



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:27 PM UTC

PDB ID : 5NMW / pdb_00005nmw
Title : Crystal Structure of the pyrrolizidine alkaloid N-oxygenase from *Zonocerus variegatus* in complex with FAD
Authors : Scheidig, A.; Kubitza, C.; Faust, A.; Ober, D.
Deposited on : 2017-04-07
Resolution : 1.89 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

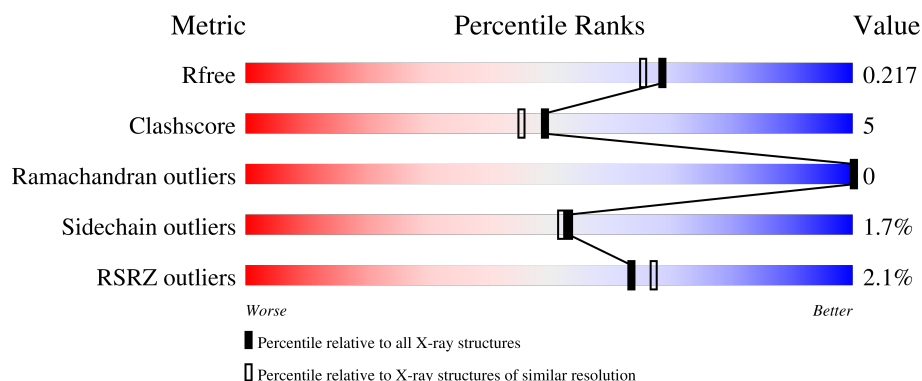
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	425	0% 81% 13% ..
1	B	425	2% 84% 10% ..
1	C	425	3% 76% 17% • 5%
1	D	425	2% 83% 11% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14660 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 Flavin-containing monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3311	2130	549	607	25			
1	B	406	Total	C	N	O	S	0	0	0
			3311	2130	549	607	25			
1	C	405	Total	C	N	O	S	0	0	0
			3303	2124	548	606	25			
1	D	405	Total	C	N	O	S	0	1	0
			3314	2130	552	607	25			

There are 48 discrepancies between the modelled and reference sequences:

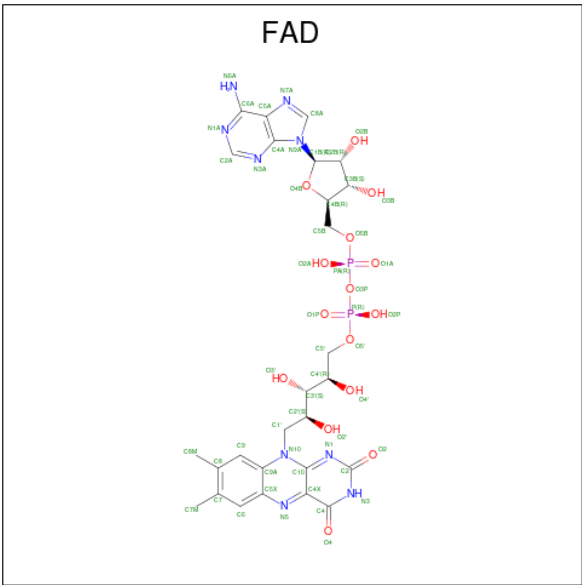
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	TYR	-	expression tag	UNP L0N8S9
A	415	ALA	-	expression tag	UNP L0N8S9
A	416	ALA	-	expression tag	UNP L0N8S9
A	417	ALA	-	expression tag	UNP L0N8S9
A	418	LEU	-	expression tag	UNP L0N8S9
A	419	GLU	-	expression tag	UNP L0N8S9
A	420	HIS	-	expression tag	UNP L0N8S9
A	421	HIS	-	expression tag	UNP L0N8S9
A	422	HIS	-	expression tag	UNP L0N8S9
A	423	HIS	-	expression tag	UNP L0N8S9
A	424	HIS	-	expression tag	UNP L0N8S9
A	425	HIS	-	expression tag	UNP L0N8S9
B	414	TYR	-	expression tag	UNP L0N8S9
B	415	ALA	-	expression tag	UNP L0N8S9
B	416	ALA	-	expression tag	UNP L0N8S9
B	417	ALA	-	expression tag	UNP L0N8S9
B	418	LEU	-	expression tag	UNP L0N8S9
B	419	GLU	-	expression tag	UNP L0N8S9
B	420	HIS	-	expression tag	UNP L0N8S9
B	421	HIS	-	expression tag	UNP L0N8S9
B	422	HIS	-	expression tag	UNP L0N8S9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	423	HIS	-	expression tag	UNP L0N8S9
B	424	HIS	-	expression tag	UNP L0N8S9
B	425	HIS	-	expression tag	UNP L0N8S9
C	414	TYR	-	expression tag	UNP L0N8S9
C	415	ALA	-	expression tag	UNP L0N8S9
C	416	ALA	-	expression tag	UNP L0N8S9
C	417	ALA	-	expression tag	UNP L0N8S9
C	418	LEU	-	expression tag	UNP L0N8S9
C	419	GLU	-	expression tag	UNP L0N8S9
C	420	HIS	-	expression tag	UNP L0N8S9
C	421	HIS	-	expression tag	UNP L0N8S9
C	422	HIS	-	expression tag	UNP L0N8S9
C	423	HIS	-	expression tag	UNP L0N8S9
C	424	HIS	-	expression tag	UNP L0N8S9
C	425	HIS	-	expression tag	UNP L0N8S9
D	414	TYR	-	expression tag	UNP L0N8S9
D	415	ALA	-	expression tag	UNP L0N8S9
D	416	ALA	-	expression tag	UNP L0N8S9
D	417	ALA	-	expression tag	UNP L0N8S9
D	418	LEU	-	expression tag	UNP L0N8S9
D	419	GLU	-	expression tag	UNP L0N8S9
D	420	HIS	-	expression tag	UNP L0N8S9
D	421	HIS	-	expression tag	UNP L0N8S9
D	422	HIS	-	expression tag	UNP L0N8S9
D	423	HIS	-	expression tag	UNP L0N8S9
D	424	HIS	-	expression tag	UNP L0N8S9
D	425	HIS	-	expression tag	UNP L0N8S9

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	354	Total	O	0	0
			354	354		
4	B	348	Total	O	0	0
			348	348		
4	C	247	Total	O	0	0
			247	247		

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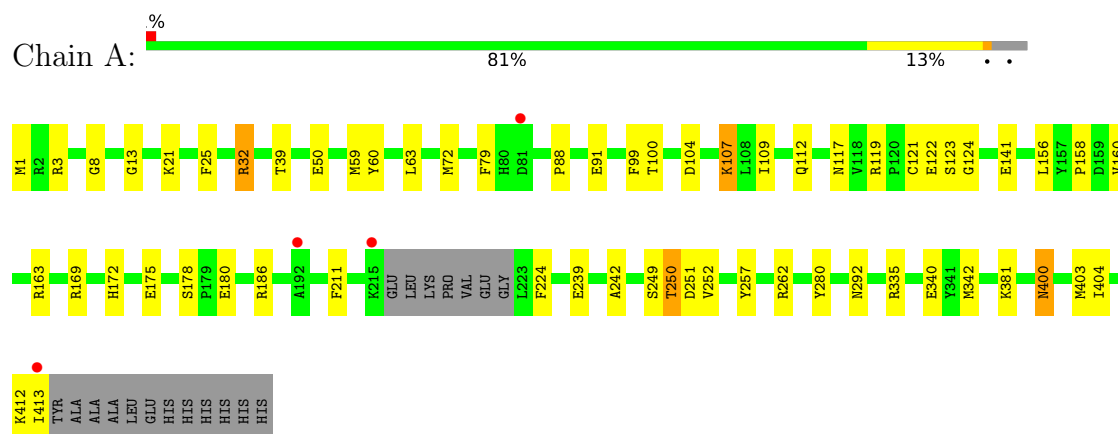
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	258	Total 258	O 258	0	0

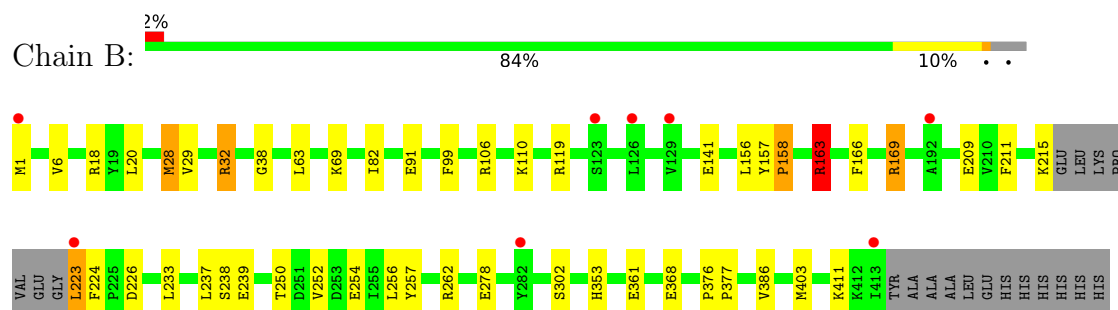
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

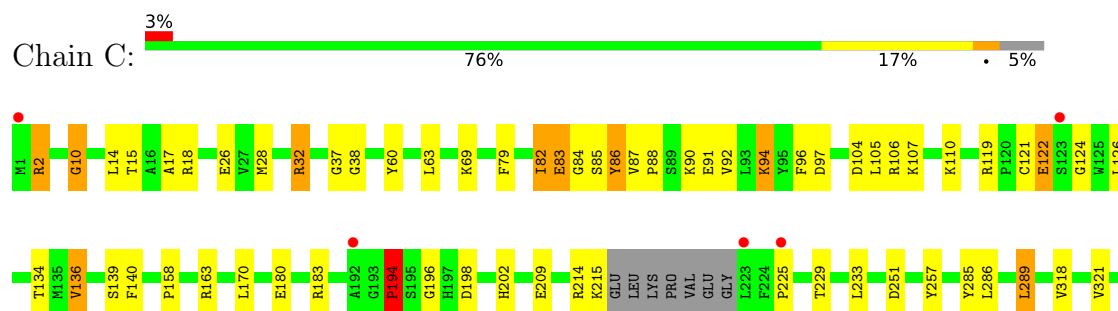
- Molecule 1: Flavin-containing monooxygenase

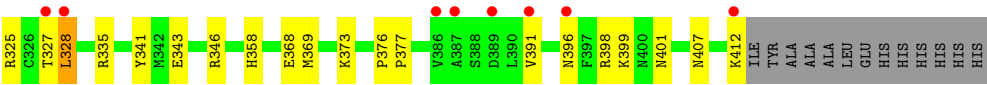


- Molecule 1: Flavin-containing monooxygenase

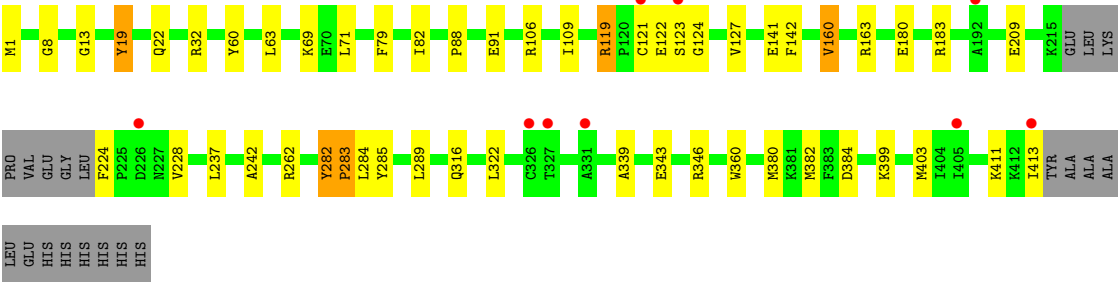
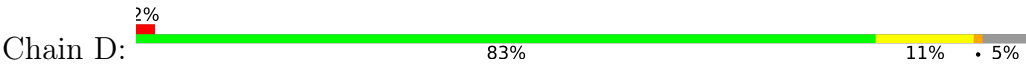


- Molecule 1: Flavin-containing monooxygenase





● Molecule 1: Flavin-containing monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.87Å 76.28Å 80.88Å 71.96° 81.45° 81.21°	Depositor
Resolution (Å)	76.46 – 1.89 76.46 – 1.89	Depositor EDS
% Data completeness (in resolution range)	89.8 (76.46-1.89) 89.9 (76.46-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.191 , 0.219 0.191 , 0.217	Depositor DCC
R_{free} test set	5969 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14660	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, MG

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	0.82	10/3406 (0.3%)	0.83	3/4618 (0.1%)
1	B	0.91	12/3406 (0.4%)	0.86	4/4618 (0.1%)
1	C	1.15	27/3398 (0.8%)	0.93	11/4607 (0.2%)
1	D	0.80	8/3409 (0.2%)	0.87	5/4621 (0.1%)
All	All	0.93	57/13619 (0.4%)	0.87	23/18464 (0.1%)

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	214	ARG	C-N	-23.05	1.01	1.33
1	C	122	GLU	C-N	-12.63	1.15	1.33
1	A	252	VAL	C-O	-6.97	1.17	1.24
1	A	239	GLU	C-O	-6.82	1.16	1.24
1	A	21	LYS	C-O	-6.68	1.16	1.24
1	C	321	VAL	C-O	-6.60	1.16	1.24
1	A	100	THR	C-O	-6.38	1.16	1.24
1	B	169	ARG	C-O	-6.37	1.16	1.24
1	B	20	LEU	C-O	-6.30	1.16	1.24
1	C	90	LYS	C-O	-6.26	1.16	1.24
1	B	256	LEU	C-O	-6.23	1.17	1.24
1	C	15	THR	C-O	-6.17	1.16	1.24
1	A	242	ALA	C-O	-5.92	1.16	1.24
1	C	87	VAL	C-N	5.90	1.40	1.33
1	D	142	PHE	C-O	-5.83	1.16	1.23
1	B	28	MET	C-O	-5.82	1.17	1.24
1	D	109	ILE	C-O	-5.74	1.17	1.24
1	D	106	ARG	C-O	-5.73	1.17	1.24
1	D	127	VAL	C-O	-5.72	1.18	1.24
1	A	251	ASP	C-O	-5.71	1.16	1.23
1	B	106	ARG	C-O	-5.69	1.17	1.24
1	B	252	VAL	C-O	-5.68	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	ASP	C-O	-5.57	1.17	1.24
1	C	289	LEU	C-O	-5.52	1.17	1.24
1	C	328	LEU	C-N	5.51	1.40	1.33
1	B	224	PHE	C-O	-5.47	1.18	1.24
1	B	99	PHE	C-O	-5.47	1.17	1.24
1	C	94	LYS	C-O	-5.46	1.17	1.24
1	C	225	PRO	N-CD	5.42	1.55	1.47
1	C	368	GLU	C-O	-5.42	1.17	1.24
1	D	283	PRO	N-CD	5.42	1.55	1.47
1	C	225	PRO	C-O	-5.40	1.16	1.23
1	C	106	ARG	C-O	-5.34	1.17	1.24
1	B	158	PRO	C-O	-5.33	1.18	1.23
1	B	158	PRO	N-CD	5.29	1.55	1.47
1	A	107	LYS	C-O	-5.29	1.17	1.24
1	C	17	ALA	C-O	-5.27	1.18	1.24
1	D	285	TYR	C-O	-5.25	1.17	1.24
1	A	249	SER	C-O	-5.24	1.17	1.23
1	C	37	GLY	C-O	-5.19	1.17	1.24
1	C	92	VAL	C-O	-5.19	1.18	1.24
1	C	86	TYR	C-O	-5.17	1.16	1.23
1	C	318	VAL	C-O	-5.15	1.18	1.24
1	C	88	PRO	N-CD	5.14	1.54	1.47
1	B	18	ARG	C-O	-5.12	1.18	1.24
1	D	19	TYR	C-O	-5.12	1.18	1.24
1	A	99	PHE	C-O	-5.10	1.18	1.24
1	B	166	PHE	C-O	-5.08	1.17	1.23
1	C	285	TYR	C-O	-5.08	1.17	1.24
1	A	224	PHE	C-O	-5.07	1.19	1.24
1	C	369	MET	C-O	-5.07	1.18	1.24
1	C	286	LEU	C-O	-5.05	1.17	1.23
1	D	282	TYR	C-O	-5.05	1.19	1.24
1	C	124	GLY	C-O	-5.02	1.19	1.24
1	C	229	THR	C-O	-5.02	1.18	1.24
1	C	69	LYS	C-O	-5.01	1.17	1.24
1	C	335	ARG	C-O	-5.00	1.18	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	GLU	O-C-N	-8.55	111.22	122.59
1	D	282	TYR	C-N-CD	7.83	137.83	120.60
1	C	121	CYS	O-C-N	-7.49	114.22	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	LEU	CA-C-N	-6.75	113.73	120.21
1	C	328	LEU	C-N-CA	-6.75	113.73	120.21
1	C	96	PHE	N-CA-C	6.49	118.44	111.36
1	D	180	GLU	CA-C-N	-6.04	113.46	119.56
1	D	180	GLU	C-N-CA	-6.04	113.46	119.56
1	B	157	TYR	CA-C-N	-5.98	113.53	119.99
1	B	157	TYR	C-N-CA	-5.98	113.53	119.99
1	C	87	VAL	CA-C-N	-5.97	114.12	120.03
1	C	87	VAL	C-N-CA	-5.97	114.12	120.03
1	C	85	SER	N-CA-C	5.62	117.48	111.36
1	B	163	ARG	CG-CD-NE	5.61	124.35	112.00
1	D	119	ARG	CA-C-N	-5.41	114.19	119.76
1	D	119	ARG	C-N-CA	-5.41	114.19	119.76
1	A	180	GLU	CA-C-N	-5.39	114.27	119.87
1	A	180	GLU	C-N-CA	-5.39	114.27	119.87
1	B	386	VAL	N-CA-C	5.20	119.09	113.43
1	C	10	GLY	CA-C-N	5.14	125.18	119.32
1	C	10	GLY	C-N-CA	5.14	125.18	119.32
1	A	109	ILE	N-CA-C	5.11	115.44	107.99
1	C	194	PRO	CA-N-CD	-5.03	104.95	112.00

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	3311	0	3201	39	2
1	B	3311	0	3201	28	2
1	C	3303	0	3188	42	2
1	D	3314	0	3202	32	2
2	A	53	0	31	1	0
2	B	53	0	31	3	0
2	C	53	0	31	3	0
2	D	53	0	31	2	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	354	0	0	14	1
4	B	348	0	0	6	1
4	C	247	0	0	8	0
4	D	258	0	0	6	0
All	All	14660	0	12916	143	5

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 5.

All (143) 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:122:GLU:HG2	1:A:123:SER:H	1.19	1.06
1:D:183:ARG:NH2	4:D:601:HOH:O	1.89	1.04
1:D:122:GLU:HG2	1:D:123:SER:H	1.22	0.98
1:B:361:GLU:OE1	4:B:601:HOH:O	1.92	0.88
1:A:403:MET:HB2	1:A:413:ILE:HD11	1.61	0.80
1:A:340:GLU:OE2	4:A:601:HOH:O	1.98	0.80
1:D:121:CYS:O	1:D:124:GLY:N	2.17	0.78
1:A:122:GLU:HG2	1:A:123:SER:N	2.00	0.75
1:A:186:ARG:NH2	4:A:603:HOH:O	2.22	0.73
1:D:160:VAL:HG13	1:D:163:ARG:HB2	1.69	0.73
1:B:278:GLU:OE2	4:B:602:HOH:O	2.07	0.72
1:C:396:ASN:HD22	1:C:399:LYS:NZ	1.87	0.72
1:A:413:ILE:O	4:A:602:HOH:O	2.07	0.71
1:B:223:LEU:N	1:B:223:LEU:HD12	2.06	0.71
1:B:1:MET:HB3	4:B:901:HOH:O	1.91	0.70
1:D:122:GLU:HG2	1:D:123:SER:N	2.01	0.70
1:A:3:ARG:NH2	4:A:604:HOH:O	2.25	0.69
1:B:91:GLU:OE2	4:B:603:HOH:O	2.12	0.68
1:B:403:MET:HE2	1:B:411:LYS:HE2	1.75	0.66
1:B:209:GLU:HG2	1:B:211:PHE:CE2	2.31	0.66
1:B:262:ARG:NH1	4:B:606:HOH:O	2.20	0.66
1:A:262:ARG:NH2	4:A:605:HOH:O	2.25	0.65
1:A:119:ARG:NH1	4:A:609:HOH:O	2.29	0.63
1:C:194:PRO:HB3	1:C:391:VAL:HG11	1.80	0.63
1:C:373:LYS:NZ	4:C:604:HOH:O	2.26	0.63
1:D:122:GLU:OE2	1:D:124:GLY:N	2.32	0.62
1:C:194:PRO:HB3	1:C:391:VAL:CG1	2.30	0.62
1:D:262:ARG:NH2	4:D:603:HOH:O	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ASP:OD2	4:C:602:HOH:O	2.16	0.61
1:B:163:ARG:HH11	1:B:163:ARG:HG3	1.66	0.61
1:C:2:ARG:NH1	1:C:26:GLU:OE1	2.33	0.61
1:B:368:GLU:OE2	4:B:604:HOH:O	2.15	0.60
1:D:384:ASP:OD1	4:D:602:HOH:O	2.17	0.60
1:B:63:LEU:HD11	2:B:501:FAD:H6	1.83	0.59
1:C:170:LEU:HD11	1:C:257:TYR:HE2	1.67	0.59
1:B:28:MET:HE2	1:B:110:LYS:HE3	1.86	0.58
1:C:325:ARG:NH2	4:C:613:HOH:O	2.37	0.57
1:D:122:GLU:CG	1:D:123:SER:H	2.06	0.57
1:A:60:TYR:CZ	1:A:63:LEU:HD12	2.40	0.56
1:B:69:LYS:NZ	1:B:82:ILE:O	2.38	0.56
1:A:160:VAL:HG13	1:A:163:ARG:HB2	1.88	0.56
1:C:134:THR:OG1	1:C:136:VAL:HG12	2.06	0.55
1:A:292:ASN:OD1	1:A:335:ARG:NH2	2.39	0.55
1:C:343:GLU:CD	1:C:346:ARG:HH21	2.15	0.55
1:A:169:ARG:NH2	4:A:616:HOH:O	2.39	0.54
1:A:122:GLU:CG	1:A:123:SER:H	2.01	0.54
1:D:71:LEU:HD21	1:D:382:MET:HB3	1.90	0.53
1:D:339:ALA:O	1:D:343:GLU:HG2	2.08	0.53
1:A:32:ARG:C	1:A:32:ARG:HD3	2.33	0.53
1:D:343:GLU:CD	1:D:346:ARG:HH21	2.17	0.53
1:A:104:ASP:OD2	1:A:107:LYS:HE2	2.08	0.53
1:A:381:LYS:CE	4:A:880:HOH:O	2.56	0.52
1:C:215:LYS:HG2	1:C:233:LEU:HD13	1.92	0.52
1:C:82:ILE:HG13	1:C:83:GLU:N	2.26	0.51
1:A:381:LYS:HE2	4:A:880:HOH:O	2.10	0.51
1:D:282:TYR:HB2	1:D:283:PRO:HA	1.93	0.51
1:C:341:TYR:OH	1:C:358:HIS:NE2	2.40	0.50
1:A:412:LYS:HE2	1:B:226:ASP:OD1	2.11	0.50
1:B:169:ARG:HD3	1:B:254:GLU:OE1	2.10	0.50
1:C:82:ILE:HD13	1:C:91:GLU:OE2	2.11	0.50
1:A:119:ARG:NE	4:A:620:HOH:O	2.43	0.50
1:C:104:ASP:OD2	1:C:107:LYS:NZ	2.44	0.50
1:D:399:LYS:NZ	4:D:610:HOH:O	2.38	0.50
1:C:63:LEU:HD11	2:C:501:FAD:H6	1.93	0.49
1:D:119:ARG:O	1:D:119:ARG:HG3	2.11	0.49
1:C:32:ARG:HD3	1:C:32:ARG:C	2.36	0.49
1:D:224:PHE:HB3	1:D:228:VAL:HB	1.95	0.49
1:A:117:ASN:OD1	1:A:119:ARG:HD3	2.14	0.48
1:C:84:GLY:HA2	1:C:401:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:HD12	1:C:140:PHE:O	2.13	0.48
1:D:69:LYS:NZ	1:D:82:ILE:O	2.46	0.48
1:B:209:GLU:HG2	1:B:211:PHE:CZ	2.49	0.48
1:B:156:LEU:C	1:B:156:LEU:HD23	2.38	0.48
1:C:396:ASN:HD22	1:C:399:LYS:HZ1	1.59	0.48
1:A:32:ARG:O	1:A:112:GLN:HA	2.13	0.48
1:C:94:LYS:NZ	4:C:622:HOH:O	2.47	0.48
1:C:158:PRO:O	1:C:163:ARG:NH1	2.47	0.48
1:B:163:ARG:HA	1:B:237:LEU:HD12	1.95	0.47
1:C:104:ASP:CG	1:C:107:LYS:HE2	2.39	0.47
1:A:156:LEU:HD12	4:A:605:HOH:O	2.15	0.47
1:B:403:MET:CE	1:B:411:LYS:HE2	2.44	0.47
1:C:28:MET:SD	1:C:110:LYS:HD2	2.55	0.47
1:A:8:GLY:O	1:A:13:GLY:HA3	2.15	0.46
1:C:196:GLY:HA2	4:C:626:HOH:O	2.14	0.46
1:B:32:ARG:HD3	1:B:32:ARG:C	2.40	0.46
1:D:22:GLN:NE2	4:D:624:HOH:O	2.48	0.46
1:D:403:MET:HB2	1:D:413:ILE:HD11	1.96	0.46
1:D:1:MET:HE1	1:D:322:LEU:HD22	1.97	0.46
1:D:60:TYR:CZ	1:D:63:LEU:HD12	2.51	0.46
1:C:407:ASN:ND2	4:C:612:HOH:O	2.37	0.45
1:C:18:ARG:HA	1:C:105:LEU:HD21	1.99	0.45
1:D:284:LEU:HA	1:D:289:LEU:O	2.16	0.44
1:A:381:LYS:HG3	4:A:880:HOH:O	2.17	0.44
1:A:63:LEU:HD11	2:A:500:FAD:H6	1.99	0.44
1:C:60:TYR:CZ	1:C:63:LEU:HD12	2.52	0.44
1:A:403:MET:CB	1:A:413:ILE:HD11	2.40	0.44
1:B:238:SER:O	1:B:239:GLU:C	2.60	0.44
1:A:172:HIS:O	1:A:175:GLU:HG2	2.18	0.44
1:C:401:ASN:O	1:C:412:LYS:HG3	2.18	0.44
1:C:202:HIS:HD2	4:C:700:HOH:O	2.00	0.43
1:D:63:LEU:HD11	2:D:500:FAD:H6	1.99	0.43
1:A:381:LYS:CG	4:A:880:HOH:O	2.66	0.43
1:C:10:GLY:O	1:C:14:LEU:HG	2.18	0.43
1:A:121:CYS:O	1:A:124:GLY:N	2.50	0.43
2:C:501:FAD:H1'1	2:C:501:FAD:H9	1.73	0.43
1:A:119:ARG:CZ	4:A:620:HOH:O	2.66	0.43
1:A:211:PHE:CZ	1:A:250:THR:HG21	2.54	0.43
1:B:215:LYS:HG2	1:B:233:LEU:HD13	2.01	0.43
1:B:223:LEU:N	1:B:223:LEU:CD1	2.76	0.43
1:C:325:ARG:NH2	4:C:601:HOH:O	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:O	1:A:59:MET:HB2	2.19	0.42
1:C:104:ASP:OD2	1:C:107:LYS:HE2	2.20	0.42
1:B:38:GLY:HA2	2:B:501:FAD:O3B	2.20	0.42
1:A:1:MET:HG3	1:A:25:PHE:HE1	1.84	0.42
1:A:280:TYR:HE1	1:A:342:MET:HE3	1.85	0.42
1:B:376:PRO:HA	1:B:377:PRO:HD3	1.97	0.42
1:C:86:TYR:CD2	1:C:398:ARG:HA	2.55	0.41
1:A:88:PRO:HG2	1:A:91:GLU:HG2	2.03	0.41
2:B:501:FAD:H1'1	2:B:501:FAD:H9	1.77	0.41
1:D:19:TYR:CD1	1:D:316:GLN:HG2	2.54	0.41
1:A:158:PRO:HD2	1:A:257:TYR:CD2	2.55	0.41
1:C:376:PRO:HA	1:C:377:PRO:HD3	1.88	0.41
1:D:122:GLU:CG	1:D:123:SER:N	2.72	0.41
1:D:8:GLY:O	1:D:13:GLY:HA3	2.20	0.41
1:D:122:GLU:OE2	1:D:124:GLY:HA3	2.20	0.41
1:D:209:GLU:OE1	4:D:604:HOH:O	2.22	0.41
1:A:400:ASN:HD22	1:A:400:ASN:H	1.69	0.41
1:C:396:ASN:HD22	1:C:399:LYS:CE	2.33	0.41
1:B:6:VAL:HB	1:B:29:VAL:HG22	2.03	0.41
1:D:282:TYR:CB	1:D:283:PRO:HA	2.51	0.41
1:A:72:MET:HE2	1:A:72:MET:HB3	1.93	0.41
1:C:289:LEU:HD22	1:C:328:LEU:HD11	2.02	0.41
1:C:180:GLU:O	1:C:183:ARG:HG2	2.21	0.41
1:D:237:LEU:HD23	1:D:242:ALA:HA	2.02	0.40
1:B:158:PRO:HD2	1:B:257:TYR:CE1	2.57	0.40
1:B:302:SER:HA	1:B:353:HIS:HB3	2.03	0.40
1:C:38:GLY:HA2	2:C:501:FAD:O3B	2.20	0.40
1:C:327:THR:O	1:C:327:THR:HG23	2.21	0.40
1:C:126:LEU:HD11	1:C:139:SER:HB3	2.03	0.40
1:D:360:TRP:CZ2	1:D:380:MET:HA	2.57	0.40
1:C:396:ASN:HA	1:C:399:LYS:HE2	2.03	0.40
1:D:88:PRO:HG2	1:D:91:GLU:HG2	2.04	0.40
2:D:500:FAD:H1'1	2:D:500:FAD:H9	1.81	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ARG:NH2	1:D:141:GLU:OE1[1_665]	1.62	0.58
1:C:122:GLU:OE2	1:D:119:ARG:NH2[1_665]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:945:HOH:O	4:B:899:HOH:O[1_655]	2.03	0.17
1:A:141:GLU:OE2	1:B:119:ARG:NH2[1_665]	2.17	0.03
1:A:119:ARG:NH1	1:B:141:GLU:OE1[1_665]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/425 (95%)	387 (96%)	15 (4%)	0	100	100
1	B	402/425 (95%)	388 (96%)	14 (4%)	0	100	100
1	C	401/425 (94%)	385 (96%)	16 (4%)	0	100	100
1	D	402/425 (95%)	386 (96%)	16 (4%)	0	100	100
All	All	1607/1700 (94%)	1546 (96%)	61 (4%)	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	363/378 (96%)	356 (98%)	7 (2%)	50	47
1	B	363/378 (96%)	359 (99%)	4 (1%)	65	67
1	C	362/378 (96%)	353 (98%)	9 (2%)	42	37
1	D	363/378 (96%)	359 (99%)	4 (1%)	65	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1451/1512 (96%)	1427 (98%)	24 (2%)	53 52

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	50	GLU
1	A	79	PHE
1	A	178	SER
1	A	250	THR
1	A	400	ASN
1	A	404	ILE
1	B	32	ARG
1	B	163	ARG
1	B	223	LEU
1	B	250	THR
1	C	2	ARG
1	C	32	ARG
1	C	79	PHE
1	C	82	ILE
1	C	83	GLU
1	C	97	ASP
1	C	136	VAL
1	C	194	PRO
1	C	209	GLU
1	D	32	ARG
1	D	79	PHE
1	D	160	VAL
1	D	411	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	98	ASN
1	B	98	ASN
1	B	202	HIS
1	B	396	ASN
1	B	409	ASN
1	C	34	HIS
1	C	98	ASN

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Mol	Chain	Res	Type
1	C	396	ASN
1	D	22	GLN
1	D	41	ASN
1	D	98	ASN
1	D	117	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	C	501	-	58,58,58	1.52	11 (18%)	85,89,89	1.60	21 (24%)
2	FAD	A	500	-	58,58,58	1.54	9 (15%)	85,89,89	1.69	18 (21%)
2	FAD	B	501	-	58,58,58	1.43	8 (13%)	85,89,89	1.70	18 (21%)
2	FAD	D	500	-	58,58,58	1.46	7 (12%)	85,89,89	1.72	18 (21%)

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
2	FAD	C	501	-	-	0/34/50/50	0/6/6/6
2	FAD	A	500	-	-	1/34/50/50	0/6/6/6
2	FAD	B	501	-	-	1/34/50/50	0/6/6/6
2	FAD	D	500	-	-	2/34/50/50	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C9A-C5X	5.29	1.49	1.41
2	B	501	FAD	C9A-C5X	5.04	1.49	1.41
2	D	500	FAD	C9A-C5X	4.88	1.49	1.41
2	C	501	FAD	C9A-C5X	4.61	1.48	1.41
2	A	500	FAD	C5A-C4A	4.59	1.47	1.39
2	C	501	FAD	C5A-C4A	4.43	1.47	1.39
2	D	500	FAD	C5A-C4A	4.31	1.46	1.39
2	B	501	FAD	C5A-C4A	3.96	1.46	1.39
2	C	501	FAD	C8-C7	3.53	1.49	1.40
2	A	500	FAD	C8-C7	3.34	1.49	1.40
2	D	500	FAD	C8-C7	3.30	1.48	1.40
2	B	501	FAD	C8-C7	3.23	1.48	1.40
2	D	500	FAD	P-O3P	3.22	1.63	1.59
2	C	501	FAD	C4-N3	-2.91	1.33	1.38
2	C	501	FAD	P-O3P	2.82	1.62	1.59
2	A	500	FAD	C5A-C6A	2.79	1.48	1.41
2	C	501	FAD	C5A-C6A	2.73	1.48	1.41
2	A	500	FAD	P-O3P	2.71	1.62	1.59
2	D	500	FAD	C5A-C6A	2.63	1.48	1.41
2	D	500	FAD	C4X-N5	2.61	1.36	1.30
2	A	500	FAD	C4X-N5	2.53	1.36	1.30
2	C	501	FAD	PA-O3P	2.52	1.62	1.59
2	B	501	FAD	P-O3P	2.50	1.62	1.59
2	D	500	FAD	C4-N3	-2.49	1.34	1.38
2	B	501	FAD	C5A-C6A	2.48	1.47	1.41
2	B	501	FAD	C4X-N5	2.46	1.36	1.30
2	B	501	FAD	C4-N3	-2.33	1.34	1.38
2	C	501	FAD	C4X-N5	2.32	1.35	1.30
2	A	500	FAD	C4-N3	-2.29	1.34	1.38
2	C	501	FAD	C8A-N7A	2.17	1.35	1.31
2	C	501	FAD	C2-N3	-2.09	1.34	1.39
2	B	501	FAD	C5X-N5	-2.09	1.35	1.39
2	A	500	FAD	C5X-N5	-2.08	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C4A-N9A	-2.05	1.33	1.37
2	A	500	FAD	C1'-C2'	-2.02	1.49	1.52

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	FAD	C5A-C4A-N3A	-5.80	118.74	126.72
2	B	501	FAD	C5A-C4A-N3A	-5.30	119.41	126.72
2	C	501	FAD	C5A-C4A-N3A	-5.16	119.61	126.72
2	A	500	FAD	C5A-C4A-N3A	-5.15	119.63	126.72
2	D	500	FAD	N3A-C4A-N9A	4.84	135.41	127.17
2	A	500	FAD	N3A-C4A-N9A	4.67	135.11	127.17
2	B	501	FAD	N3A-C4A-N9A	4.56	134.92	127.17
2	A	500	FAD	N3A-C2A-N1A	-4.09	122.39	128.58
2	C	501	FAD	N3A-C4A-N9A	4.09	134.12	127.17
2	A	500	FAD	C2A-N3A-C4A	3.79	121.09	111.83
2	D	500	FAD	C2A-N3A-C4A	3.79	121.08	111.83
2	A	500	FAD	C4A-N9A-C8A	3.76	109.69	105.74
2	D	500	FAD	N3A-C2A-N1A	-3.73	122.94	128.58
2	B	501	FAD	C2A-N3A-C4A	3.65	120.75	111.83
2	D	500	FAD	C9A-C5X-N5	-3.59	118.64	122.45
2	B	501	FAD	N3A-C2A-N1A	-3.58	123.16	128.58
2	B	501	FAD	C4A-N9A-C8A	3.50	109.41	105.74
2	C	501	FAD	C2A-N3A-C4A	3.46	120.27	111.83
2	C	501	FAD	C4A-C5A-N7A	-3.37	106.73	110.58
2	D	500	FAD	C4A-C5A-N7A	-3.34	106.76	110.58
2	B	501	FAD	C4A-C5A-N7A	-3.33	106.77	110.58
2	C	501	FAD	N3A-C2A-N1A	-3.32	123.56	128.58
2	A	500	FAD	C4A-C5A-N7A	-3.27	106.84	110.58
2	D	500	FAD	C4-C4X-N5	3.24	122.69	118.21
2	C	501	FAD	C4-C4X-N5	3.22	122.66	118.21
2	A	500	FAD	C4-C4X-N5	3.21	122.64	118.21
2	B	501	FAD	C5'-C4'-C3'	-3.19	106.19	112.22
2	D	500	FAD	C4A-N9A-C8A	3.17	109.07	105.74
2	B	501	FAD	C9A-C5X-N5	-3.15	119.12	122.45
2	B	501	FAD	C4-C4X-N5	3.08	122.46	118.21
2	C	501	FAD	C4A-N9A-C8A	2.99	108.88	105.74
2	C	501	FAD	C9A-C5X-N5	-2.95	119.33	122.45
2	B	501	FAD	C5A-N7A-C8A	2.89	107.99	103.45
2	A	500	FAD	C9A-C5X-N5	-2.88	119.39	122.45
2	D	500	FAD	C5A-N7A-C8A	2.79	107.84	103.45
2	A	500	FAD	C5A-N7A-C8A	2.76	107.79	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C5'-C4'-C3'	-2.72	107.09	112.22
2	D	500	FAD	O4-C4-C4X	-2.72	119.36	126.53
2	B	501	FAD	O2P-P-O1P	2.68	124.93	112.44
2	B	501	FAD	N9A-C8A-N7A	-2.66	110.16	113.94
2	D	500	FAD	C5X-C9A-N10	2.65	120.37	117.97
2	C	501	FAD	C4'-C3'-C2'	-2.64	109.18	113.57
2	C	501	FAD	C5'-C4'-C3'	-2.61	107.29	112.22
2	C	501	FAD	C4X-C10-N1	-2.56	118.30	124.59
2	A	500	FAD	O4-C4-C4X	-2.55	119.79	126.53
2	C	501	FAD	C5A-N7A-C8A	2.55	107.45	103.45
2	A	500	FAD	N9A-C8A-N7A	-2.50	110.39	113.94
2	A	500	FAD	C6A-C5A-N7A	2.47	136.85	132.09
2	D	500	FAD	N9A-C8A-N7A	-2.46	110.45	113.94
2	D	500	FAD	C5'-C4'-C3'	-2.45	107.60	112.22
2	B	501	FAD	O4-C4-C4X	-2.42	120.14	126.53
2	D	500	FAD	C9-C9A-N10	-2.33	118.73	121.85
2	D	500	FAD	C6-C5X-N5	2.32	122.30	118.44
2	C	501	FAD	C5X-N5-C4X	2.32	121.84	118.09
2	B	501	FAD	C6A-C5A-N7A	2.32	136.55	132.09
2	C	501	FAD	N9A-C8A-N7A	-2.31	110.66	113.94
2	A	500	FAD	C2A-N1A-C6A	2.29	122.50	118.73
2	A	500	FAD	C5X-C9A-N10	2.24	120.00	117.97
2	B	501	FAD	C4X-C4-N3	2.24	118.96	113.25
2	C	501	FAD	C10-N1-C2	2.23	121.69	116.85
2	B	501	FAD	C5X-N5-C4X	2.23	121.69	118.09
2	C	501	FAD	C4X-C4-N3	2.19	118.83	113.25
2	D	500	FAD	O2-C2-N1	-2.19	118.17	121.80
2	A	500	FAD	C4X-C4-N3	2.19	118.82	113.25
2	B	501	FAD	C4X-C10-N1	-2.17	119.27	124.59
2	C	501	FAD	C6A-C5A-N7A	2.15	136.23	132.09
2	A	500	FAD	C4X-C10-N1	-2.11	119.42	124.59
2	D	500	FAD	C5X-N5-C4X	2.10	121.48	118.09
2	C	501	FAD	C5B-C4B-C3B	-2.08	107.72	115.21
2	D	500	FAD	C4X-C4-N3	2.08	118.55	113.25
2	C	501	FAD	C2A-N1A-C6A	2.07	122.13	118.73
2	B	501	FAD	C10-N1-C2	2.06	121.30	116.85
2	C	501	FAD	O2P-P-O1P	2.04	121.94	112.44
2	A	500	FAD	O4B-C1B-N9A	-2.04	104.17	108.09
2	C	501	FAD	C5X-C9A-N10	2.02	119.79	117.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

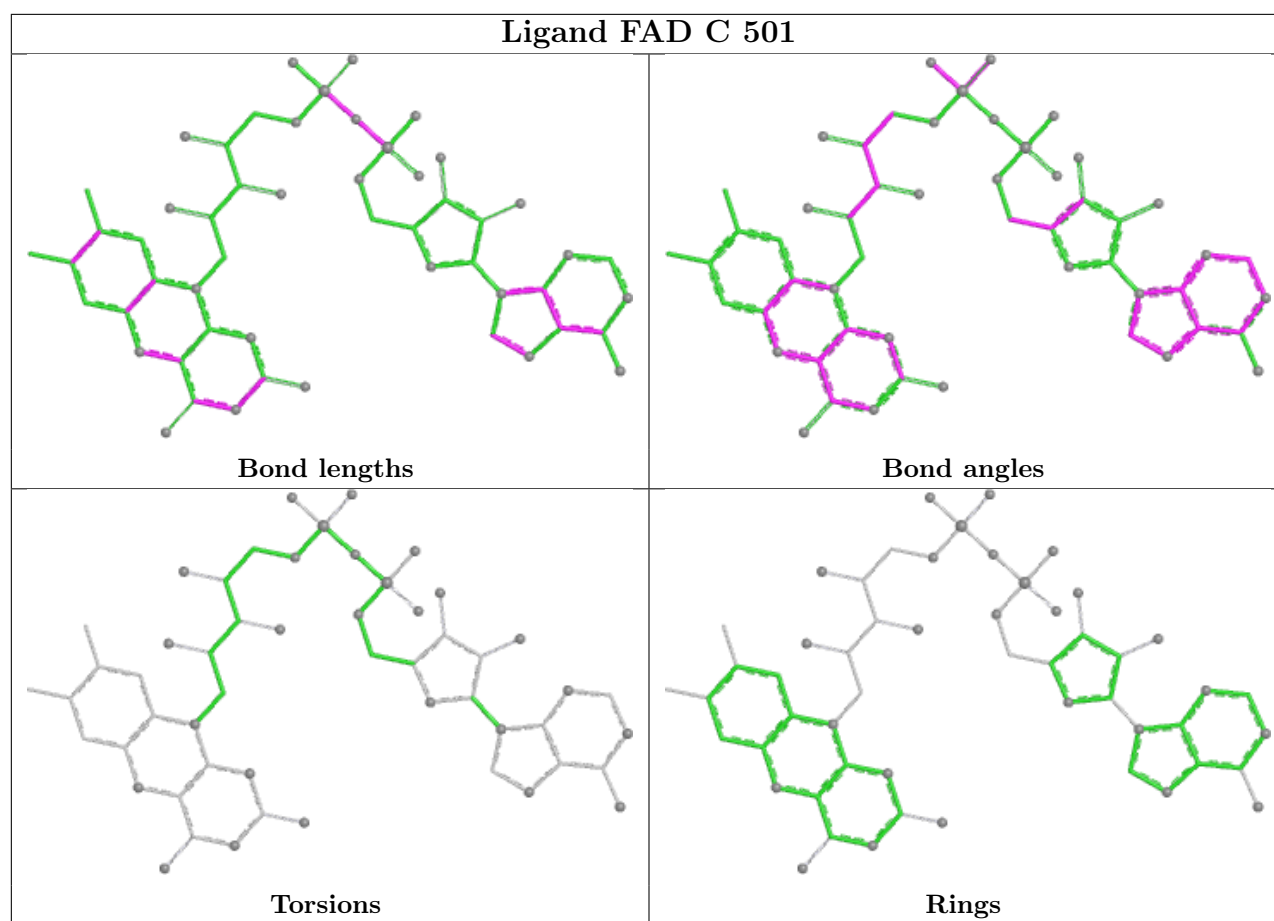
Mol	Chain	Res	Type	Atoms
2	A	500	FAD	O3'-C3'-C4'-C5'
2	D	500	FAD	PA-O3P-P-O5'
2	D	500	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	O3'-C3'-C4'-C5'

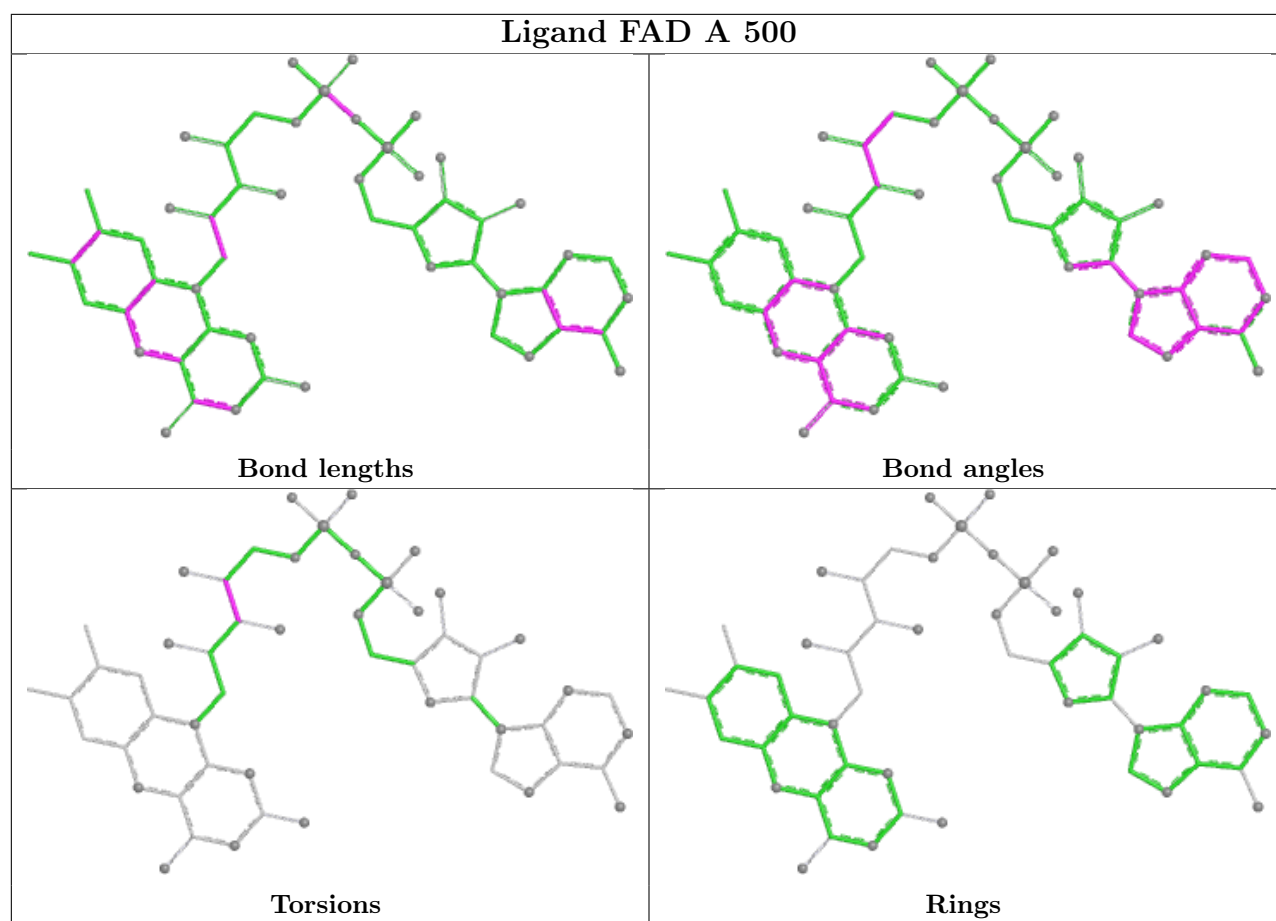
There are no ring outliers.

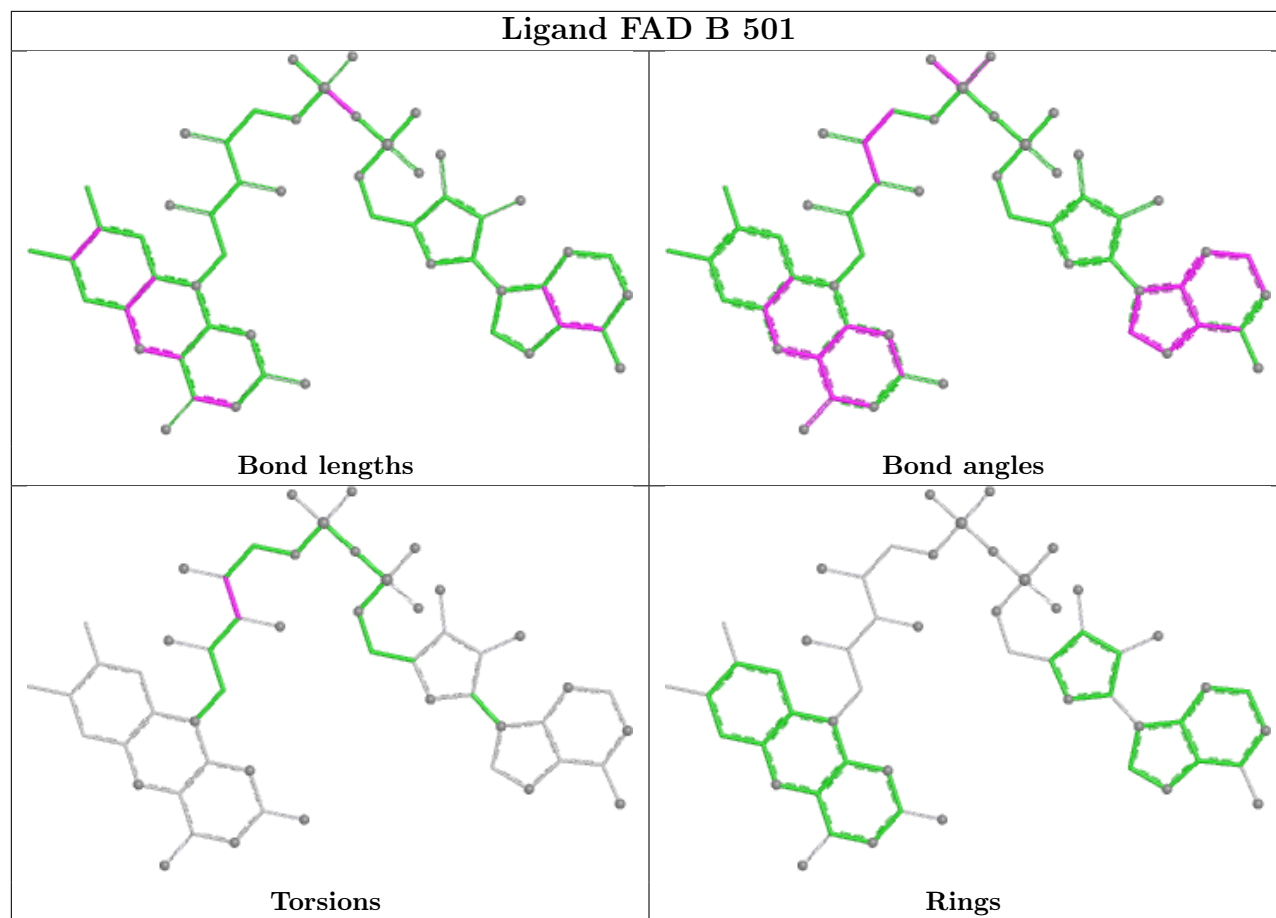
4 monomers are involved in 9 short contacts:

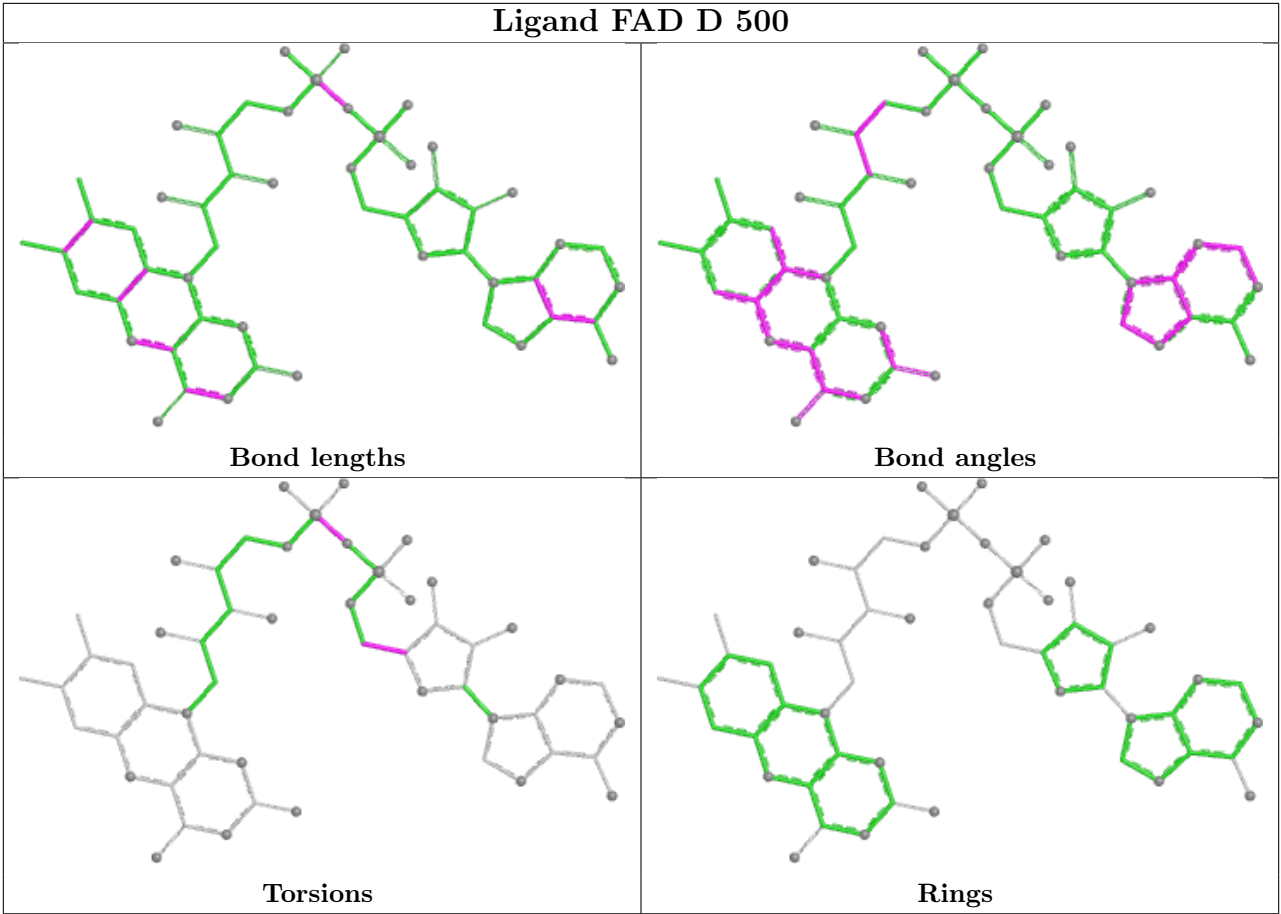
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	FAD	3	0
2	A	500	FAD	1	0
2	B	501	FAD	3	0
2	D	500	FAD	2	0

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 than 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.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	122:GLU	C	123:SER	N	1.15
1	C	214:ARG	C	215:LYS	N	1.01

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	406/425 (95%)	-0.01	4 (0%) 79 82	16, 27, 41, 55	1 (0%)
1	B	406/425 (95%)	0.09	8 (1%) 65 69	19, 27, 42, 59	2 (0%)
1	C	405/425 (95%)	0.34	13 (3%) 50 54	21, 32, 50, 63	0
1	D	405/425 (95%)	0.33	9 (2%) 62 66	15, 32, 45, 65	2 (0%)
All	All	1622/1700 (95%)	0.19	34 (2%) 63 67	15, 30, 46, 65	5 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	LEU	4.0
1	D	413	ILE	3.8
1	B	1	MET	3.7
1	C	1	MET	3.4
1	C	391	VAL	3.3
1	C	328	LEU	3.2
1	A	413	ILE	3.0
1	B	192	ALA	2.9
1	C	192	ALA	2.9
1	C	412	LYS	2.8
1	A	192	ALA	2.7
1	D	123	SER	2.7
1	B	126	LEU	2.6
1	C	123	SER	2.5
1	C	327	THR	2.5
1	C	223	LEU	2.5
1	D	192	ALA	2.4
1	D	226	ASP	2.4
1	D	327	THR	2.4
1	C	387	ALA	2.4
1	B	282	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	225	PRO	2.3
1	B	123	SER	2.3
1	A	215	LYS	2.2
1	A	81	ASP	2.2
1	B	413	ILE	2.2
1	D	121	CYS	2.2
1	C	396	ASN	2.1
1	D	326	CYS	2.1
1	D	331	ALA	2.1
1	D	405	ILE	2.0
1	C	386	VAL	2.0
1	C	389	ASP	2.0
1	B	129	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

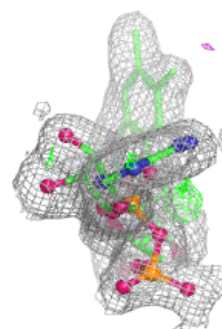
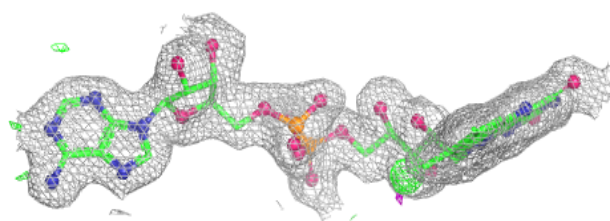
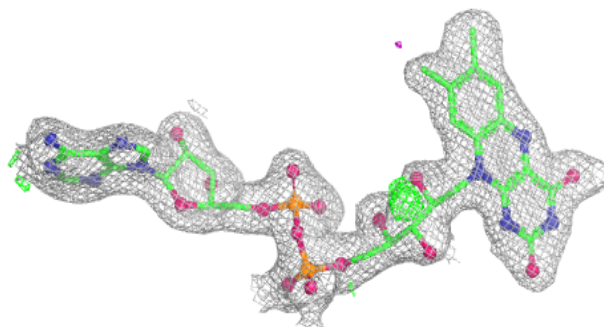
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	502	1/1	0.95	0.06	34,34,34,34	0
2	FAD	C	501	53/53	0.96	0.07	20,27,36,37	0
3	MG	C	502	1/1	0.96	0.04	35,35,35,35	0
2	FAD	D	500	53/53	0.97	0.07	20,25,32,35	0
2	FAD	B	501	53/53	0.97	0.06	17,24,32,34	0
2	FAD	A	500	53/53	0.97	0.06	16,22,29,32	0

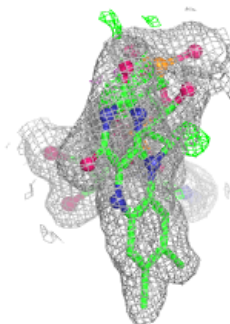
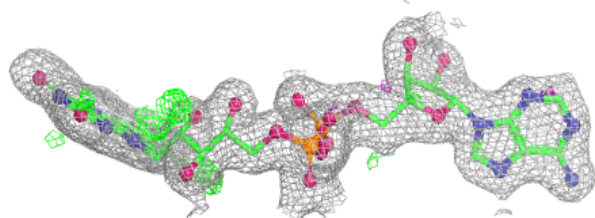
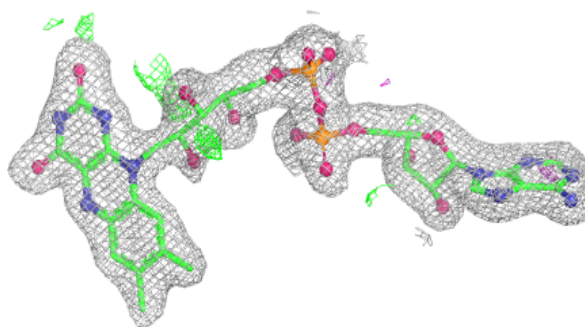
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 501:

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

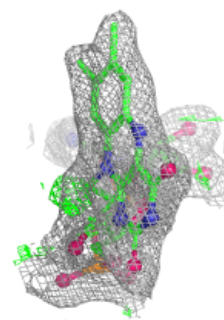
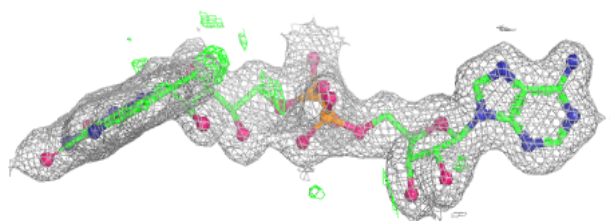
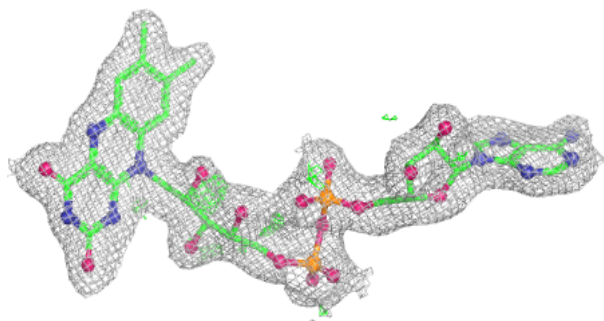
**Electron density around FAD D 500:**

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

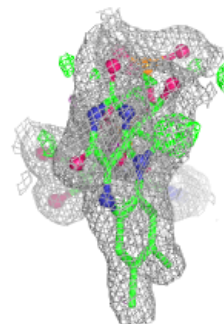
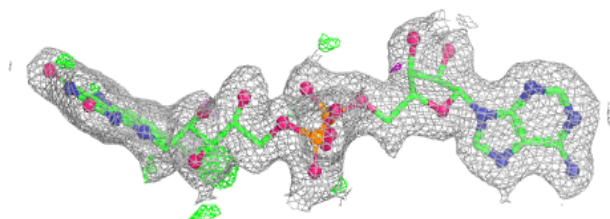
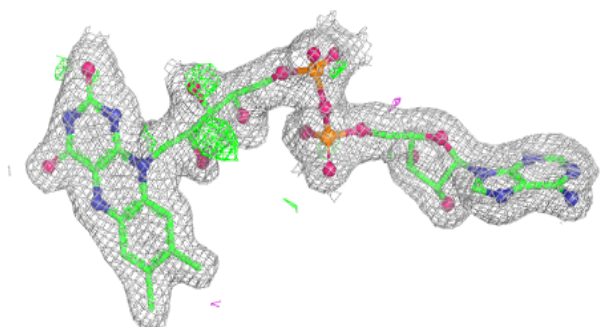


Electron density around FAD B 501:

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

**Electron density around FAD A 500:**

$2mF_o-DF_c$ (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.