



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 24, 2017 – 09:05 PM EST

PDB ID : 1FO4
Title : CRYSTAL STRUCTURE OF XANTHINE DEHYDROGENASE ISOLATED FROM BOVINE MILK
Authors : Enroth, C.; Eger, B.T.; Okamoto, K.; Nishino, T.; Nishino, T.; Pai, E.F.
Deposited on : 2000-08-24
Resolution : 2.10 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	:	1.7.1 (RC1), CSD as537be (2016)
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)	:	rb-20028442

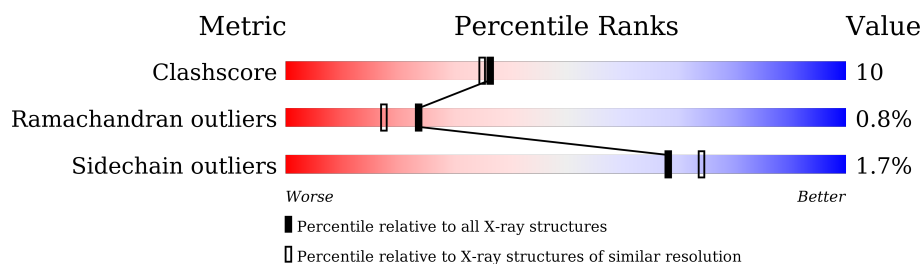
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	1332	<div> <div style="width: 78%; background-color: green;"></div> <div style="width: 18%; background-color: yellow;"></div> <div style="width: 4%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>78% 18% ..</div>
1	B	1332	<div> <div style="width: 79%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 4%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>79% 17% ..</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
5	MOS	A	3004	-	-	X	-
5	MOS	B	4004	-	-	X	-
7	FAD	A	3006	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FAD	B	4006	X	-	-	-
8	GOL	A	3007	-	X	X	-
8	GOL	A	3008	-	X	-	-
8	GOL	B	4007	-	X	X	-
8	GOL	B	4008	-	X	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 22402 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.

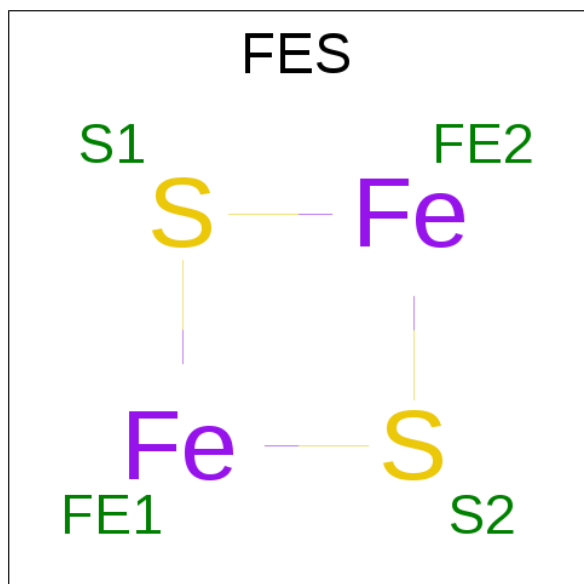
- Molecule 1 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1299	Total	C	N	O	S	0	0	0
			10077	6404	1728	1884	61			
1	B	1296	Total	C	N	O	S	0	0	0
			10054	6391	1724	1878	61			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

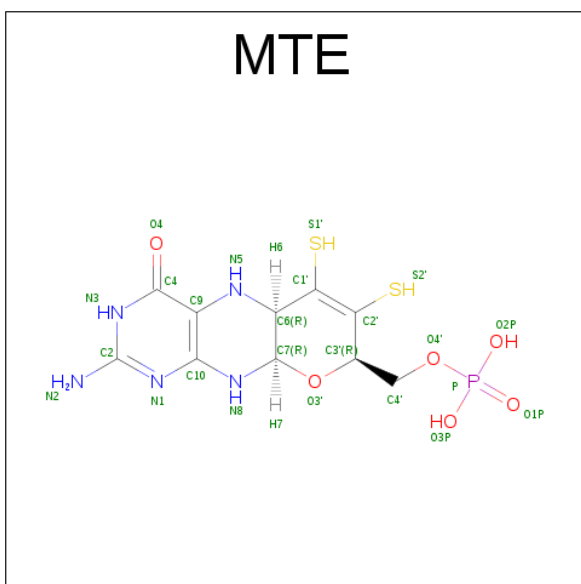
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

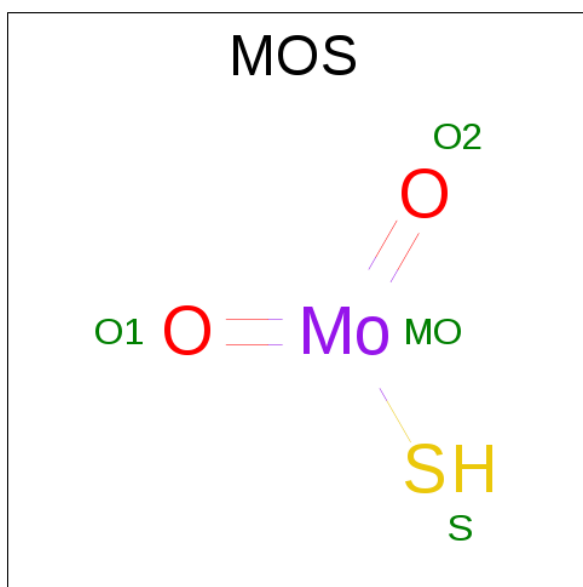
- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

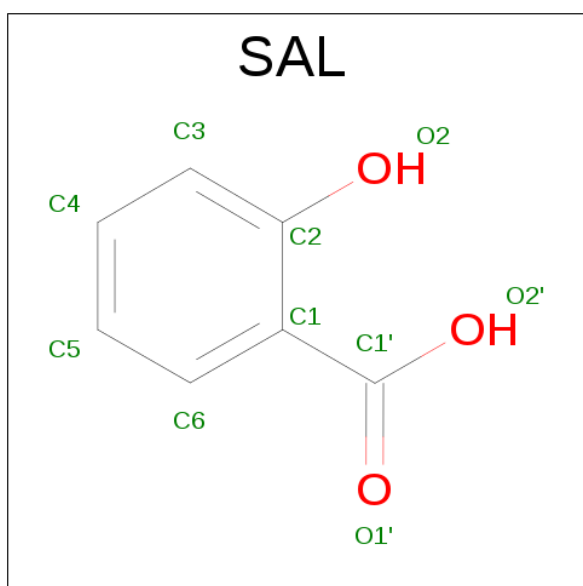
- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6P_2S_2$).





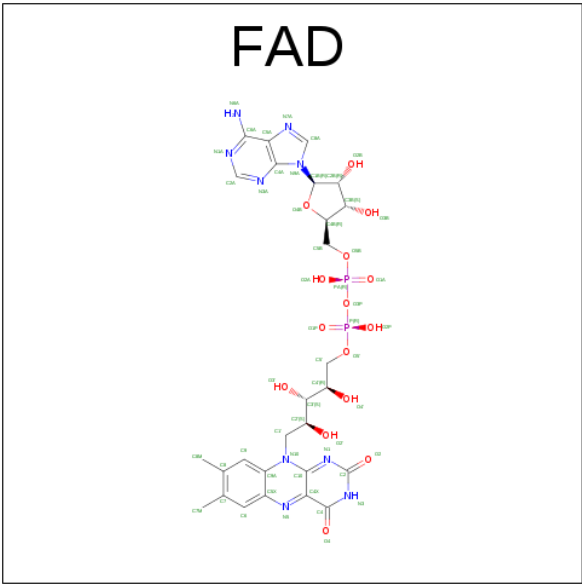
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 6 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



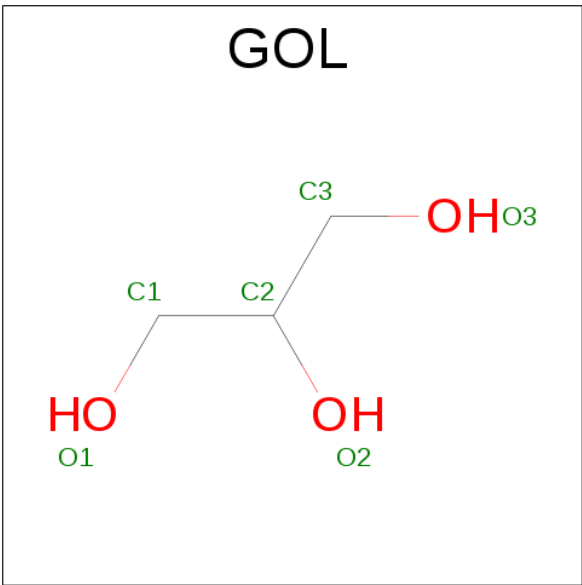
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

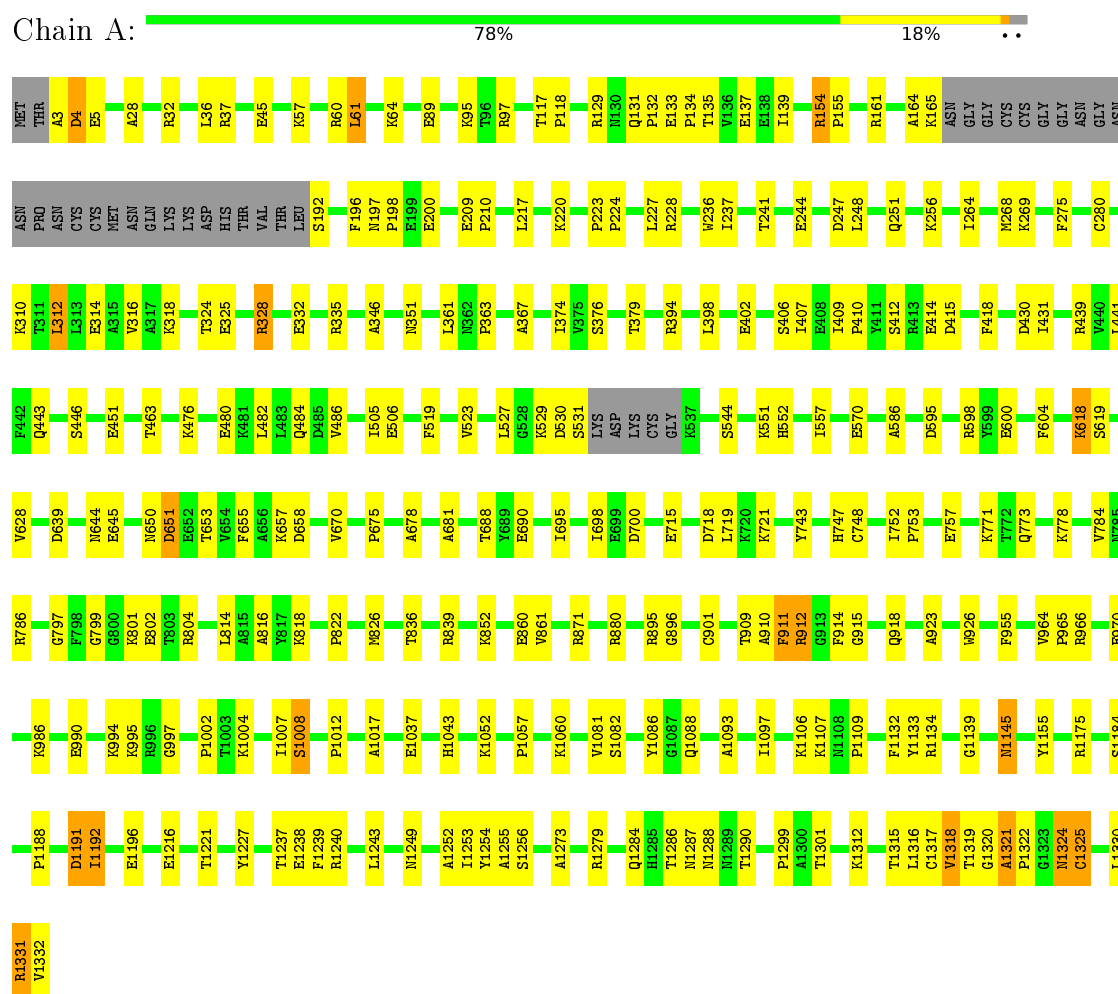
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1047	Total	O	0	0
			1047	1047		
9	B	1000	Total	O	0	0
			1000	1000		

3 Residue-property plots

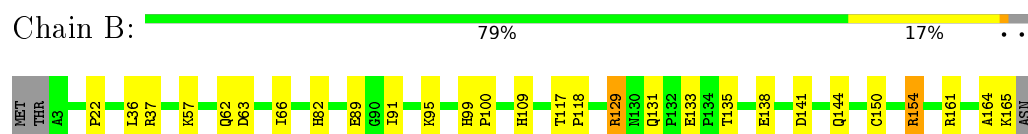
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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 DEHYDROGENASE



• Molecule 1: XANTHINE DEHYDROGENASE



L1313	GLY	L313	E508	G837	L1054	F1239
ASN	ASN	E314	R509	G838	K1055	
GLY	GLY	R328	T512	R839	P1072	N1249
ASN	ASN	L331	L527	R840	V1081	A1252
ASN	PRO	E332	G528	A844	S1082	A1255
CYS	CYS	R335	LYS	K847	I1085	S1256
CYS	CYS	W336	ASP	K852	Q1088	E1261
MET	MET	F337	SER	E860	P1262	
ASN	ASN	A338	LYS	E879	A1093	A1281
GLN	GLN	G339	ASP	R880	I1097	Q1284
LYS	LYS	K340	CYS	M885	N1108	H1285
LYS	LYS	A346	GLY	K894	P1109	T1286
ASP	HIS	A351	L538	R895	R1124	N1287
THR	THR	N351	L548	G896	V1125	N1288
THR	THR	L361	H552	R899	S1126	N1289
LEU	LEU	I374	R565	R899	T1129	T1290
S192	S192	S376	R569	I900	Y1133	K1291
N197	N197	R377	K567	C901	R1134	E1292
E200	E200	G378	A586	T909	G1139	I1293
E209	E209	T379	D595	A910	F1142	F1294
P210	P210	R394	R598	A911	N1145	P1299
L217	L217	L398	R599	R912	K1172	A1300
R218	R218	E402	R606	G913	N1173	T1301
L219	L219	I407	L607	F914	F1174	P1302
K220	K220	R427	V608	G915	R1175	V1310
G231	G231	E429	T609	I922	S1184	D1311
T241	T241	L441	A615	R942	S1185	K1312
K243	K243	M447	K616	F955	L1186	F1313
E244	E244	E451	S619	V964	N1187	L1316
K256	K256	Q471	V628	P965	P1188	C1317
V258	V258	K472	F634	R980	A1189	V1318
I264	I264	Q473	L788	D1191	I1190	A1321
F275	F275	K476	G797	K986	I1192	P1322
I279	I279	E480	E645	F987	V1195	G1323
C280	C280	K481	R650	E990	E1196	M1324
P281	P281	L482	D651	R995	T1207	C1325
L284	L284	Q483	T659	R996	L1208	K1326
L287	L287	L483	P822	I1007	T1221	L1330
R310	R310	Q484	M833	S1008	Y1227	R1331
T311	T311	V485	L834	A1017	P1236	V1332
L312	L312	V486	T836			

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.45Å 124.49Å 148.33Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10	Depositor
% Data completeness (in resolution range)	86.9 (25.00-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22402	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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, SAL, MOS, CA, 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	0.37	0/10298	0.64	1/13939 (0.0%)
1	B	0.37	0/10275	0.64	1/13909 (0.0%)
All	All	0.37	0/20573	0.64	2/27848 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1191	ASP	N-CA-C	-5.23	96.89	111.00
1	B	243	LYS	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

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	10077	0	10075	203	0
1	B	10054	0	10054	181	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	24	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	10	2	0
5	A	4	0	0	2	0
5	B	4	0	0	2	0
6	A	10	0	4	0	0
6	B	10	0	4	1	0
7	A	53	0	29	3	0
7	B	53	0	30	2	0
8	A	12	0	5	7	0
8	B	12	0	7	11	0
9	A	1047	0	0	21	0
9	B	1000	0	0	11	0
All	All	22402	0	20228	386	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 10.

The worst 5 of 386 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)
8:A:3008:GOL:C1	8:A:3008:GOL:O1	1.68	1.39
8:B:4008:GOL:C1	8:B:4008:GOL:O1	1.71	1.36
1:A:3:ALA:HB1	1:A:228:ARG:H	1.19	1.07
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.19	1.07
5:B:4004:MOS:MO	5:B:4004:MOS:S	1.66	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	1293/1332 (97%)	1228 (95%)	54 (4%)	11 (1%)	21 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1290/1332 (97%)	1236 (96%)	45 (4%)	9 (1%)	26	21
All	All	2583/2664 (97%)	2464 (95%)	99 (4%)	20 (1%)	24	17

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	A	1331	ARG
1	B	244	GLU
1	B	1008	SER
1	B	1287	ASN

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	1101/1128 (98%)	1084 (98%)	17 (2%)	72	78
1	B	1098/1128 (97%)	1078 (98%)	20 (2%)	66	72
All	All	2199/2256 (98%)	2162 (98%)	37 (2%)	68	74

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1325	CYS
1	B	328	ARG
1	B	1325	CYS
1	B	100	PRO
1	B	129	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1284	GLN
1	A	1324	ASN

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Mol	Chain	Res	Type
1	B	650	ASN
1	A	1212	HIS
1	B	1145	ASN

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 ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	21,26,26	7.33	16 (76%)	18,40,40	3.20	7 (38%)
5	MOS	A	3004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	SAL	A	3005	-	7,10,10	1.76	3 (42%)	10,13,13	1.22	0
7	FAD	A	3006	-	52,58,58	4.50	33 (63%)	52,89,89	2.94	20 (38%)
8	GOL	A	3007	-	5,5,5	7.07	4 (80%)	5,5,5	5.78	4 (80%)
8	GOL	A	3008	-	5,5,5	4.46	4 (80%)	5,5,5	5.72	3 (60%)
3	FES	B	4001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	B	4002	1	0,4,4	0.00	-	0,4,4	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MTE	B	4003	5	21,26,26	7.38	14 (66%)	18,40,40	3.17	7 (38%)
5	MOS	B	4004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	SAL	B	4005	-	7,10,10	1.74	3 (42%)	10,13,13	1.33	1 (10%)
7	FAD	B	4006	-	52,58,58	4.33	33 (63%)	52,89,89	3.01	19 (36%)
8	GOL	B	4007	-	5,5,5	6.66	5 (100%)	5,5,5	5.69	3 (60%)
8	GOL	B	4008	-	5,5,5	4.34	3 (60%)	5,5,5	5.84	3 (60%)

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	SAL	A	3005	-	-	0/0/4/4	0/1/1/1
7	FAD	A	3006	-	2/2/9/9	0/30/50/50	0/6/6/6
8	GOL	A	3007	-	-	0/4/4/4	0/0/0/0
8	GOL	A	3008	-	-	0/4/4/4	0/0/0/0
3	FES	B	4001	1	-	0/0/4/4	0/1/1/1
3	FES	B	4002	1	-	0/0/4/4	0/1/1/1
4	MTE	B	4003	5	-	0/6/34/34	0/3/3/3
5	MOS	B	4004	4	-	0/0/0/0	0/0/0/0
6	SAL	B	4005	-	-	0/0/4/4	0/1/1/1
7	FAD	B	4006	-	2/2/9/9	0/30/50/50	0/6/6/6
8	GOL	B	4007	-	-	0/4/4/4	0/0/0/0
8	GOL	B	4008	-	-	0/4/4/4	0/0/0/0

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	3007	GOL	C3-C2	-13.06	1.00	1.52
8	B	4007	GOL	C3-C2	-12.20	1.03	1.52
7	A	3006	FAD	C5'-C4'	-8.84	1.38	1.51
7	B	4006	FAD	C5'-C4'	-7.37	1.40	1.51
8	A	3008	GOL	C3-C2	-7.02	1.24	1.52

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4006	FAD	C4-C4X-C10	-7.92	114.87	119.94
7	A	3006	FAD	C4-C4X-C10	-7.76	114.98	119.94
7	A	3006	FAD	N3A-C2A-N1A	-7.29	123.14	128.87
7	B	4006	FAD	O5B-PA-O1A	-5.64	86.14	109.21
7	A	3006	FAD	C5X-C9A-N10	-5.44	113.50	117.58

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	4006	FAD	C2'
7	B	4006	FAD	C3'
7	A	3006	FAD	C2'
7	A	3006	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3003	MTE	1	0
5	A	3004	MOS	2	0
7	A	3006	FAD	3	0
8	A	3007	GOL	4	0
8	A	3008	GOL	3	0
4	B	4003	MTE	2	0
5	B	4004	MOS	2	0
6	B	4005	SAL	1	0
7	B	4006	FAD	2	0
8	B	4007	GOL	7	0
8	B	4008	GOL	4	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.