wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 10:29 pm BST

PDB ID	:	5G5G / pdb_00005g5g
Title	:	Escherichia coli Periplasmic Aldehyde Oxidase
Authors	:	Correia, M.A.S.; Otrelo-Cardoso, A.R.; Romao, M.J.; Santos-Silva, T.
Deposited on	:	2016-05-25
Resolution	:	1.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

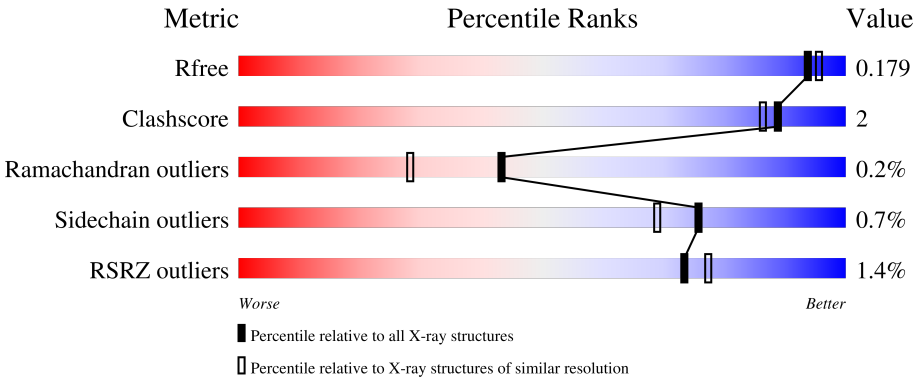
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	229	2% 73% 24%
2	B	318	2% 95%
3	C	732	% 96%

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
6	CL	A	1229	-	-	X	-
7	ACT	B	1321	-	-	X	-
9	SF4	B	320	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 10479 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 PUTATIVE XANTHINE DEHYDROGENASE YAGT IRON-SULFUR-BINDING SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	175	1341	820	239	269	13	0	7	0

- Molecule 2 is a protein called PUTATIVE XANTHINE DEHYDROGENASE YAGR MOLYBDENUM-BINDING SU SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	316	2400	1509	439	444	8	0	4	0

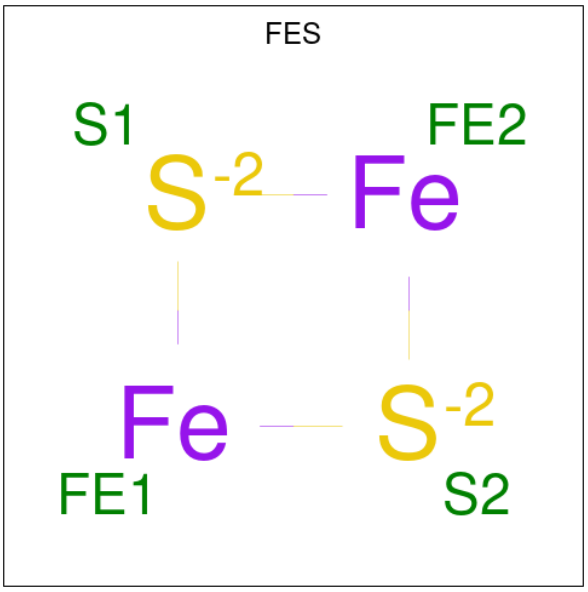
- Molecule 3 is a protein called PUTATIVE XANTHINE DEHYDROGENASE YAGS FAD-BINDING SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	731	5569	3477	989	1076	27	0	14	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	VAL	ALA	cloning artifact	UNP P77489
C	391	GLY	ASP	cloning artifact	UNP P77489

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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

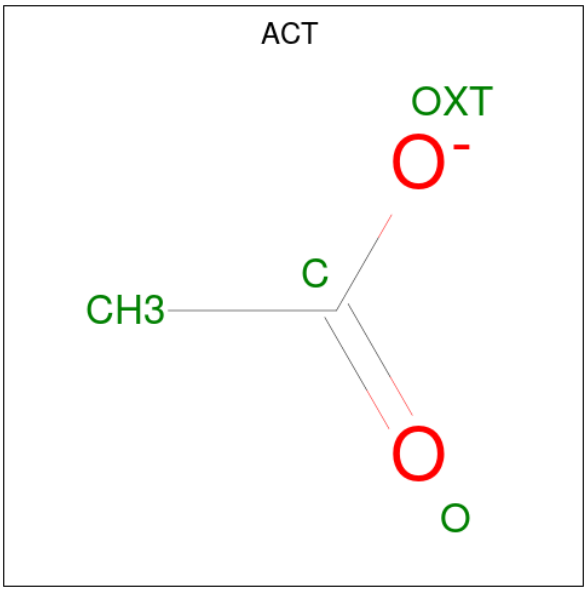
- Molecule 5 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total I 2 2	0	0
5	B	2	Total I 2 2	0	0
5	C	3	Total I 3 3	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

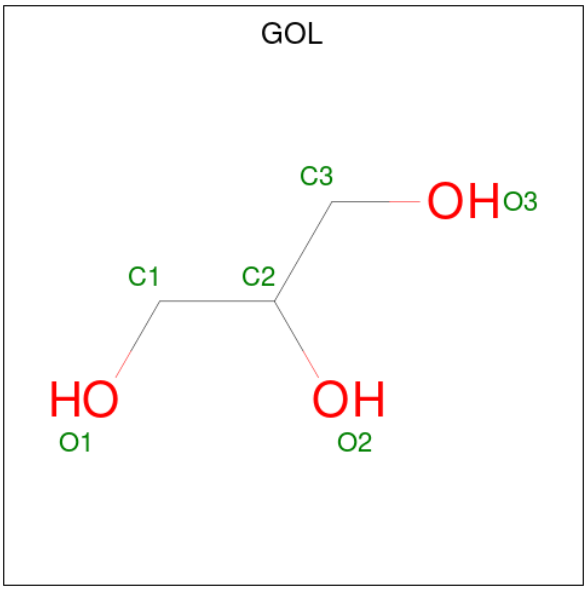
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Cl 3 3	0	0
6	B	4	Total Cl 4 4	0	0
6	C	5	Total Cl 5 5	0	0

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



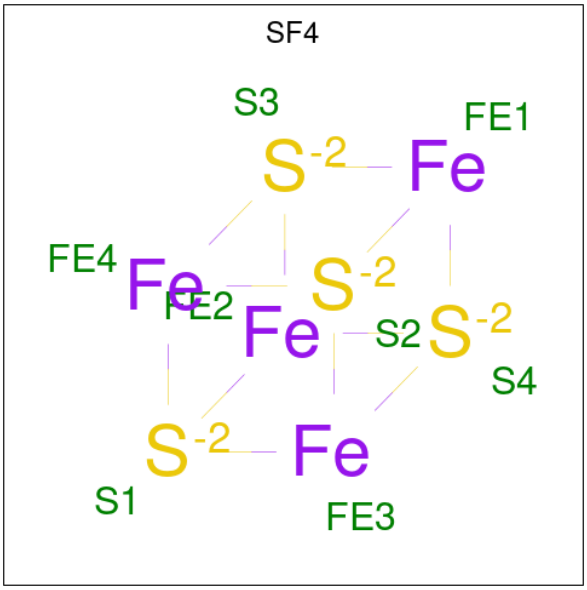
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



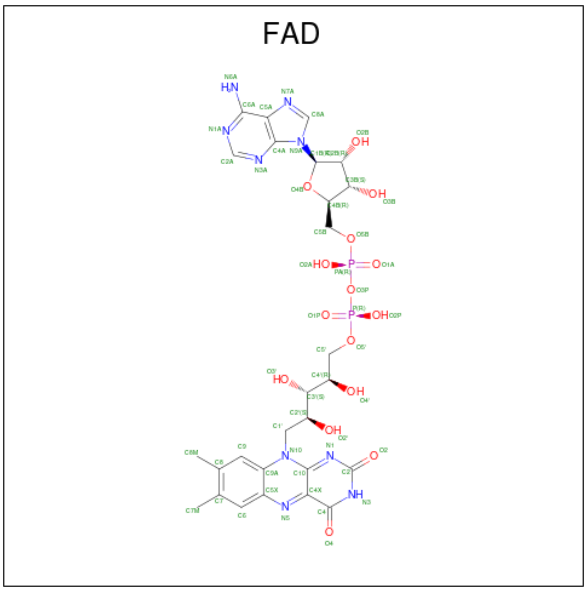
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



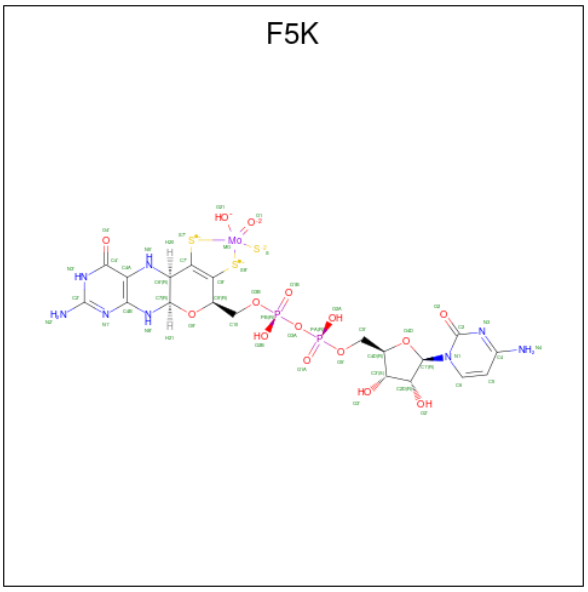
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 8 4 4	0	0

- Molecule 10 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 11 is Molybdopterin cytosine dinucleotide hydroxy-oxo-sulfido-molybdenum (CCD ID: F5K) (formula: $C_{19}H_{25}MoN_8O_{15}P_2S_3$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
11	C	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	15	2	3		

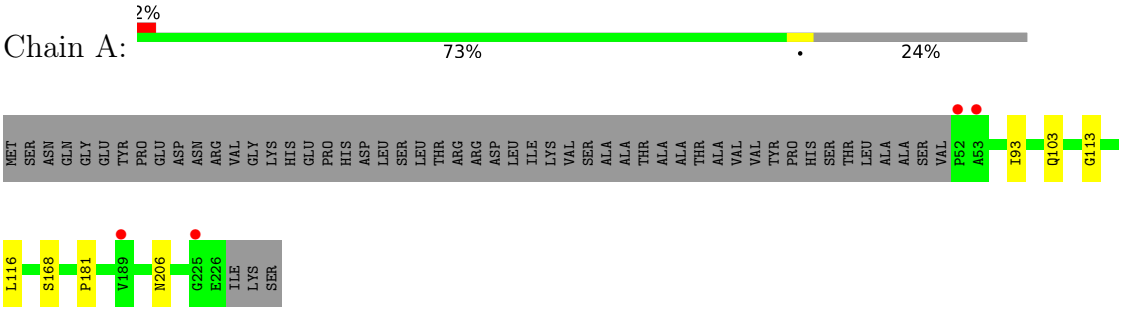
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	175	Total O 175 175	0	0
12	B	248	Total O 248 248	0	0
12	C	558	Total O 558 558	0	0

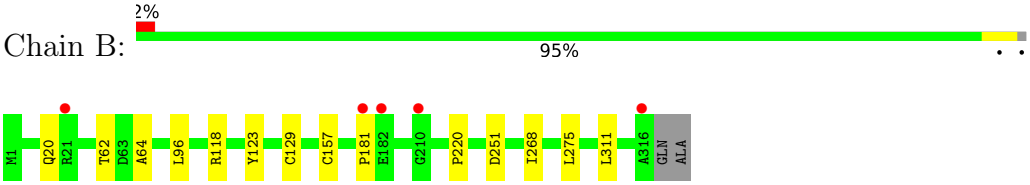
3 Residue-property plots (i)

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.

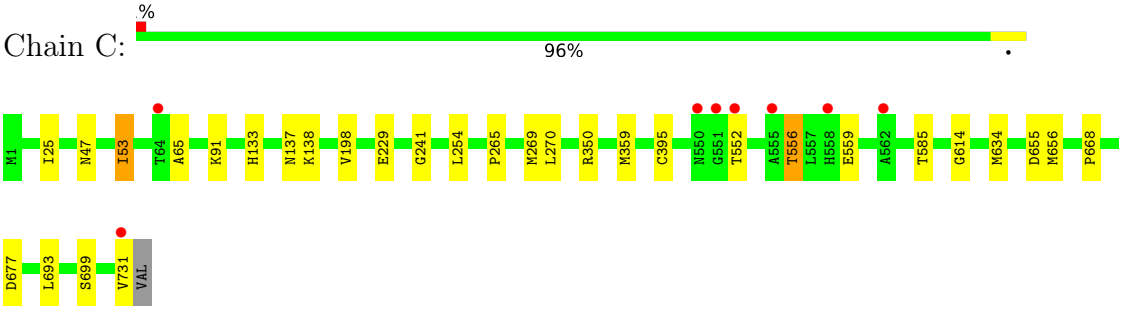
• Molecule 1: PUTATIVE XANTHINE DEHYDROGENASE YAGT IRON-SULFUR-BINDING SUBUNIT



• Molecule 2: PUTATIVE XANTHINE DEHYDROGENASE YAGR MOLYBDENUM-BINDING SU SUBUNIT



• Molecule 3: PUTATIVE XANTHINE DEHYDROGENASE YAGS FAD-BINDING SUBUNIT



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	109.68Å 78.34Å 151.91Å 90.00° 99.69° 90.00°	Depositor
Resolution (Å)	48.32 – 1.70 48.32 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.32-1.70) 98.5 (48.32-1.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.138 , 0.167 0.153 , 0.179	Depositor DCC
R_{free} test set	6835 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10479	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: GOL, FES, SF4, CSD, F5K, IOD, FAD, ACT, CL

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	0.99	1/1364 (0.1%)	0.89	0/1850
2	B	0.93	1/2447 (0.0%)	0.91	0/3327
3	C	0.98	0/5693	0.96	0/7730
All	All	0.97	2/9504 (0.0%)	0.94	0/12907

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	ASN	C-O	-7.92	1.15	1.24
2	B	220	PRO	CA-C	5.12	1.54	1.51

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	1341	0	1319	5	0
2	B	2400	0	2449	12	0
3	C	5569	0	5522	18	0
4	A	8	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	3	0	0	1	0
6	A	3	0	0	3	0
6	B	4	0	0	0	0
6	C	5	0	0	0	0
7	A	4	0	3	0	0
7	B	4	0	3	3	0
7	C	8	0	6	0	0
8	A	12	0	16	1	0
8	B	12	0	16	1	0
8	C	12	0	16	1	0
9	B	8	0	0	2	0
10	B	53	0	31	0	0
11	C	48	0	0	0	0
12	A	175	0	0	1	1
12	B	248	0	0	0	0
12	C	558	0	0	1	1
All	All	10479	0	9381	34	1

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 2.

The worst 5 of 34 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)
2:B:157:CYS:HG	9:B:320:SF4:FE4	0.74	0.97
2:B:129:CYS:HG	9:B:320:SF4:FE2	0.63	0.89
1:A:103:GLN:OE1	6:A:1229:CL:CL	2.30	0.86
3:C:53[A]:ILE:HD11	3:C:254:LEU:HD12	1.73	0.70
3:C:25:ILE:HD12	8:C:1742:GOL:H31	1.79	0.65

All (1) 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)
12:A:2030:HOH:O	12:C:2076:HOH:O[3_445]	2.18	0.02

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	180/229 (79%)	177 (98%)	3 (2%)	0	100	100
2	B	318/318 (100%)	315 (99%)	3 (1%)	0	100	100
3	C	742/732 (101%)	727 (98%)	13 (2%)	2 (0%)	36	22
All	All	1240/1279 (97%)	1219 (98%)	19 (2%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	241	GLY
3	C	350	ARG

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	148/186 (80%)	147 (99%)	1 (1%)	76	69
2	B	247/244 (101%)	247 (100%)	0	100	100
3	C	578/565 (102%)	571 (99%)	7 (1%)	63	51
All	All	973/995 (98%)	965 (99%)	8 (1%)	76	65

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	731	VAL

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Mol	Chain	Res	Type
3	C	556	THR
3	C	229	GLU
3	C	91	LYS
3	C	552	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	151	ASN
3	C	152	GLN
3	C	625	GLN
3	C	321	GLN
3	C	14	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
3	CSD	C	395	3	3,7,8	0.74	0	1,8,10	6.34	1 (100%)

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
3	CSD	C	395	3	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	395	CSD	OD1-SG-CB	-6.34	93.47	105.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	395	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 19 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
4	FES	A	231	1	0,4,4	-	-	-		
8	GOL	A	1233	-	5,5,5	0.32	0	5,5,5	0.84	0
8	GOL	B	1322	-	5,5,5	0.54	0	5,5,5	0.39	0
10	FAD	B	321	-	56,58,58	3.28	26 (46%)	81,89,89	3.48	37 (45%)
7	ACT	A	1231	-	3,3,3	0.79	0	3,3,3	0.69	0
7	ACT	C	1740	-	3,3,3	0.88	0	3,3,3	0.34	0
11	F5K	C	4001	-	43,53,53	3.84	23 (53%)	48,86,86	3.61	25 (52%)
8	GOL	B	1323	-	5,5,5	0.38	0	5,5,5	0.40	0
8	GOL	C	1742	-	5,5,5	0.41	0	5,5,5	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SF4	B	320	2	0,12,12	-	-	-		
8	GOL	C	1741	-	5,5,5	0.54	0	5,5,5	0.69	0
8	GOL	A	1232	-	5,5,5	0.47	0	5,5,5	0.93	0
4	FES	A	230	1	0,4,4	-	-	-		
7	ACT	C	1739	-	3,3,3	0.78	0	3,3,3	0.73	0
7	ACT	B	1321	-	3,3,3	0.92	0	3,3,3	1.08	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
4	FES	A	231	1	-	-	0/1/1/1
8	GOL	B	1322	-	-	1/4/4/4	-
10	FAD	B	321	-	-	0/34/50/50	0/6/6/6
11	F5K	C	4001	-	-	2/22/78/78	0/6/6/6
8	GOL	B	1323	-	-	0/4/4/4	-
8	GOL	C	1742	-	-	2/4/4/4	-
9	SF4	B	320	2	-	-	0/6/5/5
8	GOL	C	1741	-	-	0/4/4/4	-
8	GOL	A	1232	-	-	3/4/4/4	-
4	FES	A	230	1	-	-	0/1/1/1
8	GOL	A	1233	-	-	2/4/4/4	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	4001	F5K	C4A-C4B	10.90	1.57	1.38
10	B	321	FAD	C2A-N3A	9.74	1.52	1.33
10	B	321	FAD	C4X-N5	9.13	1.48	1.30
11	C	4001	F5K	C7-C6'	8.85	1.60	1.53
10	B	321	FAD	C9-C8	8.69	1.52	1.39

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	321	FAD	C2A-N1A-C6A	11.79	139.01	118.77
10	B	321	FAD	N3A-C2A-N1A	-11.36	110.83	128.60
11	C	4001	F5K	N1-C2-N3	-8.40	103.51	118.81
10	B	321	FAD	C4A-N9A-C8A	-8.31	96.72	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	4001	F5K	C4-N3-C2	8.09	133.32	120.25

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1232	GOL	O1-C1-C2-C3
8	A	1233	GOL	O1-C1-C2-C3
8	A	1232	GOL	O1-C1-C2-O2
8	A	1233	GOL	O1-C1-C2-O2
11	C	4001	F5K	C3'-C4D-C5'-O5'

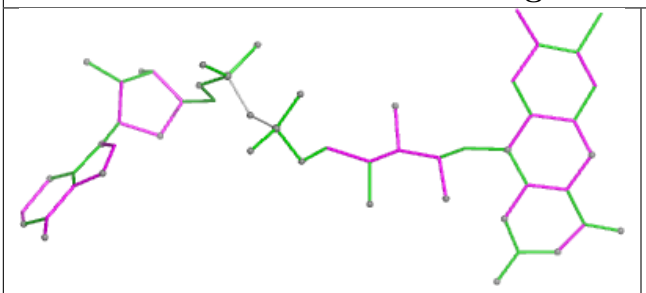
There are no ring outliers.

5 monomers are involved in 8 short contacts:

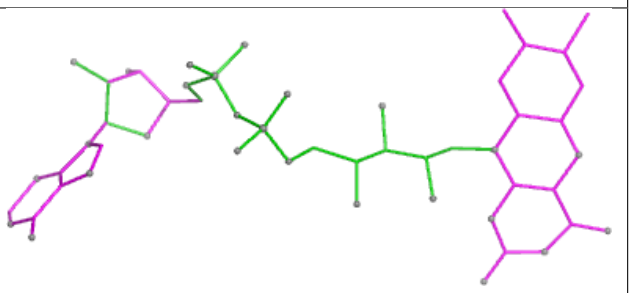
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1322	GOL	1	0
8	C	1742	GOL	1	0
9	B	320	SF4	2	0
8	A	1232	GOL	1	0
7	B	1321	ACT	3	0

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.

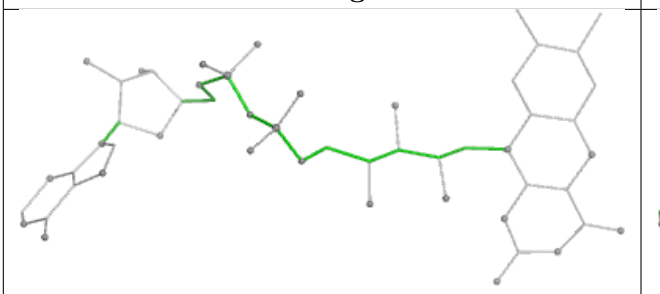
Ligand FAD B 321



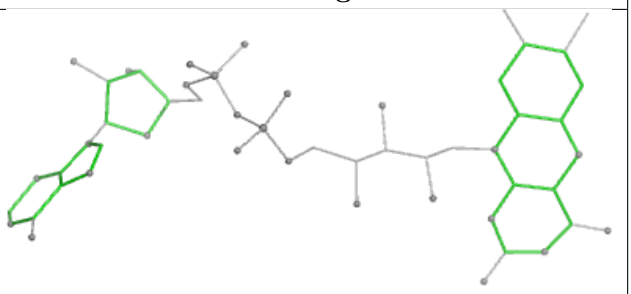
Bond lengths



Bond angles

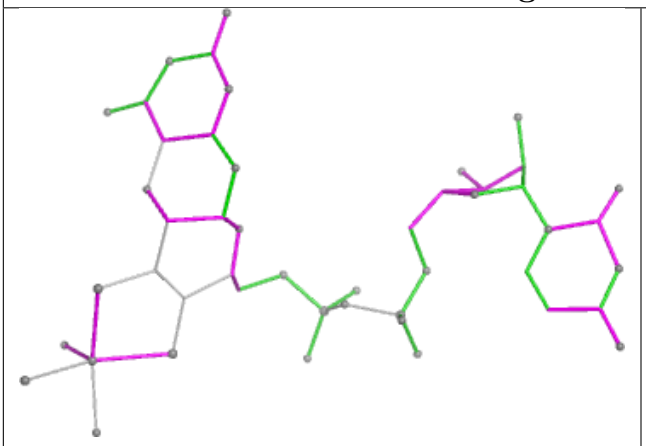


Torsions

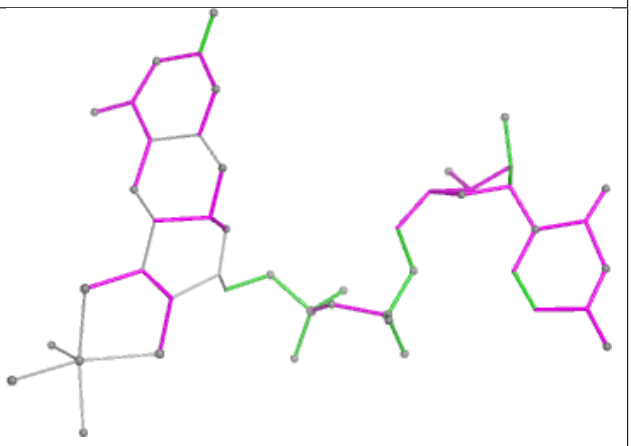


Rings

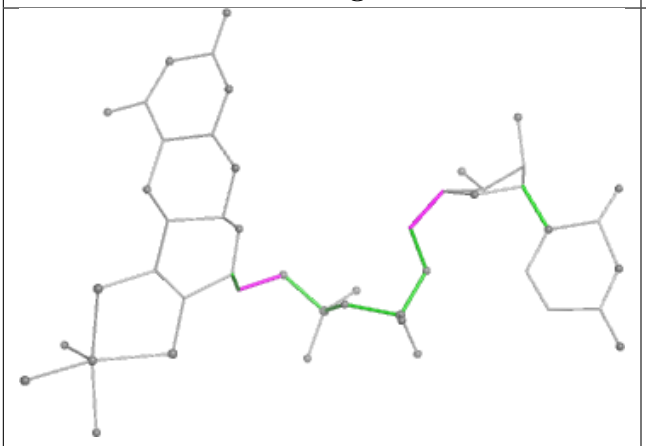
Ligand F5K C 4001



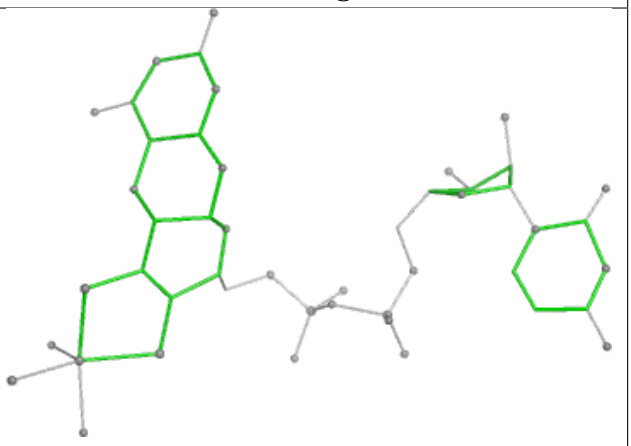
Bond lengths



Bond angles



Torsions



Rings

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, 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	175/229 (76%)	-0.39	4 (2%)	61	65	8, 15, 31, 60	7 (4%)
2	B	316/318 (99%)	-0.25	5 (1%)	70	75	8, 20, 36, 62	4 (1%)
3	C	730/732 (99%)	-0.35	8 (1%)	78	81	7, 17, 35, 61	14 (1%)
All	All	1221/1279 (95%)	-0.33	17 (1%)	73	77	7, 17, 35, 62	25 (2%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	PRO	4.6
3	C	552	THR	4.2
3	C	731	VAL	3.4
3	C	558	HIS	3.4
1	A	225	GLY	2.9

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

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, 95th 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
3	CSD	C	395	8/9	0.96	0.07	17,20,26,27	0

6.3 Carbohydrates

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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.

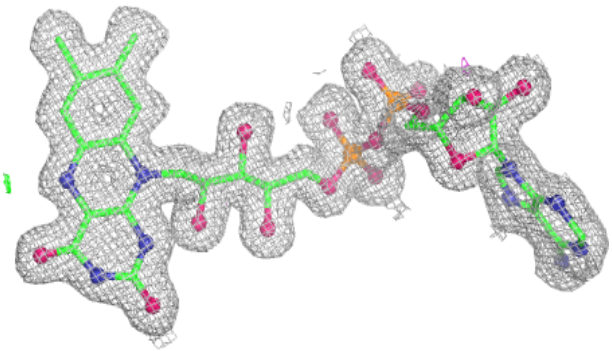
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	ACT	C	1739	4/4	0.80	0.17	53,53,58,58	0
8	GOL	A	1233	6/6	0.80	0.16	35,40,42,46	0
7	ACT	B	1321	4/4	0.81	0.16	20,23,34,38	0
9	SF4	B	320	8/8	0.82	0.14	15,17,19,20	0
8	GOL	C	1742	6/6	0.85	0.14	34,39,41,43	0
7	ACT	C	1740	4/4	0.86	0.11	34,37,38,39	0
8	GOL	A	1232	6/6	0.87	0.13	26,31,32,40	0
8	GOL	C	1741	6/6	0.87	0.12	28,39,43,43	0
8	GOL	B	1322	6/6	0.88	0.10	39,41,43,45	0
7	ACT	A	1231	4/4	0.88	0.13	27,33,34,36	0
6	CL	A	1230	1/1	0.91	0.11	43,43,43,43	0
6	CL	C	1737	1/1	0.92	0.12	36,36,36,36	0
6	CL	A	1229	1/1	0.92	0.10	27,27,27,27	0
8	GOL	B	1323	6/6	0.92	0.11	21,37,40,42	0
4	FES	A	230	4/4	0.93	0.09	10,10,11,11	0
6	CL	B	1320	1/1	0.93	0.12	37,37,37,37	0
5	IOD	A	3000	1/1	0.94	0.07	30,30,30,30	1
6	CL	B	4000	1/1	0.94	0.09	29,29,29,29	0
6	CL	B	1319	1/1	0.95	0.09	39,39,39,39	0
6	CL	C	4000	1/1	0.96	0.07	26,26,26,26	0
6	CL	C	1735	1/1	0.96	0.06	24,24,24,24	0
6	CL	C	1736	1/1	0.97	0.08	37,37,37,37	0
5	IOD	B	3000	1/1	0.97	0.05	30,30,30,30	1
5	IOD	C	1734	1/1	0.98	0.04	27,27,27,27	1
5	IOD	B	1317	1/1	0.98	0.05	28,28,28,28	1
5	IOD	C	1732	1/1	0.98	0.03	23,23,23,23	1
5	IOD	C	1733	1/1	0.99	0.03	25,25,25,25	1
6	CL	A	1228	1/1	0.99	0.05	29,29,29,29	0
6	CL	B	1318	1/1	0.99	0.04	25,25,25,25	0
6	CL	C	1738	1/1	0.99	0.03	33,33,33,33	0
10	FAD	B	321	53/53	0.99	0.03	10,12,14,14	0
11	F5K	C	4001	48/48	0.99	0.04	9,10,12,14	1
5	IOD	A	1227	1/1	1.00	0.02	13,13,13,13	1
4	FES	A	231	4/4	1.00	0.01	9,9,10,10	0

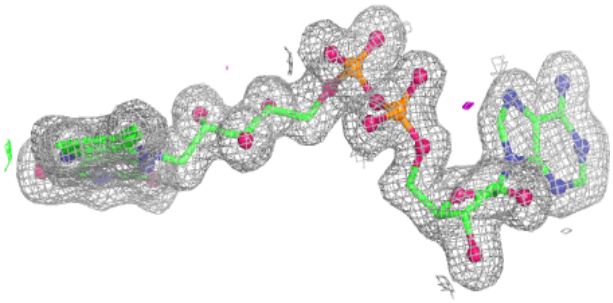
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

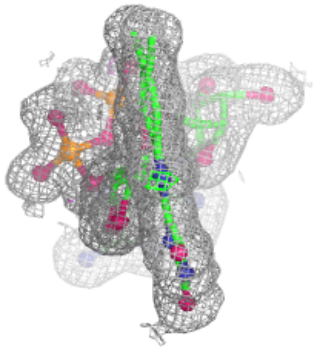
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD B 321:

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

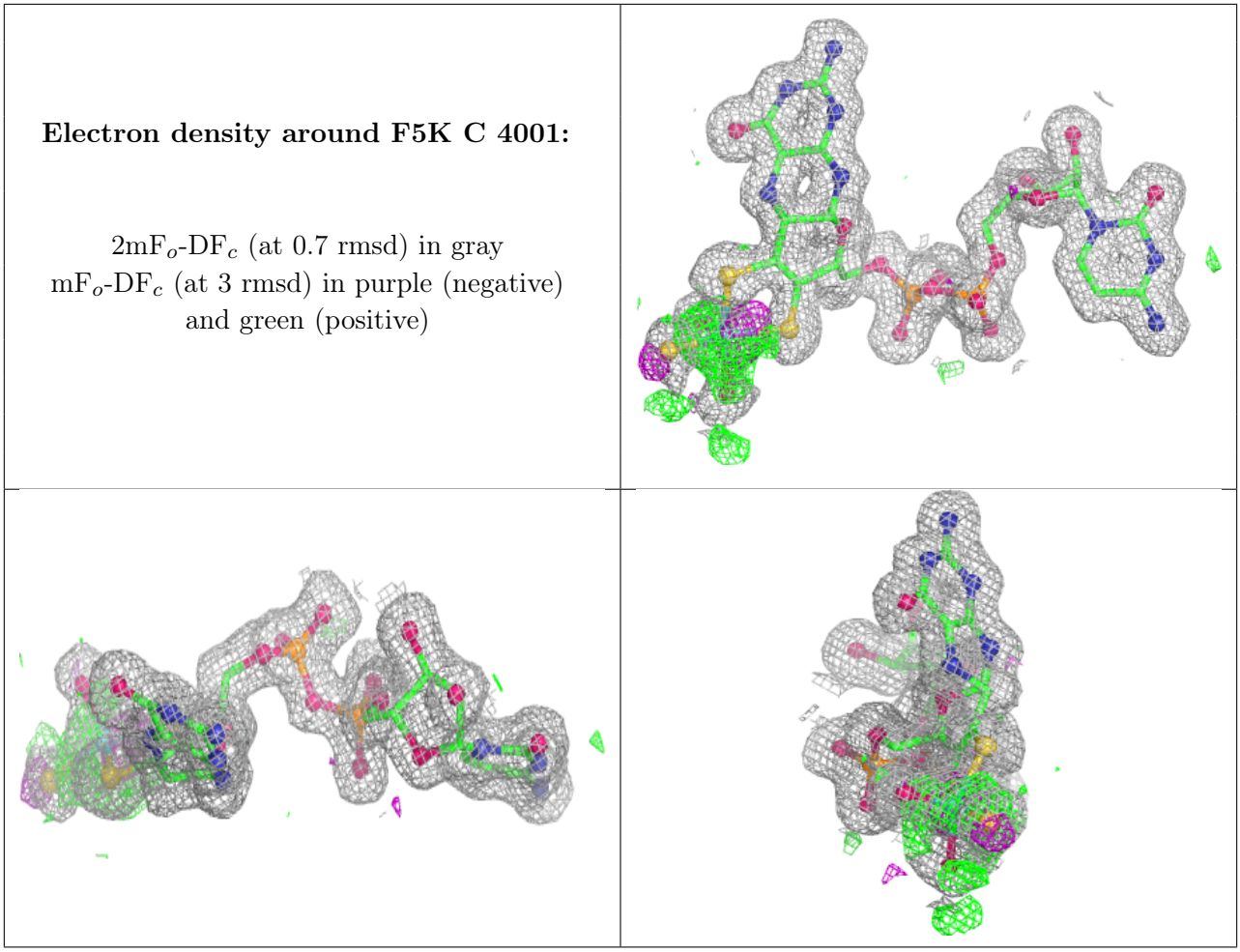






Electron density around F5K C 4001:

$2mF_o$-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.