



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:01 PM GMT

PDB ID : 1N5X  
Title : Xanthine Dehydrogenase from Bovine Milk with Inhibitor TEI-6720 Bound  
Authors : Okamoto, K.; Eger, B.T.; Nishino, T.; Kondo, S.; Pai, E.F.; Nishino, T.  
Deposited on : 2002-11-07  
Resolution : 2.80 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

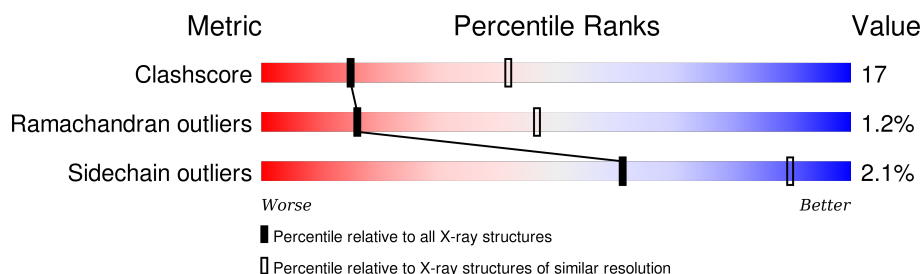
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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	1331	
1	B	1331	

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
4	MOS	A	3004	-	-	X	-
4	MOS	B	4004	-	-	X	-

## 2 Entry composition [i](#)

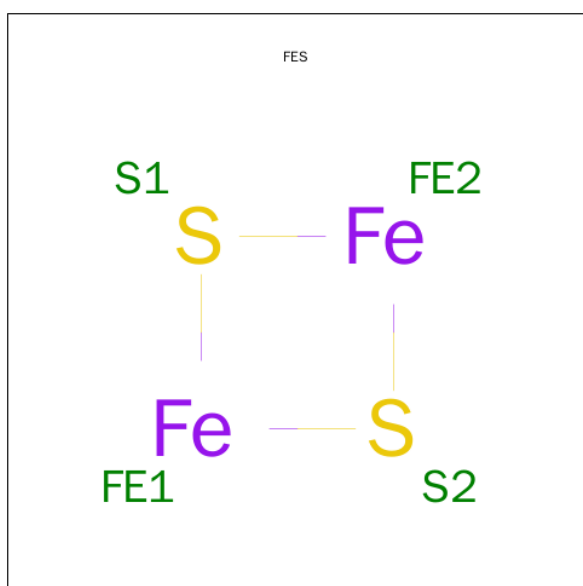
There are 6 unique types of molecules in this entry. The entry contains 20268 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

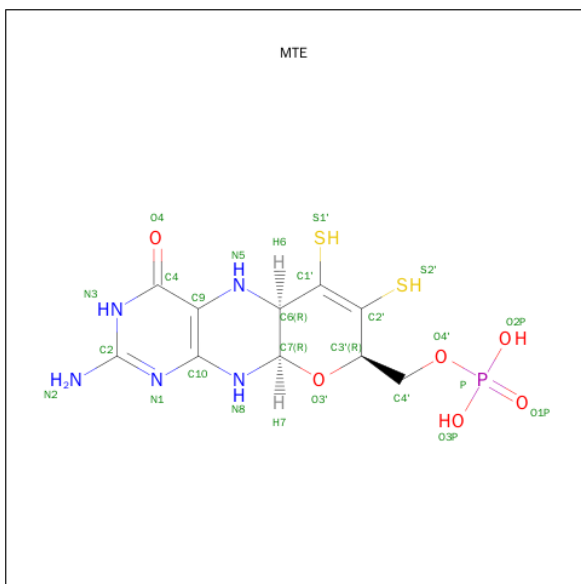
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			
1	B	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



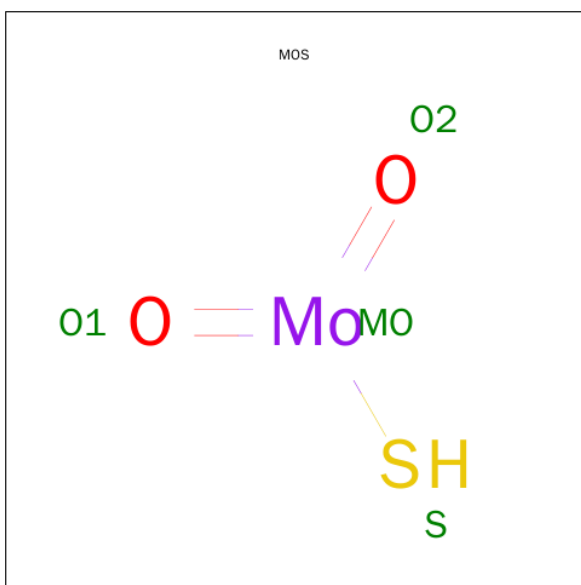
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 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:  $C_{10}H_{14}N_5O_6P S_2$ ).



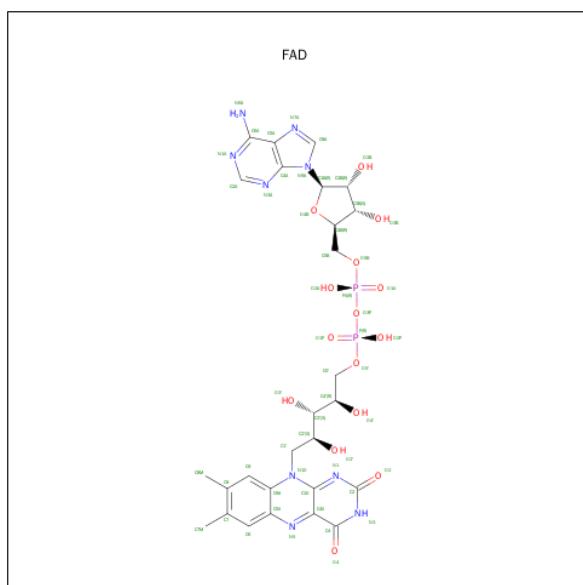
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $HMoO_2S$ ).



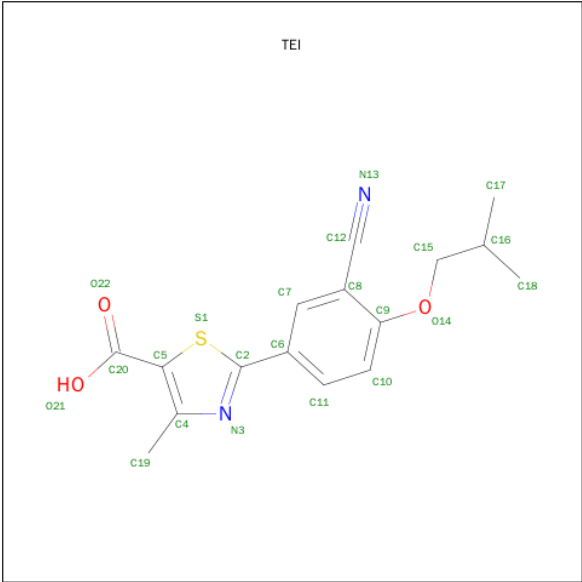
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 6 is 2-(3-CYANO-4-ISOBUTOXY-PHENYL)-4-METHYL-5-THIAZOLE-CARBOXYLIC ACID (three-letter code: TEI) (formula:  $C_{16}H_{16}N_2O_3S$ ).



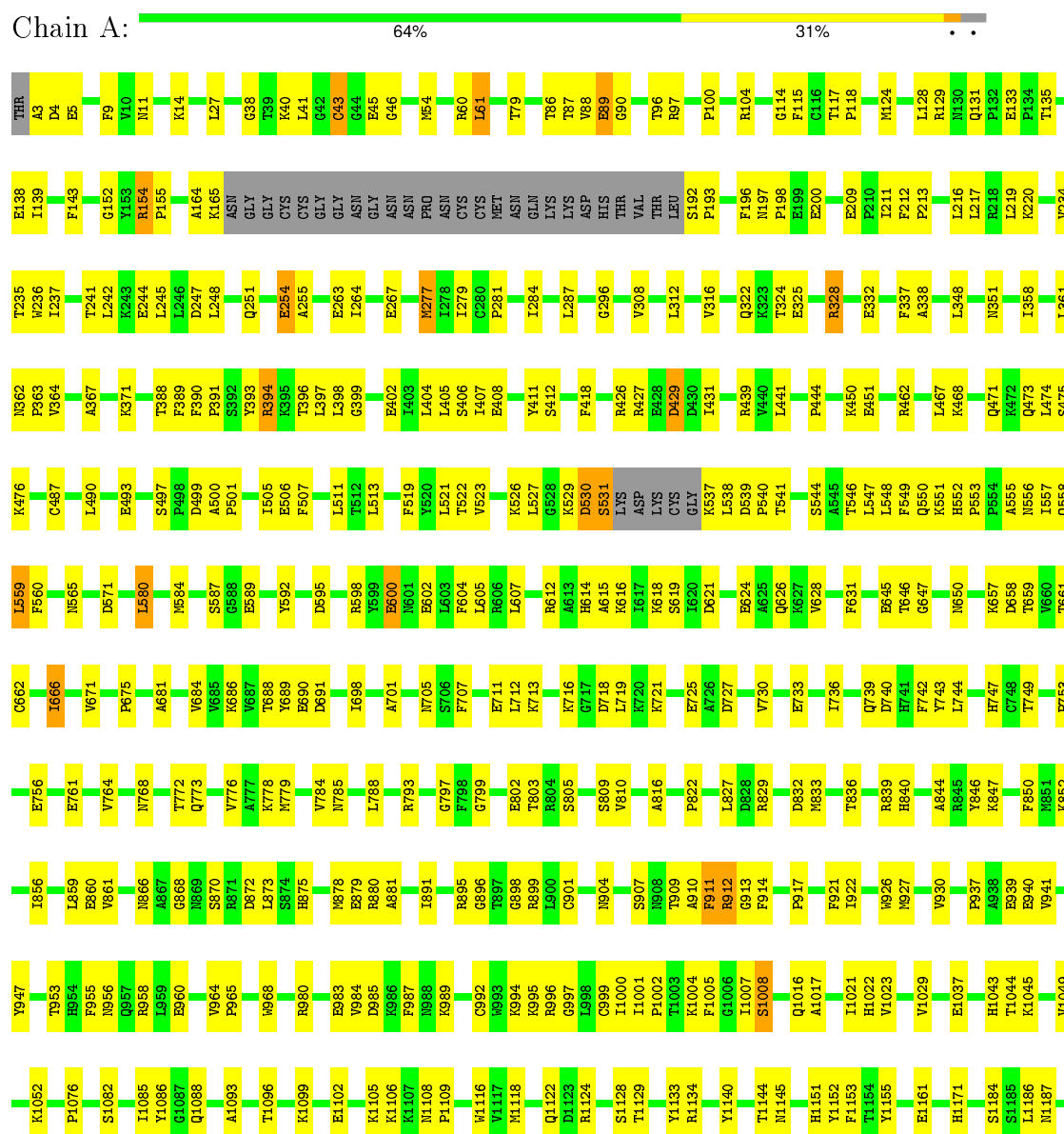
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			22	16	2	3	1		
6	B	1	Total	C	N	O	S	0	0
			22	16	2	3	1		

### 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 ( $RSRZ > 2$ ). 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



I1190	D1311
D1191	K1312
I1192	F1313
E1196	T1314
V1200	T1315
L1203	L1316
Y1213	CYS
S1214	VAL
P1215	THR
E1216	GLY
P1224	ALA
K1228	PRO
I1235	GLY
E1238	ASN
F1239	K1326
N1249	L1330
K1250	R1331
K1251	V1332
Y1254	
A1255	
S1256	
K1257	
A1258	
V1259	
P1262	
P1263	
L1264	
F1271	
F1272	
A1273	
A1280	
A1281	
Q1284	
H1285	
T1286	
N1287	
R1295	
S1298	
P1299	
A1300	
T1301	
P1302	
V1310	

• Molecule 1: Xanthine Dehydrogenase

Chain B:  64% 31%

THR	F143	T241	A367	E493	H584	V685	T772	G868	L959	I1085	L1203	L1316
A3	G152	L242	K371	S497	S587	K686	Q773	S870	E960	Y1086	L1203	CYS
E5	Y153	F243	T388	A500	E589	T688	V776	R871	V964	Q1088	S1214	VAL
F9	P155	E244	F389	I505	Y592	E689	A777	D872	P965	A1093	S1215	GLY
Y10	A164	L245	F390	E506	F595	D691	K778	S874	W968	T1096	E1216	ALA
N11	K165	L246	P391	F507	D595	I695	K779	H875	R980	K1099	P1224	PRO
K14	ASN	Q251	S392	F507	R598	L698	V784	M878	E983	E1102	K1228	GLY
G38	GLY	E252	R394	L511	R599	E699	L788	R879	V984	E1102	I1235	ALA
T39	CYS	A255	K395	T512	E600	D700	R880	R880	D985	K1105	E1238	PRO
K40	CYS	E263	T396	L513	H601	A701	R793	A881	K986	K1106	F1239	ASN
C43	GLY	I264	L397	F519	B602	N705	G797	I891	F987	N1108	K1249	CYS
G44	ASN	I264	L398	Y520	F604	S706	F798	R895	K988	P1109	K1250	THR
E45	ASN	E267	C399	L521	L605	F707	G799	G896	K989	N1116	K1251	GLY
G46	ASN	E277	E402	T522	R606	E711	E802	T897	K994	V1117	Y1254	ALA
M54	PRO	P277	L403	V823	L607	L712	T803	G898	K995	M1118	A1255	PRO
R60	ASN	I278	L404	K526	R612	K713	R804	R899	R996	Q1122	K1257	GLY
L61	CYS	I279	S406	L527	A613	K716	S805	C901	L998	D1123	A1258	ALA
T79	CYS	C280	E408	K528	H614	G717	S809	N904	C999	R1124	V1259	ASN
T86	MET	P281	E408	D530	A615	D718	V810	I1000	I1000			
T87	GLN	I284	Y411	S531	A616	L719	A816	I1001	I1002			
V88	LYS	L287	S412	L538	R617	K720	R816	S907	T1003	S1128	P1262	
E89	ASP	G296	F418	D639	S619	K721	P822	T909	K1004	T1129	P1263	
G90	HIS	V308	R426	D639	L620	E725	P822	A910	F1005	Y1133	L1264	
THR	THR	V316	R427	P540	D621	A726	L927	F911	G1006	R1134	F1271	
VAL	THR	Q322	R427	T541	B624	D727	D828	R912	S1008	Y1140	F1272	
THR	THR	E325	E428	T541	D626	V730	R829	F914	Q1016	T1144	A1273	
P192	P193	R328	D430	T541	R627	E733	D832	P917	A1017	N1145	A1280	
F196	M197	Q322	I431	S544	V628	I736	T836	F921	I1021	H1151	A1281	
M197	T324	T323	R439	A545	F631	Q739	R836	I922	H1022	Y1152	R1282	
E199	F115	E325	L441	T547	B545	D740	R839	W926	V1023	F1153	A1283	
E200	G116	E325	P444	L548	N650	H741	H840	M927	S1028	T1154	H1285	
E209	P118	R328	K450	F549	R657	F742	A844	V930	V1029	Y1155	T1286	
T211	M124	E332	E451	Q550	D658	Y743	R845	P937	L1030	E1161	N1287	
T211	P213	F337	R462	H552	T659	L744	R847	A938	V1031	H1171	R1295	
P213	L128	A338	K462	P553	V660	H747	F850	E939	E1037	S1184	S1298	
L216	R129	L348	L467	A555	C662	T749	R851	V941	H1043	L1185	A1300	
L217	H130	N351	K468	N557	C662	P753	K852	Y947	T1044	N1187	T1301	
R218	Q131	N351	Q471	Q558	V671	E756	R856	K948	V1049	I1190	A1308	
E133	E133	I358	Q473	L559	V671	E761	R859	T953	K1052	D1191	V1310	
P134	P134	I361	L474	F560	P675	V764	P861	H954	P1076	I1192	D1311	
T135	T135	N362	S475	D571	A681	V764	R866	F955	Y957	E1196	K1312	
I139	I139	W364	K476	L580	V684	N768	A867	N956	S1082	T1314	F1313	
I237	I237	V364	C487					R958		V1200	T1315	



## 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, $\alpha$ , $\beta$ , $\gamma$	168.27Å 124.66Å 147.32Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	93.7 (20.00-2.80)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.244 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MOS, TEI, 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	0.43	0/10242	0.66	0/13860
1	B	0.43	0/10242	0.66	0/13860
All	All	0.43	0/20484	0.66	0/27720

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 [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	10023	0	10026	349	5
1	B	10023	0	10026	348	4
2	A	8	0	0	2	0
2	B	8	0	0	2	0
3	A	24	0	10	4	0
3	B	24	0	10	4	0
4	A	4	0	0	8	0
4	B	4	0	0	8	0
5	A	53	0	29	2	0
5	B	53	0	29	2	0
6	A	22	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	22	0	15	0	0
All	All	20268	0	20160	706	5

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 17.

The worst 5 of 706 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:A:1330:LEU:HD22	1:A:1331:ARG:N	1.62	1.14
1:B:1330:LEU:HD22	1:B:1331:ARG:N	1.62	1.13
1:A:537:LYS:HG3	1:A:538:LEU:H	1.18	1.07
1:A:1286:THR:HG22	1:A:1287:ASN:H	1.19	1.07
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.19	1.04

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ASP:OD2	1:B:1326:LYS:O[1_545]	1.88	0.32
1:A:501:PRO:CA	1:B:1328:TRP:CB[1_545]	1.96	0.24
1:A:1213:TYR:CB	1:B:1332:VAL:CG1[1_545]	2.09	0.11
1:A:565:ASN:CB	1:A:565:ASN:CB[2_655]	2.17	0.03
1:A:501:PRO:CB	1:B:1328:TRP:CG[1_545]	2.19	0.01

## 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	1282/1331 (96%)	1173 (92%)	94 (7%)	15 (1%)	16 47
1	B	1282/1331 (96%)	1172 (91%)	95 (7%)	15 (1%)	16 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2564/2662 (96%)	2345 (92%)	189 (7%)	30 (1%)	16	47

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	530	ASP
1	A	1008	SER
1	A	1192	ILE
1	A	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	1095/1127 (97%)	1072 (98%)	23 (2%)	61	90
1	B	1095/1127 (97%)	1072 (98%)	23 (2%)	61	90
All	All	2190/2254 (97%)	2144 (98%)	46 (2%)	61	90

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1310	VAL
1	B	254	GLU
1	B	1284	GLN
1	A	1330	LEU
1	B	89	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1145	ASN
1	B	131	GLN
1	B	1145	ASN

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Mol	Chain	Res	Type
1	A	1284	GLN
1	A	1287	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 ⓘ

12 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	MTE	A	3003	4	19,26,26	6.07	11 (57%)	19,40,40	2.79	9 (47%)
4	MOS	A	3004	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	A	3005	-	48,58,58	4.83	34 (70%)	54,89,89	3.06	27 (50%)
6	TEI	A	3006	-	17,23,23	3.81	5 (29%)	16,32,32	1.77	4 (25%)
2	FES	B	4001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	B	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
3	MTE	B	4003	4	19,26,26	6.07	11 (57%)	19,40,40	2.79	8 (42%)
4	MOS	B	4004	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	B	4005	-	48,58,58	4.83	34 (70%)	54,89,89	3.07	27 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	TEI	B	4006	-	17,23,23	3.81	5 (29%)	16,32,32	1.76	4 (25%)

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	MTE	A	3003	4	-	0/6/34/34	0/3/3/3
4	MOS	A	3004	3	-	0/0/0/0	0/0/0/0
5	FAD	A	3005	-	-	0/30/50/50	0/6/6/6
6	TEI	A	3006	-	-	0/11/15/15	0/2/2/2
2	FES	B	4001	1	-	0/0/4/4	0/1/1/1
2	FES	B	4002	1	-	0/0/4/4	0/1/1/1
3	MTE	B	4003	4	-	0/6/34/34	0/3/3/3
4	MOS	B	4004	3	-	0/0/0/0	0/0/0/0
5	FAD	B	4005	-	-	0/30/50/50	0/6/6/6
6	TEI	B	4006	-	-	0/11/15/15	0/2/2/2

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3005	FAD	C5'-C4'	-9.42	1.37	1.51
5	B	4005	FAD	C5'-C4'	-9.38	1.37	1.51
3	A	3003	MTE	P-O4'	-7.39	1.35	1.60
3	B	4003	MTE	P-O4'	-7.38	1.35	1.60
3	B	4003	MTE	P-O3P	-5.60	1.34	1.54

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4005	FAD	C5X-C9A-N10	-6.65	112.57	117.62
5	A	3005	FAD	C5X-C9A-N10	-6.62	112.58	117.62
5	B	4005	FAD	C4-C4X-C10	-6.25	115.94	119.94
5	A	3005	FAD	C4-C4X-C10	-6.21	115.96	119.94
5	B	4005	FAD	O4'-C4'-C5'	-6.00	97.12	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	FES	1	0
2	A	3002	FES	1	0
3	A	3003	MTE	4	0
4	A	3004	MOS	8	0
5	A	3005	FAD	2	0
2	B	4001	FES	1	0
2	B	4002	FES	1	0
3	B	4003	MTE	4	0
4	B	4004	MOS	8	0
5	B	4005	FAD	2	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.