



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 01:04 am BST

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)

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A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

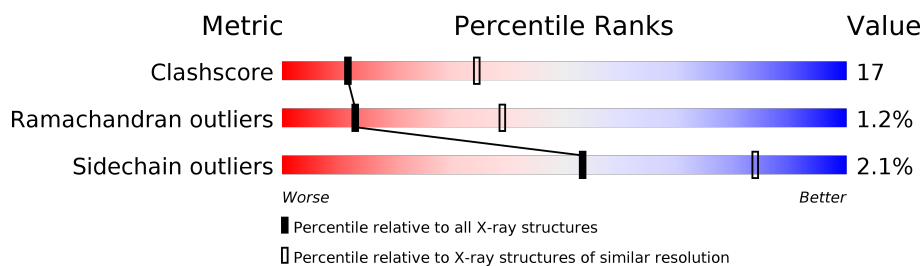
# 1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 respectively. 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  $\leq 5\%$ .

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](#)

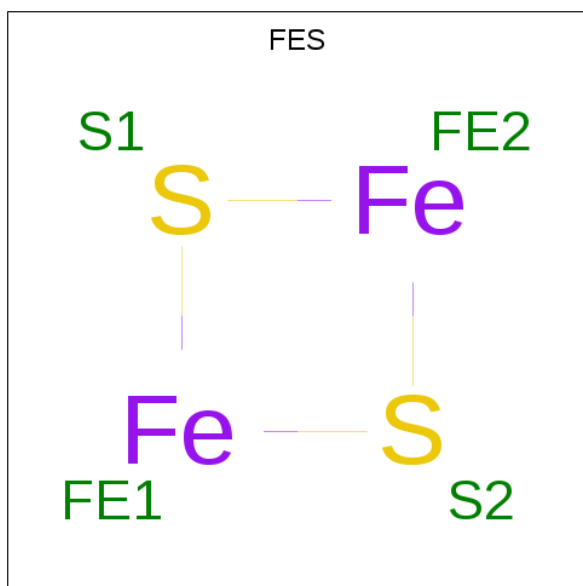
There are 6 unique types of molecules in this entry. The entry contains 20268 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

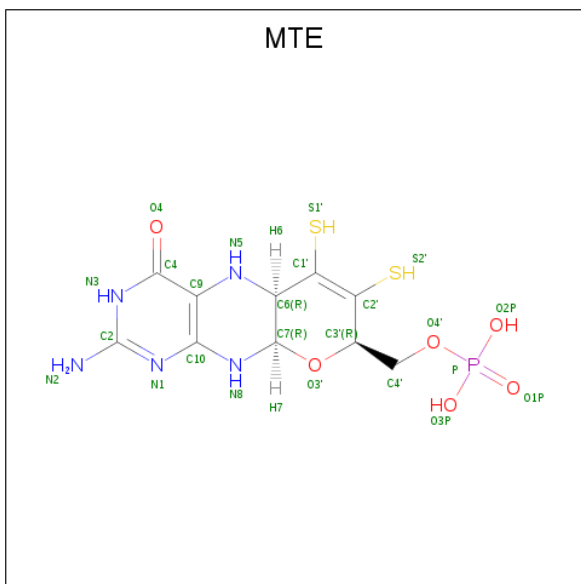
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			
1	B	1290	Total	C	N	O	S	0	0	0
			10023	6373	1718	1873	59			

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



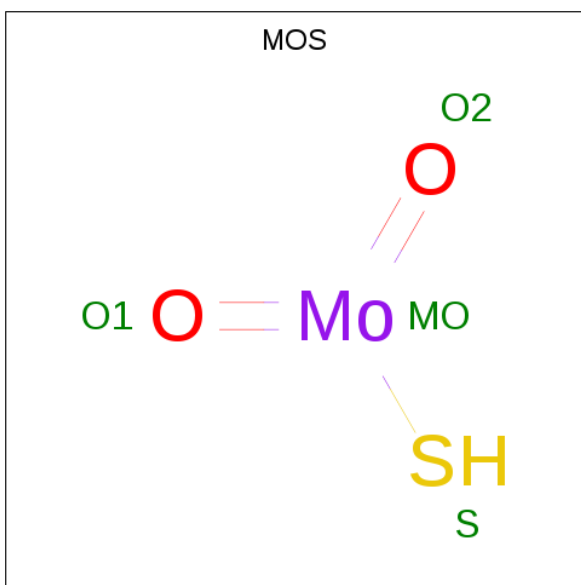
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- 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:  $C_{10}H_{14}N_5O_6PS_2$ ).



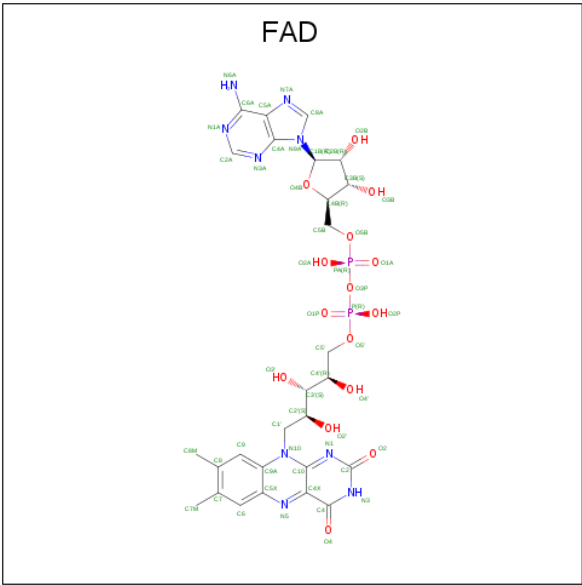
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
3	B	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

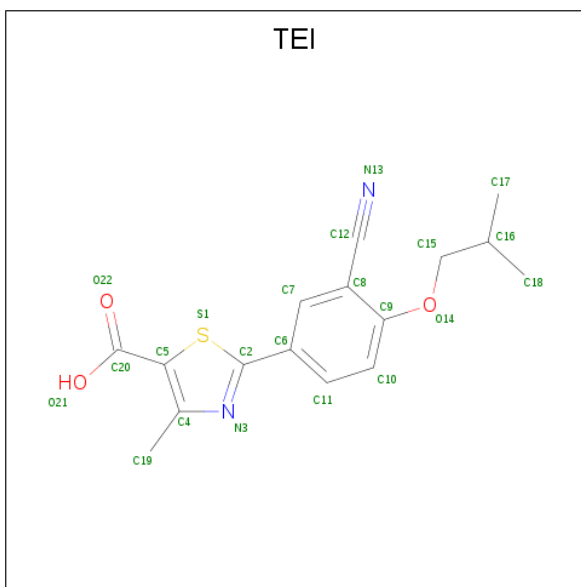
- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $\text{HMoO}_2\text{S}$ ).



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<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).





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		



T1190	D1311
D1191	K1312
T1192	F1313
E1196	T1314
T1315	L1316
V1200	CYS
L1203	VAL
Y1213	THR
S1214	GLY
P1215	ALA
E1216	PRO
P1224	GLY
K1228	ASN
T1235	K1326
E1238	L1330
F1239	R1331
L1264	V1332
H1269	
K1260	
K1251	
Y1254	
A1255	
S1256	
K1257	
A1258	
V1259	
P1262	
P1263	
L1264	
F1271	
F1272	
A1273	
A1280	
A1281	
Q1284	
H1285	
T1286	
H1287	
R1295	
S1298	
P1299	
A1300	
T1301	
P1302	
V1310	

• Molecule 1: Xanthine Dehydrogenase

Chain B:  64% 31%

THR	F143	T241	A367	E493	V584	V685	T772	G668	L959	I1085	L1203
A3	G152	T242	A371	S497	S587	K686	Q773	R669	E960	Y1086	L1203
E5	Y153	K243	K371	S497	E589	T688	A776	R671	V964	Q1088	S1214
F9	P155	E244	T388	A500	E592	V689	A777	D872	P965	A1093	P1215
Y10	A164	L246	F389	I505	V592	D691	K773	S874	W968	T1096	E1216
H11	K165	L248	F390	E506	V595	T695	H779	H575	R980	K1099	P1224
K14	ASN	Q251	P391	F507	E598	T698	V784	R878	E983	E1102	K1228
GLY	GLY	K251	S392	F519	V599	D700	L788	R880	E984	K1105	I1235
ALA	CYS	E256	K394	V512	E601	A701	R793	A881	D985	K1107	E1238
PRO	CYS	A255	T396	L513	E602	F705	G797	T891	K986	K1108	F1239
GLY	GLY	E263	L397	V520	E606	S706	F798	R895	N988	P1109	N1249
ASN	GLY	L264	G399	L521	V607	F707	G799	G896	K989	P1109	K1250
ASN	ASN	E267	E402	T522	V608	E711	E802	T897	K994	V1116	K1251
PRO	ASN	K277	L404	V523	L607	L712	T803	G898	K995	Y1117	Y1254
ASN	ASN	L278	L405	K526	R612	K713	S805	R899	R996	M1118	A1255
CYS	CYS	L279	S406	L527	V614	G716	S809	L900	G997	L900	S1256
CYS	CYS	G280	L407	V528	R614	K717	V810	C901	C999	Q1122	K1257
MET	MET	P281	E408	K529	V616	D718	P822	N904	I1000	D1123	A1258
ASN	ASN	L284	Y411	S531	R617	L719	L827	S907	I1001	R1124	V1259
GLN	LYS	L287	S412	LYS	V618	K720	A816	S908	P1002	S1128	P1262
LYS	LYS	L287	F418	ASP	S619	K721	K828	T909	K1004	T1129	P1263
ASP	ASP	L296	V418	LYS	V620	K725	R829	F914	F1005	A910	L1264
HIS	HIS	G296	R426	CYS	D621	E726	L827	F911	G1006	Y1133	F1271
THR	THR	V308	R427	GLY	E624	A728	D828	R912	I1007	R1134	F1272
VAL	VAL	L312	E428	L538	V625	D727	R829	G913	S1008	Y1140	A1273
THR	THR	V316	D429	D539	V626	V730	V833	F914	Q1016	T1144	A1280
S192	S192	P193	D430	P540	V627	E733	V836	F917	A1017	N1145	A1281
P193	P193	F196	I431	T541	V628	E736	T836	P921	I1021	H1151	A1282
F196	F196	M197	R439	S544	V631	I736	T836	I922	H1022	Y1152	A1283
M197	M197	P198	V440	A545	E645	Q739	H839	N926	V1023	F1153	Q1284
P198	P198	E325	L441	T546	V645	D740	H840	N927	S1028	T1154	H1285
E199	E199	E325	P444	L547	N650	H741	H844	V930	V1029	Y1155	T1286
E200	E200	R328	P444	L548	V650	F742	A844	V930	I1030	E1161	H1287
E209	E209	E332	K450	F549	V657	I742	R845	V937	V1031	H1171	R1295
F210	F210	E332	E451	K551	D658	L744	Y846	P937	E1037	S1298	S1298
I211	I211	F337	R462	H552	T659	H747	K847	E939	E1037	P1299	P1299
P213	P213	A338	P553	P553	V660	C748	F650	R940	H1043	A1300	A1300
L216	L216	L348	A555	A555	C662	I749	N651	V941	T1044	T1301	T1301
L217	L217	N351	N556	N556	C662	P753	K852	Y947	K1045	P1302	P1302
R218	R218	N351	I557	I557	T666	E756	L856	K948	V1049	A1308	A1308
E133	E133	I358	Q558	Q558	V671	E756	L856	K948	K1052	C1309	C1309
P194	P194	T135	F560	F560	P675	E761	L859	T953	V1310	D1311	D1311
T135	T135	L361	D571	D571	V681	V764	E854	P955	P1076	E1196	E1196
E138	E138	N362	L580	L580	A681	N866	H957	N956	F1313	T1314	T1314
I139	I139	V364	V684	V684	V684	A867	A867	N958	V1200	T1315	T1315



L1316	CYS
	VAL
	THR
	GLY
	ALA
	PRO
	GLY
	ASN
	CYS
K1326	
P1327	
H1328	
S1329	
L1330	
R1331	
V1332	

## 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, $\alpha$ , $\beta$ , $\gamma$	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:1286:THR:HG22	1:A:1287:ASN:H	1.19	1.07
1:A:537:LYS:HG3	1:A:538:LEU:H	1.18	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%)	13 39
1	B	1282/1331 (96%)	1172 (91%)	95 (7%)	15 (1%)	13 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2564/2662 (96%)	2345 (92%)	189 (7%)	30 (1%)	13	39

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%)	53	84
1	B	1095/1127 (97%)	1072 (98%)	23 (2%)	53	84
All	All	2190/2254 (97%)	2144 (98%)	46 (2%)	53	84

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	$\# Z  > 2$
4	MOS	B	4004	3	0,3,3	0.00	-	-		
6	TEI	A	3006	-	16,23,23	3.98	6 (37%)	16,32,32	1.48	3 (18%)
3	MTE	A	3003	4	21,26,26	6.04	12 (57%)	21,40,40	3.27	8 (38%)
3	MTE	B	4003	4	21,26,26	6.04	12 (57%)	21,40,40	3.27	8 (38%)
6	TEI	B	4006	-	16,23,23	3.97	6 (37%)	16,32,32	1.48	3 (18%)
5	FAD	B	4005	-	51,58,58	5.26	37 (72%)	60,89,89	3.11	30 (50%)
5	FAD	A	3005	-	51,58,58	5.26	37 (72%)	60,89,89	3.10	30 (50%)
2	FES	B	4001	1	0,4,4	0.00	-	-		
2	FES	A	3002	1	0,4,4	0.00	-	-		
4	MOS	A	3004	3	0,3,3	0.00	-	-		

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	-	-		
2	FES	B	4002	1	0,4,4	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
6	TEI	A	3006	-	-	0/11/15/15	0/2/2/2
3	MTE	A	3003	4	-	0/6/34/34	0/3/3/3
3	MTE	B	4003	4	-	0/6/34/34	0/3/3/3
6	TEI	B	4006	-	-	0/11/15/15	0/2/2/2
5	FAD	B	4005	-	-	7/30/50/50	0/6/6/6
5	FAD	A	3005	-	-	7/30/50/50	0/6/6/6
2	FES	B	4001	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	B	4002	1	-	-	0/1/1/1

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3003	MTE	C7-C6	17.21	1.67	1.53
3	B	4003	MTE	C7-C6	17.21	1.67	1.53
5	B	4005	FAD	C9A-N10	14.88	1.58	1.38
5	A	3005	FAD	C9A-N10	14.82	1.58	1.38
5	B	4005	FAD	C4X-C10	12.59	1.51	1.38

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3003	MTE	C4-C9-N5	10.14	127.63	119.12
3	B	4003	MTE	C4-C9-N5	10.12	127.62	119.12
5	B	4005	FAD	C5X-C9A-N10	-7.10	112.57	117.72
5	A	3005	FAD	C5X-C9A-N10	-7.08	112.58	117.72
5	B	4005	FAD	C1'-N10-C9A	7.02	123.82	118.29

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	4005	FAD	N10-C1'-C2'-O2'
5	B	4005	FAD	C2'-C3'-C4'-O4'
5	B	4005	FAD	O3'-C3'-C4'-O4'
5	B	4005	FAD	O3'-C3'-C4'-C5'
5	A	3005	FAD	N10-C1'-C2'-O2'

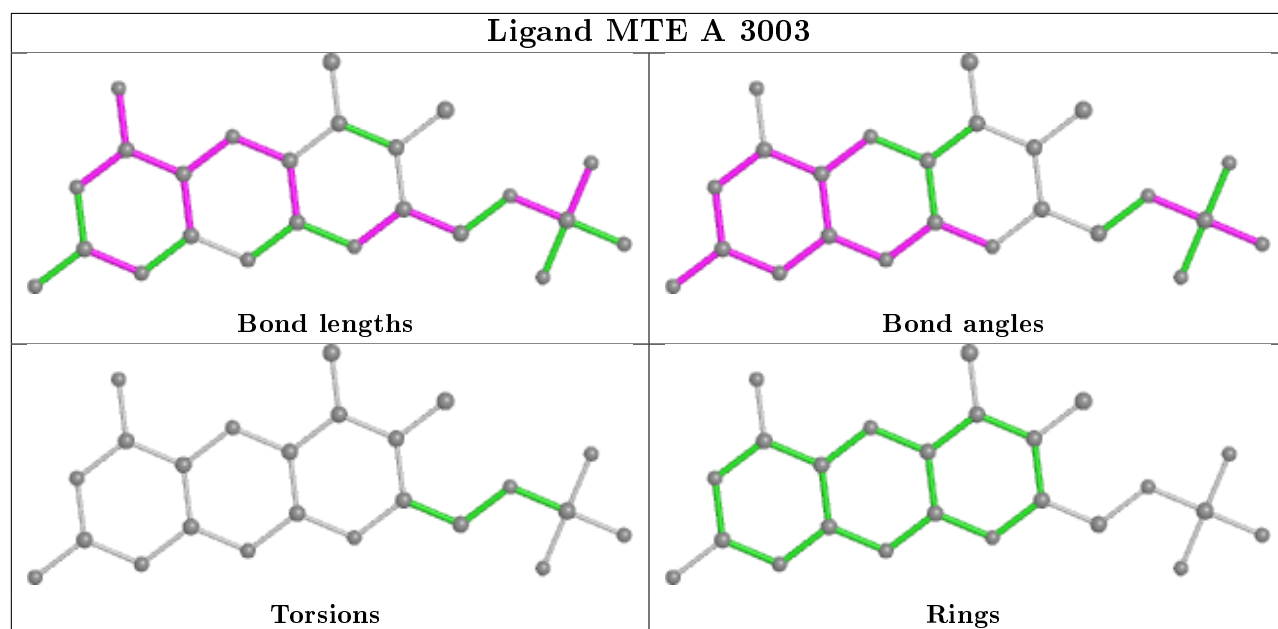
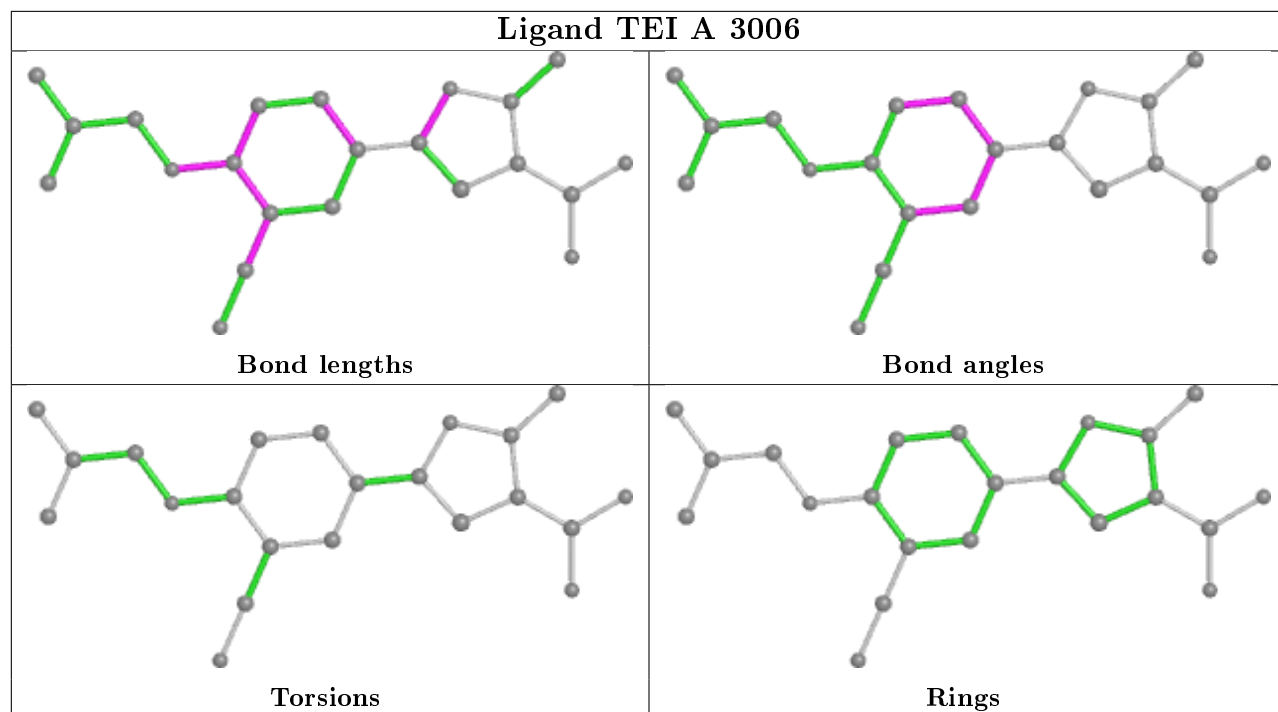
There are no ring outliers.

10 monomers are involved in 28 short contacts:

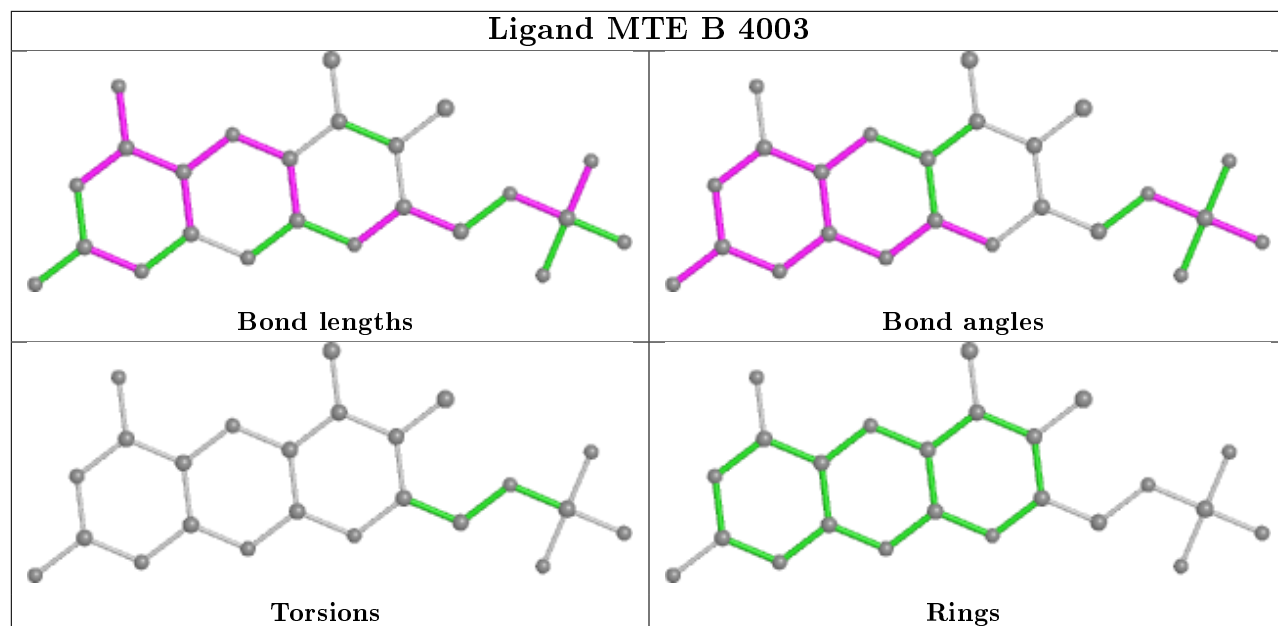
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4004	MOS	8	0
3	A	3003	MTE	4	0
3	B	4003	MTE	4	0
5	B	4005	FAD	2	0
5	A	3005	FAD	2	0
2	B	4001	FES	1	0
2	A	3002	FES	1	0
4	A	3004	MOS	8	0
2	A	3001	FES	1	0
2	B	4002	FES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

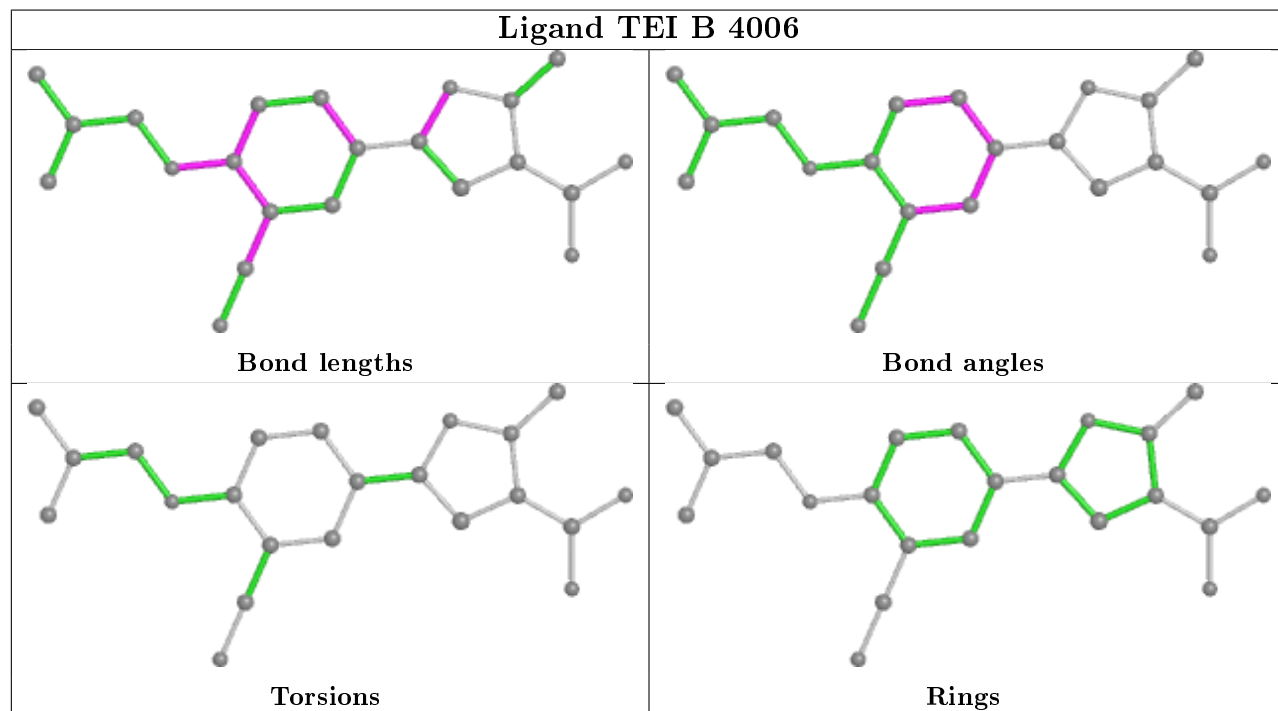


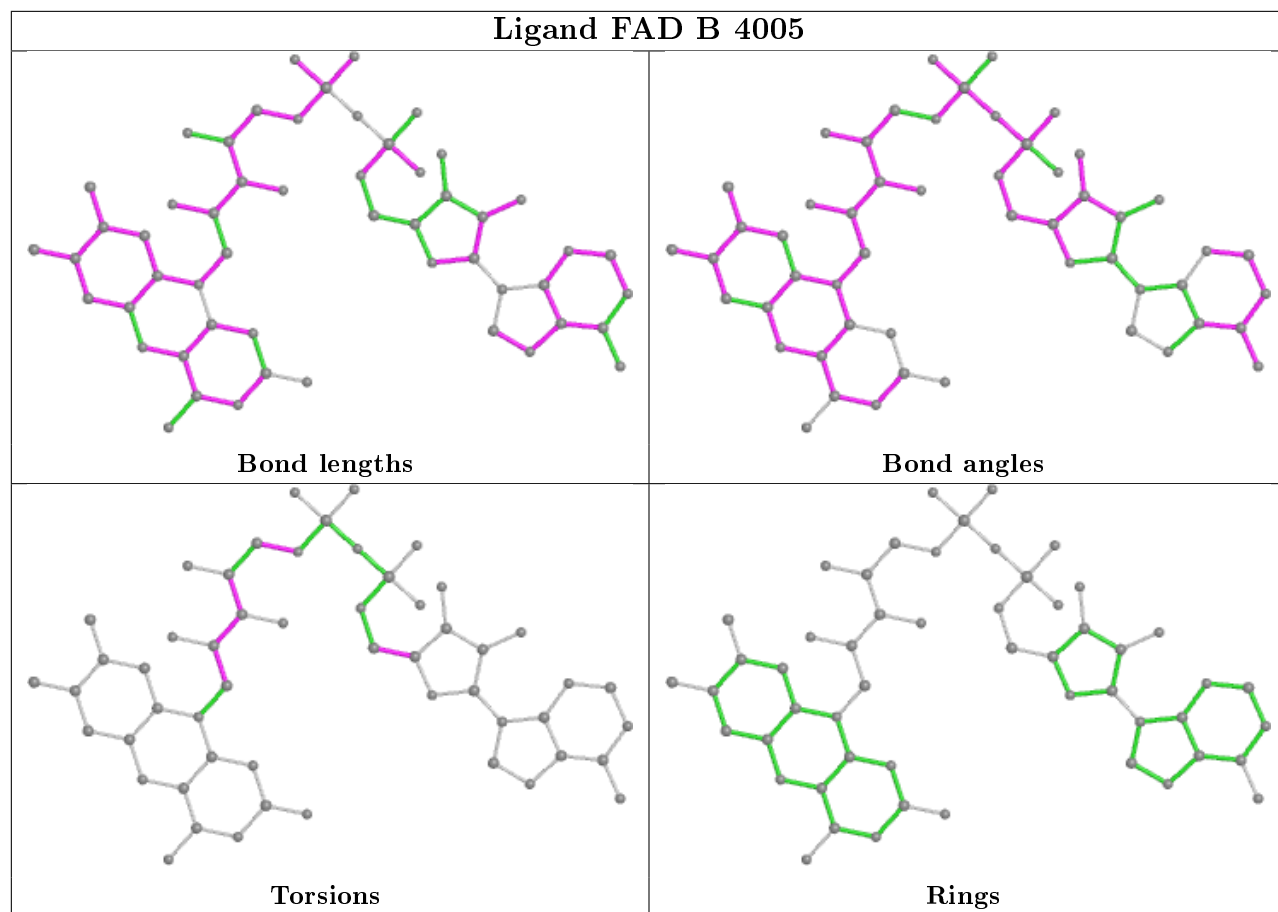


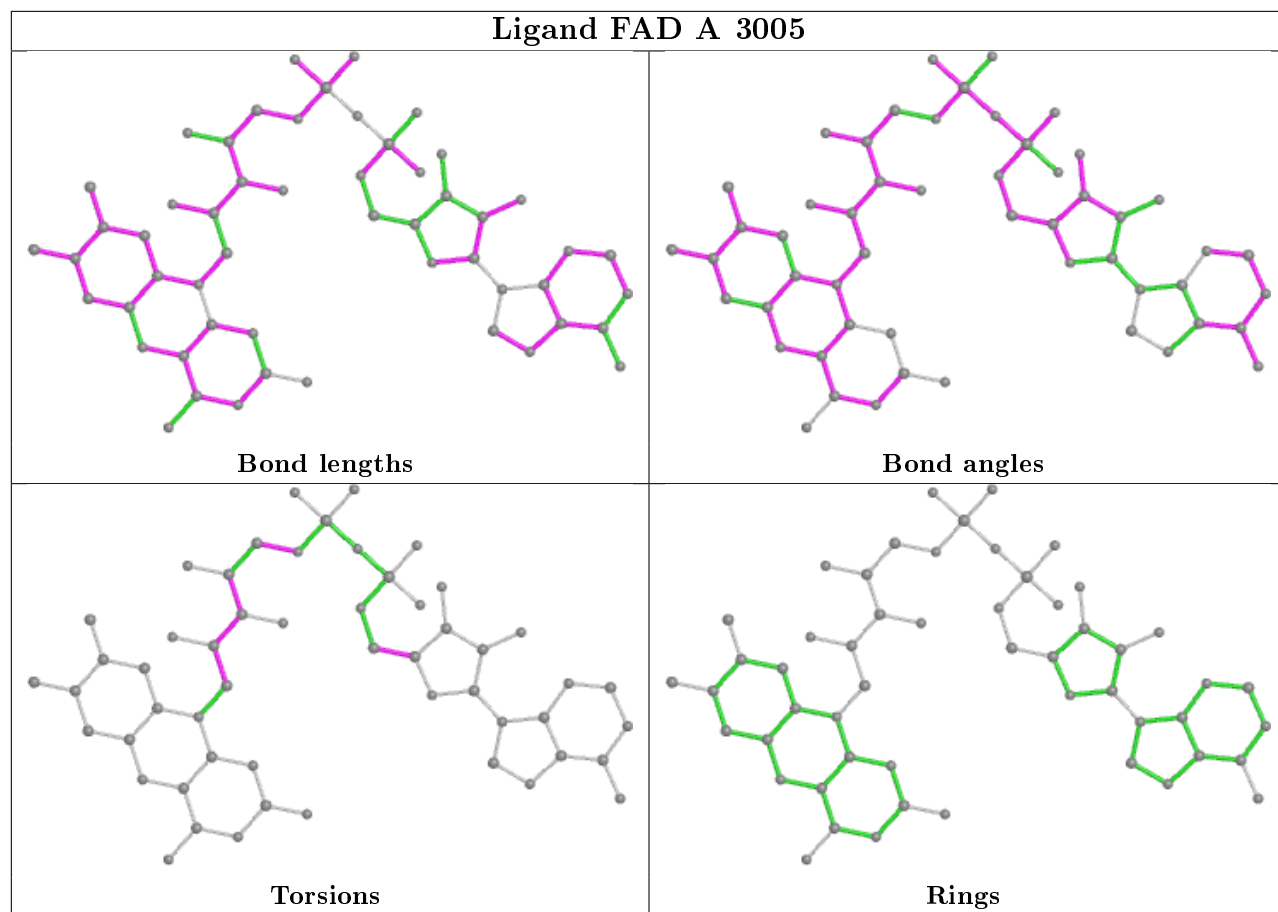
## Ligand MTE B 4003



## Ligand TEI B 4006







## 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.