Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2018 – 04:27 am GMT

PDB ID	:	1YRX
Title	:	Structure of a novel photoreceptor: the BLUF domain of AppA from Rhodobacter sphaeroides
Authors	:	Anderson, S.; Dragnea, V.; Masuda, S.; Ybe, J.; Moffat, K.; Bauer, C.
Deposited on	:	2005-02-05
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

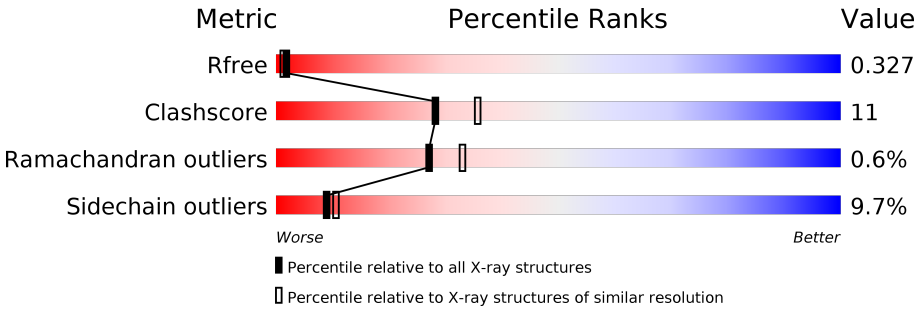
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	(not set)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

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 2.30 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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)

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%

Mol	Chain	Length	Quality of chain
1	A	121	79% 15% • •
1	B	121	62% 28% 6% •
1	C	121	76% 18% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2962 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.

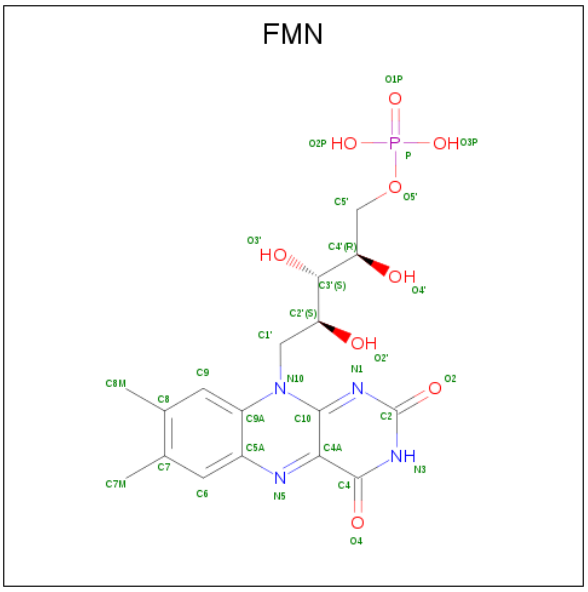
- Molecule 1 is a protein called hypothetical protein Rsph03001874.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			918	570	172	169	7			
1	B	116	Total	C	N	O	S	0	0	0
			909	565	170	167	7			
1	C	115	Total	C	N	O	S	0	0	0
			869	543	155	164	7			

There are 12 discrepancies between the modelled and reference sequences:

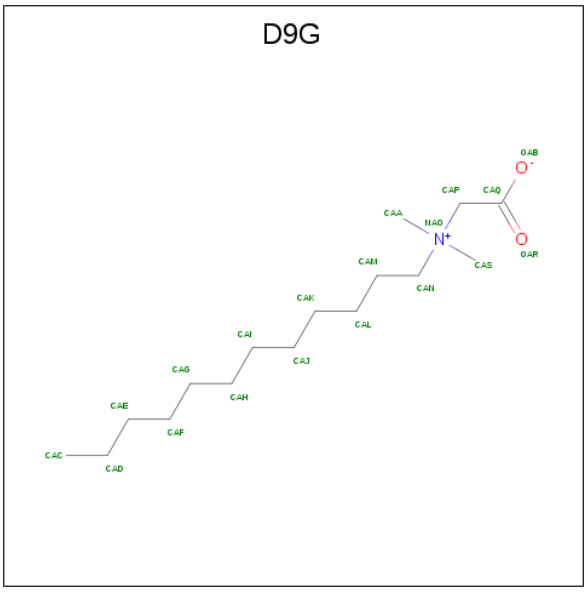
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ALA	-	CLONING ARTIFACT	UNP Q53119
A	14	GLY	-	CLONING ARTIFACT	UNP Q53119
A	15	HIS	-	CLONING ARTIFACT	UNP Q53119
A	16	MET	-	CLONING ARTIFACT	UNP Q53119
B	13	ALA	-	CLONING ARTIFACT	UNP Q53119
B	14	GLY	-	CLONING ARTIFACT	UNP Q53119
B	15	HIS	-	CLONING ARTIFACT	UNP Q53119
B	16	MET	-	CLONING ARTIFACT	UNP Q53119
C	13	ALA	-	CLONING ARTIFACT	UNP Q53119
C	14	GLY	-	CLONING ARTIFACT	UNP Q53119
C	15	HIS	-	CLONING ARTIFACT	UNP Q53119
C	16	MET	-	CLONING ARTIFACT	UNP Q53119

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is N-DODECYL-N,N-DIMETHYLGLYCINATE (three-letter code: D9G) (formula: $C_{16}H_{33}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 19 16 1 2	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 6 6	0	0
3	C	1	Total C N O 19 16 1 2	0	0
3	C	1	Total C 10 10	0	0
3	C	1	Total C 10 10	0	0

- Molecule 4 is water.

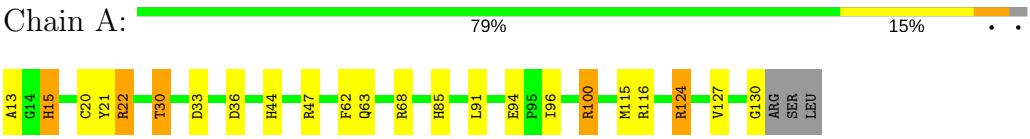
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	30	Total O 30 30	0	0
4	C	21	Total O 21 21	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

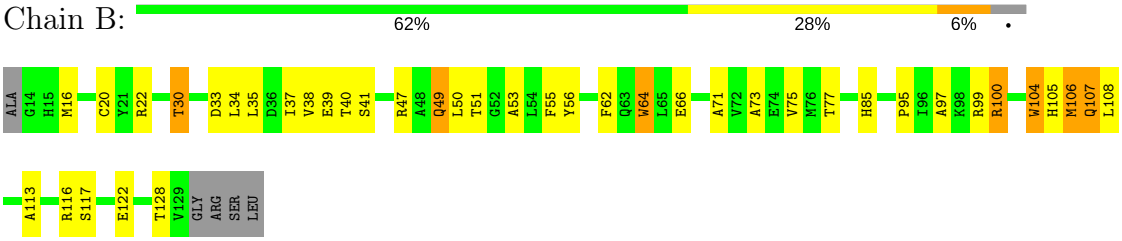
- Molecule 1: hypothetical protein Rsph03001874

Chain A:



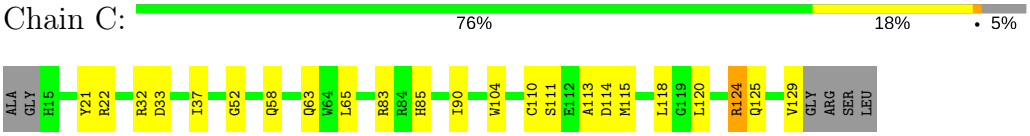
- Molecule 1: hypothetical protein Rsph03001874

Chain B:



- Molecule 1: hypothetical protein Rsph03001874

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.67Å 98.67Å 127.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 46.01 – 2.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.30) 95.4 (46.01-2.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.29Å)	Xtriage
Refinement program	XTALVIEW, REFMAC 5.1	Depositor
R, R_{free}	0.241 , 0.273 0.310 , 0.327	Depositor DCC
R_{free} test set	1387 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.5	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	0.91	EDS
Total number of atoms	2962	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: FMN, D9G

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	0.72	0/935	0.73	0/1265
1	B	0.80	3/926 (0.3%)	0.77	0/1253
1	C	0.48	0/885	0.58	0/1203
All	All	0.68	3/2746 (0.1%)	0.70	0/3721

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	ALA	C-O	8.98	1.40	1.23
1	B	20	CYS	CB-SG	-5.31	1.73	1.81
1	B	49	GLN	CD-NE2	5.17	1.45	1.32

There are no bond angle outliers.

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	918	0	896	24	1
1	B	909	0	888	27	0
1	C	869	0	823	13	1
2	A	31	0	19	0	0
2	B	31	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	19	0	0
3	A	37	0	67	0	0
3	C	39	0	71	1	0
4	A	46	0	0	5	0
4	B	30	0	0	3	0
4	C	21	0	0	1	0
All	All	2962	0	2802	60	1

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 11.

All (60) 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:B:104:TRP:HZ3	4:B:226:HOH:O	1.33	1.11
1:A:100:ARG:HH11	1:A:100:ARG:HG3	1.27	0.97
1:B:30:THR:HG22	1:B:33:ASP:H	1.34	0.92
1:A:30:THR:HG21	4:A:345:HOH:O	1.71	0.89
1:B:37:ILE:O	1:B:41:SER:HB2	1.79	0.81
1:A:100:ARG:HH11	1:A:100:ARG:CG	1.94	0.80
1:A:22:ARG:HG2	1:A:91:LEU:HD11	1.63	0.79
1:A:20:CYS:SG	1:A:62:PHE:CE2	2.80	0.74
1:B:62:PHE:CZ	1:B:64:TRP:CZ3	2.79	0.70
1:C:115:MET:HE2	1:C:118:LEU:HD12	1.81	0.63
1:A:130:GLY:HA3	4:A:350:HOH:O	1.97	0.63
1:A:30:THR:HG23	4:A:325:HOH:O	1.98	0.62
1:B:34:LEU:O	1:B:38:VAL:HG23	1.99	0.62
1:A:30:THR:HG22	1:A:33:ASP:H	1.66	0.61
1:C:21:TYR:CE1	1:C:63:GLN:HB3	2.36	0.60
1:A:100:ARG:NH1	4:A:346:HOH:O	2.35	0.59
1:B:113:ALA:O	1:B:117:SER:HB3	2.02	0.59
1:A:22:ARG:NH2	1:B:100:ARG:O	2.36	0.58
1:B:55:PHE:HD1	1:B:107:GLN:HG2	1.68	0.58
1:B:62:PHE:CZ	1:B:64:TRP:HZ3	2.20	0.58
1:A:100:ARG:NH1	1:A:100:ARG:HG3	2.08	0.57
1:B:55:PHE:CD1	1:B:107:GLN:HG2	2.39	0.57
1:B:62:PHE:HZ	1:B:64:TRP:CZ3	2.22	0.56
1:C:52:GLY:O	1:C:104:TRP:HA	2.04	0.56
1:C:124:ARG:HH11	1:C:124:ARG:HB2	1.71	0.55
1:A:13:ALA:HB3	1:A:15:HIS:CE1	2.43	0.54
1:C:33:ASP:O	1:C:37:ILE:HG13	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:THR:OG1	1:B:66:GLU:HG3	2.08	0.52
1:A:21:TYR:CE1	1:A:63:GLN:HB3	2.45	0.52
1:B:73:ALA:HB2	4:B:220:HOH:O	2.10	0.52
1:A:115:MET:HA	1:A:115:MET:CE	2.40	0.51
1:A:91:LEU:HD23	1:B:100:ARG:HG3	1.94	0.50
1:A:20:CYS:SG	1:A:62:PHE:CZ	3.03	0.50
1:B:38:VAL:HG22	1:B:106:MET:SD	2.51	0.50
1:C:58:GLN:O	1:C:58:GLN:HG3	2.12	0.49
1:A:124:ARG:C	1:A:124:ARG:HD2	2.34	0.48
1:C:125:GLN:NE2	4:C:309:HOH:O	2.46	0.48
1:A:100:ARG:HB3	1:B:22:ARG:HH12	1.79	0.48
1:B:117:SER:HA	4:B:224:HOH:O	2.15	0.47
1:B:35:LEU:O	1:B:39:GLU:HG2	2.14	0.47
1:B:53:ALA:HA	1:B:105:HIS:O	2.16	0.46
1:B:56:TYR:HB3	1:B:108:LEU:HD23	1.99	0.45
1:B:49:GLN:O	1:B:99:ARG:NH2	2.50	0.45
1:C:110:CYS:SG	1:C:115:MET:CE	3.05	0.45
1:C:111:SER:OG	1:C:114:ASP:OD1	2.30	0.44
1:A:44:HIS:HD2	1:A:47:ARG:NH1	2.15	0.44
1:C:120:LEU:HD21	3:C:301:D9G:HAJ2	1.99	0.43
1:A:68:ARG:NH2	1:C:33:ASP:OD1	2.51	0.43
1:B:56:TYR:HB3	1:B:108:LEU:CD2	2.49	0.43
1:B:16:MET:O	1:B:95:PRO:HA	2.19	0.43
1:B:50:LEU:HD13	1:B:75:VAL:HG11	2.00	0.43
1:B:40:THR:HG21	2:B:202:FMN:H4'	2.00	0.42
1:B:71:ALA:O	1:B:75:VAL:HG12	2.19	0.42
1:A:100:ARG:NH1	1:A:100:ARG:CG	2.62	0.42
1:A:96:ILE:HG22	1:A:100:ARG:NH2	2.35	0.41
1:C:124:ARG:HG3	1:C:125:GLN:N	2.35	0.41
1:A:20:CYS:SG	1:A:62:PHE:HE2	2.41	0.41
1:C:124:ARG:HH11	1:C:124:ARG:CB	2.34	0.41
1:B:62:PHE:CE1	1:B:64:TRP:HZ3	2.39	0.41
1:A:44:HIS:HE1	4:A:308:HOH:O	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:OD1	1:C:32:ARG:NH2[7_555]	2.10	0.10

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	116/121 (96%)	112 (97%)	4 (3%)	0	100 100
1	B	114/121 (94%)	109 (96%)	4 (4%)	1 (1%)	19 22
1	C	113/121 (93%)	106 (94%)	6 (5%)	1 (1%)	19 22
All	All	343/363 (94%)	327 (95%)	14 (4%)	2 (1%)	27 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	ARG
1	C	113	ALA

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	95/99 (96%)	86 (90%)	9 (10%)	9 11
1	B	95/99 (96%)	84 (88%)	11 (12%)	6 6
1	C	88/99 (89%)	81 (92%)	7 (8%)	13 16
All	All	278/297 (94%)	251 (90%)	27 (10%)	9 10

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	HIS

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Mol	Chain	Res	Type
1	A	22	ARG
1	A	30	THR
1	A	85	HIS
1	A	94	GLU
1	A	100	ARG
1	A	116	ARG
1	A	124	ARG
1	A	127	VAL
1	B	30	THR
1	B	64	TRP
1	B	77	THR
1	B	85	HIS
1	B	100	ARG
1	B	104	TRP
1	B	106	MET
1	B	107	GLN
1	B	116	ARG
1	B	122	GLU
1	B	128	THR
1	C	22	ARG
1	C	65	LEU
1	C	83	ARG
1	C	85	HIS
1	C	90	ILE
1	C	124	ARG
1	C	129	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	44	HIS
1	A	63	GLN
1	B	58	GLN
1	B	63	GLN
1	C	63	GLN
1	C	78	HIS
1	C	87	ASN

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

9 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	FMN	A	201	-	31,33,33	1.47	4 (12%)	39,50,50	1.68	7 (17%)
3	D9G	A	302	-	15,18,18	1.86	3 (20%)	18,21,21	1.69	1 (5%)
3	D9G	A	303	-	11,11,18	0.48	0	10,10,21	0.42	0
3	D9G	A	306	-	5,5,18	0.38	0	4,4,21	0.38	0
2	FMN	B	202	-	31,33,33	1.49	4 (12%)	39,50,50	1.62	6 (15%)
2	FMN	C	203	-	31,33,33	1.47	5 (16%)	39,50,50	1.62	5 (12%)
3	D9G	C	301	-	15,18,18	1.96	3 (20%)	18,21,21	1.85	2 (11%)
3	D9G	C	304	-	9,9,18	0.37	0	8,8,21	0.53	0
3	D9G	C	305	-	9,9,18	0.36	0	8,8,21	0.49	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	FMN	A	201	-	-	0/16/18/18	0/3/3/3
3	D9G	A	302	-	-	0/16/18/18	0/0/0/0
3	D9G	A	303	-	-	0/9/9/18	0/0/0/0
3	D9G	A	306	-	-	0/3/3/18	0/0/0/0
2	FMN	B	202	-	-	0/16/18/18	0/3/3/3
2	FMN	C	203	-	-	0/16/18/18	0/3/3/3
3	D9G	C	301	-	-	0/16/18/18	0/0/0/0
3	D9G	C	304	-	-	0/7/7/18	0/0/0/0
3	D9G	C	305	-	-	0/7/7/18	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	D9G	CAN-NAO	-5.69	1.40	1.52
3	A	302	D9G	CAN-NAO	-4.47	1.43	1.52
3	C	301	D9G	CAS-NAO	-3.91	1.41	1.50
3	A	302	D9G	CAS-NAO	-3.86	1.41	1.50
3	A	302	D9G	CAA-NAO	-3.76	1.41	1.50
3	C	301	D9G	CAA-NAO	-2.76	1.44	1.50
2	B	202	FMN	C5'-C4'	2.10	1.54	1.51
2	C	203	FMN	C1'-N10	2.35	1.50	1.48
2	A	201	FMN	C4-N3	2.45	1.37	1.33
2	A	201	FMN	C1'-N10	3.05	1.51	1.48
2	C	203	FMN	C4-N3	3.17	1.38	1.33
2	A	201	FMN	C4A-N5	3.25	1.38	1.33
2	C	203	FMN	C10-N1	3.26	1.37	1.33
2	C	203	FMN	C5A-N5	3.30	1.40	1.35
2	B	202	FMN	C4-N3	3.46	1.39	1.33
2	B	202	FMN	C4A-N5	3.74	1.38	1.33
2	C	203	FMN	C4A-N5	4.29	1.39	1.33
2	A	201	FMN	C10-N1	4.33	1.39	1.33
2	B	202	FMN	C10-N1	4.45	1.39	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	FMN	C4A-C4-N3	-3.19	118.93	123.47
2	B	202	FMN	C4A-C4-N3	-2.86	119.41	123.47
2	C	203	FMN	C4A-C4-N3	-2.31	120.19	123.47
2	A	201	FMN	C9A-N10-C10	-2.19	118.85	121.77
3	C	301	D9G	CAM-CAN-NAO	-2.17	110.73	115.34
2	B	202	FMN	C5A-C9A-N10	2.11	119.33	117.71
2	B	202	FMN	C4-C4A-N5	2.49	121.50	118.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	FMN	P-O5'-C5'	2.54	125.29	118.30
2	C	203	FMN	C1'-N10-C9A	2.69	120.70	118.31
2	B	202	FMN	C1'-N10-C9A	2.84	120.84	118.31
2	A	201	FMN	C5A-C9A-N10	2.98	119.98	117.71
2	A	201	FMN	C1'-N10-C9A	3.55	121.47	118.31
2	C	203	FMN	C4-C4A-N5	3.68	122.83	118.70
2	C	203	FMN	C4A-N5-C5A	3.76	120.70	116.76
2	A	201	FMN	C4A-N5-C5A	3.77	120.71	116.76
2	B	202	FMN	C4A-N5-C5A	4.57	121.55	116.76
2	A	201	FMN	C4-N3-C2	5.70	119.99	115.14
2	C	203	FMN	C4-N3-C2	5.83	120.11	115.14
2	B	202	FMN	C4-N3-C2	5.94	120.20	115.14
3	A	302	D9G	CAQ-CAP-NAO	6.09	119.63	114.64
3	C	301	D9G	CAQ-CAP-NAO	6.85	120.26	114.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	202	FMN	1	0
3	C	301	D9G	1	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.