



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:45 AM UTC

PDB ID : 1RSG / pdb_00001rsg
Title : Crystal structure of the polyamine oxidase Fms1 from yeast
Authors : Huang, Q.; Liu, Q.; Hao, Q.
Deposited on : 2003-12-09
Resolution : 1.90 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 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

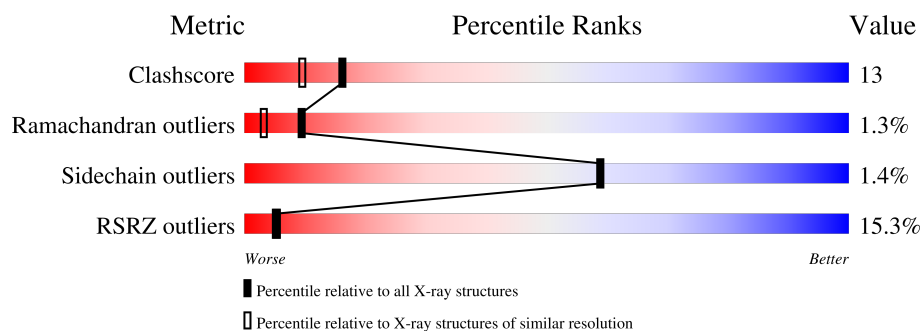
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 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	516	
1	B	516	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8861 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 FMS1 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	Se	0	0	0
			3855	2443	670	720	11	11			
1	B	491	Total	C	N	O	S	Se	0	0	0
			3931	2486	683	740	11	11			

There are 40 discrepancies between the modelled and reference sequences:

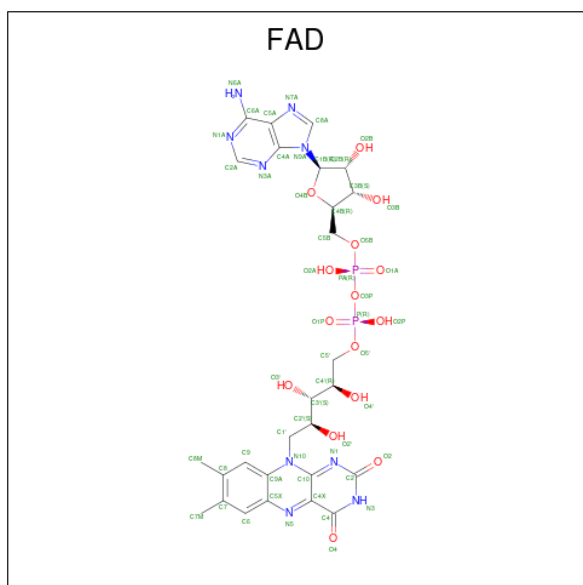
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P50264
A	122	MSE	MET	modified residue	UNP P50264
A	146	MSE	MET	modified residue	UNP P50264
A	339	MSE	MET	modified residue	UNP P50264
A	373	MSE	MET	modified residue	UNP P50264
A	374	MSE	MET	modified residue	UNP P50264
A	376	MSE	MET	modified residue	UNP P50264
A	406	MSE	MET	modified residue	UNP P50264
A	418	MSE	MET	modified residue	UNP P50264
A	462	MSE	MET	modified residue	UNP P50264
A	466	MSE	MET	modified residue	UNP P50264
A	483	MSE	MET	modified residue	UNP P50264
A	509	LEU	-	cloning artifact	UNP P50264
A	510	GLU	-	cloning artifact	UNP P50264
A	511	HIS	-	cloning artifact	UNP P50264
A	512	HIS	-	cloning artifact	UNP P50264
A	513	HIS	-	cloning artifact	UNP P50264
A	514	HIS	-	cloning artifact	UNP P50264
A	515	HIS	-	cloning artifact	UNP P50264
A	516	HIS	-	cloning artifact	UNP P50264
B	1	MSE	MET	modified residue	UNP P50264
B	122	MSE	MET	modified residue	UNP P50264
B	146	MSE	MET	modified residue	UNP P50264
B	339	MSE	MET	modified residue	UNP P50264
B	373	MSE	MET	modified residue	UNP P50264

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Chain	Residue	Modelled	Actual	Comment	Reference
B	374	MSE	MET	modified residue	UNP P50264
B	376	MSE	MET	modified residue	UNP P50264
B	406	MSE	MET	modified residue	UNP P50264
B	418	MSE	MET	modified residue	UNP P50264
B	462	MSE	MET	modified residue	UNP P50264
B	466	MSE	MET	modified residue	UNP P50264
B	483	MSE	MET	modified residue	UNP P50264
B	509	LEU	-	cloning artifact	UNP P50264
B	510	GLU	-	cloning artifact	UNP P50264
B	511	HIS	-	cloning artifact	UNP P50264
B	512	HIS	-	cloning artifact	UNP P50264
B	513	HIS	-	cloning artifact	UNP P50264
B	514	HIS	-	cloning artifact	UNP P50264
B	515	HIS	-	cloning artifact	UNP P50264
B	516	HIS	-	cloning artifact	UNP P50264

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



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

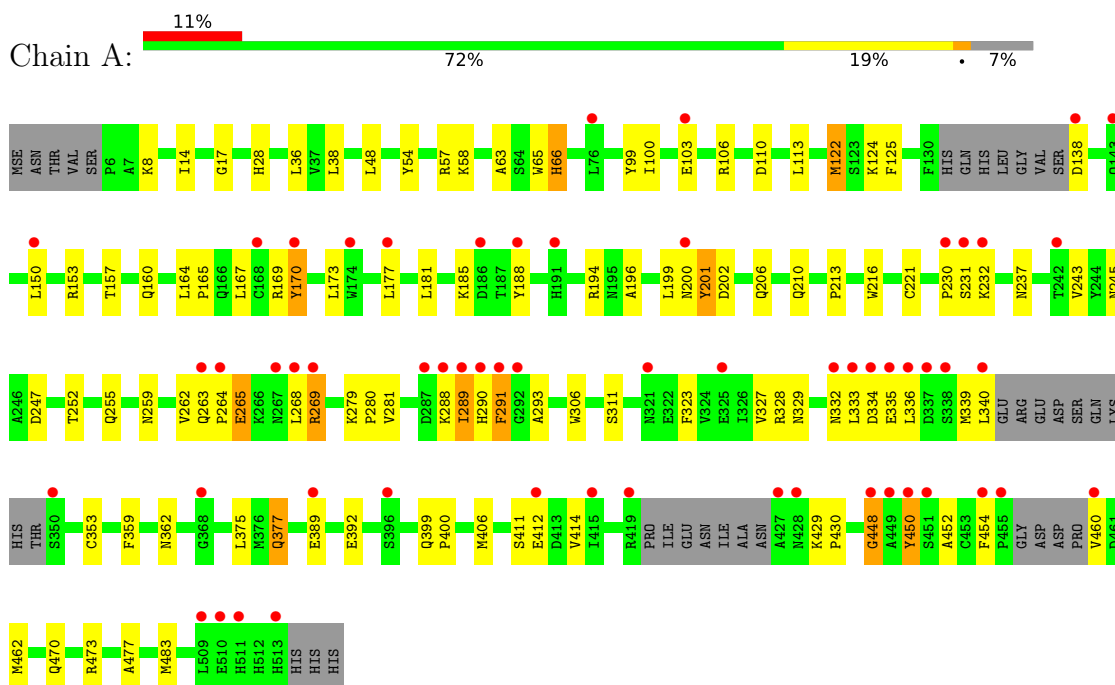
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	528	Total 528	O 528	0	0
3	B	441	Total 441	O 441	0	0

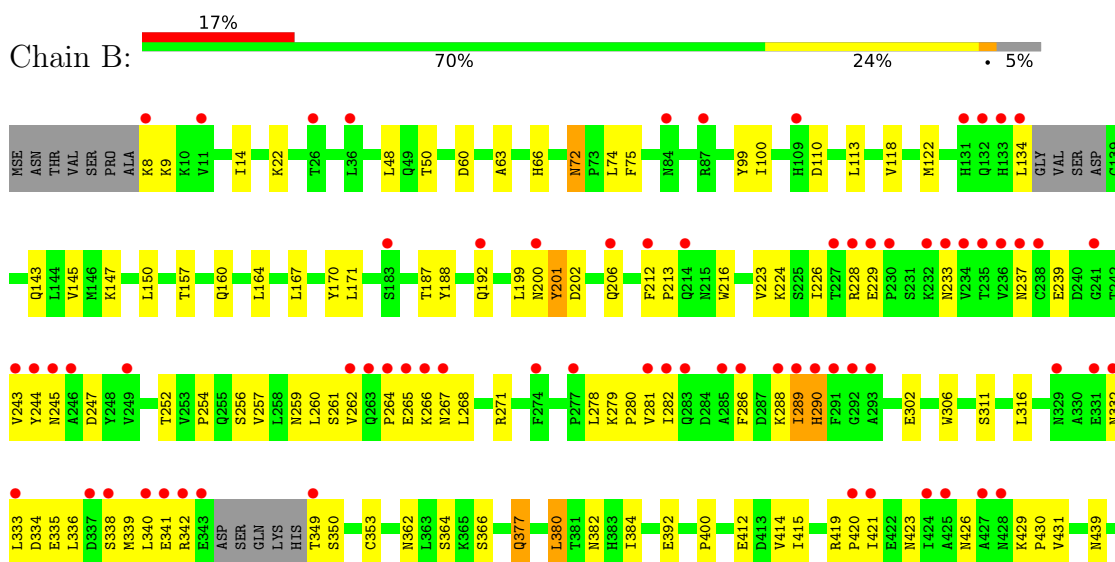
3 Residue-property plots [i](#)

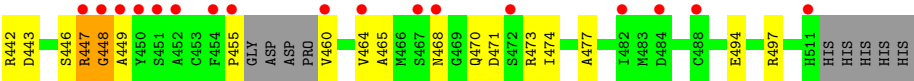
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: FMS1 protein



• Molecule 1: FMS1 protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.38Å 103.13Å 77.59Å 90.00° 94.98° 90.00°	Depositor
Resolution (Å)	35.95 – 1.90 35.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (35.95-1.90) 93.6 (35.95-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.245 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8861	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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	0.37	0/3922	0.83	6/5278 (0.1%)
1	B	0.34	0/3998	0.83	8/5385 (0.1%)
All	All	0.35	0/7920	0.83	14/10663 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	ARG	CA-C-N	7.23	127.26	119.89
1	B	419	ARG	C-N-CA	7.23	127.26	119.89
1	A	201	TYR	N-CA-C	-6.96	104.05	112.54
1	B	201	TYR	N-CA-C	-6.42	104.71	112.54
1	A	17	GLY	N-CA-C	-6.37	102.19	112.31
1	B	420	PRO	N-CA-C	5.53	119.90	111.11
1	A	66	HIS	N-CA-C	-5.42	98.93	108.20
1	B	366	SER	N-CA-C	5.41	118.35	111.69
1	A	100	ILE	N-CA-C	5.25	115.68	108.12
1	B	170	TYR	N-CA-C	-5.16	106.25	112.54
1	B	100	ILE	N-CA-C	5.10	115.25	108.11
1	A	170	TYR	N-CA-C	-5.07	106.19	112.38
1	A	65	TRP	N-CA-C	5.01	117.92	109.95
1	B	66	HIS	N-CA-C	-5.01	99.63	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3778	93	0
1	B	3931	0	3841	112	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
3	A	528	0	0	18	0
3	B	441	0	0	10	0
All	All	8861	0	7681	204	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 13.

All (204) 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:278:LEU:HA	1:B:470:GLN:HE22	1.15	1.05
1:A:353:CYS:SG	1:A:400:PRO:HG2	2.05	0.96
1:B:353:CYS:SG	1:B:400:PRO:HG2	2.13	0.88
1:B:470:GLN:HB3	1:B:474:ILE:HB	1.55	0.86
1:A:269:ARG:HA	1:A:269:ARG:CZ	2.05	0.85
1:B:290:HIS:HA	1:B:449:ALA:HB3	1.57	0.84
1:A:377:GLN:NE2	1:A:377:GLN:H	1.78	0.81
1:B:282:ILE:HD13	1:B:465:ALA:HB1	1.63	0.81
1:B:278:LEU:HA	1:B:470:GLN:NE2	1.96	0.81
1:B:150:LEU:HD12	1:B:333:LEU:HD23	1.62	0.80
1:A:406:MSE:HE2	1:A:430:PRO:HB3	1.65	0.79
1:B:192:GLN:HE21	1:B:455:PRO:HB2	1.47	0.78
1:B:14:ILE:HD12	1:B:226:ILE:HD11	1.70	0.74
1:B:8:LYS:HG3	1:B:9:LYS:HG2	1.67	0.73
1:B:72:ASN:C	1:B:72:ASN:HD22	1.99	0.71
1:A:289:ILE:HD11	1:A:462:MSE:HE2	1.74	0.70
1:B:289:ILE:HG22	1:B:290:HIS:N	2.06	0.70
1:B:289:ILE:HG23	3:B:2165:HOH:O	1.90	0.70
1:B:377:GLN:NE2	1:B:377:GLN:H	1.90	0.69
1:A:237:ASN:OD1	1:A:243:VAL:HG22	1.92	0.68
1:A:406:MSE:HE3	1:A:411:SER:OG	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASP:OD1	1:A:185:LYS:HD2	1.93	0.67
1:A:332:ASN:HD21	1:A:334:ASP:HB2	1.60	0.67
1:A:448:GLY:HA2	3:A:1861:HOH:O	1.94	0.67
1:A:150:LEU:HD12	1:A:333:LEU:HD23	1.77	0.67
1:B:289:ILE:HG22	1:B:290:HIS:H	1.60	0.67
1:A:252:THR:HG22	1:A:477:ALA:HB3	1.76	0.66
1:A:406:MSE:HE2	1:A:430:PRO:CB	2.25	0.66
1:B:256:SER:CB	1:B:448:GLY:HA3	2.25	0.66
1:B:14:ILE:CD1	1:B:226:ILE:HD11	2.26	0.65
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.26	0.65
1:B:261:SER:HA	1:B:271:ARG:NH1	2.12	0.65
1:B:380:LEU:HD22	1:B:384:ILE:HG12	1.78	0.65
1:B:122:MSE:HE2	1:B:145:VAL:HG22	1.78	0.65
1:A:306:TRP:HE3	1:A:406:MSE:HE1	1.62	0.65
1:B:143:GLN:O	1:B:147:LYS:HG3	1.96	0.64
1:B:260:LEU:HD22	1:B:268:LEU:HD13	1.79	0.64
1:B:8:LYS:HE2	1:B:245:ASN:H	1.63	0.64
1:A:265:GLU:CG	1:A:268:LEU:HG	2.29	0.63
1:A:291:PHE:HA	3:A:2117:HOH:O	1.99	0.63
1:A:268:LEU:HD12	3:A:2161:HOH:O	1.99	0.63
1:B:259:ASN:O	1:B:262:VAL:HG22	1.98	0.63
1:B:122:MSE:CE	1:B:145:VAL:HG22	2.29	0.62
1:A:58:LYS:HE2	3:A:2013:HOH:O	1.99	0.62
1:A:289:ILE:HD13	1:A:462:MSE:HB2	1.81	0.62
1:A:259:ASN:O	1:A:262:VAL:HG22	2.01	0.61
1:B:256:SER:HB2	1:B:448:GLY:HA3	1.82	0.61
1:A:288:LYS:O	1:A:289:ILE:HG23	2.01	0.60
1:B:302:GLU:HG3	1:B:431:VAL:HB	1.83	0.60
1:A:264:PRO:O	1:A:265:GLU:CB	2.50	0.59
1:B:122:MSE:HE3	1:B:188:TYR:OH	2.02	0.58
1:B:63:ALA:HA	2:B:1802:FAD:N5	2.19	0.58
1:B:171:LEU:HD13	1:B:187:THR:HG22	1.86	0.57
1:A:202:ASP:O	1:A:206:GLN:HG2	2.05	0.57
1:B:289:ILE:O	1:B:290:HIS:HB2	2.04	0.57
1:B:439:ASN:HD21	1:B:442:ARG:HD3	1.69	0.57
1:A:36:LEU:HD12	1:A:216:TRP:O	2.03	0.57
1:B:311:SER:HA	1:B:362:ASN:HB3	1.87	0.57
1:A:63:ALA:HA	2:A:1801:FAD:N5	2.20	0.57
1:A:412:GLU:OE1	1:A:429:LYS:HG2	2.05	0.57
1:B:228:ARG:HD3	1:B:471:ASP:OD2	2.05	0.57
1:B:290:HIS:HA	1:B:449:ALA:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:CD2	1:A:63:ALA:HB3	2.35	0.56
1:A:265:GLU:HG3	1:A:268:LEU:HG	1.87	0.56
1:A:206:GLN:O	1:A:210:GLN:HG3	2.05	0.56
1:A:311:SER:HA	1:A:362:ASN:HB3	1.87	0.56
1:A:247:ASP:O	1:A:473:ARG:HD2	2.05	0.56
1:B:392:GLU:HG3	3:B:2083:HOH:O	2.06	0.56
1:A:122:MSE:HE2	1:A:188:TYR:OH	2.05	0.56
1:B:279:LYS:HG3	1:B:281:VAL:HG12	1.87	0.56
1:A:460:VAL:N	3:A:1955:HOH:O	2.39	0.55
1:B:237:ASN:OD1	1:B:243:VAL:HG13	2.06	0.55
1:A:232:LYS:HG2	3:A:2155:HOH:O	2.07	0.55
1:B:349:THR:HB	3:B:2186:HOH:O	2.07	0.55
1:A:377:GLN:H	1:A:377:GLN:HE21	1.52	0.54
1:B:439:ASN:ND2	1:B:442:ARG:HD3	2.22	0.54
1:A:231:SER:O	1:A:232:LYS:HB2	2.07	0.53
1:A:306:TRP:CE3	1:A:406:MSE:HE1	2.41	0.53
1:B:447:ARG:HG3	1:B:448:GLY:H	1.73	0.53
1:B:332:ASN:HD21	1:B:334:ASP:HB2	1.73	0.53
1:A:290:HIS:O	1:A:291:PHE:HB2	2.09	0.53
1:B:72:ASN:C	1:B:72:ASN:ND2	2.67	0.53
1:B:110:ASP:HB3	1:B:113:LEU:HB2	1.92	0.52
1:B:254:PRO:HG2	1:B:257:VAL:HG23	1.91	0.52
1:B:282:ILE:HG22	1:B:286:PHE:HE1	1.74	0.52
1:B:289:ILE:CG2	1:B:290:HIS:H	2.21	0.52
1:B:447:ARG:HG3	1:B:448:GLY:N	2.24	0.52
1:A:36:LEU:HD21	1:A:38:LEU:HD21	1.91	0.52
1:B:212:PHE:HB2	1:B:213:PRO:HD2	1.92	0.52
1:A:177:LEU:HD11	1:A:181:LEU:HB2	1.93	0.51
1:B:256:SER:HB3	1:B:448:GLY:HA3	1.92	0.51
1:A:150:LEU:O	1:A:153:ARG:HD2	2.11	0.51
1:A:14:ILE:HD12	1:A:14:ILE:N	2.25	0.51
1:B:460:VAL:HG22	3:B:2101:HOH:O	2.09	0.51
1:A:54:TYR:O	1:A:57:ARG:HG3	2.10	0.51
1:A:452:ALA:HB3	1:A:454:PHE:CZ	2.46	0.51
1:B:423:ASN:HB3	1:B:426:ASN:ND2	2.26	0.51
1:B:289:ILE:CG2	1:B:290:HIS:N	2.73	0.51
1:B:266:LYS:HA	1:B:271:ARG:HE	1.76	0.50
1:A:323:PHE:O	1:A:327:VAL:HG23	2.10	0.50
1:A:414:VAL:HA	1:A:430:PRO:HG2	1.93	0.50
1:B:286:PHE:C	1:B:288:LYS:H	2.19	0.50
1:A:265:GLU:HG2	1:A:268:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:MSE:HE3	1:A:411:SER:CB	2.42	0.50
1:B:264:PRO:O	1:B:265:GLU:HB2	2.12	0.50
1:B:278:LEU:CA	1:B:470:GLN:HE22	2.05	0.50
1:A:289:ILE:CD1	1:A:462:MSE:HB2	2.42	0.49
1:B:157:THR:OG1	1:B:160:GLN:HG3	2.13	0.49
1:A:230:PRO:C	1:A:232:LYS:H	2.20	0.49
1:B:8:LYS:HG2	1:B:245:ASN:OD1	2.13	0.49
1:B:415:ILE:HD11	1:B:429:LYS:HD2	1.93	0.49
1:A:157:THR:OG1	1:A:160:GLN:HG3	2.13	0.49
1:B:63:ALA:HA	2:B:1802:FAD:C4X	2.43	0.49
1:A:288:LYS:C	1:A:289:ILE:HG12	2.37	0.48
1:A:406:MSE:HE2	1:A:430:PRO:CG	2.43	0.48
1:A:167:LEU:C	1:A:167:LEU:HD23	2.38	0.48
1:B:447:ARG:CG	1:B:448:GLY:H	2.24	0.48
1:A:359:PHE:HD2	1:A:375:LEU:HD22	1.78	0.48
1:B:8:LYS:NZ	1:B:244:TYR:HA	2.28	0.48
1:B:335:GLU:O	1:B:339:MSE:HG3	2.14	0.48
1:A:329:ASN:HB2	1:A:339:MSE:HE1	1.94	0.48
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.95	0.48
1:A:165:PRO:O	1:A:169:ARG:HG3	2.13	0.48
1:B:342:ARG:HB3	3:B:2184:HOH:O	2.14	0.48
1:A:280:PRO:HG2	3:A:1916:HOH:O	2.12	0.47
1:B:118:VAL:HG23	1:B:164:LEU:HD13	1.95	0.47
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.75	0.47
1:B:332:ASN:ND2	1:B:334:ASP:HB2	2.28	0.47
1:B:414:VAL:HA	1:B:430:PRO:HG2	1.96	0.47
1:A:58:LYS:HD3	3:A:2282:HOH:O	2.13	0.47
1:A:255:GLN:NE2	1:A:289:ILE:HD12	2.30	0.47
1:B:134:LEU:HA	3:B:2019:HOH:O	2.15	0.47
1:B:338:SER:HA	1:B:341:GLU:OE2	2.14	0.47
1:B:377:GLN:H	1:B:377:GLN:HE21	1.60	0.47
1:B:415:ILE:HD13	1:B:426:ASN:OD1	2.15	0.47
1:A:164:LEU:N	1:A:165:PRO:HD2	2.30	0.47
1:A:281:VAL:HG13	3:A:1916:HOH:O	2.15	0.47
1:A:264:PRO:O	1:A:265:GLU:HB3	2.15	0.47
1:B:289:ILE:HD12	3:B:2167:HOH:O	2.14	0.46
1:A:28:HIS:HD2	3:A:1835:HOH:O	1.98	0.46
1:A:122:MSE:O	1:A:125:PHE:HB3	2.15	0.46
1:A:406:MSE:HE2	1:A:430:PRO:HG3	1.97	0.46
1:A:138:ASP:HB3	3:A:1993:HOH:O	2.15	0.46
1:A:269:ARG:HA	1:A:269:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:THR:OG1	1:B:202:ASP:HB3	2.14	0.45
1:B:464:VAL:O	1:B:468:ASN:HB2	2.16	0.45
1:A:263:GLN:HB2	3:A:2161:HOH:O	2.15	0.45
1:B:229:GLU:OE1	1:B:233:ASN:HB2	2.16	0.45
1:B:224:LYS:HD3	1:B:239:GLU:OE1	2.16	0.45
1:A:306:TRP:HE1	1:A:362:ASN:HD21	1.65	0.45
1:B:316:LEU:HD12	1:B:316:LEU:N	2.31	0.45
1:B:202:ASP:O	1:B:206:GLN:HG3	2.17	0.45
1:B:213:PRO:HG2	1:B:216:TRP:CE2	2.52	0.45
1:A:293:ALA:HA	1:A:450:TYR:HB3	1.99	0.44
1:A:399:GLN:N	1:A:400:PRO:HD2	2.32	0.44
1:B:60:ASP:HB3	1:B:63:ALA:O	2.17	0.44
1:B:306:TRP:HE1	1:B:362:ASN:HD21	1.65	0.44
1:A:8:LYS:HD2	1:A:245:ASN:HD22	1.81	0.44
1:B:167:LEU:C	1:B:167:LEU:HD23	2.43	0.44
1:A:269:ARG:HA	1:A:269:ARG:NE	2.32	0.44
1:B:494:GLU:OE1	1:B:497:ARG:NH2	2.51	0.43
1:B:281:VAL:HG13	1:B:282:ILE:N	2.33	0.43
1:A:173:LEU:HD22	1:A:173:LEU:N	2.34	0.43
1:A:336:LEU:O	1:A:340:LEU:HG	2.18	0.43
1:A:279:LYS:HG3	1:A:470:GLN:OE1	2.19	0.43
1:A:483:MSE:HE2	3:A:2195:HOH:O	2.19	0.43
1:A:124:LYS:HG2	1:B:192:GLN:HA	2.01	0.42
1:A:335:GLU:O	1:A:339:MSE:HG3	2.19	0.42
1:A:483:MSE:HG3	3:A:2063:HOH:O	2.17	0.42
1:B:412:GLU:HB2	3:B:1919:HOH:O	2.18	0.42
1:B:72:ASN:HD21	1:B:74:LEU:HB3	1.85	0.42
1:B:213:PRO:HG2	1:B:216:TRP:CD1	2.54	0.42
1:B:447:ARG:O	1:B:448:GLY:C	2.63	0.42
1:B:254:PRO:HG2	1:B:257:VAL:CG2	2.49	0.42
1:B:382:ASN:HB3	3:B:2080:HOH:O	2.18	0.42
1:B:260:LEU:O	1:B:271:ARG:NH1	2.52	0.42
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.72	0.42
1:B:446:SER:O	1:B:447:ARG:C	2.62	0.42
1:B:288:LYS:O	1:B:289:ILE:HB	2.19	0.42
1:B:192:GLN:NE2	1:B:455:PRO:HB2	2.24	0.42
1:B:447:ARG:CG	1:B:448:GLY:N	2.83	0.42
1:B:279:LYS:HB2	1:B:280:PRO:HD2	2.02	0.41
1:A:194:ARG:NH1	3:A:1821:HOH:O	2.50	0.41
1:A:66:HIS:HB2	1:A:196:ALA:HB3	2.02	0.41
1:B:443:ASP:HB3	1:B:446:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:NH2	1:A:328:ARG:O	2.52	0.41
1:A:99:TYR:O	1:A:106:ARG:HA	2.20	0.41
1:B:336:LEU:O	1:B:340:LEU:HG	2.20	0.41
1:B:362:ASN:HD21	1:B:364:SER:HB3	1.86	0.41
1:A:103:GLU:HG3	3:A:2227:HOH:O	2.19	0.41
1:B:8:LYS:HB2	3:B:2030:HOH:O	2.20	0.41
1:A:110:ASP:HB3	1:A:113:LEU:HB2	2.03	0.41
1:B:72:ASN:ND2	1:B:75:PHE:H	2.18	0.41
1:A:167:LEU:O	1:A:170:TYR:CD2	2.74	0.41
1:B:261:SER:C	1:B:271:ARG:HH12	2.29	0.41
1:A:28:HIS:CD2	1:A:213:PRO:HD3	2.55	0.40
1:B:278:LEU:HD23	1:B:470:GLN:NE2	2.36	0.40
1:B:247:ASP:O	1:B:473:ARG:HD2	2.21	0.40
1:A:392:GLU:HG3	3:A:1999:HOH:O	2.21	0.40
1:A:138:ASP:N	3:A:2140:HOH:O	2.54	0.40
1:B:14:ILE:HD13	1:B:223:VAL:HG11	2.03	0.40
1:A:255:GLN:CD	1:A:290:HIS:CD2	3.00	0.40
1:B:99:TYR:HB3	1:B:316:LEU:HD11	2.03	0.40
1:B:265:GLU:C	1:B:267:ASN:H	2.29	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	471/516 (91%)	446 (95%)	20 (4%)	5 (1%)	11	4
1	B	483/516 (94%)	456 (94%)	20 (4%)	7 (1%)	9	3
All	All	954/1032 (92%)	902 (94%)	40 (4%)	12 (1%)	9	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	265	GLU
1	A	291	PHE
1	A	448	GLY
1	A	450	TYR
1	B	200	ASN
1	B	289	ILE
1	B	290	HIS
1	B	350	SER
1	B	447	ARG
1	B	448	GLY
1	B	421	ILE

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	422/445 (95%)	415 (98%)	7 (2%)	53	52
1	B	431/445 (97%)	426 (99%)	5 (1%)	63	63
All	All	853/890 (96%)	841 (99%)	12 (1%)	59	59

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	MSE
1	A	201	TYR
1	A	221	CYS
1	A	269	ARG
1	A	289	ILE
1	A	377	GLN
1	A	389	GLU
1	B	22	LYS
1	B	72	ASN
1	B	201	TYR
1	B	377	GLN
1	B	380	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	151	GLN
1	A	214	GLN
1	A	233	ASN
1	A	245	ASN
1	A	255	GLN
1	A	329	ASN
1	A	332	ASN
1	A	356	GLN
1	A	362	ASN
1	A	377	GLN
1	A	434	ASN
1	A	513	HIS
1	B	72	ASN
1	B	80	GLN
1	B	109	HIS
1	B	192	GLN
1	B	233	ASN
1	B	259	ASN
1	B	275	GLN
1	B	329	ASN
1	B	332	ASN
1	B	362	ASN
1	B	377	GLN
1	B	382	ASN
1	B	439	ASN
1	B	470	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

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	1802	-	58,58,58	1.18	4 (6%)	85,89,89	1.09	9 (10%)
2	FAD	A	1801	-	58,58,58	1.10	5 (8%)	85,89,89	1.04	6 (7%)

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	1802	-	-	0/34/50/50	0/6/6/6
2	FAD	A	1801	-	-	0/34/50/50	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1802	FAD	C4X-N5	4.51	1.40	1.30
2	A	1801	FAD	C4X-N5	4.21	1.39	1.30
2	B	1802	FAD	C10-N1	2.62	1.38	1.33
2	B	1802	FAD	C2A-N1A	2.49	1.38	1.33
2	A	1801	FAD	C10-N1	2.33	1.37	1.33
2	B	1802	FAD	C9A-C5X	2.24	1.44	1.41
2	A	1801	FAD	C9-C8	2.20	1.42	1.39
2	A	1801	FAD	C2A-N1A	2.04	1.37	1.33
2	A	1801	FAD	C9A-C5X	2.01	1.44	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1802	FAD	C9A-C5X-N5	-2.70	119.59	122.45
2	B	1802	FAD	O3'-C3'-C4'	-2.66	102.89	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1802	FAD	O4B-C1B-C2B	-2.54	101.18	106.62
2	A	1801	FAD	O3'-C3'-C4'	-2.54	103.16	108.93
2	A	1801	FAD	C9A-C5X-N5	-2.49	119.82	122.45
2	A	1801	FAD	N3A-C2A-N1A	-2.35	125.02	128.58
2	B	1802	FAD	C5'-C4'-C3'	-2.29	107.89	112.22
2	B	1802	FAD	C4'-C3'-C2'	2.28	117.37	113.57
2	B	1802	FAD	N3A-C2A-N1A	-2.23	125.20	128.58
2	A	1801	FAD	O4B-C1B-C2B	-2.19	101.92	106.62
2	B	1802	FAD	C4-C4X-N5	2.18	121.22	118.21
2	A	1801	FAD	C5'-C4'-C3'	-2.13	108.19	112.22
2	B	1802	FAD	O3P-PA-O1A	-2.03	104.59	110.70
2	A	1801	FAD	C4'-C3'-C2'	2.02	116.93	113.57
2	B	1802	FAD	C10-C4X-N5	-2.02	120.69	124.81

There are no chirality outliers.

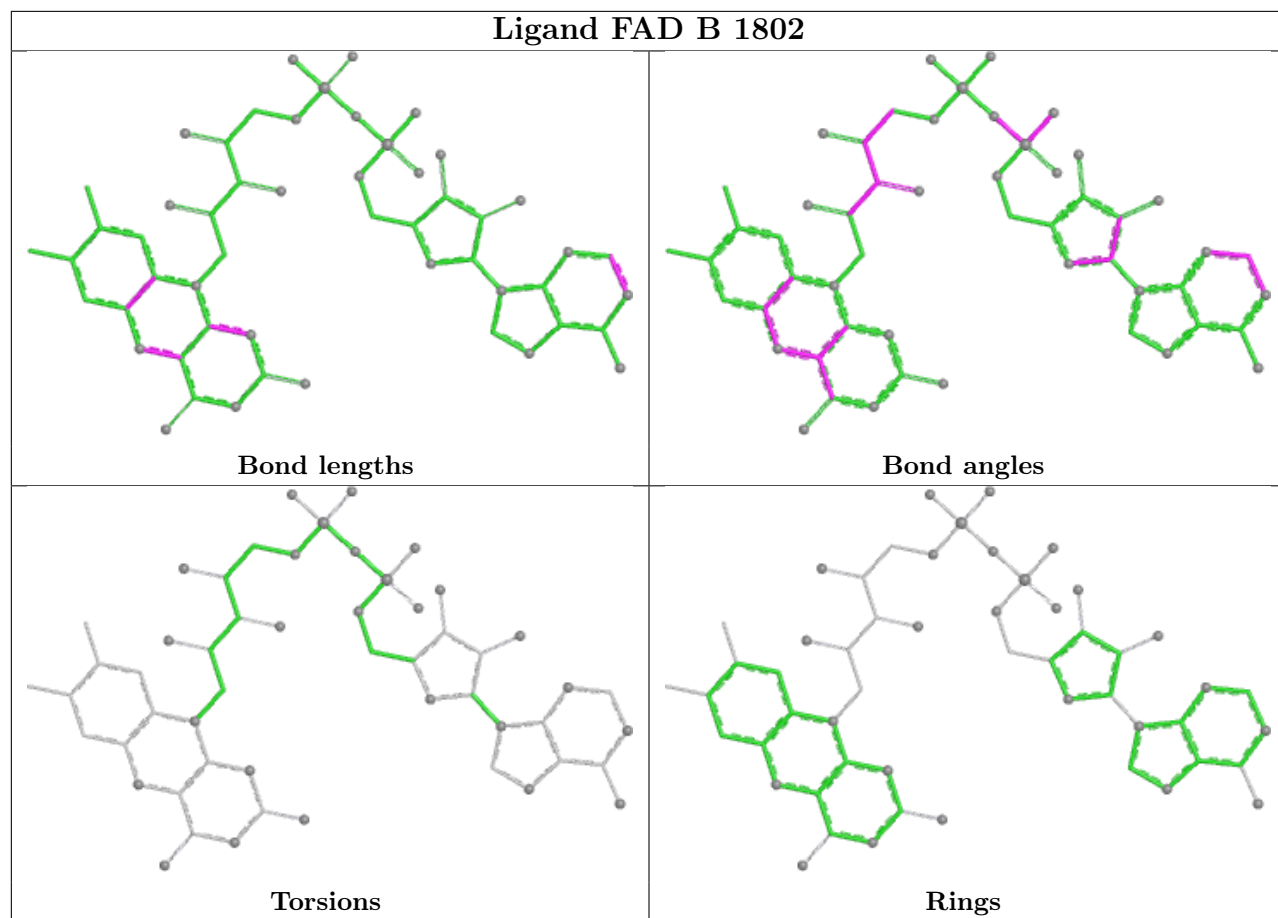
There are no torsion outliers.

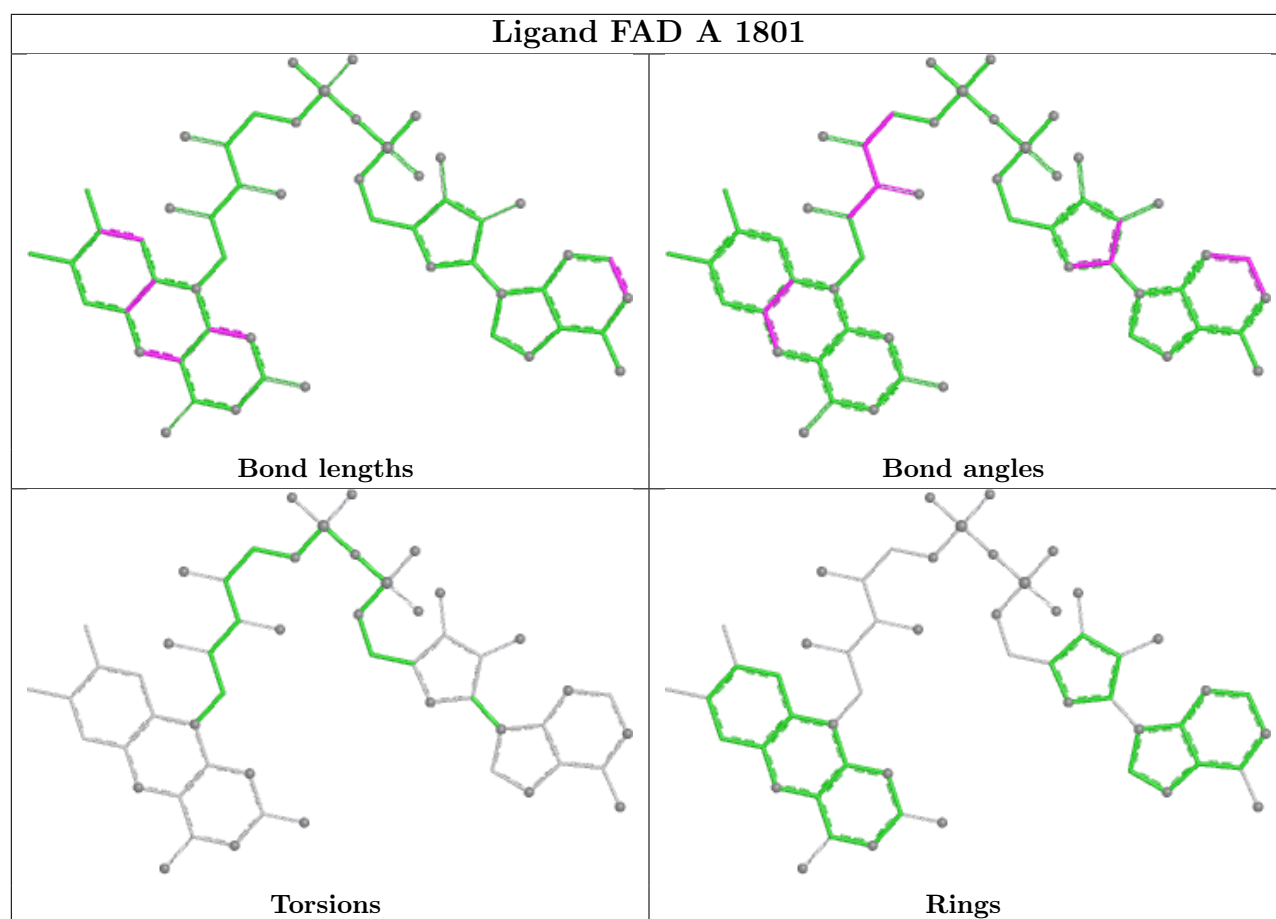
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1802	FAD	2	0
2	A	1801	FAD	1	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	470/516 (91%)	0.82	58 (12%) 8 9	16, 30, 54, 71	0
1	B	480/516 (93%)	1.04	87 (18%) 3 3	20, 33, 59, 73	0
All	All	950/1032 (92%)	0.93	145 (15%) 5 5	16, 32, 57, 73	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	PHE	7.7
1	A	449	ALA	7.3
1	B	448	GLY	6.9
1	B	449	ALA	6.8
1	B	291	PHE	6.5
1	A	264	PRO	5.9
1	A	289	ILE	5.8
1	A	290	HIS	5.6
1	B	454	PHE	5.6
1	B	342	ARG	5.5
1	B	290	HIS	5.4
1	B	341	GLU	5.2
1	B	281	VAL	5.0
1	B	132	GLN	4.8
1	A	454	PHE	4.6
1	B	349	THR	4.5
1	B	289	ILE	4.5
1	A	450	TYR	4.4
1	A	337	ASP	4.4
1	B	511	HIS	4.4
1	B	229	GLU	4.4
1	B	266	LYS	4.3
1	B	265	GLU	4.2
1	B	263	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	4.0
1	A	448	GLY	4.0
1	B	425	ALA	4.0
1	B	428	ASN	4.0
1	A	460	VAL	4.0
1	A	333	LEU	3.9
1	B	460	VAL	3.9
1	B	340	LEU	3.9
1	A	336	LEU	3.9
1	A	138	ASP	3.9
1	B	230	PRO	3.8
1	B	228	ARG	3.7
1	B	262	VAL	3.7
1	A	350	SER	3.7
1	B	206	GLN	3.6
1	A	230	PRO	3.6
1	B	286	PHE	3.6
1	A	338	SER	3.5
1	A	455	PRO	3.5
1	B	8	LYS	3.3
1	B	11	VAL	3.3
1	A	427	ALA	3.3
1	A	150	LEU	3.3
1	A	174	TRP	3.3
1	A	428	ASN	3.3
1	B	264	PRO	3.3
1	A	200	ASN	3.3
1	B	282	ILE	3.2
1	B	343	GLU	3.2
1	A	232	LYS	3.2
1	A	321	ASN	3.1
1	B	235	THR	3.1
1	B	424	ILE	3.1
1	A	288	LYS	3.1
1	A	267	ASN	3.1
1	A	269	ARG	3.0
1	A	332	ASN	3.0
1	B	245	ASN	3.0
1	A	510	GLU	3.0
1	B	237	ASN	3.0
1	A	334	ASP	2.9
1	B	233	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	285	ALA	2.9
1	B	452	ALA	2.9
1	B	232	LYS	2.9
1	B	331	GLU	2.9
1	B	451	SER	2.9
1	A	103	GLU	2.8
1	A	335	GLU	2.8
1	B	244	TYR	2.8
1	A	287	ASP	2.8
1	B	293	ALA	2.8
1	B	427	ALA	2.8
1	B	212	PHE	2.7
1	A	263	GLN	2.7
1	B	472	SER	2.7
1	A	511	HIS	2.7
1	B	464	VAL	2.7
1	B	246	ALA	2.6
1	A	231	SER	2.6
1	A	292	GLY	2.6
1	A	509	LEU	2.6
1	B	134	LEU	2.6
1	B	338	SER	2.5
1	B	337	ASP	2.5
1	B	332	ASN	2.5
1	B	26	THR	2.5
1	B	234	VAL	2.5
1	A	168	CYS	2.5
1	B	241	GLY	2.5
1	A	419	ARG	2.5
1	B	421	ILE	2.5
1	A	412	GLU	2.5
1	B	84	ASN	2.4
1	B	267	ASN	2.4
1	A	177	LEU	2.4
1	B	36	LEU	2.4
1	B	333	LEU	2.4
1	A	451	SER	2.4
1	B	183	SER	2.4
1	B	467	SER	2.4
1	B	243	VAL	2.4
1	B	484	ASP	2.4
1	B	488	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	214	GLN	2.3
1	A	186	ASP	2.3
1	B	249	VAL	2.3
1	B	238	CYS	2.3
1	B	277	PRO	2.3
1	B	227	THR	2.3
1	B	288	LYS	2.3
1	B	420	PRO	2.2
1	B	192	GLN	2.2
1	B	236	VAL	2.2
1	B	131	HIS	2.2
1	B	455	PRO	2.2
1	A	188	TYR	2.2
1	B	450	TYR	2.2
1	B	329	ASN	2.2
1	A	76	LEU	2.2
1	A	368	GLY	2.2
1	A	415	ILE	2.2
1	B	482	ILE	2.2
1	B	109	HIS	2.2
1	A	191	HIS	2.1
1	B	200	ASN	2.1
1	B	468	ASN	2.1
1	A	170	TYR	2.1
1	A	389	GLU	2.1
1	A	513	HIS	2.1
1	B	133	HIS	2.1
1	A	242	THR	2.1
1	A	143	GLN	2.1
1	B	283	GLN	2.1
1	B	274	PHE	2.0
1	A	268	LEU	2.0
1	B	447	ARG	2.0
1	A	325	GLU	2.0
1	A	396	SER	2.0
1	B	292	GLY	2.0
1	B	87	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

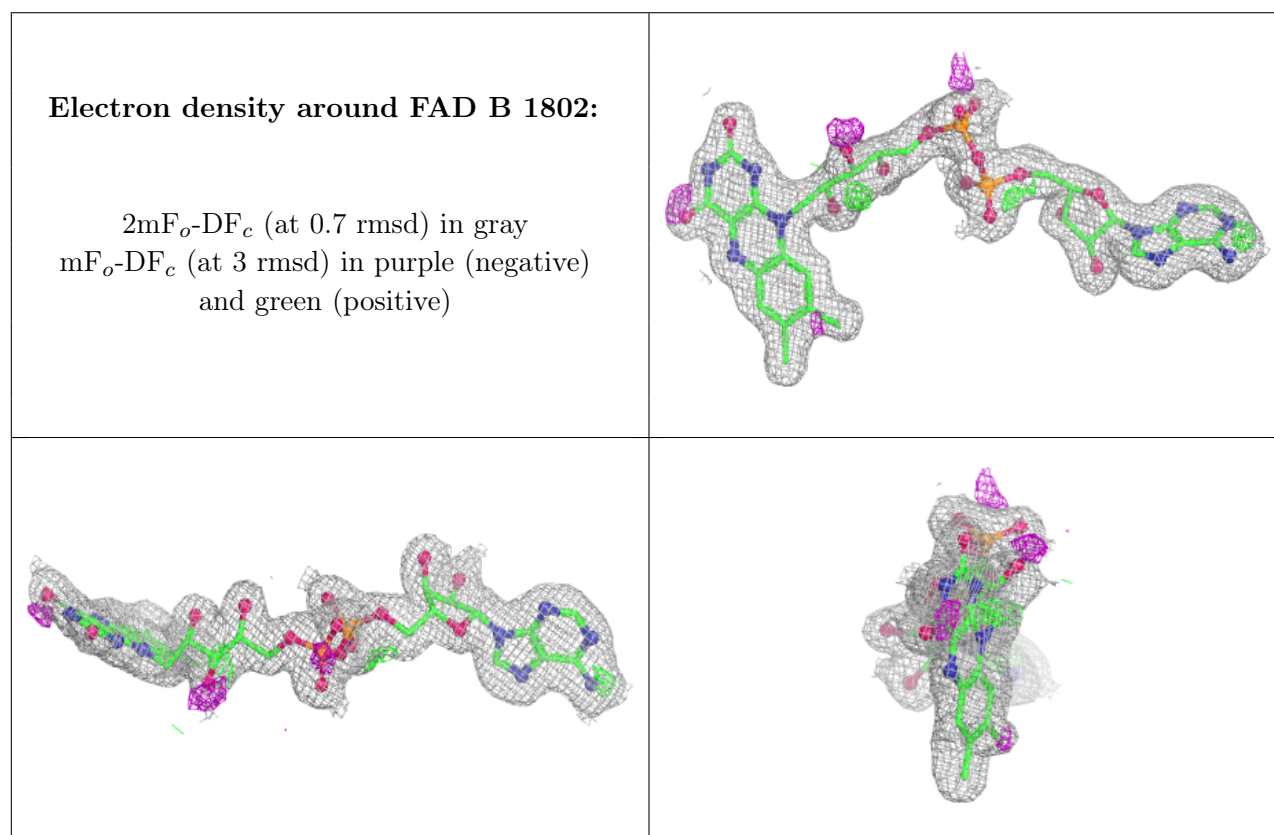
There are no oligosaccharides in this entry.

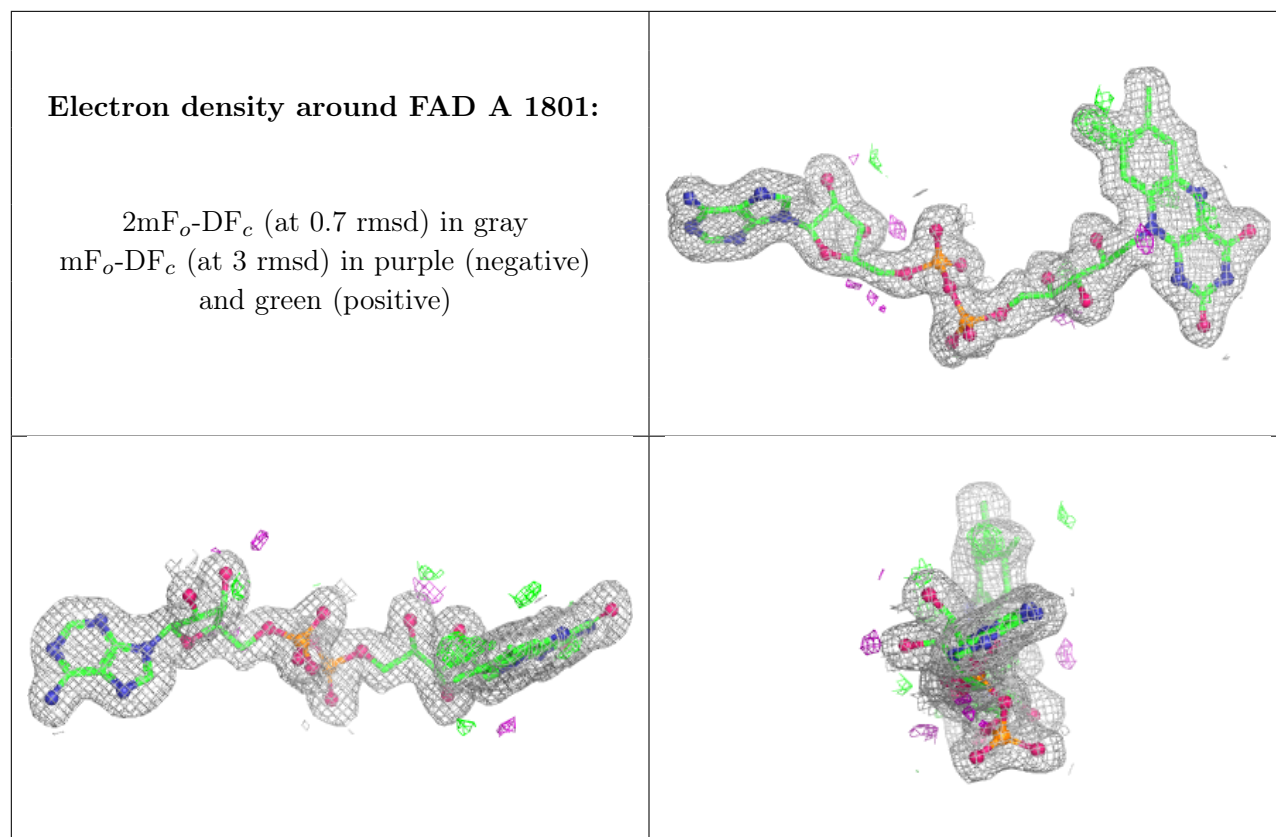
6.4 Ligands [i](#)

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	B	1802	53/53	0.94	0.09	23,27,30,33	0
2	FAD	A	1801	53/53	0.97	0.06	13,17,21,23	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 [i](#)

There are no such residues in this entry.