Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 11:37 PM EST

PDB ID	:	1C0I
Title	:	CRYSTAL STRUCTURE OF D-AMINO ACID OXIDASE IN COMPLEX WITH TWO ANTHRANYLATE MOLECULES
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Deposited on	:	1999-07-16
Resolution	:	1.90 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:

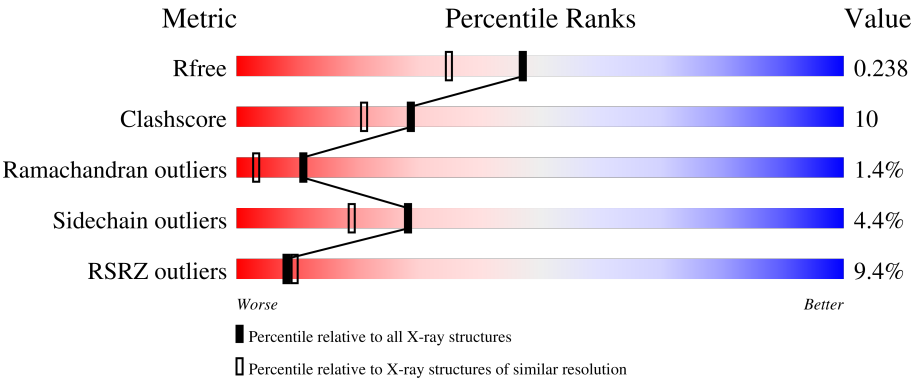
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	363	9% 80% 17% .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3232 atoms, of which 1 is hydrogen 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.

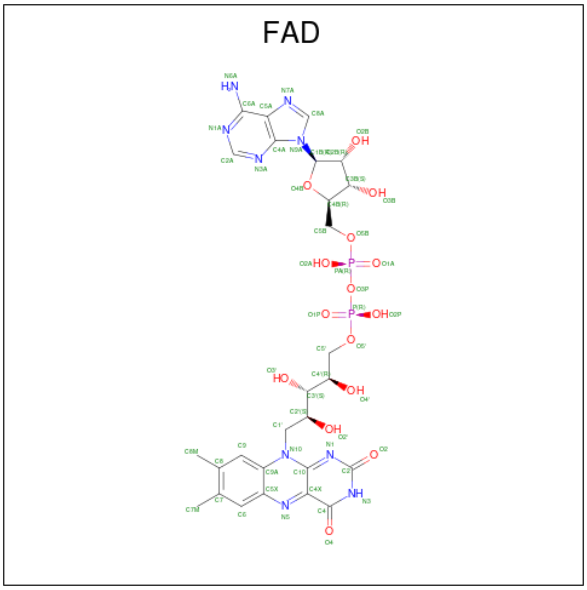
- Molecule 1 is a protein called D-AMINO ACID OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2786	1754	500	521	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

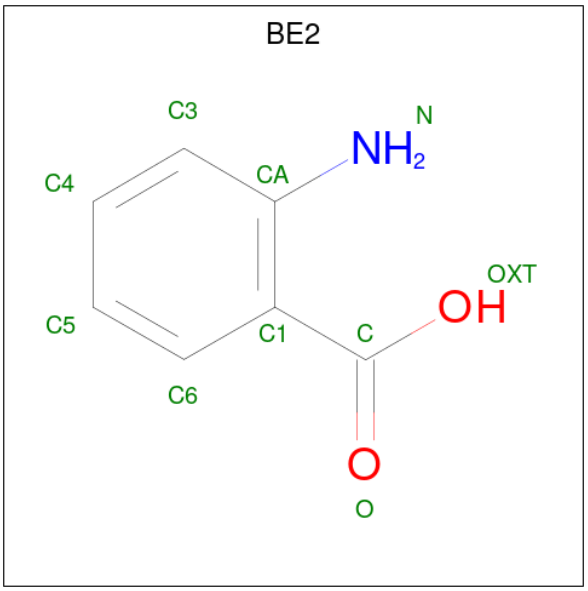
Chain	Residue	Modelled	Actual	Comment	Reference
A	999	LEU	-	conflict	UNP P80324
A	1000	MET	-	conflict	UNP P80324

- 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	H	N	O	P		
2	A	1	54	27	1	9	15	2	0	0

- Molecule 3 is 2-AMINOBENZOIC ACID (three-letter code: BE2) (formula: $C_7H_7NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 7 1 2	0	0
3	A	1	Total C N O 10 7 1 2	0	0

- Molecule 4 is water.

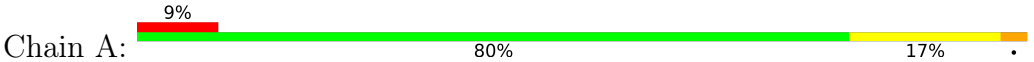
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	372	Total O 372 372	0	0

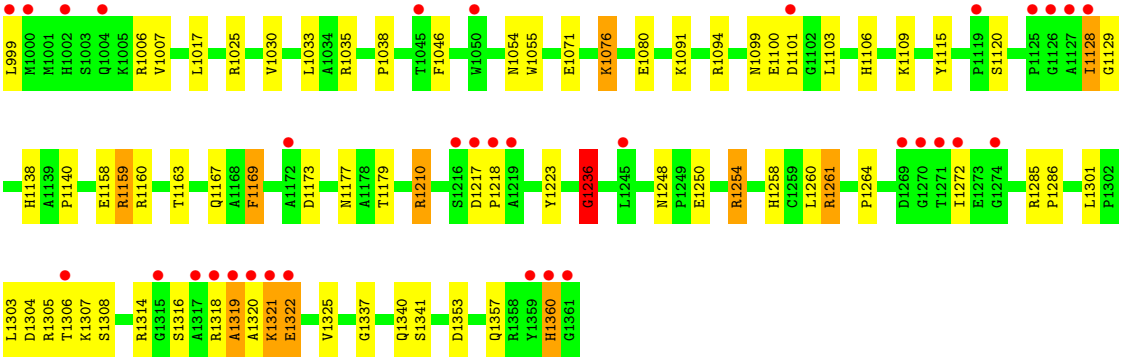
3 Residue-property plots (i)

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: D-AMINO ACID OXIDASE

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.83Å 120.83Å 136.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 45.28 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.90) 97.1 (45.28-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.89Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.199 , 0.249 0.198 , 0.238	Depositor DCC
R_{free} test set	1998 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 111.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3232	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BE2

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	0/2852	1.08	11/3876 (0.3%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1254	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	A	1254	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	A	1261	ARG	CD-NE-CZ	6.72	133.01	123.60
1	A	1159	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	1261	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	1169	PHE	C-N-CA	6.18	137.15	121.70
1	A	1236	GLY	CA-C-N	5.56	129.43	117.20
1	A	1035	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	1094	ARG	CD-NE-CZ	-5.05	116.52	123.60
1	A	1236	GLY	CA-C-O	-5.03	111.55	120.60
1	A	1055	TRP	CA-CB-CG	5.01	123.22	113.70

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	2786	0	2767	49	0
2	A	53	1	31	9	0
3	A	20	0	6	3	0
4	A	372	0	0	7	0
All	All	3231	1	2804	55	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 (55) 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:1363:FAD:C1'	2:A:1363:FAD:N10	1.68	1.55
1:A:1163:THR:H	1:A:1167:GLN:HE22	1.26	0.84
2:A:1363:FAD:N10	2:A:1363:FAD:C2'	2.46	0.78
2:A:1363:FAD:C1'	2:A:1363:FAD:C9A	2.65	0.72
1:A:1258:HIS:O	1:A:1261:ARG:HB2	1.94	0.68
1:A:1099:ASN:OD1	1:A:1101:ASP:HB2	1.96	0.66
2:A:1363:FAD:C1'	2:A:1363:FAD:C10	2.66	0.65
1:A:1223:TYR:CE2	3:A:1364:BE2:H6	2.33	0.63
1:A:1163:THR:H	1:A:1167:GLN:NE2	1.95	0.62
1:A:1301:LEU:O	1:A:1322:GLU:HA	2.00	0.61
1:A:1337:GLY:O	1:A:1341:SER:HB3	2.02	0.60
1:A:1179:THR:HB	2:A:1363:FAD:H8A	1.82	0.59
1:A:1071:GLU:HG3	1:A:1340:GLN:HG2	1.85	0.58
1:A:1007:VAL:CG2	1:A:1030:VAL:HG22	2.34	0.58
1:A:1318:ARG:HG2	1:A:1319:ALA:H	1.69	0.58
1:A:1353:ASP:O	1:A:1357:GLN:HG2	2.03	0.58
1:A:1100:GLU:OE1	1:A:1106:HIS:HE1	1.87	0.57
1:A:1320:ALA:O	1:A:1321:LYS:HB2	2.04	0.57
1:A:1179:THR:O	2:A:1363:FAD:H8A	2.05	0.56
1:A:1076:LYS:O	1:A:1080:GLU:HG3	2.06	0.55
1:A:1360:HIS:H	1:A:1360:HIS:CD2	2.25	0.53
1:A:1106:HIS:HD2	1:A:1115:TYR:OH	1.90	0.52
1:A:1173:ASP:O	1:A:1360:HIS:HE1	1.92	0.52
1:A:1318:ARG:O	1:A:1319:ALA:O	2.29	0.51
1:A:1304:ASP:OD1	1:A:1306:THR:HG23	2.11	0.50
1:A:1303:LEU:HD22	1:A:1307:LYS:HG2	1.94	0.49
1:A:1314:ARG:HH11	1:A:1314:ARG:HG3	1.78	0.48
1:A:1033:LEU:HD23	1:A:1158:GLU:HB3	1.95	0.48
1:A:1264:PRO:HG3	4:A:2283:HOH:O	2.14	0.47
1:A:1314:ARG:HG3	1:A:1314:ARG:NH1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1364:BE2:C	3:A:1365:BE2:H4	2.44	0.47
1:A:1138:HIS:CE1	1:A:1140:PRO:HG2	2.51	0.46
1:A:1138:HIS:HE1	1:A:1140:PRO:HG2	1.81	0.45
1:A:1076:LYS:HG2	4:A:2068:HOH:O	2.16	0.45
1:A:1091:LYS:HG2	4:A:2275:HOH:O	2.17	0.45
1:A:1177:ASN:HD22	1:A:1179:THR:HG23	1.81	0.44
1:A:1025:ARG:NE	4:A:2291:HOH:O	2.50	0.44
1:A:1128:ILE:HG12	1:A:1129:GLY:N	2.33	0.44
1:A:1217:ASP:HA	1:A:1218:PRO:HD2	1.76	0.44
1:A:1017:LEU:HD11	1:A:1038:PRO:HG3	2.00	0.43
1:A:1103:LEU:HD11	1:A:1128:ILE:HD13	2.00	0.43
1:A:1236:GLY:O	1:A:1254:ARG:NH2	2.49	0.43
1:A:1006:ARG:NH2	4:A:2084:HOH:O	2.50	0.43
1:A:1304:ASP:OD1	1:A:1306:THR:OG1	2.30	0.43
2:A:1363:FAD:C1'	2:A:1363:FAD:C9	2.97	0.43
1:A:1179:THR:HB	2:A:1363:FAD:C8A	2.49	0.42
1:A:1305:ARG:HD3	1:A:1308:SER:O	2.19	0.42
1:A:1223:TYR:CZ	3:A:1364:BE2:H6	2.55	0.42
1:A:1304:ASP:OD1	1:A:1306:THR:N	2.50	0.41
1:A:1285:ARG:HA	1:A:1286:PRO:HD3	1.84	0.41
1:A:1160:ARG:O	2:A:1363:FAD:H2A	2.20	0.41
1:A:1210:ARG:HG3	4:A:2296:HOH:O	2.20	0.41
1:A:1260:LEU:HD12	1:A:1264:PRO:HA	2.01	0.41
1:A:1006:ARG:NH2	4:A:2156:HOH:O	2.53	0.40
1:A:1169:PHE:CE2	1:A:1325:VAL:HB	2.57	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	361/363 (99%)	336 (93%)	20 (6%)	5 (1%)	11 3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1319	ALA
1	A	1322	GLU
1	A	1321	LYS
1	A	1236	GLY
1	A	1360	HIS

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	295/295 (100%)	282 (96%)	13 (4%)	28 19

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	999	LEU
1	A	1046	PHE
1	A	1054	ASN
1	A	1076	LYS
1	A	1109	LYS
1	A	1120	SER
1	A	1128	ILE
1	A	1159	ARG
1	A	1210	ARG
1	A	1248	ASN
1	A	1250	GLU
1	A	1272	ILE
1	A	1316	SER

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	1002	HIS
1	A	1031	HIS

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Mol	Chain	Res	Type
1	A	1054	ASN
1	A	1106	HIS
1	A	1167	GLN
1	A	1177	ASN
1	A	1248	ASN

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)

3 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	1363	-	53,58,58	5.45	34 (64%)	-		

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1363	FAD	C8-C7	13.07	1.73	1.40
2	A	1363	FAD	C9A-C5X	12.39	1.61	1.41
2	A	1363	FAD	O4B-C1B	11.62	1.57	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1363	FAD	C8A-N7A	-10.25	1.16	1.34
2	A	1363	FAD	C2-N1	9.36	1.59	1.36
2	A	1363	FAD	C9-C9A	-9.34	1.24	1.39
2	A	1363	FAD	C8M-C8	9.17	1.69	1.51
2	A	1363	FAD	C2A-N3A	8.81	1.46	1.32
2	A	1363	FAD	C1'-N10	8.20	1.68	1.48
2	A	1363	FAD	O2-C2	-7.84	1.09	1.24
2	A	1363	FAD	C6A-C5A	7.57	1.71	1.43
2	A	1363	FAD	C2'-C3'	7.57	1.67	1.53
2	A	1363	FAD	C6-C7	-7.51	1.28	1.39
2	A	1363	FAD	C5B-C4B	6.92	1.73	1.51
2	A	1363	FAD	C4-N3	6.02	1.50	1.38
2	A	1363	FAD	C6-C5X	5.99	1.49	1.40
2	A	1363	FAD	C4X-C10	5.99	1.61	1.44
2	A	1363	FAD	C7M-C7	-5.18	1.40	1.51
2	A	1363	FAD	C1'-C2'	4.81	1.59	1.52
2	A	1363	FAD	PA-O5B	4.57	1.77	1.59
2	A	1363	FAD	O4-C4	-4.35	1.15	1.23
2	A	1363	FAD	C10-N1	3.56	1.40	1.33
2	A	1363	FAD	C5X-N5	-3.43	1.32	1.39
2	A	1363	FAD	O3'-C3'	3.29	1.50	1.43
2	A	1363	FAD	C4X-N5	3.04	1.36	1.30
2	A	1363	FAD	O5B-C5B	2.84	1.55	1.44
2	A	1363	FAD	C4A-N3A	-2.75	1.31	1.35
2	A	1363	FAD	C6A-N6A	-2.63	1.24	1.34
2	A	1363	FAD	O4'-C4'	2.45	1.48	1.43
2	A	1363	FAD	C9-C8	-2.38	1.36	1.39
2	A	1363	FAD	PA-O2A	-2.18	1.45	1.55
2	A	1363	FAD	P-O2P	-2.17	1.45	1.55
2	A	1363	FAD	C10-N10	-2.15	1.32	1.37
2	A	1363	FAD	O4B-C4B	2.10	1.49	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1363	FAD	9	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, 95^{th} 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	363/363 (100%)	0.57	34 (9%) 8 9	19, 30, 65, 158	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1320	ALA	9.2
1	A	1319	ALA	9.1
1	A	1317	ALA	8.7
1	A	1321	LYS	7.4
1	A	1002	HIS	4.9
1	A	1318	ARG	4.5
1	A	1360	HIS	4.2
1	A	1361	GLY	4.2
1	A	999	LEU	4.1
1	A	1359	TYR	3.9
1	A	1306	THR	3.6
1	A	1219	ALA	3.5
1	A	1004	GLN	3.5
1	A	1315	GLY	3.4
1	A	1270	GLY	3.2
1	A	1274	GLY	2.8
1	A	1245	LEU	2.8
1	A	1000	MET	2.6
1	A	1216	SER	2.6
1	A	1322	GLU	2.5
1	A	1045	THR	2.5
1	A	1128	ILE	2.5
1	A	1127	ALA	2.4
1	A	1119	PRO	2.4
1	A	1125	PRO	2.4
1	A	1218	PRO	2.3
1	A	1272	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1269	ASP	2.2
1	A	1050	TRP	2.2
1	A	1126	GLY	2.2
1	A	1271	THR	2.2
1	A	1101	ASP	2.1
1	A	1172	ALA	2.1
1	A	1217	ASP	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, 95^{th} 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	BE2	A	1365	10/10	0.64	0.21	53,62,67,67	0
3	BE2	A	1364	10/10	0.93	0.17	31,38,42,42	0
2	FAD	A	1363	53/53	0.97	0.11	13,23,32,45	0

6.5 Other polymers (i)

There are no such residues in this entry.