Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 05:01 PM EST

PDB ID	:	4P8N
Title	:	Crystal structure of M. tuberculosis DprE1 in complex with the non-covalent inhibitor QN118
Authors	:	Neres, J.; Pojer, F.; Cole, S.T.
Deposited on	:	2014-03-31
Resolution	:	1.79 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:

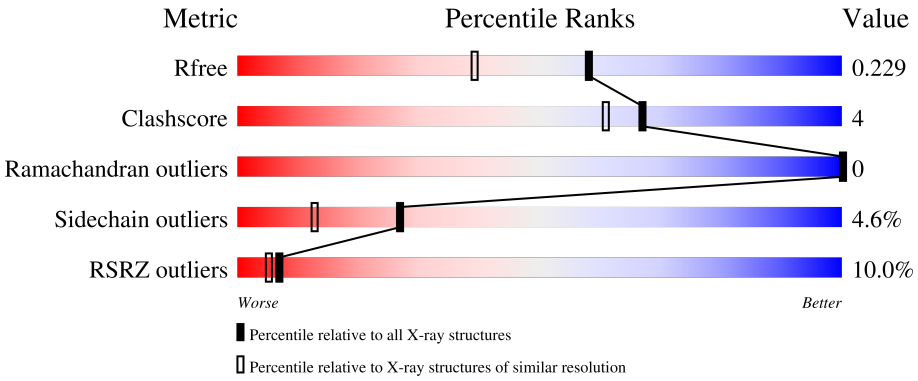
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	480	9% 84% 10% • 5%
1	B	480	9% 77% 9% • 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7246 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 Probable decaprenylphosphoryl-beta-D-ribose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	1	0
			3502	2230	616	645	11			
1	B	419	Total	C	N	O	S	0	2	0
			3230	2049	574	596	11			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP P72056
A	-17	SER	-	expression tag	UNP P72056
A	-16	SER	-	expression tag	UNP P72056
A	-15	HIS	-	expression tag	UNP P72056
A	-14	HIS	-	expression tag	UNP P72056
A	-13	HIS	-	expression tag	UNP P72056
A	-12	HIS	-	expression tag	UNP P72056
A	-11	HIS	-	expression tag	UNP P72056
A	-10	HIS	-	expression tag	UNP P72056
A	-9	SER	-	expression tag	UNP P72056
A	-8	SER	-	expression tag	UNP P72056
A	-7	GLY	-	expression tag	UNP P72056
A	-6	LEU	-	expression tag	UNP P72056
A	-5	VAL	-	expression tag	UNP P72056
A	-4	PRO	-	expression tag	UNP P72056
A	-3	ARG	-	expression tag	UNP P72056
A	-2	GLY	-	expression tag	UNP P72056
A	-1	SER	-	expression tag	UNP P72056
A	0	HIS	-	expression tag	UNP P72056
B	-18	GLY	-	expression tag	UNP P72056
B	-17	SER	-	expression tag	UNP P72056
B	-16	SER	-	expression tag	UNP P72056
B	-15	HIS	-	expression tag	UNP P72056
B	-14	HIS	-	expression tag	UNP P72056
B	-13	HIS	-	expression tag	UNP P72056

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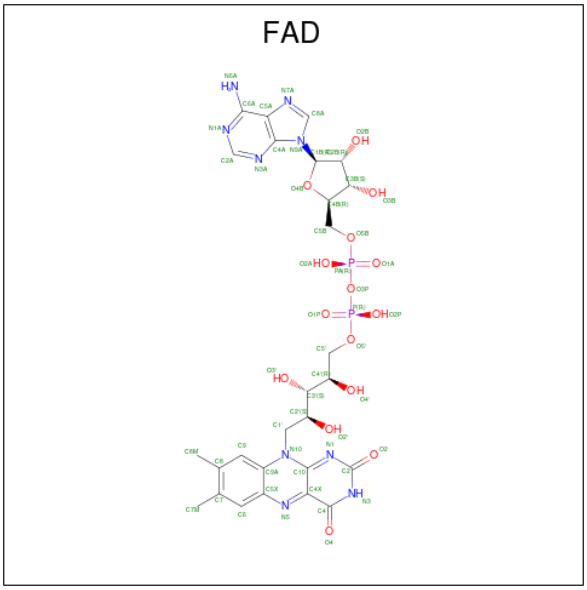
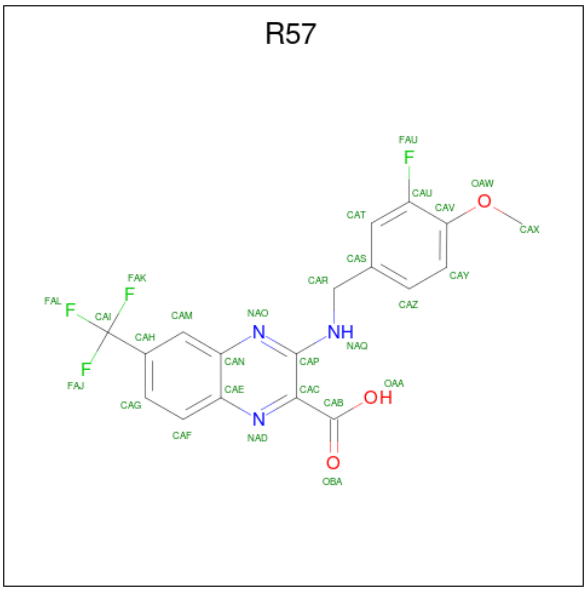
Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP P72056
B	-11	HIS	-	expression tag	UNP P72056
B	-10	HIS	-	expression tag	UNP P72056
B	-9	SER	-	expression tag	UNP P72056
B	-8	SER	-	expression tag	UNP P72056
B	-7	GLY	-	expression tag	UNP P72056
B	-6	LEU	-	expression tag	UNP P72056
B	-5	VAL	-	expression tag	UNP P72056
B	-4	PRO	-	expression tag	UNP P72056
B	-3	ARG	-	expression tag	UNP P72056
B	-2	GLY	-	expression tag	UNP P72056
B	-1	SER	-	expression tag	UNP P72056
B	0	HIS	-	expression tag	UNP P72056

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



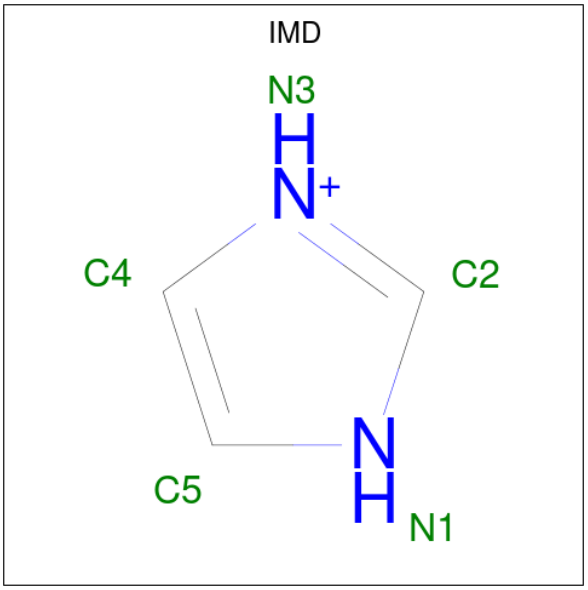
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-[(3-fluoro-4-methoxybenzyl)amino]-6-(trifluoromethyl)quinoxaline-2-carboxylic acid (three-letter code: R57) (formula: $C_{18}H_{13}F_4N_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	1
			56	36	8	6	6		
3	B	1	Total	C	F	N	O	0	0
			28	18	4	3	3		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N		0	0
			5	3	2			

- Molecule 5 is water.

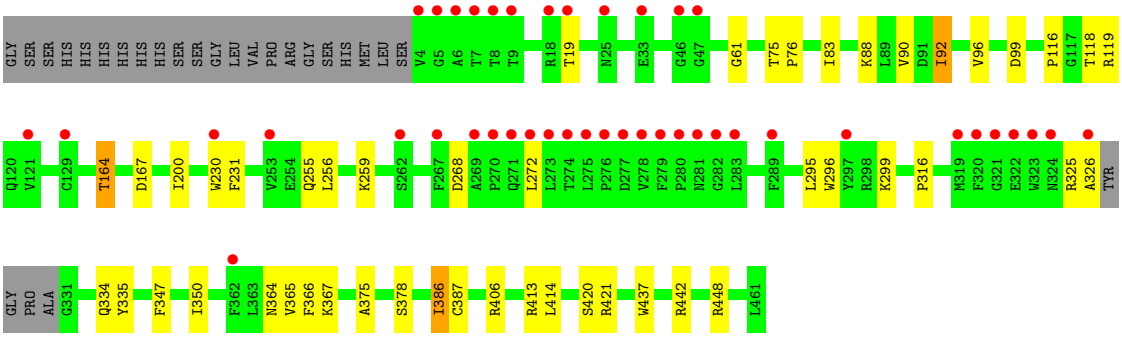
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	198	Total O 198 198	0	0
5	B	121	Total O 121 121	0	0

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.

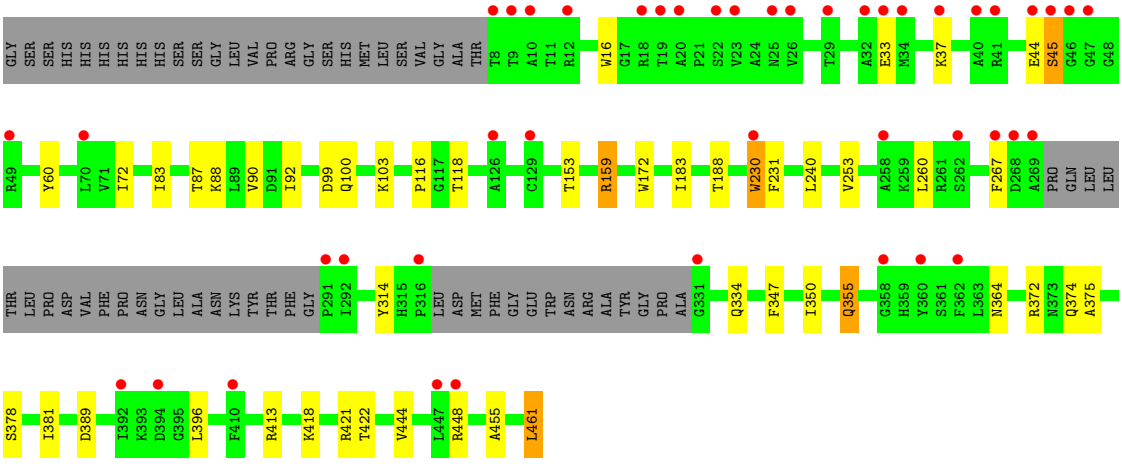
• Molecule 1: Probable decaprenylphosphoryl-beta-D-ribose oxidase

Chain A:



• Molecule 1: Probable decaprenylphosphoryl-beta-D-ribose oxidase

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	77.24Å 83.22Å 80.75Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	41.60 – 1.79 41.61 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.60-1.79) 98.3 (41.61-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.203 , 0.230 0.202 , 0.229	Depositor DCC
R_{free} test set	4600 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7246	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, FAD, R57

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	0.53	3/3590 (0.1%)	0.60	0/4878
1	B	0.52	4/3309 (0.1%)	0.56	0/4488
All	All	0.53	7/6899 (0.1%)	0.58	0/9366

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	SER	CB-OG	9.37	1.54	1.42
1	A	326	ALA	C-O	5.68	1.34	1.23
1	B	172	TRP	CD2-CE2	5.19	1.47	1.41
1	B	230	TRP	CD2-CE2	5.16	1.47	1.41
1	B	16	TRP	CD2-CE2	5.05	1.47	1.41
1	A	437	TRP	CD2-CE2	5.04	1.47	1.41
1	A	296	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

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	3502	0	3471	27	0
1	B	3230	0	3216	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	56	0	24	7	0
3	B	28	0	12	0	0
4	B	5	0	5	0	0
5	A	198	0	0	1	0
5	B	121	0	0	2	0
All	All	7246	0	6790	53	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 4.

All (53) 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:159:ARG:HG2	1:B:159:ARG:HH11	1.08	1.12
1:B:159:ARG:HG2	1:B:159:ARG:NH1	1.86	0.89
1:A:230[B]:TRP:CD1	3:A:502[B]:R57:CAX	2.57	0.87
1:A:442:ARG:HH11	1:A:442:ARG:HG2	1.49	0.78
1:A:230[B]:TRP:CD1	3:A:502[B]:R57:OAW	2.41	0.73
1:A:230[B]:TRP:CD1	3:A:502[B]:R57:H1	2.25	0.71
1:B:372[B]:ARG:HD3	1:B:381:ILE:HG22	1.73	0.70
1:A:230[B]:TRP:CG	3:A:502[B]:R57:H1	2.29	0.68
1:A:334:GLN:HE22	1:A:387:CYS:HB3	1.58	0.68
1:A:442:ARG:HH11	1:A:442:ARG:CG	2.10	0.64
1:B:99:ASP:O	1:B:103:LYS:HG3	1.97	0.63
1:A:99:ASP:HB2	1:A:119:ARG:HB3	1.81	0.62
1:A:366:PHE:CD2	1:A:386:ILE:HD11	2.34	0.62
1:A:230[B]:TRP:NE1	3:A:502[B]:R57:OAW	2.33	0.61
1:B:240:LEU:HD22	1:B:355:GLN:HG2	1.87	0.57
1:A:347:PHE:O	1:A:350:ILE:HG22	2.05	0.56
3:A:502[B]:R57:FAU	3:A:502[B]:R57:H2	1.95	0.56
1:A:347:PHE:CE1	1:A:386:ILE:HD13	2.43	0.54
1:A:366:PHE:HD2	1:A:386:ILE:HD11	1.74	0.53
1:A:347:PHE:CZ	1:A:386:ILE:HD13	2.43	0.53
1:A:375:ALA:HB3	1:A:378:SER:HB2	1.91	0.52
1:B:33:GLU:O	1:B:37:LYS:HG2	2.11	0.50
1:B:347:PHE:O	1:B:350:ILE:HG22	2.11	0.50
1:B:374:GLN:HG2	5:B:689:HOH:O	2.12	0.48
1:A:164:THR:HG22	5:A:756:HOH:O	2.13	0.48
1:B:375:ALA:HB3	1:B:378:SER:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:O	1:A:299:LYS:HG3	2.15	0.47
1:B:230:TRP:HA	1:B:364:ASN:O	2.14	0.47
1:B:153:THR:HG21	1:B:159:ARG:HD3	1.96	0.47
1:A:200:ILE:HD11	1:A:255:GLN:OE1	2.16	0.46
1:A:231:PHE:CE1	1:A:364:ASN:HB3	2.50	0.46
3:A:502[B]:R57:CAX	3:A:502[B]:R57:FAU	2.54	0.46
1:B:116:PRO:HG2	1:B:118:THR:O	2.16	0.45
1:B:83:ILE:HG12	1:B:90:VAL:HG12	1.99	0.45
1:A:61:GLY:HA2	1:A:420:SER:HB3	1.98	0.45
1:B:334:GLN:HG2	1:B:389:ASP:OD1	2.16	0.45
1:B:72:ILE:HD12	1:B:183:ILE:HD11	1.98	0.44
1:B:231:PHE:CE1	1:B:364:ASN:HB3	2.53	0.43
1:A:116:PRO:HG2	1:A:118:THR:O	2.18	0.43
1:A:83:ILE:HG12	1:A:90:VAL:HG12	1.99	0.43
1:A:335:TYR:CZ	1:A:414:LEU:HD21	2.54	0.43
1:A:230[B]:TRP:HZ2	1:A:316:PRO:HG2	1.84	0.43
1:B:455:ALA:HB1	1:B:461:LEU:HD13	2.02	0.42
1:B:60:TYR:CD2	1:B:418:LYS:HD3	2.54	0.42
1:B:100:GLN:HA	1:B:103:LYS:HE2	2.00	0.42
1:B:87:THR:O	1:B:88:LYS:HB2	2.20	0.41
1:A:92:ILE:HB	1:A:96:VAL:HG21	2.02	0.41
1:B:103:LYS:HG2	1:B:267:PHE:CE1	2.56	0.41
1:B:159:ARG:NH1	1:B:159:ARG:CG	2.66	0.41
1:B:90:VAL:O	1:B:188:THR:HA	2.21	0.41
1:A:75:THR:N	1:A:76:PRO:CD	2.84	0.41
1:A:442:ARG:CG	1:A:442:ARG:NH1	2.74	0.40
1:B:88:LYS:HE3	5:B:648:HOH:O	2.22	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	451/480 (94%)	448 (99%)	3 (1%)	0	100	100
1	B	415/480 (86%)	410 (99%)	5 (1%)	0	100	100
All	All	866/960 (90%)	858 (99%)	8 (1%)	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	364/384 (95%)	347 (95%)	17 (5%)	26	12
1	B	337/384 (88%)	322 (96%)	15 (4%)	27	13
All	All	701/768 (91%)	669 (95%)	32 (5%)	27	13

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

Mol	Chain	Res	Type
1	A	19	THR
1	A	88	LYS
1	A	92	ILE
1	A	164	THR
1	A	167	ASP
1	A	256	LEU
1	A	259	LYS
1	A	268	ASP
1	A	272	LEU
1	A	325	ARG
1	A	365	VAL
1	A	367	LYS
1	A	386	ILE
1	A	406	ARG
1	A	413	ARG
1	A	421	ARG
1	A	448	ARG
1	B	44	GLU

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Mol	Chain	Res	Type
1	B	45	SER
1	B	92	ILE
1	B	159	ARG
1	B	253	VAL
1	B	260	LEU
1	B	314	TYR
1	B	355	GLN
1	B	396	LEU
1	B	413	ARG
1	B	421	ARG
1	B	422	THR
1	B	444	VAL
1	B	448	ARG
1	B	461	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	334	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)

6 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	R57	A	502[A]	-	30,30,30	1.08	1 (3%)	43,44,44	1.50	5 (11%)
2	FAD	B	501	-	53,58,58	1.30	4 (7%)	68,89,89	1.33	12 (17%)
4	IMD	B	503	-	3,5,5	0.36	0	4,5,5	0.57	0
3	R57	A	502[B]	-	30,30,30	1.04	1 (3%)	43,44,44	1.56	3 (6%)
3	R57	B	502	-	30,30,30	1.09	2 (6%)	43,44,44	1.59	3 (6%)
2	FAD	A	501	-	53,58,58	1.27	5 (9%)	68,89,89	1.24	7 (10%)

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	R57	A	502[A]	-	-	0/17/17/17	0/3/3/3
2	FAD	B	501	-	-	2/30/50/50	0/6/6/6
4	IMD	B	503	-	-	-	0/1/1/1
3	R57	A	502[B]	-	-	2/17/17/17	0/3/3/3
3	R57	B	502	-	-	2/17/17/17	0/3/3/3
2	FAD	A	501	-	-	2/30/50/50	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C9A-C5X	5.20	1.49	1.41
2	A	501	FAD	C9A-C5X	5.15	1.49	1.41
3	A	502[A]	R57	CAP-NAO	3.69	1.36	1.31
3	B	502	R57	CAP-NAO	3.60	1.36	1.31
2	B	501	FAD	C8-C7	3.56	1.49	1.40
2	A	501	FAD	C8-C7	3.36	1.49	1.40
3	A	502[B]	R57	CAP-NAO	3.22	1.35	1.31
2	B	501	FAD	C4X-N5	2.68	1.36	1.30
2	A	501	FAD	C4X-N5	2.59	1.35	1.30
3	B	502	R57	CAC-NAD	2.38	1.36	1.32
2	A	501	FAD	C4-N3	-2.36	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C5A-C4A	2.35	1.47	1.40
2	A	501	FAD	C5A-C4A	2.32	1.47	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	R57	OAW-CAV-CAU	6.41	120.71	116.26
3	A	502[B]	R57	OAW-CAV-CAU	6.06	120.47	116.26
3	A	502[A]	R57	OAW-CAV-CAU	4.98	119.72	116.26
2	B	501	FAD	N3A-C2A-N1A	-3.99	122.45	128.68
2	A	501	FAD	N3A-C2A-N1A	-3.84	122.68	128.68
2	B	501	FAD	C4-C4X-N5	3.08	122.62	118.23
2	A	501	FAD	C4-C4X-N5	2.97	122.47	118.23
3	B	502	R57	OAW-CAV-CAY	-2.96	119.30	124.37
3	A	502[B]	R57	OAW-CAV-CAY	-2.89	119.42	124.37
2	B	501	FAD	O4-C4-C4X	-2.84	119.08	126.60
2	A	501	FAD	O4-C4-C4X	-2.70	119.43	126.60
2	B	501	FAD	O2-C2-N1	-2.46	117.76	121.83
2	B	501	FAD	C4X-C10-N1	-2.43	119.10	124.73
2	B	501	FAD	C4A-C5A-N7A	-2.42	106.88	109.40
2	B	501	FAD	C10-N1-C2	2.41	121.71	116.90
3	A	502[A]	R57	OAW-CAV-CAY	-2.37	120.31	124.37
3	A	502[A]	R57	FAL-CAI-CAH	-2.35	107.77	112.93
2	A	501	FAD	C4X-C4-N3	2.28	118.97	113.19
3	A	502[A]	R57	CAC-CAP-NAQ	-2.28	117.86	121.69
2	B	501	FAD	C4X-C4-N3	2.27	118.96	113.19
2	A	501	FAD	C10-N1-C2	2.25	121.40	116.90
2	A	501	FAD	C2A-N1A-C6A	2.22	122.56	118.75
2	B	501	FAD	C2A-N1A-C6A	2.20	122.51	118.75
2	B	501	FAD	C4X-C10-N10	2.16	119.64	116.48
3	A	502[A]	R57	CAC-CAP-NAO	-2.15	119.54	121.63
3	B	502	R57	CAP-NAO-CAN	2.05	120.52	116.56
2	A	501	FAD	C4X-C10-N1	-2.05	119.98	124.73
2	B	501	FAD	C4-N3-C2	-2.03	121.90	125.64
2	B	501	FAD	P-O3P-PA	-2.02	125.91	132.83
3	A	502[B]	R57	CAC-CAP-NAO	-2.01	119.67	121.63

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[B]	R57	CAU-CAV-OAW-CAX

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Mol	Chain	Res	Type	Atoms
3	B	502	R57	CAU-CAV-OAW-CAX
3	A	502[B]	R57	CAY-CAV-OAW-CAX
3	B	502	R57	CAY-CAV-OAW-CAX
2	A	501	FAD	PA-O3P-P-O2P
2	B	501	FAD	PA-O3P-P-O2P
2	A	501	FAD	PA-O3P-P-O1P
2	B	501	FAD	PA-O3P-P-O1P

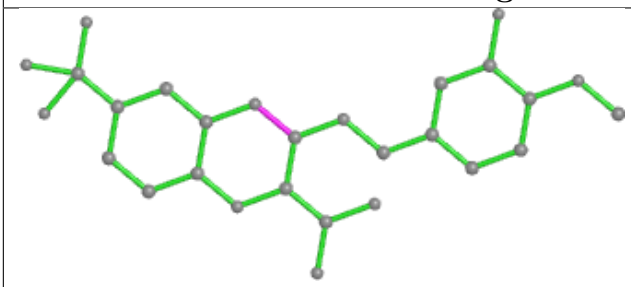
There are no ring outliers.

1 monomer is involved in 7 short contacts:

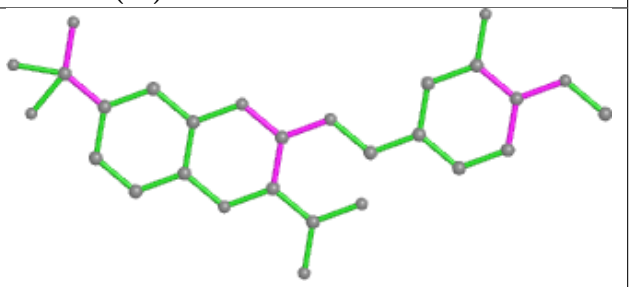
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502[B]	R57	7	0

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.

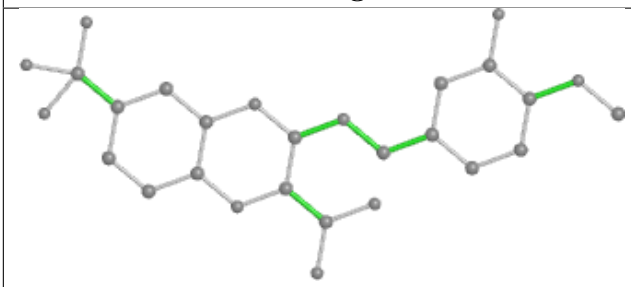
Ligand R57 A 502 (A)



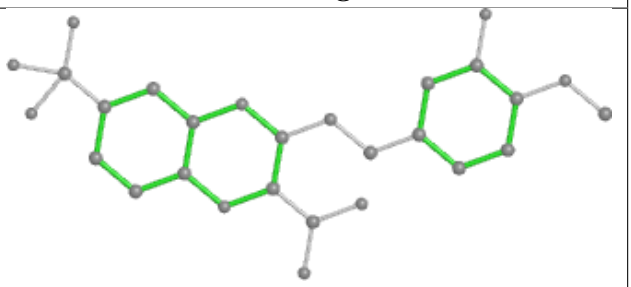
Bond lengths



Bond angles

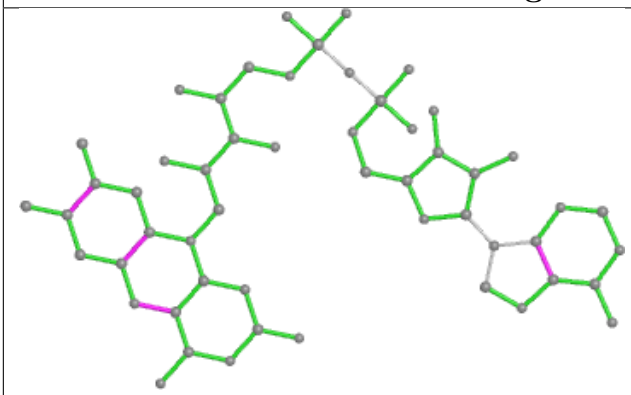


Torsions

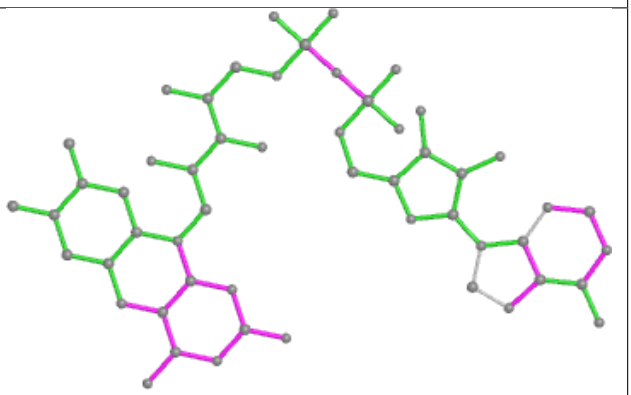


Rings

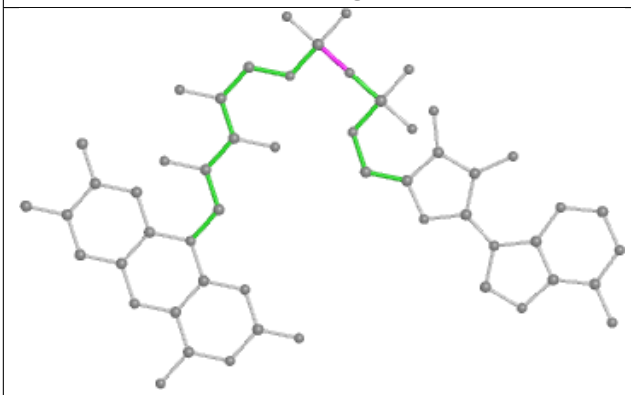
Ligand FAD B 501



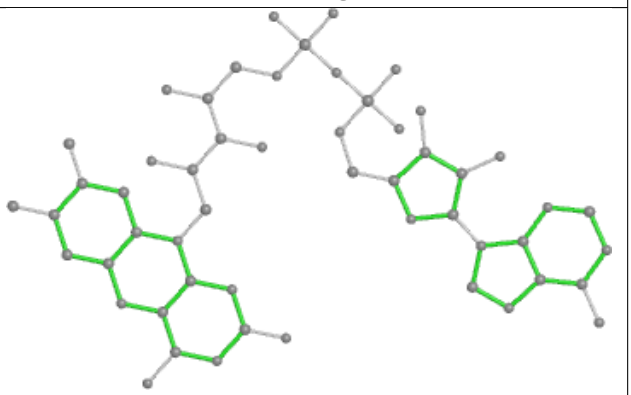
Bond lengths



Bond angles

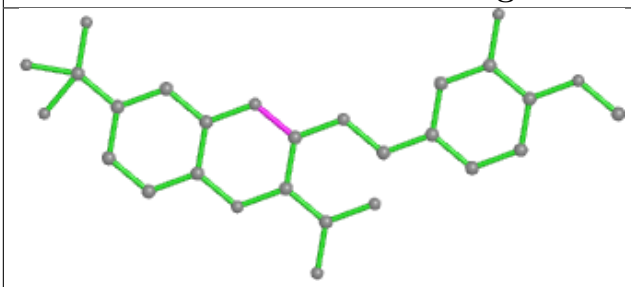


Torsions

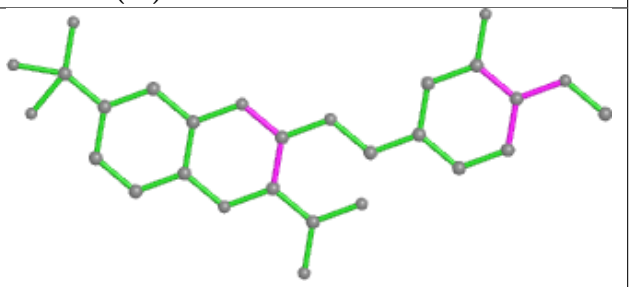


Rings

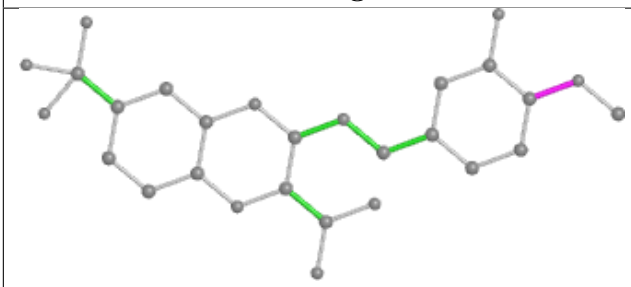
Ligand R57 A 502 (B)



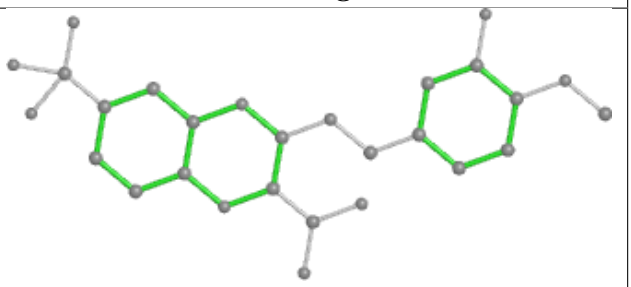
Bond lengths



Bond angles

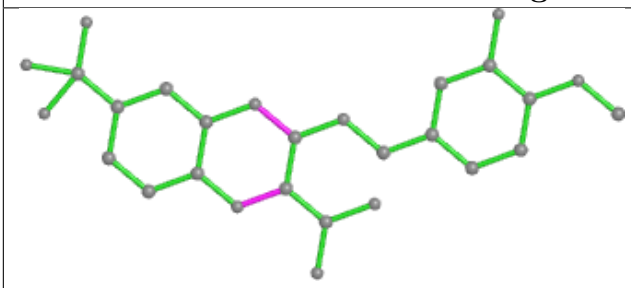


Torsions

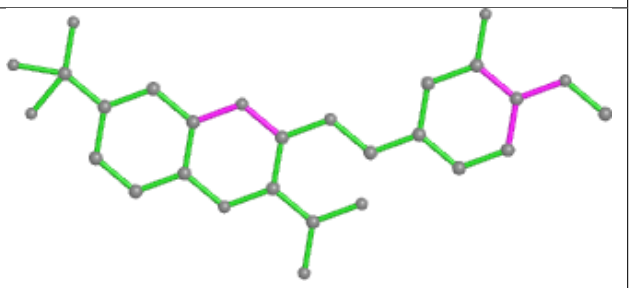


Rings

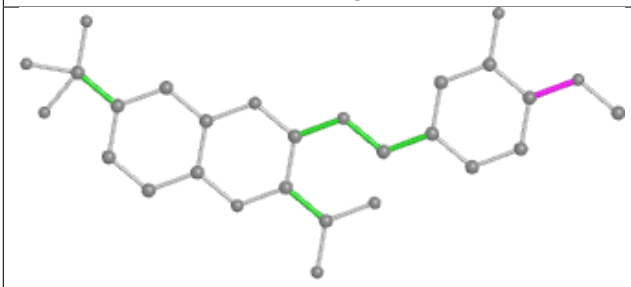
Ligand R57 B 502



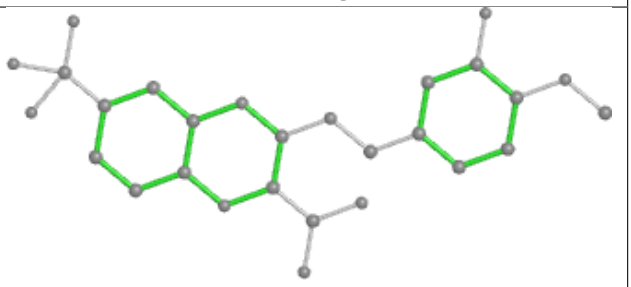
Bond lengths



Bond angles

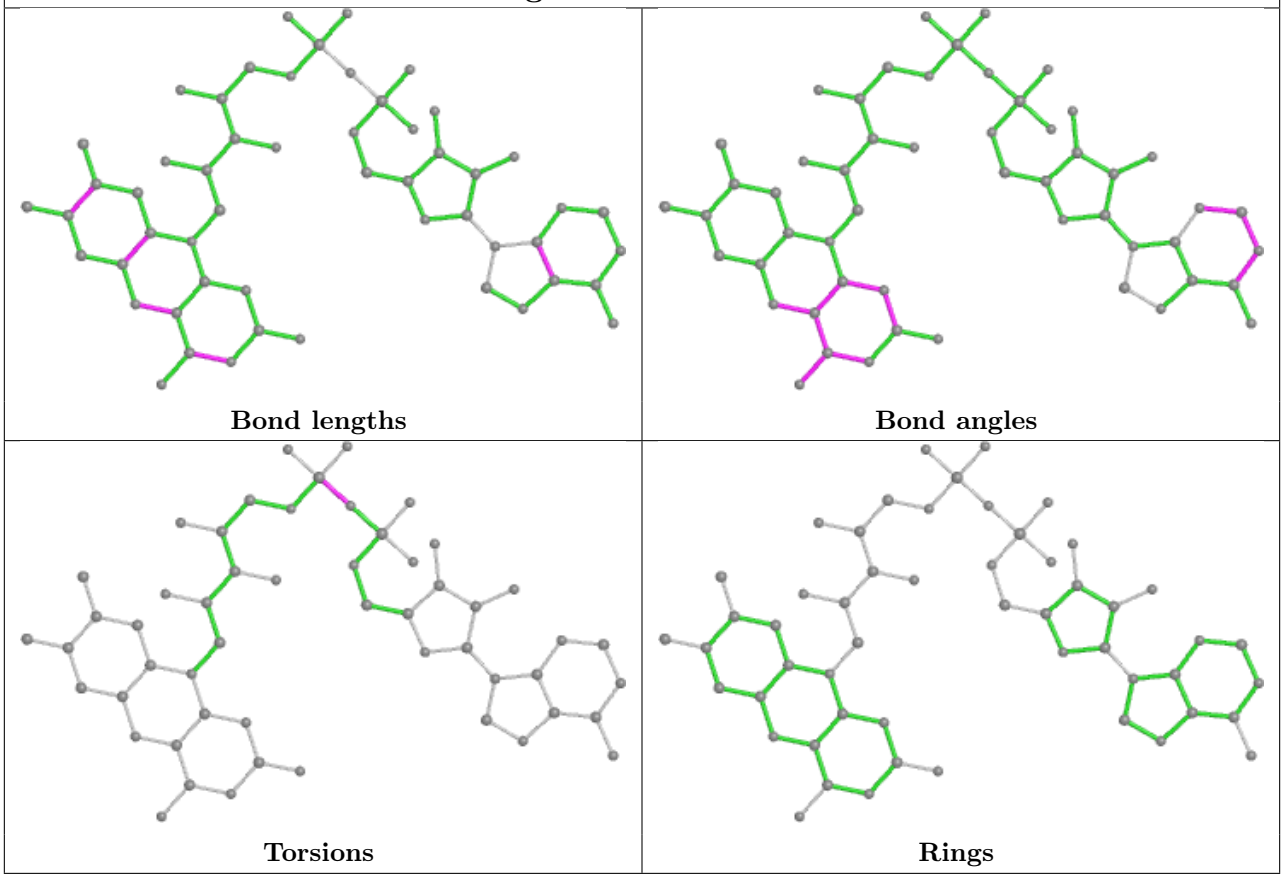


Torsions



Rings

Ligand FAD A 501



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	454/480 (94%)	0.39	43 (9%) 8 6	17, 27, 53, 70	0
1	B	419/480 (87%)	0.55	44 (10%) 6 4	20, 33, 55, 75	0
All	All	873/960 (90%)	0.46	87 (9%) 7 5	17, 30, 55, 75	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	TRP	8.0
1	B	46	GLY	7.6
1	B	47	GLY	7.3
1	B	291	PRO	5.9
1	A	4	VAL	5.8
1	A	279	PHE	5.5
1	A	5	GLY	5.4
1	A	283	LEU	5.1
1	A	281	ASN	4.9
1	A	47	GLY	4.8
1	B	362	PHE	4.8
1	B	267	PHE	4.7
1	A	280	PRO	4.7
1	B	44	GLU	4.7
1	A	272	LEU	4.7
1	B	8	THR	4.5
1	A	320	PHE	4.5
1	A	273	LEU	4.4
1	B	20	ALA	4.2
1	B	292	ILE	4.2
1	B	447	LEU	4.2
1	B	18	ARG	3.9
1	B	269	ALA	3.9
1	B	316	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	362	PHE	3.7
1	B	12	ARG	3.7
1	A	278	VAL	3.7
1	A	326	ALA	3.6
1	B	230	TRP	3.5
1	A	6	ALA	3.4
1	B	41	ARG	3.4
1	A	297	TYR	3.3
1	B	25	ASN	3.3
1	B	10	ALA	3.3
1	B	392	ILE	3.3
1	A	319	MET	3.2
1	B	9	THR	3.2
1	B	29	THR	3.2
1	A	269	ALA	3.2
1	A	275	LEU	3.1
1	B	394	ASP	3.1
1	A	7	THR	3.1
1	B	360	TYR	3.1
1	A	282	GLY	3.1
1	A	46	GLY	3.0
1	A	230[A]	TRP	3.0
1	A	324	ASN	3.0
1	A	277	ASP	2.9
1	B	331	GLY	2.9
1	B	37	LYS	2.9
1	B	19	THR	2.8
1	A	322	GLU	2.7
1	B	34	MET	2.7
1	A	270	PRO	2.7
1	B	45	SER	2.7
1	B	262	SER	2.7
1	A	321	GLY	2.7
1	A	276	PRO	2.6
1	B	268	ASP	2.6
1	B	33	GLU	2.6
1	A	18	ARG	2.6
1	A	8	THR	2.5
1	A	9	THR	2.5
1	A	289	PHE	2.5
1	A	274	THR	2.4
1	B	40	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	19	THR	2.3
1	A	267	PHE	2.3
1	A	25	ASN	2.3
1	A	262	SER	2.3
1	B	32	ALA	2.2
1	A	271	GLN	2.2
1	B	258	ALA	2.2
1	A	253	VAL	2.2
1	B	70	LEU	2.2
1	B	410	PHE	2.2
1	A	129	CYS	2.2
1	A	121	VAL	2.1
1	B	49	ARG	2.1
1	B	22	SER	2.1
1	B	126	ALA	2.1
1	B	358	GLY	2.1
1	B	26	VAL	2.1
1	B	129	CYS	2.1
1	B	448	ARG	2.1
1	A	33	GLU	2.1
1	B	23	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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	R57	B	502	28/28	0.93	0.11	33,37,44,44	8
3	R57	A	502[A]	28/28	0.96	0.12	27,28,33,33	28

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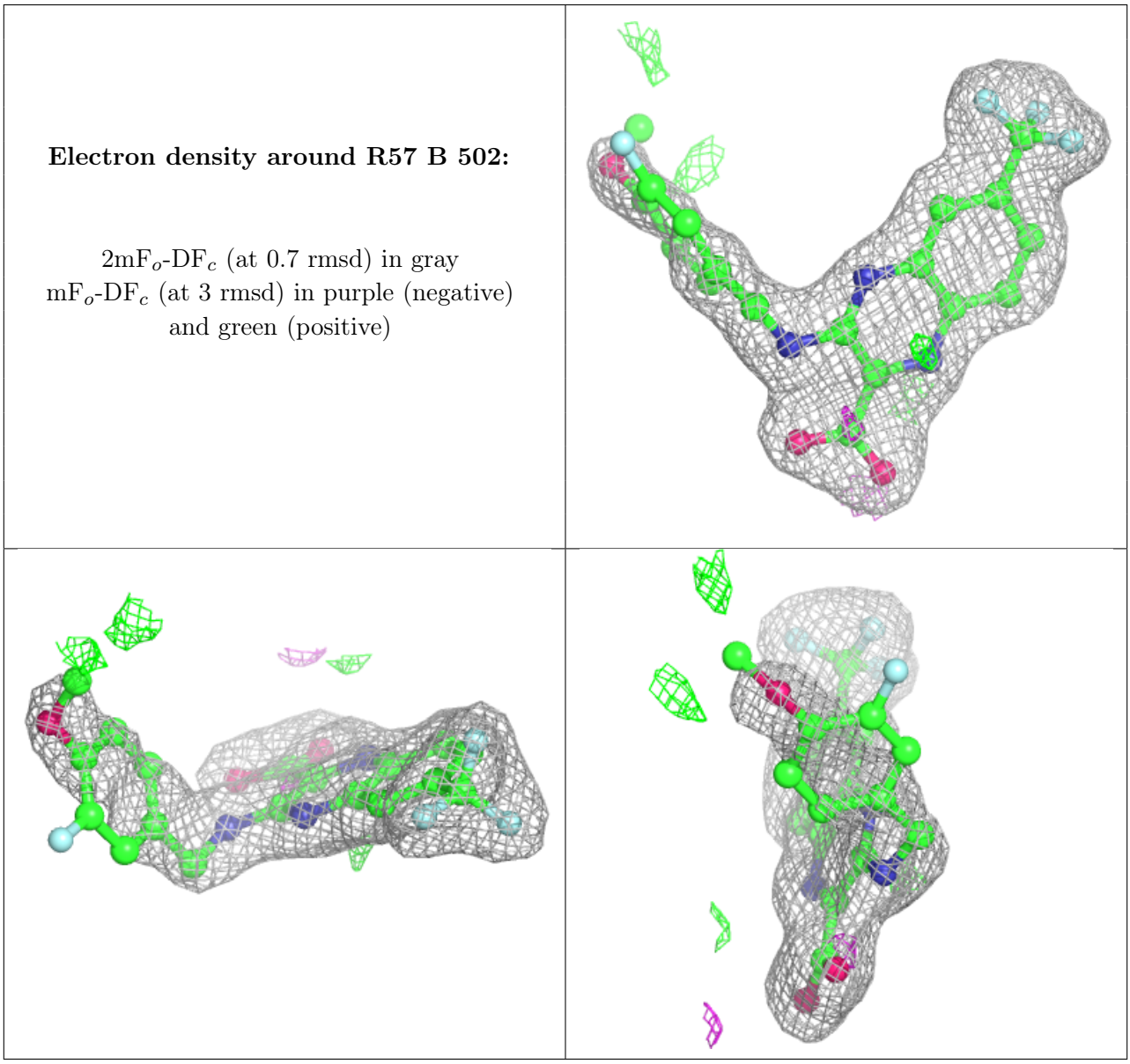
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	R57	A	502[B]	28/28	0.96	0.12	28,30,39,39	28
2	FAD	B	501	53/53	0.96	0.11	21,27,29,31	0
2	FAD	A	501	53/53	0.97	0.14	18,20,22,22	0
4	IMD	B	503	5/5	0.97	0.09	36,36,37,37	0

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.

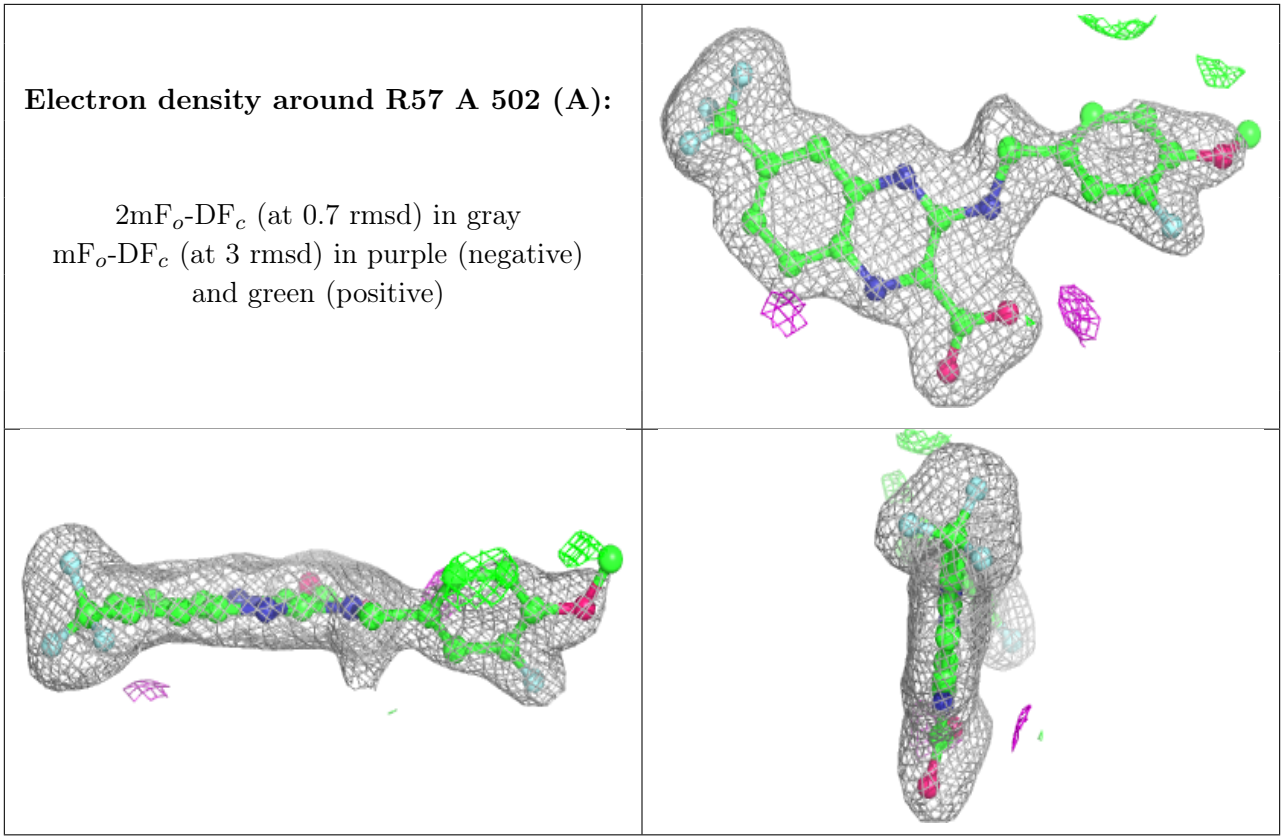
Electron density around R57 B 502:

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



Electron density around R57 A 502 (A):

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



Electron density around R57 A 502 (B):

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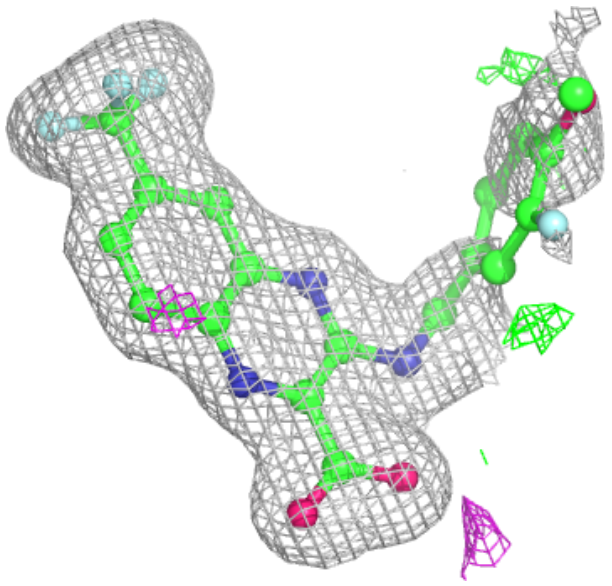
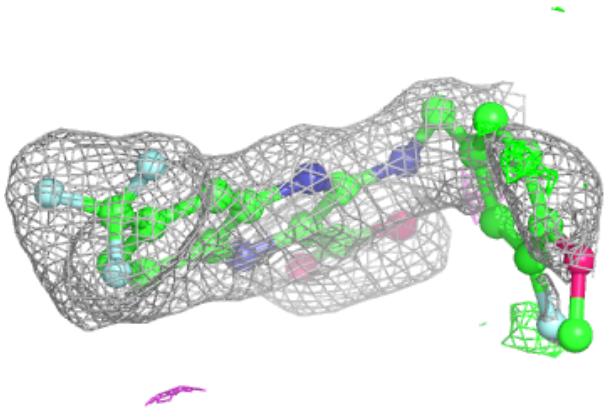
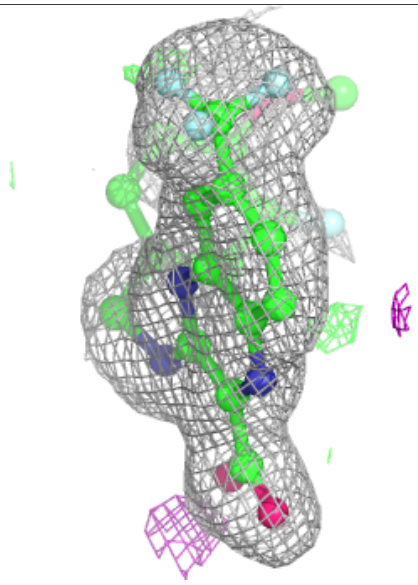
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

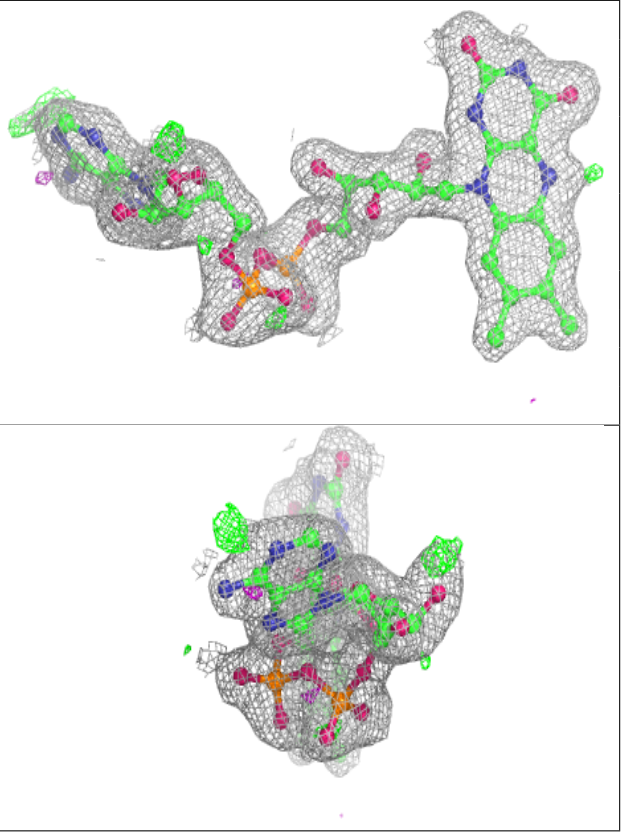


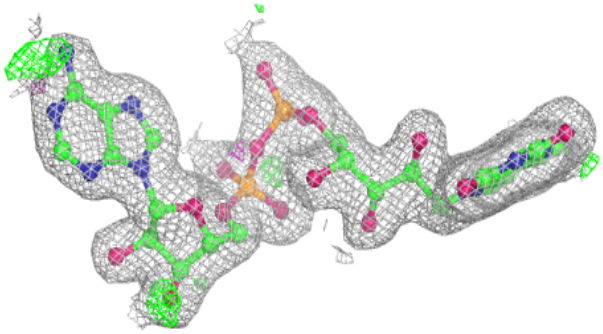




Electron density around FAD B 501:

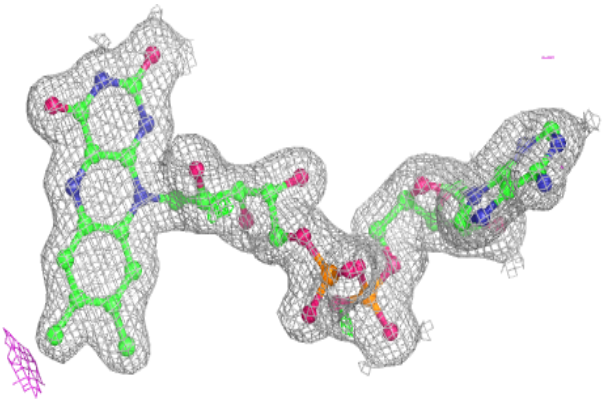
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

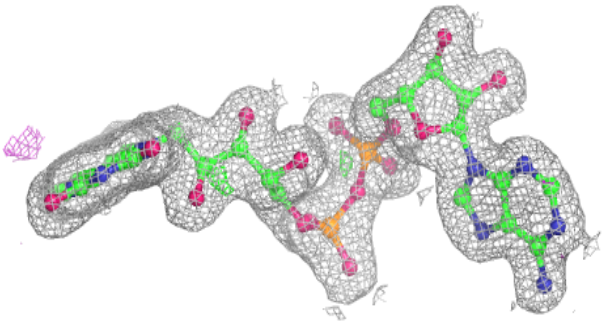


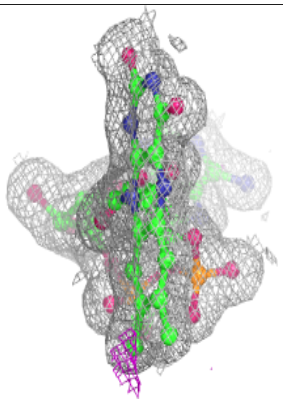


Electron density around FAD A 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.