



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 PM GMT

PDB ID : 4I6G
Title : a vertebrate cryptochrome with FAD
Authors : Xing, W.; Busino, L.; Hinds, T.R.; Marionni, S.T.; Saifee, N.H.; Bush, M.F.; Pagano, M.; Zheng, N.
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

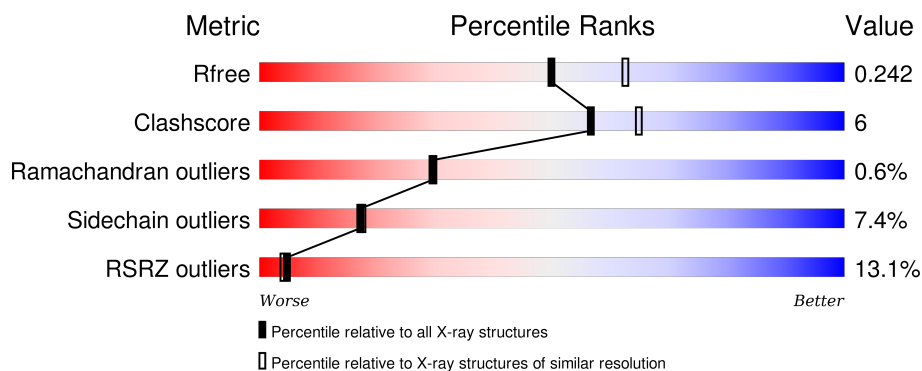
1 Overall quality at a glance

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>10%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div> </div>
1	B	512	<div> <div>15%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 7%</div> </div> </div>

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 (three-letter code: 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		

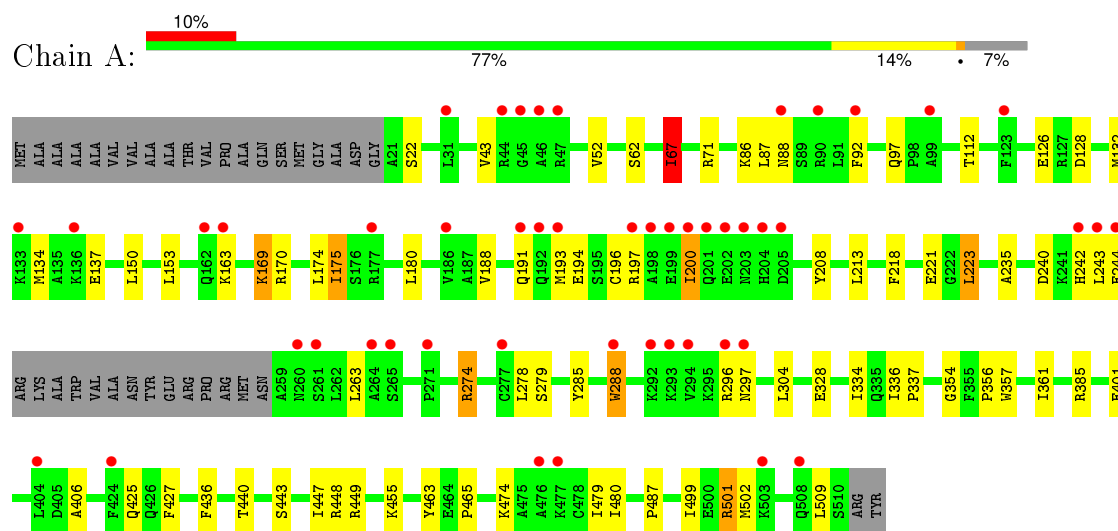
- Molecule 3 is water.

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

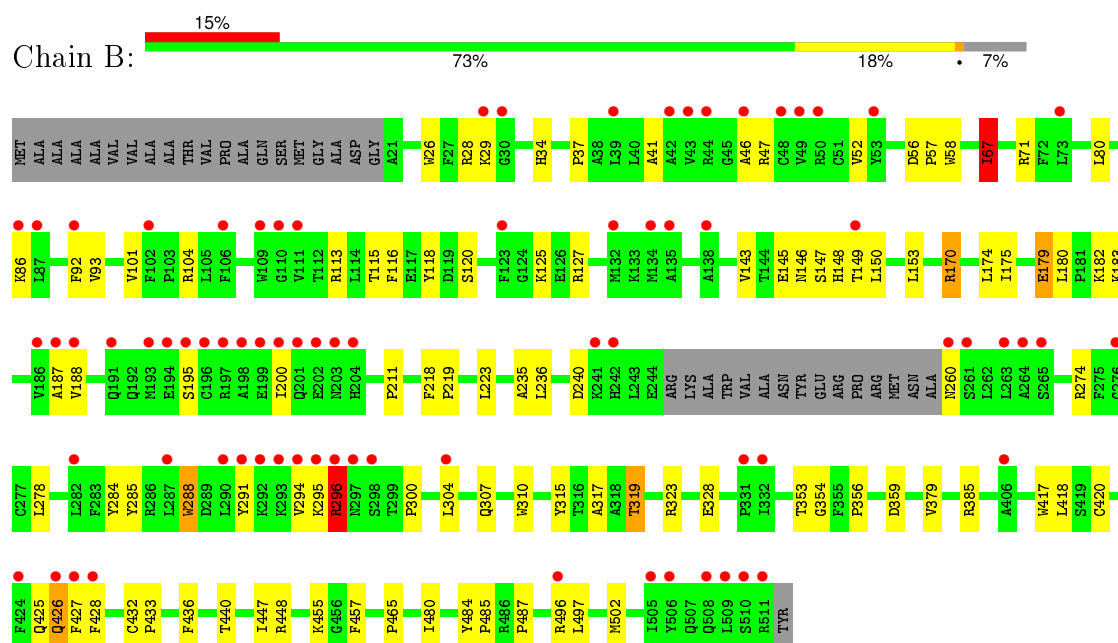
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 43.61 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.62-2.20) 96.0 (43.61-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (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	2004 reflections (3.53%)	DCC
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.8	EDS
Estimated twinning fraction	0.052 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 61191 reflections	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 1.6032e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	0/3979	0.58	1/5399 (0.0%)
1	B	0.40	0/3985	0.56	1/5406 (0.0%)
All	All	0.43	0/7964	0.57	2/10805 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ILE	CB-CA-C	-5.22	101.15	111.60
1	A	67	ILE	CB-CA-C	-5.00	101.59	111.60

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	3867	0	3797	41	0
1	B	3873	0	3805	52	0
2	A	53	0	31	0	0
2	B	53	0	31	5	0
3	A	150	0	0	5	0
3	B	113	0	0	8	0
All	All	8109	0	7664	94	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 (94) 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:HG3	1:A:501:ARG:HH11	1.64	0.61
1:A:436:PHE:O	1:A:440:THR:HG23	2.00	0.61
1:B:34:HIS:HA	1:B:187:ALA:HB2	1.83	0.60
1:A:401:GLU:OE2	3:A:1103:HOH:O	2.16	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:H	1:A:200:ILE:HD13	1.70	0.56
1:B:385:ARG:CZ	1:B:428:PHE:HB3	2.35	0.55
1:A:194:GLU:OE2	1:A:197:ARG:NH2	2.39	0.55
1:A:67:ILE:HG23	1:A:218:PHE:CD1	2.42	0.55
1:B:356:PRO:HB2	1:B:447:ILE:HD13	1.88	0.55
1:A:501:ARG:HG3	1:A:501:ARG:NH1	2.22	0.54
1:A:357:TRP:O	1:A:361:ILE:HG12	2.07	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:41:ALA:O	1:B:113:ARG:NH1	2.42	0.53
1:B:26:TRP:HB3	1:B:116:PHE:HB3	1.89	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:385:ARG:HH21	1:B:428:PHE:HD2	1.58	0.51
1:B:307:GLN:HG3	2:B:900:FAD:H51A	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:NH2	3:A:1071:HOH:O	2.29	0.51
1:A:501:ARG:CG	1:A:501:ARG:HH11	2.23	0.51
1:B:149:THR:OG1	3:B:1035:HOH:O	2.19	0.51
1:B:67:ILE:HG23	1:B:218:PHE:CD1	2.46	0.50
1:A:499:ILE:HD13	1:B:58:TRP:HE1	1.77	0.50
1:B:310:TRP:HH2	1:B:417:TRP:CH2	2.31	0.49
1:A:235:ALA:HB1	1:A:278:LEU:HB2	1.94	0.49
1:A:208:TYR:O	3:A:1056:HOH:O	2.19	0.49
1:B:34:HIS:CE1	1:B:236:LEU:HD21	2.48	0.48
1:A:22:SER:H	1:A:112:THR:HB	1.78	0.48
2:B:900:FAD:O3'	2:B:900:FAD:H2B	2.14	0.48
1:A:128:ASP:O	1:A:132:MET:HG2	2.13	0.48
1:A:169:LYS:HE3	1:A:169:LYS:HB3	1.63	0.48
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:354:GLY:HA3	1:B:487:PRO:CA	2.42	0.46
1:B:71:ARG:NH2	3:B:1041:HOH:O	2.32	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:A:188:VAL:HB	1:A:193:MET:HE3	1.98	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:420:CYS:SG	1:B:428:PHE:HB2	2.57	0.45
1:B:71:ARG:NE	3:B:1041:HOH:O	2.40	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
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:426:GLN:CD	1:B:426:GLN:H	2.21	0.43
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:67:ILE:H	1:B:67:ILE:HG13	1.62	0.41
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: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:A:263:LEU:HA	1:A:263:LEU:HD13	1.84	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:B:284:TYR:CE2	1:B:288:TRP:HD1	2.38	0.41
2:B:900:FAD:N6A	3:B:1018:HOH:O	2.36	0.41
1:A:425:GLN:NE2	3:A:1134:HOH:O	2.52	0.41
1:A:447:ILE:HD11	1:A:463:TYR:CD1	2.55	0.41
1:A:52:VAL:HG12	1:A:92:PHE:HB2	2.03	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 [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	472/512 (92%)	450 (95%)	18 (4%)	4 (1%)	24	22
1	B	472/512 (92%)	442 (94%)	28 (6%)	2 (0%)	39	42
All	All	944/1024 (92%)	892 (94%)	46 (5%)	6 (1%)	30	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	ARG
1	A	243	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	410/434 (94%)	382 (93%)	28 (7%)	20	21
1	B	411/434 (95%)	378 (92%)	33 (8%)	15	15
All	All	821/868 (95%)	760 (93%)	61 (7%)	17	17

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	67	ILE
1	A	86	LYS
1	A	88	ASN
1	A	97	GLN
1	A	126	GLU
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	191	GLN
1	A	200	ILE
1	A	223	LEU
1	A	240	ASP
1	A	274	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	279	SER
1	A	288	TRP
1	A	296	ARG
1	A	304	LEU
1	A	328	GLU
1	A	385	ARG
1	A	449	ARG
1	A	501	ARG
1	A	502	MET
1	B	28	ARG
1	B	47	ARG
1	B	67	ILE
1	B	80	LEU
1	B	86	LYS
1	B	101	VAL
1	B	104	ARG
1	B	150	LEU
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	240	ASP
1	B	260	ASN
1	B	274	ARG
1	B	288	TRP
1	B	295	LYS
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	427	PHE
1	B	496	ARG
1	B	497	LEU
1	B	502	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 carbohydrates 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	-	48,58,58	1.46	8 (16%)	54,89,89	2.07	9 (16%)
2	FAD	B	900	-	48,58,58	1.39	7 (14%)	54,89,89	2.33	11 (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	900	-	-	0/30/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	900	-	-	0/30/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	FAD	C6-C5X	-3.04	1.37	1.41
2	A	900	FAD	C6-C5X	-3.04	1.37	1.41
2	A	900	FAD	C1'-N10	-2.95	1.45	1.48
2	A	900	FAD	C10-N1	-2.42	1.31	1.35
2	B	900	FAD	C5'-C4'	-2.20	1.48	1.51
2	A	900	FAD	C5A-N7A	-2.19	1.32	1.39
2	B	900	FAD	C1'-N10	-2.11	1.46	1.48
2	A	900	FAD	C8-C7	2.04	1.46	1.41
2	A	900	FAD	C9A-C5X	2.20	1.47	1.42
2	B	900	FAD	C9A-C5X	2.24	1.47	1.42
2	B	900	FAD	C4X-C10	2.42	1.45	1.41
2	B	900	FAD	C5A-C4A	2.57	1.46	1.40
2	A	900	FAD	C4-C4X	2.63	1.46	1.41
2	B	900	FAD	C4-C4X	2.66	1.46	1.41
2	A	900	FAD	C4X-C10	2.85	1.46	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	FAD	O4'-C4'-C5'	-7.61	93.62	110.19
2	A	900	FAD	N3A-C2A-N1A	-7.09	123.47	128.89
2	B	900	FAD	N3A-C2A-N1A	-6.18	124.16	128.89
2	B	900	FAD	C4-C4X-C10	-5.13	116.66	119.94
2	A	900	FAD	C4X-C4-N3	-4.45	117.51	123.59
2	A	900	FAD	C4-C4X-C10	-4.17	117.27	119.94
2	B	900	FAD	C4X-C4-N3	-3.41	118.93	123.59
2	B	900	FAD	O3P-PA-O5B	-3.01	94.94	102.94
2	B	900	FAD	C4A-C5A-N7A	-2.79	106.91	109.48
2	A	900	FAD	O3P-PA-O5B	-2.52	96.24	102.94
2	B	900	FAD	C4-C4X-N5	2.60	121.88	118.72
2	A	900	FAD	C5X-C9A-N10	2.64	119.62	117.62
2	A	900	FAD	C4-C4X-N5	2.76	122.07	118.72
2	A	900	FAD	C4X-N5-C5X	3.18	120.42	116.76
2	B	900	FAD	C5X-C9A-N10	3.29	120.12	117.62
2	A	900	FAD	C1'-N10-C9A	3.39	122.67	118.86
2	B	900	FAD	C4X-N5-C5X	3.53	120.82	116.76
2	B	900	FAD	C1'-N10-C9A	4.10	123.47	118.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	FAD	C4-N3-C2	7.38	121.63	115.25
2	A	900	FAD	C4-N3-C2	8.04	122.19	115.25

There are no chirality outliers.

There are no torsion outliers.

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

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%)	0.51	49 (10%) 9 8	30, 57, 115, 148	0
1	B	476/512 (92%)	0.93	76 (15%) 3 2	33, 72, 131, 161	0
All	All	952/1024 (92%)	0.72	125 (13%) 5 4	30, 65, 125, 161	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	510	SER	12.9
1	B	202	GLU	8.7
1	B	511	ARG	7.2
1	B	290	LEU	7.2
1	B	204	HIS	7.0
1	B	44	ARG	7.0
1	B	191	GLN	6.8
1	B	506	TYR	6.6
1	B	296	ARG	6.4
1	B	50	ARG	6.3
1	B	200	ILE	6.3
1	B	199	GLU	5.8
1	B	203	ASN	5.8
1	B	509	LEU	5.8
1	A	203	ASN	5.7
1	B	198	ALA	5.7
1	A	202	GLU	5.6
1	B	424	PHE	5.6
1	B	242	HIS	5.4
1	A	199	GLU	5.3
1	B	264	ALA	5.3
1	B	293	LYS	5.2
1	B	426	GLN	5.2
1	B	291	TYR	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	200	ILE	5.1
1	A	264	ALA	5.0
1	A	296	ARG	4.9
1	B	505	ILE	4.8
1	A	297	ASN	4.7
1	B	294	VAL	4.7
1	B	297	ASN	4.7
1	B	295	LYS	4.4
1	B	86	LYS	4.2
1	B	193	MET	4.2
1	A	92	PHE	4.0
1	B	197	ARG	4.0
1	A	260	ASN	3.9
1	A	503	LYS	3.9
1	B	195	SER	3.7
1	B	46	ALA	3.7
1	B	111	VAL	3.7
1	B	188	VAL	3.7
1	B	201	GLN	3.7
1	A	162	GLN	3.7
1	B	427	PHE	3.7
1	A	204	HIS	3.7
1	B	109	TRP	3.6
1	B	102	PHE	3.6
1	A	476	ALA	3.6
1	A	294	VAL	3.6
1	B	292	LYS	3.5
1	B	106	PHE	3.4
1	B	287	LEU	3.4
1	A	293	LYS	3.4
1	A	88	ASN	3.3
1	A	193	MET	3.3
1	B	194	GLU	3.2
1	A	508	GLN	3.2
1	B	49	VAL	3.2
1	A	292	LYS	3.2
1	A	191	GLN	3.1
1	B	260	ASN	3.1
1	B	298	SER	3.1
1	A	45	GLY	3.1
1	B	92	PHE	3.1
1	B	132	MET	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	39	LEU	3.0
1	B	134	MET	3.0
1	A	205	ASP	2.9
1	B	304	LEU	2.9
1	A	424	PHE	2.9
1	A	123	PHE	2.9
1	A	198	ALA	2.9
1	B	428	PHE	2.8
1	A	201	GLN	2.8
1	A	197	ARG	2.8
1	B	73	LEU	2.8
1	B	110	GLY	2.8
1	A	177	ARG	2.7
1	A	186	VAL	2.7
1	A	244	GLU	2.7
1	A	242	HIS	2.7
1	A	47	ARG	2.6
1	A	288	TRP	2.6
1	B	265	SER	2.6
1	A	31	LEU	2.6
1	B	135	ALA	2.6
1	A	133	LYS	2.6
1	B	29	LYS	2.6
1	A	44	ARG	2.5
1	B	30	GLY	2.5
1	B	48	CYS	2.5
1	B	123	PHE	2.5
1	B	261	SER	2.4
1	A	192	GLN	2.4
1	A	477	LYS	2.4
1	B	496	ARG	2.4
1	B	138	ALA	2.4
1	B	332	ILE	2.4
1	B	331	PRO	2.4
1	A	261	SER	2.4
1	B	42	ALA	2.4
1	B	282	LEU	2.3
1	A	99	ALA	2.3
1	A	136	LYS	2.3
1	B	43	VAL	2.2
1	B	263	LEU	2.2
1	A	46	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	243	LEU	2.2
1	A	265	SER	2.2
1	B	149	THR	2.2
1	B	187	ALA	2.2
1	B	508	GLN	2.2
1	B	196	CYS	2.2
1	A	163	LYS	2.2
1	B	406	ALA	2.2
1	A	90	ARG	2.2
1	B	186	VAL	2.1
1	B	276	GLY	2.1
1	A	271	PRO	2.1
1	B	241	LYS	2.1
1	A	404	LEU	2.0
1	B	87	LEU	2.0
1	B	53	TYR	2.0
1	A	277	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	FAD	B	900	53/53	0.86	0.18	-0.00	63,83,123,183	0
2	FAD	A	900	53/53	0.93	0.15	-0.52	43,65,92,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.