Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 07:57 pm GMT

PDB ID	:	3ZDN
Title	:	D11-C mutant of monoamine oxidase from Aspergillus niger
Authors	:	Frank, A.; Ghislieri, D.; Willies, S.; Turner, N.J.; Grogan, G.
Deposited on	:	2012-11-29
Resolution	:	2.55 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:

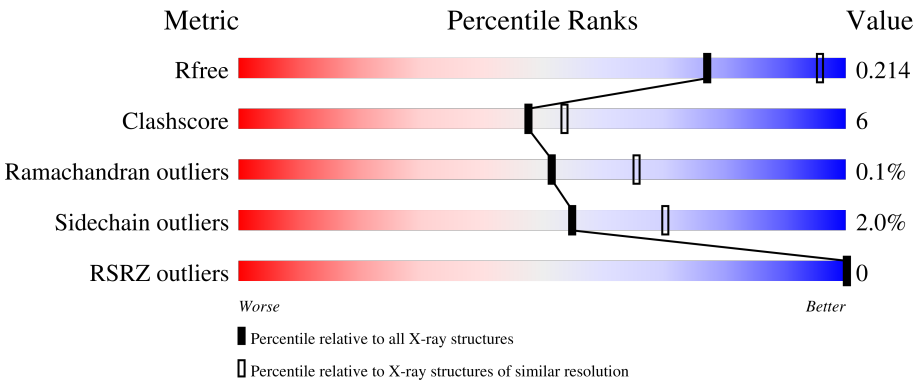
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	495	82% 13% • •
1	B	495	85% 11% • •
1	C	495	85% 10% • •
1	D	495	82% 14% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15560 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 MONOAMINE OXIDASE N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	478	3713	2346	653	693	21	0	0	0
1	B	477	3707	2342	654	690	21	0	0	0
1	C	477	3687	2336	645	685	21	0	0	0
1	D	476	3686	2332	646	687	21	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

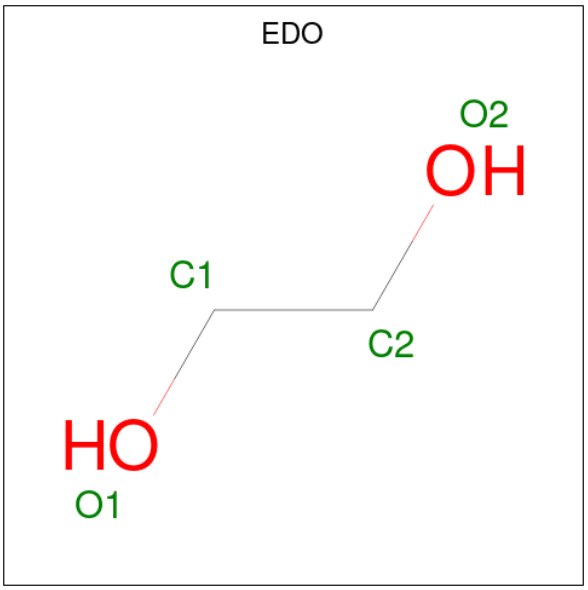
Chain	Residue	Modelled	Actual	Comment	Reference
A	210	LEU	PHE	engineered mutation	UNP P46882
A	213	THR	LEU	engineered mutation	UNP P46882
A	242	GLN	MET	engineered mutation	UNP P46882
A	246	THR	ILE	engineered mutation	UNP P46882
A	300	VAL	ALA	engineered mutation	UNP P46882
A	304	VAL	LEU	engineered mutation	UNP P46882
A	336	SER	ASN	engineered mutation	UNP P46882
A	384	ASN	THR	engineered mutation	UNP P46882
A	385	SER	ASP	engineered mutation	UNP P46882
A	430	GLY	TRP	engineered mutation	UNP P46882
A	450	GLY	ARG	engineered mutation	UNP P46882
B	210	LEU	PHE	engineered mutation	UNP P46882
B	213	THR	LEU	engineered mutation	UNP P46882
B	242	GLN	MET	engineered mutation	UNP P46882
B	246	THR	ILE	engineered mutation	UNP P46882
B	300	VAL	ALA	engineered mutation	UNP P46882
B	304	VAL	LEU	engineered mutation	UNP P46882
B	336	SER	ASN	engineered mutation	UNP P46882
B	384	ASN	THR	engineered mutation	UNP P46882
B	385	SER	ASP	engineered mutation	UNP P46882
B	430	GLY	TRP	engineered mutation	UNP P46882

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	450	GLY	ARG	engineered mutation	UNP P46882
C	210	LEU	PHE	engineered mutation	UNP P46882
C	213	THR	LEU	engineered mutation	UNP P46882
C	242	GLN	MET	engineered mutation	UNP P46882
C	246	THR	ILE	engineered mutation	UNP P46882
C	300	VAL	ALA	engineered mutation	UNP P46882
C	304	VAL	LEU	engineered mutation	UNP P46882
C	336	SER	ASN	engineered mutation	UNP P46882
C	384	ASN	THR	engineered mutation	UNP P46882
C	385	SER	ASP	engineered mutation	UNP P46882
C	430	GLY	TRP	engineered mutation	UNP P46882
C	450	GLY	ARG	engineered mutation	UNP P46882
D	210	LEU	PHE	engineered mutation	UNP P46882
D	213	THR	LEU	engineered mutation	UNP P46882
D	242	GLN	MET	engineered mutation	UNP P46882
D	246	THR	ILE	engineered mutation	UNP P46882
D	300	VAL	ALA	engineered mutation	UNP P46882
D	304	VAL	LEU	engineered mutation	UNP P46882
D	336	SER	ASN	engineered mutation	UNP P46882
D	384	ASN	THR	engineered mutation	UNP P46882
D	385	SER	ASP	engineered mutation	UNP P46882
D	430	GLY	TRP	engineered mutation	UNP P46882
D	450	GLY	ARG	engineered mutation	UNP P46882

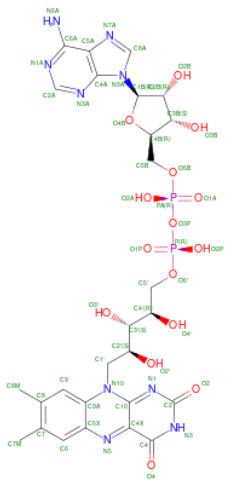
- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	180	180	180	0	0

Continued on next page...

Continued from previous page...

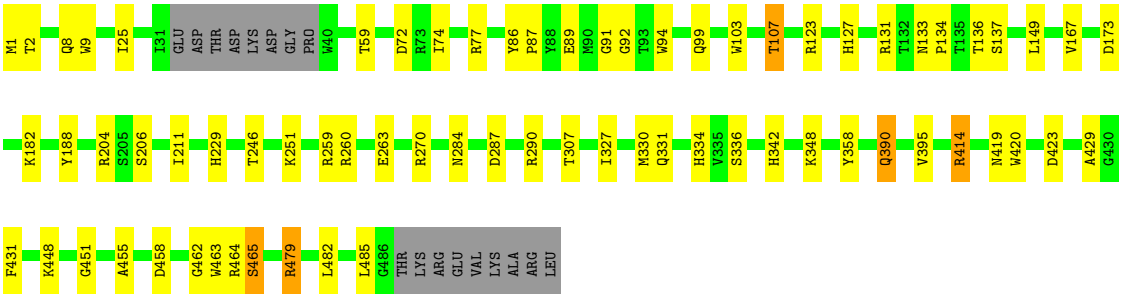
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	150	150	150	0	0
			Total	O		
4	C	126	126	126	0	0
			Total	O		
4	D	83	83	83	0	0

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: MONOAMINE OXIDASE N

Chain A: 82% 13%

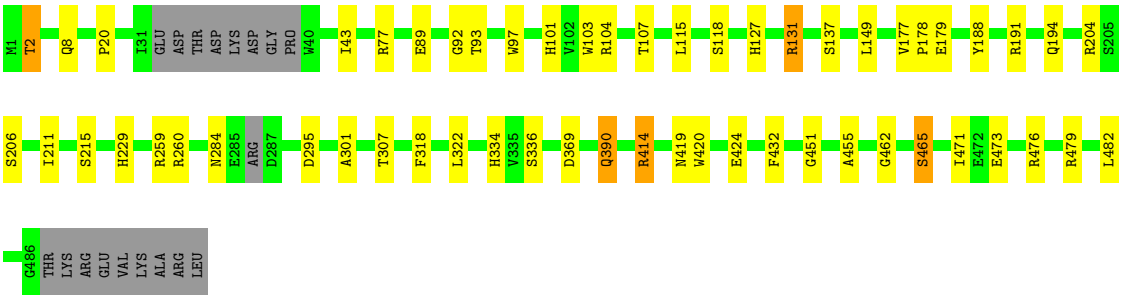


• Molecule 1: MONOAMINE OXIDASE N

Chain B: 85% 11%

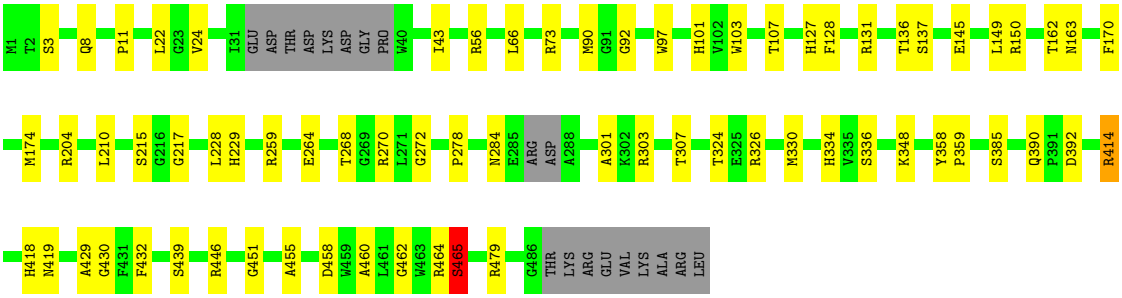
• Molecule 1: MONOAMINE OXIDASE N

Chain C: 85% 10%



• Molecule 1: MONOAMINE OXIDASE N

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.60Å 119.34Å 178.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.26 – 2.55 99.26 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.26-2.55) 100.0 (99.26-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.153 , 0.214 0.152 , 0.214	Depositor DCC
R_{free} test set	4844 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15560	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: EDO, 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	0.85	0/3810	0.95	10/5173 (0.2%)
1	B	0.83	0/3801	0.90	5/5158 (0.1%)
1	C	0.78	0/3782	0.88	7/5135 (0.1%)
1	D	0.74	0/3782	0.86	10/5136 (0.2%)
All	All	0.80	0/15175	0.90	32/20602 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	B	260	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	C	414	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	414	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	D	414	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	C	131	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	C	260	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	423	ASP	CB-CG-OD1	6.37	124.03	118.30
1	D	73	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	150	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	204	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	72	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	290	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	290	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	72	ASP	CB-CG-OD1	5.94	123.64	118.30
1	C	131	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	414	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	173	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	414	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	458	ASP	CB-CG-OD1	5.74	123.46	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	104	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	73	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	204	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	D	446	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	182	LYS	CA-CB-CG	5.40	125.28	113.40
1	D	446	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	140	MET	CB-CA-C	-5.30	99.80	110.40
1	D	204	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	228	LEU	CA-CB-CG	5.23	127.32	115.30
1	C	295	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	414	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	123	ARG	NE-CZ-NH1	5.01	122.80	120.30

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	3713	0	3522	50	0
1	B	3707	0	3509	43	0
1	C	3687	0	3484	38	0
1	D	3686	0	3486	47	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	2	0
2	D	4	0	6	0	0
3	A	53	0	31	4	0
3	B	53	0	31	4	0
3	C	53	0	31	2	0
3	D	53	0	31	4	0
4	A	180	0	0	6	0
4	B	150	0	0	4	0
4	C	126	0	0	4	0
4	D	83	0	0	1	0
All	All	15560	0	14149	177	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 6.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:CB	1:B:181:ARG:N	2.03	1.22
1:B:181:ARG:CB	1:B:181:ARG:C	2.20	1.09
1:A:8:GLN:HE21	1:A:414:ARG:HE	1.14	0.93
1:B:181:ARG:N	1:B:181:ARG:C	2.29	0.86
1:A:8:GLN:NE2	1:A:414:ARG:HE	1.74	0.85
1:B:8:GLN:HE21	1:B:414:ARG:HE	1.25	0.84
1:B:334:HIS:HD2	1:B:336:SER:H	1.25	0.82
1:D:334:HIS:HD2	1:D:336:SER:H	1.27	0.82
1:B:390:GLN:HE21	1:B:419:ASN:HD21	1.28	0.81
1:C:179:GLU:HB2	4:C:2071:HOH:O	1.82	0.79
1:A:25:ILE:CD1	1:A:74:ILE:HG23	2.12	0.79
1:C:390:GLN:NE2	1:C:419:ASN:HD21	1.81	0.79
1:D:464:ARG:O	1:D:465:SER:HB3	1.84	0.78
1:D:390:GLN:NE2	1:D:419:ASN:HD21	1.82	0.76
1:B:390:GLN:NE2	1:B:419:ASN:HD21	1.86	0.74
1:C:334:HIS:HD2	1:C:336:SER:H	1.35	0.73
1:D:22:LEU:O	1:D:259:ARG:HD3	1.90	0.71
1:C:390:GLN:HE21	1:C:419:ASN:HD21	1.38	0.70
1:A:390:GLN:HE21	1:A:390:GLN:HA	1.57	0.69
1:D:390:GLN:HE21	1:D:390:GLN:HA	1.57	0.69
1:C:118:SER:HB3	1:C:369:ASP:OD1	1.92	0.69
1:C:191:ARG:HH11	1:C:194:GLN:HE21	1.41	0.69
1:D:429:ALA:HB1	3:D:1487:FAD:HM83	1.75	0.69
1:A:334:HIS:HD2	1:A:336:SER:H	1.39	0.68
1:A:25:ILE:HD11	1:A:74:ILE:HG23	1.76	0.68
1:D:149:LEU:HD22	1:D:210:LEU:HD13	1.74	0.68
1:C:284:ASN:ND2	1:C:451:GLY:H	1.92	0.68
1:D:465:SER:O	3:D:1487:FAD:H1'2	1.94	0.67
1:A:229:HIS:HE1	1:A:462:GLY:O	1.77	0.66
1:D:229:HIS:HE1	1:D:462:GLY:O	1.79	0.66
1:A:284:ASN:HD21	1:A:451:GLY:H	1.42	0.65
1:A:149:LEU:HD21	1:A:206:SER:HB3	1.78	0.65
1:A:259:ARG:O	1:A:263:GLU:HG2	1.99	0.63
1:B:8:GLN:NE2	1:B:414:ARG:HE	1.95	0.63
1:C:284:ASN:HD21	1:C:451:GLY:H	1.44	0.63
1:C:188:TYR:CD2	1:C:211:ILE:HD12	2.33	0.63
1:C:473:GLU:OE1	1:C:476:ARG:NH2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:THR:O	1:A:270:ARG:NH1	2.33	0.61
1:C:334:HIS:CD2	1:C:336:SER:H	2.18	0.60
1:B:131:ARG:NH1	1:B:136:THR:O	2.34	0.60
1:D:8:GLN:NE2	1:D:414:ARG:HE	1.99	0.60
1:A:479:ARG:HG2	4:B:2014:HOH:O	2.02	0.59
1:A:429:ALA:HB1	3:A:1487:FAD:HM83	1.84	0.59
1:D:131:ARG:NH1	1:D:136:THR:O	2.36	0.59
1:B:429:ALA:HB1	3:B:1486:FAD:HM83	1.85	0.58
1:C:8:GLN:NE2	1:C:414:ARG:HE	2.01	0.58
1:B:334:HIS:CD2	1:B:336:SER:H	2.13	0.58
1:A:103:TRP:O	1:A:107:THR:HG23	2.03	0.58
1:B:229:HIS:HE1	1:B:462:GLY:O	1.87	0.57
1:D:390:GLN:HE21	1:D:419:ASN:HD21	1.53	0.57
1:A:92:GLY:HA2	3:A:1487:FAD:C4X	2.35	0.57
1:D:326:ARG:HG2	1:D:330:MET:HE3	1.86	0.57
1:D:307:THR:HA	1:D:455:ALA:O	2.05	0.57
1:C:307:THR:HA	1:C:455:ALA:O	2.06	0.56
1:D:390:GLN:NE2	1:D:390:GLN:HA	2.20	0.56
1:B:8:GLN:NE2	1:B:414:ARG:HH21	2.03	0.56
1:D:3:SER:HB2	1:D:24:VAL:CG2	2.35	0.55
1:D:92:GLY:HA2	3:D:1487:FAD:C4X	2.37	0.55
1:D:131:ARG:HD2	1:D:137:SER:OG	2.05	0.55
1:D:43:ILE:HG13	1:D:301:ALA:HB2	1.89	0.55
1:C:229:HIS:HE1	1:C:462:GLY:O	1.90	0.55
1:C:465:SER:O	3:C:1487:FAD:H1'2	2.06	0.54
1:D:326:ARG:HG2	1:D:330:MET:CE	2.38	0.53
1:A:25:ILE:HD11	1:A:74:ILE:CG2	2.38	0.53
1:D:429:ALA:CB	3:D:1487:FAD:HM83	2.37	0.53
1:B:92:GLY:HA2	3:B:1486:FAD:C4X	2.38	0.53
1:A:25:ILE:HD12	1:A:74:ILE:HG23	1.89	0.53
1:D:174:MET:HE1	1:D:439:SER:HB3	1.91	0.53
1:D:334:HIS:CD2	1:D:336:SER:H	2.18	0.53
1:D:464:ARG:O	1:D:465:SER:CB	2.57	0.53
1:B:149:LEU:HD21	1:B:206:SER:HB3	1.90	0.52
1:A:327:ILE:O	1:A:331:GLN:HG3	2.09	0.52
1:B:336:SER:HB3	1:B:430:GLY:O	2.10	0.52
1:A:229:HIS:HD2	4:A:2086:HOH:O	1.92	0.52
1:B:181:ARG:C	1:B:181:ARG:CG	2.78	0.52
1:B:259:ARG:O	1:B:263:GLU:HG2	2.11	0.51
1:D:56:ARG:HD3	1:D:264:GLU:OE1	2.09	0.51
1:D:460:ALA:HB3	1:D:464:ARG:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:HA	1:C:420:TRP:CH2	2.46	0.51
1:D:268:THR:HB	1:D:270:ARG:NH1	2.26	0.51
1:A:77:ARG:HA	1:A:420:TRP:CH2	2.45	0.50
1:B:307:THR:HA	1:B:455:ALA:O	2.11	0.50
1:A:9:TRP:CD1	1:A:395:VAL:HG11	2.47	0.50
1:B:10:THR:HG1	1:B:13:THR:HG1	1.59	0.50
1:C:92:GLY:HA2	3:C:1487:FAD:C4X	2.42	0.50
1:A:465:SER:O	3:A:1487:FAD:H1'2	2.12	0.49
1:D:174:MET:CE	1:D:439:SER:HB3	2.42	0.49
1:D:336:SER:HB3	1:D:430:GLY:O	2.12	0.49
1:B:334:HIS:HB2	1:B:432:PHE:O	2.12	0.49
1:B:465:SER:HA	4:B:2018:HOH:O	2.11	0.49
1:D:284:ASN:HD21	1:D:451:GLY:H	1.61	0.49
1:A:448:LYS:CB	4:A:2175:HOH:O	2.60	0.49
1:D:11:PRO:HD2	4:D:2002:HOH:O	2.12	0.49
1:B:149:LEU:CD2	1:B:206:SER:HB3	2.43	0.48
1:D:90:MET:CE	1:D:418:HIS:HB2	2.42	0.48
1:A:287:ASP:CB	4:A:2129:HOH:O	2.60	0.48
1:A:390:GLN:NE2	1:A:419:ASN:HD21	2.11	0.48
1:D:128:PHE:CD2	1:D:145:GLU:HG3	2.48	0.48
1:B:8:GLN:HE22	1:B:414:ARG:HH21	1.60	0.48
1:B:388:HIS:HD2	4:B:2131:HOH:O	1.94	0.48
1:D:103:TRP:O	1:D:107:THR:HG23	2.13	0.48
1:A:133:ASN:HB2	1:A:134:PRO:CD	2.44	0.48
1:A:94:TRP:CG	1:A:246:THR:HA	2.49	0.47
1:B:42:VAL:HG11	1:B:58:LEU:HD13	1.96	0.47
1:A:131:ARG:HD3	1:A:137:SER:OG	2.14	0.47
1:C:191:ARG:HH11	1:C:194:GLN:NE2	2.08	0.47
1:A:429:ALA:CB	3:A:1487:FAD:HM83	2.45	0.47
1:B:284:ASN:HD21	1:B:451:GLY:H	1.63	0.47
1:C:424:GLU:HG2	4:C:2121:HOH:O	2.15	0.47
1:A:94:TRP:CD2	1:A:246:THR:HA	2.49	0.47
1:D:8:GLN:HE21	1:D:414:ARG:HE	1.62	0.46
1:D:66:LEU:HA	1:D:272:GLY:O	2.15	0.46
1:A:358:TYR:HA	4:A:2153:HOH:O	2.15	0.46
1:C:2:THR:HA	1:C:20:PRO:HA	1.97	0.46
1:B:303:ARG:HH11	1:B:303:ARG:HG2	1.80	0.46
1:A:464:ARG:O	1:A:465:SER:CB	2.63	0.46
1:B:390:GLN:HE21	1:B:419:ASN:ND2	2.04	0.46
1:B:429:ALA:CB	3:B:1486:FAD:HM83	2.45	0.46
1:C:107:THR:OG1	1:D:101:HIS:HE1	1.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASN:OD1	1:A:136:THR:HG22	2.16	0.45
1:D:303:ARG:HG2	1:D:303:ARG:HH11	1.81	0.45
1:B:97:TRP:HB3	1:B:103:TRP:CE2	2.51	0.45
1:A:99:GLN:HG2	1:A:463:TRP:CE2	2.52	0.45
1:C:334:HIS:HE1	4:C:2017:HOH:O	1.98	0.44
2:C:601:EDO:H12	1:D:170:PHE:CG	2.52	0.44
1:D:97:TRP:HB3	1:D:103:TRP:CE2	2.52	0.44
1:B:215:SER:HB2	1:B:432:PHE:CD1	2.53	0.44
1:C:318:PHE:CD2	1:C:322:LEU:HD11	2.53	0.44
1:A:131:ARG:CD	1:A:137:SER:OG	2.66	0.44
1:C:43:ILE:HD12	1:C:301:ALA:CB	2.48	0.44
1:C:149:LEU:CD2	1:C:206:SER:HB3	2.48	0.44
1:B:465:SER:O	3:B:1486:FAD:H1'2	2.18	0.43
1:C:177:VAL:HA	1:C:178:PRO:HD2	1.91	0.43
1:C:97:TRP:HB3	1:C:103:TRP:CE2	2.54	0.43
1:C:131:ARG:HD3	1:C:137:SER:OG	2.18	0.43
1:C:149:LEU:HD21	1:C:206:SER:HB3	2.01	0.43
1:D:217:GLY:C	1:D:385:SER:HB2	2.38	0.43
1:A:431:PHE:HB2	1:A:458:ASP:OD1	2.19	0.43
1:B:154:HIS:O	1:B:158:ASN:HB2	2.19	0.43
1:C:131:ARG:CD	1:C:137:SER:OG	2.67	0.43
1:C:465:SER:HA	4:C:2016:HOH:O	2.18	0.43
1:B:196:ARG:HG2	4:B:2080:HOH:O	2.19	0.43
1:D:136:THR:CG2	1:D:137:SER:N	2.82	0.43
1:A:465:SER:HA	4:A:2020:HOH:O	2.19	0.42
1:B:103:TRP:O	1:B:107:THR:HG23	2.19	0.42
1:A:149:LEU:CD2	1:A:206:SER:HB3	2.48	0.42
1:B:327:ILE:H	1:B:327:ILE:HG12	1.68	0.42
1:A:8:GLN:HE21	1:A:414:ARG:NE	1.98	0.42
1:A:348:LYS:HZ2	1:A:348:LYS:HG2	1.69	0.42
1:C:115:LEU:O	2:C:601:EDO:H22	2.20	0.42
1:D:90:MET:HE2	1:D:418:HIS:HB2	2.01	0.42
1:A:77:ARG:O	1:A:91:GLY:HA3	2.20	0.42
1:A:229:HIS:CD2	4:A:2086:HOH:O	2.70	0.42
1:B:92:GLY:O	1:B:254:GLN:HG3	2.19	0.42
1:C:43:ILE:HD12	1:C:301:ALA:HB3	2.01	0.42
1:B:9:TRP:CD1	1:B:395:VAL:HG11	2.54	0.42
1:C:89:GLU:HG3	1:C:93:THR:HG23	2.02	0.42
1:B:284:ASN:ND2	1:B:451:GLY:H	2.18	0.42
1:C:259:ARG:HA	1:C:259:ARG:HD2	1.83	0.42
1:D:162:THR:O	1:D:163:ASN:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:SER:HB2	1:D:432:PHE:CD1	2.55	0.42
1:A:89:GLU:O	1:A:342:HIS:NE2	2.43	0.41
1:A:307:THR:HA	1:A:455:ALA:O	2.20	0.41
1:A:259:ARG:HD2	1:A:259:ARG:HA	1.82	0.41
1:B:63:PHE:CE2	1:B:482:LEU:HD23	2.56	0.41
1:B:131:ARG:HH11	1:B:131:ARG:HG2	1.85	0.41
1:B:152:ALA:HB1	1:B:207:LEU:HB2	2.01	0.41
1:A:188:TYR:CD2	1:A:211:ILE:HD12	2.55	0.41
1:C:188:TYR:CG	1:C:211:ILE:HD12	2.55	0.41
1:C:101:HIS:HB3	1:C:471:ILE:HG22	2.01	0.41
1:D:392:ASP:OD1	1:D:392:ASP:N	2.53	0.41
1:A:251:LYS:HB2	1:A:251:LYS:HE3	1.52	0.41
1:A:464:ARG:O	1:A:465:SER:HB3	2.21	0.41
1:A:86:TYR:HA	1:A:87:PRO:HD3	1.88	0.40
1:A:330:MET:HB3	1:A:330:MET:HE2	1.65	0.40
1:C:215:SER:HA	1:C:432:PHE:CD2	2.55	0.40
1:D:358:TYR:HA	1:D:359:PRO:HA	1.83	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	474/495 (96%)	460 (97%)	14 (3%)	0	100	100
1	B	472/495 (95%)	458 (97%)	14 (3%)	0	100	100
1	C	471/495 (95%)	449 (95%)	22 (5%)	0	100	100
1	D	470/495 (95%)	454 (97%)	15 (3%)	1 (0%)	47	60
All	All	1887/1980 (95%)	1821 (96%)	65 (3%)	1 (0%)	51	65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	465	SER

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	385/413 (93%)	375 (97%)	10 (3%)	46	61
1	B	383/413 (93%)	375 (98%)	8 (2%)	53	68
1	C	377/413 (91%)	370 (98%)	7 (2%)	57	72
1	D	380/413 (92%)	374 (98%)	6 (2%)	62	77
All	All	1525/1652 (92%)	1494 (98%)	31 (2%)	55	70

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	107	THR
1	A	127	HIS
1	A	167	VAL
1	A	390	GLN
1	A	465	SER
1	A	479	ARG
1	A	482	LEU
1	A	485	LEU
1	B	2	THR
1	B	67	LEU
1	B	193	ASP
1	B	280	ARG
1	B	327	ILE
1	B	447	GLU
1	B	479	ARG
1	B	482	LEU
1	C	2	THR
1	C	127	HIS
1	C	204	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	390	GLN
1	C	465	SER
1	C	479	ARG
1	C	482	LEU
1	D	127	HIS
1	D	278	PRO
1	D	324	THR
1	D	348	LYS
1	D	465	SER
1	D	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	101	HIS
1	A	229	HIS
1	A	284	ASN
1	A	334	HIS
1	A	390	GLN
1	B	8	GLN
1	B	101	HIS
1	B	154	HIS
1	B	163	ASN
1	B	229	HIS
1	B	284	ASN
1	B	331	GLN
1	B	334	HIS
1	B	388	HIS
1	B	390	GLN
1	B	404	GLN
1	C	8	GLN
1	C	101	HIS
1	C	154	HIS
1	C	163	ASN
1	C	194	GLN
1	C	229	HIS
1	C	242	GLN
1	C	284	ASN
1	C	334	HIS
1	C	388	HIS
1	C	390	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	8	GLN
1	D	101	HIS
1	D	154	HIS
1	D	163	ASN
1	D	229	HIS
1	D	284	ASN
1	D	334	HIS
1	D	390	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	FAD	A	1487	-	53,58,58	1.77	8 (15%)	68,89,89	1.65	17 (25%)
2	EDO	B	601	-	3,3,3	0.49	0	2,2,2	0.64	0
2	EDO	C	601	-	3,3,3	0.42	0	2,2,2	0.43	0
3	FAD	B	1486	-	53,58,58	2.08	12 (22%)	68,89,89	1.82	16 (23%)
2	EDO	D	601	-	3,3,3	0.44	0	2,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	A	601	-	3,3,3	0.25	0	2,2,2	0.51	0
3	FAD	C	1487	-	53,58,58	1.96	9 (16%)	68,89,89	1.64	14 (20%)
3	FAD	D	1487	-	53,58,58	2.16	12 (22%)	68,89,89	1.63	14 (20%)

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	FAD	A	1487	-	-	2/30/50/50	0/6/6/6
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
3	FAD	B	1486	-	-	3/30/50/50	0/6/6/6
2	EDO	D	601	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
3	FAD	C	1487	-	-	2/30/50/50	0/6/6/6
3	FAD	D	1487	-	-	2/30/50/50	0/6/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1486	FAD	C4X-N5	6.38	1.43	1.30
3	C	1487	FAD	C4X-N5	6.08	1.42	1.30
3	B	1486	FAD	C2A-N3A	6.06	1.41	1.32
3	D	1487	FAD	C2A-N3A	6.01	1.41	1.32
3	A	1487	FAD	C4X-N5	5.92	1.42	1.30
3	C	1487	FAD	C8M-C8	-5.87	1.39	1.51
3	D	1487	FAD	C8M-C8	-5.78	1.39	1.51
3	D	1487	FAD	C4X-N5	5.58	1.41	1.30
3	B	1486	FAD	C8M-C8	-5.52	1.40	1.51
3	D	1487	FAD	C10-N1	5.36	1.44	1.33
3	A	1487	FAD	C2A-N3A	5.14	1.40	1.32
3	B	1486	FAD	C7M-C7	-5.08	1.40	1.51
3	C	1487	FAD	C2A-N3A	4.59	1.39	1.32
3	D	1487	FAD	C7M-C7	-4.30	1.42	1.51
3	C	1487	FAD	C10-N1	4.26	1.41	1.33
3	A	1487	FAD	C7M-C7	-4.18	1.42	1.51
3	C	1487	FAD	C7M-C7	-4.08	1.42	1.51
3	C	1487	FAD	C2A-N1A	3.90	1.41	1.33
3	A	1487	FAD	C8M-C8	-3.85	1.43	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1487	FAD	C2A-N1A	3.66	1.40	1.33
3	C	1487	FAD	P-O1P	3.41	1.63	1.50
3	D	1487	FAD	P-O1P	3.12	1.62	1.50
3	A	1487	FAD	C2A-N1A	3.08	1.39	1.33
3	D	1487	FAD	C2-N1	2.94	1.43	1.36
3	B	1486	FAD	O3B-C3B	2.72	1.49	1.43
3	B	1486	FAD	C5A-C4A	-2.71	1.33	1.40
3	A	1487	FAD	P-O1P	2.70	1.60	1.50
3	B	1486	FAD	P-O1P	2.68	1.60	1.50
3	B	1486	FAD	C10-N1	2.57	1.38	1.33
3	B	1486	FAD	C2'-C3'	2.50	1.58	1.53
3	C	1487	FAD	C4'-C3'	-2.49	1.48	1.53
3	D	1487	FAD	C2B-C1B	-2.46	1.50	1.53
3	D	1487	FAD	O4B-C1B	2.43	1.44	1.41
3	D	1487	FAD	PA-O1A	2.42	1.59	1.50
3	B	1486	FAD	C4-N3	2.40	1.43	1.38
3	B	1486	FAD	C2A-N1A	2.35	1.38	1.33
3	D	1487	FAD	C5A-C4A	-2.24	1.35	1.40
3	A	1487	FAD	O4B-C1B	2.15	1.44	1.41
3	B	1486	FAD	O4B-C4B	-2.14	1.40	1.45
3	C	1487	FAD	C5A-C4A	-2.08	1.35	1.40
3	A	1487	FAD	C5A-C4A	-2.00	1.35	1.40

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1487	FAD	N3A-C2A-N1A	-6.66	118.27	128.68
3	B	1486	FAD	N3A-C2A-N1A	-6.63	118.32	128.68
3	C	1487	FAD	N3A-C2A-N1A	-6.38	118.70	128.68
3	A	1487	FAD	N3A-C2A-N1A	-5.61	119.92	128.68
3	B	1486	FAD	O4B-C1B-C2B	-4.31	100.62	106.93
3	A	1487	FAD	C4X-C10-N10	3.68	121.86	116.48
3	C	1487	FAD	P-O3P-PA	-3.58	120.53	132.83
3	B	1486	FAD	C4-N3-C2	-3.51	119.16	125.64
3	B	1486	FAD	C4X-C10-N10	3.49	121.58	116.48
3	B	1486	FAD	C5'-C4'-C3'	-3.30	105.82	112.20
3	A	1487	FAD	O4B-C1B-C2B	-3.25	102.17	106.93
3	B	1486	FAD	C4X-C4-N3	3.14	121.16	113.19
3	A	1487	FAD	O2A-PA-O5B	3.14	122.31	107.75
3	A	1487	FAD	C5X-C9A-N10	3.08	121.13	117.95
3	B	1486	FAD	C10-N1-C2	3.02	122.94	116.90
3	D	1487	FAD	C10-C4X-N5	-2.96	118.58	124.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1486	FAD	C1B-N9A-C4A	-2.92	121.51	126.64
3	A	1487	FAD	C4-N3-C2	-2.91	120.26	125.64
3	C	1487	FAD	C5'-C4'-C3'	-2.85	106.70	112.20
3	C	1487	FAD	C6-C5X-C9A	2.84	122.96	118.94
3	B	1486	FAD	C6-C5X-C9A	2.84	122.95	118.94
3	D	1487	FAD	C4X-C4-N3	2.81	120.33	113.19
3	D	1487	FAD	C4-N3-C2	-2.80	120.47	125.64
3	D	1487	FAD	C9A-C5X-N5	-2.75	119.44	122.43
3	A	1487	FAD	C6-C5X-C9A	2.73	122.79	118.94
3	B	1486	FAD	C4A-C5A-N7A	-2.71	106.57	109.40
3	A	1487	FAD	C9A-C5X-N5	-2.68	119.52	122.43
3	C	1487	FAD	C9A-C5X-N5	-2.67	119.53	122.43
3	D	1487	FAD	P-O3P-PA	-2.67	123.67	132.83
3	C	1487	FAD	C10-C4X-N5	-2.65	119.23	124.86
3	D	1487	FAD	C4-C4X-C10	2.58	121.12	116.79
3	B	1486	FAD	C10-C4X-N5	-2.57	119.40	124.86
3	A	1487	FAD	C9A-N10-C10	-2.55	116.80	120.77
3	C	1487	FAD	C4X-C10-N1	-2.54	118.84	124.73
3	D	1487	FAD	O4-C4-C4X	-2.52	119.90	126.60
3	B	1486	FAD	C4-C4X-N5	2.49	121.77	118.23
3	D	1487	FAD	C5'-C4'-C3'	-2.48	107.40	112.20
3	D	1487	FAD	C4X-C10-N1	-2.48	118.98	124.73
3	C	1487	FAD	C1B-N9A-C4A	-2.43	122.37	126.64
3	C	1487	FAD	O2A-PA-O5B	2.42	118.98	107.75
3	C	1487	FAD	C4X-C4-N3	2.37	119.20	113.19
3	D	1487	FAD	C6-C5X-C9A	2.36	122.27	118.94
3	D	1487	FAD	C9-C9A-N10	2.36	125.02	121.84
3	B	1486	FAD	C4'-C3'-C2'	-2.34	108.49	113.36
3	B	1486	FAD	C4X-C10-N1	-2.28	119.45	124.73
3	B	1486	FAD	C1'-N10-C9A	2.24	124.25	120.51
3	C	1487	FAD	C4-C4X-C10	2.24	120.55	116.79
3	A	1487	FAD	C1B-N9A-C4A	-2.24	122.71	126.64
3	A	1487	FAD	C4-C4X-C10	2.22	120.53	116.79
3	A	1487	FAD	C4A-C5A-N7A	-2.22	107.09	109.40
3	A	1487	FAD	O3'-C3'-C4'	-2.19	103.51	108.81
3	C	1487	FAD	C4X-C10-N10	2.18	119.67	116.48
3	A	1487	FAD	C4X-C4-N3	2.17	118.70	113.19
3	B	1486	FAD	O4-C4-C4X	-2.14	120.92	126.60
3	A	1487	FAD	C10-C4X-N5	-2.12	120.35	124.86
3	A	1487	FAD	C4X-C10-N1	-2.11	119.84	124.73
3	A	1487	FAD	O5B-PA-O1A	-2.10	100.87	109.07
3	C	1487	FAD	C4A-C5A-N7A	-2.09	107.22	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1487	FAD	C9-C9A-C5X	-2.04	116.25	120.11
3	C	1487	FAD	C4-N3-C2	-2.04	121.88	125.64
3	D	1487	FAD	C5A-C6A-N6A	-2.03	117.26	120.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

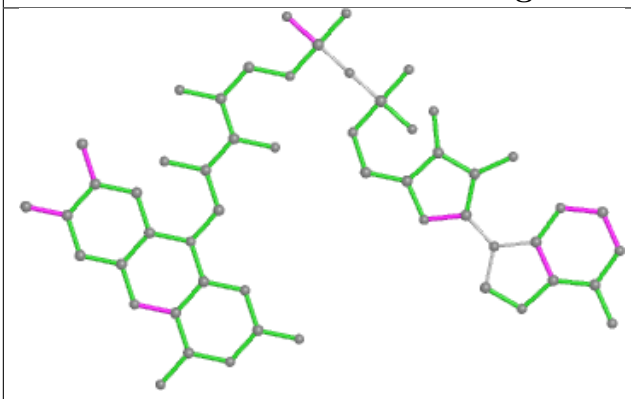
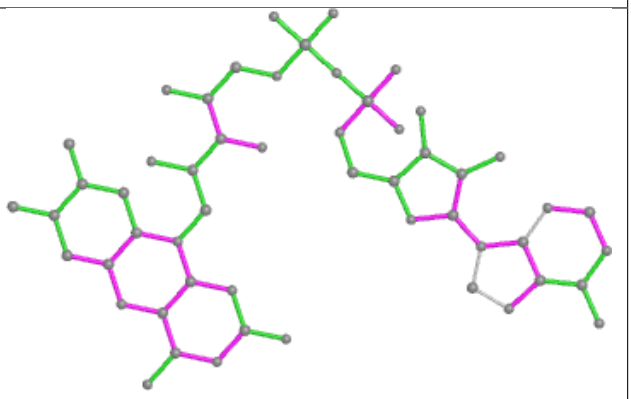
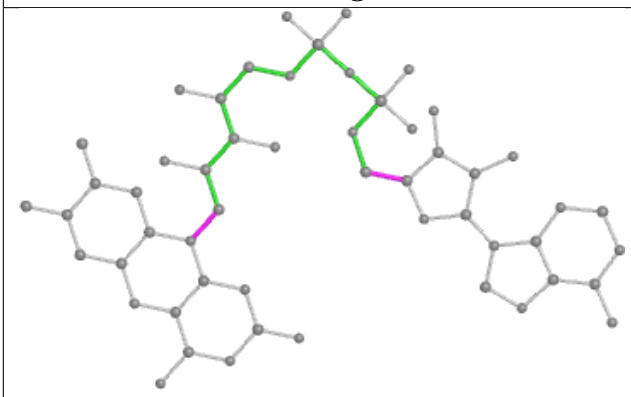
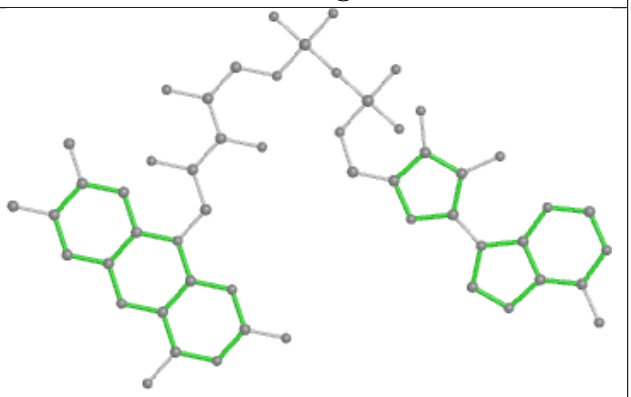
Mol	Chain	Res	Type	Atoms
3	B	1486	FAD	C5'-O5'-P-O1P
3	B	1486	FAD	C5'-O5'-P-O3P
3	A	1487	FAD	C2'-C1'-N10-C10
3	A	1487	FAD	O4B-C4B-C5B-O5B
3	B	1486	FAD	O4B-C4B-C5B-O5B
3	C	1487	FAD	O4B-C4B-C5B-O5B
3	D	1487	FAD	O4B-C4B-C5B-O5B
3	C	1487	FAD	P-O3P-PA-O2A
3	D	1487	FAD	C5'-O5'-P-O1P

There are no ring outliers.

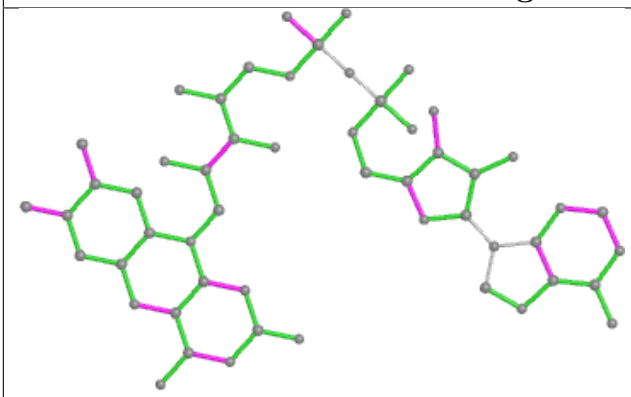
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1487	FAD	4	0
2	C	601	EDO	2	0
3	B	1486	FAD	4	0
3	C	1487	FAD	2	0
3	D	1487	FAD	4	0

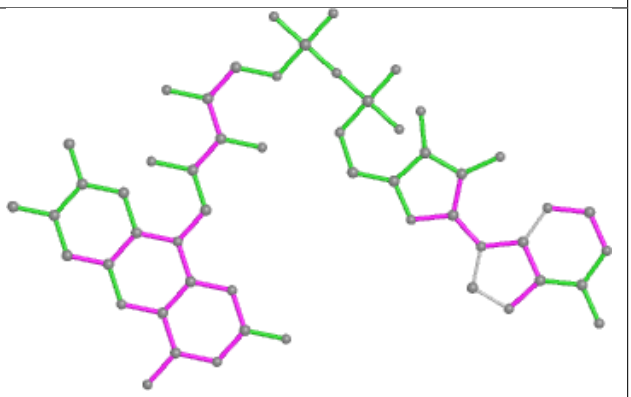
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A 1487	
 Bond lengths	 Bond angles
 Torsions	 Rings

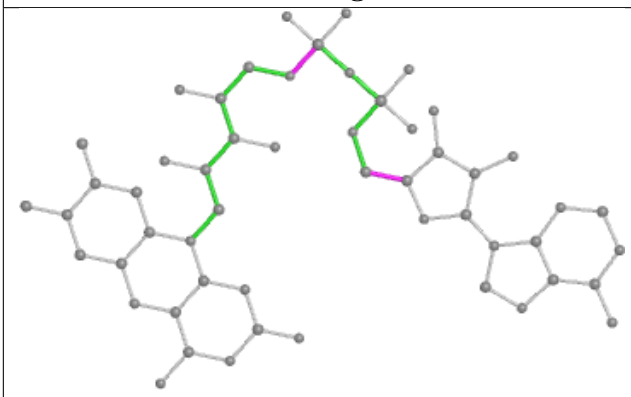
Ligand FAD B 1486



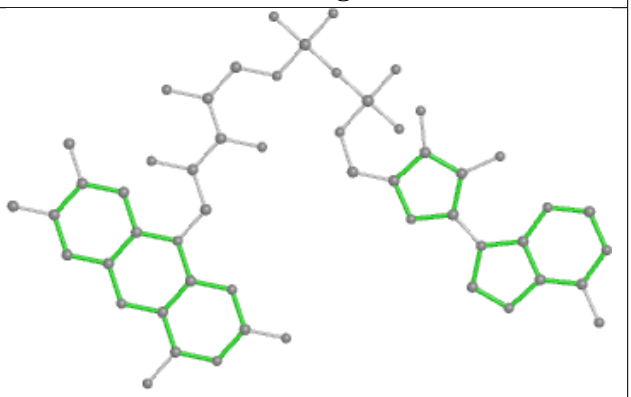
Bond lengths



Bond angles

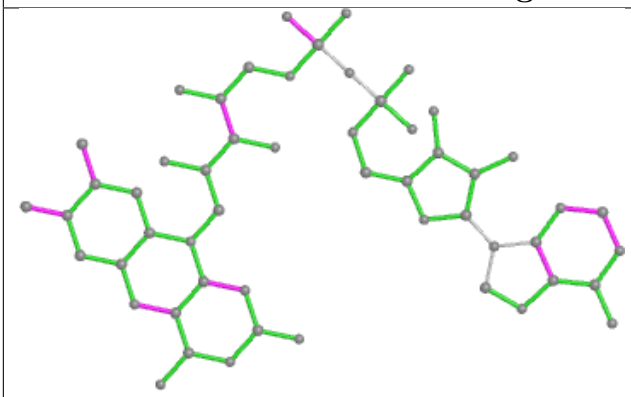


Torsions

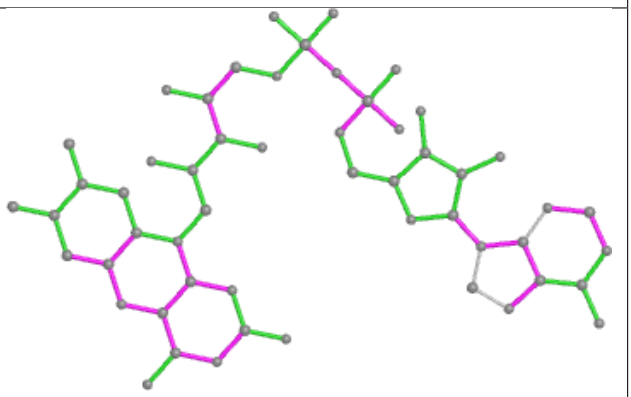


Rings

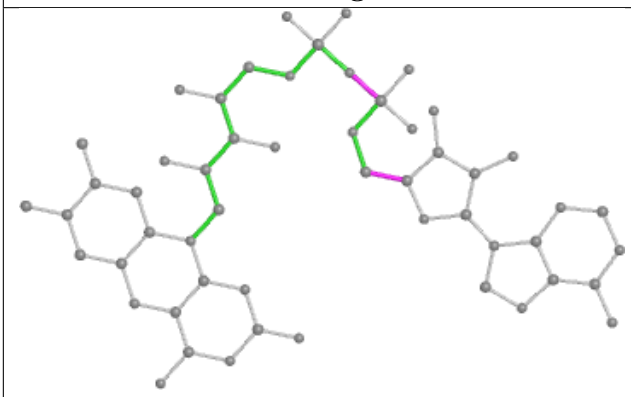
Ligand FAD C 1487



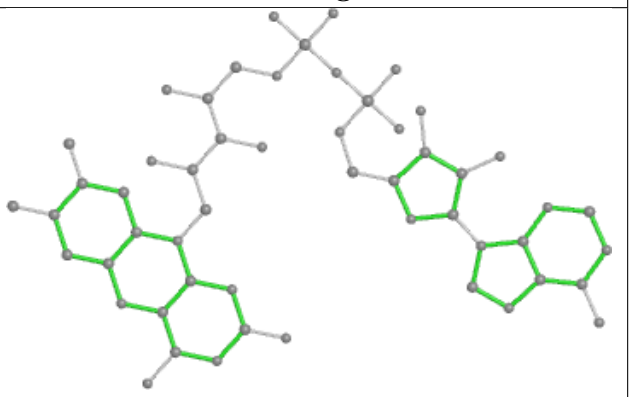
Bond lengths



Bond angles

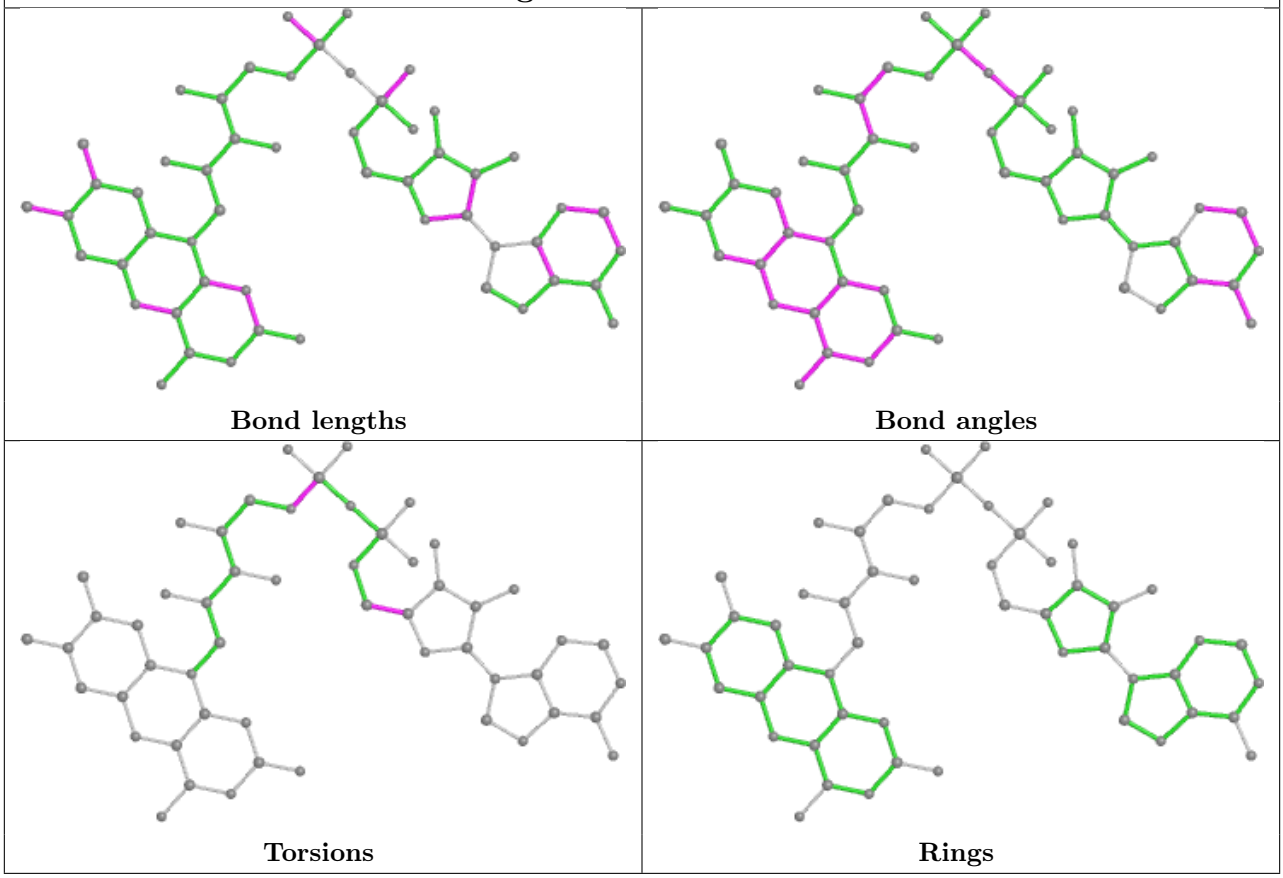


Torsions



Rings

Ligand FAD D 1487



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	478/495 (96%)	-0.65	0	100	100	13, 23, 40, 66	0
1	B	477/495 (96%)	-0.66	0	100	100	13, 25, 42, 63	0
1	C	477/495 (96%)	-0.61	0	100	100	16, 32, 51, 74	0
1	D	476/495 (96%)	-0.58	0	100	100	17, 34, 52, 74	0
All	All	1908/1980 (96%)	-0.62	0	100	100	13, 28, 48, 74	0

There are no RSRZ outliers to report.

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
2	EDO	C	601	4/4	0.97	0.15	36,36,38,39	0
3	FAD	D	1487	53/53	0.97	0.12	24,32,43,44	0
2	EDO	A	601	4/4	0.98	0.15	26,27,27,29	0
2	EDO	D	601	4/4	0.98	0.13	33,36,37,42	0

Continued on next page...

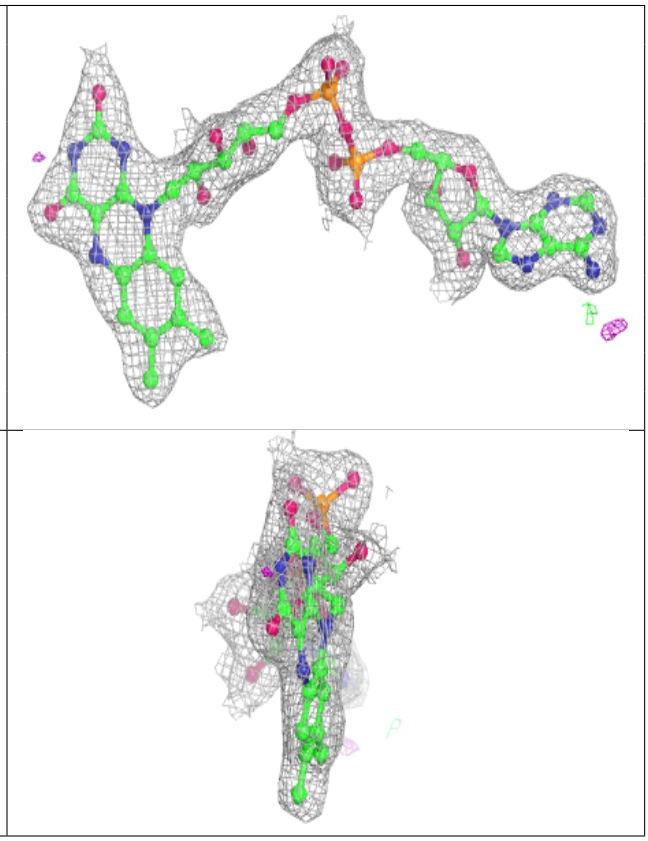
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FAD	C	1487	53/53	0.98	0.11	19,27,34,38	0
2	EDO	B	601	4/4	0.98	0.16	34,35,36,37	0
3	FAD	A	1487	53/53	0.99	0.11	16,18,20,21	0
3	FAD	B	1486	53/53	0.99	0.12	16,22,24,26	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.

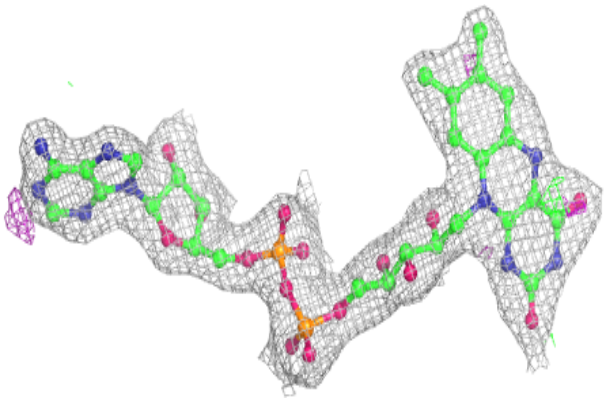
Electron density around FAD D 1487:

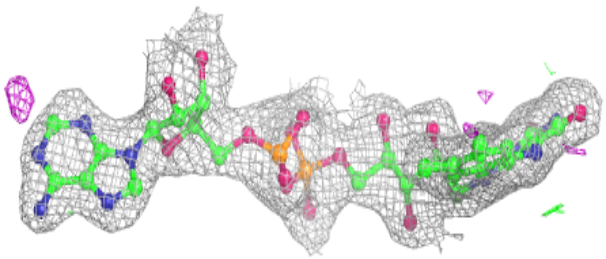
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

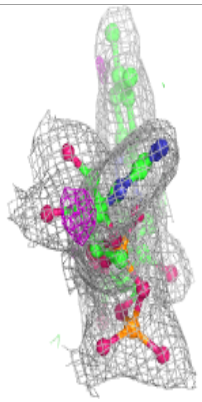


Electron density around FAD C 1487:

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

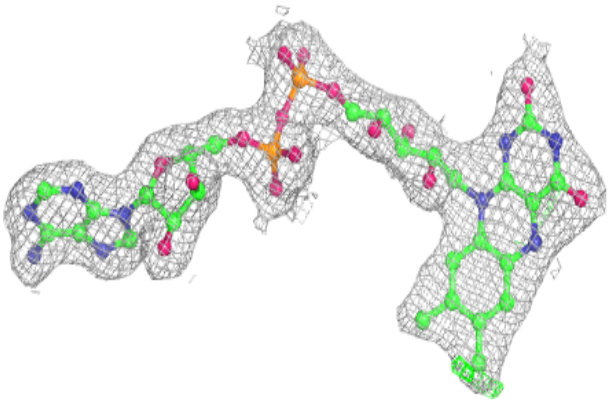


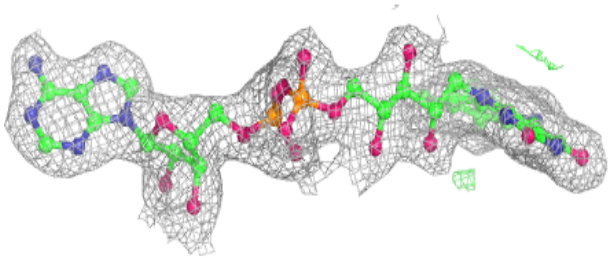


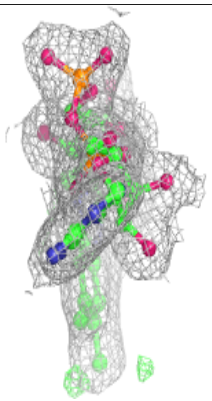


Electron density around FAD A 1487:

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

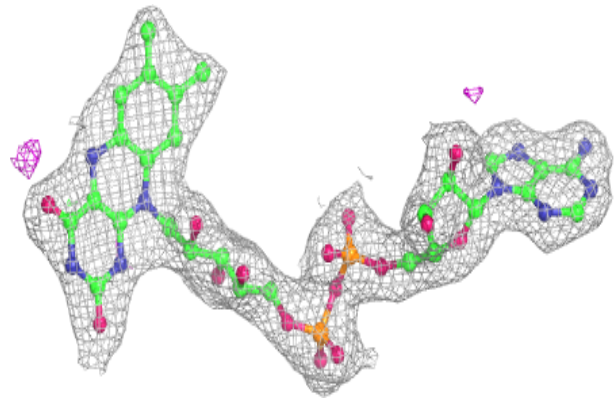


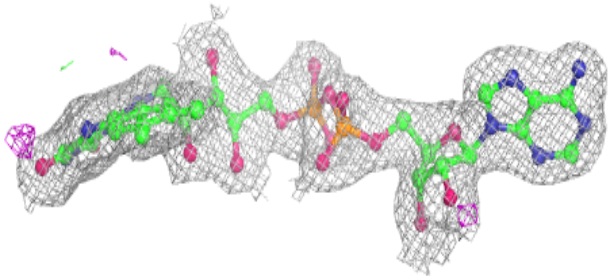


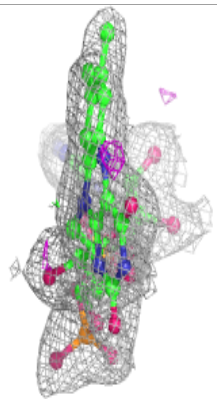


Electron density around FAD B 1486:

$2mF_o$-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.