



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:20 AM GMT

PDB ID : 2CKJ
Title : HUMAN MILK XANTHINE OXIDOREDUCTASE
Authors : Pearson, A.R.; Godber, B.L.J.; Eisenthal, 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

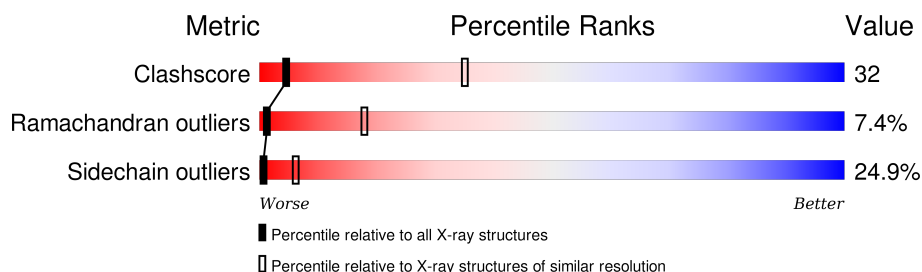
1 Overall quality at a glance

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	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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](#)

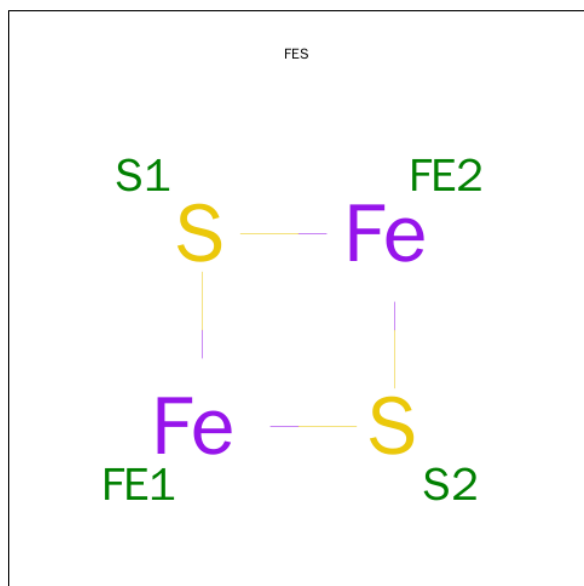
There are 6 unique types of molecules in this entry. The entry contains 39807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: FES) (formula: Fe₂S₂).



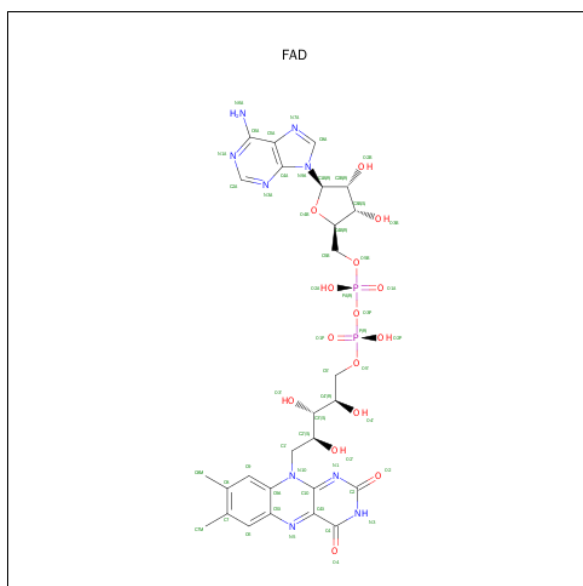
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



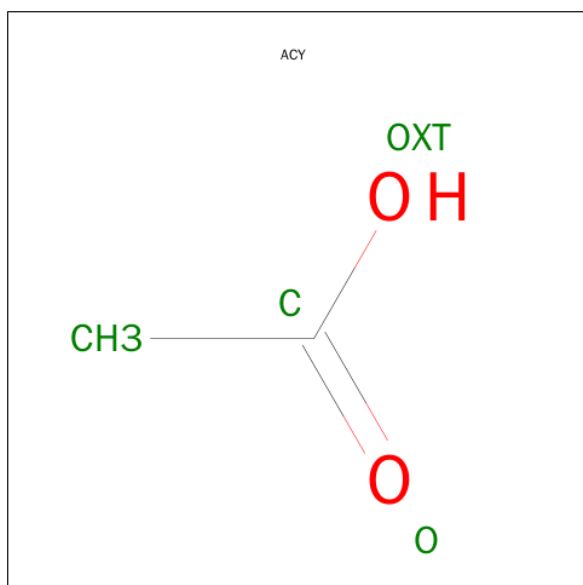
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



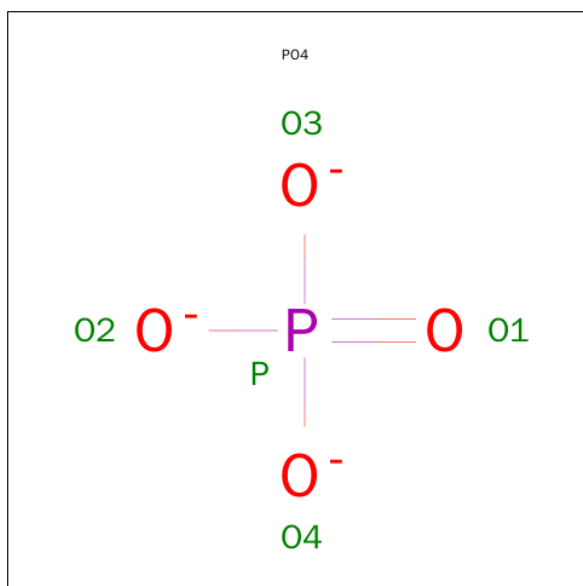
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- 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).



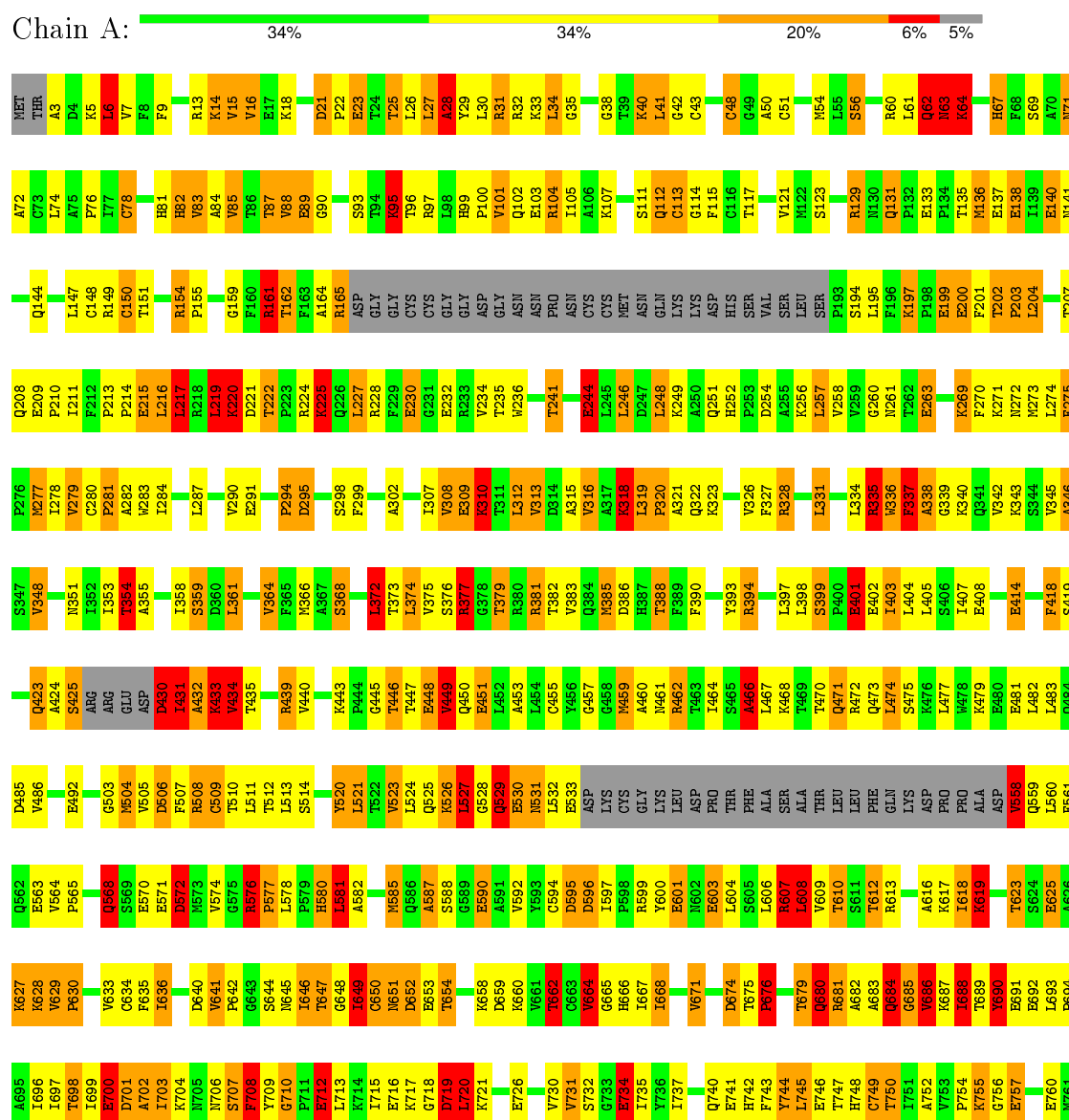
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			5	4	1		

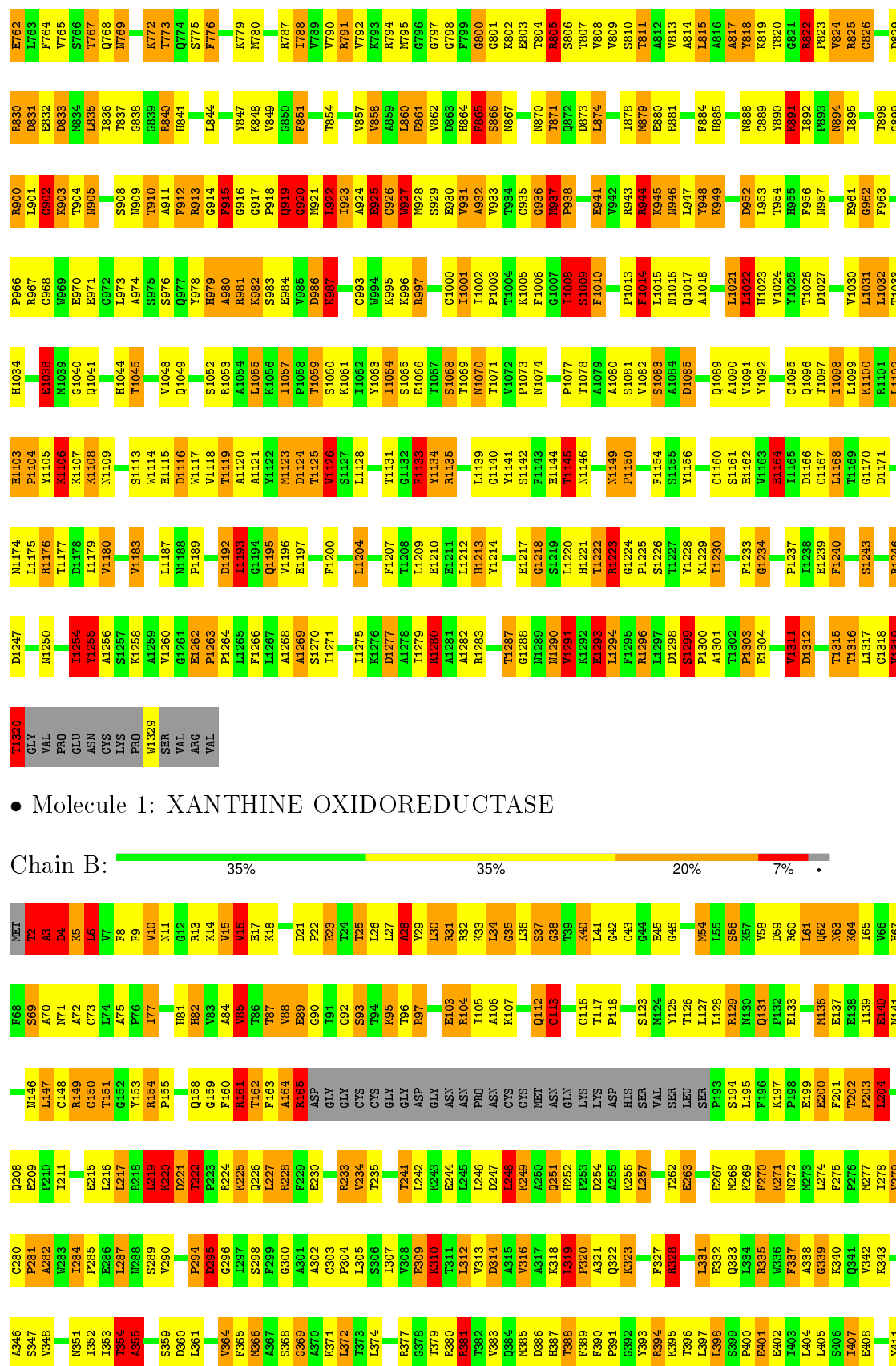
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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



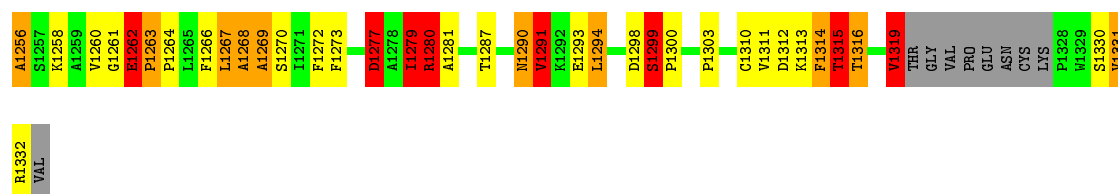


- Molecule 1: XANTHINE OXIDOREDUCTASE

Chain C:  35% 36% 18% 8% .

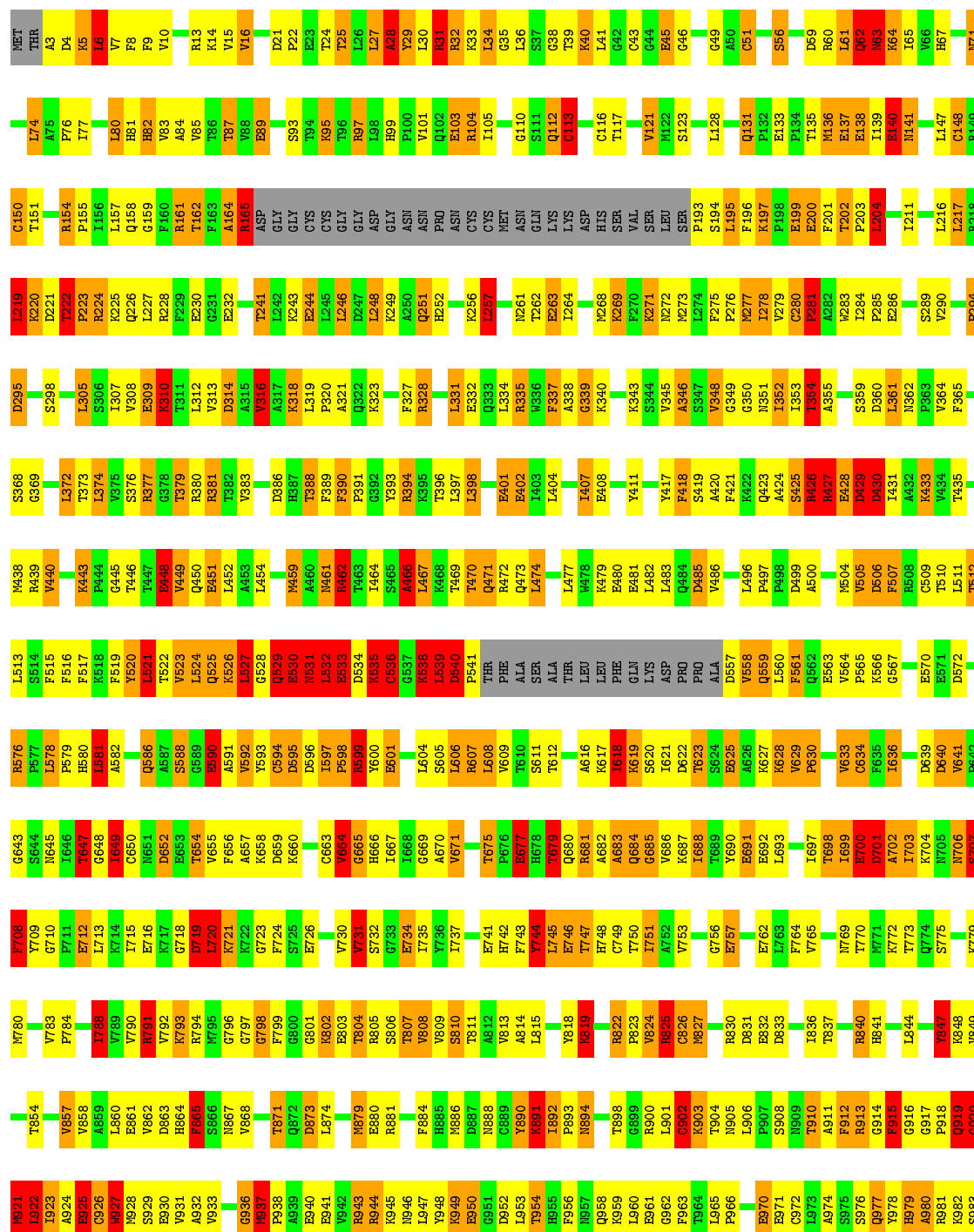
MET	THR	A3	K5	K6	V7	F8	F9	V10	N11	G12	R13	K14	V15	V16	E17	D21	T24	T25	L26	L27	A28	Y29	L30	R31	R32	R33	L34	L36	S37	G38	T39	K40	L41	G42	C43	G44	E45	G46	G47	C48	R49	L61	G62	R63	R64	G65	V66	W67
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L1179	E1103	H1034	R967	R900	D831	E757	K687	A616	PHE	Q484	E414	V248	C280	D205	A142	N71
V1180	P1104	E1038	E970	L901	E832	E757	I688	K617	GLN	D485	G415	G349	P281	D205	F143	N71
M1181	Y1105	E1038	E970	C902	D833	E760	T690	K618	LYS	D485	G416	G350	A282	D211	F143	L74
D1182	K1106	M1039	E971	K903	D833	E761	T690	K619	ASP	C487	Y417	G351	W283	D211	L147	L74
V1183	K1107	Q1040	C972	S908	T836	E762	E692	K620	PRO	L490	F418	I352	I284	D215	C148	A75
L1187	K1108	Q1041	L973	S909	T837	E763	L693	K621	ALA	L491	S419	I353	L287	D216	C150	A76
			A974	N909	T838	L763	L694	K622	D557	L492	Q423	K354	L287	D217	G151	I77
			S975	T910	R840	F764	P694	K623	D558	E492	A424	A355	E291	D218	T151	H81
D1192	W1114	L1043	S976	A911	B841	F765	A695	K624	D559	E493	A425	I358	E291	D219	G152	H81
E1193	E1115	T1045	S977	R912	B842	F766	L696	K625	D560	E494	R426	S359	P284	D220	Y153	H82
G1194	D1116	R913	Q978	R913	F843	T767	L697	K626	D561	E495	R427	S360	P285	D221	Y154	H83
Q1195	V1117	V1048	H979	G914	F844	Q768	T698	K627	D562	E496	R428	I361	D286	D222	P155	A84
Q1196	V1118	L844	A980	F915	A845	Q769	L699	K628	D563	E497	A429	I362	D287	D223	I156	H85
E1197	T1119	Q1049	R981	G916	B846	M769	E700	K629	D564	E498	ASP	K363	I287	D224	L157	H86
G1198	S1052	S1052	K982	G917	T847	T773	D701	K630	D565	E499	ASP	K364	S298	D225	Q158	H87
	R1053	R1053	S983	G918	T848	Q774	A702	K631	D566	E500	ASP	I365	S298	D226	Q159	H88
V1201	A1122	A1054	S984	P918	K848	Q775	I703	K632	D567	E501	ILE	I366	Q226	D227	F160	E89
	Y1201	E984	S985	Q919	B849	F776	R704	K633	D568	E502	A432	I367	Q227	D228	F161	E89
L1204	M1123	L1055	D986	G920	F850	Q777	I705	K634	D569	E503	V434	I368	Q228	D229	T162	S93
	D1124	K1056	D987	N921	F851	Q778	I706	K635	D570	E504	T435	I369	Q229	D230	T163	S94
T1208	T1125	I1057	K988	L922	T854	Q779	N707	K636	D571	E505	M438	I370	Q230	D231	T164	S95
L1209	S1127	P1059	N989	A924	T855	Q780	F708	K637	D572	E506	R439	I371	Q232	D232	T165	S96
		S1060	E991	E925	L860	Q781	Y709	K638	D573	E507	V440	I372	Q233	D233	T166	S97
L1212	G1132	I1064	E992	C926	B861	Q782	G710	K639	D574	E508	V441	I373	Q234	D234	T167	S98
L1213	F1133	S1065	K995	N927	B862	Q783	E711	K640	D575	E509	V442	I374	Q235	D235	T168	S99
Y1214	Y1134	S1066	K996	N928	B863	Q784	E712	K641	D576	E510	V443	I375	Q236	D236	T169	S100
	R1135	S1067	K997	N929	B864	Q785	E713	K642	D577	E511	V444	I376	Q237	D237	T170	S101
G1218	L1139	S1068	R998	E930	B865	Q786	G711	K643	D578	E512	V445	I377	Q238	D238	T171	S102
S1219	S1219	L1069	R999	E931	B866	Q787	G712	K644	D579	E513	V446	I378	Q239	D239	T172	S103
L1220	G1140	N1070	G998	N931	B867	Q788	G713	K645	D580	E514	V447	I379	Q240	D240	T173	S104
H1221	H1141	T1071		A932	B868	Q789	G714	K646	D581	E515	V448	I380	Q241	D241	T174	S105
T1222	Y1141	T1072	I1001	V933	B869	Q790	G715	K647	D582	E516	V449	I381	Q242	D242	T175	S106
		P1073	I1002	G936	B870	Q791	G716	K648	D583	E517	V450	I382	Q243	D243	T176	S107
L1223	E1144	P1074	P1003	N937	B871	Q792	G717	K649	D584	E518	V451	I383	Q244	D244	T177	S108
	T1145	N1074	P1004	N938	B872	Q793	G718	K650	D585	E519	V452	I384	Q245	D245	T178	S109
Y1228	N1149	P1075	K1005	P938	B873	Q794	G719	K651	D586	E520	V453	I385	Q246	D246	T179	S110
I1230	P1150	L1076	I1006	E939	B874	Q795	G720	K652	D587	E521	V454	I386	Q247	D247	T180	S111
P1231	F1151	A1079	S1008	E941	B875	Q796	G721	K653	D588	E522	V455	I387	Q248	D248	T181	S112
A1232	F1152	A1080	F1010	N942	B876	Q797	G722	K654	D589	E523	V456	I388	Q249	D249	T182	S113
F1233	F1153	S1081	T1011	R943	B877	Q798	G723	K655	D590	E524	V457	I389	Q250	D250	T183	S114
G1234	G1157	V1082		R944	B878	Q799	G724	K656	D591	E525	V458	I390	Q251	D251	T184	S115
S1235	G1158	F1014	F1014	K945	B879	Q800	G725	K657	D592	E526	V459	I391	Q252	D252	T185	S116
	A1159	L1015	L1015	N946	B880	Q801	G726	K658	D593	E527	V460	I392	Q253	D253	T186	S117
E1239	F1240	D1085	Q1017	N947	B881	Q802	G727	K659	D594	E528	V461	I393	Q254	D254	T187	S118
R1241	R1241	L1086	Q1017	E950	B882	Q803	G728	K660	D595	E529	V462	I394	Q255	D255	T188	S119
S1243	S1243	L1087	A1018	G951	B883	Q804	G729	K661	D596	E530	V463	I395	Q256	D256	T189	S120
L1245	L1245	A1030	A1019	D952	B884	Q805	G730	K662	D597	E531	V464	I396	Q257	D257	T190	S121
R1246	R1246	A1031	G1019	E953	B885	Q806	G731	K663	D598	E532	V465	I397	Q258	D258	T191	S122
D1247	D1247	A1032	A1020	L953	B886	Q807	G732	K664	D599	E533	V466	I398	Q259	D259	T192	S123
C1248	C1248	A1033	L1021	T954	B887	Q808	G733	K665	D600	E534	V467	I399	Q260	D260	T193	S124
P1249	P1249	A1034	L1022	F956	B888	Q809	G734	K666	D601	E535	V468	I400	Q261	D261	T194	S125
		C1095	Y1025		B889	Q810	G735	K667	D602	E536	V469	I401	Q262	D262	T195	S126
		Q1096	T1026		B890	Q811	G736	K668	D603	E537	V470	I402	Q263	D263	T196	S127
		L1098	D1027		B891	Q812	G737	K669	D604	E538	V471	I403	Q264	D264	T197	S128
		L1099	L1030		B892	Q813	G738	K670	D605	E539	V472	I404	Q265	D265	T198	S129
		L1100	L1031		B893	Q814	G739	K671	D606	E540	V473	I405	Q266	D266	T199	S130
		L1101	L1032		B894	Q815	G740	K672	D607	E541	V474	I406	Q267	D267	T200	S131
		L1102	L1033		B895	Q816	G741	K673	D608	E542	V475	I407	Q268	D268	T201	S132
					B896	Q817	G742	K674	D609	E543	V476	I408	Q269	D269	T202	S133
					B897	Q818	G743	K675	D610	E544	V477	I409	Q270	D270	T203	S134
					B898	Q819	G744	K676	D611	E545	V478	I410	Q271	D271	T204	S135
					B899	Q820	G745	K677	D612	E546	V479	I411	Q272	D272	T205	S136
					B900	Q821	G746	K678	D613	E547	V480	I412	Q273	D273	T206	S137
					B901	Q822	G747	K679	D614	E548	V481	I413	Q274	D274	T207	S138
					B902	Q823	G748	K680	D615	E549	V482	I414	Q275	D275	T208	S139
					B903	Q824	G749	K681	D616	E550	V483	I415	Q276	D276	T209	S140
					B904	Q825	G750	K682	D617	E551	V484	I416	Q277	D277	T210	S141
					B905	Q826	G751	K683	D618	E552	V485	I417	Q278	D278	T211	S142
					B906	Q827	G752	K684	D619	E553	V486	I418	Q279	D279	T212	S143
					B907	Q828	G753	K685	D620	E554	V487	I419	Q280	D280	T213	S144
					B908	Q829	G754	K686	D621	E555	V488	I420	Q281	D281	T214	S145
					B909	Q830	G755	K687	D622	E556	V489	I421	Q282	D282	T215	S146
					B910	Q831	G756	K688	D623	E557	V490	I422	Q283	D283	T216	S147
					B911	Q832	G757	K689	D624	E558	V491	I423	Q284	D284	T217	S148
					B912	Q833	G758	K690	D625	E559	V492	I424	Q285	D285	T218	S149
					B913	Q834	G759	K691	D626	E560	V493	I425	Q286	D286	T219	S150
					B914	Q835	G760	K692	D627	E561	V494	I426	Q287	D287	T220	S151
					B915	Q836	G761	K693	D628	E562	V495	I427	Q288	D288	T221	S152
					B916	Q837	G762	K694	D629	E563	V496	I428	Q289	D289	T222	S153
					B917	Q838	G763	K695	D630	E564	V497	I429	Q290	D290	T223	S154
					B918	Q839	G764	K696	D631	E565	V498	I430	Q291	D291	T224	S155
					B919	Q840	G765	K697	D632	E566	V499	I431	Q292	D292	T225	S156
					B920	Q841	G766	K698	D633	E567	V500	I432	Q293	D293	T226	S157
					B921	Q842	G767	K699	D634	E568	V501	I433	Q294	D294	T227	S158
					B922	Q843	G768	K700	D635	E569	V502	I434	Q295	D295	T228	S159
					B923	Q844	G769	K701	D636	E570	V503	I435	Q296	D296	T229	S160
					B924	Q845	G770	K702	D637	E571	V504	I436	Q297	D297	T230	S161
					B925	Q846	G771	K703	D638	E572	V505	I437	Q298	D298	T231	S162
					B926	Q847	G772	K704	D639	E573	V506	I438	Q299	D299	T232	S163
					B927	Q848	G773	K705	D640	E574	V507	I439	Q			



• Molecule 1: XANTHINE OXIDOREDUCTASE

Chain D: 36% 34% 20% 7% .



F1272	F1273	D1277	A1278	I1279	R1280	T1287	G1288	N1289	N1290	Y1291	K1292	E1293	L1294	D1298	S1299	P1300	T1302	P1303	E1304	K1305	I1306	R1307	N1308	V1311	D1312	K1313	F1314	T1315	T1316	L1317	G1318	V1319	T1320	GLY	VAL	PRO	GLU	ASN	C1326	K1327	P1328	W1329	S1330	V1331	R1332	VAL										
F1200	L1204	G1205	L1206	L1209	E1210	E1211	L1212	H1213	Y1214	G1218	H1221	T1222	R1223	G1224	P1225	S1226	T1227	Y1228	K1229	I1230	G1234	P1237	I1238	E1239	F1240	R1241	V1242	S1243	L1244	L1245	R1246	D1247	N1250	I1254	Y1255	A1256	S1257	K1258	A1259	V1260	G1261	E1262	P1263	P1264	L1265	F1266	L1267	A1268	A1269	S1270	I1271					
M1123	D1124	T1125	V1126	S1127	T1131	G1132	F1133	Y1134	R1135	L1139	S1142	F1143	E1144	T1145	N1146	N1149	F1154	S1155	Y1156	G1157	V1158	A1159	C1160	S1161	E1162	V1163	E1164	I1165	D1166	C1167	G1170	D1171	H1172	K1173	N1174	L1175	R1176	T1177	D1178	V1183	G1184	S1185	S1186	L1187	D1192	I1193	G1194	Q1195	V1196	E1197						
E984	V985	D986	K987	F988	N989	K990	E991	K995	K996	R997	I1001	I1002	P1003	T1004	K1005	I1008	S1009	F1010	F1014	L1015	N1016	Q1017	A1018	L1021	L1022	H1023	T1026	V1030	L1031	L1032	T1033	H1034	E1038	M1039	G1040	Q1041	H1044	T1045	V1048	Q1049	V1050	A1051	S1052	R1053	A1054	L1055	K1056	I1057	P1058							
T1059	S1060	K1061	I1062	Y1063	I1064	S1065	E1066	T1067	S1068	T1069	M1070	T1071	V1072	P1073	N1074	P1077	T1078	A1079	A1080	S1081	V1082	S1083	A1084	D1085	L1086	Q1089	A1090	V1091	C1095	Q1096	T1097	I1098	L1099	K1100	R1101	L1102	E1103	P1104	Y1105	K1106	K1107	K1108	N1109	P1110	S1111	G1112	S1113	W1114	E1115	D1116	W1117	V1118	T1119	A1120	A1121	Y1122

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

5.3.1 Protein backbone

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	21
1	B	1281/1333 (96%)	1021 (80%)	158 (12%)	102 (8%)	1	16
1	C	1273/1333 (96%)	1011 (79%)	168 (13%)	94 (7%)	1	18
1	D	1275/1333 (96%)	1006 (79%)	174 (14%)	95 (8%)	1	17
All	All	5084/5332 (95%)	4040 (80%)	668 (13%)	376 (7%)	1	18

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%)	1	6
1	B	1088/1126 (97%)	812 (75%)	276 (25%)	1	6
1	C	1082/1126 (96%)	814 (75%)	268 (25%)	1	6
1	D	1084/1126 (96%)	813 (75%)	271 (25%)	1	6
All	All	4321/4504 (96%)	3246 (75%)	1075 (25%)	1	6

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	A	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FAD	A	3006	-	48,58,58	2.20	11 (22%)	54,89,89	2.98	21 (38%)
4	GOL	A	3007	-	5,5,5	0.53	0	5,5,5	1.02	0
2	FES	B	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	B	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FAD	B	3006	-	48,58,58	2.39	13 (27%)	54,89,89	3.37	21 (38%)
4	GOL	B	3007	-	5,5,5	0.60	0	5,5,5	0.77	0
2	FES	C	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	C	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FAD	C	3006	-	48,58,58	2.22	14 (29%)	54,89,89	3.55	25 (46%)
4	GOL	C	3007	-	5,5,5	0.48	0	5,5,5	0.57	0
2	FES	D	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	D	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FAD	D	3006	-	48,58,58	2.33	10 (20%)	54,89,89	3.72	24 (44%)
4	GOL	D	3007	-	5,5,5	0.81	0	5,5,5	1.31	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACY	D	3008	-	1,3,3	4.97	1 (100%)	0,3,3	0.00	-
6	PO4	D	3009	-	4,4,4	0.47	0	6,6,6	0.34	0

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	A	3001	1	-	0/0/4/4	0/1/1/1
2	FES	A	3002	1	-	0/0/4/4	0/1/1/1
3	FAD	A	3006	-	-	0/30/50/50	0/6/6/6
4	GOL	A	3007	-	-	0/4/4/4	0/0/0/0
2	FES	B	3001	1	-	0/0/4/4	0/1/1/1
2	FES	B	3002	1	-	0/0/4/4	0/1/1/1
3	FAD	B	3006	-	-	0/30/50/50	0/6/6/6
4	GOL	B	3007	-	-	0/4/4/4	0/0/0/0
2	FES	C	3001	1	-	0/0/4/4	0/1/1/1
2	FES	C	3002	1	-	0/0/4/4	0/1/1/1
3	FAD	C	3006	-	-	0/30/50/50	0/6/6/6
4	GOL	C	3007	-	-	0/4/4/4	0/0/0/0
2	FES	D	3001	1	-	0/0/4/4	0/1/1/1
2	FES	D	3002	1	-	0/0/4/4	0/1/1/1
3	FAD	D	3006	-	-	0/30/50/50	0/6/6/6
4	GOL	D	3007	-	-	0/4/4/4	0/0/0/0
5	ACY	D	3008	-	-	0/0/0/0	0/0/0/0
6	PO4	D	3009	-	-	0/0/0/0	0/0/0/0

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3006	FAD	O4B-C1B	-5.22	1.34	1.41
3	C	3006	FAD	O2'-C2'	-3.66	1.35	1.43
3	C	3006	FAD	C6-C5X	-3.65	1.36	1.41
3	B	3006	FAD	O2'-C2'	-3.06	1.36	1.43
3	A	3006	FAD	C4-C4X	-2.84	1.35	1.41

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3006	FAD	N3A-C2A-N1A	-9.39	121.71	128.89
3	C	3006	FAD	N3A-C2A-N1A	-8.94	122.05	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3006	FAD	N3A-C2A-N1A	-7.61	123.07	128.89
3	D	3006	FAD	C4X-C4-N3	-6.94	114.10	123.59
3	D	3006	FAD	N3A-C2A-N1A	-6.39	124.00	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 81 short contacts:

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

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.