Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:34 PM GMT

PDB ID	:	4P9S
Title	:	Crystal structure of the mature form of rat DMGDH
Authors	:	Luka, Z.; Pakhomova, S.; Loukachevitch, L.V.; Newcomer, M.E.; Wagner, C.
Deposited on	:	2014-04-04
Resolution	:	2.32 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:

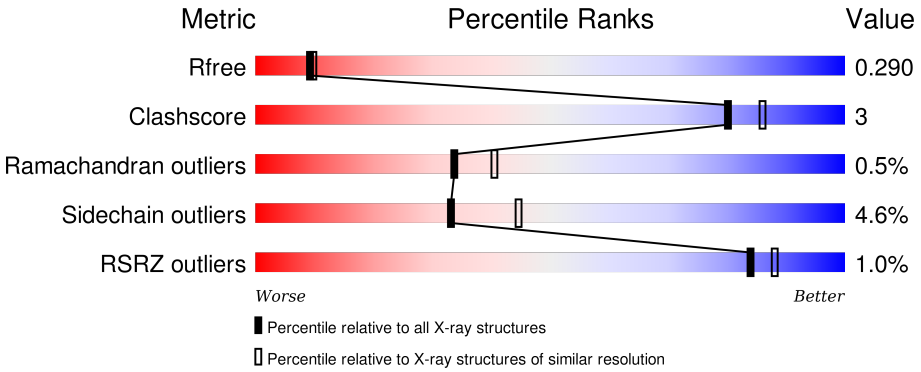
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.32 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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% 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	848	% 86% 10%
1	B	848	% 84% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13162 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.

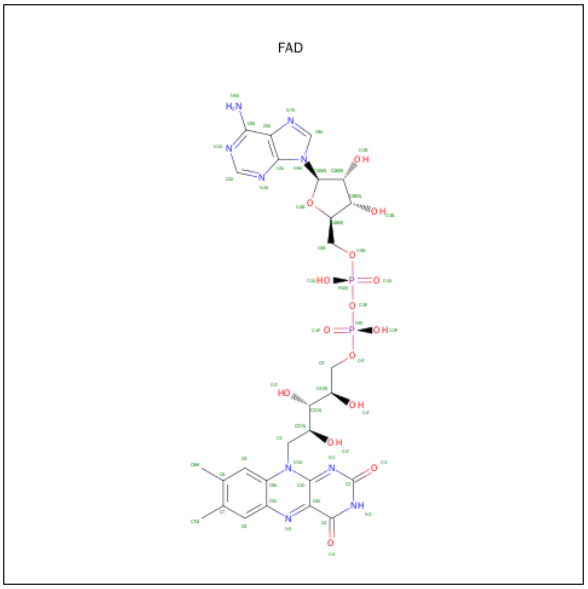
- Molecule 1 is a protein called Dimethylglycine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	816	Total	C	N	O	S	0	0	0
			6476	4143	1111	1203	19			
1	B	816	Total	C	N	O	S	0	0	0
			6476	4143	1111	1203	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	expression tag	UNP Q5RKL4
A	21	ALA	-	expression tag	UNP Q5RKL4
A	858	ALA	-	expression tag	UNP Q5RKL4
A	859	ALA	-	expression tag	UNP Q5RKL4
A	860	LEU	-	expression tag	UNP Q5RKL4
A	861	GLU	-	expression tag	UNP Q5RKL4
A	862	HIS	-	expression tag	UNP Q5RKL4
A	863	HIS	-	expression tag	UNP Q5RKL4
A	864	HIS	-	expression tag	UNP Q5RKL4
A	865	HIS	-	expression tag	UNP Q5RKL4
A	866	HIS	-	expression tag	UNP Q5RKL4
A	867	HIS	-	expression tag	UNP Q5RKL4
B	20	MET	-	expression tag	UNP Q5RKL4
B	21	ALA	-	expression tag	UNP Q5RKL4
B	858	ALA	-	expression tag	UNP Q5RKL4
B	859	ALA	-	expression tag	UNP Q5RKL4
B	860	LEU	-	expression tag	UNP Q5RKL4
B	861	GLU	-	expression tag	UNP Q5RKL4
B	862	HIS	-	expression tag	UNP Q5RKL4
B	863	HIS	-	expression tag	UNP Q5RKL4
B	864	HIS	-	expression tag	UNP Q5RKL4
B	865	HIS	-	expression tag	UNP Q5RKL4
B	866	HIS	-	expression tag	UNP Q5RKL4
B	867	HIS	-	expression tag	UNP Q5RKL4

- 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.

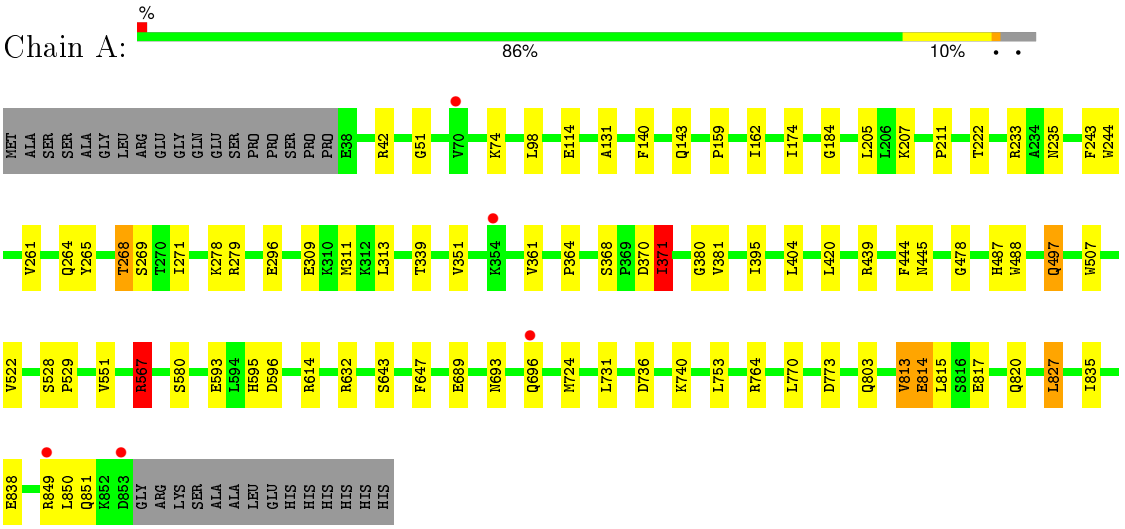
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	57	Total	O	0	0
			57	57		

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.

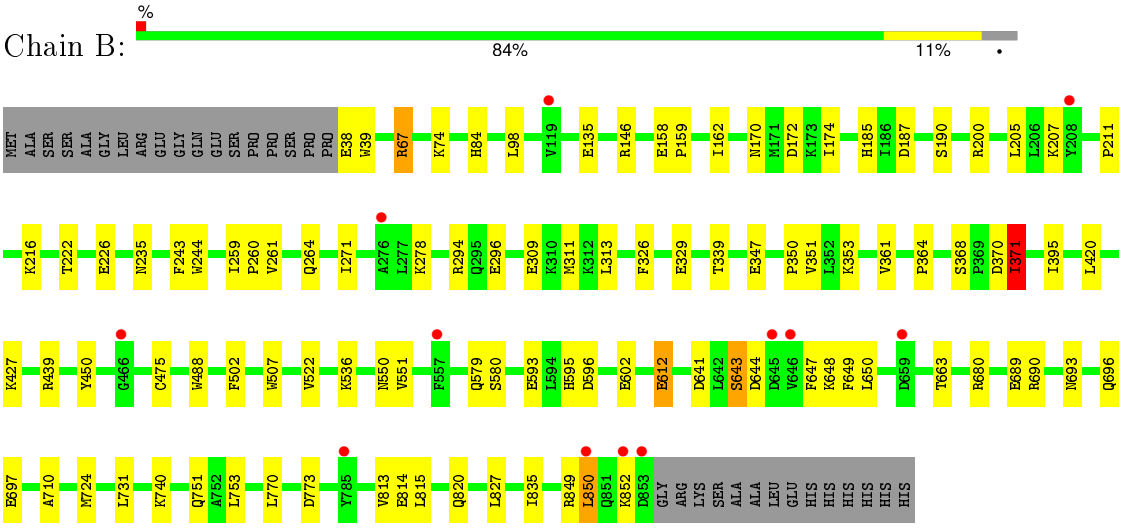
- Molecule 1: Dimethylglycine dehydrogenase

Chain A:



- Molecule 1: Dimethylglycine dehydrogenase

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	85.21Å 131.44Å 171.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.32 39.45 – 2.33	Depositor EDS
% Data completeness (in resolution range)	89.7 (40.00-2.32) 89.8 (39.45-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.71 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.253 , 0.295 0.255 , 0.290	Depositor DCC
R_{free} test set	1517 reflections (2.06%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 75123 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13162	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: 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	0.59	0/6641	0.73	2/9015 (0.0%)
1	B	0.59	0/6641	0.73	4/9015 (0.0%)
All	All	0.59	0/13282	0.73	6/18030 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	567	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	827	LEU	CA-CB-CG	5.58	128.13	115.30
1	B	850	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	146	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	200	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	B	680	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	6476	0	6409	42	0
1	B	6476	0	6409	46	0
2	A	53	0	29	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	30	2	0
3	A	47	0	0	3	0
3	B	57	0	0	1	0
All	All	13162	0	12877	87	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 3.

All (87) 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:159:PRO:HA	1:A:162:ILE:HD12	1.62	0.80
1:B:159:PRO:HA	1:B:162:ILE:HD12	1.62	0.79
1:A:271:ILE:HG21	1:A:351:VAL:CG1	2.13	0.78
1:B:271:ILE:HG21	1:B:351:VAL:CG1	2.14	0.78
1:A:268:THR:HG21	1:A:271:ILE:HD11	1.72	0.69
1:A:271:ILE:HG21	1:A:351:VAL:HG11	1.75	0.67
1:B:271:ILE:HG21	1:B:351:VAL:HG11	1.77	0.67
1:B:39:TRP:CZ3	1:B:207:LYS:HD3	2.32	0.65
1:B:595:HIS:HD2	1:B:596:ASP:OD1	1.82	0.62
1:A:595:HIS:HD2	1:A:596:ASP:OD1	1.82	0.62
1:A:98:LEU:HD21	1:A:420:LEU:HD11	1.83	0.60
1:A:205:LEU:HD11	1:A:207:LYS:HD3	1.83	0.60
1:B:271:ILE:HG21	1:B:351:VAL:HG13	1.83	0.60
1:A:271:ILE:HG21	1:A:351:VAL:HG13	1.84	0.60
1:B:98:LEU:HD21	1:B:420:LEU:HD11	1.83	0.59
1:A:567:ARG:HD2	3:A:1044:HOH:O	2.04	0.58
1:B:39:TRP:CE3	1:B:207:LYS:HD3	2.39	0.57
1:A:264:GLN:HA	1:A:361:VAL:O	2.04	0.57
1:B:264:GLN:HA	1:B:361:VAL:O	2.05	0.57
1:B:187:ASP:HB3	1:B:190:SER:OG	2.05	0.57
1:A:268:THR:HG22	1:A:269:SER:O	2.06	0.56
1:B:205:LEU:HG	1:B:207:LYS:HE3	1.88	0.55
1:A:551:VAL:HG13	1:A:740:LYS:HG3	1.89	0.55
1:A:497:GLN:H	1:A:497:GLN:HE21	1.55	0.54
1:A:296:GLU:HA	1:A:296:GLU:OE1	2.07	0.53
1:B:296:GLU:HA	1:B:296:GLU:OE1	2.08	0.53
1:B:261:VAL:O	1:B:364:PRO:HA	2.10	0.52
1:B:551:VAL:HG13	1:B:740:LYS:HG3	1.90	0.52
1:B:536:LYS:HE3	1:B:612:GLU:OE2	2.10	0.52
1:A:143:GLN:NE2	3:A:1039:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:O	1:A:364:PRO:HA	2.10	0.51
1:B:135:GLU:OE2	1:B:450:TYR:OH	2.24	0.51
1:B:488:TRP:CE2	1:B:507:TRP:HB3	2.47	0.50
1:A:820:GLN:HB3	1:A:835:ILE:HD12	1.95	0.48
1:A:488:TRP:CE2	1:A:507:TRP:HB3	2.48	0.48
1:B:74:LYS:HG3	1:B:211:PRO:HB3	1.94	0.48
1:A:370:ASP:O	1:A:371:ILE:HG22	2.15	0.47
1:A:74:LYS:HG3	1:A:211:PRO:HB3	1.96	0.46
1:B:820:GLN:HB3	1:B:835:ILE:HD12	1.98	0.46
1:B:364:PRO:O	2:B:901:FAD:HM81	2.16	0.46
1:B:502:PHE:HB3	1:B:827:LEU:HD21	1.98	0.45
1:B:162:ILE:HD13	1:B:174:ILE:HG21	1.98	0.45
1:B:326:PHE:HA	1:B:329:GLU:OE1	2.15	0.45
1:A:311:MET:SD	1:A:439:ARG:HG3	2.57	0.45
1:B:710:ALA:O	3:B:1047:HOH:O	2.20	0.45
1:B:814:GLU:HG2	1:B:815:LEU:HG	1.99	0.45
1:B:370:ASP:O	1:B:371:ILE:HG22	2.17	0.44
1:B:170:ASN:OD1	1:B:172:ASP:OD2	2.35	0.44
1:A:309:GLU:HG3	1:B:309:GLU:HG3	2.01	0.43
1:A:814:GLU:HG2	1:A:815:LEU:HG	2.00	0.43
1:A:567:ARG:HE	1:A:567:ARG:HB2	1.72	0.43
1:A:497:GLN:H	1:A:497:GLN:NE2	2.15	0.43
1:A:380:GLY:O	1:A:381:VAL:HG13	2.18	0.43
1:A:222:THR:HG22	1:A:235:ASN:HA	2.01	0.43
1:B:641:ASP:OD1	1:B:643:SER:HB2	2.19	0.43
1:B:243:PHE:CE1	1:B:244:TRP:CZ3	3.06	0.43
1:B:395:ILE:HD12	1:B:395:ILE:O	2.18	0.43
1:A:764:ARG:HD3	1:A:813:VAL:HG12	2.00	0.43
1:A:268:THR:CG2	1:A:269:SER:O	2.66	0.43
1:A:444:PHE:O	1:A:445:ASN:C	2.57	0.43
1:A:478:GLY:HA3	1:A:487:HIS:NE2	2.34	0.42
1:B:475:CYS:HB2	1:B:488:TRP:O	2.20	0.42
1:B:693:ASN:O	1:B:696:GLN:HG2	2.20	0.42
1:B:350:PRO:O	1:B:353:LYS:HG3	2.19	0.42
1:A:243:PHE:CZ	1:A:244:TRP:CZ3	3.07	0.42
1:B:311:MET:SD	1:B:439:ARG:HG3	2.59	0.42
1:A:51:GLY:HA2	3:A:1022:HOH:O	2.19	0.42
1:B:222:THR:HG22	1:B:235:ASN:HA	2.02	0.42
1:A:395:ILE:HD12	1:A:395:ILE:O	2.19	0.42
1:A:131:ALA:HB2	1:A:140:PHE:CE2	2.55	0.42
1:B:243:PHE:CE1	1:B:244:TRP:CH2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:GLN:NE2	1:B:663:THR:HG21	2.35	0.41
1:A:488:TRP:CD2	1:A:507:TRP:HB3	2.55	0.41
1:B:650:LEU:HD23	1:B:650:LEU:HA	1.90	0.41
1:B:67:ARG:CZ	1:B:67:ARG:HB3	2.50	0.41
1:A:243:PHE:CE1	1:A:244:TRP:CZ3	3.08	0.41
1:B:84:HIS:CD2	2:B:901:FAD:C7	3.04	0.41
1:A:162:ILE:HD13	1:A:174:ILE:HG21	2.02	0.41
1:B:649:PHE:O	1:B:650:LEU:HB2	2.21	0.41
1:A:265:TYR:CE2	2:A:901:FAD:HM72	2.55	0.41
1:A:693:ASN:O	1:A:696:GLN:HG2	2.21	0.41
1:B:259:ILE:HA	1:B:260:PRO:HD3	1.97	0.41
1:B:550:ASN:HD21	1:B:740:LYS:HE2	1.86	0.41
1:B:185:HIS:CD2	1:B:294:ARG:HD2	2.56	0.40
1:A:243:PHE:CE1	1:A:244:TRP:CH2	3.09	0.40
1:A:528:SER:N	1:A:529:PRO:CD	2.85	0.40
1:B:644:ASP:O	1:B:648:LYS:NZ	2.41	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	814/848 (96%)	778 (96%)	31 (4%)	5 (1%)	30	35
1	B	814/848 (96%)	784 (96%)	27 (3%)	3 (0%)	39	48
All	All	1628/1696 (96%)	1562 (96%)	58 (4%)	8 (0%)	34	40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	ILE
1	B	371	ILE

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Mol	Chain	Res	Type
1	A	593	GLU
1	B	593	GLU
1	A	522	VAL
1	A	814	GLU
1	B	522	VAL
1	A	184	GLY

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	689/714 (96%)	656 (95%)	33 (5%)	31	42
1	B	689/714 (96%)	659 (96%)	30 (4%)	35	47
All	All	1378/1428 (96%)	1315 (95%)	63 (5%)	33	44

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	114	GLU
1	A	233	ARG
1	A	268	THR
1	A	278	LYS
1	A	279	ARG
1	A	313	LEU
1	A	339	THR
1	A	368	SER
1	A	371	ILE
1	A	404	LEU
1	A	497	GLN
1	A	567	ARG
1	A	580	SER
1	A	614	ARG
1	A	632	ARG
1	A	643	SER

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Mol	Chain	Res	Type
1	A	647	PHE
1	A	689	GLU
1	A	724	MET
1	A	731	LEU
1	A	736	ASP
1	A	753	LEU
1	A	770	LEU
1	A	773	ASP
1	A	803	GLN
1	A	813	VAL
1	A	817	GLU
1	A	827	LEU
1	A	838	GLU
1	A	849	ARG
1	A	850	LEU
1	A	851	GLN
1	B	38	GLU
1	B	67	ARG
1	B	158	GLU
1	B	216	LYS
1	B	226	GLU
1	B	278	LYS
1	B	313	LEU
1	B	339	THR
1	B	347	GLU
1	B	368	SER
1	B	371	ILE
1	B	427	LYS
1	B	580	SER
1	B	602	GLU
1	B	612	GLU
1	B	643	SER
1	B	647	PHE
1	B	689	GLU
1	B	690	ARG
1	B	697	GLU
1	B	724	MET
1	B	731	LEU
1	B	751	GLN
1	B	753	LEU
1	B	770	LEU
1	B	773	ASP

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Mol	Chain	Res	Type
1	B	813	VAL
1	B	849	ARG
1	B	850	LEU
1	B	852	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	497	GLN
1	A	579	GLN
1	A	595	HIS
1	A	803	GLN
1	B	150	HIS
1	B	462	GLN
1	B	579	GLN
1	B	595	HIS

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

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	901	1	48,58,58	1.33	10 (20%)	54,89,89	2.44	14 (25%)
2	FAD	B	901	1	48,58,58	1.37	7 (14%)	54,89,89	2.15	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	901	1	-	0/30/50/50	0/6/6/6
2	FAD	B	901	1	-	0/30/50/50	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	FAD	C1'-N10	-3.76	1.44	1.48
2	A	901	FAD	C1'-N10	-3.55	1.44	1.48
2	A	901	FAD	C5A-N7A	-2.08	1.32	1.39
2	A	901	FAD	C8-C7	2.02	1.46	1.41
2	A	901	FAD	O4B-C1B	2.11	1.43	1.41
2	A	901	FAD	C4-C4X	2.18	1.45	1.41
2	A	901	FAD	C9A-C5X	2.26	1.47	1.42
2	B	901	FAD	C8-C7	2.36	1.47	1.41
2	A	901	FAD	C10-N10	2.43	1.42	1.39
2	B	901	FAD	C4-C4X	2.44	1.46	1.41
2	A	901	FAD	C5A-C4A	2.57	1.46	1.40
2	B	901	FAD	C9A-C5X	2.78	1.48	1.42
2	A	901	FAD	C9A-N10	2.78	1.42	1.38
2	B	901	FAD	C5A-C4A	3.02	1.47	1.40
2	B	901	FAD	C2A-N3A	3.17	1.37	1.32
2	B	901	FAD	C4X-C10	3.32	1.47	1.41
2	A	901	FAD	C4X-C10	3.70	1.47	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	FAD	N3A-C2A-N1A	-7.95	122.81	128.89
2	B	901	FAD	N3A-C2A-N1A	-7.73	122.98	128.89
2	A	901	FAD	C4X-C10-N10	-5.65	117.19	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	FAD	C4-C4X-C10	-5.07	116.70	119.94
2	B	901	FAD	C4A-C5A-N7A	-4.07	105.73	109.48
2	A	901	FAD	C2B-C1B-N9A	-3.85	108.41	114.29
2	A	901	FAD	C4B-O4B-C1B	-3.82	105.52	109.72
2	A	901	FAD	C4X-C4-N3	-3.75	118.47	123.59
2	B	901	FAD	C4X-C10-N10	-3.52	118.44	120.52
2	B	901	FAD	C4X-C4-N3	-2.54	120.12	123.59
2	B	901	FAD	C1'-C2'-C3'	-2.31	103.21	109.82
2	B	901	FAD	O2'-C2'-C1'	-2.28	104.33	109.94
2	A	901	FAD	C9A-C5X-N5	-2.17	119.15	122.36
2	A	901	FAD	C2A-N1A-C6A	2.15	122.61	118.77
2	A	901	FAD	O4B-C4B-C3B	2.33	109.84	105.15
2	A	901	FAD	N6A-C6A-N1A	2.62	124.84	119.20
2	A	901	FAD	C1'-N10-C9A	3.06	122.30	118.86
2	B	901	FAD	C4-C4X-N5	3.14	122.53	118.72
2	B	901	FAD	C1'-N10-C9A	3.53	122.82	118.86
2	A	901	FAD	C4X-N5-C5X	3.54	120.84	116.76
2	B	901	FAD	C4X-N5-C5X	4.29	121.69	116.76
2	A	901	FAD	O4B-C1B-N9A	4.31	117.11	108.10
2	A	901	FAD	C5X-C9A-N10	5.03	121.44	117.62
2	B	901	FAD	C4-N3-C2	6.71	121.05	115.25
2	A	901	FAD	C4-N3-C2	7.18	121.45	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	FAD	1	0
2	B	901	FAD	2	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	816/848 (96%)	0.08	5 (0%) 90 93	16, 28, 45, 81	0
1	B	816/848 (96%)	0.17	12 (1%) 76 82	16, 30, 50, 83	0
All	All	1632/1696 (96%)	0.12	17 (1%) 84 88	16, 29, 48, 83	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	853	ASP	4.6
1	B	850	LEU	4.2
1	A	696	GLN	3.3
1	B	557	PHE	3.1
1	A	853	ASP	2.9
1	B	466	GLY	2.7
1	A	354	LYS	2.7
1	B	646	VAL	2.7
1	B	659	ASP	2.3
1	B	119	VAL	2.3
1	B	645	ASP	2.3
1	B	852	LYS	2.3
1	B	208	TYR	2.2
1	B	785	TYR	2.2
1	A	849	ARG	2.2
1	B	276	ALA	2.1
1	A	70	VAL	2.1

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 (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
2	FAD	A	901	53/53	0.94	0.14	0.11	19,23,26,29	0
2	FAD	B	901	53/53	0.96	0.10	-1.07	15,18,21,25	0

6.5 Other polymers (i)

There are no such residues in this entry.