Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:53 AM GMT

PDB ID	:	3NFR
Title	:	Casimiroin analog inhibitor of quinone reductase 2
Authors	:	Sturdy, M.; Mesecar, A.D.; Jermihov, K.; Cushman, M.; Maiti, A.
Deposited on	:	2010-06-10
Resolution	:	1.57 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

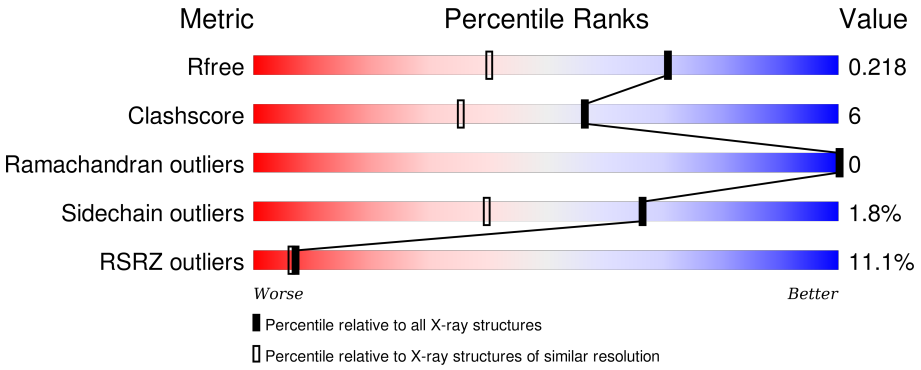
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.57 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	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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 <=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	230	13% 78% 20%
1	B	230	9% 88% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4086 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.

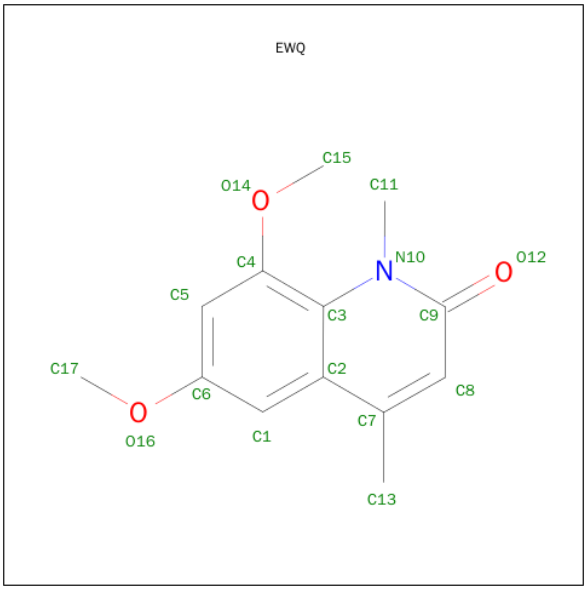
- Molecule 1 is a protein called Ribosyldihydronicotinamide dehydrogenase [quinone].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1824	1174	304	338	8			
1	B	230	Total	C	N	O	S	0	0	0
			1824	1174	304	338	8			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

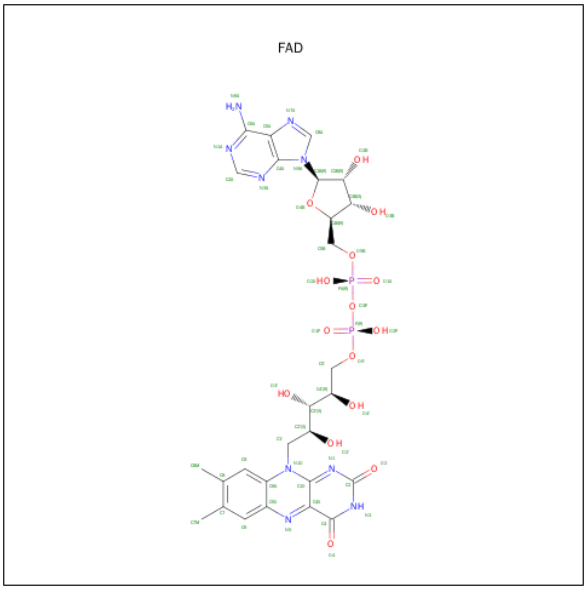
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 6,8-DIMETHOXY-1,4-DIMETHYLQUINOLIN-2(1H)-ONE (three-letter code: EWQ) (formula: $C_{13}H_{15}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	13	1	3		
3	B	1	Total	C	N	O	0	0
			17	13	1	3		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is water.

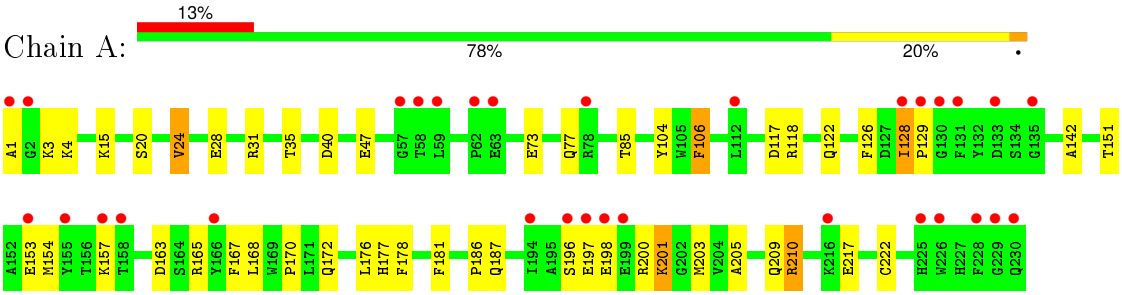
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		
5	B	176	Total	O	0	0
			176	176		

3 Residue-property plots (i)

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.

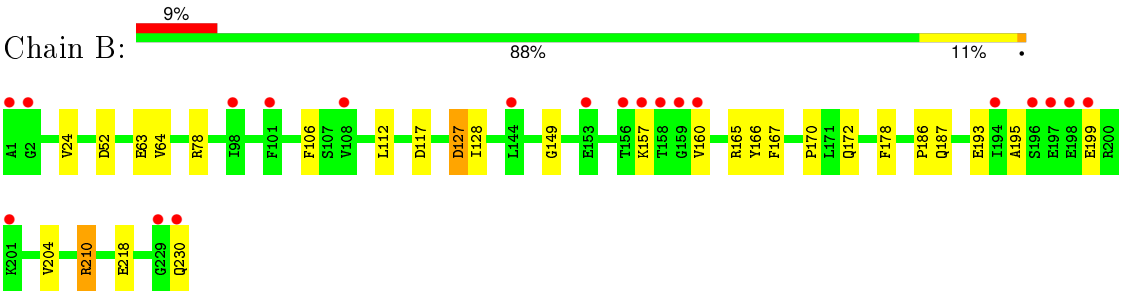
- Molecule 1: Ribosyldihydronicotinamide dehydrogenase [quinone]

Chain A:



- Molecule 1: Ribosyldihydronicotinamide dehydrogenase [quinone]

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.06Å 83.21Å 106.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.56 – 1.57 29.98 – 1.57	Depositor EDS
% Data completeness (in resolution range)	90.7 (65.56-1.57) 90.7 (29.98-1.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.15 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.194 , 0.219 0.194 , 0.218	Depositor DCC
R_{free} test set	3227 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 63789 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4086	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, EWQ, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.35	5/1874 (0.3%)	1.20	13/2542 (0.5%)
1	B	1.32	2/1874 (0.1%)	1.21	12/2542 (0.5%)
All	All	1.34	7/3748 (0.2%)	1.21	25/5084 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	GLU	CB-CG	-6.82	1.39	1.52
1	A	178	PHE	CE2-CZ	6.80	1.50	1.37
1	A	24	VAL	CB-CG2	-5.91	1.40	1.52
1	A	176	LEU	N-CA	5.47	1.57	1.46
1	A	106	PHE	CD1-CE1	5.46	1.50	1.39
1	B	64	VAL	CB-CG2	5.13	1.63	1.52
1	B	106	PHE	CD1-CE1	5.01	1.49	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	52	ASP	CB-CG-OD1	9.98	127.28	118.30
1	A	210	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	B	78	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	B	117	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	47	GLU	OE1-CD-OE2	-6.88	115.05	123.30
1	B	78	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	117	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	118	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	40	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	112	LEU	CB-CG-CD2	-6.00	100.80	111.00
1	B	106	PHE	CB-CG-CD2	-5.89	116.68	120.80
1	B	165	ARG	NE-CZ-NH2	-5.68	117.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	VAL	CG1-CB-CG2	5.49	119.68	110.90
1	B	178	PHE	CB-CG-CD2	5.45	124.62	120.80
1	A	31	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	127	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	210	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	117	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	118	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	128	ILE	CB-CA-C	5.25	122.11	111.60
1	B	218	GLU	CB-CA-C	-5.19	100.03	110.40
1	A	106	PHE	CB-CG-CD2	-5.02	117.28	120.80
1	B	167	PHE	CB-CG-CD1	5.02	124.32	120.80
1	A	28	GLU	OE1-CD-OE2	5.02	129.32	123.30
1	A	203	MET	CG-SD-CE	-5.02	92.17	100.20

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	1824	0	1779	28	0
1	B	1824	0	1779	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	17	0	15	2	0
3	B	17	0	15	4	0
4	A	53	0	31	10	0
4	B	53	0	31	0	0
5	A	120	0	0	2	0
5	B	176	0	0	4	0
All	All	4086	0	3650	45	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 (45) 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:200:ARG:HD2	4:A:233:FAD:N3A	2.04	0.73
1:A:200:ARG:NH1	4:A:233:FAD:N3A	2.39	0.69
1:A:205:ALA:O	1:A:209:GLN:HG3	1.93	0.69
1:A:200:ARG:HB3	4:A:233:FAD:C2A	2.28	0.64
1:A:172:GLN:HE22	1:A:186:PRO:HD3	1.64	0.63
3:A:232:EWQ:C11	3:A:232:EWQ:O14	2.48	0.62
1:B:24:VAL:HG11	1:B:204:VAL:CG1	2.31	0.60
1:A:200:ARG:HH11	4:A:233:FAD:C2A	2.15	0.60
3:B:231:EWQ:C11	3:B:231:EWQ:O14	2.48	0.60
1:B:187:GLN:HE21	1:B:210:ARG:HH11	1.50	0.59
1:A:196:SER:O	1:A:198:GLU:O	2.20	0.59
1:A:157:LYS:HG2	1:A:163:ASP:HB2	1.86	0.58
1:A:165:ARG:HA	1:A:168:LEU:HD12	1.87	0.56
1:A:198:GLU:O	1:A:200:ARG:N	2.38	0.55
1:A:85:THR:HG21	5:A:288:HOH:O	2.07	0.53
4:A:233:FAD:HM72	5:B:385:HOH:O	2.11	0.50
4:A:233:FAD:HM81	5:B:278:HOH:O	2.10	0.50
1:B:24:VAL:HG13	5:B:328:HOH:O	2.12	0.49
1:A:200:ARG:HB3	4:A:233:FAD:H2A	1.94	0.49
1:A:187:GLN:HE21	1:A:210:ARG:HH11	1.59	0.49
1:A:4:LYS:HG2	1:A:35:THR:HB	1.94	0.48
1:A:24:VAL:HG13	5:A:350:HOH:O	2.16	0.46
3:B:231:EWQ:H11B	3:B:231:EWQ:O14	2.15	0.46
1:A:128:ILE:HA	1:A:129:PRO:HA	1.75	0.46
1:B:157:LYS:HG3	1:B:166:TYR:OH	2.16	0.45
1:B:187:GLN:NE2	1:B:210:ARG:HH11	2.15	0.45
1:A:1:ALA:HA	1:A:3:LYS:H	1.81	0.45
1:A:142:ALA:HB2	1:A:181:PHE:CD1	2.52	0.44
1:A:73:GLU:O	1:A:77:GLN:HG2	2.17	0.44
3:B:231:EWQ:H17B	3:B:231:EWQ:H1	1.62	0.44
1:B:24:VAL:HG11	1:B:204:VAL:HG12	2.00	0.43
1:A:106:PHE:HB3	1:B:170:PRO:HB3	2.00	0.43
1:A:201:LYS:HD3	4:A:233:FAD:N1A	2.34	0.43
1:A:151:THR:OG1	1:A:154:MET:HG3	2.18	0.42
1:B:193:GLU:HB2	5:B:398:HOH:O	2.18	0.42
1:B:149:GLY:C	3:B:231:EWQ:H11B	2.40	0.42
1:A:177:HIS:ND1	1:A:222:CYS:HB3	2.35	0.42
1:A:104:TYR:HA	4:A:233:FAD:C5X	2.49	0.41
1:A:20:SER:OG	4:A:233:FAD:N7A	2.45	0.41
1:B:172:GLN:HE22	1:B:186:PRO:HD3	1.85	0.41
1:A:15:LYS:NZ	1:B:63:GLU:HG2	2.36	0.41
1:B:195:ALA:HB1	1:B:199:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:HB2	1:A:126:PHE:CZ	2.56	0.40
1:A:167:PHE:O	1:A:170:PRO:HD2	2.21	0.40
3:A:232:EWQ:O14	3:A:232:EWQ:H11B	2.18	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	228/230 (99%)	215 (94%)	13 (6%)	0	100	100
1	B	228/230 (99%)	221 (97%)	7 (3%)	0	100	100
All	All	456/460 (99%)	436 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	194/194 (100%)	191 (98%)	3 (2%)	72	48
1	B	194/194 (100%)	190 (98%)	4 (2%)	61	32
All	All	388/388 (100%)	381 (98%)	7 (2%)	66	40

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	GLU
1	A	197	GLU
1	A	201	LYS
1	B	127	ASP
1	B	128	ILE
1	B	160	VAL
1	B	230	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	172	GLN
1	A	187	GLN
1	A	212	GLN
1	B	172	GLN
1	B	187	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EWQ	A	232	-	16,18,18	1.24	4 (25%)	21,26,26	1.56	4 (19%)
4	FAD	A	233	-	48,58,58	1.88	11 (22%)	54,89,89	2.66	16 (29%)
3	EWQ	B	231	-	16,18,18	1.83	4 (25%)	21,26,26	1.68	4 (19%)
4	FAD	B	233	-	48,58,58	1.68	8 (16%)	54,89,89	2.62	19 (35%)

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
3	EWQ	A	232	-	-	0/4/4/4	0/2/2/2
4	FAD	A	233	-	-	0/30/50/50	0/6/6/6
3	EWQ	B	231	-	-	0/4/4/4	0/2/2/2
4	FAD	B	233	-	-	0/30/50/50	0/6/6/6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	233	FAD	O2'-C2'	-2.89	1.36	1.43
4	A	233	FAD	C4-C4X	-2.89	1.35	1.41
4	A	233	FAD	P-O2P	-2.84	1.42	1.54
4	B	233	FAD	P-O1P	-2.22	1.43	1.51
4	A	233	FAD	O4-C4	-2.18	1.19	1.24
4	B	233	FAD	C9-C8	2.01	1.43	1.37
4	A	233	FAD	P-O1P	2.02	1.58	1.51
3	A	232	EWQ	C7-C2	2.09	1.46	1.42
4	A	233	FAD	C2A-N1A	2.15	1.38	1.33
3	A	232	EWQ	C4-C3	2.18	1.45	1.42
3	A	232	EWQ	C2-C3	2.19	1.47	1.42
3	B	231	EWQ	C4-C3	2.70	1.46	1.42
3	A	232	EWQ	C1-C6	2.80	1.42	1.37
3	B	231	EWQ	C8-C7	2.88	1.44	1.39
3	B	231	EWQ	C2-C3	2.90	1.49	1.42
4	B	233	FAD	C2A-N1A	3.03	1.39	1.33
4	B	233	FAD	C10-N1	3.26	1.41	1.35
3	B	231	EWQ	C7-C2	3.41	1.49	1.42
4	B	233	FAD	C9A-N10	3.52	1.43	1.38
4	A	233	FAD	C4-N3	3.63	1.39	1.33
4	A	233	FAD	C2A-N3A	3.76	1.38	1.32
4	B	233	FAD	C4-N3	4.24	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	233	FAD	C1'-N10	4.36	1.53	1.48
4	B	233	FAD	C2A-N3A	4.49	1.40	1.32
4	A	233	FAD	C10-N1	4.77	1.43	1.35
4	B	233	FAD	C4X-N5	5.77	1.42	1.33
4	A	233	FAD	C4X-N5	6.07	1.42	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	233	FAD	N3A-C2A-N1A	-12.42	119.38	128.89
4	A	233	FAD	N3A-C2A-N1A	-11.44	120.13	128.89
4	A	233	FAD	O3P-P-O5'	-4.20	91.81	102.94
3	A	232	EWQ	C9-N10-C3	-4.03	118.01	121.75
4	A	233	FAD	C4X-C4-N3	-4.00	118.12	123.59
3	B	231	EWQ	O16-C6-C1	-3.94	114.70	124.62
4	B	233	FAD	C4B-O4B-C1B	-3.53	105.84	109.72
4	B	233	FAD	O4'-C4'-C5'	-3.43	102.72	110.19
4	A	233	FAD	C7M-C7-C6	-3.39	111.06	120.28
4	B	233	FAD	O3P-PA-O5B	-3.32	94.13	102.94
4	A	233	FAD	O4'-C4'-C3'	-3.18	101.02	109.02
4	B	233	FAD	C4A-C5A-N7A	-3.14	106.59	109.48
4	A	233	FAD	C4A-C5A-N7A	-3.13	106.60	109.48
3	B	231	EWQ	C17-O16-C6	-2.88	110.78	117.51
4	A	233	FAD	O3B-C3B-C4B	-2.83	102.55	111.05
4	B	233	FAD	O3P-P-O5'	-2.78	95.56	102.94
4	A	233	FAD	C1B-N9A-C4A	-2.63	122.97	126.94
4	B	233	FAD	C1B-N9A-C4A	-2.59	123.03	126.94
4	B	233	FAD	O4'-C4'-C3'	-2.54	102.63	109.02
4	B	233	FAD	C7M-C7-C6	-2.51	113.45	120.28
4	B	233	FAD	C4X-C4-N3	-2.45	120.24	123.59
4	B	233	FAD	P-O3P-PA	-2.32	126.21	132.73
4	B	233	FAD	C8M-C8-C9	-2.14	114.47	120.28
4	B	233	FAD	O2A-PA-O3P	2.02	114.24	105.09
3	A	232	EWQ	C11-N10-C9	2.19	121.23	118.19
4	A	233	FAD	O2B-C2B-C3B	2.35	119.47	111.83
4	B	233	FAD	O5'-P-O1P	2.36	118.79	109.62
4	A	233	FAD	C9A-C5X-N5	2.40	125.90	122.36
4	A	233	FAD	C6-C7-C8	2.55	124.91	120.04
3	A	232	EWQ	C1-C6-C5	2.58	124.61	121.29
4	A	233	FAD	C1'-N10-C9A	2.60	121.78	118.86
3	B	231	EWQ	C15-O14-C4	2.61	121.59	117.77
4	A	233	FAD	C8M-C8-C7	2.73	126.72	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	232	EWQ	C8-C9-N10	2.76	124.11	119.75
4	A	233	FAD	C4X-C10-N10	2.80	122.17	120.52
4	B	233	FAD	O4B-C1B-N9A	2.88	114.13	108.10
4	B	233	FAD	C4-C4X-N5	3.51	122.98	118.72
3	B	231	EWQ	C1-C6-C5	3.61	125.94	121.29
4	B	233	FAD	C8M-C8-C7	3.62	128.68	120.73
4	A	233	FAD	C2B-C1B-N9A	4.72	121.51	114.29
4	B	233	FAD	C4X-C10-N10	4.82	123.36	120.52
4	B	233	FAD	C4-N3-C2	4.82	119.41	115.25
4	A	233	FAD	C4-N3-C2	7.91	122.09	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	232	EWQ	2	0
4	A	233	FAD	10	0
3	B	231	EWQ	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	230/230 (100%)	0.76	31 (13%) 4 4	10, 25, 48, 62	0
1	B	230/230 (100%)	0.36	20 (8%) 13 11	9, 18, 41, 54	0
All	All	460/460 (100%)	0.56	51 (11%) 7 6	9, 20, 45, 62	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	7.1
1	A	230	GLN	6.5
1	B	194	ILE	6.4
1	A	194	ILE	5.6
1	A	59	LEU	4.9
1	A	58	THR	4.8
1	B	157	LYS	4.7
1	B	230	GLN	4.7
1	A	1	ALA	4.6
1	A	197	GLU	4.4
1	A	128	ILE	4.3
1	B	197	GLU	4.2
1	B	198	GLU	4.0
1	A	131	PHE	3.8
1	A	198	GLU	3.8
1	A	2	GLY	3.8
1	B	160	VAL	3.7
1	A	229	GLY	3.6
1	A	133	ASP	3.4
1	A	57	GLY	3.2
1	A	157	LYS	3.2
1	B	156	THR	3.2
1	A	225	HIS	3.1
1	A	196	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	62	PRO	2.9
1	B	158	THR	2.9
1	A	78	ARG	2.8
1	A	129	PRO	2.8
1	B	144	LEU	2.8
1	A	158	THR	2.8
1	A	130	GLY	2.8
1	B	196	SER	2.7
1	A	226	TRP	2.7
1	B	108	VAL	2.7
1	A	135	GLY	2.6
1	A	228	PHE	2.6
1	B	159	GLY	2.6
1	A	199	GLU	2.4
1	A	155	TYR	2.4
1	A	153	GLU	2.4
1	B	2	GLY	2.3
1	B	98	ILE	2.2
1	B	153	GLU	2.2
1	B	199	GLU	2.2
1	A	112	LEU	2.1
1	A	63	GLU	2.1
1	B	229	GLY	2.1
1	B	101	PHE	2.1
1	A	216	LYS	2.1
1	A	166	TYR	2.0
1	B	201	LYS	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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	EWQ	B	231	17/17	0.85	0.13	1.12	23,30,36,39	0
4	FAD	A	233	53/53	0.86	0.16	0.65	15,25,58,59	0
4	FAD	B	233	53/53	0.88	0.14	0.34	16,26,53,57	0
3	EWQ	A	232	17/17	0.90	0.10	-0.13	18,22,29,33	0
2	ZN	A	231	1/1	0.97	0.07	-1.86	29,29,29,29	0
2	ZN	B	232	1/1	0.99	0.04	-3.69	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.