



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 01:46 AM EDT

PDB ID : 3EWK
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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.20.1
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

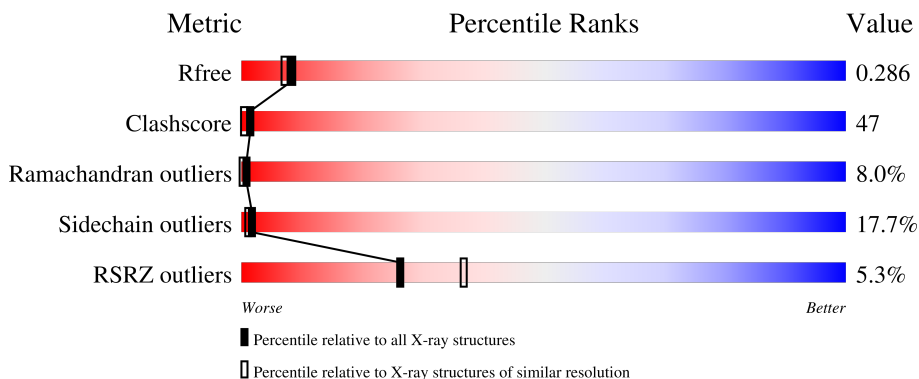
1 Overall quality at a glance

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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	

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	-	-	-

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
			Total	C	N	O	S			
1	A	227	1793	1110	334	340	9	0	0	0

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



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

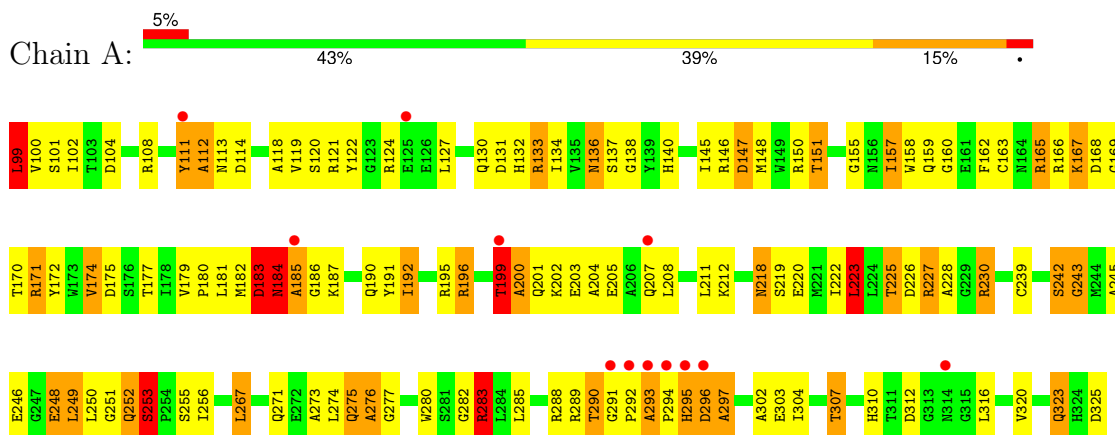
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	59	Total O 59 59	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: 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 40.69 – 2.34	Depositor EDS
% Data completeness (in resolution range)	81.6 (40.80-2.34) 82.1 (40.69-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.34Å)	Xtrriage
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 (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.14	1/1828 (0.1%)	1.32	20/2475 (0.8%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	GLU	CD-OE1	5.54	1.31	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	NE-CZ-NH1	-13.18	113.71	120.30
1	A	223	LEU	CA-CB-CG	9.34	136.78	115.30
1	A	131	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	99	LEU	CA-CB-CG	7.02	131.44	115.30
1	A	171	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	111	TYR	C-N-CA	6.17	137.13	121.70
1	A	133	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	A	131	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	283	ARG	N-CA-C	5.86	126.82	111.00
1	A	253	SER	N-CA-C	5.86	126.81	111.00
1	A	243	GLY	N-CA-C	-5.79	98.63	113.10
1	A	223	LEU	CB-CG-CD2	5.70	120.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	276	ALA	CA-C-N	5.40	127.00	116.20
1	A	248	GLU	N-CA-C	-5.34	96.58	111.00
1	A	296	ASP	C-N-CA	5.15	134.58	121.70
1	A	111	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	104	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	183	ASP	CA-C-N	5.04	128.28	117.20
1	A	242	SER	N-CA-C	5.01	124.53	111.00

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
1	A	252	GLN	Peptide
1	A	276	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1793	0	1747	162	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	170	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 47.

All (170) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:248:GLU:O	1:A:249:LEU:HB2	1.74	0.85
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
1:A:293:ALA:C	1:A:295:HIS:HB2	2.02	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:184:ASN:O	1:A:185:ALA:C	2.27	0.72
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:183:ASP:HB2	1:A:184:ASN:C	2.12	0.70
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: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
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:184:ASN:C	5:A:374:HOH:O	2.37	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:283:ARG:HA	1:A:302:ALA:O	2.02	0.59
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:LYS:C	1:A:169:GLY:H	2.10	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:291:GLY:C	1:A:293:ALA:HB2	2.27	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
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: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:148:MET:HG2	1:A:158:TRP:CD2	2.47	0.50
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: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
1:A:148:MET:SD	1:A:148:MET:C	2.92	0.47
2:A:326:FAD:O4B	5:A:373:HOH:O	2.20	0.47
1:A:183:ASP:CB	1:A:184:ASN:C	2.83	0.47
1:A:225:THR:CG2	5:A:338:HOH:O	2.63	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:250:LEU:O	1:A:251:GLY:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:183:ASP:C	1:A:184:ASN:O	2.55	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:196:ARG:CG	1:A:196:ARG:NH1	2.62	0.44
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:168:ASP:OD1	1:A:168:ASP:C	2.55	0.44
1:A:146:ARG:HD3	5:A:383:HOH:O	2.16	0.44
1:A:122:TYR:HA	1:A:167:LYS:HZ3	1.82	0.43
1:A:248:GLU:O	1:A:249:LEU:CG	2.65	0.43
1:A:228:ALA:C	5:A:376:HOH:O	2.57	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: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:275:GLN:CD	5:A:376:HOH:O	2.57	0.42
1:A:159:GLN:CD	1:A:177:THR:HG22	2.40	0.42
1:A:294:PRO:C	1:A:296:ASP:HB2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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Mol	Chain	Res	Type
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	186/186 (100%)	153 (82%)	33 (18%)	2 1

All (33) 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	136	ASN
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	182	MET
1	A	184	ASN
1	A	192	ILE
1	A	196	ARG

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Mol	Chain	Res	Type
1	A	199	THR
1	A	202	LYS
1	A	211	LEU
1	A	218	ASN
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	275	GLN
1	A	285	LEU
1	A	290	THR
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
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 monosaccharides 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
2	FAD	A	326	-	54,58,58	4.16	29 (53%)	71,89,89	3.66	34 (47%)
3	GOL	A	386	-	5,5,5	1.03	0	5,5,5	1.59	1 (20%)

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	326	-	3/3/9/9	16/30/50/50	0/6/6/6
3	GOL	A	386	-	-	0/4/4/4	-

All (29) 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	C2A-N3A	10.06	1.47	1.32
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	O2-C2	7.06	1.38	1.24
2	A	326	FAD	C1'-C2'	6.42	1.61	1.52
2	A	326	FAD	O4B-C1B	5.84	1.48	1.40
2	A	326	FAD	O4B-C4B	5.70	1.57	1.45
2	A	326	FAD	C8A-N7A	5.58	1.44	1.34
2	A	326	FAD	C6-C5X	5.36	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	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	C6A-N6A	3.49	1.46	1.34
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	C2'-C3'	-2.78	1.48	1.53
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	PA-O2A	-2.08	1.45	1.55

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	326	FAD	O4B-C1B-N9A	17.01	131.30	108.75
2	A	326	FAD	N3A-C2A-N1A	-10.70	114.14	128.67
2	A	326	FAD	O3'-C3'-C4'	-7.86	91.06	108.93
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	C1B-N9A-C4A	-4.96	117.93	126.64
2	A	326	FAD	O2A-PA-O3P	-4.87	94.11	107.27
2	A	326	FAD	O4'-C4'-C5'	4.49	119.89	109.99
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	C4A-C5A-N7A	3.27	112.79	109.34
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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	N6A-C6A-N1A	2.21	123.06	118.33
2	A	326	FAD	O2-C2-N1	-2.14	118.24	121.80

All (3) chirality outliers are listed below:

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

All (16) torsion outliers are listed below:

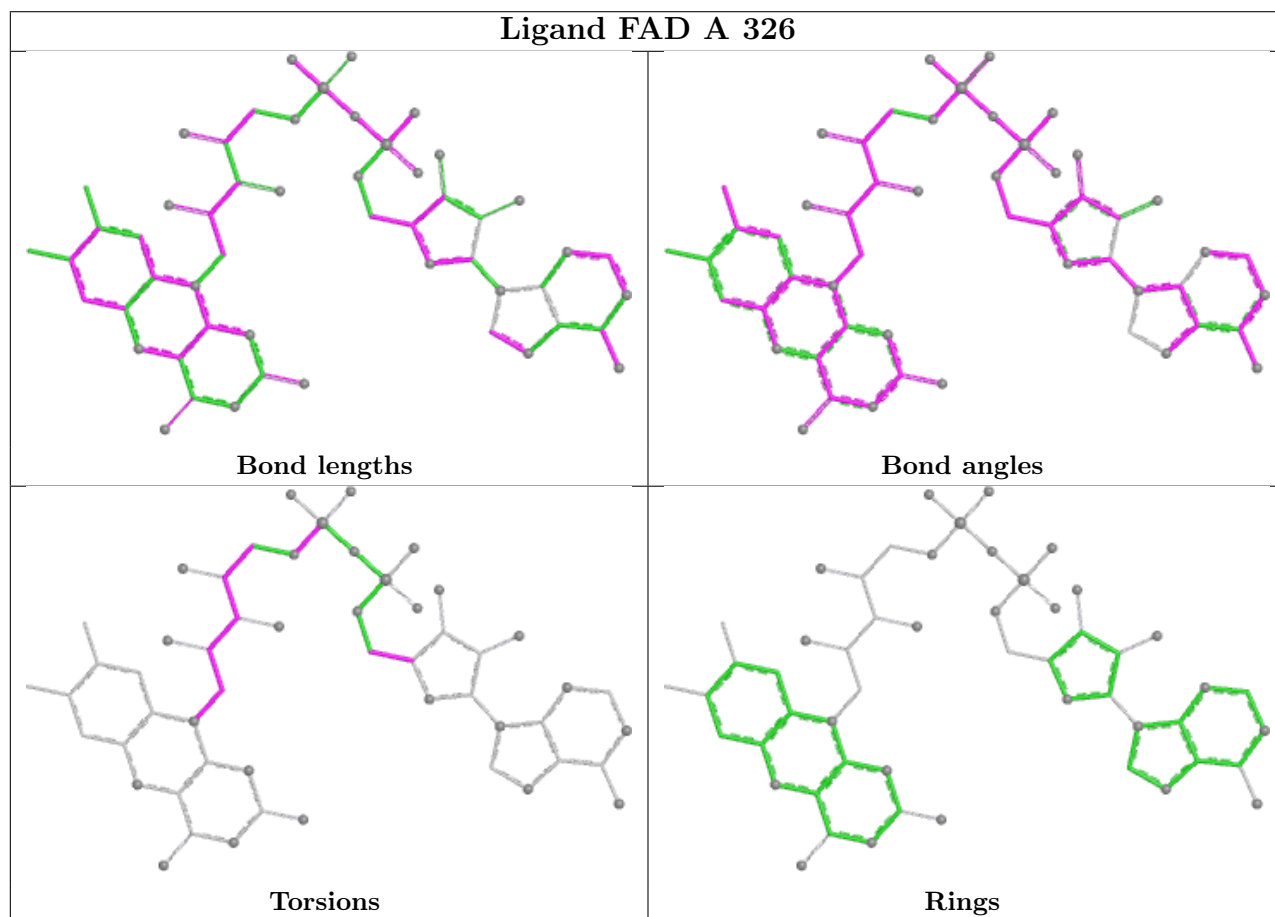
Mol	Chain	Res	Type	Atoms
2	A	326	FAD	C2'-C1'-N10-C10
2	A	326	FAD	N10-C1'-C2'-C3'
2	A	326	FAD	O2'-C2'-C3'-O3'
2	A	326	FAD	C3'-C4'-C5'-O5'
2	A	326	FAD	O4'-C4'-C5'-O5'
2	A	326	FAD	C5'-O5'-P-O3P
2	A	326	FAD	O3'-C3'-C4'-C5'
2	A	326	FAD	O3'-C3'-C4'-O4'
2	A	326	FAD	O2'-C2'-C3'-C4'
2	A	326	FAD	C2'-C3'-C4'-O4'
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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/227 (100%)	0.40	12 (5%) 26 37	33, 53, 78, 96	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	ALA	6.1
1	A	291	GLY	4.9
1	A	296	ASP	4.4
1	A	292	PRO	3.8
1	A	199	THR	3.1
1	A	125	GLU	3.0
1	A	294	PRO	2.9
1	A	295	HIS	2.6
1	A	185	ALA	2.4
1	A	207	GLN	2.1
1	A	314	ASN	2.1
1	A	111	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

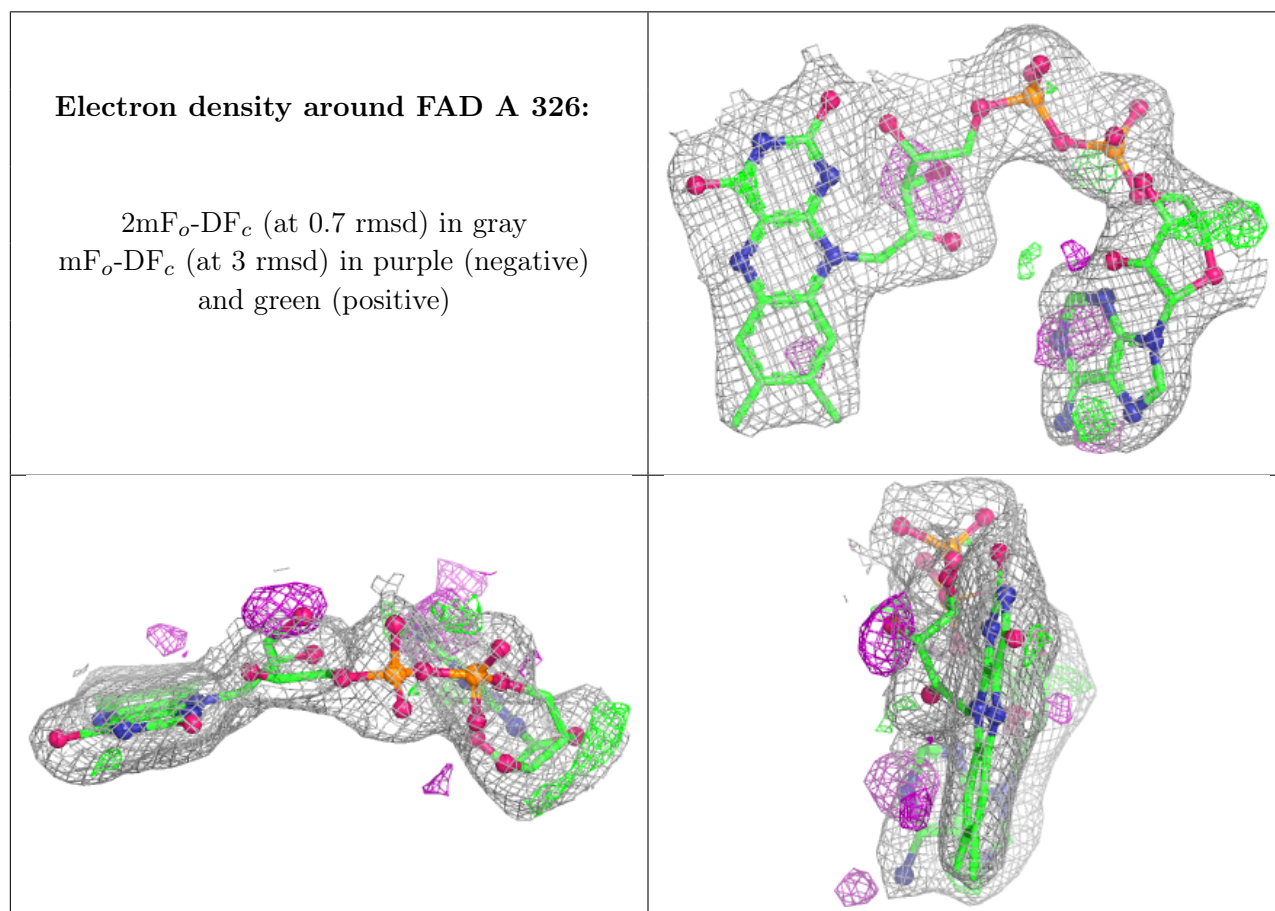
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	386	6/6	0.74	0.16	52,59,63,67	0
4	CL	A	327	1/1	0.75	0.23	86,86,86,86	0
2	FAD	A	326	53/53	0.94	0.17	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 [i](#)

There are no such residues in this entry.