



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:38 PM GMT

PDB ID : 3ZYV
Title : Crystal structure of the mouse liver Aldehyde Oxidase 3 (mAOX3)
Authors : Trincao, J.; Coelho, C.; Mahro, M.; Rodrigues, D.; Terao, M.; Garattini, E.;
Leimkuehler, S.; Romao, M.J.
Deposited on : 2011-08-27
Resolution : 2.54 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

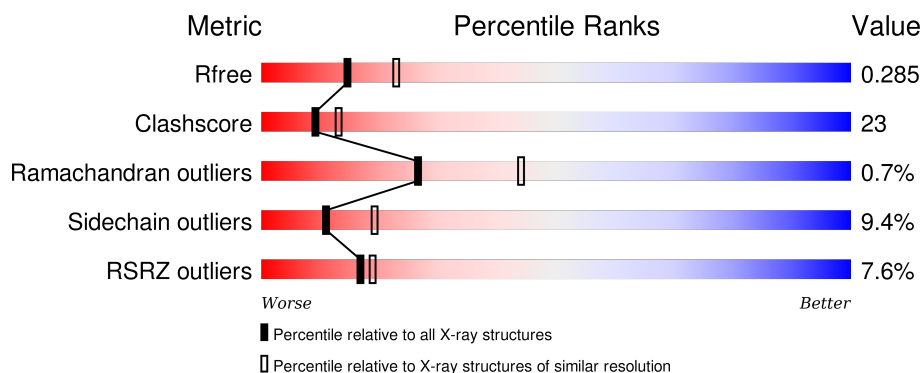
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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))
R_{free}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Mol	Chain	Length	Quality of chain
1	A	1335	<div> <div>6%</div> <div>58% 32% 6%</div> </div>
1	B	1335	<div> <div>6%</div> <div>57% 33% 5% 5%</div> </div>
1	C	1335	<div> <div>7%</div> <div>59% 30% 7%</div> </div>
1	D	1335	<div> <div>10%</div> <div>58% 32% 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	D	3002	-	-	X	-
5	MOS	A	3004	-	-	X	-
5	MOS	B	3004	-	-	X	-
5	MOS	C	3004	-	-	X	-
5	MOS	D	3004	-	-	X	-
6	FAD	C	3005	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 38315 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.

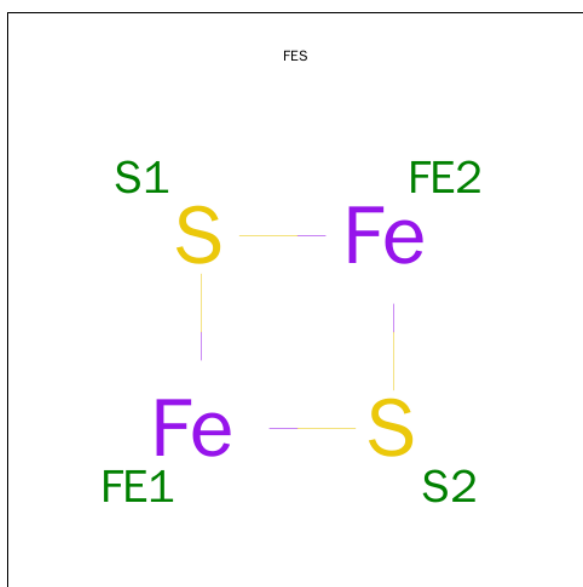
- Molecule 1 is a protein called AOX3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1253	Total	C	N	O	S	0	0	0
			9314	5905	1602	1747	60			
1	B	1262	Total	C	N	O	S	0	0	0
			9471	6016	1621	1774	60			
1	C	1244	Total	C	N	O	S	0	0	0
			9231	5865	1579	1728	59			
1	D	1257	Total	C	N	O	S	0	0	0
			9289	5892	1602	1739	56			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

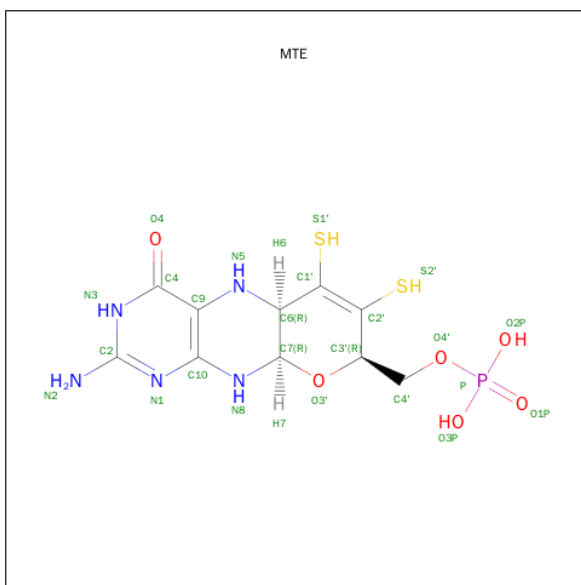
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



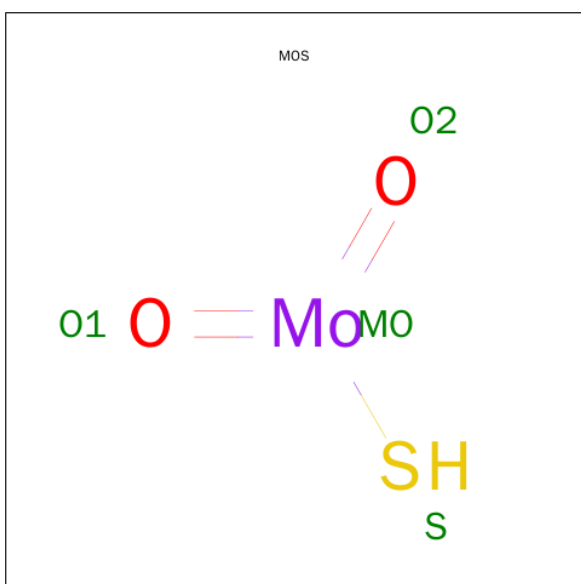
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C₁₀H₁₄N₅O₆P S₂).



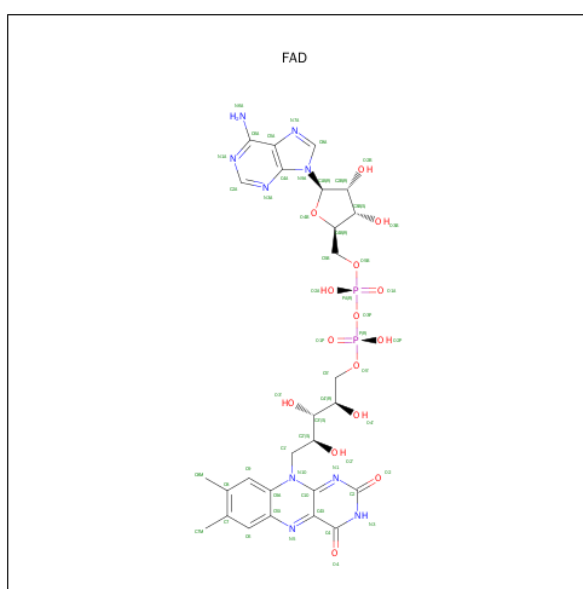
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
4	B	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
4	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
4	D	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO_2S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	B	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	C	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	D	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

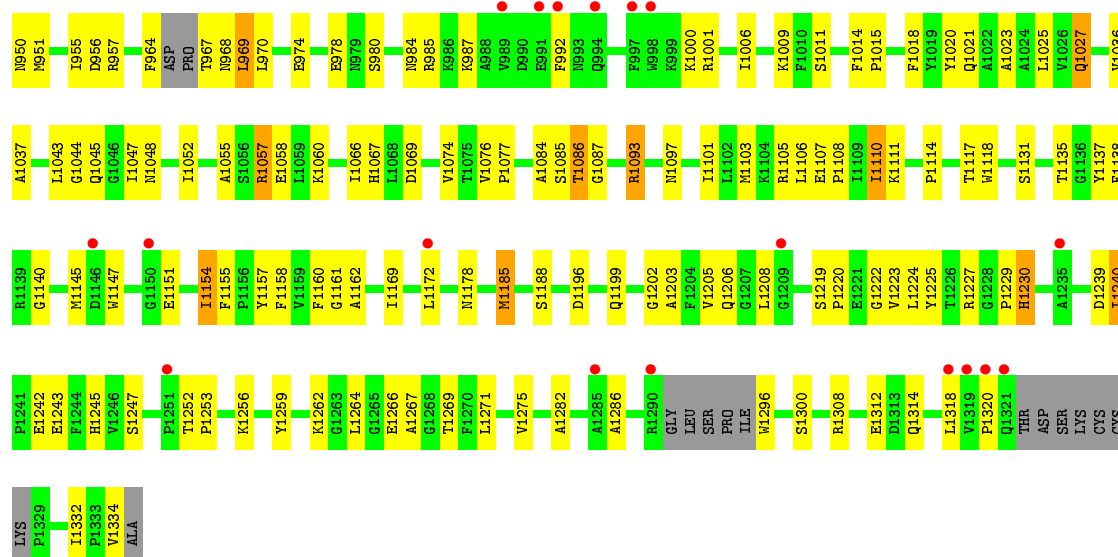
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	182	Total	O	0	0
			182	182		

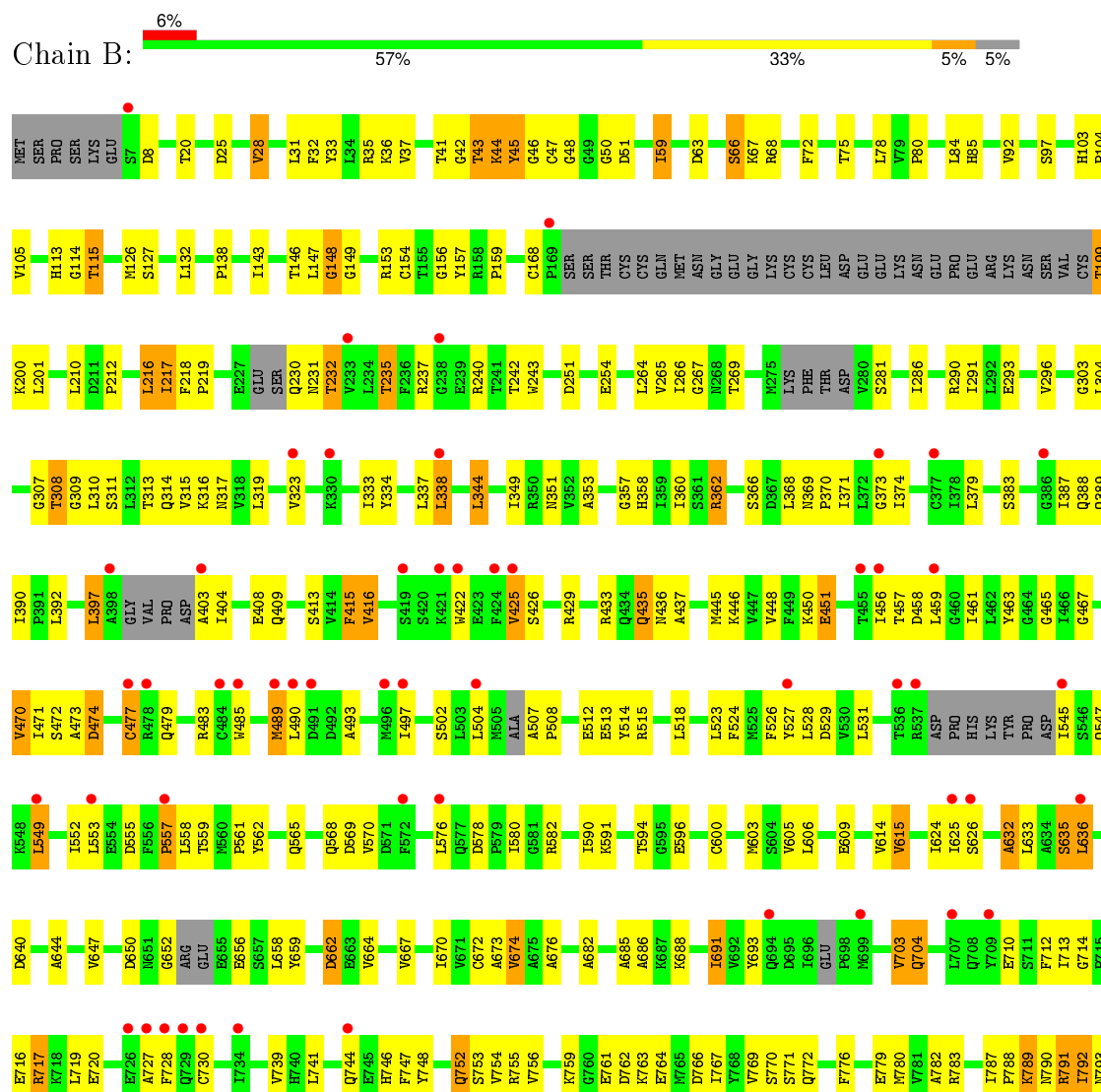
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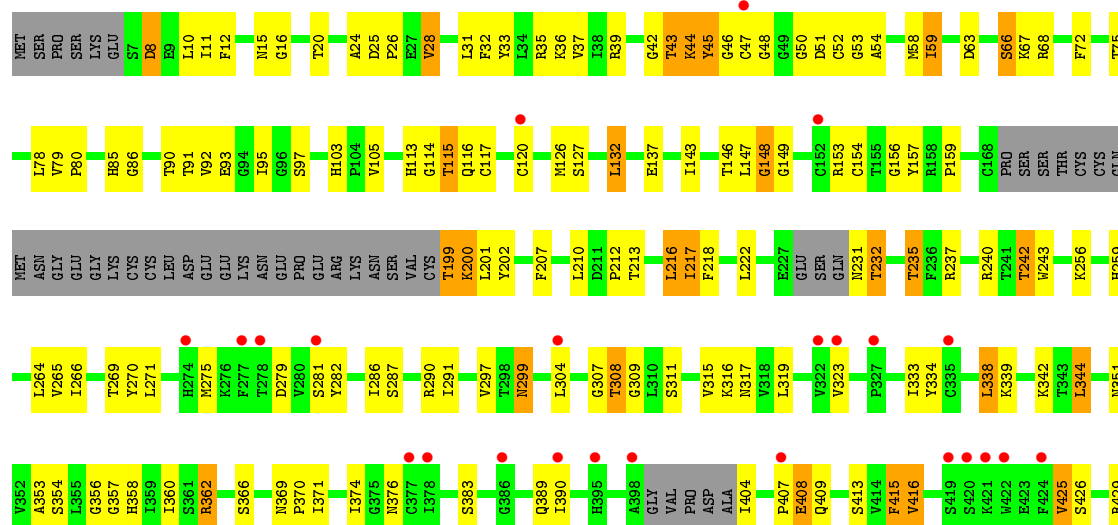
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	166	Total 166	O 166	0	0
7	C	147	Total 147	O 147	0	0
7	D	155	Total 155	O 155	0	0



• Molecule 1: AOX3







A1267	G1268	T1269	F1270	L1271	V1275	A1282	A1286	R1287	E1288	E1289	R1290	G1291	LEU	SER	P1294	I1295	S1300	P1301	R1308	E1312	D1313	T1316	N1317	L1318	VAL	PRO	GLN	K1233	I1234	V1237	T1238	D1239	I1240	E1243	F1244	H1245	V1246	S1247	T1250	P1251	T1252	P1253	Y1259	K1262	G1263	L1264	G1265	E1266			
W1185	S1188	F1189	P1193	D1196	I1197	G1202	A1203	F1204	V1205	Q1206	L1208	Y1211	S1219	P1220	E1221	G1222	V1223	L1224	V1225	T1226	G1227	G1228	P1229	H1230	Q1231	Y1232	K1233	I1234	V1237	T1238	D1239	I1240	E1243	F1244	H1245	V1246	S1247	T1250	P1251	T1252	P1253	Y1259	K1262	G1263	L1264	G1265	E1266				
G1087	R1093	N1097	I1101	L1102	M1103	K1104	R1105	L1106	E1107	P1108	I1109	K1111	Q1112	M1113	P1114	S1115	G1116	T1117	W1118	V1127	S1131	T1135	G1136	Y1137	F1138	R1139	G1140	Y1141	Q1142	W1147	E1148	K1149	G1150	E1151	G1152	D1153	I1154	P1155	F1156	Y1157	F1158	V1159	F1160	G1161	I1169	L1172	N1178				
R996	K1000	R1001	I1006	K1009	S1011	P1015	F1018	Q1021	A1022	A1023	A1024	V1026	Q1027	I1028	Y1029	L1035	V1036	A1037	L1043	G1044	Q1045	G1046	I1047	N1048	I1052	A1055	S1056	R1057	E1058	L1059	K1060	I1066	H1067	D1068	D1069	V1074	T1075	V1076	P1077	G1083	A1084	S1085	T1086								
G903	R904	V905	C906	K907	T908	N909	L910	A915	F916	R917	G918	F919	G920	F921	P922	Q923	V927	T928	L929	G932	G934	R937	R938	A963	L964	S966	P967	R968	L969	L970	N973	E974	V977	E978	S981	N984	K987	A1084	S1085	T1086											
K809	L813	V819	R826	P827	I831	L832	E833	R834	R835	D836	M838	L839	T841	G842	G843	R844	N857	N858	A863	D865	I866	Q867	L868	Y869	I870	N871	G872	G873	S879	E880	L881	V882	I883	E884	L887	L888	K889	L890	E891	N892	A893	Y894	N898	L899	R900	V901	R902				
L735	E736	E737	V739	L741	G742	G743	Q744	E745	H746	F747	Y748	Q752	S753	V756	G760	E761	D762	K763	E764	I767	S770	S771	D772	D773	F776	E779	W780	W781	A782	W783	I787	P788	K789	N790	K791	I792	N793	V796	K797	K798	A802	F803	G804	G805	R806	A807	S808				
I665	C666	V667	I670	G672	A673	V674	A675	E676	D677	A682	A685	A686	K687	K688	R689	G690	E691	V692	Y693	I696	GLU	M699	T702	Y703	Q704	D705	Q708	Y709	E710	S711	I712	I713	G714	P715	E716	R717	K718	L719	E720	Q721	G722	N723	V724	E725	E726	A727	F728	Q729	C730	I734	
ALA	A507	P508	E512	E513	Y514	L518	A519	I520	L523	F524	M525	F526	Y527	L528	D529	V530	L531	K532	G533	T536	R537	D538	HIS	LYS	TYR	PRO	ASP	I545	S546	Q547	K548	L549	L550	H551	L552	L553	P557	LEU	THR	PRO	Y562	Q565	Q568	I569	C569	V570	D571	F572	P575	L576	MET
R433	Q434	Q435	N436	A437	M445	K446	V447	V448	F449	D452	T453	T454	T455	T456	T457	D458	L459	G460	I461	L462	Y463	G467	I470	I471	K475	S476	C477	R478	Q479	L480	I481	G482	R483	V484	D485	E486	E488	M489	D492	A493	G494	K495	M496	I497	C498	V501	S502	L503	LEU	MET	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.88Å 135.27Å 147.37Å 78.16° 77.72° 89.90°	Depositor
Resolution (Å)	49.91 – 2.54 49.91 – 2.55	Depositor EDS
% Data completeness (in resolution range)	75.0 (49.91-2.54) 72.5 (49.91-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.256 , 0.285 0.257 , 0.285	Depositor DCC
R_{free} test set	8336 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.770	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 164929 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	38315	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MOS, NA, FES, FAD, MTE

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	0.31	0/9482	0.50	1/12869 (0.0%)
1	B	0.32	0/9650	0.50	2/13097 (0.0%)
1	C	0.31	0/9398	0.51	1/12757 (0.0%)
1	D	0.31	0/9460	0.49	0/12852
All	All	0.31	0/37990	0.50	4/51575 (0.0%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	619	LYS	CB-CG-CD	7.44	130.95	111.60
1	A	697	GLU	C-N-CD	-6.60	106.07	120.60
1	B	558	LEU	N-CA-C	-6.30	93.99	111.00
1	B	561	PRO	N-CA-CB	5.06	109.37	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	557	PRO	Peptide
1	B	557	PRO	Peptide
1	C	226	ALA	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	9314	0	9046	438	0
1	B	9471	0	9271	446	0
1	C	9231	0	8962	414	0
1	D	9289	0	8958	438	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	1	0
3	C	8	0	0	1	0
3	D	8	0	0	2	0
4	A	24	0	10	4	0
4	B	24	0	10	1	0
4	C	24	0	10	3	0
4	D	24	0	10	3	0
5	A	4	0	0	2	0
5	B	4	0	0	2	0
5	C	4	0	0	2	0
5	D	4	0	0	2	0
6	A	53	0	31	8	0
6	B	53	0	31	14	0
6	C	53	0	31	21	0
6	D	53	0	31	15	0
7	A	182	0	0	93	0
7	B	166	0	0	65	0
7	C	147	0	0	57	0
7	D	155	0	0	90	0
All	All	38315	0	36401	1701	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 23.

The worst 5 of 1701 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)
6:B:3005:FAD:H9	6:B:3005:FAD:O2'	1.48	1.12
1:A:308:THR:HG21	6:A:3005:FAD:N6A	1.62	1.11
1:B:308:THR:HG21	6:B:3005:FAD:N6A	1.67	1.09
1:A:496:MET:SD	7:A:2076:HOH:O	2.12	1.07
1:D:12:PHE:HB3	7:D:2002:HOH:O	1.55	1.06

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	1221/1335 (92%)	1123 (92%)	89 (7%)	9 (1%)	26	44
1	B	1238/1335 (93%)	1137 (92%)	93 (8%)	8 (1%)	30	48
1	C	1210/1335 (91%)	1111 (92%)	88 (7%)	11 (1%)	21	36
1	D	1231/1335 (92%)	1120 (91%)	104 (8%)	7 (1%)	30	48
All	All	4900/5340 (92%)	4491 (92%)	374 (8%)	35 (1%)	26	44

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ALA
1	B	762	ASP
1	C	398	ALA
1	C	474	ASP
1	A	762	ASP

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	958/1129 (85%)	869 (91%)	89 (9%)	11	19
1	B	988/1129 (88%)	891 (90%)	97 (10%)	10	17
1	C	948/1129 (84%)	862 (91%)	86 (9%)	12	20
1	D	941/1129 (83%)	854 (91%)	87 (9%)	11	20
All	All	3835/4516 (85%)	3476 (91%)	359 (9%)	11	19

5 of 359 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	880	GLU
1	C	217	ILE
1	D	747	PHE
1	B	978	GLU
1	B	1247	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	733	GLN
1	B	1100	GLN
1	D	708	GLN
1	B	1067	HIS
1	C	208	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	FES	A	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	A	3003	5	19,26,26	0.89	1 (5%)	19,40,40	2.05	6 (31%)
5	MOS	A	3004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	A	3005	-	48,58,58	1.27	5 (10%)	54,89,89	2.05	11 (20%)
3	FES	B	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	B	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	B	3003	5	19,26,26	0.95	1 (5%)	19,40,40	2.26	7 (36%)
5	MOS	B	3004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	B	3005	-	48,58,58	1.27	6 (12%)	54,89,89	2.49	10 (18%)
3	FES	C	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	C	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	C	3003	5	19,26,26	0.97	1 (5%)	19,40,40	2.59	8 (42%)
5	MOS	C	3004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	C	3005	-	48,58,58	1.28	5 (10%)	54,89,89	2.13	11 (20%)
3	FES	D	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	D	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	D	3003	5	19,26,26	0.93	1 (5%)	19,40,40	2.31	6 (31%)
5	MOS	D	3004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	D	3005	-	48,58,58	1.29	6 (12%)	54,89,89	2.05	11 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	3001	1	-	0/0/4/4	0/1/1/1
3	FES	A	3002	1	-	0/0/4/4	0/1/1/1
4	MTE	A	3003	5	-	0/6/34/34	0/3/3/3
5	MOS	A	3004	4	-	0/0/0/0	0/0/0/0
6	FAD	A	3005	-	-	0/30/50/50	0/6/6/6
3	FES	B	3001	1	-	0/0/4/4	0/1/1/1
3	FES	B	3002	1	-	0/0/4/4	0/1/1/1
4	MTE	B	3003	5	-	0/6/34/34	0/3/3/3
5	MOS	B	3004	4	-	0/0/0/0	0/0/0/0
6	FAD	B	3005	-	-	0/30/50/50	0/6/6/6
3	FES	C	3001	1	-	0/0/4/4	0/1/1/1
3	FES	C	3002	1	-	0/0/4/4	0/1/1/1
4	MTE	C	3003	5	-	0/6/34/34	0/3/3/3
5	MOS	C	3004	4	-	0/0/0/0	0/0/0/0
6	FAD	C	3005	-	-	0/30/50/50	0/6/6/6
3	FES	D	3001	1	-	0/0/4/4	0/1/1/1
3	FES	D	3002	1	-	0/0/4/4	0/1/1/1
4	MTE	D	3003	5	-	0/6/34/34	0/3/3/3
5	MOS	D	3004	4	-	0/0/0/0	0/0/0/0
6	FAD	D	3005	-	-	0/30/50/50	0/6/6/6

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3005	FAD	C9A-N10	2.13	1.41	1.38
6	B	3005	FAD	C9A-N10	2.30	1.41	1.38
6	D	3005	FAD	C5A-C4A	2.77	1.46	1.40
6	B	3005	FAD	C5A-C4A	2.80	1.46	1.40
6	A	3005	FAD	C8-C7	2.86	1.48	1.41

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3005	FAD	N3A-C2A-N1A	-7.37	123.25	128.89
4	C	3003	MTE	O3'-C7-C6	-7.06	104.14	108.96
6	D	3005	FAD	N3A-C2A-N1A	-6.93	123.59	128.89
6	C	3005	FAD	N3A-C2A-N1A	-6.71	123.76	128.89
6	A	3005	FAD	N3A-C2A-N1A	-6.51	123.91	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002	FES	1	0
4	A	3003	MTE	4	0
5	A	3004	MOS	2	0
6	A	3005	FAD	8	0
3	B	3002	FES	1	0
4	B	3003	MTE	1	0
5	B	3004	MOS	2	0
6	B	3005	FAD	14	0
3	C	3002	FES	1	0
4	C	3003	MTE	3	0
5	C	3004	MOS	2	0
6	C	3005	FAD	21	0
3	D	3002	FES	2	0
4	D	3003	MTE	3	0
5	D	3004	MOS	2	0
6	D	3005	FAD	15	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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1253/1335 (93%)	0.48	74 (5%) 26 30	12, 40, 70, 88	0
1	B	1262/1335 (94%)	0.49	75 (5%) 26 30	10, 39, 67, 87	0
1	C	1244/1335 (93%)	0.53	98 (7%) 15 17	18, 43, 73, 99	0
1	D	1257/1335 (94%)	0.72	133 (10%) 8 9	20, 45, 79, 97	0
All	All	5016/5340 (93%)	0.55	380 (7%) 17 19	10, 42, 73, 99	0

The worst 5 of 380 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	477	CYS	7.1
1	C	937	ALA	6.7
1	D	492	ASP	5.5
1	C	497	ILE	5.3
1	D	494	GLY	5.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NA	D	2337	1/1	0.98	0.18	-0.18	17,17,17,17	0
6	FAD	B	3005	53/53	0.94	0.16	-0.35	7,31,43,51	0
2	NA	B	2337	1/1	0.95	0.16	-0.50	12,12,12,12	0
6	FAD	C	3005	53/53	0.94	0.15	-0.57	9,31,49,50	0
2	NA	A	2337	1/1	0.90	0.14	-0.83	26,26,26,26	0
4	MTE	C	3003	24/24	0.97	0.16	-0.86	7,32,46,61	0
6	FAD	D	3005	53/53	0.94	0.15	-0.90	6,33,46,53	0
4	MTE	B	3003	24/24	0.96	0.17	-0.92	15,35,49,67	0
4	MTE	D	3003	24/24	0.97	0.18	-1.04	13,33,49,53	0
4	MTE	A	3003	24/24	0.97	0.17	-1.08	12,27,37,42	0
2	NA	C	2337	1/1	0.89	0.15	-1.24	50,50,50,50	0
5	MOS	D	3004	4/4	0.98	0.16	-1.55	42,55,69,77	0
3	FES	B	3001	4/4	0.99	0.14	-1.63	7,20,22,26	0
6	FAD	A	3005	53/53	0.96	0.14	-1.64	9,28,45,49	0
3	FES	A	3001	4/4	0.99	0.14	-1.77	19,20,23,26	0
3	FES	B	3002	4/4	0.99	0.11	-2.13	20,21,34,38	0
3	FES	D	3002	4/4	0.99	0.10	-2.13	15,24,25,41	0
3	FES	C	3001	4/4	0.98	0.12	-2.33	24,24,31,39	0
3	FES	C	3002	4/4	0.97	0.08	-2.48	29,33,36,38	0
3	FES	D	3001	4/4	0.99	0.14	-2.70	15,23,23,26	0
5	MOS	B	3004	4/4	0.98	0.15	-2.86	42,55,69,77	0
3	FES	A	3002	4/4	0.99	0.09	-2.89	16,23,33,38	0
5	MOS	C	3004	4/4	0.99	0.09	-3.17	42,55,69,77	0
5	MOS	A	3004	4/4	0.99	0.12	-3.95	42,55,69,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.