



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 03:23 AM JST

PDB ID : 4YRW / pdb_00004yrw
Title : rat xanthine oxidoreductase, C-terminal deletion protein variant
Authors : Okamoto, K.
Deposited on : 2015-03-16
Resolution : 1.99 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

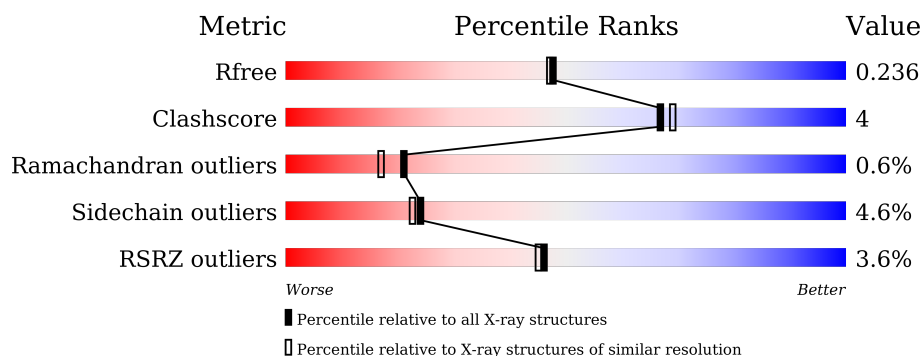
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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))</
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2 Entry composition [i](#)

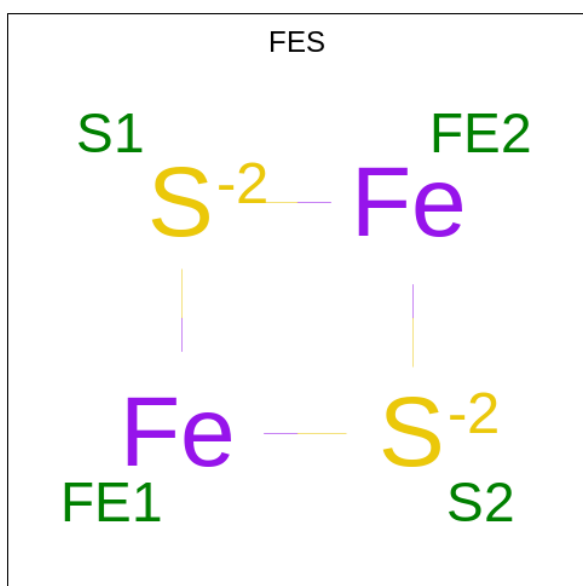
There are 8 unique types of molecules in this entry. The entry contains 20715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

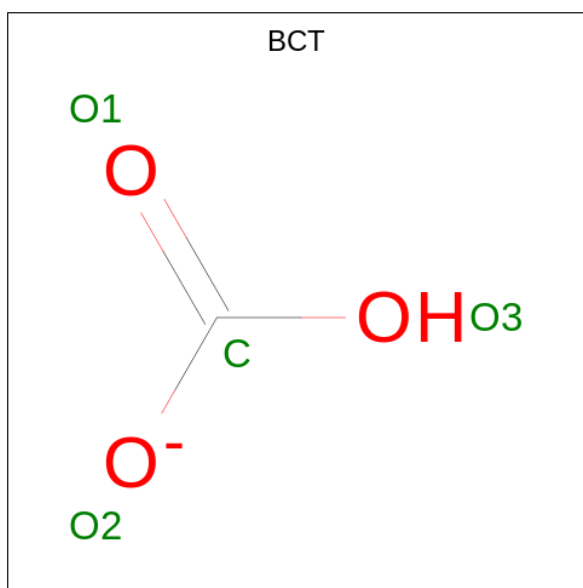
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1289	Total	C	N	O	S	0	0	0
			9964	6314	1714	1873	63			
1	B	1286	Total	C	N	O	S	0	0	0
			9939	6298	1711	1867	63			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



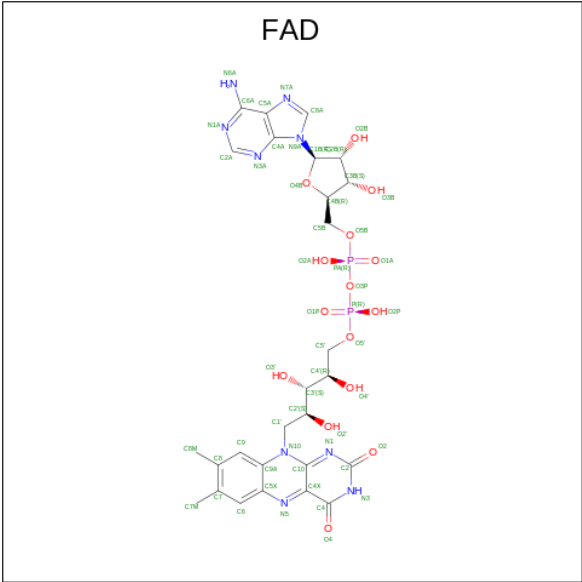
- Molecule 3 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		

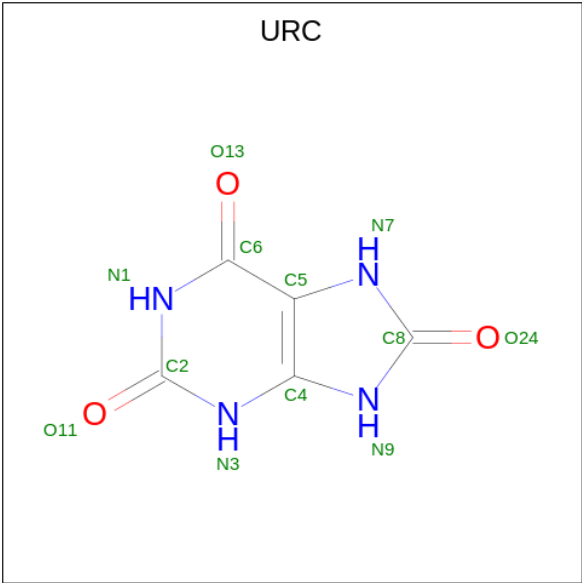
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0

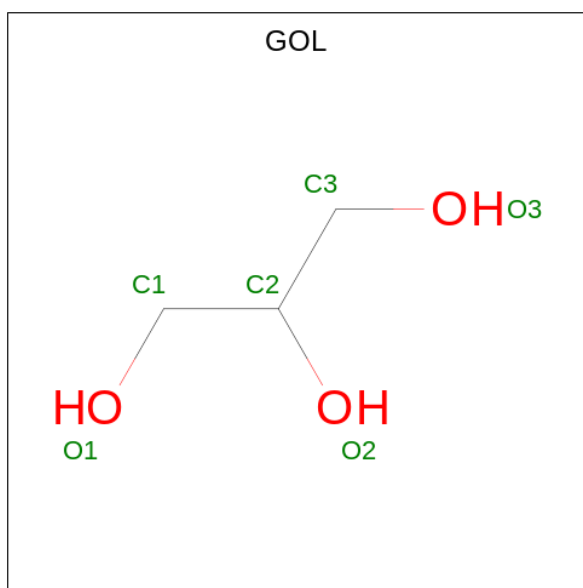


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is URIC ACID (CCD ID: URC) (formula: C₅H₄N₄O₃).



- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

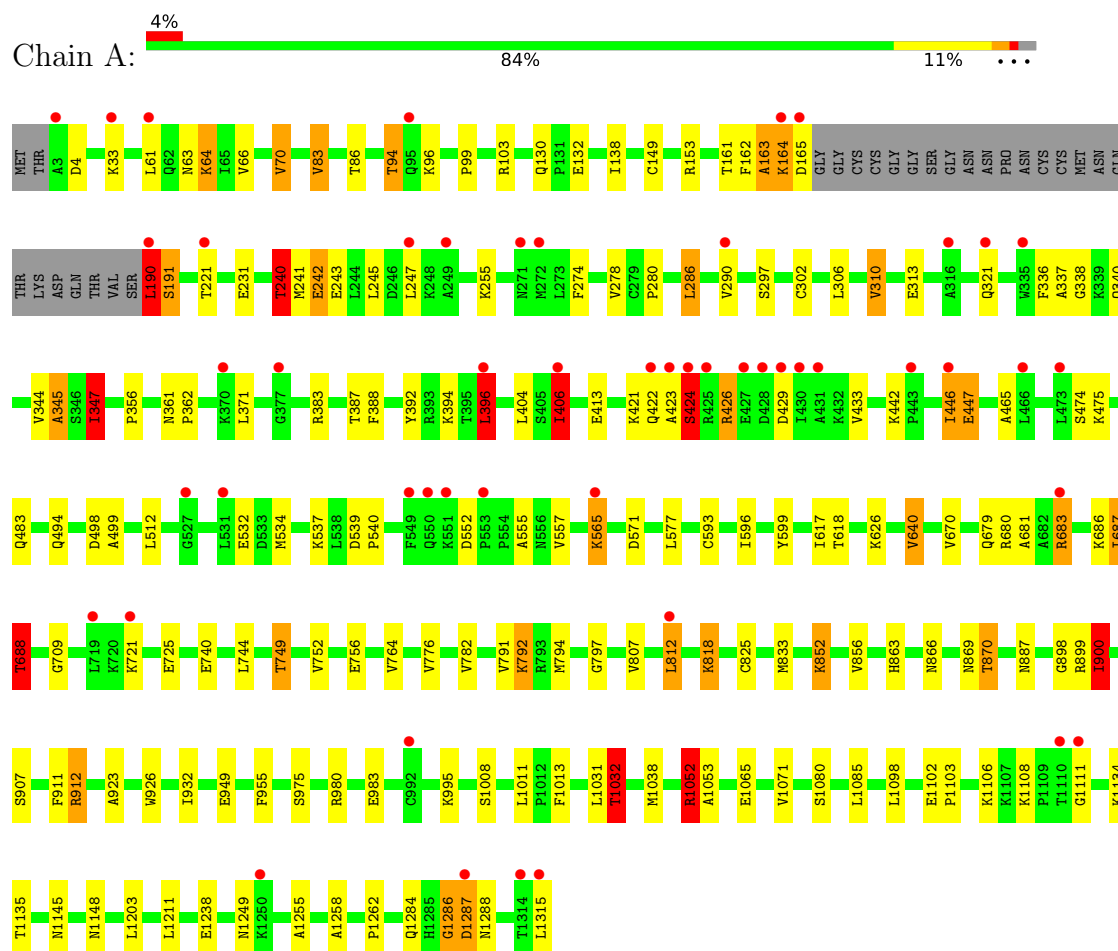
- Molecule 8 is water.

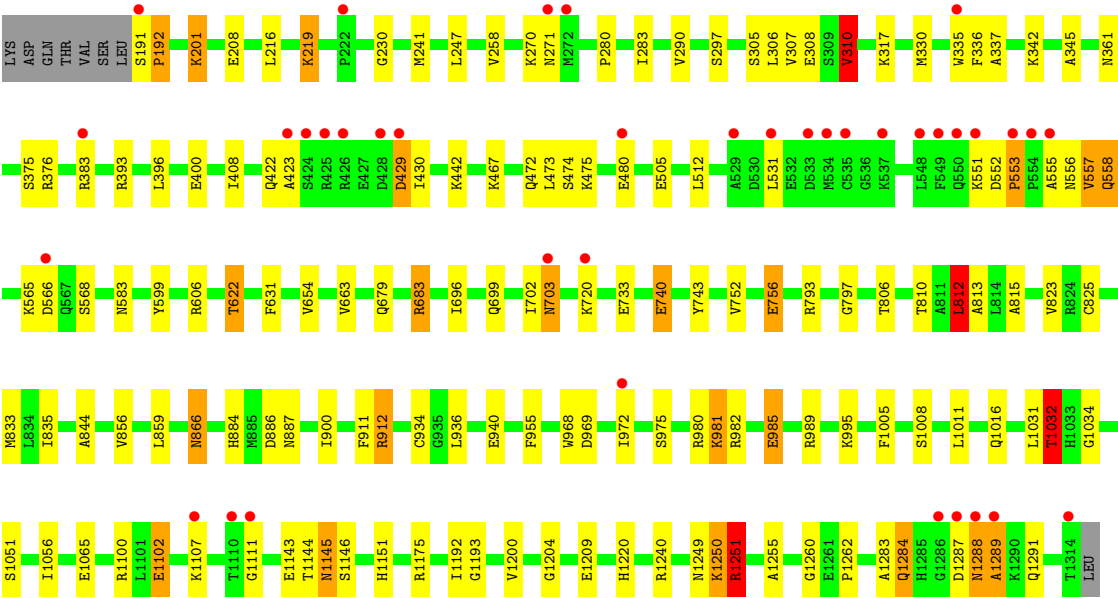
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	250	Total	O	0	0

3 Residue-property plots

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.50Å 138.47Å 222.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.33 – 1.99 43.33 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.33-1.99) 99.7 (43.33-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.229 0.194 , 0.236	Depositor DCC
R_{free} test set	10396 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning		

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: FES, BCT, URC, CA, GOL, 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	1.27	22/10174 (0.2%)	1.21	40/13767 (0.3%)
1	B	1.40	46/10149 (0.5%)	1.22	40/13734 (0.3%)
All	All	1.34	68/20323 (0.3%)	1.21	80/27501 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain
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There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	886	ASP	Peptide

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	9964	0	9967	85	0
1	B	9939	0	9942	65	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	53	0	31	1	

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:THR:OG1	1:A:688:THR:HG22	1.71	0.89

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	1285/1315 (98%)	1239 (96%)	38 (3%)	8 (1%)	21	17
1	B	1282/1315 (98%)	1242 (97%)	32 (2%)	8 (1%)	21	17
All	All	2567/2630 (98%)	2481 (97%)	70 (3%)	16 (1%)	21	17

5 of 16 Ramachandran outliers are listed below:

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1085/1109 (98%)	1044 (96%)	41 (4%)	29	29
All	All	2173/2218 (98%)	2072 (95%)	101 (5%)	24	22

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1134	LYS
1	B	310	VAL
1	B	1262	PRO
1	A	1315	LEU
1	B	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	869	ASN
1	B	1145	ASN
1	B	1288	ASN
1	A	1284	GLN
1	A	1220	HIS

5

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).

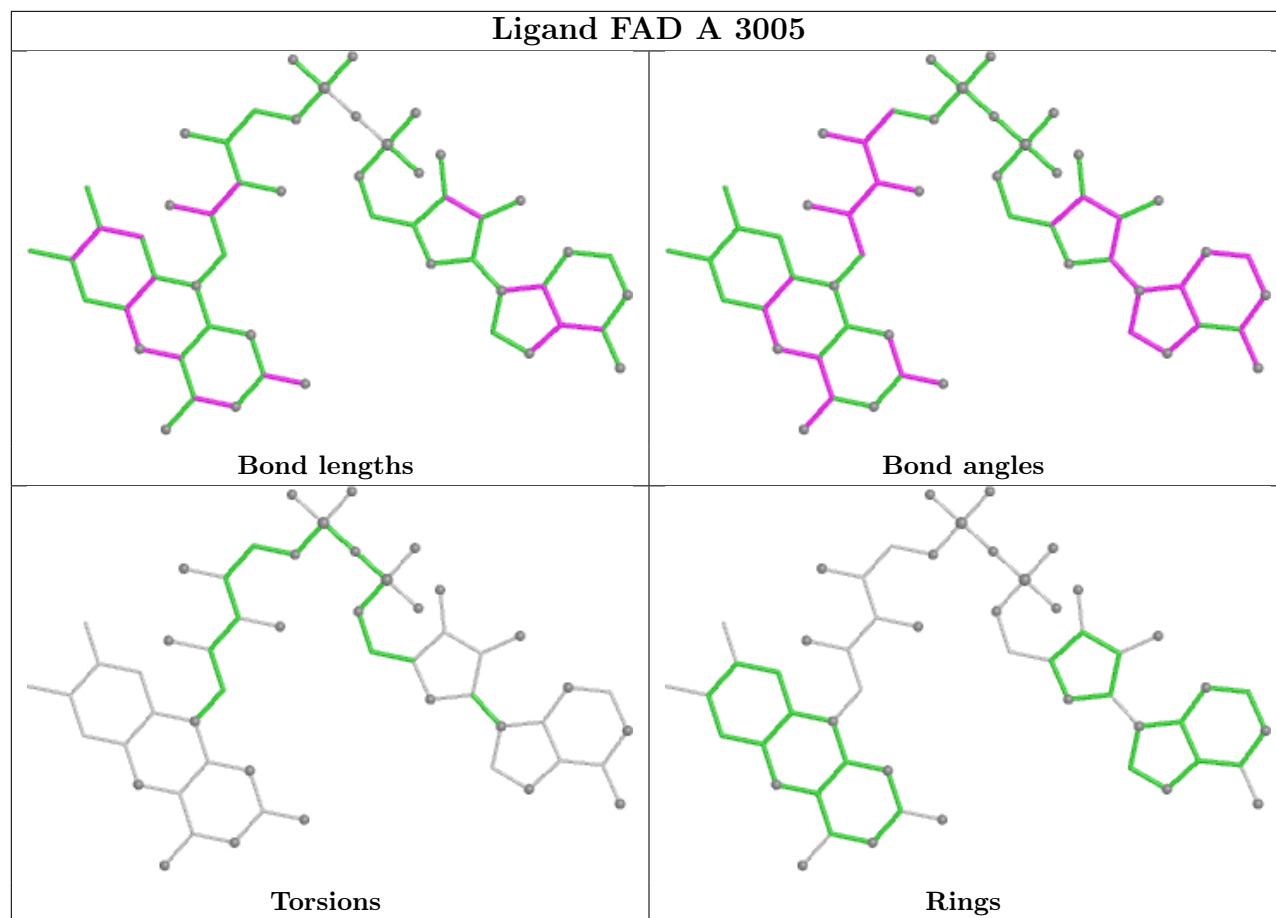
Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	A	3005	-	56,58,58	1.61	14 (25%)	81,89,89	1.83	20 (24%)
7	GOL	A	3007	-	5,5,5	0.68	0	5,5,5	0.69	0
2	FES	A	3002	1	0,4,4	-	-	-	-	-
7	GOL	B	4007	-	5,5,5	0.59	0	5,5,5	0.38	0
3	BCT	B	4005	-	2,3,3	0.63	0	2,3,3	1.35	0
6	URC	B	4006	-	11,					

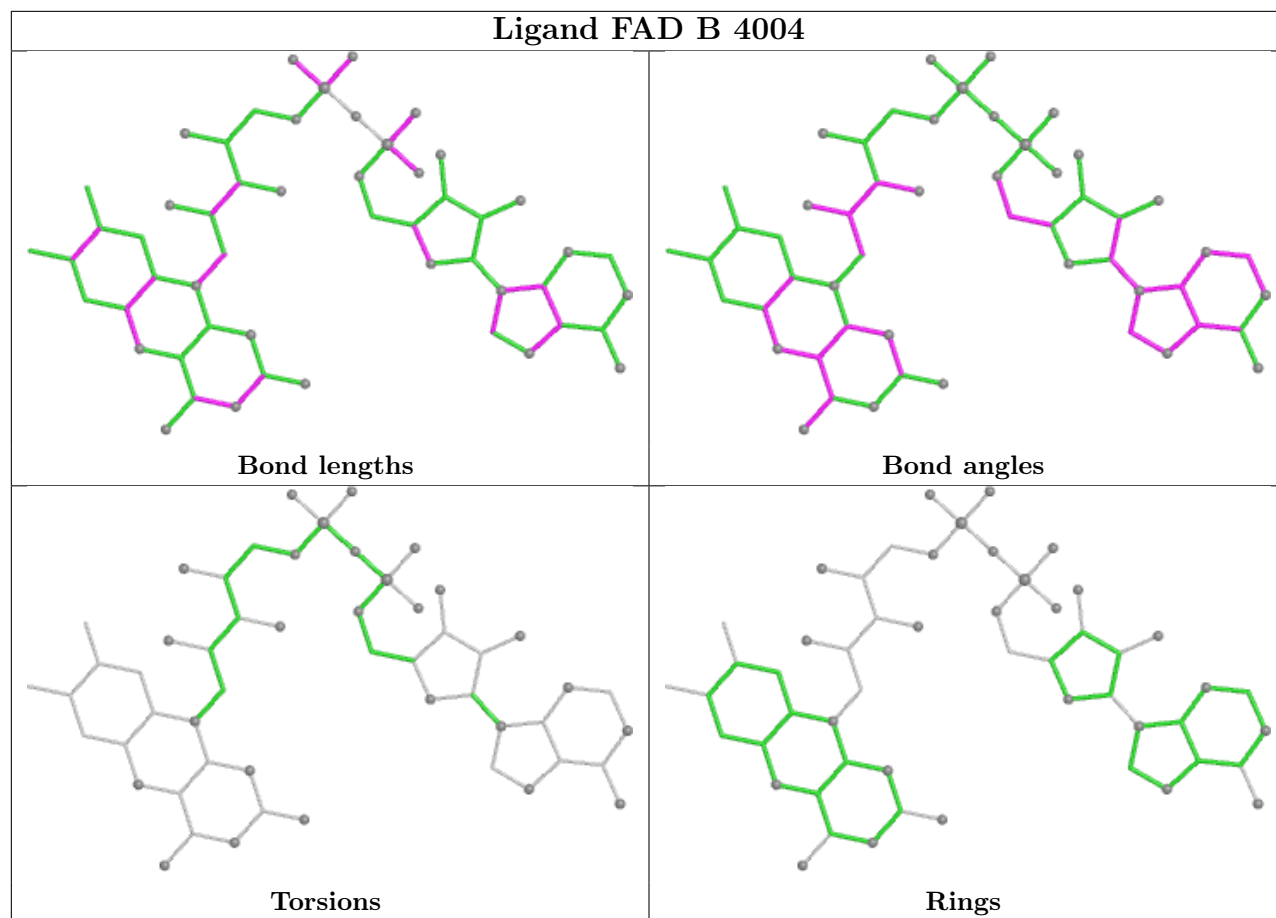
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4004	FAD	C5A-N7A	-4.30	1.30	1.39
5	B	4004	FAD	C9A-C5X	4.00	1.47	1.41
5	B	4004	FAD	C8A-N9A	-3.90	1.30	1.37
5	B	4004	FAD	C5X-N5	-3.84	1.32	1.39

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4004	FAD	C5A-C4A-N3A	-5.89	119.06	126.75
6	B	4006	URC	N7-C8-N9	5.87	116.48	107.19
5	B	4004	FAD	N3A-C4A-N9A	5.35	135.89	127.08
5	A	3005	FAD	N3A-C4A-N9A	4.93	135.21	127.08
5	A	3005	FAD	C5A-C4A-N3A	-4.92		





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](#)

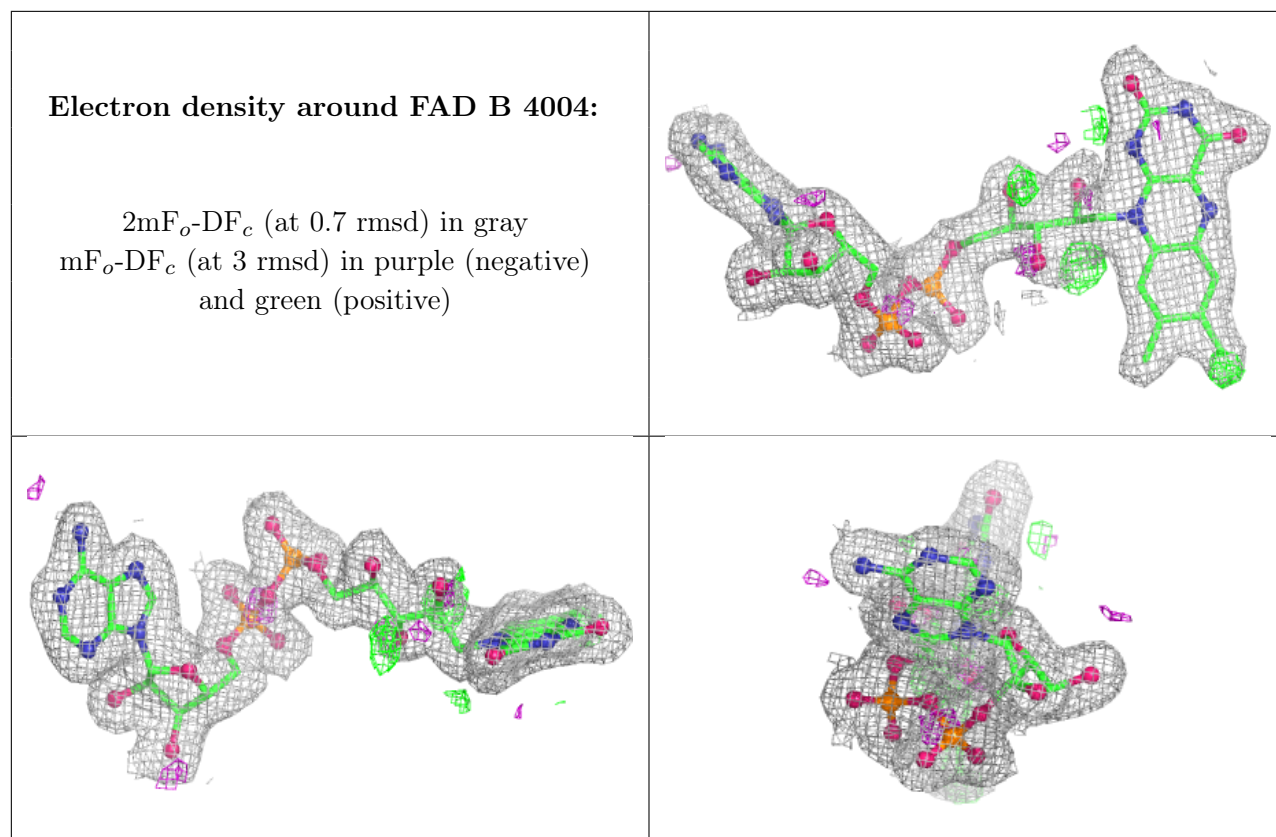
In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile 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	1289/1315 (98%)	0.30	51 (3%) 42 41	17, 30, 51, 86	0
1	B	1286/1315 (97%)	-0.00	42 (3%) 49 48	15, 24, 46, 85	0
All	All	2575/2630 (97%)	0.15	93 (3%) 46 45	15, 27, 49, 86	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	ALA	7.7
1	A	190	LEU	5.7
1	A	1315	LEU	

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	3007	6/6	0.92	0.12	25,27,28,29	0
7	GOL	B	4007	6/6	0.94	0.08	26,30,31,31	0
7	GOL	B	4008	6/6	0.94	0.09	23,27,28,28	0
6	URC	B	4006	12/12	0.96	0.06	22,24,28,29	0
5	FAD	A	3005	53/53	0.96	0.07	23,30,34,36	0
5	FAD	B	4004	53/53	0.96	0.07	16,21,25,27	0
6	URC	A	3006	12/12	0.96	0.06	24,27,31,31	0
4	CA	A	3004	1/1	0.97	0.10	34,34,34,34	0
3	BCT	A	3003	4/4	0.97	0.07	26,28,28,29	0
3	BCT	B	4005	4/4	0.98	0.04	19,20,21,	



6.5 Other polymers [i](#)

There are no such residues in this entry.