



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2026 – 02:02 pm BST

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 : 1.8.4, CSD as541be (2020)
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) : 2.50

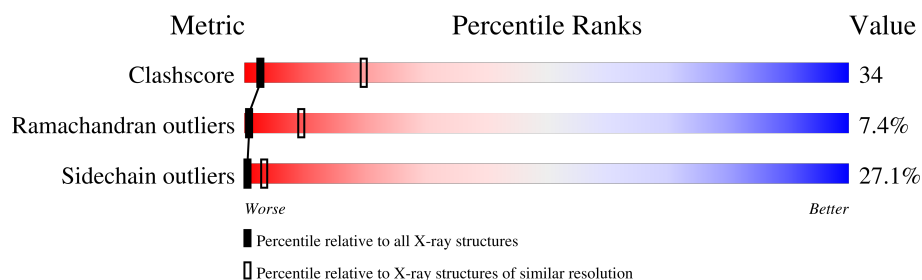
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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](#)

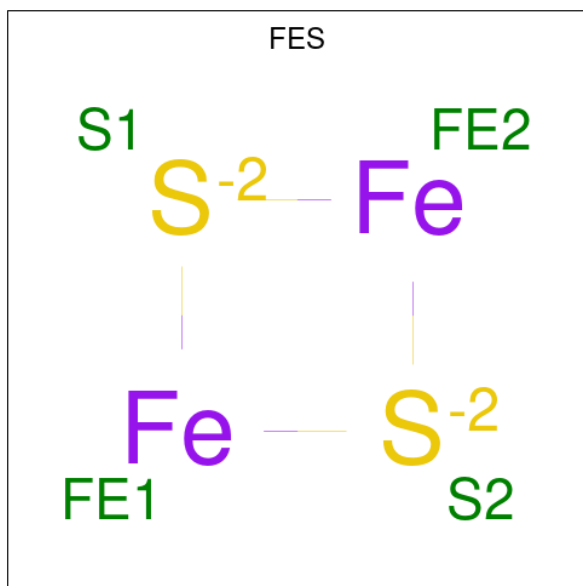
There are 6 unique types of molecules in this entry. The entry contains 39807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).



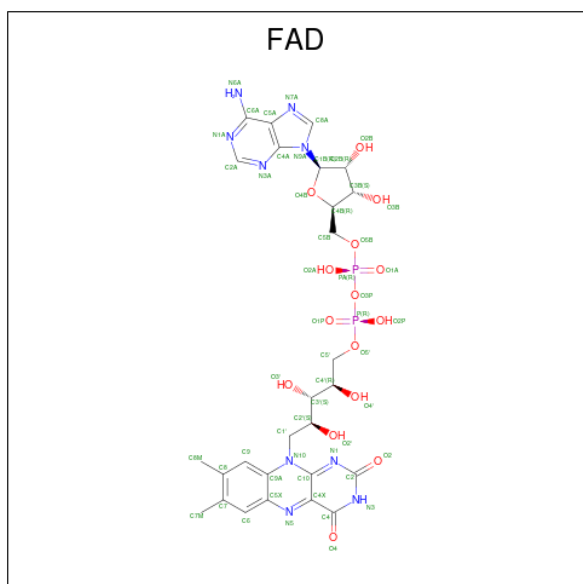
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		

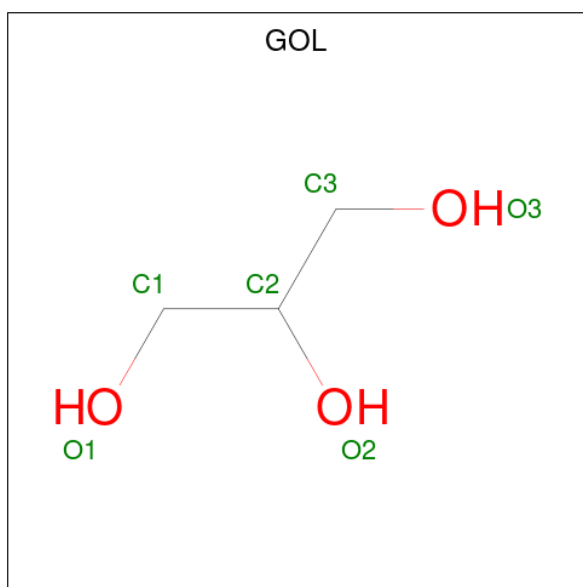
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		
2	D	1	Total	Fe	S	0	0
			4	2	2		
2	D	1	Total	Fe	S	0	0
			4	2	2		

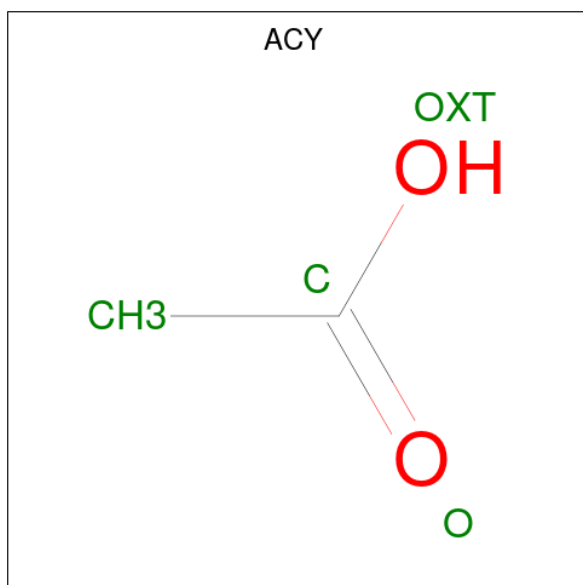
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).





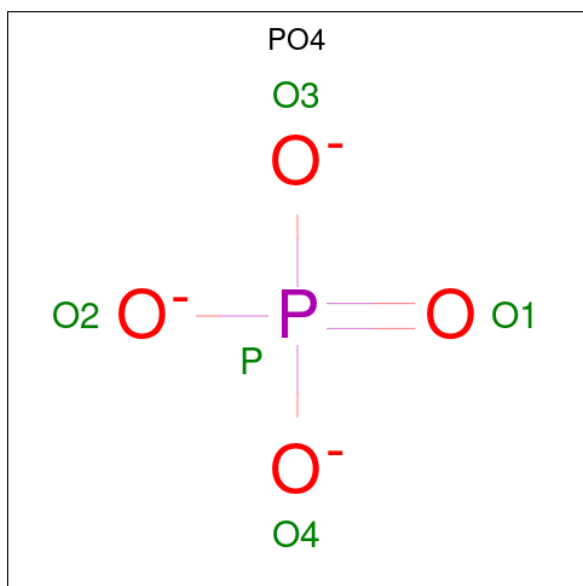
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- 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).



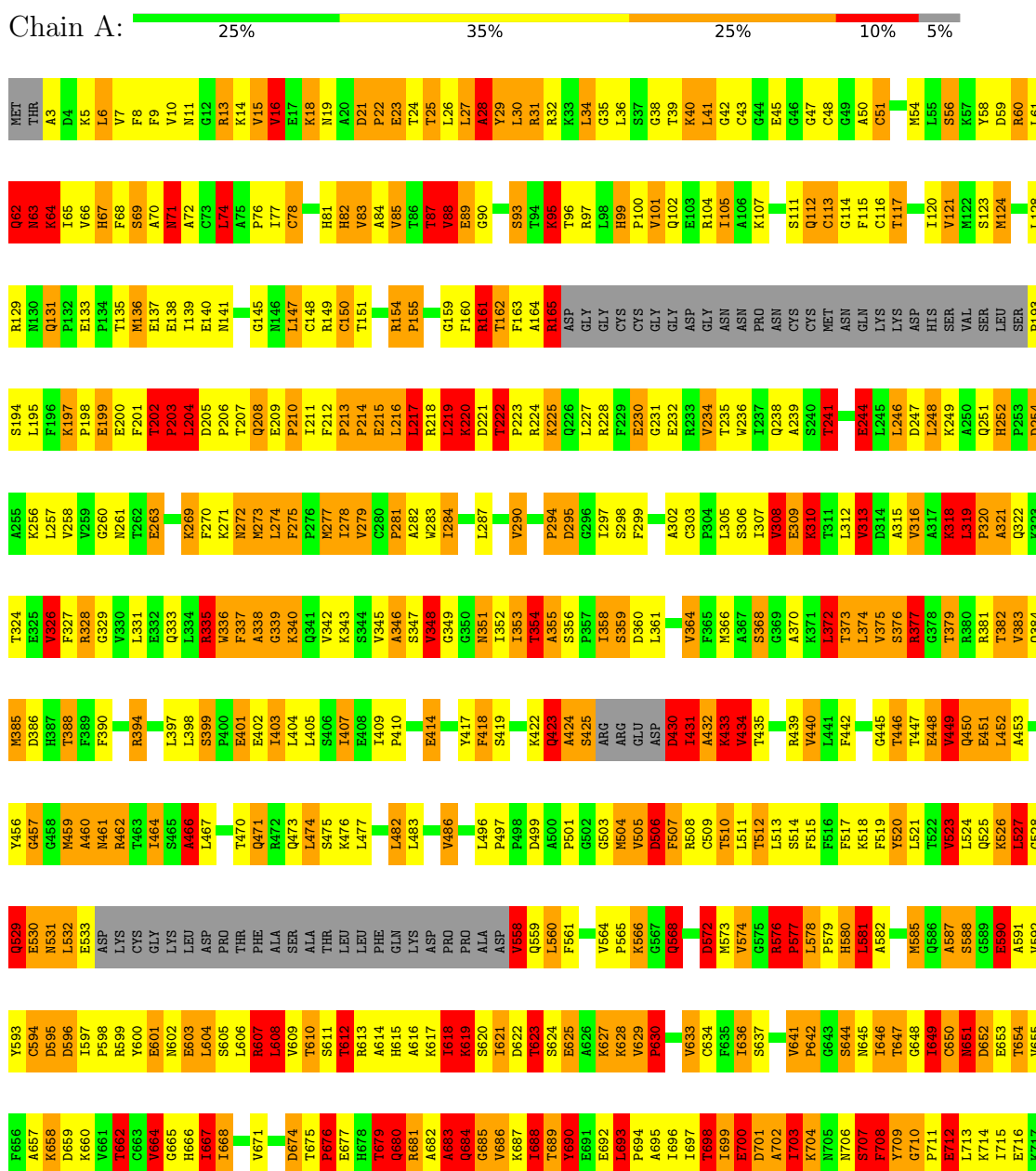
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			5	4	1		

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



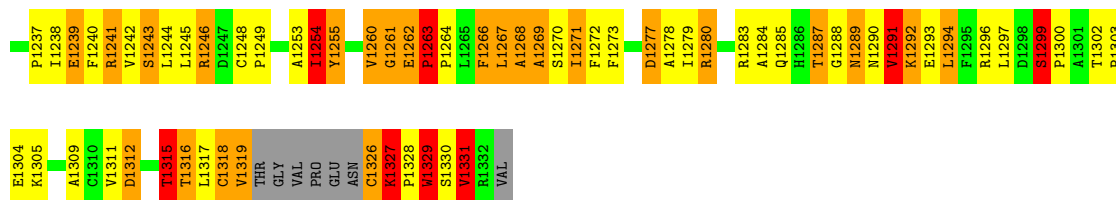
A1301	C1167	L1102	Q1041	G977	A911	P842	L781	G718
T1302	T1168	E1103	H1044	Y978	F912	F843	L781	D719
P1303	T1169	P1104	H1044	H979	F913	F843	L781	D719
E1304	E1239	Y1105	T1045	A980	G914	Y847	L781	K721
K1305	F1240	K1106	K1046	R981	F915	K848	N786	K722
I1306	R1241	K1107	R1047	K982	G916	V849	R787	G723
V1311	K1173	K1108	V1048	S983	G917	G850	L788	
D1312	N1174	N1109	Q1049	E984	P918	F851	L788	D728
	L1175		V1050	V985	Q919	G917	L788	N729
T1315	R1176	S1113	A1051	D986	G920	T854	L788	V730
T1316	T1177	V1114	S1052	K987	M921		L788	V731
L1317	D1178	E1115	R1053		L922	V857	L788	S732
C1318	L1179	D1116	A1054	E991	L923	V858	L788	G733
V1319	V1180	W1117	A1054	N992	A924	A859	L788	E734
T1320	M1181	V1118	K1056	C993	E925	L860	G796	E735
GLY	D1182	T1119	I1057	W994	C926	E861	G797	V736
VAL	V1183	A1120	P1058	K985	A927	V862	G798	L737
PRO		A1121	T1059	K996	M928	D863	F799	G738
ASN	L1187	Y1122	S1060	R997	S929	H864	G800	G739
CYS	M1188	M1123	K1061		E930	F865	G801	Q740
LYS	P1189	D1124	I1062	C1000	E931	S866	K802	E741
PRO	A1190	T1125	Y1063	T1001	A932	N867	E803	H742
SER	E1259	V1126	I1064	T1002	V933	V868	L815	L743
VAL	V1260	S1127	S1065	P1003	T834	G869	R805	L744
ARG	E1262	L1128	E1066	T1004	C935	N870	S806	L745
VAL	P1263	S1129	T1067	K1005	G936	T871	S806	E746
ARG	P1264	A1130	S1068	T1008	M937	D873	V808	T747
		T1131	T1069	S1009	P938	L874	V809	H748
A1268		G1132	N1070	I1010			S810	C749
A1269	F1200	F1133	T1071	F1010	E941		T811	T750
S1270	Y1134	Y1134	V1072	T1011	V942	I878	A812	T751
I1271	R1135	P1073	P1073	V1012	R942	M879	V813	A752
	L1204	T1136	N1074	P1013	R944	E880	A814	L753
A1274	G1205	P1137	T1075	F1014	K945	R881	L815	P754
I1275	L1206	M1138	S1076	L1015	N946	A882	L816	L755
K1276		L1139	P1077	N1016	L947	L883	A817	K755
D1277	L1209	G1140	T1078	Q1017	Y948	F884	E757	G756
A1278	E1210	Y1141	A1079	A1018	K949	L885	E757	E758
I1279	E1211	S1142	A1080	G1019	E950		T820	A758
R1280	L1212	F1143	S1081	G1019	G951		G821	G759
A1281	H1213	E1144	V1082	L1021	D952	N888	G821	E760
A1282		T1145	S1083	L1022	L953	C889	R822	M761
R1283	G1218	N1146	A1084	H1023	L953	X930	P823	E762
S1219	S1219	P1153	D1085	V1024	P954	R891	P823	L763
Q1285	L1220	F1154	L1086	V1025	H955	I892	V824	L763
L1286	H1221	N1149	N1087	T1026	F956	P893	R825	F764
T1287	P1222	F1151	N1087	T1026	F956	P893	C826	V765
G1288	R1223	H1152	G1088	D1027	K959	N894	M827	S766
N1289	G1224	Y1153	Q1089	G1028	K959	I895	L828	T767
V1290	P1225	F1154	A1090	S1029	G962		D829	Q768
L1291	S1226	F1154	Y1091	V1030	F963		R830	N769
K1292	T1227	G1157	Y1092	L1031	P963		D831	T770
E1293	L1228	V1158	A1093	T1033	P966		E832	M771
L1294	K1229	A1159	C1095	H1034	R967		D833	L772
F1295	I1230	C1160	Q1096	G1035	C902		L901	K773
R1296	P1231	S1161	T1097	G1036	X903		L835	Q774
L1297	A1232	E1164	I1098	T1037	T904		L835	Q774
D1298	F1233	I1164	L1099	E1038	E970		S775	F776
S1299	G1234	T1165	K1100	T1037	E971		T837	V777
	S1235	D1166	K1101	A1039	A974		G838	A778
							G339	N779
							N909	K779
							H841	

● Molecule 1: XANTHINE OXIDOREDUCTASE

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

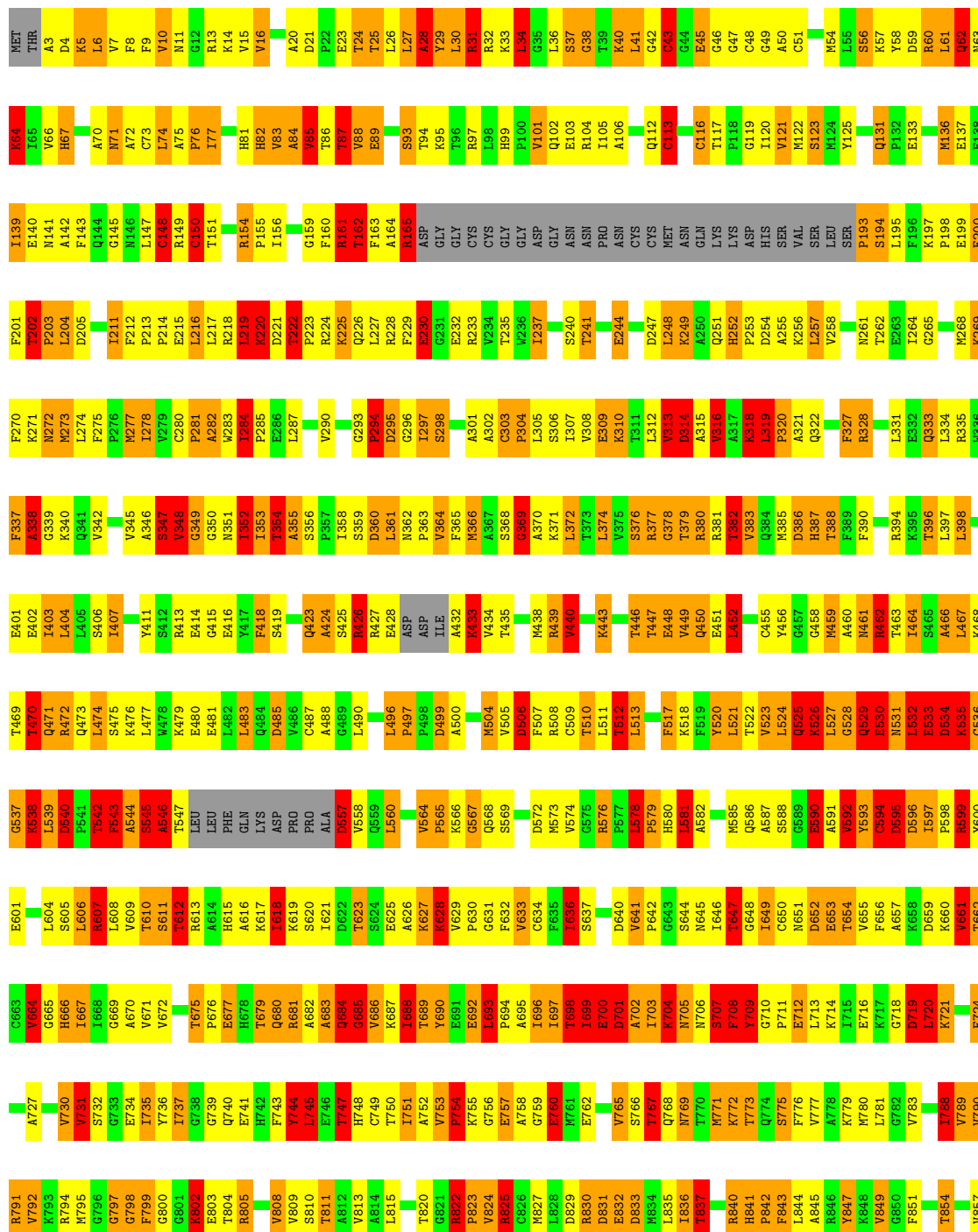
SER	P193	S194	L195	F196	K197	P198	E199	E200	F201	T202	P203	L204	D205	E209	P210	L211	L212	F212	C213	P213	P214	E215	L216	L217	R218	L219	K220	D221	T222	P223	K224	K225	Q226	L227	R228	F229	E230	G231	E232	R233	R234	T235	W236	A239	S240	T241	E244	L245	L246	D247	L248	K249	A250	Q251	H252	P253	D254	A255
	Q131	P132	E133	P134	T135	M136	E137	E138	L139	N140	A141	A142	F143	Q144	G145	N146	L147	C148	R149	C150	T151	G152	Y153	R154	P155	Q158	G159	F160	P161	T162	F163	A164	R165	ASP	GLY	GLY	CYS	CYS	GLY	ASP	GLY	ASN	ASN	PRD	ASN	CYS	MET	ASN	GLN	LYS	LYS	ASP	HIS	SER	VAL	L128	R129	N130
MET	T2	A3	D4	K5	L6	V7	F8	N7	V10	N11	G12	R13	K14	V15	V16	E17	K18	N19	A20	D21	P22	E23	T24	T25	L26	L27	A28	Y29	L30	R31	K32	K33	L34	G35	L36	S37	G38	T39	K40	L41	G42	C43	G44	E45	G46	A50	C51	V53	M54	L55	S56	K57	Y58	D59	R60	L61	Q62	

H1172	K1107	G1041	Q977	R813	G850	A785	R719	V655	A591	Q529	C455	F389	K323	K256
K1173	G1112	G1042	T978	G914	F851	M786	L720	F656	V592	E530	Y456	F390	V326	L257
L1175	L1043	L1044	H979	F915	R852	M787	K721	A657	Y593	N531	M459	F391	L532	T262
R1176	T1045	H1045	A980	G916	R853	T788	K722	K658	C594	L532	A460	G392	R328	E263
T1177	K1046	K1046	R981	G917	T854	T789	F723	D659	D595	E533	N461	R394	D596	I264
D1178	D1107	M1047	S983	Q919	T856	R791	F724	V661	F597	K535	R462	K395	L331	M268
I1179	V1048	V1048	E984	G920	V857	V792	V730	T662	F598	C836	T463	T396	E332	K269
L1180	Q1049	V985	V985	N921	R858	K793	V731	G663	R599	G537	L464	L398	L334	F270
V1183	V1050	R794	D986	L922	A859	M795	G733	V664	Y600	K538	A465	L399	L334	K271
T1118	A1051	L860	R794	R937	L860	M795	G733	G665	E601	L539	A466	G399	L334	M272
A1120	S1052	A924	F988	E918	E861	G796	E734	H666	N602	D540	L467	P400	F337	L274
S1185	R1053	E925	R989	E925	V862	G797	L735	L667	E603	P541	K468	E401	A338	M273
A1054	A1054	C926	G798	C926	D863	G798	V736	M671	L604	T842	T469	E401	G339	L274
L1155	A1055	A927	F799	A927	H864	F799	I737	V672	S605	F543	T470	L404	K340	F275
K1056	K1056	N928	G800	N928	F865	G800	G738	V672	L606	A544	Q471	L405	K340	F276
P1058	T1057	S929	C801	S929	S866	C801	G739	A673	R607	S845	Q472	S406	V342	M277
T1059	E930	E930	K802	E930	N867	D674	Q740	A673	L608	A546	Q473	I407	K343	L278
S1060	V931	V868	E741	V931	V868	T675	E741	P676	V609	T547	L474	E408	S344	V279
G997	A932	H871	H742	A932	H871	T604	H742	P676	T610	LEU	S475	I409	V345	C280
G998	V933	Q872	F743	V933	Q872	R805	F743	P676	S611	PHE	K476	P410	A346	P281
L999	G936	D873	L744	G936	D873	S806	L744	Q680	T612	GLN	L482	Y411	S347	A282
C1000	R937	L874	T745	R937	L874	R681	T745	Q680	H615	LYS	L483	S412	V348	W283
I1001	P938	S875	T747	P938	S875	A682	T747	A682	A616	ASP	Q484	E414	N351	I284
I1002	A939	Q876	H748	A939	Q876	A683	H748	A683	K617	PRO	D485	I352	I352	E286
P1003	E940	S877	C749	E940	S877	Q684	C749	Q684	L618	PRO	V486	I353	I353	L287
T1004	E941	T878	T750	E941	T878	G685	T750	G685	K619	ALA	C487	A420	A355	S289
S1009	R944	E881	A752	R944	E881	K687	A752	K687	D622	V583	F421	F421	A355	V290
F1010	K945	A882	V753	K945	A882	L688	V753	L688	T623	D557	K422	K422	I358	P284
T1011	R946	L883	R754	R946	L883	T689	R754	T689	S624	L560	Q423	Q423	S359	D284
F1014	L947	F884	G756	L947	F884	Y690	G756	Y690	E625	F561	L496	Q423	D360	D295
L1015	G949	N886	E757	G949	N886	E691	E757	E691	K626	Q562	P497	S425	L361	G296
Q1017	E951	N888	G759	E951	N888	L693	G759	L693	V629	E563	P498	R426	I297	I297
G1019	D952	C889	G759	D952	C889	P694	G759	P694	V630	V564	D499	E428	F365	S298
A1020	L953	Y890	E760	L953	Y890	A695	E760	A695	P630	K566	A500	D429	M366	P289
L1021	F956	R892	R761	F956	R892	L696	R761	L696	V633	G567	V505	D430	A367	G300
L1022	G951	N888	E762	G951	N888	T697	E762	T697	Q568	Q568	I431	I431	A301	A301
H1023	R959	N888	R766	R959	N888	T697	R766	T697	C634	S569	A432	G369	S368	A302
V1024	L960	T898	Q768	L960	T898	T698	Q768	T698	F635	C509	K433	A370	C303	C303
Y1025	G961	G899	N769	G961	G899	D833	N769	D833	E570	F635	C509	V434	A370	P304
T1026	G962	R900	T770	G962	R900	E700	T770	E700	D701	E571	T510	L372	K371	L305
D1027	F963	L901	M834	F963	L901	D701	M834	D701	S637	D572	T435	T373	L372	S306
G1028	P966	C902	L835	P966	C902	A702	L835	A702	A638	M573	T511	T373	L372	S306
S1028	A967	K903	T836	S1028	A967	T703	T836	T703	D639	V574	T511	T373	L372	S306
V1030	G968	N905	T837	V1030	G968	T709	T837	T709	Y641	F515	T511	T373	L372	S306
L1031	E968	T904	R837	L1031	E968	G710	R837	G710	P642	F516	T511	T373	L372	S306
T1032	Q969	N905	R840	T1032	Q969	P711	R840	P711	L578	F516	T511	T373	L372	S306
T1033	E970	L906	R840	T1033	E970	E712	R840	E712	P642	F516	T511	T373	L372	S306
H1034	E971	P907	H841	H1034	E971	L713	H841	L713	G643	P579	T511	T373	L372	S306
G1035	C972	S908	P842	G1035	C972	K714	P842	K714	L578	F516	T511	T373	L372	S306
E1038	L973	N909	P842	E1038	L973	I715	P842	I715	G643	P579	T511	T373	L372	S306
P1039	A974	T910	R847	P1039	A974	E716	R847	E716	L578	F516	T511	T373	L372	S306
M1039	S975	A911	K848	M1039	S975	K717	K848	K717	G643	P579	T511	T373	L372	S306
G1040	S976	F912	V849	G1040	S976	G718	V849	G718	L578	F516	T511	T373	L372	S306
K1172	K1107	G1041	Q977	R813	G850	A785	R719	V655	A591	Q529	C455	F389	K323	K256
K1173	G1112	G1042	T978	G914	F851	M786	L720	F656	V592	E530	Y456	F390	V326	L257
L1175	L1043	L1044	H979	F915	R852	M787	K721	A657	Y593	N531	M459	F391	L532	T262
R1176	T1045	H1045	A980	G916	R853	T788	K722	K658	C594	L532	A460	G392	R328	E263
T1177	K1046	K1046	R981	G917	T854	T789	F723	D659	D595	E533	N461	R394	D596	I264
D1178	D1107	M1047	S983	Q919	T856	R791	F724	V661	F597	K535	R462	K395	L331	M268
I1179	V1048	V1048	E984	G920	V857	V792	V730	T662	F598	C836	T463	T396	E332	K269
L1180	Q1049	V985	V985	N921	R858	K793	V731	G663	R599	G537	L464	L398	L334	F270
V1183	V1050	R794	D986	L922	A859	M795	G733	V664	Y600	K538	A465	L399	L334	K271
T1118	A1051	L860	R794	R937	L860	M795	G733	G665	E601	L539	A466	G399	L334	M272
A1120	S1052	A924	F988	E918	E861	G796	E734	H666	N602	D540	L467	P400	F337	L274
S1185	R1053	E925	R989	E925	V862	G797	L735	L667	E603	P541	K468	E401	A338	M273
A1054	A1054	C926	G798	C926	D863	G798	V736	M671	L604	T842	T469	E401	G339	L274
L1155	A1055	A927	F799	A927	H864	F799	I737	V672	S605	F543	T470	L404	K340	F275
K1056	K1056	N928	G800	N928	F865	G800	G738	V672	L606	A544	Q471	L405	K340	F276
P1058	T1057	S929	C801	S929	S866	C801	G739	A673	R607	S845	Q472	S406	V342	M277
T1059	E930	E930	K802	E930	N867	D674	Q740	A673	L608	A546	Q473	I407	K343	L278
S1060	V931	V868	E741	V931	V868	T675	E741	P676	V609	T547	L474	E408	S344	V279
G997	A932	H871	H742	A932	H871	T604	H742	P676	T610	LEU	S475	I409	V345	C280
G998	V933	Q872	F743	V933	Q872	R805	F743	P676	S611	PHE	K476	P410	A346	P281
L999	G936	D873	L744	G936	D873	S806	L744	Q680	T612	GLN	L482	Y411	S347	A282
C1000	R937	L874	T745	R937	L874	R681	T745	Q680	H615	LYS	L483	S412	V348	W283
I1001	P938	S875	T747	P938	S875	A682	T747	A682	A616	ASP	Q484	E414	N351	I284
I1002	A939	Q876	H748	A939	Q876	A683	H748	A683	K617	PRO	D485	I352	I352	E286
P1003	E940	S877	C749	E940	S877	Q684	C749	Q684	L618	PRO	V486	I353	I353	L287
T1004	E941	T878	T750	E941	T878	G685	T750	G685	K619	ALA	C487	A420	A355	S289
S1009	R944	E881	A752	R944	E881	K687	A752	K687	D622	V583	F421	F421	A355	V290
F1010	K945	A882	V753	K945	A882	L688	V753	L688	T623	D557	K422	K422	I358	P284
T1011	R946	L883	R754	R946	L883	T689	R754	T689	S624	L560	Q423	Q423	S359	D284
F1014	L947	F884	G756	L947	F884	Y690	G756	Y690	E625	F561	L496	Q423	D360	D295
L1015	G949	N886	E757	G949	N886	E691	E757	E691	K626	Q562	P497	S425	L361	G296
Q1017	E951	N888	G759	E951	N888	L693	G759	L693	V629	E563	P498	R426	I297	I297
G1019	D952	C889	G759	D952	C889	P694	G759	P694	V630	V564	D499	E428	F365	S298
A1020	L953	Y890	E760	L953	Y890	A695	E760	A695	P630	K566	A500	D429	M366	P289
L1021	F956	R892	R761	F956	R892	L696	R761	L696	V633	G567	V505	D430	A367	G300
L1022	G951	N888	E762	G951	N888	T697	E762	T697	Q568	Q568	I431	I431	A301	A301
H1023	R959	N888	R766	R959	N888	T697	R766	T697	C634	S569	A432	G369	S368	A302
V1024	L960	T898	Q768	L960	T898	T698	Q768	T698	F635	C509	K433	A370	C303	C303
Y1025	G961	G899	N769	G961	G899	D833	N769	D833	E570	F635	C509	V434	A370	P304
T1026	G962	R900	T770	G962	R900	E700	T770	E700	D701	E571	T510	L372	K371	L305
D1027	F963	L901	M834	F963	L901	D701	M834	D701	S637	D572	T435	T373	L372	S306
G1028	P966	C902	L835	P966	C902	A702	L835	A702	A638	M573	T511	T373	L372	S306
S1028	A967	K903	T836	S1028	A967	T703	T836	T703	D639	V574	T511	T373	L372	S306
V1030	G968	N905	T837	V1030	G968	T709	T837	T709	Y641	F515	T511	T373	L372	S306
L1031	E968	T904												



• Molecule 1: XANTHINE OXIDOREDUCTASE

Chain C: 26% 36% 24% 11%



L1297	F1233	I1165	K1100	M1039	E971	S908	R840	S775	E712	G589	K526	Y456	F390
D1296	G1234	D1166	R1101	Q1040	C972	T909	H841	F776	L713	E590	L527		P391
S1299	S1235	C1167	L1102	Q1041	L973	A911	P842	W777	K714	E653	G528	M459	
P1300	L1236	E1103	E1103	G1042	A974	F912	R846	A778	L715	V592	Q529	A460	R394
A1301	P1237	G1170	P1104	L1043	S975	A911	R846	R779	E716	V593	Q530	N461	K395
T1302	L1238	D1171	Y1105	H1044	S976	R913	Y847	W780	T717	C594	N531	R462	T396
E1239	P1303	H1172	K1106	T1045	Q977	G914	K846		G718	D595	L532	T463	L398
F1240	F1240	K1173	K1107	V1048	Y978	F915	W849	V783	D719	D596	E533	L464	
R1241	M1174	K1108	L1108	Q1049	A990	G916	P784		L720	D659	D540	S465	
V1242	L1175	A1109	A990	G917	G917	S918	T854		K721	R660	Q471	S406	L405
S1243	R1176	P1110	P1110	V1050	R981	P918		V768	G722	R599	Q536	L467	E402
L1244	T1177	S1111	L1101	A1051	K982	Q919	W857	I768	G723	V769	G537	K468	I403
L1245	D1178	G1112	G1112	S1082	S983	G320	W858	V790	F724	E601		T469	L404
R1246		S1113	S1113	R1053	E984	M921		R791					L405
D1247		M1181	W1114	A1054	V985	L922	L860	V792		L604	L604		S406
N1250		D1182	D1182	L1055	D986	I923	E861	R793		S605	P541		Q471
K1251		V1183	D1116	K1056	K987	A924	V662	R794		L606	THR		I407
		G1184	V1117	I1057	F983	E925	D863	V795		R607	PHE		E408
		S1185	V1118	T1058	N989	C926	H664	G796		L608			
		S1186	T1119	T1059	K990	W927	F865	G797		V609	ALA		Y411
		L1187	A1120	S1080	E991	M928	S866	G798		T610	SER		S412
		N1188	A1121	K1061		S929	N867			W672	ALA		R413
		P1189	Y1122	Y1062	R997	E930	V668	G801		T612	LEU		E414
		A1190	M1123	Y1063		V931	G869	X802		T675	LEU		F418
		I1191	D1124	I1064	I1001	A932	R870	E803		P676	PHE		S419
		L1192	T1125	S1065	T1002	V933	T871	T804		E677	GLN		A420
		T1193	Y1126	E1066	P1003		L872	R805		H678	LYS		A420
		E1194	S1127	T1067	T1004	G936	D873	S806		T679	ASP		F421
		K1195	L1128	S1068	K937	L874	T807	H742		Q680	PRO		Q422
		Q1196	S1129	T1069	K1005	P938	S875	V808		R681	PRO		Q423
		E1197	L1265	L1060		A939		V809		S620	ALA		A424
		G1198	T1131	T1071	I1008	R940	T878	S810		A683			S425
		A1199	F1132	P1072	S1009	E940	N879	T811		L976	L496		R426
			F1133	T1073	F1010	E941	E880	A812		D622	V558		R427
			Y1134	N1074	T1011	V942	R881	V813		Q685	Q559		E428
			R1135	T1075	P1013	R943	A882	A814		S624	D499		D429
			T1136	S1076	F1014	R944	L883	L815		E625	F561		D430
			P1137	P1077	L1015	N946	F884	A816		K627			I431
			M1138	T1078	N1016	L947	H885	A817		V690	V564	M504	A432
			L1139	A1079	Q1017	Y948	N886	Y818		E691	K566	V505	K433
			G1140	A1080	A1018	K949	D887	X819		P690	G567	T434	T435
			Y1141	S1081	G1019	E950	N888	T820		G631	Q568	F507	
			S1142	T1082	A1020	G951	C889	G821		F632	S569	R508	M438
			F1143	S1083	L1021	D952	X890	R822		V633	E570	C509	R439
			E1144	A1084	L1022	L953	K891	A823		C634	E571	T510	V440
			T1145	D1085	H1023	T954	L892	W824		P696	L697	L511	F440
			N1146	L1086	Y1024	H955	P893	R825		T698	D572	L441	F442
				N1087	Y1025	F956	N894	C826		L699	R576	L513	K443
				G1088	T1026	N957		R827		E700	P577	S514	P444
				Q1089	D1027	Q958	C897	L828		D640	L578	F515	G445
				A1090		K959	T898	D829		W701	P579	F516	T446
				Y1091	V1030	E961	R830	C899		A702	H580	F517	T447
				L1092	L1031	N961	R900	D831		T703	L581	K618	E448
				A1093	L1032	G962	L901	E832		G643	A582	F519	V449
				C1095	T1033	F963	C902	D833		N705	E533	Y520	
				Q1096	H1034	T964	K903	R834		T706	D584	Q450	E451
				T1097	G1035	L965	T904	L835		S707	L521	T522	L452
				L1098	L1036	P966	N905	T836		F708	G648	V523	A453
				L1099	T1037	E963	L906	T837		T773	L454	L524	
				L1099	E1038	F967				D650	P588	C656	
										T711			

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: FES, PO4, GOL, ACY, FAD

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	$\# Z > 2$
4	GOL	A	3007	-	5,5,5	0.59	0	5,5,5	0.95	0
2	FES	B	3002	1	0,4,4	-	-	-		
2	FES	D	3002	1	0,4,4	-	-	-		
4	GOL	D	3007	-	5,5,5	0.85	0	5,5,5	1.30	1 (20%)
2	FES	D	3001	1	0,4,4	-	-	-		
2	FES	A	3002	1	0,4,4	-	-	-		
2	FES	C	3002	1	0,4,4	-	-	-		
3	FAD	C	3006	-	56,58,58	2.01	17 (30%)	81,89,89	2.78	39 (48%)
3	FAD	D	3006	-	56,58,58	2.27	14 (25%)	81,89,89	2.86	39 (48%)
5	ACY	D	3008	-	3,3,3	1.13	0	3,3,3	1.52	0
6	PO4	D	3009	-	4,4,4	1.07	0	6,6,6	1.86	1 (16%)
2	FES	A	3001	1	0,4,4	-	-	-		
3	FAD	A	3006	-	56,58,58	1.79	11 (19%)	81,89,89	2.13	33 (40%)
4	GOL	B	3007	-	5,5,5	0.61	0	5,5,5	0.75	0
4	GOL	C	3007	-	5,5,5	0.52	0	5,5,5	0.53	0
2	FES	B	3001	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	B	3006	-	56,58,58	1.93	14 (25%)	81,89,89	2.78	36 (44%)
2	FES	C	3001	1	0,4,4	-	-	-		

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	GOL	A	3007	-	-	2/4/4/4	-
2	FES	B	3002	1	-	-	0/1/1/1
2	FES	D	3002	1	-	-	0/1/1/1
4	GOL	D	3007	-	-	0/4/4/4	-
2	FES	D	3001	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
3	FAD	C	3006	-	-	9/34/50/50	0/6/6/6
3	FAD	D	3006	-	-	11/34/50/50	0/6/6/6
2	FES	C	3002	1	-	-	0/1/1/1
4	GOL	B	3007	-	-	2/4/4/4	-
3	FAD	A	3006	-	-	8/34/50/50	0/6/6/6
4	GOL	C	3007	-	-	2/4/4/4	-
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	B	3001	1	-	-	0/1/1/1
3	FAD	B	3006	-	-	10/34/50/50	0/6/6/6
2	FES	C	3001	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	8.12	1.49	1.33
3	D	3006	FAD	C2A-N1A	7.07	1.47	1.33
3	D	3006	FAD	C5A-C4A	6.22	1.50	1.39
3	A	3006	FAD	C2A-N1A	5.43	1.44	1.33
3	C	3006	FAD	C2A-N1A	5.23	1.43	1.33

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3006	FAD	C2B-C1B-N9A	8.80	135.59	113.30
3	B	3006	FAD	C5A-C4A-N3A	-8.10	116.18	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3006	FAD	C2B-C1B-N9A	7.43	132.11	113.30
3	C	3006	FAD	C5A-C4A-N3A	-7.15	117.42	126.75
3	B	3006	FAD	C6A-C5A-C4A	7.01	126.60	117.18

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

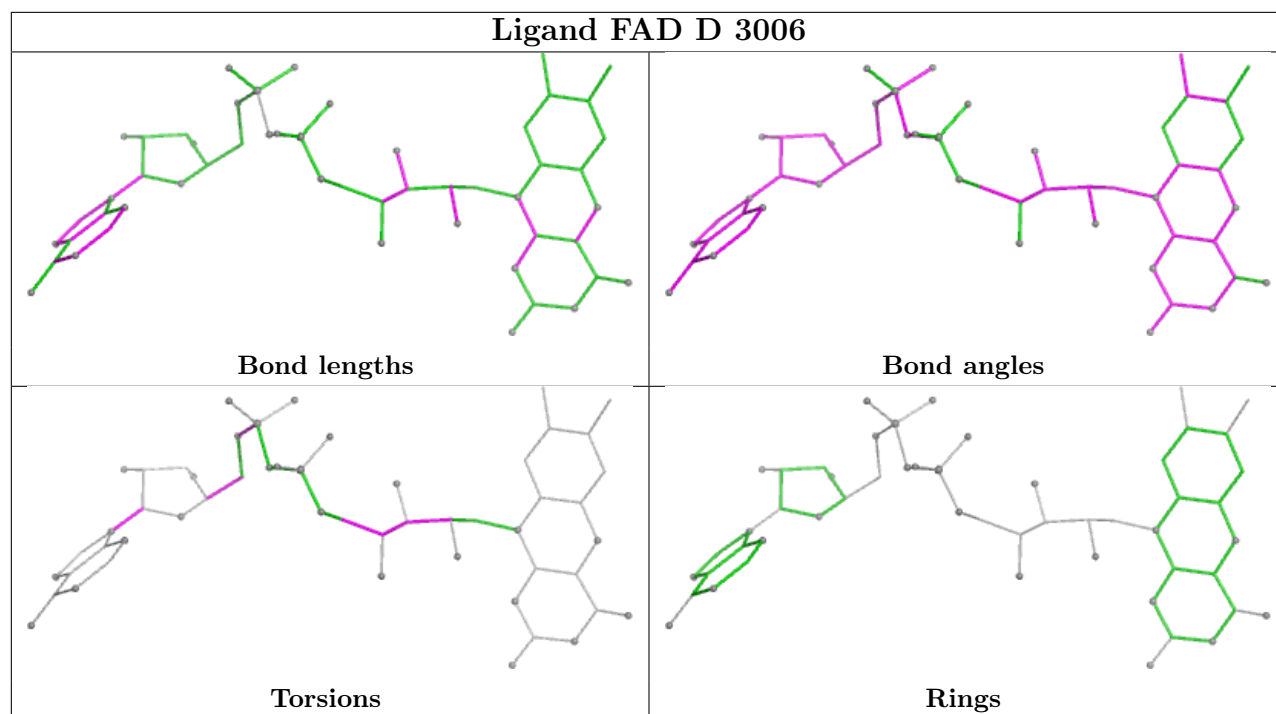
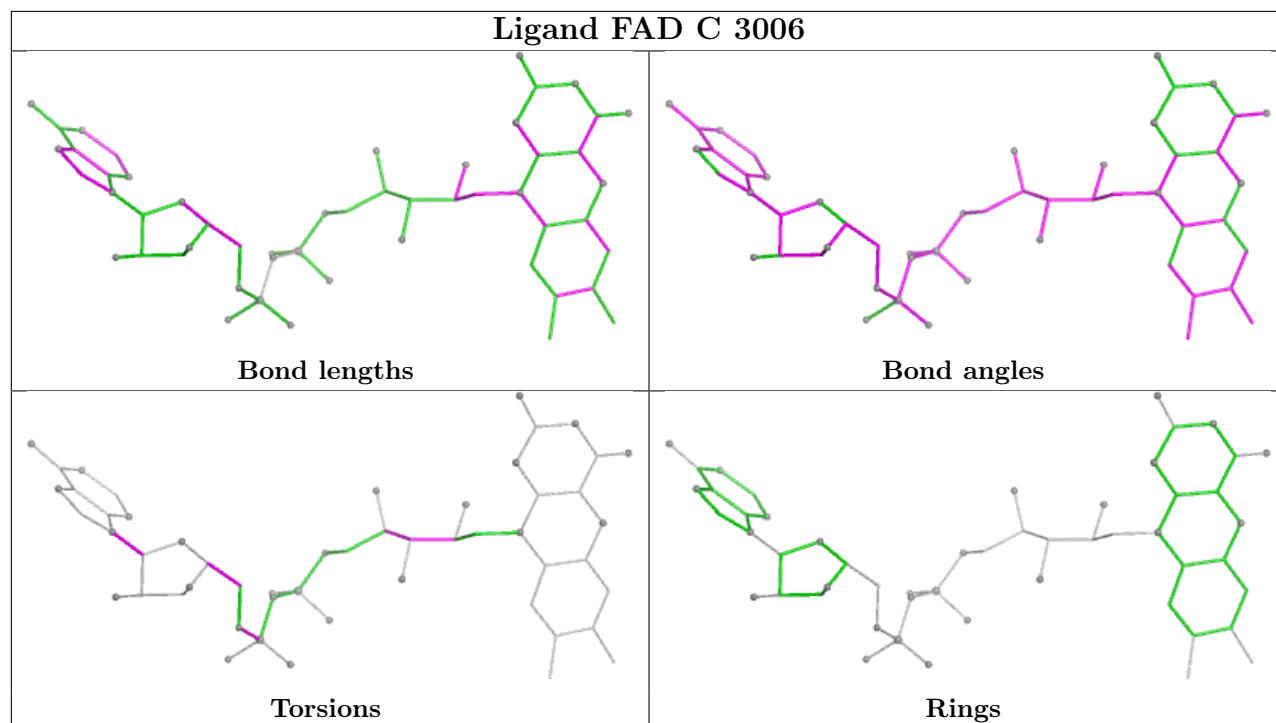
Mol	Chain	Res	Type	Atoms
3	A	3006	FAD	C5B-O5B-PA-O3P
3	B	3006	FAD	C5B-O5B-PA-O1A
3	B	3006	FAD	C5B-O5B-PA-O2A
3	B	3006	FAD	C5B-O5B-PA-O3P
3	B	3006	FAD	O4B-C1B-N9A-C4A

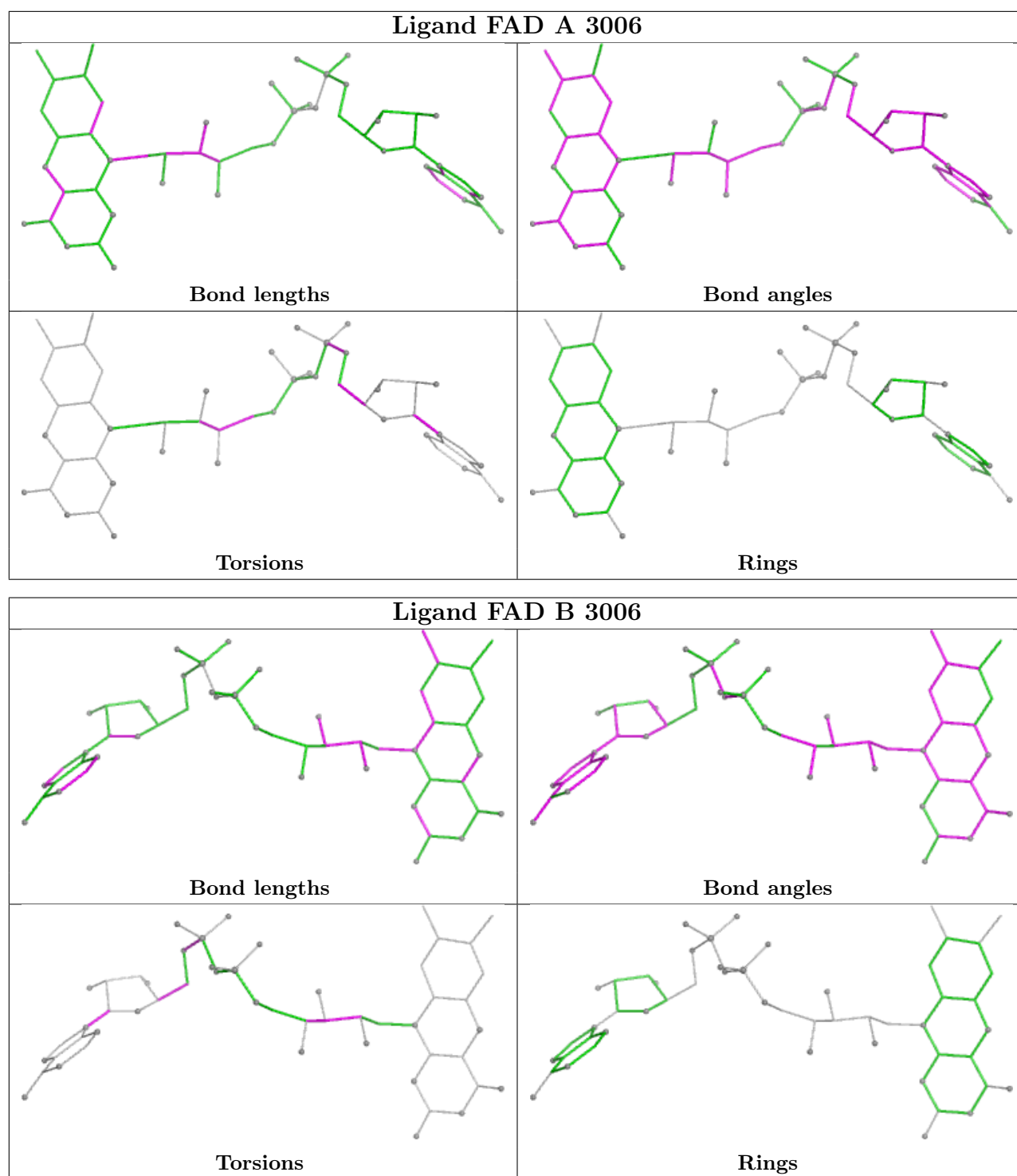
There are no ring outliers.

11 monomers are involved in 79 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.