Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:27 PM GMT

PDB ID	:	4OYR
Title	:	Competition of the small inhibitor PT91 with large fatty acyl substrate of the Mycobacterium tuberculosis enoyl-ACP reductase InhA by induced substrate-binding loop refolding
Authors	:	Li, H.J.; Pan, P.; Lai, C.T.; Liu, N.; Garcia-Diaz, M.; Simmerling, C.; Tonge, P.J.
Deposited on	:	2014-02-13
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
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:

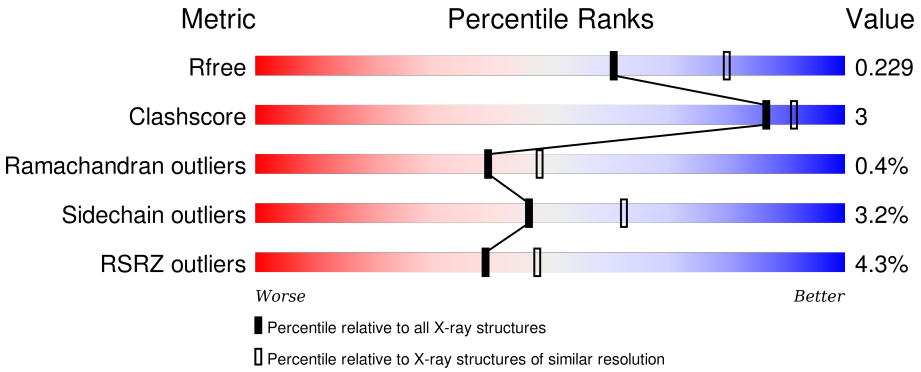
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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% 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	289	3% 83% 10% 8%
1	B	289	% 85% 7% 8%
1	C	289	7% 86% 7% 7%
1	D	289	4% 82% 5% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7944 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	3	0
			1967	1258	334	365	10			
1	B	267	Total	C	N	O	S	0	0	0
			1942	1234	339	359	10			
1	C	268	Total	C	N	O	S	0	6	0
			1932	1232	339	350	11			
1	D	254	Total	C	N	O	S	0	2	3
			1738	1111	307	309	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P0A5Y6
A	-18	GLY	-	expression tag	UNP P0A5Y6
A	-17	SER	-	expression tag	UNP P0A5Y6
A	-16	SER	-	expression tag	UNP P0A5Y6
A	-15	HIS	-	expression tag	UNP P0A5Y6
A	-14	HIS	-	expression tag	UNP P0A5Y6
A	-13	HIS	-	expression tag	UNP P0A5Y6
A	-12	HIS	-	expression tag	UNP P0A5Y6
A	-11	HIS	-	expression tag	UNP P0A5Y6
A	-10	HIS	-	expression tag	UNP P0A5Y6
A	-9	SER	-	expression tag	UNP P0A5Y6
A	-8	SER	-	expression tag	UNP P0A5Y6
A	-7	GLY	-	expression tag	UNP P0A5Y6
A	-6	LEU	-	expression tag	UNP P0A5Y6
A	-5	VAL	-	expression tag	UNP P0A5Y6
A	-4	PRO	-	expression tag	UNP P0A5Y6
A	-3	ARG	-	expression tag	UNP P0A5Y6
A	-2	GLY	-	expression tag	UNP P0A5Y6
A	-1	SER	-	expression tag	UNP P0A5Y6
A	0	HIS	-	expression tag	UNP P0A5Y6
B	-19	MET	-	expression tag	UNP P0A5Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P0A5Y6
B	-17	SER	-	expression tag	UNP P0A5Y6
B	-16	SER	-	expression tag	UNP P0A5Y6
B	-15	HIS	-	expression tag	UNP P0A5Y6
B	-14	HIS	-	expression tag	UNP P0A5Y6
B	-13	HIS	-	expression tag	UNP P0A5Y6
B	-12	HIS	-	expression tag	UNP P0A5Y6
B	-11	HIS	-	expression tag	UNP P0A5Y6
B	-10	HIS	-	expression tag	UNP P0A5Y6
B	-9	SER	-	expression tag	UNP P0A5Y6
B	-8	SER	-	expression tag	UNP P0A5Y6
B	-7	GLY	-	expression tag	UNP P0A5Y6
B	-6	LEU	-	expression tag	UNP P0A5Y6
B	-5	VAL	-	expression tag	UNP P0A5Y6
B	-4	PRO	-	expression tag	UNP P0A5Y6
B	-3	ARG	-	expression tag	UNP P0A5Y6
B	-2	GLY	-	expression tag	UNP P0A5Y6
B	-1	SER	-	expression tag	UNP P0A5Y6
B	0	HIS	-	expression tag	UNP P0A5Y6
C	-19	MET	-	expression tag	UNP P0A5Y6
C	-18	GLY	-	expression tag	UNP P0A5Y6
C	-17	SER	-	expression tag	UNP P0A5Y6
C	-16	SER	-	expression tag	UNP P0A5Y6
C	-15	HIS	-	expression tag	UNP P0A5Y6
C	-14	HIS	-	expression tag	UNP P0A5Y6
C	-13	HIS	-	expression tag	UNP P0A5Y6
C	-12	HIS	-	expression tag	UNP P0A5Y6
C	-11	HIS	-	expression tag	UNP P0A5Y6
C	-10	HIS	-	expression tag	UNP P0A5Y6
C	-9	SER	-	expression tag	UNP P0A5Y6
C	-8	SER	-	expression tag	UNP P0A5Y6
C	-7	GLY	-	expression tag	UNP P0A5Y6
C	-6	LEU	-	expression tag	UNP P0A5Y6
C	-5	VAL	-	expression tag	UNP P0A5Y6
C	-4	PRO	-	expression tag	UNP P0A5Y6
C	-3	ARG	-	expression tag	UNP P0A5Y6
C	-2	GLY	-	expression tag	UNP P0A5Y6
C	-1	SER	-	expression tag	UNP P0A5Y6
C	0	HIS	-	expression tag	UNP P0A5Y6
D	-19	MET	-	expression tag	UNP P0A5Y6
D	-18	GLY	-	expression tag	UNP P0A5Y6
D	-17	SER	-	expression tag	UNP P0A5Y6

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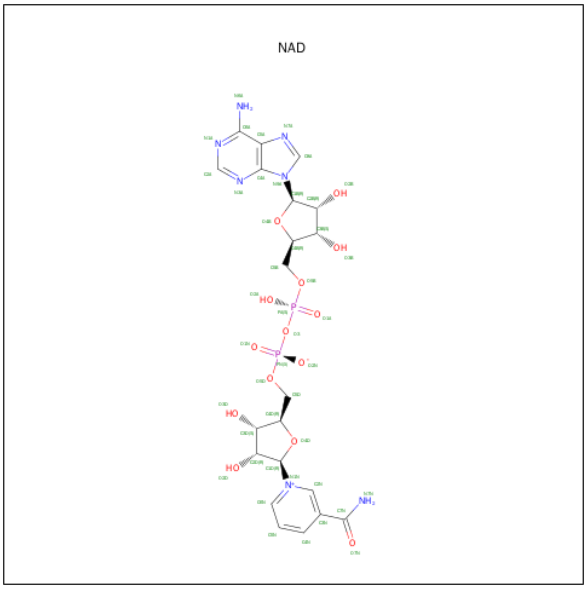
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P0A5Y6
D	-15	HIS	-	expression tag	UNP P0A5Y6
D	-14	HIS	-	expression tag	UNP P0A5Y6
D	-13	HIS	-	expression tag	UNP P0A5Y6
D	-12	HIS	-	expression tag	UNP P0A5Y6
D	-11	HIS	-	expression tag	UNP P0A5Y6
D	-10	HIS	-	expression tag	UNP P0A5Y6
D	-9	SER	-	expression tag	UNP P0A5Y6
D	-8	SER	-	expression tag	UNP P0A5Y6
D	-7	GLY	-	expression tag	UNP P0A5Y6
D	-6	LEU	-	expression tag	UNP P0A5Y6
D	-5	VAL	-	expression tag	UNP P0A5Y6
D	-4	PRO	-	expression tag	UNP P0A5Y6
D	-3	ARG	-	expression tag	UNP P0A5Y6
D	-2	GLY	-	expression tag	UNP P0A5Y6
D	-1	SER	-	expression tag	UNP P0A5Y6
D	0	HIS	-	expression tag	UNP P0A5Y6

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

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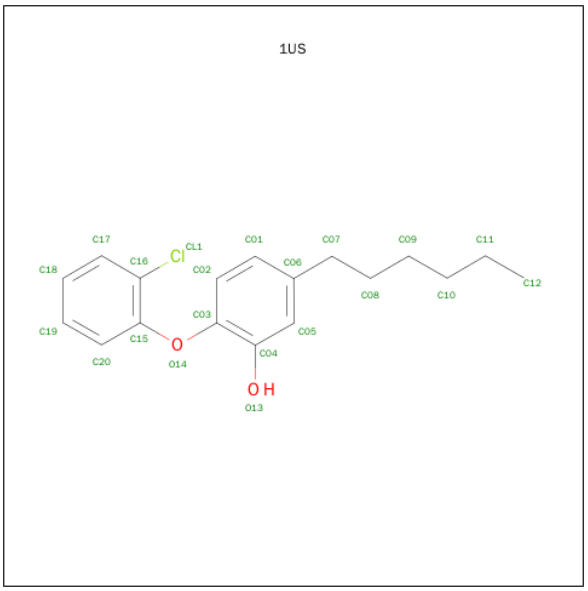
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 2-(2-chloranylphenoxy)-5-hexyl-phenol (three-letter code: 1US) (formula: $C_{18}H_{21}ClO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			19	16	1	2		
3	B	1	Total	C	Cl	O	0	0
			20	17	1	2		
3	C	1	Total	C	Cl	O	0	0
			19	16	1	2		
3	D	1	Total	C	Cl	O	0	0
			20	17	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	31	Total	O	0	0
			31	31		
4	C	28	Total	O	0	0
			28	28		

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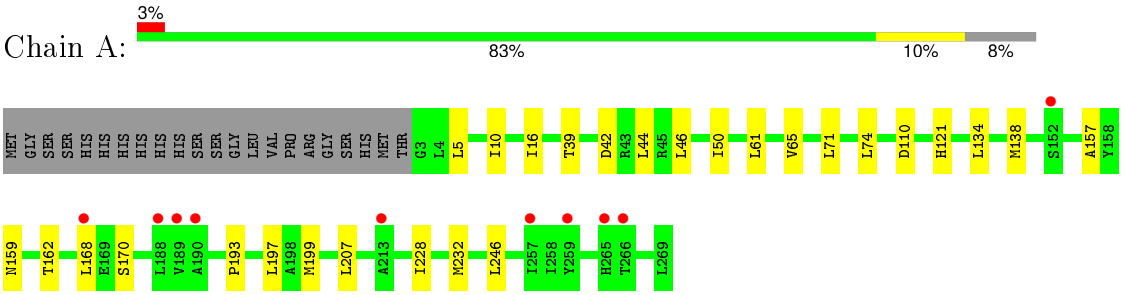
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	8	Total O 8 8	0	0

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 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.

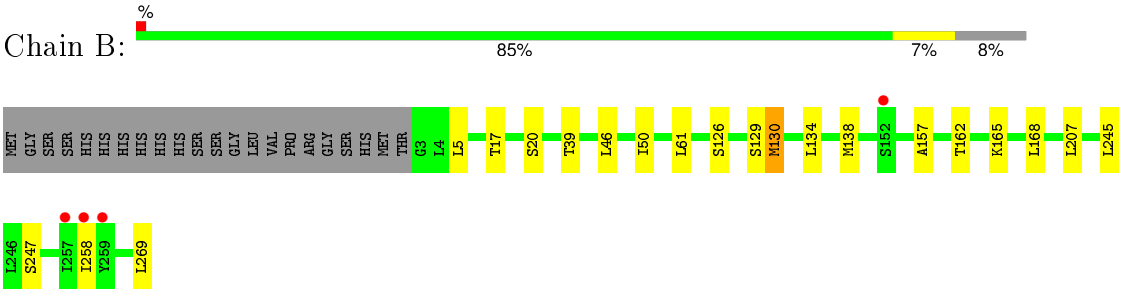
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain A:



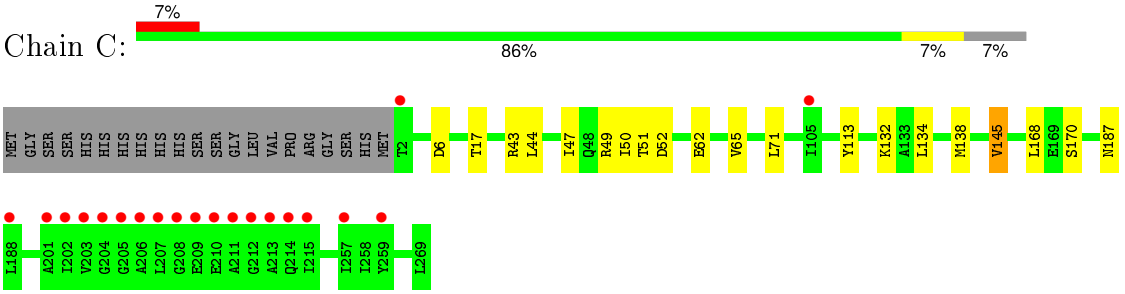
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain B:



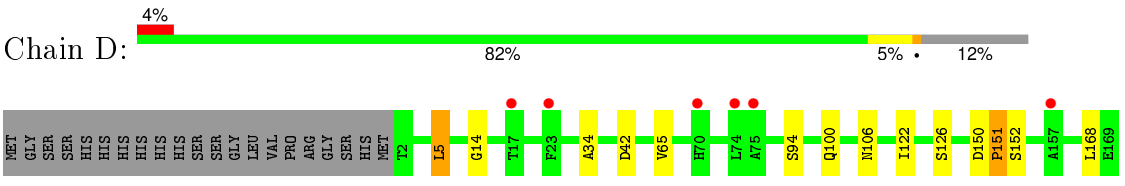
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

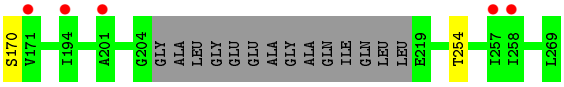
Chain C:



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain D:




S170
V171
I194
A201
G204
GLY
ALA
LEU
GLY
GLU
GLU
ALA
GLY
ALA
GLN
ILE
GLN
LEU
LEU
E219
T254
I257
I258
L269

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.84Å 90.65Å 164.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.70 – 2.30 43.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.8 (43.70-2.30) 80.0 (43.70-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.194 , 0.244 0.186 , 0.229	Depositor DCC
R_{free} test set	2284 reflections (5.94%)	DCC
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.918	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 45509 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7944	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: 1US, NAD

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	0.38	0/2005	0.55	0/2727
1	B	0.37	0/1980	0.53	0/2691
1	C	0.36	0/1970	0.53	0/2668
1	D	0.29	0/1774	0.47	0/2396
All	All	0.35	0/7729	0.52	0/10482

There are no bond length outliers.

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	1967	0	1955	14	0
1	B	1942	0	1923	11	0
1	C	1932	0	1873	9	0
1	D	1738	0	1633	8	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	2	0
3	A	19	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	16	0	0
3	C	19	0	14	0	0
3	D	20	0	16	0	0
4	A	44	0	0	0	0
4	B	31	0	0	0	0
4	C	28	0	0	0	0
4	D	8	0	0	0	0
All	All	7944	0	7548	41	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 (41) 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:C:17:THR:HA	1:C:50:ILE:HD13	1.73	0.69
1:D:5:LEU:HB3	1:D:34:ALA:HB2	1.76	0.68
1:B:17:THR:HA	1:B:50:ILE:HD13	1.79	0.63
1:B:157:ALA:HB2	1:B:207:LEU:HD21	1.81	0.61
1:C:44:LEU:HD11	1:C:62:GLU:HB2	1.83	0.60
2:D:301:NAD:H2N	2:D:301:NAD:O1N	2.02	0.59
1:C:49:ARG:O	1:C:52:ASP:HB2	2.07	0.53
1:A:16:ILE:O	1:A:50:ILE:HD13	2.10	0.51
1:B:134:LEU:O	1:B:138:MET:HG3	2.11	0.50
2:C:301:NAD:H2N	2:C:301:NAD:O1N	2.10	0.50
1:A:157:ALA:HB2	1:A:207:LEU:HD21	1.94	0.49
1:B:20:SER:OG	2:B:301:NAD:O1A	2.27	0.48
1:C:47:ILE:O	1:C:51:THR:HG23	2.13	0.47
1:A:46[A]:LEU:O	1:A:50:ILE:HD12	2.15	0.46
1:A:121:HIS:HB2	1:C:113:TYR:CE2	2.50	0.46
1:A:10:ILE:HD13	1:A:246:LEU:HD13	1.99	0.45
1:C:65:VAL:HG22	2:C:301:NAD:N1A	2.32	0.45
1:A:193:PRO:O	1:A:232:MET:HG3	2.17	0.45
1:B:130:MET:HE3	1:B:130:MET:HB3	1.91	0.44
1:A:46[B]:LEU:O	1:A:50:ILE:HD12	2.17	0.44
1:B:245:LEU:HD21	1:B:258:ILE:HD13	2.00	0.44
1:C:145[A]:VAL:HA	1:C:187:ASN:O	2.18	0.43
1:A:110:ASP:OD1	1:C:132:LYS:NZ	2.52	0.43
1:C:134:LEU:O	1:C:138:MET:HG3	2.19	0.43
1:D:122:ILE:O	1:D:126:SER:OG	2.28	0.43
1:B:245:LEU:HD11	1:B:258:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:HG22	2:A:301:NAD:N1A	2.33	0.42
1:D:150:ASP:OD1	1:D:152:SER:OG	2.34	0.42
1:D:65:VAL:HG22	2:D:301:NAD:N1A	2.34	0.42
1:D:14:GLY:HA3	1:D:94:SER:O	2.19	0.42
1:B:165:LYS:HD3	1:B:165:LYS:HA	1.69	0.42
1:A:199:MET:HE3	3:A:302:1US:H6	2.02	0.42
1:A:199:MET:CE	3:A:302:1US:H6	2.50	0.42
1:A:228:ILE:HG23	1:D:254:THR:HG21	2.01	0.42
1:B:126:SER:HA	1:B:129:SER:HB2	2.02	0.42
1:D:150:ASP:HA	1:D:151:PRO:HD3	1.86	0.41
1:D:100:GLN:O	1:D:106:ASN:ND2	2.53	0.41
1:A:39:THR:HA	1:A:61:LEU:O	2.21	0.41
1:B:39:THR:HA	1:B:61:LEU:O	2.20	0.41
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.90	0.40
1:A:134:LEU:O	1:A:138:MET:HG3	2.21	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	268/289 (93%)	257 (96%)	9 (3%)	2 (1%)	26	31
1	B	265/289 (92%)	254 (96%)	11 (4%)	0	100	100
1	C	272/289 (94%)	261 (96%)	11 (4%)	0	100	100
1	D	250/289 (86%)	236 (94%)	12 (5%)	2 (1%)	24	27
All	All	1055/1156 (91%)	1008 (96%)	43 (4%)	4 (0%)	39	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	ASP
1	A	42	ASP
1	A	159	ASN
1	D	151	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	193/222 (87%)	183 (95%)	10 (5%)	29	38
1	B	190/222 (86%)	184 (97%)	6 (3%)	46	62
1	C	182/222 (82%)	172 (94%)	10 (6%)	27	36
1	D	155/222 (70%)	151 (97%)	4 (3%)	54	71
All	All	720/888 (81%)	690 (96%)	30 (4%)	46	49

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	44	LEU
1	A	71	LEU
1	A	74	LEU
1	A	162	THR
1	A	168[A]	LEU
1	A	168[B]	LEU
1	A	170	SER
1	A	197[A]	LEU
1	A	197[B]	LEU
1	B	5	LEU
1	B	130	MET
1	B	162	THR
1	B	168	LEU
1	B	247	SER
1	B	269	LEU
1	C	6	ASP
1	C	43[A]	ARG

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Mol	Chain	Res	Type
1	C	43[B]	ARG
1	C	71[A]	LEU
1	C	71[B]	LEU
1	C	145[A]	VAL
1	C	145[B]	VAL
1	C	168[A]	LEU
1	C	168[B]	LEU
1	C	170	SER
1	D	5	LEU
1	D	168[A]	LEU
1	D	168[B]	LEU
1	D	170	SER

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

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)

8 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	NAD	A	301	-	38,48,48	2.89	17 (44%)	47,73,73	2.42	7 (14%)
3	1US	A	302	-	20,20,22	0.79	1 (5%)	26,26,28	0.88	1 (3%)
2	NAD	B	301	-	38,48,48	2.83	18 (47%)	47,73,73	2.49	11 (23%)
3	1US	B	302	-	21,21,22	0.77	1 (4%)	27,27,28	0.92	0
2	NAD	C	301	-	38,48,48	2.94	19 (50%)	47,73,73	2.58	10 (21%)
3	1US	C	302	-	20,20,22	0.91	1 (5%)	26,26,28	0.67	0
2	NAD	D	301	-	38,48,48	2.90	16 (42%)	47,73,73	2.30	10 (21%)
3	1US	D	302	-	21,21,22	0.90	1 (4%)	27,27,28	0.77	1 (3%)

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	NAD	A	301	-	-	0/22/62/62	0/5/5/5
3	1US	A	302	-	-	0/8/8/10	0/2/2/2
2	NAD	B	301	-	-	0/22/62/62	0/5/5/5
3	1US	B	302	-	-	0/9/9/10	0/2/2/2
2	NAD	C	301	-	-	0/22/62/62	0/5/5/5
3	1US	C	302	-	-	0/8/8/10	0/2/2/2
2	NAD	D	301	-	-	0/22/62/62	0/5/5/5
3	1US	D	302	-	-	0/9/9/10	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAD	O7N-C7N	-2.87	1.18	1.24
2	D	301	NAD	O7N-C7N	-2.76	1.18	1.24
2	A	301	NAD	O7N-C7N	-2.36	1.19	1.24
2	B	301	NAD	O7N-C7N	-2.23	1.19	1.24
2	C	301	NAD	PN-O2N	-2.10	1.46	1.54
2	C	301	NAD	PA-O2A	-2.09	1.46	1.54
2	D	301	NAD	PN-O2N	-2.08	1.46	1.54
2	B	301	NAD	PN-O2N	-2.05	1.46	1.54
2	B	301	NAD	PA-O2A	-2.02	1.46	1.54
2	A	301	NAD	PN-O2N	-2.01	1.46	1.54
3	A	302	1US	O13-C04	2.01	1.40	1.36
2	C	301	NAD	C3D-C4D	2.07	1.58	1.53
2	C	301	NAD	O4B-C4B	2.08	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	1US	C16-CL1	2.11	1.78	1.73
3	C	302	1US	C16-CL1	2.11	1.78	1.73
2	B	301	NAD	C3D-C4D	2.12	1.58	1.53
3	D	302	1US	C16-CL1	2.12	1.78	1.73
2	A	301	NAD	C3D-C4D	2.15	1.58	1.53
2	C	301	NAD	C3N-C7N	2.22	1.54	1.50
2	B	301	NAD	C3N-C7N	2.28	1.54	1.50
2	B	301	NAD	C5N-C4N	2.49	1.44	1.38
2	D	301	NAD	C3N-C7N	2.64	1.54	1.50
2	B	301	NAD	C3B-C4B	2.68	1.60	1.53
2	A	301	NAD	C3N-C7N	2.84	1.55	1.50
2	D	301	NAD	C3B-C4B	2.89	1.60	1.53
2	D	301	NAD	C5N-C4N	2.93	1.44	1.38
2	A	301	NAD	C3B-C4B	2.94	1.60	1.53
2	A	301	NAD	C5N-C4N	2.97	1.45	1.38
2	B	301	NAD	PN-O1N	3.11	1.62	1.51
2	C	301	NAD	C3B-C4B	3.12	1.61	1.53
2	C	301	NAD	C5N-C4N	3.16	1.45	1.38
2	B	301	NAD	C6N-C5N	3.16	1.45	1.38
2	D	301	NAD	C6N-C5N	3.28	1.46	1.38
2	A	301	NAD	C6N-C5N	3.41	1.46	1.38
2	C	301	NAD	C6N-C5N	3.53	1.46	1.38
2	D	301	NAD	PN-O1N	3.71	1.64	1.51
2	C	301	NAD	PN-O1N	3.72	1.64	1.51
2	C	301	NAD	C6A-N6A	3.77	1.46	1.34
2	A	301	NAD	C6A-N6A	3.78	1.46	1.34
2	D	301	NAD	C6A-N6A	3.78	1.46	1.34
2	B	301	NAD	C6A-N6A	3.78	1.46	1.34
2	A	301	NAD	PA-O1A	3.90	1.65	1.51
2	C	301	NAD	PA-O1A	3.91	1.65	1.51
2	A	301	NAD	PN-O1N	3.92	1.65	1.51
2	D	301	NAD	C2N-C3N	3.94	1.45	1.39
2	A	301	NAD	C2A-N1A	3.99	1.41	1.33
2	B	301	NAD	PA-O1A	4.02	1.65	1.51
2	D	301	NAD	PA-O1A	4.05	1.66	1.51
2	B	301	NAD	C2N-C3N	4.15	1.45	1.39
2	B	301	NAD	C2A-N1A	4.48	1.42	1.33
2	C	301	NAD	C2A-N1A	4.57	1.42	1.33
2	A	301	NAD	C8A-N7A	4.66	1.43	1.34
2	C	301	NAD	C2N-C3N	4.68	1.46	1.39
2	D	301	NAD	C2A-N1A	4.72	1.42	1.33
2	A	301	NAD	C2N-C3N	4.80	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAD	C8A-N7A	4.83	1.43	1.34
2	C	301	NAD	C8A-N7A	4.85	1.43	1.34
2	D	301	NAD	C6N-N1N	4.94	1.48	1.35
2	B	301	NAD	C2A-N3A	4.94	1.40	1.32
2	A	301	NAD	C2A-N3A	5.02	1.41	1.32
2	A	301	NAD	C6N-N1N	5.10	1.49	1.35
2	B	301	NAD	C6N-N1N	5.17	1.49	1.35
2	B	301	NAD	C8A-N7A	5.23	1.44	1.34
2	C	301	NAD	C6N-N1N	5.28	1.49	1.35
2	D	301	NAD	C2A-N3A	5.45	1.41	1.32
2	C	301	NAD	C2A-N3A	5.52	1.41	1.32
2	A	301	NAD	C4N-C3N	5.81	1.49	1.39
2	B	301	NAD	C4N-C3N	6.13	1.49	1.39
2	C	301	NAD	C4N-C3N	6.37	1.50	1.39
2	D	301	NAD	C4N-C3N	6.43	1.50	1.39
2	C	301	NAD	C7N-N7N	6.57	1.46	1.33
2	D	301	NAD	C7N-N7N	6.60	1.46	1.33
2	B	301	NAD	C7N-N7N	6.72	1.46	1.33
2	A	301	NAD	C7N-N7N	7.15	1.47	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	NAD	N3A-C2A-N1A	-12.08	119.64	128.89
2	A	301	NAD	N3A-C2A-N1A	-11.97	119.73	128.89
2	B	301	NAD	N3A-C2A-N1A	-11.88	119.80	128.89
2	D	301	NAD	N3A-C2A-N1A	-11.45	120.13	128.89
2	B	301	NAD	C4B-O4B-C1B	-7.53	101.44	109.72
2	A	301	NAD	C4B-O4B-C1B	-6.56	102.51	109.72
2	C	301	NAD	C4B-O4B-C1B	-6.42	102.66	109.72
2	D	301	NAD	PN-O3-PA	-5.42	117.51	132.73
2	C	301	NAD	C2B-C1B-N9A	-4.61	107.25	114.29
2	C	301	NAD	PN-O3-PA	-4.52	120.04	132.73
2	A	301	NAD	C2B-C1B-N9A	-4.34	107.66	114.29
2	A	301	NAD	PN-O3-PA	-4.07	121.29	132.73
2	B	301	NAD	PN-O3-PA	-3.92	121.71	132.73
2	D	301	NAD	C2B-C1B-N9A	-3.25	109.33	114.29
2	B	301	NAD	C2B-C1B-N9A	-2.90	109.86	114.29
2	D	301	NAD	C4B-O4B-C1B	-2.69	106.76	109.72
2	A	301	NAD	C1B-N9A-C4A	-2.15	123.70	126.94
2	B	301	NAD	C1B-N9A-C4A	-2.04	123.86	126.94
2	C	301	NAD	O3B-C3B-C4B	2.04	117.16	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	NAD	O3D-C3D-C4D	2.09	117.31	111.05
2	A	301	NAD	O4B-C4B-C5B	2.09	116.81	109.32
2	C	301	NAD	O3-PN-O5D	2.16	108.67	102.94
2	C	301	NAD	C2N-C3N-C4N	2.17	120.70	118.29
2	B	301	NAD	O3D-C3D-C4D	2.18	117.60	111.05
2	B	301	NAD	C2N-C3N-C4N	2.26	120.81	118.29
2	B	301	NAD	O3-PA-O5B	2.27	108.95	102.94
2	D	301	NAD	O3B-C3B-C2B	2.27	119.22	111.83
2	D	301	NAD	O4D-C4D-C5D	2.29	117.49	109.32
2	C	301	NAD	C3N-C7N-N7N	2.29	120.32	117.82
2	D	301	NAD	O3B-C3B-C4B	2.30	117.94	111.05
2	B	301	NAD	O3B-C3B-C2B	2.33	119.40	111.83
3	A	302	1US	O14-C03-C04	2.33	120.70	116.12
2	B	301	NAD	O4B-C4B-C5B	2.36	117.76	109.32
3	D	302	1US	O14-C03-C04	2.40	120.84	116.12
2	D	301	NAD	O4D-C1D-N1N	2.75	111.15	108.13
2	C	301	NAD	O3-PA-O5B	2.80	110.36	102.94
2	A	301	NAD	O4D-C1D-N1N	2.81	111.22	108.13
2	B	301	NAD	O4D-C1D-N1N	3.01	111.44	108.13
2	D	301	NAD	O3-PN-O5D	3.12	111.22	102.94
2	C	301	NAD	O4D-C1D-N1N	4.52	113.10	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	1	0
3	A	302	1US	2	0
2	B	301	NAD	1	0
2	C	301	NAD	2	0
2	D	301	NAD	2	0

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, 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	267/289 (92%)	-0.09	10 (3%) 45 54	23, 38, 53, 64	0
1	B	267/289 (92%)	-0.07	4 (1%) 76 81	26, 43, 58, 75	0
1	C	268/289 (92%)	0.26	20 (7%) 17 24	26, 44, 74, 93	0
1	D	254/289 (87%)	0.28	11 (4%) 39 48	31, 57, 79, 91	0
All	All	1056/1156 (91%)	0.09	45 (4%) 39 48	23, 44, 72, 93	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	213	ALA	6.4
1	C	211	ALA	5.3
1	C	212	GLY	4.6
1	C	208	GLY	4.2
1	C	202	ILE	3.7
1	C	201	ALA	3.5
1	C	203	VAL	3.5
1	C	205	GLY	3.2
1	C	210	GLU	3.1
1	C	207	LEU	3.0
1	C	209	GLU	3.0
1	D	201	ALA	3.0
1	A	257	ILE	2.9
1	C	215	ILE	2.9
1	C	259	TYR	2.9
1	A	259	TYR	2.7
1	A	266	THR	2.6
1	C	204	GLY	2.6
1	D	257	ILE	2.5
1	C	188	LEU	2.4
1	B	257	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	157	ALA	2.4
1	D	70	HIS	2.4
1	A	152	SER	2.4
1	B	258	ILE	2.4
1	D	23	PHE	2.4
1	C	206	ALA	2.4
1	B	152	SER	2.3
1	B	259	TYR	2.3
1	C	257	ILE	2.3
1	D	258	ILE	2.3
1	A	213	ALA	2.3
1	A	265	HIS	2.2
1	D	75	ALA	2.2
1	C	214	GLN	2.2
1	D	17	THR	2.2
1	D	171	VAL	2.2
1	A	188	LEU	2.1
1	C	105	ILE	2.1
1	D	194	ILE	2.1
1	A	189	VAL	2.1
1	C	2	THR	2.1
1	A	168[A]	LEU	2.1
1	A	190	ALA	2.0
1	D	74	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	1US	D	302	20/21	0.88	0.25	1.52	52,59,75,78	0
3	1US	B	302	20/21	0.95	0.13	0.41	31,36,42,48	0
2	NAD	D	301	44/44	0.93	0.19	0.40	54,65,76,103	0
3	1US	A	302	19/21	0.96	0.13	0.28	24,32,39,42	0
2	NAD	A	301	44/44	0.96	0.13	0.13	20,32,41,50	0
2	NAD	B	301	44/44	0.97	0.12	-0.16	27,38,46,49	0
3	1US	C	302	19/21	0.94	0.14	-0.39	34,42,52,55	0
2	NAD	C	301	44/44	0.97	0.11	-0.74	29,41,52,58	0

6.5 Other polymers (i)

There are no such residues in this entry.