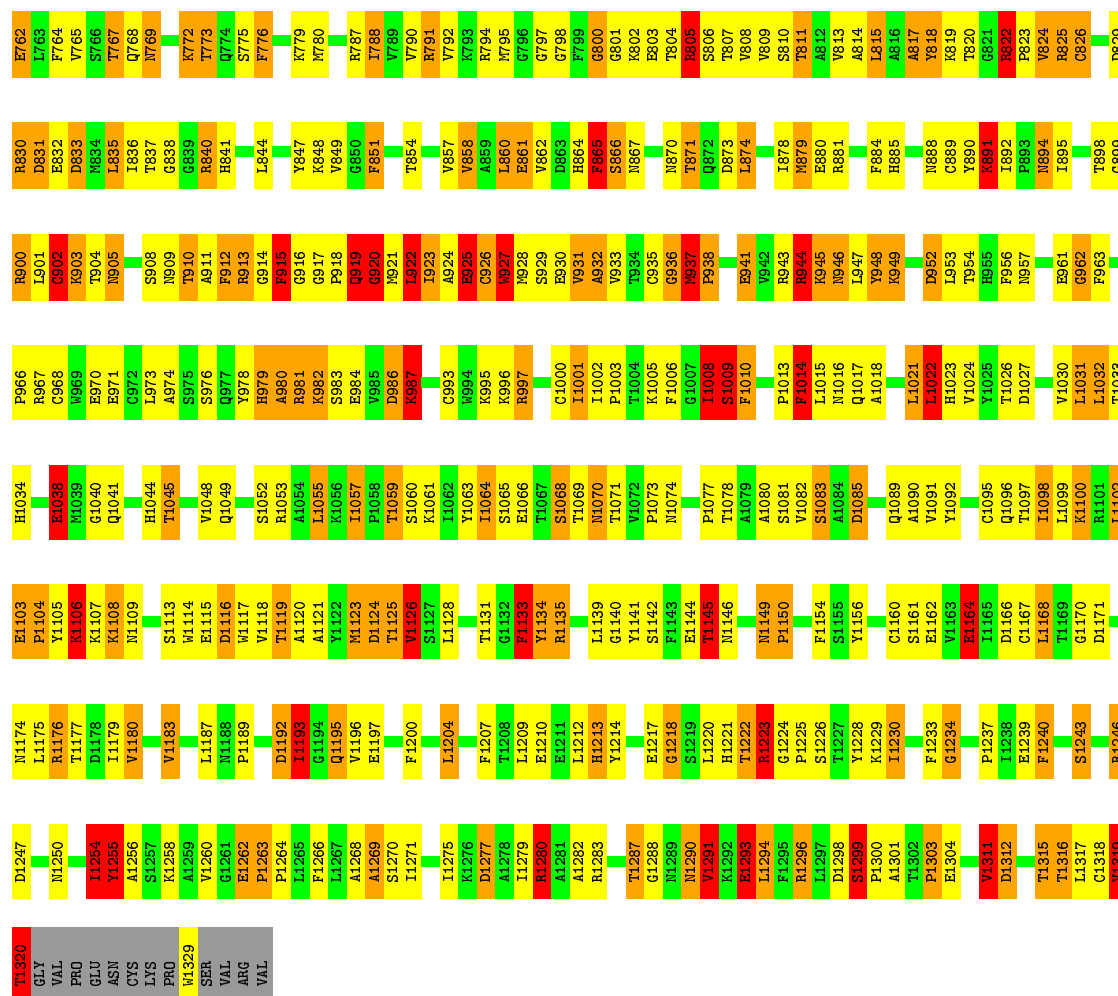
3 Residue-property plots

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.

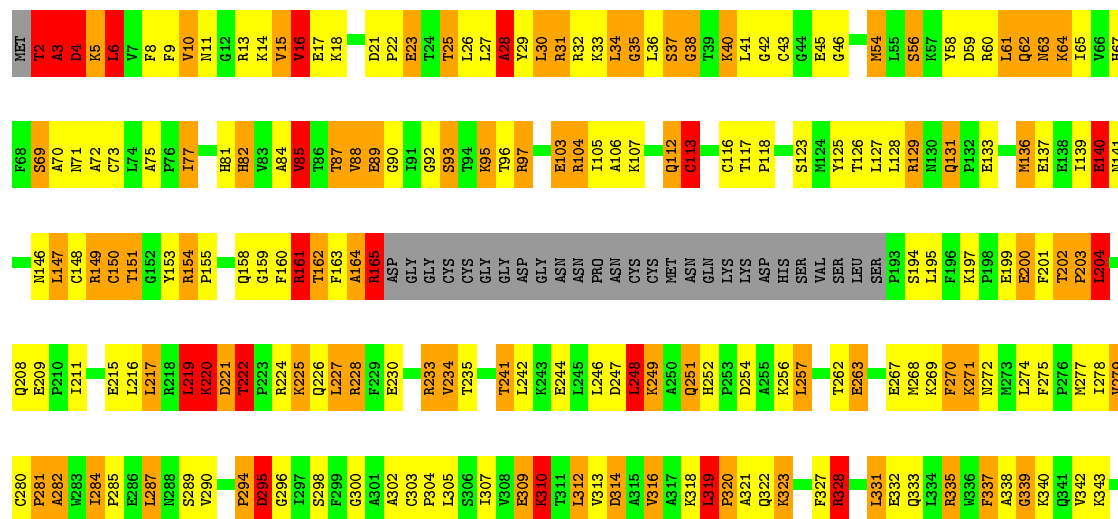
• Molecule 1: XANTHINE OXIDOREDUCTASE





• Molecule 1: XANTHINE OXIDOREDUCTASE

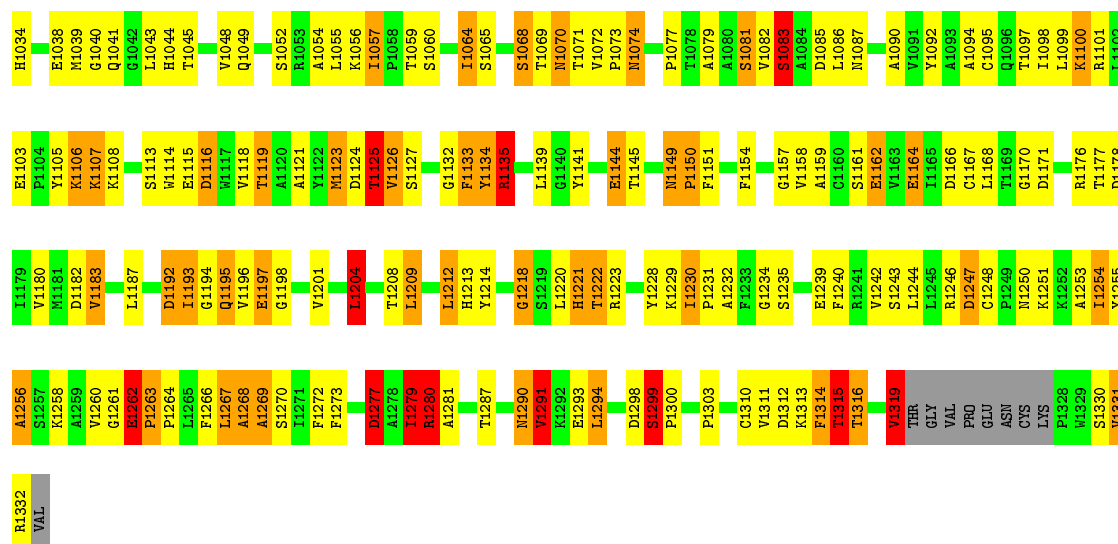
Chain B: 35% 35% 20% 7%



VAL	P1249	R1101	T1026	L960	R895	C826	P754	V686	LEU	L477	S412	A346	
	K1251	L1102	D1027	G962	R896	M827	K755	K687	LEU	E480	E414	V348	
	I1254	M1174	E1103	S1029	G899	D829	E757	T689	GLN	E481			
		L1175	Y1105	V1030	R900	R830	R831	E691	L618	LYS	L482	Y417	K351
		T1177	K1106	L1031	L901	D831	E760	E692	K619	ASP	L483	F418	I352
	V1260	K1107	L1032	R967	C902	E832	M761	E692	PRG	V486	S419	I353	
	E1262	I1179	T1033	C968	K903	D833	E762	L693	ALA	V486	T354	T354	
	P1263	V1180	H1034	N969	T904	M834	P694	P694	ALA	C487	F421	A355	
	P1264	S1111	E1038	E970	N905	L835	T767	E695	S624		K422		
	P1265	G1112	E971	E971	S908	I836	Q768	I696	E625	Y490	Q423	S359	
VAL	P1266	S1113	M1039	C972	R909	T837	M769	I697	Q559	E424	A424	S360	
	L1267	W1114	G1040	A974	N909	R840	K772	T698	Q559	E425	S425	L361	
	E1268	D1115	Q1041	S975	A911	H841	T773	E699	Q562	E993			
	P1269	D1116	H1044	S976	R912	R841	Q774	D701	Q562	L496	V364	V364	
	S1270	V1117	T1045	O977	E913	Y847	S775	A702	V564	P497	E428	F365	
	I1271	T1118	V1048	R979	G914	K848	F776	I703	V564	E498	R429	K366	
	F1272	A1120	Q1049	H979	F915	V849	M780	N706	K566	D499	D430	A367	
	F1273	A1121	V1050	A980	G916	G850	S707	S707	E570		I431	S368	
	E1274	Y1122	K981	R981	G917	F851	V783	F708	E571	A432	R427	G369	
	P1275	M1123	A1051	K982	P918	R852	P784	Y709	R508	K430	V434	K371	
VAL	V1276	S1052	S983	S983	Q919	K853	P784	G710	D572	C509	T435		
	Q1277	D1124	E984	E984	G920	T854	R791	P711	H573	T510		T373	
	A1278	T1125	V985	V985	R921	V857	R787	E712	V574	L511	M438	L374	
	I1279	D986	I1057	I987	I923	V858	R789	E712	G643	T512	R439		
	R1280	S1127	K987	K987	I924	K714	V790	L713	R576	T513	V440		
	Q1285	T1131	K990	K990	A924	A859	R791	I715	P577	S514	R377	R377	
	E1286	G1132	E1066	K996	E930	L860	R791	I715	L578	P577	G378	G378	
	T1287	F1133	T1067	R997	R931	E861	E716	E716	R579	P515	T379	R380	
	L1288	Y1134	S1068	I999	M928	V862	R794	K717	H590	F516	T447	R381	
	M1289	R1135	E1065	K995	S929	H864	G796	D719	L581	T382	E448	V383	
VAL	N1290	H1212	S1065	E1066	E930	R865	G797	L720	A582	Y620	Q384	Q384	
	E1291	L1139	T1067	K996	E930	R865	G797	L720	L521	V449	V449	V449	
	E1292	G1140	E1066	K996	E930	R865	G797	L720	L521	Q450	K385	K385	
	E1293	Y1141	S1068	G996	A932	R867	G798	T722	E587	E451	D386	D386	
	F1295	S1142	T1069	I999	R937	R871	G801	S725	S888	L524	L452	D387	
	L1296	F1143	M1070	C1000	K802	I878	K802	Q525	E590	T388	T388	T388	
	L1297	E1144	T1071	T1001	D873	R878	E803	E726	K326	L454	F389	F389	
	H1298	T1145	V1072	P1003	P938	L874	T804	E726	A591	C455	F390	F390	
	E1298	H1146	P1003	P1003	P938	L874	T804	E726	V592	Y456	P391	P391	
	S1299	N1146	S1076	T1004	A859	S875	R805	V730	Y593	Q529	G392	G392	
VAL	P1300	P1077	P1077	L1005	R896	Q876	S806	V731	C594	Q529	M459	R393	
	P1303	T1227	S1081	F1006	E941	R877	T807	E663	C594	E530	K394	K394	
	K1304	Y1153	V1082	L1007	R897	R878	V808	I735	D595	N531	N461	T396	
	K1309	F1154	E1083	T1008	R943	M879	R809	E666	D596	L532	R462	K396	
	L1307	S1155	S1083	S1009	R944	E881	S810	E741	E533	E533	K462	T397	
	N1308	T1156	A1084	F1010	K945	R881	T811	E741	P598	D534	L463	L397	
	A1309	K1157	D1085	T1011	N946	A882	E812	H742	R899	K335	I464	L398	
	C1310	L1158	Q1089	F1014	Y948	F884	A814	F743	Y600	C536	S465	S399	
	V1311	A1159	Q1089	Y1015	K949	H885	L815	P676	E601	G537	A466	P400	
	D1312	C1160	Y1092	M1016	R950				N602	K538	L467	E401	
VAL	E1239	S1161		M1016	K950				E603	L539	K468	E403	
	F1240	E1162	Y1092	Q1017	G951	M888	T747	T747	L604	D540	L404	L404	
	R1241	V1163	C1095	Q1017	D952	H748	Q880	H748	P541	T470	L404	L404	
	L1242	E1164	Q1096	G1019	L953	Y890	R819	C749	T542	Q471	S406	S406	
	S1243	I1165	T1097	E1019	R822	K391	R822	T750	F543	R472	L407	L407	
	V1319	D1166	I1098	L1021	F956	I892	P823	I751	A544	Q473	E408	E408	
	THR	C1167	L1099	L1022	L1022	P950	P824	R752	A546	T610	S475	S475	Y411
		GLY	E1169	E1169	E1169					G485	K476	K476	Y411

- Molecule 1: XANTHINE OXIDOREDUCTASE







4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.73Å 197.73Å 285.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.76 – 3.59	Depositor
% Data completeness (in resolution range)	98.2 (30.76-3.59)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	39807	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: GOL, ACY, PO4, 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	2.11	336/9969 (3.4%)	1.70	184/13492 (1.4%)
1	B	2.14	334/10160 (3.3%)	1.73	211/13751 (1.5%)
1	C	2.10	326/10113 (3.2%)	1.72	202/13685 (1.5%)
1	D	2.06	304/10118 (3.0%)	1.70	175/13693 (1.3%)
All	All	2.10	1300/40360 (3.2%)	1.71	772/54621 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	40
1	B	1	54
1	C	1	49
1	D	0	55
All	All	2	198

The worst 5 of 1300 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1318	CYS	CB-SG	17.07	2.11	1.82
1	A	762	GLU	CG-CD	16.49	1.76	1.51
1	A	78	CYS	CB-SG	16.00	2.09	1.82
1	B	3	ALA	N-CA	15.65	1.77	1.46
1	B	762	GLU	CD-OE1	15.23	1.42	1.25

The worst 5 of 772 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	794	ARG	NE-CZ-NH2	-14.57	113.02	120.30
1	A	830	ARG	NE-CZ-NH1	13.47	127.04	120.30
1	C	825	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	B	599	ARG	CG-CD-NE	13.40	139.94	111.80
1	C	599	ARG	NE-CZ-NH1	13.04	126.82	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	165	ARG	CA
1	C	165	ARG	CA

5 of 198 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	GLU	Peptide
1	A	164	ALA	Peptide
1	A	202	THR	Peptide
1	A	222	THR	Peptide
1	A	294	PRO	Peptide

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	9764	0	9788	628	0
1	B	9951	0	9967	711	0
1	C	9905	0	9922	648	0
1	D	9910	0	9929	634	0
2	A	8	0	0	2	0
2	B	8	0	0	2	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	53	0	30	12	0
3	B	53	0	29	6	0
3	C	53	0	29	10	0
3	D	53	0	29	14	0
4	A	6	0	8	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	14	0
4	C	6	0	8	4	0
4	D	6	0	8	10	0
5	D	4	0	3	0	0
6	D	5	0	0	1	0
All	All	39807	0	39758	2568	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 32.

The worst 5 of 2568 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:D:793:LYS:CD	1:D:793:LYS:CG	1.74	1.62
1:C:1319:VAL:CA	1:C:1319:VAL:CB	1.77	1.61
1:D:903:LYS:CD	1:D:903:LYS:CE	1.75	1.61
1:B:1319:VAL:CA	1:B:1319:VAL:CB	1.78	1.61
1:A:318:LYS:CE	1:A:318:LYS:CD	1.76	1.61

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	1255/1333 (94%)	1002 (80%)	168 (13%)	85 (7%)	1	15
1	B	1281/1333 (96%)	1021 (80%)	158 (12%)	102 (8%)	1	11
1	C	1273/1333 (96%)	1011 (79%)	168 (13%)	94 (7%)	1	13
1	D	1275/1333 (96%)	1006 (79%)	174 (14%)	95 (8%)	1	12
All	All	5084/5332 (95%)	4040 (80%)	668 (13%)	376 (7%)	1	13

5 of 376 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ALA
1	A	219	LEU
1	A	220	LYS
1	A	272	ASN
1	A	449	VAL

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	1067/1126 (95%)	807 (76%)	260 (24%)	0	4
1	B	1088/1126 (97%)	812 (75%)	276 (25%)	0	4
1	C	1082/1126 (96%)	814 (75%)	268 (25%)	0	4
1	D	1084/1126 (96%)	813 (75%)	271 (25%)	0	4
All	All	4321/4504 (96%)	3246 (75%)	1075 (25%)	0	4

5 of 1075 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1057	ILE
1	C	379	THR
1	D	921	MET
1	B	1126	VAL
1	C	62	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1195	GLN
1	C	423	GLN
1	D	992	ASN
1	B	1213	HIS
1	C	251	GLN

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 ⓘ

18 ligands are modelled in this entry.

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$
2	FES	C	3002	1	0,4,4	0.00	-	-		
2	FES	A	3001	1	0,4,4	0.00	-	-		
3	FAD	A	3006	-	51,58,58	2.27	12 (23%)	60,89,89	2.57	26 (43%)
5	ACY	D	3008	-	1,3,3	5.46	1 (100%)	0,3,3	0.00	-
3	FAD	D	3006	-	51,58,58	2.42	13 (25%)	60,89,89	3.34	27 (45%)
2	FES	B	3002	1	0,4,4	0.00	-	-		
3	FAD	B	3006	-	51,58,58	2.48	15 (29%)	60,89,89	2.76	23 (38%)
3	FAD	C	3006	-	51,58,58	2.47	15 (29%)	60,89,89	3.22	29 (48%)
2	FES	D	3002	1	0,4,4	0.00	-	-		
2	FES	B	3001	1	0,4,4	0.00	-	-		
4	GOL	A	3007	-	5,5,5	0.59	0	5,5,5	0.95	0
4	GOL	B	3007	-	5,5,5	0.61	0	5,5,5	0.75	0
2	FES	C	3001	1	0,4,4	0.00	-	-		
4	GOL	D	3007	-	5,5,5	0.85	0	5,5,5	1.30	1 (20%)
4	GOL	C	3007	-	5,5,5	0.52	0	5,5,5	0.53	0
2	FES	D	3001	1	0,4,4	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FES	A	3002	1	0,4,4	0.00	-	-		
6	PO4	D	3009	-	4,4,4	1.07	0	6,6,6	1.86	1 (16%)

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
2	FES	C	3002	1	-	-	0/1/1/1
3	FAD	C	3006	-	-	8/30/50/50	0/6/6/6
3	FAD	A	3006	-	-	6/30/50/50	0/6/6/6
2	FES	D	3001	1	-	-	0/1/1/1
3	FAD	D	3006	-	-	9/30/50/50	0/6/6/6
3	FAD	B	3006	-	-	8/30/50/50	0/6/6/6
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	D	3002	1	-	-	0/1/1/1
2	FES	B	3001	1	-	-	0/1/1/1
2	FES	C	3001	1	-	-	0/1/1/1
4	GOL	B	3007	-	-	2/4/4/4	-
4	GOL	A	3007	-	-	2/4/4/4	-
4	GOL	D	3007	-	-	0/4/4/4	-
4	GOL	C	3007	-	-	2/4/4/4	-
2	FES	B	3002	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3006	FAD	C2A-N3A	10.49	1.49	1.32
3	A	3006	FAD	C1'-N10	8.94	1.57	1.48
3	B	3006	FAD	C1'-N10	7.48	1.55	1.48
3	D	3006	FAD	C2A-N1A	7.07	1.47	1.33
3	B	3006	FAD	C2A-N3A	7.04	1.43	1.32

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3006	FAD	C1'-N10-C9A	10.72	126.73	118.29
3	D	3006	FAD	C4-C4X-C10	9.79	126.43	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	3006	FAD	C4-N3-C2	8.62	122.42	115.14
3	D	3006	FAD	C1'-N10-C10	8.46	125.98	118.41
3	D	3006	FAD	C10-C4X-N5	-7.63	115.98	121.26

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

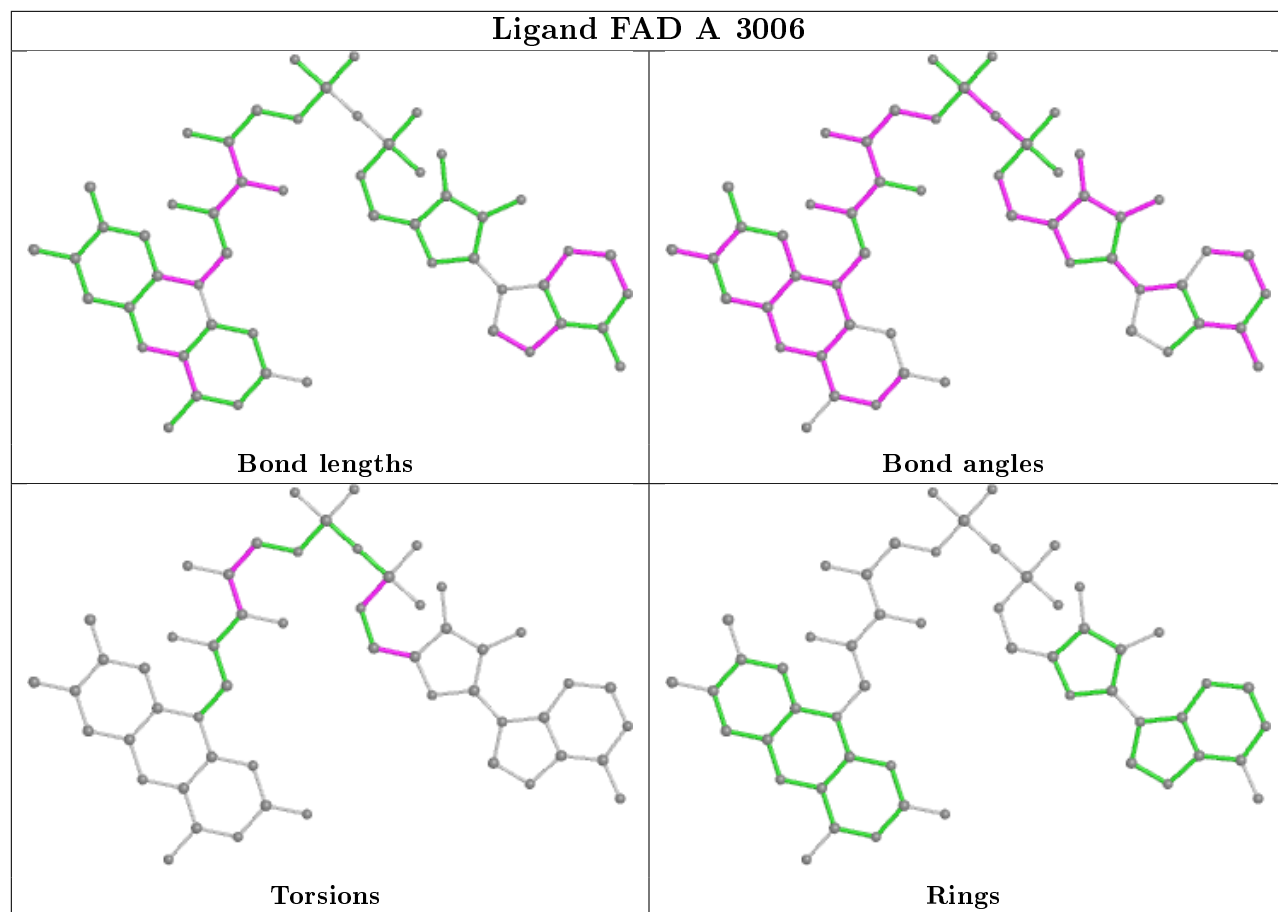
Mol	Chain	Res	Type	Atoms
4	C	3007	GOL	C1-C2-C3-O3
3	A	3006	FAD	C5B-O5B-PA-O3P
3	D	3006	FAD	C5B-O5B-PA-O3P
3	D	3006	FAD	C1'-C2'-C3'-O3'
3	D	3006	FAD	O4'-C4'-C5'-O5'

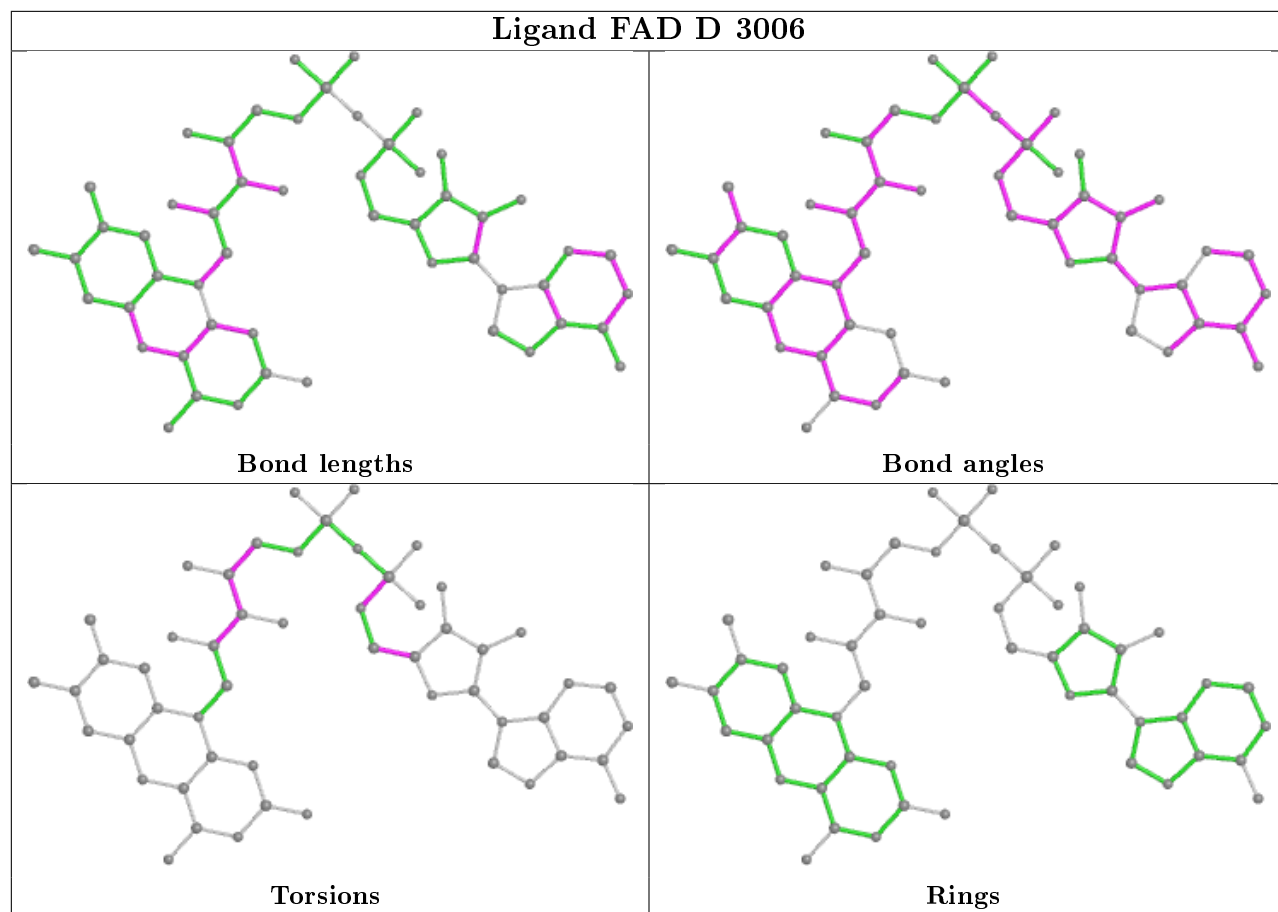
There are no ring outliers.

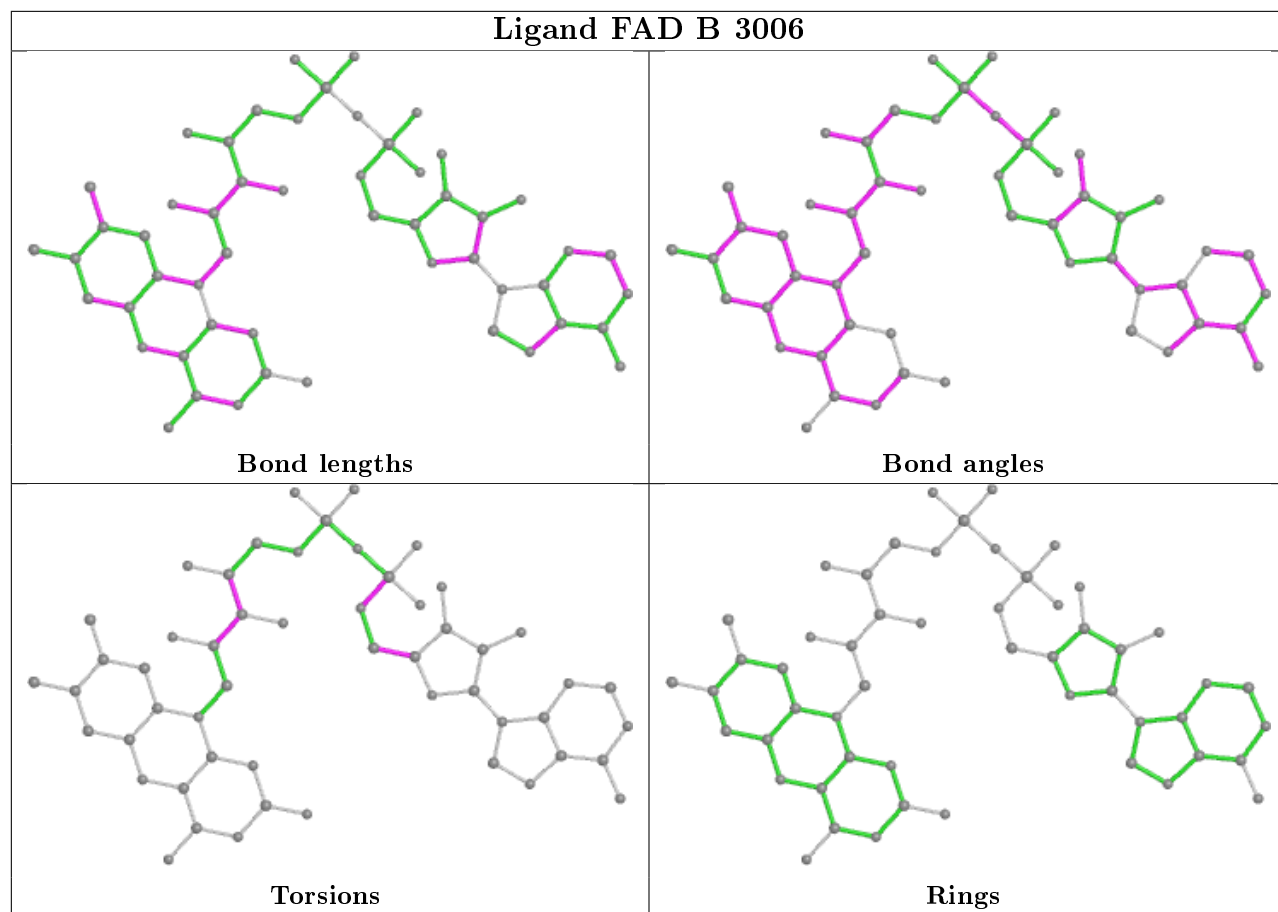
11 monomers are involved in 81 short contacts:

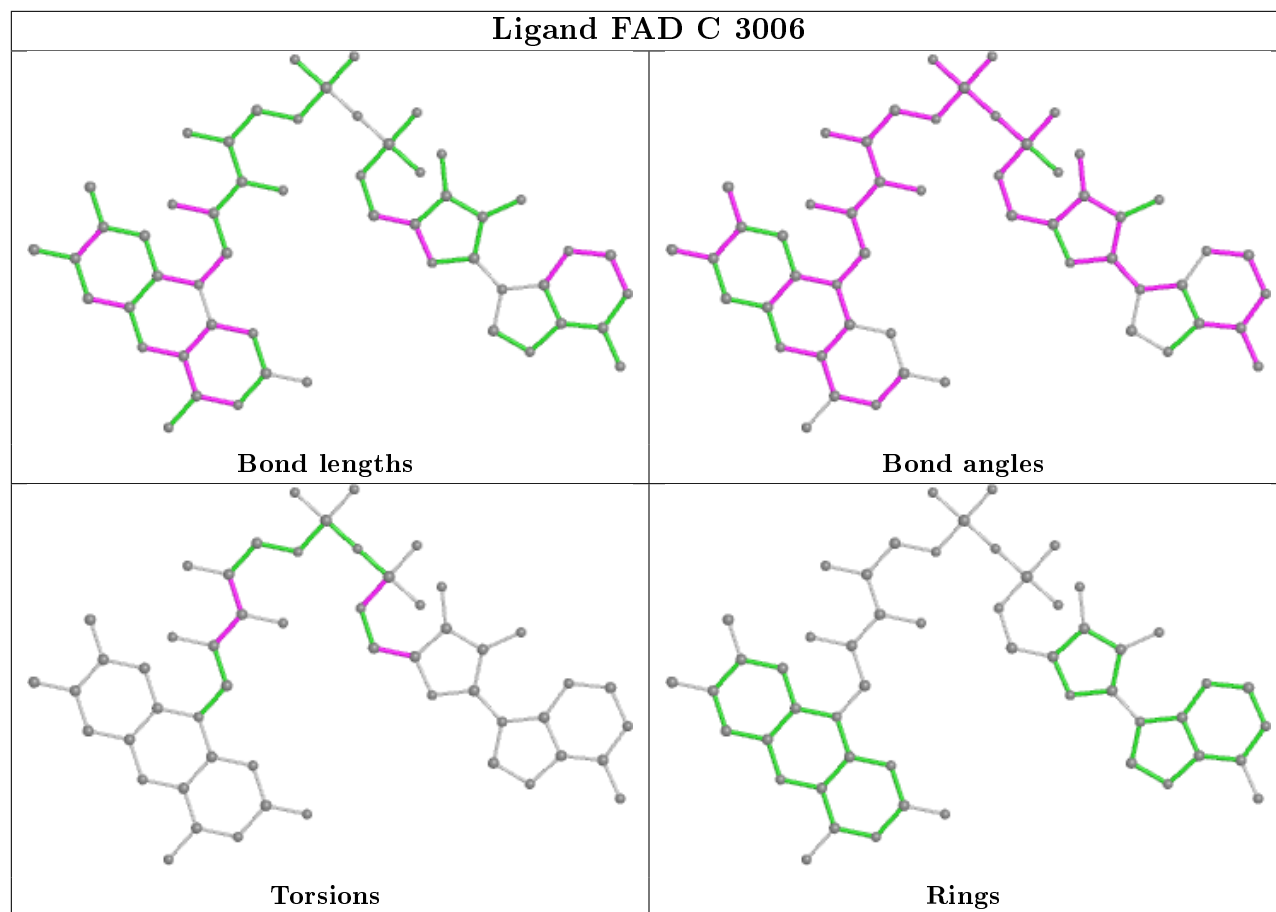
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3006	FAD	12	0
3	D	3006	FAD	14	0
2	B	3002	FES	2	0
3	B	3006	FAD	6	0
3	C	3006	FAD	10	0
4	A	3007	GOL	6	0
4	B	3007	GOL	14	0
4	D	3007	GOL	10	0
4	C	3007	GOL	4	0
2	A	3002	FES	2	0
6	D	3009	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.