



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:34 AM BST

PDB ID : 2C4C
Title : Crystal structure of the NADPH-treated monooxygenase domain of MICAL
Authors : Siebold, C.; Berrow, N.; Walter, T.S.; Harlos, K.; Owens, R.J.; Terman, J.R.;
Stuart, D.I.; Kolodkin, A.L.; Pasterkamp, R.J.; Jones, E.Y.
Deposited on : 2005-10-18
Resolution : 2.90 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 : 2.13.1
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) : 2.13.1

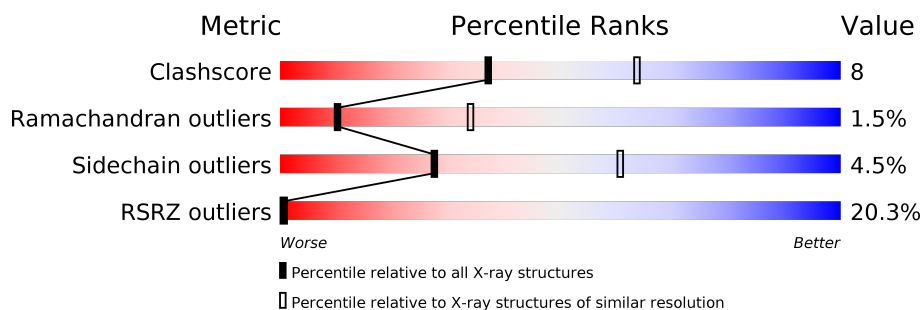
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	497	
1	B	497	

2 Entry composition [i](#)

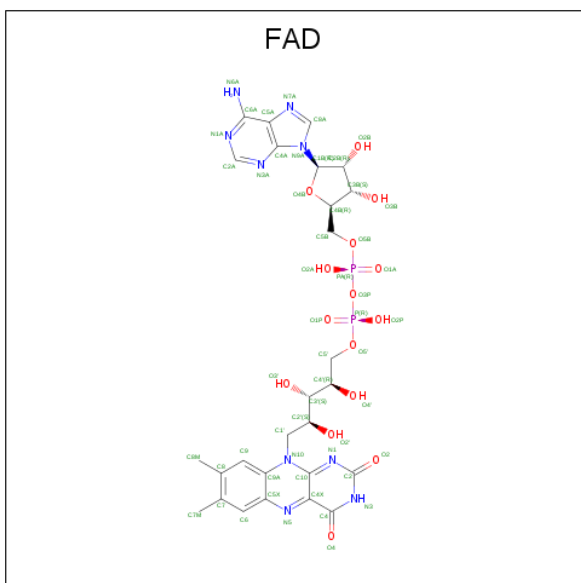
There are 4 unique types of molecules in this entry. The entry contains 7620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEDD9-INTERACTING PROTEIN WITH CALPONIN HO-MOLOGY AND LIM DOMAINS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	476	Total 3719	C 2374	N 665	O 664	S 16	0	0	0
1	B	477	Total 3723	C 2376	N 666	O 665	S 16	0	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 83	C 44	N 13	O 23	P 3	0	1

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

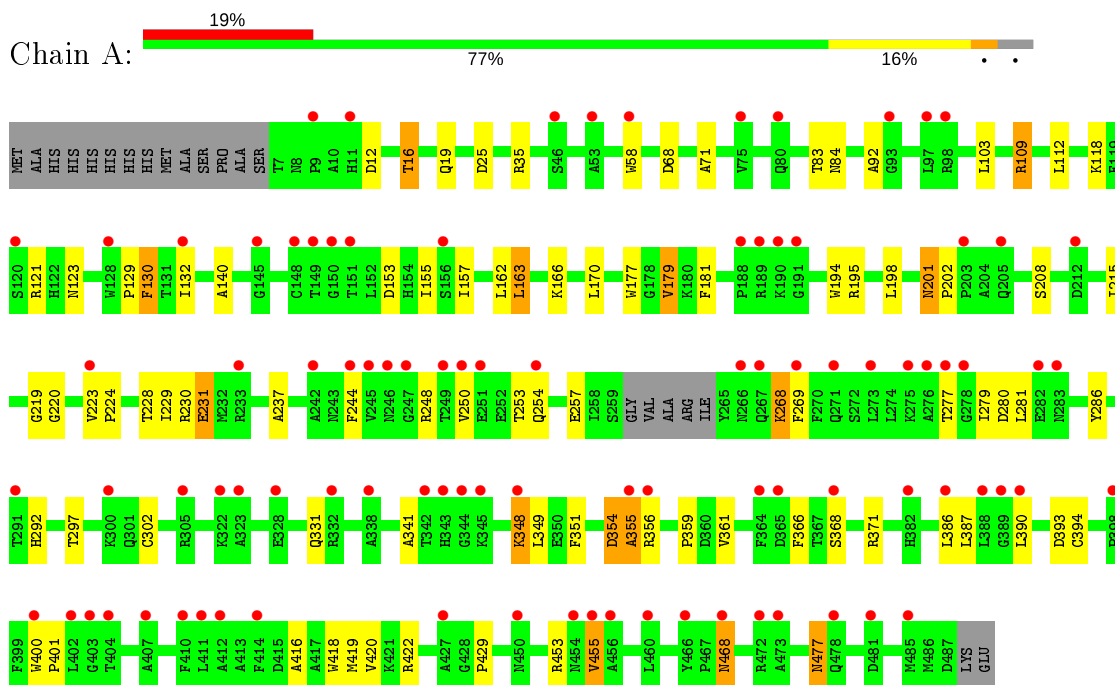
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	21	Total O 21 21	0	0
4	B	19	Total O 19 19	0	0

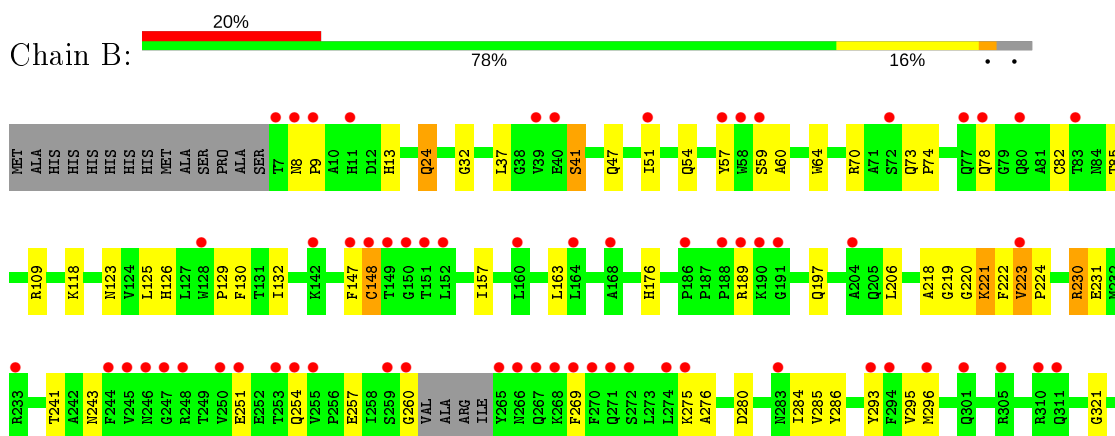
3 Residue-property plots [i](#)

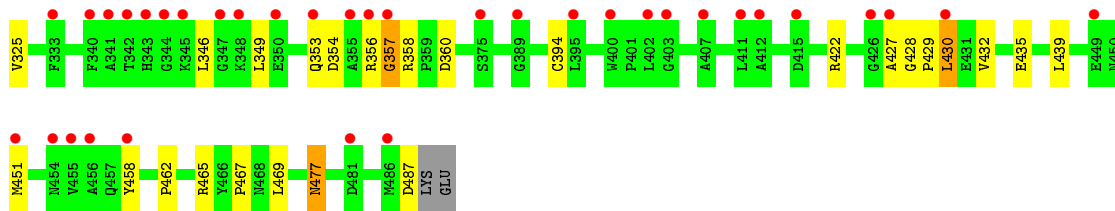
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NEDD9-INTERACTING PROTEIN WITH CALPONIN HOMOLGY AND LIM DOMAINS



• Molecule 1: NEDD9-INTERACTING PROTEIN WITH CALPONIN HOMOLGY AND LIM DOMAINS





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.71Å 89.92Å 83.57Å 90.00° 113.82° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 25.48 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.90) 98.5 (25.48-2.68)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.68Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.294 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtrriage
Anisotropy	0.340	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 79.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7620	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/3801	0.52	0/5146
1	B	0.33	0/3805	0.51	0/5151
All	All	0.33	0/7606	0.51	0/10297

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	3719	0	3740	63	0
1	B	3723	0	3743	54	0
2	A	53	0	31	3	0
2	B	83	0	38	7	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
4	A	21	0	0	1	0
4	B	19	0	0	0	0
All	All	7620	0	7552	118	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 8.

All (118) 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:220:GLY:HA3	1:B:221:LYS:HB2	1.35	1.08
1:A:354:ASP:HB3	1:A:355:ALA:HB3	1.06	1.05
1:A:354:ASP:HB3	1:A:355:ALA:CB	1.86	1.05
1:B:222:PHE:HA	1:B:223:VAL:HB	1.48	0.93
1:A:354:ASP:CB	1:A:355:ALA:HB3	1.97	0.93
1:B:220:GLY:CA	1:B:221:LYS:HB2	2.11	0.80
1:A:354:ASP:HB2	1:A:356:ARG:N	2.04	0.72
1:B:220:GLY:HA3	1:B:221:LYS:CB	2.18	0.72
1:A:354:ASP:HB2	1:A:356:ARG:H	1.52	0.71
1:B:123:ASN:HB3	2:B:600[B]:FAD:O4	1.94	0.68
1:B:284:ILE:HG13	1:B:296:MET:HB3	1.74	0.68
1:A:230:ARG:HH12	1:A:371:ARG:HD2	1.61	0.64
1:A:269:PHE:HZ	1:A:341:ALA:HA	1.63	0.63
1:A:331:GLN:OE1	1:A:359:PRO:HG3	1.99	0.63
2:B:600[A]:FAD:H9	2:B:600[A]:FAD:O2'	1.98	0.63
1:A:250:VAL:O	1:A:254:GLN:HG2	2.00	0.60
1:A:400:TRP:N	1:A:401:PRO:HD2	2.15	0.60
1:B:222:PHE:HA	1:B:223:VAL:CB	2.25	0.60
1:A:123:ASN:O	1:A:157:ILE:HG13	2.02	0.59
1:A:132:ILE:HD11	1:A:153:ASP:HB2	1.84	0.59
1:A:166:LYS:O	1:A:170:LEU:HG	2.03	0.58
1:A:351:PHE:HE1	1:A:361:VAL:HB	1.69	0.58
1:A:195:ARG:HH11	1:A:208:SER:HA	1.68	0.58
1:B:435:GLU:O	1:B:439:LEU:HD12	2.04	0.57
1:A:103:LEU:HD11	1:A:215:ILE:HD12	1.86	0.56
1:A:268:LYS:HE3	1:A:268:LYS:H	1.71	0.56
1:B:47:GLN:O	1:B:51:ILE:HG12	2.05	0.56
1:B:241:THR:HG21	2:B:600[A]:FAD:HM73	1.86	0.56
1:A:477:ASN:N	1:A:477:ASN:HD22	2.05	0.55
1:A:354:ASP:HB3	1:A:355:ALA:CA	2.37	0.55
1:B:176:HIS:CD2	1:B:206:LEU:HD13	2.43	0.53
1:B:220:GLY:CA	1:B:221:LYS:CB	2.80	0.53
1:A:228:THR:HG21	1:B:230:ARG:NH1	2.23	0.53
1:A:219:GLY:O	1:A:394:CYS:HB3	2.08	0.53
1:B:430:LEU:HD23	1:B:430:LEU:H	1.74	0.53
1:B:70:ARG:O	1:B:73:GLN:HB2	2.09	0.52
1:A:68:ASP:HA	1:A:71:ALA:HB3	1.92	0.51
1:B:41:SER:HA	1:B:47:GLN:HE21	1.76	0.51
1:A:257:GLU:HA	1:A:286:TYR:HD2	1.76	0.51
2:A:600:FAD:O2'	2:A:600:FAD:C9	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:ALA:HB3	1:B:432:VAL:HG13	1.93	0.50
1:A:228:THR:HA	1:B:231:GLU:O	2.12	0.49
1:A:130:PHE:HA	1:A:455:VAL:CG2	2.42	0.49
1:A:16:THR:HA	1:A:19:GLN:HG2	1.95	0.49
1:A:130:PHE:HA	1:A:455:VAL:HG23	1.94	0.49
2:A:600:FAD:O2'	2:A:600:FAD:H9	2.13	0.49
1:A:387:LEU:HD21	1:A:419:MET:HG2	1.95	0.48
1:A:416:ALA:O	1:A:420:VAL:HG23	2.12	0.48
1:B:57:TYR:CE1	1:B:59:SER:HB3	2.48	0.48
1:B:243:ASN:HB2	1:B:360:ASP:HB3	1.95	0.48
1:B:257:GLU:HA	1:B:286:TYR:HD2	1.78	0.48
1:A:231:GLU:OE2	1:A:368:SER:HB3	2.14	0.48
1:A:92:ALA:HB2	1:A:112:LEU:HD21	1.96	0.47
1:A:280:ASP:HB3	1:A:302:CYS:SG	2.55	0.47
1:A:244:PHE:CD1	1:A:349:LEU:HB3	2.50	0.47
1:B:126:HIS:H	2:B:600[A]:FAD:C4	2.28	0.47
1:B:356:ARG:HH11	1:B:358:ARG:HH22	1.63	0.46
1:A:140:ALA:HA	1:A:163:LEU:HD13	1.96	0.46
1:A:257:GLU:HA	1:A:286:TYR:CD2	2.50	0.46
1:A:223:VAL:HG13	1:A:229:ILE:HD13	1.97	0.46
1:A:121:ARG:HB3	1:A:157:ILE:HD12	1.98	0.46
1:B:37:LEU:HB3	1:B:54:GLN:NE2	2.31	0.46
1:B:147:PHE:O	1:B:148:CYS:C	2.54	0.46
1:B:353:GLN:HG3	1:B:357:GLY:HA2	1.98	0.45
1:B:439:LEU:HD21	1:B:462:PRO:HB3	1.98	0.45
1:B:125:LEU:HD21	1:B:157:ILE:HG12	1.98	0.45
1:B:477:ASN:N	1:B:477:ASN:OD1	2.48	0.45
1:A:83:THR:HG23	1:A:84:ASN:HD22	1.82	0.45
1:A:220:GLY:N	1:A:393:ASP:HB3	2.32	0.44
1:A:109:ARG:HD2	4:A:2015:HOH:O	2.17	0.44
1:B:285:VAL:HB	1:B:295:VAL:HG13	1.99	0.44
1:B:260:GLY:HA2	1:B:285:VAL:HG22	2.00	0.44
1:B:243:ASN:OD1	1:B:293:TYR:HD1	2.00	0.44
1:A:201:ASN:HA	1:A:202:PRO:HD2	1.91	0.44
1:B:223:VAL:N	1:B:224:PRO:HD3	2.33	0.43
1:A:224:PRO:HG2	1:A:390:LEU:HD21	1.98	0.43
1:A:348:LYS:H	1:A:348:LYS:HE2	1.84	0.43
1:A:354:ASP:CB	1:A:355:ALA:CA	2.96	0.43
1:A:468:ASN:HD22	1:A:468:ASN:HA	1.62	0.43
1:B:428:GLY:O	1:B:432:VAL:HG22	2.18	0.43
1:A:118:LYS:HB2	3:A:601:CL:CL	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:O	1:A:166:LYS:HG3	2.19	0.43
1:A:12:ASP:O	1:A:16:THR:HG23	2.19	0.43
1:B:219:GLY:O	1:B:394:CYS:HB3	2.19	0.42
1:A:279:ILE:HG22	1:A:281:LEU:HG	2.01	0.42
1:A:393:ASP:OD1	2:A:600:FAD:O3'	2.35	0.42
1:B:346:LEU:HB3	1:B:349:LEU:HD21	2.01	0.42
1:A:248:ARG:HA	1:A:253:THR:HG23	2.02	0.42
1:A:418:TRP:O	1:A:422:ARG:HG2	2.19	0.42
1:B:451:MET:HA	1:B:467:PRO:HD3	2.01	0.42
1:A:194:TRP:CD1	1:A:386:LEU:HB2	2.54	0.42
1:A:237:ALA:O	1:A:366:PHE:HB2	2.20	0.42
1:B:123:ASN:ND2	2:B:600[B]:FAD:H6	2.35	0.42
1:A:181:PHE:HA	1:A:198:LEU:HD23	2.01	0.42
1:B:123:ASN:O	1:B:157:ILE:HG13	2.20	0.42
1:A:244:PHE:HB2	1:A:292:HIS:HB2	2.02	0.41
1:B:13:HIS:CE1	1:B:32:GLY:HA3	2.55	0.41
1:A:277:THR:HB	1:A:279:ILE:HG12	2.02	0.41
1:B:125:LEU:HD22	2:B:600[A]:FAD:H2'	2.03	0.41
1:B:82:CYS:HB3	1:B:85:THR:OG1	2.20	0.41
1:B:321:GLY:O	1:B:325:VAL:HG22	2.21	0.41
1:A:177:TRP:O	1:A:179:VAL:HG22	2.20	0.41
1:B:60:ALA:HB1	1:B:64:TRP:NE1	2.36	0.41
1:B:8:ASN:HA	1:B:9:PRO:HD3	1.94	0.41
1:A:351:PHE:CE1	1:A:361:VAL:HB	2.52	0.41
1:B:60:ALA:HB1	1:B:64:TRP:CE2	2.56	0.41
1:B:24:GLN:OE1	1:B:24:GLN:HA	2.21	0.41
1:B:223:VAL:H	1:B:224:PRO:HD3	1.85	0.41
1:A:354:ASP:CB	1:A:355:ALA:CB	2.76	0.41
1:B:73:GLN:HA	1:B:74:PRO:HD3	1.93	0.41
1:B:125:LEU:HD11	1:B:157:ILE:HG23	2.04	0.40
1:A:123:ASN:HB2	1:A:157:ILE:HD11	2.04	0.40
1:B:129:PRO:HA	1:B:132:ILE:HD12	2.03	0.40
1:A:129:PRO:HA	1:A:132:ILE:HD12	2.03	0.40
1:B:353:GLN:CG	1:B:357:GLY:HA2	2.51	0.40
1:B:458:TYR:CD2	1:B:465:ARG:HG2	2.57	0.40
1:A:228:THR:HG21	1:B:230:ARG:HH11	1.84	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	472/497 (95%)	436 (92%)	31 (7%)	5 (1%)	14	42
1	B	473/497 (95%)	442 (93%)	22 (5%)	9 (2%)	8	28
All	All	945/994 (95%)	878 (93%)	53 (6%)	14 (2%)	10	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASP
1	B	276	ALA
1	B	148	CYS
1	B	221	LYS
1	B	275	LYS
1	A	58	TRP
1	A	355	ALA
1	A	429	PRO
1	B	41	SER
1	B	218	ALA
1	B	357	GLY
1	B	223	VAL
1	A	201	ASN
1	B	429	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/403 (96%)	370 (96%)	16 (4%)	30	64
1	B	386/403 (96%)	367 (95%)	19 (5%)	25	57
All	All	772/806 (96%)	737 (96%)	35 (4%)	27	61

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	25	ASP
1	A	35	ARG
1	A	109	ARG
1	A	130	PHE
1	A	155	ILE
1	A	163	LEU
1	A	179	VAL
1	A	231	GLU
1	A	268	LYS
1	A	297	THR
1	A	348	LYS
1	A	453	ARG
1	A	455	VAL
1	A	468	ASN
1	A	477	ASN
1	B	24	GLN
1	B	78	GLN
1	B	109	ARG
1	B	118	LYS
1	B	130	PHE
1	B	163	LEU
1	B	189	ARG
1	B	197	GLN
1	B	230	ARG
1	B	251	GLU
1	B	254	GLN
1	B	269	PHE
1	B	280	ASP
1	B	354	ASP
1	B	422	ARG
1	B	430	LEU
1	B	469	LEU
1	B	477	ASN
1	B	487	ASP

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

Mol	Chain	Res	Type
1	A	19	GLN
1	A	84	ASN
1	A	205	GLN
1	A	353	GLN
1	A	468	ASN
1	A	477	ASN
1	B	13	HIS
1	B	19	GLN
1	B	47	GLN
1	B	49	HIS
1	B	176	HIS
1	B	254	GLN
1	B	301	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	600	-	51,58,58	1.46	6 (11%)	60,89,89	1.77	13 (21%)
2	FAD	B	600[B]	-	51,58,58	1.56	7 (13%)	60,89,89	1.78	11 (18%)
2	FAD	B	600[A]	-	51,58,58	1.48	6 (11%)	60,89,89	1.73	11 (18%)

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	A	600	-	-	10/30/50/50	0/6/6/6
2	FAD	B	600[B]	-	-	14/30/50/50	0/6/6/6
2	FAD	B	600[A]	-	-	11/30/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600[B]	FAD	C10-N1	5.33	1.40	1.33
2	B	600[A]	FAD	C10-N1	4.60	1.39	1.33
2	B	600[B]	FAD	C2A-N3A	4.50	1.39	1.32
2	B	600[A]	FAD	C2A-N3A	4.50	1.39	1.32
2	A	600	FAD	C10-N1	4.34	1.38	1.33
2	B	600[B]	FAD	C4X-N5	4.20	1.39	1.33
2	A	600	FAD	C2A-N3A	4.11	1.38	1.32
2	A	600	FAD	C4X-N5	3.91	1.38	1.33
2	B	600[B]	FAD	C4-N3	3.83	1.39	1.33
2	B	600[A]	FAD	C4X-N5	3.62	1.38	1.33
2	A	600	FAD	C1'-N10	3.61	1.51	1.48
2	B	600[A]	FAD	C1'-N10	3.48	1.51	1.48
2	B	600[A]	FAD	C4-N3	3.17	1.38	1.33
2	A	600	FAD	C4-N3	3.17	1.38	1.33
2	B	600[B]	FAD	C2A-N1A	2.60	1.38	1.33
2	B	600[A]	FAD	C2A-N1A	2.60	1.38	1.33
2	A	600	FAD	C2A-N1A	2.46	1.38	1.33
2	B	600[B]	FAD	C5X-N5	2.45	1.39	1.35
2	B	600[B]	FAD	C1'-N10	2.42	1.50	1.48

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600[B]	FAD	C4-N3-C2	6.09	120.28	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600[A]	FAD	C4-N3-C2	6.02	120.23	115.14
2	A	600	FAD	C4-N3-C2	5.99	120.20	115.14
2	A	600	FAD	N3A-C2A-N1A	-5.87	119.51	128.68
2	B	600[B]	FAD	N3A-C2A-N1A	-5.62	119.89	128.68
2	B	600[A]	FAD	N3A-C2A-N1A	-5.62	119.89	128.68
2	B	600[A]	FAD	C9A-N10-C10	-4.42	116.12	121.91
2	B	600[B]	FAD	C4X-N5-C5X	4.30	121.07	116.77
2	A	600	FAD	C9A-N10-C10	-4.15	116.47	121.91
2	B	600[B]	FAD	C10-C4X-N5	-4.00	118.49	121.26
2	A	600	FAD	C10-C4X-N5	-3.72	118.68	121.26
2	B	600[B]	FAD	C4-C4X-N5	3.08	122.12	118.60
2	B	600[B]	FAD	C5X-C9A-N10	3.03	119.91	117.72
2	B	600[B]	FAD	P-O3P-PA	-2.96	122.68	132.83
2	A	600	FAD	C1B-N9A-C4A	-2.87	121.59	126.64
2	B	600[A]	FAD	C10-C4X-N5	-2.85	119.28	121.26
2	B	600[B]	FAD	O3B-C3B-C4B	-2.82	102.90	111.05
2	B	600[A]	FAD	O3B-C3B-C4B	-2.82	102.90	111.05
2	A	600	FAD	C4X-C4-N3	-2.77	119.65	123.43
2	B	600[A]	FAD	C4X-C4-N3	-2.75	119.67	123.43
2	B	600[A]	FAD	P-O3P-PA	-2.63	123.79	132.83
2	B	600[B]	FAD	C3B-C2B-C1B	2.56	104.84	100.98
2	B	600[A]	FAD	C3B-C2B-C1B	2.56	104.84	100.98
2	B	600[A]	FAD	C5X-C9A-N10	2.52	119.54	117.72
2	B	600[B]	FAD	C4X-C4-N3	-2.46	120.06	123.43
2	A	600	FAD	C5X-C9A-N10	2.45	119.49	117.72
2	B	600[A]	FAD	C9A-C5X-N5	-2.43	118.56	122.36
2	A	600	FAD	C9A-C5X-N5	-2.41	118.59	122.36
2	A	600	FAD	C4-C4X-N5	2.34	121.27	118.60
2	A	600	FAD	P-O3P-PA	-2.29	124.96	132.83
2	A	600	FAD	O3B-C3B-C4B	-2.20	104.67	111.05
2	A	600	FAD	C2B-C3B-C4B	2.20	106.91	102.64
2	B	600[B]	FAD	C2B-C3B-C4B	2.09	106.71	102.64
2	B	600[A]	FAD	C2B-C3B-C4B	2.09	106.71	102.64
2	A	600	FAD	C3B-C2B-C1B	2.07	104.10	100.98

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	O4'-C4'-C5'-O5'
2	B	600[B]	FAD	C2'-C1'-N10-C10
2	B	600[B]	FAD	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
2	B	600[B]	FAD	O3'-C3'-C4'-C5'
2	B	600[B]	FAD	C3'-C4'-C5'-O5'
2	B	600[B]	FAD	O4'-C4'-C5'-O5'
2	B	600[B]	FAD	C5'-O5'-P-O1P
2	B	600[B]	FAD	C5'-O5'-P-O3P
2	B	600[B]	FAD	PA-O3P-P-O5'
2	B	600[A]	FAD	C2'-C3'-C4'-O4'
2	B	600[A]	FAD	O3'-C3'-C4'-O4'
2	B	600[A]	FAD	C3'-C4'-C5'-O5'
2	B	600[A]	FAD	O4'-C4'-C5'-O5'
2	B	600[A]	FAD	C5'-O5'-P-O1P
2	B	600[B]	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	C3B-C4B-C5B-O5B
2	B	600[B]	FAD	O4B-C4B-C5B-O5B
2	B	600[A]	FAD	O4B-C4B-C5B-O5B
2	B	600[B]	FAD	C2'-C3'-C4'-O4'
2	B	600[A]	FAD	O3'-C3'-C4'-C5'
2	B	600[A]	FAD	C2'-C3'-C4'-C5'
2	B	600[B]	FAD	C3B-C4B-C5B-O5B
2	B	600[A]	FAD	C3B-C4B-C5B-O5B
2	A	600	FAD	O3'-C3'-C4'-C5'
2	A	600	FAD	C2'-C3'-C4'-C5'
2	A	600	FAD	C2'-C3'-C4'-O4'
2	A	600	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	C5B-O5B-PA-O3P
2	A	600	FAD	C5B-O5B-PA-O1A
2	B	600[A]	FAD	N10-C1'-C2'-O2'
2	B	600[B]	FAD	O2'-C2'-C3'-C4'
2	B	600[B]	FAD	C5B-O5B-PA-O1A
2	B	600[A]	FAD	C5B-O5B-PA-O1A

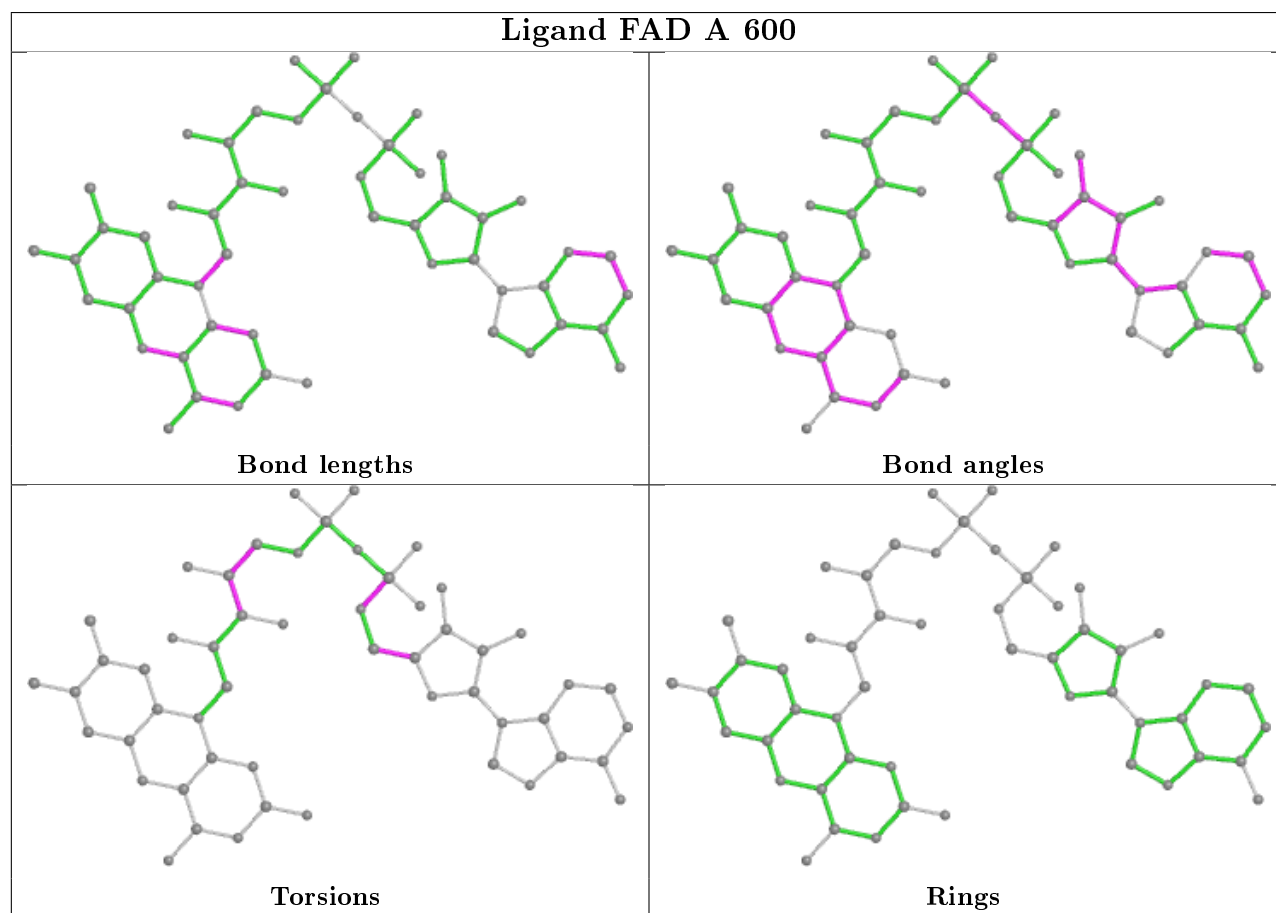
There are no ring outliers.

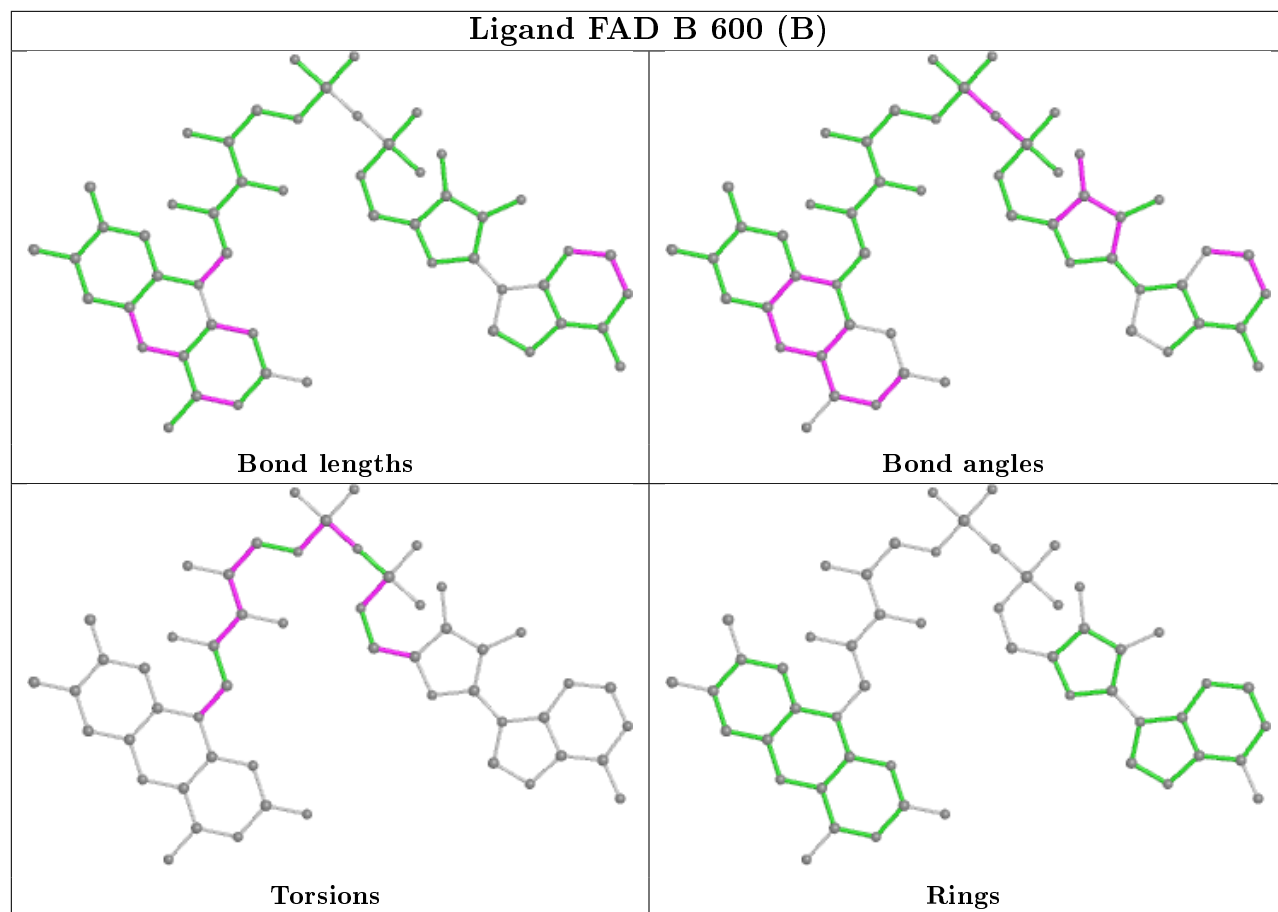
3 monomers are involved in 10 short contacts:

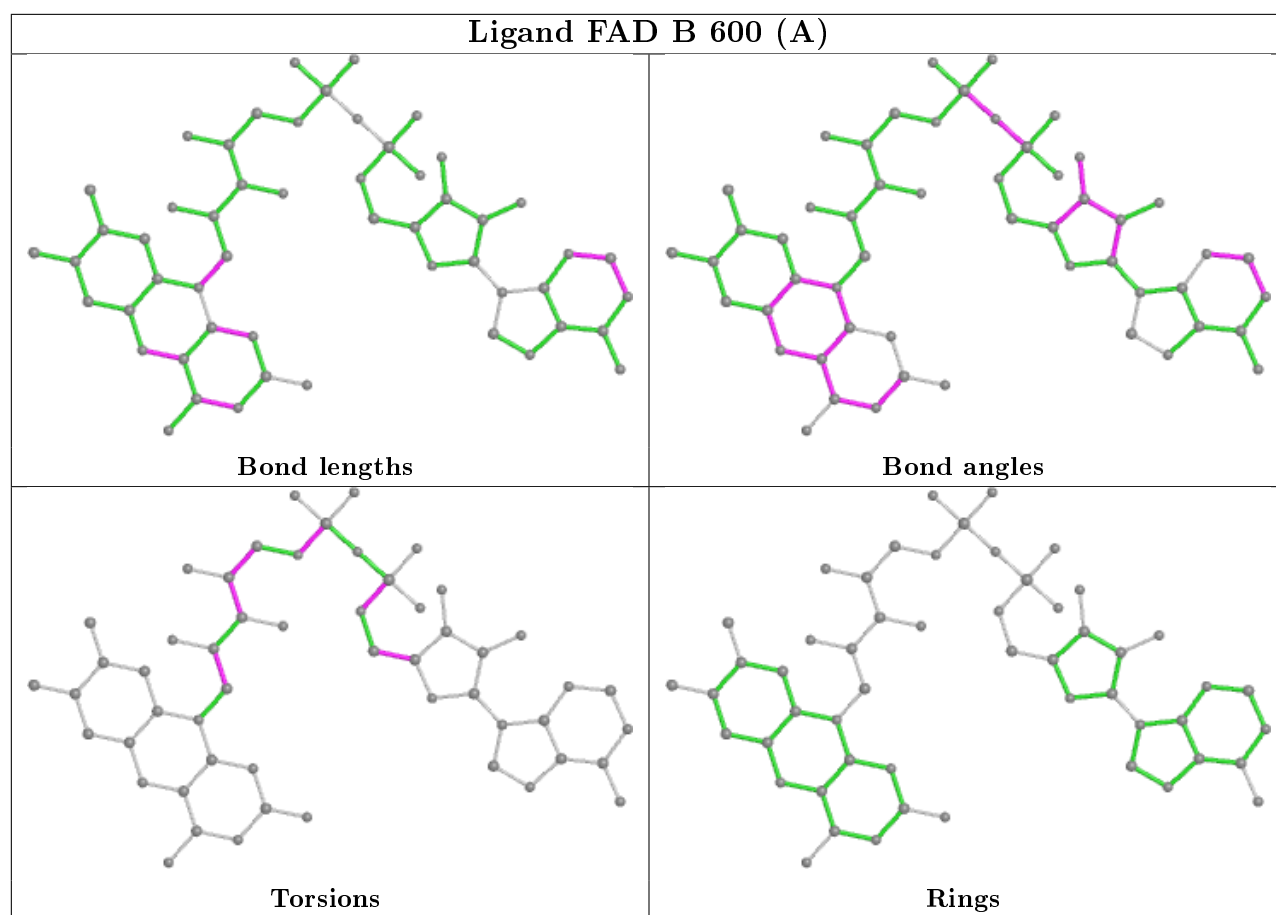
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	3	0
2	B	600[B]	FAD	2	0
2	B	600[A]	FAD	5	0

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	476/497 (95%)	1.25	94 (19%) 1 0	72, 81, 89, 97	0
1	B	477/497 (95%)	1.29	99 (20%) 1 0	72, 81, 88, 98	0
All	All	953/994 (95%)	1.27	193 (20%) 1 0	72, 81, 89, 98	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	ALA	13.5
1	B	150	GLY	10.1
1	B	148	CYS	9.7
1	B	151	THR	7.4
1	A	191	GLY	7.1
1	B	254	GLN	7.1
1	A	323	ALA	6.7
1	B	250	VAL	6.6
1	A	250	VAL	6.6
1	B	265	TYR	6.4
1	B	267	GLN	6.0
1	B	251	GLU	5.7
1	A	485	MET	5.5
1	A	271	GLN	5.5
1	A	266	ASN	5.4
1	B	269	PHE	5.4
1	B	344	GLY	5.3
1	A	148	CYS	5.1
1	A	267	GLN	5.1
1	A	345	LYS	5.1
1	A	151	THR	5.0
1	A	454	ASN	4.9
1	B	149	THR	4.9
1	B	274	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	402	LEU	4.9
1	B	59	SER	4.8
1	B	58	TRP	4.7
1	B	426	GLY	4.7
1	A	149	THR	4.6
1	B	266	ASN	4.5
1	B	348	LYS	4.5
1	B	301	GLN	4.5
1	B	271	GLN	4.4
1	B	486	MET	4.4
1	B	83	THR	4.3
1	B	343	HIS	4.2
1	A	190	LYS	4.2
1	B	255	VAL	4.2
1	B	456	ALA	4.2
1	A	223	VAL	4.2
1	A	277	THR	4.1
1	B	8	ASN	4.0
1	B	40	GLU	3.9
1	A	407	ALA	3.8
1	B	270	PHE	3.8
1	A	481	ASP	3.7
1	A	282	GLU	3.7
1	A	427	ALA	3.7
1	A	189	ARG	3.7
1	B	7	THR	3.7
1	B	80	GLN	3.7
1	B	353	GLN	3.6
1	A	456	ALA	3.6
1	A	188	PRO	3.6
1	B	189	ARG	3.6
1	B	345	LYS	3.6
1	B	186	PRO	3.5
1	A	342	THR	3.4
1	A	251	GLU	3.4
1	A	404	THR	3.4
1	A	120	SER	3.4
1	B	342	THR	3.4
1	A	468	ASN	3.3
1	B	245	VAL	3.3
1	B	403	GLY	3.2
1	B	340	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	454	ASN	3.2
1	B	11	HIS	3.2
1	A	382	HIS	3.2
1	A	247	GLY	3.2
1	A	273	LEU	3.2
1	B	268	LYS	3.1
1	A	300	LYS	3.1
1	B	305	ARG	3.1
1	A	246	ASN	3.1
1	A	455	VAL	3.1
1	B	458	TYR	3.1
1	B	356	ARG	3.1
1	A	203	PRO	3.0
1	A	478	GLN	3.0
1	A	245	VAL	3.0
1	A	412	ALA	3.0
1	B	259	SER	3.0
1	A	473	ALA	3.0
1	A	269	PHE	3.0
1	B	272	SER	3.0
1	B	333	PHE	2.9
1	A	80	GLN	2.9
1	A	128	TRP	2.9
1	B	78	GLN	2.9
1	B	9	PRO	2.9
1	B	275	LYS	2.9
1	A	410	PHE	2.9
1	B	389	GLY	2.9
1	A	278	GLY	2.8
1	B	455	VAL	2.8
1	B	164	LEU	2.8
1	A	212	ASP	2.8
1	B	481	ASP	2.8
1	A	58	TRP	2.8
1	B	188	PRO	2.8
1	A	348	LYS	2.7
1	B	341	ALA	2.7
1	B	147	PHE	2.7
1	A	249	THR	2.7
1	A	338	ALA	2.7
1	B	253	THR	2.7
1	A	53	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	51	ILE	2.6
1	A	275	LYS	2.6
1	A	322	LYS	2.6
1	B	190	LYS	2.6
1	A	205	GLN	2.6
1	B	310	ARG	2.6
1	A	305	ARG	2.6
1	B	233	ARG	2.6
1	B	247	GLY	2.6
1	B	411	LEU	2.6
1	B	128	TRP	2.6
1	A	9	PRO	2.6
1	A	343	HIS	2.6
1	A	390	LEU	2.6
1	A	75	VAL	2.5
1	B	244	PHE	2.5
1	B	246	ASN	2.5
1	A	11	HIS	2.5
1	B	355	ALA	2.5
1	A	364	PHE	2.5
1	B	72	SER	2.4
1	A	411	LEU	2.4
1	B	152	LEU	2.4
1	A	365	ASP	2.4
1	A	356	ARG	2.4
1	B	412	ALA	2.4
1	B	77	GLN	2.4
1	A	368	SER	2.4
1	B	168	ALA	2.4
1	A	150	GLY	2.3
1	A	460	LEU	2.3
1	B	400	TRP	2.3
1	A	355	ALA	2.3
1	B	160	LEU	2.3
1	A	450	ASN	2.3
1	B	294	PHE	2.3
1	B	357	GLY	2.3
1	B	248	ARG	2.3
1	A	328	GLU	2.3
1	B	57	TYR	2.3
1	A	156	SER	2.3
1	A	472	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	347	GLY	2.3
1	A	254	GLN	2.3
1	B	39	VAL	2.2
1	B	142	LYS	2.2
1	B	260	GLY	2.2
1	A	466	TYR	2.2
1	B	204	ALA	2.2
1	A	98	ARG	2.2
1	A	388	LEU	2.2
1	A	414	PHE	2.2
1	B	415	ASP	2.2
1	B	427	ALA	2.2
1	A	46	SER	2.2
1	B	375	SER	2.2
1	B	293	TYR	2.2
1	A	97	LEU	2.1
1	A	242	ALA	2.1
1	A	389	GLY	2.1
1	A	93	GLY	2.1
1	B	395	LEU	2.1
1	A	132	ILE	2.1
1	A	400	TRP	2.1
1	A	291	THR	2.1
1	A	145	GLY	2.1
1	A	332	ARG	2.1
1	B	407	ALA	2.1
1	A	344	GLY	2.1
1	A	403	GLY	2.1
1	B	430	LEU	2.1
1	B	296	MET	2.1
1	B	451	MET	2.1
1	A	386	LEU	2.1
1	B	191	GLY	2.1
1	B	350	GLU	2.1
1	A	283	ASN	2.1
1	A	233	ARG	2.0
1	B	223	VAL	2.0
1	A	398	PRO	2.0
1	A	402	LEU	2.0
1	B	311	GLN	2.0
1	A	244	PHE	2.0
1	B	449	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	283	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

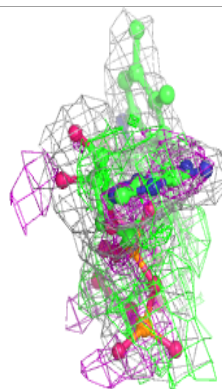
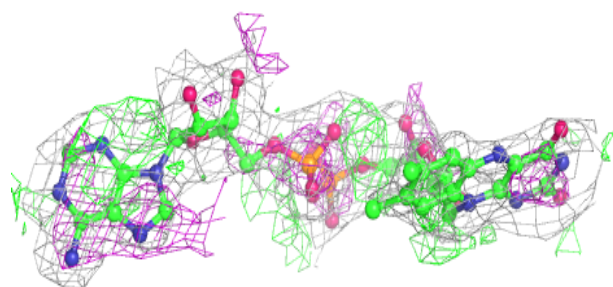
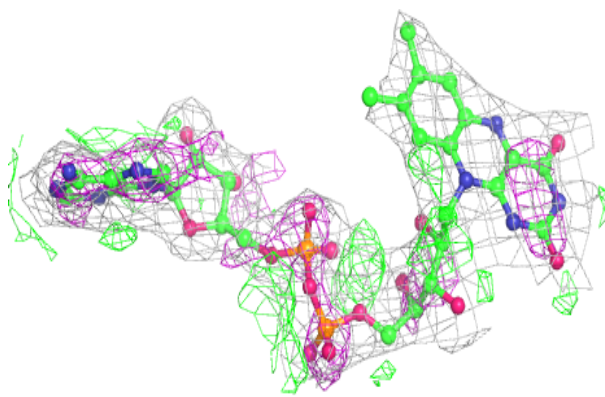
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	600[B]	53/53	0.88	0.24	37,41,47,48	30
2	FAD	B	600[A]	53/53	0.88	0.24	45,49,60,60	30
2	FAD	A	600	53/53	0.91	0.21	48,54,69,69	0
3	CL	B	601	1/1	0.97	0.17	65,65,65,65	0
3	CL	A	601	1/1	0.98	0.32	64,64,64,64	0

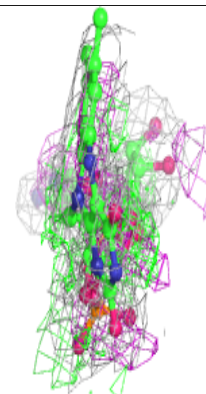
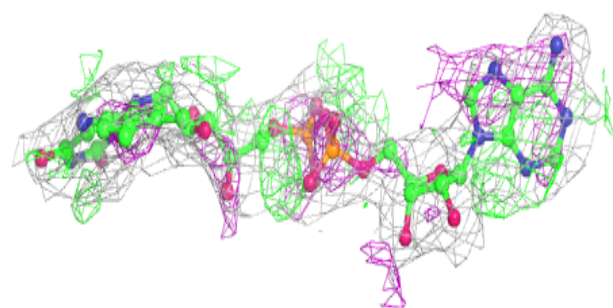
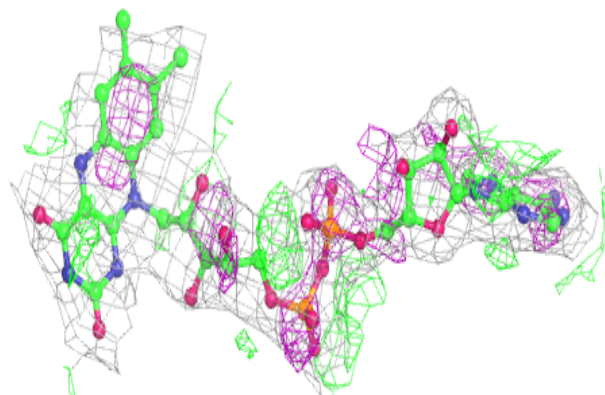
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

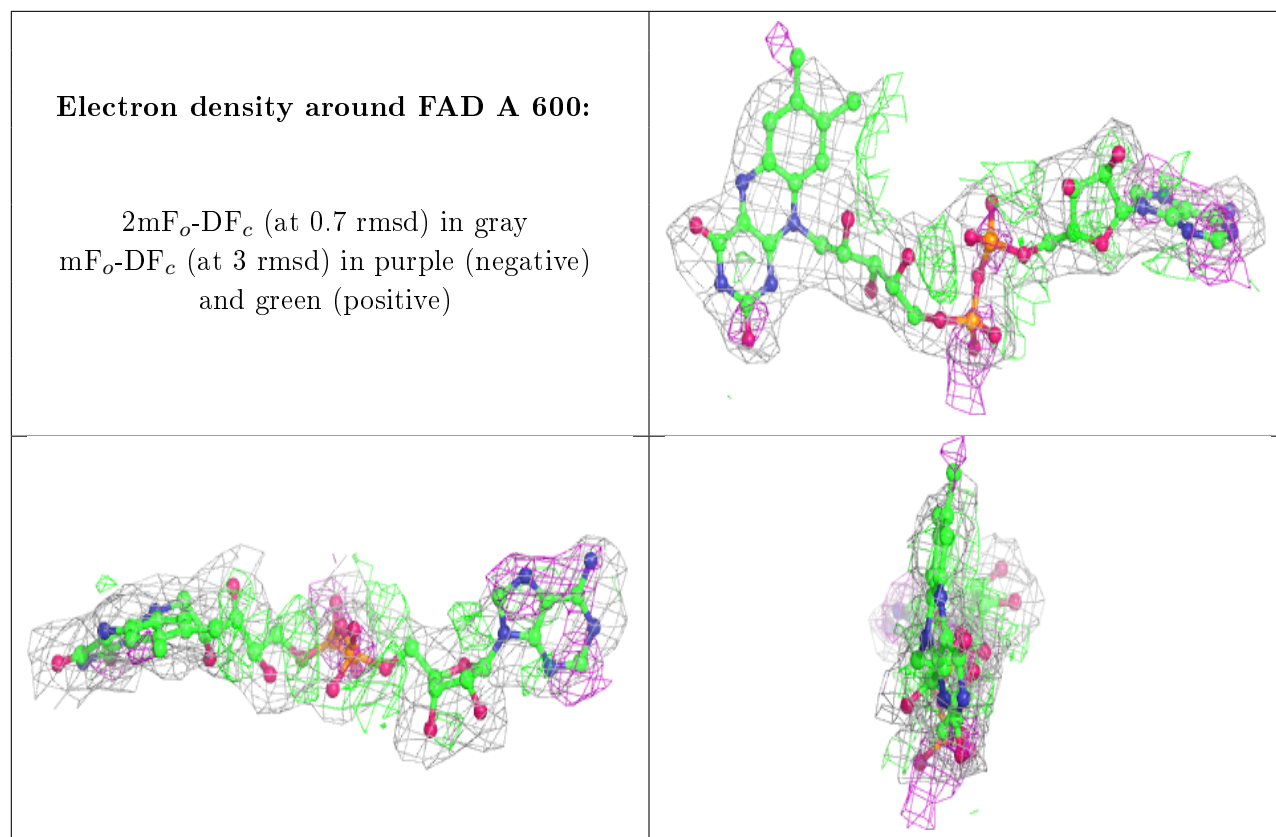
Electron density around FAD B 600 (B):

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

**Electron density around FAD B 600 (A):**

$2mF_o-DF_c$ (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.