Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 01:44 AM EDT

PDB ID	:	1RYI
Title	:	STRUCTURE OF GLYCINE OXIDASE WITH BOUND INHIBITOR GLYCOLATE
Authors	:	Moertl, M.; Diederichs, K.; Welte, W.; Pollegioni, L.; Molla, G.; Motteran, L.; Andriolo, G.; Pilone, M.S.
Deposited on	:	2003-12-22
Resolution	:	1.80 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 (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:

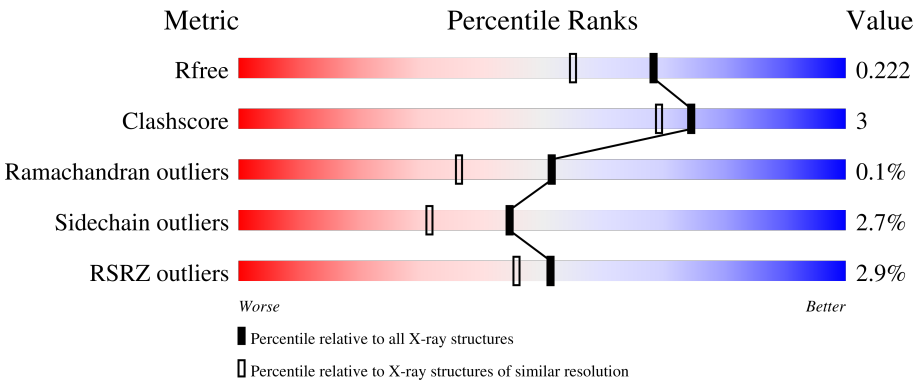
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	382	3% 84% 10% • 5%
1	B	382	2% 88% 6% • 5%
1	C	382	2% 87% 8% • 5%
1	D	382	4% 86% 9% 5%

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	GOA	A	9110	-	X	-	-
3	GOA	B	9210	-	X	-	-
3	GOA	C	9310	-	-	X	-
3	GOA	D	9410	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12720 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 OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	2855	1826	489	523	17	0	1	0
1	B	364	2866	1835	490	524	17	0	2	0
1	C	364	2855	1826	489	523	17	0	1	0
1	D	364	2866	1835	490	524	17	0	2	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP O31616
A	-11	HIS	-	expression tag	UNP O31616
A	-10	HIS	-	expression tag	UNP O31616
A	-9	HIS	-	expression tag	UNP O31616
A	-8	HIS	-	expression tag	UNP O31616
A	-7	HIS	-	expression tag	UNP O31616
A	-6	HIS	-	expression tag	UNP O31616
A	-5	MET	-	expression tag	UNP O31616
A	-4	ALA	-	expression tag	UNP O31616
A	-3	ARG	-	expression tag	UNP O31616
A	-2	ILE	-	expression tag	UNP O31616
A	-1	ARG	-	expression tag	UNP O31616
A	0	ALA	-	expression tag	UNP O31616
B	-12	MET	-	expression tag	UNP O31616
B	-11	HIS	-	expression tag	UNP O31616
B	-10	HIS	-	expression tag	UNP O31616
B	-9	HIS	-	expression tag	UNP O31616
B	-8	HIS	-	expression tag	UNP O31616
B	-7	HIS	-	expression tag	UNP O31616
B	-6	HIS	-	expression tag	UNP O31616
B	-5	MET	-	expression tag	UNP O31616

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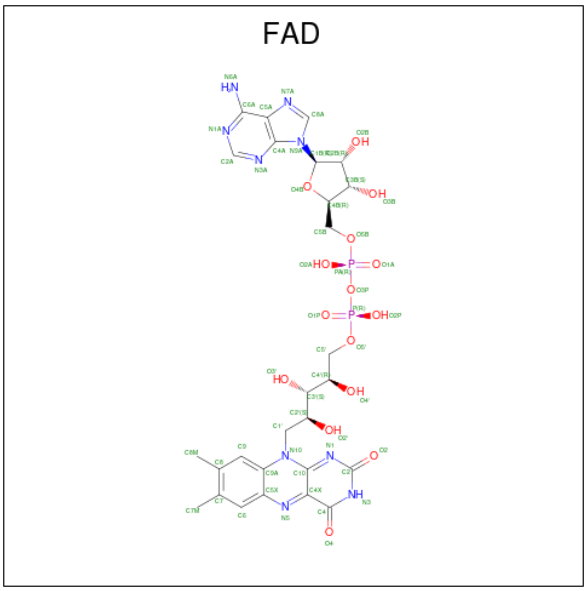
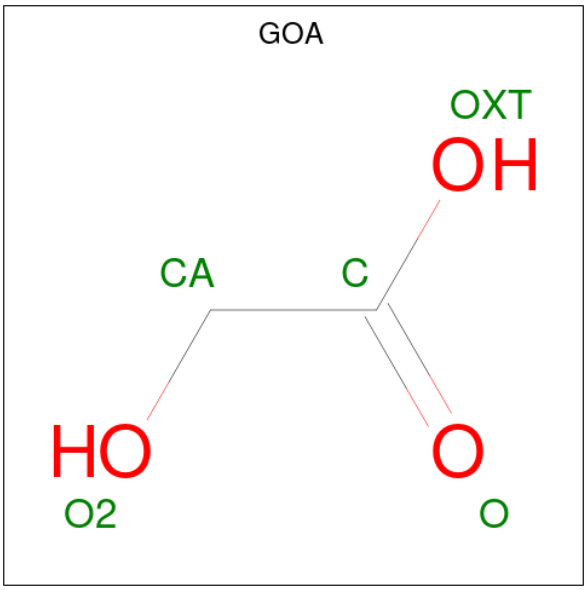
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ALA	-	expression tag	UNP O31616
B	-3	ARG	-	expression tag	UNP O31616
B	-2	ILE	-	expression tag	UNP O31616
B	-1	ARG	-	expression tag	UNP O31616
B	0	ALA	-	expression tag	UNP O31616
C	-12	MET	-	expression tag	UNP O31616
C	-11	HIS	-	expression tag	UNP O31616
C	-10	HIS	-	expression tag	UNP O31616
C	-9	HIS	-	expression tag	UNP O31616
C	-8	HIS	-	expression tag	UNP O31616
C	-7	HIS	-	expression tag	UNP O31616
C	-6	HIS	-	expression tag	UNP O31616
C	-5	MET	-	expression tag	UNP O31616
C	-4	ALA	-	expression tag	UNP O31616
C	-3	ARG	-	expression tag	UNP O31616
C	-2	ILE	-	expression tag	UNP O31616
C	-1	ARG	-	expression tag	UNP O31616
C	0	ALA	-	expression tag	UNP O31616
D	-12	MET	-	expression tag	UNP O31616
D	-11	HIS	-	expression tag	UNP O31616
D	-10	HIS	-	expression tag	UNP O31616
D	-9	HIS	-	expression tag	UNP O31616
D	-8	HIS	-	expression tag	UNP O31616
D	-7	HIS	-	expression tag	UNP O31616
D	-6	HIS	-	expression tag	UNP O31616
D	-5	MET	-	expression tag	UNP O31616
D	-4	ALA	-	expression tag	UNP O31616
D	-3	ARG	-	expression tag	UNP O31616
D	-2	ILE	-	expression tag	UNP O31616
D	-1	ARG	-	expression tag	UNP O31616
D	0	ALA	-	expression tag	UNP O31616

- Molecule 2 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		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0
2	C	1	53	27	9	15	2	0	0
2	D	1	53	27	9	15	2	0	0

- Molecule 3 is GLYCOLIC ACID (three-letter code: GOA) (formula: $C_2H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	5	2	3	0	0
			Total	C	O		
3	B	1	5	2	3	0	0
			Total	C	O		
3	C	1	5	2	3	0	0
			Total	C	O		
3	D	1	5	2	3	0	0

- Molecule 4 is water.

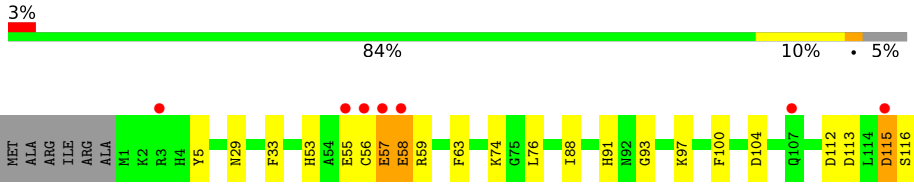
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	267	267	267	0	0
			Total	O		
4	B	262	262	262	0	0
			Total	O		
4	C	298	298	298	0	0
			Total	O		
4	D	219	219	219	0	0

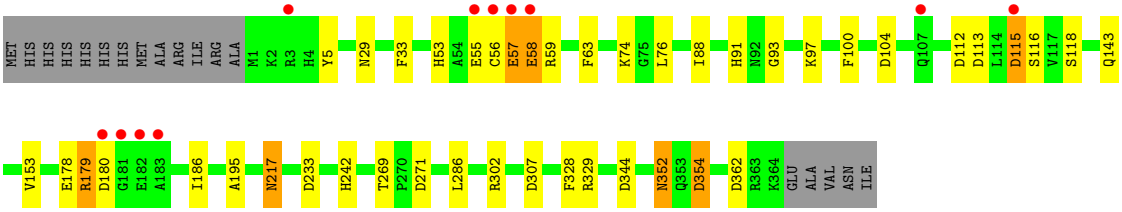
3 Residue-property plots (i)

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 OXIDASE

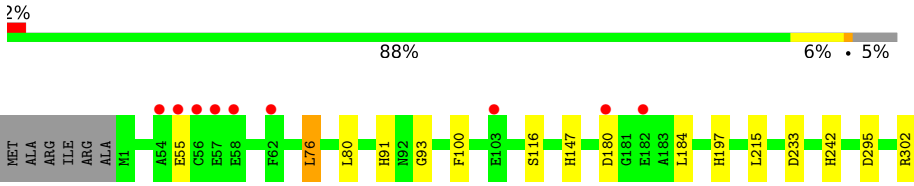
Chain A:

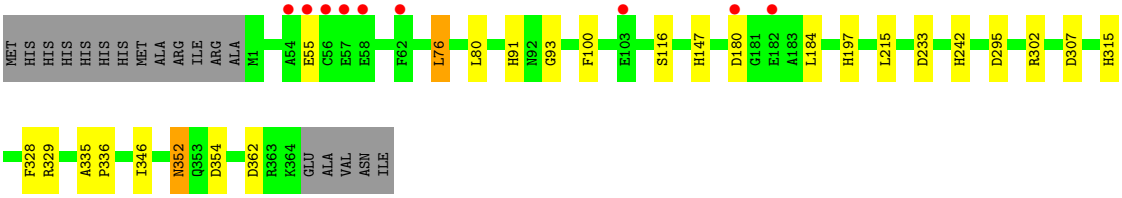




- Molecule 1: GLYCINE OXIDASE

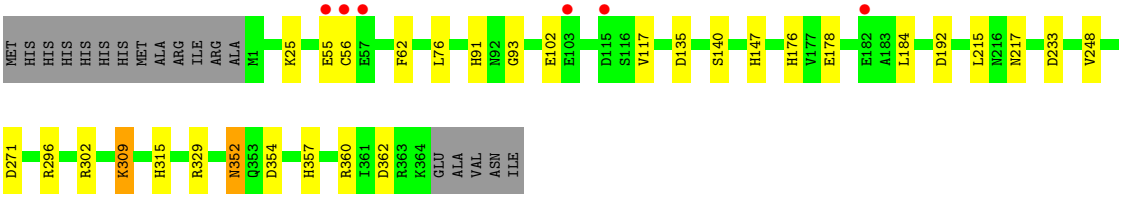
Chain B:





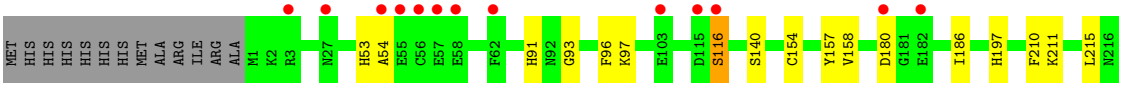
- Molecule 1: GLYCINE OXIDASE

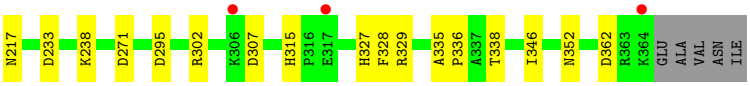
Chain C:



- Molecule 1: GLYCINE OXIDASE

Chain D:




N217
D233
K238
D271
D295
R302
K306
D307
H315
P316
E317
H327
F328
R329
A335
P336
A337
T338
I346
N352
D362
R363
K364
GLU
ALA
VAL
ASN
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	73.71Å 218.76Å 217.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 1.80 19.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.92-1.80) 98.3 (19.92-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.177 , 0.214 0.189 , 0.222	Depositor DCC
R_{free} test set	8006 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.6	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	0.96	EDS
Total number of atoms	12720	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, GOA

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	0.51	0/2926	0.78	9/3952 (0.2%)
1	B	0.52	0/2938	0.75	5/3968 (0.1%)
1	C	0.52	0/2926	0.76	5/3952 (0.1%)
1	D	0.50	0/2938	0.74	5/3968 (0.1%)
All	All	0.51	0/11728	0.76	24/15840 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	307	ASP	CB-CG-OD2	6.93	124.54	118.30
1	D	271	ASP	CB-CG-OD2	6.75	124.38	118.30
1	D	362	ASP	CB-CG-OD2	6.55	124.20	118.30
1	C	271	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	233	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	233	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	354	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	362	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	295	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	362	ASP	CB-CG-OD2	6.04	123.73	118.30
1	D	295	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	192	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	113	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	307	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	307	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	112	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	344	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	104	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	180	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	233	ASP	CB-CG-OD2	5.16	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	ASP	CB-CG-OD2	5.13	122.91	118.30
1	C	135	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	233	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	362	ASP	CB-CG-OD2	5.01	122.81	118.30

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	2855	0	2803	25	0
1	B	2866	0	2811	12	0
1	C	2855	0	2803	19	0
1	D	2866	0	2811	18	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	2	0
3	D	5	0	0	1	0
4	A	267	0	0	5	0
4	B	262	0	0	1	0
4	C	298	0	0	0	0
4	D	219	0	0	3	0
All	All	12720	0	11352	74	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 3.

All (74) 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:C:147:HIS:CD2	1:C:248:VAL:HG13	2.02	0.95
1:C:91:HIS:HB3	1:C:147:HIS:CE1	2.17	0.80
1:A:178:GLU:HA	1:A:179:ARG:CB	2.17	0.74
1:D:197:HIS:CD2	1:D:346:ILE:HG23	2.28	0.69
1:C:62:PHE:CE1	1:C:309:LYS:HG2	2.28	0.69
1:B:215:LEU:HD11	1:B:315:HIS:CD2	2.29	0.68
1:A:302:ARG:HE	3:A:9110:GOA:CA	2.06	0.67
1:D:302:ARG:HE	3:D:9410:GOA:CA	2.07	0.67
1:D:91:HIS:HD2	1:D:93:GLY:H	1.43	0.67
1:A:271:ASP:OD2	4:A:9253:HOH:O	2.15	0.64
1:C:147:HIS:CD2	1:C:248:VAL:CG1	2.80	0.64
1:A:178:GLU:HA	1:A:179:ARG:HB2	1.79	0.63
1:A:217:ASN:HD22	1:A:217:ASN:H	1.46	0.63
1:C:147:HIS:HD2	1:C:248:VAL:HG13	1.60	0.61
1:B:302:ARG:HE	3:B:9210:GOA:CA	2.13	0.61
1:A:100:PHE:HD1	1:A:242:HIS:CD2	2.19	0.60
1:B:197:HIS:CD2	1:B:346:ILE:HG23	2.36	0.60
1:D:215:LEU:HD11	1:D:315:HIS:CD2	2.37	0.60
1:C:352:ASN:HD21	1:C:354:ASP:HB2	1.66	0.59
1:A:91:HIS:HD2	1:A:93:GLY:H	1.50	0.59
1:B:91:HIS:HD2	1:B:93:GLY:H	1.50	0.58
1:C:217:ASN:HD22	1:C:217:ASN:H	1.51	0.57
1:A:180:ASP:HA	4:A:9333:HOH:O	2.05	0.55
1:A:56:CYS:HB3	1:A:63:PHE:CE1	2.42	0.55
1:B:147:HIS:HD2	4:B:9241:HOH:O	1.90	0.55
1:A:178:GLU:HA	1:A:179:ARG:HB3	1.88	0.55
1:C:352:ASN:C	1:C:352:ASN:HD22	2.12	0.53
1:D:53:HIS:CE1	1:D:116:SER:HB2	2.43	0.53
1:C:302:ARG:HE	3:C:9310:GOA:CA	2.22	0.53
1:B:91:HIS:HB3	1:B:147:HIS:CE1	2.45	0.51
1:C:117:VAL:CG1	1:C:140:SER:OG	2.58	0.51
1:C:91:HIS:CB	1:C:147:HIS:CE1	2.90	0.51
1:C:91:HIS:HD2	1:C:93:GLY:H	1.59	0.51
1:A:352:ASN:C	1:A:352:ASN:HD22	2.14	0.50
1:A:33:PHE:CE1	1:A:186:ILE:HD11	2.47	0.49
1:B:352:ASN:HD21	1:B:354:ASP:HB2	1.77	0.49
1:A:53:HIS:HE1	1:A:116:SER:OG	1.96	0.48
1:D:97:LYS:NZ	4:D:9606:HOH:O	2.46	0.48
1:D:54:ALA:HA	1:D:97:LYS:NZ	2.28	0.48
1:D:217:ASN:H	1:D:217:ASN:HD22	1.61	0.48
1:A:57:GLU:O	1:A:58:GLU:CB	2.62	0.48
1:D:54:ALA:HA	1:D:97:LYS:HZ1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:PHE:HD1	1:B:242:HIS:CD2	2.33	0.47
1:A:5:TYR:O	1:A:195:ALA:HA	2.15	0.47
1:A:328:PHE:CD2	1:A:329:ARG:HG3	2.51	0.46
1:C:91:HIS:CD2	1:C:93:GLY:H	2.34	0.45
1:A:29:ASN:OD1	4:A:9270:HOH:O	2.21	0.45
1:A:100:PHE:CD1	1:A:242:HIS:CD2	3.02	0.45
1:D:154:CYS:O	1:D:158:VAL:HG23	2.17	0.45
1:C:357:HIS:HD2	1:C:360:ARG:HD3	1.82	0.45
1:B:76:LEU:HD22	1:B:80:LEU:HG	2.00	0.44
1:A:178:GLU:CA	1:A:179:ARG:CB	2.93	0.44
1:D:96:PHE:CE1	1:D:238:LYS:HD3	2.54	0.43
1:C:215:LEU:HD11	1:C:315:HIS:CD2	2.53	0.43
1:D:335:ALA:HB3	1:D:336:PRO:HD3	2.01	0.43
1:A:57:GLU:O	1:A:58:GLU:HB2	2.19	0.42
1:B:352:ASN:C	1:B:352:ASN:HD22	2.21	0.42
1:B:328:PHE:CD2	1:B:329:ARG:HG3	2.53	0.42
1:D:53:HIS:HE1	1:D:116:SER:HB2	1.83	0.42
1:C:117:VAL:CG1	1:C:140:SER:HG	2.32	0.42
1:D:328:PHE:CD2	1:D:329:ARG:HG3	2.54	0.42
1:C:91:HIS:HB3	1:C:147:HIS:ND1	2.35	0.42
1:D:91:HIS:HE1	4:D:9431:HOH:O	2.02	0.42
1:C:176:HIS:HE1	1:C:178:GLU:OE2	2.02	0.42
1:B:335:ALA:HB3	1:B:336:PRO:HD3	2.02	0.42
1:D:210:PHE:CD2	1:D:217:ASN:HB2	2.55	0.42
1:A:352:ASN:HD21	1:A:354:ASP:HB2	1.85	0.42
1:D:116:SER:HB3	4:D:9569:HOH:O	2.19	0.41
1:A:88:ILE:HG22	1:A:153:VAL:HA	2.01	0.41
1:A:143:GLN:HG3	4:A:9354:HOH:O	2.20	0.41
1:C:329:ARG:HG2	3:C:9310:GOA:CA	2.51	0.41
1:A:97:LYS:NZ	4:A:9374:HOH:O	2.51	0.40
1:A:352:ASN:ND2	1:A:354:ASP:H	2.20	0.40
1:D:327:HIS:HE1	1:D:338:THR:OG1	2.05	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	363/382 (95%)	353 (97%)	8 (2%)	2 (1%)	25	12
1	B	364/382 (95%)	350 (96%)	14 (4%)	0	100	100
1	C	363/382 (95%)	353 (97%)	10 (3%)	0	100	100
1	D	364/382 (95%)	350 (96%)	14 (4%)	0	100	100
All	All	1454/1528 (95%)	1406 (97%)	46 (3%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ARG
1	A	58	GLU

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	296/310 (96%)	285 (96%)	11 (4%)	34	19
1	B	297/310 (96%)	292 (98%)	5 (2%)	60	51
1	C	296/310 (96%)	287 (97%)	9 (3%)	41	27
1	D	297/310 (96%)	290 (98%)	7 (2%)	49	36
All	All	1186/1240 (96%)	1154 (97%)	32 (3%)	44	31

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	57	GLU
1	A	59	ARG
1	A	74	LYS

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Mol	Chain	Res	Type
1	A	76	LEU
1	A	115	ASP
1	A	118	SER
1	A	217	ASN
1	A	269	THR
1	A	286	LEU
1	A	352	ASN
1	B	55	GLU
1	B	76	LEU
1	B	116	SER
1	B	184	LEU
1	B	352	ASN
1	C	25	LYS
1	C	55	GLU
1	C	56	CYS
1	C	76	LEU
1	C	102	GLU
1	C	184	LEU
1	C	296	ARG
1	C	309	LYS
1	C	352	ASN
1	D	116	SER
1	D	140	SER
1	D	157	TYR
1	D	180	ASP
1	D	186	ILE
1	D	211	LYS
1	D	352	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	53	HIS
1	A	70	GLN
1	A	91	HIS
1	A	110	GLN
1	A	147	HIS
1	A	197	HIS
1	A	217	ASN
1	A	327	HIS
1	A	352	ASN

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Mol	Chain	Res	Type
1	B	90	GLN
1	B	91	HIS
1	B	147	HIS
1	B	197	HIS
1	B	216	ASN
1	B	217	ASN
1	B	352	ASN
1	C	29	ASN
1	C	53	HIS
1	C	91	HIS
1	C	147	HIS
1	C	176	HIS
1	C	197	HIS
1	C	217	ASN
1	C	352	ASN
1	C	357	HIS
1	D	53	HIS
1	D	70	GLN
1	D	91	HIS
1	D	217	ASN
1	D	290	GLN
1	D	327	HIS
1	D	352	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)

8 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	$\#\|Z\| > 2$
3	GOA	D	9410	-	4,4,4	3.21	2 (50%)	4,4,4	1.56	1 (25%)
2	FAD	D	9400	-	53,58,58	1.19	5 (9%)	68,89,89	1.52	11 (16%)
2	FAD	B	9200	-	53,58,58	1.16	4 (7%)	68,89,89	1.29	5 (7%)
2	FAD	A	9100	-	53,58,58	1.13	4 (7%)	68,89,89	1.30	6 (8%)
3	GOA	C	9310	-	4,4,4	2.97	2 (50%)	4,4,4	1.42	0
3	GOA	A	9110	-	4,4,4	3.19	2 (50%)	4,4,4	1.14	0
3	GOA	B	9210	-	4,4,4	3.18	2 (50%)	4,4,4	1.34	0
2	FAD	C	9300	-	53,58,58	1.12	3 (5%)	68,89,89	1.45	10 (14%)

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	GOA	D	9410	-	-	2/2/2/2	-
2	FAD	D	9400	-	-	1/30/50/50	0/6/6/6
2	FAD	B	9200	-	-	1/30/50/50	0/6/6/6
2	FAD	A	9100	-	-	1/30/50/50	0/6/6/6
3	GOA	C	9310	-	-	1/2/2/2	-
3	GOA	A	9110	-	-	2/2/2/2	-
3	GOA	B	9210	-	-	2/2/2/2	-
2	FAD	C	9300	-	-	1/30/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9110	GOA	CA-C	-5.67	1.31	1.51
3	D	9410	GOA	CA-C	-5.59	1.31	1.51
3	B	9210	GOA	CA-C	-5.59	1.31	1.51
3	C	9310	GOA	CA-C	-5.27	1.32	1.51
2	B	9200	FAD	C4X-N5	4.56	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9300	FAD	C4X-N5	4.53	1.39	1.30
2	A	9100	FAD	C4X-N5	4.12	1.38	1.30
2	D	9400	FAD	C4X-N5	4.10	1.38	1.30
2	D	9400	FAD	C2A-N3A	3.99	1.38	1.32
2	C	9300	FAD	C2A-N3A	3.74	1.38	1.32
2	A	9100	FAD	C2A-N3A	3.55	1.37	1.32
2	B	9200	FAD	C2A-N3A	3.23	1.37	1.32
2	D	9400	FAD	C10-N1	3.18	1.39	1.33
2	B	9200	FAD	C2A-N1A	2.95	1.39	1.33
3	D	9410	GOA	O2-CA	-2.89	1.31	1.41
2	A	9100	FAD	C10-N1	2.88	1.39	1.33
3	B	9210	GOA	O2-CA	-2.68	1.32	1.41
2	D	9400	FAD	C2A-N1A	2.67	1.38	1.33
3	A	9110	GOA	O2-CA	-2.58	1.32	1.41
2	B	9200	FAD	C10-N1	2.49	1.38	1.33
2	C	9300	FAD	C10-N1	2.45	1.38	1.33
3	C	9310	GOA	O2-CA	-2.44	1.33	1.41
2	A	9100	FAD	C2A-N1A	2.24	1.38	1.33
2	D	9400	FAD	C1'-N10	2.18	1.53	1.48

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	9400	FAD	N3A-C2A-N1A	-6.86	117.95	128.68
2	C	9300	FAD	N3A-C2A-N1A	-6.06	119.20	128.68
2	A	9100	FAD	N3A-C2A-N1A	-5.66	119.83	128.68
2	B	9200	FAD	N3A-C2A-N1A	-5.11	120.69	128.68
2	D	9400	FAD	C4X-C10-N10	3.20	121.16	116.48
2	C	9300	FAD	C4X-C10-N10	3.17	121.12	116.48
2	D	9400	FAD	C4X-C4-N3	2.89	120.53	113.19
2	C	9300	FAD	C5A-C6A-N6A	2.81	124.62	120.35
2	A	9100	FAD	C4X-C10-N10	2.79	120.56	116.48
2	D	9400	FAD	C4-N3-C2	-2.77	120.53	125.64
2	B	9200	FAD	C4X-C10-N10	2.76	120.51	116.48
2	C	9300	FAD	C4A-C5A-N7A	-2.75	106.53	109.40
2	C	9300	FAD	C2A-N1A-C6A	2.60	123.20	118.75
2	C	9300	FAD	O4B-C1B-C2B	-2.56	103.18	106.93
2	B	9200	FAD	C4-N3-C2	-2.53	120.97	125.64
2	D	9400	FAD	C3B-C2B-C1B	2.53	104.78	100.98
2	C	9300	FAD	C4X-C4-N3	2.50	119.53	113.19
2	C	9300	FAD	C4-N3-C2	-2.47	121.08	125.64
2	B	9200	FAD	C10-C4X-N5	-2.45	119.66	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	9200	FAD	C4X-C4-N3	2.36	119.19	113.19
3	D	9410	GOA	O-C-CA	-2.36	113.60	122.45
2	A	9100	FAD	C5X-C9A-N10	2.33	120.36	117.95
2	D	9400	FAD	C1'-N10-C9A	2.33	124.39	120.51
2	D	9400	FAD	C10-C4X-N5	-2.23	120.13	124.86
2	A	9100	FAD	C10-C4X-N5	-2.22	120.14	124.86
2	C	9300	FAD	C10-C4X-N5	-2.21	120.16	124.86
2	D	9400	FAD	C4-C4X-N5	2.18	121.33	118.23
2	A	9100	FAD	C1'-N10-C9A	2.10	124.01	120.51
2	C	9300	FAD	C4X-C10-N1	-2.06	119.96	124.73
2	D	9400	FAD	O4B-C1B-C2B	-2.05	103.93	106.93
2	A	9100	FAD	C4X-C4-N3	2.04	118.37	113.19
2	D	9400	FAD	C4X-C10-N1	-2.04	120.01	124.73
2	D	9400	FAD	O4-C4-C4X	-2.02	121.23	126.60

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	9110	GOA	O-C-CA-O2
3	A	9110	GOA	OXT-C-CA-O2
3	B	9210	GOA	O-C-CA-O2
3	B	9210	GOA	OXT-C-CA-O2
3	D	9410	GOA	O-C-CA-O2
3	D	9410	GOA	OXT-C-CA-O2
3	C	9310	GOA	OXT-C-CA-O2
2	A	9100	FAD	O4B-C4B-C5B-O5B
2	B	9200	FAD	O4B-C4B-C5B-O5B
2	D	9400	FAD	O4B-C4B-C5B-O5B
2	C	9300	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

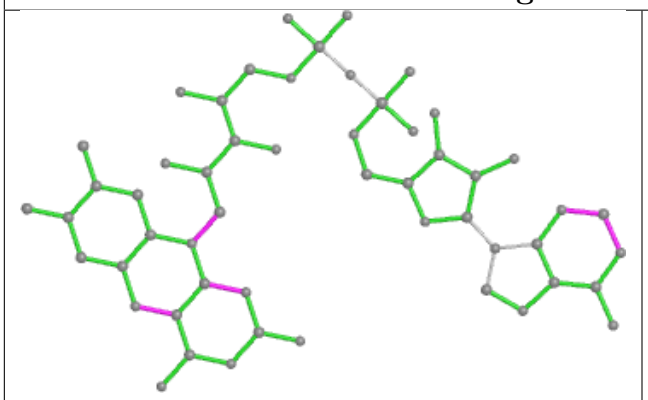
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	9410	GOA	1	0
3	C	9310	GOA	2	0
3	A	9110	GOA	1	0
3	B	9210	GOA	1	0

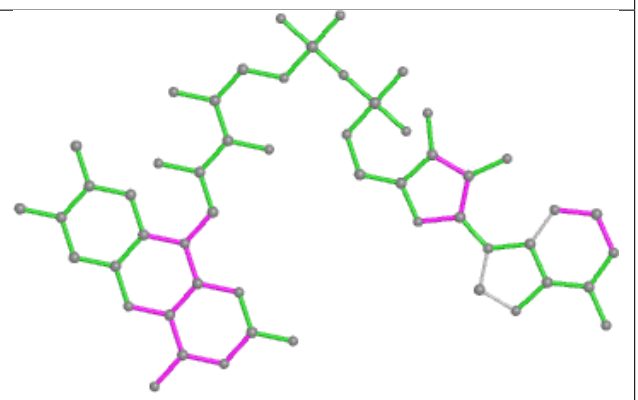
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

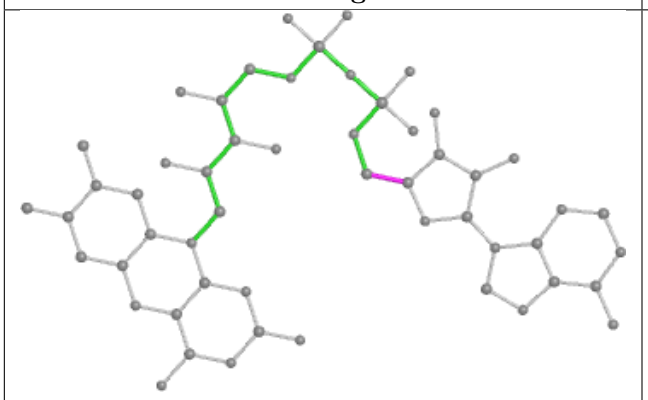
Ligand FAD D 9400



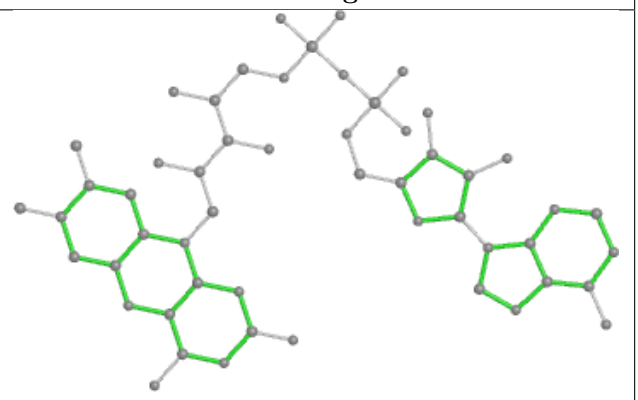
Bond lengths



Bond angles

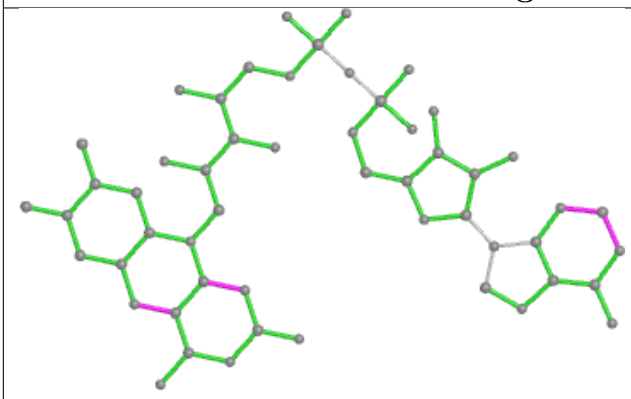


Torsions

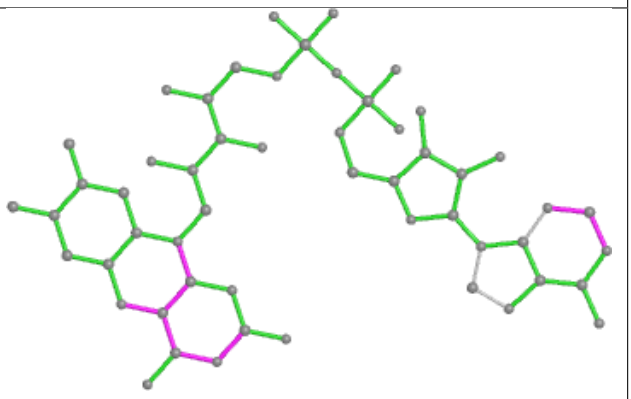


Rings

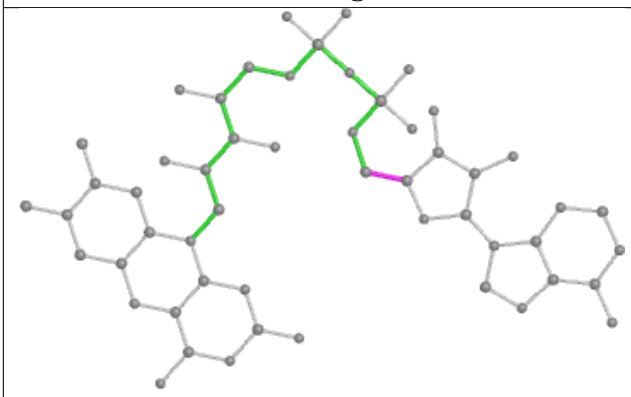
Ligand FAD B 9200



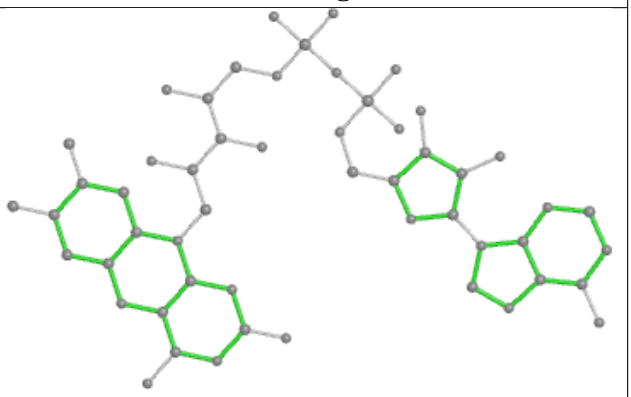
Bond lengths



Bond angles

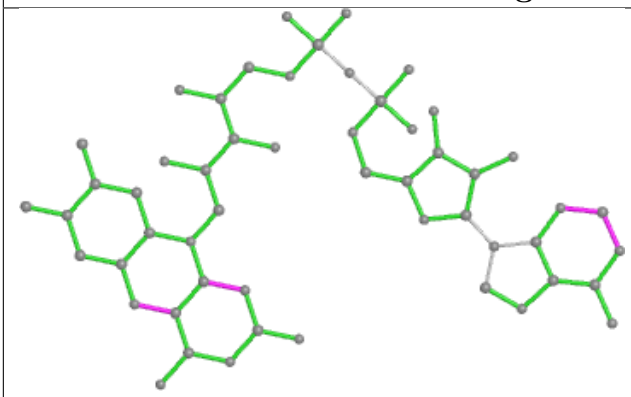


Torsions

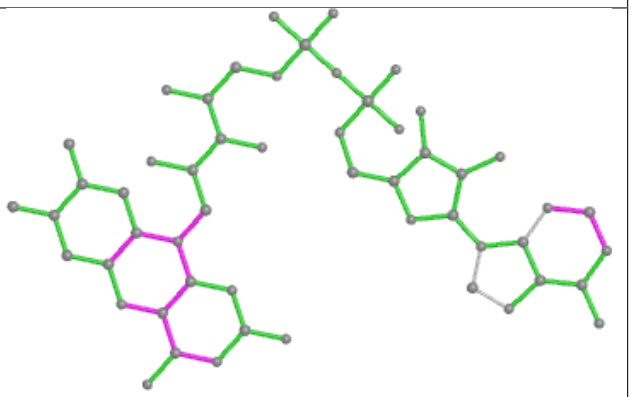


Rings

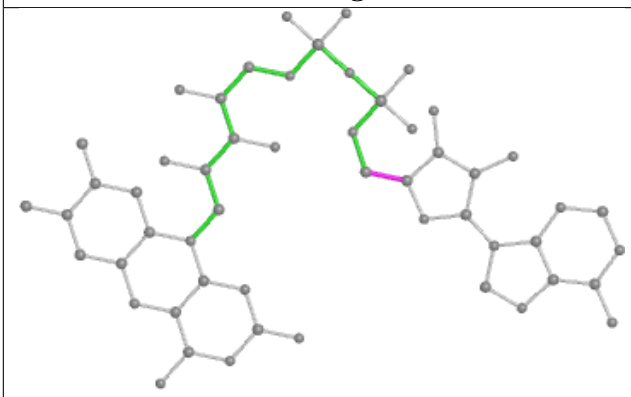
Ligand FAD A 9100



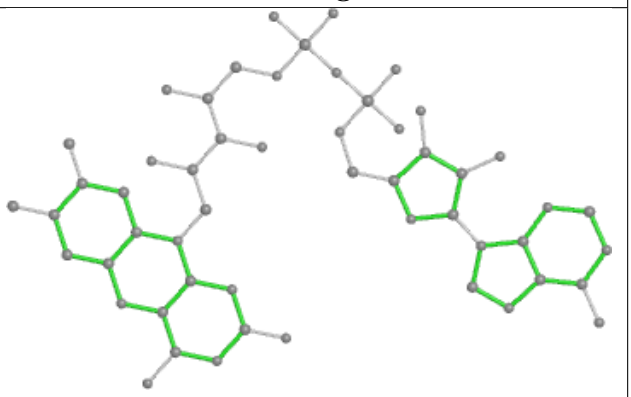
Bond lengths



Bond angles

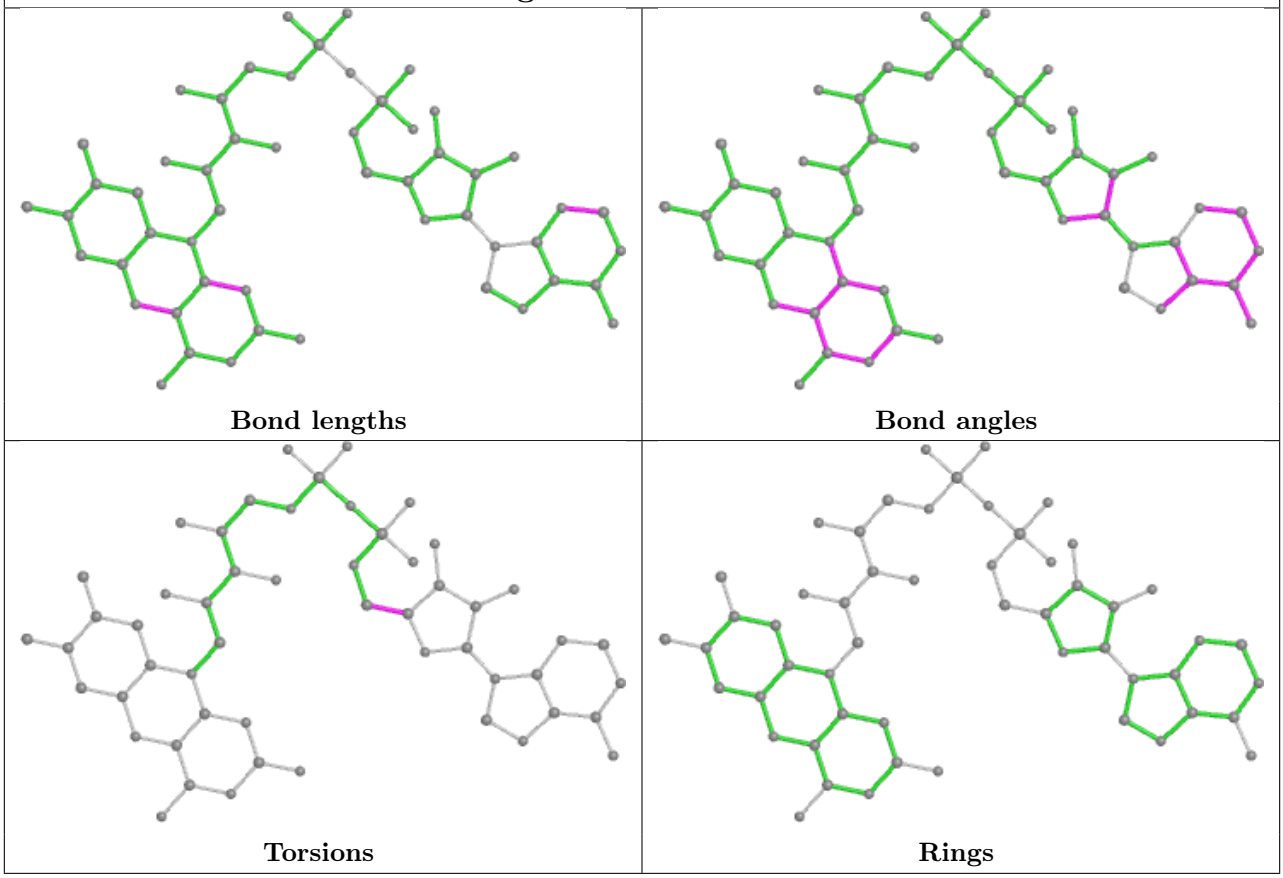


Torsions



Rings

Ligand FAD C 9300



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	364/382 (95%)	-0.07	11 (3%)	50	44	17, 26, 50, 71	0
1	B	364/382 (95%)	-0.06	9 (2%)	57	52	17, 25, 44, 83	0
1	C	364/382 (95%)	-0.15	6 (1%)	72	68	15, 23, 44, 75	0
1	D	364/382 (95%)	0.10	16 (4%)	34	28	17, 28, 49, 83	0
All	All	1456/1528 (95%)	-0.04	42 (2%)	51	46	15, 26, 48, 83	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	CYS	12.0
1	C	56	CYS	8.0
1	B	58	GLU	7.2
1	B	56	CYS	6.7
1	D	54	ALA	5.9
1	C	57	GLU	4.7
1	A	56	CYS	4.4
1	A	58	GLU	4.2
1	D	62[A]	PHE	4.1
1	D	182	GLU	3.9
1	B	55	GLU	3.8
1	D	180	ASP	3.7
1	B	54	ALA	3.6
1	B	57	GLU	3.5
1	A	57	GLU	3.4
1	B	62[A]	PHE	3.3
1	A	182	GLU	3.3
1	D	55	GLU	3.3
1	A	180	ASP	3.3
1	D	57	GLU	3.0
1	D	58	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	115	ASP	3.0
1	A	55	GLU	2.9
1	A	183	ALA	2.9
1	A	3	ARG	2.8
1	A	181	GLY	2.7
1	D	3	ARG	2.6
1	D	116	SER	2.6
1	A	107	GLN	2.6
1	C	55	GLU	2.6
1	C	182	GLU	2.5
1	A	115	ASP	2.4
1	B	103	GLU	2.4
1	D	103	GLU	2.4
1	B	180	ASP	2.3
1	D	306	LYS	2.3
1	D	27	ASN	2.2
1	C	115	ASP	2.2
1	C	103	GLU	2.2
1	B	182	GLU	2.1
1	D	364	LYS	2.1
1	D	317	GLU	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, 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	GOA	B	9210	5/5	0.89	0.18	26,30,36,55	0
3	GOA	C	9310	5/5	0.92	0.21	21,26,34,51	0

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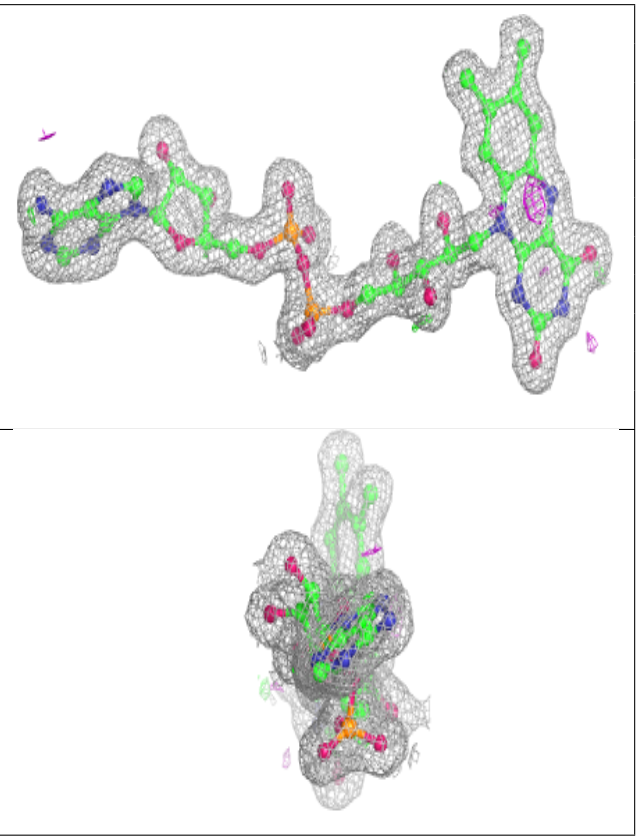
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOA	D	9410	5/5	0.94	0.17	28,29,35,41	0
3	GOA	A	9110	5/5	0.95	0.15	22,25,32,44	0
2	FAD	B	9200	53/53	0.97	0.07	13,18,22,23	0
2	FAD	D	9400	53/53	0.97	0.07	14,21,27,29	0
2	FAD	C	9300	53/53	0.98	0.07	12,16,19,20	0
2	FAD	A	9100	53/53	0.98	0.07	14,18,20,26	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.

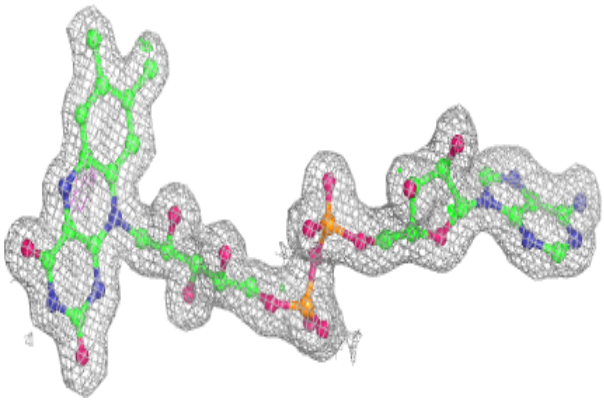
Electron density around FAD B 9200:

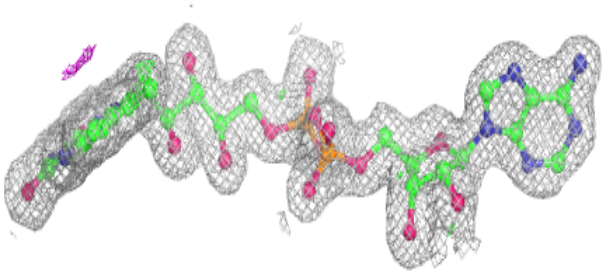
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

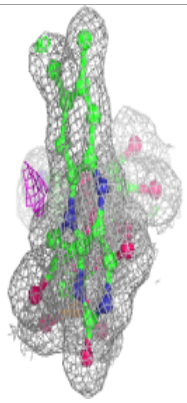


Electron density around FAD D 9400:

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

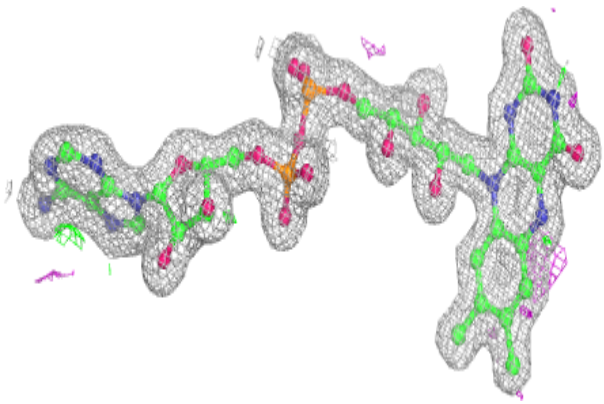


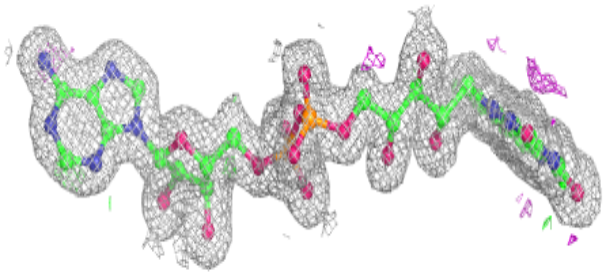


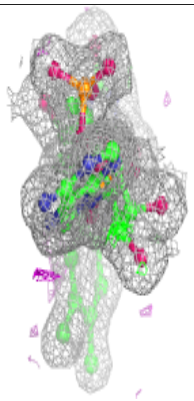


Electron density around FAD C 9300:

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

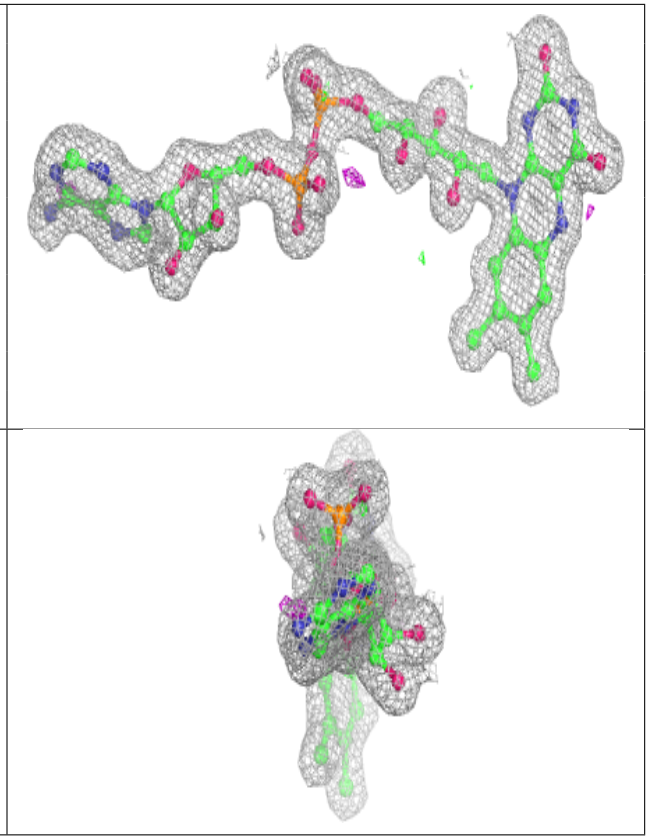






Electron density around FAD A 9100:

$2mF_o$-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.