wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2021 – 08:08 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

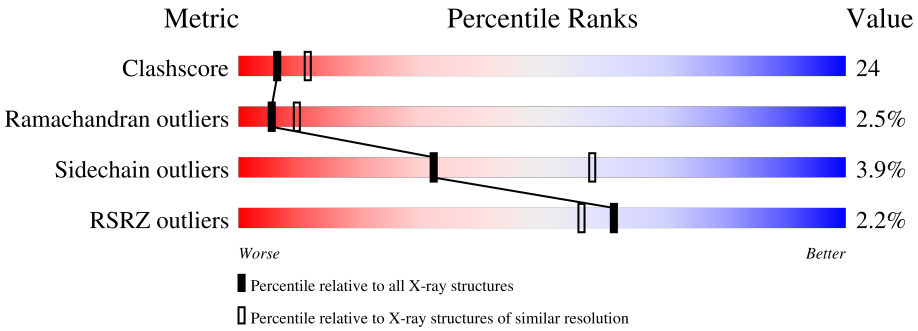
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	2% 57% 37%

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	-

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.

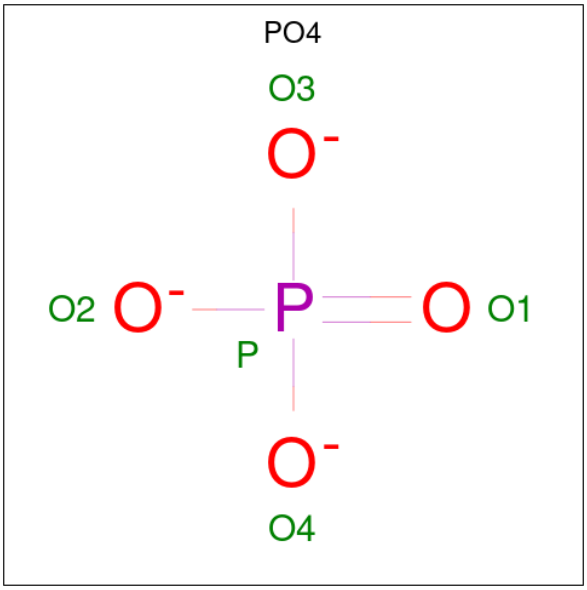
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

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 mutation	UNP P22985
A	992	ARG	CYS	engineered mutation	UNP P22985
A	1324	SER	CYS	engineered mutation	UNP P22985

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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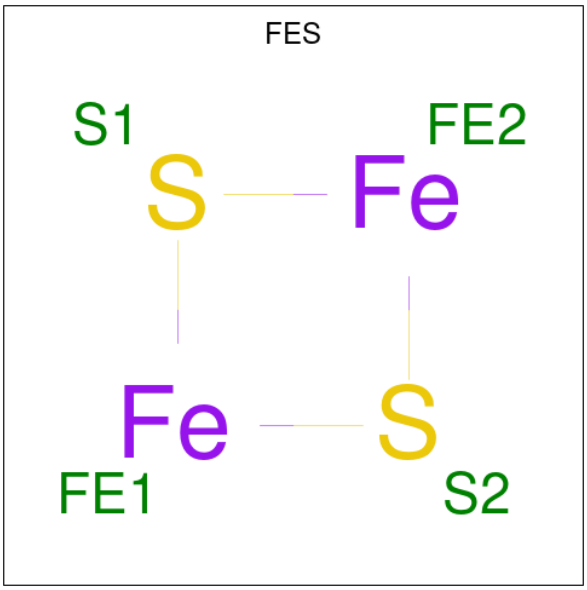
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0

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

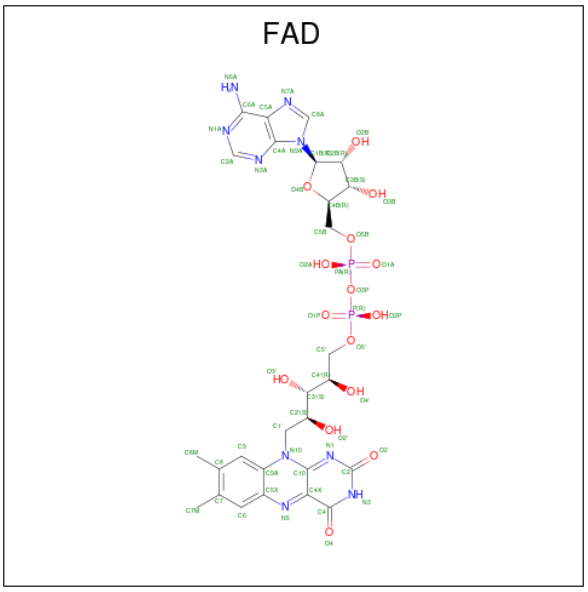
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



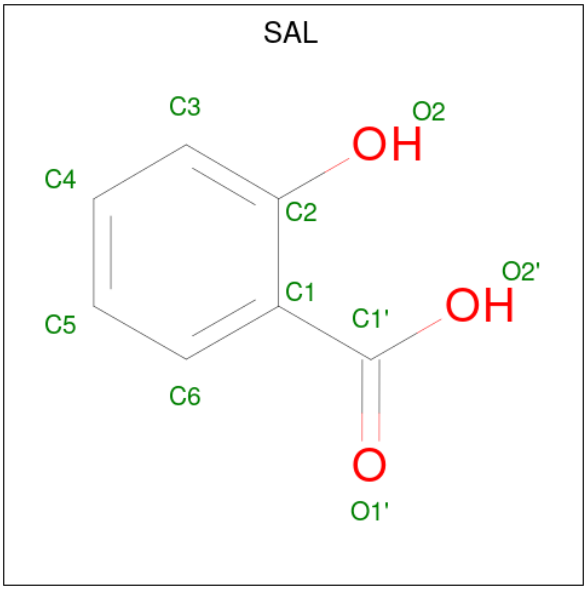
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	A	1	Total Fe S 4 2 2	0	0

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



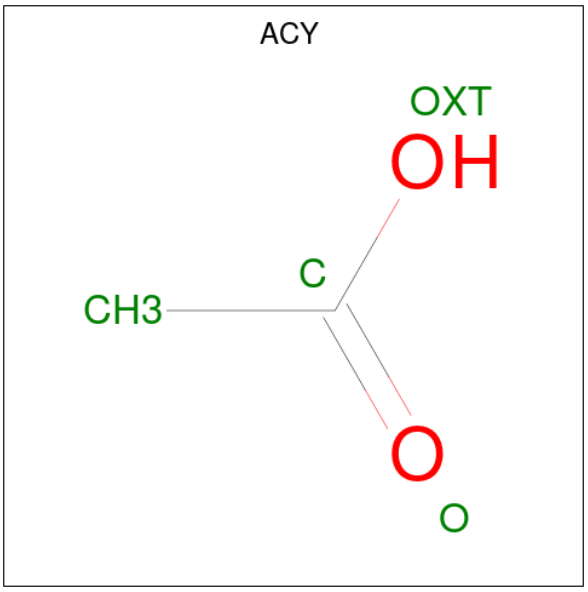
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0

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



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

- 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 4 2 2	0	0

- Molecule 8 is water.

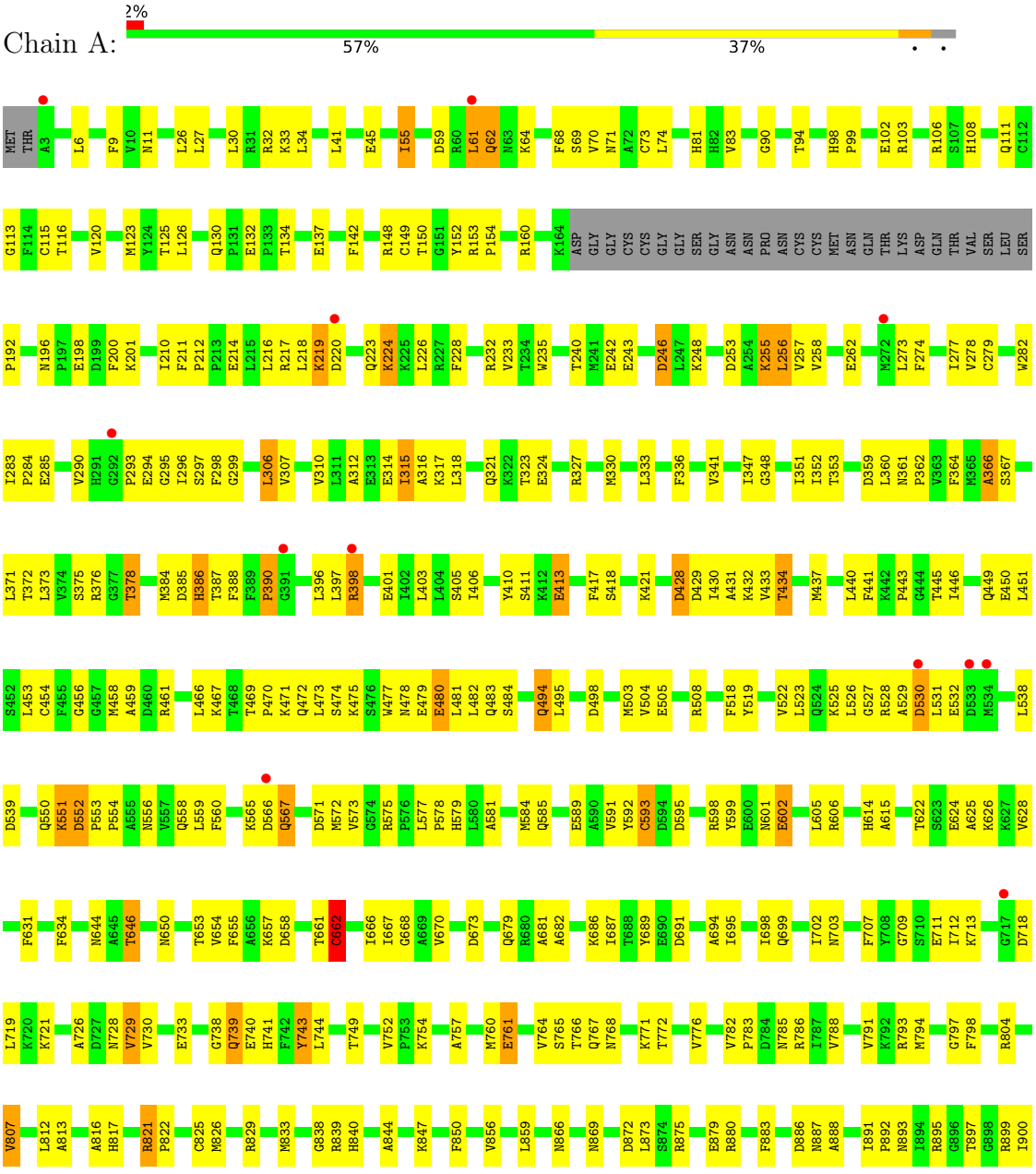
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	206	Total O 206 206	0	0

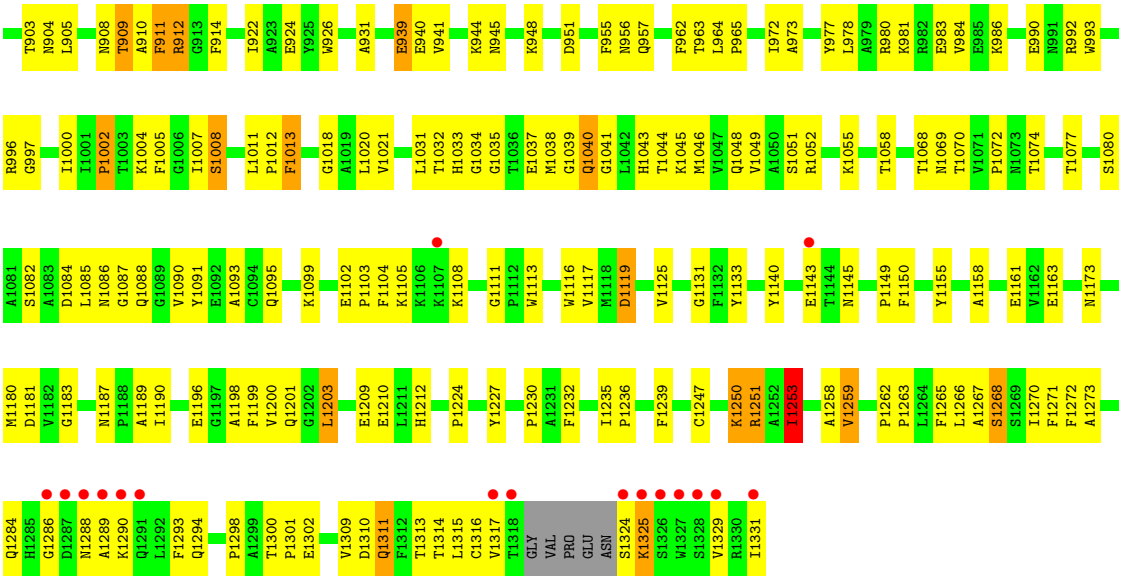
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

- Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:




T903 N904 L905 N908 T909 A910 F911 R912 G913 F914 I922 A923 E924 Y925 W926 A931 E939 E940 V941 K944 N945 K948 D951 F955 N956 Q957 F962 T963 L964 P965 I972 A973 Y977 L978 A979 R980 K981 R982 E983 V984 E985 K986 E990 N991 R992 W993
R996 G997 I1000 I1001 P1002 T1003 K1004 F1005 G1006 I1007 S1008 L1011 P1012 F1013 G1018 A1019 L1020 V1021 L1031 T1032 H1033 G1034 G1035 T1036 E1037 M1038 G1039 Q1040 G1041 L1042 H1043 T1044 K1045 M1046 V1047 Q1048 V1049 A1050 S1051 R1052 K1055 T1058 T1068 N1069 T1070 V1071 P1072 N1073 T1074 T1077 S1080
A1081 S1082 A1083 D1084 L1085 N1086 G1087 Q1088 G1089 V1090 Y1091 E1092 A1093 C1094 Q1095 K1099 E1102 P1103 F1104 K1105 K1106 K1107 K1108 G1111 P1112 W1113 W1116 V1117 M1118 D1119 V1125 G1131 F1132 Y1133 Y1140 E1143 T1144 N1145 P1149 F1150 Y1155 A1158 E1161 V1162 E1163 N1173
M1180 D1181 Y1182 G1183 N1187 P1188 A1189 I1190 E1196 G1197 A1198 F1199 V1200 Q1201 G1202 L1203 E1209 E1210 L1211 H1212 P1224 Y1227 P1230 A1231 F1232 I1235 P1236 F1239 C1247 K1250 R1251 A1252 I1253 A1258 V1259 P1262 P1263 L1264 F1265 L1266 A1267 S1268 S1269 I1270 F1271 F1272 A1273
Q1284 H1285 G1286 D1287 N1288 A1289 K1290 Q1291 L1292 F1293 Q1294 P1298 A1299 T1300 P1301 E1302 V1309 D1310 Q1311 F1312 T1313 T1314 L1315 C1316 V1317 T1318 GLY VAL PRO GLU ASN S1324 K1325 S1326 W1327 S1328 V1329 R1330 I1331

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	6.04 (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.	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10330	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

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:HH11	1:A:398:ARG:HB3	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%)	5 9

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%)	32 58

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

Mol	Chain	Res	Type
1	A	983	GLU
1	A	1119	ASP
1	A	1002	PRO
1	A	1072	PRO
1	A	1203	LEU

Sometimes 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	699	GLN
1	A	1311	GLN
1	A	817	HIS
1	A	1086	ASN
1	A	768	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
7	ACY	A	3001	-	1,3,3	2.12	1 (100%)	0,3,3	-	-
4	FES	A	4003	1	0,4,4	-	-	-		
2	PO4	A	2001	-	4,4,4	1.67	0	6,6,6	0.44	0
5	FAD	A	4004	-	51,58,58	3.37	20 (39%)	60,89,89	2.80	20 (33%)
6	SAL	A	4005	-	8,10,10	2.10	4 (50%)	9,13,13	1.14	0
2	PO4	A	2003	-	4,4,4	1.74	1 (25%)	6,6,6	0.42	0
2	PO4	A	2002	-	4,4,4	1.65	0	6,6,6	0.44	0
4	FES	A	4002	1	0,4,4	-	-	-		

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
4	FES	A	4003	1	-	-	0/1/1/1
5	FAD	A	4004	-	-	6/30/50/50	0/6/6/6
4	FES	A	4002	1	-	-	0/1/1/1
6	SAL	A	4005	-	-	0/0/4/4	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4004	FAD	C4X-C10	12.54	1.51	1.38
5	A	4004	FAD	C9A-N10	8.79	1.50	1.38
5	A	4004	FAD	O4B-C1B	7.37	1.51	1.41
5	A	4004	FAD	C4-N3	5.64	1.42	1.33
5	A	4004	FAD	C10-N1	5.58	1.40	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	4004	FAD	C4-N3-C2	10.99	124.42	115.14
5	A	4004	FAD	C5X-C9A-N10	-8.07	111.87	117.72
5	A	4004	FAD	C4-C4X-C10	-7.63	114.90	119.95
5	A	4004	FAD	C4-C4X-N5	5.97	125.42	118.60
5	A	4004	FAD	C4X-N5-C5X	5.03	121.80	116.77

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	4004	FAD	N10-C1'-C2'-O2'
5	A	4004	FAD	N10-C1'-C2'-C3'
5	A	4004	FAD	C2'-C3'-C4'-C5'
5	A	4004	FAD	C2'-C3'-C4'-O4'
5	A	4004	FAD	O3'-C3'-C4'-C5'

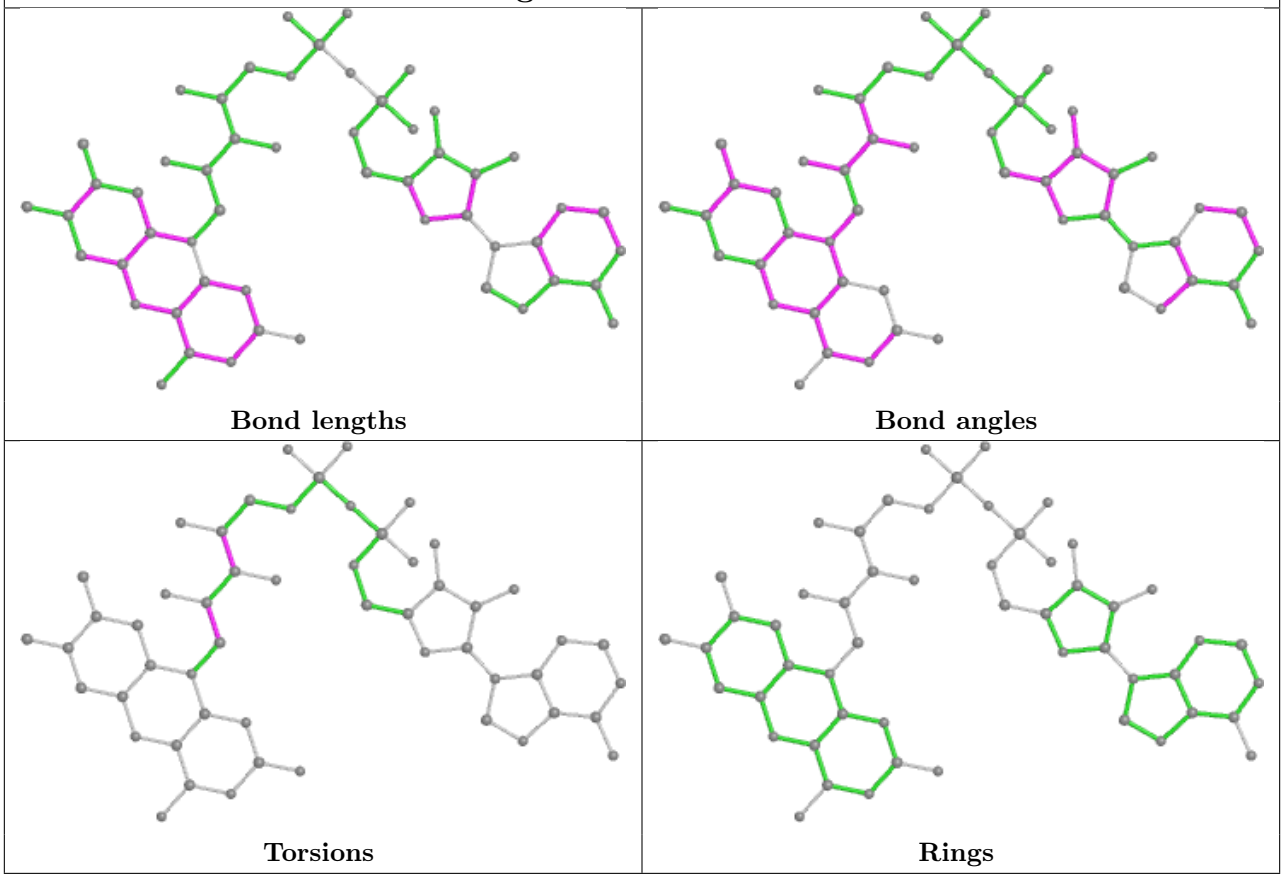
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4003	FES	1	0
5	A	4004	FAD	3	0
4	A	4002	FES	2	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 then 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 FAD A 4004



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

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^{th} 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^2)	Q<0.9
1	A	1297/1331 (97%)	-0.33	29 (2%) 62 56	9, 35, 61, 88	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1324	SER	7.0
1	A	1318	THR	5.4
1	A	1325	LYS	4.7
1	A	1326	SER	4.5
1	A	1289	ALA	4.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
6	SAL	A	4005	10/10	0.87	0.20	31,33,42,42	0
7	ACY	A	3001	4/4	0.90	0.22	55,55,56,56	0

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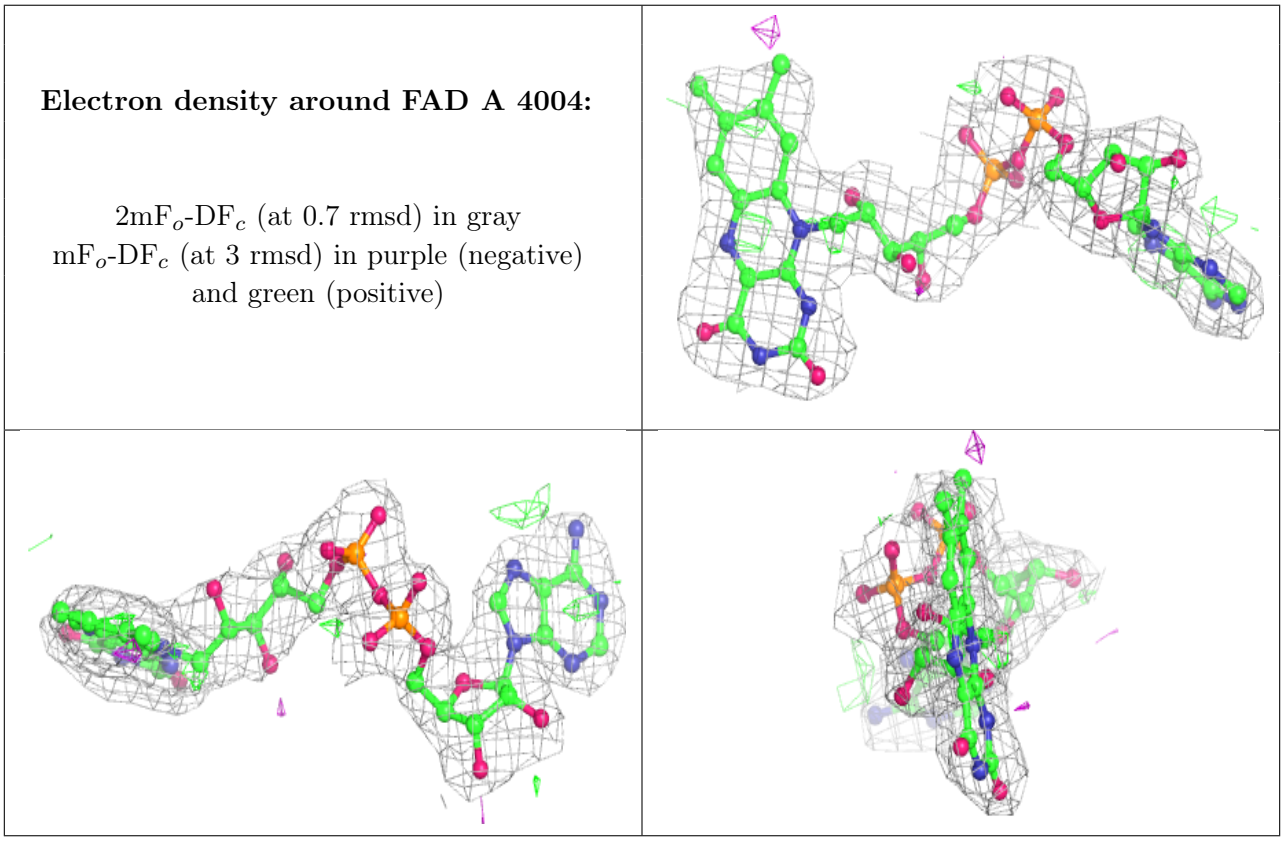
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	A	2002	5/5	0.95	0.12	68,68,69,70	0
5	FAD	A	4004	53/53	0.96	0.15	25,36,44,45	0
2	PO4	A	2003	5/5	0.96	0.12	70,70,71,72	0
3	CA	A	4001	1/1	0.96	0.06	28,28,28,28	0
2	PO4	A	2001	5/5	0.98	0.11	41,42,44,45	0
4	FES	A	4002	4/4	0.98	0.05	31,31,34,36	0
4	FES	A	4003	4/4	0.98	0.09	22,23,23,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 4004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.