



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:44 AM UTC

PDB ID : 4I6G / pdb_00004i6g
Title : a vertebrate cryptochrome with FAD
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Deposited on : 2012-11-29
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

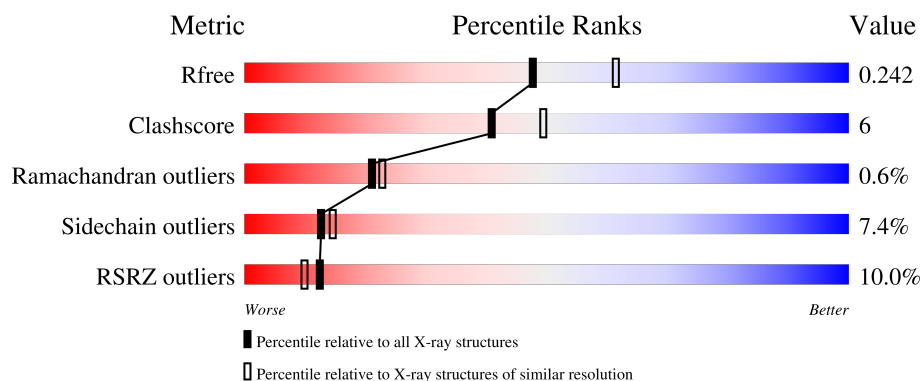
1 Overall quality at a glance

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))
R_{free}	180053	6164 (2.20-2.20)
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	512	6% 76% 15% • 7%
1	B	512	12% 73% 18% • 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8109 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	476	Total	C	N	O	S	0	0	0
			3867	2484	681	683	19			
1	B	476	Total	C	N	O	S	0	0	0
			3873	2487	684	683	19			

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



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

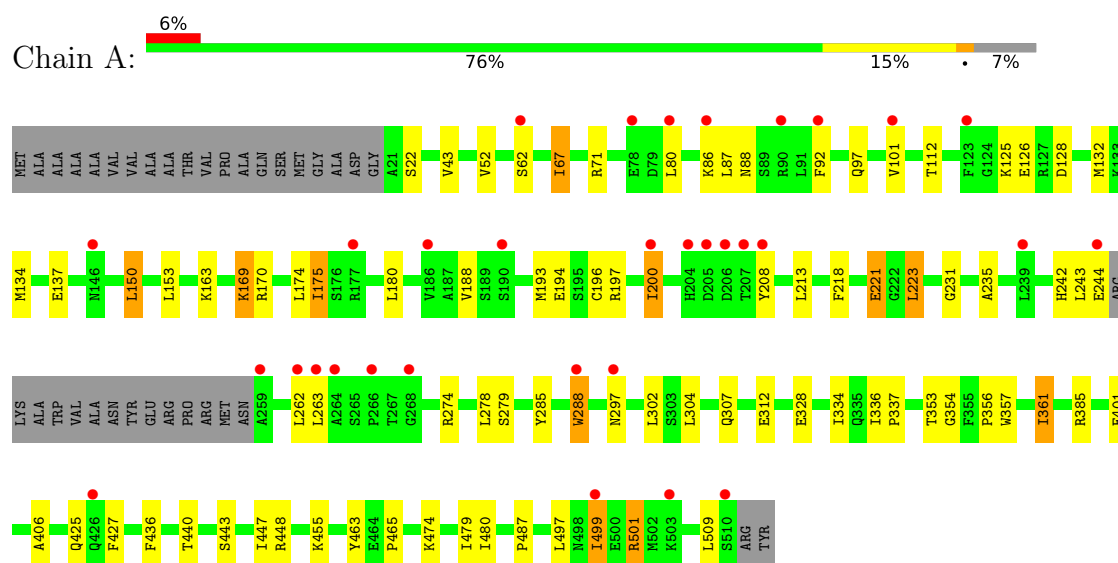
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total 150	O 150	0	0
3	B	113	Total 113	O 113	0	0

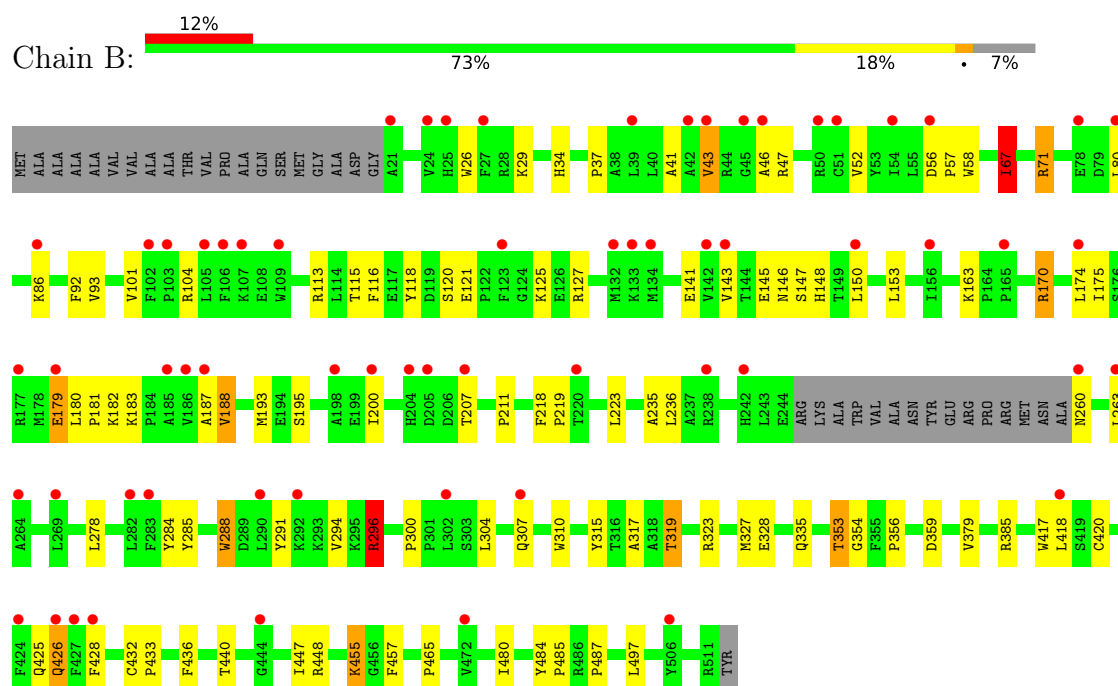
3 Residue-property plots [i](#)

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: Cryptochrome-2



• Molecule 1: Cryptochrome-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	97.53Å 97.53Å 128.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.62 – 2.20 43.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.62-2.20) 96.1 (43.62-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.197 , 0.238 0.205 , 0.242	Depositor DCC
R_{free} test set	2010 reflections (3.18%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8109	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6016e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/3979	0.86	4/5399 (0.1%)
1	B	0.51	0/3985	0.87	5/5406 (0.1%)
All	All	0.54	0/7964	0.87	9/10805 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	GLY	N-CA-C	8.93	120.43	111.95
1	B	207	THR	N-CA-C	-8.03	102.95	114.12
1	B	67	ILE	CB-CA-C	-7.10	101.15	112.16
1	A	67	ILE	CB-CA-C	-6.82	101.59	112.16
1	B	353	THR	N-CA-C	-6.70	101.88	110.53
1	A	353	THR	N-CA-C	-6.57	101.28	110.35
1	A	361	ILE	CB-CA-C	-5.75	104.61	111.97
1	B	121	GLU	CA-C-N	5.05	124.22	118.97
1	B	121	GLU	C-N-CA	5.05	124.22	118.97

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	3867	0	3797	44	0
1	B	3873	0	3805	55	0
2	A	53	0	31	0	0
2	B	53	0	31	5	0
3	A	150	0	0	6	0
3	B	113	0	0	7	0
All	All	8109	0	7664	100	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 6.

All (100) 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:354:GLY:HA3	1:A:487:PRO:HA	1.56	0.87
1:A:87:LEU:HD13	1:A:193:MET:HG3	1.68	0.75
1:B:354:GLY:HA3	1:B:487:PRO:HA	1.67	0.74
1:B:127:ARG:NH1	3:B:1111:HOH:O	2.20	0.73
1:A:443:SER:O	1:A:448:ARG:NH2	2.24	0.70
1:B:29:LYS:HD3	1:B:148:HIS:CE1	2.27	0.69
1:B:448:ARG:HG2	1:B:455:LYS:HA	1.77	0.66
1:A:334:ILE:HD12	1:A:509:LEU:HD11	1.79	0.65
1:A:427:PHE:O	3:A:1148:HOH:O	2.13	0.65
1:B:120:SER:HB2	1:B:319:THR:HG23	1.78	0.65
1:B:179:GLU:OE2	3:B:1070:HOH:O	2.15	0.64
1:B:46:ALA:HB1	1:B:195:SER:HB2	1.81	0.63
1:A:474:LYS:HG3	1:A:479:ILE:HD11	1.81	0.62
1:B:436:PHE:O	1:B:440:THR:HG23	2.00	0.61
1:A:501:ARG:HH11	1:A:501:ARG:HG3	1.64	0.61
1:A:436:PHE:O	1:A:440:THR:HG23	2.00	0.61
1:A:401:GLU:OE2	3:A:1103:HOH:O	2.16	0.60
1:B:34:HIS:HA	1:B:187:ALA:HB2	1.83	0.60
1:B:93:VAL:HG11	1:B:211:PRO:HD3	1.82	0.60
1:A:448:ARG:HG2	1:A:455:LYS:HA	1.84	0.59
1:B:118:TYR:HB3	1:B:146:ASN:HA	1.87	0.57
1:B:294:VAL:O	1:B:296:ARG:NH2	2.38	0.57
1:A:200:ILE:HD13	1:A:200:ILE:H	1.70	0.56
1:A:194:GLU:OE2	1:A:197:ARG:NH2	2.39	0.55
1:B:385:ARG:CZ	1:B:428:PHE:HB3	2.35	0.55
1:A:67:ILE:HG23	1:A:218:PHE:CD1	2.42	0.55
1:A:188:VAL:HB	1:A:193:MET:HE3	1.88	0.55
1:B:356:PRO:HB2	1:B:447:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TRP:O	1:A:361:ILE:HG12	2.07	0.54
1:A:501:ARG:HG3	1:A:501:ARG:NH1	2.22	0.54
1:B:118:TYR:OH	1:B:125:LYS:HD3	2.06	0.54
1:A:274:ARG:HD2	1:A:406:ALA:O	2.08	0.54
1:B:26:TRP:HB3	1:B:116:PHE:HB3	1.89	0.53
1:B:41:ALA:O	1:B:113:ARG:NH1	2.42	0.53
1:B:307:GLN:HB2	2:B:900:FAD:O4B	2.09	0.53
1:B:317:ALA:O	3:B:1053:HOH:O	2.19	0.51
1:B:307:GLN:HG3	2:B:900:FAD:H51A	1.91	0.51
1:B:385:ARG:HH21	1:B:428:PHE:HD2	1.58	0.51
1:A:71:ARG:NH2	3:A:1071:HOH:O	2.29	0.51
1:B:43:VAL:HG21	1:B:193:MET:HE2	1.93	0.51
1:A:501:ARG:HH11	1:A:501:ARG:CG	2.23	0.51
1:A:499:ILE:HD13	1:B:58:TRP:HE1	1.77	0.50
1:B:67:ILE:HG23	1:B:218:PHE:CD1	2.46	0.50
1:B:310:TRP:HH2	1:B:417:TRP:CH2	2.31	0.49
1:B:181:PRO:O	1:B:285:TYR:OH	2.25	0.49
1:A:208:TYR:O	3:A:1056:HOH:O	2.19	0.49
1:A:235:ALA:HB1	1:A:278:LEU:HB2	1.94	0.49
1:A:125:LYS:NZ	3:A:1104:HOH:O	2.42	0.49
1:A:22:SER:H	1:A:112:THR:HB	1.78	0.48
1:B:34:HIS:CE1	1:B:236:LEU:HD21	2.48	0.48
2:B:900:FAD:H2B	2:B:900:FAD:O3'	2.14	0.48
1:A:128:ASP:O	1:A:132:MET:HG2	2.13	0.48
1:A:169:LYS:HB3	1:A:169:LYS:HE3	1.63	0.48
1:B:426:GLN:H	1:B:426:GLN:CD	2.21	0.47
1:B:323:ARG:NH2	1:B:328:GLU:O	2.39	0.47
1:A:354:GLY:CA	1:A:487:PRO:HA	2.38	0.47
1:B:385:ARG:NH2	1:B:428:PHE:HB3	2.30	0.46
1:B:71:ARG:NH2	3:B:1041:HOH:O	2.32	0.46
1:B:354:GLY:HA3	1:B:487:PRO:CA	2.42	0.46
1:A:354:GLY:HA3	1:A:487:PRO:CA	2.35	0.45
1:A:43:VAL:HG23	1:A:196:CYS:SG	2.57	0.45
1:B:484:TYR:CD1	1:B:485:PRO:HD2	2.51	0.45
1:A:242:HIS:O	1:A:244:GLU:N	2.50	0.45
1:B:71:ARG:NE	3:B:1041:HOH:O	2.40	0.45
1:B:420:CYS:SG	1:B:428:PHE:HB2	2.57	0.45
1:B:448:ARG:NH1	1:B:457:PHE:O	2.51	0.44
1:B:465:PRO:HB2	1:B:480:ILE:HD11	1.98	0.44
1:A:71:ARG:HD3	1:A:213:LEU:HD11	1.99	0.44
1:B:153:LEU:HD21	1:B:315:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:TYR:HA	1:B:288:TRP:HB2	1.98	0.44
1:A:285:TYR:HA	1:A:288:TRP:HB2	1.99	0.44
1:A:356:PRO:HB2	1:A:447:ILE:HD13	1.99	0.44
1:B:432:CYS:HA	1:B:433:PRO:HD2	1.87	0.44
1:B:115:THR:HG22	1:B:143:VAL:HB	2.00	0.43
1:B:291:TYR:CG	1:B:300:PRO:HB3	2.54	0.43
1:B:327:MET:HE3	1:B:335:GLN:HE22	1.82	0.43
1:A:465:PRO:HB2	1:A:480:ILE:HD11	2.00	0.43
1:B:235:ALA:HB1	1:B:278:LEU:HB2	2.01	0.42
1:B:359:ASP:OD2	1:B:484:TYR:OH	2.32	0.42
1:A:175:ILE:HD12	1:A:175:ILE:HA	1.85	0.42
1:B:182:LYS:HG3	3:B:1029:HOH:O	2.19	0.42
1:A:307:GLN:H	1:A:307:GLN:CD	2.27	0.42
1:B:353:THR:O	1:B:359:ASP:OD2	2.38	0.42
1:B:56:ASP:HA	1:B:57:PRO:HD3	1.85	0.42
1:A:336:ILE:HA	1:A:337:PRO:HD3	1.91	0.41
1:B:37:PRO:HB2	1:B:145:GLU:HG3	2.01	0.41
1:B:67:ILE:H	1:B:67:ILE:HG13	1.62	0.41
1:A:263:LEU:HD13	1:A:263:LEU:HA	1.84	0.41
1:A:440:THR:HG22	1:B:219:PRO:HG3	2.01	0.41
1:B:52:VAL:HG12	1:B:92:PHE:HB2	2.02	0.41
1:B:188:VAL:HG21	1:B:193:MET:HE3	2.02	0.41
1:B:170:ARG:NH1	1:B:170:ARG:HA	2.35	0.41
2:B:900:FAD:H3B	2:B:900:FAD:O3P	2.21	0.41
1:A:150:LEU:HB2	1:A:312:GLU:CD	2.46	0.41
1:B:284:TYR:CE2	1:B:288:TRP:HD1	2.38	0.41
1:A:425:GLN:NE2	3:A:1134:HOH:O	2.52	0.41
2:B:900:FAD:N6A	3:B:1018:HOH:O	2.36	0.41
1:A:52:VAL:HG12	1:A:92:PHE:HB2	2.03	0.41
1:A:447:ILE:HD11	1:A:463:TYR:CD1	2.55	0.41
1:A:134:MET:O	1:A:137:GLU:HG2	2.21	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	472/512 (92%)	450 (95%)	18 (4%)	4 (1%)	16	16
1	B	472/512 (92%)	442 (94%)	28 (6%)	2 (0%)	30	34
All	All	944/1024 (92%)	892 (94%)	46 (5%)	6 (1%)	21	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	ARG
1	A	243	LEU
1	A	223	LEU
1	A	297	ASN
1	B	147	SER
1	A	221	GLU

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	398/434 (92%)	370 (93%)	28 (7%)	14	16
1	B	411/434 (95%)	379 (92%)	32 (8%)	11	13
All	All	809/868 (93%)	749 (93%)	60 (7%)	13	14

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	80	LEU
1	A	86	LYS
1	A	88	ASN
1	A	97	GLN
1	A	101	VAL
1	A	126	GLU

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Mol	Chain	Res	Type
1	A	150	LEU
1	A	153	LEU
1	A	163	LYS
1	A	169	LYS
1	A	170	ARG
1	A	174	LEU
1	A	175	ILE
1	A	180	LEU
1	A	200	ILE
1	A	221	GLU
1	A	223	LEU
1	A	262	LEU
1	A	279	SER
1	A	288	TRP
1	A	302	LEU
1	A	304	LEU
1	A	328	GLU
1	A	385	ARG
1	A	497	LEU
1	A	499	ILE
1	A	501	ARG
1	B	43	VAL
1	B	47	ARG
1	B	67	ILE
1	B	71	ARG
1	B	80	LEU
1	B	86	LYS
1	B	101	VAL
1	B	104	ARG
1	B	141	GLU
1	B	150	LEU
1	B	163	LYS
1	B	170	ARG
1	B	174	LEU
1	B	175	ILE
1	B	179	GLU
1	B	180	LEU
1	B	183	LYS
1	B	188	VAL
1	B	200	ILE
1	B	223	LEU
1	B	260	ASN

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Mol	Chain	Res	Type
1	B	263	LEU
1	B	288	TRP
1	B	296	ARG
1	B	304	LEU
1	B	319	THR
1	B	379	VAL
1	B	418	LEU
1	B	425	GLN
1	B	426	GLN
1	B	455	LYS
1	B	497	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	411	ASN
1	B	260	ASN
1	B	411	ASN
1	B	426	GLN

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	A	900	-	58,58,58	1.76	10 (17%)	85,89,89	1.63	20 (23%)
2	FAD	B	900	-	58,58,58	1.74	10 (17%)	85,89,89	1.86	23 (27%)

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	900	-	-	2/34/50/50	0/6/6/6
2	FAD	B	900	-	-	9/34/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	FAD	C4-N3	-5.04	1.29	1.38
2	A	900	FAD	C4-N3	-4.73	1.30	1.38
2	B	900	FAD	C5A-C4A	4.05	1.46	1.39
2	A	900	FAD	C5A-N7A	-3.89	1.32	1.39
2	A	900	FAD	C4A-N9A	-3.78	1.29	1.37
2	B	900	FAD	C2-N3	-3.77	1.30	1.39
2	B	900	FAD	C9A-C5X	3.74	1.47	1.41
2	B	900	FAD	C5X-N5	-3.73	1.32	1.39
2	A	900	FAD	C5X-N5	-3.72	1.32	1.39
2	A	900	FAD	C9A-C5X	3.67	1.47	1.41
2	A	900	FAD	C2-N3	-3.26	1.31	1.39
2	B	900	FAD	C5A-N7A	-3.25	1.33	1.39
2	A	900	FAD	C5A-C4A	2.95	1.44	1.39
2	B	900	FAD	C4A-N9A	-2.83	1.31	1.37
2	A	900	FAD	C8A-N9A	-2.75	1.32	1.37
2	B	900	FAD	C5'-C4'	-2.59	1.48	1.51
2	A	900	FAD	C6-C7	-2.31	1.36	1.39
2	A	900	FAD	C8-C7	2.29	1.46	1.40
2	B	900	FAD	C8A-N9A	-2.22	1.33	1.37
2	B	900	FAD	O4B-C4B	-2.06	1.40	1.45

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	FAD	O4'-C4'-C5'	-7.42	93.62	109.99
2	B	900	FAD	C5A-C4A-N3A	-5.01	119.82	126.72
2	A	900	FAD	C5A-C4A-N3A	-4.73	120.20	126.72
2	A	900	FAD	N3A-C4A-N9A	4.36	134.57	127.17
2	B	900	FAD	N3A-C4A-N9A	4.13	134.19	127.17
2	B	900	FAD	O5'-C5'-C4'	-4.02	98.64	109.36
2	A	900	FAD	C4A-N9A-C8A	3.62	109.54	105.74
2	A	900	FAD	N3A-C2A-N1A	-3.38	123.47	128.58
2	A	900	FAD	C2A-N3A-C4A	3.35	120.02	111.83
2	B	900	FAD	C2A-N3A-C4A	3.24	119.75	111.83
2	B	900	FAD	C4A-C5A-N7A	-3.21	106.91	110.58
2	A	900	FAD	C4'-C3'-C2'	-3.13	108.37	113.57
2	A	900	FAD	C4X-C10-N10	3.07	120.88	116.48
2	B	900	FAD	N3A-C2A-N1A	-2.92	124.16	128.58
2	B	900	FAD	C4A-N9A-C8A	2.89	108.77	105.74
2	A	900	FAD	C4-C4X-N5	2.80	122.07	118.21
2	B	900	FAD	C4X-C10-N1	-2.79	117.76	124.59
2	A	900	FAD	C2'-C1'-N10	2.66	122.79	110.20
2	B	900	FAD	C4-C4X-N5	2.66	121.88	118.21
2	B	900	FAD	C4'-C3'-C2'	-2.61	109.22	113.57
2	A	900	FAD	C4X-C10-N1	-2.61	118.19	124.59
2	A	900	FAD	C4A-C5A-N7A	-2.48	107.74	110.58
2	B	900	FAD	C4X-C10-N10	2.43	119.95	116.48
2	A	900	FAD	C9A-N10-C10	-2.40	117.09	120.75
2	B	900	FAD	C5A-N7A-C8A	2.40	107.22	103.45
2	B	900	FAD	C5X-C9A-N10	2.38	120.12	117.97
2	B	900	FAD	C2'-C1'-N10	2.37	121.42	110.20
2	B	900	FAD	C9A-N10-C10	-2.32	117.21	120.75
2	A	900	FAD	N3-C2-N1	2.29	124.38	119.50
2	A	900	FAD	N9A-C8A-N7A	-2.28	110.71	113.94
2	B	900	FAD	C4-N3-C2	-2.26	121.63	125.64
2	A	900	FAD	O2-C2-N1	-2.26	118.05	121.80
2	B	900	FAD	C4X-C4-N3	2.23	118.93	113.25
2	B	900	FAD	C6A-C5A-N7A	2.14	136.22	132.09
2	B	900	FAD	N3-C2-N1	2.14	124.04	119.50
2	A	900	FAD	C5A-N7A-C8A	2.12	106.78	103.45
2	A	900	FAD	O2P-P-O1P	2.11	122.24	112.44
2	B	900	FAD	C2A-N1A-C6A	2.10	122.19	118.73
2	B	900	FAD	O4-C4-C4X	-2.09	121.02	126.53
2	A	900	FAD	O3B-C3B-C4B	-2.05	105.19	111.08
2	A	900	FAD	C10-C4X-N5	-2.03	120.65	124.81
2	A	900	FAD	C6A-C5A-N7A	2.03	136.00	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	FAD	C5'-C4'-C3'	2.01	116.00	112.22

There are no chirality outliers.

All (11) torsion outliers are listed below:

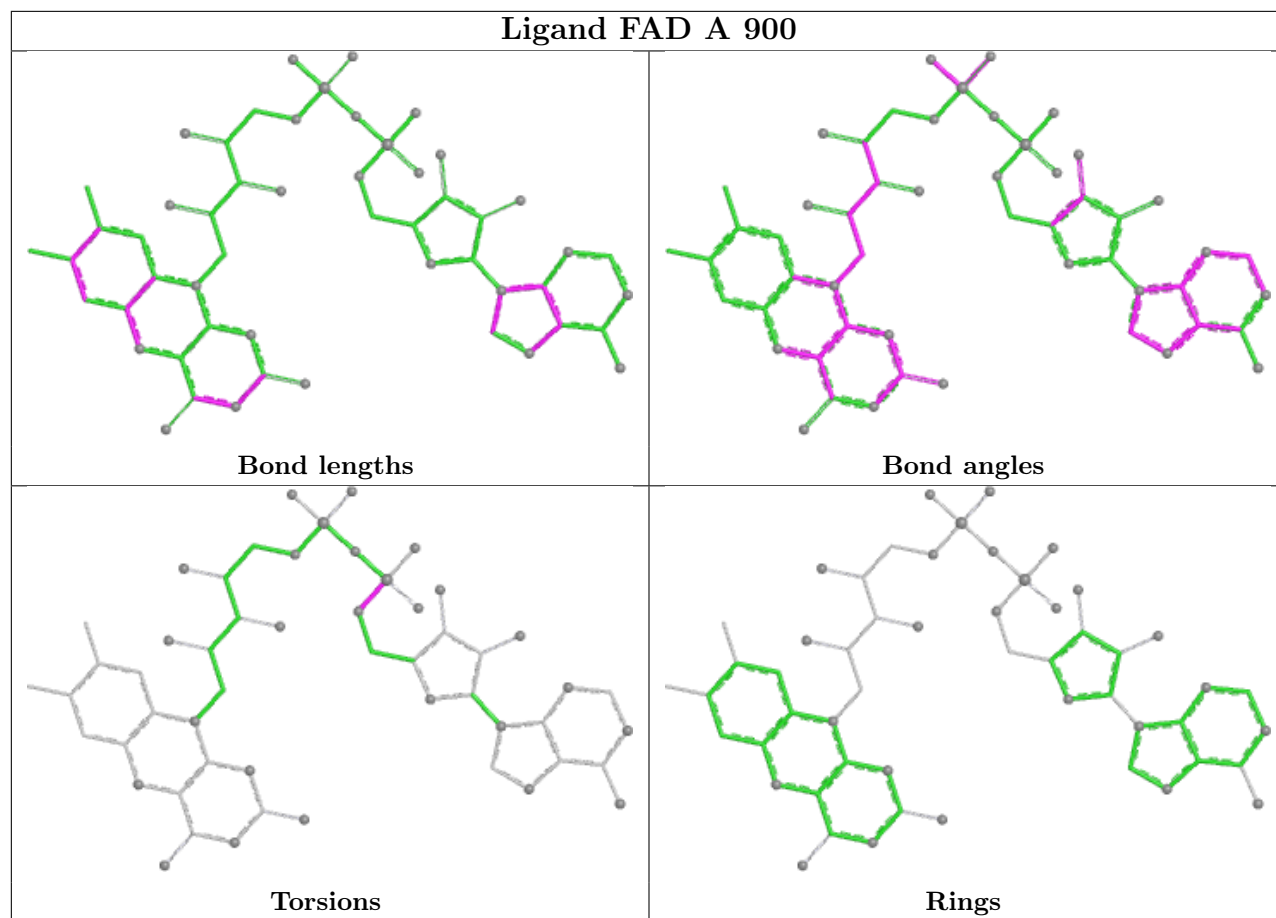
Mol	Chain	Res	Type	Atoms
2	A	900	FAD	C5B-O5B-PA-O2A
2	B	900	FAD	C3'-C4'-C5'-O5'
2	B	900	FAD	O4'-C4'-C5'-O5'
2	B	900	FAD	C5'-O5'-P-O1P
2	B	900	FAD	C5'-O5'-P-O2P
2	B	900	FAD	O3'-C3'-C4'-C5'
2	B	900	FAD	C2'-C3'-C4'-C5'
2	A	900	FAD	C5B-O5B-PA-O3P
2	B	900	FAD	C5'-O5'-P-O3P
2	B	900	FAD	O4B-C4B-C5B-O5B
2	B	900	FAD	PA-O3P-P-O1P

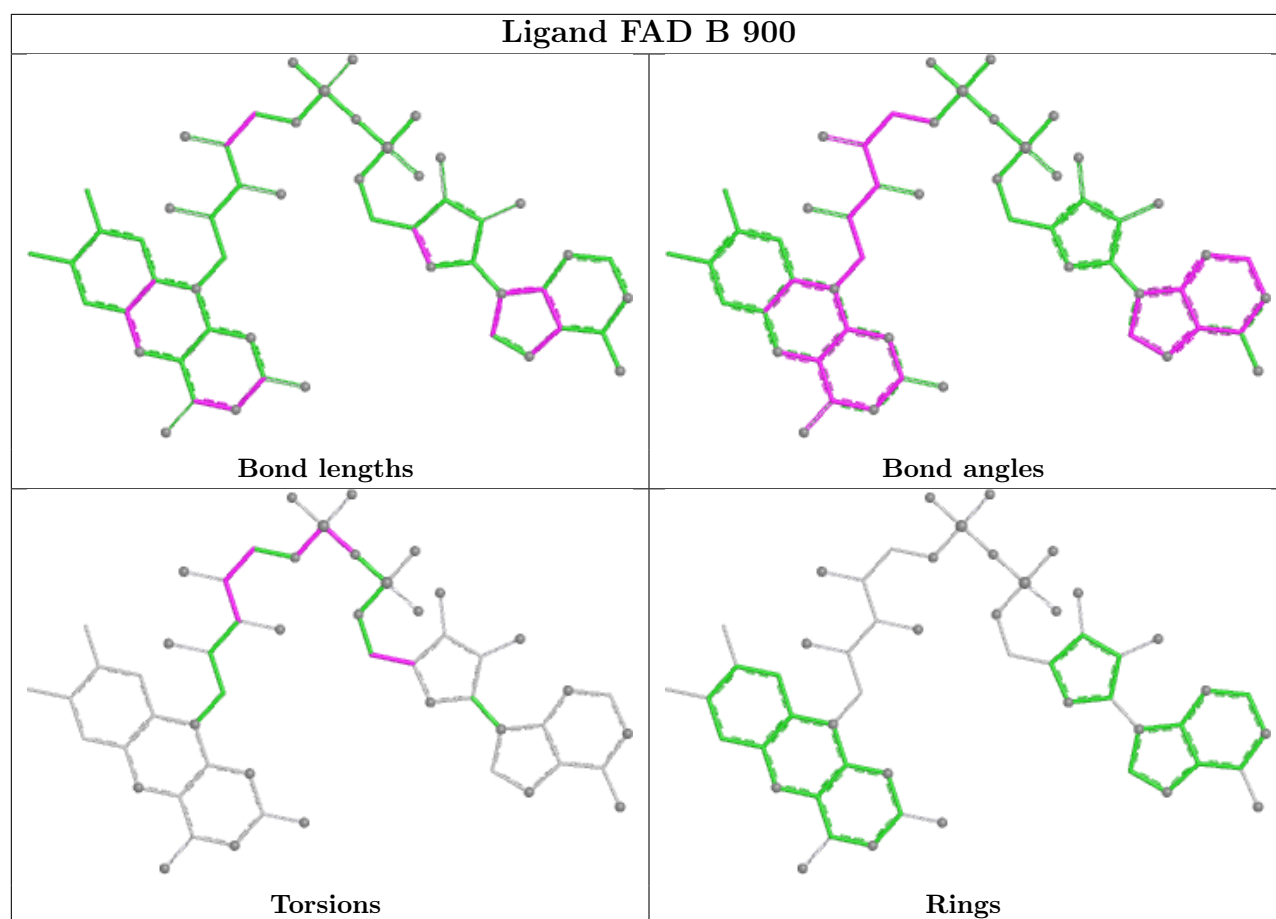
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	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	476/512 (92%)	0.49	32 (6%) 24 21	30, 57, 115, 148	0
1	B	476/512 (92%)	0.89	63 (13%) 7 5	33, 72, 131, 161	0
All	All	952/1024 (92%)	0.69	95 (9%) 12 10	30, 65, 125, 161	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ALA	6.2
1	A	259	ALA	5.1
1	B	427	PHE	4.8
1	B	200	ILE	4.7
1	A	262	LEU	4.1
1	B	242	HIS	4.0
1	B	102	PHE	4.0
1	A	207	THR	3.7
1	B	204	HIS	3.6
1	A	200	ILE	3.6
1	A	288	TRP	3.6
1	B	177	ARG	3.6
1	B	207	THR	3.5
1	B	39	LEU	3.5
1	A	205	ASP	3.5
1	B	424	PHE	3.5
1	B	428	PHE	3.5
1	B	45	GLY	3.3
1	A	503	LYS	3.1
1	B	185	ALA	3.1
1	B	25	HIS	3.0
1	A	123	PHE	3.0
1	A	499	ILE	3.0
1	A	204	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	187	ALA	2.9
1	A	268	GLY	2.9
1	B	198	ALA	2.8
1	A	297	ASN	2.8
1	B	123	PHE	2.8
1	B	292	LYS	2.8
1	B	46	ALA	2.8
1	B	426	GLN	2.8
1	B	506	TYR	2.8
1	B	264	ALA	2.8
1	A	177	ARG	2.8
1	B	24	VAL	2.8
1	A	264	ALA	2.7
1	A	244	GLU	2.7
1	B	107	LYS	2.7
1	B	269	LEU	2.7
1	B	302	LEU	2.7
1	B	283	PHE	2.6
1	B	186	VAL	2.6
1	A	266	PRO	2.6
1	B	205	ASP	2.6
1	B	472	VAL	2.6
1	A	510	SER	2.6
1	B	42	ALA	2.6
1	A	206	ASP	2.6
1	B	103	PRO	2.6
1	A	86	LYS	2.6
1	B	106	PHE	2.5
1	B	56	ASP	2.5
1	B	179	GLU	2.5
1	B	50	ARG	2.5
1	B	105	LEU	2.5
1	A	146	ASN	2.4
1	B	418	LEU	2.4
1	B	220	THR	2.4
1	B	142	VAL	2.4
1	B	143	VAL	2.4
1	A	263	LEU	2.4
1	B	78	GLU	2.4
1	A	92	PHE	2.3
1	B	132	MET	2.3
1	B	54	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	239	LEU	2.3
1	B	80	LEU	2.3
1	A	186	VAL	2.3
1	B	43	VAL	2.3
1	B	133	LYS	2.3
1	B	282	LEU	2.2
1	B	444	GLY	2.2
1	A	78	GLU	2.2
1	A	426	GLN	2.2
1	A	80	LEU	2.2
1	B	263	LEU	2.2
1	B	165	PRO	2.2
1	A	190	SER	2.2
1	A	90	ARG	2.2
1	B	134	MET	2.1
1	B	27	PHE	2.1
1	B	86	LYS	2.1
1	B	156	ILE	2.1
1	B	260	ASN	2.1
1	B	290	LEU	2.1
1	A	101	VAL	2.1
1	A	62	SER	2.1
1	B	238	ARG	2.1
1	B	307	GLN	2.0
1	B	150	LEU	2.0
1	B	174	LEU	2.0
1	A	208	TYR	2.0
1	B	109	TRP	2.0
1	B	51	CYS	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 ⓘ

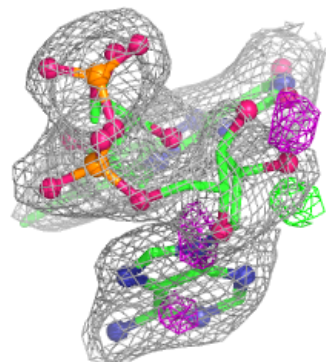
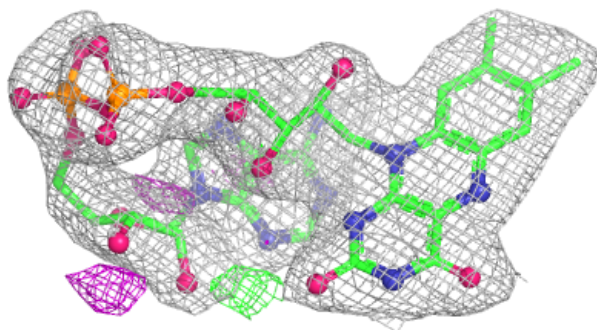
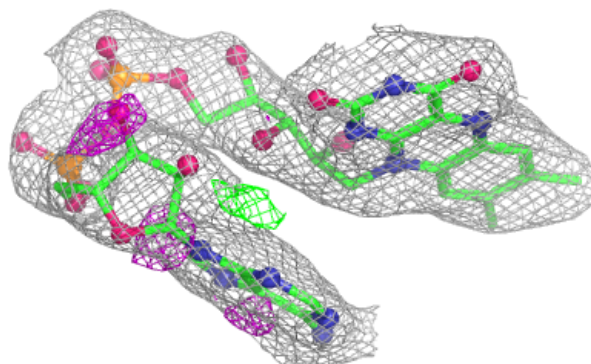
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

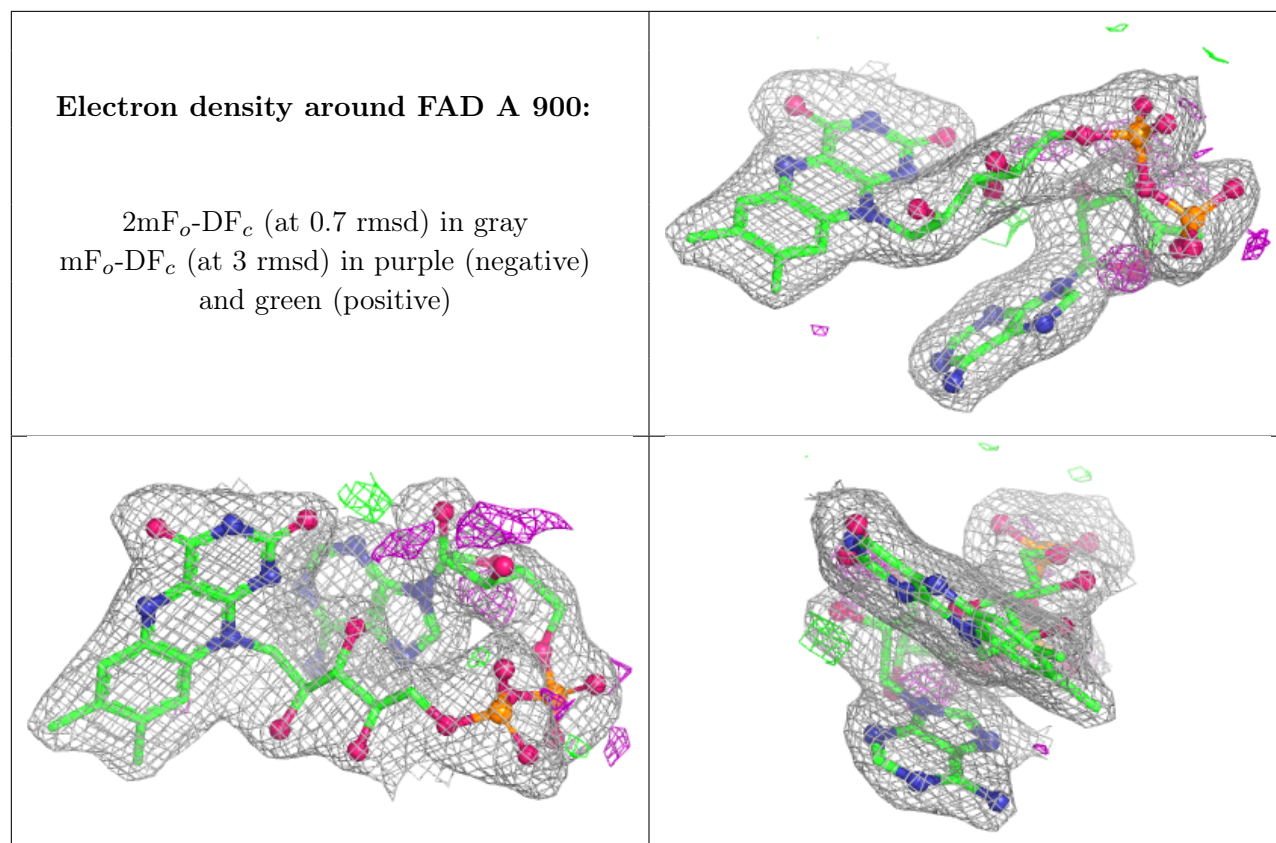
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	900	53/53	0.91	0.13	63,83,123,183	0
2	FAD	A	900	53/53	0.94	0.10	43,65,92,137	0

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 900:

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.