



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:46 AM UTC

PDB ID : 6SEK / pdb_00006sek
Title : Crystal Structure of Ancestral Flavin-containing monooxygenase (FMO) 5
Authors : Nicoll, C.; Bailleul, G.; Fiorentini, F.; Mascotti, M.L.; Fraaije, M.; Mattevi, A.
Deposited on : 2019-07-30
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

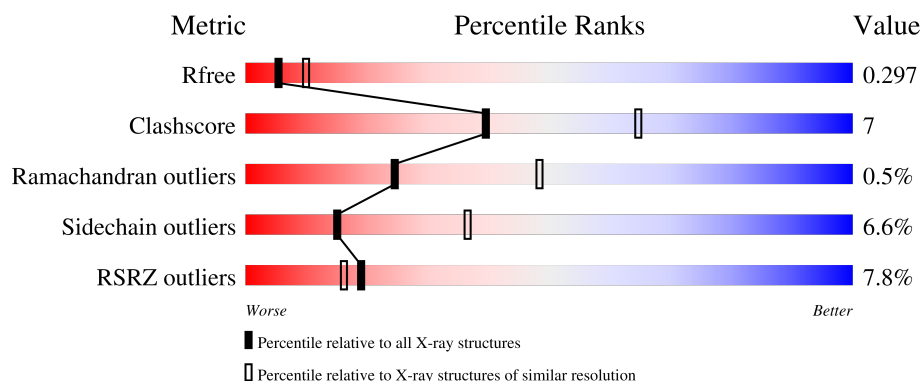
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	533	7% 77% 17% • 5%
1	B	533	8% 74% 18% • 5%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8329 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 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4010	2568	680	740	22			
1	B	504	Total	C	N	O	S	0	0	0
			4010	2568	680	740	22			

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



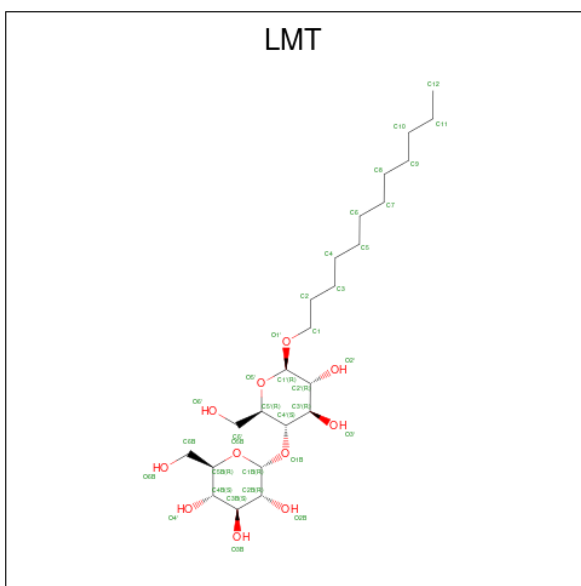
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



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

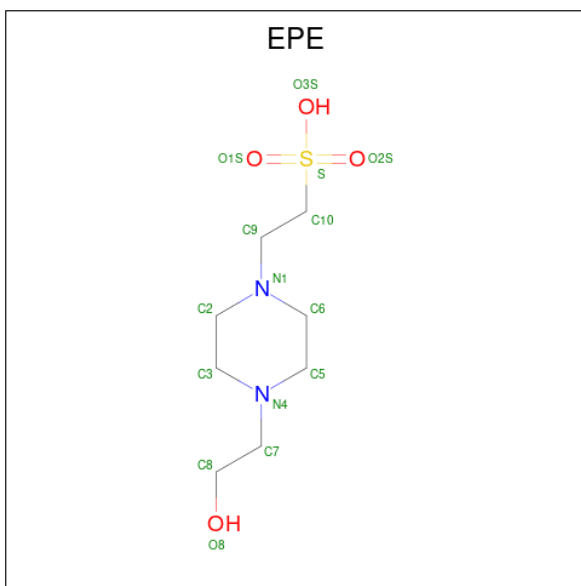
- Molecule 4 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			26	15	11		

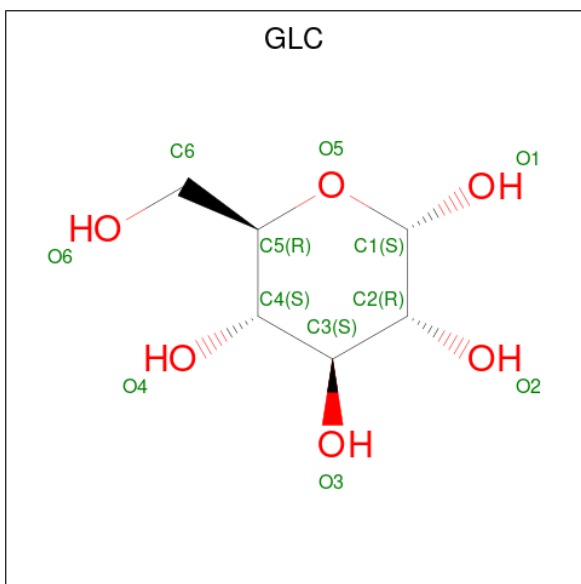
- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD

ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 6 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	6	6		

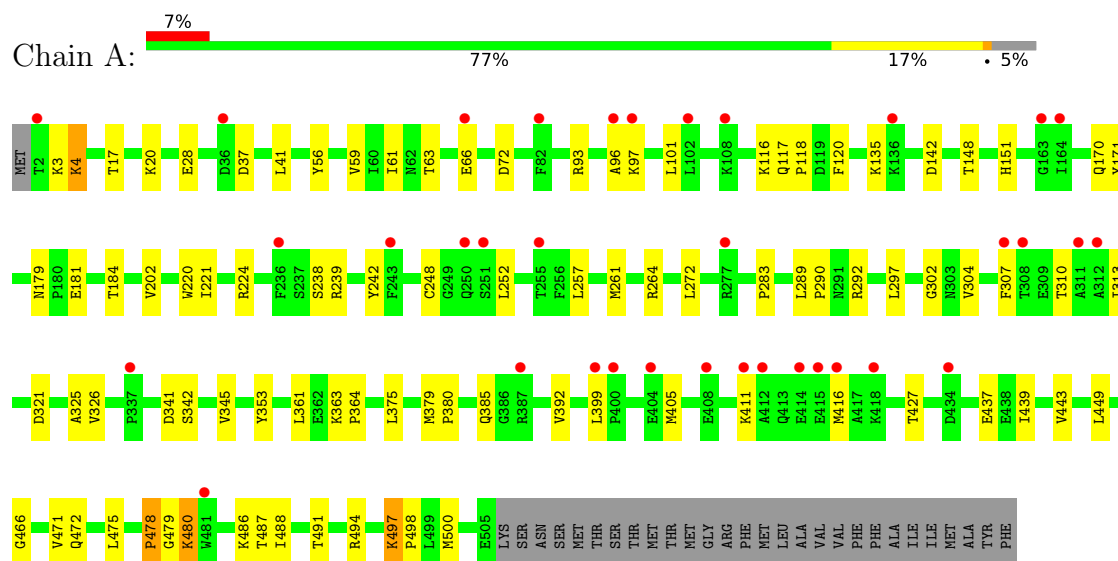
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	O	0	0
			17	17		
7	B	10	Total	O	0	0
			10	10		

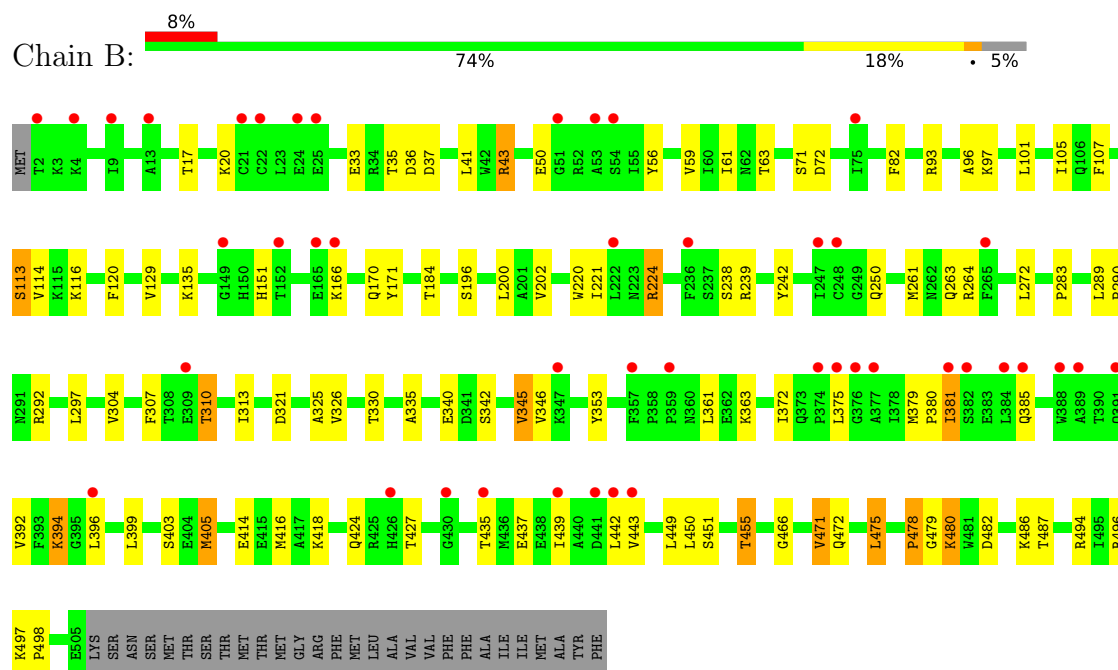
3 Residue-property plots

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 5



- Molecule 1: Ancestral Flavin-containing monooxygenase 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.78Å 100.07Å 143.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.70 49.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.00-2.70) 99.7 (49.00-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.222 , 0.295 0.227 , 0.297	Depositor DCC
R_{free} test set	1964 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 19.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8329	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAP, EPE, LMT, GLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.04	0/4104	1.43	7/5539 (0.1%)
1	B	1.05	0/4104	1.44	9/5539 (0.2%)
All	All	1.04	0/8208	1.44	16/11078 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	THR	CA-CB-OG1	-6.35	100.08	109.60
1	B	224	ARG	CB-CA-C	-6.04	100.76	110.79
1	A	310	THR	CA-CB-OG1	-6.04	100.54	109.60
1	A	385	GLN	CA-C-N	5.32	125.85	120.00
1	A	385	GLN	C-N-CA	5.32	125.85	120.00
1	B	340	GLU	CA-C-N	5.25	127.57	120.38
1	B	340	GLU	C-N-CA	5.25	127.57	120.38
1	B	482	ASP	CA-C-O	-5.21	114.90	120.42
1	A	63	THR	CA-C-N	5.21	128.47	120.82
1	A	63	THR	C-N-CA	5.21	128.47	120.82
1	B	63	THR	CA-C-N	5.20	128.47	120.82
1	B	63	THR	C-N-CA	5.20	128.47	120.82
1	A	148	THR	CA-C-O	-5.17	115.93	121.56
1	B	385	GLN	CA-C-N	5.11	125.62	120.00
1	B	385	GLN	C-N-CA	5.11	125.62	120.00
1	A	302	GLY	CA-C-O	-5.04	117.12	122.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4010	0	4007	48	0
1	B	4010	0	4007	60	0
2	A	53	0	31	7	0
2	B	53	0	31	9	0
3	A	48	0	25	2	0
3	B	48	0	25	3	0
4	A	26	0	25	0	0
5	A	15	0	18	1	0
5	B	15	0	18	0	0
6	A	24	0	24	0	0
7	A	17	0	0	0	0
7	B	10	0	0	0	0
All	All	8329	0	8211	111	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 (111) 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:399:LEU:HD13	1:A:405:MET:HE1	1.71	0.71
1:A:488:ILE:O	1:A:491:THR:HG22	1.91	0.69
2:A:601:FAD:C6	3:A:602:NAP:C2N	2.74	0.66
1:B:151:HIS:CD2	2:B:601:FAD:H1'1	2.31	0.65
1:A:20:LYS:NZ	1:A:72:ASP:OD2	2.30	0.65
1:B:335:ALA:HA	1:B:345:VAL:HG21	1.78	0.64
1:A:416:MET:HE1	1:A:427:THR:O	1.98	0.64
1:B:221:ILE:HD12	1:B:272:LEU:HD13	1.79	0.64
1:B:416:MET:HE1	1:B:427:THR:O	1.98	0.63
1:B:394:LYS:HB2	1:B:396:LEU:HD23	1.80	0.63
1:B:239:ARG:HE	1:B:472:GLN:NE2	1.98	0.62
1:A:239:ARG:HE	1:A:472:GLN:NE2	1.98	0.61
1:B:399:LEU:HD13	1:B:405:MET:HE1	1.81	0.61
2:B:601:FAD:C6	3:B:602:NAP:C2N	2.79	0.60
1:B:41:LEU:HD11	2:B:601:FAD:HM82	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LEU:HD22	1:B:396:LEU:N	2.16	0.59
1:A:171:TYR:HA	1:A:326:VAL:O	2.03	0.59
1:B:20:LYS:NZ	1:B:72:ASP:OD2	2.35	0.59
1:B:41:LEU:HD11	2:B:601:FAD:C8M	2.33	0.58
1:A:399:LEU:HD13	1:A:405:MET:CE	2.33	0.58
1:B:33:GLU:OE1	2:B:601:FAD:O3B	2.20	0.58
1:B:71:SER:O	1:B:471:VAL:HG12	2.04	0.58
1:B:151:HIS:HD2	2:B:601:FAD:H1'1	1.67	0.57
1:B:171:TYR:HA	1:B:326:VAL:O	2.03	0.57
1:A:151:HIS:CD2	2:A:601:FAD:H1'1	2.40	0.56
1:B:399:LEU:HD13	1:B:405:MET:CE	2.36	0.56
1:B:220:TRP:HB3	1:B:261:MET:HE1	1.88	0.55
1:A:487:THR:O	1:A:494:ARG:NH2	2.39	0.55
1:A:4:LYS:HG2	1:A:142:ASP:CB	2.37	0.54
1:A:221:ILE:HD12	1:A:272:LEU:HD13	1.88	0.54
1:A:239:ARG:HE	1:A:472:GLN:HE21	1.54	0.53
1:B:487:THR:O	1:B:494:ARG:NH2	2.42	0.53
1:A:116:LYS:HB2	1:A:120:PHE:CG	2.44	0.53
1:A:41:LEU:HD11	2:A:601:FAD:HM82	1.92	0.52
1:B:239:ARG:HH12	1:B:437:GLU:CD	2.17	0.52
1:A:4:LYS:HG2	1:A:142:ASP:HB3	1.90	0.52
1:B:396:LEU:N	1:B:396:LEU:CD2	2.72	0.52
1:B:239:ARG:HE	1:B:472:GLN:HE21	1.56	0.52
1:B:439:ILE:O	1:B:443:VAL:HG23	2.10	0.51
1:A:353:TYR:CG	1:A:405:MET:HG2	2.45	0.51
1:A:220:TRP:HB3	1:A:261:MET:HE1	1.92	0.51
1:A:96:ALA:HA	1:A:101:LEU:HD12	1.92	0.50
1:A:353:TYR:HB3	1:A:405:MET:HE2	1.93	0.50
1:A:283:PRO:HD3	1:A:375:LEU:HD22	1.94	0.50
1:B:304:VAL:HG11	1:B:307:PHE:CZ	2.47	0.49
1:B:116:LYS:HB2	1:B:120:PHE:CG	2.48	0.49
1:B:396:LEU:CD2	1:B:396:LEU:H	2.25	0.49
1:B:35:THR:HG22	1:B:36:ASP:H	1.77	0.49
1:A:439:ILE:O	1:A:443:VAL:HG23	2.14	0.48
1:B:105:ILE:HG21	1:B:107:PHE:CE1	2.47	0.48
1:B:353:TYR:CG	1:B:405:MET:HG2	2.48	0.48
1:B:82:PHE:CD1	1:B:224:ARG:HD2	2.49	0.48
1:B:96:ALA:HA	1:B:101:LEU:HD12	1.96	0.48
1:A:283:PRO:CD	1:A:375:LEU:HD22	2.44	0.48
1:A:304:VAL:HG11	1:A:307:PHE:CZ	2.48	0.48
1:B:353:TYR:HB3	1:B:405:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:OE1	1:A:494:ARG:NH1	2.47	0.47
1:B:239:ARG:O	1:B:242:TYR:HB3	2.15	0.47
1:A:170:GLN:O	1:A:325:ALA:HA	2.14	0.47
1:A:151:HIS:HD2	2:A:601:FAD:H1'1	1.80	0.47
1:B:82:PHE:CZ	1:B:224:ARG:HB3	2.50	0.46
1:A:117:GLN:HB3	1:A:118:PRO:HD2	1.97	0.46
1:B:497:LYS:N	1:B:498:PRO:CD	2.78	0.46
1:A:239:ARG:HH12	1:A:437:GLU:CD	2.23	0.46
1:A:41:LEU:HD11	2:A:601:FAD:C8M	2.45	0.46
1:A:497:LYS:N	1:A:498:PRO:CD	2.79	0.46
1:B:61:ILE:HG13	2:B:601:FAD:O4	2.15	0.46
1:A:364:PRO:HB3	1:A:399:LEU:HD12	1.98	0.46
1:B:170:GLN:O	1:B:325:ALA:HA	2.16	0.45
1:A:379:MET:N	1:A:380:PRO:HD2	2.32	0.45
1:A:61:ILE:HG13	2:A:601:FAD:O4	2.16	0.45
1:B:379:MET:N	1:B:380:PRO:HD2	2.32	0.44
1:A:37:ASP:OD2	1:A:93:ARG:NH2	2.50	0.44
2:A:601:FAD:H6	3:A:602:NAP:C3N	2.48	0.44
1:A:257:LEU:HD11	5:A:604:EPE:H82	2.00	0.44
1:A:239:ARG:HH21	1:A:472:GLN:HE21	1.65	0.44
1:B:238:SER:HB2	1:B:466:GLY:O	2.18	0.44
1:B:113:SER:HB3	1:B:129:VAL:CG1	2.48	0.43
1:A:292:ARG:NH2	1:A:297:LEU:HD13	2.34	0.43
1:A:471:VAL:HG11	1:A:487:THR:OG1	2.19	0.43
1:B:239:ARG:HH21	1:B:472:GLN:HE21	1.66	0.43
1:B:82:PHE:CE2	1:B:224:ARG:HB3	2.54	0.43
1:B:283:PRO:HD3	1:B:375:LEU:HD22	2.00	0.43
1:B:56:TYR:CE2	1:B:59:VAL:HG22	2.54	0.43
1:B:330:THR:HA	3:B:602:NAP:O4B	2.19	0.43
1:A:248:CYS:HB3	1:A:252:LEU:HD23	1.99	0.42
1:B:381:ILE:HD12	1:B:435:THR:HG21	2.02	0.42
1:B:35:THR:HG21	1:B:43:ARG:HH12	1.83	0.42
1:A:238:SER:HB2	1:A:466:GLY:O	2.19	0.42
1:B:479:GLY:O	1:B:480:LYS:C	2.63	0.42
1:B:41:LEU:HD13	2:B:601:FAD:H2'	2.02	0.42
1:B:61:ILE:CG1	2:B:601:FAD:O4	2.68	0.42
1:B:151:HIS:CE1	3:B:602:NAP:H4D	2.55	0.42
1:A:479:GLY:O	1:A:480:LYS:C	2.63	0.42
1:A:135:LYS:O	1:A:135:LYS:CG	2.67	0.41
1:A:361:LEU:HB3	1:A:363:LYS:O	2.20	0.41
1:B:475:LEU:HD12	1:B:475:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:MET:O	1:A:500:MET:HG3	2.20	0.41
1:A:289:LEU:N	1:A:290:PRO:CD	2.82	0.41
1:A:239:ARG:O	1:A:242:TYR:HB3	2.21	0.41
1:B:379:MET:HB2	1:B:380:PRO:HD3	2.01	0.41
1:B:292:ARG:NH2	1:B:297:LEU:HD13	2.35	0.41
1:A:56:TYR:CE2	1:A:59:VAL:HG22	2.55	0.41
1:B:361:LEU:HB3	1:B:363:LYS:O	2.20	0.41
1:B:220:TRP:HB3	1:B:261:MET:CE	2.51	0.40
1:A:353:TYR:CB	1:A:405:MET:HE2	2.51	0.40
1:B:196:SER:O	1:B:200:LEU:HG	2.21	0.40
1:B:289:LEU:N	1:B:290:PRO:CD	2.84	0.40
1:B:451:SER:O	1:B:455:THR:HG23	2.21	0.40
1:B:496:ARG:C	1:B:498:PRO:HD2	2.47	0.40
1:B:37:ASP:OD2	1:B:93:ARG:NH2	2.54	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	502/533 (94%)	477 (95%)	23 (5%)	2 (0%)	30	54
1	B	502/533 (94%)	478 (95%)	21 (4%)	3 (1%)	21	44
All	All	1004/1066 (94%)	955 (95%)	44 (4%)	5 (0%)	24	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	LYS
1	B	480	LYS
1	B	394	LYS
1	A	478	PRO

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Mol	Chain	Res	Type
1	B	478	PRO

5.3.2 Protein sidechains ⓘ

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	441/466 (95%)	418 (95%)	23 (5%)	21	47
1	B	441/466 (95%)	406 (92%)	35 (8%)	11	28
All	All	882/932 (95%)	824 (93%)	58 (7%)	15	36

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	LYS
1	A	17	THR
1	A	28	GLU
1	A	97	LYS
1	A	179	ASN
1	A	181	GLU
1	A	184	THR
1	A	202	VAL
1	A	224	ARG
1	A	264	ARG
1	A	313	ILE
1	A	321	ASP
1	A	341	ASP
1	A	342	SER
1	A	345	VAL
1	A	392	VAL
1	A	411	LYS
1	A	449	LEU
1	A	475	LEU
1	A	478	PRO
1	A	486	LYS

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Mol	Chain	Res	Type
1	A	497	LYS
1	B	17	THR
1	B	43	ARG
1	B	50	GLU
1	B	97	LYS
1	B	113	SER
1	B	114	VAL
1	B	135	LYS
1	B	166	LYS
1	B	184	THR
1	B	202	VAL
1	B	250	GLN
1	B	263	GLN
1	B	264	ARG
1	B	310	THR
1	B	313	ILE
1	B	321	ASP
1	B	342	SER
1	B	345	VAL
1	B	346	VAL
1	B	372	ILE
1	B	381	ILE
1	B	392	VAL
1	B	403	SER
1	B	405	MET
1	B	414	GLU
1	B	418	LYS
1	B	424	GLN
1	B	442	LEU
1	B	449	LEU
1	B	450	LEU
1	B	455	THR
1	B	471	VAL
1	B	475	LEU
1	B	478	PRO
1	B	486	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	151	HIS

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Mol	Chain	Res	Type
1	A	153	ASN
1	A	155	HIS
1	A	291	ASN
1	A	424	GLN
1	A	472	GLN
1	B	117	GLN
1	B	151	HIS
1	B	155	HIS
1	B	228	HIS
1	B	424	GLN
1	B	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EPE	A	604	-	15,15,15	2.44	1 (6%)	19,20,20	1.53	5 (26%)
5	EPE	B	603	-	15,15,15	2.18	1 (6%)	19,20,20	1.46	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	601	-	58,58,58	0.76	2 (3%)	85,89,89	0.77	2 (2%)
6	GLC	A	606	-	12,12,12	0.87	0	17,17,17	1.17	2 (11%)
3	NAP	A	602	-	50,52,52	1.24	6 (12%)	71,80,80	1.78	14 (19%)
2	FAD	B	601	-	58,58,58	0.64	1 (1%)	85,89,89	0.83	4 (4%)
4	LMT	A	603	-	27,27,36	1.15	1 (3%)	38,38,47	1.61	10 (26%)
3	NAP	B	602	-	50,52,52	1.47	6 (12%)	71,80,80	1.99	19 (26%)
6	GLC	A	605	-	12,12,12	1.28	1 (8%)	17,17,17	1.26	3 (17%)

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	A	604	-	-	2/9/19/19	0/1/1/1
5	EPE	B	603	-	-	6/9/19/19	0/1/1/1
2	FAD	A	601	-	-	10/34/50/50	0/6/6/6
6	GLC	A	606	-	-	2/2/22/22	0/1/1/1
3	NAP	A	602	-	-	11/35/67/67	0/5/5/5
2	FAD	B	601	-	-	5/34/50/50	0/6/6/6
4	LMT	A	603	-	-	9/12/52/61	0/2/2/2
3	NAP	B	602	-	-	4/35/67/67	0/5/5/5
6	GLC	A	605	-	-	2/2/22/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	EPE	C10-S	-8.61	1.65	1.77
5	B	603	EPE	C10-S	-7.71	1.66	1.77
3	B	602	NAP	PA-O3	5.19	1.65	1.59
3	A	602	NAP	C5A-C4A	4.51	1.47	1.39
3	B	602	NAP	PN-O3	4.17	1.64	1.59
3	B	602	NAP	O4D-C1D	3.90	1.46	1.40
4	A	603	LMT	O1'-C1'	3.80	1.46	1.40
2	A	601	FAD	P-O3P	3.44	1.63	1.59
3	B	602	NAP	C5A-C4A	2.78	1.44	1.39
3	A	602	NAP	C5A-N7A	-2.74	1.34	1.39
3	A	602	NAP	O4D-C1D	2.70	1.44	1.40
3	A	602	NAP	P2B-O2B	2.42	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	NAP	C8A-N7A	2.42	1.36	1.31
3	B	602	NAP	C4A-N9A	-2.37	1.32	1.37
6	A	605	GLC	C1-C2	2.09	1.57	1.52
3	A	602	NAP	C8A-N7A	2.08	1.35	1.31
2	A	601	FAD	PA-O3P	2.07	1.61	1.59
2	B	601	FAD	P-O3P	2.05	1.61	1.59
3	A	602	NAP	C5A-C6A	2.02	1.46	1.41

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAP	N3A-C4A-N9A	5.87	137.15	127.17
3	A	602	NAP	C5A-C4A-N3A	-5.85	118.67	126.72
3	B	602	NAP	C5A-C4A-N3A	-5.47	119.18	126.72
3	B	602	NAP	N3A-C4A-N9A	5.31	136.20	127.17
3	B	602	NAP	N3A-C2A-N1A	-4.96	121.07	128.58
3	B	602	NAP	C4A-N9A-C8A	4.85	110.83	105.74
3	B	602	NAP	C2A-N3A-C4A	4.28	122.27	111.83
3	A	602	NAP	C4A-N9A-C8A	3.65	109.57	105.74
5	A	604	EPE	C6-N1-C2	3.64	116.69	108.84
3	A	602	NAP	N3A-C2A-N1A	-3.53	123.24	128.58
3	A	602	NAP	C2A-N3A-C4A	3.45	120.25	111.83
3	B	602	NAP	N9A-C8A-N7A	-3.44	109.06	113.94
3	A	602	NAP	N6A-C6A-N1A	3.40	125.95	118.38
5	B	603	EPE	O1S-S-C10	3.21	111.58	106.73
3	B	602	NAP	C6N-N1N-C2N	-3.16	119.19	121.88
4	A	603	LMT	O1'-C1'-C2'	3.14	113.04	108.27
3	A	602	NAP	C5A-C6A-N6A	-3.12	115.55	123.29
5	B	603	EPE	C6-N1-C2	3.11	115.55	108.84
3	B	602	NAP	C5A-C6A-N6A	-3.09	115.63	123.29
3	B	602	NAP	C4D-O4D-C1D	-3.05	107.14	109.92
3	A	602	NAP	C2D-C3D-C4D	3.03	108.47	102.61
3	B	602	NAP	O3-PA-O1A	-2.93	101.88	110.70
3	B	602	NAP	C5N-C4N-C3N	-2.86	117.55	120.36
4	A	603	LMT	O5B-C1B-C2B	2.85	116.23	110.37
4	A	603	LMT	C3'-C4'-C5'	2.83	117.20	110.93
5	A	604	EPE	O1S-S-C10	2.69	110.79	106.73
3	B	602	NAP	O5D-PN-O1N	2.52	118.94	108.94
3	A	602	NAP	O3-PA-O1A	-2.52	103.12	110.70
4	A	603	LMT	C2'-C3'-C4'	2.51	115.38	109.68
4	A	603	LMT	O5'-C1'-C2'	-2.51	105.21	110.37
4	A	603	LMT	O4'-C4B-C3B	-2.48	104.54	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAP	N6A-C6A-N1A	2.47	123.87	118.38
4	A	603	LMT	C1-O1'-C1'	2.42	117.81	113.68
3	A	602	NAP	O7N-C7N-C3N	-2.42	116.64	119.60
2	B	601	FAD	C4'-C3'-C2'	2.38	117.54	113.57
6	A	605	GLC	C1-C2-C3	2.36	115.17	110.36
3	B	602	NAP	C2N-C3N-C4N	2.36	121.00	118.26
2	A	601	FAD	O2P-P-O3P	2.30	113.50	107.27
4	A	603	LMT	O5B-C5B-C4B	2.29	113.82	109.70
3	B	602	NAP	C3N-C7N-N7N	2.27	120.53	117.74
2	B	601	FAD	O2P-P-O1P	2.27	122.99	112.44
2	B	601	FAD	C4-N3-C2	-2.23	121.68	125.64
6	A	606	GLC	O5-C5-C6	2.21	111.92	106.44
3	A	602	NAP	O2A-PA-O1A	2.15	122.46	112.44
4	A	603	LMT	C3B-C4B-C5B	2.14	114.11	110.23
3	A	602	NAP	C5A-N7A-C8A	2.12	106.79	103.45
3	B	602	NAP	O3D-C3D-C2D	-2.12	105.03	111.82
3	A	602	NAP	N9A-C8A-N7A	-2.11	110.95	113.94
3	A	602	NAP	O2B-C2B-C1B	2.10	117.45	110.05
6	A	606	GLC	O5-C5-C4	-2.10	105.92	109.70
6	A	605	GLC	C1-O5-C5	2.10	117.71	113.65
2	A	601	FAD	C4-N3-C2	-2.09	121.93	125.64
5	A	604	EPE	C6-C5-N4	2.09	114.86	110.65
3	B	602	NAP	O4B-C1B-N9A	2.08	112.08	108.09
3	B	602	NAP	O2A-PA-O3	2.08	112.89	107.27
3	B	602	NAP	O3X-P2B-O2X	2.04	115.46	107.80
5	A	604	EPE	C8-C7-N4	2.03	120.55	113.44
5	A	604	EPE	O3S-S-C10	2.02	109.95	106.00
4	A	603	LMT	C4B-C3B-C2B	2.02	114.37	110.83
2	B	601	FAD	C4X-C4-N3	2.01	118.36	113.25
6	A	605	GLC	O5-C5-C6	2.01	111.41	106.44

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5B-O5B-PA-O1A
3	A	602	NAP	C5B-O5B-PA-O1A
3	A	602	NAP	C5B-O5B-PA-O2A
3	A	602	NAP	C5B-O5B-PA-O3
3	A	602	NAP	C5D-O5D-PN-O3
3	A	602	NAP	C5D-O5D-PN-O1N
3	A	602	NAP	C5D-O5D-PN-O2N
5	A	604	EPE	C8-C7-N4-C3
5	A	604	EPE	N4-C7-C8-O8
5	B	603	EPE	C9-C10-S-O1S
5	B	603	EPE	C9-C10-S-O2S
4	A	603	LMT	O5B-C1B-O1B-C4'
4	A	603	LMT	O5'-C5'-C6'-O6'
6	A	606	GLC	C4-C5-C6-O6
3	A	602	NAP	O4D-C4D-C5D-O5D
4	A	603	LMT	O5'-C1'-O1'-C1
4	A	603	LMT	C4'-C5'-C6'-O6'
4	A	603	LMT	C2'-C1'-O1'-C1
6	A	606	GLC	O5-C5-C6-O6
4	A	603	LMT	C2B-C1B-O1B-C4'
3	A	602	NAP	O4B-C4B-C5B-O5B
4	A	603	LMT	O1'-C1-C2-C3
5	B	603	EPE	C9-C10-S-O3S
3	A	602	NAP	C3B-C4B-C5B-O5B
4	A	603	LMT	O5B-C5B-C6B-O6B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
3	A	602	NAP	C3D-C4D-C5D-O5D
3	B	602	NAP	O4D-C4D-C5D-O5D
5	B	603	EPE	C10-C9-N1-C6
5	B	603	EPE	C8-C7-N4-C3
6	A	605	GLC	C4-C5-C6-O6
4	A	603	LMT	C4B-C5B-C6B-O6B
3	A	602	NAP	PN-O3-PA-O5B
3	B	602	NAP	C3D-C4D-C5D-O5D
2	A	601	FAD	C5'-O5'-P-O1P
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C5B-O5B-PA-O3P
5	B	603	EPE	C10-C9-N1-C2
6	A	605	GLC	O5-C5-C6-O6
2	A	601	FAD	O4B-C4B-C5B-O5B

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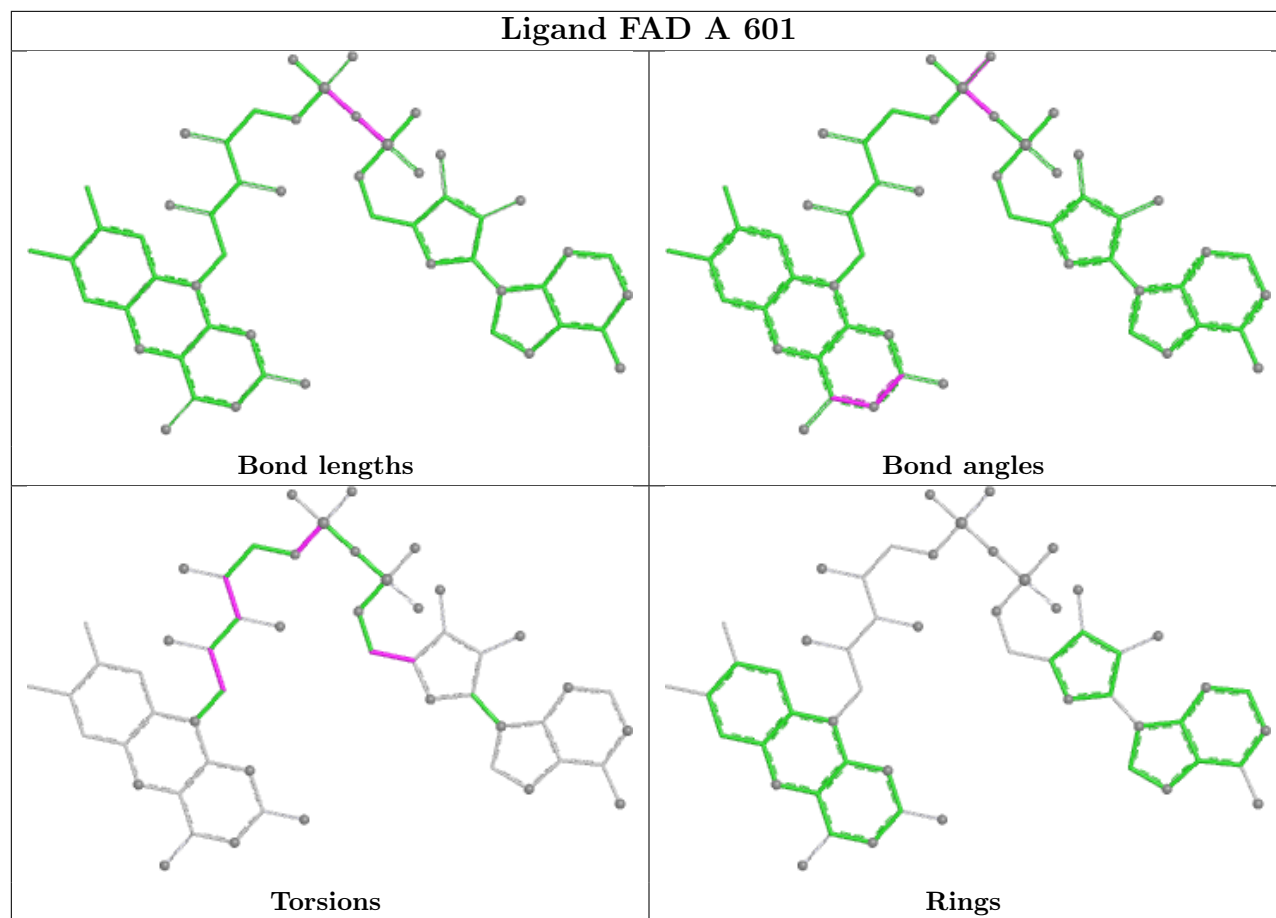
Mol	Chain	Res	Type	Atoms
3	B	602	NAP	C2B-O2B-P2B-O1X
3	B	602	NAP	C4N-C3N-C7N-N7N

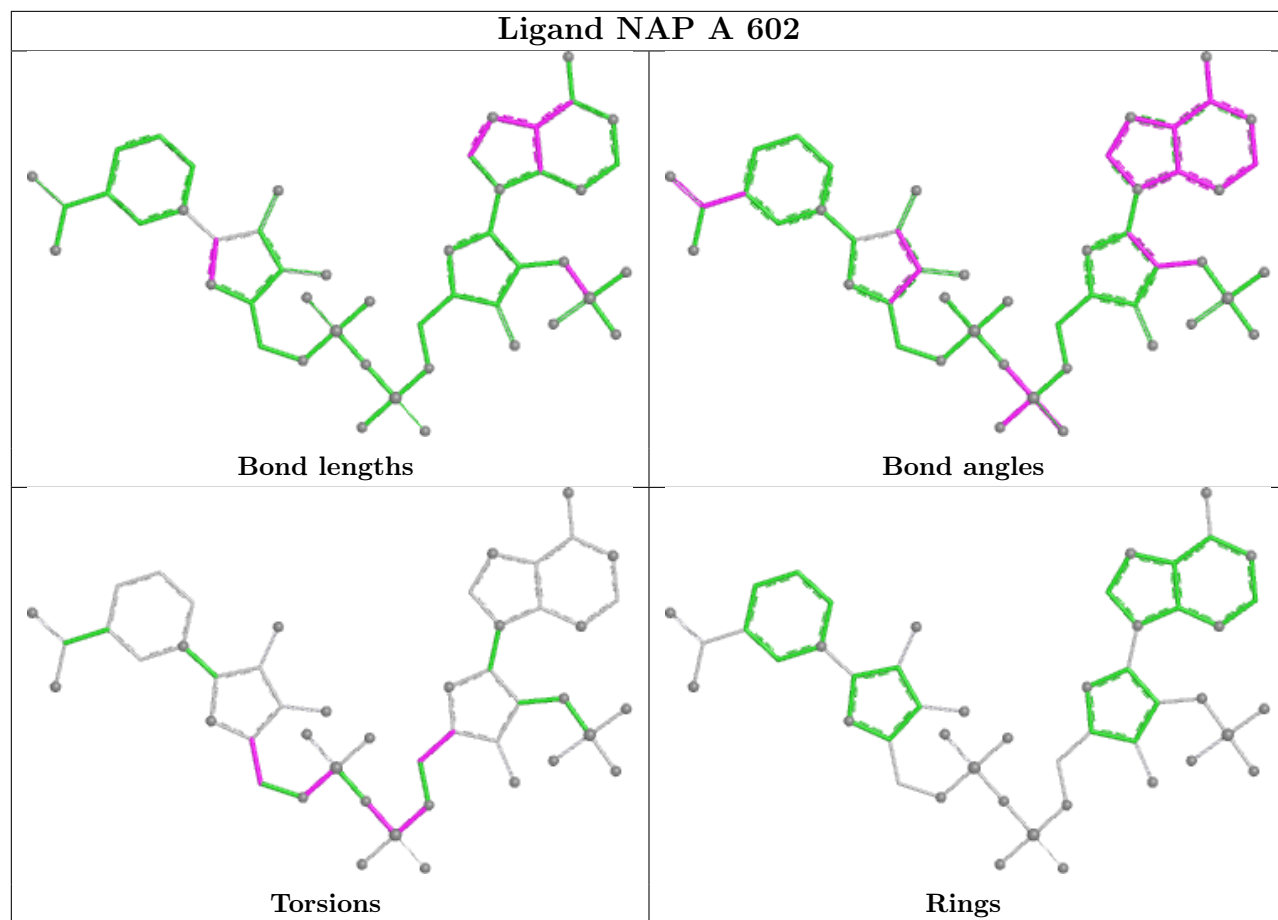
There are no ring outliers.

5 monomers are involved in 19 short contacts:

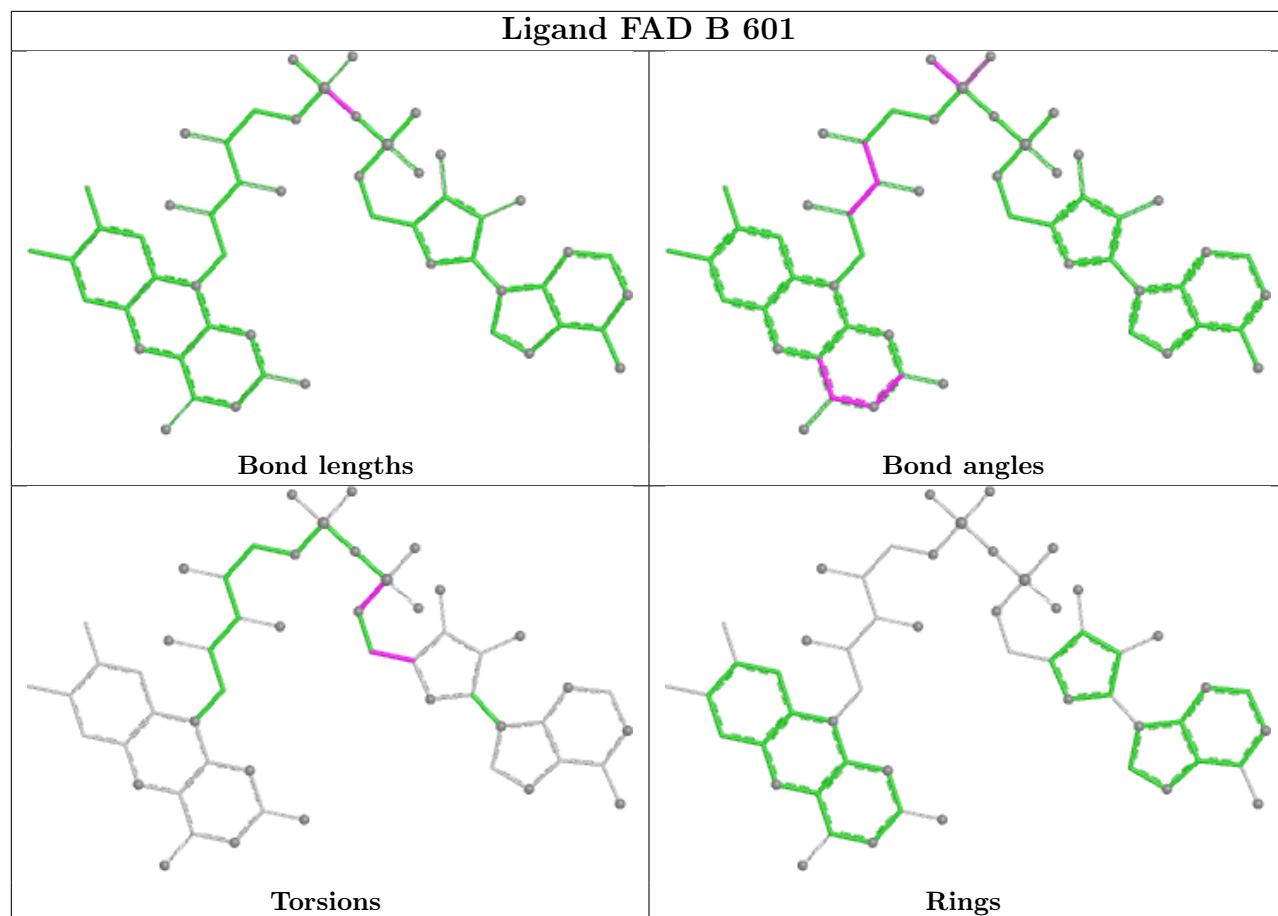
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	EPE	1	0
2	A	601	FAD	7	0
3	A	602	NAP	2	0
2	B	601	FAD	9	0
3	B	602	NAP	3	0

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 than 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.

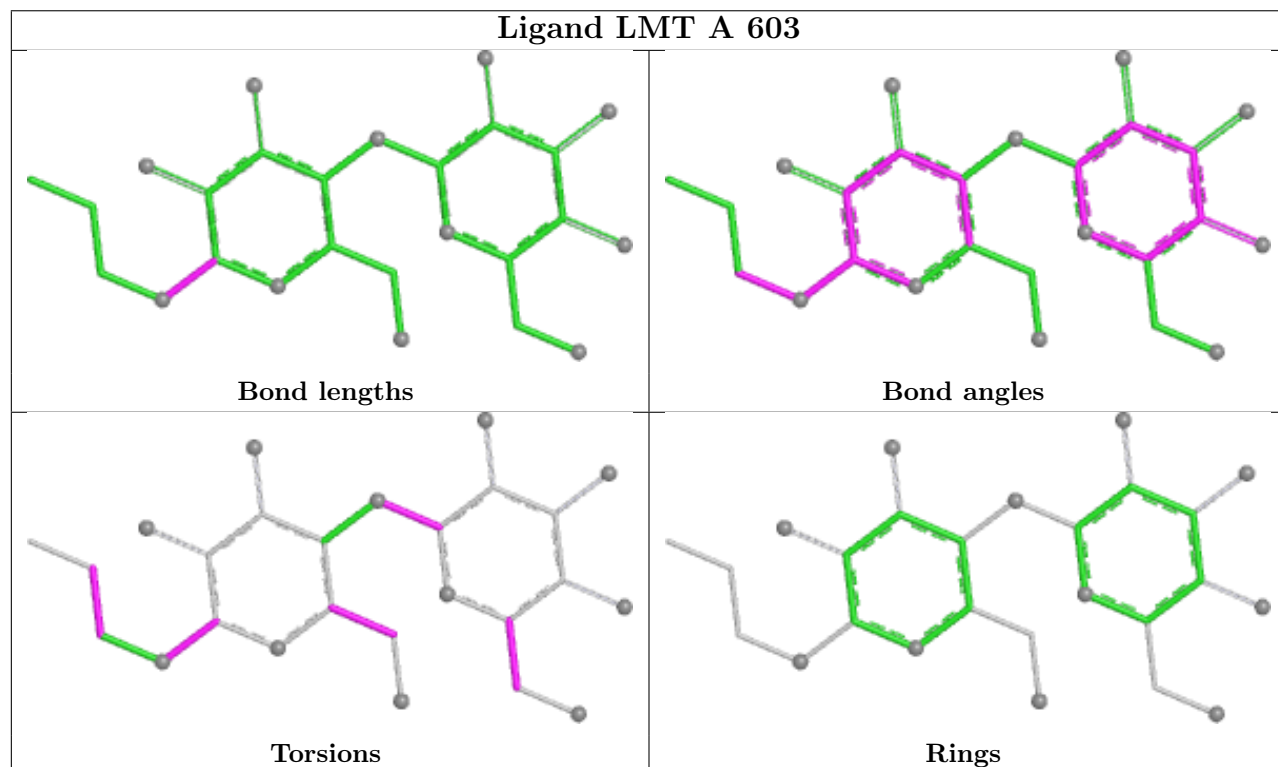


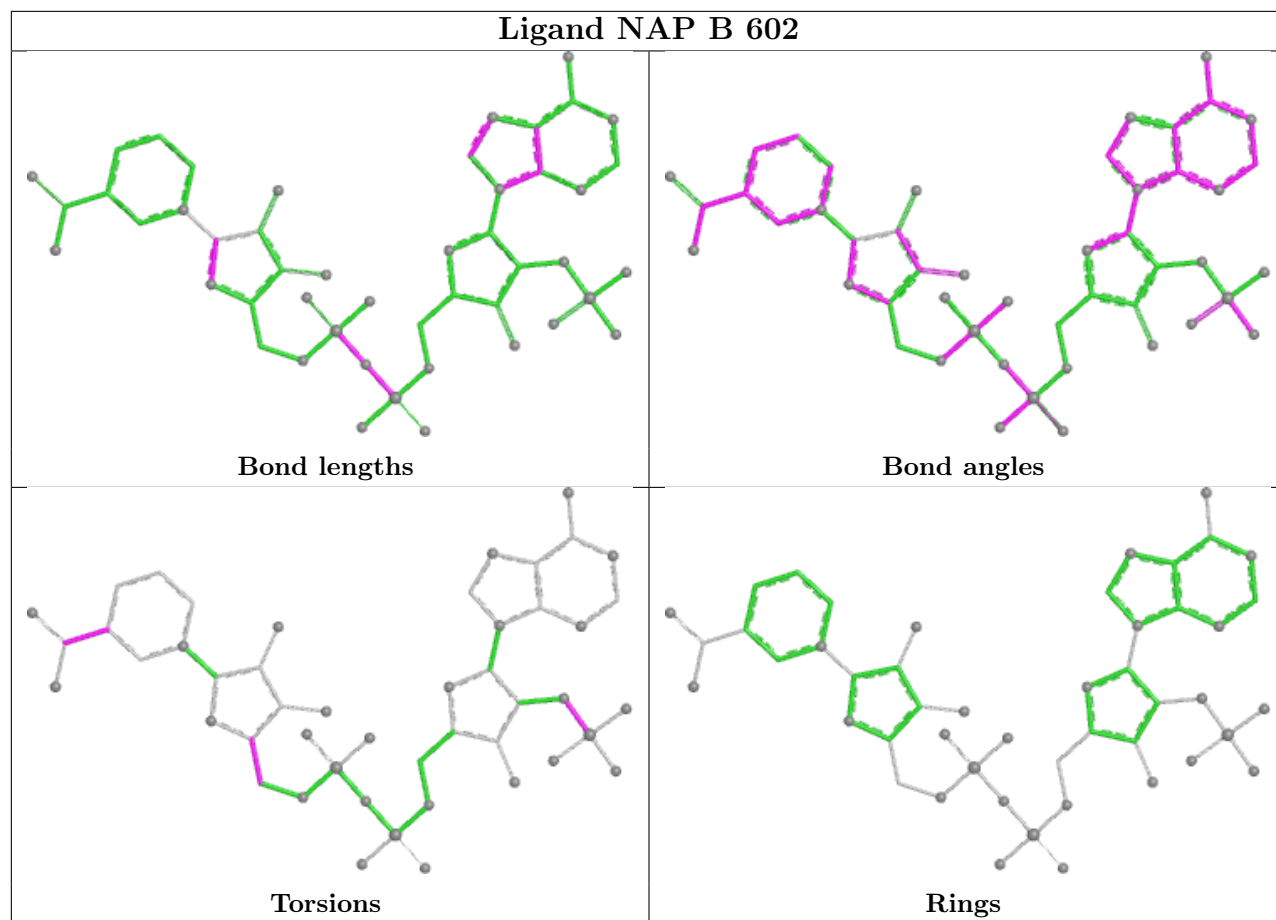


Ligand FAD B 601



Ligand LMT A 603





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	504/533 (94%)	0.28	35 (6%)	23 20	59, 83, 114, 132	0
1	B	504/533 (94%)	0.44	44 (8%)	16 13	61, 93, 122, 150	0
All	All	1008/1066 (94%)	0.36	79 (7%)	19 16	59, 87, 119, 150	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	LYS	8.3
1	B	382	SER	6.6
1	A	400	PRO	5.9
1	A	411	LYS	5.6
1	A	415	GLU	5.4
1	B	24	GLU	5.3
1	A	277	ARG	5.3
1	B	248	CYS	5.3
1	A	312	ALA	5.0
1	B	385	GLN	5.0
1	A	408	GLU	4.6
1	B	430	GLY	4.4
1	A	251	SER	4.4
1	B	53	ALA	4.3
1	B	152	THR	4.3
1	A	307	PHE	4.2
1	A	404	GLU	4.0
1	B	222	LEU	4.0
1	B	374	PRO	4.0
1	A	311	ALA	3.9
1	B	166	LYS	3.9
1	B	381	ILE	3.8
1	B	391	GLN	3.7
1	B	51	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	389	ALA	3.6
1	A	308	THR	3.5
1	B	22	CYS	3.4
1	B	384	LEU	3.4
1	B	21	CYS	3.4
1	A	36	ASP	3.4
1	A	66	GLU	3.2
1	A	102	LEU	3.1
1	B	388	TRP	3.1
1	B	359	PRO	3.1
1	A	250	GLN	3.0
1	B	2	THR	3.0
1	A	108	LYS	2.9
1	B	375	LEU	2.9
1	B	347	LYS	2.8
1	B	396	LEU	2.8
1	A	96	ALA	2.7
1	B	13	ALA	2.7
1	B	377	ALA	2.7
1	A	412	ALA	2.7
1	B	54	SER	2.7
1	A	236	PHE	2.6
1	B	435	THR	2.6
1	A	164	ILE	2.5
1	B	25	GLU	2.5
1	A	416	MET	2.5
1	A	97	LYS	2.5
1	B	443	VAL	2.5
1	A	481	TRP	2.5
1	A	337	PRO	2.5
1	A	255	THR	2.4
1	A	82	PHE	2.4
1	A	243	PHE	2.4
1	A	434	ASP	2.4
1	B	236	PHE	2.4
1	A	414	GLU	2.4
1	B	165	GLU	2.4
1	B	442	LEU	2.3
1	B	309	GLU	2.3
1	B	9	ILE	2.3
1	B	4	LYS	2.3
1	B	441	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	399	LEU	2.3
1	A	163	GLY	2.3
1	B	247	ILE	2.2
1	B	357	PHE	2.2
1	A	2	THR	2.2
1	B	149	GLY	2.2
1	B	265	PHE	2.2
1	A	136	LYS	2.1
1	B	426	HIS	2.1
1	B	439	ILE	2.1
1	B	75	ILE	2.0
1	B	376	GLY	2.0
1	A	387	ARG	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](#)

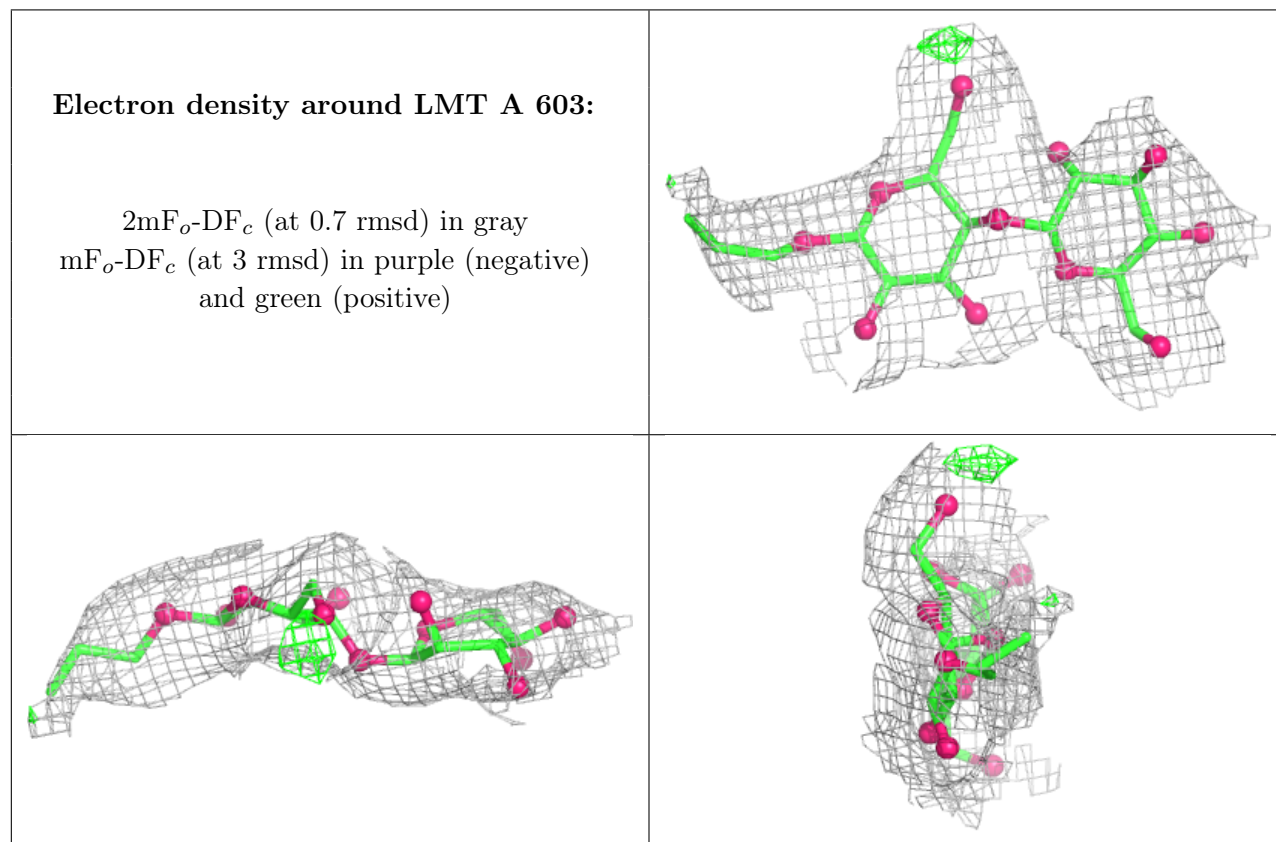
There are no oligosaccharides in this entry.

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.

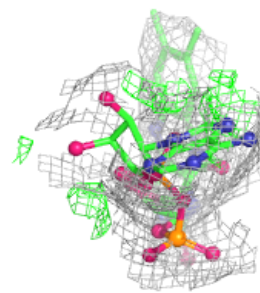
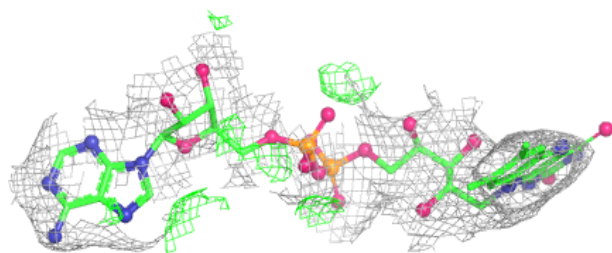
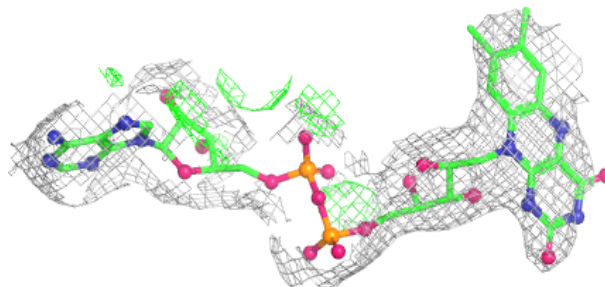
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GLC	A	605	12/12	0.69	0.11	107,121,135,138	0
4	LMT	A	603	26/35	0.70	0.13	105,146,169,176	0
5	EPE	A	604	15/15	0.72	0.16	68,99,158,165	0
6	GLC	A	606	12/12	0.82	0.10	111,131,145,153	0
5	EPE	B	603	15/15	0.89	0.11	100,121,145,147	0
2	FAD	B	601	53/53	0.91	0.11	72,99,147,161	0
3	NAP	A	602	48/48	0.95	0.07	63,74,83,85	0
2	FAD	A	601	53/53	0.95	0.08	67,83,121,126	0
3	NAP	B	602	48/48	0.96	0.06	57,73,91,101	0

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

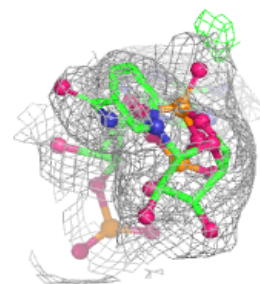
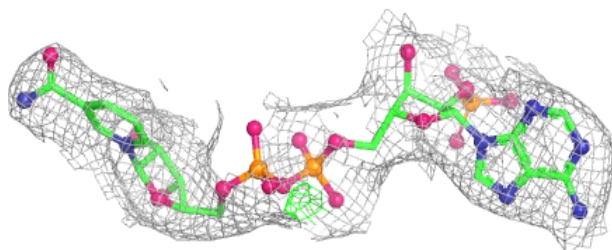
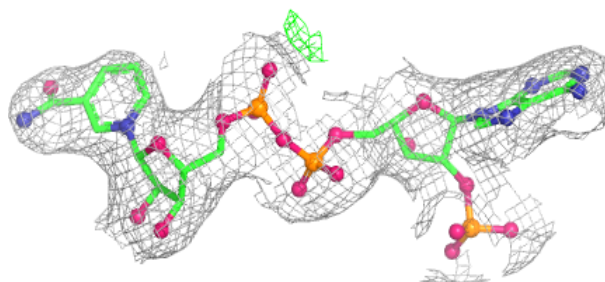


Electron density around FAD B 601:

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

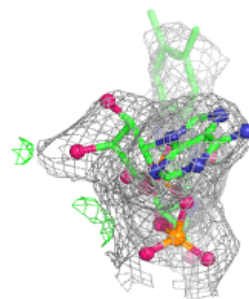
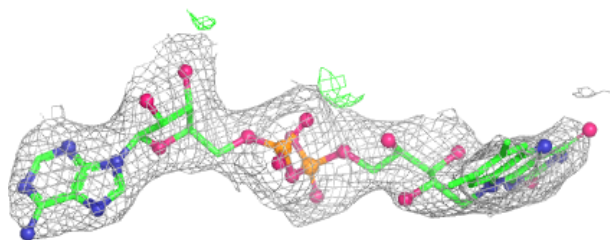
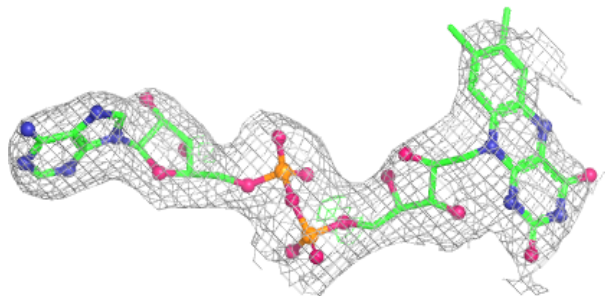
**Electron density around NAP A 602:**

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

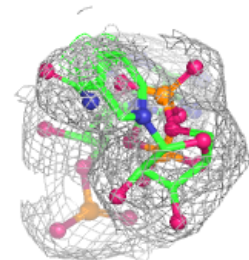
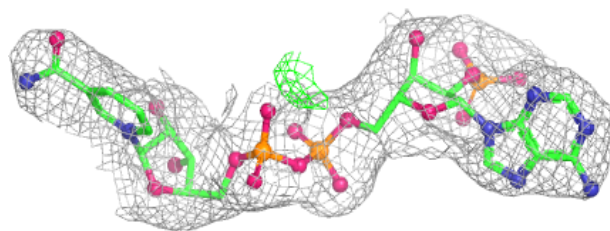
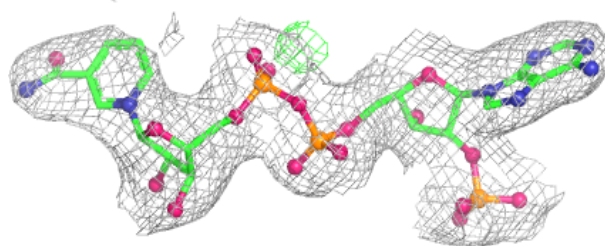


Electron density around FAD A 601:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.