Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 06:12 PM EDT

PDB ID	:	2TPR
Title	:	X-RAY STRUCTURE OF TRYPANOTHIONE REDUCTASE FROM CRITHIDIA FASCICULATA AT 2.4 ANGSTROMS RESOLUTION
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Deposited on	:	1991-08-22
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

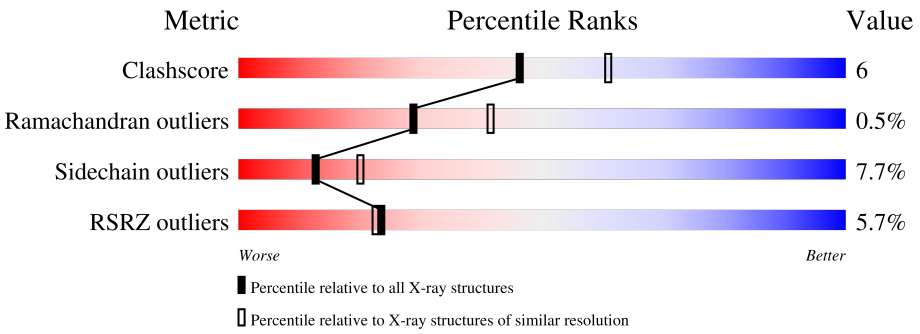
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	490	6% 76% 19% • • •
1	B	490	6% 78% 17% • • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7772 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.

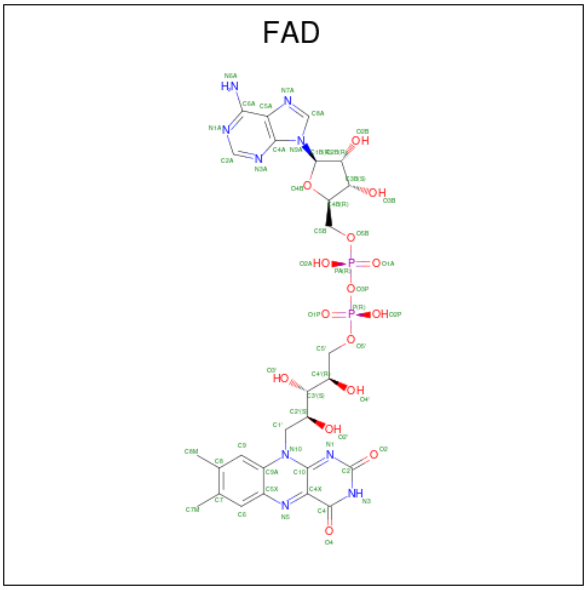
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	482	3658	2301	634	703	20	0	0	0
1	B	482	3658	2301	634	703	20	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	GLU	ASP	conflict	UNP P39040
A	453	VAL	PHE	conflict	UNP P39040
A	478	GLU	GLN	conflict	UNP P39040
B	296	GLU	ASP	conflict	UNP P39040
B	453	VAL	PHE	conflict	UNP P39040
B	478	GLU	GLN	conflict	UNP P39040

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



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

- Molecule 3 is water.

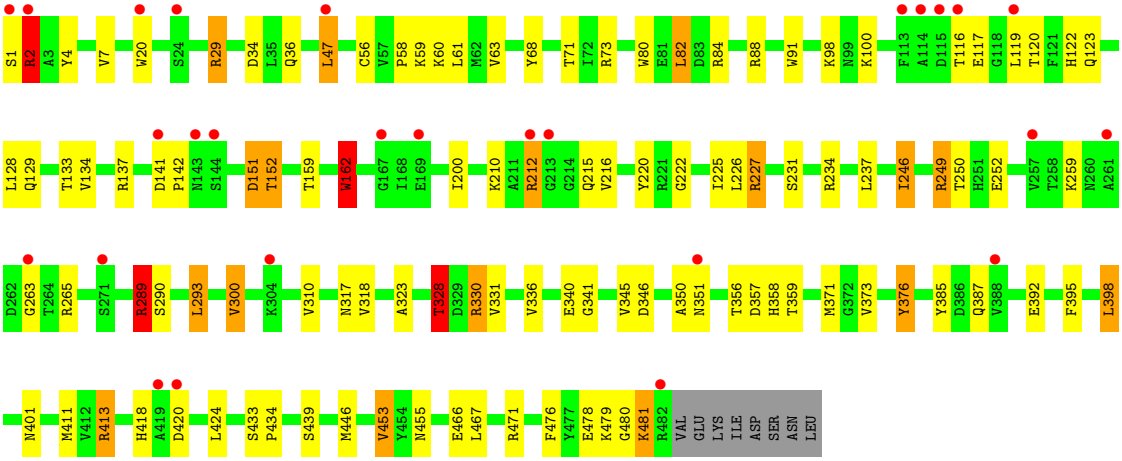
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	154	154	154	0	0
			Total	O		
3	B	196	196	196	0	0

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.

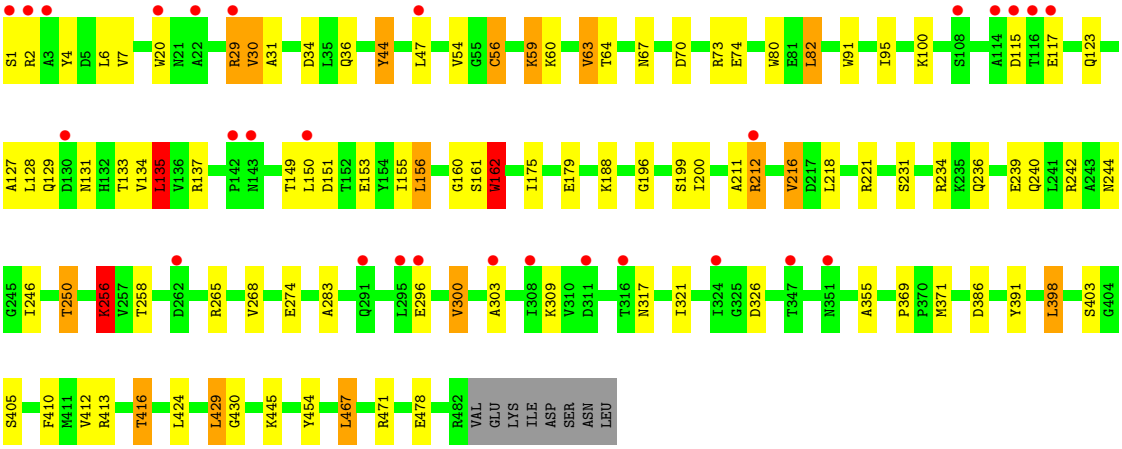
- Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A:



- Molecule 1: TRYPANOTHIONE REDUCTASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.00Å 161.80Å 61.50Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40 14.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40) 55.4 (14.91-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available) 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 109.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7772	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: 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	0.72	0/3730	1.40	39/5057 (0.8%)
1	B	0.75	1/3730 (0.0%)	1.35	30/5057 (0.6%)
All	All	0.74	1/7460 (0.0%)	1.38	69/10114 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	VAL	CA-CB	5.66	1.66	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	413	ARG	NE-CZ-NH1	12.98	126.79	120.30
1	B	413	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	A	84	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	A	289	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	84	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	A	91	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	A	413	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	B	20	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	A	20	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	80	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	B	80	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	A	162	TRP	CD1-CG-CD2	7.86	112.58	106.30
1	B	91	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	A	20	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	B	20	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	A	91	TRP	CE2-CD2-CG	-7.44	101.34	107.30
1	B	80	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	A	289	ARG	NE-CZ-NH2	-7.34	116.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	91	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	A	227	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	80	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	B	242	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	29	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	328	THR	N-CA-CB	-7.03	96.94	110.30
1	A	453	VAL	CG1-CB-CG2	-6.91	99.84	110.90
1	B	162	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	162	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	A	2	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	250	THR	N-CA-CB	-6.58	97.80	110.30
1	A	29	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	454	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	A	330	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	471	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	256	LYS	CA-CB-CG	5.91	126.39	113.40
1	B	391	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	A	88	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	162	TRP	NE1-CE2-CZ2	-5.81	124.01	130.40
1	B	471	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	29	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	371	MET	CG-SD-CE	-5.67	91.12	100.20
1	A	91	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	A	420	ASP	N-CA-CB	-5.65	100.42	110.60
1	A	330	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	249	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	478	GLU	N-CA-C	-5.53	96.07	111.00
1	B	135	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	429	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	221	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	227	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	220	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	A	385	TYR	CA-C-N	-5.44	105.22	117.20
1	A	73	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	47	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	56	CYS	CA-CB-SG	5.41	123.73	114.00
1	B	29	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	2	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	137	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	153	GLU	CA-CB-CG	5.24	124.92	113.40
1	B	20	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	A	137	ARG	NE-CZ-NH1	5.21	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	20	TRP	CG-CD1-NE1	-5.20	104.91	110.10
1	B	80	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	B	212	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	405	SER	N-CA-C	5.11	124.81	111.00
1	A	373	VAL	N-CA-CB	-5.10	100.28	111.50
1	A	411	MET	CA-CB-CG	5.07	121.92	113.30
1	B	137	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	82	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	376	TYR	CB-CG-CD2	-5.00	118.00	121.00

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	3658	0	3598	54	0
1	B	3658	0	3598	41	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	154	0	0	0	0
3	B	196	0	0	1	0
All	All	7772	0	7258	92	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 (92) 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:340:GLU:HG2	1:A:356:THR:HG21	1.57	0.86
1:B:188:LYS:HD3	1:B:211:ALA:HB3	1.64	0.79
1:B:7:VAL:HG11	1:B:134:VAL:HG11	1.65	0.77
1:B:60:LYS:O	1:B:64:THR:HG23	1.93	0.68
1:A:259:LYS:HE3	1:A:263:GLY:HA2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HD22	1:B:155:ILE:HD13	1.78	0.66
1:A:328:THR:HG23	1:A:330:ARG:HE	1.61	0.65
1:A:200:ILE:HD12	1:A:226:LEU:HD13	1.78	0.65
1:A:395:PHE:CE2	1:A:466:GLU:HG3	2.32	0.64
1:A:4:TYR:HB2	1:A:152:THR:HG23	1.80	0.64
1:B:199:SER:HB3	1:B:283:ALA:HB3	1.82	0.62
1:A:129:GLN:HB3	1:A:133:THR:HG23	1.82	0.61
1:A:300:VAL:HA	1:A:317:ASN:HD21	1.65	0.61
1:B:196:GLY:O	1:B:200:ILE:HG12	2.03	0.59
1:A:395:PHE:HE2	1:A:466:GLU:HG3	1.67	0.59
1:B:74:GLU:HG2	1:B:403:SER:HB2	1.84	0.58
1:B:160:GLY:HA2	1:B:326:ASP:HB2	1.85	0.58
1:B:129:GLN:HB3	1:B:133:THR:HG23	1.86	0.58
1:A:249:ARG:HB3	1:A:252:GLU:HG3	1.87	0.56
1:A:290:SER:HA	1:A:293:LEU:HD22	1.87	0.56
1:A:36:GLN:HA	1:A:123:GLN:OE1	2.06	0.54
1:B:240:GLN:OE1	1:B:369:PRO:HG3	2.07	0.54
1:B:268:VAL:HG22	1:B:274:GLU:HG2	1.89	0.54
1:A:357:ASP:OD1	1:A:359:THR:HB	2.07	0.53
1:A:328:THR:CG2	1:A:330:ARG:HE	2.21	0.53
1:B:416:THR:HG21	3:B:594:HOH:O	2.07	0.53
1:B:410:PHE:CD2	1:B:430:GLY:HA3	2.46	0.51
1:B:2:ARG:HB2	1:B:4:TYR:HE2	1.76	0.51
1:A:376:TYR:HD2	1:A:424:LEU:HB3	1.74	0.51
1:A:480:GLY:O	1:A:481:LYS:HB2	2.11	0.51
1:A:231:SER:HA	1:A:234:ARG:HD3	1.93	0.50
1:A:159:THR:HG21	1:A:293:LEU:HD11	1.92	0.50
1:A:356:THR:HG23	1:A:358:HIS:CE1	2.45	0.50
1:B:2:ARG:HB2	1:B:4:TYR:CE2	2.47	0.49
1:B:73:ARG:HH11	1:B:73:ARG:HG2	1.77	0.49
1:B:34:ASP:O	1:B:123:GLN:HA	2.11	0.49
1:A:2:ARG:O	1:A:151:ASP:HB3	2.12	0.49
1:B:236:GLN:HE22	1:B:240:GLN:HE21	1.61	0.49
1:B:303:ALA:HB2	1:B:309:LYS:HG3	1.94	0.49
1:A:162:TRP:HB2	1:A:289:ARG:HG3	1.95	0.48
1:A:212:ARG:HA	1:A:212:ARG:HE	1.79	0.48
1:B:231:SER:HA	1:B:234:ARG:HD3	1.94	0.48
1:A:346:ASP:HA	1:A:350:ALA:HB3	1.95	0.48
1:A:210:LYS:HZ3	1:A:212:ARG:NH2	2.12	0.47
1:A:116:THR:HG23	1:A:119:LEU:HB3	1.95	0.47
1:A:455:ASN:O	1:B:445:LYS:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:PHE:O	1:A:481:LYS:HB3	2.14	0.47
1:B:7:VAL:HG22	1:B:31:ALA:HB3	1.97	0.47
1:A:216:VAL:HG13	1:A:246:ILE:HB	1.97	0.46
1:B:412:VAL:HG21	1:B:467:LEU:HD13	1.97	0.46
1:A:222:GLY:HA3	1:A:227:ARG:HH21	1.81	0.45
1:A:227:ARG:HD3	1:A:234:ARG:NH2	2.32	0.45
1:A:331:VAL:HB	1:A:336:VAL:HG11	1.99	0.45
1:A:82:LEU:HD13	1:B:82:LEU:HD13	2.00	0.44
1:A:227:ARG:HD3	1:A:234:ARG:HH22	1.81	0.44
1:B:300:VAL:HA	1:B:317:ASN:OD1	2.18	0.44
1:A:433:SER:OG	1:A:434:PRO:HD3	2.18	0.44
1:A:200:ILE:HD11	1:A:225:ILE:HB	1.99	0.43
1:B:161:SER:O	1:B:162:TRP:HD1	2.01	0.43
1:A:398:LEU:O	1:A:401:ASN:HB2	2.18	0.43
1:B:36:GLN:HA	1:B:123:GLN:NE2	2.33	0.43
1:B:256:LYS:HE2	1:B:268:VAL:HG21	1.99	0.43
1:A:61:LEU:HD21	1:B:398:LEU:HB2	2.01	0.42
1:A:210:LYS:HZ3	1:A:212:ARG:HH21	1.66	0.42
1:A:59:LYS:O	1:A:63:VAL:HG23	2.19	0.42
1:B:59:LYS:O	1:B:63:VAL:HG13	2.18	0.42
1:B:44:TYR:HB3	1:B:54:VAL:HG11	2.01	0.42
1:B:2:ARG:HD2	1:B:150:LEU:HD23	2.00	0.42
1:A:7:VAL:HG23	1:A:152:THR:HG21	2.01	0.42
1:A:100:LYS:HD2	1:A:100:LYS:HA	1.92	0.42
1:B:1:SER:HA	1:B:151:ASP:HB2	2.01	0.42
1:A:58:PRO:HB3	1:A:98:LYS:HD3	2.01	0.42
1:A:341:GLY:O	1:A:345:VAL:HG23	2.19	0.42
1:A:387:GLN:HB3	1:A:418:HIS:HB3	2.02	0.42
1:B:131:ASN:HB2	1:B:321:ILE:HD11	2.01	0.42
1:B:59:LYS:HE2	1:B:59:LYS:HB3	1.82	0.41
1:A:34:ASP:O	1:A:123:GLN:HA	2.21	0.41
1:A:392:GLU:CD	1:A:413:ARG:HH11	2.23	0.41
1:A:453:VAL:HG12	1:A:467:LEU:O	2.19	0.41
1:A:120:THR:OG1	1:A:122:HIS:HE1	2.04	0.41
1:A:356:THR:HG23	1:A:358:HIS:HE1	1.85	0.41
1:A:68:TYR:HA	1:A:71:THR:OG1	2.20	0.41
1:A:310:VAL:HG11	1:A:323:ALA:HB3	2.03	0.41
1:A:141:ASP:HA	1:A:142:PRO:HD3	1.88	0.41
1:B:6:LEU:HD11	1:B:156:LEU:HB2	2.03	0.41
1:B:175:ILE:HB	1:B:179:GLU:HB2	2.02	0.41
1:B:127:ALA:O	1:B:135:LEU:HD23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLN:HB3	1:B:133:THR:CG2	2.51	0.40
1:A:318:VAL:O	1:A:318:VAL:HG12	2.20	0.40
1:B:200:ILE:HD13	1:B:218:LEU:HD21	2.02	0.40
1:A:478:GLU:O	1:A:479:LYS:HB2	2.22	0.40
1:B:6:LEU:O	1:B:30:VAL:HA	2.21	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	480/490 (98%)	454 (95%)	23 (5%)	3 (1%)	25	36
1	B	480/490 (98%)	455 (95%)	23 (5%)	2 (0%)	34	48
All	All	960/980 (98%)	909 (95%)	46 (5%)	5 (0%)	29	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	MET
1	A	481	LYS
1	A	117	GLU
1	B	355	ALA
1	B	44	TYR

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	384/393 (98%)	359 (94%)	25 (6%)	17 27
1	B	384/393 (98%)	350 (91%)	34 (9%)	9 14
All	All	768/786 (98%)	709 (92%)	59 (8%)	13 20

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	ARG
1	A	29	ARG
1	A	47	LEU
1	A	56	CYS
1	A	60	LYS
1	A	128	LEU
1	A	134	VAL
1	A	151	ASP
1	A	152	THR
1	A	162	TRP
1	A	212	ARG
1	A	215	GLN
1	A	237	LEU
1	A	246	ILE
1	A	250	THR
1	A	265	ARG
1	A	289	ARG
1	A	293	LEU
1	A	300	VAL
1	A	328	THR
1	A	351	ASN
1	A	371	MET
1	A	398	LEU
1	A	439	SER
1	B	29	ARG
1	B	30	VAL
1	B	47	LEU
1	B	56	CYS
1	B	59	LYS
1	B	63	VAL
1	B	67	ASN
1	B	70	ASP
1	B	82	LEU

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Mol	Chain	Res	Type
1	B	95	ILE
1	B	100	LYS
1	B	115	ASP
1	B	117	GLU
1	B	135	LEU
1	B	149	THR
1	B	156	LEU
1	B	162	TRP
1	B	212	ARG
1	B	216	VAL
1	B	239	GLU
1	B	244	ASN
1	B	246	ILE
1	B	250	THR
1	B	256	LYS
1	B	258	THR
1	B	265	ARG
1	B	296	GLU
1	B	300	VAL
1	B	386	ASP
1	B	398	LEU
1	B	416	THR
1	B	424	LEU
1	B	429	LEU
1	B	467	LEU

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	122	HIS
1	A	129	GLN
1	A	207	ASN
1	A	244	ASN
1	A	317	ASN
1	B	39	HIS
1	B	123	GLN
1	B	207	ASN
1	B	236	GLN
1	B	244	ASN
1	B	251	HIS
1	B	339	ASN
1	B	401	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	FAD	A	500	-	53,58,58	0.87	1 (1%)	68,89,89	0.97	3 (4%)
2	FAD	B	500	-	53,58,58	0.87	0	68,89,89	1.06	4 (5%)

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	A	500	-	-	4/30/50/50	0/6/6/6
2	FAD	B	500	-	-	4/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	O4B-C1B	2.52	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	FAD	O4B-C1B-C2B	-3.23	102.21	106.93
2	B	500	FAD	C4'-C3'-C2'	2.87	119.34	113.36
2	A	500	FAD	O4B-C1B-C2B	-2.76	102.90	106.93
2	A	500	FAD	C5A-C6A-N6A	2.37	123.95	120.35
2	B	500	FAD	O4B-C4B-C3B	2.17	109.41	105.11
2	A	500	FAD	C4'-C3'-C2'	2.10	117.73	113.36
2	B	500	FAD	O3'-C3'-C2'	-2.05	103.85	108.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

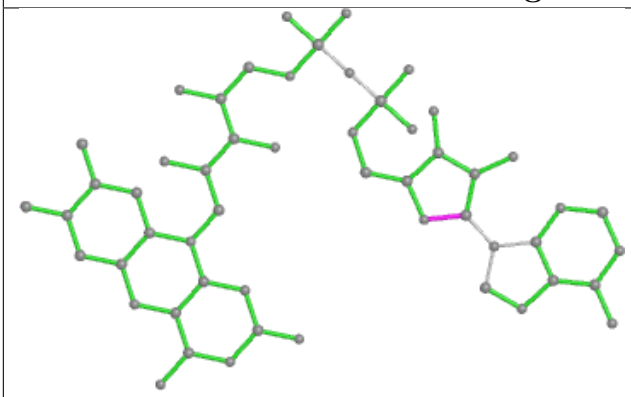
Mol	Chain	Res	Type	Atoms
2	A	500	FAD	PA-O3P-P-O5'
2	B	500	FAD	PA-O3P-P-O5'
2	A	500	FAD	P-O3P-PA-O2A
2	A	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	O4B-C4B-C5B-O5B
2	A	500	FAD	P-O3P-PA-O1A
2	B	500	FAD	P-O3P-PA-O1A
2	B	500	FAD	PA-O3P-P-O2P

There are no ring outliers.

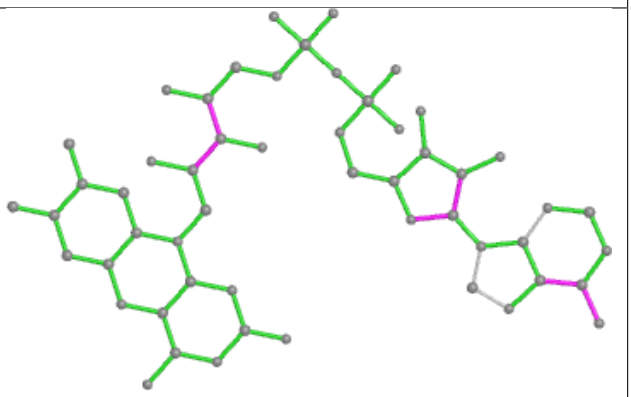
No monomer is involved in short contacts.

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.

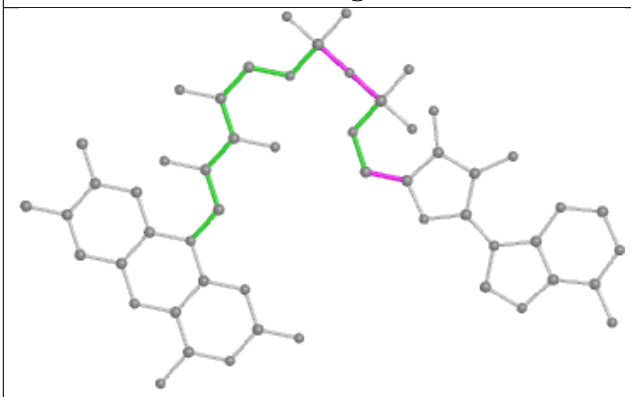
Ligand FAD A 500



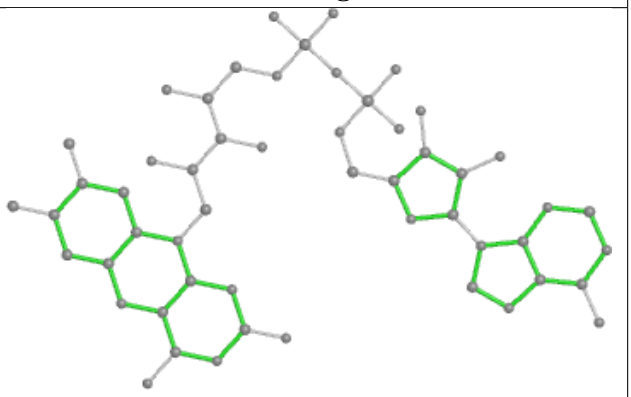
Bond lengths



Bond angles

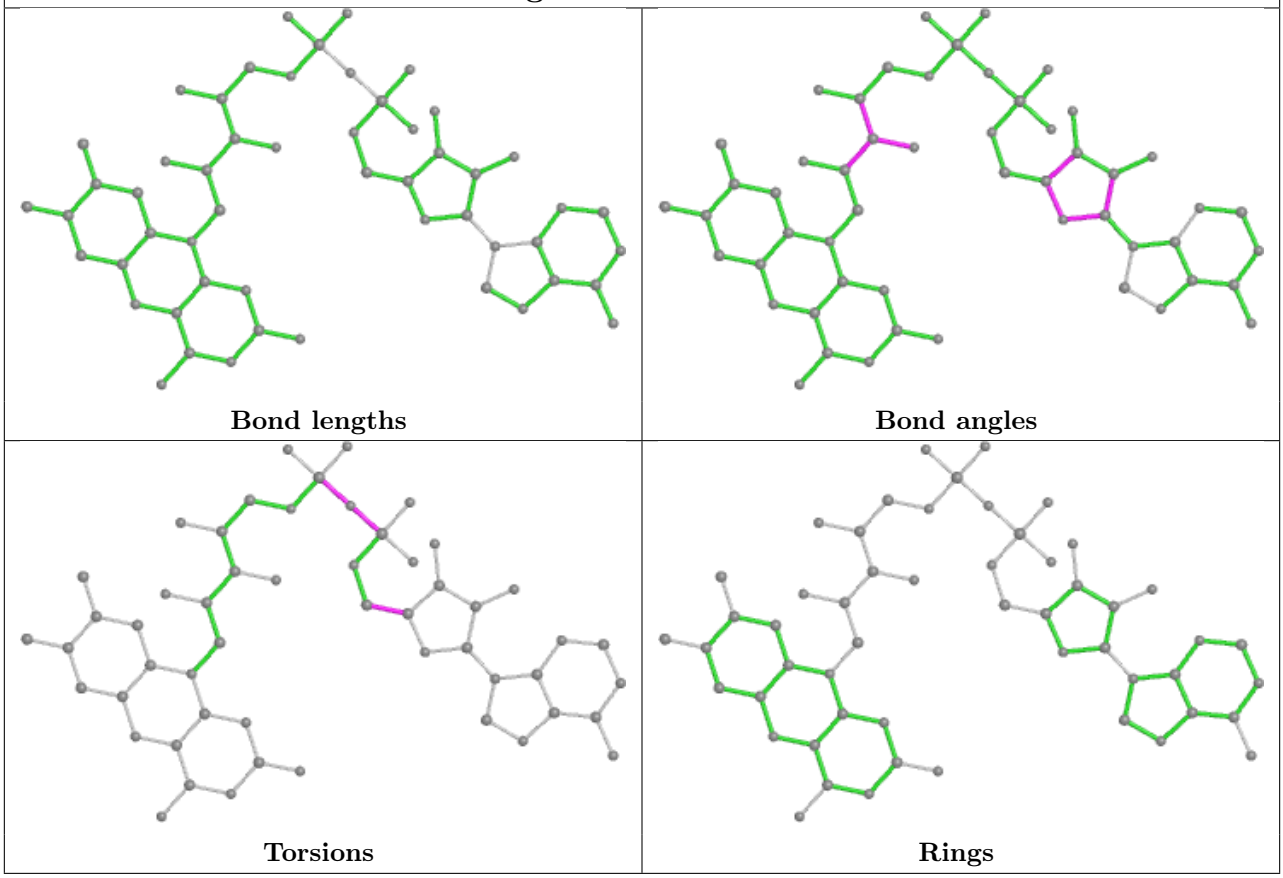


Torsions



Rings

Ligand FAD B 500



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	482/490 (98%)	0.04	27 (5%)	24	23	10, 30, 60, 101	0
1	B	482/490 (98%)	0.02	28 (5%)	23	22	11, 29, 64, 120	0
All	All	964/980 (98%)	0.03	55 (5%)	23	22	10, 30, 63, 120	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	SER	8.7
1	B	2	ARG	6.3
1	A	1	SER	5.6
1	A	351	ASN	5.3
1	B	114	ALA	4.6
1	A	2	ARG	4.3
1	A	212	ARG	4.2
1	B	3	ALA	3.8
1	B	150	LEU	3.7
1	A	115	ASP	3.7
1	A	167	GLY	3.7
1	B	115	ASP	3.4
1	A	388	VAL	3.4
1	B	351	ASN	3.3
1	B	303	ALA	3.3
1	A	141	ASP	3.1
1	A	304	LYS	3.0
1	B	117	GLU	3.0
1	A	169	GLU	2.9
1	A	119	LEU	2.9
1	A	213	GLY	2.8
1	B	22	ALA	2.6
1	B	316	THR	2.6
1	A	116	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	263	GLY	2.6
1	A	24	SER	2.5
1	A	114	ALA	2.5
1	A	47	LEU	2.5
1	A	261	ALA	2.4
1	A	482	ARG	2.4
1	B	347	THR	2.4
1	A	143	ASN	2.4
1	B	295	LEU	2.4
1	B	116	THR	2.4
1	A	144	SER	2.4
1	B	20	TRP	2.4
1	B	291	GLN	2.3
1	A	257	VAL	2.3
1	B	108	SER	2.3
1	B	296	GLU	2.3
1	B	311	ASP	2.3
1	B	47	LEU	2.3
1	B	29	ARG	2.3
1	A	113	PHE	2.2
1	B	324	ILE	2.2
1	A	20	TRP	2.2
1	B	143	ASN	2.2
1	B	212	ARG	2.2
1	A	271	SER	2.2
1	B	142	PRO	2.1
1	B	308	ILE	2.1
1	B	262	ASP	2.1
1	A	419	ALA	2.1
1	A	420	ASP	2.1
1	B	130	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

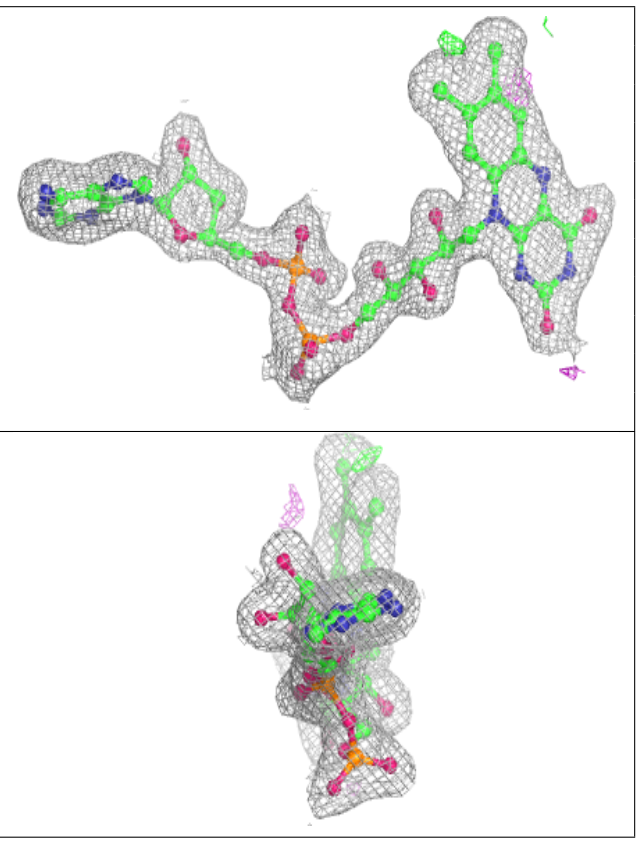
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	B	500	53/53	0.95	0.11	8,20,28,28	0
2	FAD	A	500	53/53	0.96	0.10	10,17,23,24	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.

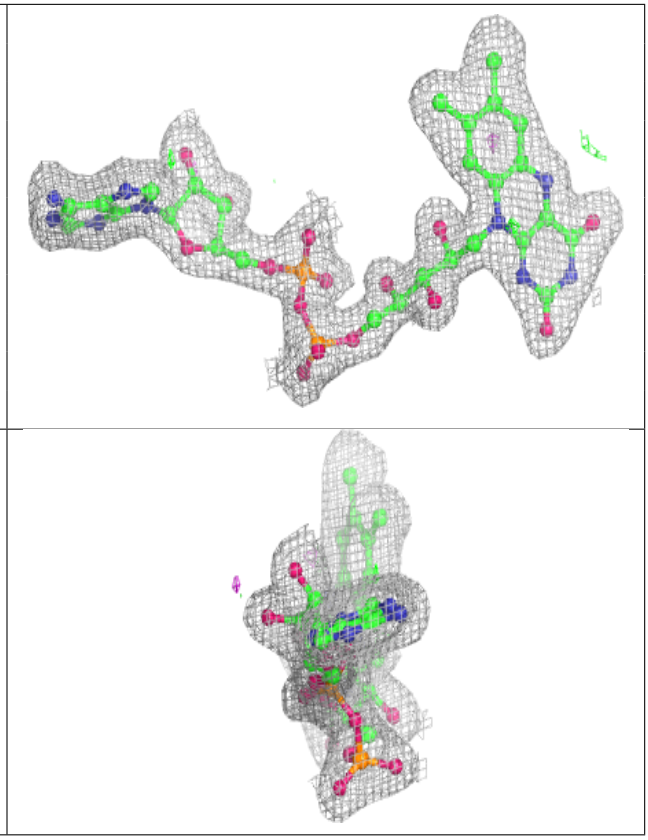
Electron density around FAD B 500:

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 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.