



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:50 PM GMT

PDB ID : 1VDV  
Title : Bovine Milk Xanthine Dehydrogenase Y-700 Bound Form  
Authors : Fukunari, A.; Okamoto, K.; Nishino, T.; Eger, B.T.; Pai, E.F.; Kamezawa, M.; Yamada, I.; Kato, N.  
Deposited on : 2004-03-25  
Resolution : 1.98 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](mailto: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.

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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

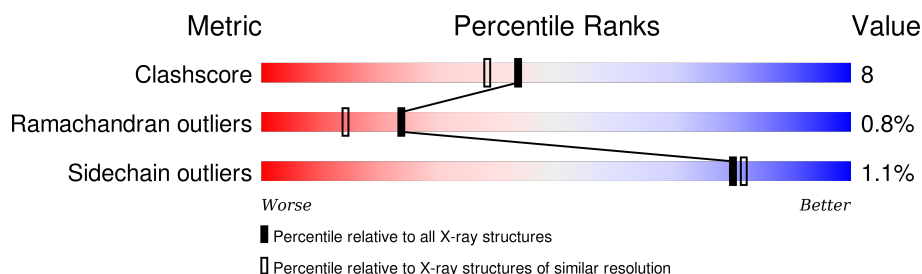
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)

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  $\geq 3$ , 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	
1	B	1332	

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	B	4004	-	-	X	-
9	ACY	A	5201	-	-	X	-
9	ACY	B	5202	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22610 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/oxidase.

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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P80457
B	1	MET	-	INITIATING METHIONINE	UNP P80457

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

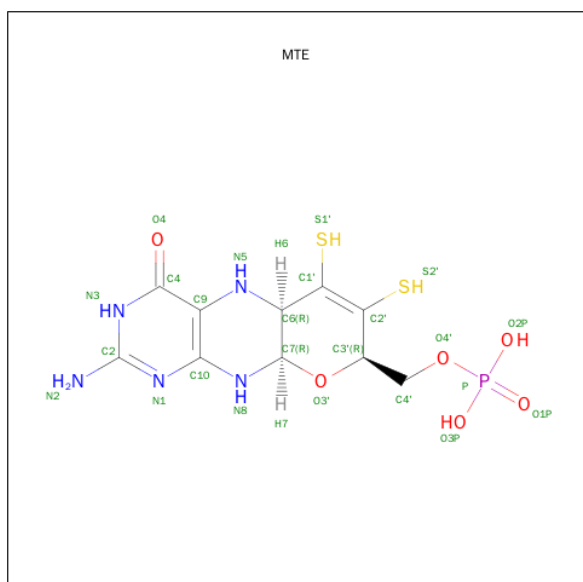
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



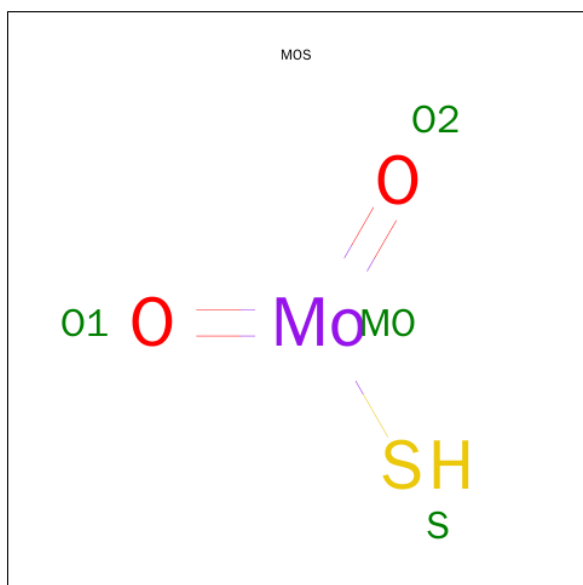
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- 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
4	A	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
4	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $\text{HMoO}_2\text{S}$ ).



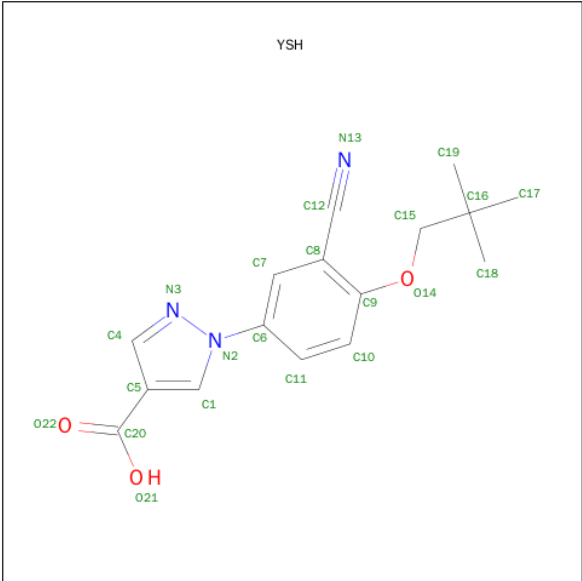
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S		
			4	1	2	1		
5	B	1	Total	Mo	O	S		
			4	1	2	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



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

- Molecule 7 is 1-[3-CYANO-4-(NEOPENTYLOXY)PHENYL]-1H-PYRAZOLE-4-CARBOXYLIC ACID (three-letter code: YSH) (formula: C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>O<sub>3</sub>).



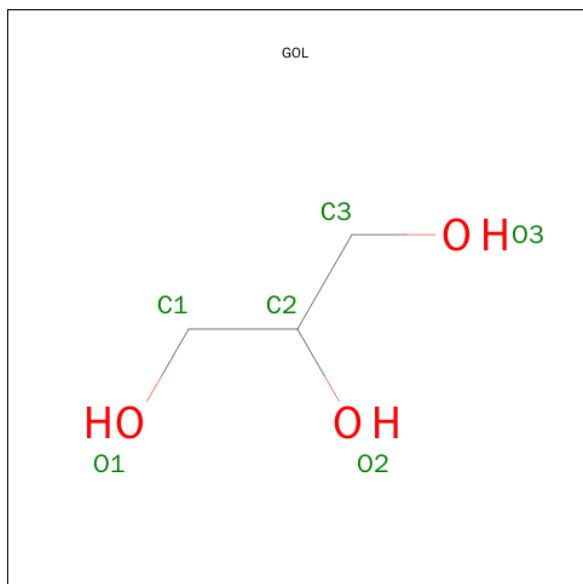
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			22	16	3	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			22	16	3	3		

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



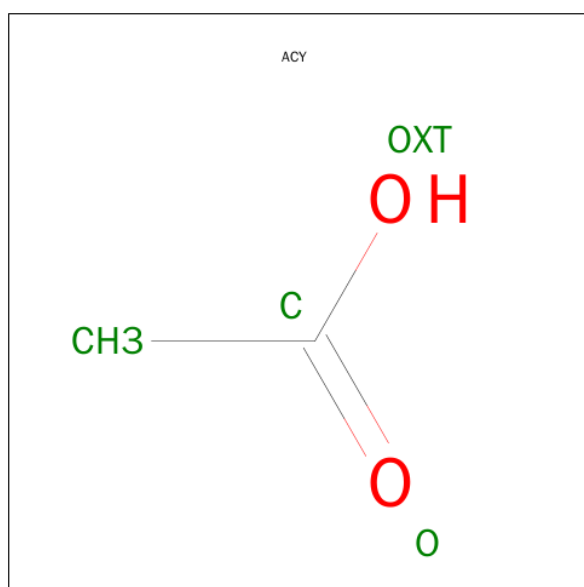
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O		0	0
			6	3	3			
8	A	1	Total	C	O		0	0
			6	3	3			
8	A	1	Total	C	O		0	0
			6	3	3			
8	A	1	Total	C	O		0	0
			6	3	3			
8	A	1	Total	C	O		0	0
			6	3	3			
8	B	1	Total	C	O		0	0
			6	3	3			
8	B	1	Total	C	O		0	0
			6	3	3			
8	B	1	Total	C	O		0	0
			6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

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

- Molecule 9 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0

- Molecule 10 is water.

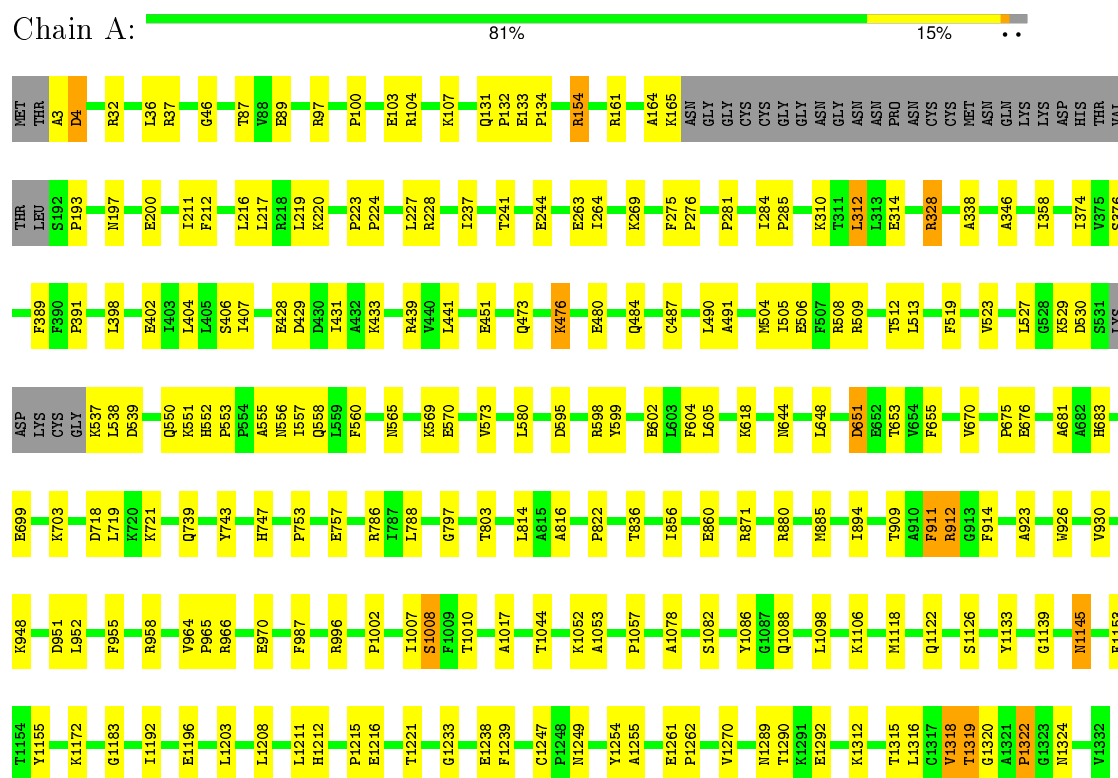
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1086	Total 1086	O 1086	0	0
10	B	1033	Total 1033	O 1033	0	0

### 3 Residue-property plots

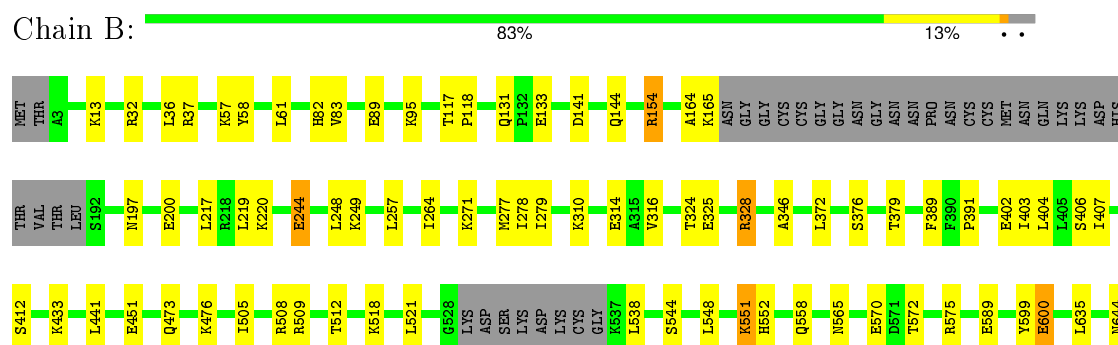
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



- Molecule 1: Xanthine dehydrogenase/oxidase



L1316	G1087	R895	M650
C1317	Q1088	G896	T653
V1318	L1098	R897	F654
T1319	M1108	G898	F655
G1320	P1109	R899	K656
A1321	F1132	T909	K657
P1322	Y1133	A910	D658
G1323	G1139	F911	E676
M1324	G1139	R912	E699
C1325	N1145	G913	F914
K1326	K1172	F914	Y926
V1332	M1173	Y926	L712
	I1192	V930	K713
	E1196	K948	L719
	F1199	D951	F723
	L1203	L952	A726
	T1221	F955	I736
	T1226	R958	Y743
	P1236	Y964	H747
	T1237	P965	P753
	E1238	F987	E757
	F1239	C992	K778
	M1249	M993	R786
	A1255	K994	G797
	E1261	R995	L814
	P1262	R996	A815
	G1267	P1002	A816
	A1281	I1007	F817
	Q1284	S1008	K818
	H1285	F1009	M826
	T1286	T1010	T836
	N1287	A1017	K847
	M1288	L1030	Y857
	M1289	Q1048	E860
	T1290	A1053	R871
	K1291	P1057	H875
	E1292	A1078	R880
	S1298	S1082	
	K1312	Y1086	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.82Å 123.94Å 148.89Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	20.00 – 1.98	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.98)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.178 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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, YSH, MOS, CA, FES, ACY, 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	0.32	0/10298	0.60	0/13939
1	B	0.31	0/10275	0.60	0/13909
All	All	0.32	0/20573	0.60	0/27848

There are no bond length outliers.

There are no bond angle outliers.

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	10076	172	0
1	B	10054	0	10053	155	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	0	0
4	A	24	0	10	1	0
4	B	24	0	10	1	0
5	A	4	0	0	1	0
5	B	4	0	0	2	0
6	A	53	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	53	0	31	3	0
7	A	22	0	16	3	0
7	B	22	0	16	3	0
8	A	66	0	88	8	0
8	B	60	0	80	8	0
9	A	4	0	3	4	0
9	B	4	0	3	4	0
10	A	1086	0	0	9	0
10	B	1033	0	0	7	0
All	All	22610	0	20417	331	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 8.

The worst 5 of 331 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)
7:B:5102:YSH:C1	7:B:5102:YSH:N2	1.70	1.52
7:A:5101:YSH:C1	7:A:5101:YSH:N2	1.68	1.51
1:A:3:ALA:HB1	1:A:228:ARG:H	1.20	1.06
1:A:537:LYS:HG2	1:A:538:LEU:H	1.28	0.98
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.30	0.97

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%)	1244 (96%)	41 (3%)	8 (1%)	30 21
1	B	1290/1332 (97%)	1234 (96%)	44 (3%)	12 (1%)	21 12
All	All	2583/2664 (97%)	2478 (96%)	85 (3%)	20 (1%)	24 14

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	B	1008	SER
1	B	1287	ASN
1	B	1324	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%)	1086 (99%)	15 (1%)	74	75
1	B	1098/1128 (97%)	1088 (99%)	10 (1%)	84	86
All	All	2199/2256 (98%)	2174 (99%)	25 (1%)	80	82

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	PRO
1	A	1208	LEU
1	B	1145	ASN
1	A	1145	ASN
1	A	1239	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1284	GLN
1	B	131	GLN
1	B	1145	ASN
1	A	1324	ASN
1	B	146	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 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 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	6.48	12 (63%)	19,40,40	3.00	8 (42%)
5	MOS	A	3004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	A	3005	-	48,58,58	2.63	21 (43%)	54,89,89	3.22	24 (44%)
8	GOL	A	5001	-	5,5,5	0.24	0	5,5,5	0.37	0
8	GOL	A	5002	-	5,5,5	0.17	0	5,5,5	0.33	0
8	GOL	A	5003	-	5,5,5	0.26	0	5,5,5	0.30	0
8	GOL	A	5004	-	5,5,5	0.23	0	5,5,5	0.30	0
8	GOL	A	5005	-	5,5,5	0.25	0	5,5,5	0.31	0
8	GOL	A	5006	-	5,5,5	0.17	0	5,5,5	0.39	0
8	GOL	A	5011	-	5,5,5	0.15	0	5,5,5	0.33	0
8	GOL	A	5016	-	5,5,5	0.21	0	5,5,5	0.46	0
8	GOL	A	5017	-	5,5,5	0.22	0	5,5,5	0.29	0
8	GOL	A	5018	-	5,5,5	0.29	0	5,5,5	0.25	0
8	GOL	A	5019	-	5,5,5	0.27	0	5,5,5	0.26	0
7	YSH	A	5101	-	18,23,23	8.56	11 (61%)	24,33,33	3.97	8 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ACY	A	5201	-	1,3,3	0.93	0	0,3,3	0.00	-
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	-
4	MTE	B	4003	5	19,26,26	6.22	12 (63%)	19,40,40	2.97	9 (47%)
5	MOS	B	4004	4	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	B	4005	-	48,58,58	2.75	23 (47%)	54,89,89	3.17	20 (37%)
8	GOL	B	5007	-	5,5,5	0.22	0	5,5,5	0.29	0
8	GOL	B	5008	-	5,5,5	0.19	0	5,5,5	0.36	0
8	GOL	B	5009	-	5,5,5	0.26	0	5,5,5	0.27	0
8	GOL	B	5012	-	5,5,5	0.16	0	5,5,5	0.41	0
8	GOL	B	5013	-	5,5,5	0.17	0	5,5,5	0.26	0
8	GOL	B	5014	-	5,5,5	0.16	0	5,5,5	0.35	0
8	GOL	B	5015	-	5,5,5	0.20	0	5,5,5	0.28	0
8	GOL	B	5020	-	5,5,5	0.20	0	5,5,5	0.31	0
8	GOL	B	5021	-	5,5,5	0.21	0	5,5,5	0.36	0
8	GOL	B	5022	-	5,5,5	0.17	0	5,5,5	0.33	0
7	YSH	B	5102	-	18,23,23	8.76	11 (61%)	24,33,33	3.94	8 (33%)
9	ACY	B	5202	-	1,3,3	1.35	0	0,3,3	0.00	-

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
8	GOL	A	5001	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5002	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5003	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5004	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5005	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5006	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5011	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5016	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5017	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5018	-	-	0/4/4/4	0/0/0/0
8	GOL	A	5019	-	-	0/4/4/4	0/0/0/0
7	YSH	A	5101	-	-	0/12/16/16	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ACY	A	5201	-	-	0/0/0/0	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	FAD	B	4005	-	-	0/30/50/50	0/6/6/6
8	GOL	B	5007	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5008	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5009	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5012	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5013	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5014	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5015	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5020	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5021	-	-	0/4/4/4	0/0/0/0
8	GOL	B	5022	-	-	0/4/4/4	0/0/0/0
7	YSH	B	5102	-	-	0/12/16/16	0/2/2/2
9	ACY	B	5202	-	-	0/0/0/0	0/0/0/0

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3003	MTE	C6-N5	-6.73	1.36	1.45
4	B	4003	MTE	P-O4'	-6.67	1.37	1.60
4	A	3003	MTE	P-O4'	-6.51	1.38	1.60
4	B	4003	MTE	P-O3P	-5.38	1.35	1.54
4	A	3003	MTE	P-O3P	-5.32	1.35	1.54

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3005	FAD	N3A-C2A-N1A	-14.65	117.67	128.89
6	B	4005	FAD	N3A-C2A-N1A	-14.48	117.81	128.89
4	A	3003	MTE	C10-C9-N5	-3.85	113.99	118.85
4	B	4003	MTE	N3-C2-N1	-3.70	119.48	125.53
4	A	3003	MTE	N3-C2-N1	-3.68	119.50	125.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002	FES	1	0
4	A	3003	MTE	1	0
5	A	3004	MOS	1	0
6	A	3005	FAD	4	0
8	A	5001	GOL	1	0
8	A	5002	GOL	2	0
8	A	5006	GOL	2	0
8	A	5011	GOL	2	0
8	A	5019	GOL	1	0
7	A	5101	YSH	3	0
9	A	5201	ACY	4	0
4	B	4003	MTE	1	0
5	B	4004	MOS	2	0
6	B	4005	FAD	3	0
8	B	5008	GOL	2	0
8	B	5013	GOL	1	0
8	B	5014	GOL	2	0
8	B	5020	GOL	1	0
8	B	5022	GOL	2	0
7	B	5102	YSH	3	0
9	B	5202	ACY	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 will therefore be empty.

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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