



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:10 pm BST

PDB ID : 5VWU
Title : Crystal structure of oxidized Aspergillus fumigatus UDP-galactopyranose mutase complexed with NADH
Authors : Tanner, J.J.
Deposited on : 2017-05-22
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

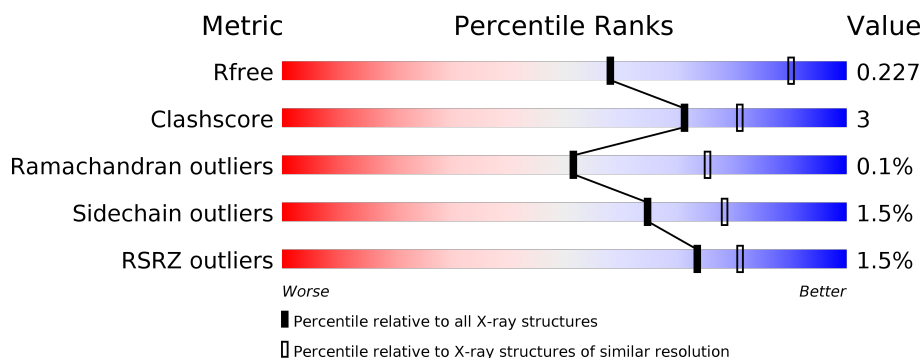
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on 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	513	<div> <div>88%</div> <div>8%</div> <div>•</div> </div>
1	B	513	<div> <div>87%</div> <div>8%</div> <div>• •</div> </div>
1	C	513	<div> <div>3%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
1	D	513	<div> <div>2%</div> <div>92%</div> <div>6%</div> <div>•</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15591 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 UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3777	2409	635	712	21			
1	B	494	Total	C	N	O	S	0	0	0
			3777	2406	633	718	20			
1	C	503	Total	C	N	O	S	0	0	0
			3826	2440	647	720	19			
1	D	504	Total	C	N	O	S	0	0	0
			3827	2442	644	721	20			

There are 24 discrepancies between the modelled and reference sequences:

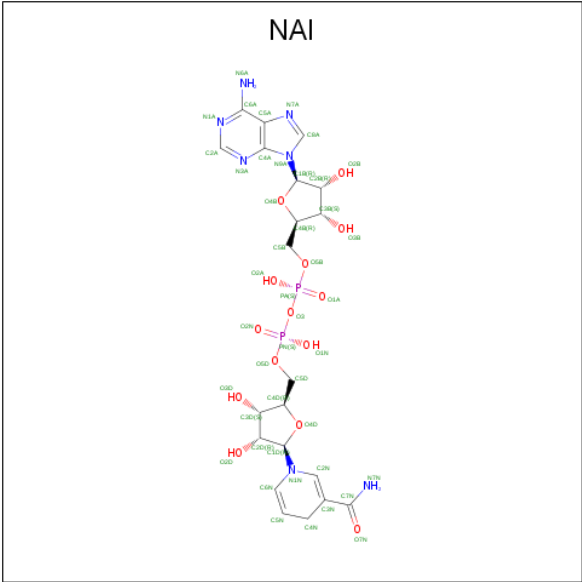
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP Q4W1X2
A	-1	ILE	-	expression tag	UNP Q4W1X2
A	0	ALA	-	expression tag	UNP Q4W1X2
A	344	ALA	LYS	engineered mutation	UNP Q4W1X2
A	345	ALA	LYS	engineered mutation	UNP Q4W1X2
A	429	THR	ALA	conflict	UNP Q4W1X2
B	-2	ALA	-	expression tag	UNP Q4W1X2
B	-1	ILE	-	expression tag	UNP Q4W1X2
B	0	ALA	-	expression tag	UNP Q4W1X2
B	344	ALA	LYS	engineered mutation	UNP Q4W1X2
B	345	ALA	LYS	engineered mutation	UNP Q4W1X2
B	429	THR	ALA	conflict	UNP Q4W1X2
C	-2	ALA	-	expression tag	UNP Q4W1X2
C	-1	ILE	-	expression tag	UNP Q4W1X2
C	0	ALA	-	expression tag	UNP Q4W1X2
C	344	ALA	LYS	engineered mutation	UNP Q4W1X2
C	345	ALA	LYS	engineered mutation	UNP Q4W1X2
C	429	THR	ALA	conflict	UNP Q4W1X2
D	-2	ALA	-	expression tag	UNP Q4W1X2
D	-1	ILE	-	expression tag	UNP Q4W1X2
D	0	ALA	-	expression tag	UNP Q4W1X2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	344	ALA	LYS	engineered mutation	UNP Q4W1X2
D	345	ALA	LYS	engineered mutation	UNP Q4W1X2
D	429	THR	ALA	conflict	UNP Q4W1X2

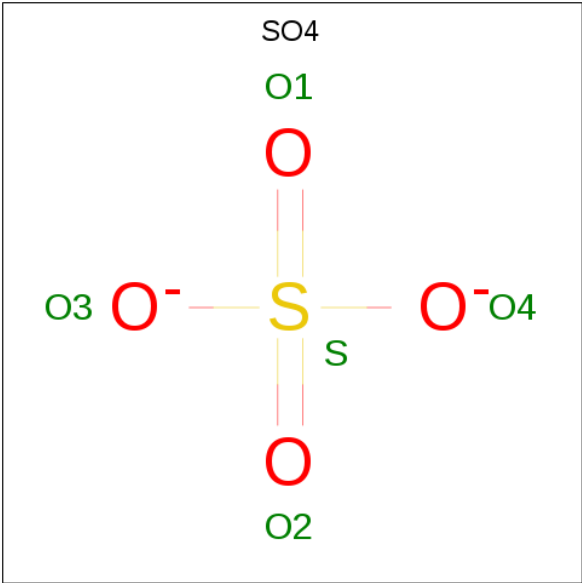
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- The chemical structure of FAD (Flavin Adenine Dinucleotide) is shown. It consists of a flavin isoalloxazine ring system (top) connected via a ribitol chain to an adenine ring system (bottom). The flavin ring is labeled with N1A, N3A, C2A, C4A, C6A, C8A, and N7A. The ribitol chain is labeled with C5B, C6B, C7B, C8B, C9B, and C10B. The adenine ring is labeled with N1, N3, C2, C4, C6, C7, C8, and N9. The structure is color-coded: blue for nitrogen atoms, red for oxygen atoms, and black for carbon atoms. The ribitol chain is shown in a zig-zag conformation, and the adenine ring is shown in a planar conformation.

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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

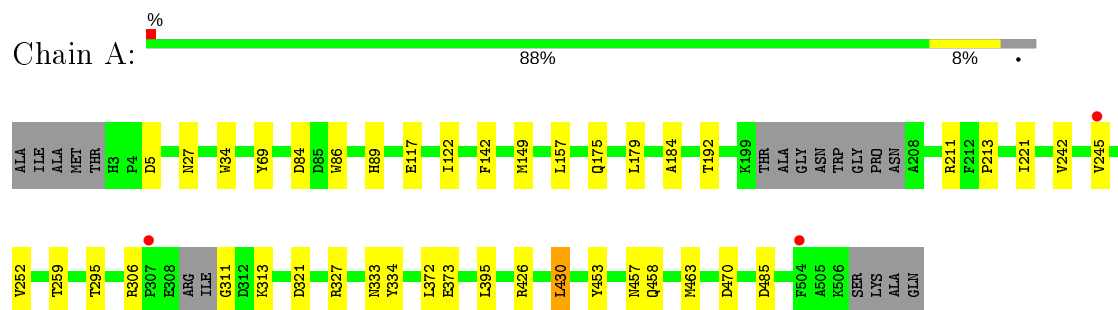
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	7	Total O 7 7	0	0
5	C	5	Total O 5 5	0	0
5	D	5	Total O 5 5	0	0

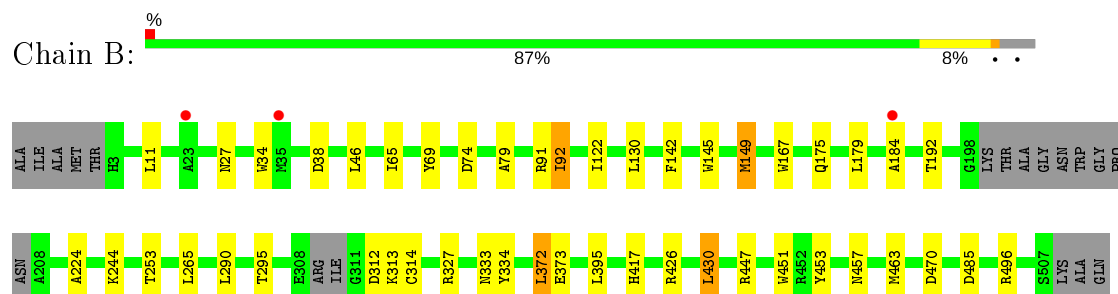
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

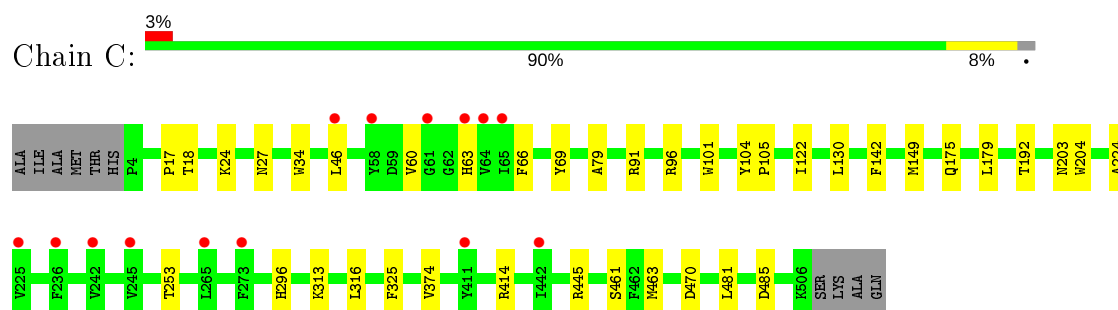
• Molecule 1: UDP-galactopyranose mutase



• Molecule 1: UDP-galactopyranose mutase

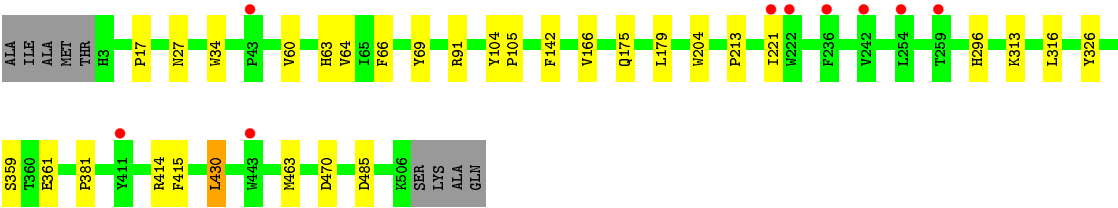


• Molecule 1: UDP-galactopyranose mutase



• Molecule 1: UDP-galactopyranose mutase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.25Å 218.25Å 318.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.59 – 2.75 162.48 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.59-2.75) 99.3 (162.48-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.73Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.194 , 0.227 0.194 , 0.227	Depositor DCC
R_{free} test set	5796 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15591	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, SO4, FAD

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	0.46	0/3870	0.62	0/5277
1	B	0.45	0/3870	0.62	0/5279
1	C	0.42	0/3924	0.59	0/5356
1	D	0.43	0/3925	0.58	0/5356
All	All	0.44	0/15589	0.60	0/21268

There are no bond length outliers.

There are no bond angle outliers.

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	3777	0	3592	26	0
1	B	3777	0	3583	31	0
1	C	3826	0	3615	23	0
1	D	3827	0	3613	17	0
2	A	53	0	31	5	0
2	B	53	0	31	7	0
2	C	53	0	31	6	0
2	D	53	0	31	3	0
3	A	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	1	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	20	0	0	0	0
4	D	20	0	0	0	0
5	A	2	0	0	0	0
5	B	7	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
All	All	15591	0	14579	104	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 3.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:NE	1:B:373:GLU:OE2	2.25	0.67
1:A:372:LEU:HD21	1:A:395:LEU:HD21	1.78	0.66
1:B:122:ILE:HD12	1:B:192:THR:HG22	1.81	0.63
1:B:149:MET:SD	1:B:184:ALA:HA	2.39	0.62
1:C:46:LEU:O	1:C:60:VAL:HG21	1.99	0.61
1:D:69:TYR:CD1	1:D:463:MET:HG3	2.37	0.60
1:B:244:LYS:HB3	1:B:253:THR:HB	1.84	0.59
1:D:313:LYS:HD3	1:D:316:LEU:HD21	1.85	0.58
1:C:325:PHE:HA	1:C:374:VAL:HG22	1.86	0.57
1:A:327:ARG:NE	1:A:373:GLU:OE2	2.25	0.57
1:C:313:LYS:HD3	1:C:316:LEU:HD21	1.86	0.56
1:B:372:LEU:HD11	1:B:395:LEU:HD21	1.89	0.55
1:B:313:LYS:HG3	1:B:333:ASN:HB3	1.89	0.55
1:B:46:LEU:HD13	2:B:601:FAD:HM81	1.87	0.55
2:B:601:FAD:H2'	2:B:601:FAD:N1	2.23	0.54
1:A:69:TYR:CD1	1:A:463:MET:HG3	2.43	0.54
1:B:453:TYR:CE1	3:B:602:NAI:H42N	2.43	0.54
1:C:296:HIS:CE1	1:C:414:ARG:HD2	2.44	0.53
1:A:457:ASN:HB2	2:A:601:FAD:O2	2.08	0.52
1:D:359:SER:OG	1:D:361:GLU:HG2	2.09	0.52
1:B:92:ILE:HG22	1:B:314:CYS:HB3	1.92	0.52
1:A:149:MET:SD	1:A:184:ALA:HA	2.50	0.51
1:D:166:VAL:HG22	1:D:326:TYR:CD1	2.46	0.51
1:B:290:LEU:HD21	1:B:430:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:O	1:C:204:TRP:HB3	2.11	0.51
1:C:17:PRO:HG2	2:C:601:FAD:O3'	2.10	0.51
1:B:142:PHE:CE1	1:B:179:LEU:HD11	2.46	0.50
1:D:91:ARG:O	1:D:204:TRP:HB3	2.10	0.50
1:B:69:TYR:CD1	1:B:463:MET:HG3	2.46	0.50
1:B:74:ASP:OD2	1:B:496:ARG:NE	2.40	0.50
1:B:69:TYR:CG	1:B:463:MET:HG3	2.47	0.50
1:C:66:PHE:HB2	1:C:91:ARG:NH1	2.26	0.50
1:B:290:LEU:HD13	1:B:451:TRP:CD2	2.46	0.50
1:A:313:LYS:HG3	1:A:333:ASN:HB3	1.94	0.50
1:C:69:TYR:CD1	1:C:463:MET:HG3	2.47	0.49
1:B:130:LEU:HD23	1:C:130:LEU:HD23	1.94	0.49
1:B:426:ARG:HG2	1:B:430:LEU:HD22	1.96	0.48
1:A:89:HIS:ND1	1:A:313:LYS:HG2	2.29	0.48
1:D:296:HIS:CE1	1:D:414:ARG:HD2	2.50	0.47
2:A:601:FAD:O2'	2:A:601:FAD:O4'	2.29	0.46
1:C:105:PRO:HD3	1:C:203:ASN:HB3	1.96	0.46
1:B:92:ILE:HG21	1:B:312:ASP:OD1	2.16	0.46
1:D:213:PRO:HG3	1:D:221:ILE:HG13	1.96	0.46
1:A:334:TYR:CD1	1:A:334:TYR:N	2.84	0.46
2:A:601:FAD:H9	2:A:601:FAD:H1'1	1.66	0.46
1:A:245:VAL:HG22	1:A:252:VAL:HG22	1.96	0.46
1:A:306:ARG:HD2	1:A:311:GLY:HA2	1.97	0.45
1:A:86:TRP:CD2	1:A:211:ARG:HD2	2.50	0.45
1:B:167:TRP:HH2	1:B:453:TYR:CD1	2.34	0.45
1:A:242:VAL:HG13	1:A:252:VAL:HG13	1.98	0.45
1:D:60:VAL:HG13	1:D:415:PHE:CE2	2.50	0.45
2:B:601:FAD:H9	2:B:601:FAD:H1'1	1.63	0.45
1:A:117:GLU:OE2	1:A:157:LEU:HD21	2.16	0.45
1:A:69:TYR:CG	1:A:463:MET:HG3	2.51	0.45
1:B:11:LEU:O	1:B:265:LEU:HD12	2.17	0.45
1:C:142:PHE:CE1	1:C:179:LEU:HD11	2.52	0.45
1:C:69:TYR:CG	1:C:463:MET:HG3	2.52	0.45
1:D:430:LEU:HD12	1:D:430:LEU:HA	1.84	0.44
1:B:145:TRP:CD2	1:B:179:LEU:HD13	2.53	0.44
1:A:122:ILE:HD12	1:A:192:THR:HG22	1.99	0.44
1:A:321:ASP:OD1	1:A:321:ASP:N	2.46	0.44
1:B:295:THR:HG21	2:B:601:FAD:C7M	2.47	0.44
1:D:69:TYR:CG	1:D:463:MET:HG3	2.52	0.44
1:A:458:GLN:HA	2:A:601:FAD:O3'	2.17	0.44
1:B:65:ILE:HB	1:B:91:ARG:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:HIS:HB3	2:C:601:FAD:N3	2.32	0.44
1:A:27:ASN:HB2	1:A:34:TRP:CZ2	2.52	0.43
1:B:457:ASN:HB2	2:B:601:FAD:O2	2.18	0.43
1:C:17:PRO:HD2	2:C:601:FAD:H4'	2.00	0.43
1:B:27:ASN:HB2	1:B:34:TRP:CZ2	2.53	0.43
1:C:122:ILE:HD12	1:C:192:THR:HG22	1.99	0.43
1:C:104:TYR:CG	1:C:105:PRO:HA	2.54	0.43
1:B:313:LYS:HD2	1:B:313:LYS:N	2.33	0.43
1:D:66:PHE:HB2	1:D:91:ARG:NH2	2.34	0.43
1:D:63:HIS:HB3	2:D:601:FAD:C4	2.50	0.42
1:D:142:PHE:CE1	1:D:179:LEU:HD11	2.53	0.42
1:C:79:ALA:HB1	1:C:224:ALA:CB	2.49	0.42
1:A:334:TYR:N	1:A:334:TYR:HD1	2.17	0.42
1:A:453:TYR:CE1	3:A:602:NAI:H42N	2.55	0.42
1:C:27:ASN:HB2	1:C:34:TRP:CZ2	2.54	0.42
1:D:69:TYR:CE1	1:D:463:MET:HG3	2.55	0.42
1:A:295:THR:HG21	2:A:601:FAD:C7M	2.50	0.42
1:B:334:TYR:CD1	1:B:334:TYR:N	2.88	0.42
1:A:5:ASP:HB2	1:A:259:THR:O	2.20	0.42
1:B:38:ASP:OD2	2:B:601:FAD:O3B	2.37	0.42
1:D:17:PRO:HD2	2:D:601:FAD:H4'	2.02	0.42
1:A:213:PRO:HG3	1:A:221:ILE:HG13	2.02	0.41
2:C:601:FAD:H1'1	2:C:601:FAD:H9	1.75	0.41
1:A:142:PHE:CE1	1:A:179:LEU:HD11	2.55	0.41
1:B:142:PHE:CD1	1:B:179:LEU:HD11	2.54	0.41
1:C:445:ARG:NE	1:C:481:LEU:HD22	2.35	0.41
1:C:96:ARG:HB2	1:C:101:TRP:CZ3	2.56	0.41
1:A:426:ARG:HG2	1:A:430:LEU:HD22	2.02	0.41
2:C:601:FAD:O4'	2:C:601:FAD:O2'	2.31	0.41
1:D:104:TYR:CG	1:D:105:PRO:HA	2.55	0.41
1:C:18:THR:OG1	1:C:461:SER:HB3	2.20	0.41
1:C:24:LYS:HA	1:C:24:LYS:HD2	1.93	0.41
1:B:79:ALA:HB1	1:B:224:ALA:CB	2.51	0.41
1:C:142:PHE:CD1	1:C:179:LEU:HD11	2.57	0.40
1:A:372:LEU:HD11	1:A:395:LEU:HD11	2.04	0.40
1:D:27:ASN:HB2	1:D:34:TRP:HZ2	1.87	0.40
2:D:601:FAD:H1'1	2:D:601:FAD:H9	1.75	0.40
1:B:447:ARG:HB2	2:B:601:FAD:H5'2	2.04	0.40
2:C:601:FAD:N1	2:C:601:FAD:H2'	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	488/513 (95%)	477 (98%)	11 (2%)	0	100	100
1	B	488/513 (95%)	476 (98%)	12 (2%)	0	100	100
1	C	501/513 (98%)	490 (98%)	11 (2%)	0	100	100
1	D	502/513 (98%)	489 (97%)	12 (2%)	1 (0%)	47	69
All	All	1979/2052 (96%)	1932 (98%)	46 (2%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	VAL

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	387/432 (90%)	382 (99%)	5 (1%)	69	81
1	B	389/432 (90%)	381 (98%)	8 (2%)	53	71
1	C	386/432 (89%)	381 (99%)	5 (1%)	69	81
1	D	385/432 (89%)	380 (99%)	5 (1%)	69	81
All	All	1547/1728 (90%)	1524 (98%)	23 (2%)	65	78

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	A	175	GLN
1	A	430	LEU
1	A	470	ASP
1	A	485	ASP
1	B	92	ILE
1	B	149	MET
1	B	175	GLN
1	B	372	LEU
1	B	417	HIS
1	B	430	LEU
1	B	470	ASP
1	B	485	ASP
1	C	149	MET
1	C	175	GLN
1	C	253	THR
1	C	470	ASP
1	C	485	ASP
1	D	175	GLN
1	D	381	PRO
1	D	430	LEU
1	D	470	ASP
1	D	485	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

19 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
4	SO4	C	602	-	4,4,4	0.13	0	6,6,6	0.26	0
4	SO4	B	604	-	4,4,4	0.12	0	6,6,6	0.19	0
4	SO4	B	605	-	4,4,4	0.14	0	6,6,6	0.26	0
4	SO4	D	605	-	4,4,4	0.18	0	6,6,6	0.32	0
4	SO4	D	603	-	4,4,4	0.17	0	6,6,6	0.25	0
4	SO4	C	605	-	4,4,4	0.13	0	6,6,6	0.22	0
4	SO4	C	604	-	4,4,4	0.14	0	6,6,6	0.42	0
3	NAI	A	602	-	42,48,48	1.61	5 (11%)	47,73,73	1.46	7 (14%)
4	SO4	B	603	-	4,4,4	0.13	0	6,6,6	0.33	0
2	FAD	B	601	-	51,58,58	1.34	4 (7%)	60,89,89	2.34	8 (13%)
4	SO4	A	604	-	4,4,4	0.22	0	6,6,6	0.29	0
4	SO4	C	603	-	4,4,4	0.16	0	6,6,6	0.46	0
2	FAD	C	601	-	51,58,58	1.26	4 (7%)	60,89,89	2.31	7 (11%)
4	SO4	A	603	-	4,4,4	0.19	0	6,6,6	0.19	0
4	SO4	D	602	-	4,4,4	0.17	0	6,6,6	0.31	0
2	FAD	A	601	-	51,58,58	1.29	5 (9%)	60,89,89	2.31	9 (15%)
3	NAI	B	602	-	42,48,48	1.65	8 (19%)	47,73,73	1.40	3 (6%)
2	FAD	D	601	-	51,58,58	1.25	5 (9%)	60,89,89	2.34	10 (16%)
4	SO4	D	604	-	4,4,4	0.16	0	6,6,6	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	A	602	-	-	12/25/72/72	0/5/5/5
2	FAD	B	601	-	-	17/30/50/50	0/6/6/6
2	FAD	C	601	-	-	21/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	-	13/30/50/50	0/6/6/6
2	FAD	D	601	-	-	18/30/50/50	0/6/6/6
3	NAI	B	602	-	-	6/25/72/72	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C4X-C10	6.28	1.45	1.38
3	A	602	NAI	PN-O5D	6.05	1.83	1.59
2	A	601	FAD	C4X-C10	5.76	1.44	1.38
2	C	601	FAD	C4X-C10	5.39	1.44	1.38
2	D	601	FAD	C4X-C10	5.34	1.44	1.38
3	B	602	NAI	PN-O5D	4.89	1.79	1.59
3	A	602	NAI	O2B-C2B	-3.90	1.33	1.43
3	B	602	NAI	O2B-C2B	-3.85	1.33	1.43
2	C	601	FAD	C4-N3	3.47	1.39	1.33
2	B	601	FAD	C4-N3	3.43	1.39	1.33
2	D	601	FAD	C4-N3	3.40	1.39	1.33
3	B	602	NAI	C4A-N3A	3.18	1.40	1.35
2	A	601	FAD	C4-C4X	3.14	1.46	1.41
2	B	601	FAD	C5X-N5	3.10	1.40	1.35
2	A	601	FAD	C5X-N5	2.85	1.40	1.35
2	A	601	FAD	C4-N3	2.79	1.37	1.33
2	B	601	FAD	C4-C4X	2.75	1.46	1.41
2	A	601	FAD	C1'-N10	-2.66	1.45	1.48
2	D	601	FAD	C1'-N10	-2.61	1.45	1.48
2	C	601	FAD	C4X-N5	-2.55	1.29	1.33
3	B	602	NAI	C2B-C1B	2.50	1.57	1.53
2	D	601	FAD	C4X-N5	-2.44	1.29	1.33
3	B	602	NAI	C3D-C4D	2.43	1.59	1.53
3	A	602	NAI	C4A-N3A	2.41	1.39	1.35
3	B	602	NAI	C7N-N7N	2.41	1.39	1.33
2	C	601	FAD	C1'-N10	-2.32	1.45	1.48
3	B	602	NAI	C2A-N1A	2.30	1.38	1.33
3	A	602	NAI	PA-O5B	2.19	1.68	1.59
3	B	602	NAI	O2D-C2D	-2.07	1.38	1.43
3	A	602	NAI	C6N-N1N	2.07	1.42	1.37
2	D	601	FAD	C5X-N5	2.04	1.38	1.35

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4-N3-C2	13.21	126.30	115.14
2	C	601	FAD	C4-N3-C2	13.18	126.27	115.14
2	A	601	FAD	C4-N3-C2	13.10	126.20	115.14
2	D	601	FAD	C4-N3-C2	13.08	126.19	115.14
2	A	601	FAD	C4X-C4-N3	-7.18	113.61	123.43
2	B	601	FAD	C4X-C4-N3	-7.12	113.69	123.43
2	D	601	FAD	C4X-C4-N3	-6.69	114.28	123.43
2	C	601	FAD	C4X-C4-N3	-6.38	114.70	123.43
2	C	601	FAD	C10-C4X-N5	5.48	125.05	121.26
3	B	602	NAI	PN-O3-PA	-5.31	114.61	132.83
2	D	601	FAD	C10-C4X-N5	5.07	124.76	121.26
2	B	601	FAD	C10-C4X-N5	4.63	124.46	121.26
3	A	602	NAI	PN-O3-PA	-4.57	117.13	132.83
2	C	601	FAD	C4X-C10-N10	-4.18	116.01	120.30
2	A	601	FAD	C10-C4X-N5	4.03	124.04	121.26
2	C	601	FAD	C4-C4X-C10	-3.94	117.35	119.95
2	D	601	FAD	C4-C4X-C10	-3.93	117.35	119.95
2	B	601	FAD	C4X-C10-N10	-3.90	116.30	120.30
2	D	601	FAD	C4X-C10-N10	-3.80	116.40	120.30
2	A	601	FAD	C4X-C10-N10	-3.71	116.48	120.30
2	B	601	FAD	O3'-C3'-C2'	3.67	117.68	108.81
2	B	601	FAD	C1'-N10-C10	3.59	121.62	118.41
2	D	601	FAD	O5'-P-O1P	-3.49	95.45	109.07
2	A	601	FAD	C4-C4X-C10	-3.46	117.66	119.95
2	B	601	FAD	C4-C4X-C10	-3.33	117.75	119.95
3	A	602	NAI	PA-O5B-C5B	-2.92	104.54	121.68
2	D	601	FAD	O2A-PA-O1A	2.92	126.67	112.24
3	B	602	NAI	PA-O5B-C5B	-2.63	106.27	121.68
2	C	601	FAD	O2P-P-O1P	2.55	124.86	112.24
3	A	602	NAI	O7N-C7N-C3N	2.52	125.65	120.90
2	A	601	FAD	O3'-C3'-C2'	2.50	114.84	108.81
2	D	601	FAD	O2P-P-O1P	2.40	124.11	112.24
2	A	601	FAD	C5A-C6A-N6A	2.37	123.95	120.35
2	B	601	FAD	C5A-C6A-N6A	2.35	123.92	120.35
2	D	601	FAD	C5A-C6A-N6A	2.32	123.88	120.35
3	A	602	NAI	C3B-C2B-C1B	-2.23	97.62	100.98
3	A	602	NAI	C2A-N1A-C6A	-2.22	114.97	118.75
2	C	601	FAD	C5A-C6A-N6A	2.18	123.67	120.35
2	A	601	FAD	C5'-C4'-C3'	-2.14	108.08	112.20
2	A	601	FAD	O5B-PA-O1A	2.12	117.35	109.07
3	A	602	NAI	C5B-C4B-C3B	-2.05	107.49	115.18
3	B	602	NAI	O5D-PN-O2N	-2.04	101.09	109.07
3	A	602	NAI	C4A-C5A-N7A	2.02	111.50	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	O3'-C3'-C2'	2.02	113.68	108.81

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAI	C5B-O5B-PA-O1A
3	A	602	NAI	O4B-C4B-C5B-O5B
3	A	602	NAI	C3B-C4B-C5B-O5B
3	A	602	NAI	C5D-O5D-PN-O2N
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C2'-C1'-N10-C9A
2	B	601	FAD	C2'-C1'-N10-C10
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'
2	B	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	C5B-O5B-PA-O1A
2	C	601	FAD	C5B-O5B-PA-O2A
2	C	601	FAD	C2'-C1'-N10-C9A
2	C	601	FAD	C1'-C2'-C3'-O3'
2	C	601	FAD	C1'-C2'-C3'-C4'
2	C	601	FAD	C2'-C3'-C4'-O4'
2	C	601	FAD	C2'-C3'-C4'-C5'
2	C	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	O3'-C3'-C4'-C5'
2	C	601	FAD	C3'-C4'-C5'-O5'
2	C	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	C5'-O5'-P-O1P
2	C	601	FAD	C5'-O5'-P-O3P
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C2'-C1'-N10-C9A
2	A	601	FAD	C1'-C2'-C3'-O3'
2	A	601	FAD	C1'-C2'-C3'-C4'
2	A	601	FAD	O2'-C2'-C3'-O3'
2	A	601	FAD	O2'-C2'-C3'-C4'
2	A	601	FAD	C3'-C4'-C5'-O5'
2	A	601	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	C5'-O5'-P-O3P
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	D	601	FAD	C2'-C1'-N10-C9A
2	D	601	FAD	C1'-C2'-C3'-O3'
2	D	601	FAD	C1'-C2'-C3'-C4'
2	D	601	FAD	C3'-C4'-C5'-O5'
2	D	601	FAD	O4'-C4'-C5'-O5'
2	D	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	C2'-C3'-C4'-O4'
3	A	602	NAI	O4D-C4D-C5D-O5D
3	A	602	NAI	C3D-C4D-C5D-O5D
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	C2'-C3'-C4'-C5'
2	C	601	FAD	O2'-C2'-C3'-O3'
2	C	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C2'-C3'-C4'-O4'
3	A	602	NAI	PA-O3-PN-O2N
2	B	601	FAD	O4B-C4B-C5B-O5B
3	A	602	NAI	O4D-C1D-N1N-C2N
3	A	602	NAI	PA-O3-PN-O5D
2	B	601	FAD	P-O3P-PA-O5B
2	C	601	FAD	P-O3P-PA-O5B
2	A	601	FAD	PA-O3P-P-O5'
2	D	601	FAD	P-O3P-PA-O5B
3	B	602	NAI	PA-O3-PN-O5D
2	C	601	FAD	C4'-C5'-O5'-P
3	A	602	NAI	C5D-O5D-PN-O3
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C5'-O5'-P-O3P
2	D	601	FAD	C5B-O5B-PA-O3P
3	B	602	NAI	O4D-C1D-N1N-C2N
3	A	602	NAI	C5D-O5D-PN-O1N
2	B	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5'-O5'-P-O2P
2	D	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	P-O3P-PA-O1A
2	C	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C3B-C4B-C5B-O5B
3	B	602	NAI	C3D-C4D-C5D-O5D
3	B	602	NAI	O4D-C4D-C5D-O5D

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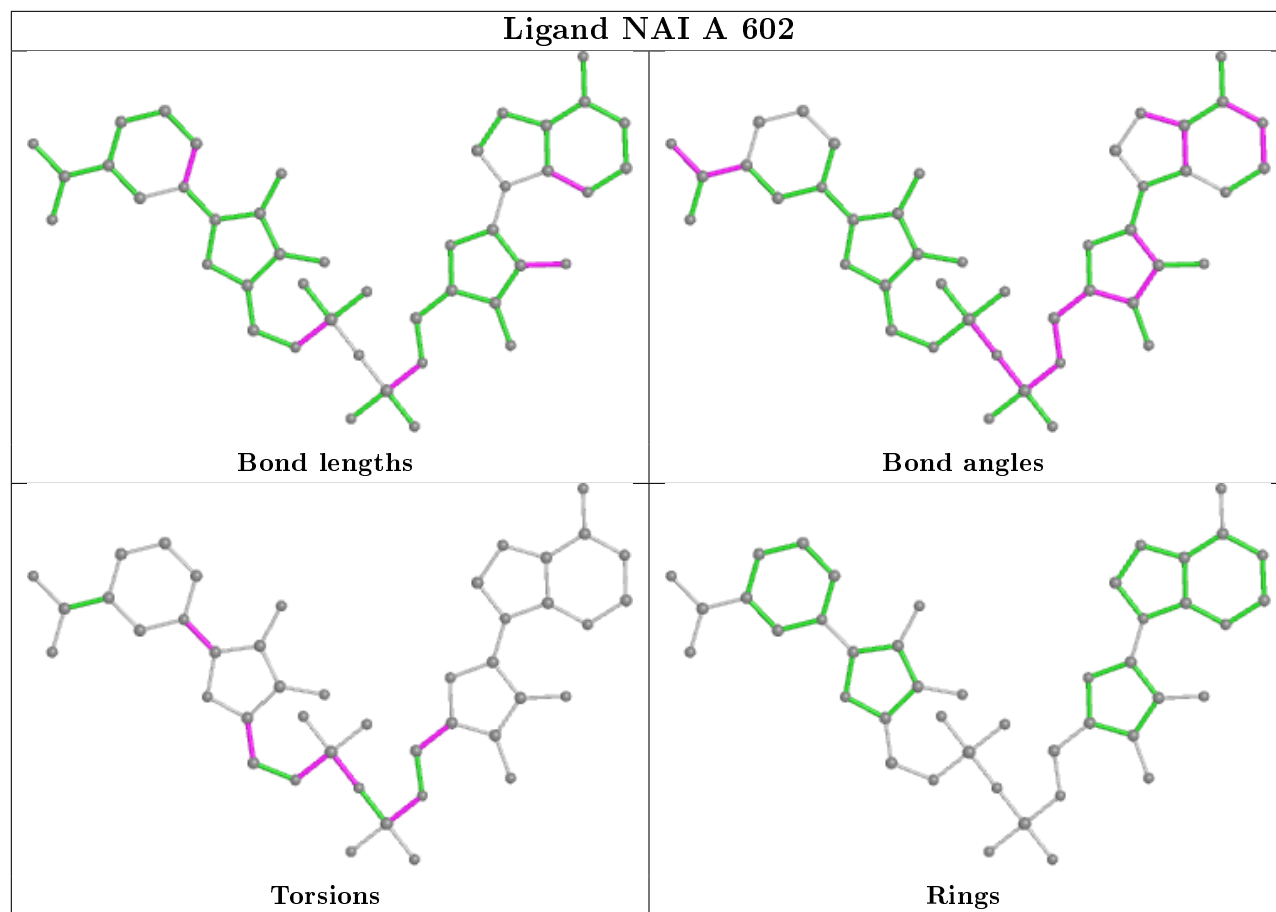
Mol	Chain	Res	Type	Atoms
2	D	601	FAD	PA-O3P-P-O1P
3	B	602	NAI	O4B-C4B-C5B-O5B
2	B	601	FAD	C2'-C3'-C4'-C5'
3	A	602	NAI	C5B-O5B-PA-O3
2	C	601	FAD	C5B-O5B-PA-O3P
2	D	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C3B-C4B-C5B-O5B
3	B	602	NAI	C3B-C4B-C5B-O5B
2	C	601	FAD	C5'-O5'-P-O2P

There are no ring outliers.

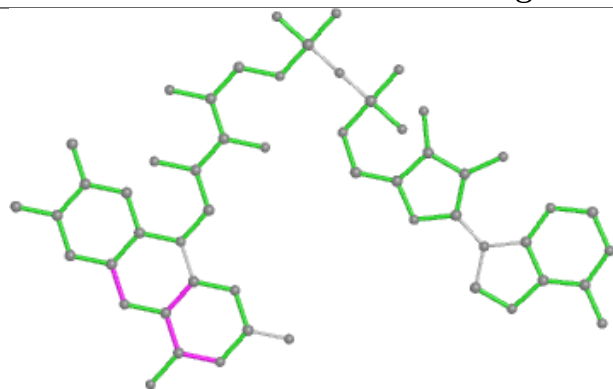
6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NAI	1	0
2	B	601	FAD	7	0
2	C	601	FAD	6	0
2	A	601	FAD	5	0
3	B	602	NAI	1	0
2	D	601	FAD	3	0

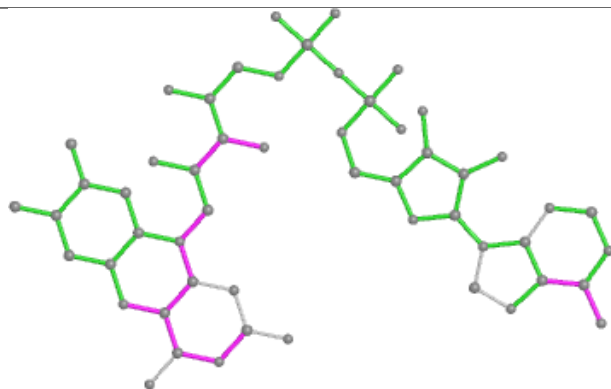
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



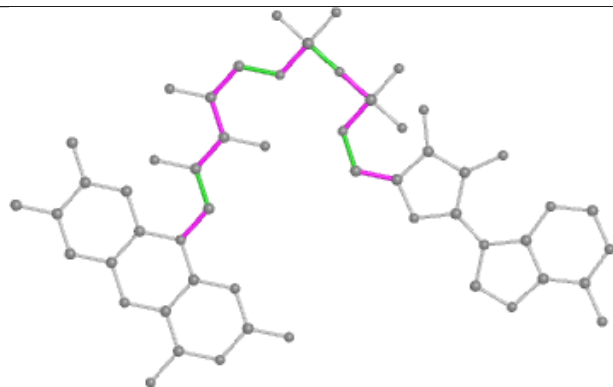
Ligand FAD B 601



Bond lengths



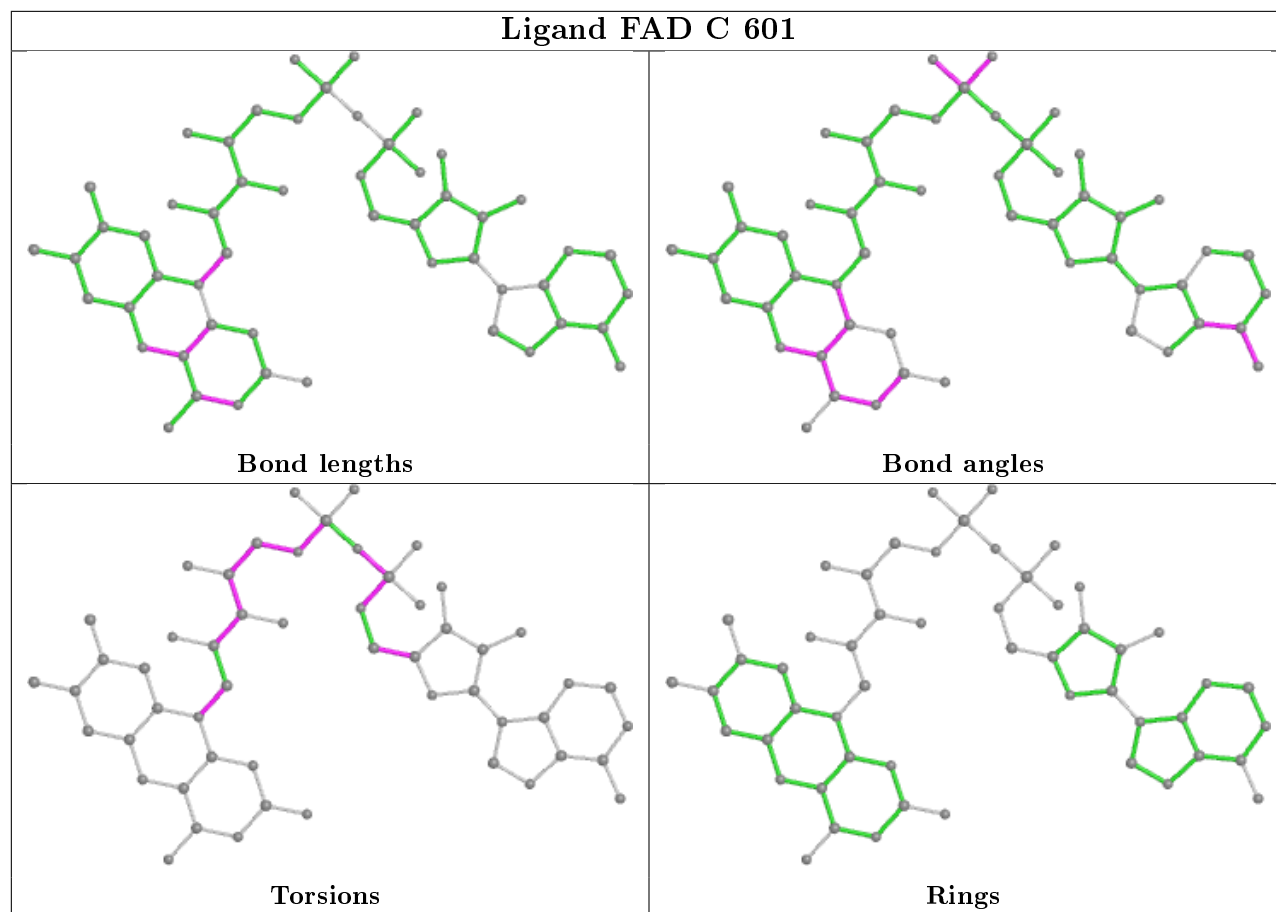
Bond angles

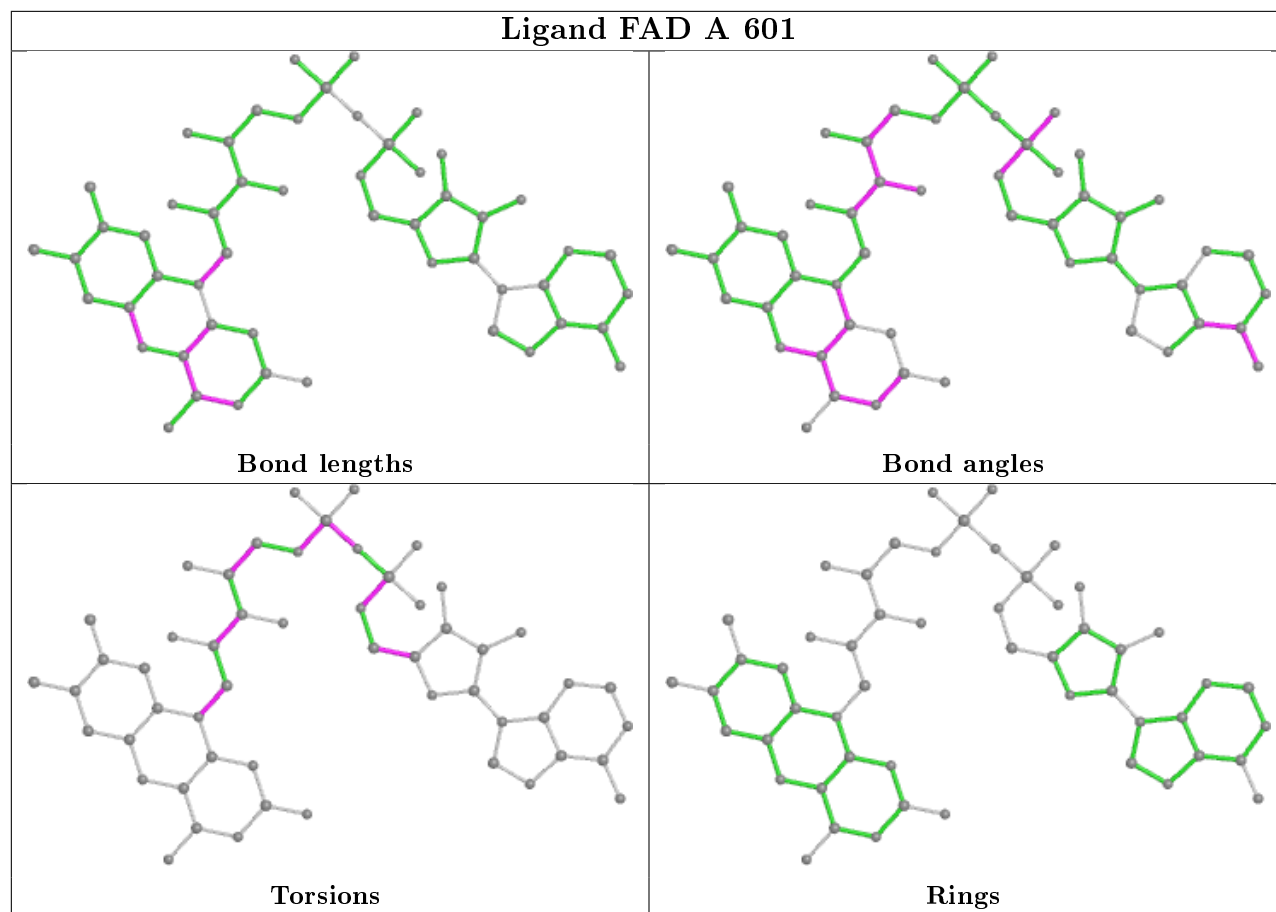


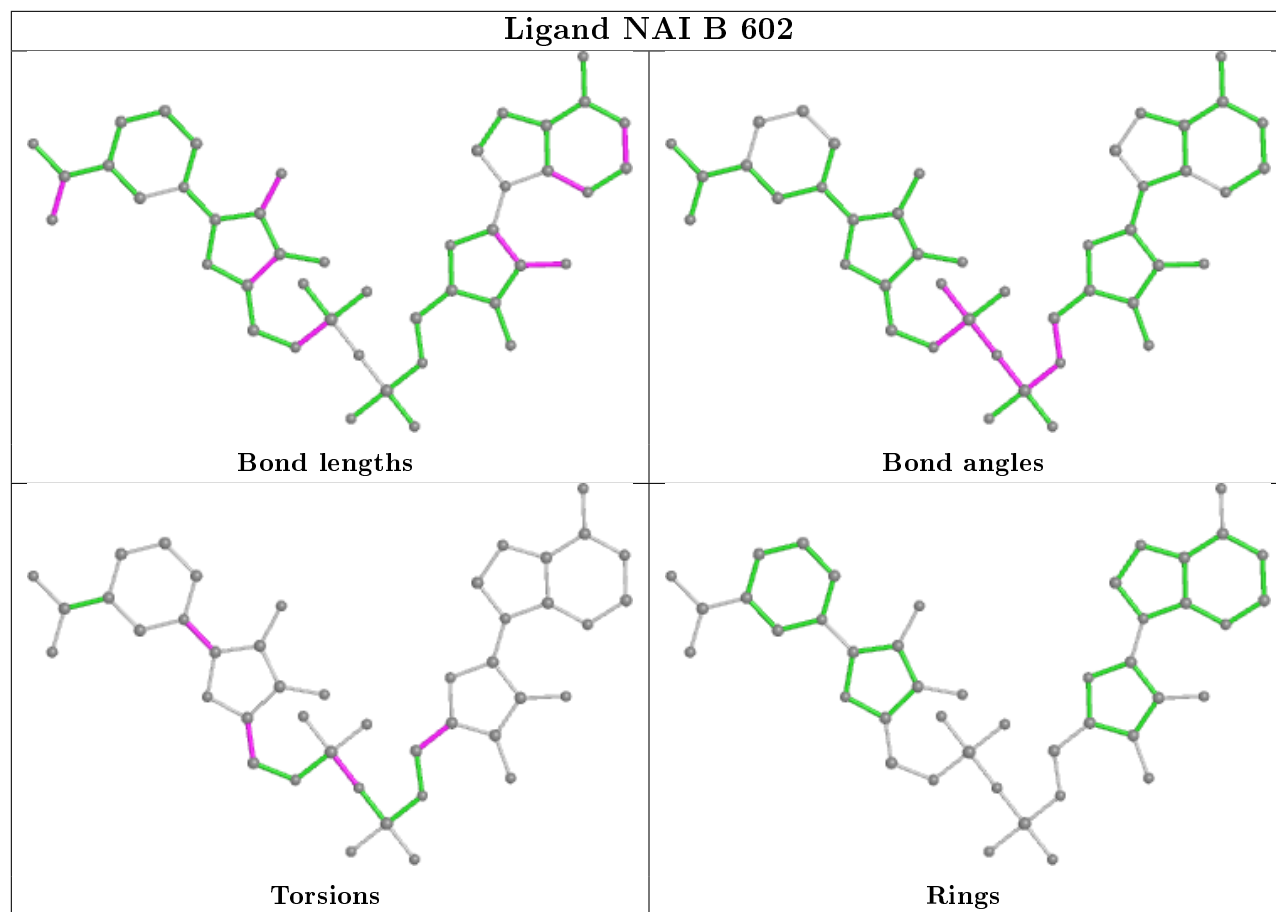
Torsions

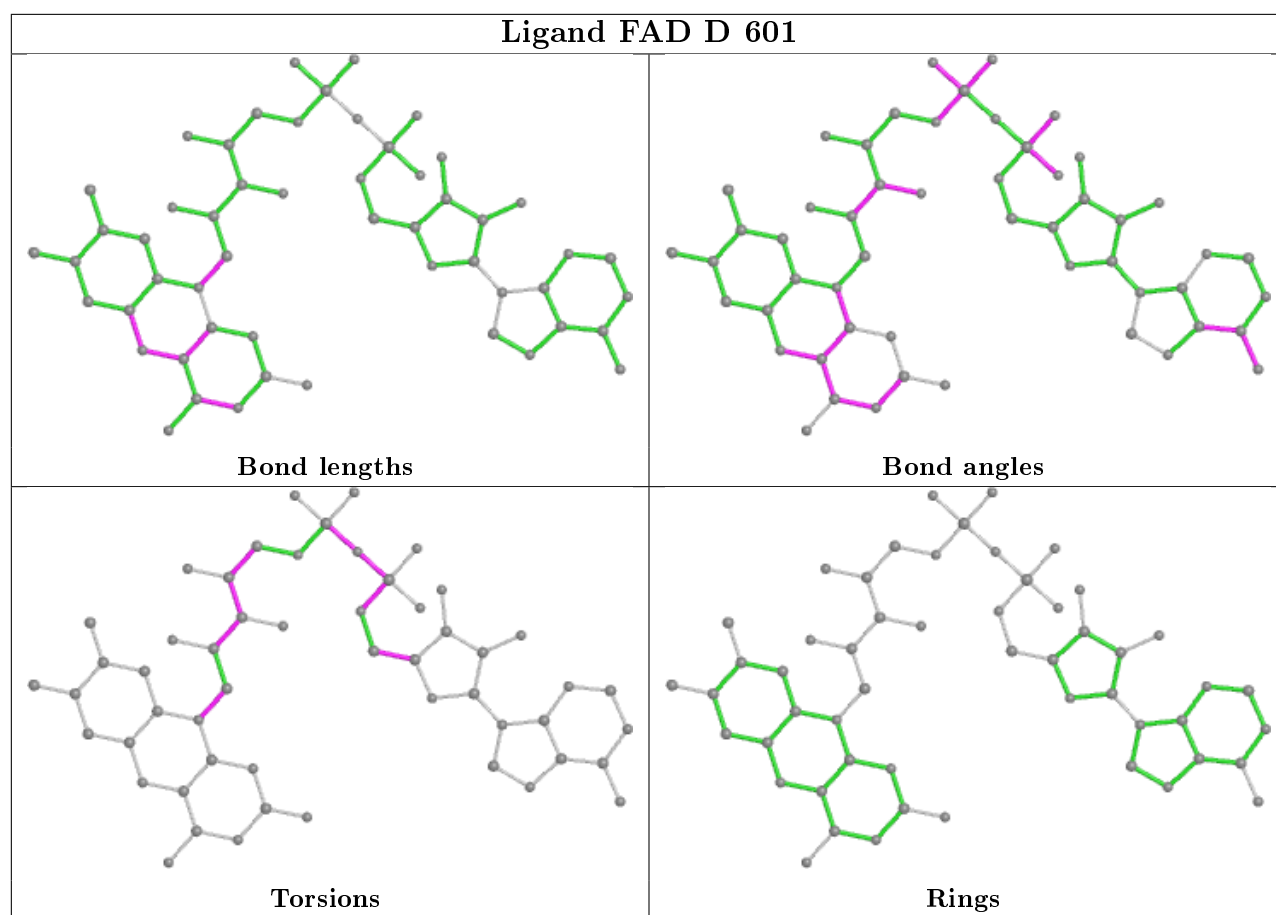


Rings









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	494/513 (96%)	0.28	3 (0%) 89 92	31, 49, 78, 108	0
1	B	494/513 (96%)	0.26	3 (0%) 89 92	33, 50, 81, 118	0
1	C	503/513 (98%)	0.42	14 (2%) 53 62	31, 56, 86, 106	0
1	D	504/513 (98%)	0.39	9 (1%) 68 76	30, 58, 90, 111	0
All	All	1995/2052 (97%)	0.34	29 (1%) 73 81	30, 53, 85, 118	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	HIS	4.5
1	B	184	ALA	3.6
1	C	273	PHE	3.6
1	C	265	LEU	2.8
1	D	236	PHE	2.8
1	C	64	VAL	2.8
1	C	236	PHE	2.8
1	C	65	ILE	2.6
1	D	259	THR	2.6
1	C	242	VAL	2.5
1	A	245	VAL	2.5
1	B	23	ALA	2.4
1	C	46	LEU	2.4
1	D	43	PRO	2.3
1	D	411	TYR	2.3
1	C	411	TYR	2.3
1	D	221	ILE	2.3
1	C	61	GLY	2.3
1	A	504	PHE	2.2
1	C	245	VAL	2.2
1	D	443	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	35	MET	2.2
1	D	242	VAL	2.2
1	A	307	PRO	2.1
1	D	222	TRP	2.1
1	C	442	ILE	2.1
1	D	254	LEU	2.1
1	C	58	TYR	2.1
1	C	225	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

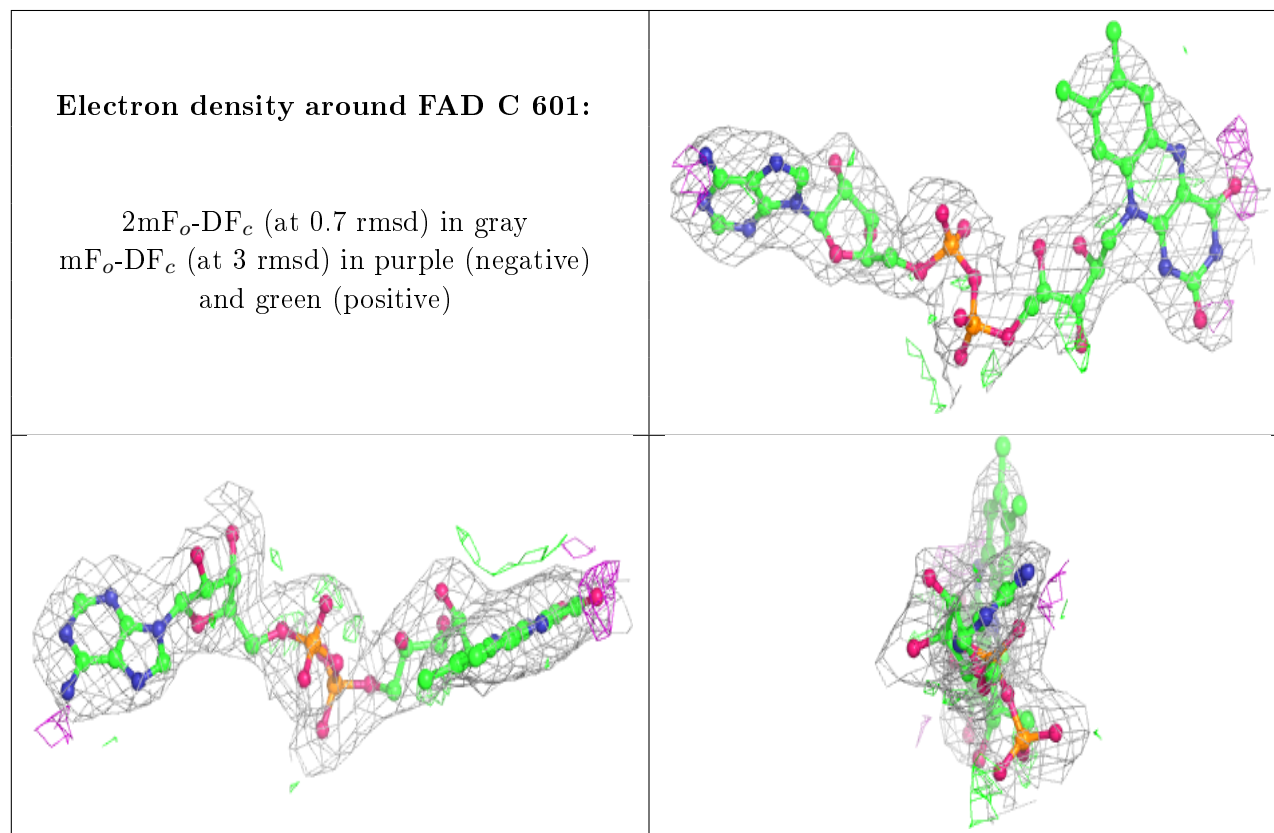
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	604	5/5	0.85	0.27	83,88,91,99	5
4	SO4	D	602	5/5	0.89	0.20	84,84,89,89	5
4	SO4	A	604	5/5	0.90	0.20	86,91,93,97	0
4	SO4	B	603	5/5	0.91	0.13	85,86,92,97	5
4	SO4	D	604	5/5	0.91	0.19	67,68,77,79	5
4	SO4	C	603	5/5	0.93	0.22	73,77,80,83	5
4	SO4	C	602	5/5	0.93	0.18	70,71,76,83	5
4	SO4	B	604	5/5	0.95	0.20	66,72,78,78	5
4	SO4	D	603	5/5	0.95	0.28	67,77,79,85	5
4	SO4	B	605	5/5	0.95	0.23	81,82,84,87	0
2	FAD	C	601	53/53	0.95	0.21	40,60,72,86	0
2	FAD	D	601	53/53	0.95	0.22	37,60,73,84	0
3	NAI	A	602	44/44	0.95	0.20	40,63,69,76	0
4	SO4	A	603	5/5	0.96	0.17	59,64,73,78	5
3	NAI	B	602	44/44	0.97	0.20	41,57,65,66	0

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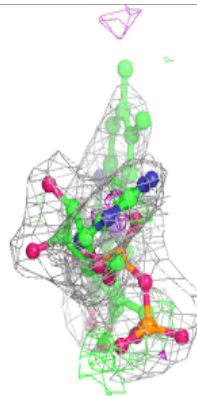
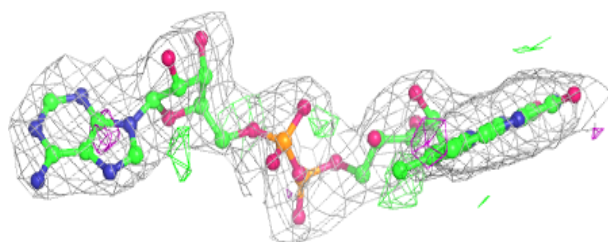
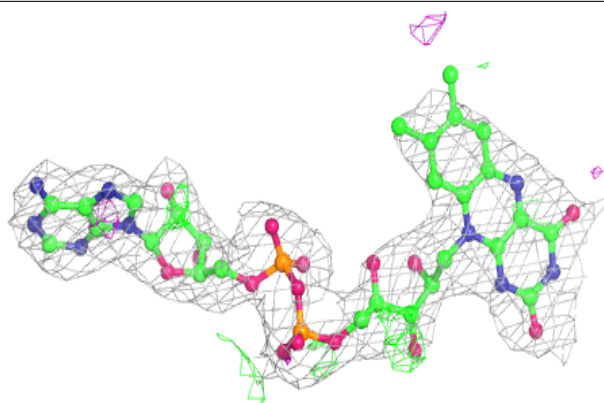
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	A	601	53/53	0.97	0.21	38,48,59,76	0
4	SO4	C	605	5/5	0.98	0.28	56,58,66,71	5
2	FAD	B	601	53/53	0.98	0.20	24,46,54,55	0
4	SO4	D	605	5/5	0.99	0.25	55,55,55,70	5

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.

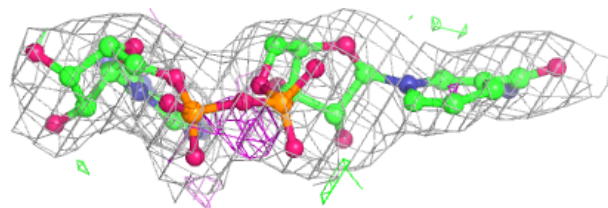
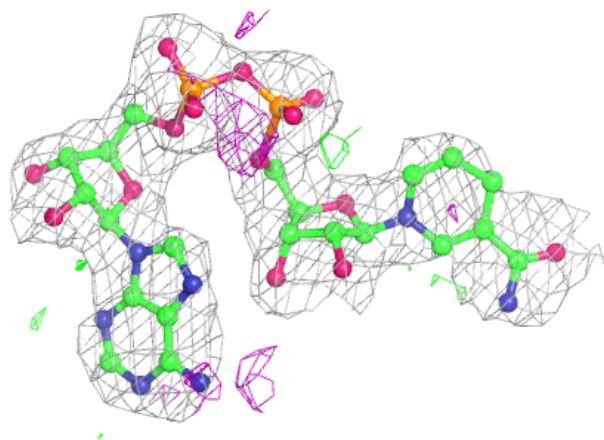


Electron density around FAD D 601:

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

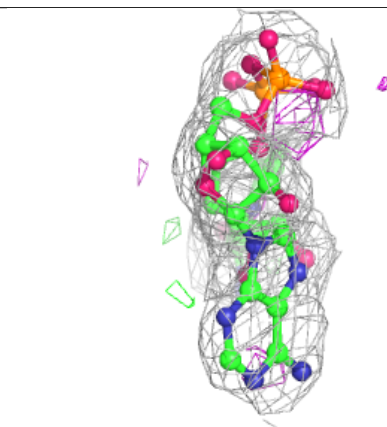
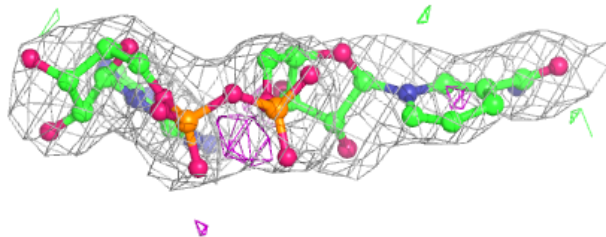
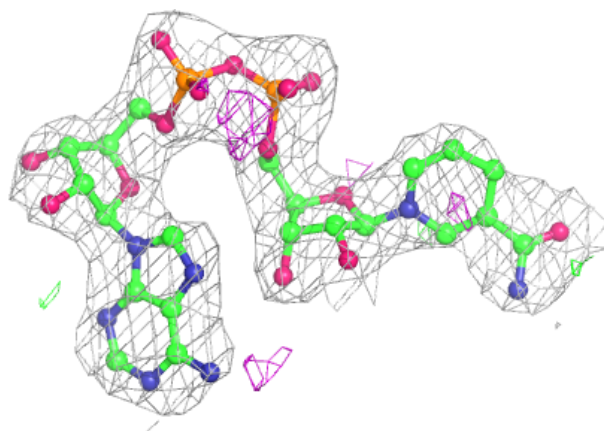
**Electron density around NAI A 602:**

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

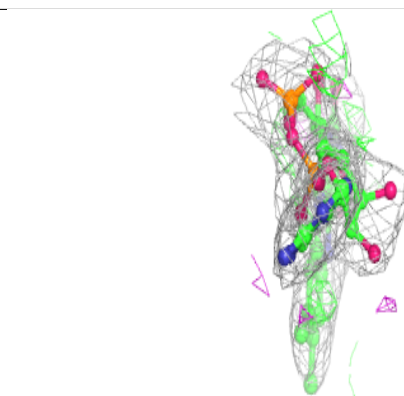
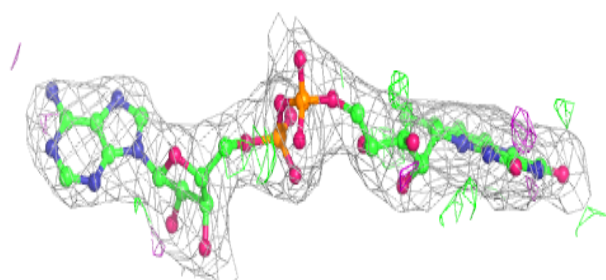
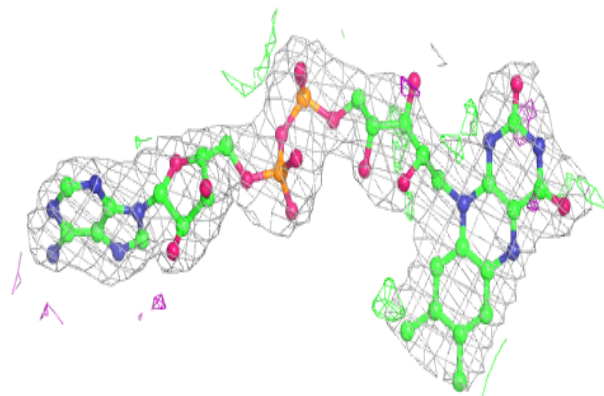


Electron density around NAI B 602:

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

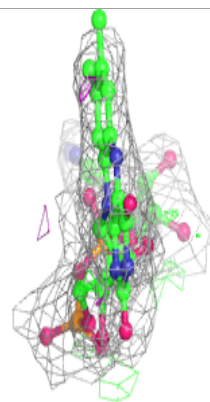
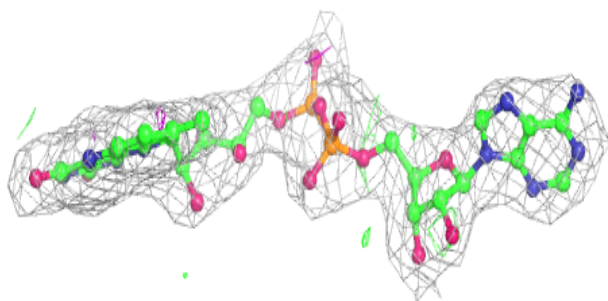
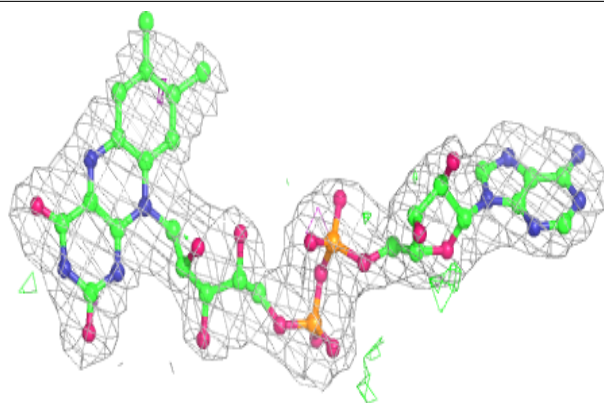
**Electron density around FAD A 601:**

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



Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.