



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 11:00 PM UTC

PDB ID : 2CKJ / pdb_00002ckj
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 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

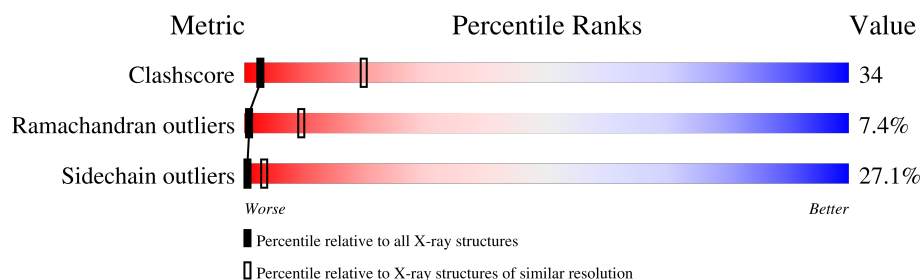
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (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 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	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	-
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](#)

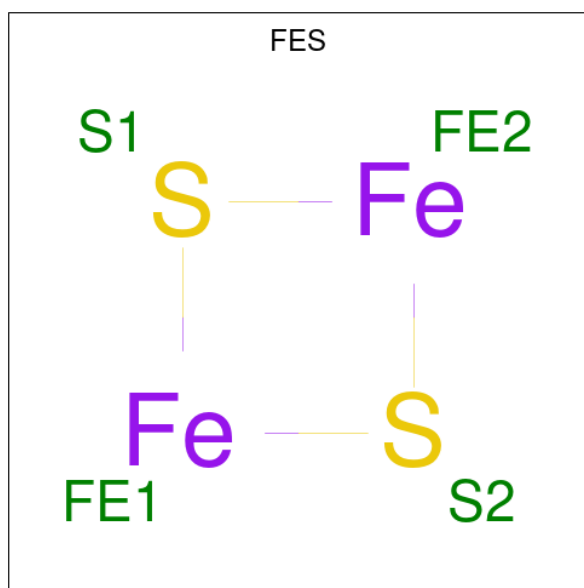
There are 6 unique types of molecules in this entry. The entry contains 39807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: FES) (formula: Fe₂S₂).



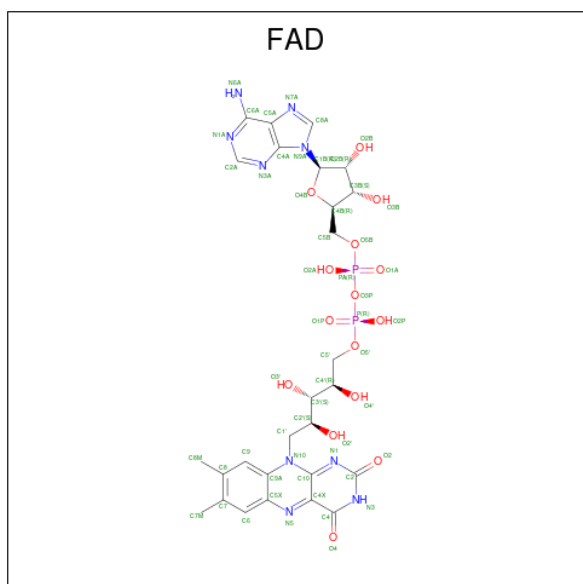
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		

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

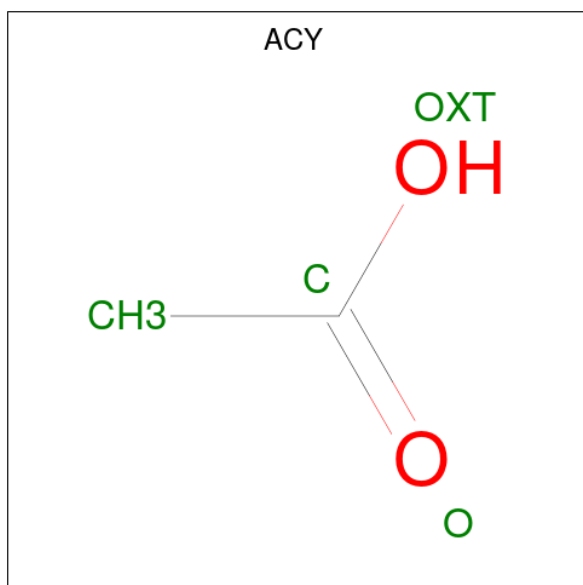
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).





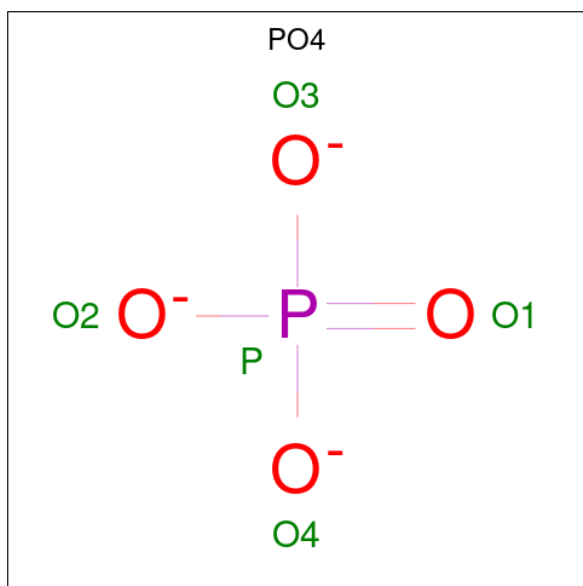
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETIC ACID (CCD ID: 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 (CCD ID: PO4) (formula: O_4P).



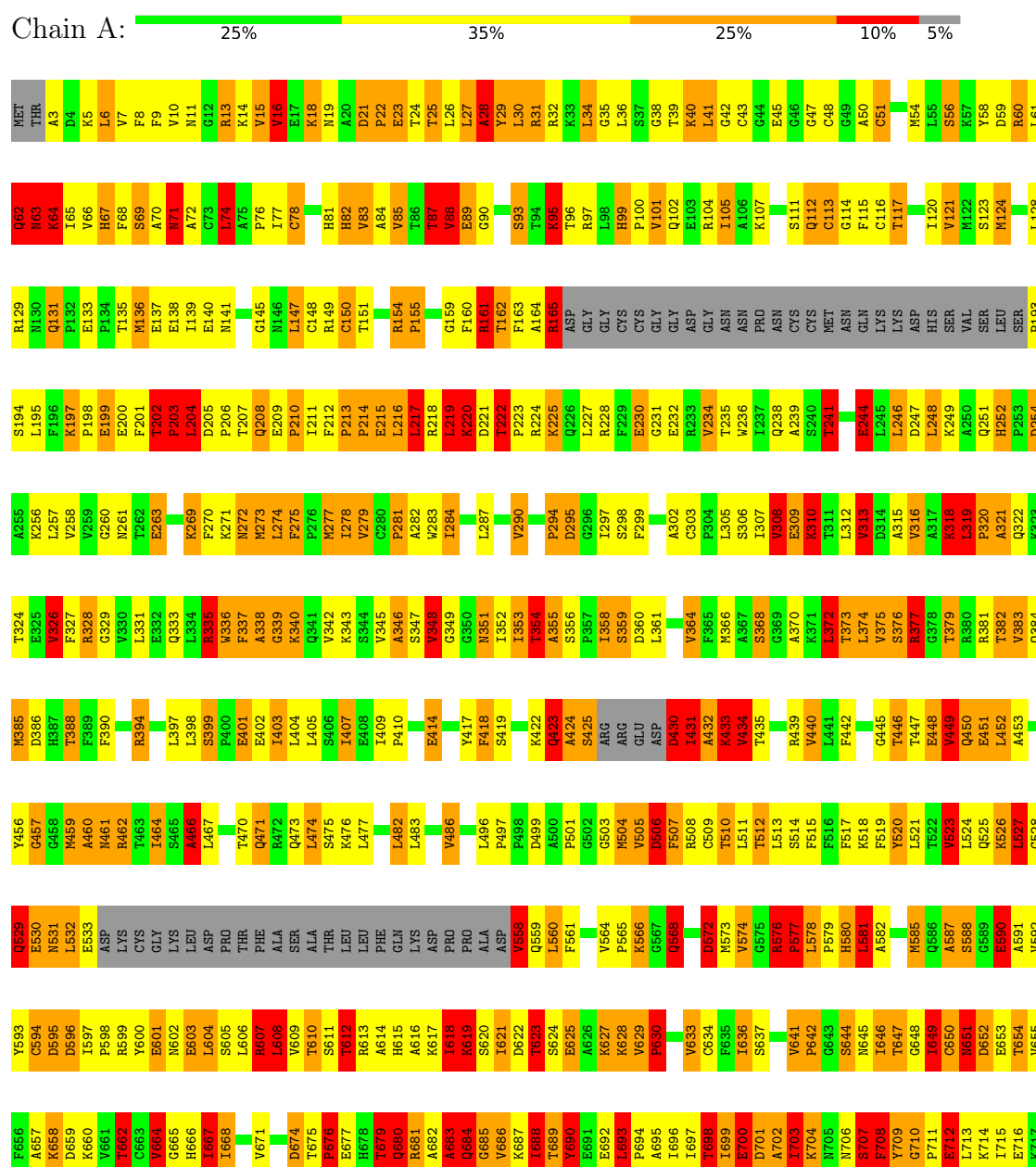
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

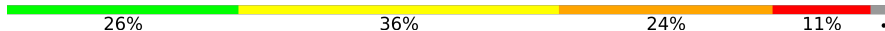
Note EDS was not executed.

• Molecule 1: XANTHINE OXIDOREDUCTASE



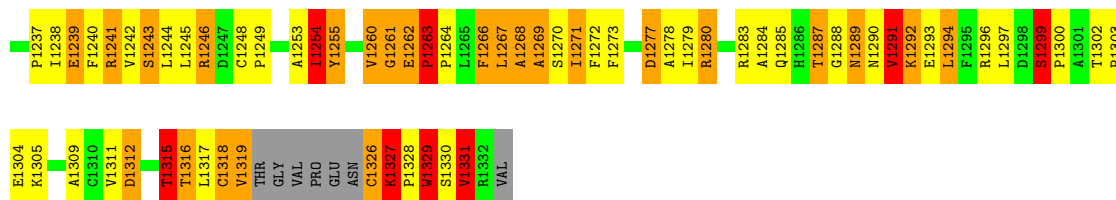
A1301	T1236	C1167	L1102	Q1041	G977	A911	P842	L781	G718
T1302	P1237	L1168	E1103		Y978	F912	F843		D719
P1303	T1238	T1169	P1104	H1044	H979	R913		G782	L720
E1304	E1239	G1170	Y1105		R981	G914	K848	G783	K721
K1305	F1240	D1171	K1106	T1046	K981	F915	Y847	N786	K722
I1306	R1241	H1172	K1107	M1047	K982	G916	V849	R787	G723
	V1242	K1173	K1108	V1048	S983	G917	G850	L788	
V1311	S1243	M1174	M1109	Q1049	E984	P918	F851	V789	D728
D1312	L1244	L1175		V1050	V985	Q919	T854	V790	N729
	L1245	R1176	S1113	A1051	V986	G920		R791	V730
T1315	D1246	T1177	W1114	S1052	A1051	M921	V792	V792	V731
T1316	D1247	D1178	E1115	R1063	K987	L922	V857	G793	S732
L1317	C1248	I1179	D1116	A1054	E991	L923	V858	G733	G733
C1318	P1249	M1180	W1117	L1055	N992	A924	A959	R794	E734
V1319	N1250	M1181	V1118	K1056	C993	E925	L860	M795	I735
T1320		D1182	T1119	I1057	W994	G926	E861	G796	I736
GLY	T1254	V1183	A1120	P1058	K995	Q927	V862	G797	V737
VAL	Y1255		A1121	T1059	K996	M828	D863	G798	G738
PRO	A1256	L1187	Y1122	S1060	R997	S929	H864	F799	
GLU	S1257	M1188	M1123	K1061		E930	F865	G800	Q740
ASN	K1258	A1189	D1124	I1062		A932	H864	G801	E740
CYS	A1259	P1190	T1125	Y1063	I1001	R931	S866	K802	G741
LYS	V1260	I1191	Y1126	I1064	I1002	V933	N867	E903	H742
PRO	G1261	D1192	S1127	S1065	P1003	T934	G869	T804	F743
	E1262	T1193	L1128	I1066	T1004	C935	M870	R805	Y744
W1329	P1263	G1194	S1129	T1067	K1005	G936	Q872	S806	L745
SER	P1264	K1195	A1130	S1068		M937	T871	T807	E746
VAL		V1196	T1131	T1069		P938	D873	V808	T747
ARG		E1197	G1132	N1070	I1008		L874	R909	H748
VAL	A1268		F1133	T1071	S1009	P938		S810	C749
	A1269	F1200	Y1134	I1072	F1010	E941		T811	T750
	T1270		R1135	V1073	T1011	V942	I878	V751	T751
		L1204	T1136	P1073	V1012	R943	M879	A812	A752
			P1137	N1074	P1013	K944	E880	V813	
A1274		G1205	T1075	T1075	F1014	K945	R881	A814	V753
T1275		L1206	N1138	S1076	L1015	N946	A882	L815	P754
D1276			L1139	P1077	M1016	L947	L883	A816	K755
		L1209	G1140	T1078	Q1017	Y948	E884	A817	G756
A1278		E1210	Y1141	T1079	A1018	K949	H885	E884	E757
T1279		E1211	S1142	A1080	G1019	E950		K819	A758
R1280		L1212	F1143	V1082	G1019	E950		G759	G759
A1281		H1213	E1144	S1083	A1020	G951		G821	E760
			T1145		L1021	R952	N888	R822	M761
A1282		G1218	N1146	S1083	L1022	L953	C889	P823	E762
R1283		S1219	Y1153	A1084	H1023	R954	Y890	V824	L763
A1284		T1219	F1154	D1085	V1024	H955	R891	R825	L763
Q1285		L1220	P1150	L1086	Y1025	F956	R893	F764	V765
		H1221	T1026	N1087	T1026		N894	C826	G766
T1287		T1222	F1151	G1088	D1027	K959	I895	M827	S766
L1288		G1223	H1152	Q1088	G1028			L828	T767
N1289		R1224	Y1153	A1090	S1029	G962	T898	D829	Q768
N1290		P1225	F1154	V1091	V1030	F963	R830	R830	M769
		S1226		Y1092	L1031		G999	D831	T770
							R900	E832	M771
K1292		T1227	G1157	A1093	P966	P966	L901	D833	K772
E1293		V1228	V1158	A1094	T1033	R967	C902	M834	V773
L1294		K1229	A1159	C1095	H1034		K903	L835	Q774
		T1230		Q1096	G1035	E970	T904	I836	
F1295		P1231	S1161	T1097	G1036	E971	N905	T837	F776
L1296		A1232		I1098	T1037			G838	V777
D1298		F1233	E1164	L1099	E1038	A974	S908	G339	A778
S1299		G1234	T1165	K1100	T1039	S975	N109	R840	K779
		S1235	D1166	L1101	G1040	S976	K910	R941	
							T910		

● Molecule 1: XANTHINE OXIDOREDUCTASE

Chain B:  26% 36% 24% 11% .

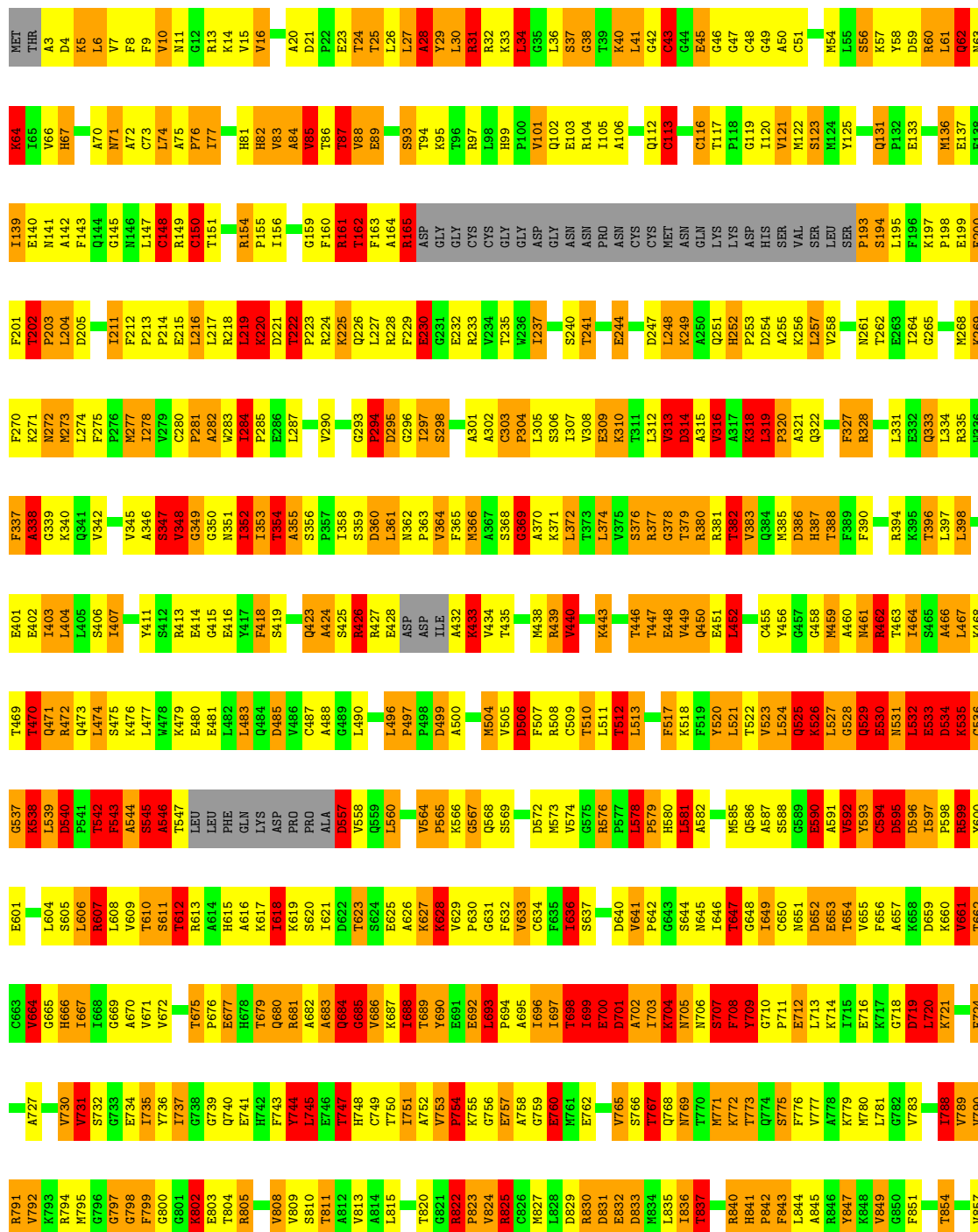
SER	P193	S194	L195	F196	K197	P198	E199	E200	F201	T202	P203	L204	D205	MET																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
	Q131	P132	E133	L134	L135	M136	E137	E138	L139	N140	N141	A142	F143		Q144	G145	N146	L147	L148	F149	T150	T151	G152	Y153	R154	P155																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														

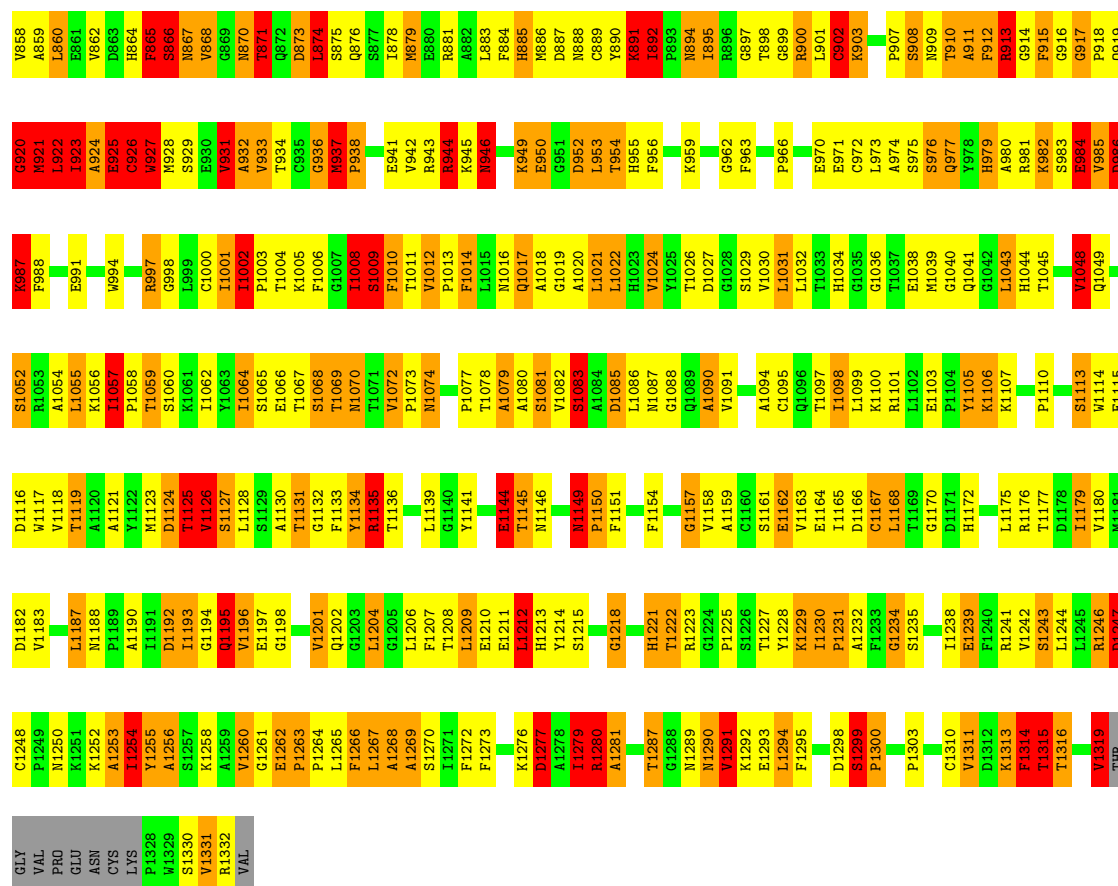
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K1173	S1111	G1042	Y978	G914	F851	N786	K721	F656	V592	Y456	F390	K257	
L1174	G1112	H1043	H979	F915	M852	K787	L720	A657	Y593	M459	G392	V326	
L1175	G1113	H1044	A980	G916	K853	V788	K722	K658	C594	A460	G393	F327	T262
L1176	S1113	T1045	R981	G917	T854	V789	G723	D659	D595	K460	R394	R328	E263
T1177	V1114	K1046	K982	P918	G855	V790	F724	K660	D596	M461	R394	I264	
D1178	E1115	M1047	S983	Q919	T856	R791		V661	L597	R462	K395	L331	G
D1179	D1116	V1048	E984	G920	V857	V792	V730	T662	P598	T463	T396	M268	
V1180	V1117	Q1049	V985	M921	R858	K793	W731	G663	R599	L464	L397	Q333	K269
	V1118	V1050	D986	L922	A859	R794	S732	V664	Y600	S465	F270	L334	F270
	T1119	A1051	F983	I923	L860	M795	G733	G665	E601	L466	S399	K271	
G1183	A1120	S1052	F988	A924	R601	G796	E734	H666	N602	L467	P400	N272	
V1184	A1121	R1053	N989	E925	V862	G797	I735	I687	E603	K468	E401	F337	
S1185	Y1122	M1054	K990	C926	D863	G798	Y736		L604	T469		A338	M273
L1186	D1123	L1055	E991	E927	H864	F799	I737	V671	S605	T542	L404	G339	M274
M1188	D1124	K1056	N992	M928	F865	G800	G738	V672	L606	Q471	L404	K340	L275
P1189	T1125	P1057	C993	S929	S866	G801	G739	A673	R607	R472	L405	Q341	P276
A1190	V1126	P1058	V994	E930	N867	K802	Q740	D674	L608	Q473	I407	K343	M277
I1191	S1127	T1059	K995	V931	V868	E803	Q741	T675	V609	Q473	E408	K343	I278
D1192	L1193	S1060	K996	A932	T804	T804	H742	P676	S611	L474	E408	S344	V279
L1193	T1131		G997	V933	T871	R805	F743		T612	PHE	Y411	S347	P281
G1194	G998	I1064	G998	G936	D873	S806	L745	T679	T612	GLN	S412	V348	A282
V1195	S1065	S1065	L999	R937	L874	V808	E746	R681	H615	L482	R413	I284	W283
F1133	E1066	T1067	C1000	P938	R875	V809	T747	A682	A616	Q484	R413	I284	K284
E1197	V1134	T1067	I1001	P938	S875	V809	H748	A682	K617	Q484	R413	P285	E286
G1198	R1135	S1068	I1002	A939	Q876	S810	H748	A683	K617	D485	F418	I353	L287
A1199	T1136	T1069	P1003	E940	S877	T811	C749	Q684	E625	V497	S425	V486	N288
F1200	P1137	M1070	T1004	E941	R878	A812	T750	G685	K619	C487	R426	T354	S289
V1201	N1138	T1071	T1004	V942	M879	V813	I751	V686	D622	A420	R427	I297	
Q1202	L1139	V1072		R943	E880	A814	A752	K687	D622	L490	F421	I297	
G1203	F1140	P1073	I1008	R944	R881	L815	V753	L688	T623	Q559	K422	S298	V290
L1204	Y1141	N1074	S1009	K945	A882	A816	P754	T689	T623	H495	Q423	P294	
G1205	S1142	T1075	T1011	R946	L883	A817	K755	V690	E625	L496	S359	D295	
	F1143	S1076		L947	F884	Y818	G756	E691	A626	P497	A424	G296	
				L953	N885	K819	E757	E692	K627	Q562	S425	G296	
T1208	E1144	P1077	F1014	K948	M886		A758	L693	K628	E563	R426	I297	
L1209	T1145		L1015	K949				L693	K628	D499	R427	S298	
E1210	N1146	A1080	L1016	E950	D887	R822	G759	P694	V629	A500	E428	F299	
E1211		S1081	Q1017	N888	N888	P823	E760	A695	V629	F365	D429	G300	
L1212	N1149	V1082	A1018	D952	C889	V824	M761	I696	K630	M366	D429	G300	
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	F1151	A1084	G1020		K891	C826	L763	T698	C634	Q568	I431	A302	
	H1152	D1085	L1021	F956	L892	M827	F764	I699	F635	E570	K433	A302	
P1216					P893	L828	V765	E700	F635	E570	K433	A302	
E1217	S1155	Q1089	H1022	K959	N894	R830	T767	A702	R639	T510	V434	L305	
S1219	Y1156		V1024	L960	T898	D831	Q768	I703	D640	T512	L374	V308	
L1220	G1157	Y1092	Y1025	E961	G899	E832	N769		D640	S514	R439	V308	
H1221	V1158	A1093	T1026	G962	R900	R833	M770	N706	E641	F515	R439	V308	
A1159	C1095	L1093	D1027	F963	L901	M834	K772	S707	P642	F516	V440	E309	
R1223	C1095												
T1222													
K1223													
G1224	S1161	Q1096	S1029	P966	G902	R833	K772	F708	G643	F517	K443	T311	
P1225	E1162	T1097	V1030	R967	K903	L835	T773	Y709	H580	F517	G378	V313	
S1226	V1163	L1098	L1031	G968	T904	T837	Q774	G710	L581	Y520	T446	D314	
T1227	E1164	I1099	L1032	W969	N905		S775	P711	T647	L521	T447	A315	
V1228	D1165	K1100	T1033	E970	L906	R840	F776	E712	G648	T522	E448	V316	
K1229	C1166	R1101	H1034	E971	P907	H841	V777	L713	I649	V523	V449	A317	
L1230	C1167	L1102	G1035	S908	P907	P842			C650	L524	Q450	K318	
P1231	L1168	E1103	L973	N909	N909	H841			R651	Q525	A851	M385	
A1232	T1169	P1104	A974	T910	T910	Y847	W780	I716	T715	R526	L452	D386	
F1233	G1170	Y1105	S975	R976	A911	K648	V783	K717	E653	L527	A453	H387	
V1234	S1174	V1105	S976	V876	V876	V840			T582	C590	L454	T399	



• Molecule 1: XANTHINE OXIDOREDUCTASE

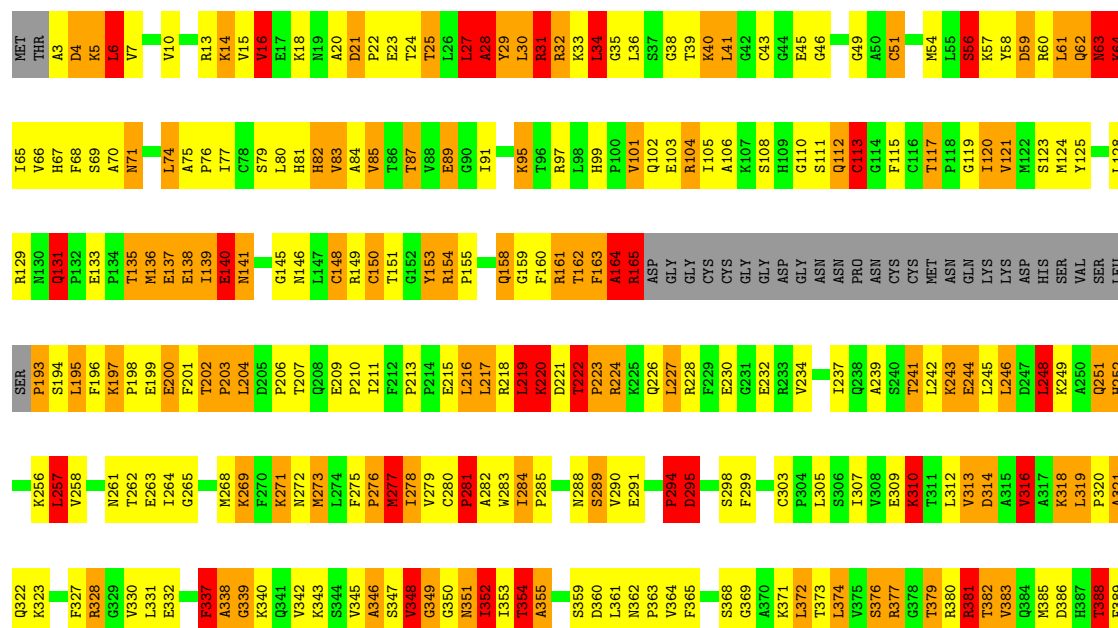
Chain C: 26% 36% 24% 11%





● Molecule 1: XANTHINE OXIDOREDUCTASE

Chain D: 25% 38% 23% 10% .



L1297	L1298	S1299	P1300	A1301	T1302	P1303	E1304	E1305	L1306	A1307	N1308	Y1311	D1312	K1313	F1314	T1315	T1316	L1317	C1318	T1319	T1320	GLY	VAL	PRO	GLU	ASN	C1326	K1327	P1328	W1329	S1330	R1332	VAL	F390	P391	R394	N461	R462	T463	L464	S465	E401	A402	K403	L404	L405	S406	E408	Y411	S412	R413	E414	F418	S419	A420	F421	Q422	Q423	A424	S425	R426	R427	E428	D429	D430	I431	A432	K433	V434	T435	M438	R439	V440	L441	F442	K443	P444	Q445	T446	T447	E448	V449	Q450	E451	L452	A453	L454	C455	Y456	M459	A460	R461	T462	L463	L464	S465	E466	L467	K468	T469	T470	Q471	R472	L473	L474	S475	K476	W478	K479	E480	E481	L482	L483	Q484	Q485	R486	P487	ALA	D557	L486	P487	P488	P498	D499	L560	A500	P501	M504	V505	D506	F507	Q508	S509	E570	E571	L510	L511	T512	L513	S514	P444	Q445	T446	T447	E448	V449	Q450	E451	L452	A453	L454	C455	K526	L527	Q528	Q529	E530	N531	L532	E533	D534	L535	K536	E537	G538	L539	D540	P541	THR	PHE	ALA	SER	ALA	THR	LEU	LEU	PHE	GLN	LYS	ASP	PRO	PRO	ALA	D557	L486	P487	P488	P498	D499	L560	A500	P501	M504	V505	D506	F507	Q508	S509	E570	E571	L510	L511	T512	L513	S514	P444	Q445	T446	T447	E448	V449	Q450	E451	L452	A453	L454	C455	E589	E590	V591	V592	C593	D594	D595	D596	L597	P598	R599	Y600	E601	L604	S605	L606	R607	R608	V609	S611	T610	T612	R613	R614	E615	A616	K617	T618	R619	R621	S620	L621	D622	T623	S624	E625	A626	K627	R628	V629	G631	G632	F633	G634	P635	L636	D639	D640	V641	G643	S644	N645	N646	T647	S648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	E712	L713	K714	L715	K716	L717	E718	G719	T720	L721	K722	G723	F724	A727	V730	W731	G732	W733	E734	T735	W736	T737	R738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E762	L763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018	E1019	E1020	E1021	E1022	E1023	E1024	E1025	E1026	E1027	E1028	E1029	E1030	E1031	E1032	E1033	E1034	E1035	E1036	E1037	E1038	E1039	E1040	E1041	E1042	E1043	E1044	E1045	E1046	E1047	E1048	E1049	E1050	E1051	E1052	E1053	E1054	E1055	E1056	E1057	E1058	E1059	E1060	E1061	E1062	E1063	E1064	E1065	E1066	E1067	E1068	E1069	E1070	E1071	E1072	E1073	E1074	E1075	E1076	E1077	E1078	E1079	E1080	E1081	E1082	E1083	E1084	E1085	E1086	E1087	E1088	E1089	E1090	E1091	E1092	E1093	E1094	E1095	E1096	E1097	E1098	E1099	E1100	E1101	E1102	E1103	E1104	E1105	E1106	E1107	E1108	E1109	E1110	E1111	E1112	E1113	E1114	E1115	E1116	E1117	E1118	E1119	E1120	E1121	E1122	E1123	E1124	E1125	E1126	E1127	E1128	E1129	E1130	E1131	E1132	E1133	E1134	E1135	E1136	E1137	E1138	E1139	E1140	E1141	E1142	E1143	E1144	E1145	E1146	E1147	E1148	E1149	E1150	E1151	E1152	E1153	E1154	E1155	E1156	E1157	E1158	E1159	E1160	E1161	E1162	E1163	E1164	E1165	E1166	E1167	E1168	E1169	E1170	E1171	E1172	E1173	E1174	E1175	E1176	E1177	E1178	E1179	E1180	E1181	E1182	E1183	E1184	E1185	E1186	E1187	E1188	E1189	E1190	E1191	E1192	E1193	E1194	E1195	E1196	E1197	E1198	E1199	E1200	E1201	E1202	E1203	E1204	E1205	E1206	E1207	E1208	E1209	E1210	E1211	E1212	E1213	E1214	E1215	E1216	E1217	E1218	E1219	E1220	E1221	E1222	E1223	E1224	E1225	E1226	E1227	E1228	E1229	E1230	E1231	E1232	E1233	E1234	E1235	E1236	E1237	E1238	E1239	E1240	E1241	E1242	E1243	E1244	E1245	E1246	E1247	E1248	E1249	E1250	E1251	E1252	E1253	E1254	E1255	E1256	E1257	E1258	E1259	E1260	E1261	E1262	E1263	E1264	E1265	E1266	E1267	E1268	E1269	E1270	E1271	E1272	E1273	E1274	E1275	E1276	E1277	E1278	E1279	E1280	E1281	E1282	E1283	E1284	E1285	E1286	E1287	E1288	E1289	E1290	E1291	E1292	E1293	E1294	E1295	E1296	F1233	G1234	S1235	I1236	P1237	I1238	E1239	F1240	R1241	S1242	R1243	L1244	L1245	R1246	D1247	N1250	K1251	L1252	L1253	L1254	L1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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 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, FAD, GOL, ACY, 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	2.46	516/9969 (5.2%)	2.19	457/13492 (3.4%)
1	B	2.51	514/10160 (5.1%)	2.20	474/13751 (3.4%)
1	C	2.45	479/10113 (4.7%)	2.19	466/13685 (3.4%)
1	D	2.41	487/10118 (4.8%)	2.15	443/13693 (3.2%)
All	All	2.46	1996/40360 (4.9%)	2.18	1840/54621 (3.4%)

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 1996 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	ALA	N-CA	24.39	1.77	1.46
1	B	431	ILE	CA-CB	23.30	1.81	1.54
1	B	1289	ASN	CA-C	19.41	1.62	1.52
1	A	1289	ASN	CA-C	17.58	1.63	1.52
1	C	355	ALA	CA-CB	-17.42	1.31	1.52

The worst 5 of 1840 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	SER	N-CA-C	18.64	134.38	110.33
1	A	216	LEU	N-CA-C	-16.47	90.15	110.41
1	C	194	SER	N-CA-C	16.14	132.30	110.35
1	A	194	SER	N-CA-C	15.94	131.31	110.43
1	B	753	VAL	N-CA-C	15.73	123.72	108.15

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

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	663	0
1	B	9951	0	9967	736	0
1	C	9905	0	9922	680	0
1	D	9910	0	9929	674	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	10	0
3	B	53	0	29	6	0
3	C	53	0	29	9	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	11	0
5	D	4	0	3	0	0
6	D	5	0	0	1	0
All	All	39807	0	39758	2697	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 34.

The worst 5 of 2697 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:CG	1:D:793:LYS:CD	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	11
1	B	1281/1333 (96%)	1021 (80%)	158 (12%)	102 (8%)	1	8
1	C	1273/1333 (96%)	1011 (79%)	168 (13%)	94 (7%)	1	9
1	D	1275/1333 (96%)	1006 (79%)	174 (14%)	95 (8%)	1	9
All	All	5084/5332 (95%)	4040 (80%)	668 (13%)	376 (7%)	1	9

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%)	781 (73%)	286 (27%)	0	3
1	B	1088/1126 (97%)	794 (73%)	294 (27%)	0	3
1	C	1082/1126 (96%)	787 (73%)	295 (27%)	0	3
1	D	1084/1126 (96%)	786 (72%)	298 (28%)	0	3
All	All	4321/4504 (96%)	3148 (73%)	1173 (27%)	0	3

5 of 1173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	290	VAL
1	D	1226	SER
1	D	403	ILE
1	D	289	SER
1	D	731	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	71	ASN
1	D	864	HIS
1	C	529	GLN
1	D	748	HIS
1	D	1044	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 ⓘ

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	B	3001	1	0,4,4	-	-	-		
3	FAD	B	3006	-	58,58,58	1.97	16 (27%)	85,89,89	2.67	32 (37%)
6	PO4	D	3009	-	4,4,4	1.13	0	6,6,6	1.92	1 (16%)
2	FES	A	3001	1	0,4,4	-	-	-		
4	GOL	B	3007	-	5,5,5	0.62	0	5,5,5	0.79	0
2	FES	B	3002	1	0,4,4	-	-	-		
2	FES	D	3001	1	0,4,4	-	-	-		
2	FES	C	3001	1	0,4,4	-	-	-		
3	FAD	A	3006	-	58,58,58	1.82	11 (18%)	85,89,89	2.19	37 (43%)
4	GOL	C	3007	-	5,5,5	0.55	0	5,5,5	0.54	0
2	FES	C	3002	1	0,4,4	-	-	-		
4	GOL	A	3007	-	5,5,5	0.61	0	5,5,5	0.99	0
2	FES	A	3002	1	0,4,4	-	-	-		
2	FES	D	3002	1	0,4,4	-	-	-		
3	FAD	D	3006	-	58,58,58	2.51	16 (27%)	85,89,89	2.74	38 (44%)
5	ACY	D	3008	-	3,3,3	1.20	0	3,3,3	1.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	3007	-	5,5,5	0.90	0	5,5,5	1.36	1 (20%)
3	FAD	C	3006	-	58,58,58	2.04	18 (31%)	85,89,89	2.71	41 (48%)

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	B	3001	1	-	-	0/1/1/1
3	FAD	B	3006	-	-	11/34/50/50	0/6/6/6
4	GOL	B	3007	-	-	2/4/4/4	-
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	B	3002	1	-	-	0/1/1/1
2	FES	D	3001	1	-	-	0/1/1/1
2	FES	C	3001	1	-	-	0/1/1/1
3	FAD	A	3006	-	-	9/34/50/50	0/6/6/6
4	GOL	C	3007	-	-	2/4/4/4	-
2	FES	C	3002	1	-	-	0/1/1/1
4	GOL	A	3007	-	-	2/4/4/4	-
2	FES	A	3002	1	-	-	0/1/1/1
2	FES	D	3002	1	-	-	0/1/1/1
3	FAD	D	3006	-	-	12/34/50/50	0/6/6/6
4	GOL	D	3007	-	-	0/4/4/4	-
3	FAD	C	3006	-	-	9/34/50/50	0/6/6/6

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3006	FAD	C2A-N3A	8.50	1.49	1.33
3	D	3006	FAD	C2A-N1A	7.39	1.47	1.33
3	D	3006	FAD	PA-O3P	7.35	1.67	1.59
3	D	3006	FAD	C5A-C4A	6.46	1.50	1.39
3	A	3006	FAD	C2A-N1A	5.68	1.44	1.33

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3006	FAD	C2B-C1B-N9A	8.97	135.59	113.30
3	B	3006	FAD	C5A-C4A-N3A	-7.65	116.18	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3006	FAD	C2B-C1B-N9A	7.57	132.11	113.30
3	B	3006	FAD	C6A-C5A-C4A	6.90	126.60	117.18
3	C	3006	FAD	C5A-C4A-N3A	-6.75	117.42	126.72

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

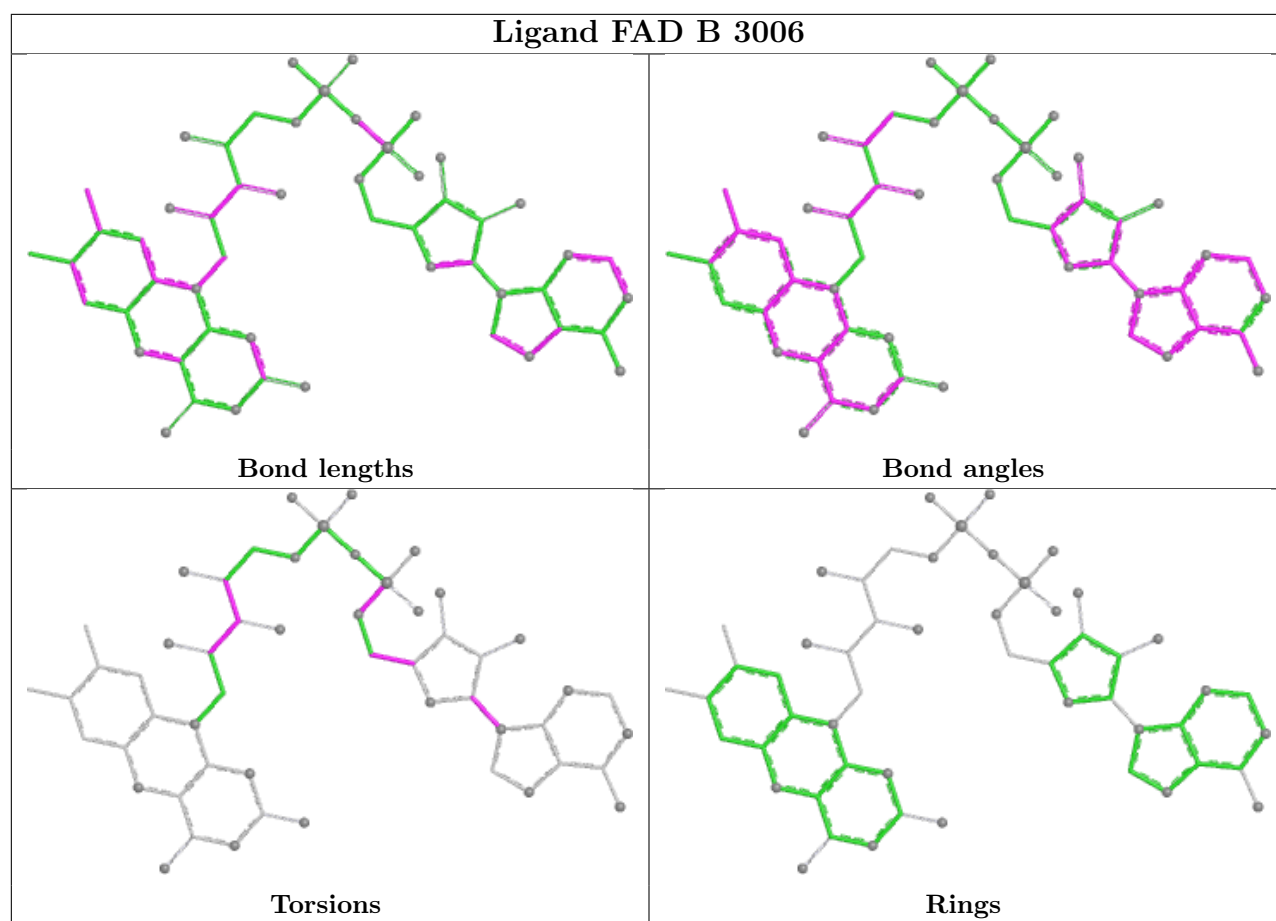
Mol	Chain	Res	Type	Atoms
3	B	3006	FAD	C5B-O5B-PA-O1A
3	B	3006	FAD	C5B-O5B-PA-O2A
3	B	3006	FAD	C5B-O5B-PA-O3P
3	B	3006	FAD	O4B-C1B-N9A-C4A
3	B	3006	FAD	C2'-C3'-C4'-O4'

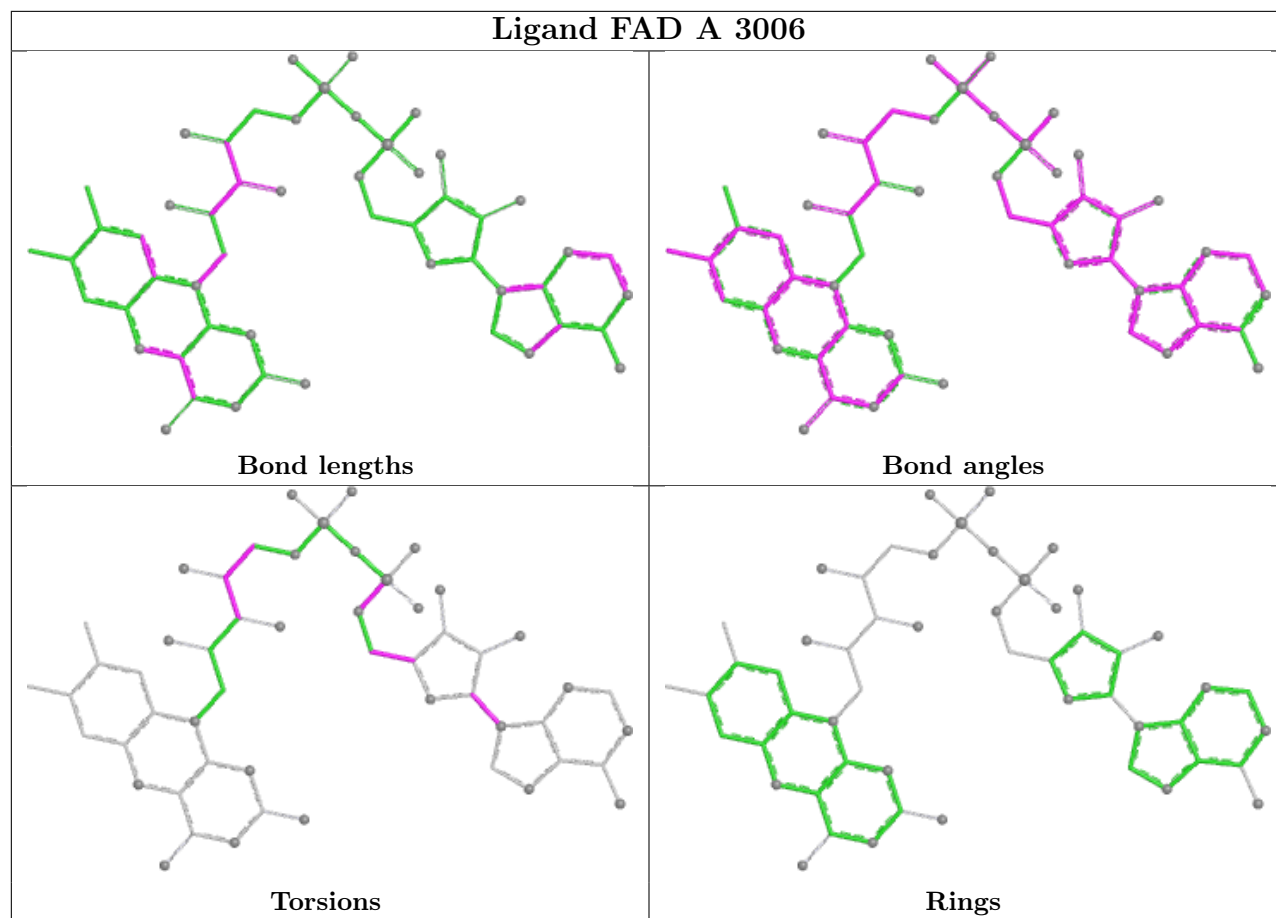
There are no ring outliers.

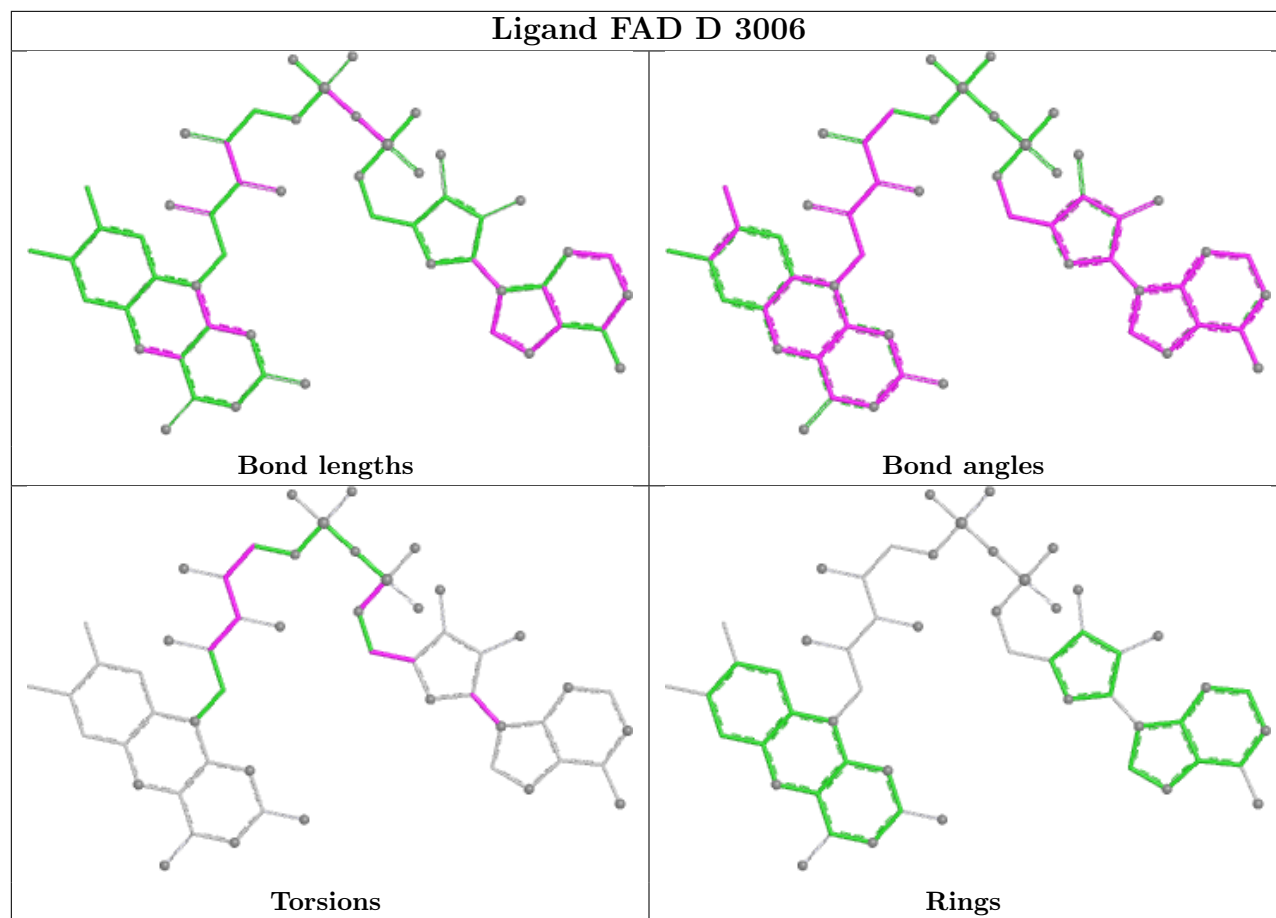
11 monomers are involved in 79 short contacts:

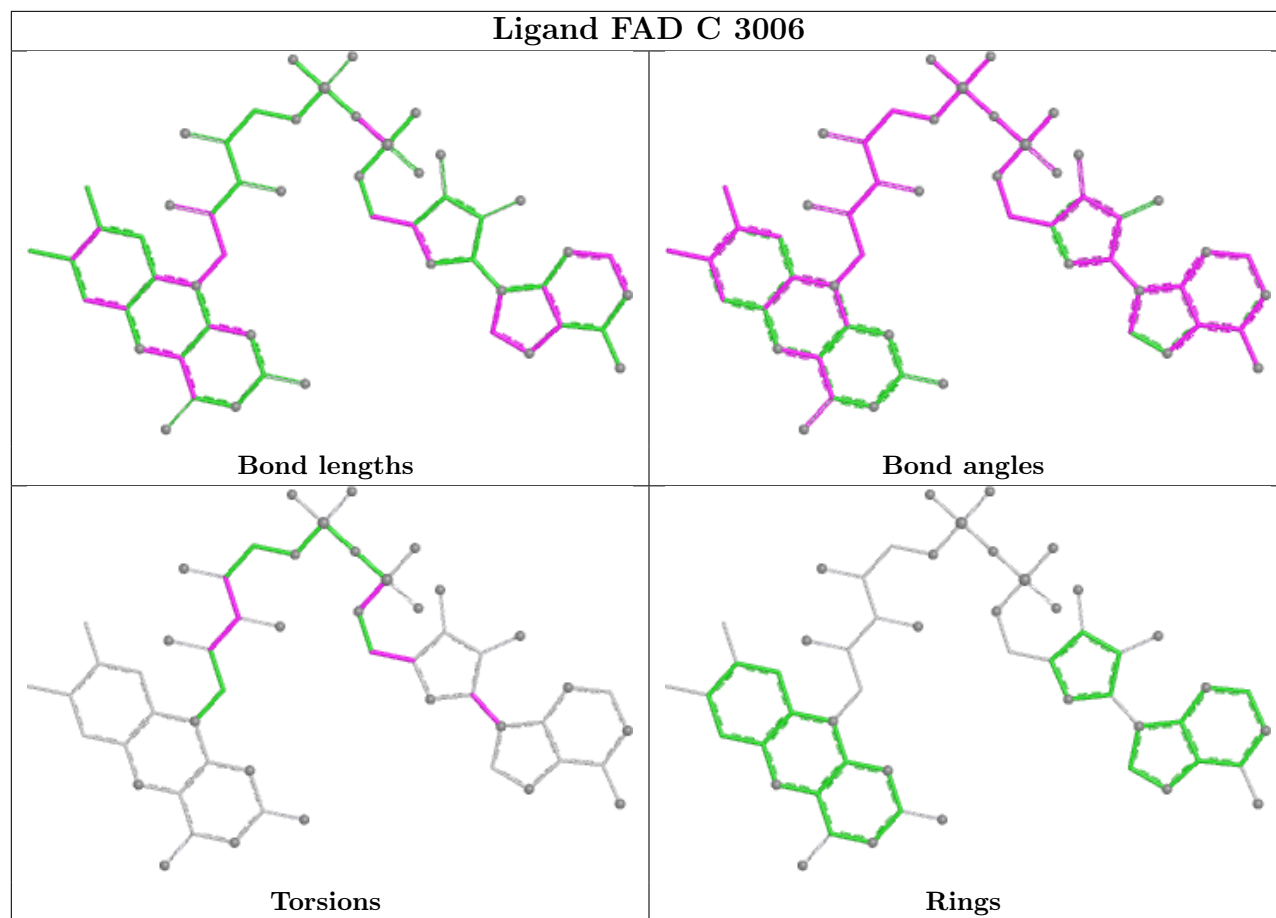
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3006	FAD	6	0
6	D	3009	PO4	1	0
4	B	3007	GOL	14	0
2	B	3002	FES	2	0
3	A	3006	FAD	10	0
4	C	3007	GOL	4	0
4	A	3007	GOL	6	0
2	A	3002	FES	2	0
3	D	3006	FAD	14	0
4	D	3007	GOL	11	0
3	C	3006	FAD	9	0

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 [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.