



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:56 PM UTC

PDB ID : 3BNU / pdb_00003bnu
Title : Crystal structure of polyamine oxidase FMS1 from *Saccharomyces cerevisiae*
in complex with bis-(3S,3'S)-methylated spermine
Authors : Huang, Q.; Hao, Q.
Deposited on : 2007-12-14
Resolution : 2.20 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

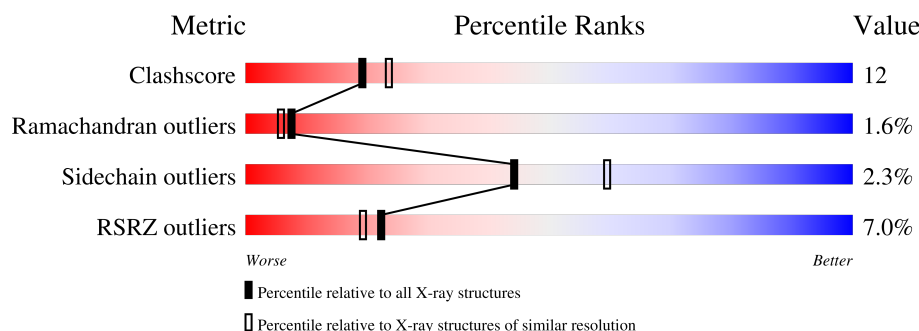
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	5% 74% 21% • •
1	B	516	9% 72% 21% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SPZ	B	803	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8193 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 Polyamine oxidase FMS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	499	Total	C	N	O	S	0	0	0
			3845	2425	668	730	22			
1	A	497	Total	C	N	O	S	0	0	0
			3905	2471	684	728	22			

There are 16 discrepancies between the modelled and reference sequences:

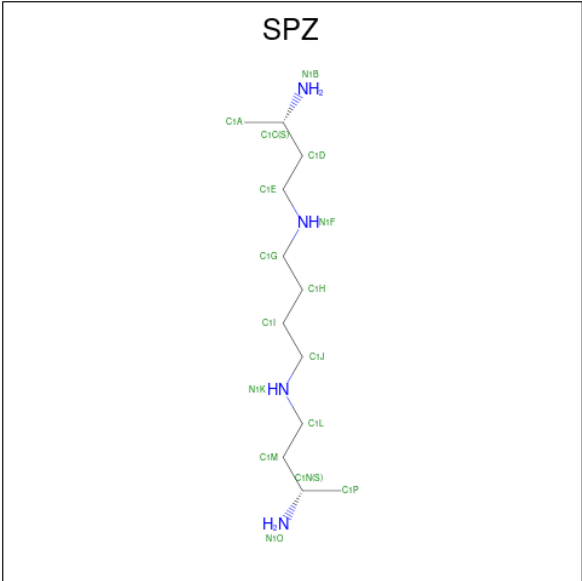
Chain	Residue	Modelled	Actual	Comment	Reference
B	509	LEU	-	expression tag	UNP P50264
B	510	GLU	-	expression tag	UNP P50264
B	511	HIS	-	expression tag	UNP P50264
B	512	HIS	-	expression tag	UNP P50264
B	513	HIS	-	expression tag	UNP P50264
B	514	HIS	-	expression tag	UNP P50264
B	515	HIS	-	expression tag	UNP P50264
B	516	HIS	-	expression tag	UNP P50264
A	509	LEU	-	expression tag	UNP P50264
A	510	GLU	-	expression tag	UNP P50264
A	511	HIS	-	expression tag	UNP P50264
A	512	HIS	-	expression tag	UNP P50264
A	513	HIS	-	expression tag	UNP P50264
A	514	HIS	-	expression tag	UNP P50264
A	515	HIS	-	expression tag	UNP P50264
A	516	HIS	-	expression tag	UNP P50264

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 3 is (3S,3'S)-N 1 ,N 1 '-butane-1,4-diyldibutane-1,3-diamine (CCD ID: SPZ) (formula: C₁₂H₃₀N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			16	12	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			16	12	4		

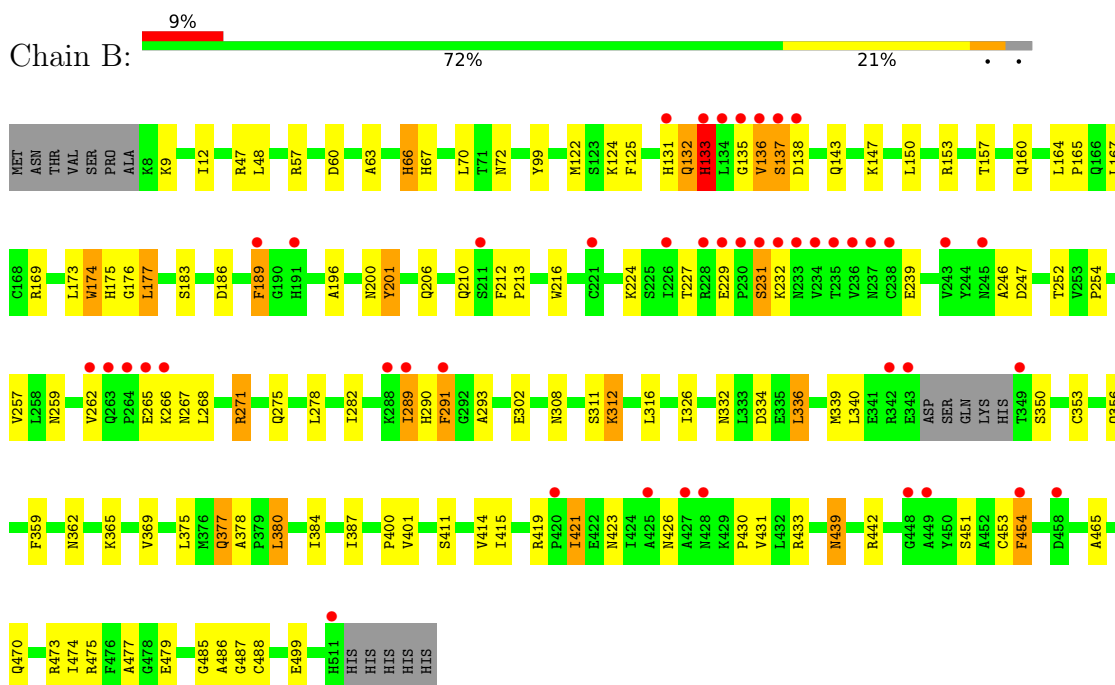
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	140	Total	O	0	0
			140	140		
4	A	165	Total	O	0	0
			165	165		

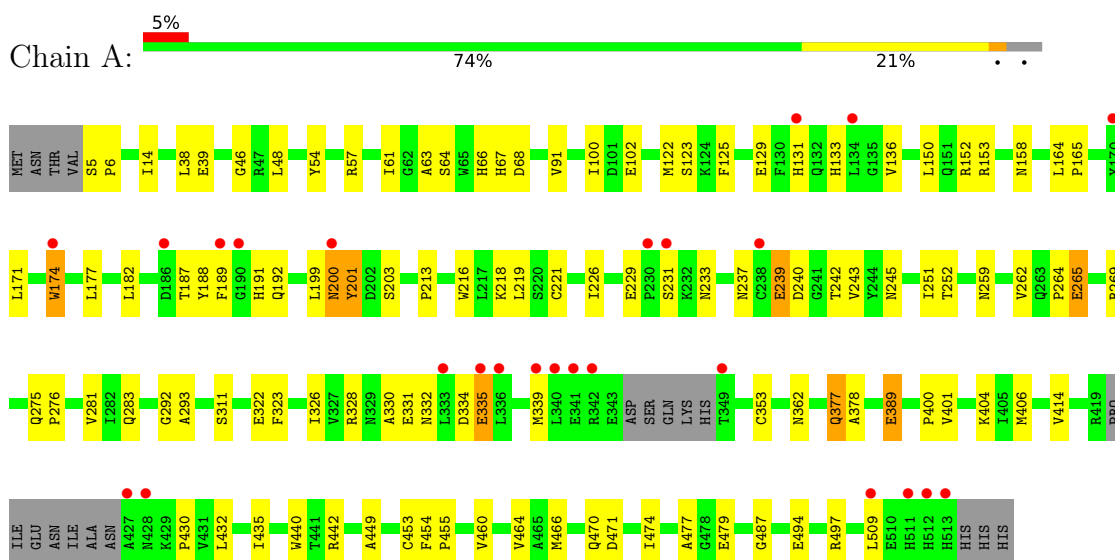
3 Residue-property plots [i](#)

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: Polyamine oxidase FMS1



• Molecule 1: Polyamine oxidase FMS1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.19Å 103.00Å 77.52Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.8 (30.00-2.20) 89.7 (30.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.268 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8193	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 3.71% 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, SPZ

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	0.44	1/3988 (0.0%)	0.89	9/5393 (0.2%)
1	B	0.42	1/3923 (0.0%)	0.88	7/5309 (0.1%)
All	All	0.43	2/7911 (0.0%)	0.89	16/10702 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	509	LEU	CB-CG	-5.84	1.41	1.53
1	B	268	LEU	CB-CG	-5.59	1.42	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	TRP	N-CA-C	6.29	118.94	111.71
1	B	454	PHE	N-CA-C	-6.18	101.76	110.29
1	A	66	HIS	N-CA-C	-5.92	99.08	108.73
1	A	201	TYR	N-CA-C	-5.85	105.03	111.82
1	A	454	PHE	N-CA-C	-5.79	102.86	110.39
1	B	419	ARG	N-CA-C	-5.72	98.56	108.97
1	A	100	ILE	N-CA-C	5.67	116.04	108.11
1	B	453	CYS	N-CA-C	5.56	118.30	109.24
1	A	182	LEU	N-CA-C	5.40	118.35	109.76
1	A	174	TRP	N-CA-C	-5.30	106.98	113.50
1	B	174	TRP	N-CA-C	-5.26	105.14	112.45
1	A	453	CYS	N-CA-C	5.25	117.53	109.07
1	B	66	HIS	N-CA-C	-5.24	100.62	108.96
1	B	201	TYR	N-CA-C	-5.16	106.25	112.54
1	A	323	PHE	N-CA-C	-5.09	105.62	111.07
1	B	289	ILE	N-CA-C	5.07	119.88	109.34

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	3905	0	3762	76	0
1	B	3845	0	3639	101	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
3	A	16	0	30	5	0
3	B	16	0	30	9	0
4	A	165	0	0	2	0
4	B	140	0	0	4	0
All	All	8193	0	7523	180	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 12.

All (180) 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:282:ILE:HD13	1:B:465:ALA:HB1	1.51	0.92
1:A:353:CYS:SG	1:A:400:PRO:HG2	2.17	0.83
1:B:377:GLN:NE2	1:B:377:GLN:H	1.78	0.81
1:B:353:CYS:SG	1:B:400:PRO:HG2	2.21	0.80
1:A:269:ARG:NE	1:A:269:ARG:HA	1.97	0.79
1:B:302:GLU:HG3	1:B:431:VAL:HB	1.64	0.79
1:B:67:HIS:NE2	3:B:803:SPZ:H1M	2.02	0.75
1:B:377:GLN:H	1:B:377:GLN:HE21	1.34	0.72
1:B:278:LEU:HA	1:B:470:GLN:HE22	1.53	0.72
1:B:174:TRP:O	3:B:803:SPZ:H1JA	1.89	0.72
1:B:439:ASN:HD21	1:B:442:ARG:HD3	1.55	0.70
1:B:189:PHE:HD2	1:B:189:PHE:H	1.38	0.70
1:A:158:ASN:HD22	1:A:328:ARG:HH21	1.39	0.69
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.24	0.68
1:B:265:GLU:C	1:B:267:ASN:H	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ILE:HD13	1:B:426:ASN:OD1	1.94	0.68
1:A:377:GLN:NE2	1:A:377:GLN:H	1.92	0.67
1:B:72:ASN:C	1:B:72:ASN:HD22	2.03	0.67
1:B:189:PHE:HD2	1:B:189:PHE:N	1.92	0.66
1:B:271:ARG:HH11	1:B:271:ARG:HG3	1.61	0.66
1:B:138:ASP:HB3	4:B:908:HOH:O	1.94	0.66
1:A:406:MET:HE2	1:A:406:MET:HA	1.78	0.66
1:A:264:PRO:O	1:A:265:GLU:HB3	1.97	0.64
1:B:470:GLN:HB3	1:B:474:ILE:HB	1.78	0.63
1:B:133:HIS:HB3	1:B:136:VAL:HG13	1.81	0.63
1:B:380:LEU:HD22	1:B:384:ILE:HG12	1.81	0.63
1:A:54:TYR:O	1:A:57:ARG:HG3	2.00	0.62
1:A:133:HIS:HB3	1:A:136:VAL:CG2	2.30	0.62
1:B:176:GLY:C	1:B:177:LEU:HD12	2.25	0.61
1:B:278:LEU:HA	1:B:470:GLN:NE2	2.15	0.61
1:A:259:ASN:O	1:A:262:VAL:HG22	2.01	0.61
1:A:332:ASN:HD21	1:A:334:ASP:HB2	1.65	0.60
1:B:189:PHE:N	1:B:189:PHE:CD2	2.64	0.60
1:A:158:ASN:ND2	1:A:328:ARG:HH21	2.00	0.60
1:B:63:ALA:HA	2:B:802:FAD:N5	2.17	0.59
1:B:213:PRO:HG2	1:B:216:TRP:CE2	2.38	0.59
1:B:67:HIS:NE2	3:B:803:SPZ:C1M	2.65	0.59
1:B:473:ARG:HH11	1:B:473:ARG:HG3	1.67	0.59
1:A:264:PRO:O	1:A:265:GLU:CB	2.51	0.58
1:A:311:SER:HA	1:A:362:ASN:HB3	1.86	0.58
1:B:224:LYS:HD2	1:B:239:GLU:OE1	2.04	0.58
1:B:377:GLN:NE2	1:B:377:GLN:N	2.49	0.58
1:A:122:MET:O	1:A:125:PHE:HB3	2.03	0.58
1:A:133:HIS:HB3	1:A:136:VAL:HG21	1.85	0.58
1:B:439:ASN:ND2	1:B:442:ARG:HD3	2.19	0.57
1:B:332:ASN:HD21	1:B:334:ASP:HB2	1.69	0.57
1:B:227:THR:HG23	1:B:275:GLN:HB3	1.86	0.57
1:A:330:ALA:CA	1:A:339:MET:HE1	2.35	0.56
1:A:174:TRP:CZ3	3:A:802:SPZ:H1AA	2.40	0.56
1:B:271:ARG:HD3	1:B:271:ARG:C	2.30	0.56
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.04	0.56
1:A:460:VAL:O	1:A:464:VAL:HG23	2.05	0.56
1:B:157:THR:OG1	1:B:160:GLN:HG3	2.06	0.56
1:B:66:HIS:HB2	1:B:196:ALA:HB3	1.86	0.55
1:B:99:TYR:HB3	1:B:316:LEU:HD11	1.87	0.55
1:A:229:GLU:C	1:A:231:SER:H	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PHE:HB2	1:B:213:PRO:HD2	1.89	0.55
1:A:164:LEU:N	1:A:165:PRO:HD2	2.22	0.55
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.88	0.55
1:B:308:ASN:O	1:B:365:LYS:HD2	2.06	0.55
1:A:67:HIS:HE1	3:A:802:SPZ:H1A	1.73	0.54
1:B:475:ARG:HB3	1:B:499:GLU:OE1	2.08	0.54
3:B:803:SPZ:C1J	3:B:803:SPZ:HN1O	2.20	0.54
1:A:63:ALA:HA	2:A:801:FAD:N5	2.23	0.54
1:B:293:ALA:HB3	1:B:378:ALA:HB2	1.91	0.53
1:A:150:LEU:O	1:A:153:ARG:HD2	2.08	0.53
1:A:189:PHE:CZ	3:A:802:SPZ:H1MA	2.43	0.53
1:A:414:VAL:HA	1:A:430:PRO:HG2	1.91	0.53
1:A:322:GLU:O	1:A:326:ILE:HG13	2.08	0.52
1:B:213:PRO:HG2	1:B:216:TRP:CD2	2.44	0.52
1:A:240:ASP:OD1	1:A:242:THR:HG23	2.10	0.52
1:A:479:GLU:OE1	1:A:487:GLY:HA2	2.10	0.52
1:A:252:THR:HG22	1:A:477:ALA:HB3	1.92	0.51
1:B:177:LEU:HD12	1:B:177:LEU:N	2.25	0.51
1:B:265:GLU:C	1:B:267:ASN:N	2.69	0.51
1:B:302:GLU:OE2	1:B:433:ARG:NH1	2.40	0.51
1:B:486:ALA:O	3:B:803:SPZ:C1E	2.58	0.51
1:B:488:CYS:SG	3:B:803:SPZ:N1F	2.82	0.51
1:B:311:SER:O	1:B:312:LYS:HE3	2.11	0.50
1:B:229:GLU:O	1:B:231:SER:N	2.44	0.50
1:A:262:VAL:CG1	1:A:283:GLN:HG2	2.41	0.50
1:B:186:ASP:HB2	4:B:855:HOH:O	2.11	0.50
1:B:486:ALA:O	3:B:803:SPZ:H1E	2.11	0.50
1:B:414:VAL:HA	1:B:430:PRO:HG2	1.94	0.49
1:A:233:ASN:HB3	1:A:245:ASN:HD21	1.77	0.49
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.43	0.49
1:A:14:ILE:HD12	1:A:14:ILE:N	2.27	0.49
1:B:173:LEU:N	1:B:173:LEU:HD22	2.28	0.49
1:A:237:ASN:OD1	1:A:243:VAL:HG22	2.13	0.49
1:B:239:GLU:OE1	1:B:239:GLU:HA	2.13	0.49
1:B:213:PRO:HG2	1:B:216:TRP:CD1	2.47	0.48
1:B:336:LEU:HD22	1:B:340:LEU:CD1	2.43	0.48
1:A:262:VAL:HG12	1:A:283:GLN:HG2	1.95	0.48
1:B:411:SER:HA	4:B:826:HOH:O	2.14	0.48
1:B:47:ARG:NH2	1:B:254:PRO:HB3	2.29	0.48
1:B:259:ASN:O	1:B:262:VAL:HG22	2.13	0.48
1:A:229:GLU:C	1:A:231:SER:N	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ASP:O	1:B:473:ARG:HD2	2.14	0.47
1:B:271:ARG:HG3	1:B:271:ARG:NH1	2.27	0.47
1:A:471:ASP:OD1	1:A:471:ASP:C	2.56	0.47
1:B:131:HIS:O	1:B:132:GLN:C	2.57	0.47
1:B:254:PRO:HG2	1:B:257:VAL:HG23	1.96	0.47
1:A:269:ARG:HA	1:A:269:ARG:CZ	2.44	0.47
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.97	0.47
1:B:70:LEU:HD23	1:A:152:ARG:CZ	2.45	0.47
1:B:165:PRO:O	1:B:169:ARG:HG3	2.14	0.47
1:A:470:GLN:HB3	1:A:474:ILE:HB	1.97	0.47
1:B:135:GLY:O	1:B:137:SER:N	2.48	0.46
1:A:432:LEU:HD21	1:A:435:ILE:HD11	1.98	0.46
1:B:332:ASN:ND2	1:B:334:ASP:HB2	2.30	0.46
1:A:269:ARG:HG2	1:A:269:ARG:HH11	1.79	0.46
1:A:48:LEU:CD2	1:A:63:ALA:HB3	2.45	0.46
1:A:226:ILE:HD13	1:A:251:ILE:HD11	1.97	0.46
1:A:213:PRO:HB2	1:A:216:TRP:CD1	2.50	0.46
1:B:9:LYS:O	1:B:246:ALA:HA	2.16	0.46
1:A:123:SER:HB3	1:A:188:TYR:CE2	2.51	0.46
1:B:167:LEU:C	1:B:167:LEU:HD23	2.41	0.46
1:A:67:HIS:NE2	3:A:802:SPZ:H1G	2.31	0.46
1:B:153:ARG:HG3	4:B:814:HOH:O	2.15	0.45
1:B:206:GLN:O	1:B:210:GLN:HG3	2.17	0.45
1:B:213:PRO:HG2	1:B:216:TRP:CG	2.52	0.45
1:A:494:GLU:OE1	1:A:497:ARG:NH2	2.50	0.45
1:A:389:GLU:HB2	4:A:861:HOH:O	2.17	0.45
1:B:213:PRO:O	1:B:216:TRP:HB2	2.17	0.45
1:B:143:GLN:O	1:B:147:LYS:HG3	2.16	0.44
1:A:229:GLU:O	1:A:231:SER:N	2.49	0.44
1:A:455:PRO:HG2	4:A:895:HOH:O	2.16	0.44
1:B:377:GLN:HE21	1:B:377:GLN:N	2.08	0.44
1:B:359:PHE:HD2	1:B:375:LEU:HD22	1.82	0.44
1:A:331:GLU:CB	1:A:335:GLU:HG3	2.48	0.44
1:A:189:PHE:CE1	1:A:191:HIS:CE1	3.06	0.44
1:B:183:SER:HB2	1:B:454:PHE:C	2.43	0.43
1:A:442:ARG:HH11	1:A:442:ARG:HG2	1.83	0.43
1:B:326:ILE:HG12	1:B:339:MET:HE2	2.01	0.43
1:A:177:LEU:HD11	1:A:292:GLY:HA2	2.00	0.43
1:A:262:VAL:O	1:A:262:VAL:HG23	2.18	0.43
1:A:102:GLU:O	1:A:404:LYS:HE2	2.18	0.43
1:B:72:ASN:C	1:B:72:ASN:ND2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HD12	1:A:61:ILE:HA	1.85	0.43
1:A:68:ASP:HB3	1:A:192:GLN:HB2	2.00	0.43
1:A:46:GLY:C	1:A:48:LEU:H	2.27	0.43
1:B:164:LEU:N	1:B:165:PRO:HD2	2.34	0.43
1:B:353:CYS:SG	1:B:401:VAL:HG13	2.59	0.43
1:A:38:LEU:HD23	1:A:218:LYS:HB3	2.01	0.42
1:B:291:PHE:H	1:B:451:SER:HA	1.83	0.42
1:B:423:ASN:HB3	1:B:426:ASN:ND2	2.35	0.42
1:A:353:CYS:SG	1:A:401:VAL:HG13	2.59	0.42
2:A:801:FAD:C4X	3:A:802:SPZ:H1GA	2.49	0.42
1:B:485:GLY:O	1:B:488:CYS:HB2	2.19	0.42
1:A:200:ASN:O	1:A:203:SER:HB3	2.19	0.42
1:B:12:ILE:HG13	1:B:246:ALA:HB2	2.02	0.42
1:A:449:ALA:HA	2:A:801:FAD:HM81	2.02	0.42
1:B:213:PRO:CG	1:B:216:TRP:CE2	3.03	0.42
1:B:356:GLN:N	1:B:356:GLN:CD	2.78	0.42
1:B:336:LEU:HD22	1:B:340:LEU:HD11	2.01	0.42
1:B:122:MET:O	1:B:125:PHE:HB3	2.20	0.42
1:A:5:SER:HB3	1:A:6:PRO:CD	2.50	0.42
1:A:466:MET:HA	1:A:466:MET:HE2	2.02	0.42
3:B:803:SPZ:N1K	3:B:803:SPZ:N1O	2.68	0.42
1:B:60:ASP:HB3	1:B:63:ALA:O	2.19	0.41
1:A:269:ARG:HG2	1:A:269:ARG:NH1	2.34	0.41
1:A:171:LEU:HD13	1:A:187:THR:HG22	2.02	0.41
1:A:239:GLU:HG3	1:A:240:ASP:N	2.35	0.41
1:B:175:HIS:HB3	1:B:177:LEU:HD13	2.01	0.41
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.76	0.41
3:B:803:SPZ:H1MA	3:B:803:SPZ:H1J	1.87	0.41
1:B:439:ASN:HD22	1:B:439:ASN:HA	1.70	0.41
1:A:91:VAL:O	1:A:91:VAL:HG13	2.20	0.41
1:B:362:ASN:ND2	1:B:362:ASN:C	2.77	0.41
1:A:269:ARG:NE	1:A:269:ARG:CA	2.75	0.41
1:B:421:ILE:O	1:B:421:ILE:HG22	2.19	0.41
1:A:39:GLU:HB3	1:A:219:LEU:HD23	2.01	0.41
1:B:332:ASN:HD22	1:B:334:ASP:H	1.69	0.41
1:B:387:ILE:O	1:B:387:ILE:HG13	2.20	0.40
1:A:129:GLU:HA	1:A:129:GLU:OE1	2.21	0.40
1:B:254:PRO:HG2	1:B:257:VAL:CG2	2.51	0.40
1:A:275:GLN:HA	1:A:276:PRO:C	2.46	0.40
1:B:150:LEU:O	1:B:153:ARG:HG2	2.22	0.40
1:B:265:GLU:O	1:B:267:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLU:CD	1:A:339:MET:HE2	2.46	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	491/516 (95%)	461 (94%)	27 (6%)	3 (1%)	21	23
1	B	495/516 (96%)	445 (90%)	37 (8%)	13 (3%)	4	2
All	All	986/1032 (96%)	906 (92%)	64 (6%)	16 (2%)	7	6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	VAL
1	B	200	ASN
1	B	231	SER
1	B	232	LYS
1	B	289	ILE
1	B	290	HIS
1	A	200	ASN
1	A	265	GLU
1	B	132	GLN
1	B	133	HIS
1	B	291	PHE
1	A	131	HIS
1	B	266	LYS
1	B	137	SER
1	B	421	ILE
1	B	350	SER

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	417/457 (91%)	409 (98%)	8 (2%)	50	66
1	B	403/457 (88%)	392 (97%)	11 (3%)	39	53
All	All	820/914 (90%)	801 (98%)	19 (2%)	44	59

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	124	LYS
1	B	133	HIS
1	B	177	LEU
1	B	189	PHE
1	B	201	TYR
1	B	271	ARG
1	B	312	LYS
1	B	336	LEU
1	B	377	GLN
1	B	380	LEU
1	B	439	ASN
1	A	64	SER
1	A	201	TYR
1	A	221	CYS
1	A	239	GLU
1	A	281	VAL
1	A	335	GLU
1	A	377	GLN
1	A	389	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	ASN
1	B	191	HIS
1	B	192	GLN

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	267	ASN
1	B	275	GLN
1	B	329	ASN
1	B	332	ASN
1	B	362	ASN
1	B	377	GLN
1	B	439	ASN
1	A	29	GLN
1	A	55	GLN
1	A	109	HIS
1	A	131	HIS
1	A	158	ASN
1	A	191	HIS
1	A	192	GLN
1	A	245	ASN
1	A	255	GLN
1	A	267	ASN
1	A	275	GLN
1	A	332	ASN
1	A	362	ASN
1	A	377	GLN
1	A	434	ASN

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	A	801	-	58,58,58	1.33	7 (12%)	85,89,89	2.27	9 (10%)
3	SPZ	A	802	-	15,15,15	0.39	0	16,16,16	1.02	2 (12%)
2	FAD	B	802	-	58,58,58	1.43	9 (15%)	85,89,89	2.21	9 (10%)
3	SPZ	B	803	-	15,15,15	0.37	0	16,16,16	0.99	1 (6%)

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	801	-	-	4/34/50/50	0/6/6/6
3	SPZ	A	802	-	-	0/13/13/13	-
2	FAD	B	802	-	-	4/34/50/50	0/6/6/6
3	SPZ	B	803	-	-	0/13/13/13	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	FAD	PA-O3P	4.24	1.64	1.59
2	B	802	FAD	C4X-N5	3.94	1.39	1.30
2	A	801	FAD	C4X-N5	3.91	1.39	1.30
2	A	801	FAD	PA-O3P	3.04	1.62	1.59
2	B	802	FAD	C2A-N1A	2.89	1.39	1.33
2	A	801	FAD	C5B-C4B	2.82	1.60	1.51
2	B	802	FAD	C10-N1	2.82	1.38	1.33
2	A	801	FAD	C2A-N1A	2.76	1.38	1.33
2	A	801	FAD	C10-N1	2.49	1.38	1.33
2	B	802	FAD	C5B-C4B	2.40	1.58	1.51
2	A	801	FAD	C9A-C5X	2.37	1.45	1.41
2	A	801	FAD	C9-C8	2.30	1.42	1.39
2	B	802	FAD	C9-C8	2.27	1.42	1.39
2	B	802	FAD	C9A-C5X	2.18	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	FAD	C9-C9A	2.14	1.43	1.39
2	B	802	FAD	P-O3P	2.13	1.61	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	O3P-PA-O1A	-12.87	71.98	110.70
2	B	802	FAD	O3P-PA-O1A	-12.31	73.68	110.70
2	A	801	FAD	O2A-PA-O5B	-7.83	72.10	107.57
2	B	802	FAD	O2A-PA-O5B	-7.46	73.76	107.57
2	A	801	FAD	O5B-PA-O1A	6.74	135.64	108.94
2	B	802	FAD	O5B-PA-O1A	6.69	135.47	108.94
2	A	801	FAD	O2A-PA-O1A	-6.57	81.90	112.44
2	B	802	FAD	O2A-PA-O3P	6.37	124.48	107.27
2	B	802	FAD	O2A-PA-O1A	-6.03	84.38	112.44
2	A	801	FAD	O2A-PA-O3P	5.21	121.36	107.27
2	A	801	FAD	O4B-C1B-C2B	-2.65	100.94	106.62
3	B	803	SPZ	C1E-C1D-C1C	-2.59	110.97	115.17
2	A	801	FAD	C9A-C5X-N5	-2.54	119.76	122.45
2	B	802	FAD	O4B-C1B-C2B	-2.50	101.26	106.62
2	A	801	FAD	O3'-C3'-C4'	-2.41	103.45	108.93
2	A	801	FAD	N3A-C2A-N1A	-2.40	124.95	128.58
2	B	802	FAD	O3'-C3'-C4'	-2.36	103.56	108.93
2	B	802	FAD	C9A-C5X-N5	-2.34	119.97	122.45
3	A	802	SPZ	C1E-C1D-C1C	-2.17	111.64	115.17
2	B	802	FAD	N3A-C2A-N1A	-2.17	125.30	128.58
3	A	802	SPZ	C1L-C1M-C1N	-2.17	111.66	115.17

There are no chirality outliers.

All (8) torsion outliers are listed below:

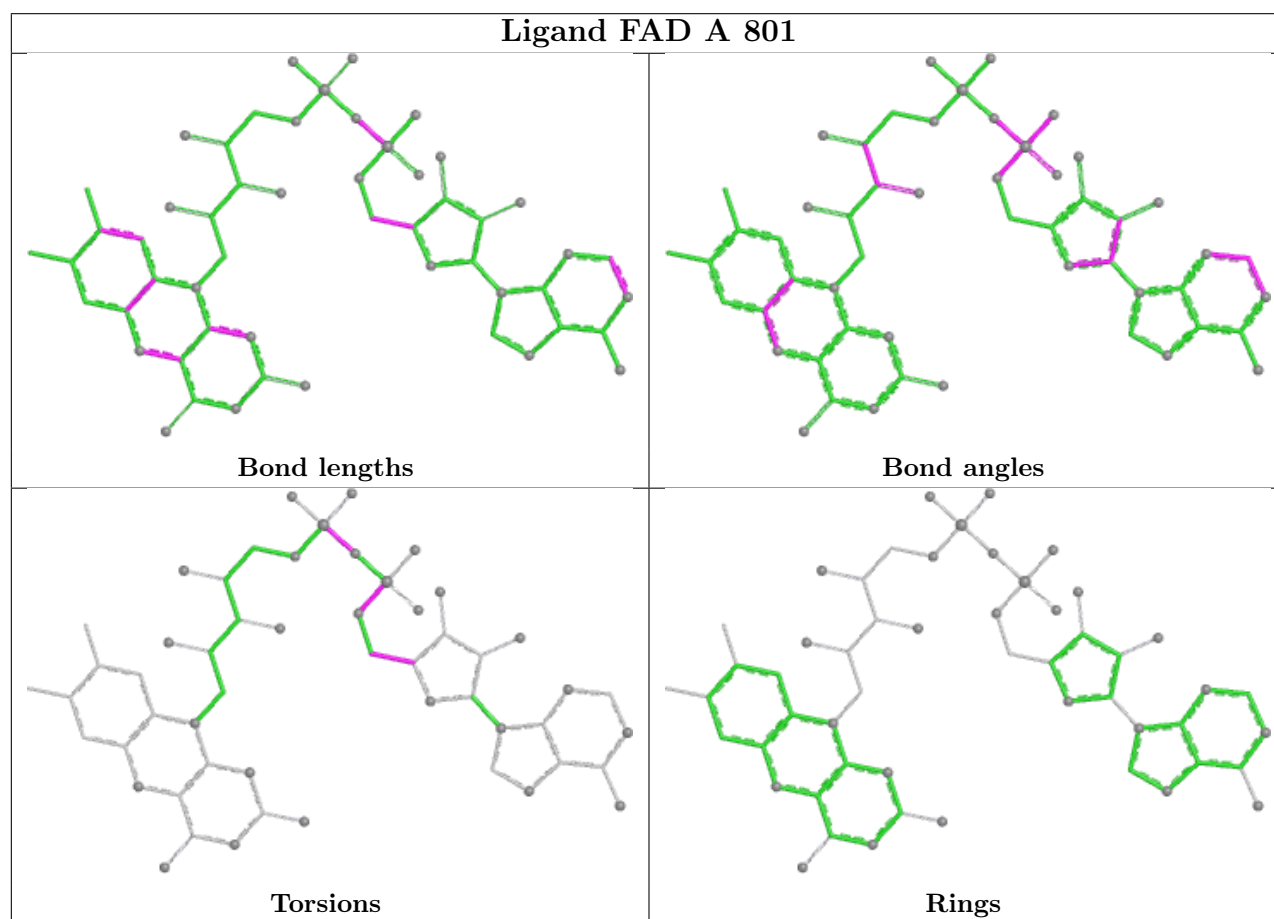
Mol	Chain	Res	Type	Atoms
2	B	802	FAD	C5B-O5B-PA-O1A
2	A	801	FAD	C5B-O5B-PA-O1A
2	A	801	FAD	PA-O3P-P-O5'
2	B	802	FAD	C3B-C4B-C5B-O5B
2	B	802	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	C3B-C4B-C5B-O5B
2	B	802	FAD	PA-O3P-P-O5'

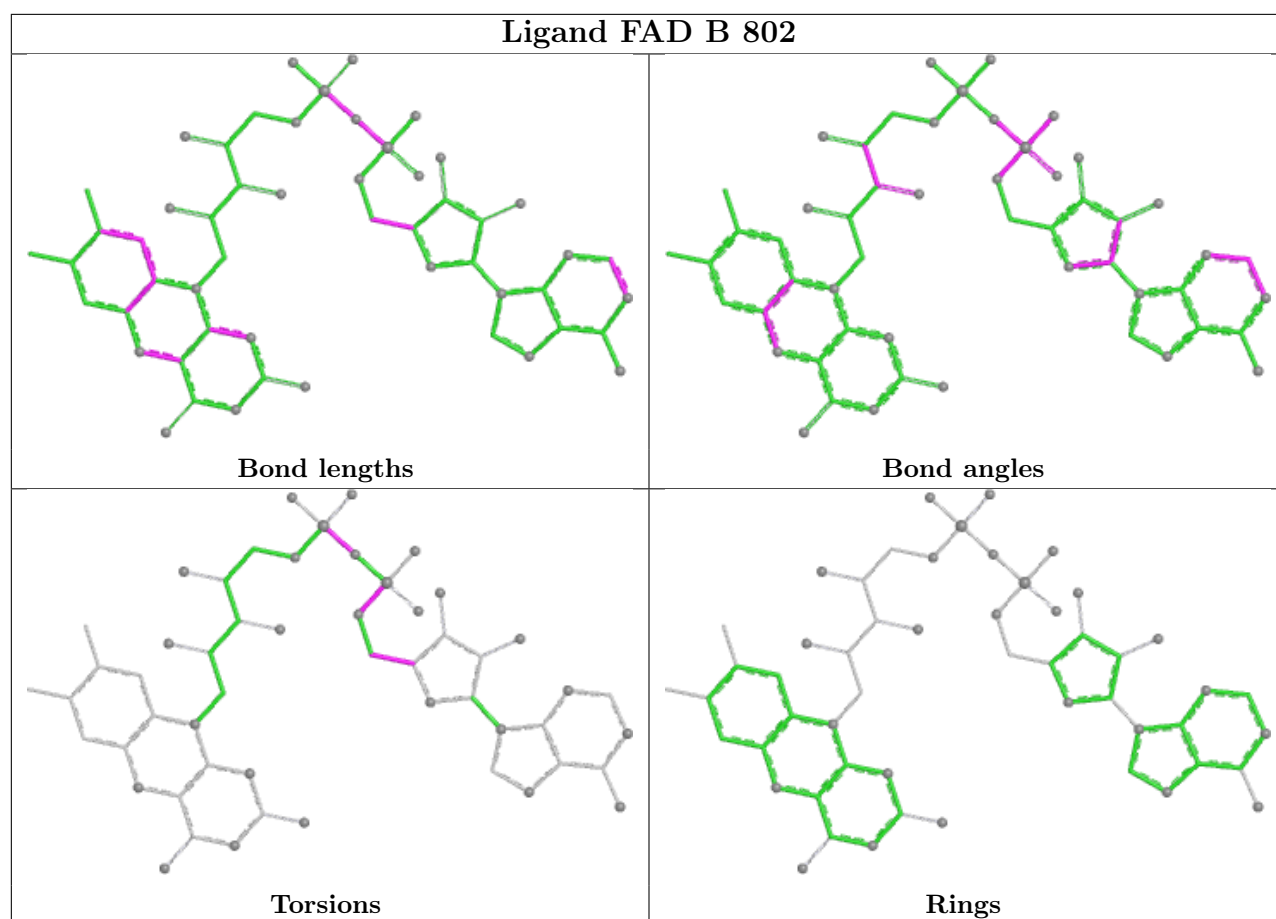
There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	3	0
3	A	802	SPZ	5	0
2	B	802	FAD	1	0
3	B	803	SPZ	9	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	497/516 (96%)	0.25	25 (5%)	34 31	18, 31, 56, 76	0
1	B	499/516 (96%)	0.54	45 (9%)	15 12	21, 35, 61, 85	0
All	All	996/1032 (96%)	0.39	70 (7%)	22 19	18, 33, 59, 85	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	LEU	6.6
1	B	289	ILE	6.2
1	B	342	ARG	4.6
1	A	349	THR	4.3
1	A	342	ARG	4.2
1	B	291	PHE	3.9
1	A	341	GLU	3.9
1	B	264	PRO	3.8
1	B	138	ASP	3.5
1	B	230	PRO	3.5
1	B	136	VAL	3.3
1	B	233	ASN	3.2
1	B	235	THR	3.2
1	B	511	HIS	3.1
1	B	211	SER	3.1
1	A	230	PRO	3.1
1	A	513	HIS	3.0
1	A	174	TRP	2.9
1	B	236	VAL	2.9
1	B	234	VAL	2.9
1	B	226	ILE	2.8
1	B	425	ALA	2.8
1	A	333	LEU	2.7
1	B	133	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	448	GLY	2.7
1	B	137	SER	2.7
1	B	265	GLU	2.7
1	B	232	LYS	2.7
1	A	190	GLY	2.7
1	B	427	ALA	2.6
1	B	262	VAL	2.6
1	B	349	THR	2.6
1	B	245	ASN	2.6
1	B	189	PHE	2.6
1	B	243	VAL	2.6
1	A	238	CYS	2.6
1	B	191	HIS	2.6
1	B	288	LYS	2.6
1	A	427	ALA	2.5
1	B	428	ASN	2.5
1	B	343	GLU	2.5
1	B	449	ALA	2.5
1	A	189	PHE	2.5
1	B	458	ASP	2.5
1	A	131	HIS	2.4
1	A	340	LEU	2.4
1	A	170	TYR	2.3
1	B	263	GLN	2.3
1	B	237	ASN	2.3
1	B	229	GLU	2.3
1	A	186	ASP	2.3
1	A	509	LEU	2.3
1	B	420	PRO	2.3
1	B	135	GLY	2.3
1	A	200	ASN	2.2
1	B	131	HIS	2.2
1	B	266	LYS	2.2
1	A	336	LEU	2.2
1	A	428	ASN	2.2
1	A	231	SER	2.2
1	A	335	GLU	2.1
1	A	512	HIS	2.1
1	B	454	PHE	2.1
1	B	231	SER	2.1
1	A	134	LEU	2.1
1	A	339	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	221	CYS	2.0
1	B	238	CYS	2.0
1	A	511	HIS	2.0
1	B	228	ARG	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](#)

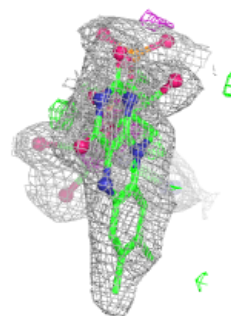
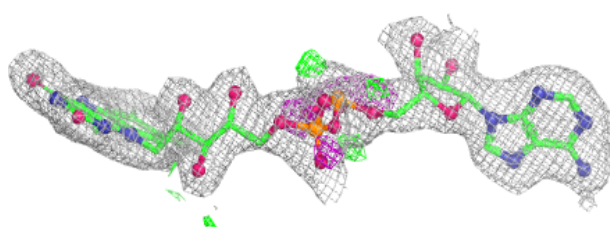
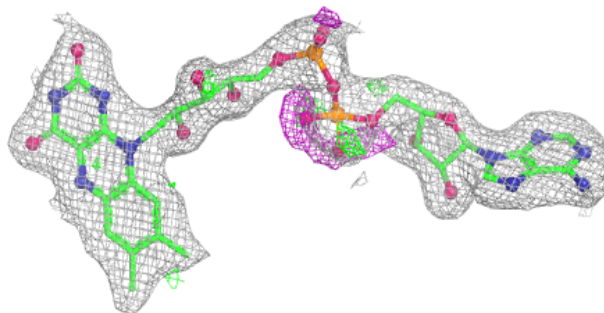
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	SPZ	B	803	16/16	0.64	0.26	54,58,60,60	0
3	SPZ	A	802	16/16	0.75	0.25	57,61,66,67	0
2	FAD	B	802	53/53	0.91	0.10	22,29,38,43	0
2	FAD	A	801	53/53	0.95	0.07	16,20,23,36	0

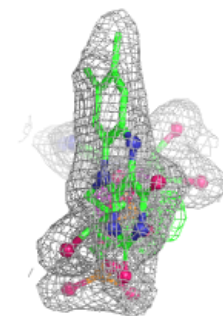
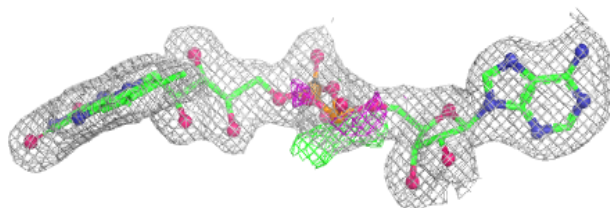
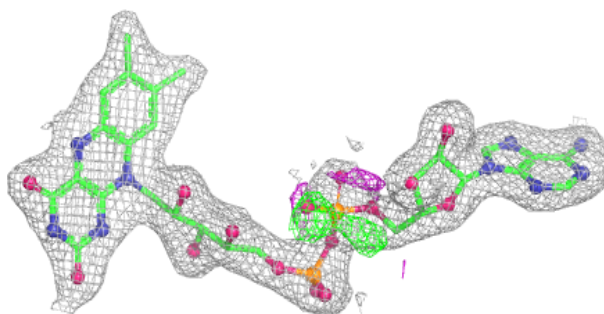
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 802:

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

**Electron density around FAD A 801:**

$2mF_o-DF_c$ (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.