



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:15 PM UTC

PDB ID : 6K8I / pdb_00006k8i
Title : Crystal structure of Arabidopsis thaliana CRY2
Authors : Ma, L.; Wang, X.; Guan, Z.; Yin, P.
Deposited on : 2019-06-12
Resolution : 2.70 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

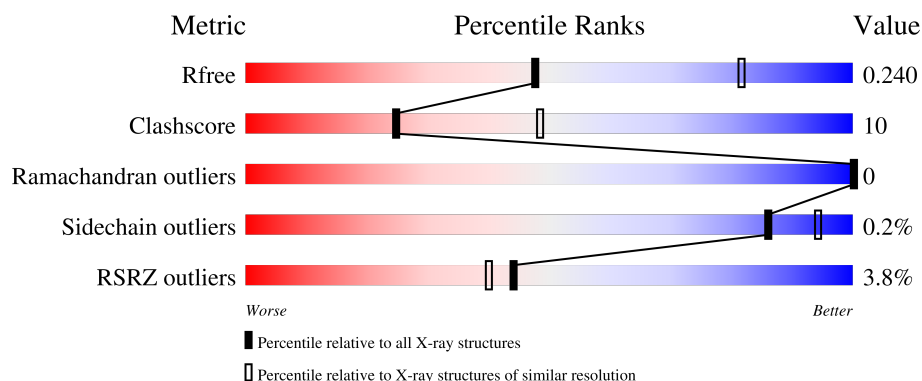
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

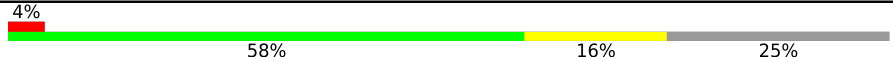
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	612	
1	B	612	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7608 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.

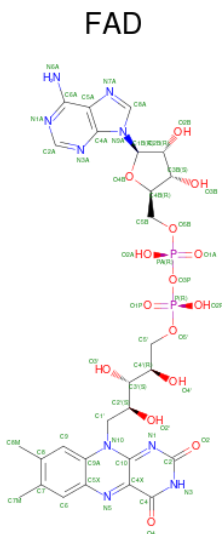
- Molecule 1 is a protein called Cryptochrome-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	1	0
			3728	2412	632	668	16			
1	B	461	Total	C	N	O	S	0	0	0
			3752	2427	638	671	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLN	LYS	See Sequence details	UNP Q96524
A	95	PRO	ALA	See Sequence details	UNP Q96524
A	366	GLY	ALA	See Sequence details	UNP Q96524
A	534	VAL	ALA	See Sequence details	UNP Q96524
B	78	GLN	LYS	See Sequence details	UNP Q96524
B	95	PRO	ALA	See Sequence details	UNP Q96524
B	366	GLY	ALA	See Sequence details	UNP Q96524
B	534	VAL	ALA	See Sequence details	UNP Q96524

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	13	Total O 13 13	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.12Å 160.37Å 139.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 2.70 49.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.03-2.70) 99.8 (49.03-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.185 , 0.237 0.189 , 0.240	Depositor DCC
R_{free} test set	1950 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7608	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: 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	0.36	0/3839	0.59	2/5219 (0.0%)
1	B	0.41	0/3863	0.65	2/5251 (0.0%)
All	All	0.39	0/7702	0.62	4/10470 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	GLU	CA-CB-CG	-6.26	101.58	114.10
1	B	422	LYS	CB-CG-CD	-5.66	98.27	111.30
1	A	459	SER	CA-C-N	-5.37	110.89	121.41
1	A	459	SER	C-N-CA	-5.37	110.89	121.41

There are no chirality outliers.

There are no planarity outliers.

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	3728	0	3657	73	0
1	B	3752	0	3690	80	0
2	A	53	0	30	5	0
2	B	53	0	30	3	0
3	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	0	0	0
All	All	7608	0	7407	147	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 10.

All (147) 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)
2:A:701:FAD:C1B	2:A:701:FAD:O4B	1.63	1.14
1:A:266:ARG:NH1	1:B:172:TRP:HE3	1.46	1.13
1:A:266:ARG:NH1	1:B:172:TRP:CE3	2.21	1.09
1:A:266:ARG:CZ	1:B:172:TRP:HE3	1.75	0.99
1:A:189:ILE:HD12	1:A:190:GLU:H	1.32	0.91
1:A:266:ARG:CZ	1:B:172:TRP:CE3	2.58	0.86
1:B:460:GLY:O	1:B:466:ASN:ND2	2.11	0.83
1:B:234:LYS:HD3	1:B:237:LYS:HE3	1.62	0.80
1:A:189:ILE:HD12	1:A:190:GLU:N	2.01	0.76
1:A:431:ARG:HG2	1:A:438:ALA:HA	1.69	0.75
1:B:431:ARG:HG2	1:B:438:ALA:HA	1.70	0.74
1:B:409:GLU:HB3	1:B:411:ASP:OD1	1.89	0.73
1:B:36:PHE:HB3	1:B:76:LEU:HD23	1.72	0.70
1:B:41:GLU:OE2	1:B:80:HIS:ND1	2.16	0.69
1:A:398:GLN:HB3	1:A:404:ILE:HG12	1.74	0.68
1:B:83:ILE:H	1:B:83:ILE:HD12	1.58	0.67
1:A:242:ASN:HB3	1:A:246:LEU:HD21	1.78	0.65
1:B:131:GLY:HA2	1:B:259:ARG:HH22	1.59	0.65
1:A:475:ASP:O	1:A:478:ARG:HB2	1.98	0.64
1:A:90:ILE:HG23	1:A:95:PRO:HD2	1.79	0.63
1:A:45:GLN:H	1:A:45:GLN:CD	2.07	0.62
1:B:205:LEU:O	1:B:208:ARG:HB2	2.00	0.62
1:A:238:LYS:HD2	1:A:240:VAL:O	2.00	0.61
1:A:232:TYR:OH	2:A:701:FAD:O1A	2.16	0.61
1:A:398:GLN:HG2	1:A:403:SER:OG	2.01	0.61
1:A:370:LEU:HB3	1:A:372:LEU:HD13	1.81	0.61
1:B:411:ASP:HA	1:B:485:ILE:HD11	1.81	0.61
1:B:98:VAL:HG11	1:B:119:LEU:HD13	1.81	0.60
1:B:248:SER:HB3	2:B:701:FAD:H5'2	1.82	0.60
1:B:188:SER:O	1:B:192:LEU:HD13	2.02	0.60
1:A:13:ARG:CZ	1:A:103:LEU:HD13	2.32	0.59
1:A:172:TRP:CZ3	1:B:266:ARG:HD3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ILE:HG13	1:B:186:ALA:H	1.67	0.59
1:B:45:GLN:H	1:B:45:GLN:CD	2.10	0.59
1:A:7:THR:HG23	1:A:97:LYS:HB3	1.85	0.58
1:A:440:LEU:HD13	1:A:445:ILE:HA	1.85	0.58
1:A:111:ARG:O	1:A:115:VAL:HG13	2.05	0.56
1:A:215:SER:HB2	1:B:271:ILE:HD12	1.88	0.56
1:A:267:MET:SD	1:B:170:PRO:HG3	2.44	0.56
1:A:266:ARG:NH2	1:B:172:TRP:HA	2.22	0.55
1:B:159:LEU:HD23	1:B:163:ILE:HD12	1.88	0.55
1:A:147:PRO:HB2	1:A:149:THR:HG23	1.88	0.55
1:B:357:ARG:HD3	1:B:423:TYR:CE2	2.42	0.55
1:B:148:PHE:CZ	1:B:157:LYS:HG2	2.42	0.54
1:B:156:LYS:NZ	1:B:289:ARG:HH12	2.06	0.54
1:A:368:LYS:HE2	1:A:410:LEU:HA	1.91	0.53
1:B:408:HIS:NE2	1:B:412:ARG:HB3	2.23	0.53
1:A:170:PRO:HG3	1:B:267:MET:SD	2.49	0.53
1:A:14:ASP:OD2	1:A:101:ASN:ND2	2.33	0.53
1:A:332:ARG:HA	1:A:345:MET:HE2	1.90	0.53
1:A:38:TRP:HH2	1:A:48:PRO:HG2	1.74	0.52
1:A:133:LEU:HB3	1:A:295:GLU:OE2	2.10	0.52
1:A:354:MET:HG3	1:A:359:ARG:HG2	1.90	0.52
1:B:155:TRP:O	1:B:158:CYS:HB2	2.10	0.52
1:B:242:ASN:HB3	1:B:246:LEU:HD11	1.91	0.51
1:B:354:MET:HE2	1:B:359:ARG:HG2	1.92	0.51
1:B:93:THR:OG1	1:B:95:PRO:HD3	2.10	0.51
1:A:415:ASN:HD22	1:A:416:PRO:HD2	1.74	0.51
1:B:134:LEU:N	1:B:295:GLU:OE2	2.44	0.51
1:A:10:TRP:HB3	1:A:100:PHE:HB3	1.92	0.50
1:B:38:TRP:HH2	1:B:48:PRO:HG2	1.76	0.50
1:B:265:ALA:HB3	1:B:288:LEU:HD21	1.93	0.50
1:A:86:ILE:O	1:A:90:ILE:HD12	2.11	0.50
1:B:408:HIS:HD2	1:B:409:GLU:O	1.94	0.50
1:B:146:LYS:HD2	1:B:146:LYS:N	2.27	0.50
1:A:83:ILE:CG1	1:A:115:VAL:HG12	2.42	0.50
1:B:94:GLY:N	1:B:95:PRO:HD3	2.26	0.49
1:B:217:ALA:HB2	1:B:250:TYR:CD1	2.47	0.49
1:A:259:ARG:O	1:A:263:GLN:HG2	2.13	0.49
1:A:374:TRP:CZ3	1:A:375:LYS:HG2	2.47	0.49
1:B:354:MET:HE3	1:B:358:ILE:HG22	1.93	0.49
1:B:90:ILE:HA	1:B:95:PRO:CD	2.42	0.49
1:B:8:ILE:HD11	1:B:95:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:TYR:CD2	1:B:407:GLY:HA2	2.48	0.48
1:A:81:ASN:HB3	1:A:84:SER:HB3	1.95	0.48
1:A:157:LYS:NZ	1:A:161:MET:HE3	2.29	0.48
1:A:223:GLU:OE1	1:A:227:LYS:HG3	2.14	0.48
1:A:378:MET:HE3	1:A:378:MET:HB2	1.75	0.48
1:B:401:SER:O	1:B:410:LEU:HD21	2.14	0.47
1:A:357:ARG:HD2	1:A:423:TYR:CE1	2.49	0.47
1:A:130:ASN:HB2	1:A:136:GLU:OE2	2.14	0.47
1:B:440:LEU:HD13	1:B:445:ILE:HA	1.97	0.47
2:A:701:FAD:H8A	2:A:701:FAD:O5B	2.14	0.47
1:B:361:ILE:HG12	1:B:419:GLN:NE2	2.29	0.47
1:B:363:SER:OG	1:B:400:ILE:HG13	2.15	0.46
1:A:370:LEU:CB	1:A:372:LEU:HD13	2.45	0.46
1:B:98:VAL:HG13	1:B:126:VAL:HG13	1.96	0.46
1:A:328:PHE:HA	1:A:372:LEU:HD21	1.97	0.46
1:A:452:PRO:HG2	1:A:455:VAL:CG2	2.45	0.46
1:A:413:LEU:HB3	1:A:478:ARG:HD2	1.98	0.46
2:B:701:FAD:O5B	2:B:701:FAD:H8A	2.16	0.46
1:B:148:PHE:HZ	1:B:157:LYS:HG2	1.80	0.46
1:B:437:LEU:HD22	1:B:440:LEU:HD12	1.98	0.46
1:B:40:PRO:HB3	1:B:47:TYR:CE1	2.51	0.45
1:B:146:LYS:HB3	1:B:147:PRO:HD2	1.98	0.45
1:A:360:VAL:HG13	1:A:400:ILE:HG22	1.98	0.45
1:B:279:GLU:HG2	1:B:280:GLY:N	2.31	0.45
1:B:387:ASP:O	2:B:701:FAD:N3	2.41	0.45
1:A:453:LEU:HD12	1:A:453:LEU:H	1.81	0.45
1:B:133:LEU:HD21	1:B:298:ARG:HD3	1.99	0.45
1:B:189:ILE:HA	1:B:192:LEU:HD13	1.98	0.45
1:B:408:HIS:CD2	1:B:409:GLU:O	2.69	0.45
1:A:45:GLN:HG2	1:A:46:PHE:CD2	2.52	0.45
1:B:242:ASN:HB3	1:B:246:LEU:HD21	1.99	0.45
1:B:72:SER:OG	1:B:73:ASP:N	2.48	0.45
1:B:104:TYR:OH	1:B:136:GLU:OE1	2.22	0.45
1:B:90:ILE:HA	1:B:95:PRO:HD2	1.99	0.44
1:B:167:MET:HE2	1:B:167:MET:HB3	1.87	0.44
1:A:136:GLU:HB2	1:A:139:GLU:HG3	2.00	0.44
1:A:357:ARG:CD	1:A:423:TYR:CZ	3.01	0.44
1:A:378:MET:HE2	1:A:397:TRP:CG	2.52	0.44
1:B:87:LEU:HD22	1:B:122:ARG:HH21	1.81	0.44
1:B:137:PRO:HB2	1:B:302:PHE:CD2	2.53	0.44
1:B:156:LYS:HZ1	1:B:289:ARG:HH12	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ASP:O	2:A:701:FAD:N3	2.42	0.43
1:A:94:GLY:N	1:A:95:PRO:HD3	2.33	0.43
1:A:248:SER:HB3	2:A:701:FAD:H5'2	2.00	0.43
1:A:431:ARG:NH1	1:A:445:ILE:HD12	2.34	0.43
1:A:68:LYS:HA	1:A:72:SER:O	2.18	0.43
1:B:363:SER:HB2	1:B:397:TRP:CZ3	2.53	0.43
1:B:117:GLU:O	1:B:121:GLU:OE1	2.37	0.43
1:B:67:LEU:HD12	1:B:74:LEU:HB2	2.00	0.43
1:B:387:ASP:O	1:B:388:ALA:C	2.62	0.43
1:A:36:PHE:HB3	1:A:76:LEU:HD23	2.01	0.42
1:B:68:LYS:HA	1:B:72:SER:O	2.19	0.42
1:B:188:SER:O	1:B:192:LEU:CD1	2.67	0.42
1:A:473[A]:ASP:OD1	1:A:476:THR:HG23	2.19	0.42
1:B:87:LEU:CD2	1:B:122:ARG:HE	2.32	0.42
1:B:205:LEU:O	1:B:208:ARG:CB	2.66	0.42
1:B:188:SER:OG	1:B:191:GLU:HG3	2.19	0.41
1:A:415:ASN:HD22	1:A:416:PRO:CD	2.33	0.41
1:B:141:TYR:CE2	1:B:146:LYS:N	2.88	0.41
1:A:55:TRP:CE3	1:A:212:PRO:HG3	2.54	0.41
1:A:137:PRO:HB3	1:A:299:TYR:HA	2.01	0.41
1:B:221:LEU:HD13	1:B:261:VAL:HG22	2.03	0.41
1:B:83:ILE:H	1:B:83:ILE:CD1	2.29	0.41
1:A:238:LYS:HE3	1:A:243:SER:HB3	2.03	0.41
1:A:164:GLU:OE1	1:A:164:GLU:HA	2.21	0.41
1:A:189:ILE:CD1	1:A:190:GLU:N	2.80	0.41
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.76	0.41
1:A:354:MET:HE3	1:A:358:ILE:HG22	2.02	0.41
1:A:265:ALA:HB3	1:A:288:LEU:HD21	2.03	0.40
1:A:90:ILE:HA	1:A:95:PRO:CD	2.52	0.40
1:A:148:PHE:CE2	1:A:157:LYS:HG2	2.56	0.40
1:B:176:PRO:O	1:B:177:ILE:HG23	2.21	0.40
1:A:474:ILE:O	1:A:478:ARG:HG2	2.22	0.40
1:B:122:ARG:HG2	1:B:122:ARG:HH11	1.86	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	450/612 (74%)	432 (96%)	18 (4%)	0	100	100
1	B	453/612 (74%)	427 (94%)	26 (6%)	0	100	100
All	All	903/1224 (74%)	859 (95%)	44 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	399/531 (75%)	396 (99%)	3 (1%)	73	88
1	B	402/531 (76%)	402 (100%)	0	100	100
All	All	801/1062 (75%)	798 (100%)	3 (0%)	86	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	LEU
1	A	473[A]	ASP
1	A	473[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	415	ASN
1	B	408	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](#)

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	701	-	58,58,58	3.22	25 (43%)	85,89,89	2.10	23 (27%)
2	FAD	A	701	-	58,58,58	3.31	25 (43%)	85,89,89	1.93	21 (24%)

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	701	-	-	4/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	701	-	-	4/34/50/50	0/6/6/6

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FAD	O4B-C1B	9.39	1.63	1.42
2	B	701	FAD	O4B-C1B	8.58	1.61	1.42
2	A	701	FAD	C4X-N5	7.12	1.46	1.30
2	B	701	FAD	P-O3P	7.09	1.67	1.59
2	A	701	FAD	C10-N1	7.06	1.47	1.33
2	B	701	FAD	C10-N1	6.93	1.47	1.33
2	B	701	FAD	C2B-C1B	-6.88	1.31	1.53
2	A	701	FAD	C9A-N10	6.79	1.52	1.41
2	A	701	FAD	C2B-C1B	-6.70	1.32	1.53
2	B	701	FAD	C4X-N5	6.57	1.44	1.30
2	B	701	FAD	PA-O3P	6.53	1.66	1.59
2	A	701	FAD	C5X-N5	6.21	1.50	1.39
2	A	701	FAD	P-O3P	6.15	1.66	1.59
2	A	701	FAD	O4B-C4B	-6.02	1.31	1.45
2	B	701	FAD	O4B-C4B	-5.87	1.31	1.45
2	A	701	FAD	PA-O3P	5.36	1.65	1.59
2	A	701	FAD	C2-N3	5.28	1.50	1.39
2	B	701	FAD	C5X-N5	5.28	1.49	1.39
2	A	701	FAD	C2-N1	5.12	1.48	1.36
2	B	701	FAD	C10-N10	5.10	1.48	1.37
2	B	701	FAD	C9A-N10	5.02	1.49	1.41
2	B	701	FAD	C2-N3	4.92	1.49	1.39
2	B	701	FAD	C2-N1	4.73	1.47	1.36
2	A	701	FAD	C10-N10	4.48	1.47	1.37
2	A	701	FAD	C4-N3	4.30	1.46	1.38
2	B	701	FAD	C4-N3	4.23	1.46	1.38
2	B	701	FAD	C6A-N6A	3.94	1.44	1.34
2	A	701	FAD	O2B-C2B	3.69	1.52	1.43
2	A	701	FAD	C6A-N6A	3.58	1.43	1.34
2	B	701	FAD	O2B-C2B	3.08	1.50	1.43
2	A	701	FAD	O3B-C3B	-3.02	1.35	1.43
2	B	701	FAD	O4-C4	-2.94	1.18	1.23
2	B	701	FAD	O3B-C3B	-2.91	1.35	1.43
2	A	701	FAD	O2-C2	-2.82	1.18	1.24
2	B	701	FAD	C1'-C2'	2.71	1.56	1.52
2	A	701	FAD	C1'-C2'	2.63	1.56	1.52
2	B	701	FAD	O2'-C2'	-2.63	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	C5A-C4A	-2.45	1.34	1.39
2	B	701	FAD	C5A-N7A	-2.44	1.34	1.39
2	A	701	FAD	C5A-N7A	-2.44	1.34	1.39
2	A	701	FAD	O2'-C2'	-2.42	1.38	1.43
2	B	701	FAD	O4'-C4'	-2.40	1.38	1.43
2	A	701	FAD	O4-C4	-2.38	1.19	1.23
2	A	701	FAD	C4X-C4	2.22	1.52	1.44
2	A	701	FAD	C5A-C4A	-2.21	1.35	1.39
2	A	701	FAD	C2A-N3A	2.19	1.37	1.33
2	B	701	FAD	O2-C2	-2.14	1.20	1.24
2	A	701	FAD	O4'-C4'	-2.09	1.39	1.43
2	B	701	FAD	C2A-N3A	2.08	1.37	1.33
2	B	701	FAD	C4'-C3'	2.02	1.56	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	C7M-C7-C6	-7.16	106.96	119.57
2	B	701	FAD	C7M-C7-C8	6.01	133.04	120.76
2	B	701	FAD	N3A-C2A-N1A	-5.64	120.04	128.58
2	A	701	FAD	N3A-C2A-N1A	-5.34	120.50	128.58
2	A	701	FAD	C7M-C7-C6	-5.30	110.23	119.57
2	A	701	FAD	N6A-C6A-N1A	-5.26	106.65	118.38
2	B	701	FAD	N6A-C6A-N1A	-4.88	107.51	118.38
2	A	701	FAD	C7M-C7-C8	4.59	130.13	120.76
2	B	701	FAD	C5A-C4A-N3A	-4.48	120.55	126.72
2	B	701	FAD	N9A-C8A-N7A	-4.31	107.82	113.94
2	A	701	FAD	C5A-C6A-N6A	4.21	133.72	123.29
2	A	701	FAD	C5A-C4A-N3A	-4.16	120.98	126.72
2	B	701	FAD	C5A-C6A-N6A	3.92	132.98	123.29
2	A	701	FAD	C5'-C4'-C3'	-3.75	105.14	112.22
2	A	701	FAD	C8M-C8-C7	-3.64	113.32	120.76
2	B	701	FAD	N3A-C4A-N9A	3.47	133.07	127.17
2	A	701	FAD	N9A-C8A-N7A	-3.45	109.05	113.94
2	A	701	FAD	C8M-C8-C9	3.33	125.44	119.57
2	B	701	FAD	C5X-C9A-N10	3.23	120.89	117.97
2	B	701	FAD	C4-N3-C2	-3.15	120.04	125.64
2	B	701	FAD	C2A-N3A-C4A	3.14	119.50	111.83
2	A	701	FAD	C4X-C10-N10	3.14	120.97	116.48
2	A	701	FAD	C4-N3-C2	-3.02	120.27	125.64
2	B	701	FAD	C4A-N9A-C8A	2.98	108.87	105.74
2	A	701	FAD	N3A-C4A-N9A	2.92	132.13	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	C10-N1-C2	2.86	123.05	116.85
2	A	701	FAD	C5X-C9A-N10	2.83	120.53	117.97
2	B	701	FAD	C5'-C4'-C3'	-2.82	106.89	112.22
2	A	701	FAD	C2A-N3A-C4A	2.75	118.54	111.83
2	B	701	FAD	C5A-N7A-C8A	2.73	107.74	103.45
2	B	701	FAD	C4X-C10-N10	2.71	120.36	116.48
2	B	701	FAD	C4X-C10-N1	-2.61	118.20	124.59
2	B	701	FAD	C4-C4X-C10	2.43	121.10	116.93
2	B	701	FAD	C4X-C4-N3	2.40	119.35	113.25
2	B	701	FAD	O4-C4-C4X	-2.38	120.26	126.53
2	B	701	FAD	C10-C4X-N5	-2.37	119.97	124.81
2	A	701	FAD	C2B-C1B-N9A	-2.36	107.45	113.30
2	A	701	FAD	C4-C4X-C10	2.32	120.91	116.93
2	B	701	FAD	C9A-C5X-N5	-2.28	120.04	122.45
2	A	701	FAD	C10-C4X-N5	-2.25	120.21	124.81
2	B	701	FAD	C6A-C5A-C4A	2.11	120.06	117.18
2	A	701	FAD	C6A-C5A-C4A	2.08	120.02	117.18
2	A	701	FAD	C4A-N9A-C8A	2.07	107.92	105.74
2	A	701	FAD	C4X-C4-N3	2.07	118.52	113.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5B-O5B-PA-O2A
2	B	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	C4'-C5'-O5'-P
2	A	701	FAD	C4'-C5'-O5'-P
2	A	701	FAD	C5'-O5'-P-O1P
2	A	701	FAD	P-O3P-PA-O2A
2	A	701	FAD	P-O3P-PA-O1A

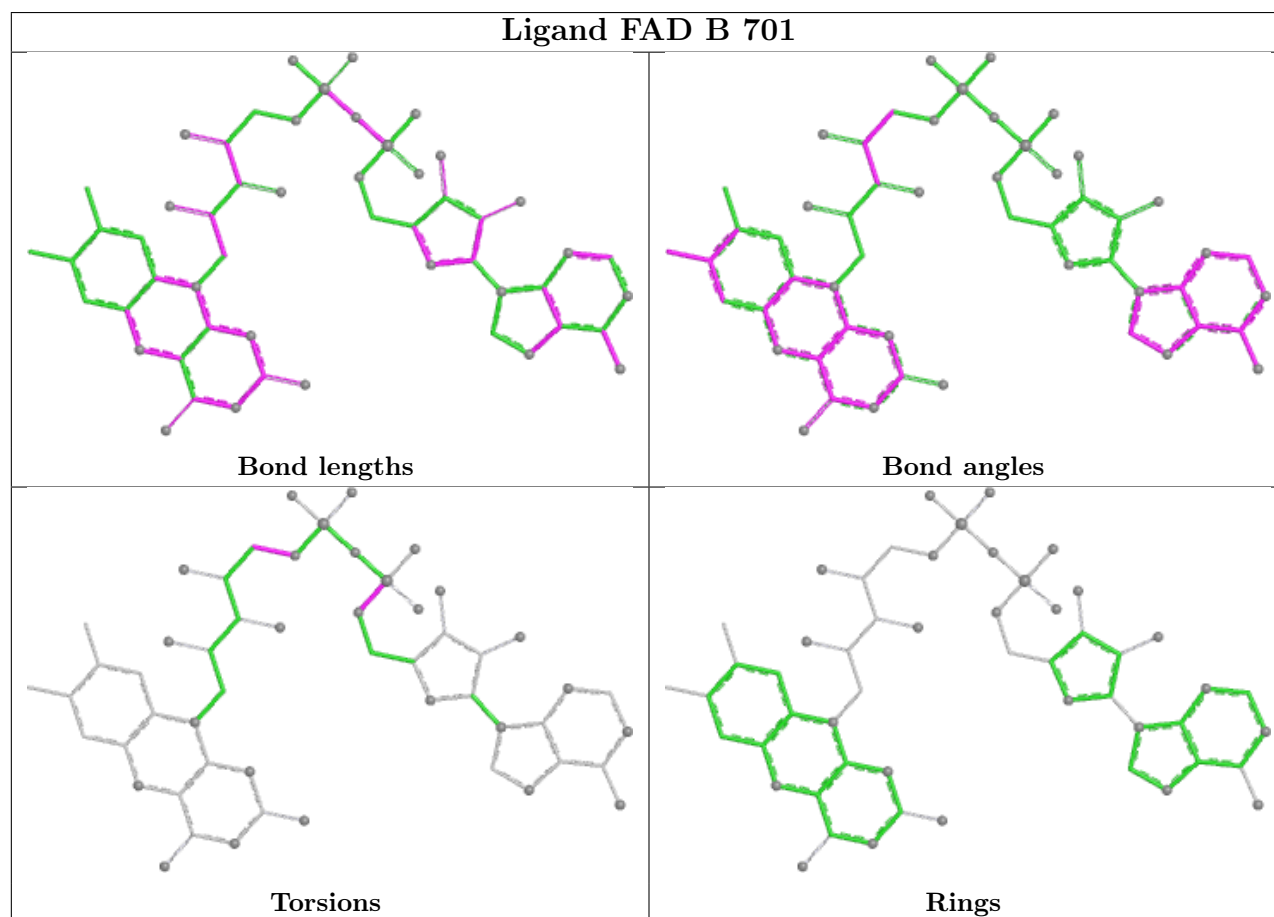
There are no ring outliers.

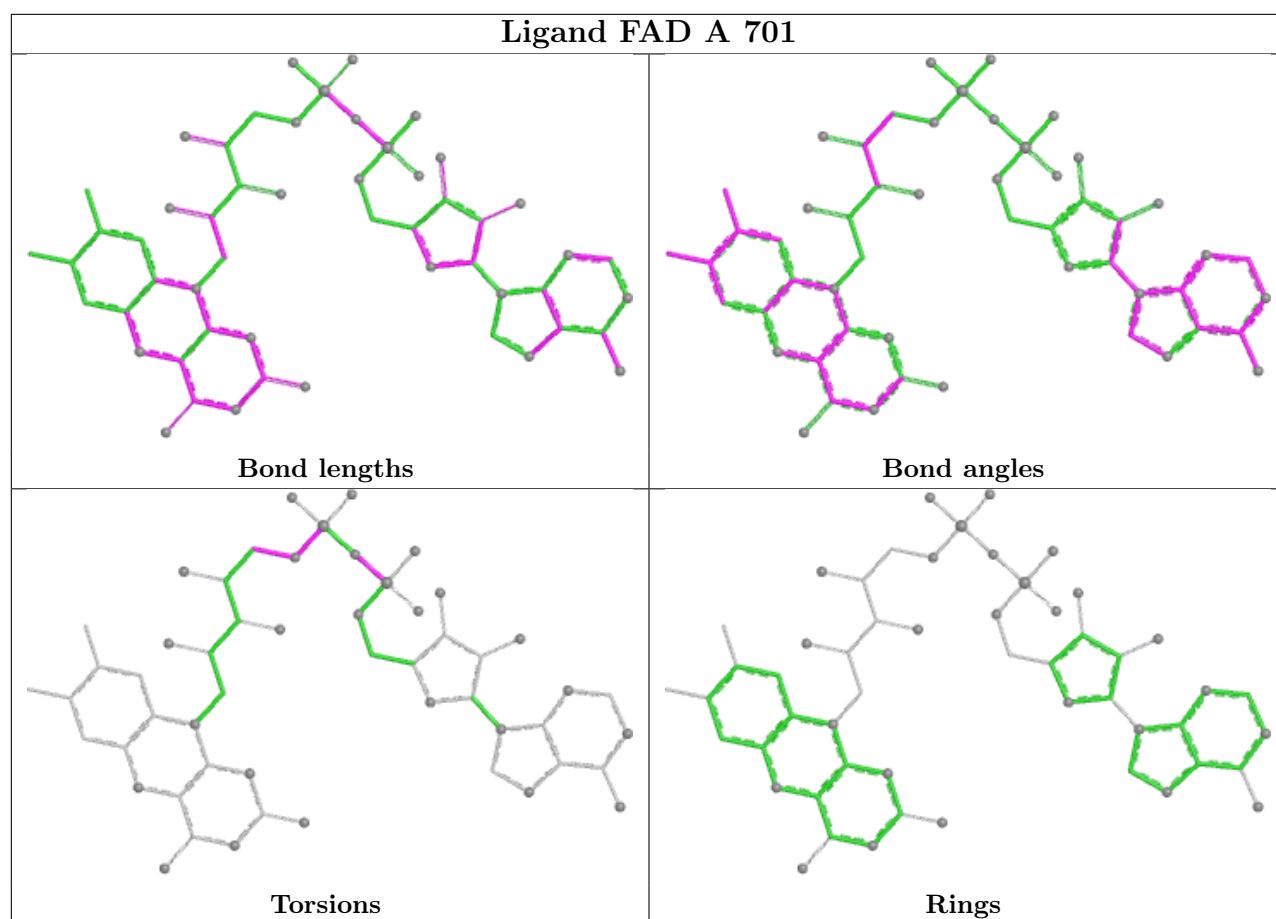
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FAD	3	0
2	A	701	FAD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	457/612 (74%)	0.05	24 (5%) 32 28	41, 69, 121, 165	1 (0%)
1	B	461/612 (75%)	-0.11	11 (2%) 59 56	42, 62, 115, 147	0
All	All	918/1224 (75%)	-0.03	35 (3%) 44 40	41, 65, 120, 165	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	ILE	5.2
1	A	484	ALA	4.3
1	B	321	TRP	4.0
1	A	408	HIS	3.8
1	B	185	TRP	3.8
1	A	184	ILE	3.5
1	A	163	ILE	3.5
1	A	165	SER	3.3
1	B	410	LEU	3.2
1	B	320	PRO	3.2
1	A	167	MET	3.2
1	A	406	ASP	3.1
1	A	414	ASP	3.0
1	B	408	HIS	2.9
1	A	147	PRO	2.8
1	A	405	PRO	2.7
1	A	164	GLU	2.7
1	A	142	CYS	2.7
1	B	121	GLU	2.6
1	A	162	SER	2.6
1	A	132	ASP	2.5
1	A	185	TRP	2.5
1	A	148	PHE	2.5
1	A	140	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	320	PRO	2.4
1	B	156	LYS	2.4
1	B	305	PRO	2.4
1	A	305	PRO	2.4
1	A	177	ILE	2.3
1	A	189	ILE	2.2
1	A	5	LYS	2.2
1	A	410	LEU	2.1
1	A	146	LYS	2.1
1	B	488	THR	2.0
1	B	208	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](#)

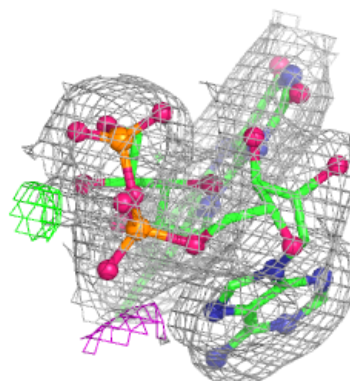
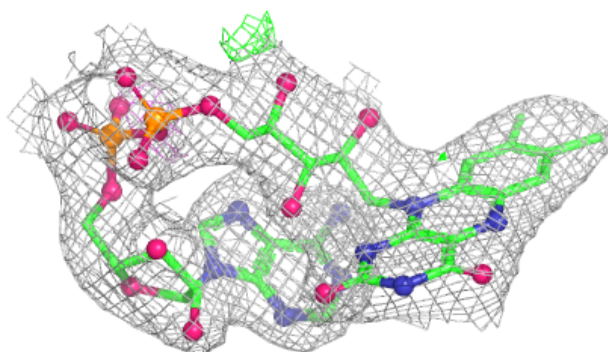
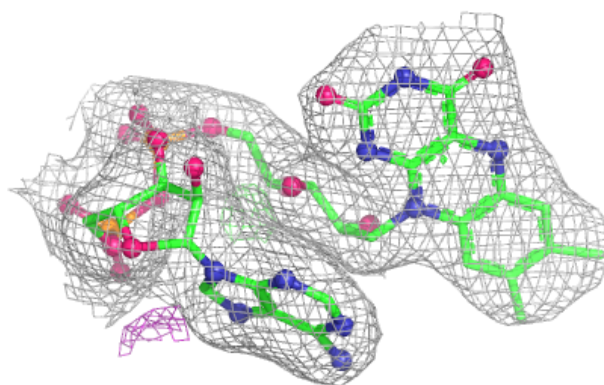
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	FAD	A	701	53/53	0.97	0.06	44,52,63,70	0
2	FAD	B	701	53/53	0.98	0.05	36,48,57,63	0

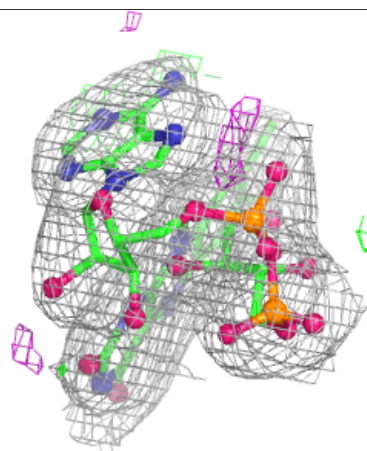
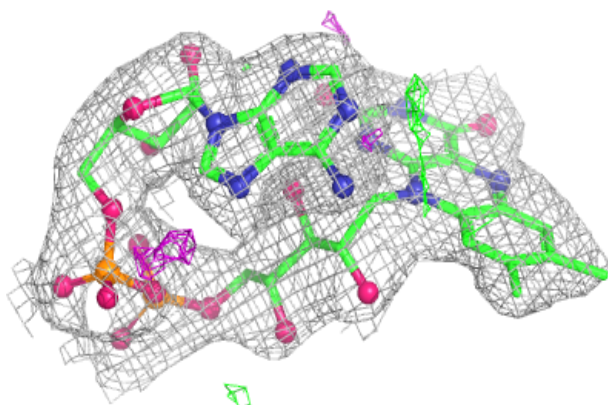
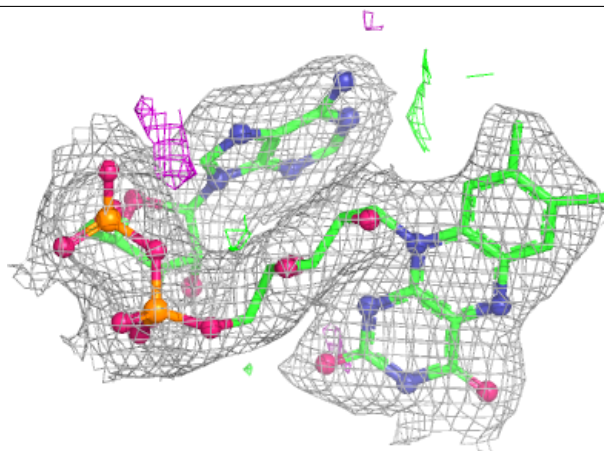
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 701:

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

**Electron density around FAD B 701:**

$2mF_o-DF_c$ (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.