Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 06:21 pm GMT

PDB ID	:	7AL4
Title	:	Ancestral Flavin-containing monooxygenase (FMO) 1 (mammalian)
Authors	:	Nicoll, C.R.; Mattevi, A.
Deposited on	:	2020-10-05
Resolution	:	3.00 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:

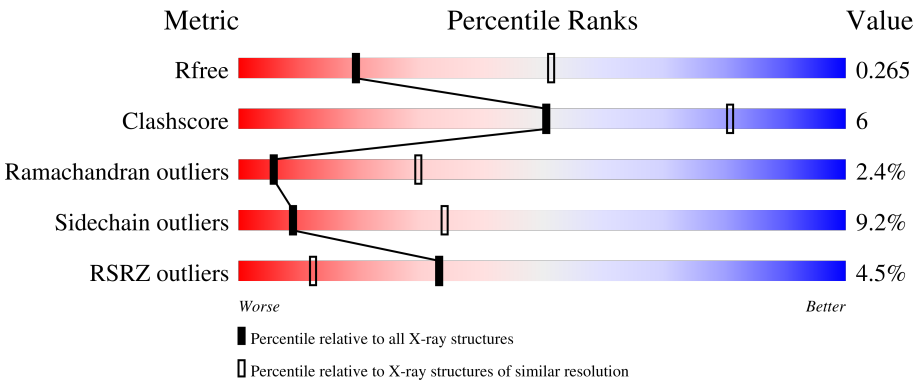
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	531	% 77% 18% • •
1	B	531	4% 79% 18% • •
1	C	531	11% 78% 18% • •
1	D	531	% 76% 20% • •

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	LMT	A	603	-	-	-	X

2 Entry composition (i)

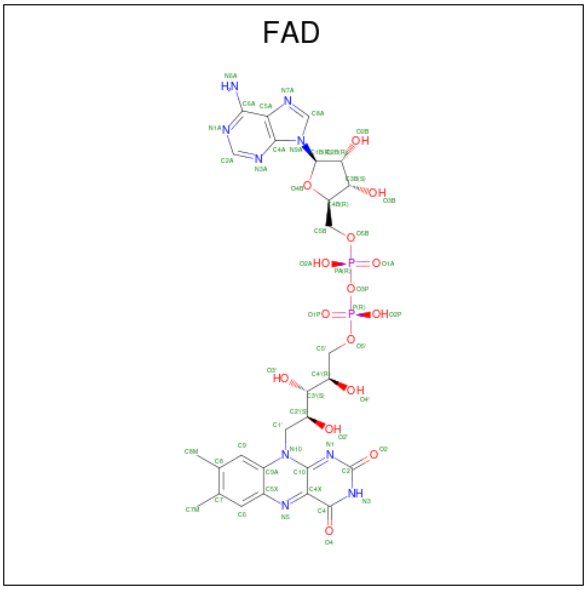
There are 7 unique types of molecules in this entry. The entry contains 17079 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ancestral Flavin-containing monooxygenase 1 (mammalian).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	524	4153	2693	687	748	25	0	0	0
			Total	C	N	O	S			
1	C	520	4081	2633	681	744	23	0	0	0
			Total	C	N	O	S			
1	B	523	4105	2650	685	747	23	0	0	0
			Total	C	N	O	S			
1	A	517	4071	2630	679	739	23	0	0	0

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



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

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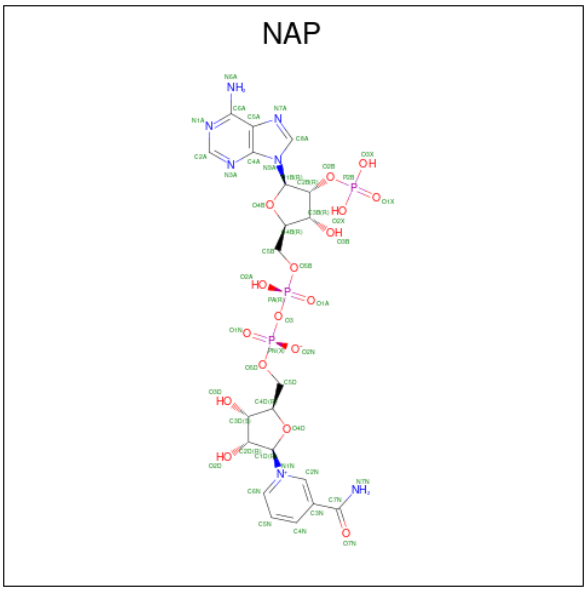
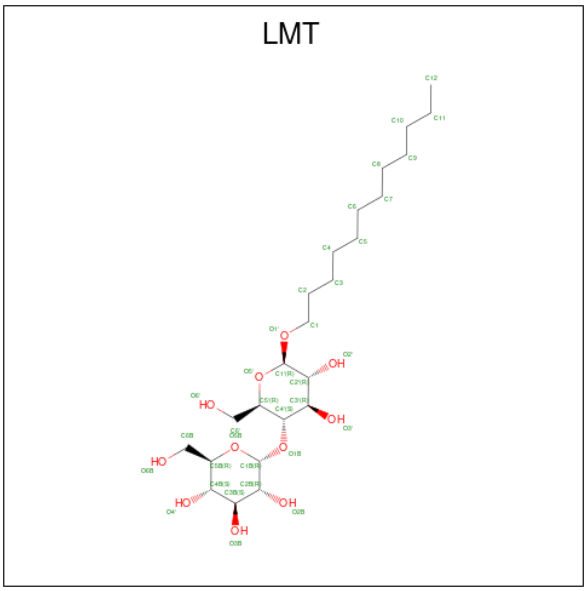
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

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



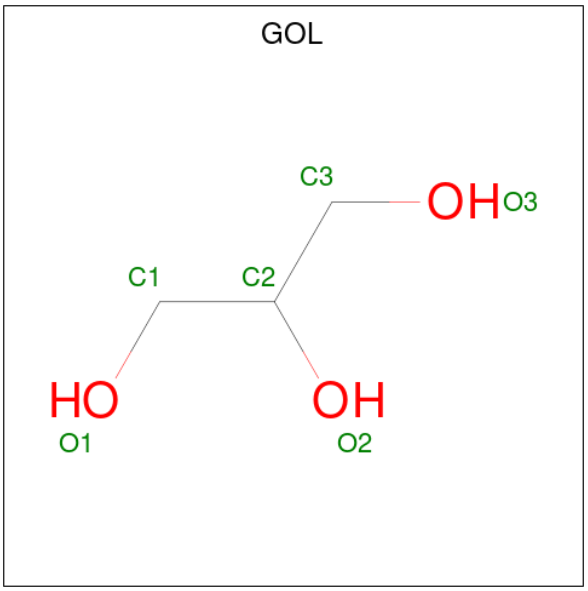
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	D	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	C	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	D	1	35	24	11	0	0
			Total	C	O		
4	B	1	35	24	11	0	0
			Total	C	O		
4	B	1	35	24	11	0	0
			Total	C	O		
4	A	1	35	24	11	0	0
			Total	C	O		
4	A	1	35	24	11	0	0
			Total	C	O		
4	A	1	35	24	11	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	D	1	6	3	3	0	0
			Total	C	O		
5	D	1	6	3	3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is water.

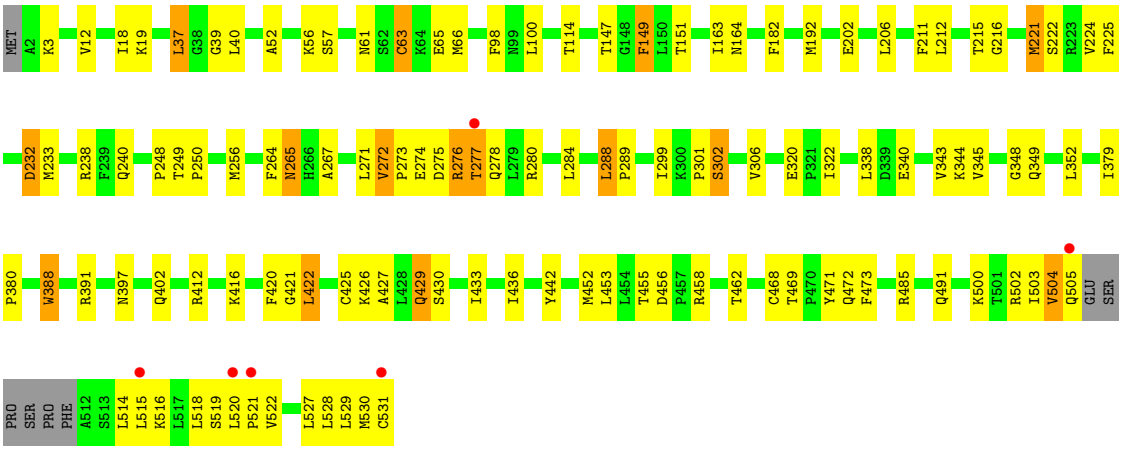
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	D	16	16	16	0	0
			Total	O		
7	C	5	5	5	0	0
			Total	O		
7	B	8	8	8	0	0
			Total	O		
7	A	11	11	11	0	0

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.

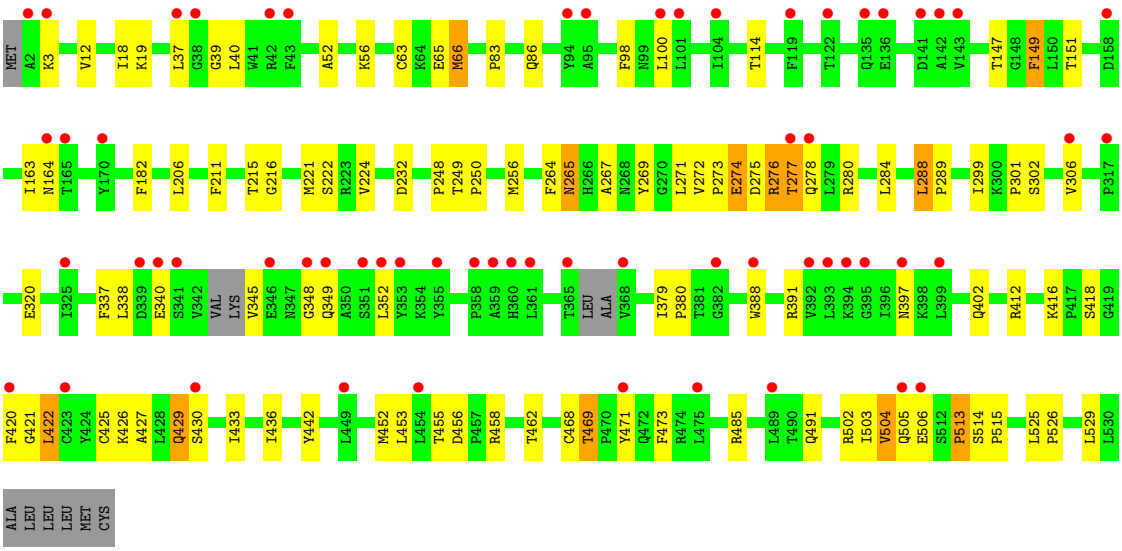
• Molecule 1: Ancestral Flavin-containing monooxygenase 1 (mammalian)

Chain D:



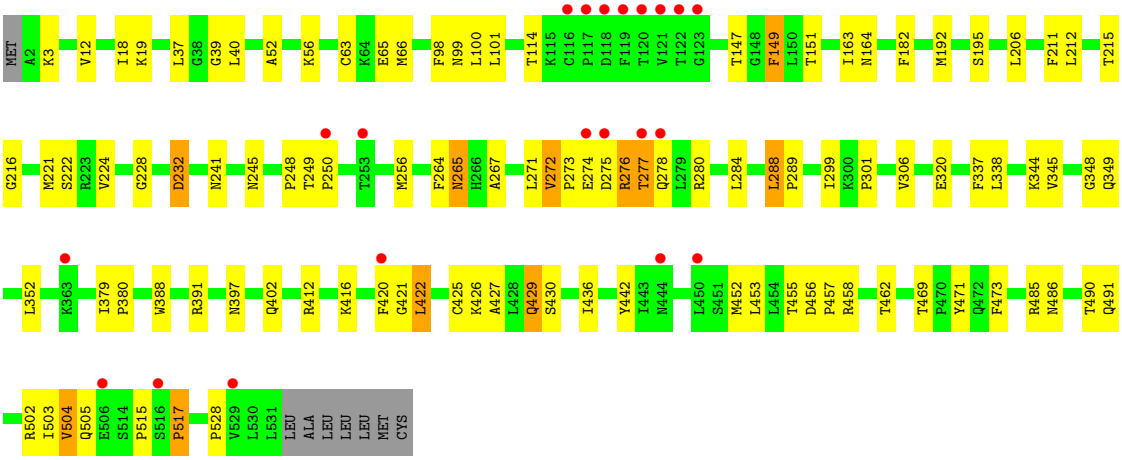
• Molecule 1: Ancestral Flavin-containing monooxygenase 1 (mammalian)

Chain C:



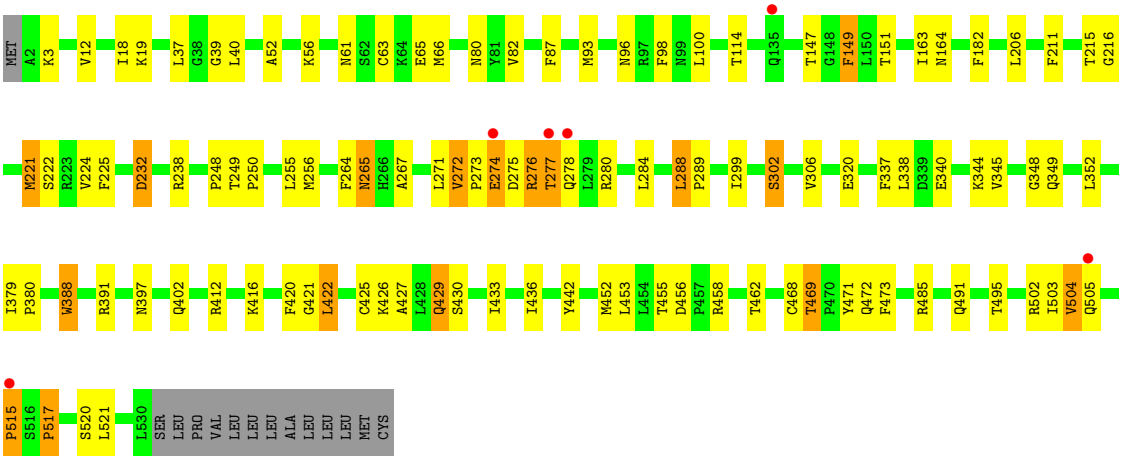
• Molecule 1: Ancestral Flavin-containing monooxygenase 1 (mammalian)

Chain B:



• Molecule 1: Ancestral Flavin-containing monooxygenase 1 (mammalian)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.92Å 92.45Å 156.69Å 90.00° 95.12° 90.00°	Depositor
Resolution (Å)	49.10 – 3.00 49.10 – 3.00	Depositor EDS
% Data completeness (in resolution range)	60.1 (49.10-3.00) 60.1 (49.10-3.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.264 0.228 , 0.265	Depositor DCC
R_{free} test set	817 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.0	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	17079	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAP, GOL, LMT, 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	0.68	0/4176	0.76	2/5672 (0.0%)
1	B	0.68	0/4211	0.76	2/5722 (0.0%)
1	C	0.69	0/4185	0.75	3/5684 (0.1%)
1	D	0.68	0/4260	0.76	0/5786
All	All	0.68	0/16832	0.76	7/22864 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	517	PRO	N-CA-CB	6.55	111.16	103.30
1	C	515	PRO	N-CA-CB	5.98	110.47	103.30
1	B	528	PRO	N-CA-CB	5.82	110.28	103.30
1	C	513	PRO	N-CA-CB	5.72	110.17	103.30
1	C	526	PRO	N-CA-CB	5.69	110.13	103.30
1	A	515	PRO	N-CA-CB	5.41	109.79	103.30
1	A	517	PRO	N-CA-CB	5.16	109.49	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4071	0	4033	54	0
1	B	4105	0	4049	53	0
1	C	4081	0	4011	45	0
1	D	4153	0	4191	52	0
2	A	53	0	31	4	0
2	B	53	0	31	3	0
2	C	53	0	31	3	0
2	D	53	0	31	2	0
3	A	48	0	25	3	0
3	B	48	0	25	6	0
3	C	48	0	25	1	0
3	D	48	0	25	1	0
4	A	105	0	138	0	0
4	B	70	0	92	2	0
4	D	35	0	46	0	0
5	D	12	0	16	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	11	0	0	0	0
7	B	8	0	0	0	0
7	C	5	0	0	1	0
7	D	16	0	0	0	0
All	All	17079	0	16800	194	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (194) 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:379:ILE:HB	1:A:380:PRO:HD3	1.66	0.77
1:D:379:ILE:HB	1:D:380:PRO:HD3	1.68	0.74
1:B:379:ILE:HB	1:B:380:PRO:HD3	1.69	0.73
1:C:379:ILE:HB	1:C:380:PRO:HD3	1.70	0.72
1:D:344:LYS:O	1:D:345:VAL:HG22	1.88	0.72
1:D:240:GLN:NE2	1:D:518:LEU:HD12	2.06	0.69
1:A:344:LYS:O	1:A:345:VAL:HG22	1.92	0.69
1:D:248:PRO:HA	1:D:420:PHE:HA	1.80	0.64
1:D:240:GLN:HE21	1:D:518:LEU:HD12	1.63	0.64
1:D:456:ASP:OD2	1:D:485:ARG:NH1	2.30	0.64
1:A:456:ASP:OD2	1:A:485:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:THR:OG1	1:C:491:GLN:NE2	2.32	0.63
1:B:456:ASP:OD2	1:B:485:ARG:NH1	2.32	0.63
1:A:248:PRO:HA	1:A:420:PHE:HA	1.79	0.63
2:A:601:FAD:HM73	3:A:602:NAP:C5N	2.30	0.62
1:B:248:PRO:HA	1:B:420:PHE:HA	1.80	0.61
1:D:301:PRO:HA	1:A:502:ARG:HD2	1.82	0.61
1:C:248:PRO:HA	1:C:420:PHE:HA	1.83	0.61
1:A:40:LEU:HD11	2:A:601:FAD:C8M	2.31	0.60
1:B:52:ALA:N	1:B:151:THR:HG22	2.17	0.60
1:C:456:ASP:OD2	1:C:485:ARG:NH1	2.34	0.60
1:D:288:LEU:HB3	1:D:289:PRO:HD3	1.84	0.60
1:D:502:ARG:NH2	1:A:272:VAL:O	2.36	0.58
1:D:40:LEU:HD11	2:D:601:FAD:C8M	2.34	0.58
1:C:288:LEU:HB3	1:C:289:PRO:HD3	1.86	0.58
1:B:65:GLU:OE1	1:B:471:TYR:OH	2.22	0.58
1:A:288:LEU:HB3	1:A:289:PRO:HD3	1.85	0.57
1:A:469:THR:OG1	1:A:491:GLN:NE2	2.38	0.57
1:B:344:LYS:O	1:B:345:VAL:HG22	2.03	0.57
1:B:288:LEU:HB3	1:B:289:PRO:HD3	1.84	0.57
2:B:601:FAD:HM73	3:B:602:NAP:C4N	2.35	0.57
1:C:40:LEU:HD11	2:C:601:FAD:C8M	2.35	0.56
1:C:505:GLN:O	1:C:506:GLU:C	2.42	0.56
1:C:502:ARG:HD2	1:B:301:PRO:HA	1.87	0.56
1:C:301:PRO:HA	1:B:502:ARG:HD2	1.87	0.56
1:D:52:ALA:N	1:D:151:THR:HG22	2.20	0.55
1:B:40:LEU:HD11	2:B:601:FAD:C8M	2.35	0.55
1:B:195:SER:OG	3:B:602:NAP:PN	2.65	0.55
1:B:469:THR:OG1	1:B:491:GLN:NE2	2.39	0.55
1:B:195:SER:OG	3:B:602:NAP:O2N	2.24	0.55
1:A:52:ALA:N	1:A:151:THR:HG22	2.22	0.54
2:C:601:FAD:HM73	3:C:602:NAP:C5N	2.36	0.54
1:C:249:THR:HB	1:C:250:PRO:HD3	1.90	0.54
1:B:457:PRO:HD2	4:B:604:LMT:O2B	2.07	0.54
1:A:216:GLY:O	1:A:273:PRO:HA	2.07	0.54
1:B:222:SER:OG	1:B:224:VAL:HB	2.08	0.54
1:C:289:PRO:HB2	1:B:224:VAL:HG21	1.88	0.53
1:B:276:ARG:O	1:B:278:GLN:N	2.41	0.53
1:D:469:THR:OG1	1:D:491:GLN:NE2	2.41	0.53
1:A:65:GLU:OE1	1:A:471:TYR:OH	2.26	0.53
1:D:276:ARG:O	1:D:278:GLN:N	2.41	0.53
1:C:52:ALA:N	1:C:151:THR:HG22	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLY:O	1:C:273:PRO:HA	2.09	0.53
1:B:249:THR:HB	1:B:250:PRO:HD3	1.90	0.53
1:D:61:ASN:ND2	3:D:602:NAP:H2N	2.24	0.53
1:D:216:GLY:O	1:D:273:PRO:HA	2.08	0.53
1:A:276:ARG:O	1:A:278:GLN:N	2.42	0.53
1:A:61:ASN:ND2	3:A:602:NAP:H2N	2.24	0.53
1:B:101:LEU:HD11	1:A:96:ASN:ND2	2.24	0.52
1:B:216:GLY:O	1:B:273:PRO:HA	2.10	0.52
1:D:249:THR:HB	1:D:250:PRO:HD3	1.91	0.52
1:C:222:SER:OG	1:C:224:VAL:HB	2.09	0.52
1:A:391:ARG:NH1	1:A:397:ASN:OD1	2.41	0.52
1:D:232:ASP:OD1	1:D:232:ASP:N	2.38	0.52
1:A:222:SER:OG	1:A:224:VAL:HB	2.09	0.52
1:A:249:THR:HB	1:A:250:PRO:HD3	1.90	0.52
1:C:149:PHE:CD2	1:C:149:PHE:N	2.77	0.51
1:D:149:PHE:N	1:D:149:PHE:CD2	2.78	0.51
1:A:211:PHE:CE2	1:A:320:GLU:HG2	2.46	0.51
1:D:519:SER:HB2	1:D:522:VAL:HB	1.92	0.51
1:C:12:VAL:CG1	1:C:379:ILE:HD13	2.41	0.51
2:A:601:FAD:HM73	3:A:602:NAP:C4N	2.40	0.51
1:A:149:PHE:N	1:A:149:PHE:CD2	2.79	0.50
1:B:12:VAL:CG1	1:B:379:ILE:HD13	2.41	0.50
1:C:276:ARG:O	1:C:278:GLN:N	2.43	0.50
1:B:388:TRP:CE3	1:B:442:TYR:HB3	2.47	0.50
1:D:12:VAL:CG1	1:D:379:ILE:HD13	2.42	0.50
1:C:388:TRP:CE3	1:C:442:TYR:HB3	2.47	0.50
1:D:265:ASN:OD1	1:D:267:ALA:HB3	2.12	0.49
1:B:149:PHE:CD2	1:B:149:PHE:N	2.80	0.49
1:A:12:VAL:CG1	1:A:379:ILE:HD13	2.42	0.49
1:A:388:TRP:CE3	1:A:442:TYR:HB3	2.47	0.49
1:B:195:SER:OG	3:B:602:NAP:O1N	2.30	0.49
2:B:601:FAD:HM73	3:B:602:NAP:C5N	2.42	0.49
1:D:388:TRP:CE3	1:D:442:TYR:HB3	2.49	0.48
1:C:211:PHE:CE2	1:C:320:GLU:HG2	2.49	0.48
1:D:65:GLU:OE1	1:D:471:TYR:OH	2.31	0.48
1:C:433:ILE:HD12	1:C:468:CYS:SG	2.53	0.48
1:C:65:GLU:OE1	1:C:471:TYR:OH	2.32	0.47
1:C:301:PRO:HA	1:B:502:ARG:HG3	1.95	0.47
1:B:211:PHE:CE2	1:B:320:GLU:HG2	2.49	0.47
1:B:271:LEU:HG	1:B:299:ILE:HD13	1.97	0.47
1:D:433:ILE:HD12	1:D:468:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:HG22	1:A:100:LEU:HD22	1.97	0.47
1:A:19:LYS:HD3	1:A:98:PHE:CD2	2.50	0.47
1:A:433:ILE:HD12	1:A:468:CYS:SG	2.54	0.47
1:D:391:ARG:NH1	1:D:397:ASN:OD1	2.48	0.46
1:D:222:SER:OG	1:D:224:VAL:HB	2.14	0.46
1:A:80:ASN:ND2	1:A:495:THR:O	2.38	0.46
1:C:274:GLU:HB2	1:B:505:GLN:HE21	1.81	0.46
1:D:19:LYS:HD3	1:D:98:PHE:CD2	2.50	0.46
1:B:195:SER:HG	3:B:602:NAP:PN	2.39	0.46
1:C:271:LEU:HG	1:C:299:ILE:HD13	1.97	0.46
1:C:345:VAL:O	1:C:345:VAL:HG23	2.15	0.45
1:D:18:ILE:HG22	1:D:100:LEU:HD22	1.98	0.45
1:D:271:LEU:HG	1:D:299:ILE:HD13	1.98	0.45
1:C:265:ASN:OD1	1:C:267:ALA:HB3	2.15	0.45
1:B:232:ASP:OD1	1:B:232:ASP:N	2.38	0.45
1:C:388:TRP:CZ3	1:C:442:TYR:HB3	2.51	0.45
1:B:388:TRP:CZ3	1:B:442:TYR:HB3	2.52	0.45
1:B:265:ASN:OD1	1:B:267:ALA:HB3	2.17	0.45
1:B:19:LYS:HD3	1:B:98:PHE:CD2	2.51	0.45
1:A:388:TRP:CZ3	1:A:442:TYR:HB3	2.51	0.45
1:D:211:PHE:CE2	1:D:320:GLU:HG2	2.52	0.45
1:D:436:ILE:HG21	1:D:473:PHE:CZ	2.52	0.44
1:C:436:ILE:HG21	1:C:473:PHE:CZ	2.52	0.44
1:D:500:LYS:CD	1:A:267:ALA:O	2.66	0.44
1:D:520:LEU:HB3	1:D:521:PRO:HD3	1.99	0.44
1:C:19:LYS:HD3	1:C:98:PHE:CD2	2.52	0.44
1:A:436:ILE:HG21	1:A:473:PHE:CZ	2.52	0.44
1:B:99:ASN:HA	1:A:93:MET:HE1	1.99	0.44
1:D:388:TRP:CZ3	1:D:442:TYR:HB3	2.52	0.44
1:A:221:MET:HE2	1:A:225:PHE:CE1	2.52	0.44
1:D:504:VAL:HG22	1:D:505:GLN:H	1.83	0.44
1:C:18:ILE:HG22	1:C:100:LEU:HD22	1.99	0.44
1:A:504:VAL:HG22	1:A:505:GLN:H	1.83	0.44
1:C:391:ARG:NH1	1:C:397:ASN:OD1	2.49	0.43
1:A:265:ASN:OD1	1:A:267:ALA:HB3	2.18	0.43
1:B:18:ILE:HG22	1:B:100:LEU:HD22	1.99	0.43
1:C:504:VAL:HG22	1:C:505:GLN:H	1.84	0.43
1:B:348:GLY:O	1:B:427:ALA:HB1	2.18	0.43
1:A:271:LEU:HG	1:A:299:ILE:HD13	2.00	0.43
1:B:421:GLY:O	1:B:422:LEU:C	2.56	0.43
1:D:345:VAL:HG23	1:D:345:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:LEU:HB3	1:D:343:VAL:HG22	2.00	0.43
1:B:504:VAL:HG22	1:B:505:GLN:H	1.84	0.43
1:C:83:PRO:HD2	1:C:86:GLN:NE2	2.33	0.42
1:B:192:MET:HE3	1:B:212:LEU:HD22	2.01	0.42
1:B:436:ILE:HG21	1:B:473:PHE:CZ	2.54	0.42
1:A:40:LEU:HD11	2:A:601:FAD:C8	2.49	0.42
1:A:264:PHE:HE1	1:A:271:LEU:HD12	1.84	0.42
1:C:348:GLY:O	1:C:427:ALA:HB1	2.19	0.42
1:B:391:ARG:NH1	1:B:397:ASN:OD1	2.51	0.42
1:A:348:GLY:O	1:A:427:ALA:HB1	2.19	0.42
1:D:63:CYS:SG	1:D:233:MET:HG3	2.60	0.42
1:C:264:PHE:CE1	1:C:271:LEU:HD12	2.55	0.42
1:B:345:VAL:O	1:B:345:VAL:HG23	2.20	0.42
1:A:82:VAL:CG2	1:A:87:PHE:CD1	3.03	0.42
1:D:12:VAL:HG13	1:D:379:ILE:HD13	2.01	0.42
1:D:505:GLN:HE21	1:A:274:GLU:HB2	1.84	0.42
1:A:421:GLY:O	1:A:422:LEU:C	2.57	0.42
1:D:421:GLY:O	1:D:422:LEU:C	2.57	0.42
1:C:301:PRO:CA	1:B:502:ARG:HG3	2.49	0.42
1:B:12:VAL:HG13	1:B:379:ILE:HD13	2.02	0.42
1:A:12:VAL:HG13	1:A:379:ILE:HD13	2.02	0.42
1:B:264:PHE:HE1	1:B:271:LEU:HD12	1.84	0.41
1:D:238:ARG:NH2	1:D:472:GLN:HE21	2.17	0.41
1:D:264:PHE:HE1	1:D:271:LEU:HD12	1.85	0.41
4:B:604:LMT:H1B	4:B:604:LMT:H3'	1.96	0.41
1:A:264:PHE:CE1	1:A:271:LEU:HD12	2.55	0.41
1:D:264:PHE:CE1	1:D:271:LEU:HD12	2.55	0.41
1:C:274:GLU:HB2	1:B:505:GLN:NE2	2.35	0.41
1:D:192:MET:HE3	1:D:212:LEU:HD22	2.00	0.41
1:C:264:PHE:HE1	1:C:271:LEU:HD12	1.84	0.41
1:A:267:ALA:N	1:A:272:VAL:HG13	2.35	0.41
1:D:57:SER:HB3	1:D:202:GLU:OE2	2.21	0.41
1:C:12:VAL:HG13	1:C:379:ILE:HD13	2.00	0.41
1:C:421:GLY:O	1:C:422:LEU:C	2.59	0.41
1:B:337:PHE:CD1	1:B:338:LEU:HD22	2.56	0.41
1:A:238:ARG:NH2	1:A:472:GLN:HE21	2.19	0.41
1:D:37:LEU:HD23	1:D:37:LEU:C	2.41	0.41
1:D:40:LEU:HD11	2:D:601:FAD:HM82	2.02	0.41
1:B:264:PHE:CE1	1:B:271:LEU:HD12	2.55	0.41
1:B:267:ALA:N	1:B:272:VAL:HG13	2.36	0.41
1:A:345:VAL:HG23	1:A:345:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PHE:CD1	1:C:338:LEU:HD22	2.55	0.41
1:C:289:PRO:CB	1:B:224:VAL:HG21	2.50	0.40
1:B:486:ASN:O	1:B:490:THR:HG22	2.22	0.40
1:C:418:SER:HA	7:C:702:HOH:O	2.21	0.40
1:A:222:SER:OG	1:A:224:VAL:N	2.52	0.40
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.97	0.40
1:D:221:MET:HE2	1:D:225:PHE:CE1	2.56	0.40
1:D:271:LEU:O	1:D:272:VAL:C	2.59	0.40
1:C:40:LEU:HD11	2:C:601:FAD:HM82	2.03	0.40
1:A:232:ASP:OD1	1:A:232:ASP:N	2.39	0.40
1:D:348:GLY:O	1:D:427:ALA:HB1	2.20	0.40
1:A:211:PHE:CZ	1:A:320:GLU:HG2	2.56	0.40
1:A:288:LEU:CB	1:A:289:PRO:HD3	2.51	0.40
1:A:337:PHE:CD1	1:A:338:LEU:HD22	2.56	0.40
1:A:520:SER:O	1:A:521:LEU:C	2.60	0.40
1:D:500:LYS:HD3	1:A:267:ALA:O	2.20	0.40
1:C:269:TYR:CE2	1:B:228:GLY:HA3	2.57	0.40
1:B:241:ASN:O	1:B:245:ASN:ND2	2.54	0.40
1:A:379:ILE:CB	1:A:380:PRO:HD3	2.44	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	511/531 (96%)	442 (86%)	57 (11%)	12 (2%)	6 30
1	B	519/531 (98%)	445 (86%)	63 (12%)	11 (2%)	7 33
1	C	512/531 (96%)	437 (85%)	61 (12%)	14 (3%)	5 26
1	D	520/531 (98%)	438 (84%)	69 (13%)	13 (2%)	5 28
All	All	2062/2124 (97%)	1762 (86%)	250 (12%)	50 (2%)	6 29

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	66	MET
1	D	422	LEU
1	D	425	CYS
1	D	514	LEU
1	C	66	MET
1	C	422	LEU
1	C	425	CYS
1	C	513	PRO
1	C	514	SER
1	C	529	LEU
1	B	66	MET
1	B	277	THR
1	B	422	LEU
1	B	425	CYS
1	B	515	PRO
1	B	517	PRO
1	A	66	MET
1	A	422	LEU
1	A	425	CYS
1	D	277	THR
1	C	277	THR
1	A	277	THR
1	A	39	GLY
1	A	517	PRO
1	D	265	ASN
1	D	276	ARG
1	D	429	GLN
1	D	530	MET
1	C	265	ASN
1	C	429	GLN
1	B	39	GLY
1	B	276	ARG
1	B	429	GLN
1	A	276	ARG
1	A	302	SER
1	A	429	GLN
1	D	39	GLY
1	D	302	SER
1	D	528	LEU
1	C	39	GLY
1	C	276	ARG
1	C	302	SER

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Mol	Chain	Res	Type
1	C	525	LEU
1	A	515	PRO
1	D	504	VAL
1	C	504	VAL
1	B	265	ASN
1	A	265	ASN
1	A	504	VAL
1	B	504	VAL

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	443/469 (94%)	402 (91%)	41 (9%)	9 33
1	B	444/469 (95%)	407 (92%)	37 (8%)	11 39
1	C	441/469 (94%)	401 (91%)	40 (9%)	9 34
1	D	461/469 (98%)	415 (90%)	46 (10%)	7 29
All	All	1789/1876 (95%)	1625 (91%)	164 (9%)	9 34

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	LYS
1	D	37	LEU
1	D	56	LYS
1	D	63	CYS
1	D	114	THR
1	D	147	THR
1	D	149	PHE
1	D	163	ILE
1	D	164	ASN
1	D	182	PHE
1	D	206	LEU
1	D	215	THR
1	D	221	MET

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Mol	Chain	Res	Type
1	D	232	ASP
1	D	256	MET
1	D	272	VAL
1	D	274	GLU
1	D	275	ASP
1	D	277	THR
1	D	280	ARG
1	D	284	LEU
1	D	288	LEU
1	D	302	SER
1	D	306	VAL
1	D	322	ILE
1	D	340	GLU
1	D	349	GLN
1	D	352	LEU
1	D	388	TRP
1	D	402	GLN
1	D	412	ARG
1	D	416	LYS
1	D	426	LYS
1	D	429	GLN
1	D	430	SER
1	D	452	MET
1	D	453	LEU
1	D	455	THR
1	D	458	ARG
1	D	462	THR
1	D	503	ILE
1	D	515	LEU
1	D	516	LYS
1	D	527	LEU
1	D	529	LEU
1	D	531	CYS
1	C	3	LYS
1	C	37	LEU
1	C	56	LYS
1	C	63	CYS
1	C	66	MET
1	C	114	THR
1	C	147	THR
1	C	149	PHE
1	C	163	ILE

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Mol	Chain	Res	Type
1	C	164	ASN
1	C	182	PHE
1	C	206	LEU
1	C	215	THR
1	C	221	MET
1	C	232	ASP
1	C	256	MET
1	C	272	VAL
1	C	274	GLU
1	C	275	ASP
1	C	277	THR
1	C	280	ARG
1	C	284	LEU
1	C	288	LEU
1	C	306	VAL
1	C	340	GLU
1	C	349	GLN
1	C	352	LEU
1	C	402	GLN
1	C	412	ARG
1	C	416	LYS
1	C	426	LYS
1	C	429	GLN
1	C	430	SER
1	C	452	MET
1	C	453	LEU
1	C	455	THR
1	C	458	ARG
1	C	462	THR
1	C	469	THR
1	C	503	ILE
1	B	3	LYS
1	B	37	LEU
1	B	56	LYS
1	B	63	CYS
1	B	114	THR
1	B	147	THR
1	B	149	PHE
1	B	163	ILE
1	B	164	ASN
1	B	182	PHE
1	B	206	LEU

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Mol	Chain	Res	Type
1	B	215	THR
1	B	221	MET
1	B	232	ASP
1	B	256	MET
1	B	272	VAL
1	B	274	GLU
1	B	275	ASP
1	B	277	THR
1	B	280	ARG
1	B	284	LEU
1	B	288	LEU
1	B	306	VAL
1	B	349	GLN
1	B	352	LEU
1	B	402	GLN
1	B	412	ARG
1	B	416	LYS
1	B	426	LYS
1	B	429	GLN
1	B	430	SER
1	B	452	MET
1	B	453	LEU
1	B	455	THR
1	B	458	ARG
1	B	462	THR
1	B	503	ILE
1	A	3	LYS
1	A	37	LEU
1	A	56	LYS
1	A	63	CYS
1	A	114	THR
1	A	147	THR
1	A	149	PHE
1	A	163	ILE
1	A	164	ASN
1	A	182	PHE
1	A	206	LEU
1	A	215	THR
1	A	221	MET
1	A	232	ASP
1	A	256	MET
1	A	272	VAL

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Mol	Chain	Res	Type
1	A	274	GLU
1	A	275	ASP
1	A	277	THR
1	A	280	ARG
1	A	284	LEU
1	A	288	LEU
1	A	302	SER
1	A	306	VAL
1	A	340	GLU
1	A	349	GLN
1	A	352	LEU
1	A	388	TRP
1	A	402	GLN
1	A	412	ARG
1	A	416	LYS
1	A	426	LYS
1	A	429	GLN
1	A	430	SER
1	A	452	MET
1	A	453	LEU
1	A	455	THR
1	A	458	ARG
1	A	462	THR
1	A	469	THR
1	A	503	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	61	ASN
1	D	84	ASN
1	D	86	GLN
1	D	172	HIS
1	D	240	GLN
1	D	268	ASN
1	D	314	ASN
1	D	347	ASN
1	D	472	GLN
1	D	486	ASN
1	D	491	GLN
1	D	505	GLN
1	C	61	ASN

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Mol	Chain	Res	Type
1	C	84	ASN
1	C	86	GLN
1	C	99	ASN
1	C	172	HIS
1	C	268	ASN
1	C	314	ASN
1	C	347	ASN
1	C	472	GLN
1	C	486	ASN
1	C	491	GLN
1	B	61	ASN
1	B	84	ASN
1	B	86	GLN
1	B	172	HIS
1	B	314	ASN
1	B	347	ASN
1	B	472	GLN
1	B	486	ASN
1	B	491	GLN
1	B	505	GLN
1	A	61	ASN
1	A	84	ASN
1	A	86	GLN
1	A	96	ASN
1	A	99	ASN
1	A	172	HIS
1	A	314	ASN
1	A	347	ASN
1	A	472	GLN
1	A	486	ASN
1	A	491	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)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
4	LMT	D	603	-	36,36,36	0.77	1 (2%)	47,47,47	1.11	4 (8%)
5	GOL	D	606	-	5,5,5	0.14	0	5,5,5	0.37	0
4	LMT	B	604	-	36,36,36	0.73	1 (2%)	47,47,47	1.41	6 (12%)
4	LMT	A	606	-	36,36,36	0.73	1 (2%)	47,47,47	1.60	5 (10%)
3	NAP	D	602	-	45,52,52	0.88	2 (4%)	56,80,80	1.25	7 (12%)
3	NAP	C	602	-	45,52,52	0.90	3 (6%)	56,80,80	1.20	6 (10%)
3	NAP	B	602	-	45,52,52	0.90	1 (2%)	56,80,80	1.37	8 (14%)
3	NAP	A	602	-	45,52,52	0.89	2 (4%)	56,80,80	1.50	9 (16%)
4	LMT	A	605	-	36,36,36	0.67	1 (2%)	47,47,47	0.88	2 (4%)
2	FAD	B	601	-	53,58,58	0.67	0	68,89,89	0.79	3 (4%)
4	LMT	B	603	-	36,36,36	0.63	1 (2%)	47,47,47	0.88	2 (4%)
2	FAD	D	601	-	53,58,58	0.66	0	68,89,89	0.78	1 (1%)
5	GOL	D	604	-	5,5,5	0.21	0	5,5,5	0.57	0
4	LMT	A	603	-	36,36,36	0.76	1 (2%)	47,47,47	1.36	7 (14%)
2	FAD	C	601	-	53,58,58	0.62	0	68,89,89	0.78	2 (2%)
2	FAD	A	601	-	53,58,58	0.65	0	68,89,89	0.88	4 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMT	D	603	-	-	8/21/61/61	0/2/2/2
5	GOL	D	606	-	-	0/4/4/4	-
4	LMT	B	604	-	-	10/21/61/61	0/2/2/2
4	LMT	A	606	-	-	12/21/61/61	0/2/2/2
3	NAP	D	602	-	-	14/31/67/67	0/5/5/5
3	NAP	C	602	-	-	13/31/67/67	0/5/5/5
3	NAP	B	602	-	-	9/31/67/67	0/5/5/5
3	NAP	A	602	-	-	10/31/67/67	0/5/5/5
4	LMT	A	605	-	-	10/21/61/61	0/2/2/2
2	FAD	B	601	-	-	12/30/50/50	0/6/6/6
4	LMT	B	603	-	-	9/21/61/61	0/2/2/2
2	FAD	D	601	-	-	12/30/50/50	0/6/6/6
5	GOL	D	604	-	-	2/4/4/4	-
4	LMT	A	603	-	-	11/21/61/61	0/2/2/2
2	FAD	C	601	-	-	12/30/50/50	0/6/6/6
2	FAD	A	601	-	-	12/30/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	LMT	O1'-C1'	2.88	1.45	1.40
4	D	603	LMT	O1'-C1'	2.87	1.45	1.40
4	A	605	LMT	O1'-C1'	2.80	1.45	1.40
4	A	603	LMT	O1'-C1'	2.73	1.44	1.40
4	B	604	LMT	O1'-C1'	2.70	1.44	1.40
3	B	602	NAP	C5A-C4A	2.67	1.48	1.40
3	C	602	NAP	C5A-C4A	2.51	1.47	1.40
3	D	602	NAP	O4D-C1D	2.40	1.44	1.41
3	A	602	NAP	C5A-C4A	2.26	1.46	1.40
3	D	602	NAP	C5A-C4A	2.26	1.46	1.40
4	B	603	LMT	O1'-C1'	2.23	1.44	1.40
3	A	602	NAP	P2B-O2B	2.13	1.63	1.59
3	C	602	NAP	P2B-O2B	2.12	1.63	1.59
3	C	602	NAP	O4D-C1D	2.09	1.44	1.41

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	LMT	O1'-C1'-C2'	7.03	119.28	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	606	LMT	C1-O1'-C1'	4.66	121.57	113.84
3	A	602	NAP	N3A-C2A-N1A	-4.51	121.63	128.68
3	D	602	NAP	N3A-C2A-N1A	-4.25	122.04	128.68
3	B	602	NAP	N3A-C2A-N1A	-4.23	122.06	128.68
3	C	602	NAP	N3A-C2A-N1A	-4.09	122.29	128.68
4	B	604	LMT	C1B-C2B-C3B	4.04	118.42	110.00
4	B	604	LMT	O1B-C4'-C3'	3.83	117.46	107.28
4	B	604	LMT	C1'-O5'-C5'	3.48	120.52	113.69
4	A	603	LMT	C1B-C2B-C3B	3.48	117.24	110.00
3	A	602	NAP	O7N-C7N-C3N	-3.46	115.49	119.63
3	A	602	NAP	C1B-N9A-C4A	-3.37	120.71	126.64
3	A	602	NAP	C4A-C5A-N7A	-3.33	105.92	109.40
4	D	603	LMT	O5'-C5'-C4'	3.32	116.75	109.75
4	A	603	LMT	C1B-O5B-C5B	3.31	120.19	113.69
3	C	602	NAP	C3D-C2D-C1D	3.12	105.68	100.98
4	A	603	LMT	C2'-C3'-C4'	3.10	116.77	109.68
4	B	604	LMT	C1B-O1B-C4'	3.10	125.64	117.96
4	B	604	LMT	C4B-C3B-C2B	3.08	116.20	110.82
3	D	602	NAP	C6N-N1N-C2N	-3.05	119.20	121.97
3	C	602	NAP	PN-O3-PA	-3.05	122.38	132.83
4	A	603	LMT	O1B-C4'-C5'	2.96	117.55	109.45
3	A	602	NAP	C3D-C2D-C1D	2.95	105.42	100.98
3	A	602	NAP	PN-O3-PA	-2.91	122.83	132.83
4	A	606	LMT	O5'-C1'-C2'	-2.91	104.19	110.35
3	B	602	NAP	PN-O3-PA	-2.78	123.30	132.83
4	A	603	LMT	C1'-C2'-C3'	2.72	115.67	110.00
3	C	602	NAP	C4A-C5A-N7A	-2.72	106.57	109.40
4	D	603	LMT	O1'-C1'-C2'	2.72	112.54	108.30
4	A	603	LMT	O1B-C1B-C2B	2.64	114.94	108.10
3	B	602	NAP	C2A-N1A-C6A	2.58	123.17	118.75
3	D	602	NAP	PN-O3-PA	-2.58	123.98	132.83
4	B	604	LMT	O5'-C5'-C4'	2.57	115.17	109.75
4	B	603	LMT	O1B-C1B-C2B	2.55	114.72	108.10
3	A	602	NAP	C2A-N1A-C6A	2.51	123.05	118.75
4	D	603	LMT	C1'-O5'-C5'	2.38	118.36	113.69
3	B	602	NAP	O7N-C7N-C3N	-2.38	116.79	119.63
2	A	601	FAD	C5A-C6A-N6A	2.36	123.94	120.35
4	A	606	LMT	O5B-C5B-C6B	2.33	112.22	106.44
4	A	605	LMT	C3'-C4'-C5'	-2.29	105.67	110.93
4	A	603	LMT	C1B-O1B-C4'	2.29	123.63	117.96
3	D	602	NAP	O2B-P2B-O1X	-2.29	100.55	109.39
3	A	602	NAP	C6N-N1N-C2N	-2.26	119.91	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	602	NAP	C2A-N1A-C6A	2.25	122.60	118.75
2	A	601	FAD	O5'-C5'-C4'	2.22	115.29	109.36
2	C	601	FAD	C5A-C6A-N6A	2.22	123.72	120.35
3	D	602	NAP	C1B-N9A-C4A	-2.21	122.75	126.64
3	C	602	NAP	C1B-N9A-C4A	-2.17	122.83	126.64
3	B	602	NAP	C4A-C5A-N7A	-2.15	107.15	109.40
4	A	605	LMT	C1-O1'-C1'	2.13	117.38	113.84
2	D	601	FAD	C4-N3-C2	-2.13	121.70	125.64
3	B	602	NAP	C3D-C2D-C1D	2.13	104.18	100.98
4	B	603	LMT	C1B-C2B-C3B	2.12	114.40	110.00
3	A	602	NAP	O2A-PA-O1A	2.10	122.65	112.24
4	A	606	LMT	C1B-O5B-C5B	2.10	117.82	113.69
3	B	602	NAP	O3X-P2B-O2X	2.10	115.67	107.64
3	C	602	NAP	C2A-N1A-C6A	2.09	122.33	118.75
2	A	601	FAD	O2A-PA-O1A	2.09	122.58	112.24
2	A	601	FAD	C4-N3-C2	-2.08	121.80	125.64
3	B	602	NAP	O2A-PA-O1A	2.08	122.52	112.24
2	B	601	FAD	C5A-C6A-N6A	2.07	123.49	120.35
2	C	601	FAD	C4-N3-C2	-2.06	121.83	125.64
2	B	601	FAD	C4-N3-C2	-2.03	121.90	125.64
3	D	602	NAP	C4A-C5A-N7A	-2.02	107.29	109.40
4	D	603	LMT	C1B-O5B-C5B	2.02	117.66	113.69
2	B	601	FAD	C4X-C4-N3	2.01	118.30	113.19

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	N10-C1'-C2'-C3'
2	D	601	FAD	C5'-O5'-P-O1P
2	D	601	FAD	C5'-O5'-P-O2P
2	C	601	FAD	N10-C1'-C2'-O2'
2	C	601	FAD	N10-C1'-C2'-C3'
2	C	601	FAD	C5'-O5'-P-O1P
2	C	601	FAD	C5'-O5'-P-O2P
2	B	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	C5'-O5'-P-O1P
2	B	601	FAD	C5'-O5'-P-O2P
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5'-O5'-P-O2P
3	D	602	NAP	C5B-O5B-PA-O1A
3	D	602	NAP	O4B-C4B-C5B-O5B
3	D	602	NAP	C5D-O5D-PN-O3
3	D	602	NAP	C2N-C3N-C7N-O7N
3	D	602	NAP	C2N-C3N-C7N-N7N
3	C	602	NAP	C5B-O5B-PA-O1A
3	C	602	NAP	O4B-C4B-C5B-O5B
3	C	602	NAP	C3B-C4B-C5B-O5B
3	C	602	NAP	C5D-O5D-PN-O3
3	C	602	NAP	C5D-O5D-PN-O1N
3	C	602	NAP	C5D-O5D-PN-O2N
3	C	602	NAP	C2N-C3N-C7N-O7N
3	C	602	NAP	C2N-C3N-C7N-N7N
3	B	602	NAP	C5B-O5B-PA-O1A
3	B	602	NAP	C2N-C3N-C7N-O7N
3	B	602	NAP	C2N-C3N-C7N-N7N
3	A	602	NAP	O4B-C4B-C5B-O5B
3	A	602	NAP	C5D-O5D-PN-O3
3	A	602	NAP	C5D-O5D-PN-O2N
3	A	602	NAP	C2N-C3N-C7N-O7N
3	A	602	NAP	C2N-C3N-C7N-N7N
4	B	604	LMT	C2'-C1'-O1'-C1
4	B	604	LMT	O5'-C1'-O1'-C1
4	A	605	LMT	C2'-C1'-O1'-C1
4	A	605	LMT	O5'-C1'-O1'-C1
4	A	606	LMT	C2'-C1'-O1'-C1
5	D	604	GOL	O1-C1-C2-C3
4	B	604	LMT	C3'-C4'-O1B-C1B
3	D	602	NAP	C4N-C3N-C7N-O7N
3	D	602	NAP	C4N-C3N-C7N-N7N
3	C	602	NAP	C4N-C3N-C7N-O7N
3	C	602	NAP	C4N-C3N-C7N-N7N
4	A	603	LMT	C5'-C4'-O1B-C1B
3	B	602	NAP	C4N-C3N-C7N-O7N
3	A	602	NAP	C4N-C3N-C7N-N7N
3	B	602	NAP	C4N-C3N-C7N-N7N
3	A	602	NAP	C4N-C3N-C7N-O7N
4	A	603	LMT	C2B-C1B-O1B-C4'
4	A	603	LMT	O5B-C1B-O1B-C4'
4	A	603	LMT	O5B-C5B-C6B-O6B
3	D	602	NAP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	D	602	NAP	C3D-C4D-C5D-O5D
4	A	605	LMT	O5'-C5'-C6'-O6'
4	A	606	LMT	C4'-C5'-C6'-O6'
4	B	604	LMT	O5'-C5'-C6'-O6'
2	D	601	FAD	O3'-C3'-C4'-C5'
2	C	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-C5'
4	D	603	LMT	C4'-C5'-C6'-O6'
2	D	601	FAD	C2'-C3'-C4'-C5'
2	C	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
4	A	606	LMT	O5'-C5'-C6'-O6'
3	D	602	NAP	C3B-C4B-C5B-O5B
3	A	602	NAP	C3B-C4B-C5B-O5B
2	D	601	FAD	C2'-C3'-C4'-O4'
4	A	606	LMT	C5'-C4'-O1B-C1B
4	A	603	LMT	C4B-C5B-C6B-O6B
4	B	604	LMT	C4'-C5'-C6'-O6'
3	C	602	NAP	C1B-C2B-O2B-P2B
4	B	604	LMT	O1'-C1-C2-C3
2	B	601	FAD	C2'-C3'-C4'-C5'
4	A	605	LMT	O5B-C5B-C6B-O6B
4	A	606	LMT	C1-C2-C3-C4
2	D	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-O4'
4	D	603	LMT	C6-C7-C8-C9
4	B	604	LMT	C5-C6-C7-C8
2	C	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-O4'
4	A	605	LMT	C3-C4-C5-C6
4	B	604	LMT	C3-C4-C5-C6
3	C	602	NAP	C3B-C2B-O2B-P2B
4	A	603	LMT	C2-C3-C4-C5
4	D	603	LMT	C1-C2-C3-C4
4	B	604	LMT	C2-C1-O1'-C1'
4	A	605	LMT	C2-C1-O1'-C1'
4	A	606	LMT	C2-C1-O1'-C1'
4	D	603	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	606	LMT	O1'-C1-C2-C3
4	A	605	LMT	C4'-C5'-C6'-O6'
5	D	604	GOL	O1-C1-C2-O2
4	B	604	LMT	C7-C8-C9-C10
4	A	606	LMT	O5'-C1'-O1'-C1
4	B	603	LMT	C1-C2-C3-C4
4	D	603	LMT	O5'-C5'-C6'-O6'
4	A	603	LMT	O1'-C1-C2-C3
4	A	605	LMT	C1-C2-C3-C4
4	A	603	LMT	C4-C5-C6-C7
4	D	603	LMT	C5-C6-C7-C8
4	A	606	LMT	C3'-C4'-O1B-C1B
4	D	603	LMT	C3-C4-C5-C6
2	B	601	FAD	O4'-C4'-C5'-O5'
4	D	603	LMT	C2-C1-O1'-C1'
2	D	601	FAD	PA-O3P-P-O5'
2	C	601	FAD	PA-O3P-P-O5'
2	B	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	PA-O3P-P-O5'
4	B	603	LMT	C5-C6-C7-C8
4	A	603	LMT	C3'-C4'-O1B-C1B
4	A	605	LMT	C2-C3-C4-C5
3	D	602	NAP	C5B-O5B-PA-O3
3	B	602	NAP	C5B-O5B-PA-O3
3	A	602	NAP	C2B-O2B-P2B-O3X
4	A	606	LMT	C3-C4-C5-C6
4	B	603	LMT	C3-C4-C5-C6
4	A	603	LMT	C3-C4-C5-C6
3	D	602	NAP	C5D-O5D-PN-O1N
3	D	602	NAP	C5D-O5D-PN-O2N
3	A	602	NAP	C5D-O5D-PN-O1N
4	A	606	LMT	C4-C5-C6-C7
4	B	603	LMT	C11-C10-C9-C8
2	B	601	FAD	N10-C1'-C2'-O2'
4	B	603	LMT	O1'-C1-C2-C3
4	B	603	LMT	C2B-C1B-O1B-C4'
4	A	605	LMT	C6-C7-C8-C9
4	A	603	LMT	C6-C7-C8-C9
4	B	603	LMT	C7-C8-C9-C10
3	B	602	NAP	PA-O3-PN-O5D
4	B	603	LMT	C9-C10-C11-C12
2	D	601	FAD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	C	601	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	O4'-C4'-C5'-O5'
4	A	606	LMT	C2-C3-C4-C5
2	D	601	FAD	C5'-O5'-P-O3P
2	C	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5'-O5'-P-O3P
2	A	601	FAD	C5'-O5'-P-O3P
3	C	602	NAP	C5B-O5B-PA-O3
3	B	602	NAP	C2B-O2B-P2B-O2X
2	A	601	FAD	O4B-C4B-C5B-O5B
3	D	602	NAP	C5B-O5B-PA-O2A
2	D	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
3	B	602	NAP	O4B-C4B-C5B-O5B
4	B	603	LMT	C4-C5-C6-C7

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	LMT	2	0
3	D	602	NAP	1	0
3	C	602	NAP	1	0
3	B	602	NAP	6	0
3	A	602	NAP	3	0
2	B	601	FAD	3	0
2	D	601	FAD	2	0
2	C	601	FAD	3	0
2	A	601	FAD	4	0

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

equivalents in the CSD to analyse the geometry.

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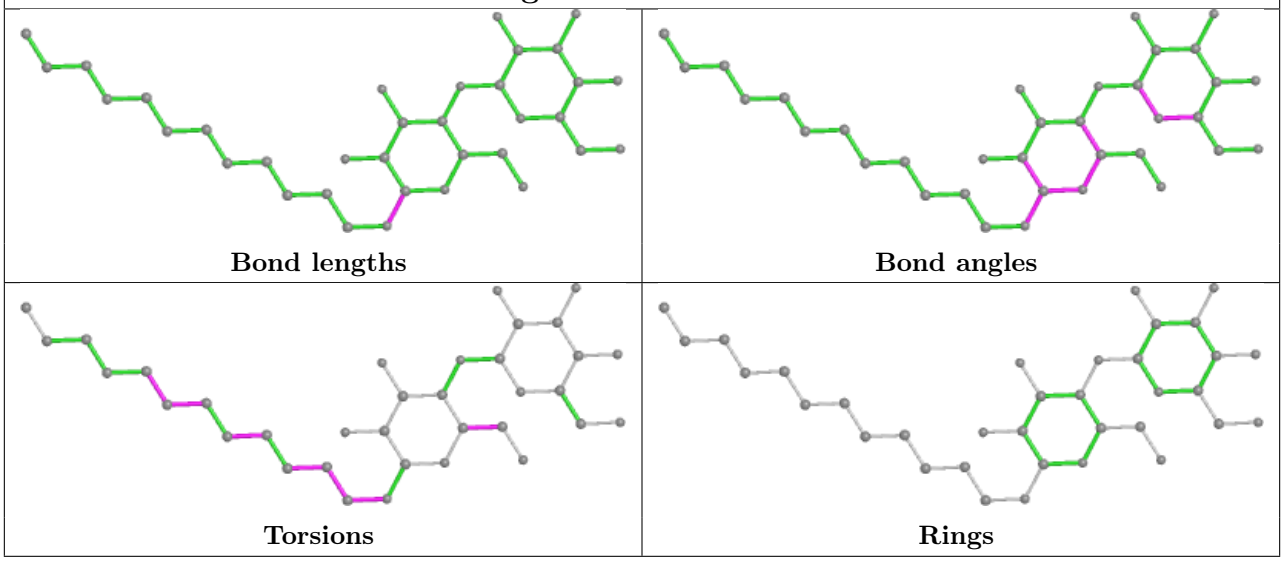
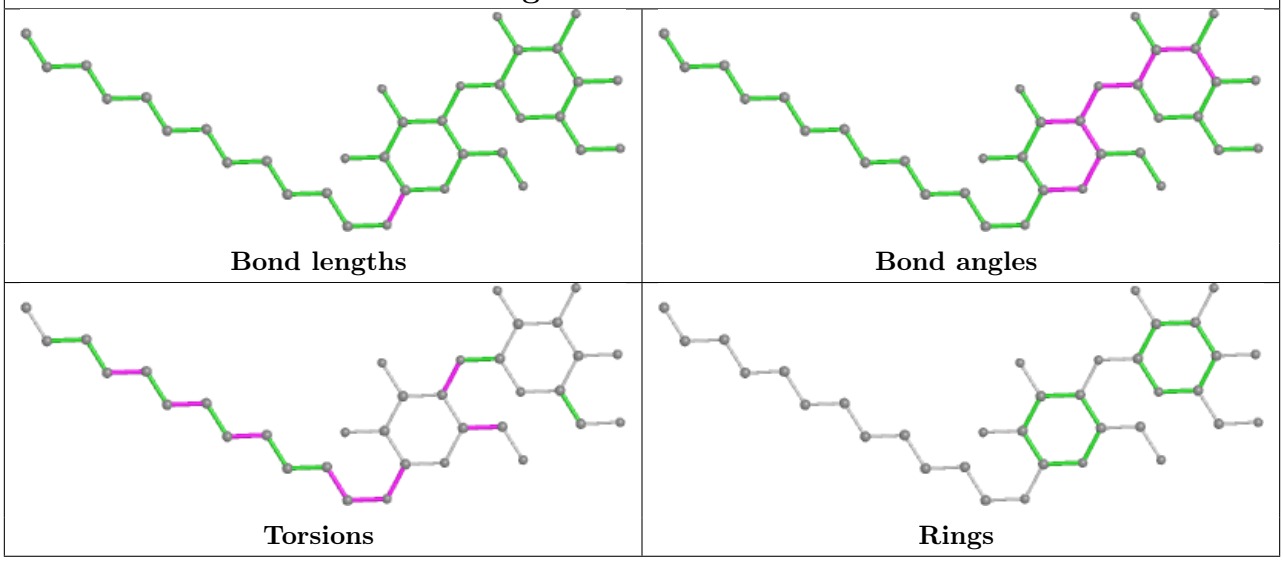


Ligand LMT B 604



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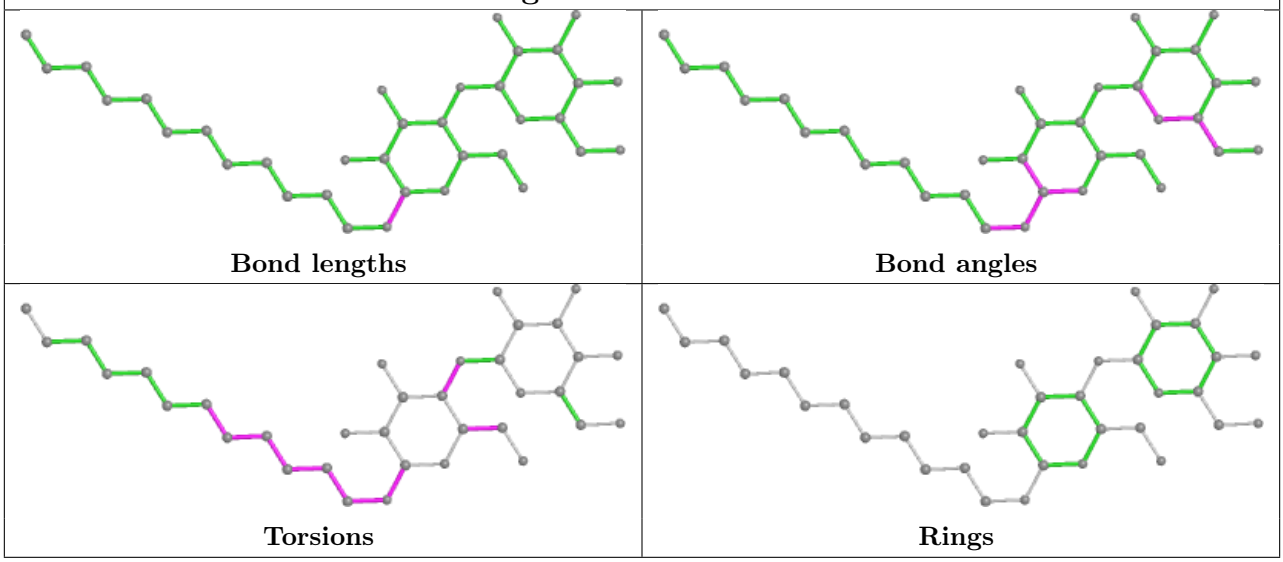

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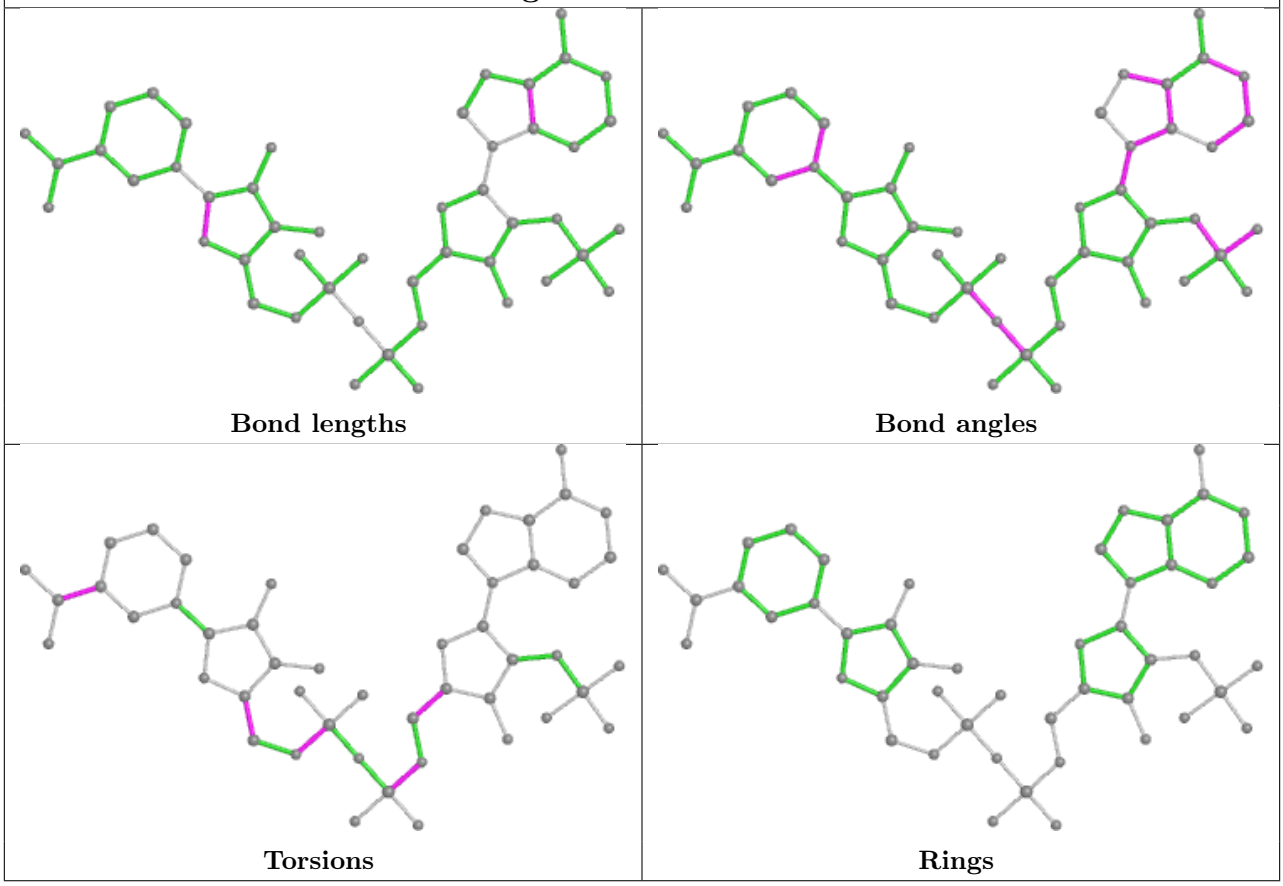

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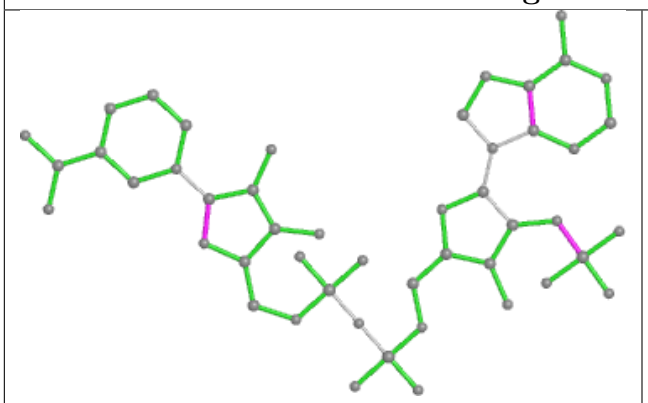
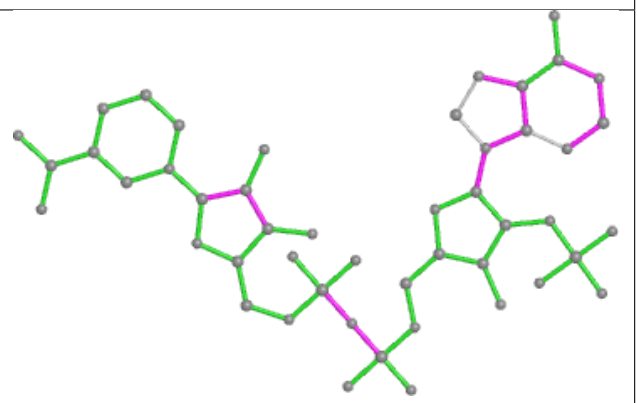
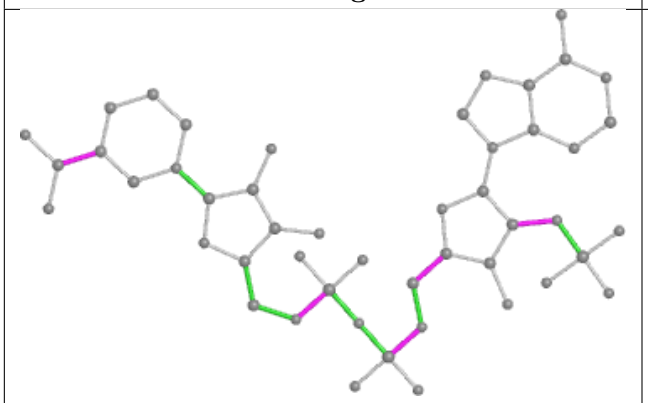


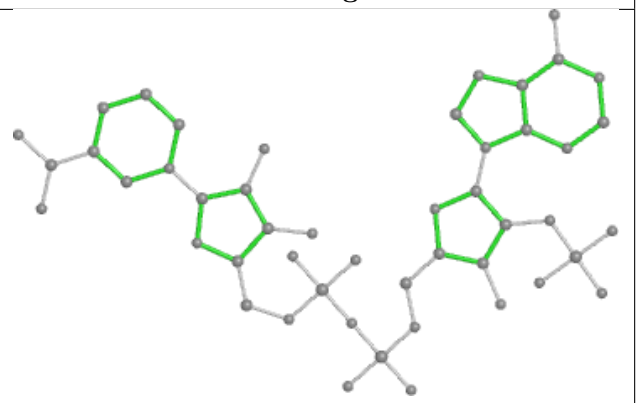
Bond lengths



Bond angles

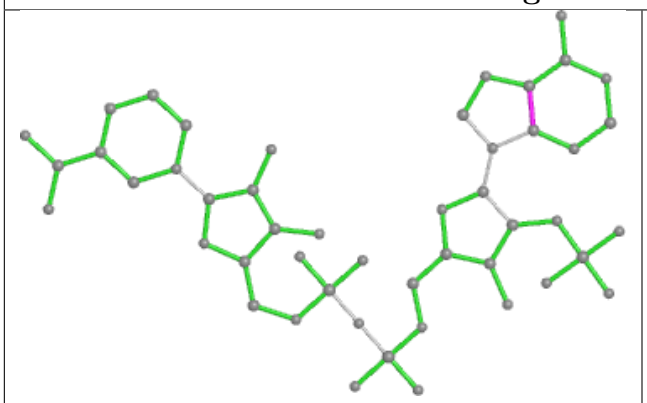


Torsions

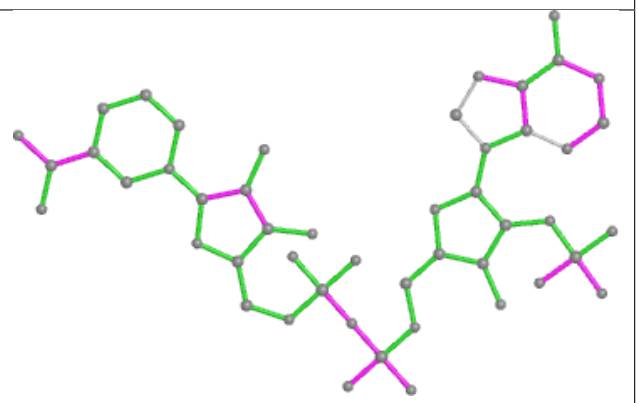


Rings

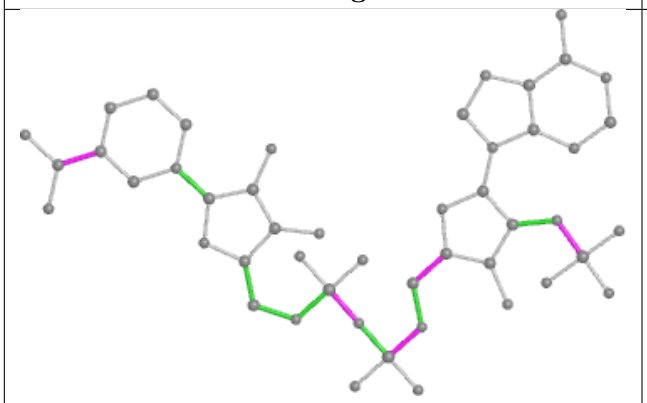
Ligand NAP B 602



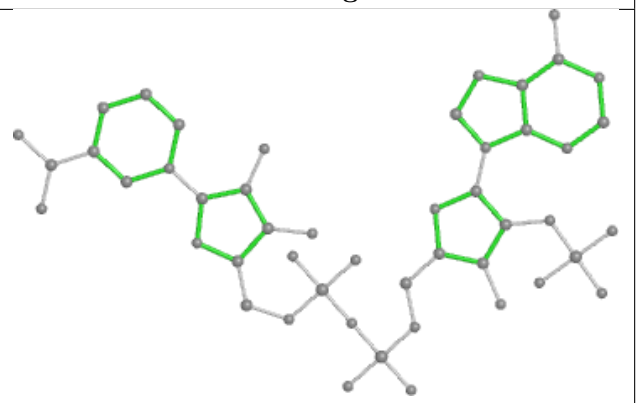
Bond lengths



Bond angles

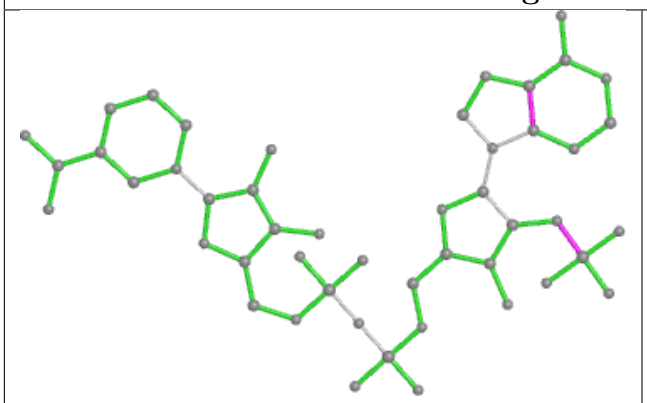


Torsions

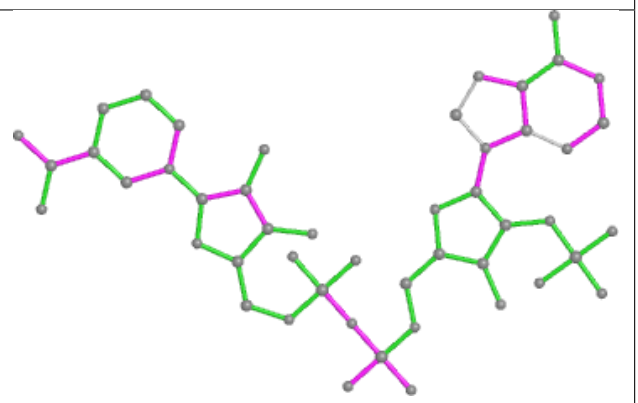


Rings

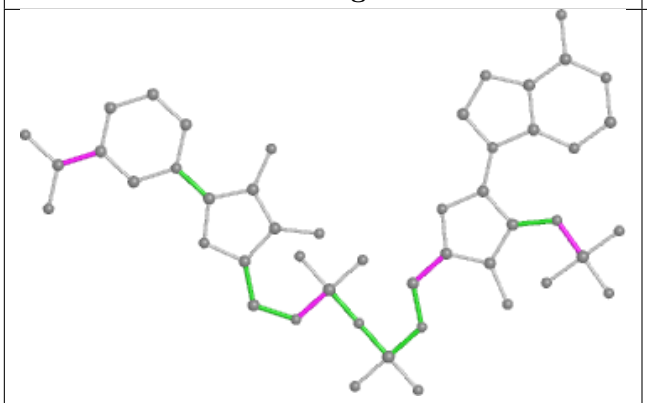
Ligand NAP A 602



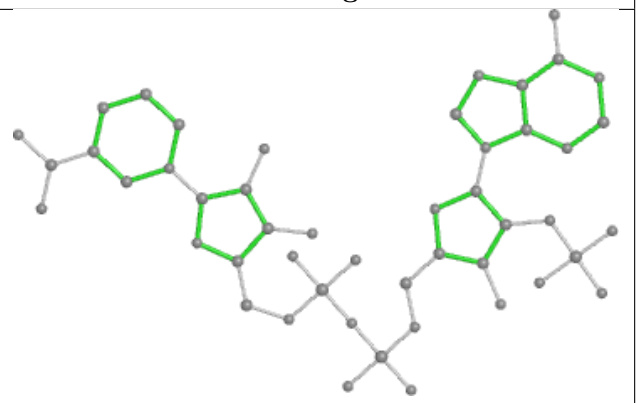
Bond lengths



Bond angles

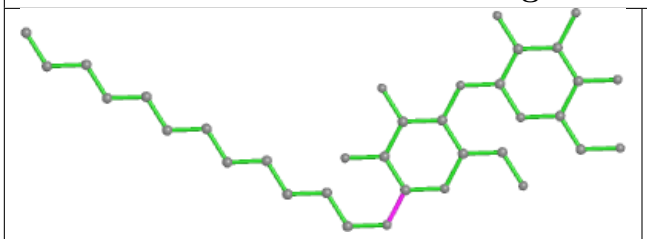


Torsions

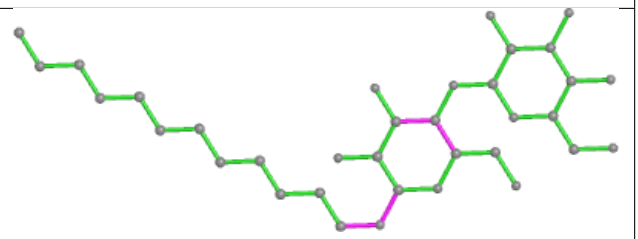


Rings

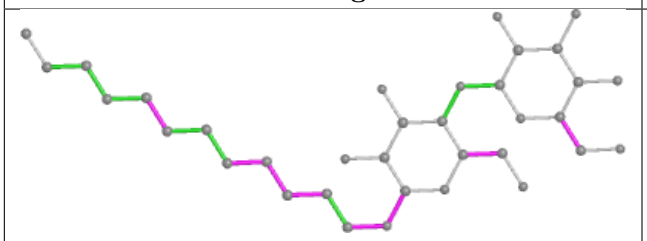
Ligand LMT A 605



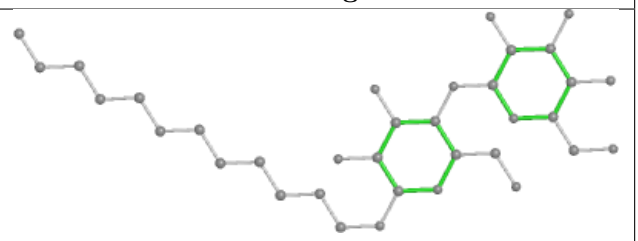
Bond lengths



Bond angles

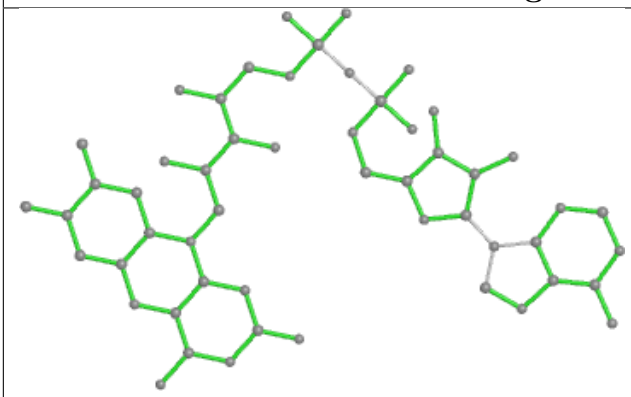


Torsions

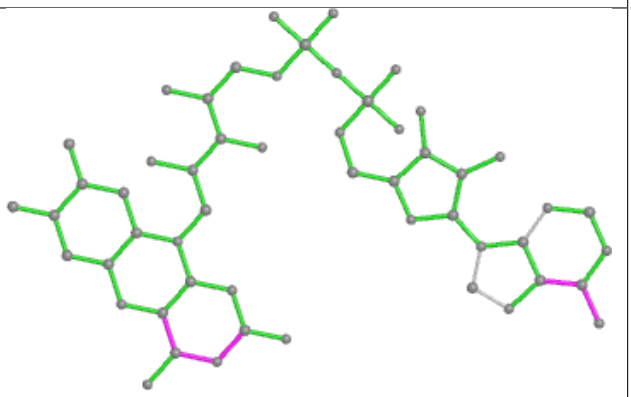


Rings

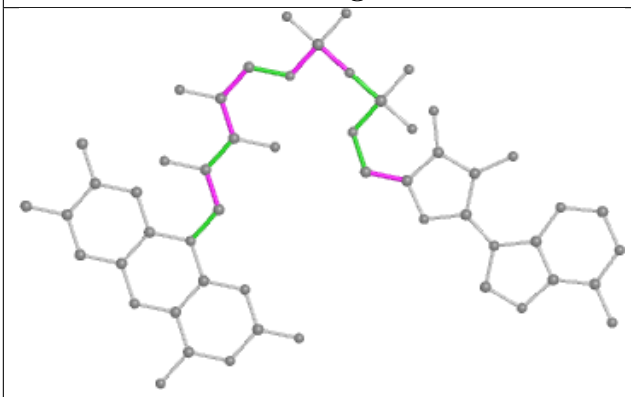
Ligand FAD B 601



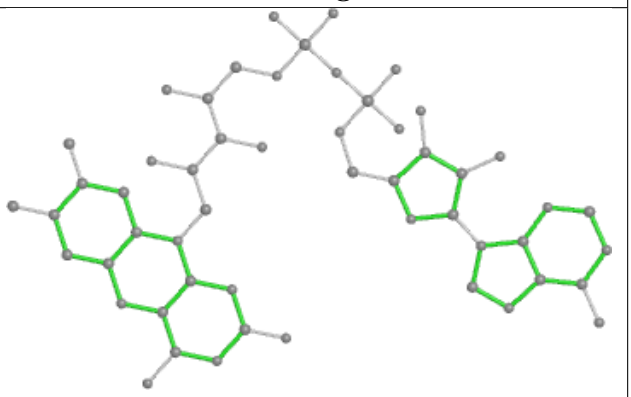
Bond lengths



Bond angles

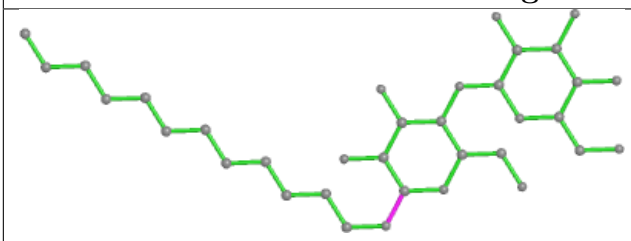


Torsions



Rings

Ligand LMT B 603



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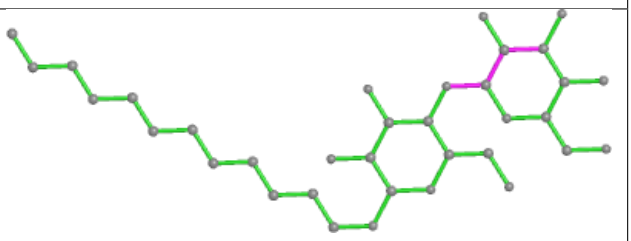
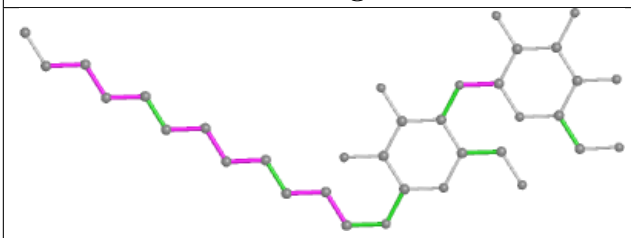
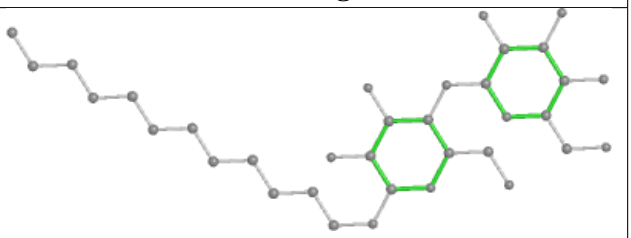


Bond angles

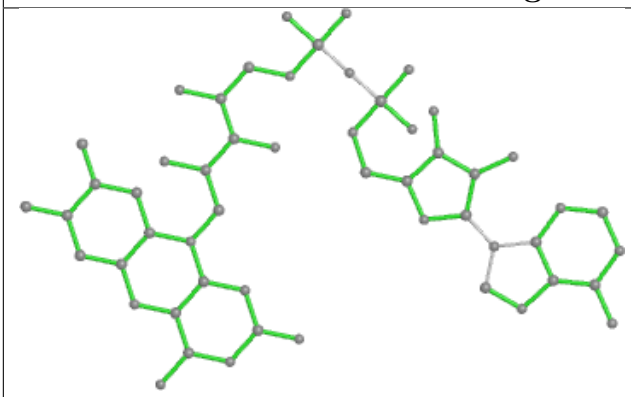


Torsions

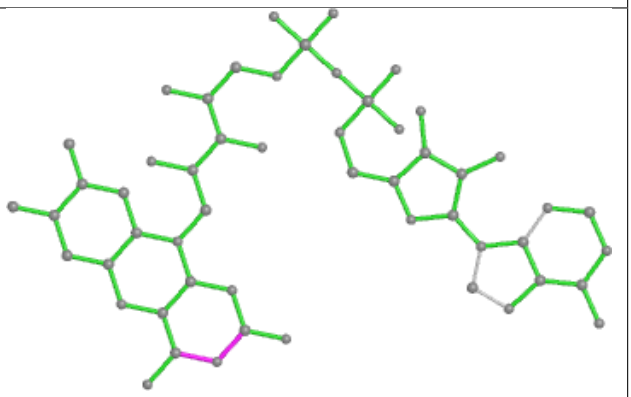


Rings

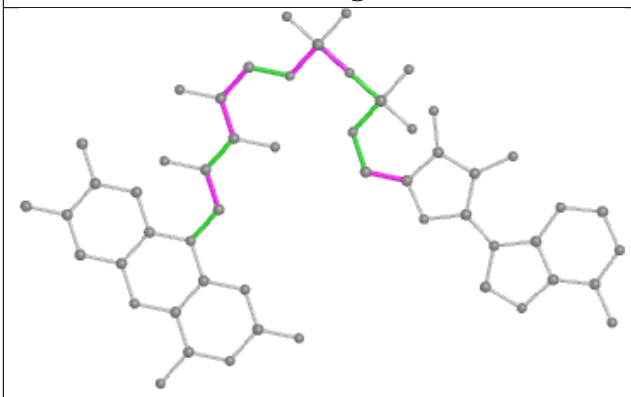
Ligand FAD D 601



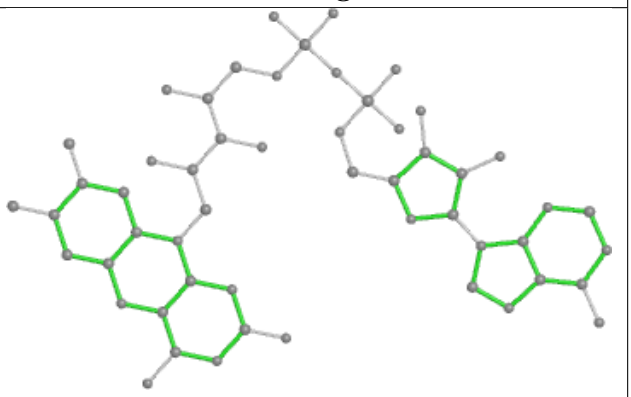
Bond lengths



Bond angles

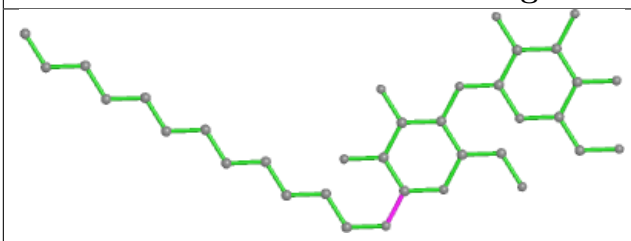


Torsions

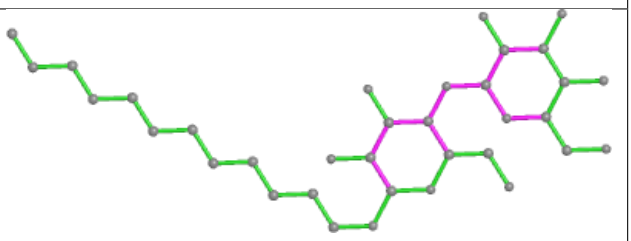


Rings

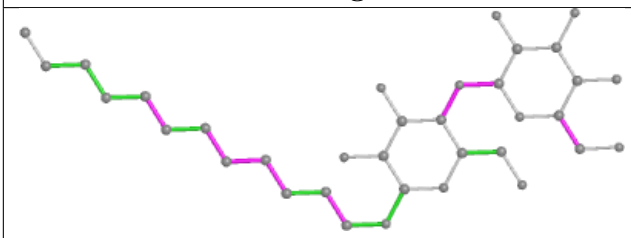
Ligand LMT A 603



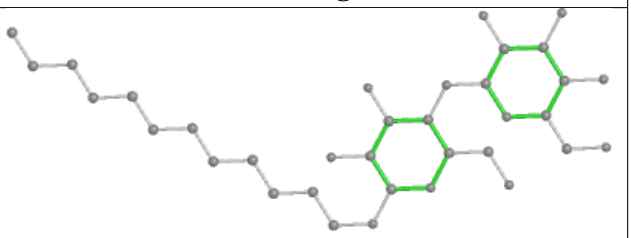
Bond lengths



Bond angles

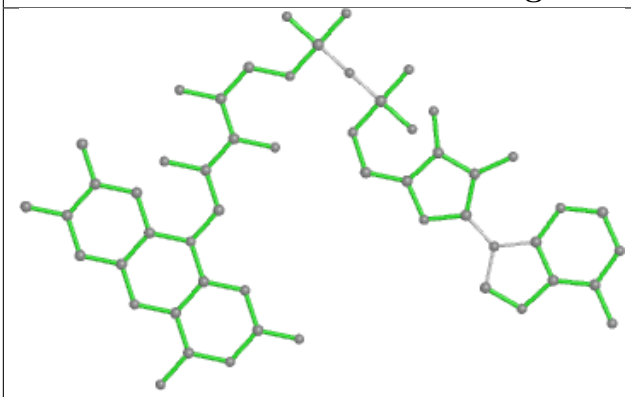


Torsions

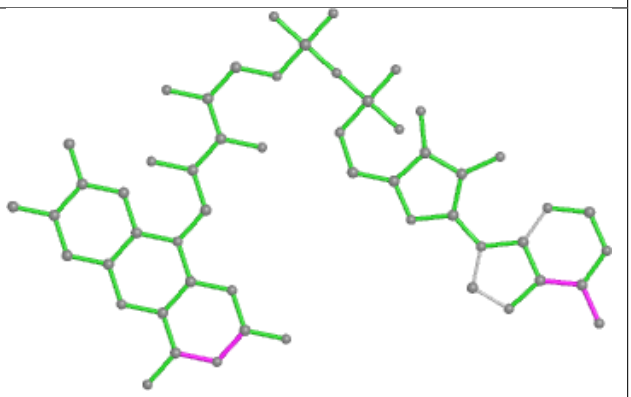


Rings

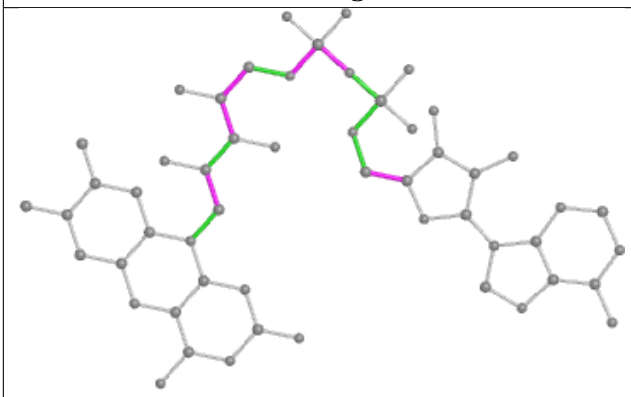
Ligand FAD C 601



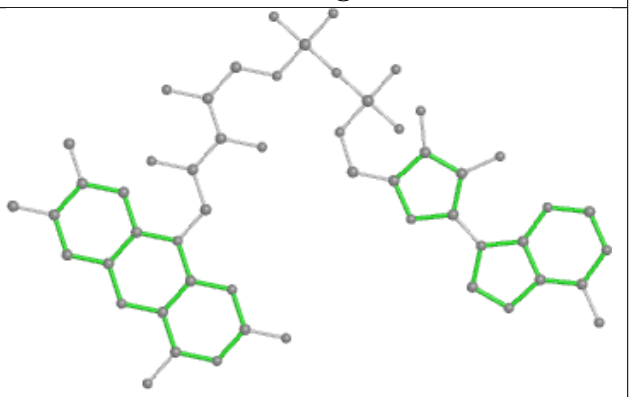
Bond lengths



Bond angles

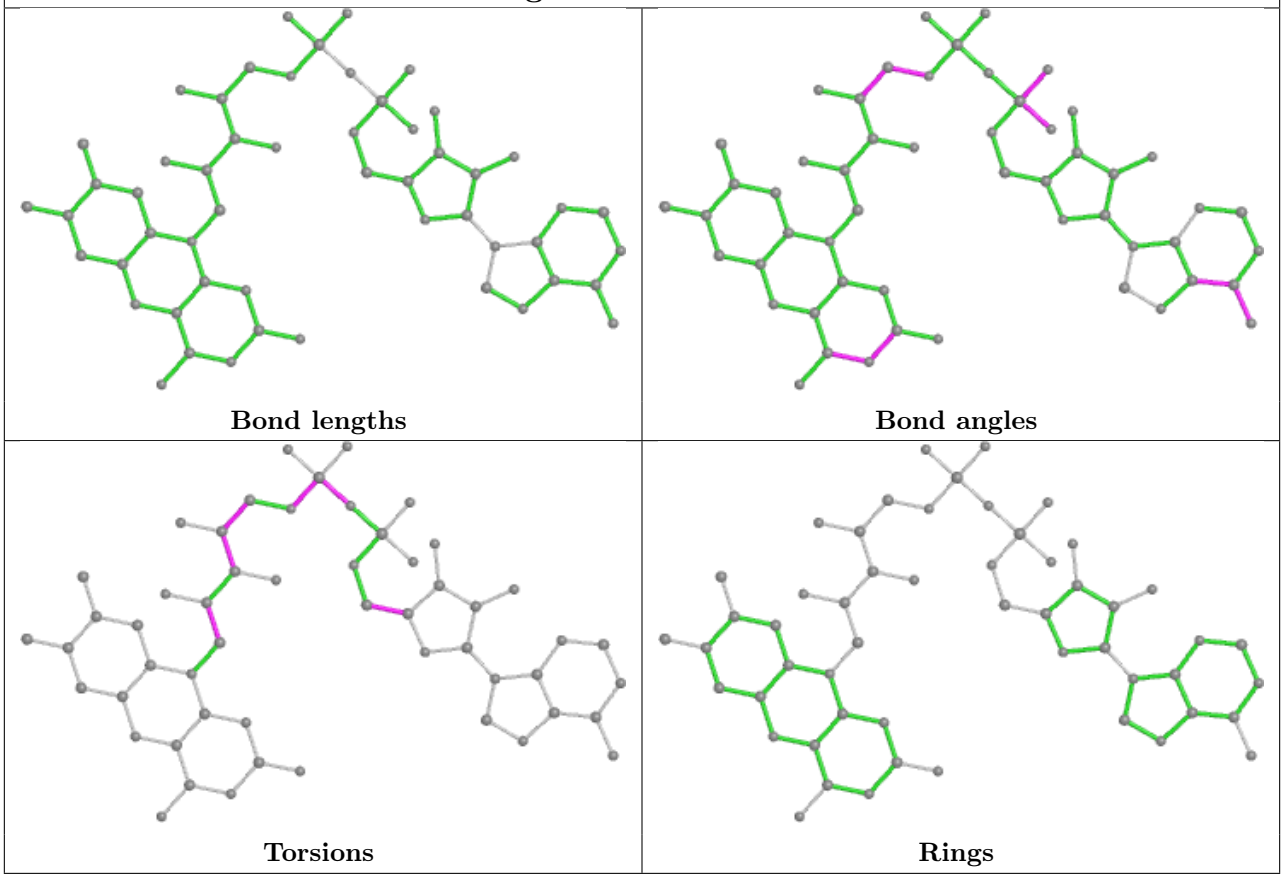


Torsions



Rings

Ligand FAD A 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	505:GLN	C	513:GLU	N	16.04
1	B	506:GLU	C	514:SER	N	15.75
1	C	506:GLU	C	512:SER	N	11.59
1	A	521:LEU	C	527:LEU	N	11.20

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	517/531 (97%)	-0.31	6 (1%) 79 54	28, 61, 116, 167	0
1	B	523/531 (98%)	-0.10	21 (4%) 38 15	38, 83, 144, 190	0
1	C	520/531 (97%)	0.51	61 (11%) 4 1	62, 136, 181, 217	0
1	D	524/531 (98%)	-0.35	6 (1%) 80 56	26, 56, 116, 222	0
All	All	2084/2124 (98%)	-0.06	94 (4%) 33 12	26, 77, 162, 222	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	THR	6.0
1	C	340	GLU	4.9
1	A	277	THR	4.8
1	C	341	SER	4.4
1	C	142	ALA	4.3
1	A	505	GLN	4.3
1	D	277	THR	4.3
1	B	117	PRO	4.0
1	C	393	LEU	4.0
1	C	489	LEU	4.0
1	C	423	CYS	3.9
1	C	505	GLN	3.9
1	C	361	LEU	3.8
1	C	365	THR	3.8
1	C	95	ALA	3.8
1	C	360	HIS	3.7
1	C	119	PHE	3.7
1	C	38	GLY	3.6
1	C	348	GLY	3.6
1	C	359	ALA	3.6
1	C	506	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	274	GLU	3.6
1	C	277	THR	3.6
1	C	368	VAL	3.5
1	C	101	LEU	3.5
1	C	3	LYS	3.5
1	C	392	VAL	3.5
1	B	506	GLU	3.4
1	C	355	TYR	3.3
1	B	121	VAL	3.3
1	C	42	ARG	3.3
1	C	165	THR	3.1
1	D	505	GLN	3.1
1	C	397	ASN	3.1
1	C	136	GLU	3.1
1	B	274	GLU	3.0
1	C	353	TYR	2.9
1	B	118	ASP	2.9
1	C	349	GLN	2.8
1	B	250	PRO	2.8
1	C	339	ASP	2.8
1	C	346	GLU	2.8
1	B	119	PHE	2.8
1	A	135	GLN	2.8
1	C	141	ASP	2.8
1	B	420	PHE	2.7
1	B	122	THR	2.7
1	C	388	TRP	2.7
1	C	471	TYR	2.7
1	C	358	PRO	2.7
1	C	351	SER	2.6
1	C	104	ILE	2.6
1	C	43	PHE	2.6
1	D	531	CYS	2.6
1	C	449	LEU	2.5
1	B	120	THR	2.5
1	C	382	GLY	2.5
1	C	306	VAL	2.5
1	B	116	CYS	2.5
1	C	135	GLN	2.5
1	B	444	ASN	2.5
1	B	275	ASP	2.5
1	C	420	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLY	2.4
1	C	170	TYR	2.4
1	C	475	LEU	2.4
1	C	100	LEU	2.3
1	B	278	GLN	2.3
1	C	164	ASN	2.3
1	D	521	PRO	2.3
1	C	37	LEU	2.3
1	B	529	VAL	2.3
1	C	122	THR	2.2
1	A	278	GLN	2.2
1	C	430	SER	2.2
1	B	253	THR	2.2
1	C	394	LYS	2.2
1	C	94	TYR	2.2
1	C	143	VAL	2.2
1	B	363	LYS	2.2
1	C	399	LEU	2.2
1	C	317	PRO	2.2
1	C	158	ASP	2.1
1	C	2	ALA	2.1
1	C	325	ILE	2.1
1	C	352	LEU	2.1
1	B	450	LEU	2.1
1	D	520	LEU	2.1
1	C	278	GLN	2.1
1	C	395	GLY	2.1
1	D	515	LEU	2.0
1	B	516	SER	2.0
1	A	515	PRO	2.0
1	C	454	LEU	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)

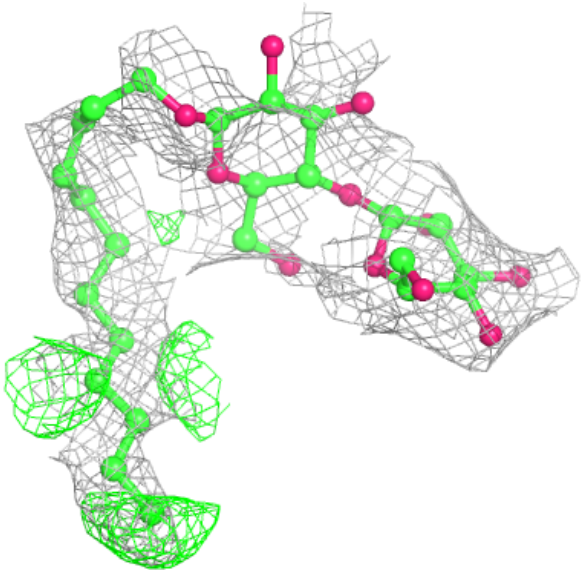
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

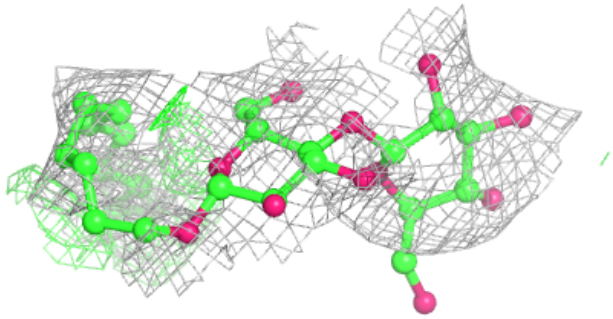
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LMT	A	605	35/35	0.68	0.29	109,147,183,190	0
4	LMT	A	603	35/35	0.69	0.42	95,139,166,169	0
4	LMT	B	603	35/35	0.72	0.29	84,146,161,163	0
4	LMT	D	603	35/35	0.75	0.27	88,129,141,146	0
4	LMT	A	606	35/35	0.75	0.24	96,153,175,179	0
4	LMT	B	604	35/35	0.76	0.36	103,134,154,157	0
3	NAP	C	602	48/48	0.84	0.22	121,138,148,151	0
5	GOL	D	606	6/6	0.84	0.40	89,93,96,96	0
2	FAD	C	601	53/53	0.92	0.20	101,125,144,148	0
6	CL	A	604	1/1	0.92	0.14	84,84,84,84	0
3	NAP	A	602	48/48	0.93	0.19	48,65,106,117	0
3	NAP	D	602	48/48	0.94	0.17	65,86,92,98	0
2	FAD	B	601	53/53	0.94	0.17	44,52,71,82	0
3	NAP	B	602	48/48	0.94	0.14	73,89,115,121	0
5	GOL	D	604	6/6	0.95	0.14	43,45,46,46	0
6	CL	B	605	1/1	0.96	0.07	56,56,56,56	0
2	FAD	A	601	53/53	0.96	0.17	33,42,56,61	0
2	FAD	D	601	53/53	0.98	0.17	32,36,43,45	0
6	CL	D	605	1/1	0.98	0.10	43,43,43,43	0

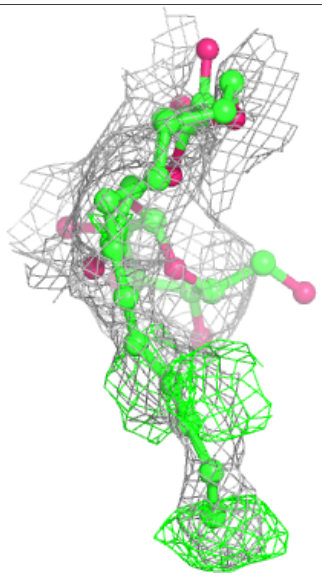
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 605:

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

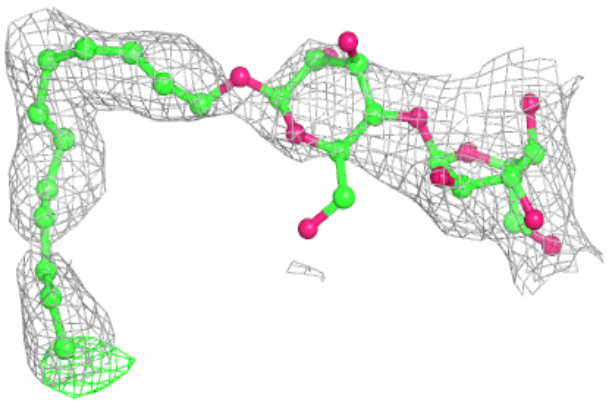


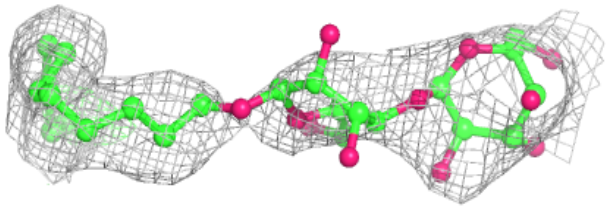


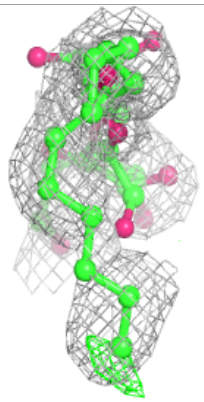


Electron density around LMT A 603:

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

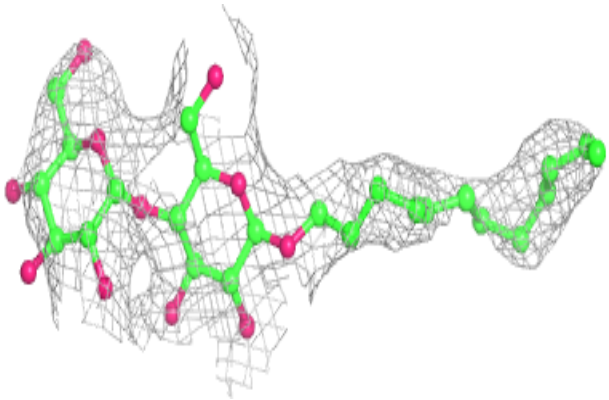


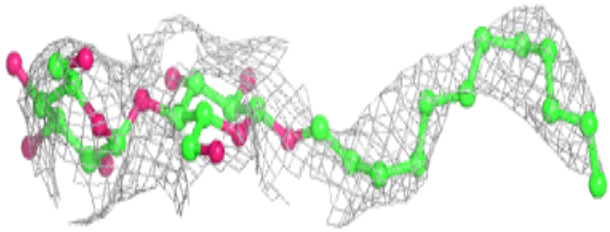


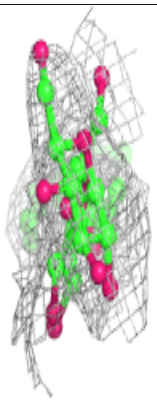


Electron density around LMT B 603:

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

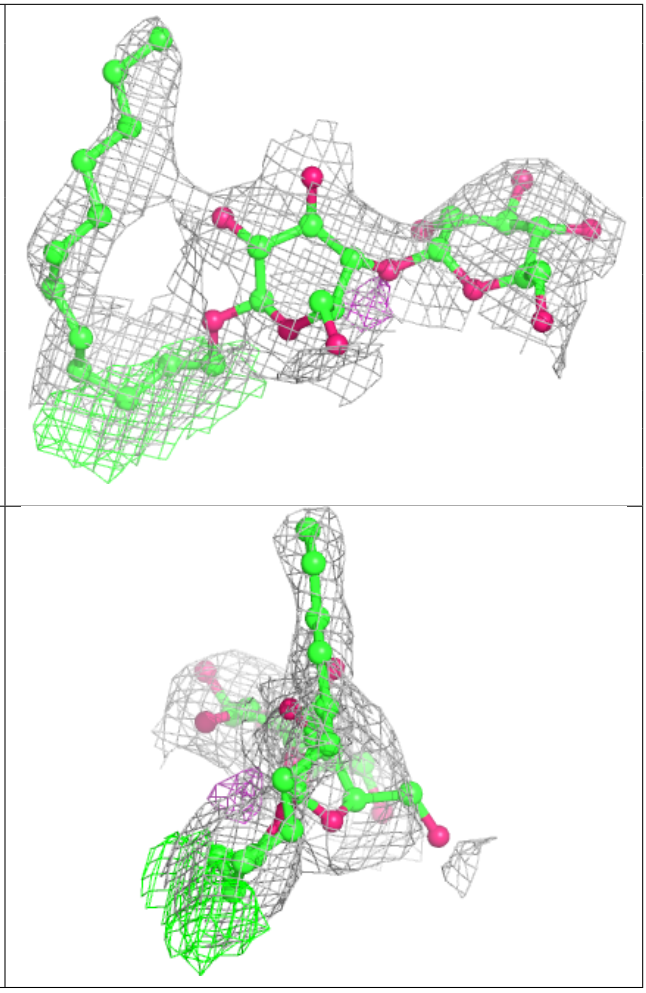






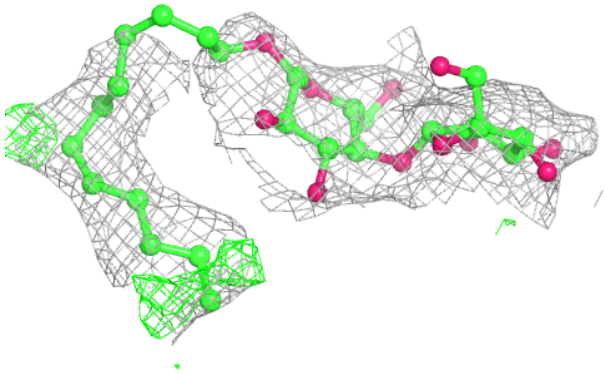
Electron density around LMT D 603:

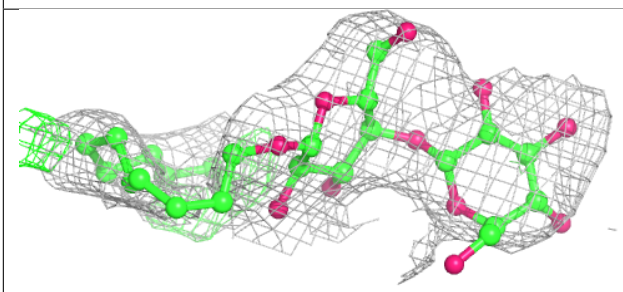
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMT A 606:

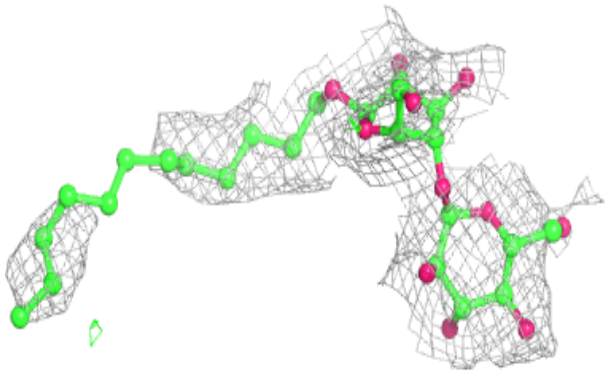
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

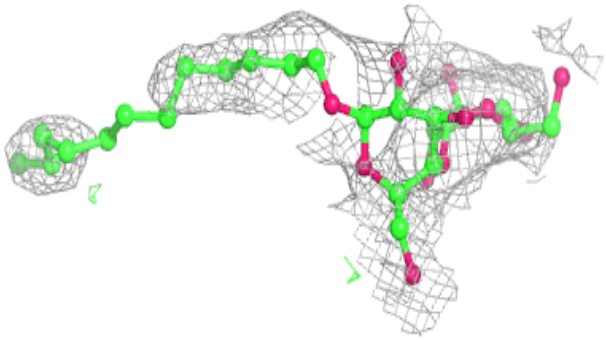


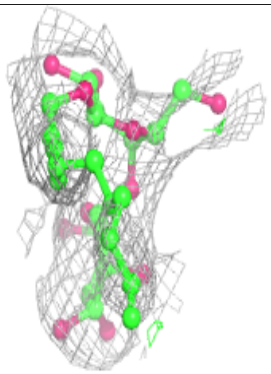


Electron density around LMT B 604:

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

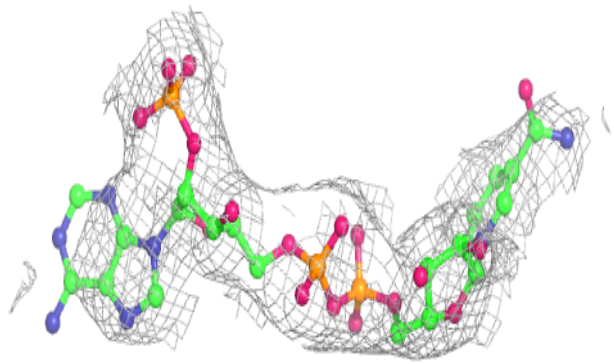


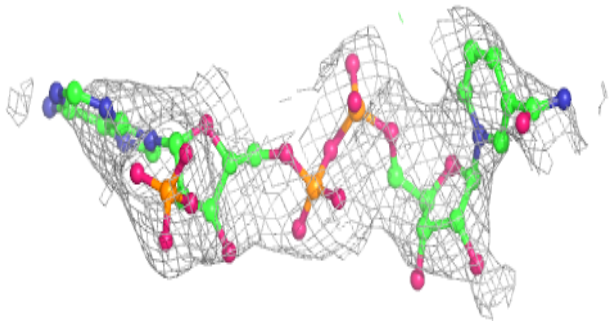


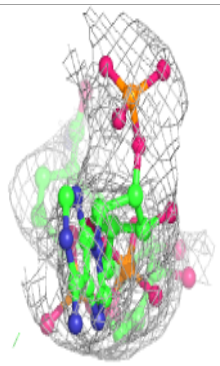


Electron density around NAP C 602:

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

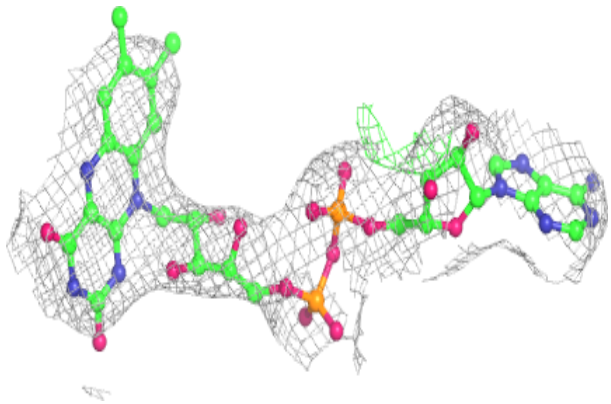


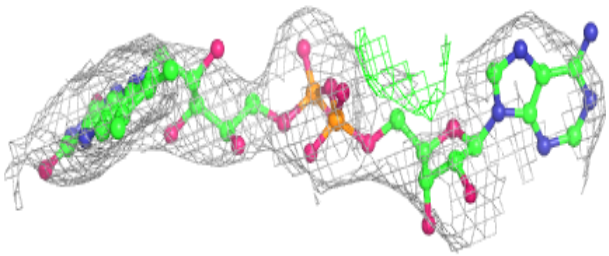


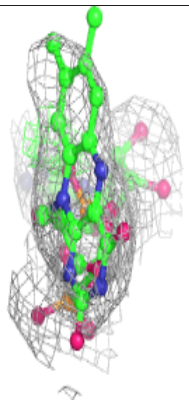


Electron density around FAD C 601:

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

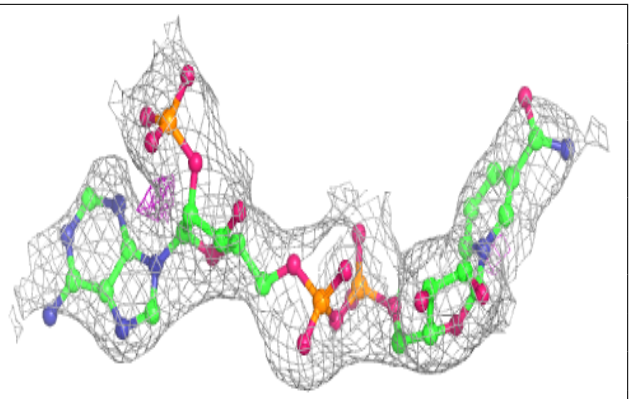


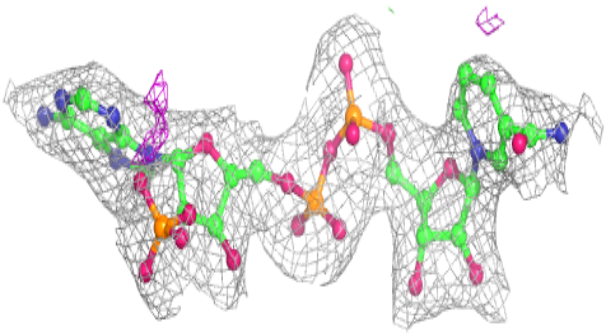


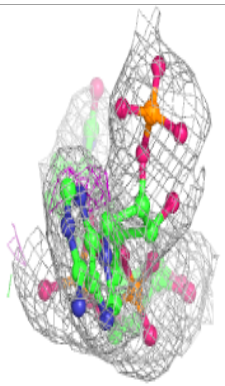


Electron density around NAP A 602:

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

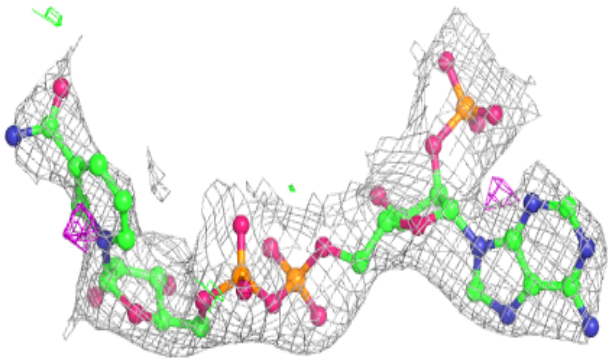


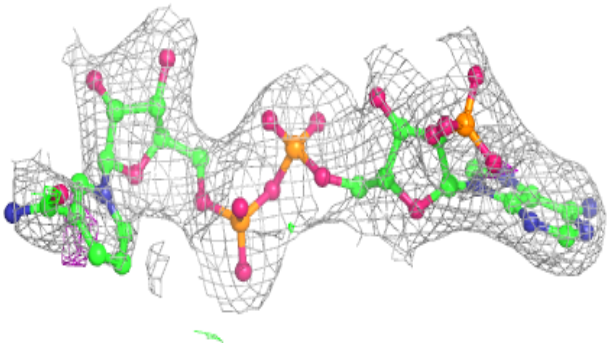


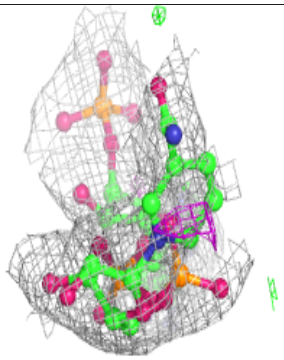


Electron density around NAP D 602:

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

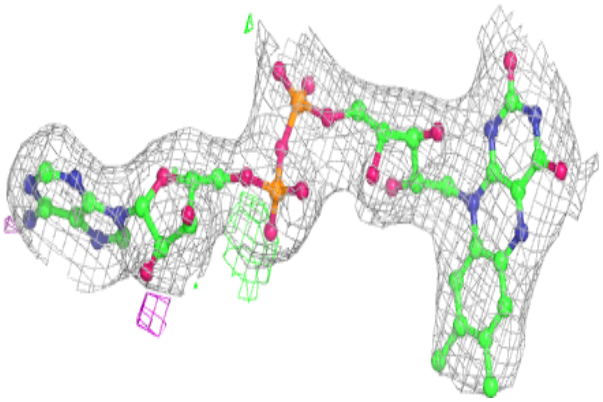


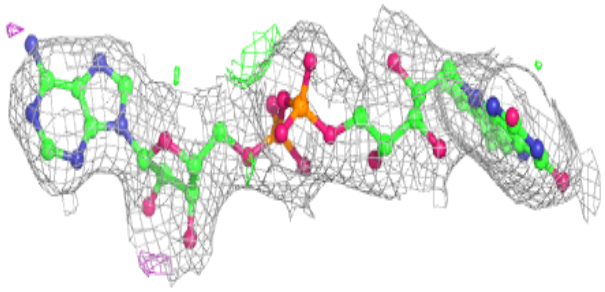


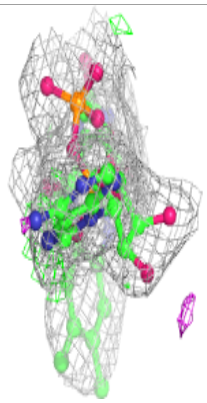


Electron density around FAD B 601:

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

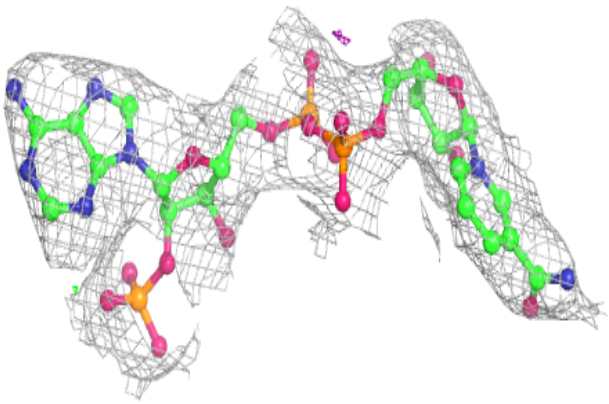


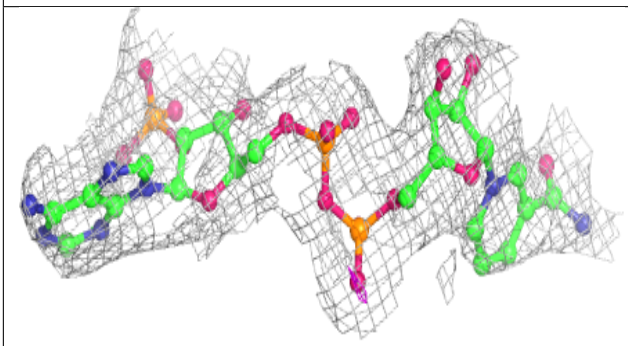


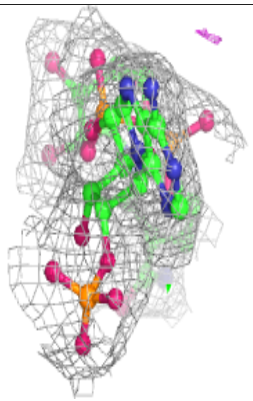


Electron density around NAP B 602:

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

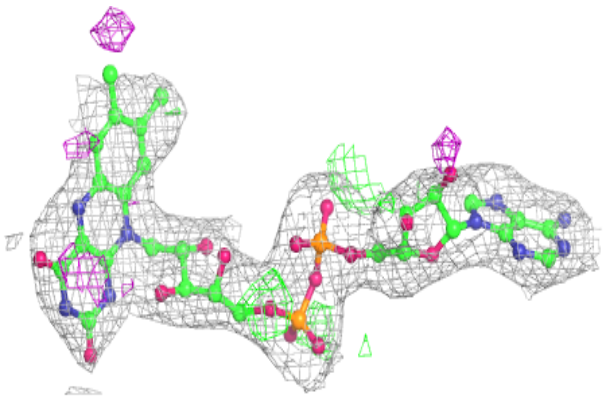


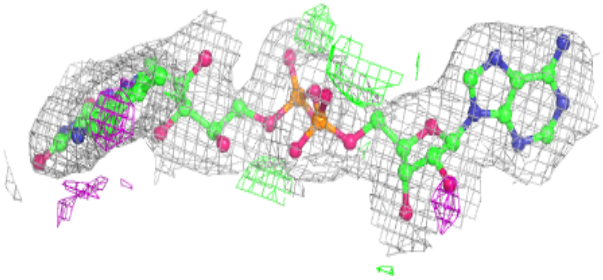


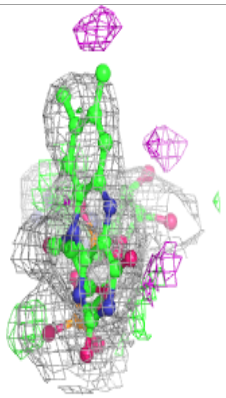


Electron density around FAD A 601:

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

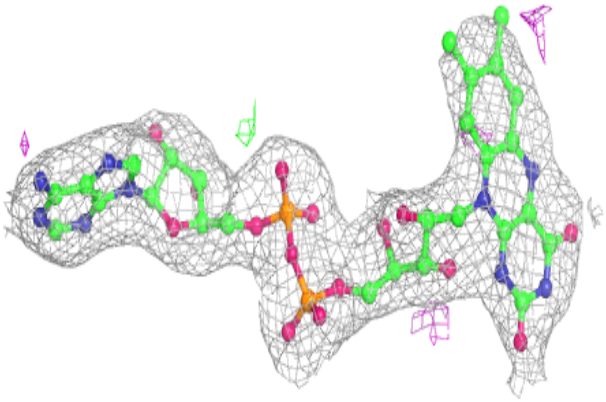


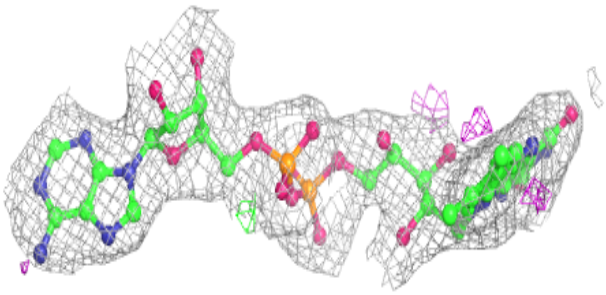


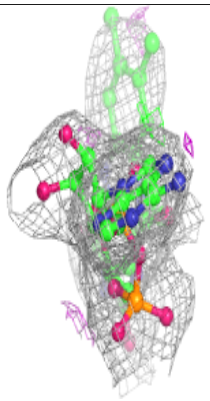


Electron density around FAD D 601:

$2mF_o$-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.