Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:36 pm BST

PDB ID	:	5J5Z
Title	:	Crystal structure of the D444V disease-causing mutant of the human dihydrolipoamide dehydrogenase
Authors	:	Szabo, E.; Mizsei, R.; Zambo, Z.; Torocsik, B.; Weiss, M.S.; Adam-Vizi, V.; Ambrus, A.
Deposited on	:	2016-04-04
Resolution	:	1.84 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 following versions of software and data (see references ⓘ) were used in the production of this report:

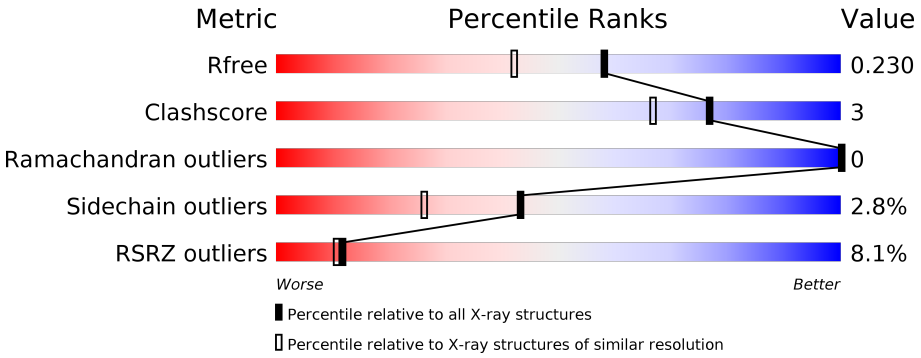
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 on 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	496	7% 83% 12% .
1	B	496	9% 88% 9% .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7848 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 Dihydrolipoyl dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	7	0
			3598	2270	624	682	22			
1	B	482	Total	C	N	O	S	0	5	0
			3611	2279	624	686	22			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P09622
A	-20	ALA	-	expression tag	UNP P09622
A	-19	SER	-	expression tag	UNP P09622
A	-18	TRP	-	expression tag	UNP P09622
A	-17	SER	-	expression tag	UNP P09622
A	-16	HIS	-	expression tag	UNP P09622
A	-15	PRO	-	expression tag	UNP P09622
A	-14	GLN	-	expression tag	UNP P09622
A	-13	PHE	-	expression tag	UNP P09622
A	-12	GLU	-	expression tag	UNP P09622
A	-11	LYS	-	expression tag	UNP P09622
A	-10	GLY	-	expression tag	UNP P09622
A	-9	ALA	-	expression tag	UNP P09622
A	-8	LEU	-	expression tag	UNP P09622
A	-7	GLU	-	expression tag	UNP P09622
A	-6	VAL	-	expression tag	UNP P09622
A	-5	LEU	-	expression tag	UNP P09622
A	-4	PHE	-	expression tag	UNP P09622
A	-3	GLN	-	expression tag	UNP P09622
A	-2	GLY	-	expression tag	UNP P09622
A	-1	PRO	-	expression tag	UNP P09622
A	0	GLY	-	expression tag	UNP P09622
A	444	VAL	ASP	engineered mutation	UNP P09622
B	-21	MET	-	initiating methionine	UNP P09622
B	-20	ALA	-	expression tag	UNP P09622

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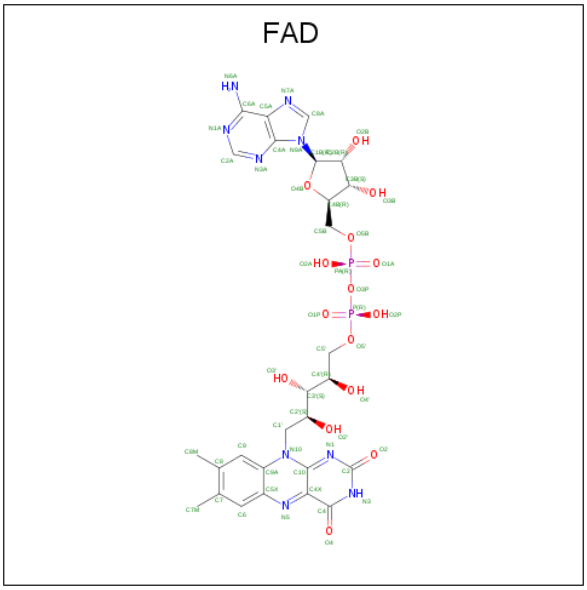
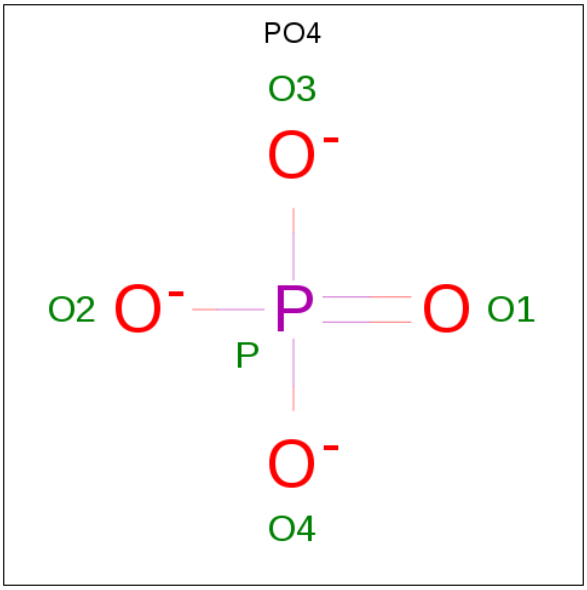
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	expression tag	UNP P09622
B	-18	TRP	-	expression tag	UNP P09622
B	-17	SER	-	expression tag	UNP P09622
B	-16	HIS	-	expression tag	UNP P09622
B	-15	PRO	-	expression tag	UNP P09622
B	-14	GLN	-	expression tag	UNP P09622
B	-13	PHE	-	expression tag	UNP P09622
B	-12	GLU	-	expression tag	UNP P09622
B	-11	LYS	-	expression tag	UNP P09622
B	-10	GLY	-	expression tag	UNP P09622
B	-9	ALA	-	expression tag	UNP P09622
B	-8	LEU	-	expression tag	UNP P09622
B	-7	GLU	-	expression tag	UNP P09622
B	-6	VAL	-	expression tag	UNP P09622
B	-5	LEU	-	expression tag	UNP P09622
B	-4	PHE	-	expression tag	UNP P09622
B	-3	GLN	-	expression tag	UNP P09622
B	-2	GLY	-	expression tag	UNP P09622
B	-1	PRO	-	expression tag	UNP P09622
B	0	GLY	-	expression tag	UNP P09622
B	444	VAL	ASP	engineered mutation	UNP P09622

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



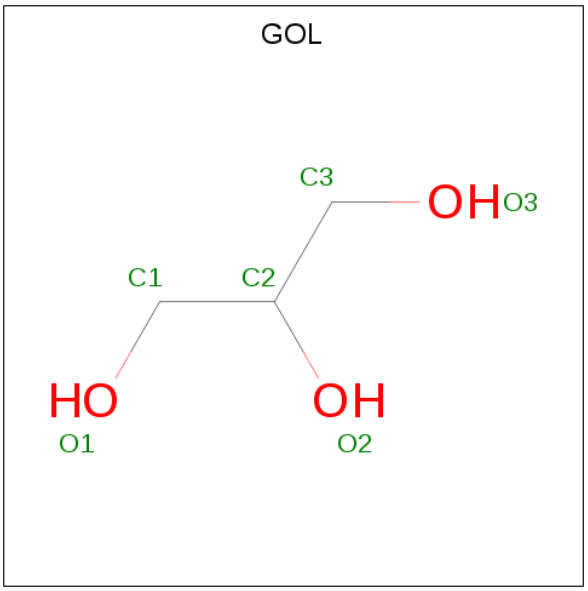
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- 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 12 6 6	0	1
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

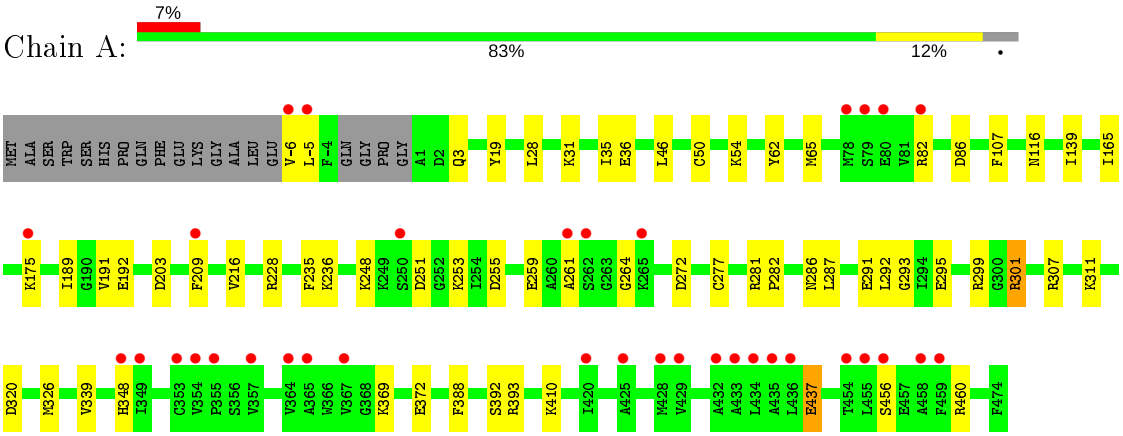
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	276	Total O 279 279	0	4
5	B	219	Total O 220 220	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

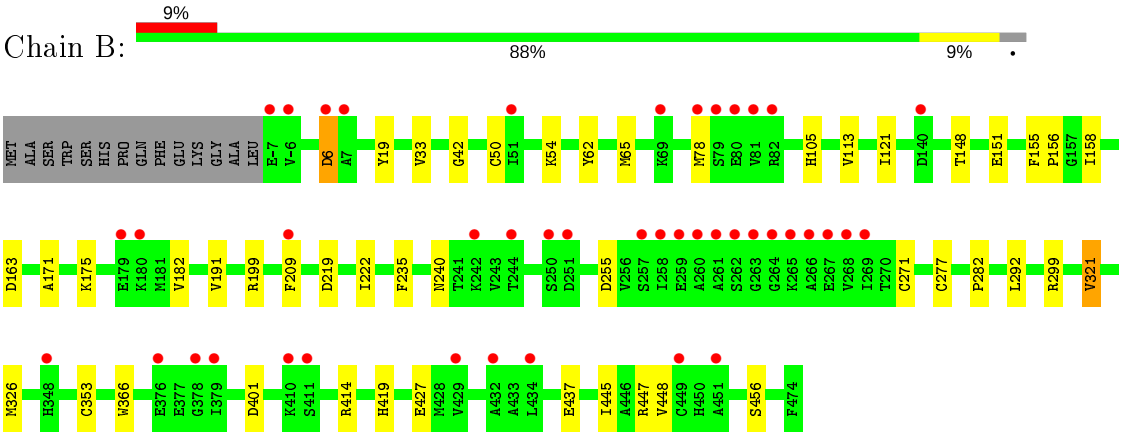
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain A:



- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.03Å 168.94Å 61.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 1.84 48.38 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.38-1.84) 98.1 (48.38-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.181 , 0.226 0.189 , 0.230	Depositor DCC
R_{free} test set	2101 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7848	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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, PO4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.35	12/3661 (0.3%)	1.20	18/4941 (0.4%)
1	B	1.29	9/3679 (0.2%)	1.17	12/4968 (0.2%)
All	All	1.32	21/7340 (0.3%)	1.19	30/9909 (0.3%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	GLU	CD-OE1	10.39	1.37	1.25
1	B	456	SER	CB-OG	9.93	1.55	1.42
1	A	437	GLU	CD-OE1	9.91	1.36	1.25
1	A	456	SER	CB-OG	8.23	1.52	1.42
1	A	191	VAL	CB-CG1	-6.62	1.39	1.52
1	B	427	GLU	CD-OE2	6.59	1.32	1.25
1	A	388	PHE	CG-CD2	6.44	1.48	1.38
1	A	291	GLU	CD-OE2	6.42	1.32	1.25
1	A	369	LYS	C-O	5.94	1.34	1.23
1	A	192	GLU	CD-OE1	5.67	1.31	1.25
1	B	156	PRO	N-CA	5.52	1.56	1.47
1	A	36	GLU	CD-OE1	5.51	1.31	1.25
1	B	299	ARG	C-O	-5.50	1.12	1.23
1	B	6	ASP	CB-CG	-5.34	1.40	1.51
1	B	42	GLY	N-CA	5.29	1.53	1.46
1	B	171	ALA	N-CA	5.25	1.56	1.46
1	B	437	GLU	CD-OE1	5.12	1.31	1.25
1	A	437	GLU	C-O	-5.11	1.13	1.23
1	A	291	GLU	CG-CD	5.10	1.59	1.51
1	A	175	LYS	C-O	-5.07	1.13	1.23
1	B	366	TRP	CD1-NE1	5.04	1.46	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	A	251	ASP	CB-CG-OD1	8.78	126.20	118.30
1	B	199	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	B	401	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	A	460	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	A	299	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	320	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	255	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	163	ASP	CB-CG-OD1	5.87	123.59	118.30
1	A	251	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	393	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	B	6	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	A	307	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	B	414	ARG	CG-CD-NE	-5.48	100.29	111.80
1	B	148	THR	CA-CB-CG2	-5.46	104.76	112.40
1	A	86	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	A	292	LEU	CB-CG-CD2	-5.39	101.83	111.00
1	A	295	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	A	255	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	287	LEU	CB-CG-CD1	5.32	120.04	111.00
1	A	107	PHE	CB-CG-CD1	5.31	124.52	120.80
1	A	372	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	A	228	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	191	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	B	151	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	B	447	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	255	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	219	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	107	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	A	46	LEU	CB-CG-CD2	-5.05	102.41	111.00

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	3598	0	3660	26	0
1	B	3611	0	3670	15	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	24	0	32	2	0
5	A	279	0	0	10	0
5	B	220	0	0	3	0
All	All	7848	0	7424	42	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 (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:HB2	1:A:264:GLY:O	1.82	0.80
1:A:82[B]:ARG:HH21	1:A:82[B]:ARG:HG2	1.51	0.75
1:B:105[B]:HIS:CD2	5:B:611:HOH:O	2.48	0.67
1:A:82[B]:ARG:CG	1:A:82[B]:ARG:HH21	2.07	0.66
1:B:155:PHE:CD1	1:B:158:ILE:HD12	2.31	0.66
1:A:326[B]:MET:HE1	5:A:824:HOH:O	1.97	0.64
1:A:437:GLU:OE1	5:A:602:HOH:O	2.16	0.61
4:A:505:GOL:O2	5:A:601:HOH:O	2.16	0.60
1:A:348[B]:HIS:ND1	5:A:603:HOH:O	2.32	0.58
1:A:65[B]:MET:HA	1:A:65[B]:MET:CE	2.33	0.58
1:B:445:ILE:N	1:B:445:ILE:HD13	2.21	0.55
1:B:326[B]:MET:HE3	5:B:811:HOH:O	2.08	0.54
1:A:65[B]:MET:HA	1:A:65[B]:MET:HE2	1.90	0.54
1:A:165:ILE:HD12	1:A:248:LYS:HE2	1.90	0.53
1:A:348[B]:HIS:HE1	5:A:848:HOH:O	1.93	0.52
1:A:82[B]:ARG:CG	1:A:82[B]:ARG:NH2	2.70	0.52
1:A:437:GLU:HG2	1:B:448:VAL:HG22	1.93	0.50
1:A:392:SER:HB2	5:A:611:HOH:O	2.11	0.49
1:B:121:ILE:HG21	1:B:292:LEU:HD11	1.95	0.49
1:B:155:PHE:CE1	1:B:158:ILE:HD12	2.47	0.49
1:A:281:ARG:HB2	1:A:282:PRO:HD2	1.94	0.49
5:A:753[B]:HOH:O	1:B:353:CYS:O	2.20	0.48
1:B:33:VAL:HG22	1:B:113:VAL:HB	1.96	0.48
4:A:503[A]:GOL:H12	5:A:642:HOH:O	2.13	0.48
1:A:209:PHE:CE1	1:A:261:ALA:HB1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326[B]:MET:HE3	5:A:862:HOH:O	2.14	0.47
1:A:236:LYS:HB2	1:A:236:LYS:HE2	1.77	0.45
1:A:253:LYS:HE2	1:A:272:ASP:OD1	2.17	0.45
1:A:286:ASN:HB3	5:A:663:HOH:O	2.17	0.45
1:A:282:PRO:HG3	1:A:301:ARG:HG3	1.99	0.44
1:A:28:LEU:HD12	1:A:339:VAL:HG12	2.00	0.44
1:A:203:ASP:OD1	1:A:236:LYS:NZ	2.31	0.44
1:B:282:PRO:HB3	1:B:321:VAL:HA	2.01	0.43
1:A:293:GLY:O	1:A:311:LYS:HE2	2.17	0.43
1:A:62:TYR:CD1	1:A:65[A]:MET:CE	3.01	0.43
1:A:189:ILE:HG22	1:A:277[B]:CYS:SG	2.58	0.43
1:B:326[B]:MET:HE1	5:B:738:HOH:O	2.19	0.43
1:B:182:VAL:HG23	1:B:271:CYS:HB3	2.03	0.41
1:B:222:ILE:HG13	1:B:419:HIS:HB3	2.03	0.41
1:B:209:PHE:O	1:B:240:ASN:HA	2.21	0.40
1:A:35:ILE:HD11	1:A:139:ILE:HD13	2.04	0.40
1:B:62:TYR:HD1	1:B:65:MET:HE2	1.87	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	480/496 (97%)	468 (98%)	12 (2%)	0	100	100
1	B	485/496 (98%)	471 (97%)	14 (3%)	0	100	100
All	All	965/992 (97%)	939 (97%)	26 (3%)	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	383/390 (98%)	371 (97%)	12 (3%)	40 23
1	B	384/390 (98%)	374 (97%)	10 (3%)	46 29
All	All	767/780 (98%)	745 (97%)	22 (3%)	43 25

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	VAL
1	A	-5	LEU
1	A	3	GLN
1	A	19	TYR
1	A	31	LYS
1	A	50	CYS
1	A	54	LYS
1	A	116	ASN
1	A	216	VAL
1	A	235	PHE
1	A	301	ARG
1	A	410	LYS
1	B	6	ASP
1	B	19	TYR
1	B	50	CYS
1	B	54	LYS
1	B	78	MET
1	B	175	LYS
1	B	235	PHE
1	B	277[A]	CYS
1	B	277[B]	CYS
1	B	321	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	GOL	A	503[A]	-	5,5,5	0.50	0	5,5,5	1.84	1 (20%)
3	PO4	B	502	-	4,4,4	0.43	0	6,6,6	1.17	1 (16%)
4	GOL	A	505	-	5,5,5	1.12	0	5,5,5	0.80	0
2	FAD	B	501	-	51,58,58	2.50	15 (29%)	60,89,89	3.20	18 (30%)
3	PO4	A	502	-	4,4,4	1.22	0	6,6,6	1.09	0
4	GOL	A	504	-	5,5,5	0.41	0	5,5,5	0.33	0
4	GOL	A	503[B]	-	5,5,5	0.69	0	5,5,5	1.52	0
2	FAD	A	501	-	51,58,58	2.08	11 (21%)	60,89,89	3.29	21 (35%)

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	A	503[A]	-	-	2/4/4/4	-
4	GOL	A	505	-	-	2/4/4/4	-
2	FAD	B	501	-	-	3/30/50/50	0/6/6/6
4	GOL	A	504	-	-	4/4/4/4	-
4	GOL	A	503[B]	-	-	4/4/4/4	-
2	FAD	A	501	-	-	2/30/50/50	0/6/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C4X-C10	9.32	1.48	1.38
2	A	501	FAD	C4-C4X	6.69	1.52	1.41
2	B	501	FAD	C4-C4X	6.43	1.52	1.41
2	A	501	FAD	C8A-N7A	6.36	1.46	1.34
2	B	501	FAD	C2A-N3A	5.16	1.40	1.32
2	A	501	FAD	O4B-C1B	4.23	1.47	1.41
2	B	501	FAD	C2B-C1B	-4.22	1.47	1.53
2	A	501	FAD	C5X-N5	4.13	1.42	1.35
2	B	501	FAD	O4B-C1B	4.08	1.46	1.41
2	A	501	FAD	C4X-C10	3.95	1.42	1.38
2	B	501	FAD	C6-C5X	-3.81	1.35	1.41
2	A	501	FAD	C9A-C5X	3.73	1.50	1.42
2	B	501	FAD	C9A-C5X	3.56	1.49	1.42
2	B	501	FAD	C5X-N5	3.37	1.40	1.35
2	B	501	FAD	C8A-N7A	3.26	1.40	1.34
2	B	501	FAD	O4-C4	3.17	1.32	1.24
2	B	501	FAD	C4X-N5	3.05	1.37	1.33
2	A	501	FAD	C2A-N1A	2.72	1.39	1.33
2	A	501	FAD	C2A-N3A	2.57	1.36	1.32
2	A	501	FAD	P-O2P	-2.45	1.43	1.55
2	A	501	FAD	C5'-C4'	-2.44	1.48	1.51
2	B	501	FAD	C4A-N3A	-2.21	1.32	1.35
2	B	501	FAD	C5A-C4A	2.17	1.46	1.40
2	B	501	FAD	PA-O1A	2.08	1.58	1.50
2	B	501	FAD	C2-N3	-2.04	1.34	1.38
2	A	501	FAD	C2B-C1B	-2.04	1.50	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FAD	C4-N3-C2	12.95	126.07	115.14
2	B	501	FAD	C1'-N10-C9A	12.38	128.03	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FAD	C1'-N10-C9A	12.19	127.88	118.29
2	A	501	FAD	C4-C4X-C10	-9.55	113.63	119.95
2	A	501	FAD	C4-N3-C2	9.39	123.07	115.14
2	A	501	FAD	C10-C4X-N5	8.66	127.24	121.26
2	B	501	FAD	C5X-C9A-N10	8.44	123.83	117.72
2	A	501	FAD	C5X-C9A-N10	5.79	121.91	117.72
2	B	501	FAD	C4X-C4-N3	-5.75	115.56	123.43
2	A	501	FAD	C1'-N10-C10	-5.36	113.61	118.41
2	B	501	FAD	C4-C4X-C10	-4.75	116.81	119.95
2	A	501	FAD	N6A-C6A-N1A	4.70	128.34	118.57
2	A	501	FAD	C4X-C4-N3	-4.43	117.38	123.43
2	A	501	FAD	C5A-C6A-N6A	-4.36	113.73	120.35
2	B	501	FAD	C5A-C6A-N6A	-4.29	113.83	120.35
2	B	501	FAD	C9A-N10-C10	-4.25	116.34	121.91
2	B	501	FAD	N6A-C6A-N1A	3.95	126.77	118.57
2	A	501	FAD	C1B-N9A-C4A	-3.82	119.94	126.64
2	A	501	FAD	O4B-C1B-C2B	-3.30	102.10	106.93
2	B	501	FAD	C1'-N10-C10	-3.14	115.60	118.41
4	A	503[A]	GOL	C3-C2-C1	-3.10	99.64	111.70
2	B	501	FAD	C1B-N9A-C4A	-3.07	121.25	126.64
2	B	501	FAD	C4X-N5-C5X	3.01	119.78	116.77
2	A	501	FAD	C4X-C10-N10	-2.96	117.26	120.30
2	A	501	FAD	O5B-PA-O1A	-2.94	97.58	109.07
2	A	501	FAD	C9A-N10-C10	-2.77	118.29	121.91
2	B	501	FAD	O2'-C2'-C1'	-2.76	102.96	109.59
2	B	501	FAD	C9-C9A-C5X	-2.74	115.19	119.88
2	B	501	FAD	C9A-C5X-N5	-2.69	118.15	122.36
2	B	501	FAD	N3A-C2A-N1A	-2.61	124.59	128.68
2	A	501	FAD	C9A-C5X-N5	-2.50	118.46	122.36
2	A	501	FAD	O3'-C3'-C2'	-2.49	102.80	108.81
2	B	501	FAD	C10-C4X-N5	2.45	122.95	121.26
2	B	501	FAD	O5B-PA-O1A	-2.44	99.53	109.07
2	A	501	FAD	C6-C5X-N5	2.33	121.62	119.05
3	B	502	PO4	O4-P-O2	2.33	115.45	107.97
2	A	501	FAD	O2'-C2'-C1'	-2.25	104.17	109.59
2	A	501	FAD	O2A-PA-O5B	2.03	117.17	107.75
2	A	501	FAD	O4B-C4B-C3B	2.03	109.12	105.11
2	B	501	FAD	O4'-C4'-C5'	2.01	114.44	109.92
2	A	501	FAD	C3B-C2B-C1B	2.00	103.99	100.98

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	GOL	O1-C1-C2-C3
4	A	503[B]	GOL	O1-C1-C2-O2
4	A	503[B]	GOL	O1-C1-C2-C3
4	A	503[B]	GOL	C1-C2-C3-O3
4	A	504	GOL	O1-C1-C2-O2
4	A	503[A]	GOL	O1-C1-C2-C3
4	A	505	GOL	C1-C2-C3-O3
4	A	504	GOL	C1-C2-C3-O3
4	A	503[B]	GOL	O2-C2-C3-O3
4	A	503[A]	GOL	O1-C1-C2-O2
2	A	501	FAD	O4B-C4B-C5B-O5B
4	A	505	GOL	O2-C2-C3-O3
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	PA-O3P-P-O5'
2	A	501	FAD	PA-O3P-P-O5'
4	A	504	GOL	O2-C2-C3-O3
2	B	501	FAD	C3B-C4B-C5B-O5B

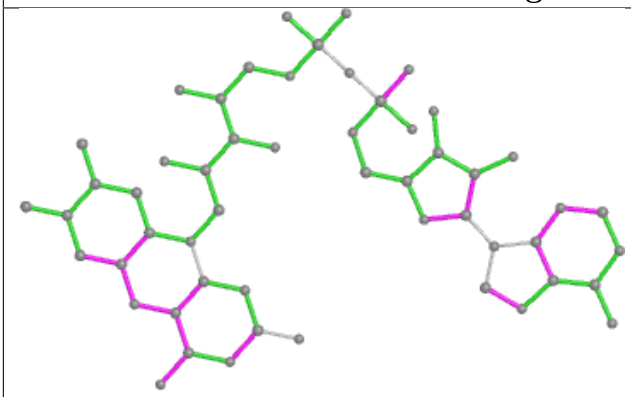
There are no ring outliers.

2 monomers are involved in 2 short contacts:

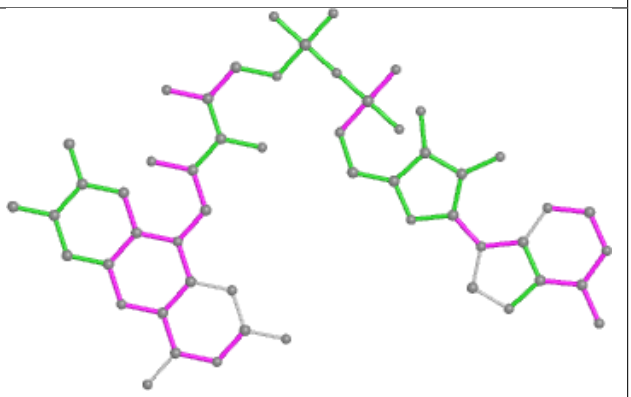
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503[A]	GOL	1	0
4	A	505	GOL	1	0

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.

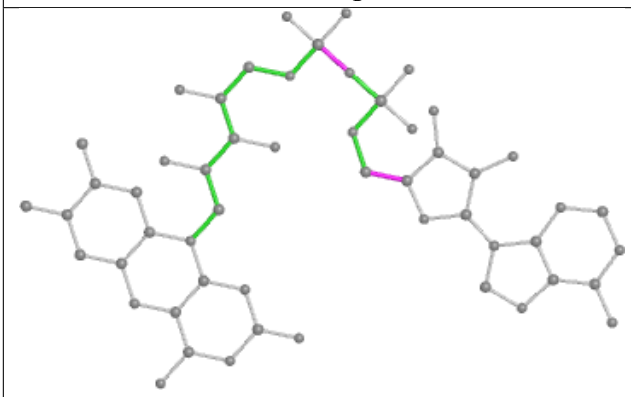
Ligand FAD B 501



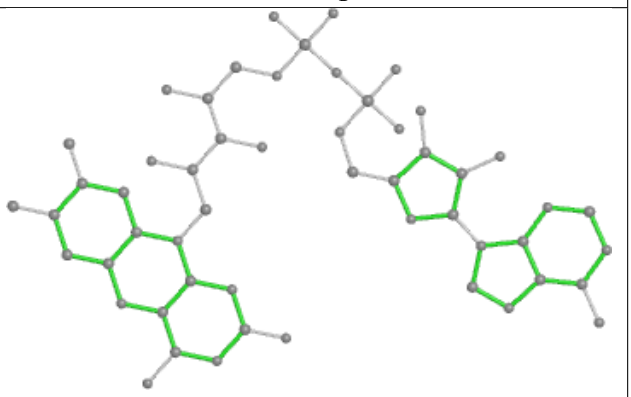
Bond lengths



Bond angles

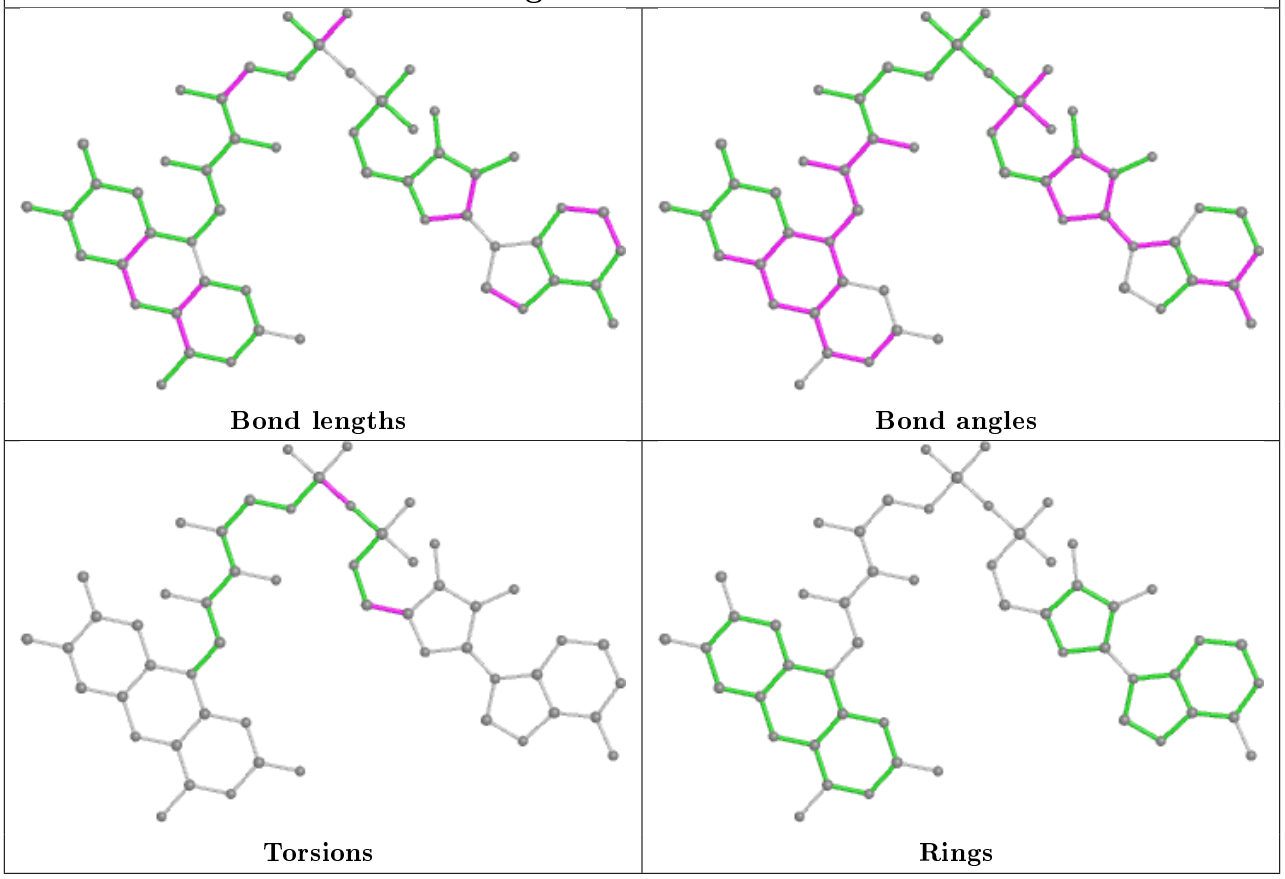


Torsions



Rings

Ligand FAD A 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	477/496 (96%)	0.19	35 (7%) 15 13	22, 34, 56, 88	0
1	B	482/496 (97%)	0.36	43 (8%) 9 8	25, 38, 65, 85	0
All	All	959/992 (96%)	0.27	78 (8%) 12 11	22, 36, 62, 88	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	SER	5.2
1	A	261	ALA	4.7
1	B	262	SER	4.4
1	B	69	LYS	4.4
1	B	261	ALA	4.4
1	B	79	SER	4.2
1	B	266	ALA	4.2
1	B	378	GLY	4.1
1	B	265	LYS	4.0
1	A	348[A]	HIS	3.9
1	B	209	PHE	3.8
1	B	379	ILE	3.8
1	B	-7	GLU	3.6
1	A	432	ALA	3.6
1	B	-6	VAL	3.6
1	A	455	LEU	3.5
1	B	376	GLU	3.5
1	B	264	GLY	3.4
1	A	82[A]	ARG	3.3
1	A	-6	VAL	3.3
1	A	80	GLU	3.2
1	B	263	GLY	3.2
1	B	244	THR	3.1
1	B	78	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	81	VAL	3.0
1	B	449	CYS	2.9
1	A	425	ALA	2.9
1	B	180	LYS	2.9
1	B	269	ILE	2.8
1	B	82	ARG	2.8
1	B	258	ILE	2.8
1	A	367	VAL	2.8
1	B	268	VAL	2.8
1	A	436	LEU	2.7
1	B	80	GLU	2.7
1	A	428	MET	2.7
1	A	349	ILE	2.7
1	B	259	GLU	2.7
1	B	267	GLU	2.7
1	A	355	PRO	2.7
1	A	454	THR	2.6
1	B	451	ALA	2.6
1	A	429	VAL	2.6
1	B	429	VAL	2.6
1	B	242	LYS	2.6
1	B	410	LYS	2.6
1	B	411	SER	2.5
1	B	6	ASP	2.5
1	A	265	LYS	2.5
1	A	433	ALA	2.5
1	A	458	ALA	2.5
1	A	250	SER	2.5
1	A	364	VAL	2.5
1	B	260	ALA	2.4
1	B	51	ILE	2.4
1	A	262	SER	2.4
1	B	434	LEU	2.4
1	B	179	GLU	2.4
1	A	434	LEU	2.4
1	A	365	ALA	2.4
1	A	353	CYS	2.3
1	A	435	ALA	2.3
1	A	209	PHE	2.2
1	A	456	SER	2.2
1	A	459	PHE	2.2
1	B	140	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	7	ALA	2.2
1	A	-5	LEU	2.2
1	B	250	SER	2.1
1	A	420	ILE	2.1
1	A	78	MET	2.1
1	A	175	LYS	2.1
1	B	251	ASP	2.1
1	B	348[A]	HIS	2.1
1	B	432	ALA	2.1
1	B	257	SER	2.0
1	A	354	VAL	2.0
1	A	357	VAL	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 carbohydrates 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.

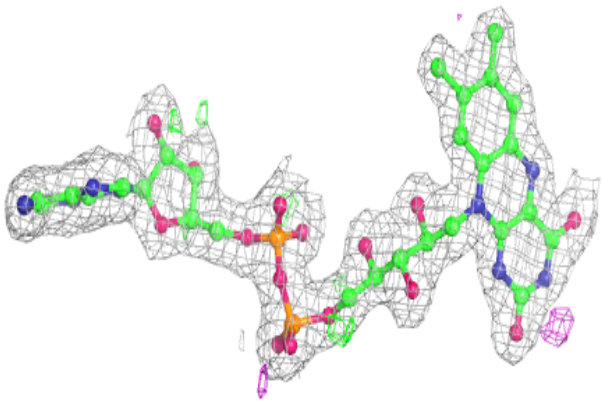
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	504	6/6	0.72	0.23	73,86,90,94	0
4	GOL	A	505	6/6	0.77	0.38	40,44,51,52	6
4	GOL	A	503[A]	6/6	0.87	0.19	26,31,33,33	6
4	GOL	A	503[B]	6/6	0.87	0.19	26,36,37,37	6
3	PO4	B	502	5/5	0.90	0.15	75,77,81,87	0
3	PO4	A	502	5/5	0.94	0.12	49,59,75,84	0
2	FAD	B	501	53/53	0.98	0.12	25,27,29,30	0
2	FAD	A	501	53/53	0.98	0.09	22,24,25,26	0

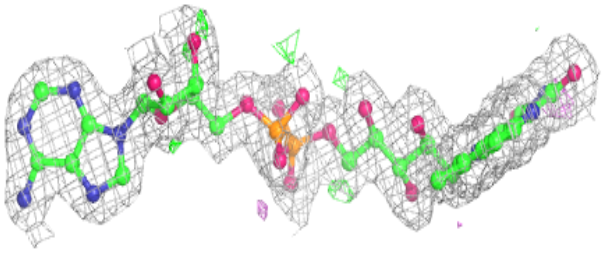
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

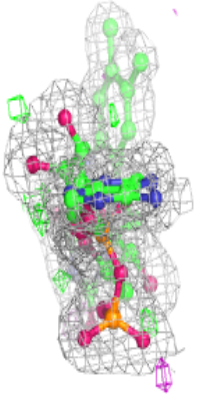
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD B 501:

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

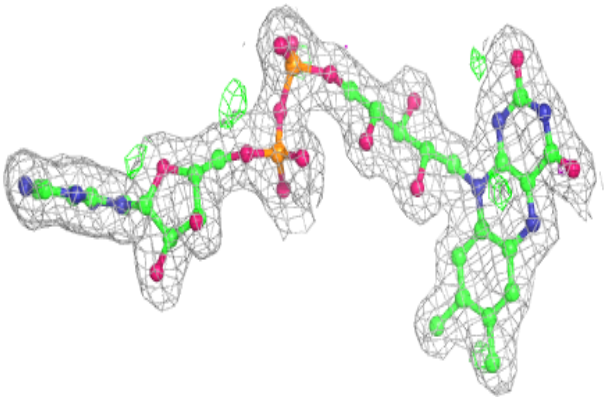


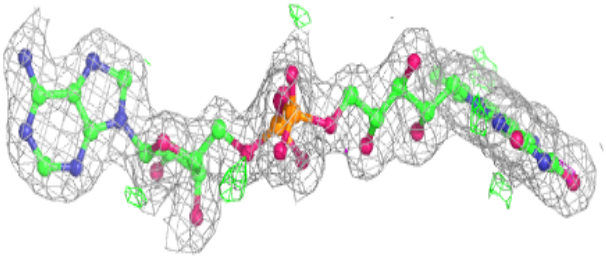


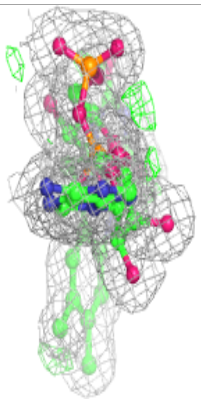


Electron density around FAD A 501:

$2mF_o$-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.