Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2022 – 06:12 PM JST

PDB ID	:	7FGP
Title	:	Crystal structure of Aureimonas altamirenisis flavin-containing opine dehydrogenase (FAD-bound form)
Authors	:	Yoshiwara, K.; Watanabe, Y.; Watanabe, S.
Deposited on	:	2021-07-27
Resolution	:	1.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

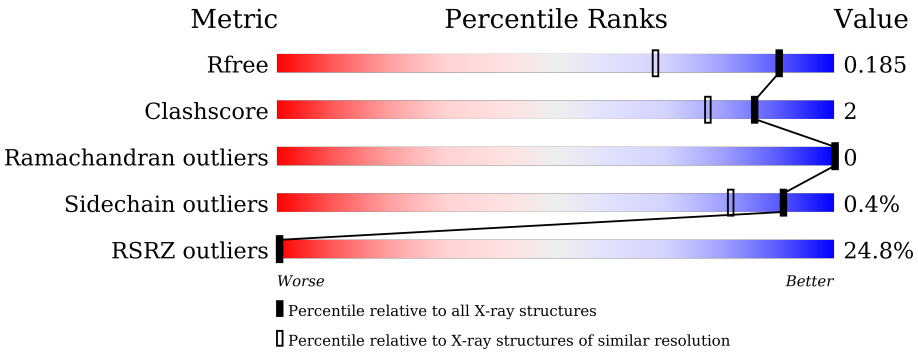
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 1.47 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}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	390	17% 94%
1	B	390	30% 88% 5% 7%

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
3	SO4	B	703	-	-	-	X
5	PEG	B	705	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6683 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 Glycine/D-amino acid oxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	Se	0	0	0
			2854	1792	517	539	4	2			
1	B	364	Total	C	N	O	S	Se	0	0	0
			2730	1723	491	510	4	2			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MSE	-	initiating methionine	UNP A0A1M6P181
A	-11	GLY	-	expression tag	UNP A0A1M6P181
A	-10	SER	-	expression tag	UNP A0A1M6P181
A	-9	SER	-	expression tag	UNP A0A1M6P181
A	-8	HIS	-	expression tag	UNP A0A1M6P181
A	-7	HIS	-	expression tag	UNP A0A1M6P181
A	-6	HIS	-	expression tag	UNP A0A1M6P181
A	-5	HIS	-	expression tag	UNP A0A1M6P181
A	-4	HIS	-	expression tag	UNP A0A1M6P181
A	-3	HIS	-	expression tag	UNP A0A1M6P181
A	-2	SER	-	expression tag	UNP A0A1M6P181
A	-1	GLN	-	expression tag	UNP A0A1M6P181
A	0	ASP	-	expression tag	UNP A0A1M6P181
A	1	LEU	-	expression tag	UNP A0A1M6P181
A	373	GLU	-	expression tag	UNP A0A1M6P181
A	374	GLN	-	expression tag	UNP A0A1M6P181
A	375	GLU	-	expression tag	UNP A0A1M6P181
A	376	PRO	-	expression tag	UNP A0A1M6P181
A	377	ALA	-	expression tag	UNP A0A1M6P181
B	-12	MSE	-	initiating methionine	UNP A0A1M6P181
B	-11	GLY	-	expression tag	UNP A0A1M6P181
B	-10	SER	-	expression tag	UNP A0A1M6P181
B	-9	SER	-	expression tag	UNP A0A1M6P181
B	-8	HIS	-	expression tag	UNP A0A1M6P181
B	-7	HIS	-	expression tag	UNP A0A1M6P181

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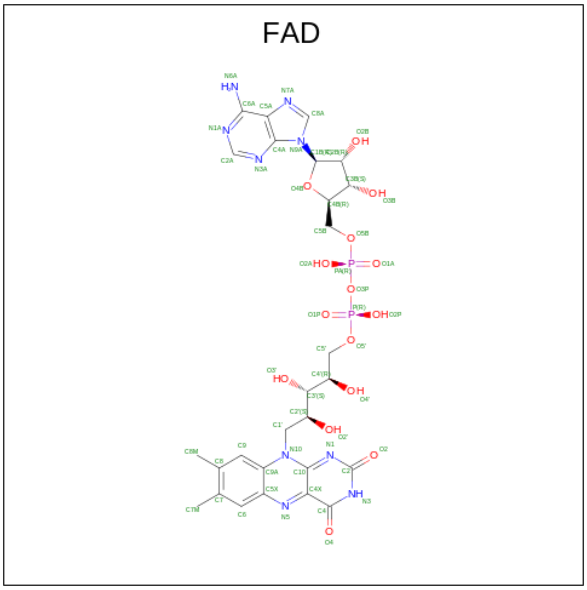
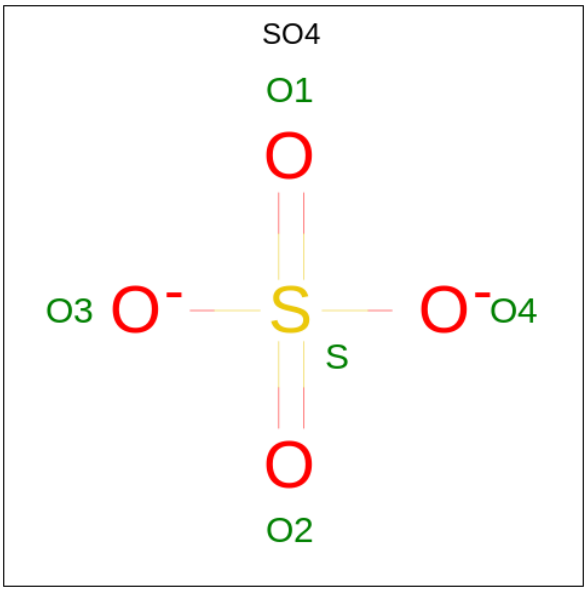
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP A0A1M6P181
B	-5	HIS	-	expression tag	UNP A0A1M6P181
B	-4	HIS	-	expression tag	UNP A0A1M6P181
B	-3	HIS	-	expression tag	UNP A0A1M6P181
B	-2	SER	-	expression tag	UNP A0A1M6P181
B	-1	GLN	-	expression tag	UNP A0A1M6P181
B	0	ASP	-	expression tag	UNP A0A1M6P181
B	1	LEU	-	expression tag	UNP A0A1M6P181
B	373	GLU	-	expression tag	UNP A0A1M6P181
B	374	GLN	-	expression tag	UNP A0A1M6P181
B	375	GLU	-	expression tag	UNP A0A1M6P181
B	376	PRO	-	expression tag	UNP A0A1M6P181
B	377	ALA	-	expression tag	UNP A0A1M6P181

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



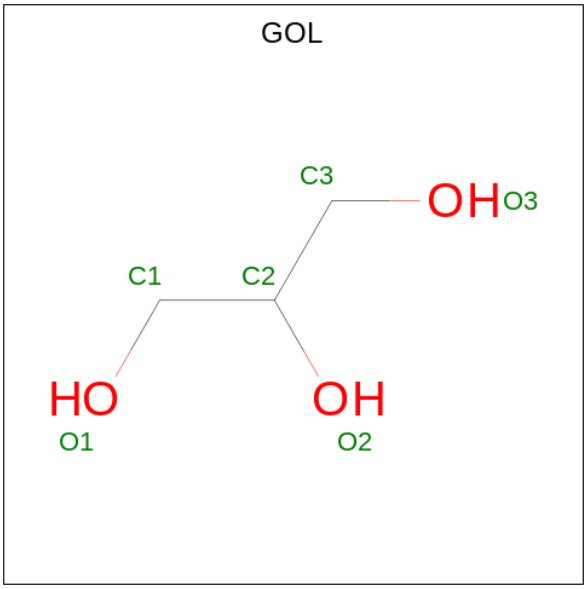
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



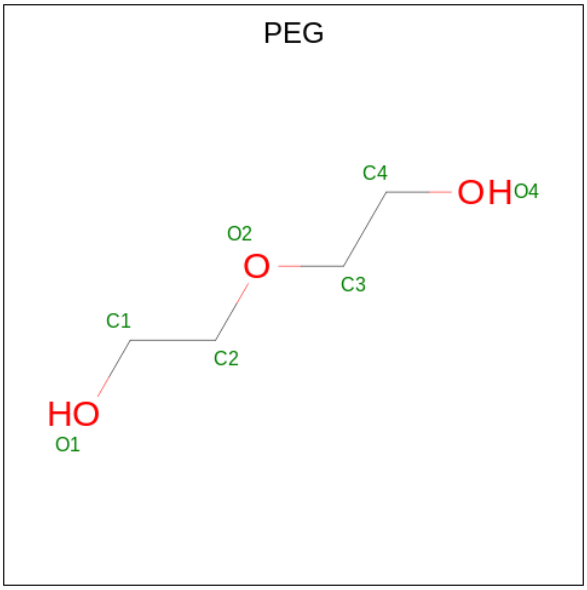
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

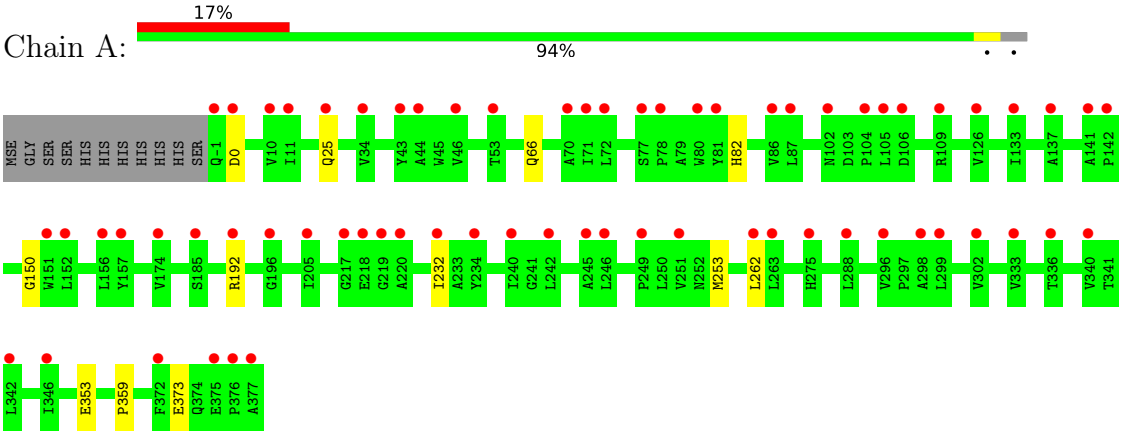
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	549	Total O 549 549	0	0
6	B	376	Total O 376 376	0	0

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.

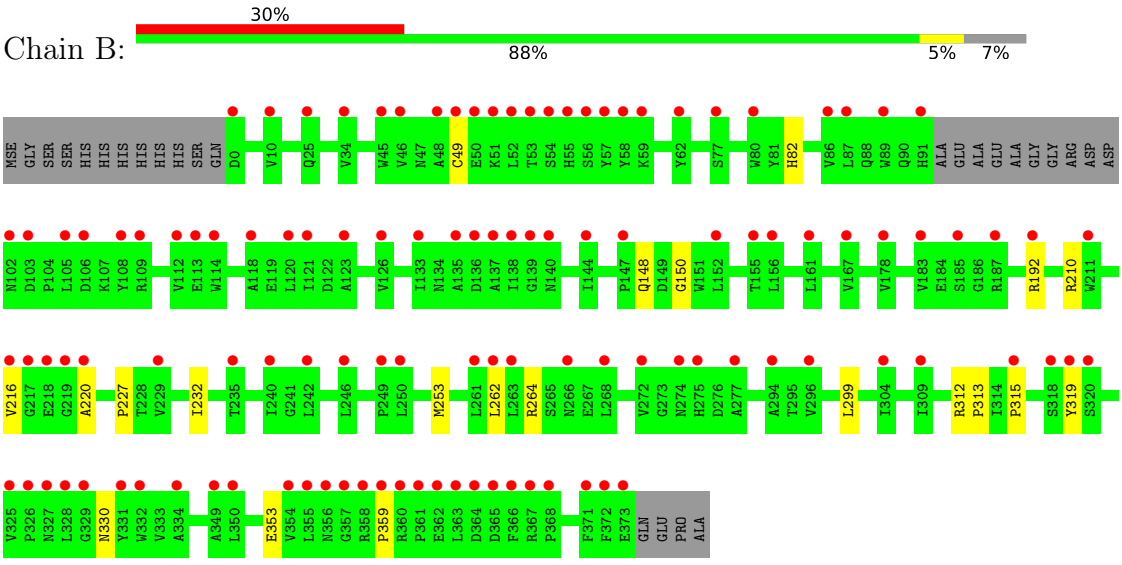
• Molecule 1: Glycine/D-amino acid oxidase

Chain A:



• Molecule 1: Glycine/D-amino acid oxidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	105.73Å 105.73Å 261.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.02 – 1.47 49.02 – 1.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.02-1.47) 100.0 (49.02-1.47)	Depositor EDS
R_{merge}	0.64	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 1.47Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.174 , 0.185 0.173 , 0.185	Depositor DCC
R_{free} test set	7341 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	16.4	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6683	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 4.41% 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: FAD, GOL, SO4, PEG

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	0.25	0/2918	0.47	0/3984
1	B	0.24	0/2792	0.47	0/3817
All	All	0.25	0/5710	0.47	0/7801

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	2854	0	2791	9	0
1	B	2730	0	2671	16	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	30	0	40	2	0
4	B	6	0	8	0	0
5	B	7	0	10	5	0
6	A	549	0	0	2	0
6	B	376	0	0	2	0
All	All	6683	0	5582	25	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 2.

All (25) 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:B:312:ARG:HH22	5:B:705:PEG:H32	1.33	0.89
1:B:192:ARG:NH1	6:B:801:HOH:O	2.18	0.74
1:A:66:GLN:NE2	6:A:501:HOH:O	2.22	0.68
1:B:353:GLU:HG2	1:B:359:PRO:HA	1.78	0.65
1:A:82:HIS:ND1	4:A:406:GOL:H31	2.16	0.60
1:B:312:ARG:NH2	5:B:705:PEG:H32	2.13	0.57
1:B:232:ILE:HD11	2:B:702:FAD:HM72	1.87	0.56
1:A:373:GLU:HA	4:A:407:GOL:H11	1.88	0.56
1:B:312:ARG:HH22	5:B:705:PEG:C3	2.12	0.55
1:B:264:ARG:HH12	5:B:705:PEG:HO1	1.55	0.55
1:B:330:ASN:ND2	6:B:809:HOH:O	2.39	0.53
1:B:210:ARG:HA	1:B:313:PRO:HB3	1.92	0.51
1:A:0:ASP:HB3	1:A:25:GLN:HG3	1.91	0.51
1:B:82:HIS:O	1:B:150:GLY:HA3	2.12	0.50
1:B:264:ARG:NH1	5:B:705:PEG:O1	2.37	0.49
1:A:82:HIS:O	1:A:150:GLY:HA3	2.12	0.48
1:A:192:ARG:NH1	6:A:509:HOH:O	2.36	0.47
1:A:353:GLU:HG3	1:A:359:PRO:HA	1.97	0.46
1:B:315:PRO:HD2	1:B:319:TYR:CD2	2.51	0.46
1:A:232:ILE:HD11	2:A:401:FAD:HM72	2.00	0.42
1:B:253:MSE:HA	1:B:262:LEU:O	2.20	0.42
1:B:227:PRO:HA	1:B:312:ARG:O	2.19	0.41
1:A:253:MSE:HA	1:A:262:LEU:O	2.21	0.41
1:B:216:VAL:HB	1:B:220:ALA:HB3	2.01	0.41
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.93	0.40

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	377/390 (97%)	371 (98%)	6 (2%)	0	100	100
1	B	360/390 (92%)	349 (97%)	11 (3%)	0	100	100
All	All	737/780 (94%)	720 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	288/298 (97%)	288 (100%)	0	100	100
1	B	276/298 (93%)	274 (99%)	2 (1%)	84	68
All	All	564/596 (95%)	562 (100%)	2 (0%)	91	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	49	CYS
1	B	148	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

14 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	GOL	B	704	-	5,5,5	0.89	0	5,5,5	1.01	0
5	PEG	B	705	-	6,6,6	0.48	0	5,5,5	0.33	0
4	GOL	A	409	-	5,5,5	0.86	0	5,5,5	1.03	0
3	SO4	B	703	-	4,4,4	0.15	0	6,6,6	0.04	0
3	SO4	B	701	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	A	407	-	5,5,5	0.93	0	5,5,5	0.98	0
4	GOL	A	408	-	5,5,5	0.89	0	5,5,5	1.03	0
4	GOL	A	405	-	5,5,5	0.90	0	5,5,5	1.03	0
3	SO4	A	404	-	4,4,4	0.13	0	6,6,6	0.05	0
3	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.04	0
4	GOL	A	406	-	5,5,5	0.89	0	5,5,5	1.01	0
2	FAD	B	702	-	53,58,58	0.46	0	68,89,89	0.49	1 (1%)
3	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	FAD	A	401	-	53,58,58	0.50	0	68,89,89	0.53	1 (1%)

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	GOL	B	704	-	-	0/4/4/4	-
5	PEG	B	705	-	-	2/4/4/4	-
4	GOL	A	409	-	-	2/4/4/4	-
4	GOL	A	407	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	408	-	-	3/4/4/4	-
4	GOL	A	405	-	-	2/4/4/4	-
4	GOL	A	406	-	-	3/4/4/4	-
2	FAD	B	702	-	-	1/30/50/50	0/6/6/6
2	FAD	A	401	-	-	1/30/50/50	0/6/6/6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	FAD	C5A-C6A-N6A	2.27	123.80	120.35
2	B	702	FAD	C5A-C6A-N6A	2.25	123.77	120.35

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	GOL	C1-C2-C3-O3
4	A	406	GOL	O1-C1-C2-C3
4	A	408	GOL	O1-C1-C2-C3
5	B	705	PEG	O1-C1-C2-O2
5	B	705	PEG	O2-C3-C4-O4
4	A	407	GOL	O1-C1-C2-C3
4	A	407	GOL	C1-C2-C3-O3
4	A	406	GOL	O1-C1-C2-O2
4	A	405	GOL	O2-C2-C3-O3
4	A	406	GOL	O2-C2-C3-O3
4	A	409	GOL	O1-C1-C2-O2
4	A	407	GOL	O1-C1-C2-O2
4	A	408	GOL	O1-C1-C2-O2
4	A	409	GOL	O1-C1-C2-C3
4	A	408	GOL	C1-C2-C3-O3
2	A	401	FAD	O4B-C4B-C5B-O5B
2	B	702	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	705	PEG	5	0

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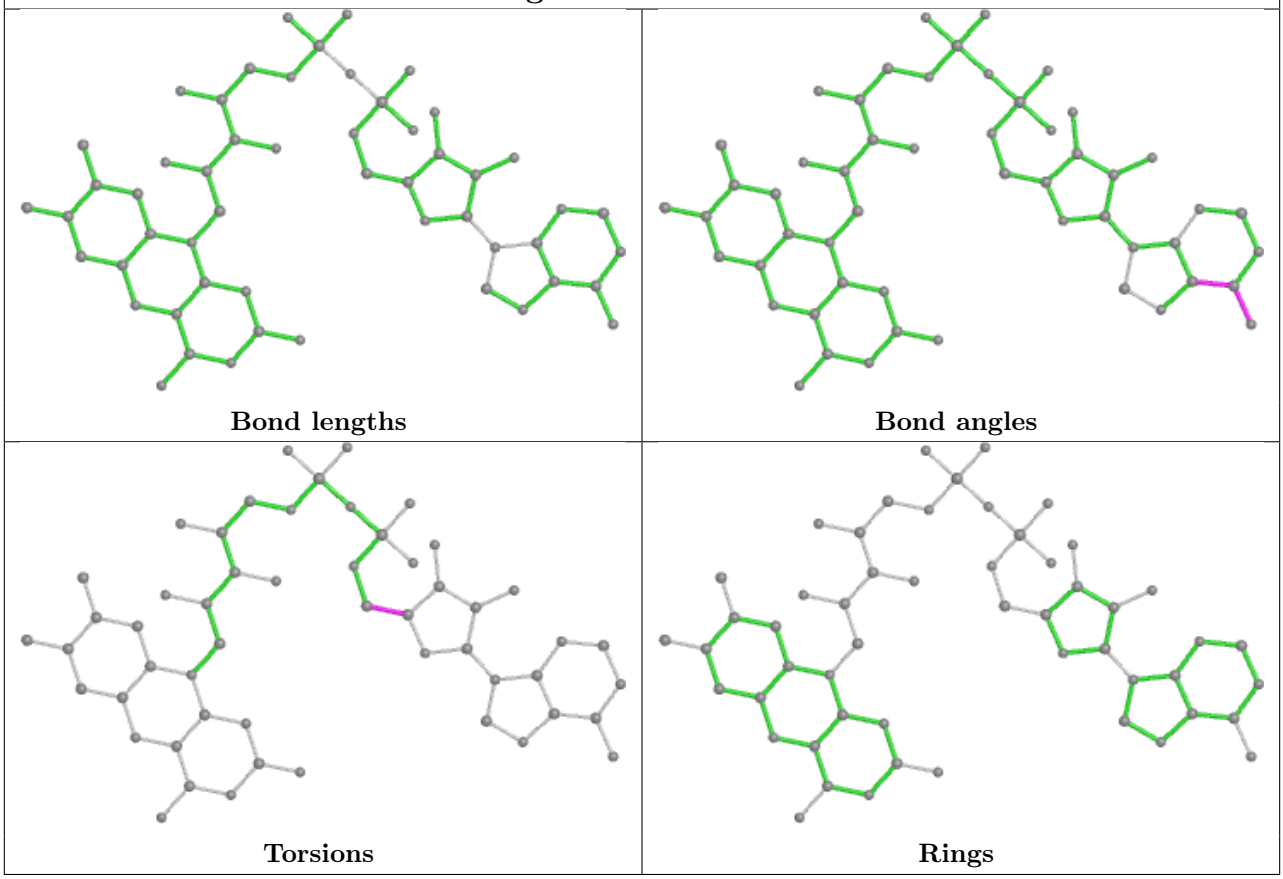
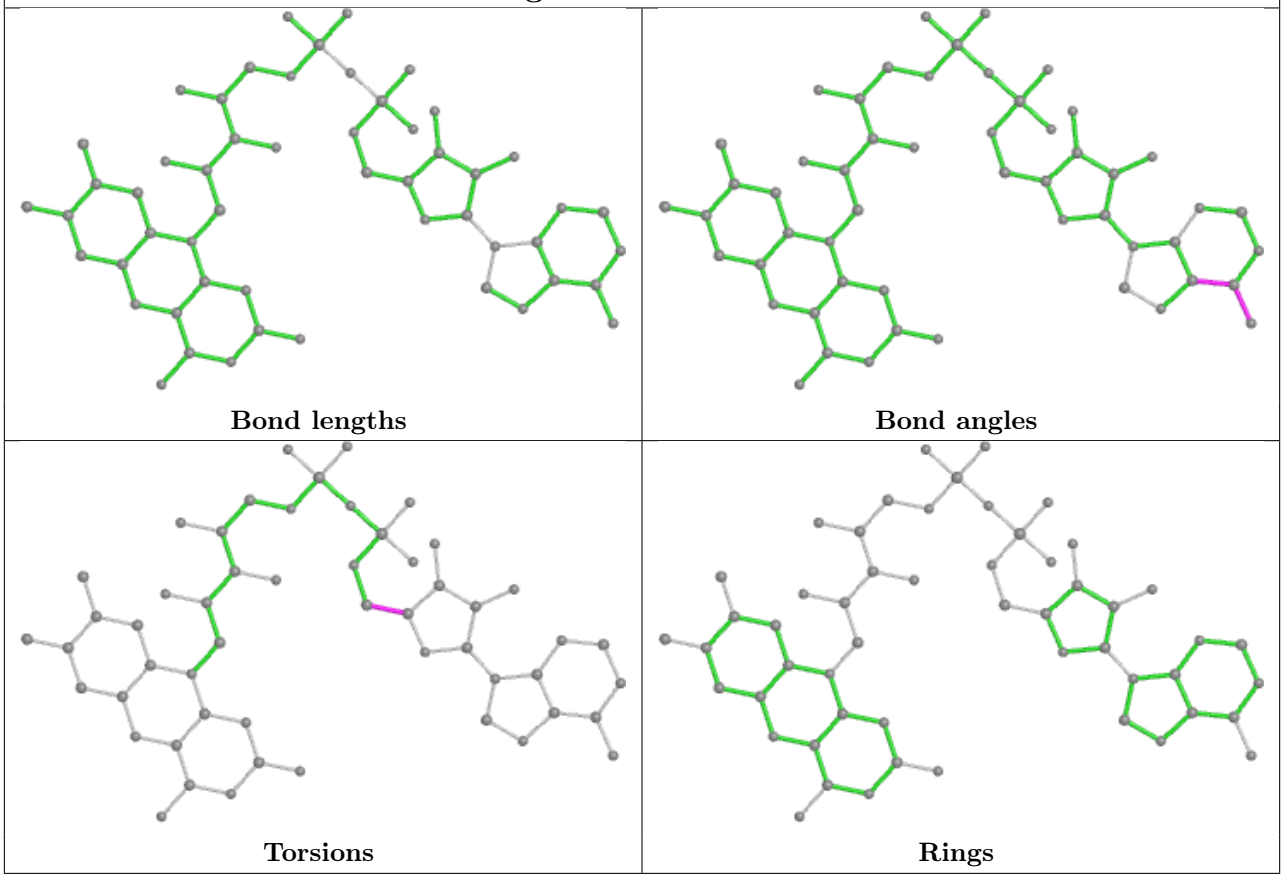
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	407	GOL	1	0
4	A	406	GOL	1	0
2	B	702	FAD	1	0
2	A	401	FAD	1	0

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 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 702



Ligand FAD A 401



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	377/390 (96%)	1.39	67 (17%)	1	1	11, 15, 25, 46	0
1	B	362/390 (92%)	1.73	116 (32%)	0	0	12, 20, 35, 53	0
All	All	739/780 (94%)	1.56	183 (24%)	0	0	11, 18, 33, 53	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	PRO	8.8
1	B	361	PRO	8.1
1	B	358	ARG	7.8
1	B	326	PRO	7.2
1	B	52	LEU	6.7
1	B	372	PHE	6.6
1	A	377	ALA	6.4
1	B	102	ASN	6.0
1	A	-1	GLN	5.7
1	B	363	LEU	5.6
1	B	112	VAL	5.5
1	B	319	TYR	5.5
1	A	376	PRO	4.8
1	A	219	GLY	4.7
1	B	53	THR	4.7
1	B	219	GLY	4.7
1	B	58	TYR	4.4
1	B	51	LYS	4.1
1	B	371	PHE	4.1
1	B	62	TYR	3.9
1	B	360	ARG	3.8
1	B	366	PHE	3.8
1	A	53	THR	3.8
1	A	105	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	108	TYR	3.7
1	B	373	GLU	3.7
1	A	106	ASP	3.6
1	B	218	GLU	3.6
1	B	49	CYS	3.5
1	B	105	LEU	3.5
1	B	220	ALA	3.5
1	B	114	TRP	3.4
1	B	54	SER	3.4
1	B	187	ARG	3.3
1	B	328	LEU	3.3
1	A	86	VAL	3.3
1	B	275	HIS	3.3
1	B	357	GLY	3.2
1	B	332	TRP	3.2
1	B	103	ASP	3.2
1	B	137	ALA	3.2
1	A	302	VAL	3.2
1	B	249	PRO	3.2
1	A	0	ASP	3.1
1	B	327	ASN	3.1
1	B	364	ASP	3.1
1	B	118	ALA	3.1
1	B	57	TYR	3.1
1	B	183	VAL	3.0
1	A	151	TRP	3.0
1	A	220	ALA	3.0
1	B	135	ALA	2.9
1	B	55	HIS	2.9
1	A	372	PHE	2.9
1	B	356	ASN	2.9
1	A	217	GLY	2.8
1	B	217	GLY	2.8
1	A	242	LEU	2.8
1	B	56	SER	2.8
1	A	46	VAL	2.7
1	A	246	LEU	2.7
1	B	138	ILE	2.7
1	B	325	VAL	2.7
1	B	355	LEU	2.7
1	B	25	GLN	2.7
1	B	121	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	277	ALA	2.6
1	A	34	VAL	2.6
1	A	185	SER	2.6
1	B	192	ARG	2.6
1	A	152	LEU	2.6
1	B	91	HIS	2.6
1	B	368	PRO	2.6
1	A	25	GLN	2.6
1	A	262	LEU	2.6
1	A	296	VAL	2.6
1	B	59	LYS	2.5
1	A	375	GLU	2.5
1	B	140	ASN	2.5
1	B	113	GLU	2.5
1	B	296	VAL	2.5
1	B	0	ASP	2.5
1	A	218	GLU	2.5
1	A	87	LEU	2.5
1	A	192	ARG	2.5
1	B	48	ALA	2.5
1	B	274	ASN	2.5
1	B	246	LEU	2.4
1	B	250	LEU	2.4
1	B	331	TYR	2.4
1	A	340	VAL	2.4
1	B	10	VAL	2.4
1	B	167	VAL	2.4
1	B	106	ASP	2.4
1	B	123	ALA	2.4
1	A	81	TYR	2.4
1	B	45	TRP	2.4
1	B	211	TRP	2.4
1	B	272	VAL	2.4
1	B	354	VAL	2.4
1	A	346	ILE	2.4
1	B	240	ILE	2.4
1	B	318	SER	2.4
1	B	263	LEU	2.4
1	A	44	ALA	2.4
1	B	365	ASP	2.4
1	A	156	LEU	2.4
1	B	87	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	2.4
1	B	185	SER	2.3
1	A	137	ALA	2.3
1	A	10	VAL	2.3
1	A	174	VAL	2.3
1	A	102	ASN	2.3
1	A	240	ILE	2.3
1	A	299	LEU	2.3
1	A	342	LEU	2.3
1	B	152	LEU	2.3
1	B	334	ALA	2.3
1	A	109	ARG	2.3
1	B	367	ARG	2.3
1	B	34	VAL	2.3
1	B	266	ASN	2.3
1	A	77	SER	2.3
1	A	133	ILE	2.3
1	A	72	LEU	2.3
1	B	261	LEU	2.3
1	B	262	LEU	2.3
1	A	333	VAL	2.3
1	A	71	ILE	2.3
1	A	232	ILE	2.3
1	B	86	VAL	2.3
1	B	126	VAL	2.3
1	B	362	GLU	2.2
1	A	205	ILE	2.2
1	B	80	TRP	2.2
1	A	336	THR	2.2
1	B	229	VAL	2.2
1	B	133	ILE	2.2
1	B	144	ILE	2.2
1	B	156	LEU	2.2
1	B	350	LEU	2.2
1	B	294	ALA	2.2
1	A	43	TYR	2.2
1	B	46	VAL	2.2
1	A	78	PRO	2.2
1	A	288	LEU	2.2
1	B	109	ARG	2.2
1	B	235	THR	2.1
1	B	161	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	11	ILE	2.1
1	B	304	ILE	2.1
1	A	80	TRP	2.1
1	A	142	PRO	2.1
1	B	320	SER	2.1
1	B	50	GLU	2.1
1	B	139	GLY	2.1
1	B	329	GLY	2.1
1	A	251	VAL	2.1
1	B	349	ALA	2.1
1	A	263	LEU	2.1
1	A	70	ALA	2.1
1	A	298	ALA	2.1
1	B	309	ILE	2.1
1	A	234	TYR	2.1
1	B	77	SER	2.1
1	B	89	TRP	2.1
1	A	245	ALA	2.1
1	A	104	PRO	2.0
1	B	147	PRO	2.0
1	B	315	PRO	2.0
1	A	157	TYR	2.0
1	A	126	VAL	2.0
1	A	196	GLY	2.0
1	B	155	THR	2.0
1	A	275	HIS	2.0
1	A	249	PRO	2.0
1	B	242	LEU	2.0
1	B	268	LEU	2.0
1	B	178	VAL	2.0
1	B	216	VAL	2.0
1	B	136	ASP	2.0
1	A	141	ALA	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

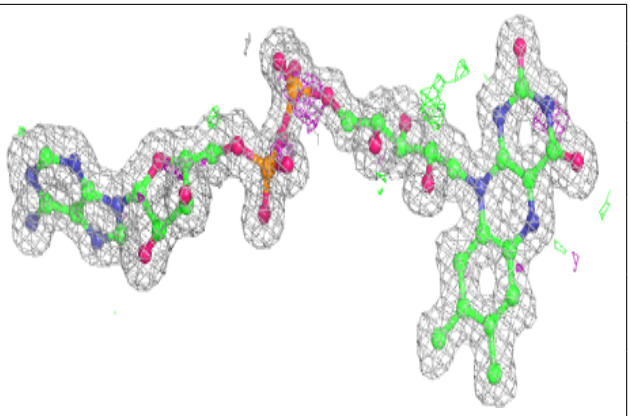
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

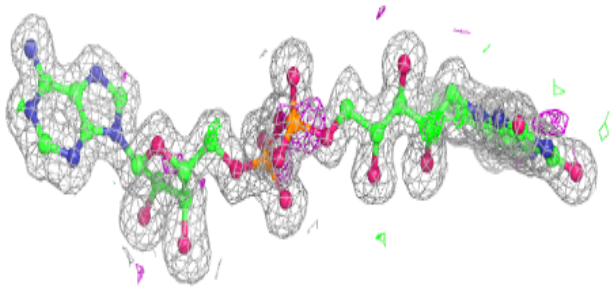
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	703	5/5	0.60	0.41	40,48,51,56	0
4	GOL	A	406	6/6	0.70	0.32	25,32,38,42	0
4	GOL	A	409	6/6	0.71	0.30	26,29,34,37	0
5	PEG	B	705	7/7	0.72	0.25	30,32,38,39	0
4	GOL	A	407	6/6	0.75	0.28	32,36,40,41	0
3	SO4	B	701	5/5	0.76	0.36	35,35,40,45	0
4	GOL	B	704	6/6	0.77	0.24	28,30,33,35	0
4	GOL	A	405	6/6	0.80	0.18	26,27,32,36	0
3	SO4	A	404	5/5	0.84	0.27	33,34,40,41	0
4	GOL	A	408	6/6	0.86	0.21	24,27,30,30	0
3	SO4	A	403	5/5	0.91	0.41	30,37,43,46	0
3	SO4	A	402	5/5	0.92	0.30	41,41,45,50	0
2	FAD	B	702	53/53	0.92	0.14	13,14,17,18	0
2	FAD	A	401	53/53	0.94	0.14	9,11,14,14	0

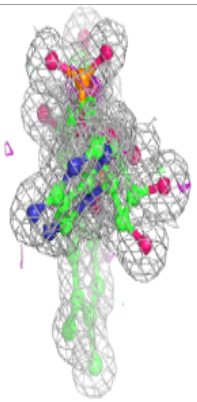
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 702:

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

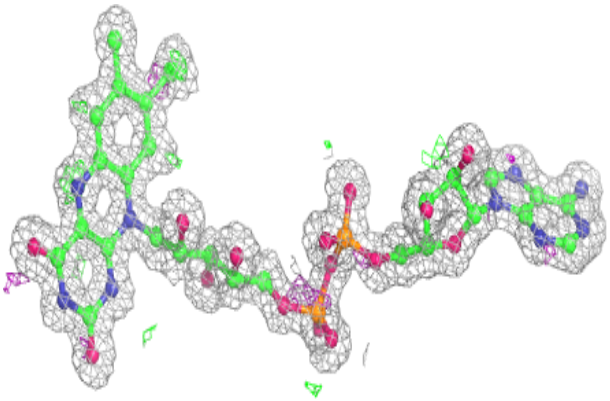


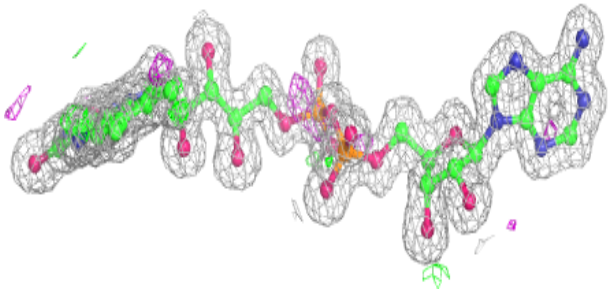


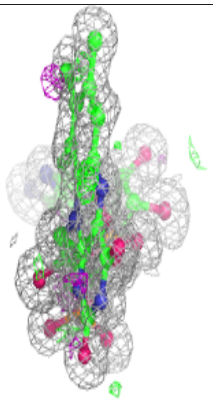


Electron density around FAD A 401:

$2mF_o$-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.