WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 26, 2014 – 03:54 PM GMT

PDB ID   :   3PM9
Title   :   Crystal structure of a Putative dehydrogenase (RPA1076) from Rhodopseu-
               domonas palustris CGA009 at 2.57 A resolution
Authors   :   Joint Center for Structural Genomics (JCSG)
Deposited on : 2010-11-16
Resolution :   2.57 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.57 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	Percentile Ranks	Value
Rfree		0.220
Clashscore		2
Ramachandran outliers		0.3%
Sidechain outliers		0.9%
RSRZ outliers		1.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
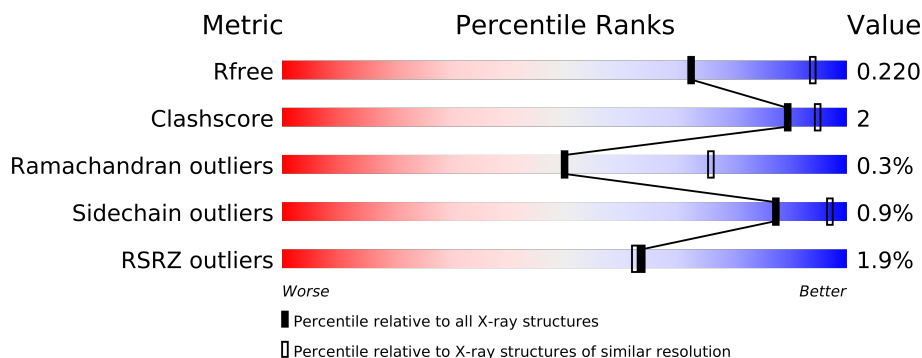
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1891 (2.60-2.56)
Clashscore	79885	2358 (2.60-2.56)
Ramachandran outliers	78287	2316 (2.60-2.56)
Sidechain outliers	78261	2316 (2.60-2.56)
RSRZ outliers	66119	1891 (2.60-2.56)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	476	
1	B	476	
1	C	476	
1	D	476	
1	E	476	
1	F	476	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	UNL	A	477	-	X
3	UNL	B	477	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	UNL	C	477	-	X
3	UNL	D	477	-	X
3	UNL	E	477	-	X
3	UNL	F	477	-	X
4	PO4	A	484	-	X
4	PO4	A	490	-	X
4	PO4	B	485	-	X
4	PO4	B	491	-	X
4	PO4	C	486	-	X
4	PO4	C	492	-	X
4	PO4	D	487	-	X
4	PO4	D	493	-	X
4	PO4	E	488	-	X
4	PO4	E	494	-	X
4	PO4	F	489	-	X
4	PO4	F	495	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 22350 atoms, of which 0 are hydrogen and 0 are deuterium.

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.
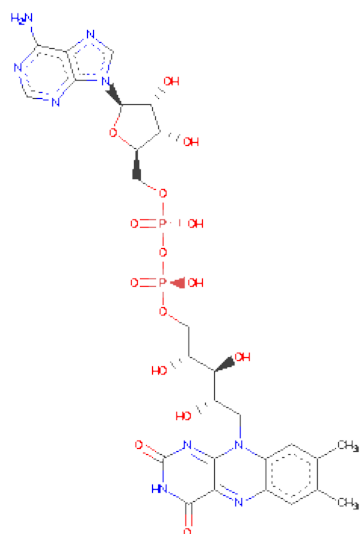
- Molecule 1 is a protein called Putative oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	Se	0	3	0
			3487	2208	600	671	2	6			
1	B	465	Total	C	N	O	S	Se	0	4	0
			3493	2212	602	671	2	6			
1	C	465	Total	C	N	O	S	Se	0	5	0
			3499	2215	602	674	2	6			
1	D	465	Total	C	N	O	S	Se	0	5	0
			3501	2216	609	668	2	6			
1	E	465	Total	C	N	O	S	Se	0	6	0
			3509	2220	608	673	2	6			
1	F	465	Total	C	N	O	S	Se	0	4	0
			3498	2213	605	672	2	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q6NAV4
B	0	GLY	-	leader sequence	UNP Q6NAV4
C	0	GLY	-	leader sequence	UNP Q6NAV4
D	0	GLY	-	leader sequence	UNP Q6NAV4
E	0	GLY	-	leader sequence	UNP Q6NAV4
F	0	GLY	-	leader sequence	UNP Q6NAV4

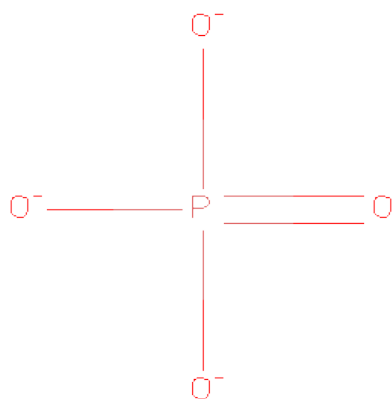- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

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

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 6	O 6	0	0
3	E	1	Total 6	O 6	0	0
3	B	1	Total 6	O 6	0	0
3	C	1	Total 6	O 6	0	0
3	A	1	Total 6	O 6	0	0
3	F	1	Total 6	O 6	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	P 1	0	0
4	A	1	Total 5	O 4	P 1	0	0
4	A	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	B	1	Total 5	O 4	P 1	0	0
4	C	1	Total 5	O 4	P 1	0	0
4	C	1	Total 5	O 4	P 1	0	0
4	C	1	Total 5	O 4	P 1	0	0
4	D	1	Total 5	O 4	P 1	0	0
4	D	1	Total 5	O 4	P 1	0	0
4	D	1	Total 5	O 4	P 1	0	0
4	E	1	Total 5	O 4	P 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total 5	O 4	P 1	0	0
4	E	1	Total 5	O 4	P 1	0	0
4	F	1	Total 5	O 4	P 1	0	0
4	F	1	Total 5	O 4	P 1	0	0
4	F	1	Total 5	O 4	P 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total 203	O 203	0	0
5	B	168	Total 168	O 168	0	0
5	C	126	Total 126	O 126	0	0
5	D	143	Total 143	O 143	0	0
5	E	145	Total 145	O 145	0	0
5	F	134	Total 134	O 134	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.
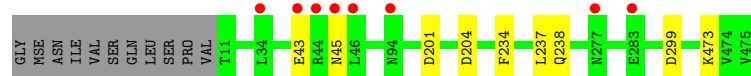
- Molecule 1: Putative oxidoreductase

Chain A:
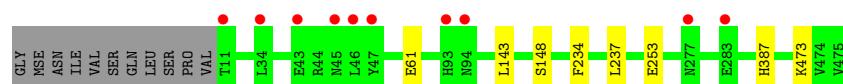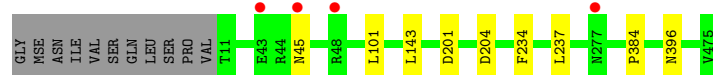
- Molecule 1: Putative oxidoreductase

Chain B:

- Molecule 1: Putative oxidoreductase

Chain C:

- Molecule 1: Putative oxidoreductase

Chain D:

- Molecule 1: Putative oxidoreductase

Chain E:

- Molecule 1: Putative oxidoreductase

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	146.09Å 250.73Å 251.71Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 90.00°	
Resolution (Å)	49.36 – 2.57	Depositor
	49.36 – 2.57	EDS
% Data completeness	98.9 (49.36-2.57)	Depositor
(in resolution range)	98.9 (49.36-2.57)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.03 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.193 , 0.227	Depositor
	0.190 , 0.220	DCC
R_{free} test set	7270 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 16.7	EDS
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
L-test for twinning	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	3 of 144702 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22350	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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 36.01 % 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 5.3365e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, UNL, 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	0.68	1/3549 (0.0%)	0.64	1/4814 (0.0%)
1	B	0.66	0/3558	0.62	0/4826
1	C	0.69	1/3567 (0.0%)	0.61	0/4838
1	D	0.66	0/3569	0.63	0/4840
1	E	0.67	1/3580 (0.0%)	0.63	0/4855
1	F	0.67	1/3563 (0.0%)	0.62	0/4833
All	All	0.67	4/21386 (0.0%)	0.63	1/29006 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	407	GLU	CG-CD	6.02	1.60	1.51
1	C	61	GLU	CG-CD	5.90	1.60	1.51
1	A	61	GLU	CG-CD	5.73	1.60	1.51
1	E	72	GLU	CG-CD	5.73	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	LEU	CA-CB-CG	7.31	132.11	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3487	0	0	2	0
1	B	3493	0	0	3	0
1	C	3499	0	0	7	0
1	D	3501	0	0	3	0
1	E	3509	0	0	3	0
1	F	3498	0	0	4	0
2	A	53	0	0	1	0
2	B	53	0	0	1	0
2	C	53	0	0	2	0
2	D	53	0	0	2	0
2	E	53	0	0	1	0
2	F	53	0	0	1	0
3	A	6	0	0	4	0
3	B	6	0	0	4	0
3	C	6	0	0	4	0
3	D	6	0	0	4	0
3	E	6	0	0	3	0
3	F	6	0	0	2	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	1	0
4	D	15	0	0	1	0
4	E	15	0	0	1	0
4	F	15	0	0	0	0
5	A	203	0	0	1	0
5	B	168	0	0	2	0
5	C	126	0	0	2	0
5	D	143	0	0	0	0
5	E	145	0	0	1	0
5	F	134	0	0	1	0
All	All	22350	0	0	48	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (48) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:477:UNL:O1	3:F:477:UNL:O3	1.64	1.15
3:B:477:UNL:O2	3:B:477:UNL:O3	1.66	1.12

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:477:UNL:O3	3:C:477:UNL:O2	1.68	1.11
3:D:477:UNL:O4	3:D:477:UNL:O3	1.78	0.99
3:A:477:UNL:O6	3:A:477:UNL:O5	1.85	0.95
3:D:477:UNL:O3	3:D:477:UNL:O2	1.90	0.89
3:E:477:UNL:O6	3:E:477:UNL:O4	1.93	0.86
3:E:477:UNL:O5	3:E:477:UNL:O4	1.96	0.84
3:B:477:UNL:O2	3:B:477:UNL:O1	1.97	0.82
3:C:477:UNL:O1	3:C:477:UNL:O2	2.08	0.70
3:B:477:UNL:O6	3:B:477:UNL:O4	2.15	0.64
3:C:477:UNL:O5	3:C:477:UNL:O4	2.17	0.62
3:F:477:UNL:O4	3:F:477:UNL:O3	2.21	0.58
1:C:473:LYS:NZ	5:C:1051:HOH:O	2.36	0.58
1:D:396:ASN:ND2	4:D:493:PO4:O2	2.38	0.56
3:D:477:UNL:O3	3:D:477:UNL:O5	2.26	0.54
3:B:477:UNL:O3	3:B:477:UNL:O4	2.25	0.53
1:C:396:ASN:ND2	4:C:492:PO4:O3	2.42	0.52
1:C:42[B]:GLU:OE1	1:C:44:ARG:N	2.43	0.51
3:E:477:UNL:O1	3:E:477:UNL:O3	2.30	0.50
1:A:473:LYS:NZ	5:A:845:HOH:O	2.45	0.50
1:C:74:ARG:NE	5:C:939:HOH:O	2.43	0.49
1:F:56:ARG:NH2	5:F:971:HOH:O	2.46	0.48
1:D:201:ASP:OD2	1:D:204:ASP:OD2	2.32	0.47
1:B:201:ASP:OD2	1:B:204:ASP:OD2	2.33	0.47
3:D:477:UNL:O4	3:D:477:UNL:O6	2.32	0.47
3:A:477:UNL:O2	3:A:477:UNL:O4	2.32	0.47
1:F:201:ASP:OD2	1:F:204:ASP:OD2	2.33	0.46
1:D:101:LEU:CD1	2:D:476:FAD:N6A	2.79	0.46
1:B:473:LYS:NZ	5:B:1320:HOH:O	2.50	0.45
1:C:201:ASP:OD2	1:C:204:ASP:OD2	2.35	0.45
1:F:201:ASP:OD1	1:F:201:ASP:C	2.56	0.44
2:F:476:FAD:C2'	2:F:476:FAD:N1	2.79	0.44
1:A:387:HIS:NE2	3:A:477:UNL:O6	2.50	0.44
2:C:476:FAD:N1	2:C:476:FAD:C2'	2.80	0.44
1:E:344:GLN:NE2	4:E:494:PO4:O1	2.51	0.44
2:A:476:FAD:N1	2:A:476:FAD:C2'	2.79	0.44
2:B:476:FAD:N1	2:B:476:FAD:C2'	2.80	0.43
1:E:473:LYS:NZ	5:E:1322:HOH:O	2.52	0.43
1:C:355:ILE:C	1:C:355:ILE:CD1	2.86	0.43
3:C:477:UNL:O3	3:C:477:UNL:O4	2.37	0.43
2:D:476:FAD:C2'	2:D:476:FAD:N1	2.82	0.42
1:F:355:ILE:C	1:F:355:ILE:CD1	2.88	0.42
2:E:476:FAD:C2'	2:E:476:FAD:N1	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:101:LEU:CD1	2:C:476:FAD:N6A	2.82	0.41
1:B:238:GLN:N	5:B:637:HOH:O	2.53	0.41
1:E:142:SER:OG	1:E:146:GLN:OE1	2.38	0.40
3:A:477:UNL:O4	3:A:477:UNL:O5	2.40	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	466/476 (98%)	453 (97%)	13 (3%)	0	100	100
1	B	467/476 (98%)	454 (97%)	12 (3%)	1 (0%)	56	81
1	C	468/476 (98%)	456 (97%)	12 (3%)	0	100	100
1	D	468/476 (98%)	450 (96%)	16 (3%)	2 (0%)	43	70
1	E	469/476 (98%)	456 (97%)	11 (2%)	2 (0%)	43	70
1	F	467/476 (98%)	453 (97%)	12 (3%)	2 (0%)	43	70
All	All	2805/2856 (98%)	2722 (97%)	76 (3%)	7 (0%)	50	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	ASN
1	E	45	ASN
1	F	146	GLN
1	D	45	ASN
1	D	384	PRO
1	E	384	PRO
1	F	384	PRO

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	362/372 (97%)	357 (99%)	5 (1%)	78	94
1	B	363/372 (98%)	359 (99%)	4 (1%)	84	96
1	C	365/372 (98%)	363 (100%)	2 (0%)	94	99
1	D	365/372 (98%)	362 (99%)	3 (1%)	89	97
1	E	366/372 (98%)	360 (98%)	6 (2%)	75	92
1	F	364/372 (98%)	362 (100%)	2 (0%)	94	99
All	All	2185/2232 (98%)	2163 (99%)	22 (1%)	87	96

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	SER
1	A	234	PHE
1	A	237	LEU
1	A	253[A]	GLU
1	A	253[B]	GLU
1	B	43	GLU
1	B	234	PHE
1	B	237	LEU
1	B	299	ASP
1	C	234	PHE
1	C	237	LEU
1	D	143	LEU
1	D	234	PHE
1	D	237	LEU
1	E	228[A]	ARG
1	E	228[B]	ARG
1	E	234	PHE
1	E	237	LEU
1	E	283	GLU
1	E	299	ASP
1	F	234	PHE
1	F	237	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 30 ligands modelled in this entry, 6 are unknown - leaving 24 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
2	FAD	A	476	-	58,58,58	1.44	6 (10%)	85,89,89	2.00	13 (15%)
4	PO4	A	478	-	4,4,4	0.28	0	6,6,6	0.31	0
4	PO4	A	484	-	4,4,4	0.16	0	6,6,6	0.30	0
4	PO4	A	490	-	4,4,4	0.41	0	6,6,6	0.31	0
2	FAD	B	476	-	58,58,58	1.30	6 (10%)	85,89,89	1.96	16 (18%)
4	PO4	B	479	-	4,4,4	0.17	0	6,6,6	0.30	0
4	PO4	B	485	-	4,4,4	0.23	0	6,6,6	0.32	0
4	PO4	B	491	-	4,4,4	0.47	0	6,6,6	0.32	0
2	FAD	C	476	-	58,58,58	1.32	6 (10%)	85,89,89	2.02	17 (20%)
4	PO4	C	480	-	4,4,4	0.13	0	6,6,6	0.31	0
4	PO4	C	486	-	4,4,4	0.16	0	6,6,6	0.32	0
4	PO4	C	492	-	4,4,4	0.37	0	6,6,6	0.31	0
2	FAD	D	476	-	58,58,58	1.43	7 (12%)	85,89,89	2.01	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	PO4	D	481	-	4,4,4	0.17	0	6,6,6	0.31	0
4	PO4	D	487	-	4,4,4	0.27	0	6,6,6	0.32	0
4	PO4	D	493	-	4,4,4	0.33	0	6,6,6	0.32	0
2	FAD	E	476	-	58,58,58	1.40	8 (13%)	85,89,89	1.97	15 (17%)
4	PO4	E	482	-	4,4,4	0.36	0	6,6,6	0.31	0
4	PO4	E	488	-	4,4,4	0.23	0	6,6,6	0.30	0
4	PO4	E	494	-	4,4,4	0.31	0	6,6,6	0.31	0
2	FAD	F	476	-	58,58,58	1.28	5 (8%)	85,89,89	1.97	15 (17%)
4	PO4	F	483	-	4,4,4	0.22	0	6,6,6	0.31	0
4	PO4	F	489	-	4,4,4	0.14	0	6,6,6	0.31	0
4	PO4	F	495	-	4,4,4	0.37	0	6,6,6	0.32	0

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	476	-	-	0/34/50/50	0/1/6/6
4	PO4	A	478	-	-	0/0/0/0	0/0/0/0
4	PO4	A	484	-	-	0/0/0/0	0/0/0/0
4	PO4	A	490	-	-	0/0/0/0	0/0/0/0
2	FAD	B	476	-	-	0/34/50/50	0/1/6/6
4	PO4	B	479	-	-	0/0/0/0	0/0/0/0
4	PO4	B	485	-	-	0/0/0/0	0/0/0/0
4	PO4	B	491	-	-	0/0/0/0	0/0/0/0
2	FAD	C	476	-	-	0/34/50/50	0/1/6/6
4	PO4	C	480	-	-	0/0/0/0	0/0/0/0
4	PO4	C	486	-	-	0/0/0/0	0/0/0/0
4	PO4	C	492	-	-	0/0/0/0	0/0/0/0
2	FAD	D	476	-	-	0/34/50/50	0/1/6/6
4	PO4	D	481	-	-	0/0/0/0	0/0/0/0
4	PO4	D	487	-	-	0/0/0/0	0/0/0/0
4	PO4	D	493	-	-	0/0/0/0	0/0/0/0
2	FAD	E	476	-	-	0/34/50/50	0/1/6/6
4	PO4	E	482	-	-	0/0/0/0	0/0/0/0
4	PO4	E	488	-	-	0/0/0/0	0/0/0/0
4	PO4	E	494	-	-	0/0/0/0	0/0/0/0
2	FAD	F	476	-	-	0/34/50/50	0/1/6/6
4	PO4	F	483	-	-	0/0/0/0	0/0/0/0
4	PO4	F	489	-	-	0/0/0/0	0/0/0/0
4	PO4	F	495	-	-	0/0/0/0	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	476	FAD	C1'-N10	5.56	1.54	1.48
2	A	476	FAD	C1'-N10	5.39	1.54	1.48
2	E	476	FAD	C1'-N10	5.39	1.54	1.48
2	F	476	FAD	C1'-N10	4.72	1.53	1.48
2	C	476	FAD	C1'-N10	4.58	1.53	1.48
2	D	476	FAD	C1'-C2'	4.49	1.55	1.51
2	B	476	FAD	C1'-N10	4.24	1.53	1.48
2	B	476	FAD	C1'-C2'	4.21	1.55	1.51
2	A	476	FAD	C1'-C2'	4.18	1.55	1.51
2	F	476	FAD	C1'-C2'	3.65	1.55	1.51
2	E	476	FAD	C1'-C2'	3.46	1.54	1.51
2	C	476	FAD	C1'-C2'	3.42	1.54	1.51
2	A	476	FAD	C2'-C3'	-3.13	1.47	1.53
2	E	476	FAD	C2A-N3A	2.99	1.38	1.32
2	A	476	FAD	C2A-N1A	2.97	1.39	1.33
2	D	476	FAD	C2A-N3A	2.95	1.38	1.32
2	A	476	FAD	C2A-N3A	2.93	1.38	1.32
2	C	476	FAD	C2A-N3A	2.83	1.37	1.32
2	E	476	FAD	C2A-N1A	2.81	1.39	1.33
2	E	476	FAD	C2'-C3'	-2.78	1.47	1.53
2	D	476	FAD	C2A-N1A	2.72	1.39	1.33
2	C	476	FAD	C5X-N5	2.71	1.39	1.35
2	D	476	FAD	C9A-N10	2.70	1.42	1.38
2	B	476	FAD	C2A-N3A	2.68	1.37	1.32
2	E	476	FAD	C9A-N10	2.63	1.42	1.38
2	C	476	FAD	C9A-N10	2.60	1.42	1.38
2	B	476	FAD	C2'-C3'	-2.60	1.48	1.53
2	C	476	FAD	C2A-N1A	2.57	1.39	1.33
2	A	476	FAD	C9A-N10	2.48	1.42	1.38
2	F	476	FAD	C9A-N10	2.40	1.42	1.38
2	B	476	FAD	C9A-N10	2.40	1.42	1.38
2	D	476	FAD	C2'-C3'	-2.35	1.48	1.53
2	F	476	FAD	C2'-C3'	-2.32	1.48	1.53
2	E	476	FAD	C4A-N9A	-2.30	1.34	1.37
2	B	476	FAD	C2A-N1A	2.23	1.38	1.33
2	F	476	FAD	C2A-N3A	2.21	1.36	1.32
2	D	476	FAD	C5X-N5	2.19	1.38	1.35
2	E	476	FAD	O4B-C4B	-2.00	1.40	1.45

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	476	FAD	N3A-C2A-N1A	-11.11	119.42	128.71
2	F	476	FAD	N3A-C2A-N1A	-10.75	119.72	128.71
2	A	476	FAD	N3A-C2A-N1A	-10.73	119.73	128.71
2	E	476	FAD	N3A-C2A-N1A	-10.57	119.87	128.71
2	D	476	FAD	N3A-C2A-N1A	-10.11	120.26	128.71
2	B	476	FAD	N3A-C2A-N1A	-9.71	120.59	128.71
2	C	476	FAD	C2-N1-C10	6.97	122.01	114.98
2	D	476	FAD	C2-N1-C10	6.40	121.43	114.98
2	F	476	FAD	C2-N1-C10	6.34	121.36	114.98
2	A	476	FAD	C2-N1-C10	6.33	121.36	114.98
2	B	476	FAD	C2-N1-C10	6.27	121.30	114.98
2	E	476	FAD	C2-N1-C10	6.16	121.18	114.98
2	B	476	FAD	C1'-N10-C9A	6.16	124.86	118.87
2	A	476	FAD	C1'-N10-C9A	6.09	124.80	118.87
2	D	476	FAD	C1'-N10-C9A	5.73	124.45	118.87
2	F	476	FAD	C1'-N10-C9A	5.65	124.37	118.87
2	E	476	FAD	C1'-N10-C9A	5.30	124.03	118.87
2	C	476	FAD	C1'-N10-C9A	5.19	123.92	118.87
2	E	476	FAD	C9A-N10-C10	-4.21	117.64	121.77
2	A	476	FAD	C9A-N10-C10	-3.84	118.00	121.77
2	D	476	FAD	C9A-N10-C10	-3.67	118.17	121.77
2	E	476	FAD	C4X-C10-N1	-3.63	119.10	122.73
2	C	476	FAD	N3A-C4A-N9A	3.59	131.91	125.43
2	A	476	FAD	C4X-C10-N1	-3.48	119.25	122.73
2	D	476	FAD	C4X-C10-N1	-3.48	119.26	122.73
2	C	476	FAD	C4X-N5-C5X	3.43	120.55	116.69
2	F	476	FAD	C9A-N10-C10	-3.41	118.42	121.77
2	C	476	FAD	C4X-C10-N1	-3.31	119.42	122.73
2	D	476	FAD	C4X-N5-C5X	3.29	120.39	116.69
2	A	476	FAD	N3A-C4A-N9A	3.28	131.35	125.43
2	D	476	FAD	N3A-C4A-N9A	3.24	131.29	125.43
2	F	476	FAD	C4X-N5-C5X	3.21	120.30	116.69
2	B	476	FAD	C9A-N10-C10	-3.19	118.64	121.77
2	F	476	FAD	C5X-C9A-N10	3.15	119.91	116.80
2	E	476	FAD	N3A-C4A-N9A	3.14	131.11	125.43
2	A	476	FAD	C4X-N5-C5X	3.12	120.19	116.69
2	F	476	FAD	N3A-C4A-N9A	3.10	131.03	125.43
2	B	476	FAD	C4X-N5-C5X	3.10	120.17	116.69
2	B	476	FAD	N3A-C4A-N9A	3.09	131.00	125.43
2	F	476	FAD	C4X-C10-N1	-3.05	119.69	122.73
2	A	476	FAD	O2'-C2'-C1'	2.97	117.08	109.71
2	E	476	FAD	C5X-C9A-N10	2.90	119.66	116.80
2	D	476	FAD	P-O3P-PA	-2.88	123.24	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	476	FAD	C9A-N10-C10	-2.85	118.97	121.77
2	E	476	FAD	C4X-N5-C5X	2.84	119.88	116.69
2	C	476	FAD	C4X-C10-N10	2.84	121.92	120.51
2	C	476	FAD	P-O3P-PA	-2.84	123.37	131.68
2	B	476	FAD	C4X-C10-N1	-2.78	119.96	122.73
2	D	476	FAD	C5X-C9A-N10	2.73	119.49	116.80
2	F	476	FAD	O4'-C4'-C3'	2.71	115.79	109.05
2	A	476	FAD	C5X-C9A-N10	2.67	119.43	116.80
2	D	476	FAD	O3'-C3'-C4'	2.59	115.28	108.74
2	B	476	FAD	C5X-C9A-N10	2.55	119.31	116.80
2	E	476	FAD	P-O3P-PA	-2.55	124.22	131.68
2	B	476	FAD	C4-N3-C2	-2.51	120.24	125.39
2	B	476	FAD	O3'-C3'-C4'	2.50	115.06	108.74
2	C	476	FAD	C4-N3-C2	-2.49	120.28	125.39
2	B	476	FAD	O4'-C4'-C3'	2.46	115.18	109.05
2	E	476	FAD	O3'-C3'-C4'	2.43	114.89	108.74
2	C	476	FAD	O4'-C4'-C3'	2.41	115.04	109.05
2	B	476	FAD	P-O3P-PA	-2.40	124.64	131.68
2	F	476	FAD	C4-N3-C2	-2.40	120.47	125.39
2	A	476	FAD	C4-N3-C2	-2.36	120.54	125.39
2	E	476	FAD	C4-N3-C2	-2.36	120.55	125.39
2	B	476	FAD	C4B-O4B-C1B	2.33	112.28	109.75
2	D	476	FAD	C4-N3-C2	-2.33	120.62	125.39
2	F	476	FAD	C2A-N3A-C4A	2.33	120.63	114.01
2	B	476	FAD	C4A-C5A-N7A	-2.32	107.53	109.52
2	A	476	FAD	O3'-C3'-C4'	2.32	114.59	108.74
2	D	476	FAD	C4A-C5A-N7A	-2.31	107.54	109.52
2	D	476	FAD	C5A-C4A-N3A	-2.30	120.70	125.70
2	A	476	FAD	P-O3P-PA	-2.29	124.97	131.68
2	F	476	FAD	P-O3P-PA	-2.27	125.02	131.68
2	B	476	FAD	C5A-C4A-N3A	-2.27	120.76	125.70
2	C	476	FAD	O4B-C1B-N9A	2.27	110.55	108.44
2	D	476	FAD	O4B-C1B-N9A	-2.26	106.34	108.44
2	F	476	FAD	O3'-C3'-C4'	2.26	114.44	108.74
2	A	476	FAD	O4'-C4'-C3'	2.24	114.63	109.05
2	C	476	FAD	N7A-C8A-N9A	-2.23	108.05	114.36
2	C	476	FAD	O3'-C3'-C4'	2.22	114.36	108.74
2	B	476	FAD	O2'-C2'-C1'	2.16	115.06	109.71
2	E	476	FAD	O2'-C2'-C1'	2.14	115.02	109.71
2	E	476	FAD	O4'-C4'-C3'	2.12	114.34	109.05
2	E	476	FAD	N7A-C8A-N9A	-2.12	108.35	114.36
2	E	476	FAD	O2A-PA-O3P	2.11	115.14	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	476	FAD	C5A-C4A-N3A	-2.10	121.12	125.70
2	D	476	FAD	C2A-N3A-C4A	2.08	119.93	114.01
2	D	476	FAD	N7A-C8A-N9A	-2.08	108.48	114.36
2	D	476	FAD	O2'-C2'-C1'	2.06	114.83	109.71
2	D	476	FAD	O4'-C4'-C3'	2.05	114.15	109.05
2	D	476	FAD	C4X-C10-N10	2.04	121.53	120.51
2	C	476	FAD	C2A-N3A-C4A	2.03	119.79	114.01
2	F	476	FAD	C5A-C4A-N3A	-2.01	121.32	125.70
2	C	476	FAD	C5X-C9A-N10	2.01	118.78	116.80
2	F	476	FAD	N7A-C8A-N9A	-2.00	108.70	114.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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, 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(Å²)	Q<0.9
1	A	465/476 (97%)	-0.04	10 (2%)	59	57	23, 35, 54, 72	0
1	B	465/476 (97%)	-0.03	8 (1%)	67	67	23, 36, 56, 73	0
1	C	465/476 (97%)	0.01	10 (2%)	59	57	26, 38, 58, 77	0
1	D	465/476 (97%)	-0.05	4 (0%)	81	83	25, 37, 57, 75	0
1	E	465/476 (97%)	-0.07	11 (2%)	56	54	24, 36, 55, 72	0
1	F	465/476 (97%)	0.01	11 (2%)	56	54	24, 38, 59, 77	0
All	All	2790/2856 (97%)	-0.03	54 (1%)	64	62	23, 37, 57, 77	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	GLU	4.9
1	F	43	GLU	4.5
1	F	11	THR	3.9
1	B	45	ASN	3.8
1	F	46	LEU	3.8
1	E	43	GLU	3.8
1	B	34	LEU	3.5
1	C	46	LEU	3.5
1	B	277	ASN	3.5
1	B	43	GLU	3.4
1	E	11	THR	3.2
1	A	283	GLU	3.2
1	E	94	ASN	3.2
1	D	43	GLU	3.1
1	C	277	ASN	3.0
1	A	47	TYR	2.9
1	C	94	ASN	2.8
1	F	283	GLU	2.8
1	A	46	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	34	LEU	2.7
1	B	94	ASN	2.7
1	A	11	THR	2.7
1	F	47	TYR	2.7
1	A	45	ASN	2.6
1	D	277	ASN	2.6
1	E	279	ARG	2.6
1	B	283	GLU	2.6
1	F	34	LEU	2.6
1	C	50	HIS	2.5
1	B	46	LEU	2.5
1	D	48	ARG	2.5
1	F	277	ASN	2.5
1	E	46	LEU	2.4
1	E	47	TYR	2.4
1	C	48	ARG	2.4
1	F	50	HIS	2.4
1	E	283	GLU	2.3
1	A	277	ASN	2.3
1	F	94	ASN	2.3
1	E	34	LEU	2.3
1	F	279	ARG	2.2
1	A	94	ASN	2.2
1	F	45	ASN	2.2
1	A	34	LEU	2.2
1	C	43	GLU	2.2
1	C	47	TYR	2.2
1	E	48	ARG	2.2
1	E	277	ASN	2.1
1	B	44	ARG	2.1
1	E	35	GLU	2.1
1	A	93	HIS	2.1
1	C	438	VAL	2.1
1	D	45	ASN	2.1
1	C	11	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PO4	B	485	5/5	0.36	16.99	35,35,35,36	5
4	PO4	F	489	5/5	0.34	13.55	42,42,43,43	5
4	PO4	E	488	5/5	0.37	13.24	36,37,38,38	5
4	PO4	C	486	5/5	0.33	11.69	33,34,34,34	5
4	PO4	A	484	5/5	0.28	9.86	32,32,33,34	5
4	PO4	B	491	5/5	0.22	9.05	29,29,30,31	5
3	UNL	F	477	6/-	0.30	8.19	30,49,54,55	0
4	PO4	E	494	5/5	0.24	8.15	43,43,44,44	5
4	PO4	D	493	5/5	0.23	7.63	40,40,41,41	5
4	PO4	D	487	5/5	0.27	7.13	41,42,43,43	5
4	PO4	A	490	5/5	0.25	6.47	35,35,36,37	5
3	UNL	E	477	6/-	0.27	6.01	25,50,56,57	0
3	UNL	A	477	6/-	0.31	5.14	36,52,57,67	0
4	PO4	F	495	5/5	0.21	4.79	43,44,44,44	5
4	PO4	C	492	5/5	0.24	4.70	40,40,41,41	5
3	UNL	D	477	6/-	0.26	4.24	29,48,51,53	0
3	UNL	B	477	6/-	0.22	4.13	38,44,50,56	0
3	UNL	C	477	6/-	0.21	3.67	33,47,51,54	0
4	PO4	B	479	5/5	0.16	1.54	49,49,50,50	0
4	PO4	E	482	5/5	0.15	1.04	50,51,51,52	0
4	PO4	C	480	5/5	0.14	0.25	51,51,52,53	0
4	PO4	D	481	5/5	0.12	-0.11	54,54,54,55	0
2	FAD	A	476	53/53	0.13	-0.23	24,29,42,44	0
2	FAD	E	476	53/53	0.12	-0.23	26,32,43,45	0
2	FAD	F	476	53/53	0.12	-0.27	26,33,45,48	0
2	FAD	B	476	53/53	0.12	-0.35	25,32,43,45	0
2	FAD	D	476	53/53	0.12	-0.38	28,33,44,46	0
2	FAD	C	476	53/53	0.11	-0.52	28,35,45,48	0
4	PO4	F	483	5/5	0.12	-0.66	46,46,47,48	0
4	PO4	A	478	5/5	0.12	-0.68	53,54,54,55	0

6.5 Other polymers (i)

There are no such residues in this entry.