



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:17 PM UTC

PDB ID : 3W8W / pdb_00003w8w
Title : The crystal structure of EncM
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Deposited on : 2013-03-22
Resolution : 1.95 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

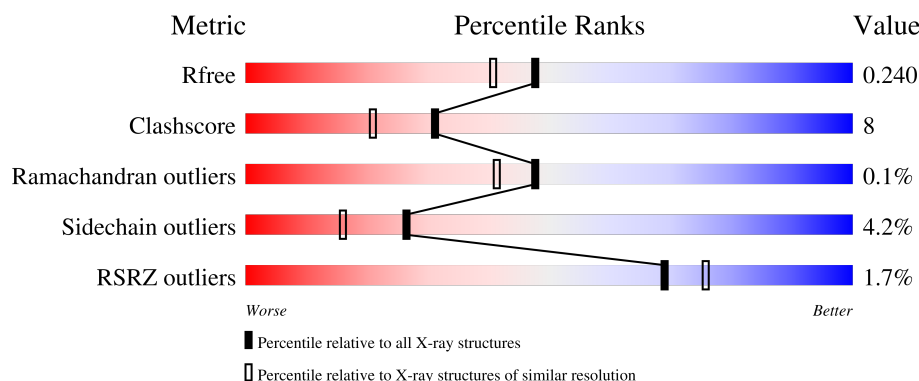
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	468	% 80% 17% ..
1	B	468	2% 80% 16% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7744 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 Putative FAD-dependent oxygenase EncM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3501	2213	625	650	13			
1	B	461	Total	C	N	O	S	0	0	0
			3507	2216	626	652	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9KHK2
A	-2	SER	-	expression tag	UNP Q9KHK2
A	-1	HIS	-	expression tag	UNP Q9KHK2
A	0	GLY	-	expression tag	UNP Q9KHK2
B	-3	GLY	-	expression tag	UNP Q9KHK2
B	-2	SER	-	expression tag	UNP Q9KHK2
B	-1	HIS	-	expression tag	UNP Q9KHK2
B	0	GLY	-	expression tag	UNP Q9KHK2

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



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

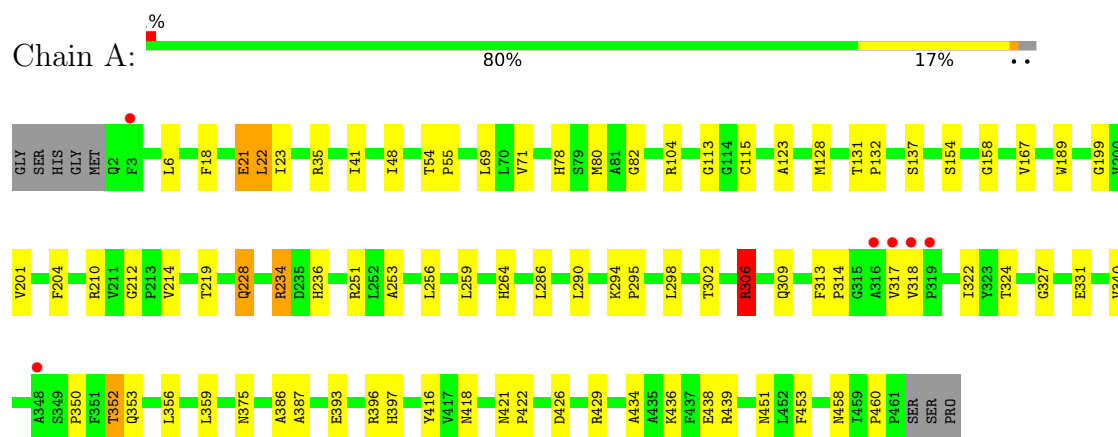
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	307	Total O 307 307	0	0
3	B	323	Total O 323 323	0	0

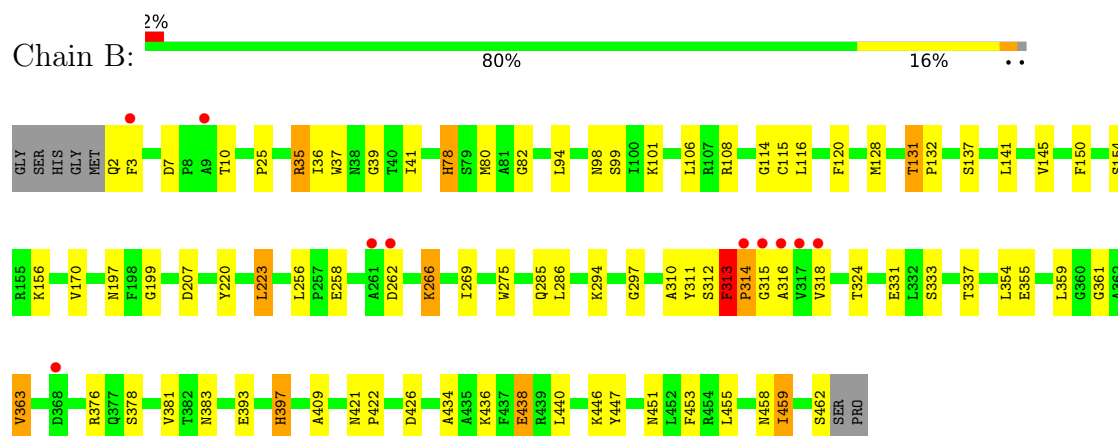
3 Residue-property plots [i](#)

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: Putative FAD-dependent oxygenase EncM



• Molecule 1: Putative FAD-dependent oxygenase EncM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.41Å 85.28Å 79.67Å 90.00° 99.84° 90.00°	Depositor
Resolution (Å)	47.72 – 1.95 47.72 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.72-1.95) 99.9 (47.72-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.243 0.189 , 0.240	Depositor DCC
R_{free} test set	3442 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	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	0.94	EDS
Total number of atoms	7744	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.30	11/3592 (0.3%)	1.27	12/4896 (0.2%)
1	B	1.23	6/3598 (0.2%)	1.28	18/4904 (0.4%)
All	All	1.26	17/7190 (0.2%)	1.28	30/9800 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	SER	N-CA	7.09	1.55	1.45
1	A	375	ASN	CG-OD1	7.03	1.36	1.23
1	A	356	LEU	C-O	6.45	1.31	1.24
1	A	436	LYS	C-O	-6.04	1.17	1.24
1	B	137	SER	C-O	-5.88	1.17	1.24
1	B	170	VAL	C-O	5.80	1.30	1.24
1	A	306	ARG	CD-NE	-5.65	1.38	1.46
1	B	361	GLY	N-CA	5.62	1.53	1.45
1	A	123	ALA	CA-C	5.51	1.59	1.52
1	B	363	VAL	C-O	5.38	1.30	1.24
1	A	132	PRO	C-O	5.37	1.29	1.23
1	A	264	HIS	CA-C	-5.31	1.46	1.52
1	A	460	PRO	C-O	-5.25	1.20	1.24
1	A	167	VAL	N-CA	-5.20	1.40	1.46
1	A	201	VAL	CA-CB	5.20	1.60	1.54
1	B	39	GLY	C-O	-5.05	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	GLY	N-CA	5.03	1.50	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	PHE	CA-C-N	17.44	141.64	119.84
1	B	313	PHE	C-N-CA	17.44	141.64	119.84
1	A	306	ARG	NE-CZ-NH2	-12.55	107.90	119.20
1	B	438	GLU	N-CA-C	8.22	119.86	111.07
1	B	154	SER	N-CA-C	7.88	119.50	111.07
1	A	306	ARG	NE-CZ-NH1	7.86	129.36	121.50
1	A	306	ARG	CD-NE-CZ	7.67	135.14	124.40
1	B	313	PHE	C-N-CD	-7.64	93.68	125.00
1	A	309	GLN	N-CA-C	6.27	118.91	111.33
1	A	212	GLY	CA-C-N	6.20	126.57	119.93
1	A	212	GLY	C-N-CA	6.20	126.57	119.93
1	B	378	SER	CA-C-N	-6.13	113.45	119.64
1	B	378	SER	C-N-CA	-6.13	113.45	119.64
1	A	306	ARG	CG-CD-NE	-6.02	98.76	112.00
1	B	78	HIS	N-CA-C	5.97	120.43	113.20
1	A	234	ARG	N-CA-CB	5.92	118.83	110.12
1	A	306	ARG	CB-CG-CD	5.81	124.66	111.30
1	B	266	LYS	CA-C-N	-5.65	113.94	119.76
1	B	266	LYS	C-N-CA	-5.65	113.94	119.76
1	A	350	PRO	N-CA-C	5.47	120.70	113.86
1	A	434	ALA	N-CA-C	5.40	116.97	111.14
1	B	397	HIS	N-CA-C	5.38	116.83	111.07
1	B	434	ALA	N-CA-C	5.35	116.80	111.07
1	A	71	VAL	N-CA-C	5.17	115.54	107.99
1	B	294	LYS	CA-C-N	-5.12	114.06	120.51
1	B	294	LYS	C-N-CA	-5.12	114.06	120.51
1	B	459	ILE	CA-C-N	-5.08	116.00	119.66
1	B	459	ILE	C-N-CA	-5.08	116.00	119.66
1	B	197	ASN	N-CA-C	5.06	118.92	112.34
1	B	409	ALA	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	313	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3501	0	3413	57	0
1	B	3507	0	3418	66	0
2	A	53	0	31	5	0
2	B	53	0	31	6	0
3	A	307	0	0	12	0
3	B	323	0	0	14	0
All	All	7744	0	6893	115	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 (115) 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:78:HIS:ND1	2:B:600:FAD:HM82	1.08	1.39
1:A:78:HIS:ND1	2:A:600:FAD:HM82	1.06	1.37
1:A:78:HIS:ND1	2:A:600:FAD:C8M	2.00	1.24
1:B:78:HIS:ND1	2:B:600:FAD:C8M	2.01	1.21
1:A:228:GLN:HE21	1:A:228:GLN:H	1.14	0.96
1:B:35:ARG:HH21	1:B:35:ARG:CG	1.85	0.89
1:B:451:ASN:HD21	1:B:458:ASN:HD21	1.18	0.86
1:A:78:HIS:CE1	2:A:600:FAD:HM82	2.11	0.84
1:B:78:HIS:CG	2:B:600:FAD:HM82	2.12	0.84
1:A:128:MET:HE2	3:B:840:HOH:O	1.78	0.84
1:A:451:ASN:HD21	1:A:458:ASN:HD21	1.27	0.82
1:B:7:ASP:HB3	1:B:10:THR:HG22	1.59	0.82
1:A:78:HIS:CG	2:A:600:FAD:HM82	2.13	0.81
1:B:128:MET:HE2	3:B:875:HOH:O	1.81	0.81
1:A:128:MET:HE1	1:B:315:GLY:O	1.82	0.80
1:A:115:CYS:HB3	3:A:920:HOH:O	1.83	0.78
1:A:352:THR:HG21	3:A:900:HOH:O	1.84	0.78
1:B:7:ASP:HB3	1:B:10:THR:CG2	2.14	0.76
1:A:396:ARG:HD3	3:A:874:HOH:O	1.85	0.76
1:B:115:CYS:HB3	3:B:919:HOH:O	1.86	0.75
1:A:352:THR:HB	1:A:386:ALA:HA	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:HH21	1:B:35:ARG:HG2	1.53	0.73
1:B:438:GLU:HB2	3:B:866:HOH:O	1.90	0.71
1:A:228:GLN:HE21	1:A:228:GLN:N	1.87	0.71
1:B:128:MET:CE	3:B:875:HOH:O	2.37	0.70
1:A:21:GLU:OE1	1:B:101:LYS:NZ	2.23	0.69
1:B:359:LEU:HD11	3:B:779:HOH:O	1.93	0.69
1:B:223:LEU:H	1:B:266:LYS:HZ1	1.40	0.68
1:B:35:ARG:HH21	1:B:35:ARG:HG3	1.58	0.68
1:A:69:LEU:O	3:A:704:HOH:O	2.12	0.68
1:A:306:ARG:HD2	1:B:310:ALA:O	1.95	0.67
1:B:311:TYR:O	1:B:314:PRO:HD3	1.98	0.64
1:A:352:THR:HG22	1:A:387:ALA:H	1.62	0.64
1:A:228:GLN:H	1:A:228:GLN:NE2	1.91	0.63
1:B:7:ASP:CB	1:B:10:THR:HG22	2.28	0.62
1:B:421:ASN:HB2	1:B:422:PRO:CD	2.29	0.62
1:A:306:ARG:NH2	3:A:986:HOH:O	2.27	0.62
1:A:236:HIS:HE1	3:A:769:HOH:O	1.81	0.61
1:A:318:VAL:HG23	1:B:128:MET:HE2	1.82	0.61
1:A:104:ARG:CD	3:A:706:HOH:O	2.49	0.60
1:B:275:TRP:CZ3	1:B:285:GLN:HG3	2.37	0.60
1:A:219:THR:CG2	1:A:298:LEU:HD13	2.31	0.59
1:A:318:VAL:HG23	3:B:875:HOH:O	2.03	0.59
1:A:18:PHE:CE2	1:A:22:LEU:HD13	2.38	0.58
1:B:131:THR:HB	1:B:132:PRO:HD2	1.86	0.58
1:A:294:LYS:HD2	1:A:295:PRO:HD2	1.85	0.57
1:B:333:SER:O	1:B:337:THR:HG23	2.06	0.56
1:B:3:PHE:HE2	3:B:740:HOH:O	1.89	0.56
1:B:35:ARG:HG2	1:B:35:ARG:NH2	2.20	0.56
1:B:421:ASN:HB2	1:B:422:PRO:HD2	1.88	0.56
1:A:219:THR:HG22	1:A:298:LEU:HD13	1.86	0.55
1:B:41:ILE:HG13	1:B:82:GLY:HA3	1.88	0.55
1:B:131:THR:HB	1:B:132:PRO:CD	2.36	0.55
1:A:219:THR:HG22	1:A:298:LEU:CD1	2.36	0.55
1:B:223:LEU:H	1:B:266:LYS:NZ	2.05	0.55
1:B:35:ARG:NH2	1:B:36:ILE:O	2.41	0.54
1:B:98:ASN:OD1	1:B:115:CYS:HA	2.07	0.54
1:A:35:ARG:HD2	3:A:711:HOH:O	2.07	0.54
1:B:78:HIS:CE1	2:B:600:FAD:HM82	2.19	0.54
1:B:363:VAL:O	1:B:376:ARG:HD3	2.07	0.53
1:B:451:ASN:HD21	1:B:458:ASN:ND2	1.99	0.53
1:A:353:GLN:NE2	3:A:990:HOH:O	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:HG13	1:A:82:GLY:HA3	1.91	0.52
1:A:78:HIS:ND1	2:A:600:FAD:C8	2.70	0.52
1:A:104:ARG:HD2	3:A:706:HOH:O	2.09	0.52
1:A:189:TRP:CH2	1:A:439:ARG:HD3	2.45	0.52
1:A:421:ASN:HB2	1:A:422:PRO:CD	2.41	0.51
1:A:322:ILE:HD12	1:A:322:ILE:C	2.35	0.50
1:A:104:ARG:HH12	1:B:35:ARG:HD3	1.77	0.50
1:B:78:HIS:ND1	2:B:600:FAD:C8	2.72	0.50
1:B:150:PHE:CE1	3:B:779:HOH:O	2.62	0.49
1:B:440:LEU:HB3	1:B:459:ILE:HD13	1.93	0.49
1:B:393:GLU:HB3	1:B:397:HIS:CD2	2.48	0.49
1:A:256:LEU:HB2	1:A:259:LEU:CD1	2.42	0.49
1:B:7:ASP:OD2	1:B:10:THR:HG22	2.12	0.49
1:B:355:GLU:CG	1:B:383:ASN:HB3	2.42	0.49
1:A:286:LEU:O	1:A:290:LEU:HG	2.13	0.49
1:A:23:ILE:HB	1:A:48:ILE:HB	1.96	0.48
1:A:210:ARG:NH2	1:B:316:ALA:O	2.46	0.47
1:B:80:MET:SD	1:B:324:THR:HG21	2.55	0.47
1:B:312:SER:HA	1:B:313:PHE:HA	1.59	0.46
1:A:251:ARG:HD2	1:A:353:GLN:HE21	1.80	0.46
1:B:131:THR:CB	1:B:132:PRO:CD	2.93	0.46
1:A:104:ARG:HD3	3:A:706:HOH:O	2.13	0.46
1:B:156:LYS:HE2	3:B:931:HOH:O	2.15	0.45
1:A:80:MET:SD	1:A:324:THR:HG21	2.56	0.45
1:B:359:LEU:HD13	1:B:381:VAL:HG23	1.98	0.44
1:B:37:TRP:CH2	2:B:600:FAD:HM81	2.52	0.44
1:A:154:SER:HA	1:A:158:GLY:O	2.18	0.44
1:B:94:LEU:O	1:B:114:GLY:HA3	2.18	0.44
1:A:313:PHE:CG	1:A:314:PRO:HD2	2.53	0.43
1:B:120:PHE:HB2	3:B:919:HOH:O	2.17	0.43
1:B:436:LYS:HB2	3:B:818:HOH:O	2.17	0.43
1:A:128:MET:CE	1:B:315:GLY:O	2.59	0.43
1:A:199:GLY:HA2	1:A:453:PHE:CE2	2.53	0.42
1:B:220:TYR:HA	1:B:269:ILE:O	2.19	0.42
1:A:393:GLU:HB3	1:A:397:HIS:CD2	2.54	0.42
1:B:199:GLY:HA2	1:B:453:PHE:CE2	2.55	0.42
1:B:258:GLU:O	1:B:297:GLY:HA2	2.18	0.42
1:A:253:ALA:HB1	1:A:259:LEU:CD2	2.50	0.42
1:A:302:THR:HG21	1:B:256:LEU:HD22	2.00	0.41
1:A:416:TYR:CZ	1:A:418:ASN:HB2	2.56	0.41
1:B:141:LEU:O	1:B:145:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLY:HA2	1:A:204:PHE:HE2	1.86	0.41
1:B:2:GLN:HE21	1:B:25:PRO:HB3	1.86	0.41
1:A:429:ARG:HD3	3:A:729:HOH:O	2.21	0.41
1:B:120:PHE:N	3:B:919:HOH:O	2.53	0.41
1:B:128:MET:HG3	1:B:128:MET:O	2.21	0.41
1:B:131:THR:CG2	1:B:207:ASP:O	2.69	0.41
1:B:446:LYS:HD3	1:B:447:TYR:CE1	2.56	0.41
1:A:54:THR:HB	1:A:55:PRO:HD3	2.03	0.41
1:A:421:ASN:HB2	1:A:422:PRO:HD2	2.03	0.41
1:B:376:ARG:HG3	3:B:885:HOH:O	2.20	0.41
1:B:393:GLU:O	1:B:397:HIS:HD2	2.04	0.40
1:A:451:ASN:HD21	1:A:458:ASN:ND2	2.06	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	458/468 (98%)	448 (98%)	10 (2%)	0	100	100
1	B	459/468 (98%)	444 (97%)	14 (3%)	1 (0%)	43	36
All	All	917/936 (98%)	892 (97%)	24 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/361 (98%)	339 (96%)	16 (4%)	24	14
1	B	356/361 (99%)	342 (96%)	14 (4%)	28	18
All	All	711/722 (98%)	681 (96%)	30 (4%)	26	16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	21	GLU
1	A	22	LEU
1	A	131	THR
1	A	137	SER
1	A	214	VAL
1	A	228	GLN
1	A	234	ARG
1	A	306	ARG
1	A	317	VAL
1	A	331	GLU
1	A	340	VAL
1	A	352	THR
1	A	359	LEU
1	A	426	ASP
1	A	438	GLU
1	B	35	ARG
1	B	106	LEU
1	B	108	ARG
1	B	116	LEU
1	B	131	THR
1	B	223	LEU
1	B	262	ASP
1	B	286	LEU
1	B	318	VAL
1	B	331	GLU
1	B	354	LEU

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Mol	Chain	Res	Type
1	B	426	ASP
1	B	455	LEU
1	B	462	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	138	HIS
1	A	228	GLN
1	A	236	HIS
1	A	264	HIS
1	A	330	ASN
1	A	353	GLN
1	A	375	ASN
1	A	418	ASN
1	A	458	ASN
1	B	2	GLN
1	B	125	GLN
1	B	163	ASN
1	B	236	HIS
1	B	264	HIS
1	B	296	HIS
1	B	330	ASN
1	B	411	HIS
1	B	441	GLN
1	B	458	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

2 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	B	600	-	58,58,58	1.91	8 (13%)	85,89,89	1.59	17 (20%)
2	FAD	A	600	-	58,58,58	1.70	8 (13%)	85,89,89	1.51	12 (14%)

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	B	600	-	-	4/34/50/50	0/6/6/6
2	FAD	A	600	-	-	6/34/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	PA-O3P	7.73	1.67	1.59
2	B	600	FAD	P-O3P	7.17	1.67	1.59
2	A	600	FAD	P-O3P	6.24	1.66	1.59
2	A	600	FAD	C8A-N7A	4.92	1.41	1.31
2	A	600	FAD	C4X-N5	4.22	1.39	1.30
2	A	600	FAD	PA-O3P	4.01	1.63	1.59
2	B	600	FAD	C8A-N7A	3.99	1.39	1.31
2	B	600	FAD	C4X-N5	3.92	1.39	1.30
2	A	600	FAD	C4-N3	-3.15	1.33	1.38
2	B	600	FAD	C2-N3	-2.79	1.32	1.39
2	B	600	FAD	C8M-C8	2.66	1.56	1.51
2	A	600	FAD	O4-C4	2.21	1.27	1.23
2	B	600	FAD	P-O2P	-2.17	1.45	1.55
2	A	600	FAD	C4X-C10	2.06	1.50	1.44
2	B	600	FAD	C5A-C4A	2.04	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C5A-N7A	-2.02	1.35	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	N3A-C2A-N1A	-4.44	121.86	128.58
2	B	600	FAD	N3A-C2A-N1A	-4.39	121.94	128.58
2	A	600	FAD	C5A-C4A-N3A	-3.94	121.29	126.72
2	A	600	FAD	O4B-C1B-N9A	-3.64	101.10	108.09
2	A	600	FAD	C4'-C3'-C2'	-3.43	107.86	113.57
2	A	600	FAD	N9A-C8A-N7A	-3.41	109.10	113.94
2	B	600	FAD	C4-C4X-N5	3.37	122.86	118.21
2	B	600	FAD	C4'-C3'-C2'	-3.30	108.07	113.57
2	B	600	FAD	C5A-C4A-N3A	-3.28	122.20	126.72
2	B	600	FAD	O3B-C3B-C4B	-3.27	101.70	111.08
2	B	600	FAD	O3P-PA-O1A	-3.25	100.91	110.70
2	B	600	FAD	O4-C4-C4X	-2.98	118.66	126.53
2	B	600	FAD	C2A-N1A-C6A	2.84	123.40	118.73
2	B	600	FAD	O2P-P-O3P	-2.84	99.60	107.27
2	B	600	FAD	O4B-C1B-N9A	-2.73	102.86	108.09
2	B	600	FAD	C5A-C4A-N9A	2.64	108.68	105.81
2	A	600	FAD	C4A-N9A-C8A	2.62	108.49	105.74
2	B	600	FAD	O4'-C4'-C3'	-2.50	103.40	109.25
2	A	600	FAD	C2A-N3A-C4A	2.40	117.70	111.83
2	A	600	FAD	C2A-N1A-C6A	2.31	122.53	118.73
2	B	600	FAD	O2-C2-N1	-2.30	117.97	121.80
2	A	600	FAD	O4-C4-C4X	-2.30	120.47	126.53
2	A	600	FAD	O3P-PA-O1A	-2.27	103.87	110.70
2	A	600	FAD	N6A-C6A-N1A	2.22	123.31	118.38
2	A	600	FAD	O2A-PA-O3P	2.18	113.17	107.27
2	B	600	FAD	C4X-C10-N10	-2.11	113.47	116.48
2	B	600	FAD	O2P-P-O1P	2.08	122.13	112.44
2	B	600	FAD	C4X-C4-N3	2.07	118.53	113.25
2	B	600	FAD	N3-C2-N1	2.05	123.85	119.50

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C2'-C3'-C4'-O4'
2	A	600	FAD	C2'-C3'-C4'-C5'
2	B	600	FAD	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	A	600	FAD	O3'-C3'-C4'-O4'
2	B	600	FAD	O3'-C3'-C4'-C5'
2	B	600	FAD	C2'-C3'-C4'-O4'
2	A	600	FAD	O3'-C3'-C4'-C5'
2	A	600	FAD	N10-C1'-C2'-O2'
2	A	600	FAD	PA-O3P-P-O2P
2	B	600	FAD	PA-O3P-P-O2P

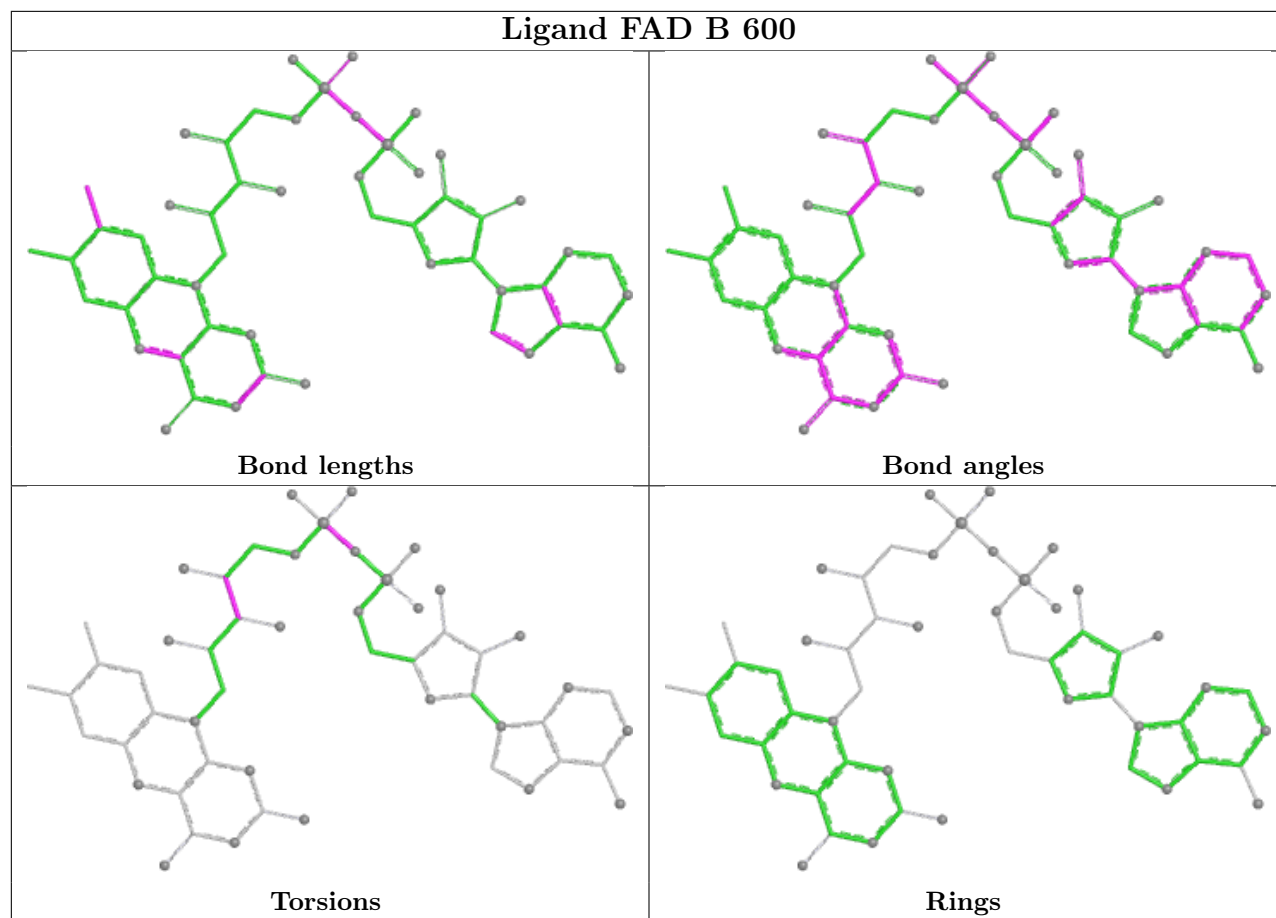
There are no ring outliers.

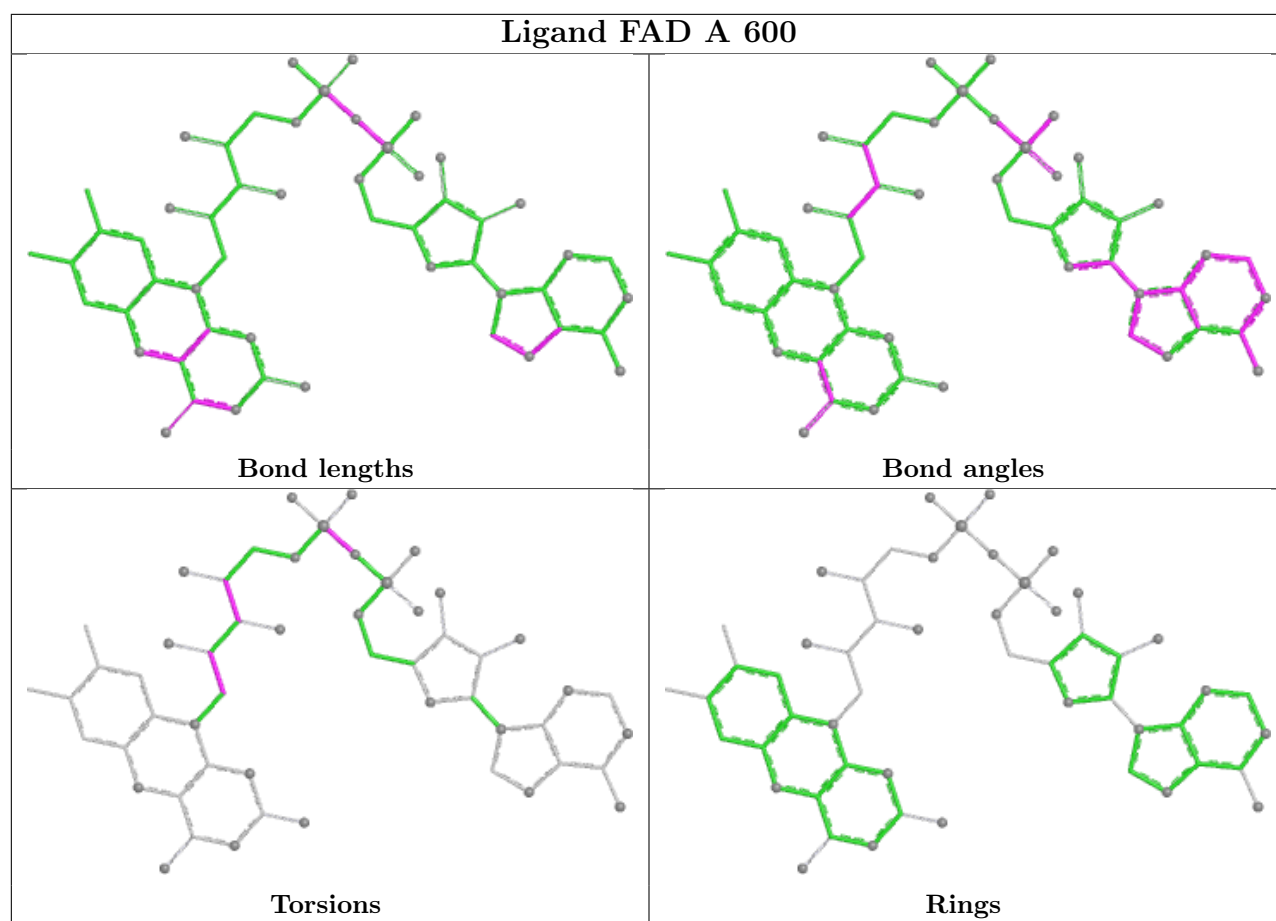
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAD	6	0
2	A	600	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.

Ligand FAD B 600





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	460/468 (98%)	0.01	6 (1%) 75 81	8, 15, 27, 44	0
1	B	461/468 (98%)	0.11	10 (2%) 62 69	8, 16, 31, 46	0
All	All	921/936 (98%)	0.06	16 (1%) 69 76	8, 15, 29, 46	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	ALA	5.1
1	A	316	ALA	4.0
1	B	315	GLY	3.6
1	B	317	VAL	3.6
1	B	314	PRO	3.4
1	B	262	ASP	3.2
1	B	3	PHE	3.0
1	A	317	VAL	2.7
1	A	348	ALA	2.6
1	A	318	VAL	2.5
1	B	368	ASP	2.5
1	A	3	PHE	2.3
1	A	319	PRO	2.2
1	B	318	VAL	2.2
1	B	9	ALA	2.0
1	B	261	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

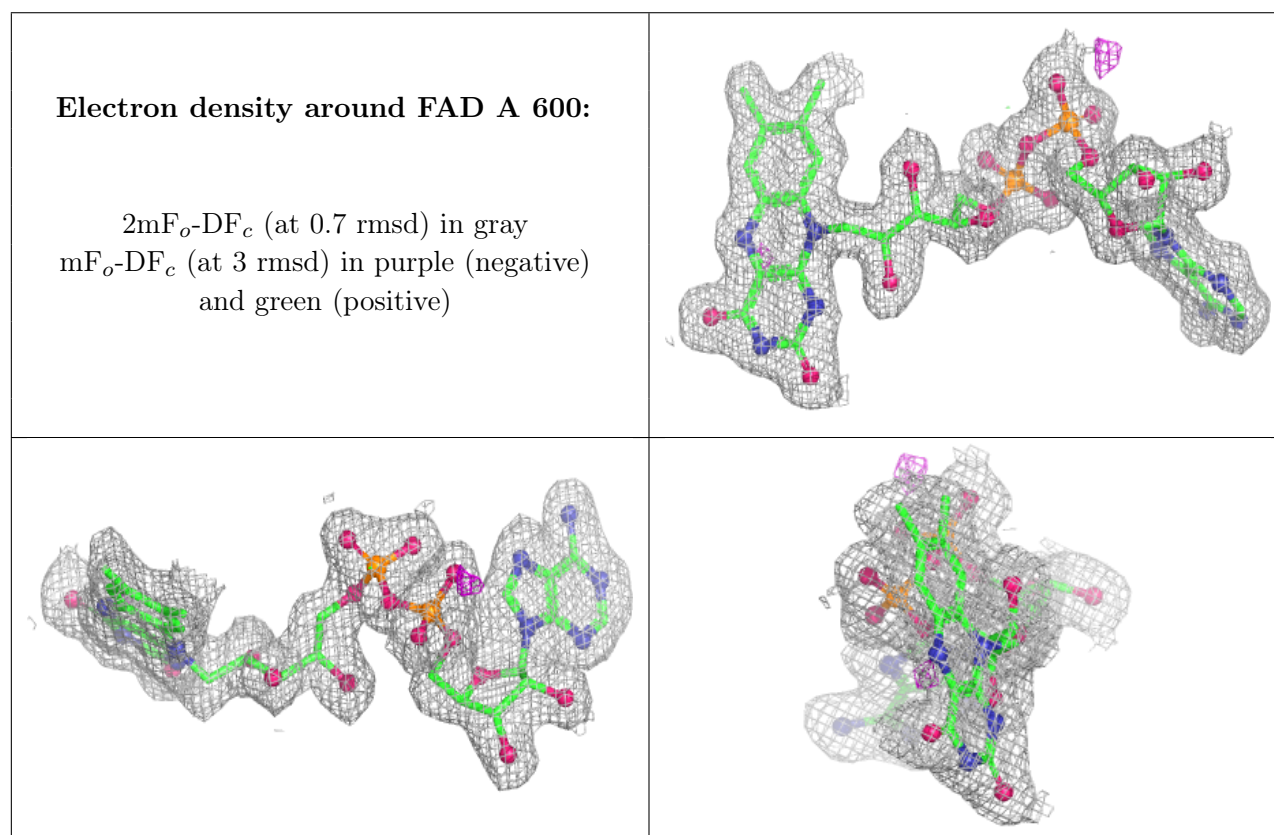
There are no oligosaccharides in this entry.

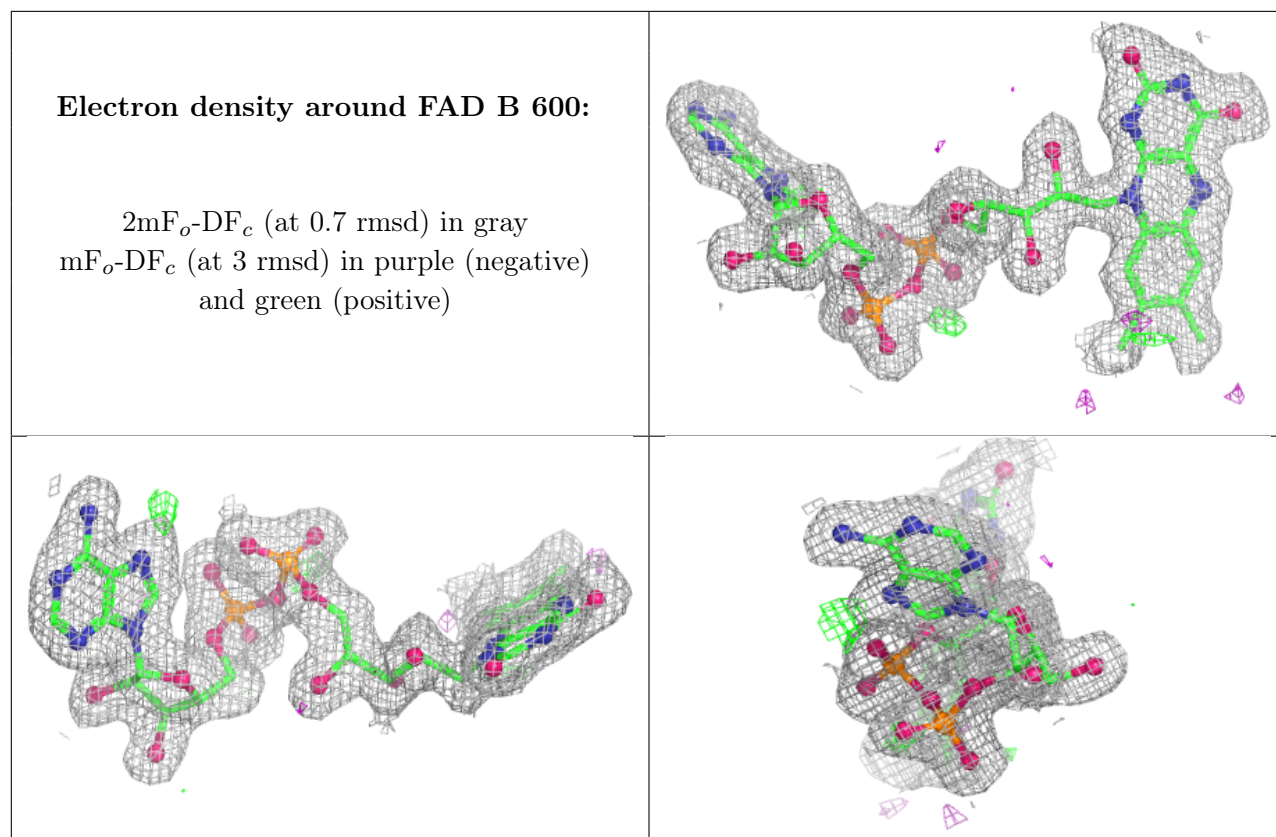
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	600	53/53	0.97	0.05	8,9,10,10	0
2	FAD	B	600	53/53	0.97	0.06	8,9,11,11	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.