



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:47 PM GMT

PDB ID : 4G6H
Title : Crystal structure of NDH with NADH
Authors : Li, W.; Feng, Y.; Ge, J.; Yang, M.
Deposited on : 2012-07-19
Resolution : 2.26 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 ⓘ 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 (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

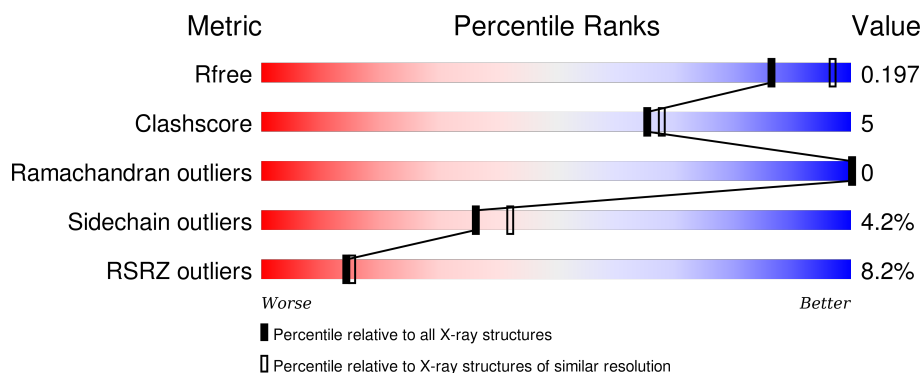
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 $\leq 5\%$. 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	502	
1	B	502	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	B	602	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8221 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 Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3738	2415	635	683	5			
1	B	472	Total	C	N	O	S	0	0	0
			3738	2415	635	683	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	EXPRESSION TAG	UNP P32340
A	13	ARG	-	EXPRESSION TAG	UNP P32340
A	14	GLY	-	EXPRESSION TAG	UNP P32340
A	15	SER	-	EXPRESSION TAG	UNP P32340
A	16	HIS	-	EXPRESSION TAG	UNP P32340
A	17	HIS	-	EXPRESSION TAG	UNP P32340
A	18	HIS	-	EXPRESSION TAG	UNP P32340
A	19	HIS	-	EXPRESSION TAG	UNP P32340
A	20	HIS	-	EXPRESSION TAG	UNP P32340
A	21	HIS	-	EXPRESSION TAG	UNP P32340
A	22	GLY	-	EXPRESSION TAG	UNP P32340
A	23	SER	-	EXPRESSION TAG	UNP P32340
B	12	MET	-	EXPRESSION TAG	UNP P32340
B	13	ARG	-	EXPRESSION TAG	UNP P32340
B	14	GLY	-	EXPRESSION TAG	UNP P32340
B	15	SER	-	EXPRESSION TAG	UNP P32340
B	16	HIS	-	EXPRESSION TAG	UNP P32340
B	17	HIS	-	EXPRESSION TAG	UNP P32340
B	18	HIS	-	EXPRESSION TAG	UNP P32340
B	19	HIS	-	EXPRESSION TAG	UNP P32340
B	20	HIS	-	EXPRESSION TAG	UNP P32340
B	21	HIS	-	EXPRESSION TAG	UNP P32340
B	22	GLY	-	EXPRESSION TAG	UNP P32340
B	23	SER	-	EXPRESSION TAG	UNP P32340

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- The chemical structure of FAD (Flavin Adenine Dinucleotide) is shown. It consists of an adenine base (blue) linked to a ribose sugar (red), which is connected via a pyrophosphate bridge (red) to another ribose sugar (red) linked to a riboflavin moiety (blue). The structure is labeled with atom numbers and includes stereochemical indicators (wedges and dashes) for the ribose sugars.

The chemical structure of NAI (Nucleoside Analog Inhibitor) is a complex molecule. It features a purine base (adenine) linked to a ribose sugar, which is further linked to a phosphate group. The phosphate group is connected to a nucleoside moiety, which consists of a ribose sugar and a nucleobase (cytosine). The structure is shown with various stereochemical configurations and atom labels.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mg	0	0
			3	3		
4	A	3	Total	Mg	0	0
			3	3		

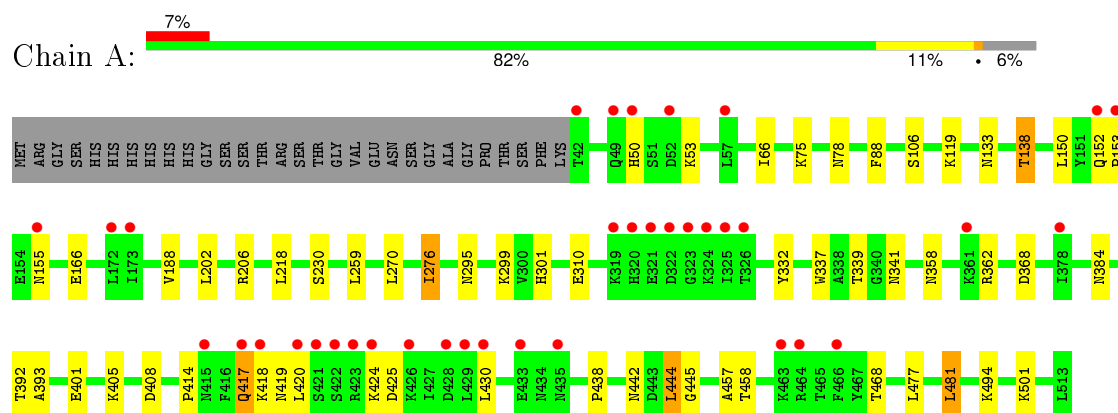
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	275	Total	O	0	0
			275	275		
5	B	270	Total	O	0	0
			270	270		

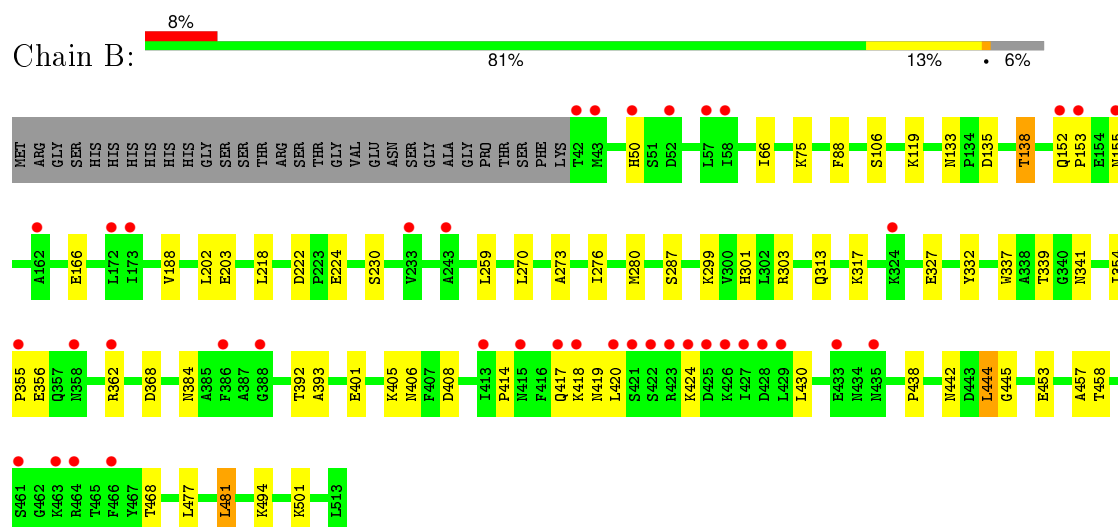
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial



- Molecule 1: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	126.19Å 229.59Å 111.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.15 – 2.26 29.89 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.15-2.26) 99.9 (29.89-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.193 , 0.225 0.195 , 0.197	Depositor DCC
R_{free} test set	3820 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.7	EDS
Estimated twinning fraction	0.003 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 77137 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8221	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, NAI, 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	0.51	0/3824	0.65	3/5177 (0.1%)
1	B	0.53	1/3824 (0.0%)	0.66	3/5177 (0.1%)
All	All	0.52	1/7648 (0.0%)	0.66	6/10354 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	CG-CD	5.16	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	ARG	NE-CZ-NH1	-13.09	113.76	120.30
1	B	362	ARG	NE-CZ-NH2	12.55	126.58	120.30
1	A	362	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	A	362	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	B	362	ARG	CD-NE-CZ	6.14	132.19	123.60
1	A	362	ARG	CD-NE-CZ	5.86	131.81	123.60

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	3738	0	3803	32	0
1	B	3738	0	3803	32	1
2	A	53	0	31	3	0
2	B	53	0	31	3	0
3	A	44	0	27	10	0
3	B	44	0	27	7	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	275	0	0	15	0
5	B	270	0	0	10	0
All	All	8221	0	7722	77	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 5.

All (77) 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:419:ASN:O	5:A:729:HOH:O	1.88	0.91
1:A:392:THR:HG22	3:A:602:NAI:H5N	1.62	0.81
1:B:392:THR:HG22	3:B:604:NAI:H5N	1.62	0.81
1:A:341:ASN:ND2	3:A:602:NAI:O3D	2.16	0.78
1:B:406:ASN:OD1	5:B:935:HOH:O	2.01	0.78
3:A:602:NAI:O2A	5:A:815:HOH:O	2.02	0.77
1:B:368:ASP:HB3	1:B:438:PRO:HB3	1.68	0.76
1:A:425:ASP:OD1	5:A:945:HOH:O	2.02	0.75
1:A:295:ASN:OD1	5:A:784:HOH:O	2.04	0.75
1:B:224:GLU:OE1	5:B:894:HOH:O	2.08	0.71
1:B:222:ASP:O	5:B:742:HOH:O	2.07	0.71
1:A:138:THR:HG21	1:A:166:GLU:OE1	1.90	0.71
1:B:453:GLU:OE1	5:B:881:HOH:O	2.08	0.71
1:A:438:PRO:O	5:A:808:HOH:O	2.08	0.70
1:B:138:THR:HG21	1:B:166:GLU:OE1	1.93	0.68
1:A:368:ASP:HB3	1:A:438:PRO:HB3	1.75	0.68
3:B:604:NAI:O2A	5:B:831:HOH:O	2.12	0.67
1:A:75:LYS:HE3	1:A:119:LYS:HD2	1.77	0.66
1:B:75:LYS:HE3	1:B:119:LYS:HD2	1.77	0.66
1:B:152:GLN:HB2	1:B:153:PRO:HD3	1.79	0.65
1:A:152:GLN:HB2	1:A:153:PRO:HD3	1.80	0.63
1:B:341:ASN:ND2	3:B:604:NAI:O3D	2.31	0.63
1:A:310:GLU:OE2	5:A:898:HOH:O	2.16	0.61
1:A:358:ASN:ND2	5:A:910:HOH:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASN:HB2	1:B:138:THR:HG22	1.83	0.60
1:A:133:ASN:HB2	1:A:138:THR:HG22	1.84	0.60
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.84	0.60
1:B:313:GLN:OE1	5:B:968:HOH:O	2.16	0.60
3:A:602:NAI:H2D	5:A:774:HOH:O	2.02	0.60
1:B:477:LEU:HG	1:B:481:LEU:HD22	1.85	0.59
1:B:419:ASN:ND2	1:B:424:LYS:O	2.37	0.57
3:A:602:NAI:H3D	5:A:774:HOH:O	2.05	0.56
1:A:299:LYS:HD3	1:A:301:HIS:NE2	2.21	0.56
3:A:602:NAI:C2D	5:A:774:HOH:O	2.54	0.55
1:A:417:GLN:NE2	5:A:919:HOH:O	1.91	0.55
1:B:299:LYS:HD3	1:B:301:HIS:NE2	2.22	0.54
1:B:106:SER:HA	1:B:494:LYS:HE3	1.89	0.54
1:A:337:TRP:HE1	1:A:339:THR:HG1	1.56	0.53
1:A:419:ASN:ND2	1:A:424:LYS:O	2.40	0.52
3:A:602:NAI:C3D	5:A:774:HOH:O	2.59	0.50
3:B:604:NAI:C3D	5:B:888:HOH:O	2.59	0.50
1:B:66:ILE:HG13	1:B:88:PHE:HB2	1.96	0.47
1:B:445:GLY:HA3	1:B:458:THR:O	2.13	0.47
1:A:106:SER:HA	1:A:494:LYS:HE3	1.96	0.47
2:A:601:FAD:C10	3:A:602:NAI:H42N	2.44	0.47
1:B:401:GLU:O	1:B:405:LYS:HG2	2.15	0.46
1:B:337:TRP:HE1	1:B:339:THR:HG1	1.63	0.46
1:A:401:GLU:O	1:A:405:LYS:HG2	2.15	0.46
1:A:206:ARG:HD2	5:A:924:HOH:O	2.16	0.46
1:A:393:ALA:HB2	2:A:601:FAD:H2'	1.97	0.46
1:A:66:ILE:HG13	1:A:88:PHE:HB2	1.98	0.46
1:A:230:SER:OG	1:A:332:TYR:HA	2.17	0.44
1:B:135:ASP:N	5:B:916:HOH:O	2.34	0.44
3:A:602:NAI:H1D	5:A:770:HOH:O	2.18	0.43
1:A:405:LYS:O	1:A:408:ASP:HB2	2.18	0.43
1:A:206:ARG:NH1	5:A:924:HOH:O	1.88	0.43
3:B:604:NAI:O1A	5:B:868:HOH:O	2.21	0.43
1:B:457:ALA:O	1:B:468:THR:HA	2.19	0.43
1:A:445:GLY:HA3	1:A:458:THR:O	2.19	0.43
1:B:230:SER:OG	1:B:332:TYR:HA	2.19	0.42
1:A:442:ASN:O	1:A:444:LEU:HD13	2.19	0.42
1:B:356:GLU:OE1	1:B:356:GLU:N	2.44	0.42
1:B:414:PRO:O	1:B:418:LYS:HG3	2.20	0.42
1:A:414:PRO:O	1:A:418:LYS:HG3	2.20	0.41
1:B:393:ALA:HB2	2:B:605:FAD:H2'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASN:ND2	5:B:963:HOH:O	2.41	0.41
1:B:354:ILE:HA	1:B:355:PRO:HD3	1.93	0.41
3:B:604:NAI:H42N	2:B:605:FAD:C10	2.51	0.41
1:B:317:LYS:HG2	1:B:327:GLU:HG2	2.03	0.41
1:A:276:ILE:HD13	1:A:276:ILE:H	1.85	0.41
1:B:273:ALA:O	1:B:303:ARG:HA	2.21	0.41
3:B:604:NAI:H42N	2:B:605:FAD:C4X	2.51	0.40
2:A:601:FAD:C4X	3:A:602:NAI:H42N	2.51	0.40
1:B:405:LYS:O	1:B:408:ASP:HB2	2.21	0.40
1:B:442:ASN:O	1:B:444:LEU:HD13	2.21	0.40
1:A:53:LYS:HD2	1:A:78:ASN:OD1	2.22	0.40
1:A:457:ALA:O	1:A:468:THR:HA	2.22	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:B:287:SER:OG	1:B:287:SER:OG[3_454]	2.19	0.01

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	470/502 (94%)	457 (97%)	13 (3%)	0	100	100
1	B	470/502 (94%)	455 (97%)	15 (3%)	0	100	100
All	All	940/1004 (94%)	912 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	403/427 (94%)	386 (96%)	17 (4%)	36	42
1	B	403/427 (94%)	386 (96%)	17 (4%)	36	42
All	All	806/854 (94%)	772 (96%)	34 (4%)	36	42

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	138	THR
1	A	150	LEU
1	A	155	ASN
1	A	188	VAL
1	A	202	LEU
1	A	218	LEU
1	A	259	LEU
1	A	270	LEU
1	A	276	ILE
1	A	384	ASN
1	A	417	GLN
1	A	420	LEU
1	A	430	LEU
1	A	444	LEU
1	A	481	LEU
1	A	501	LYS
1	B	50	HIS
1	B	138	THR
1	B	155	ASN
1	B	188	VAL
1	B	202	LEU
1	B	218	LEU
1	B	259	LEU
1	B	270	LEU
1	B	276	ILE
1	B	280	MET

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Mol	Chain	Res	Type
1	B	384	ASN
1	B	417	GLN
1	B	420	LEU
1	B	430	LEU
1	B	444	LEU
1	B	481	LEU
1	B	501	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	B	341	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 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
2	FAD	A	601	-	48,58,58	1.13	4 (8%)	54,89,89	2.39	11 (20%)
3	NAI	A	602	-	38,48,48	1.23	3 (7%)	48,73,73	1.59	5 (10%)
3	NAI	B	604	-	38,48,48	1.24	3 (7%)	48,73,73	1.61	5 (10%)
2	FAD	B	605	-	48,58,58	1.21	5 (10%)	54,89,89	2.39	9 (16%)

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	601	-	-	0/30/50/50	0/6/6/6
3	NAI	A	602	-	-	0/25/72/72	0/5/5/5
3	NAI	B	604	-	-	0/25/72/72	0/5/5/5
2	FAD	B	605	-	-	0/30/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	604	NAI	C4N-C5N	-4.64	1.39	1.49
3	A	602	NAI	C4N-C5N	-4.56	1.39	1.49
2	A	601	FAD	C4-N3	2.22	1.37	1.33
2	B	605	FAD	C10-N1	2.38	1.39	1.35
2	A	601	FAD	C2A-N1A	2.60	1.38	1.33
2	A	601	FAD	C4X-N5	2.64	1.37	1.33
2	B	605	FAD	C4-N3	2.64	1.38	1.33
2	B	605	FAD	C2A-N1A	2.67	1.39	1.33
3	B	604	NAI	C5A-C4A	2.92	1.47	1.40
3	A	602	NAI	C5A-C4A	3.00	1.47	1.40
3	B	604	NAI	C6N-C5N	3.13	1.39	1.33
3	A	602	NAI	C6N-C5N	3.13	1.39	1.33
2	B	605	FAD	C2A-N3A	3.13	1.37	1.32
2	A	601	FAD	C2A-N3A	3.27	1.38	1.32
2	B	605	FAD	C4X-N5	3.69	1.39	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	N3A-C2A-N1A	-13.29	118.72	128.89
2	B	605	FAD	N3A-C2A-N1A	-12.57	119.27	128.89
3	B	604	NAI	N3A-C2A-N1A	-6.87	123.64	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAI	N3A-C2A-N1A	-6.81	123.68	128.89
3	B	604	NAI	PN-O3-PA	-4.28	120.70	132.73
3	A	602	NAI	PN-O3-PA	-4.13	121.14	132.73
3	B	604	NAI	C4A-C5A-N7A	-3.33	106.42	109.48
2	A	601	FAD	P-O3P-PA	-3.31	123.43	132.73
3	A	602	NAI	C4A-C5A-N7A	-3.30	106.44	109.48
2	A	601	FAD	C1B-N9A-C4A	-3.26	122.03	126.94
2	B	605	FAD	P-O3P-PA	-3.21	123.72	132.73
2	B	605	FAD	C4X-C4-N3	-3.14	119.30	123.59
2	A	601	FAD	C4X-C4-N3	-3.05	119.42	123.59
2	B	605	FAD	C4X-C10-N10	-2.97	118.77	120.52
2	B	605	FAD	C4A-C5A-N7A	-2.57	107.12	109.48
2	B	605	FAD	C9A-C5X-N5	-2.29	118.96	122.36
2	A	601	FAD	C4A-C5A-N7A	-2.11	107.54	109.48
2	A	601	FAD	C4-C4X-C10	2.09	121.28	119.94
3	A	602	NAI	C3D-C2D-C1D	2.12	105.66	101.40
3	B	604	NAI	C5N-C4N-C3N	2.20	118.59	112.52
3	A	602	NAI	C5N-C4N-C3N	2.23	118.66	112.52
2	A	601	FAD	O3'-C3'-C2'	2.36	114.69	108.75
3	B	604	NAI	C3D-C2D-C1D	2.45	106.33	101.40
2	B	605	FAD	C4X-N5-C5X	3.21	120.45	116.76
2	A	601	FAD	C1'-N10-C9A	3.25	122.51	118.86
2	A	601	FAD	C4X-N5-C5X	3.25	120.50	116.76
2	A	601	FAD	C5X-C9A-N10	3.47	120.26	117.62
2	B	605	FAD	C5X-C9A-N10	4.27	120.86	117.62
2	A	601	FAD	C4-N3-C2	4.40	119.05	115.25
2	B	605	FAD	C4-N3-C2	6.54	120.90	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	3	0
3	A	602	NAI	10	0
3	B	604	NAI	7	0
2	B	605	FAD	3	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, 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(Å ²)	Q<0.9
1	A	472/502 (94%)	0.08	37 (7%)	16 17	20, 34, 75, 103	0
1	B	472/502 (94%)	0.15	40 (8%)	13 14	20, 35, 76, 103	0
All	All	944/1004 (94%)	0.12	77 (8%)	14 15	20, 35, 76, 103	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	GLN	8.9
1	B	423	ARG	7.7
1	A	152	GLN	7.4
1	B	463	LYS	7.4
1	B	420	LEU	5.8
1	B	421	SER	5.4
1	A	324	LYS	5.3
1	A	50	HIS	5.3
1	B	422	SER	5.2
1	B	358	ASN	5.1
1	B	424	LYS	5.1
1	A	42	THR	4.9
1	B	42	THR	4.6
1	A	418	LYS	4.5
1	A	433	GLU	4.5
1	B	162	ALA	4.4
1	B	425	ASP	4.4
1	A	155	ASN	4.4
1	A	49	GLN	4.3
1	B	427	ILE	4.3
1	B	52	ASP	4.1
1	B	429	LEU	4.0
1	A	322	ASP	3.9
1	A	463	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	326	THR	3.8
1	A	424	LYS	3.7
1	B	426	LYS	3.7
1	A	423	ARG	3.6
1	A	52	ASP	3.6
1	B	155	ASN	3.6
1	A	417	GLN	3.5
1	A	321	GLU	3.5
1	A	429	LEU	3.5
1	B	153	PRO	3.4
1	B	362	ARG	3.3
1	A	421	SER	3.3
1	B	435	ASN	3.3
1	B	433	GLU	3.3
1	A	422	SER	3.2
1	A	320	HIS	3.1
1	A	378	ILE	3.0
1	A	464	ARG	3.0
1	A	153	PRO	2.9
1	A	319	LYS	2.9
1	B	415	ASN	2.9
1	A	323	GLY	2.9
1	A	426	LYS	2.9
1	B	418	LYS	2.9
1	A	428	ASP	2.9
1	A	466	PHE	2.9
1	A	172	LEU	2.9
1	B	428	ASP	2.9
1	B	417	GLN	2.8
1	A	420	LEU	2.7
1	B	464	ARG	2.7
1	B	386	PHE	2.6
1	A	57	LEU	2.5
1	B	172	LEU	2.5
1	A	415	ASN	2.5
1	B	388	GLY	2.4
1	B	413	ILE	2.4
1	B	58	ILE	2.4
1	A	325	ILE	2.4
1	B	50	HIS	2.4
1	B	243	ALA	2.4
1	B	43	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	466	PHE	2.3
1	B	461	SER	2.3
1	A	435	ASN	2.3
1	A	173	ILE	2.2
1	A	361	LYS	2.2
1	B	324	LYS	2.2
1	B	355	PRO	2.2
1	B	233	VAL	2.1
1	B	173	ILE	2.1
1	B	57	LEU	2.1
1	A	430	LEU	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	B	602	1/1	0.99	0.15	2.02	20,20,20,20	0
3	NAI	B	604	44/44	0.92	0.14	0.54	26,42,63,65	0
3	NAI	A	602	44/44	0.93	0.14	0.27	34,44,60,66	0
4	MG	B	603	1/1	0.93	0.12	0.13	50,50,50,50	0
2	FAD	B	605	53/53	0.98	0.14	0.12	21,28,33,41	0
4	MG	A	603	1/1	0.96	0.11	-0.20	34,34,34,34	0
2	FAD	A	601	53/53	0.98	0.12	-0.25	17,23,31,35	0
4	MG	A	604	1/1	0.96	0.09	-0.49	46,46,46,46	0
4	MG	A	605	1/1	0.81	0.12	-0.65	71,71,71,71	0
4	MG	B	601	1/1	0.82	0.34	-	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.