



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:00 PM UTC

PDB ID : 5WED / pdb_00005wed
Title : Structure of bacterial type II NADH dehydrogenase from *Caldalkalibacillus thermarum* at 2.15Å resolution
Authors : Nakatani, Y.; Aragao, D.; Cook, G.M.
Deposited on : 2017-07-09
Resolution : 2.15 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

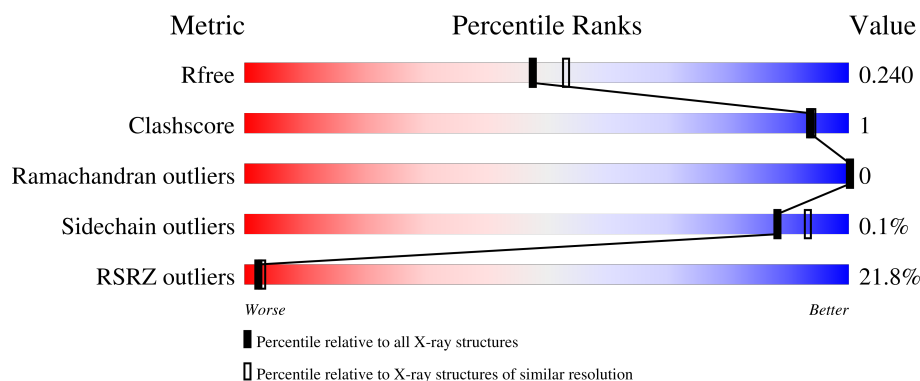
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	405	20% 94%
1	B	405	14% 93%
1	C	405	20% 94%
1	D	405	31% 95%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12435 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 FAD-dependent pyridine nucleotide-disulfide oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	394	Total	C	N	O	S	0	0	0
			2948	1882	509	549	8			
1	A	394	Total	C	N	O	S	0	0	0
			2946	1880	509	549	8			
1	C	394	Total	C	N	O	S	0	0	0
			2933	1876	496	552	9			
1	D	394	Total	C	N	O	S	0	0	0
			2894	1855	506	525	8			

There are 24 discrepancies between the modelled and reference sequences:

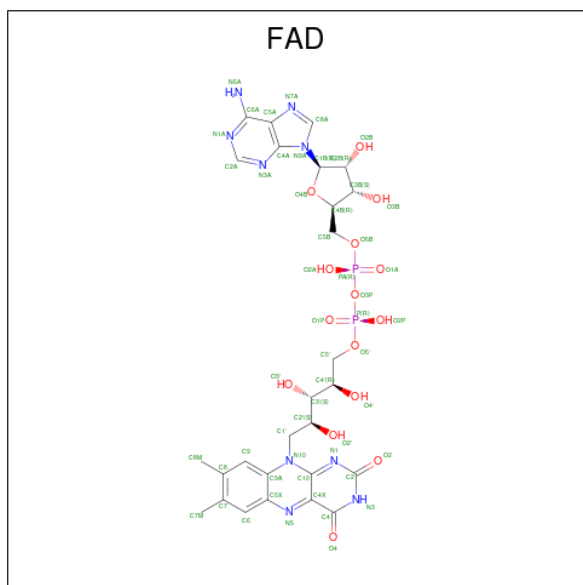
Chain	Residue	Modelled	Actual	Comment	Reference
B	400	HIS	-	expression tag	UNP F5L3B8
B	401	HIS	-	expression tag	UNP F5L3B8
B	402	HIS	-	expression tag	UNP F5L3B8
B	403	HIS	-	expression tag	UNP F5L3B8
B	404	HIS	-	expression tag	UNP F5L3B8
B	405	HIS	-	expression tag	UNP F5L3B8
A	400	HIS	-	expression tag	UNP F5L3B8
A	401	HIS	-	expression tag	UNP F5L3B8
A	402	HIS	-	expression tag	UNP F5L3B8
A	403	HIS	-	expression tag	UNP F5L3B8
A	404	HIS	-	expression tag	UNP F5L3B8
A	405	HIS	-	expression tag	UNP F5L3B8
C	400	HIS	-	expression tag	UNP F5L3B8
C	401	HIS	-	expression tag	UNP F5L3B8
C	402	HIS	-	expression tag	UNP F5L3B8
C	403	HIS	-	expression tag	UNP F5L3B8
C	404	HIS	-	expression tag	UNP F5L3B8
C	405	HIS	-	expression tag	UNP F5L3B8
D	400	HIS	-	expression tag	UNP F5L3B8
D	401	HIS	-	expression tag	UNP F5L3B8
D	402	HIS	-	expression tag	UNP F5L3B8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	403	HIS	-	expression tag	UNP F5L3B8
D	404	HIS	-	expression tag	UNP F5L3B8
D	405	HIS	-	expression tag	UNP F5L3B8

- 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	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

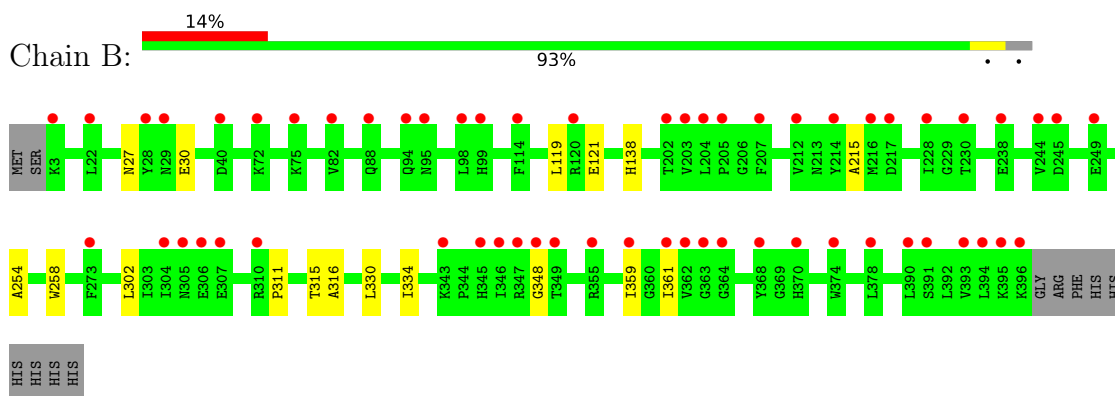
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	154	Total	O	0	0
			154	154		
3	A	122	Total	O	0	0
			122	122		
3	C	127	Total	O	0	0
			127	127		
3	D	99	Total	O	0	0
			99	99		

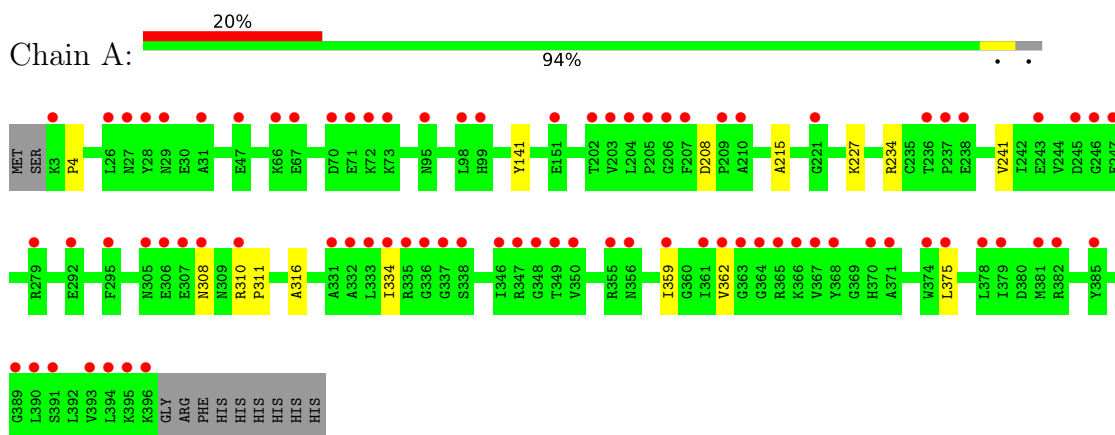
3 Residue-property plots

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.

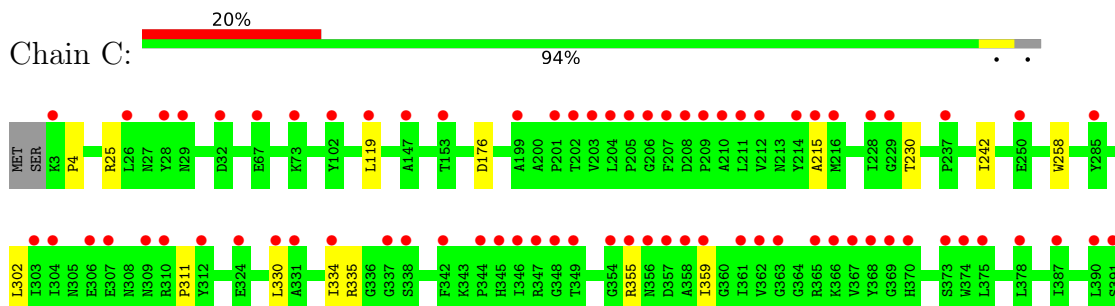
- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase

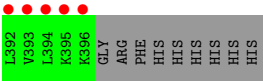


- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase

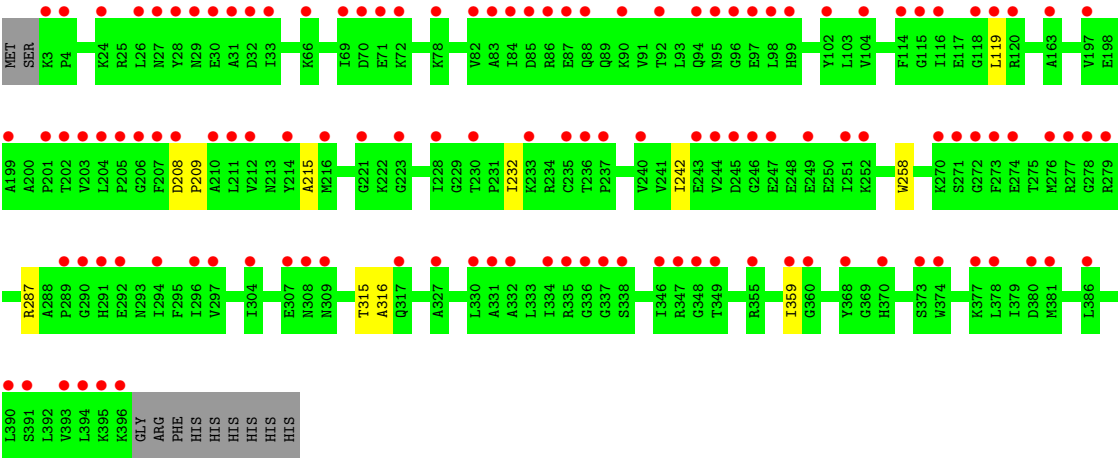
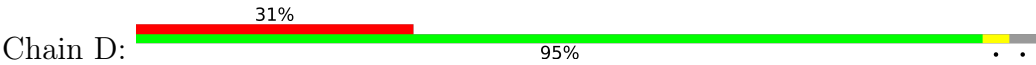


- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase





● Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.80Å 113.57Å 129.78Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	48.87 – 2.15 48.87 – 2.15	Depositor EDS
% Data completeness (in resolution range)	91.7 (48.87-2.15) 91.8 (48.87-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.238 0.213 , 0.240	Depositor DCC
R_{free} test set	5261 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12435	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: 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	0.30	0/3004	0.71	2/4088 (0.0%)
1	B	0.30	0/3005	0.73	0/4089
1	C	0.30	0/2989	0.72	0/4068
1	D	0.29	0/2952	0.72	0/4022
All	All	0.30	0/11950	0.72	2/16267 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASP	CA-C-N	5.04	125.06	119.32
1	A	208	ASP	C-N-CA	5.04	125.06	119.32

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	2946	0	2899	9	0
1	B	2948	0	2914	10	0
1	C	2933	0	2891	8	0
1	D	2894	0	2844	7	0
2	A	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	2	0
2	C	53	0	31	0	0
2	D	53	0	31	2	0
3	A	122	0	0	1	0
3	B	154	0	0	0	0
3	C	127	0	0	0	0
3	D	99	0	0	1	0
All	All	12435	0	11672	33	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 1.

All (33) 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:215:ALA:HB2	1:A:359:ILE:HD13	1.84	0.58
1:B:302:LEU:HD11	1:B:311:PRO:HB3	1.86	0.57
1:D:215:ALA:HB2	1:D:359:ILE:HD13	1.86	0.57
1:B:215:ALA:HB2	1:B:359:ILE:HD13	1.85	0.57
1:A:227:LYS:NZ	3:A:702:HOH:O	2.37	0.57
1:D:232:ILE:HD13	1:D:242:ILE:HG22	1.87	0.56
1:D:316:ALA:HB2	2:D:601:FAD:H2'	1.93	0.51
1:C:4:PRO:HG3	1:C:334:ILE:HD12	1.93	0.51
1:C:215:ALA:HB2	1:C:359:ILE:HD13	1.93	0.51
1:B:27:ASN:N	1:B:30:GLU:OE2	2.35	0.49
1:C:230:THR:HG21	1:C:242:ILE:HD12	1.94	0.48
1:C:330:LEU:O	1:C:334:ILE:HG12	2.13	0.48
1:A:234:ARG:HG2	1:A:241:VAL:HB	1.98	0.46
1:C:25:ARG:O	1:C:335:ARG:NH2	2.48	0.46
1:A:316:ALA:HB2	2:A:601:FAD:H2'	1.97	0.46
1:C:302:LEU:HD11	1:C:311:PRO:HB3	1.97	0.45
1:B:330:LEU:O	1:B:334:ILE:HG12	2.17	0.45
1:D:119:LEU:HD21	1:D:258:TRP:CE3	2.53	0.44
1:B:315:THR:HB	2:B:601:FAD:O2	2.17	0.44
1:C:176:ASP:OD2	1:C:355:ARG:N	2.42	0.44
1:B:316:ALA:HB2	2:B:601:FAD:H2'	1.99	0.44
1:B:119:LEU:HD21	1:B:258:TRP:CE3	2.52	0.43
1:A:4:PRO:HG3	1:A:334:ILE:HD12	1.99	0.43
1:A:310:ARG:HA	1:A:311:PRO:HD3	1.92	0.42
1:B:348:GLY:HA3	1:B:361:ILE:O	2.18	0.42
1:C:119:LEU:HD21	1:C:258:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:HG21	1:A:375:LEU:HD13	2.01	0.41
1:D:287:ARG:NH1	3:D:703:HOH:O	2.41	0.41
1:A:308:ASN:OD1	1:A:310:ARG:HG2	2.21	0.41
1:D:315:THR:HB	2:D:601:FAD:O2	2.20	0.41
1:B:138:HIS:HE1	1:B:254:ALA:O	2.04	0.41
1:D:208:ASP:HA	1:D:209:PRO:HD3	1.96	0.41
1:B:138:HIS:HD2	1:A:141:TYR:OH	2.04	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	392/405 (97%)	383 (98%)	9 (2%)	0	100	100
1	B	392/405 (97%)	382 (97%)	10 (3%)	0	100	100
1	C	392/405 (97%)	382 (97%)	10 (3%)	0	100	100
1	D	392/405 (97%)	384 (98%)	8 (2%)	0	100	100
All	All	1568/1620 (97%)	1531 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	297/329 (90%)	297 (100%)	0	100	100
1	B	298/329 (91%)	297 (100%)	1 (0%)	86	91
1	C	297/329 (90%)	297 (100%)	0	100	100
1	D	283/329 (86%)	283 (100%)	0	100	100
All	All	1175/1316 (89%)	1174 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	ASN
1	B	89	GLN
1	B	122	HIS
1	B	138	HIS
1	B	196	ASN
1	B	213	ASN
1	A	89	GLN
1	A	99	HIS
1	A	122	HIS
1	A	142	GLN
1	A	196	ASN
1	A	213	ASN
1	C	89	GLN
1	C	196	ASN
1	C	213	ASN
1	D	89	GLN
1	D	95	ASN
1	D	122	HIS
1	D	142	GLN
1	D	196	ASN
1	D	213	ASN
1	D	317	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 ⓘ

4 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$
2	FAD	D	601	-	58,58,58	2.81	20 (34%)	85,89,89	2.20	23 (27%)
2	FAD	C	601	-	58,58,58	2.81	20 (34%)	85,89,89	2.18	21 (24%)
2	FAD	A	601	-	58,58,58	2.81	20 (34%)	85,89,89	2.18	22 (25%)
2	FAD	B	601	-	58,58,58	2.79	18 (31%)	85,89,89	2.19	23 (27%)

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
2	FAD	D	601	-	-	2/34/50/50	0/6/6/6
2	FAD	C	601	-	-	6/34/50/50	0/6/6/6
2	FAD	A	601	-	-	2/34/50/50	0/6/6/6
2	FAD	B	601	-	-	2/34/50/50	0/6/6/6

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	O4B-C1B	8.20	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	O4B-C1B	8.08	1.60	1.42
2	A	601	FAD	O4B-C1B	8.07	1.60	1.42
2	D	601	FAD	O4B-C1B	8.06	1.60	1.42
2	D	601	FAD	C2B-C1B	-7.75	1.29	1.53
2	C	601	FAD	C2B-C1B	-7.74	1.29	1.53
2	A	601	FAD	C2B-C1B	-7.67	1.29	1.53
2	B	601	FAD	C2B-C1B	-7.62	1.29	1.53
2	D	601	FAD	O4B-C4B	-7.09	1.29	1.45
2	C	601	FAD	O4B-C4B	-7.02	1.29	1.45
2	A	601	FAD	O4B-C4B	-6.98	1.29	1.45
2	B	601	FAD	O4B-C4B	-6.95	1.29	1.45
2	C	601	FAD	C4X-N5	5.66	1.43	1.30
2	A	601	FAD	C4X-N5	5.66	1.43	1.30
2	D	601	FAD	C4X-N5	5.51	1.42	1.30
2	B	601	FAD	C4X-N5	5.48	1.42	1.30
2	A	601	FAD	C5X-N5	5.27	1.49	1.39
2	D	601	FAD	C5X-N5	5.09	1.48	1.39
2	C	601	FAD	C5X-N5	5.08	1.48	1.39
2	B	601	FAD	C5X-N5	5.07	1.48	1.39
2	C	601	FAD	C10-N1	5.03	1.43	1.33
2	B	601	FAD	C10-N1	4.99	1.43	1.33
2	D	601	FAD	C10-N1	4.98	1.43	1.33
2	A	601	FAD	C10-N1	4.96	1.43	1.33
2	A	601	FAD	C6A-N6A	4.65	1.46	1.34
2	B	601	FAD	C6A-N6A	4.63	1.46	1.34
2	D	601	FAD	C6A-N6A	4.58	1.45	1.34
2	C	601	FAD	C6A-N6A	4.57	1.45	1.34
2	D	601	FAD	C2-N1	4.57	1.47	1.36
2	B	601	FAD	C2-N1	4.53	1.46	1.36
2	C	601	FAD	C2-N1	4.52	1.46	1.36
2	A	601	FAD	C2-N1	4.42	1.46	1.36
2	B	601	FAD	O4-C4	-4.36	1.15	1.23
2	A	601	FAD	O4-C4	-4.35	1.15	1.23
2	D	601	FAD	O4-C4	-4.30	1.15	1.23
2	C	601	FAD	O4-C4	-4.30	1.15	1.23
2	B	601	FAD	O2B-C2B	4.23	1.53	1.43
2	A	601	FAD	O2B-C2B	4.18	1.53	1.43
2	D	601	FAD	O2B-C2B	4.17	1.53	1.43
2	C	601	FAD	O2B-C2B	4.16	1.53	1.43
2	D	601	FAD	C10-N10	3.74	1.45	1.37
2	A	601	FAD	C10-N10	3.74	1.45	1.37
2	C	601	FAD	C10-N10	3.70	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C10-N10	3.65	1.45	1.37
2	A	601	FAD	C2-N3	3.44	1.46	1.39
2	C	601	FAD	C2-N3	3.44	1.46	1.39
2	B	601	FAD	C2-N3	3.41	1.46	1.39
2	D	601	FAD	C2-N3	3.36	1.46	1.39
2	A	601	FAD	C8M-C8	3.35	1.57	1.51
2	C	601	FAD	C8M-C8	3.26	1.57	1.51
2	D	601	FAD	C8M-C8	3.23	1.57	1.51
2	B	601	FAD	C8M-C8	3.22	1.57	1.51
2	C	601	FAD	C7M-C7	2.95	1.56	1.51
2	A	601	FAD	C7M-C7	2.93	1.56	1.51
2	D	601	FAD	C7M-C7	2.90	1.56	1.51
2	B	601	FAD	C7M-C7	2.89	1.56	1.51
2	B	601	FAD	C9A-N10	2.84	1.46	1.41
2	D	601	FAD	C9A-N10	2.81	1.46	1.41
2	C	601	FAD	C9A-N10	2.81	1.46	1.41
2	D	601	FAD	O4'-C4'	-2.80	1.37	1.43
2	A	601	FAD	O4'-C4'	-2.73	1.37	1.43
2	B	601	FAD	O4'-C4'	-2.72	1.37	1.43
2	C	601	FAD	O4'-C4'	-2.69	1.37	1.43
2	A	601	FAD	C9A-N10	2.69	1.45	1.41
2	A	601	FAD	C8A-N7A	2.47	1.36	1.31
2	B	601	FAD	C8A-N7A	2.42	1.36	1.31
2	D	601	FAD	C8A-N7A	2.37	1.36	1.31
2	A	601	FAD	C4-N3	2.31	1.43	1.38
2	C	601	FAD	C4-N3	2.29	1.43	1.38
2	C	601	FAD	C8A-N7A	2.29	1.36	1.31
2	D	601	FAD	C4-N3	2.23	1.43	1.38
2	D	601	FAD	C5'-C4'	2.12	1.54	1.51
2	A	601	FAD	C5'-C4'	2.11	1.54	1.51
2	B	601	FAD	C4-N3	2.10	1.42	1.38
2	C	601	FAD	C5'-C4'	2.08	1.54	1.51
2	D	601	FAD	C2A-N1A	2.06	1.37	1.33
2	C	601	FAD	C2A-N1A	2.03	1.37	1.33
2	A	601	FAD	C2A-N1A	2.01	1.37	1.33

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C7M-C7-C6	-9.11	103.53	119.57
2	A	601	FAD	C7M-C7-C6	-9.05	103.63	119.57
2	D	601	FAD	C7M-C7-C6	-9.01	103.70	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C7M-C7-C6	-8.77	104.13	119.57
2	B	601	FAD	C7M-C7-C8	7.77	136.63	120.76
2	D	601	FAD	C7M-C7-C8	7.58	136.25	120.76
2	A	601	FAD	C7M-C7-C8	7.58	136.23	120.76
2	C	601	FAD	C7M-C7-C8	7.42	135.91	120.76
2	C	601	FAD	N3A-C2A-N1A	-5.80	119.81	128.58
2	A	601	FAD	N3A-C2A-N1A	-5.62	120.07	128.58
2	B	601	FAD	N3A-C2A-N1A	-5.61	120.09	128.58
2	D	601	FAD	N3A-C2A-N1A	-5.60	120.11	128.58
2	B	601	FAD	N6A-C6A-N1A	-5.39	106.38	118.38
2	D	601	FAD	N6A-C6A-N1A	-5.29	106.59	118.38
2	A	601	FAD	N6A-C6A-N1A	-5.26	106.67	118.38
2	C	601	FAD	N6A-C6A-N1A	-5.18	106.83	118.38
2	A	601	FAD	C5A-C4A-N3A	-4.95	119.90	126.72
2	B	601	FAD	C5A-C4A-N3A	-4.92	119.94	126.72
2	C	601	FAD	C5A-C4A-N3A	-4.71	120.23	126.72
2	D	601	FAD	C5A-C4A-N3A	-4.68	120.27	126.72
2	D	601	FAD	N9A-C8A-N7A	-4.27	107.88	113.94
2	B	601	FAD	C5A-C6A-N6A	4.22	133.74	123.29
2	C	601	FAD	N9A-C8A-N7A	-4.22	107.95	113.94
2	D	601	FAD	C5A-C6A-N6A	4.13	133.51	123.29
2	A	601	FAD	C5A-C6A-N6A	4.08	133.38	123.29
2	A	601	FAD	N9A-C8A-N7A	-4.07	108.16	113.94
2	C	601	FAD	C5A-C6A-N6A	4.04	133.28	123.29
2	B	601	FAD	N9A-C8A-N7A	-3.92	108.38	113.94
2	A	601	FAD	C2A-N3A-C4A	3.35	120.02	111.83
2	B	601	FAD	C2A-N3A-C4A	3.34	119.98	111.83
2	C	601	FAD	C2A-N3A-C4A	3.32	119.94	111.83
2	D	601	FAD	C4-N3-C2	-3.27	119.83	125.64
2	C	601	FAD	C4-N3-C2	-3.27	119.84	125.64
2	C	601	FAD	C8M-C8-C9	3.25	125.30	119.57
2	D	601	FAD	C8M-C8-C9	3.23	125.26	119.57
2	B	601	FAD	C4-N3-C2	-3.22	119.93	125.64
2	D	601	FAD	C2A-N3A-C4A	3.21	119.68	111.83
2	A	601	FAD	C4-N3-C2	-3.20	119.96	125.64
2	C	601	FAD	C8M-C8-C7	-3.13	114.37	120.76
2	D	601	FAD	C8M-C8-C7	-3.11	114.41	120.76
2	C	601	FAD	C4'-C3'-C2'	-3.00	108.58	113.57
2	B	601	FAD	C8M-C8-C9	2.97	124.81	119.57
2	A	601	FAD	N3A-C4A-N9A	2.96	132.21	127.17
2	C	601	FAD	N3A-C4A-N9A	2.89	132.09	127.17
2	D	601	FAD	N3A-C4A-N9A	2.89	132.08	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C8M-C8-C7	-2.89	114.87	120.76
2	B	601	FAD	C4'-C3'-C2'	-2.88	108.77	113.57
2	A	601	FAD	C8M-C8-C9	2.88	124.65	119.57
2	B	601	FAD	N3A-C4A-N9A	2.85	132.01	127.17
2	D	601	FAD	C5A-N7A-C8A	2.76	107.79	103.45
2	C	601	FAD	C5A-N7A-C8A	2.72	107.72	103.45
2	A	601	FAD	C8M-C8-C7	-2.71	115.22	120.76
2	A	601	FAD	C5A-N7A-C8A	2.69	107.68	103.45
2	C	601	FAD	C5X-C9A-N10	2.67	120.38	117.97
2	B	601	FAD	C5A-N7A-C8A	2.66	107.62	103.45
2	A	601	FAD	C4'-C3'-C2'	-2.65	109.17	113.57
2	A	601	FAD	C9A-C5X-N5	-2.58	119.72	122.45
2	A	601	FAD	C5X-C9A-N10	2.56	120.28	117.97
2	D	601	FAD	C4A-N9A-C8A	2.53	108.39	105.74
2	C	601	FAD	C4X-C4-N3	2.51	119.64	113.25
2	C	601	FAD	C9A-C5X-N5	-2.50	119.80	122.45
2	B	601	FAD	C5X-C9A-N10	2.48	120.21	117.97
2	A	601	FAD	C4X-C4-N3	2.48	119.56	113.25
2	D	601	FAD	C5X-C9A-N10	2.46	120.19	117.97
2	D	601	FAD	C4'-C3'-C2'	-2.45	109.49	113.57
2	B	601	FAD	C4X-C4-N3	2.44	119.48	113.25
2	D	601	FAD	C4X-C4-N3	2.44	119.47	113.25
2	C	601	FAD	C4A-N9A-C8A	2.44	108.30	105.74
2	D	601	FAD	C9A-C5X-N5	-2.43	119.87	122.45
2	A	601	FAD	C10-C4X-N5	-2.42	119.86	124.81
2	C	601	FAD	O4-C4-C4X	-2.42	120.15	126.53
2	B	601	FAD	C9A-C5X-N5	-2.41	119.90	122.45
2	A	601	FAD	C4X-C10-N10	2.40	119.92	116.48
2	D	601	FAD	O4-C4-C4X	-2.40	120.19	126.53
2	B	601	FAD	O4-C4-C4X	-2.39	120.23	126.53
2	A	601	FAD	O4-C4-C4X	-2.38	120.25	126.53
2	C	601	FAD	C4X-C10-N10	2.37	119.87	116.48
2	C	601	FAD	C10-C4X-N5	-2.35	120.00	124.81
2	D	601	FAD	C10-C4X-N5	-2.35	120.01	124.81
2	B	601	FAD	C4X-C10-N10	2.33	119.81	116.48
2	B	601	FAD	C10-C4X-N5	-2.32	120.08	124.81
2	D	601	FAD	C4X-C10-N10	2.31	119.79	116.48
2	A	601	FAD	C4A-N9A-C8A	2.13	107.97	105.74
2	D	601	FAD	C3B-C2B-C1B	2.12	105.48	101.46
2	B	601	FAD	C4A-C5A-N7A	-2.09	108.20	110.58
2	A	601	FAD	C6A-C5A-C4A	2.05	119.98	117.18
2	B	601	FAD	C5A-C4A-N9A	2.05	108.05	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C6A-C5A-C4A	2.03	119.95	117.18
2	D	601	FAD	C4A-C5A-N7A	-2.00	108.29	110.58

There are no chirality outliers.

All (12) torsion outliers are listed below:

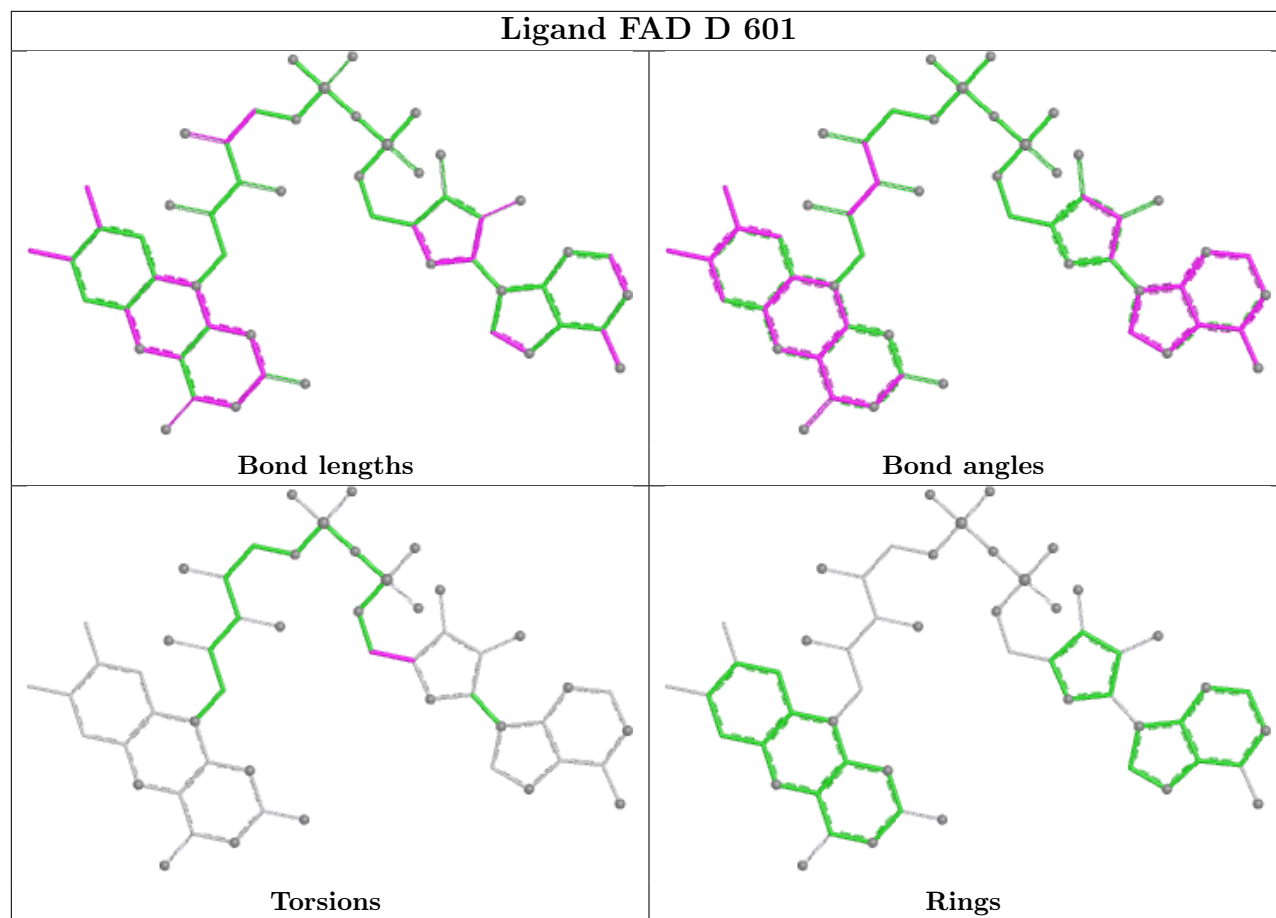
Mol	Chain	Res	Type	Atoms
2	D	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	C2'-C3'-C4'-O4'
2	C	601	FAD	O3'-C3'-C4'-C5'
2	C	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	C2'-C3'-C4'-C5'

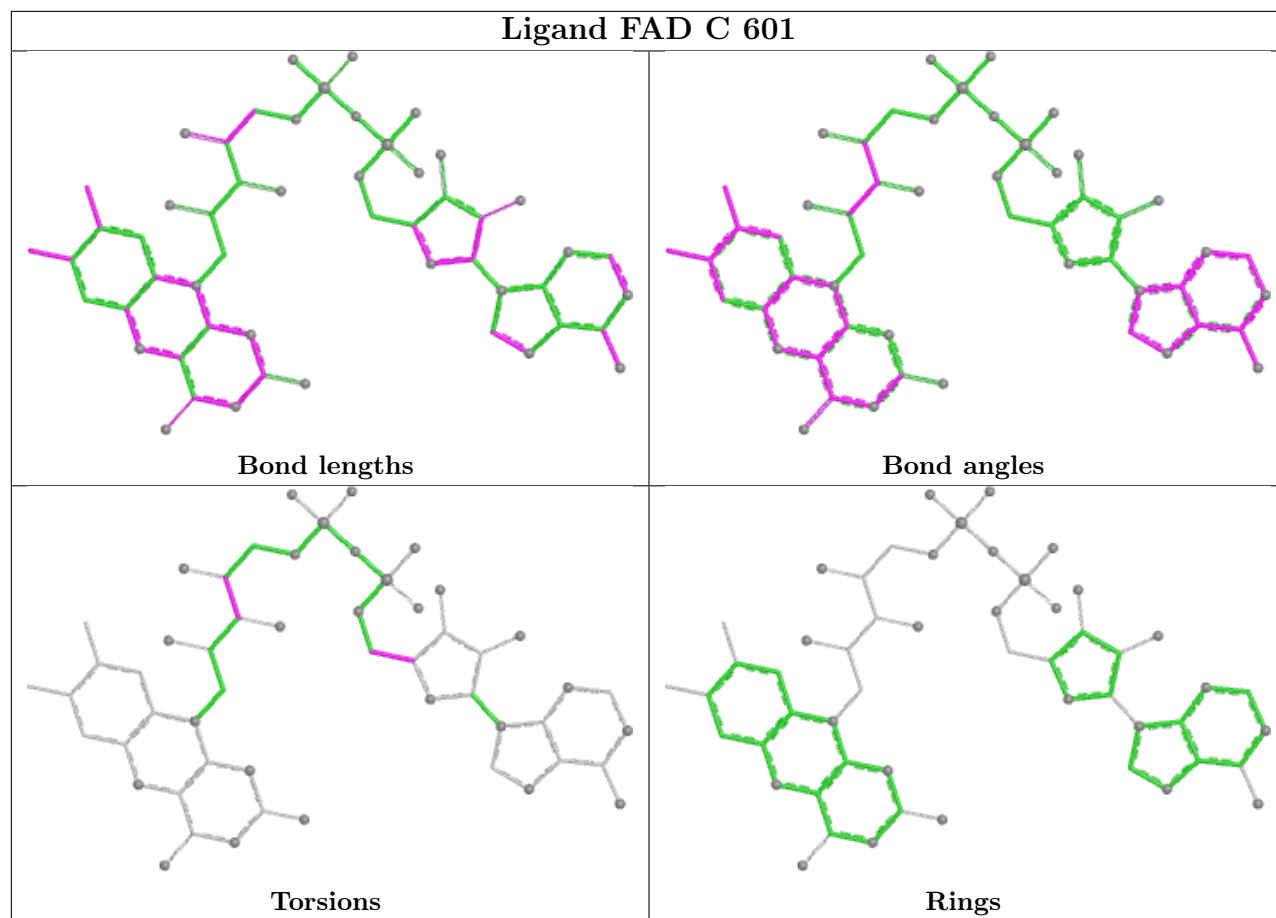
There are no ring outliers.

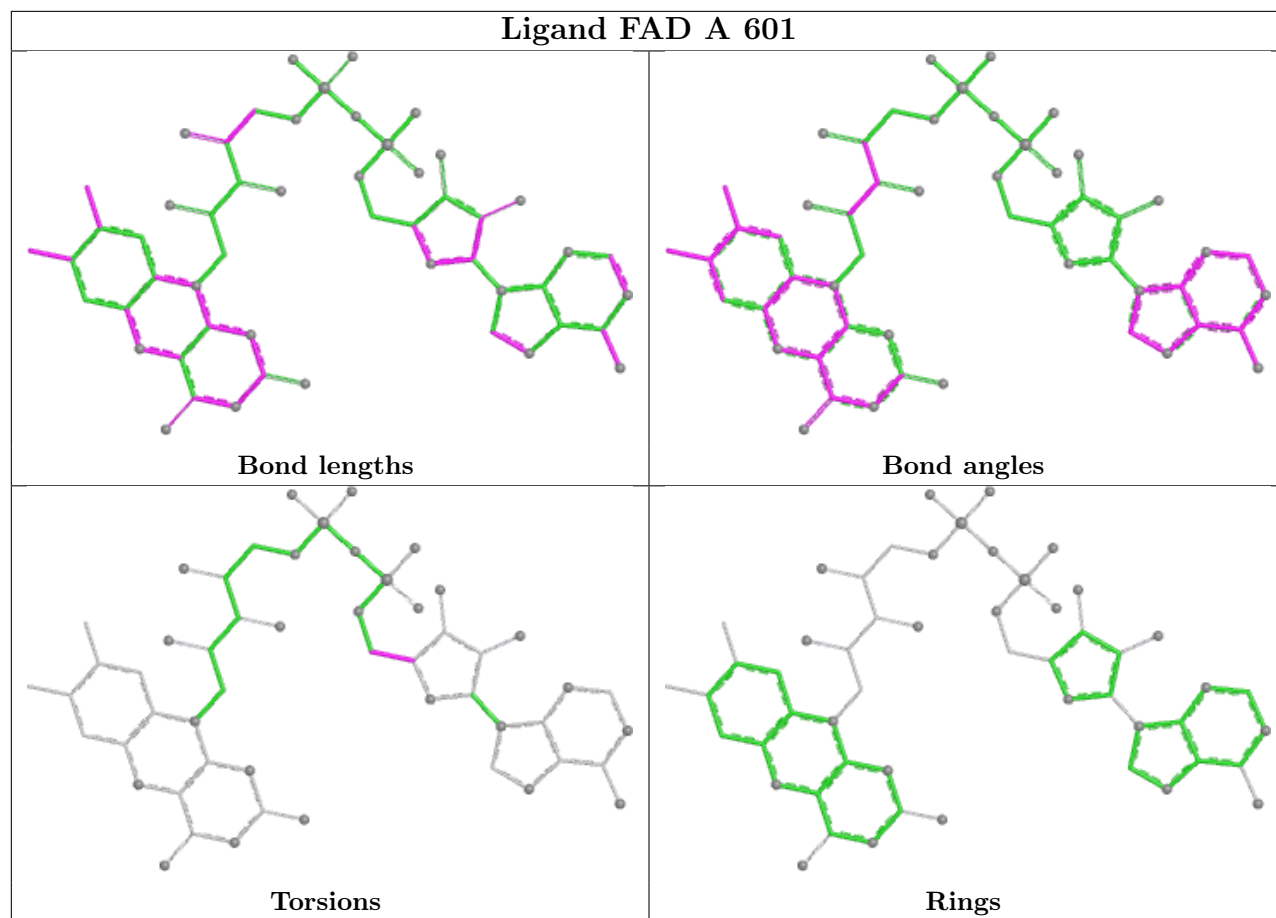
3 monomers are involved in 5 short contacts:

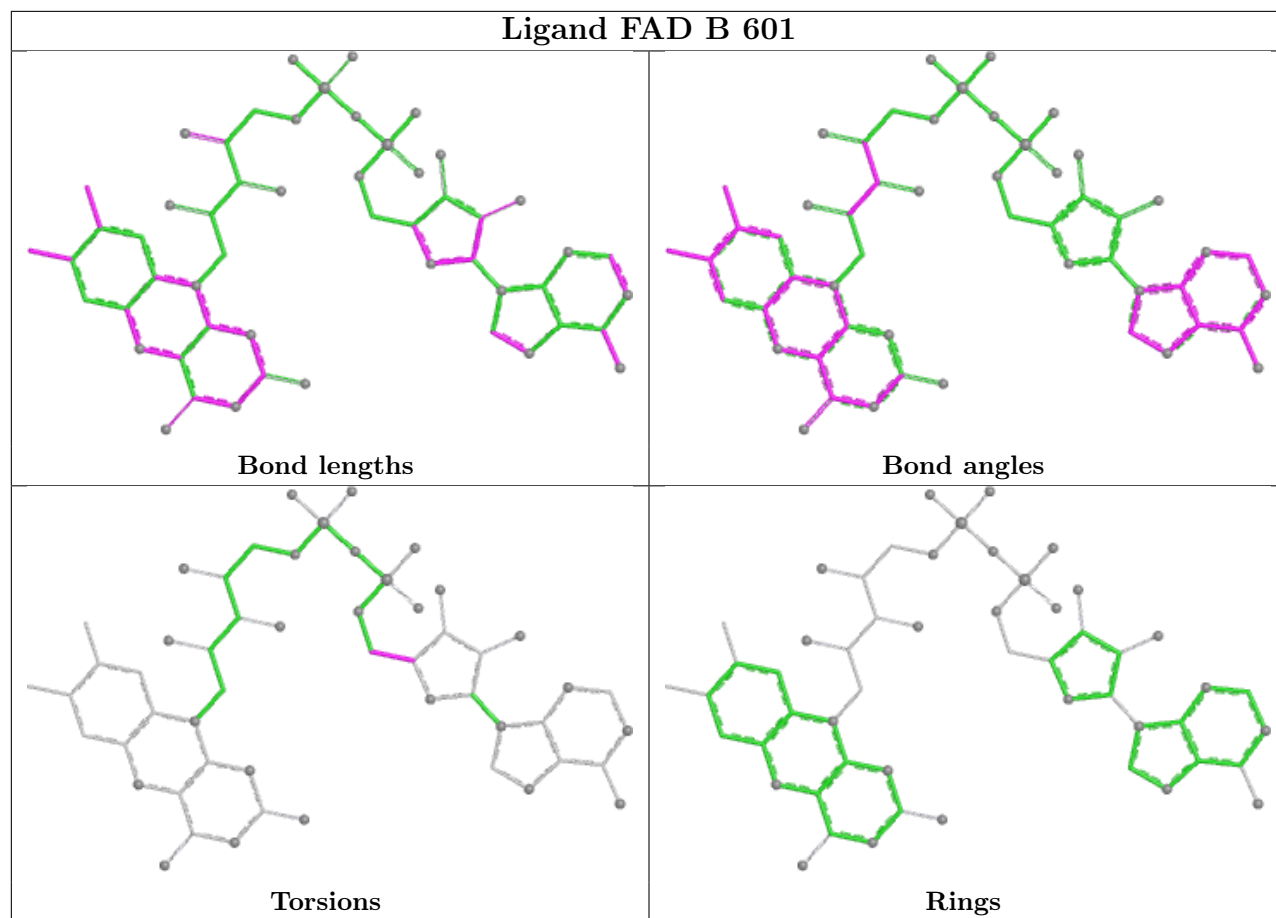
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	FAD	2	0
2	A	601	FAD	1	0
2	B	601	FAD	2	0

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









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	394/405 (97%)	1.27	81 (20%) 2 3	29, 51, 83, 114	0
1	B	394/405 (97%)	1.02	58 (14%) 6 6	29, 47, 79, 97	0
1	C	394/405 (97%)	1.20	79 (20%) 3 3	33, 50, 84, 112	0
1	D	394/405 (97%)	1.62	125 (31%) 1 1	34, 57, 92, 113	0
All	All	1576/1620 (97%)	1.28	343 (21%) 2 3	29, 51, 86, 114	0

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	TYR	7.7
1	D	346	ILE	7.6
1	C	28	TYR	7.4
1	D	205	PRO	7.1
1	C	365	ARG	6.7
1	B	205	PRO	6.7
1	A	29	ASN	6.3
1	A	374	TRP	6.0
1	A	207	PHE	5.9
1	A	394	LEU	5.6
1	B	3	LYS	5.6
1	B	368	TYR	5.1
1	B	363	GLY	5.1
1	B	207	PHE	5.1
1	D	3	LYS	5.0
1	D	334	ILE	5.0
1	D	85	ASP	5.0
1	A	307	GLU	4.9
1	C	348	GLY	4.9
1	D	27	ASN	4.9
1	B	204	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	204	LEU	4.8
1	D	336	GLY	4.8
1	D	396	LYS	4.7
1	A	348	GLY	4.7
1	C	374	TRP	4.7
1	B	349	THR	4.6
1	D	28	TYR	4.6
1	A	337	GLY	4.6
1	D	204	LEU	4.6
1	C	355	ARG	4.6
1	D	368	TYR	4.6
1	D	370	HIS	4.6
1	D	202	THR	4.5
1	B	396	LYS	4.5
1	A	203	VAL	4.5
1	D	394	LEU	4.5
1	A	361	ILE	4.4
1	A	390	LEU	4.4
1	C	396	LYS	4.4
1	C	394	LEU	4.3
1	D	203	VAL	4.3
1	D	207	PHE	4.3
1	C	346	ILE	4.3
1	D	247	GLU	4.3
1	A	371	ALA	4.2
1	C	206	GLY	4.2
1	A	202	THR	4.2
1	C	207	PHE	4.2
1	D	359	ILE	4.2
1	A	368	TYR	4.2
1	B	374	TRP	4.2
1	D	290	GLY	4.2
1	D	276	MET	4.2
1	B	203	VAL	4.2
1	D	244	VAL	4.2
1	C	29	ASN	4.1
1	A	206	GLY	4.1
1	C	208	ASP	4.1
1	D	88	GLN	4.1
1	D	245	ASP	4.0
1	D	97	GLU	4.0
1	A	347	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	228	ILE	4.0
1	B	346	ILE	3.9
1	B	348	GLY	3.9
1	A	27	ASN	3.9
1	D	374	TRP	3.8
1	D	84	ILE	3.8
1	A	3	LYS	3.8
1	D	29	ASN	3.8
1	C	347	ARG	3.8
1	D	292	GLU	3.8
1	D	332	ALA	3.8
1	B	202	THR	3.8
1	D	32	ASP	3.8
1	A	335	ARG	3.8
1	D	289	PRO	3.7
1	D	277	ARG	3.7
1	D	114	PHE	3.7
1	D	69	ILE	3.7
1	A	99	HIS	3.6
1	C	307	GLU	3.6
1	D	206	GLY	3.6
1	D	92	THR	3.6
1	C	324	GLU	3.6
1	A	245	ASP	3.5
1	B	394	LEU	3.5
1	A	375	LEU	3.5
1	D	271	SER	3.5
1	A	362	VAL	3.5
1	C	362	VAL	3.5
1	B	120	ARG	3.5
1	A	205	PRO	3.4
1	D	390	LEU	3.4
1	C	356	ASN	3.4
1	D	201	PRO	3.4
1	A	378	LEU	3.4
1	C	359	ILE	3.4
1	C	395	LYS	3.4
1	B	359	ILE	3.4
1	C	392	LEU	3.4
1	B	345	HIS	3.3
1	B	362	VAL	3.3
1	B	364	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	391	SER	3.3
1	A	366	LYS	3.3
1	B	304	ILE	3.3
1	A	247	GLU	3.3
1	D	381	MET	3.3
1	A	338	SER	3.3
1	A	349	THR	3.2
1	D	243	GLU	3.2
1	B	40	ASP	3.2
1	C	330	LEU	3.2
1	D	94	GLN	3.2
1	B	370	HIS	3.2
1	C	205	PRO	3.2
1	A	308	ASN	3.2
1	A	385	TYR	3.2
1	A	306	GLU	3.2
1	D	118	GLY	3.2
1	D	237	PRO	3.2
1	D	72	LYS	3.2
1	D	331	ALA	3.1
1	B	390	LEU	3.1
1	C	310	ARG	3.1
1	D	86	ARG	3.1
1	D	119	LEU	3.1
1	A	379	ILE	3.1
1	D	71	GLU	3.1
1	D	83	ALA	3.1
1	D	24	LYS	3.1
1	A	356	ASN	3.0
1	B	245	ASP	3.0
1	D	99	HIS	3.0
1	D	330	LEU	3.0
1	C	363	GLY	3.0
1	D	274	GLU	3.0
1	A	31	ALA	3.0
1	D	279	ARG	2.9
1	D	31	ALA	2.9
1	D	327	ALA	2.9
1	A	305	ASN	2.9
1	C	26	LEU	2.9
1	A	151	GLU	2.9
1	A	238	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	95	ASN	2.9
1	B	378	LEU	2.9
1	A	396	LYS	2.9
1	C	361	ILE	2.9
1	C	331	ALA	2.9
1	B	217	ASP	2.9
1	A	367	VAL	2.9
1	C	334	ILE	2.9
1	D	236	THR	2.9
1	C	391	SER	2.9
1	D	70	ASP	2.8
1	D	96	GLY	2.9
1	D	347	ARG	2.8
1	C	338	SER	2.8
1	A	364	GLY	2.8
1	A	350	VAL	2.8
1	A	334	ILE	2.8
1	D	360	GLY	2.8
1	C	202	THR	2.8
1	C	345	HIS	2.8
1	D	273	PHE	2.8
1	B	75	LYS	2.8
1	D	349	THR	2.8
1	C	303	ILE	2.8
1	B	249	GLU	2.7
1	A	389	GLY	2.7
1	A	210	ALA	2.7
1	C	368	TYR	2.7
1	A	236	THR	2.7
1	A	279	ARG	2.7
1	A	382	ARG	2.7
1	C	393	VAL	2.7
1	B	216	MET	2.7
1	A	336	GLY	2.7
1	A	98	LEU	2.7
1	C	209	PRO	2.7
1	B	29	ASN	2.7
1	B	244	VAL	2.7
1	D	212	VAL	2.7
1	D	208	ASP	2.7
1	D	115	GLY	2.7
1	A	47	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	358	ALA	2.6
1	A	26	LEU	2.6
1	C	119	LEU	2.6
1	D	373	SER	2.6
1	D	377	LYS	2.6
1	B	395	LYS	2.6
1	C	285	TYR	2.6
1	C	203	VAL	2.6
1	C	304	ILE	2.6
1	C	354	GLY	2.6
1	A	71	GLU	2.6
1	A	370	HIS	2.6
1	C	349	THR	2.6
1	D	120	ARG	2.6
1	D	338	SER	2.6
1	D	391	SER	2.6
1	C	214	TYR	2.6
1	D	116	ILE	2.6
1	A	221	GLY	2.6
1	D	272	GLY	2.6
1	C	3	LYS	2.6
1	B	355	ARG	2.6
1	C	201	PRO	2.6
1	C	378	LEU	2.6
1	A	66	LYS	2.5
1	C	309	ASN	2.5
1	C	366	LYS	2.5
1	D	355	ARG	2.5
1	D	98	LEU	2.5
1	A	67	GLU	2.5
1	A	292	GLU	2.5
1	D	249	GLU	2.5
1	B	82	VAL	2.5
1	A	346	ILE	2.5
1	D	251	ILE	2.5
1	D	348	GLY	2.5
1	D	393	VAL	2.5
1	B	343	LYS	2.5
1	A	72	LYS	2.5
1	C	312	TYR	2.5
1	C	306	GLU	2.5
1	D	210	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	363	GLY	2.5
1	D	233	LYS	2.5
1	B	310	ARG	2.5
1	A	243	GLU	2.5
1	B	347	ARG	2.5
1	B	228	ILE	2.5
1	D	30	GLU	2.4
1	B	214	TYR	2.4
1	C	102	TYR	2.4
1	C	237	PRO	2.4
1	A	332	ALA	2.4
1	C	147	ALA	2.4
1	D	163	ALA	2.4
1	D	378	LEU	2.4
1	C	370	HIS	2.4
1	D	291	HIS	2.4
1	B	94	GLN	2.4
1	B	307	GLU	2.4
1	C	387	ILE	2.4
1	C	344	PRO	2.4
1	A	310	ARG	2.4
1	D	246	GLY	2.4
1	D	380	ASP	2.4
1	C	367	VAL	2.4
1	A	391	SER	2.4
1	D	335	ARG	2.4
1	B	98	LEU	2.4
1	D	211	LEU	2.4
1	A	359	ILE	2.4
1	C	216	MET	2.4
1	D	82	VAL	2.4
1	D	66	LYS	2.4
1	C	153	THR	2.4
1	D	214	TYR	2.3
1	C	204	LEU	2.3
1	D	309	ASN	2.3
1	D	221	GLY	2.3
1	A	365	ARG	2.3
1	D	297	VAL	2.3
1	D	230	THR	2.3
1	B	238	GLU	2.3
1	B	306	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	199	ALA	2.3
1	D	26	LEU	2.3
1	A	70	ASP	2.3
1	D	104	VAL	2.3
1	D	308	ASN	2.3
1	A	331	ALA	2.3
1	D	278	GLY	2.3
1	C	73	LYS	2.3
1	B	99	HIS	2.3
1	B	88	GLN	2.3
1	A	355	ARG	2.3
1	D	235	CYS	2.3
1	D	78	LYS	2.3
1	C	373	SER	2.2
1	B	273	PHE	2.2
1	D	294	ILE	2.2
1	D	296	ILE	2.2
1	B	393	VAL	2.2
1	D	252	LYS	2.2
1	D	223	GLY	2.2
1	C	211	LEU	2.2
1	D	386	LEU	2.2
1	D	87	GLU	2.2
1	D	102	TYR	2.2
1	B	72	LYS	2.2
1	B	95	ASN	2.2
1	B	361	ILE	2.2
1	A	237	PRO	2.2
1	D	304	ILE	2.2
1	C	357	ASP	2.2
1	D	216	MET	2.2
1	A	246	GLY	2.2
1	C	369	GLY	2.2
1	A	333	LEU	2.2
1	C	390	LEU	2.2
1	B	28	TYR	2.2
1	B	230	THR	2.2
1	B	212	VAL	2.2
1	C	212	VAL	2.2
1	D	337	GLY	2.2
1	B	305	ASN	2.2
1	C	32	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	33	ILE	2.1
1	C	210	ALA	2.1
1	C	215	ALA	2.1
1	D	395	LYS	2.1
1	D	95	ASN	2.1
1	D	307	GLU	2.1
1	C	228	ILE	2.1
1	C	375	LEU	2.1
1	C	67	GLU	2.1
1	A	393	VAL	2.1
1	A	395	LYS	2.1
1	D	199	ALA	2.1
1	A	381	MET	2.1
1	C	250	GLU	2.1
1	A	73	LYS	2.1
1	D	270	LYS	2.1
1	B	114	PHE	2.1
1	C	342	PHE	2.1
1	B	22	LEU	2.0
1	A	209	PRO	2.0
1	D	90	LYS	2.0
1	A	295	PHE	2.0
1	D	197	VAL	2.0
1	D	240	VAL	2.0
1	D	317	GLN	2.0
1	D	4	PRO	2.0
1	C	229	GLY	2.0
1	C	337	GLY	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,

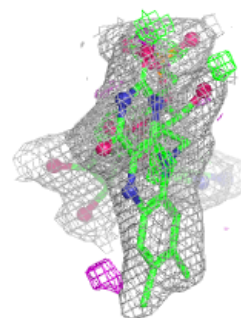
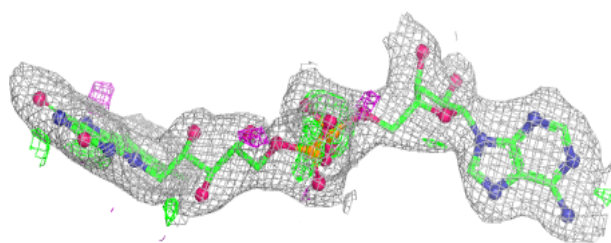
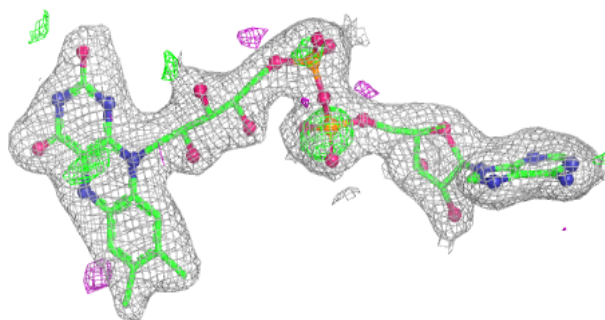
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	601	53/53	0.92	0.11	31,36,47,59	0
2	FAD	D	601	53/53	0.94	0.10	30,45,51,58	0
2	FAD	A	601	53/53	0.95	0.10	31,38,43,76	0
2	FAD	C	601	53/53	0.96	0.09	32,39,49,57	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.

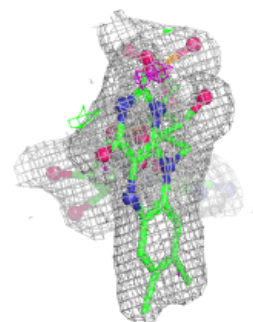
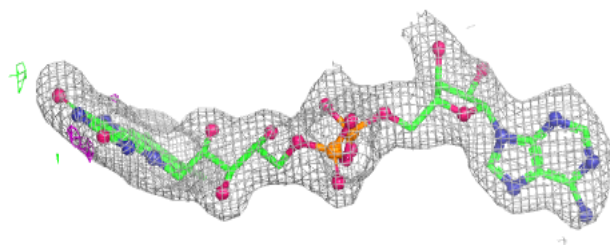
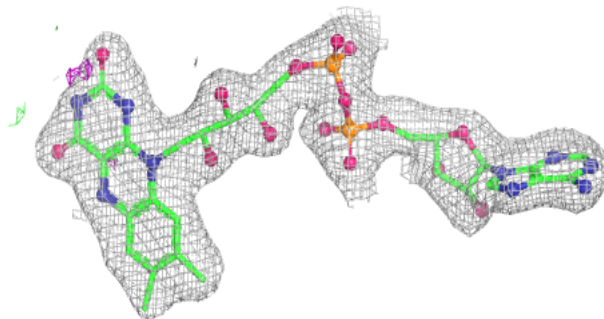
Electron density around FAD B 601:

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

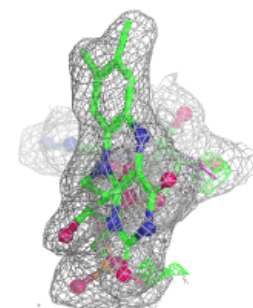
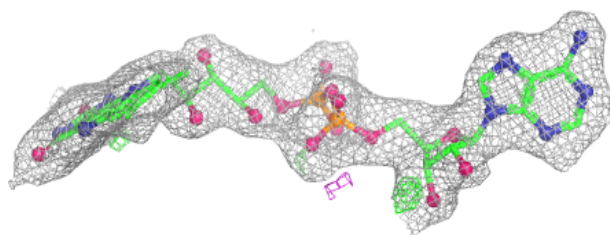
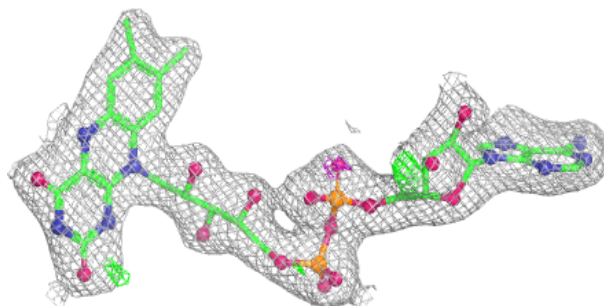


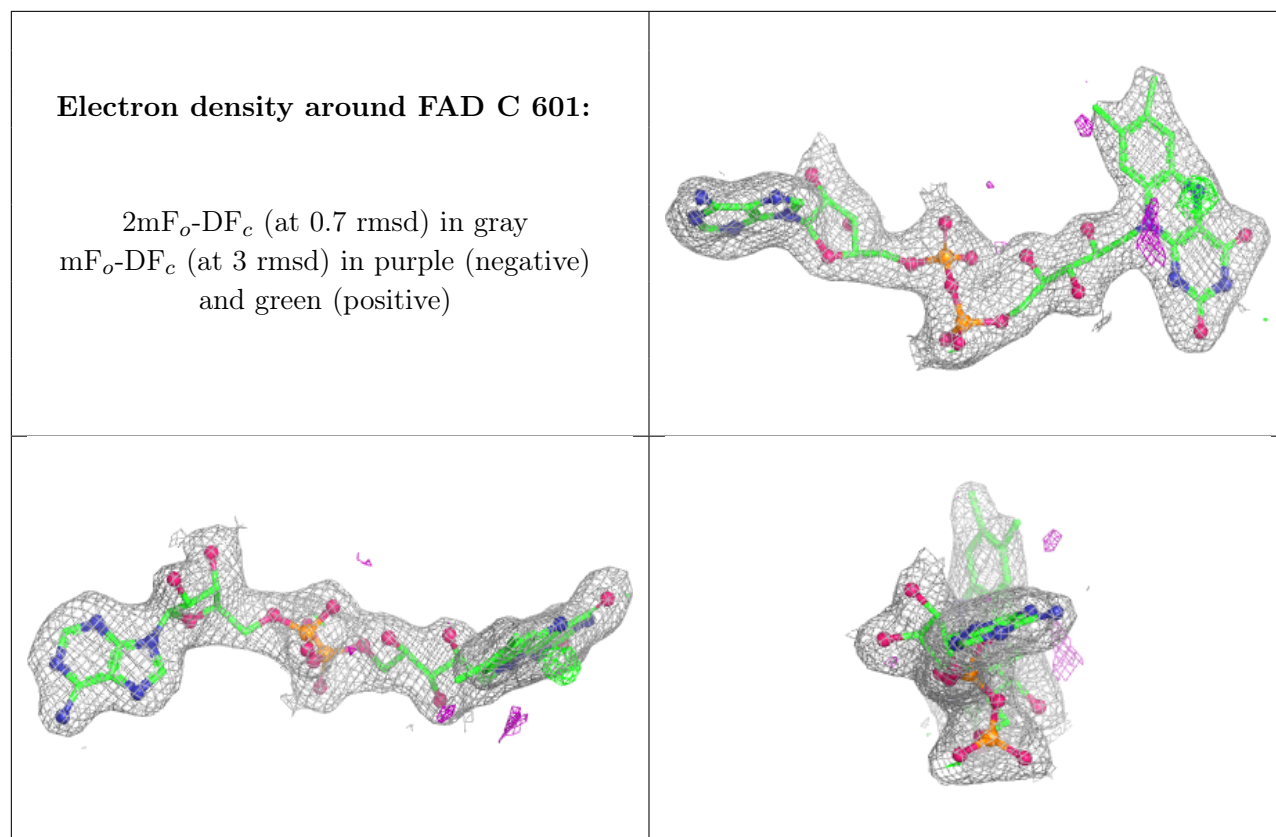
Electron density around FAD D 601:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.