Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 01:30 pm GMT

PDB ID	:	2VQB
Title	:	Bacterial flavin-containing monooxygenase in complex with NADP: soaking in aerated solution
Authors	:	Alfieri, A.; Malito, E.; Orru, R.; Fraaije, M.W.; Mattevi, A.
Deposited on	:	2008-03-12
Resolution	:	2.80 Å(reported)

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

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

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

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

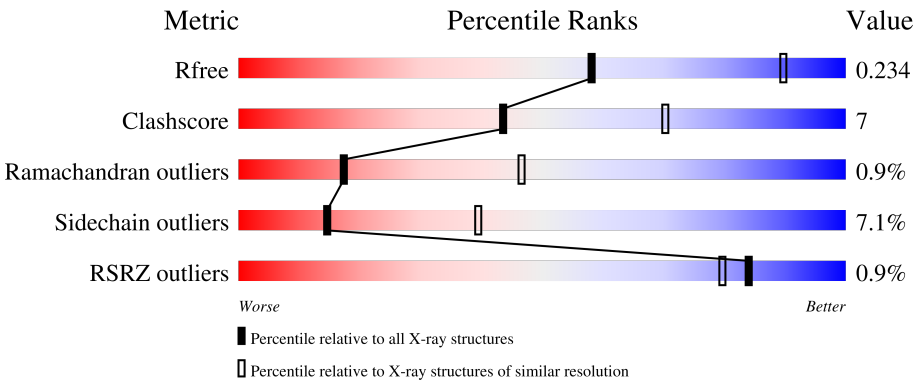
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

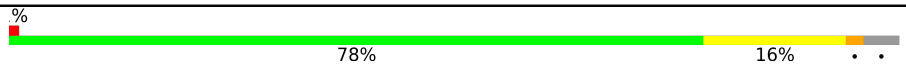
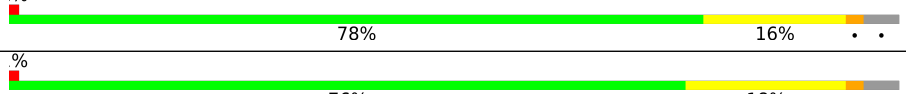
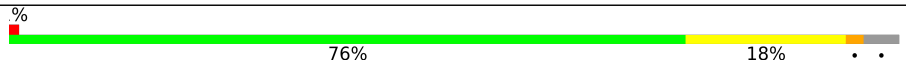
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	461	
1	B	461	
1	C	461	
1	D	461	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15036 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FLAVIN-CONTAINING MONOOXYGENASE.

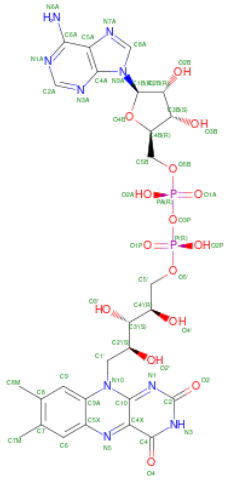
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	3638	2335	603	680	20	0	0	0
1	B	443	3638	2335	603	680	20	0	0	0
1	C	443	3638	2335	603	680	20	0	0	0
1	D	443	3638	2335	603	680	20	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	ALA	GLU	engineered mutation	UNP Q83XK4
A	159	ALA	GLU	engineered mutation	UNP Q83XK4
B	158	ALA	GLU	engineered mutation	UNP Q83XK4
B	159	ALA	GLU	engineered mutation	UNP Q83XK4
C	158	ALA	GLU	engineered mutation	UNP Q83XK4
C	159	ALA	GLU	engineered mutation	UNP Q83XK4
D	158	ALA	GLU	engineered mutation	UNP Q83XK4
D	159	ALA	GLU	engineered mutation	UNP Q83XK4

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

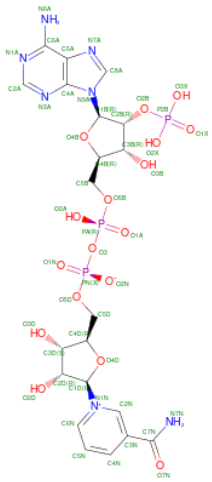
FAD



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

NAP

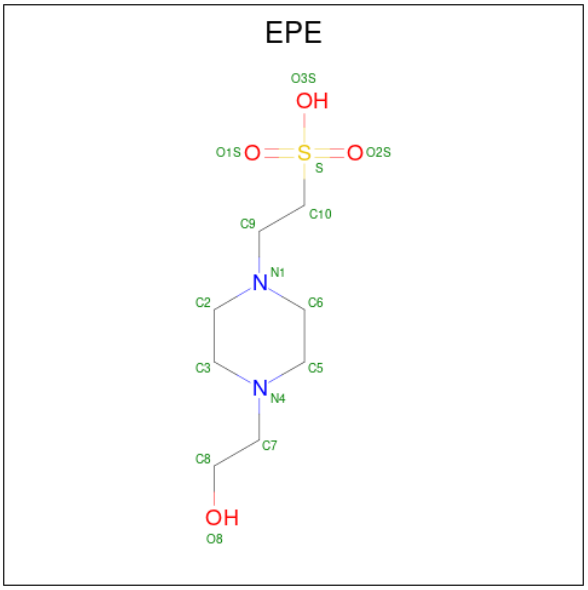


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
3	B	1	48	21	7	17	3	0	0
3	C	1	48	21	7	17	3	0	0
3	D	1	48	21	7	17	3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	15	8	2	4	1	0	0

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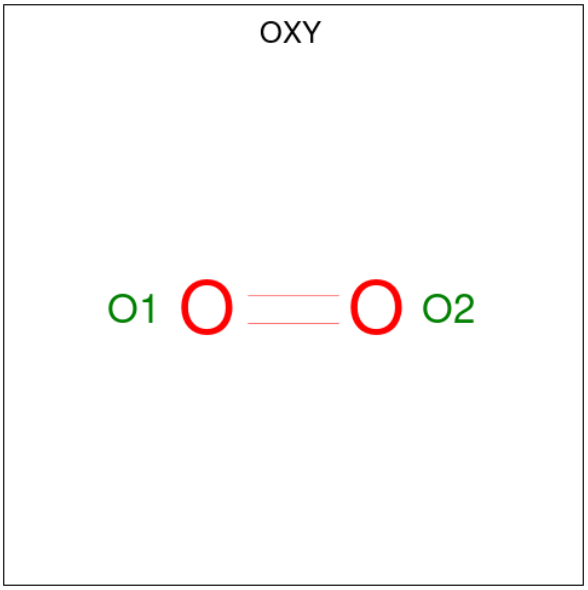
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	C	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	D	1	15	8	2	4	1	0	0

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



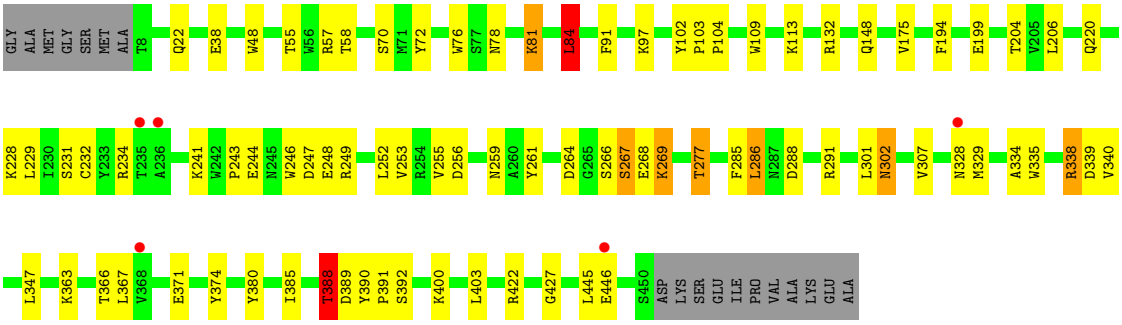
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	1	2	2	0	0
			Total	O		
6	A	1	2	2	0	0
			Total	O		
6	B	1	2	2	0	0
			Total	O		
6	B	1	2	2	0	0
			Total	O		
6	C	1	2	2	0	0
			Total	O		
6	C	1	2	2	0	0
			Total	O		
6	D	1	2	2	0	0
			Total	O		
6	D	1	2	2	0	0

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.

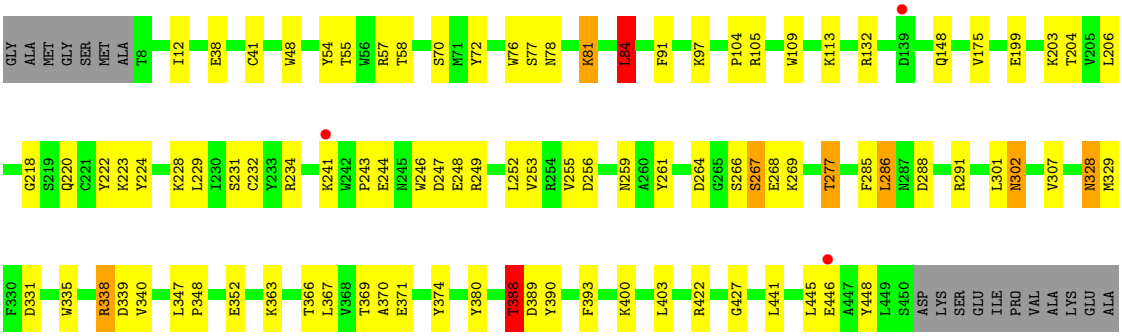
• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain A:



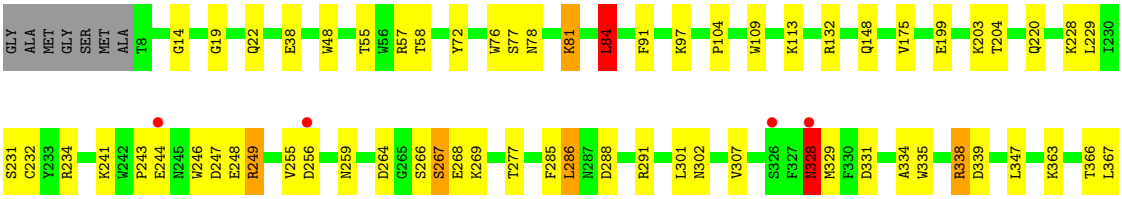
• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

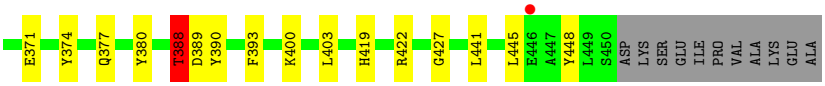
Chain B:



• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

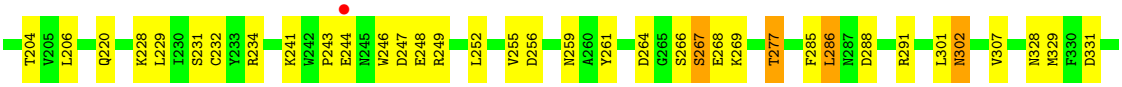
Chain C:

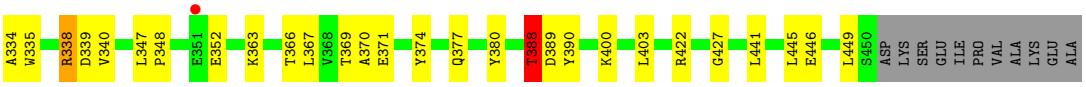




• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	218.66Å 218.66Å 130.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.72 – 2.80 29.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.72-2.80) 99.6 (29.72-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.242 0.219 , 0.234	Depositor DCC
R_{free} test set	4332 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 21.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15036	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: EPE, OXY, NAP, FAD, CL

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	0.61	0/3752	0.67	2/5095 (0.0%)
1	B	0.63	0/3752	0.68	2/5095 (0.0%)
1	C	0.61	0/3752	0.68	2/5095 (0.0%)
1	D	0.59	0/3752	0.66	2/5095 (0.0%)
All	All	0.61	0/15008	0.67	8/20380 (0.0%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	LEU	CA-CB-CG	7.13	131.71	115.30
1	C	445	LEU	CA-CB-CG	6.65	130.59	115.30
1	D	445	LEU	CA-CB-CG	6.61	130.50	115.30
1	D	84	LEU	CA-CB-CG	6.54	130.34	115.30
1	C	84	LEU	CA-CB-CG	6.41	130.05	115.30
1	B	84	LEU	CA-CB-CG	6.38	129.98	115.30
1	A	445	LEU	CA-CB-CG	6.34	129.88	115.30
1	B	445	LEU	CA-CB-CG	6.11	129.34	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	388	THR	Peptide
1	B	388	THR	Peptide
1	C	388	THR	Peptide
1	D	388	THR	Peptide

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	3638	0	3428	46	0
1	B	3638	0	3428	55	0
1	C	3638	0	3428	47	0
1	D	3638	0	3428	49	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
3	A	48	0	25	2	0
3	B	48	0	25	3	0
3	C	48	0	25	2	0
3	D	48	0	25	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	15	0	17	4	0
5	B	15	0	17	5	0
5	C	15	0	17	0	0
5	D	15	0	17	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
All	All	15036	0	14004	195	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 7.

All (195) 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)
5:A:1452:EPE:H21	5:B:1452:EPE:H21	1.21	1.17
1:C:388:THR:HG22	1:C:390:TYR:H	1.36	0.89
1:C:422:ARG:HD3	1:C:427:GLY:O	1.79	0.82
1:D:422:ARG:HD3	1:D:427:GLY:O	1.80	0.81
1:A:335:TRP:HB3	1:A:388:THR:HG21	1.63	0.81
1:A:388:THR:HG22	1:A:390:TYR:H	1.46	0.80
1:B:422:ARG:HD3	1:B:427:GLY:O	1.81	0.79
1:A:338:ARG:NH1	1:A:339:ASP:OD1	2.15	0.79
1:D:388:THR:HG22	1:D:390:TYR:H	1.48	0.78
1:B:335:TRP:HB3	1:B:388:THR:HG21	1.65	0.77
1:C:335:TRP:HB3	1:C:388:THR:HG21	1.66	0.76
1:B:388:THR:HG22	1:B:390:TYR:H	1.51	0.75
1:A:285:PHE:CD1	1:A:286:LEU:HD13	2.21	0.75
1:D:335:TRP:HB3	1:D:388:THR:HG21	1.69	0.74
1:B:57:ARG:NH2	1:C:175:VAL:O	2.20	0.74
1:D:285:PHE:CD1	1:D:286:LEU:HD13	2.23	0.73
1:A:422:ARG:HD3	1:A:427:GLY:O	1.88	0.72
1:D:338:ARG:NH1	1:D:339:ASP:OD1	2.23	0.71
1:B:338:ARG:NH1	1:B:339:ASP:OD1	2.23	0.71
1:A:57:ARG:NH2	1:D:175:VAL:O	2.24	0.71
1:A:301:LEU:O	1:A:302:ASN:HB2	1.89	0.70
1:B:175:VAL:O	1:C:57:ARG:NH2	2.25	0.70
1:B:329:MET:HE2	1:B:380:TYR:HE2	1.55	0.70
1:C:329:MET:HE2	1:C:380:TYR:HE2	1.57	0.69
1:B:285:PHE:CD1	1:B:286:LEU:HD13	2.27	0.69
1:D:329:MET:HE2	1:D:380:TYR:HE2	1.58	0.68
1:C:285:PHE:CD1	1:C:286:LEU:HD13	2.28	0.68
1:C:338:ARG:NH1	1:C:339:ASP:OD1	2.28	0.67
1:D:301:LEU:O	1:D:302:ASN:HB2	1.96	0.65
1:A:329:MET:HE2	1:A:380:TYR:HE2	1.62	0.65
1:C:301:LEU:O	1:C:302:ASN:HB2	1.96	0.65
1:C:388:THR:CG2	1:C:390:TYR:H	2.09	0.64
1:A:175:VAL:O	1:D:57:ARG:NH2	2.31	0.63
1:B:264:ASP:HB3	1:B:266:SER:H	1.63	0.63
1:B:301:LEU:O	1:B:302:ASN:HB2	1.97	0.63
1:A:264:ASP:HB3	1:A:266:SER:H	1.64	0.62
1:C:264:ASP:HB3	1:C:266:SER:H	1.65	0.62
1:B:256:ASP:HB3	1:B:259:ASN:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:CD	1:B:427:GLY:O	2.47	0.61
1:D:264:ASP:HB3	1:D:266:SER:H	1.65	0.61
1:C:422:ARG:CD	1:C:427:GLY:O	2.48	0.61
1:C:81:LYS:HG2	1:C:91:PHE:CE2	2.37	0.60
1:D:256:ASP:HB3	1:D:259:ASN:H	1.67	0.60
1:D:204:THR:HG23	1:D:228:LYS:HB3	1.83	0.60
1:A:204:THR:HG23	1:A:228:LYS:HB3	1.85	0.59
5:A:1452:EPE:H102	5:B:1452:EPE:H62	1.84	0.59
1:C:256:ASP:HB3	1:C:259:ASN:H	1.67	0.59
1:A:256:ASP:HB3	1:A:259:ASN:H	1.66	0.59
1:B:329:MET:HE2	1:B:380:TYR:CE2	2.37	0.59
1:D:388:THR:CG2	1:D:390:TYR:H	2.14	0.59
1:A:388:THR:CG2	1:A:390:TYR:H	2.14	0.58
1:B:204:THR:HG23	1:B:228:LYS:HB3	1.85	0.58
1:C:363:LYS:O	1:C:366:THR:HB	2.03	0.58
1:D:81:LYS:HG2	1:D:91:PHE:CE2	2.39	0.58
1:D:422:ARG:CD	1:D:427:GLY:O	2.50	0.58
1:B:81:LYS:HG2	1:B:91:PHE:CE2	2.39	0.57
1:B:277:THR:HG22	3:B:501:NAP:C4A	2.34	0.57
1:D:363:LYS:O	1:D:366:THR:HB	2.03	0.57
1:A:363:LYS:O	1:A:366:THR:HB	2.05	0.57
1:B:363:LYS:O	1:B:366:THR:HB	2.04	0.57
1:A:76:TRP:HA	1:A:104:PRO:HA	1.87	0.56
1:C:277:THR:HG22	3:C:501:NAP:C4A	2.35	0.56
1:B:76:TRP:HA	1:B:104:PRO:HA	1.88	0.56
5:A:1452:EPE:H21	5:B:1452:EPE:C2	2.15	0.56
1:B:338:ARG:HG3	1:B:339:ASP:N	2.21	0.56
1:B:388:THR:CG2	1:B:390:TYR:H	2.17	0.56
1:C:329:MET:HE2	1:C:380:TYR:CE2	2.38	0.55
1:D:285:PHE:HD1	1:D:286:LEU:HD13	1.70	0.55
1:D:329:MET:HE2	1:D:380:TYR:CE2	2.38	0.55
1:D:277:THR:HG22	3:D:501:NAP:C4A	2.37	0.55
1:A:55:THR:OG1	1:A:57:ARG:HG3	2.07	0.54
1:A:232:CYS:HA	1:A:249:ARG:O	2.07	0.54
1:D:76:TRP:HA	1:D:104:PRO:HA	1.90	0.54
1:C:109:TRP:CE2	1:C:113:LYS:HD2	2.43	0.54
1:A:329:MET:HE2	1:A:380:TYR:CE2	2.42	0.53
1:A:422:ARG:CD	1:A:427:GLY:O	2.54	0.53
1:C:76:TRP:HA	1:C:104:PRO:HA	1.90	0.53
1:C:204:THR:HG23	1:C:228:LYS:HB3	1.91	0.53
1:A:285:PHE:HD1	1:A:286:LEU:HD13	1.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:TRP:CE2	1:B:113:LYS:HD2	2.44	0.52
1:D:109:TRP:CE2	1:D:113:LYS:HD2	2.45	0.52
1:A:81:LYS:HG2	1:A:91:PHE:CE2	2.45	0.51
1:A:277:THR:HG22	3:A:501:NAP:C4A	2.40	0.51
1:B:132:ARG:HH21	1:B:148:GLN:HE21	1.58	0.51
1:D:72:TYR:OH	3:D:501:NAP:H4N	2.10	0.51
1:A:229:LEU:O	1:A:246:TRP:HA	2.10	0.51
1:B:253:VAL:HG22	1:B:261:TYR:O	2.11	0.51
1:A:109:TRP:CE2	1:A:113:LYS:HD2	2.46	0.51
1:D:338:ARG:HG3	1:D:339:ASP:N	2.26	0.51
1:C:267:SER:O	1:C:268:GLU:HG2	2.11	0.50
1:C:371:GLU:HA	1:C:374:TYR:CZ	2.47	0.50
1:B:132:ARG:HH21	1:B:148:GLN:NE2	2.09	0.50
1:A:338:ARG:HG3	1:A:339:ASP:N	2.27	0.50
1:B:288:ASP:OD1	1:B:291:ARG:NH1	2.44	0.50
1:C:132:ARG:HH21	1:C:148:GLN:NE2	2.10	0.49
1:D:288:ASP:OD1	1:D:291:ARG:NH1	2.45	0.49
1:C:72:TYR:OH	3:C:501:NAP:H4N	2.12	0.49
5:A:1452:EPE:C2	5:B:1452:EPE:H21	2.15	0.49
1:A:288:ASP:OD1	1:A:291:ARG:NH1	2.46	0.49
1:C:232:CYS:HA	1:C:249:ARG:O	2.13	0.49
1:C:288:ASP:OD1	1:C:291:ARG:NH1	2.46	0.49
1:B:81:LYS:O	1:B:84:LEU:HD22	2.13	0.48
1:B:231:SER:HB2	1:B:248:GLU:HG2	1.94	0.48
1:D:206:LEU:HD21	1:D:252:LEU:HD22	1.96	0.48
1:D:256:ASP:HB2	1:D:261:TYR:HE1	1.76	0.48
1:D:371:GLU:HA	1:D:374:TYR:CZ	2.49	0.48
1:C:338:ARG:HG3	1:C:339:ASP:N	2.29	0.48
1:D:81:LYS:O	1:D:84:LEU:HD22	2.14	0.48
1:B:203:LYS:HZ2	1:C:203:LYS:HZ1	1.61	0.48
1:B:285:PHE:HD1	1:B:286:LEU:HD13	1.76	0.48
1:C:388:THR:HG22	1:C:390:TYR:N	2.18	0.48
1:D:14:GLY:O	1:D:19:GLY:HA3	2.14	0.47
1:B:371:GLU:HA	1:B:374:TYR:CZ	2.49	0.47
1:A:72:TYR:OH	3:A:501:NAP:H4N	2.15	0.47
1:B:55:THR:OG1	1:B:57:ARG:HG3	2.14	0.47
1:D:232:CYS:HA	1:D:249:ARG:O	2.14	0.47
1:C:109:TRP:NE1	1:C:113:LYS:HD2	2.29	0.47
1:A:253:VAL:HG22	1:A:261:TYR:O	2.15	0.47
1:C:285:PHE:HD1	1:C:286:LEU:HD13	1.79	0.47
1:D:55:THR:OG1	1:D:57:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TYR:HB3	1:A:194:PHE:O	2.15	0.46
1:B:256:ASP:HB2	1:B:261:TYR:HE1	1.79	0.46
1:C:81:LYS:O	1:C:84:LEU:HD22	2.15	0.46
1:D:231:SER:HB2	1:D:248:GLU:HG2	1.96	0.46
1:B:232:CYS:HA	1:B:249:ARG:O	2.15	0.46
1:B:331:ASP:HB3	1:B:390:TYR:CE1	2.51	0.46
1:B:206:LEU:HD21	1:B:252:LEU:HD22	1.97	0.46
1:B:104:PRO:HD3	1:B:448:TYR:CE1	2.51	0.46
1:D:229:LEU:O	1:D:246:TRP:HA	2.15	0.46
1:C:335:TRP:HD1	1:C:388:THR:HG23	1.81	0.46
1:B:277:THR:HG22	3:B:501:NAP:C5A	2.46	0.45
1:A:335:TRP:HB3	1:A:388:THR:CG2	2.42	0.45
1:A:256:ASP:HB2	1:A:261:TYR:HE1	1.81	0.45
5:B:1452:EPE:H31	5:B:1452:EPE:H81	1.85	0.45
1:D:132:ARG:HH21	1:D:148:GLN:HE21	1.65	0.45
1:B:223:LYS:HE2	1:B:224:TYR:CE1	2.52	0.45
1:B:335:TRP:HB3	1:B:388:THR:CG2	2.41	0.45
1:C:231:SER:HB2	1:C:248:GLU:HG2	1.98	0.44
1:C:104:PRO:HD3	1:C:448:TYR:CE1	2.51	0.44
1:A:206:LEU:HD21	1:A:252:LEU:HD22	1.99	0.44
1:B:328:ASN:OD1	1:B:393:PHE:CZ	2.71	0.44
1:A:132:ARG:HH21	1:A:148:GLN:NE2	2.16	0.44
1:B:109:TRP:NE1	1:B:113:LYS:HD2	2.32	0.44
1:A:335:TRP:HD1	1:A:388:THR:HG23	1.83	0.44
1:B:267:SER:O	1:B:268:GLU:HG2	2.17	0.44
1:D:109:TRP:NE1	1:D:113:LYS:HD2	2.33	0.43
1:B:229:LEU:O	1:B:246:TRP:HA	2.18	0.43
1:B:70:SER:HB2	2:B:500:FAD:HM82	2.00	0.43
1:B:203:LYS:NZ	1:C:203:LYS:NZ	2.66	0.43
1:C:76:TRP:O	1:C:77:SER:C	2.56	0.43
1:D:267:SER:O	1:D:268:GLU:HG2	2.18	0.43
1:B:203:LYS:NZ	1:C:203:LYS:HZ1	2.15	0.43
1:A:371:GLU:HA	1:A:374:TYR:CZ	2.54	0.43
1:B:72:TYR:OH	3:B:501:NAP:H4N	2.19	0.43
1:D:132:ARG:HH21	1:D:148:GLN:NE2	2.16	0.43
1:D:9:ARG:HG3	1:D:38:GLU:HB2	2.01	0.43
1:A:81:LYS:O	1:A:84:LEU:HD22	2.18	0.43
1:A:301:LEU:O	1:A:302:ASN:CB	2.62	0.43
1:C:229:LEU:O	1:C:246:TRP:HA	2.19	0.42
1:B:222:TYR:HB2	1:B:229:LEU:HD11	2.02	0.42
1:B:76:TRP:O	1:B:77:SER:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLY:HA3	1:B:246:TRP:CH2	2.55	0.42
1:B:369:THR:O	1:B:370:ALA:C	2.56	0.42
1:D:331:ASP:HB3	1:D:390:TYR:CE1	2.54	0.42
1:A:267:SER:O	1:A:268:GLU:HG2	2.19	0.42
1:B:335:TRP:HD1	1:B:388:THR:HG23	1.85	0.42
1:C:14:GLY:O	1:C:19:GLY:HA3	2.19	0.42
1:D:348:PRO:HB2	1:D:352:GLU:HB2	2.01	0.42
1:B:54:TYR:HB2	1:B:105:ARG:CZ	2.50	0.42
1:C:331:ASP:HB3	1:C:390:TYR:CE1	2.55	0.42
1:A:385:ILE:HD12	1:A:392:SER:HA	2.01	0.42
1:C:419:HIS:CD2	1:C:419:HIS:N	2.88	0.42
1:D:369:THR:O	1:D:370:ALA:C	2.58	0.42
1:A:70:SER:HB2	2:A:500:FAD:HM82	2.02	0.41
1:A:132:ARG:HH21	1:A:148:GLN:HE21	1.68	0.41
1:B:12:ILE:O	1:B:41:CYS:HA	2.20	0.41
1:C:328:ASN:OD1	1:C:393:PHE:CZ	2.73	0.41
1:D:70:SER:HB2	2:D:500:FAD:HM82	2.03	0.41
1:B:348:PRO:HB2	1:B:352:GLU:HB2	2.03	0.41
1:D:76:TRP:O	1:D:77:SER:C	2.57	0.41
1:A:22:GLN:HA	1:A:334:ALA:HB1	2.02	0.41
1:D:335:TRP:HD1	1:D:388:THR:HG23	1.86	0.41
1:C:55:THR:OG1	1:C:57:ARG:HG3	2.21	0.41
1:C:132:ARG:HH21	1:C:148:GLN:HE21	1.67	0.41
1:D:335:TRP:HB3	1:D:388:THR:CG2	2.44	0.41
1:A:269:LYS:HE3	1:A:269:LYS:HB2	1.87	0.41
1:C:329:MET:HE3	1:C:377:GLN:HG3	2.03	0.41
1:D:97:LYS:NZ	1:D:449:LEU:O	2.54	0.41
1:A:390:TYR:HA	1:A:391:PRO:HD3	1.96	0.41
1:A:102:TYR:N	1:A:103:PRO:HD3	2.36	0.40
1:D:12:ILE:O	1:D:41:CYS:HA	2.21	0.40
1:C:22:GLN:HA	1:C:334:ALA:HB1	2.03	0.40
1:D:22:GLN:HA	1:D:334:ALA:HB1	2.03	0.40
1:A:231:SER:HB2	1:A:248:GLU:HG2	2.03	0.40
1:D:329:MET:HE3	1:D:377:GLN:HG3	2.03	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	441/461 (96%)	410 (93%)	27 (6%)	4 (1%)	17	46
1	B	441/461 (96%)	408 (92%)	29 (7%)	4 (1%)	17	46
1	C	441/461 (96%)	408 (92%)	29 (7%)	4 (1%)	17	46
1	D	441/461 (96%)	407 (92%)	30 (7%)	4 (1%)	17	46
All	All	1764/1844 (96%)	1633 (93%)	115 (6%)	16 (1%)	17	46

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	ASP
1	B	389	ASP
1	C	389	ASP
1	D	389	ASP
1	A	81	LYS
1	B	81	LYS
1	C	81	LYS
1	D	81	LYS
1	B	446	GLU
1	D	446	GLU
1	A	446	GLU
1	C	243	PRO
1	C	328	ASN
1	B	243	PRO
1	A	243	PRO
1	D	243	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	385/397 (97%)	358 (93%)	27 (7%)	15	40
1	B	385/397 (97%)	357 (93%)	28 (7%)	14	38
1	C	385/397 (97%)	359 (93%)	26 (7%)	16	42
1	D	385/397 (97%)	357 (93%)	28 (7%)	14	38
All	All	1540/1588 (97%)	1431 (93%)	109 (7%)	14	39

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	48	TRP
1	A	58	THR
1	A	78	ASN
1	A	84	LEU
1	A	97	LYS
1	A	199	GLU
1	A	220	GLN
1	A	234	ARG
1	A	241	LYS
1	A	244	GLU
1	A	247	ASP
1	A	255	VAL
1	A	267	SER
1	A	269	LYS
1	A	277	THR
1	A	286	LEU
1	A	302	ASN
1	A	307	VAL
1	A	328	ASN
1	A	338	ARG
1	A	340	VAL
1	A	347	LEU
1	A	367	LEU
1	A	388	THR
1	A	400	LYS
1	A	403	LEU
1	B	38	GLU
1	B	48	TRP
1	B	58	THR

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Mol	Chain	Res	Type
1	B	78	ASN
1	B	84	LEU
1	B	97	LYS
1	B	199	GLU
1	B	220	GLN
1	B	234	ARG
1	B	241	LYS
1	B	244	GLU
1	B	247	ASP
1	B	255	VAL
1	B	267	SER
1	B	269	LYS
1	B	277	THR
1	B	286	LEU
1	B	302	ASN
1	B	307	VAL
1	B	328	ASN
1	B	338	ARG
1	B	340	VAL
1	B	347	LEU
1	B	367	LEU
1	B	388	THR
1	B	400	LYS
1	B	403	LEU
1	B	441	LEU
1	C	38	GLU
1	C	48	TRP
1	C	58	THR
1	C	78	ASN
1	C	84	LEU
1	C	97	LYS
1	C	199	GLU
1	C	220	GLN
1	C	234	ARG
1	C	241	LYS
1	C	244	GLU
1	C	247	ASP
1	C	249	ARG
1	C	255	VAL
1	C	267	SER
1	C	269	LYS
1	C	286	LEU

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Mol	Chain	Res	Type
1	C	307	VAL
1	C	328	ASN
1	C	338	ARG
1	C	347	LEU
1	C	367	LEU
1	C	388	THR
1	C	400	LYS
1	C	403	LEU
1	C	441	LEU
1	D	38	GLU
1	D	48	TRP
1	D	58	THR
1	D	78	ASN
1	D	84	LEU
1	D	97	LYS
1	D	199	GLU
1	D	220	GLN
1	D	234	ARG
1	D	241	LYS
1	D	244	GLU
1	D	247	ASP
1	D	255	VAL
1	D	267	SER
1	D	269	LYS
1	D	277	THR
1	D	286	LEU
1	D	302	ASN
1	D	307	VAL
1	D	328	ASN
1	D	338	ARG
1	D	340	VAL
1	D	347	LEU
1	D	367	LEU
1	D	388	THR
1	D	400	LYS
1	D	403	LEU
1	D	441	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	128	ASN
1	A	148	GLN
1	A	220	GLN
1	A	328	ASN
1	A	419	HIS
1	B	63	ASN
1	B	78	ASN
1	B	128	ASN
1	B	133	HIS
1	B	148	GLN
1	B	220	GLN
1	B	328	ASN
1	C	63	ASN
1	C	78	ASN
1	C	128	ASN
1	C	148	GLN
1	C	220	GLN
1	C	328	ASN
1	D	63	ASN
1	D	128	ASN
1	D	148	GLN
1	D	220	GLN
1	D	328	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)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	D	500	-	53,58,58	1.24	5 (9%)	68,89,89	1.42	13 (19%)
6	OXY	D	1453	-	1,1,1	0.26	0	-		
2	FAD	C	500	-	53,58,58	1.11	3 (5%)	68,89,89	1.39	10 (14%)
6	OXY	A	1453	-	1,1,1	0.27	0	-		
2	FAD	A	500	-	53,58,58	1.16	5 (9%)	68,89,89	1.48	12 (17%)
3	NAP	C	501	-	45,52,52	1.37	5 (11%)	56,80,80	1.31	5 (8%)
5	EPE	B	1452	-	15,15,15	1.11	1 (6%)	18,20,20	2.21	7 (38%)
3	NAP	A	501	-	45,52,52	1.36	6 (13%)	56,80,80	1.43	7 (12%)
3	NAP	B	501	-	45,52,52	1.31	4 (8%)	56,80,80	1.37	7 (12%)
6	OXY	C	1453	-	1,1,1	0.27	0	-		
5	EPE	D	1452	-	15,15,15	0.86	1 (6%)	18,20,20	2.18	5 (27%)
2	FAD	B	500	-	53,58,58	1.21	5 (9%)	68,89,89	1.40	15 (22%)
5	EPE	C	1451	-	15,15,15	1.18	1 (6%)	18,20,20	2.22	7 (38%)
6	OXY	A	1454	-	1,1,1	0.24	0	-		
5	EPE	A	1452	-	15,15,15	0.91	1 (6%)	18,20,20	2.22	7 (38%)
6	OXY	D	1454	-	1,1,1	0.24	0	-		
6	OXY	B	1453	-	1,1,1	0.23	0	-		
6	OXY	C	1452	-	1,1,1	0.25	0	-		
3	NAP	D	501	-	45,52,52	1.26	5 (11%)	56,80,80	1.34	6 (10%)
6	OXY	B	1454	-	1,1,1	0.29	0	-		

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
5	EPE	D	1452	-	-	1/9/19/19	0/1/1/1
3	NAP	D	501	-	-	9/31/67/67	0/5/5/5
2	FAD	B	500	-	-	3/30/50/50	0/6/6/6
2	FAD	D	500	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	C	1451	-	-	7/9/19/19	0/1/1/1
3	NAP	C	501	-	-	9/31/67/67	0/5/5/5
5	EPE	A	1452	-	-	6/9/19/19	0/1/1/1
5	EPE	B	1452	-	-	8/9/19/19	0/1/1/1
2	FAD	C	500	-	-	3/30/50/50	0/6/6/6
3	NAP	A	501	-	-	9/31/67/67	0/5/5/5
3	NAP	B	501	-	-	11/31/67/67	0/5/5/5
2	FAD	A	500	-	-	3/30/50/50	0/6/6/6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAP	O4D-C1D	4.64	1.47	1.41
3	C	501	NAP	O4D-C1D	4.57	1.47	1.41
5	C	1451	EPE	C10-S	4.17	1.83	1.77
2	C	500	FAD	C4X-N5	3.98	1.38	1.30
2	D	500	FAD	C4X-N5	3.96	1.38	1.30
2	B	500	FAD	C4X-N5	3.93	1.38	1.30
5	B	1452	EPE	C10-S	3.83	1.82	1.77
2	C	500	FAD	C2A-N3A	3.81	1.38	1.32
2	A	500	FAD	C2A-N3A	3.80	1.38	1.32
2	D	500	FAD	C2A-N3A	3.78	1.38	1.32
3	A	501	NAP	O4B-C1B	3.77	1.46	1.41
2	B	500	FAD	C2A-N3A	3.67	1.38	1.32
3	A	501	NAP	O4D-C1D	3.44	1.45	1.41
2	A	500	FAD	C4X-N5	3.42	1.37	1.30
3	C	501	NAP	O4B-C1B	3.41	1.45	1.41
3	B	501	NAP	O4B-C1B	3.39	1.45	1.41
3	D	501	NAP	O4D-C1D	3.36	1.45	1.41
3	D	501	NAP	O4B-C1B	3.31	1.45	1.41
5	A	1452	EPE	C10-S	3.04	1.81	1.77
5	D	1452	EPE	C10-S	3.03	1.81	1.77
2	D	500	FAD	C10-N1	2.85	1.39	1.33
2	B	500	FAD	C10-N1	2.78	1.38	1.33
2	C	500	FAD	C10-N1	2.63	1.38	1.33
2	D	500	FAD	C2A-N1A	2.45	1.38	1.33
2	B	500	FAD	C2A-N1A	2.45	1.38	1.33
2	A	500	FAD	C10-N1	2.42	1.38	1.33
3	C	501	NAP	C7N-N7N	2.34	1.37	1.33
3	D	501	NAP	C2N-C3N	2.32	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C4X-C10	-2.27	1.37	1.44
3	A	501	NAP	C7N-N7N	2.24	1.37	1.33
3	A	501	NAP	P2B-O2X	2.17	1.63	1.54
3	D	501	NAP	C4N-C3N	2.15	1.43	1.39
3	B	501	NAP	C7N-N7N	2.14	1.37	1.33
3	C	501	NAP	P2B-O2X	2.13	1.63	1.54
3	A	501	NAP	C8A-N7A	-2.12	1.30	1.34
3	B	501	NAP	P2B-O2X	2.11	1.63	1.54
3	C	501	NAP	P2B-O3X	2.11	1.63	1.54
3	D	501	NAP	C8A-N7A	-2.10	1.31	1.34
2	A	500	FAD	C2A-N1A	2.09	1.37	1.33
3	A	501	NAP	PN-O1N	2.04	1.58	1.50
2	D	500	FAD	C4X-C10	-2.03	1.38	1.44
2	B	500	FAD	O2'-C2'	-2.01	1.39	1.43

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1452	EPE	C5-N4-C3	6.64	123.78	108.83
5	A	1452	EPE	C5-N4-C3	5.84	121.97	108.83
5	B	1452	EPE	C5-N4-C3	5.72	121.70	108.83
5	C	1451	EPE	C5-N4-C3	5.03	120.14	108.83
2	A	500	FAD	N3A-C2A-N1A	-4.86	121.09	128.68
2	C	500	FAD	N3A-C2A-N1A	-4.67	121.37	128.68
2	D	500	FAD	N3A-C2A-N1A	-4.60	121.49	128.68
3	D	501	NAP	PN-O3-PA	-4.50	117.39	132.83
3	A	501	NAP	PN-O3-PA	-4.30	118.07	132.83
3	B	501	NAP	PN-O3-PA	-4.27	118.16	132.83
3	C	501	NAP	PN-O3-PA	-4.27	118.18	132.83
5	A	1452	EPE	O1S-S-C10	4.23	112.01	106.92
2	B	500	FAD	N3A-C2A-N1A	-3.98	122.47	128.68
3	A	501	NAP	N3A-C2A-N1A	-3.85	122.66	128.68
3	A	501	NAP	C3N-C7N-N7N	3.82	122.34	117.75
2	A	500	FAD	P-O3P-PA	-3.62	120.41	132.83
5	C	1451	EPE	O2S-S-C10	3.56	111.21	106.92
3	B	501	NAP	N3A-C2A-N1A	-3.55	123.13	128.68
3	C	501	NAP	C3N-C7N-N7N	3.43	121.87	117.75
5	C	1451	EPE	O3S-S-C10	3.39	111.25	105.77
2	A	500	FAD	C4-N3-C2	-3.32	119.50	125.64
3	D	501	NAP	N3A-C2A-N1A	-3.32	123.49	128.68
2	C	500	FAD	C4-N3-C2	-3.30	119.54	125.64
2	D	500	FAD	C4-N3-C2	-3.29	119.57	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	FAD	P-O3P-PA	-3.15	122.03	132.83
2	A	500	FAD	C4X-C4-N3	3.03	120.89	113.19
5	C	1451	EPE	C7-N4-C3	3.03	118.99	111.23
3	B	501	NAP	C3N-C7N-N7N	3.02	121.38	117.75
2	D	500	FAD	C4X-C4-N3	3.00	120.80	113.19
5	B	1452	EPE	O3S-S-C10	2.98	110.59	105.77
2	C	500	FAD	P-O3P-PA	-2.97	122.64	132.83
2	D	500	FAD	C9A-C5X-N5	-2.93	119.25	122.43
3	C	501	NAP	C3B-C2B-C1B	-2.92	97.39	102.89
5	B	1452	EPE	C7-N4-C3	2.92	118.71	111.23
2	B	500	FAD	C4-N3-C2	-2.91	120.27	125.64
2	C	500	FAD	C4X-C4-N3	2.89	120.53	113.19
2	D	500	FAD	P-O3P-PA	-2.85	123.03	132.83
2	C	500	FAD	C4A-C5A-N7A	-2.82	106.47	109.40
3	C	501	NAP	C5N-C4N-C3N	-2.79	117.04	120.34
2	A	500	FAD	C4X-C10-N10	2.78	120.55	116.48
2	B	500	FAD	C9A-C5X-N5	-2.77	119.42	122.43
2	D	500	FAD	O4-C4-C4X	-2.76	119.27	126.60
5	A	1452	EPE	C7-N4-C3	2.76	118.30	111.23
2	C	500	FAD	O4-C4-C4X	-2.76	119.28	126.60
2	A	500	FAD	O4-C4-C4X	-2.74	119.34	126.60
5	D	1452	EPE	O3S-S-C10	2.71	110.16	105.77
3	A	501	NAP	C5N-C4N-C3N	-2.70	117.15	120.34
5	B	1452	EPE	C6-C5-N4	2.66	116.10	110.64
2	A	500	FAD	C9A-C5X-N5	-2.65	119.55	122.43
5	D	1452	EPE	C7-N4-C3	2.65	118.00	111.23
5	D	1452	EPE	C7-N4-C5	2.62	117.92	111.23
3	D	501	NAP	C3N-C7N-N7N	2.60	120.87	117.75
2	C	500	FAD	C4X-C10-N10	2.53	120.19	116.48
5	C	1451	EPE	C6-N1-C2	2.48	114.41	108.83
2	A	500	FAD	C4A-C5A-N7A	-2.47	106.82	109.40
2	B	500	FAD	C10-C4X-N5	-2.46	119.63	124.86
2	B	500	FAD	C4X-C4-N3	2.46	119.44	113.19
2	A	500	FAD	O2'-C2'-C1'	-2.46	103.86	109.80
5	A	1452	EPE	O2S-S-C10	2.44	109.86	106.92
2	B	500	FAD	O2'-C2'-C1'	-2.43	103.91	109.80
5	B	1452	EPE	C7-N4-C5	2.41	117.39	111.23
5	A	1452	EPE	C7-N4-C5	2.40	117.36	111.23
2	B	500	FAD	O4-C4-C4X	-2.38	120.29	126.60
3	D	501	NAP	O7N-C7N-N7N	-2.37	119.22	122.58
2	B	500	FAD	C6-C5X-C9A	2.35	122.27	118.94
3	A	501	NAP	C4A-C5A-N7A	-2.34	106.96	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1452	EPE	C6-C5-N4	2.32	115.41	110.64
5	B	1452	EPE	O2S-S-C10	2.32	109.71	106.92
2	B	500	FAD	O4B-C1B-C2B	-2.32	103.53	106.93
3	B	501	NAP	C4A-C5A-N7A	-2.32	106.99	109.40
2	D	500	FAD	C10-C4X-N5	-2.31	119.95	124.86
2	B	500	FAD	C4A-C5A-N7A	-2.31	106.99	109.40
5	C	1451	EPE	C6-C5-N4	2.31	115.37	110.64
2	B	500	FAD	C4X-C10-N1	-2.30	119.38	124.73
3	B	501	NAP	O7N-C7N-N7N	-2.30	119.31	122.58
5	B	1452	EPE	C6-N1-C2	2.27	113.93	108.83
2	B	500	FAD	C4X-C10-N10	2.27	119.79	116.48
2	A	500	FAD	C10-C4X-N5	-2.26	120.06	124.86
3	C	501	NAP	N3A-C2A-N1A	-2.23	125.19	128.68
5	A	1452	EPE	C6-N1-C2	2.23	113.84	108.83
2	D	500	FAD	O2'-C2'-C1'	-2.23	104.41	109.80
2	A	500	FAD	C4X-C10-N1	-2.19	119.64	124.73
2	B	500	FAD	C4-C4X-C10	2.19	120.48	116.79
3	B	501	NAP	C3B-C2B-C1B	-2.19	98.77	102.89
2	D	500	FAD	C4A-C5A-N7A	-2.19	107.12	109.40
2	D	500	FAD	C4X-C10-N10	2.18	119.67	116.48
2	C	500	FAD	C4X-C10-N1	-2.16	119.71	124.73
3	A	501	NAP	PN-O5D-C5D	-2.14	109.14	121.68
5	D	1452	EPE	C2-C3-N4	2.12	115.00	110.64
3	D	501	NAP	C3B-C2B-C1B	-2.12	98.90	102.89
2	C	500	FAD	C9A-C5X-N5	-2.12	120.13	122.43
3	B	501	NAP	O3D-C3D-C4D	-2.07	105.07	111.05
2	D	500	FAD	C4X-C10-N1	-2.06	119.95	124.73
2	A	500	FAD	C6-C5X-C9A	2.05	121.84	118.94
2	D	500	FAD	C6-C5X-C9A	2.04	121.83	118.94
2	B	500	FAD	C5X-N5-C4X	2.03	121.45	118.07
3	D	501	NAP	C5N-C4N-C3N	-2.03	117.94	120.34
3	A	501	NAP	C3B-C2B-C1B	-2.02	99.08	102.89
5	C	1451	EPE	C2-C3-N4	2.02	114.78	110.64
2	C	500	FAD	C10-C4X-N5	-2.00	120.60	124.86
2	D	500	FAD	C1'-N10-C9A	2.00	123.85	120.51

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	FAD	N10-C1'-C2'-O2'
2	A	500	FAD	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	B	500	FAD	N10-C1'-C2'-O2'
2	B	500	FAD	N10-C1'-C2'-C3'
2	C	500	FAD	N10-C1'-C2'-O2'
2	C	500	FAD	N10-C1'-C2'-C3'
2	D	500	FAD	N10-C1'-C2'-O2'
2	D	500	FAD	N10-C1'-C2'-C3'
3	A	501	NAP	C5D-O5D-PN-O3
3	A	501	NAP	C5D-O5D-PN-O1N
3	A	501	NAP	C5D-O5D-PN-O2N
3	B	501	NAP	C5D-O5D-PN-O3
3	B	501	NAP	C5D-O5D-PN-O1N
3	B	501	NAP	C5D-O5D-PN-O2N
3	C	501	NAP	C5D-O5D-PN-O3
3	C	501	NAP	C5D-O5D-PN-O1N
3	C	501	NAP	C5D-O5D-PN-O2N
3	D	501	NAP	C5D-O5D-PN-O3
3	D	501	NAP	C5D-O5D-PN-O1N
3	D	501	NAP	C5D-O5D-PN-O2N
5	A	1452	EPE	C8-C7-N4-C3
5	A	1452	EPE	S-C10-C9-N1
5	B	1452	EPE	C8-C7-N4-C3
5	B	1452	EPE	S-C10-C9-N1
5	B	1452	EPE	C9-C10-S-O2S
5	B	1452	EPE	C9-C10-S-O3S
5	C	1451	EPE	C8-C7-N4-C3
5	C	1451	EPE	S-C10-C9-N1
5	C	1451	EPE	C9-C10-S-O2S
5	C	1451	EPE	C9-C10-S-O3S
5	D	1452	EPE	C8-C7-N4-C3
3	A	501	NAP	O4B-C4B-C5B-O5B
3	A	501	NAP	C3B-C4B-C5B-O5B
3	A	501	NAP	O4D-C4D-C5D-O5D
3	B	501	NAP	O4B-C4B-C5B-O5B
3	B	501	NAP	C3B-C4B-C5B-O5B
3	B	501	NAP	O4D-C4D-C5D-O5D
3	C	501	NAP	O4B-C4B-C5B-O5B
3	C	501	NAP	C3B-C4B-C5B-O5B
3	C	501	NAP	O4D-C4D-C5D-O5D
3	D	501	NAP	O4B-C4B-C5B-O5B
3	D	501	NAP	C3B-C4B-C5B-O5B
3	A	501	NAP	C3D-C4D-C5D-O5D
3	B	501	NAP	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	C	501	NAP	C3D-C4D-C5D-O5D
3	D	501	NAP	O4D-C4D-C5D-O5D
3	D	501	NAP	C3D-C4D-C5D-O5D
3	C	501	NAP	C1B-C2B-O2B-P2B
3	D	501	NAP	C1B-C2B-O2B-P2B
3	D	501	NAP	C3B-C2B-O2B-P2B
5	A	1452	EPE	C9-C10-S-O3S
3	A	501	NAP	C1B-C2B-O2B-P2B
3	C	501	NAP	C3B-C2B-O2B-P2B
3	B	501	NAP	C1B-C2B-O2B-P2B
5	B	1452	EPE	N4-C7-C8-O8
5	A	1452	EPE	C10-C9-N1-C2
5	B	1452	EPE	C10-C9-N1-C2
5	B	1452	EPE	C10-C9-N1-C6
5	C	1451	EPE	C10-C9-N1-C6
3	A	501	NAP	C3B-C2B-O2B-P2B
5	A	1452	EPE	C9-C10-S-O1S
5	A	1452	EPE	C9-C10-S-O2S
5	B	1452	EPE	C9-C10-S-O1S
5	C	1451	EPE	C9-C10-S-O1S
5	C	1451	EPE	C10-C9-N1-C2
2	A	500	FAD	O4B-C4B-C5B-O5B
2	C	500	FAD	O4B-C4B-C5B-O5B
3	B	501	NAP	C3B-C2B-O2B-P2B
3	B	501	NAP	C2B-O2B-P2B-O2X
2	B	500	FAD	O4B-C4B-C5B-O5B
2	D	500	FAD	O4B-C4B-C5B-O5B
3	B	501	NAP	C5B-O5B-PA-O1A

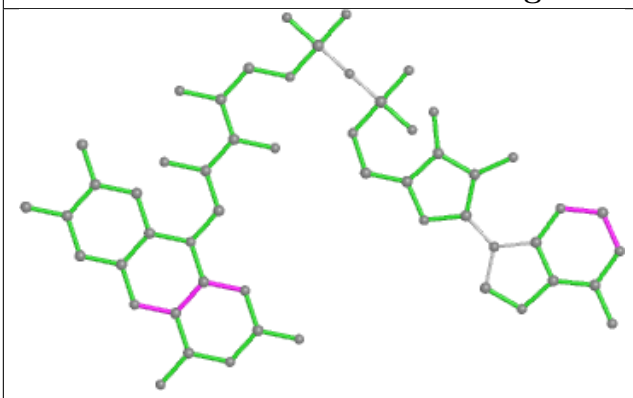
There are no ring outliers.

9 monomers are involved in 17 short contacts:

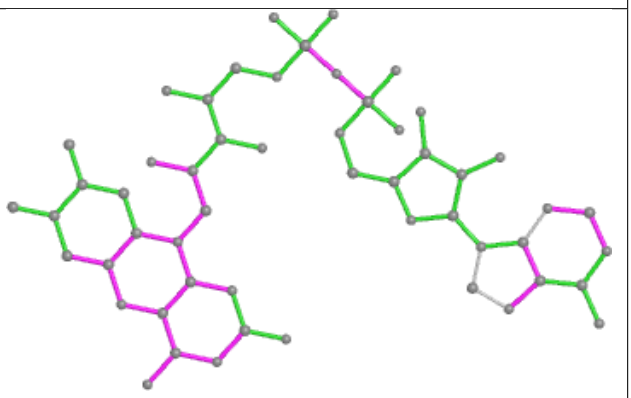
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	FAD	1	0
2	A	500	FAD	1	0
3	C	501	NAP	2	0
5	B	1452	EPE	5	0
3	A	501	NAP	2	0
3	B	501	NAP	3	0
2	B	500	FAD	1	0
5	A	1452	EPE	4	0
3	D	501	NAP	2	0

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

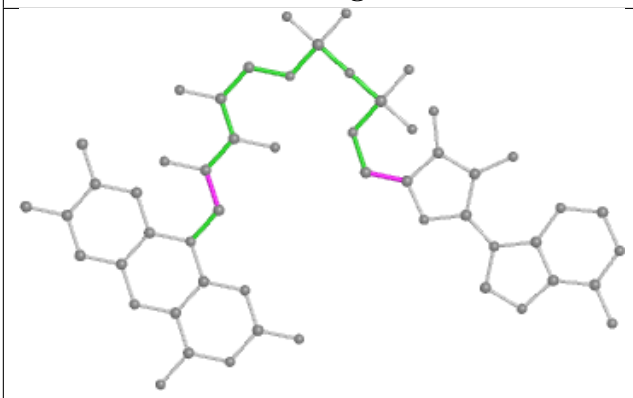
Ligand FAD D 500



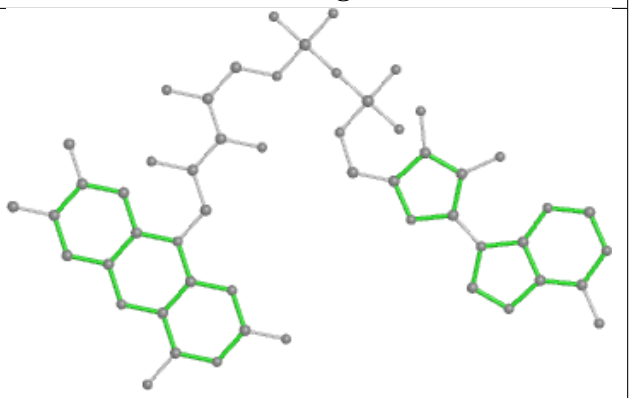
Bond lengths



Bond angles

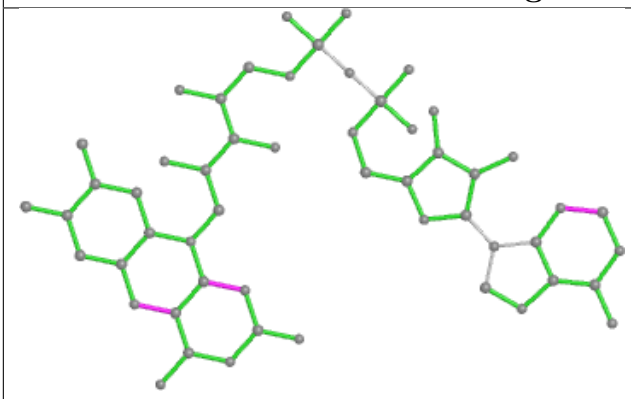


Torsions

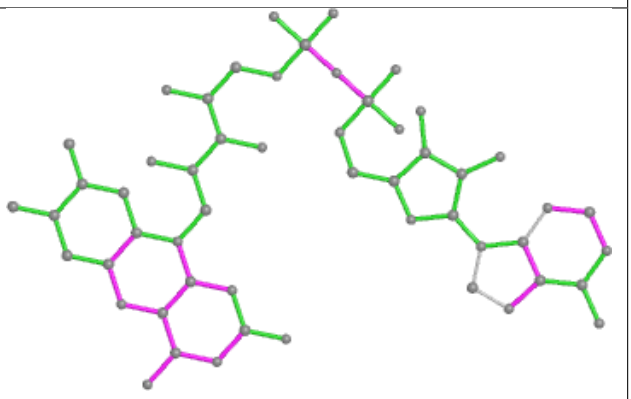


Rings

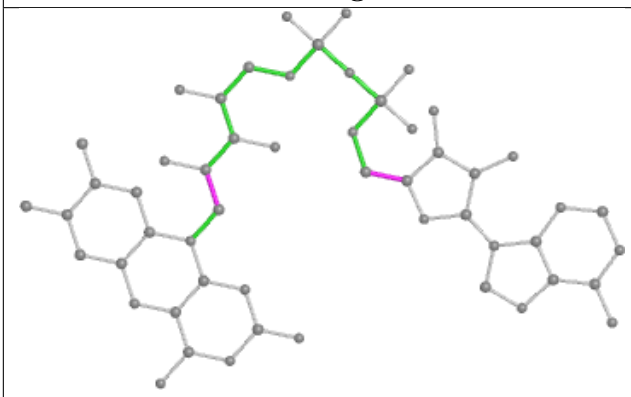
Ligand FAD C 500



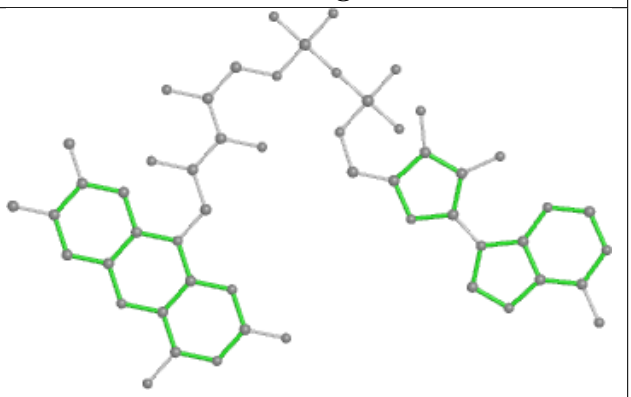
Bond lengths



Bond angles

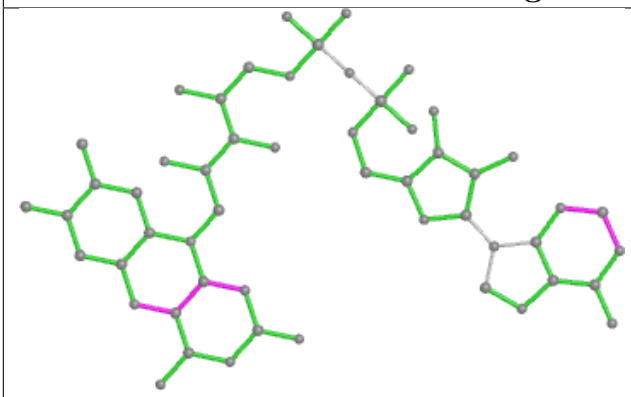


Torsions

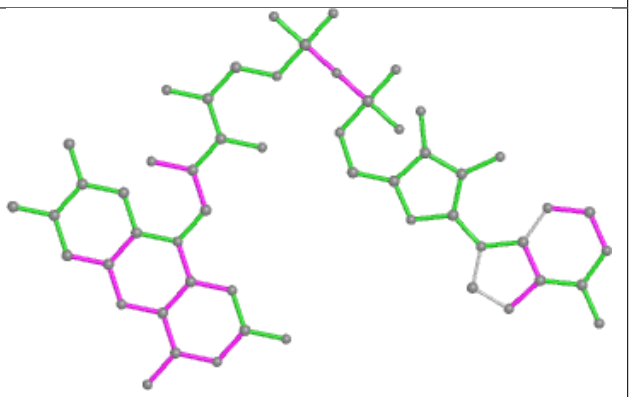


Rings

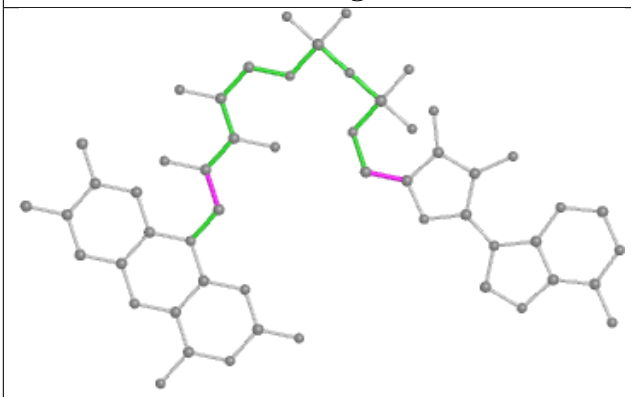
Ligand FAD A 500



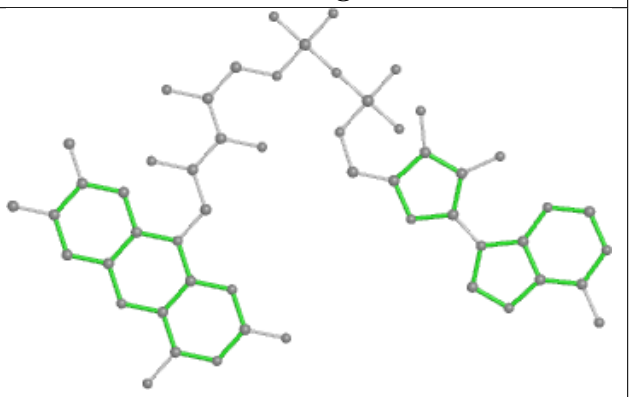
Bond lengths



Bond angles

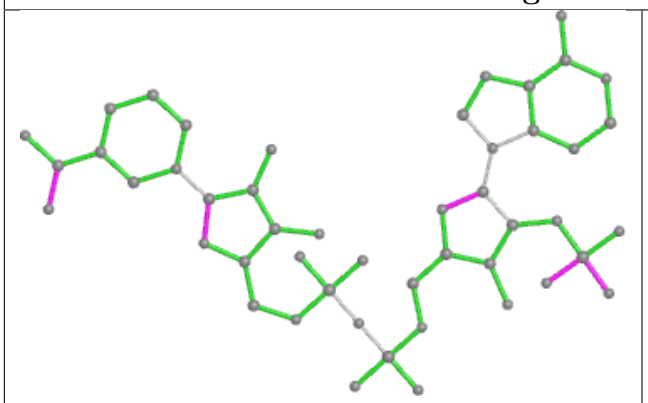


Torsions



Rings

Ligand NAP C 501



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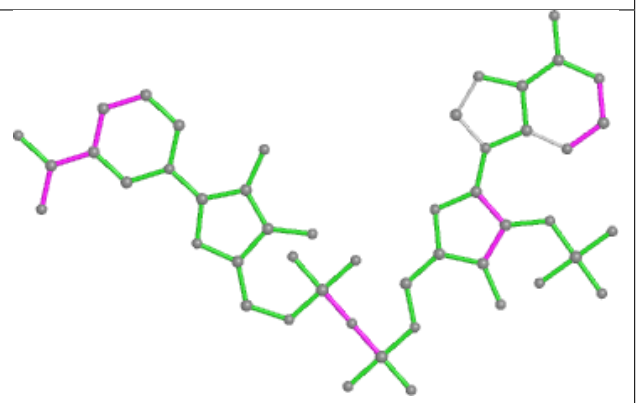
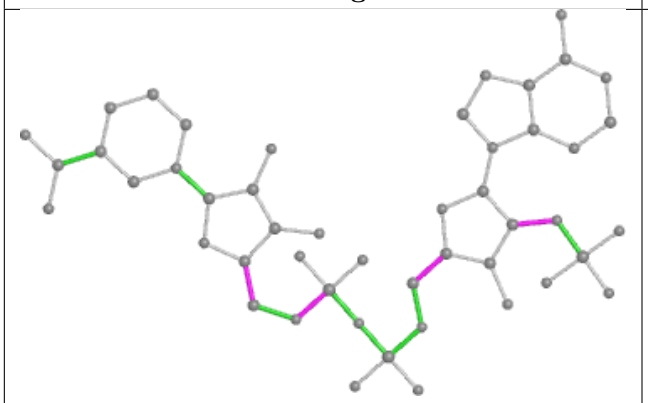


Bond angles



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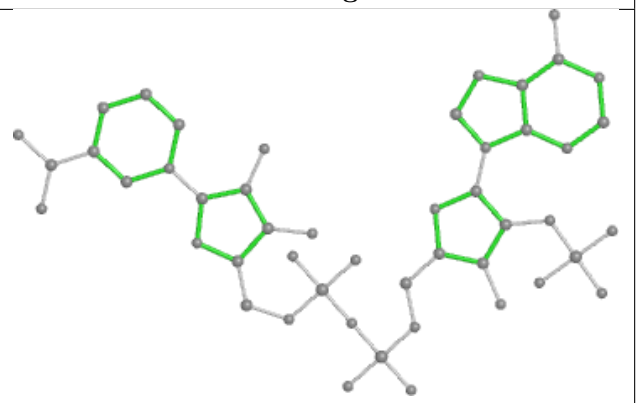
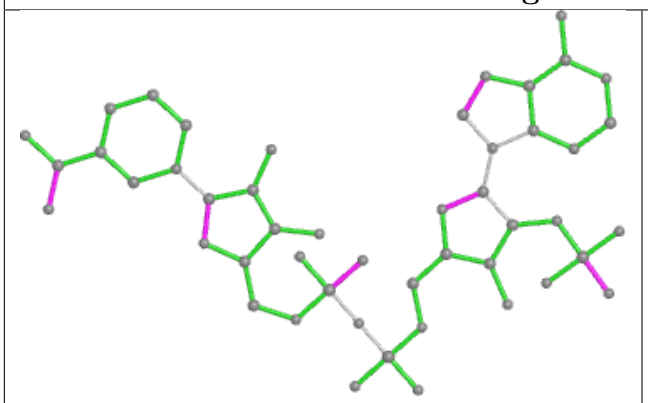


Rings

Ligand NAP A 501



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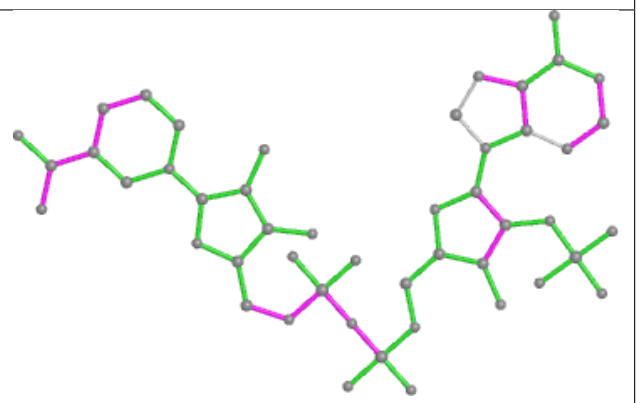
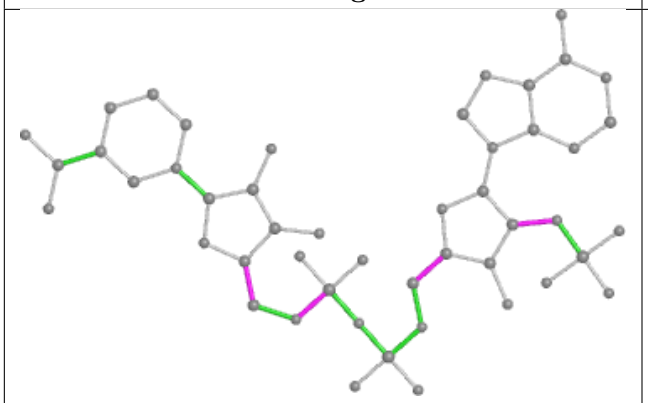


Bond angles



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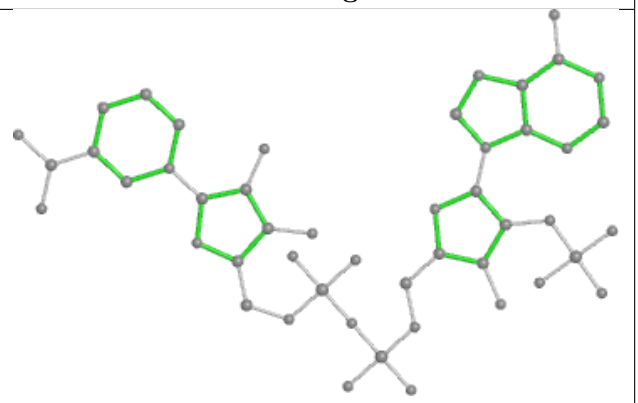
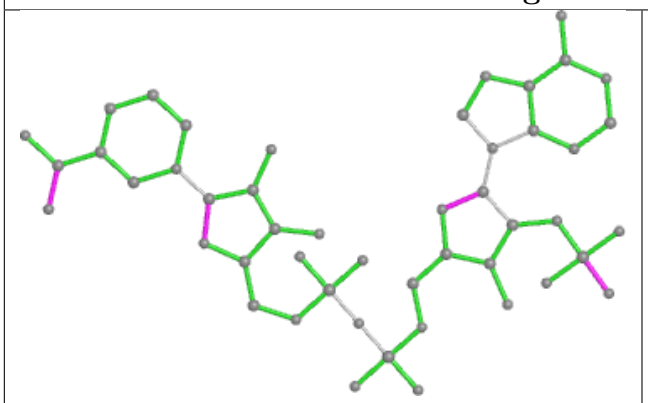


Rings

Ligand NAP B 501



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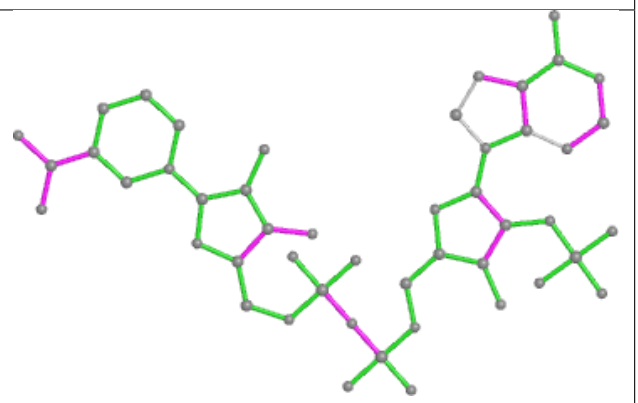
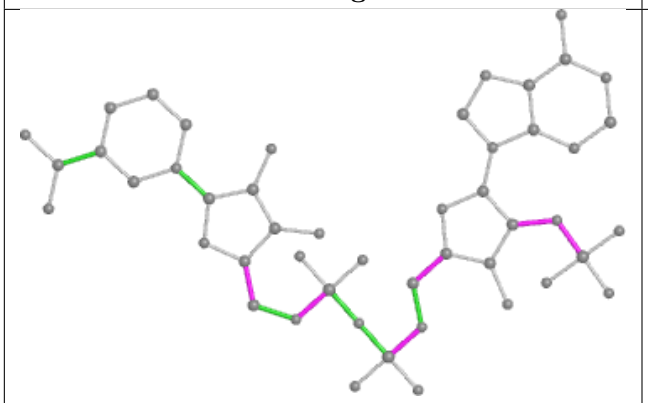


Bond angles



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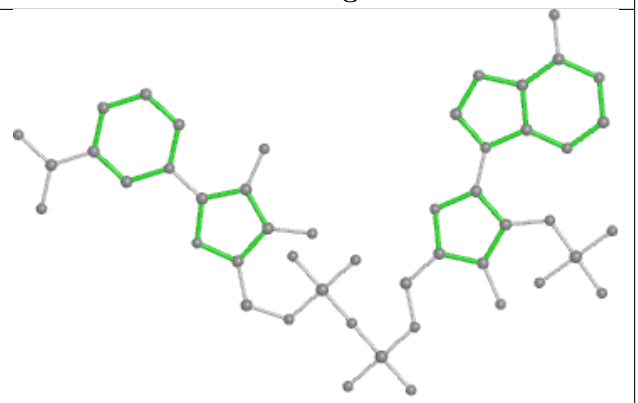
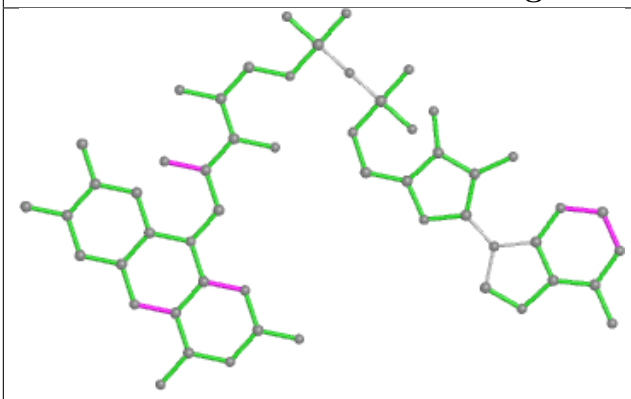
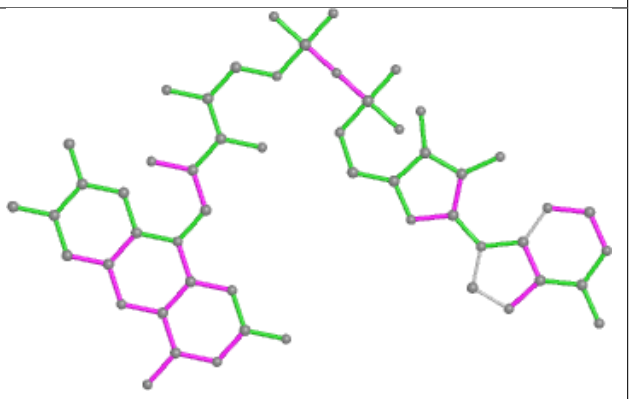


Rings

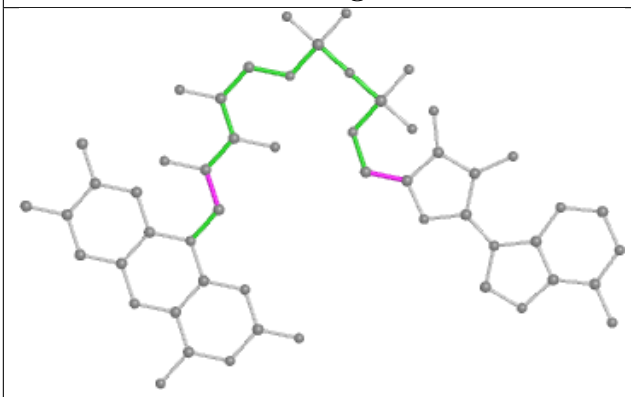
Ligand FAD B 500



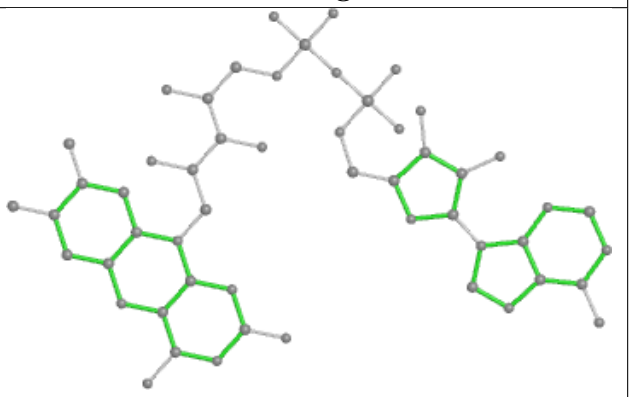
Bond lengths



Bond angles

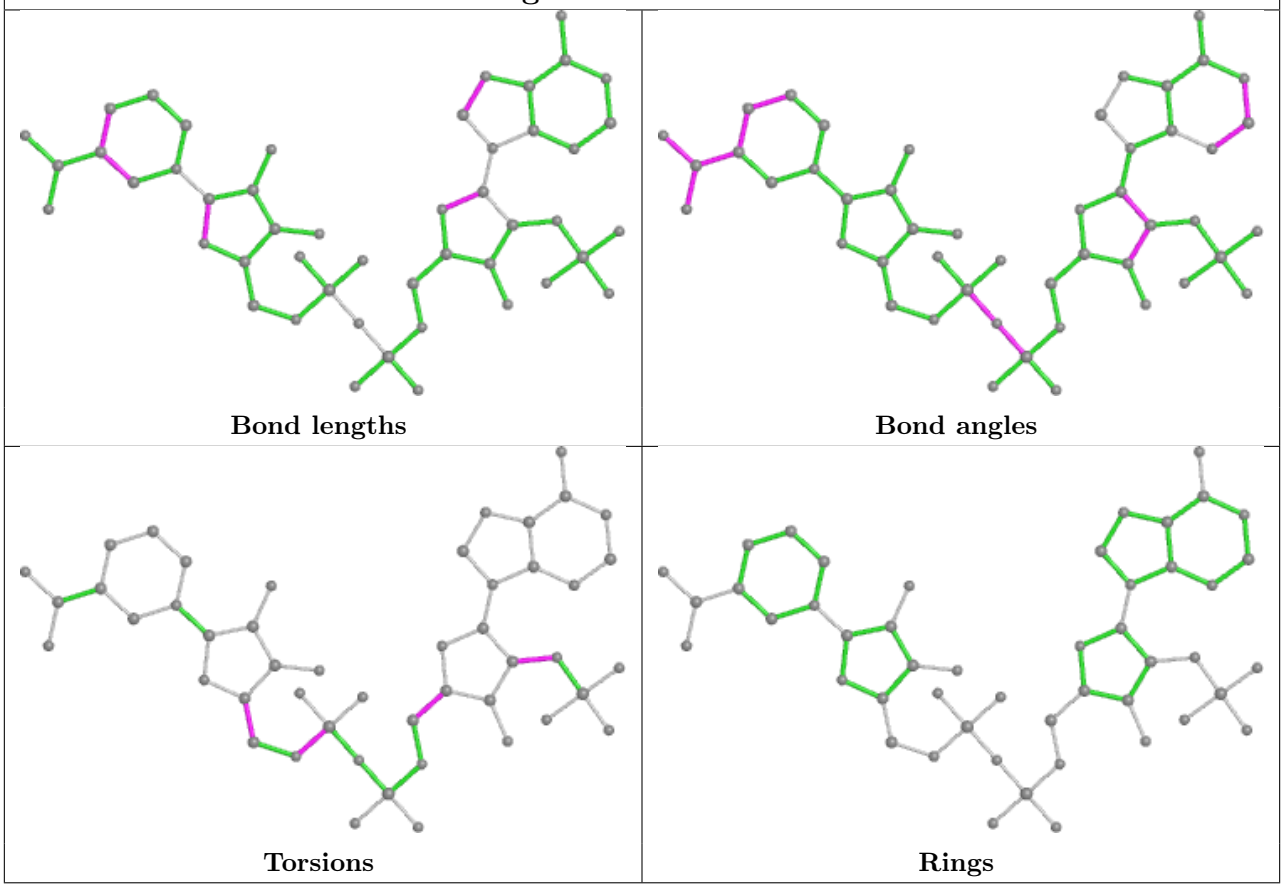


Torsions



Rings

Ligand NAP D 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 (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	443/461 (96%)	-0.23	5 (1%)	80	75	40, 52, 67, 74	0
1	B	443/461 (96%)	-0.16	3 (0%)	87	84	40, 52, 67, 74	0
1	C	443/461 (96%)	-0.21	5 (1%)	80	75	40, 52, 67, 74	0
1	D	443/461 (96%)	-0.27	3 (0%)	87	84	40, 52, 67, 74	0
All	All	1772/1844 (96%)	-0.22	16 (0%)	84	80	40, 52, 67, 74	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	GLU	3.8
1	A	236	ALA	3.4
1	A	235	THR	3.2
1	B	241	LYS	2.6
1	C	446	GLU	2.4
1	B	139	ASP	2.4
1	D	139	ASP	2.4
1	A	368	VAL	2.3
1	D	244	GLU	2.3
1	C	326	SER	2.3
1	C	328	ASN	2.3
1	A	446	GLU	2.2
1	C	256	ASP	2.2
1	D	351	GLU	2.2
1	B	446	GLU	2.1
1	A	328	ASN	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)

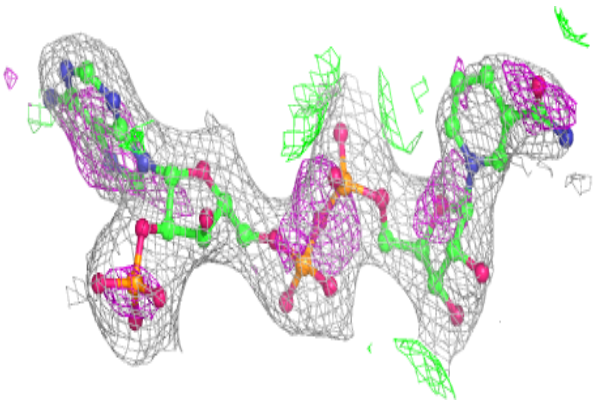
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

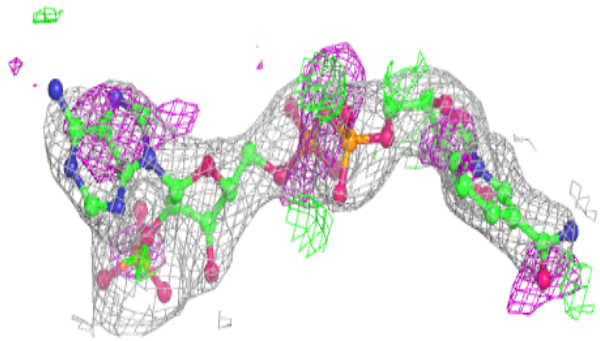
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EPE	C	1451	15/15	0.75	0.31	102,104,110,111	0
5	EPE	D	1452	15/15	0.81	0.26	103,104,107,107	0
5	EPE	B	1452	15/15	0.83	0.23	106,107,108,108	0
5	EPE	A	1452	15/15	0.86	0.24	97,103,107,108	0
6	OXY	B	1453	2/2	0.89	0.17	68,68,68,68	0
6	OXY	C	1452	2/2	0.89	0.24	50,50,50,51	0
4	CL	B	1451	1/1	0.91	0.12	60,60,60,60	0
3	NAP	C	501	48/48	0.92	0.20	41,44,50,52	0
3	NAP	B	501	48/48	0.93	0.19	41,44,50,51	0
6	OXY	A	1454	2/2	0.94	0.18	55,55,55,55	0
3	NAP	D	501	48/48	0.94	0.17	41,44,50,51	0
6	OXY	B	1454	2/2	0.94	0.66	53,53,53,54	0
3	NAP	A	501	48/48	0.94	0.19	41,44,50,51	0
6	OXY	D	1453	2/2	0.96	0.12	45,45,45,46	0
6	OXY	D	1454	2/2	0.96	0.70	52,52,52,54	0
2	FAD	B	500	53/53	0.97	0.19	37,41,46,48	0
4	CL	D	1451	1/1	0.97	0.10	56,56,56,56	0
6	OXY	C	1453	2/2	0.97	0.57	51,51,51,51	0
2	FAD	C	500	53/53	0.97	0.18	37,40,46,48	0
2	FAD	A	500	53/53	0.97	0.18	37,41,46,48	0
4	CL	A	1451	1/1	0.98	0.13	52,52,52,52	0
6	OXY	A	1453	2/2	0.98	0.57	49,49,49,50	0
2	FAD	D	500	53/53	0.98	0.20	37,41,46,48	0
4	CL	C	1454	1/1	0.99	0.15	58,58,58,58	0

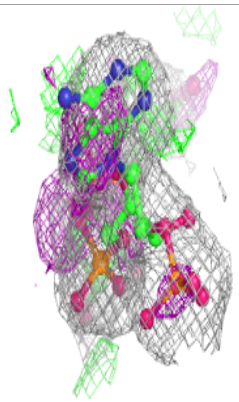
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP C 501:

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

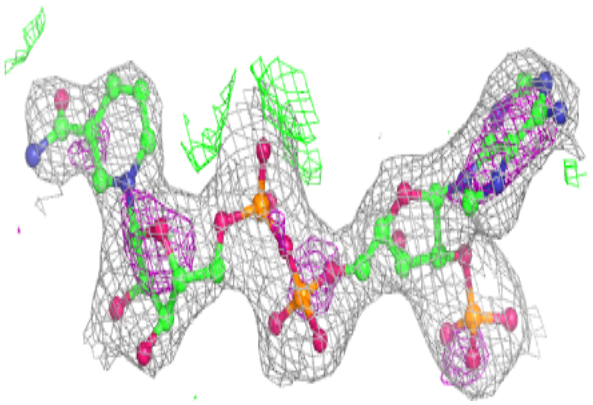


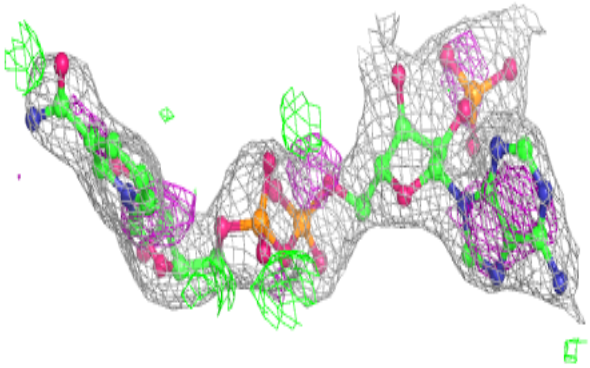


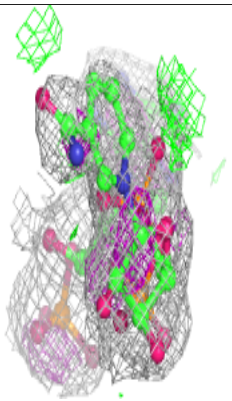


Electron density around NAP B 501:

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

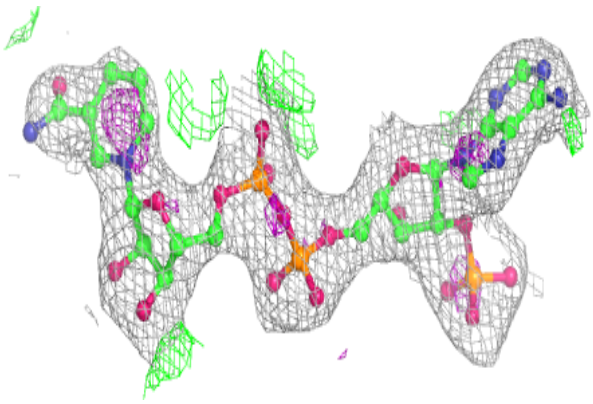


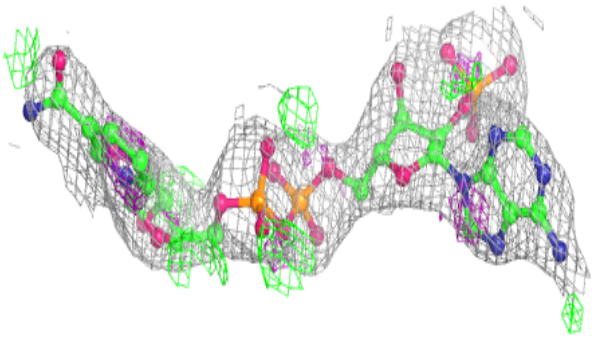


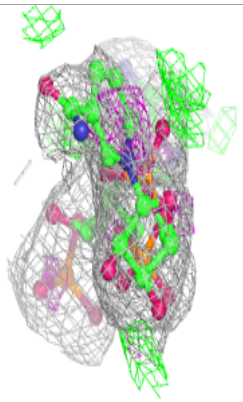


Electron density around NAP D 501:

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

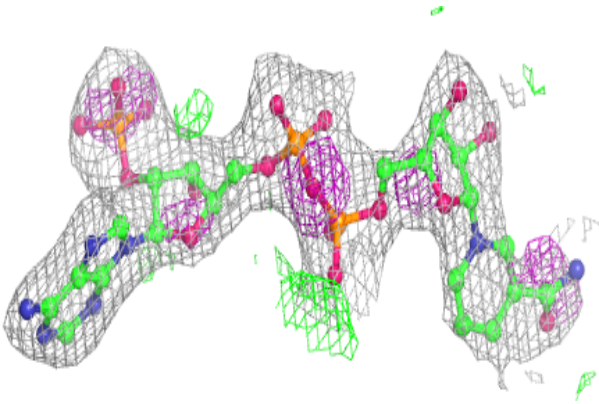


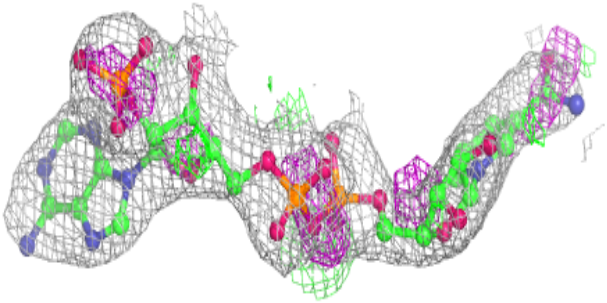


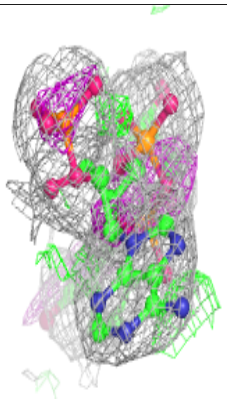


Electron density around NAP A 501:

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

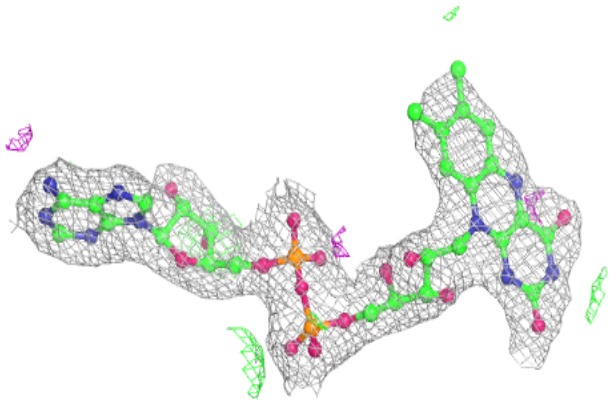


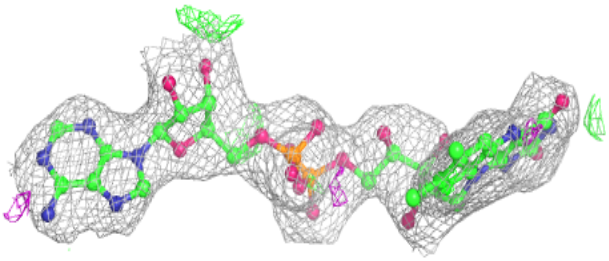


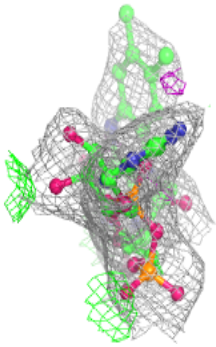


Electron density around FAD B 500:

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

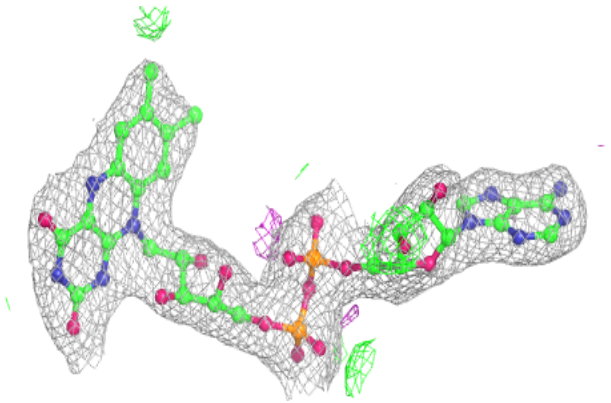


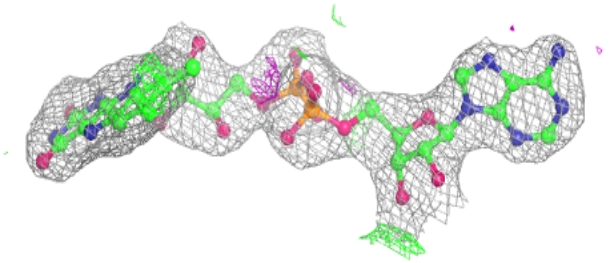


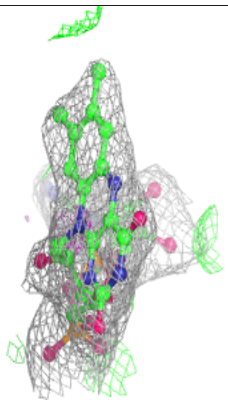


Electron density around FAD C 500:

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

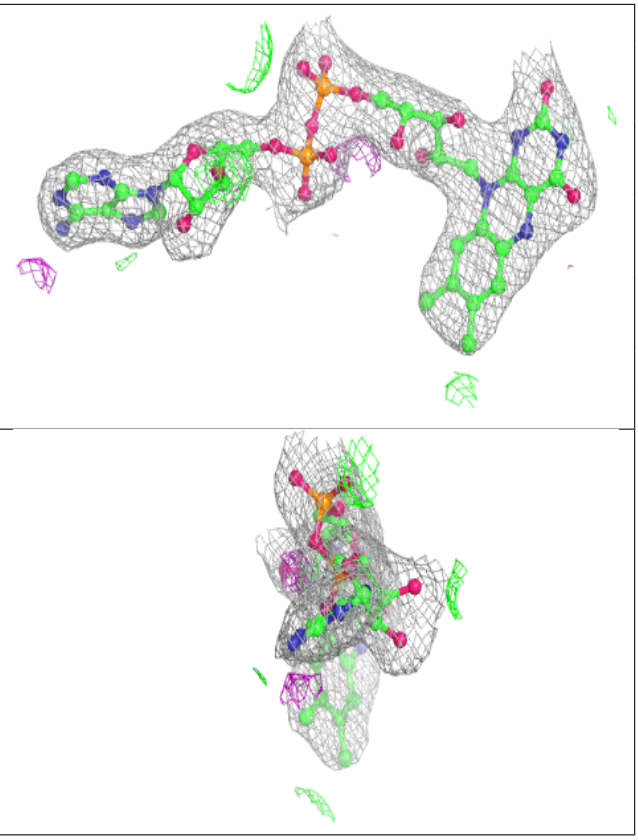






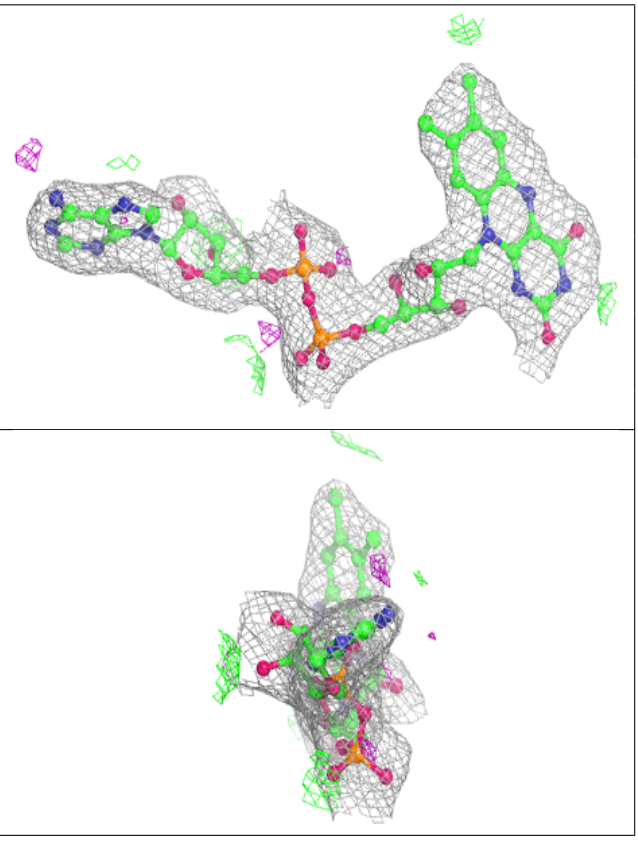
Electron density around FAD A 500:

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



Electron density around FAD D 500:

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



6.5 Other polymers (i)

There are no such residues in this entry.