



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:43 AM UTC

PDB ID : 3EWK / pdb_00003ewk
Title : Structure of the redox sensor domain of Methylococcus capsulatus (Bath) MmoS
Authors : Ukaegbu, U.E.; Rosenzweig, A.C.
Deposited on : 2008-10-15
Resolution : 2.34 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

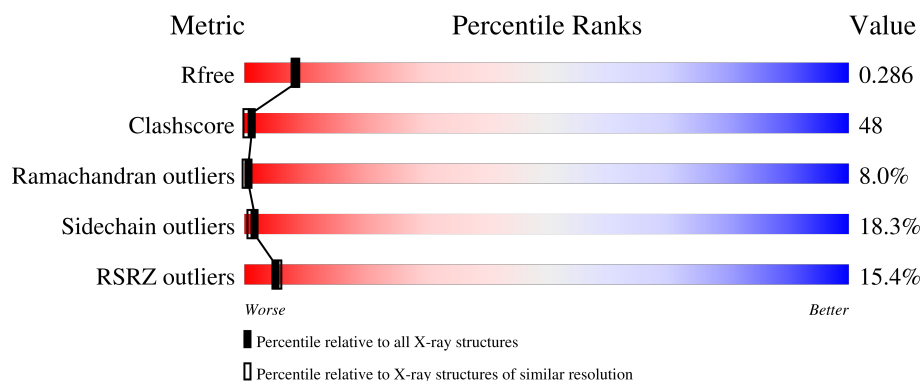
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	227	15% 41% 35% 19% .

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
2	FAD	A	326	X	X	-	-

2 Entry composition [i](#)

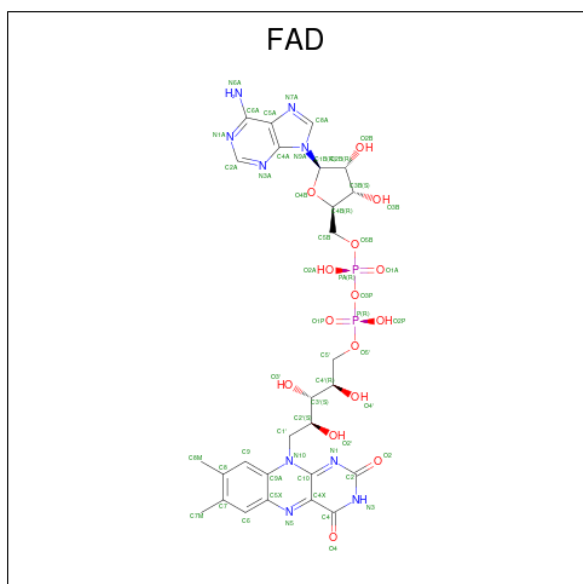
There are 5 unique types of molecules in this entry. The entry contains 1912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sensor protein.

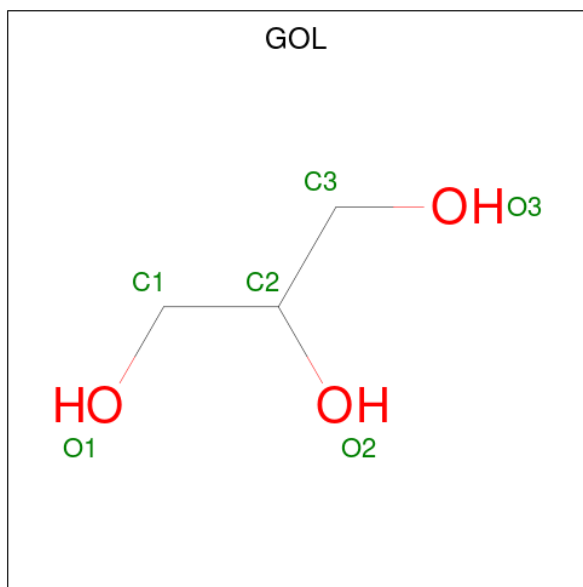
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1793	1110	334	340	9			

- 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		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

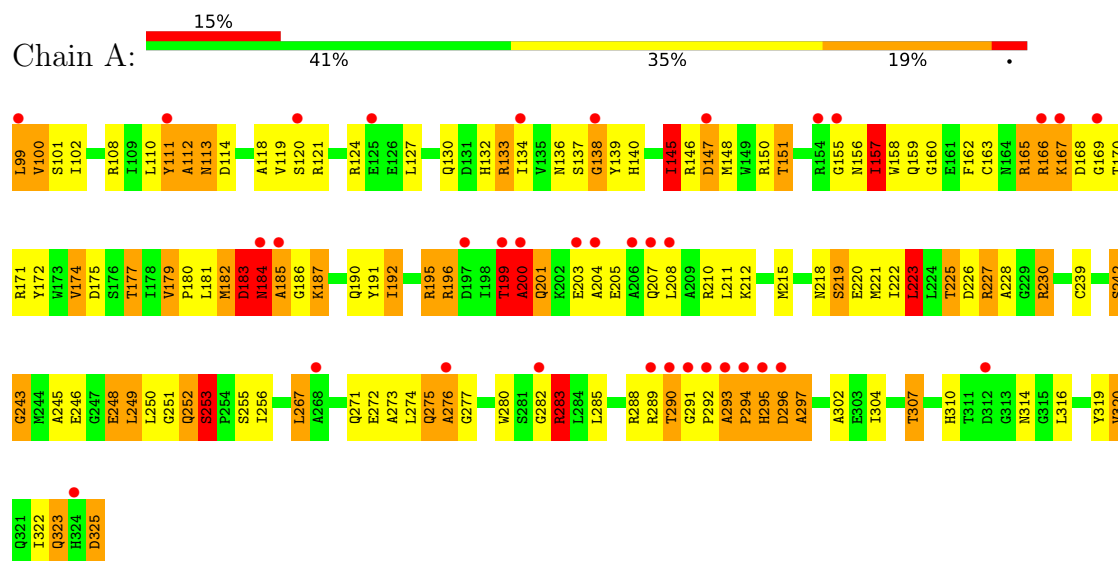
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		

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: Sensor protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.71Å 146.71Å 43.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.80 – 2.34 40.80 – 2.34	Depositor EDS
% Data completeness (in resolution range)	81.6 (40.80-2.34) 82.0 (40.80-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.283 0.245 , 0.286	Depositor DCC
R_{free} test set	852 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	1912	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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, GOL, 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	1.43	10/1828 (0.5%)	1.60	38/2475 (1.5%)

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	A	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	VAL	CA-CB	8.58	1.61	1.54
1	A	145	ILE	CA-CB	7.25	1.63	1.54
1	A	199	THR	CA-CB	6.43	1.64	1.53
1	A	283	ARG	N-CA	6.05	1.53	1.46
1	A	320	VAL	CA-CB	5.69	1.61	1.54
1	A	319	TYR	CA-C	-5.61	1.46	1.52
1	A	177	THR	C-O	5.42	1.30	1.24
1	A	200	ALA	N-CA	5.10	1.55	1.46
1	A	276	ALA	CA-C	5.06	1.59	1.52
1	A	100	VAL	CA-CB	5.01	1.61	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	SER	N-CA-C	9.39	124.53	112.89
1	A	276	ALA	N-CA-C	9.35	124.48	112.89
1	A	248	GLU	N-CA-C	-8.85	96.58	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TYR	CA-C-N	8.57	137.13	121.70
1	A	111	TYR	C-N-CA	8.57	137.13	121.70
1	A	156	ASN	N-CA-C	8.20	121.80	110.24
1	A	166	ARG	N-CA-C	7.84	122.10	112.54
1	A	133	ARG	NE-CZ-NH1	-7.79	113.71	121.50
1	A	253	SER	N-CA-C	7.70	126.81	109.81
1	A	283	ARG	N-CA-C	7.52	126.82	110.80
1	A	138	GLY	N-CA-C	-7.35	105.94	114.69
1	A	296	ASP	CA-C-N	7.16	134.58	121.70
1	A	296	ASP	C-N-CA	7.16	134.58	121.70
1	A	195	ARG	CA-C-N	-6.76	112.57	122.65
1	A	195	ARG	C-N-CA	-6.76	112.57	122.65
1	A	294	PRO	CA-C-N	6.10	132.68	121.70
1	A	294	PRO	C-N-CA	6.10	132.68	121.70
1	A	199	THR	CA-C-N	6.09	132.66	121.70
1	A	199	THR	C-N-CA	6.09	132.66	121.70
1	A	183	ASP	CA-C-N	5.88	132.28	121.70
1	A	183	ASP	C-N-CA	5.88	132.28	121.70
1	A	223	LEU	CA-CB-CG	5.85	136.78	116.30
1	A	276	ALA	CA-C-N	5.78	132.11	121.70
1	A	276	ALA	C-N-CA	5.78	132.11	121.70
1	A	219	SER	CA-CB-OG	-5.72	99.67	111.10
1	A	182	MET	N-CA-C	5.69	118.88	110.46
1	A	113	ASN	N-CA-C	5.61	117.15	110.19
1	A	199	THR	CA-C-O	-5.45	112.72	120.51
1	A	111	TYR	O-C-N	-5.40	117.58	123.52
1	A	314	ASN	N-CA-C	-5.38	106.08	113.56
1	A	320	VAL	N-CA-C	5.25	115.47	108.11
1	A	283	ARG	N-CA-CB	5.24	119.34	110.49
1	A	111	TYR	CA-CB-CG	-5.21	104.51	113.90
1	A	100	VAL	N-CA-C	5.19	115.75	108.17
1	A	215	MET	N-CA-C	-5.12	105.78	111.36
1	A	157	ILE	CB-CA-C	-5.09	104.26	111.28
1	A	243	GLY	N-CA-C	-5.06	98.63	113.30
1	A	110	LEU	N-CA-C	-5.03	107.27	113.41

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	ASP	Peptide
1	A	242	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	252	GLN	Peptide
1	A	276	ALA	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	1793	0	1747	167	5
2	A	53	0	28	14	0
3	A	6	0	8	0	0
4	A	1	0	0	0	0
5	A	59	0	0	21	0
All	All	1912	0	1783	175	5

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 48.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLN:HG2	1:A:177:THR:HG22	1.26	1.17
1:A:295:HIS:HB3	1:A:296:ASP:CA	1.80	1.10
1:A:295:HIS:CB	1:A:296:ASP:HA	1.75	1.10
1:A:230:ARG:HG2	1:A:230:ARG:HH11	1.12	1.09
1:A:293:ALA:HB1	1:A:295:HIS:CB	1.83	1.08
1:A:293:ALA:HB1	1:A:295:HIS:HB3	1.39	1.05
1:A:199:THR:HB	5:A:360:HOH:O	1.58	1.01
1:A:199:THR:HG22	1:A:200:ALA:HB2	1.37	1.00
1:A:293:ALA:CB	1:A:294:PRO:HA	1.91	0.99
1:A:293:ALA:HB3	1:A:294:PRO:HA	1.40	0.98
1:A:159:GLN:HE21	1:A:177:THR:CG2	1.79	0.95
1:A:140:HIS:HE1	1:A:163:CYS:H	1.08	0.93
2:A:326:FAD:C2'	5:A:332:HOH:O	2.15	0.92
1:A:130:GLN:HG2	1:A:134:ILE:HD12	1.51	0.92
1:A:159:GLN:CG	1:A:177:THR:HG22	1.99	0.90
1:A:296:ASP:HB3	1:A:297:ALA:HB2	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:O	1:A:249:LEU:HB2	1.74	0.85
1:A:293:ALA:C	1:A:295:HIS:HB2	2.02	0.84
1:A:199:THR:CG2	1:A:200:ALA:HB2	2.08	0.83
2:A:326:FAD:O2B	2:A:326:FAD:N3A	2.11	0.82
1:A:114:ASP:HA	5:A:345:HOH:O	1.77	0.82
1:A:157:ILE:HD13	1:A:179:VAL:HG22	1.59	0.82
1:A:293:ALA:HB1	1:A:295:HIS:HB2	1.62	0.82
1:A:100:VAL:HB	1:A:113:ASN:ND2	1.95	0.82
1:A:185:ALA:O	1:A:187:LYS:N	2.11	0.82
1:A:159:GLN:HE21	1:A:177:THR:HG21	1.43	0.81
1:A:307:THR:HG23	5:A:387:HOH:O	1.79	0.80
1:A:230:ARG:HG2	1:A:230:ARG:NH1	1.91	0.80
1:A:196:ARG:HH11	1:A:196:ARG:CG	1.95	0.80
1:A:230:ARG:HH11	1:A:230:ARG:CG	1.92	0.80
1:A:102:ILE:N	1:A:111:TYR:O	2.14	0.80
1:A:146:ARG:HA	2:A:326:FAD:H2B	1.64	0.80
1:A:296:ASP:HB3	1:A:297:ALA:CB	2.12	0.79
2:A:326:FAD:C1'	5:A:332:HOH:O	2.29	0.79
1:A:248:GLU:O	1:A:249:LEU:CB	2.30	0.78
1:A:184:ASN:O	1:A:185:ALA:C	2.27	0.77
1:A:223:LEU:HD22	1:A:320:VAL:HB	1.64	0.77
1:A:140:HIS:CE1	1:A:163:CYS:H	1.97	0.76
1:A:165:ARG:HG2	1:A:165:ARG:HH11	1.49	0.76
1:A:183:ASP:HB2	1:A:184:ASN:C	2.12	0.74
1:A:147:ASP:O	1:A:151:THR:HG23	1.87	0.74
1:A:253:SER:O	1:A:256:ILE:HG22	1.87	0.74
1:A:121:ARG:NH2	1:A:168:ASP:OD2	2.16	0.74
1:A:293:ALA:HB3	1:A:294:PRO:CA	2.16	0.74
1:A:159:GLN:HE21	1:A:177:THR:HG22	1.52	0.73
1:A:295:HIS:HB3	1:A:296:ASP:HA	0.86	0.73
1:A:291:GLY:HA2	1:A:296:ASP:O	1.90	0.72
1:A:196:ARG:HH11	1:A:196:ARG:HG3	1.53	0.71
1:A:203:GLU:O	1:A:207:GLN:HG2	1.91	0.71
2:A:326:FAD:O3B	2:A:326:FAD:O2A	2.09	0.71
1:A:165:ARG:HH11	1:A:165:ARG:CG	2.05	0.69
1:A:228:ALA:HA	5:A:376:HOH:O	1.92	0.69
1:A:293:ALA:CB	1:A:294:PRO:CA	2.69	0.69
1:A:199:THR:HG22	1:A:200:ALA:CB	2.22	0.68
1:A:184:ASN:C	5:A:374:HOH:O	2.37	0.67
1:A:195:ARG:NH1	5:A:353:HOH:O	2.27	0.67
1:A:291:GLY:O	1:A:293:ALA:HB2	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:O	1:A:201:GLN:HG2	1.98	0.64
1:A:159:GLN:NE2	1:A:177:THR:HG22	2.13	0.64
1:A:293:ALA:CB	1:A:295:HIS:HB2	2.27	0.63
1:A:162:PHE:HB2	1:A:174:VAL:HG12	1.81	0.63
1:A:146:ARG:HB2	2:A:326:FAD:H3B	1.80	0.62
1:A:99:LEU:HD13	1:A:113:ASN:HD21	1.65	0.61
1:A:102:ILE:CG1	1:A:192:ILE:HG12	2.30	0.61
1:A:179:VAL:HB	1:A:192:ILE:HG22	1.83	0.60
1:A:165:ARG:HG2	1:A:165:ARG:NH1	2.15	0.60
1:A:218:ASN:HD22	1:A:219:SER:N	2.00	0.60
1:A:293:ALA:HB1	1:A:294:PRO:HA	1.81	0.60
1:A:183:ASP:HB2	1:A:184:ASN:O	2.02	0.60
1:A:181:LEU:HD12	1:A:190:GLN:HB2	1.83	0.59
1:A:294:PRO:N	1:A:295:HIS:HB2	2.16	0.59
1:A:102:ILE:HG12	1:A:192:ILE:HG12	1.82	0.59
1:A:291:GLY:C	1:A:293:ALA:HB2	2.27	0.59
1:A:283:ARG:HA	1:A:302:ALA:O	2.02	0.59
1:A:167:LYS:C	1:A:169:GLY:H	2.10	0.58
1:A:99:LEU:HA	1:A:195:ARG:O	2.04	0.58
1:A:168:ASP:OD1	1:A:170:THR:HG23	2.04	0.58
1:A:146:ARG:CA	2:A:326:FAD:H2B	2.35	0.56
1:A:275:GLN:HB3	5:A:376:HOH:O	2.05	0.56
1:A:291:GLY:H	1:A:292:PRO:HD3	1.71	0.56
1:A:239:CYS:O	1:A:243:GLY:HA2	2.05	0.56
1:A:155:GLY:HA2	1:A:182:MET:HE1	1.88	0.56
1:A:183:ASP:HB3	1:A:184:ASN:HB2	1.87	0.55
1:A:136:ASN:ND2	1:A:137:SER:N	2.54	0.55
1:A:218:ASN:HD22	1:A:219:SER:H	1.55	0.54
1:A:127:LEU:O	1:A:130:GLN:HB2	2.07	0.54
1:A:199:THR:CB	1:A:200:ALA:HB2	2.37	0.54
1:A:255:SER:CB	1:A:267:LEU:HD21	2.38	0.54
1:A:140:HIS:HE1	1:A:163:CYS:N	1.91	0.54
1:A:136:ASN:HB2	2:A:326:FAD:O4'	2.08	0.54
1:A:223:LEU:HD22	1:A:320:VAL:CB	2.35	0.53
1:A:133:ARG:NH1	2:A:326:FAD:O1P	2.42	0.53
1:A:111:TYR:HA	1:A:112:ALA:HB3	1.91	0.53
1:A:166:ARG:O	1:A:167:LYS:HB2	2.09	0.53
1:A:130:GLN:HG2	1:A:134:ILE:CD1	2.33	0.53
1:A:246:GLU:O	1:A:249:LEU:HB2	2.08	0.53
1:A:310:HIS:HD2	5:A:384:HOH:O	1.92	0.53
1:A:293:ALA:CA	1:A:295:HIS:HB2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:MET:SD	1:A:148:MET:C	2.92	0.52
1:A:307:THR:CG2	5:A:387:HOH:O	2.45	0.52
1:A:293:ALA:HB1	1:A:296:ASP:HA	1.90	0.52
1:A:289:ARG:HG3	5:A:377:HOH:O	2.09	0.51
1:A:255:SER:HB3	1:A:267:LEU:HD21	1.91	0.51
1:A:250:LEU:O	1:A:251:GLY:C	2.53	0.51
1:A:273:ALA:CB	1:A:280:TRP:HB2	2.41	0.50
1:A:248:GLU:O	1:A:249:LEU:HG	2.12	0.50
1:A:296:ASP:CB	1:A:297:ALA:HB2	2.38	0.50
1:A:296:ASP:HB3	1:A:297:ALA:HB3	1.92	0.50
1:A:183:ASP:C	1:A:184:ASN:O	2.55	0.50
1:A:148:MET:HG2	1:A:158:TRP:CD2	2.47	0.50
1:A:183:ASP:CB	1:A:184:ASN:C	2.83	0.49
1:A:111:TYR:HE1	1:A:124:ARG:NH1	2.10	0.49
2:A:326:FAD:H1'1	5:A:332:HOH:O	2.06	0.49
1:A:168:ASP:OD1	1:A:168:ASP:C	2.55	0.48
1:A:221:MET:HE3	1:A:322:ILE:O	2.13	0.48
1:A:228:ALA:C	5:A:376:HOH:O	2.57	0.48
1:A:165:ARG:HH12	1:A:167:LYS:H	1.61	0.48
1:A:200:ALA:CB	5:A:360:HOH:O	2.61	0.48
1:A:166:ARG:O	1:A:167:LYS:CB	2.62	0.48
1:A:101:SER:OG	1:A:132:HIS:HE1	1.96	0.48
1:A:296:ASP:CB	1:A:297:ALA:CB	2.89	0.47
2:A:326:FAD:O4B	5:A:373:HOH:O	2.20	0.47
1:A:159:GLN:CD	1:A:177:THR:HG22	2.40	0.47
1:A:275:GLN:CD	5:A:376:HOH:O	2.57	0.47
1:A:225:THR:CG2	5:A:338:HOH:O	2.63	0.47
1:A:294:PRO:C	1:A:296:ASP:HB2	2.40	0.47
1:A:290:THR:N	1:A:291:GLY:CA	2.78	0.46
1:A:159:GLN:HG2	1:A:177:THR:CG2	2.18	0.46
1:A:245:ALA:O	1:A:248:GLU:O	2.33	0.46
1:A:184:ASN:O	1:A:185:ALA:O	2.33	0.46
1:A:226:ASP:HB2	1:A:227:ARG:HE	1.81	0.46
1:A:291:GLY:N	1:A:292:PRO:CD	2.79	0.46
1:A:225:THR:HG21	1:A:274:LEU:HD22	1.96	0.46
1:A:183:ASP:OD2	1:A:187:LYS:HB3	2.16	0.46
1:A:208:LEU:O	1:A:212:LYS:HB3	2.16	0.45
1:A:136:ASN:ND2	1:A:138:GLY:H	2.15	0.45
1:A:294:PRO:CA	1:A:295:HIS:HB2	2.46	0.45
1:A:325:ASP:OD1	1:A:325:ASP:C	2.59	0.45
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.62	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:O	1:A:277:GLY:HA2	2.17	0.44
2:A:326:FAD:H1'1	2:A:326:FAD:H9	1.66	0.44
1:A:227:ARG:NH1	1:A:316:LEU:H	2.16	0.44
1:A:120:SER:O	1:A:166:ARG:O	2.35	0.44
1:A:146:ARG:HD3	5:A:383:HOH:O	2.16	0.44
1:A:248:GLU:O	1:A:249:LEU:CG	2.65	0.43
1:A:133:ARG:O	1:A:134:ILE:C	2.61	0.43
1:A:147:ASP:O	1:A:151:THR:CG2	2.61	0.43
1:A:288:ARG:O	1:A:297:ALA:HA	2.18	0.43
1:A:291:GLY:H	1:A:292:PRO:CD	2.31	0.43
1:A:158:TRP:CH2	1:A:160:GLY:HA3	2.53	0.43
1:A:174:VAL:HG22	1:A:195:ARG:HB3	2.00	0.43
1:A:218:ASN:ND2	1:A:220:GLU:H	2.16	0.43
1:A:230:ARG:NH1	1:A:230:ARG:CG	2.65	0.43
1:A:183:ASP:HB3	1:A:184:ASN:CB	2.49	0.43
1:A:252:GLN:H	1:A:252:GLN:HG2	1.42	0.43
1:A:167:LYS:C	1:A:169:GLY:N	2.75	0.42
1:A:175:ASP:O	1:A:195:ARG:HA	2.20	0.42
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.89	0.42
1:A:139:TYR:CD1	1:A:139:TYR:C	2.97	0.42
1:A:200:ALA:HB3	5:A:360:HOH:O	2.19	0.42
1:A:295:HIS:CB	1:A:296:ASP:CA	2.59	0.42
1:A:323:GLN:N	1:A:323:GLN:HE21	2.18	0.42
1:A:323:GLN:NE2	5:A:347:HOH:O	2.20	0.42
1:A:121:ARG:HG3	1:A:166:ARG:HD3	2.01	0.41
1:A:155:GLY:O	1:A:180:PRO:HG2	2.20	0.41
1:A:166:ARG:HG3	1:A:172:TYR:CD2	2.56	0.41
1:A:145:ILE:HG12	2:A:326:FAD:H5'2	2.02	0.41
1:A:102:ILE:HA	1:A:191:TYR:O	2.19	0.41
1:A:203:GLU:OE1	1:A:203:GLU:HA	2.20	0.41
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.78	0.41
1:A:230:ARG:NH1	1:A:251:GLY:O	2.54	0.41
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.91	0.41
2:A:326:FAD:HO3A	2:A:326:FAD:PA	2.42	0.41
1:A:159:GLN:NE2	1:A:177:THR:CG2	2.60	0.40
1:A:271:GLN:O	1:A:275:GLN:HG2	2.20	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASP:O	1:A:219:SER:OG[4_545]	1.79	0.41
1:A:111:TYR:OH	1:A:207:GLN:OE1[4_545]	1.83	0.37
1:A:111:TYR:OH	1:A:207:GLN:NE2[4_545]	1.92	0.28
1:A:111:TYR:OH	1:A:207:GLN:CD[4_545]	2.02	0.18
1:A:183:ASP:O	1:A:219:SER:CB[4_545]	2.18	0.02

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	225/227 (99%)	187 (83%)	20 (9%)	18 (8%)	1 0

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ALA
1	A	167	LYS
1	A	184	ASN
1	A	200	ALA
1	A	283	ARG
1	A	293	ALA
1	A	295	HIS
1	A	297	ALA
1	A	186	GLY
1	A	249	LEU
1	A	253	SER
1	A	183	ASP
1	A	185	ALA
1	A	118	ALA
1	A	199	THR
1	A	204	ALA
1	A	205	GLU
1	A	282	GLY

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	186/186 (100%)	152 (82%)	34 (18%)	2 1

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	108	ARG
1	A	119	VAL
1	A	145	ILE
1	A	147	ASP
1	A	150	ARG
1	A	151	THR
1	A	157	ILE
1	A	165	ARG
1	A	171	ARG
1	A	174	VAL
1	A	184	ASN
1	A	187	LYS
1	A	192	ILE
1	A	196	ARG
1	A	199	THR
1	A	201	GLN
1	A	210	ARG
1	A	211	LEU
1	A	222	ILE
1	A	223	LEU
1	A	225	THR
1	A	227	ARG
1	A	230	ARG
1	A	253	SER
1	A	267	LEU
1	A	272	GLU
1	A	275	GLN
1	A	285	LEU
1	A	290	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	304	ILE
1	A	307	THR
1	A	323	GLN
1	A	325	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	132	HIS
1	A	136	ASN
1	A	140	HIS
1	A	156	ASN
1	A	159	GLN
1	A	218	ASN
1	A	295	HIS

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 [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
3	GOL	A	386	-	5,5,5	1.03	0	5,5,5	1.59	1 (20%)
2	FAD	A	326	-	58,58,58	4.08	32 (55%)	85,89,89	3.31	42 (49%)

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
3	GOL	A	386	-	-	0/4/4/4	-
2	FAD	A	326	-	3/3/9/9	16/34/50/50	0/6/6/6

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	326	FAD	O2'-C2'	-10.95	1.20	1.43
2	A	326	FAD	O4-C4	8.64	1.39	1.23
2	A	326	FAD	C4X-N5	8.38	1.48	1.30
2	A	326	FAD	C2A-N1A	7.91	1.48	1.33
2	A	326	FAD	C2A-N3A	7.75	1.47	1.33
2	A	326	FAD	O2-C2	7.06	1.38	1.24
2	A	326	FAD	C8A-N9A	6.94	1.49	1.37
2	A	326	FAD	C8A-N7A	6.89	1.44	1.31
2	A	326	FAD	C1'-C2'	6.42	1.61	1.52
2	A	326	FAD	O4B-C4B	5.70	1.57	1.45
2	A	326	FAD	C6-C5X	5.36	1.48	1.40
2	A	326	FAD	C9A-N10	5.29	1.50	1.41
2	A	326	FAD	C9-C9A	5.21	1.48	1.39
2	A	326	FAD	P-O3P	4.88	1.64	1.59
2	A	326	FAD	C3B-C4B	-4.87	1.40	1.53
2	A	326	FAD	C6A-N6A	4.85	1.46	1.34
2	A	326	FAD	P-O1P	4.38	1.66	1.50
2	A	326	FAD	C10-N1	4.07	1.41	1.33
2	A	326	FAD	C8-C7	3.64	1.49	1.40
2	A	326	FAD	C10-N10	3.55	1.45	1.37
2	A	326	FAD	C5A-N7A	3.29	1.45	1.39
2	A	326	FAD	C5'-C4'	3.27	1.56	1.51
2	A	326	FAD	PA-O1A	3.22	1.62	1.50
2	A	326	FAD	C5B-C4B	3.04	1.60	1.51
2	A	326	FAD	PA-O3P	2.97	1.62	1.59
2	A	326	FAD	O4B-C1B	2.83	1.48	1.42
2	A	326	FAD	C2'-C3'	-2.78	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	326	FAD	O4'-C4'	-2.64	1.37	1.43
2	A	326	FAD	C6-C7	2.54	1.43	1.39
2	A	326	FAD	C4X-C10	-2.20	1.37	1.44
2	A	326	FAD	C5A-C6A	2.17	1.47	1.41
2	A	326	FAD	PA-O2A	-2.08	1.45	1.55

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	326	FAD	O4B-C1B-N9A	12.09	131.30	108.09
2	A	326	FAD	N3A-C2A-N1A	-9.54	114.14	128.58
2	A	326	FAD	O3'-C3'-C4'	-7.86	91.06	108.93
2	A	326	FAD	C3B-C2B-C1B	7.26	115.20	101.46
2	A	326	FAD	C4'-C3'-C2'	-6.65	102.50	113.57
2	A	326	FAD	C1'-C2'-C3'	5.39	124.28	109.66
2	A	326	FAD	O5B-C5B-C4B	5.28	126.99	108.99
2	A	326	FAD	C2'-C1'-N10	5.23	134.90	110.20
2	A	326	FAD	O2P-P-O3P	5.19	121.30	107.27
2	A	326	FAD	C5'-C4'-C3'	-4.98	102.82	112.22
2	A	326	FAD	C5X-C9A-N10	4.98	122.47	117.97
2	A	326	FAD	C2B-C1B-N9A	4.95	125.61	113.30
2	A	326	FAD	O2A-PA-O3P	-4.87	94.11	107.27
2	A	326	FAD	C1B-N9A-C8A	4.57	137.24	127.09
2	A	326	FAD	O4'-C4'-C5'	4.49	119.89	109.99
2	A	326	FAD	C2A-N1A-C6A	3.77	124.93	118.73
2	A	326	FAD	C4A-N9A-C1B	-3.72	117.93	126.63
2	A	326	FAD	O4B-C4B-C5B	3.66	121.06	109.33
2	A	326	FAD	O4'-C4'-C3'	-3.64	100.72	109.25
2	A	326	FAD	C5B-C4B-C3B	-3.41	102.95	115.21
2	A	326	FAD	O2'-C2'-C1'	3.40	124.19	110.20
2	A	326	FAD	O2B-C2B-C1B	-3.24	98.96	110.10
2	A	326	FAD	O4B-C1B-C2B	-3.21	99.74	106.62
2	A	326	FAD	C5A-C4A-N9A	3.17	109.27	105.81
2	A	326	FAD	C9A-N10-C10	-3.17	115.91	120.75
2	A	326	FAD	O4-C4-C4X	-3.06	118.46	126.53
2	A	326	FAD	C2A-N3A-C4A	3.04	119.25	111.83
2	A	326	FAD	C4X-C10-N10	3.01	120.79	116.48
3	A	386	GOL	O2-C2-C3	2.99	121.54	109.18
2	A	326	FAD	O2A-PA-O5B	-2.97	94.12	107.57
2	A	326	FAD	C8M-C8-C9	-2.77	114.69	119.57
2	A	326	FAD	C4-N3-C2	-2.62	121.00	125.64
2	A	326	FAD	O3B-C3B-C2B	2.57	120.05	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	326	FAD	C9A-C5X-N5	-2.55	119.75	122.45
2	A	326	FAD	C4X-C4-N3	2.54	119.71	113.25
2	A	326	FAD	O5'-P-O1P	-2.51	99.00	108.94
2	A	326	FAD	O5B-PA-O1A	2.50	118.83	108.94
2	A	326	FAD	C6-C5X-C9A	2.48	122.45	119.05
2	A	326	FAD	O2-C2-N3	2.39	123.17	118.58
2	A	326	FAD	C1'-N10-C9A	-2.36	116.05	120.63
2	A	326	FAD	O2-C2-N1	-2.14	118.24	121.80
2	A	326	FAD	N6A-C6A-N1A	2.10	123.06	118.38
2	A	326	FAD	C5A-C6A-N6A	-2.02	118.28	123.29

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	326	FAD	C2'
2	A	326	FAD	C1B
2	A	326	FAD	C4B

All (16) torsion outliers are listed below:

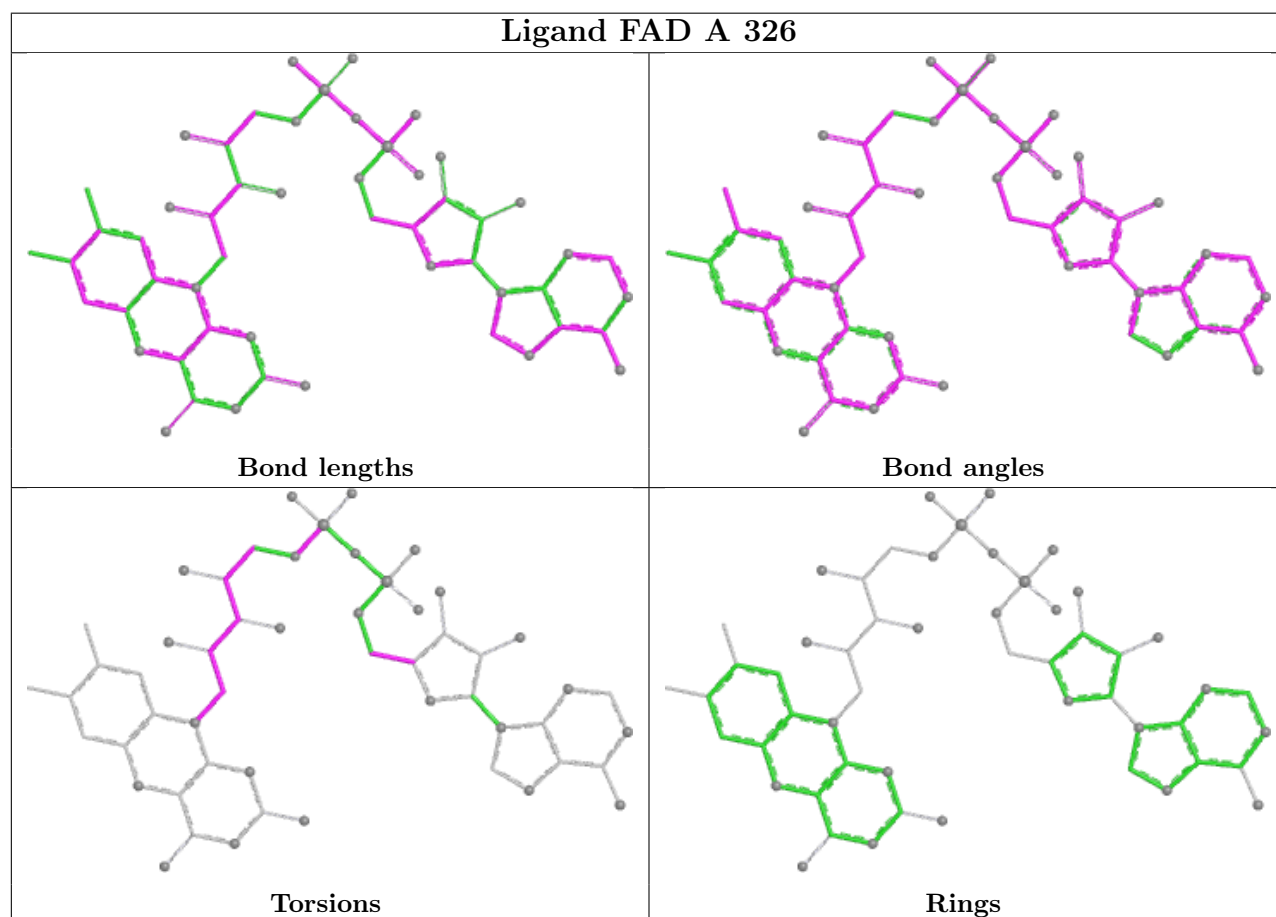
Mol	Chain	Res	Type	Atoms
2	A	326	FAD	C2'-C1'-N10-C10
2	A	326	FAD	N10-C1'-C2'-C3'
2	A	326	FAD	O2'-C2'-C3'-O3'
2	A	326	FAD	C3'-C4'-C5'-O5'
2	A	326	FAD	O4'-C4'-C5'-O5'
2	A	326	FAD	C5'-O5'-P-O3P
2	A	326	FAD	O3'-C3'-C4'-C5'
2	A	326	FAD	O3'-C3'-C4'-O4'
2	A	326	FAD	O2'-C2'-C3'-C4'
2	A	326	FAD	C2'-C3'-C4'-O4'
2	A	326	FAD	C2'-C3'-C4'-C5'
2	A	326	FAD	C5'-O5'-P-O1P
2	A	326	FAD	C5'-O5'-P-O2P
2	A	326	FAD	C3B-C4B-C5B-O5B
2	A	326	FAD	C1'-C2'-C3'-C4'
2	A	326	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	326	FAD	14	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	227/227 (100%)	1.11	35 (15%) 5 5	31, 53, 78, 96	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	PRO	6.2
1	A	199	THR	5.7
1	A	324	HIS	5.1
1	A	125	GLU	5.1
1	A	293	ALA	4.8
1	A	134	ILE	4.7
1	A	200	ALA	4.3
1	A	111	TYR	4.1
1	A	294	PRO	4.0
1	A	185	ALA	4.0
1	A	290	THR	3.7
1	A	295	HIS	3.7
1	A	207	GLN	3.6
1	A	208	LEU	3.5
1	A	296	ASP	3.0
1	A	99	LEU	3.0
1	A	204	ALA	2.8
1	A	276	ALA	2.7
1	A	291	GLY	2.7
1	A	155	GLY	2.6
1	A	312	ASP	2.5
1	A	203	GLU	2.5
1	A	138	GLY	2.5
1	A	282	GLY	2.4
1	A	184	ASN	2.3
1	A	167	LYS	2.3
1	A	197	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	289	ARG	2.2
1	A	206	ALA	2.2
1	A	166	ARG	2.1
1	A	268	ALA	2.1
1	A	147	ASP	2.1
1	A	154	ARG	2.1
1	A	120	SER	2.0
1	A	169	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

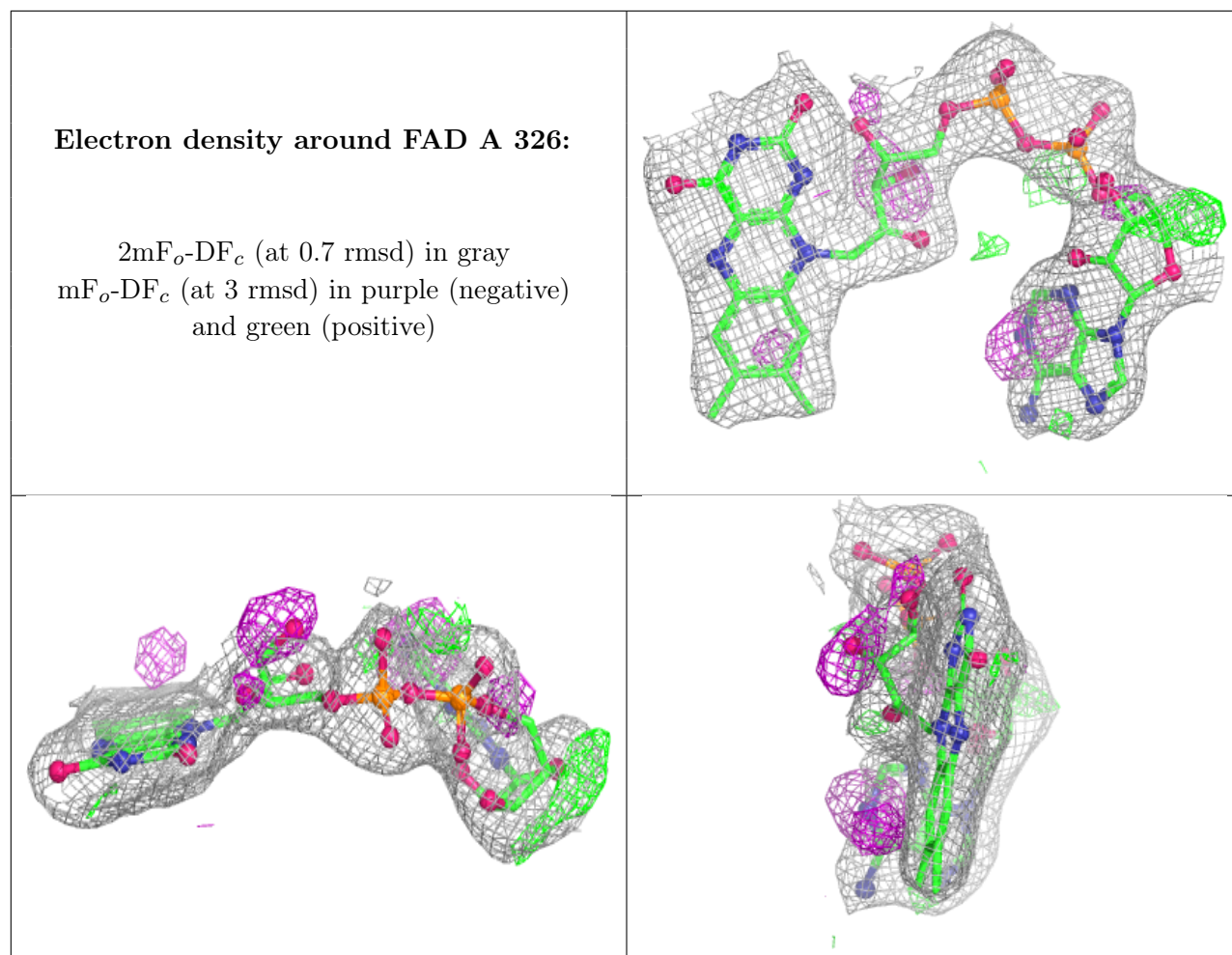
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	386	6/6	0.80	0.17	52,59,63,67	0
4	CL	A	327	1/1	0.81	0.21	86,86,86,86	0
2	FAD	A	326	53/53	0.93	0.11	30,41,60,64	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.