Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2022 – 09:48 pm BST

PDB ID	:	7P9A
Title	:	Structure of cyclohex-1-ene-1-carboxyl-CoA dehydrogenase complexed with cyclohex-1,5-diene-1-carboxyl-CoA
Authors	:	Ermler, U.; Weidenweber, S.; Boll, M.
Deposited on	:	2021-07-26
Resolution	:	1.50 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:

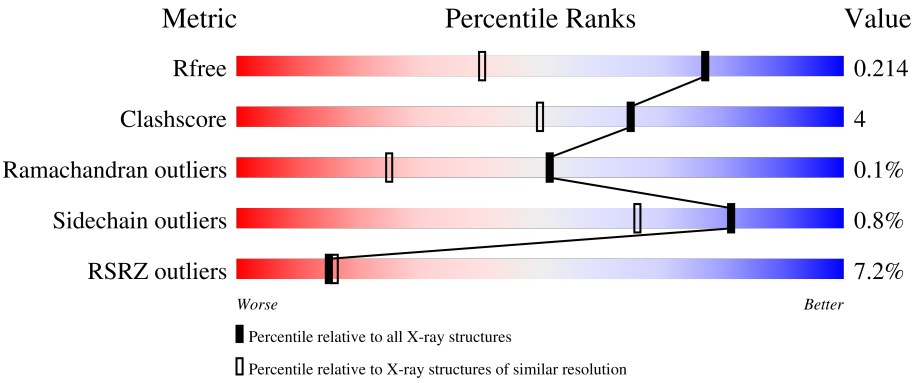
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	412	5% 81% 10% • 8%
1	B	412	8% 84% 7% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	504	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6631 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 Short-chain acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	10	0
			2949	1850	514	561	24			
1	B	379	Total	C	N	O	S	0	9	0
			2940	1845	516	557	22			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	LYS	-	expression tag	UNP Q39QF5
A	382	GLY	-	expression tag	UNP Q39QF5
A	383	GLU	-	expression tag	UNP Q39QF5
A	384	LEU	-	expression tag	UNP Q39QF5
A	385	ASN	-	expression tag	UNP Q39QF5
A	386	SER	-	expression tag	UNP Q39QF5
A	387	LYS	-	expression tag	UNP Q39QF5
A	388	LEU	-	expression tag	UNP Q39QF5
A	389	GLU	-	expression tag	UNP Q39QF5
A	390	GLY	-	expression tag	UNP Q39QF5
A	391	LYS	-	expression tag	UNP Q39QF5
A	392	PRO	-	expression tag	UNP Q39QF5
A	393	ILE	-	expression tag	UNP Q39QF5
A	394	PRO	-	expression tag	UNP Q39QF5
A	395	ASN	-	expression tag	UNP Q39QF5
A	396	PRO	-	expression tag	UNP Q39QF5
A	397	LEU	-	expression tag	UNP Q39QF5
A	398	LEU	-	expression tag	UNP Q39QF5
A	399	GLY	-	expression tag	UNP Q39QF5
A	400	LEU	-	expression tag	UNP Q39QF5
A	401	ASP	-	expression tag	UNP Q39QF5
A	402	SER	-	expression tag	UNP Q39QF5
A	403	THR	-	expression tag	UNP Q39QF5
A	404	ARG	-	expression tag	UNP Q39QF5
A	405	THR	-	expression tag	UNP Q39QF5

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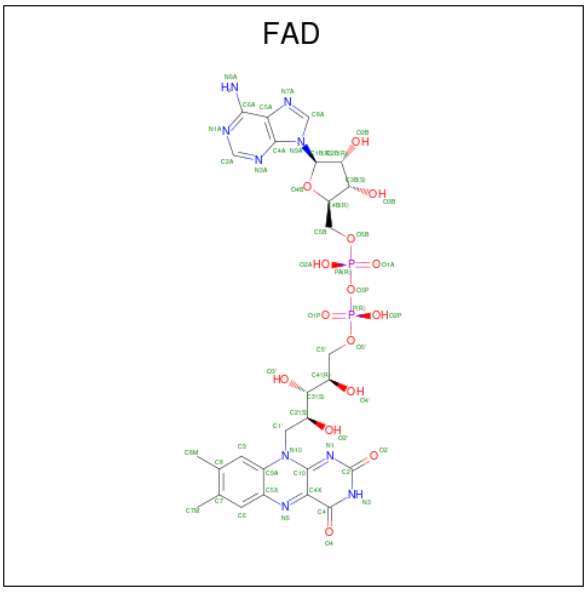
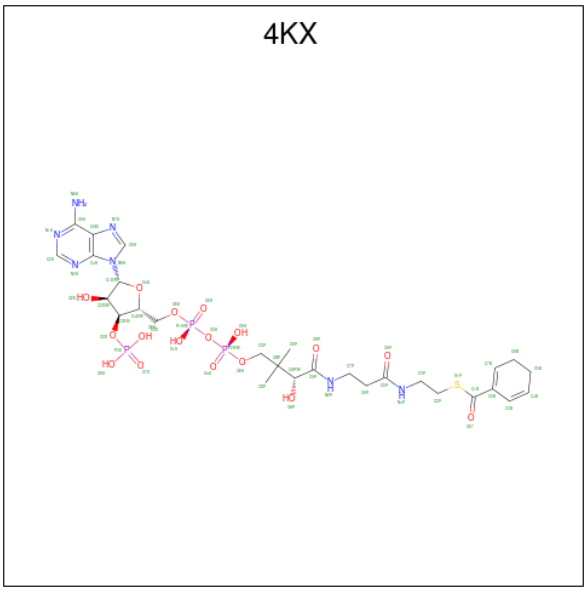
Chain	Residue	Modelled	Actual	Comment	Reference
A	406	GLY	-	expression tag	UNP Q39QF5
A	407	HIS	-	expression tag	UNP Q39QF5
A	408	HIS	-	expression tag	UNP Q39QF5
A	409	HIS	-	expression tag	UNP Q39QF5
A	410	HIS	-	expression tag	UNP Q39QF5
A	411	HIS	-	expression tag	UNP Q39QF5
A	412	HIS	-	expression tag	UNP Q39QF5
B	381	LYS	-	expression tag	UNP Q39QF5
B	382	GLY	-	expression tag	UNP Q39QF5
B	383	GLU	-	expression tag	UNP Q39QF5
B	384	LEU	-	expression tag	UNP Q39QF5
B	385	ASN	-	expression tag	UNP Q39QF5
B	386	SER	-	expression tag	UNP Q39QF5
B	387	LYS	-	expression tag	UNP Q39QF5
B	388	LEU	-	expression tag	UNP Q39QF5
B	389	GLU	-	expression tag	UNP Q39QF5
B	390	GLY	-	expression tag	UNP Q39QF5
B	391	LYS	-	expression tag	UNP Q39QF5
B	392	PRO	-	expression tag	UNP Q39QF5
B	393	ILE	-	expression tag	UNP Q39QF5
B	394	PRO	-	expression tag	UNP Q39QF5
B	395	ASN	-	expression tag	UNP Q39QF5
B	396	PRO	-	expression tag	UNP Q39QF5
B	397	LEU	-	expression tag	UNP Q39QF5
B	398	LEU	-	expression tag	UNP Q39QF5
B	399	GLY	-	expression tag	UNP Q39QF5
B	400	LEU	-	expression tag	UNP Q39QF5
B	401	ASP	-	expression tag	UNP Q39QF5
B	402	SER	-	expression tag	UNP Q39QF5
B	403	THR	-	expression tag	UNP Q39QF5
B	404	ARG	-	expression tag	UNP Q39QF5
B	405	THR	-	expression tag	UNP Q39QF5
B	406	GLY	-	expression tag	UNP Q39QF5
B	407	HIS	-	expression tag	UNP Q39QF5
B	408	HIS	-	expression tag	UNP Q39QF5
B	409	HIS	-	expression tag	UNP Q39QF5
B	410	HIS	-	expression tag	UNP Q39QF5
B	411	HIS	-	expression tag	UNP Q39QF5
B	412	HIS	-	expression tag	UNP Q39QF5

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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 1,5 Dienoyl-CoA (three-letter code: 4KX) (formula: $C_{28}H_{42}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		

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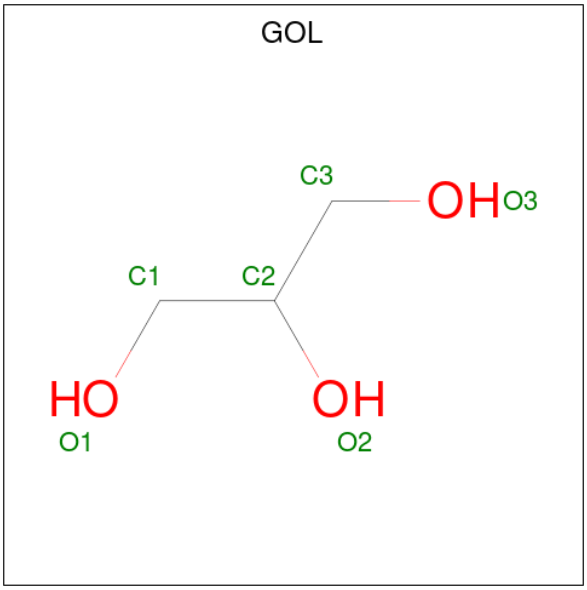
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	A	1	Total	C	O		0	0
			6	3	3			
4	B	1	Total	C	O		0	0
			6	3	3			
4	B	1	Total	C	O		0	0
			6	3	3			

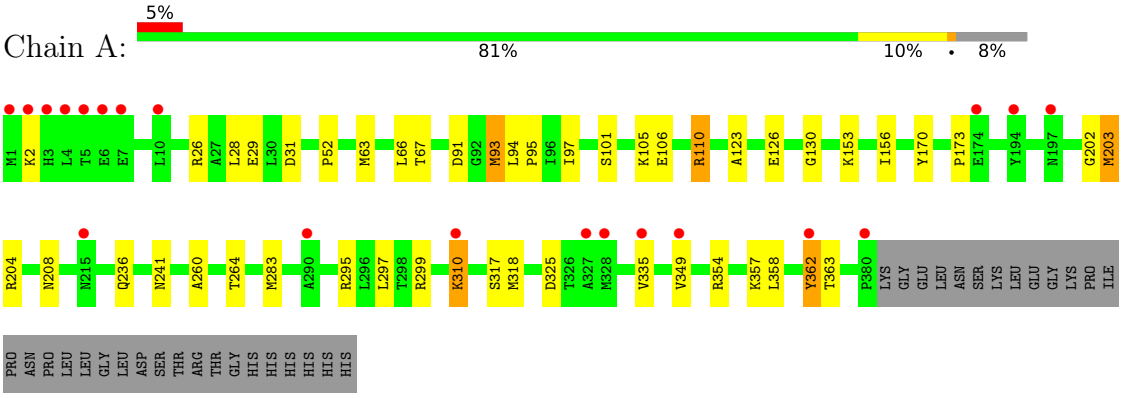
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total	O	0	0
			265	265		
5	B	234	Total	O	0	1
			235	235		

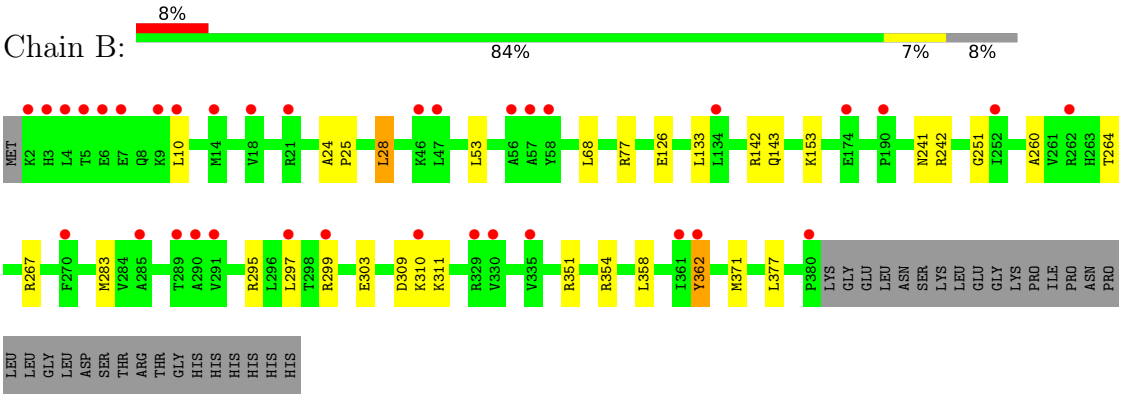
3 Residue-property plots (i)

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: Short-chain acyl-CoA dehydrogenase



• Molecule 1: Short-chain acyl-CoA dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	76.26Å 173.59Å 331.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.61 – 1.50 48.08 – 1.50	Depositor EDS
% Data completeness (in resolution range)	82.5 (46.61-1.50) 82.6 (48.08-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.185 , 0.205 0.195 , 0.214	Depositor DCC
R_{free} test set	2000 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6631	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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: FAD, GOL, 4KX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.04	1/2987 (0.0%)	1.14	11/4030 (0.3%)
1	B	0.91	0/2978	1.10	12/4018 (0.3%)
All	All	0.97	1/5965 (0.0%)	1.12	23/8048 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	CD-OE2	-5.88	1.19	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	B	295	ARG	NE-CZ-NH1	10.43	125.51	120.30
1	A	358	LEU	CB-CG-CD1	10.19	128.32	111.00
1	B	354	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	110	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	242	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	297	LEU	CB-CG-CD1	-7.16	98.83	111.00
1	B	351	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	351	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	B	377	LEU	CB-CG-CD2	-6.88	99.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	267	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	325	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	283	MET	CG-SD-CE	-6.48	89.83	100.20
1	B	283	MET	CG-SD-CE	-6.45	89.89	100.20
1	A	354	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	26	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	B	371	MET	CG-SD-CE	6.05	109.89	100.20
1	A	93	MET	CA-CB-CG	6.03	123.56	113.30
1	B	28	LEU	CB-CG-CD2	6.00	121.20	111.00
1	A	31	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	A	295	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	362	TYR	CB-CA-C	5.85	122.09	110.40
1	A	362	TYR	CB-CG-CD1	5.14	124.09	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	MET	Mainchain

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	2949	0	3011	35	0
1	B	2940	0	3004	16	0
2	A	53	0	30	1	0
2	B	53	0	29	1	0
3	A	56	0	37	0	0
3	B	56	0	38	1	0
4	A	12	0	15	0	0
4	B	12	0	16	0	0
5	A	265	0	0	8	0
5	B	235	0	0	2	0
All	All	6631	0	6180	51	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 (51) 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:63[A]:MET:HE3	1:A:67:THR:HG22	1.55	0.89
1:B:311:LYS:NZ	5:B:601:HOH:O	2.20	0.74
1:B:28:LEU:HD23	5:B:753:HOH:O	1.94	0.67
1:A:63[A]:MET:HE3	1:A:67:THR:CG2	2.24	0.67
1:A:66:LEU:CD1	1:A:299[B]:ARG:HD2	2.26	0.66
1:A:204[B]:ARG:CZ	5:A:605:HOH:O	2.45	0.63
1:A:66:LEU:HD11	1:A:299[B]:ARG:HD2	1.81	0.62
1:A:28:LEU:HD12	5:A:643:HOH:O	1.99	0.62
1:A:204[B]:ARG:NH2	5:A:605:HOH:O	2.36	0.58
1:A:310:LYS:HE2	5:A:713:HOH:O	2.03	0.58
1:A:204[B]:ARG:NH1	5:A:605:HOH:O	2.37	0.56
1:A:236:GLN:NE2	5:A:601:HOH:O	2.25	0.54
1:A:106:GLU:OE2	1:A:110:ARG:HD2	2.09	0.53
1:A:106:GLU:OE2	1:A:110:ARG:CD	2.57	0.53
1:A:241[A]:ASN:ND2	1:A:363:THR:HG22	2.24	0.52
1:B:309:ASP:HA	1:B:310:LYS:HE2	1.92	0.51
1:A:317[B]:SER:HB3	5:A:634:HOH:O	2.10	0.50
1:A:93:MET:HG2	1:A:97:ILE:HD11	1.93	0.50
1:A:335:VAL:CG2	1:A:349[B]:VAL:HG12	2.42	0.50
1:A:66:LEU:HD13	1:A:299[B]:ARG:HD2	1.94	0.50
1:B:24:ALA:HB3	1:B:25:PRO:HD3	1.94	0.49
1:A:66:LEU:HD11	1:A:299[B]:ARG:CD	2.42	0.49
1:A:260:ALA:O	1:A:264:THR:HG23	2.13	0.49
1:B:126:GLU:HG2	1:B:153:LYS:HD3	1.96	0.47
1:A:310:LYS:CE	1:A:310:LYS:H	2.29	0.46
1:A:91[A]:ASP:OD2	1:A:241[A]:ASN:OD1	2.33	0.45
1:B:142:ARG:O	1:B:143[B]:GLN:HG2	2.17	0.44
1:B:310:LYS:HE2	1:B:310:LYS:N	2.32	0.44
1:B:260:ALA:O	1:B:264:THR:HG23	2.18	0.44
1:A:63[A]:MET:HB2	1:A:63[A]:MET:HE2	1.76	0.43
1:A:101:SER:O	1:A:105:LYS:HG3	2.19	0.43
1:A:123:ALA:HA	1:A:156:ILE:HD12	1.99	0.43
1:B:358:LEU:HD21	2:B:501:FAD:HM73	2.01	0.43
1:A:93:MET:HG2	1:A:97:ILE:CD1	2.49	0.43
1:A:318[A]:MET:HB2	1:A:318[A]:MET:HE2	1.81	0.42
1:B:142:ARG:C	1:B:143[B]:GLN:HG2	2.38	0.42
1:A:208:ASN:HB2	5:A:819:HOH:O	2.19	0.42
1:A:130:GLY:HA3	2:A:501:FAD:O2P	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:VAL:HG22	1:A:349[B]:VAL:HG12	2.00	0.42
1:A:126:GLU:HG2	1:A:153:LYS:HD3	2.02	0.42
1:B:133:LEU:HD11	3:B:502:4KX:H6P	2.01	0.41
1:A:106:GLU:OE2	1:A:110:ARG:HD3	2.20	0.41
1:B:77:ARG:HA	1:B:251:GLY:O	2.20	0.41
1:B:10:LEU:HD23	1:B:10:LEU:HA	1.88	0.41
1:B:299[B]:ARG:NE	1:B:303:GLU:OE2	2.52	0.41
1:A:52:PRO:HB3	1:A:63[A]:MET:HE1	2.01	0.41
1:B:53:LEU:HD13	1:B:68:LEU:HD22	2.02	0.40
1:A:170:TYR:CD1	1:A:173:PRO:HA	2.56	0.40
1:B:297[B]:LEU:HD23	1:B:297[B]:LEU:HA	1.90	0.40
1:A:94:LEU:N	1:A:95:PRO:CD	2.85	0.40
1:A:202:GLY:O	1:A:203:MET:C	2.60	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	388/412 (94%)	381 (98%)	6 (2%)	1 (0%)	41 18
1	B	386/412 (94%)	380 (98%)	6 (2%)	0	100 100
All	All	774/824 (94%)	761 (98%)	12 (2%)	1 (0%)	51 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LYS

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	310/328 (94%)	307 (99%)	3 (1%)	76 57
1	B	308/328 (94%)	305 (99%)	3 (1%)	76 57
All	All	618/656 (94%)	612 (99%)	6 (1%)	81 57

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LYS
1	A	357	LYS
1	A	362	TYR
1	B	241[A]	ASN
1	B	241[B]	ASN
1	B	362	TYR

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

Mol	Chain	Res	Type
1	B	367	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	4KX	A	502	-	49,59,59	2.38	17 (34%)	58,87,87	2.01	16 (27%)
4	GOL	A	504	-	5,5,5	1.21	1 (20%)	5,5,5	1.31	1 (20%)
3	4KX	B	502	-	49,59,59	2.57	17 (34%)	58,87,87	2.34	18 (31%)
4	GOL	A	503	-	5,5,5	1.35	1 (20%)	5,5,5	0.44	0
4	GOL	B	503	-	5,5,5	1.30	0	5,5,5	0.91	0
2	FAD	A	501	-	53,58,58	1.95	8 (15%)	68,89,89	2.10	23 (33%)
2	FAD	B	501	-	53,58,58	2.23	15 (28%)	68,89,89	1.87	20 (29%)
4	GOL	B	504	-	5,5,5	2.48	4 (80%)	5,5,5	1.71	2 (40%)

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	4KX	A	502	-	-	2/48/79/79	0/4/4/4
4	GOL	A	504	-	-	2/4/4/4	-
3	4KX	B	502	-	-	2/48/79/79	0/4/4/4
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	B	503	-	-	0/4/4/4	-
2	FAD	A	501	-	-	7/30/50/50	0/6/6/6
2	FAD	B	501	-	-	6/30/50/50	0/5/6/6
4	GOL	B	504	-	-	1/4/4/4	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C2'-C3'	-7.63	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C4X-N5	7.55	1.45	1.30
3	A	502	4KX	C3B-C4B	7.45	1.53	1.33
3	B	502	4KX	C3B-C4B	7.35	1.52	1.33
2	B	501	FAD	C2'-C3'	-7.27	1.39	1.53
3	B	502	4KX	O4D-C1D	-7.14	1.31	1.41
2	A	501	FAD	C4X-N5	6.59	1.43	1.30
3	B	502	4KX	C5P-N4P	5.98	1.47	1.33
3	A	502	4KX	O4D-C1D	-5.70	1.33	1.41
3	B	502	4KX	C7B-C2B	5.64	1.49	1.34
3	A	502	4KX	C7B-C2B	5.37	1.48	1.34
2	A	501	FAD	C10-N10	4.84	1.47	1.37
3	A	502	4KX	C6B-C7B	-4.71	1.37	1.50
3	B	502	4KX	C6B-C7B	-4.64	1.38	1.50
2	B	501	FAD	C10-N1	4.49	1.42	1.33
3	A	502	4KX	C1B-S1P	3.98	1.88	1.77
3	A	502	4KX	OAP-CAP	3.87	1.49	1.42
3	A	502	4KX	C9P-N8P	3.73	1.41	1.33
3	B	502	4KX	C4A-N3A	-3.69	1.30	1.35
3	A	502	4KX	C5P-N4P	3.63	1.41	1.33
4	B	504	GOL	C1-C2	3.36	1.65	1.51
2	B	501	FAD	O2'-C2'	-3.30	1.36	1.43
2	B	501	FAD	C7M-C7	3.29	1.57	1.51
3	A	502	4KX	C6A-N6A	3.26	1.46	1.34
3	B	502	4KX	C3B-C2B	-3.20	1.36	1.43
3	B	502	4KX	C9P-N8P	3.19	1.40	1.33
3	A	502	4KX	O57-C1B	3.17	1.29	1.22
3	B	502	4KX	C6P-C5P	-3.09	1.45	1.51
2	B	501	FAD	C3B-C4B	-3.07	1.45	1.53
3	B	502	4KX	C6A-N6A	3.06	1.45	1.34
2	A	501	FAD	O4-C4	3.05	1.29	1.23
3	B	502	4KX	OAP-CAP	3.04	1.47	1.42
2	B	501	FAD	C9-C8	2.95	1.43	1.39
2	B	501	FAD	O2-C2	2.91	1.29	1.24
2	B	501	FAD	C10-N10	2.89	1.43	1.37
3	B	502	4KX	C2P-S1P	-2.87	1.69	1.81
2	B	501	FAD	O3'-C3'	-2.86	1.36	1.43
2	A	501	FAD	C5X-N5	2.85	1.45	1.39
2	A	501	FAD	C1'-C2'	-2.83	1.48	1.52
3	A	502	4KX	O2D-C2D	-2.81	1.36	1.43
4	B	504	GOL	O1-C1	2.76	1.54	1.42
2	B	501	FAD	O4B-C1B	2.65	1.44	1.41
4	B	504	GOL	O3-C3	2.60	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	4KX	C3B-C2B	-2.54	1.38	1.43
3	A	502	4KX	P3D-O3D	-2.51	1.54	1.59
2	A	501	FAD	C4A-N3A	-2.50	1.32	1.35
3	B	502	4KX	O2D-C2D	-2.50	1.37	1.43
3	B	502	4KX	O3D-C3D	-2.48	1.35	1.44
3	B	502	4KX	O57-C1B	2.46	1.28	1.22
2	B	501	FAD	C4A-N3A	-2.46	1.32	1.35
2	B	501	FAD	C1'-C2'	2.46	1.56	1.52
2	B	501	FAD	C2-N1	2.45	1.42	1.36
4	A	503	GOL	O1-C1	2.45	1.52	1.42
4	A	504	GOL	O3-C3	-2.44	1.32	1.42
3	B	502	4KX	C1B-S1P	2.40	1.84	1.77
2	A	501	FAD	O2'-C2'	-2.32	1.38	1.43
4	B	504	GOL	C3-C2	2.23	1.60	1.51
3	A	502	4KX	O9P-C9P	-2.21	1.19	1.23
2	B	501	FAD	O3B-C3B	2.13	1.48	1.43
3	B	502	4KX	P3D-O3D	-2.10	1.55	1.59
3	A	502	4KX	C5B-C4B	2.09	1.56	1.48
3	A	502	4KX	C6P-C5P	-2.04	1.47	1.51
3	A	502	4KX	O3D-C3D	-2.01	1.36	1.44

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	4KX	C2P-S1P-C1B	7.83	109.63	99.80
3	A	502	4KX	C2P-S1P-C1B	7.29	108.96	99.80
2	A	501	FAD	N3A-C2A-N1A	-5.52	120.05	128.68
2	B	501	FAD	C10-C4X-N5	-5.18	113.87	124.86
3	B	502	4KX	O6A-CCP-CBP	-5.15	102.27	110.55
2	A	501	FAD	O4'-C4'-C5'	-4.93	98.85	109.92
2	A	501	FAD	C6-C5X-C9A	4.89	125.85	118.94
2	A	501	FAD	C9A-C5X-N5	-4.71	117.31	122.43
3	B	502	4KX	N3A-C2A-N1A	-4.61	121.47	128.68
3	A	502	4KX	O4D-C1D-C2D	-4.47	100.39	106.93
2	A	501	FAD	C5X-C9A-N10	4.43	122.53	117.95
3	B	502	4KX	C3P-N4P-C5P	-4.30	114.85	122.84
3	A	502	4KX	CEP-CBP-CCP	4.19	115.06	108.23
2	A	501	FAD	O3'-C3'-C2'	4.19	118.93	108.81
3	A	502	4KX	O6A-CCP-CBP	-4.13	103.91	110.55
3	B	502	4KX	CEP-CBP-CCP	4.09	114.91	108.23
3	B	502	4KX	C2P-C3P-N4P	-3.97	104.08	112.42
3	B	502	4KX	C5B-C4B-C3B	-3.96	115.08	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	4KX	C5B-C4B-C3B	-3.92	115.17	122.99
3	B	502	4KX	O4D-C1D-C2D	-3.89	101.24	106.93
3	A	502	4KX	N3A-C2A-N1A	-3.86	122.64	128.68
3	B	502	4KX	O57-C1B-S1P	-3.75	111.77	122.29
2	A	501	FAD	O2-C2-N1	-3.71	115.69	121.83
2	B	501	FAD	P-O3P-PA	-3.70	120.13	132.83
2	B	501	FAD	C4X-C10-N1	-3.68	116.19	124.73
3	B	502	4KX	C7P-C6P-C5P	3.67	118.47	112.36
2	A	501	FAD	C2A-N1A-C6A	3.65	125.00	118.75
2	B	501	FAD	C3B-C2B-C1B	-3.57	95.61	100.98
2	B	501	FAD	O2'-C2'-C3'	3.51	117.62	109.10
3	B	502	4KX	O5D-P1A-O2A	3.18	121.49	109.07
2	B	501	FAD	C1'-N10-C9A	-3.17	115.22	120.51
3	B	502	4KX	C5B-C6B-C7B	-3.16	112.13	119.32
4	B	504	GOL	O2-C2-C3	3.15	122.99	109.12
3	A	502	4KX	C3P-N4P-C5P	-3.07	117.13	122.84
2	B	501	FAD	O2'-C2'-C1'	3.03	117.14	109.80
3	B	502	4KX	C6P-C7P-N8P	-2.98	105.89	111.90
3	A	502	4KX	CEP-CBP-CAP	2.97	113.98	108.82
2	B	501	FAD	C4-C4X-C10	2.96	121.77	116.79
3	B	502	4KX	O8A-P3D-O7A	2.84	121.80	110.68
2	A	501	FAD	C4-C4X-N5	-2.82	114.23	118.23
2	B	501	FAD	C9A-N10-C10	-2.79	116.42	120.77
2	B	501	FAD	N3A-C2A-N1A	-2.78	124.33	128.68
2	A	501	FAD	C9-C9A-C5X	-2.77	114.87	120.11
2	A	501	FAD	O5'-C5'-C4'	2.76	116.72	109.36
2	A	501	FAD	C1'-N10-C9A	-2.70	116.01	120.51
3	A	502	4KX	C4A-C5M-N7A	-2.69	106.59	109.40
3	B	502	4KX	O2D-C2D-C3D	2.66	118.72	111.17
2	B	501	FAD	C5A-C6A-N1A	-2.66	114.33	120.35
3	B	502	4KX	C7P-N8P-C9P	-2.64	117.89	122.59
2	A	501	FAD	O2P-P-O1P	2.63	125.23	112.24
2	A	501	FAD	O2'-C2'-C3'	2.62	115.47	109.10
2	A	501	FAD	O2-C2-N3	2.60	123.71	118.65
2	A	501	FAD	O4'-C4'-C3'	2.60	115.42	109.10
3	A	502	4KX	C2P-C3P-N4P	-2.59	106.97	112.42
2	B	501	FAD	C4'-C3'-C2'	2.57	118.70	113.36
4	A	504	GOL	C3-C2-C1	-2.57	101.72	111.70
3	A	502	4KX	O2D-C2D-C3D	2.55	118.41	111.17
2	B	501	FAD	O3B-C3B-C2B	-2.55	103.59	111.82
2	A	501	FAD	C9A-N10-C10	-2.49	116.89	120.77
3	A	502	4KX	O57-C1B-S1P	-2.46	115.39	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FAD	N6A-C6A-N1A	2.43	123.61	118.57
2	B	501	FAD	O2-C2-N1	-2.42	117.82	121.83
2	B	501	FAD	C4X-C10-N10	2.41	120.00	116.48
2	B	501	FAD	C2B-C3B-C4B	2.40	107.30	102.64
2	A	501	FAD	C3B-C2B-C1B	-2.38	97.39	100.98
3	A	502	4KX	CDP-CBP-CCP	2.35	112.06	108.23
2	B	501	FAD	O2A-PA-O1A	2.32	123.69	112.24
2	A	501	FAD	C5A-C6A-N1A	-2.27	115.20	120.35
2	B	501	FAD	C4-N3-C2	-2.22	121.54	125.64
3	B	502	4KX	O5P-C5P-N4P	-2.21	118.84	123.01
3	A	502	4KX	C3D-C2D-C1D	2.21	104.79	99.89
2	A	501	FAD	O3B-C3B-C4B	2.21	117.44	111.05
2	B	501	FAD	N6A-C6A-N1A	2.19	123.11	118.57
2	A	501	FAD	O3B-C3B-C2B	-2.16	104.84	111.82
2	A	501	FAD	C4X-C10-N10	-2.12	113.38	116.48
4	B	504	GOL	C3-C2-C1	-2.12	103.47	111.70
3	A	502	4KX	O8A-P3D-O7A	2.09	118.88	110.68
3	B	502	4KX	O9P-C9P-N8P	2.05	127.39	122.99
3	A	502	4KX	C7P-N8P-C9P	-2.03	118.97	122.59
2	B	501	FAD	O5'-P-O1P	-2.02	101.16	109.07

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C2'-C1'-N10-C10
2	B	501	FAD	C5B-O5B-PA-O1A
2	B	501	FAD	C2'-C1'-N10-C10
2	B	501	FAD	O2'-C2'-C3'-C4'
3	A	502	4KX	O57-C1B-C2B-C7B
3	A	502	4KX	C5P-C6P-C7P-N8P
3	B	502	4KX	O57-C1B-C2B-C7B
3	B	502	4KX	C5P-C6P-C7P-N8P
4	A	504	GOL	C1-C2-C3-O3
2	A	501	FAD	O3'-C3'-C4'-O4'
2	A	501	FAD	O2'-C2'-C3'-C4'
4	A	504	GOL	O2-C2-C3-O3
4	B	504	GOL	O1-C1-C2-C3
2	B	501	FAD	O2'-C2'-C3'-O3'
2	A	501	FAD	C5B-O5B-PA-O3P
2	B	501	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	B	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	O3'-C3'-C4'-C5'
2	A	501	FAD	C5B-O5B-PA-O2A

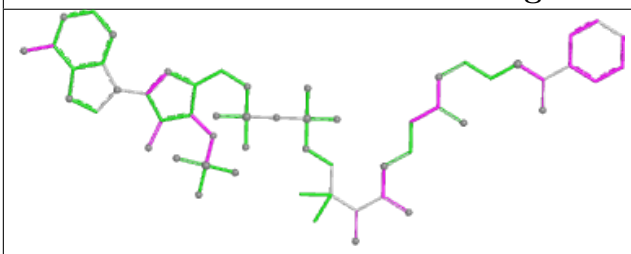
There are no ring outliers.

3 monomers are involved in 3 short contacts:

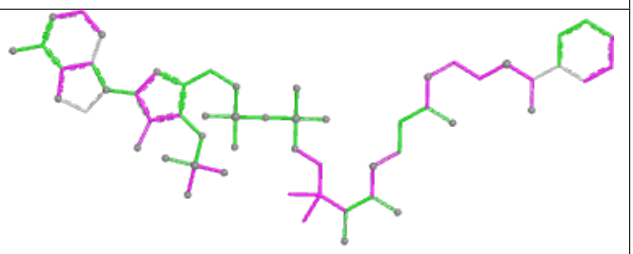
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	4KX	1	0
2	A	501	FAD	1	0
2	B	501	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

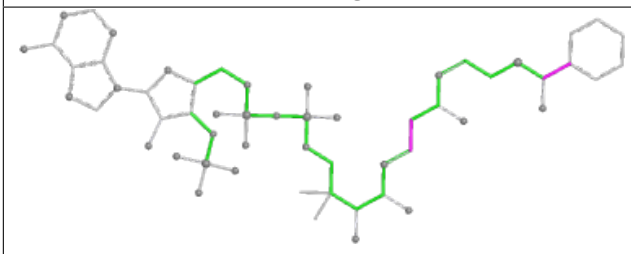
Ligand 4KX A 502



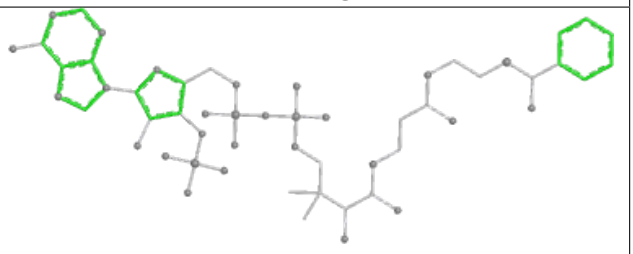
Bond lengths



Bond angles

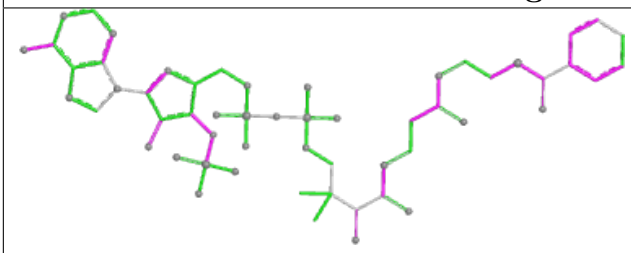


Torsions

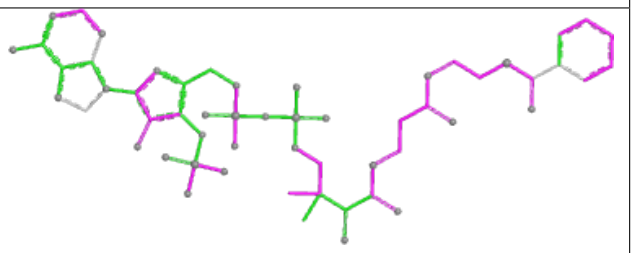


Rings

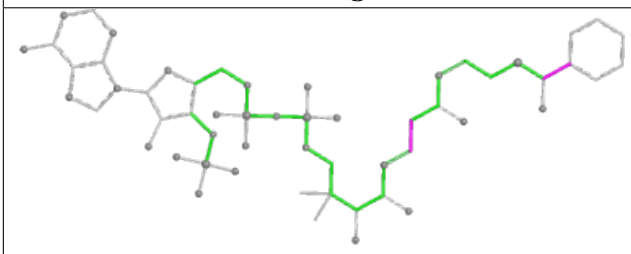
Ligand 4KX B 502



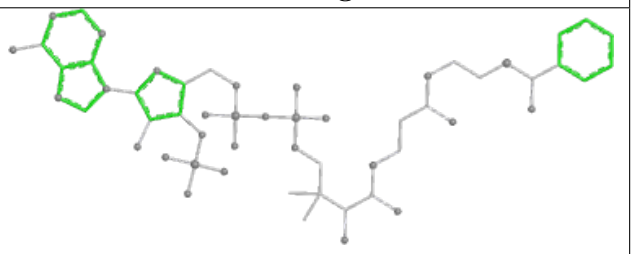
Bond lengths



Bond angles

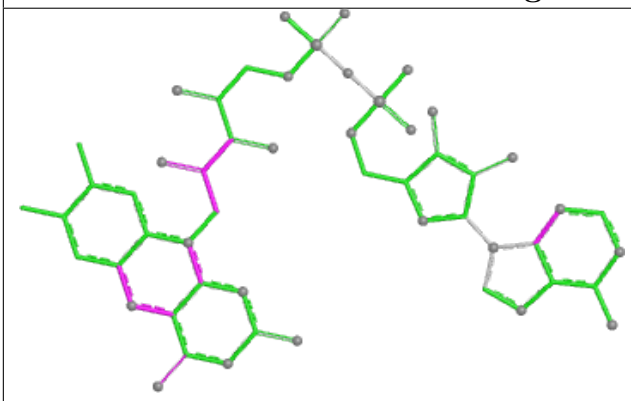


Torsions

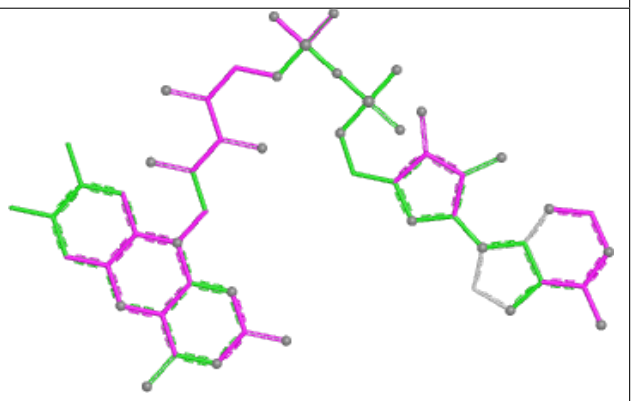


Rings

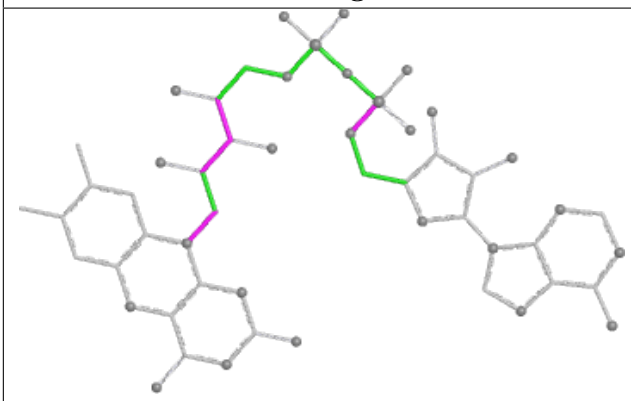
Ligand FAD A 501



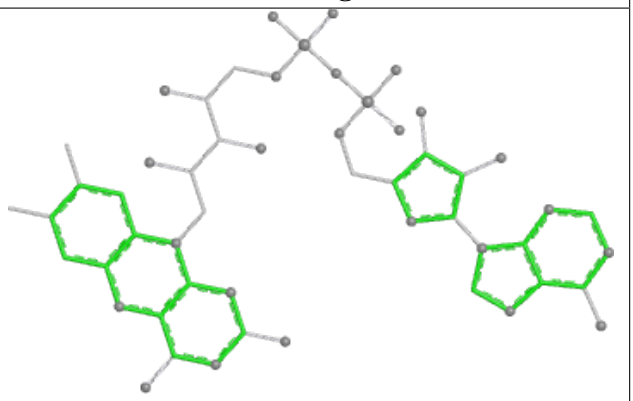
Bond lengths



Bond angles

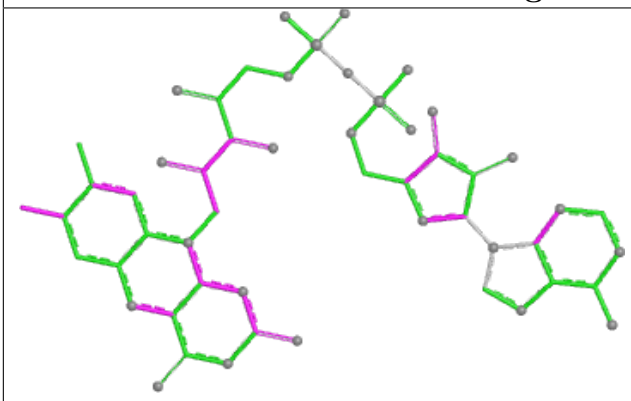


Torsions

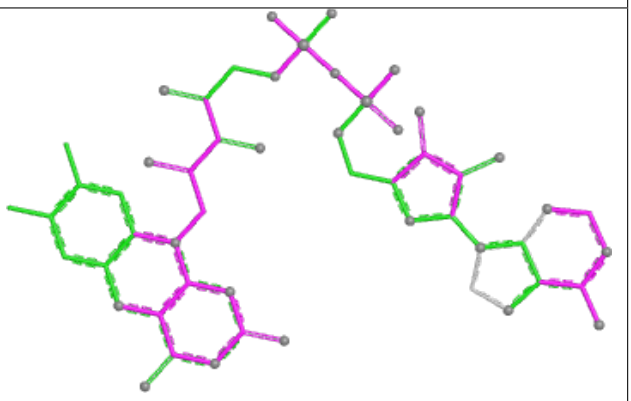


Rings

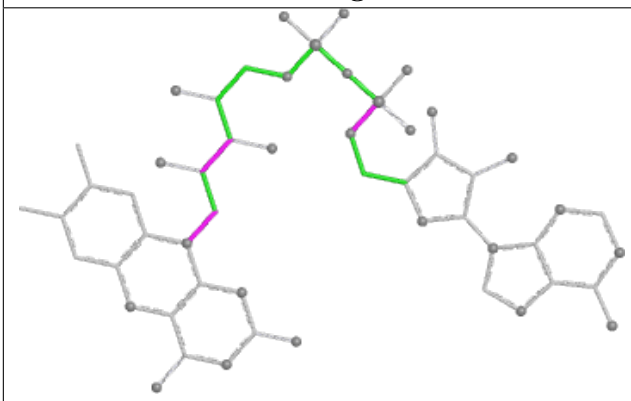
Ligand FAD B 501



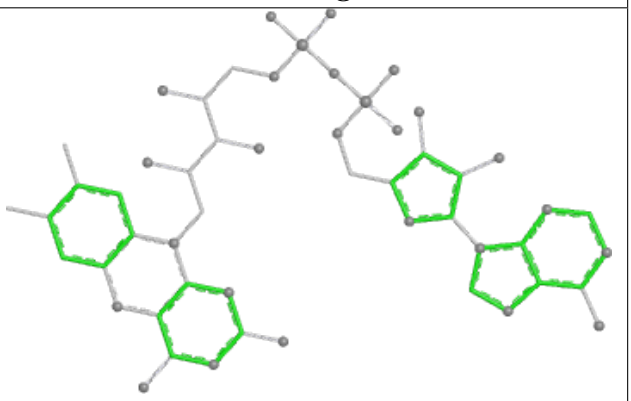
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	380/412 (92%)	0.72	20 (5%) 26 29	13, 24, 46, 80	0
1	B	379/412 (91%)	0.78	35 (9%) 9 9	16, 27, 47, 75	0
All	All	759/824 (92%)	0.75	55 (7%) 15 16	13, 25, 46, 80	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	HIS	6.1
1	B	10	LEU	5.8
1	B	6	GLU	5.5
1	A	5	THR	5.4
1	B	310	LYS	5.3
1	B	7	GLU	5.2
1	A	4	LEU	5.1
1	B	329[A]	ARG	4.7
1	A	7	GLU	4.7
1	A	310	LYS	4.6
1	B	5	THR	4.5
1	A	1	MET	4.4
1	A	6	GLU	4.2
1	B	3	HIS	4.0
1	B	174	GLU	3.9
1	B	2	LYS	3.8
1	B	380	PRO	3.6
1	B	47	LEU	3.5
1	B	190	PRO	3.1
1	A	10	LEU	3.0
1	B	9	LYS	3.0
1	A	290	ALA	3.0
1	A	2	LYS	2.9
1	A	215	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	4	LEU	2.8
1	B	290	ALA	2.8
1	A	335	VAL	2.7
1	B	335	VAL	2.6
1	B	297[A]	LEU	2.6
1	B	252	ILE	2.6
1	A	349[A]	VAL	2.6
1	B	291	VAL	2.5
1	B	362	TYR	2.5
1	B	14	MET	2.5
1	A	380	PRO	2.5
1	B	58	TYR	2.5
1	B	330	VAL	2.4
1	B	285	ALA	2.3
1	B	21	ARG	2.3
1	B	262	ARG	2.3
1	A	362	TYR	2.3
1	B	18	VAL	2.3
1	A	327	ALA	2.2
1	A	197	ASN	2.2
1	A	194	TYR	2.2
1	B	57	ALA	2.1
1	B	299[A]	ARG	2.1
1	B	289	THR	2.1
1	B	270	PHE	2.1
1	B	361	ILE	2.1
1	B	46	LYS	2.1
1	B	56	ALA	2.1
1	A	174	GLU	2.0
1	B	134	LEU	2.0
1	A	328	MET	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)

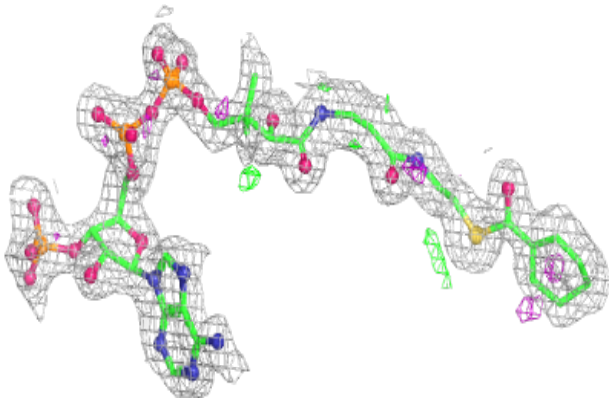
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

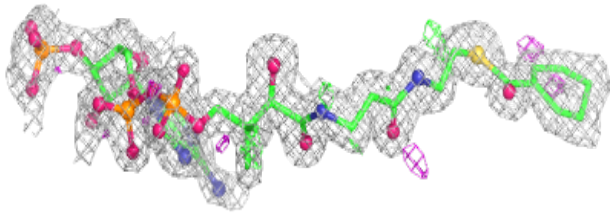
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	504	6/6	0.74	0.18	36,42,43,44	0
4	GOL	B	504	6/6	0.76	0.15	38,41,42,42	0
3	4KX	B	502	56/56	0.77	0.22	21,36,66,70	0
3	4KX	A	502	56/56	0.81	0.17	21,30,66,71	0
4	GOL	B	503	6/6	0.89	0.17	27,30,31,32	0
4	GOL	A	503	6/6	0.89	0.16	23,24,27,27	0
2	FAD	A	501	53/53	0.92	0.10	18,21,24,28	0
2	FAD	B	501	53/53	0.92	0.10	18,21,24,26	0

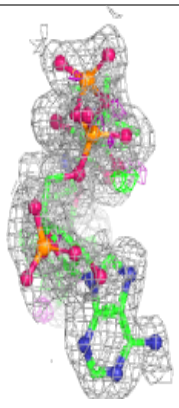
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4KX 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)

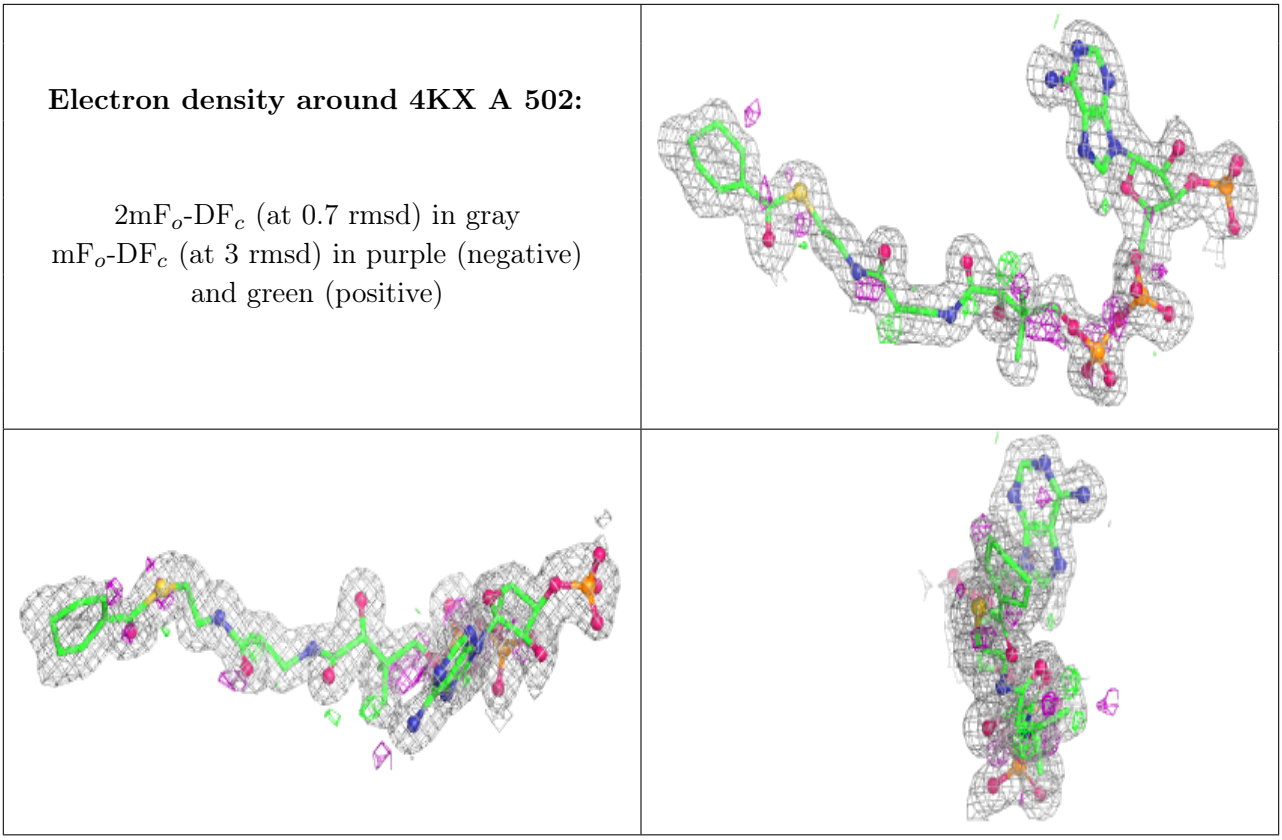






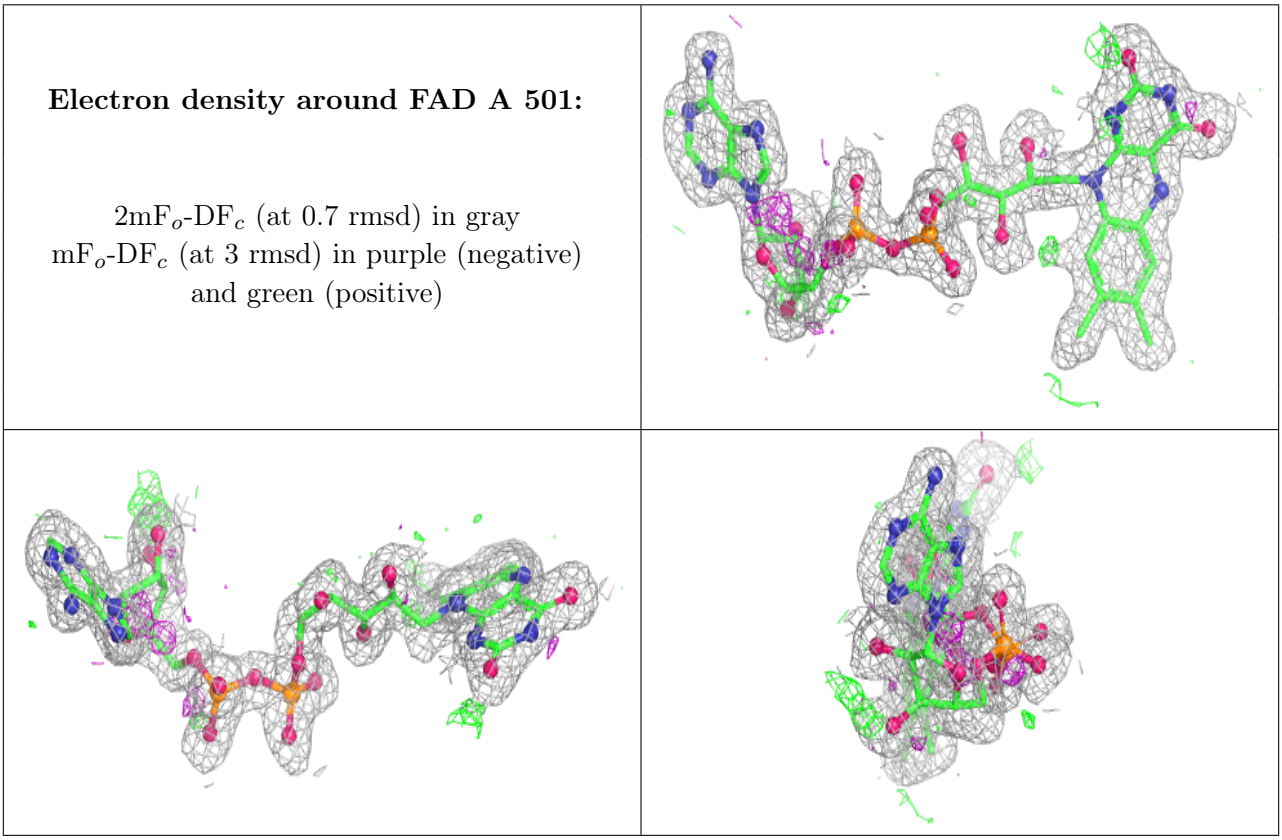
Electron density around 4KX A 502:

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



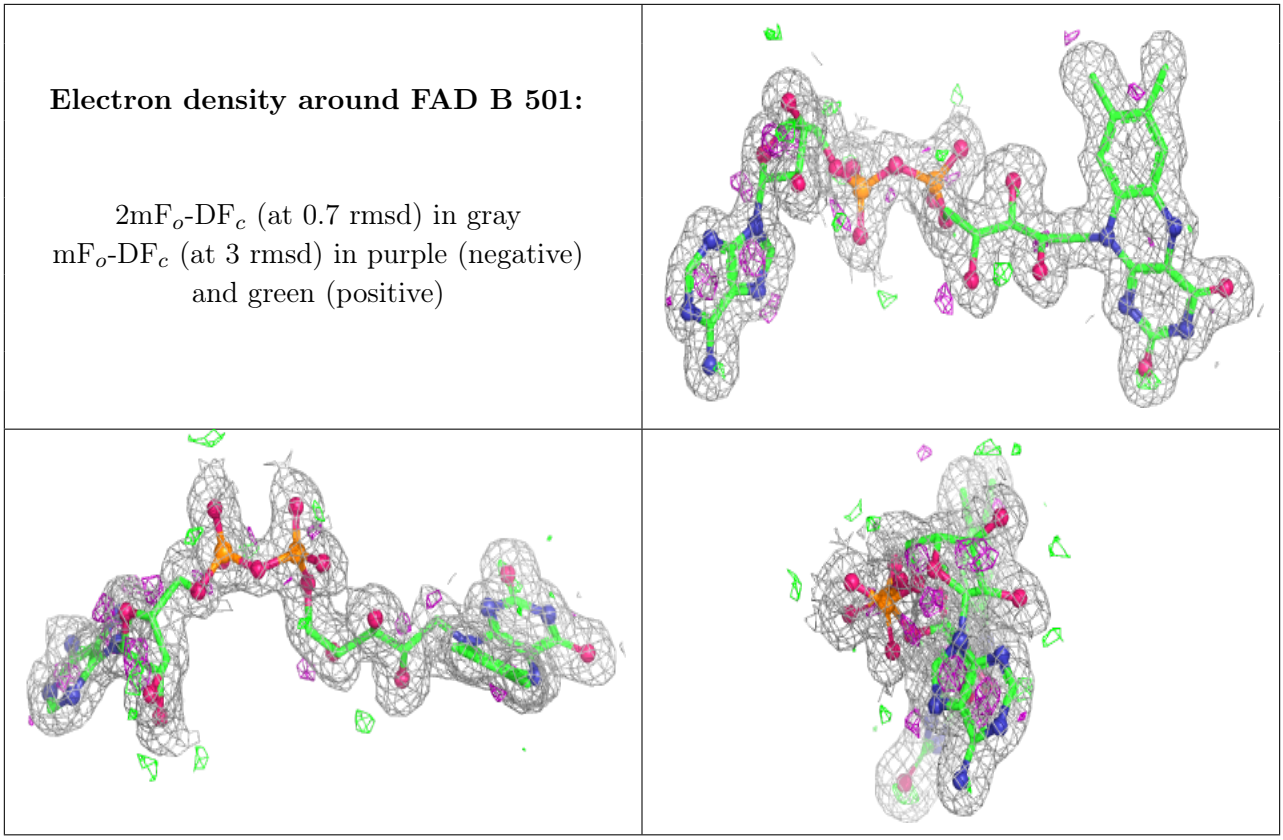
Electron density around FAD A 501:

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



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)



6.5 Other polymers

There are no such residues in this entry.