



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:16 PM GMT

PDB ID : 1WYG  
Title : Crystal Structure of a Rat Xanthine Dehydrogenase Triple Mutant (C535A, C992R and C1324S)  
Authors : Nishino, T.; Okamoto, K.; Kawaguchi, Y.; Hori, H.; Matsumura, T.; Eger, B.T.; Pai, E.F.; Nishino, T.  
Deposited on : 2005-02-14  
Resolution : 2.60 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.

---

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

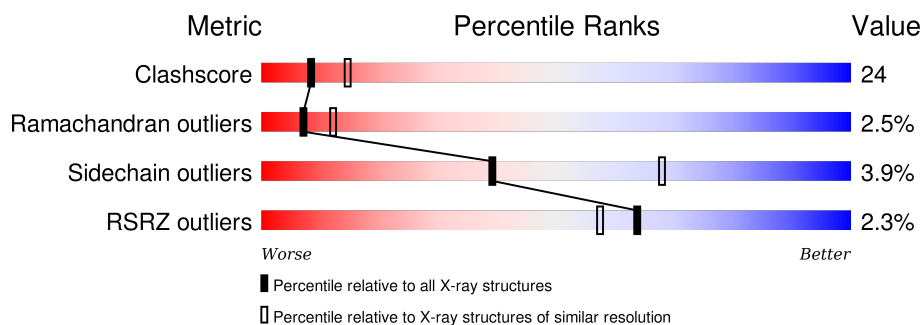
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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.

Mol	Chain	Length	Quality of chain
1	A	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	FES	A	4002	-	-	X	-
6	SAL	A	4005	-	-	-	X
7	ACY	A	3001	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10330 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	1297	Total	C	N	O	S	0	0	0
			10033	6359	1730	1882	62			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P22985
A	535	ALA	CYS	ENGINEERED	UNP P22985
A	992	ARG	CYS	ENGINEERED	UNP P22985
A	1324	SER	CYS	ENGINEERED	UNP P22985

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

*Continued on next page...*

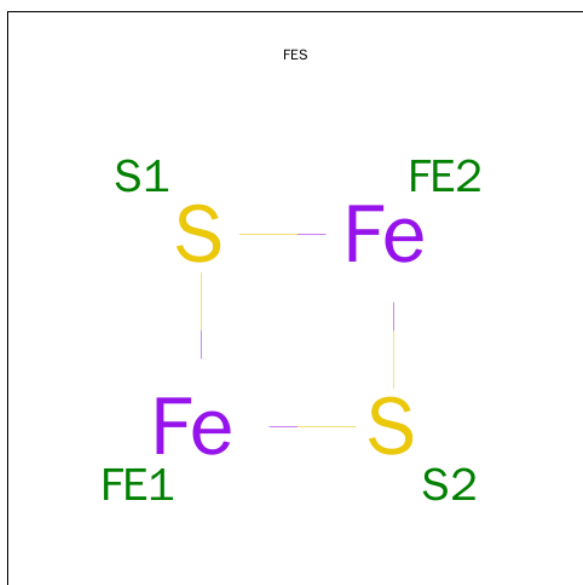
*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



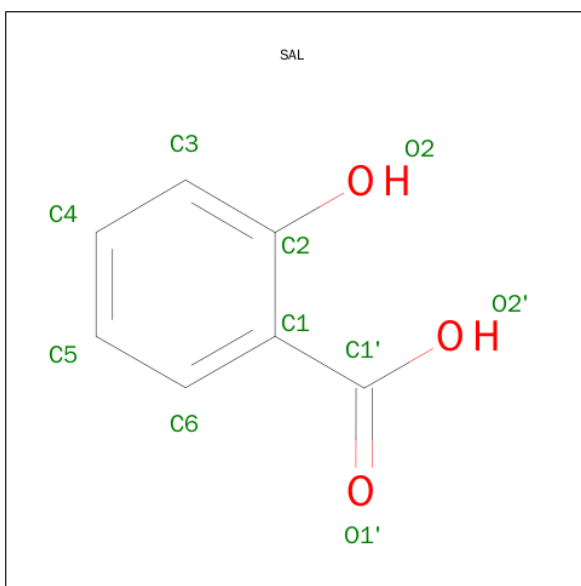
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		

- 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>).



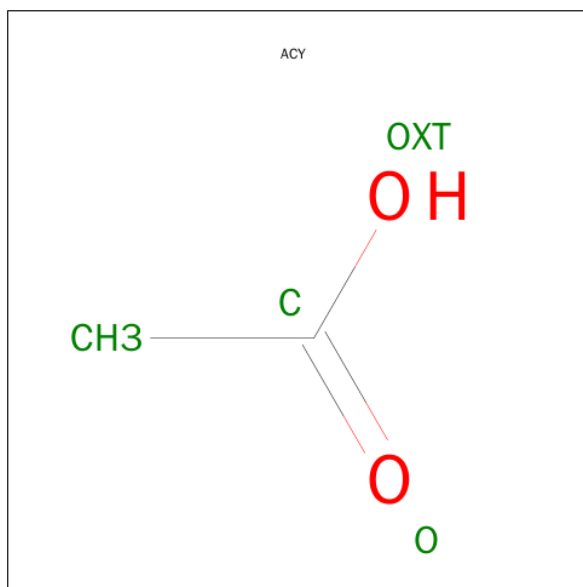
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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		

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	206	Total	O	0	0
			206	206		



R996	A1081	M1180	Q1284
G997	S1082	D1181	H1285
	A1083	V1182	G1286
I1000	D1084	G1183	D1287
I1001	L1085		N1288
P1002	M1086	N1187	A1289
T1003	G1087	P1188	K1290
K1004	Q1088	A1189	Q1291
F1005	G1089	I1190	L1292
G1006	V1090		F1293
I1007	Y1091	E1196	Q1294
S1008	E1092	G1197	
	A1093	A1198	P1298
L1011	G1094	F1199	A1299
P1012	Q1095	V1200	T1300
F1013		Q1201	P1301
	K1099	G1202	E1302
		L1203	
G1018	E1102		V1309
A1019	P1103	E1209	D1310
L1020	F1104	E1210	Q1311
V1021	K1105	L1211	F1312
	K1106	H1212	T1313
L1031	K1107		T1314
T1032	K1108	P1224	L1315
H1033			C1316
G1034		Y1227	V1317
	G1111		T1318
G1035	P1112	P1230	GLY
T1036	W1113	A1231	VAL
E1037		F1232	PRO
M1038	W1116		GLU
G1039	V1117	I1235	ASN
Q1040	M1118	P1236	S1324
G1041	D1119		K1325
L1042		F1239	S1326
H1043	V1125		W1327
T1044		C1247	S1328
K1045	G1131		V1329
M1046	F1132	K1250	M1330
V1047	Y1133	A1251	I1331
Q1048		R1252	
V1049	Y1140	S1253	
A1050		A1258	
S1051	E1143	V1259	
R1052	T1144		
	N1145	P1262	
K1055		P1263	
	P1149	L1264	
T1058	F1150	F1265	
		L1266	
T1068	Y1155	A1267	
M1069		S1268	
T1070	A1158	S1269	
V1071		I1270	
P1072	E1161	F1271	
N1073	V1162	F1272	
T1074	E1163	A1273	
T1077	N1173		
S1080			



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.25Å 134.25Å 523.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 19.91 – 2.63	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.60) 91.9 (19.91-2.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.61 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.203 , 0.248 0.228 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 71082 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SAL, PO4, FES, ACY, CA, FAD

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	0.38	0/10244	0.64	0/13859

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	10033	0	10046	485	0
2	A	15	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	0	3	0
5	A	53	0	31	3	0
6	A	10	0	5	0	0
7	A	4	0	3	0	0
8	A	206	0	0	5	0
All	All	10330	0	10085	486	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 24.

The worst 5 of 486 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:766:THR:HG22	1:A:768:ASN:H	0.99	1.08
1:A:1038:MET:H	1:A:1040:GLN:NE2	1.56	1.02
1:A:398:ARG:HB3	1:A:398:ARG:HH11	1.27	0.99
1:A:196:ASN:OD1	1:A:198:GLU:HB3	1.63	0.97
1:A:602:GLU:HG2	1:A:822:PRO:HB2	1.45	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	1291/1331 (97%)	1142 (88%)	117 (9%)	32 (2%)	<b>7</b> <b>12</b>

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	602	GLU
1	A	1008	SER
1	A	1325	LYS
1	A	152	TYR

### 5.3.2 Protein sidechains [i](#)

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	1095/1123 (98%)	1052 (96%)	43 (4%)	39 68

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	743	TYR
1	A	826	MET
1	A	1250	LYS
1	A	761	GLU
1	A	798	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	585	GLN
1	A	703	ASN
1	A	1173	ASN
1	A	642	ASN
1	A	699	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z  > 2$
2	PO4	A	2001	-	4,4,4	1.14	0	6,6,6	0.27	0
2	PO4	A	2002	-	4,4,4	1.12	0	6,6,6	0.27	0
2	PO4	A	2003	-	4,4,4	1.20	0	6,6,6	0.27	0
7	ACY	A	3001	-	1,3,3	1.89	0	0,3,3	0.00	-
4	FES	A	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	A	4003	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FAD	A	4004	-	48,58,58	2.80	17 (35%)	54,89,89	3.14	19 (35%)
6	SAL	A	4005	-	7,10,10	1.91	3 (42%)	10,13,13	1.19	0

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	PO4	A	2001	-	-	0/0/0/0	0/0/0/0
2	PO4	A	2002	-	-	0/0/0/0	0/0/0/0
2	PO4	A	2003	-	-	0/0/0/0	0/0/0/0
7	ACY	A	3001	-	-	0/0/0/0	0/0/0/0
4	FES	A	4002	1	-	0/0/4/4	0/1/1/1
4	FES	A	4003	1	-	0/0/4/4	0/1/1/1
5	FAD	A	4004	-	-	0/30/50/50	0/6/6/6
6	SAL	A	4005	-	-	0/0/4/4	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4005	SAL	C3-C2	2.31	1.43	1.39
6	A	4005	SAL	C6-C1	2.59	1.44	1.39
5	A	4004	FAD	C5A-C4A	2.63	1.46	1.40
5	A	4004	FAD	C10-N1	2.89	1.40	1.35
5	A	4004	FAD	O4B-C4B	2.94	1.51	1.45

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4004	FAD	N3A-C2A-N1A	-9.98	121.25	128.89
5	A	4004	FAD	C4-C4X-C10	-7.88	114.90	119.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4004	FAD	C5X-C9A-N10	-7.57	111.87	117.62
5	A	4004	FAD	C4X-C10-N10	-5.51	117.28	120.52
5	A	4004	FAD	O4B-C1B-N9A	-4.24	99.22	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4002	FES	2	0
4	A	4003	FES	1	0
5	A	4004	FAD	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1297/1331 (97%)	-0.29	30 (2%) 64 57	9, 35, 61, 88	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1324	SER	7.1
1	A	1318	THR	5.4
1	A	1325	LYS	4.7
1	A	1326	SER	4.6
1	A	1289	ALA	4.3

### 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
7	ACY	A	3001	4/4	0.90	0.22	4.41	55,55,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SAL	A	4005	10/10	0.87	0.20	3.26	31,33,42,42	0
5	FAD	A	4004	53/53	0.96	0.15	0.54	25,36,44,45	0
2	PO4	A	2001	5/5	0.98	0.11	-0.11	41,42,44,45	0
2	PO4	A	2002	5/5	0.96	0.12	-1.25	68,68,69,70	0
4	FES	A	4003	4/4	0.98	0.09	-1.30	22,23,23,26	0
3	CA	A	4001	1/1	0.96	0.06	-3.74	28,28,28,28	0
4	FES	A	4002	4/4	0.98	0.05	-4.07	31,31,34,36	0
2	PO4	A	2003	5/5	0.96	0.12	-	70,70,71,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.