Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:02 AM GMT

PDB ID	:	3NT2
Title	:	Crystal structure of myo-inositol dehydrogenase from Bacillus subtilis with bound cofactor
Authors	:	Van Straaten, K.E.; Palmer, D.R.J.; Sanders, D.A.R.
Deposited on	:	2010-07-02
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:

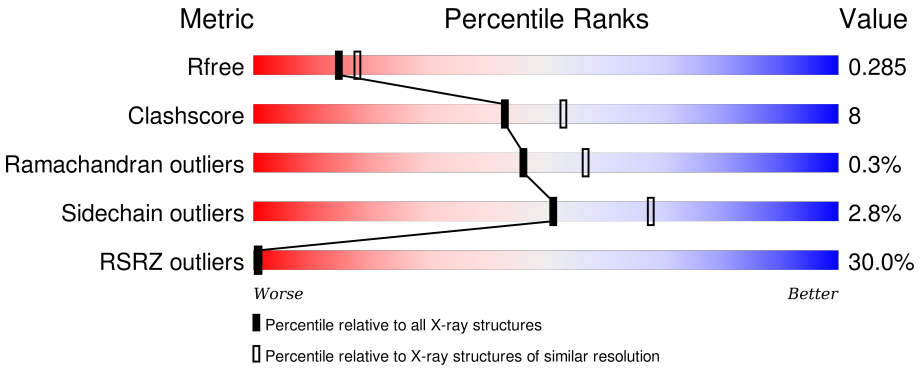
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	344	26% 80% 17%
1	B	344	32% 76% 21%

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
2	NAD	A	400	-	-	-	X

2 Entry composition

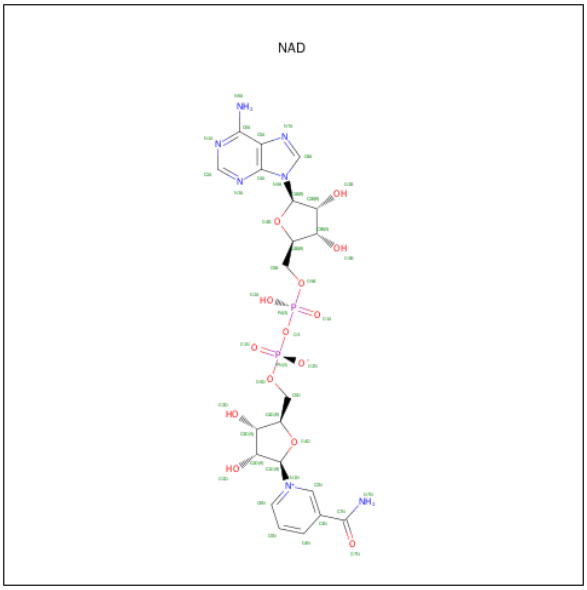
There are 4 unique types of molecules in this entry. The entry contains 5492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inositol 2-dehydrogenase/D-chiro-inositol 3-dehydrogenase.

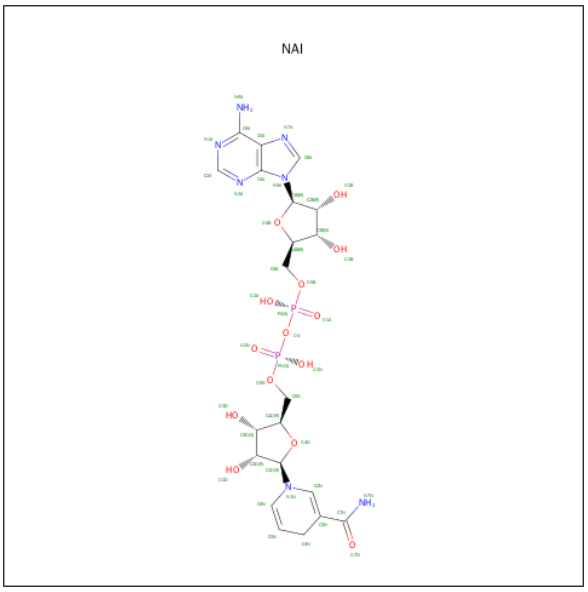
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2640	1670	444	514	12			
1	B	337	Total	C	N	O	S	0	0	0
			2640	1670	444	514	12			

- 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		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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

- Molecule 4 is water.

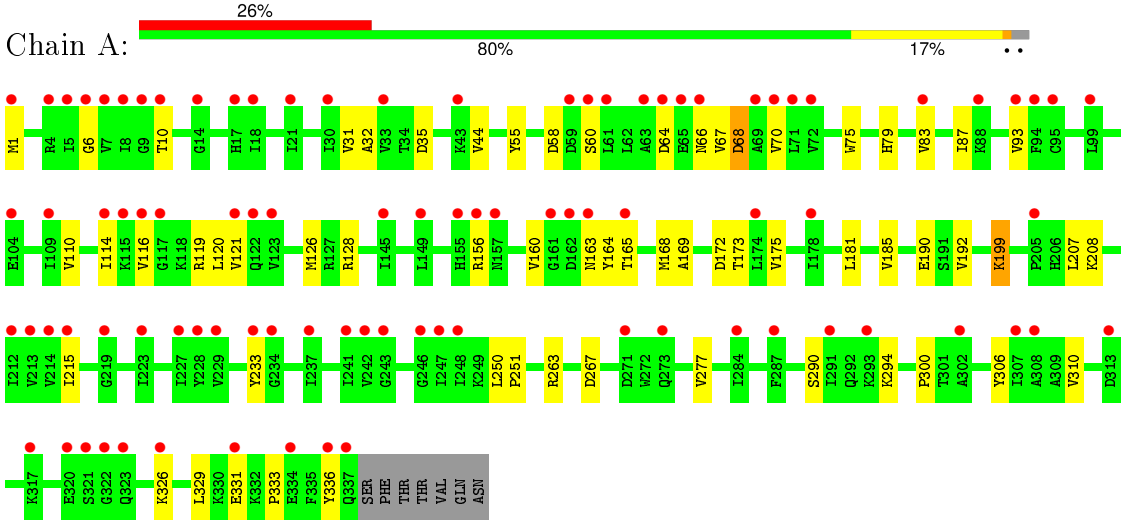
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		
4	B	55	Total	O	0	0
			55	55		

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.

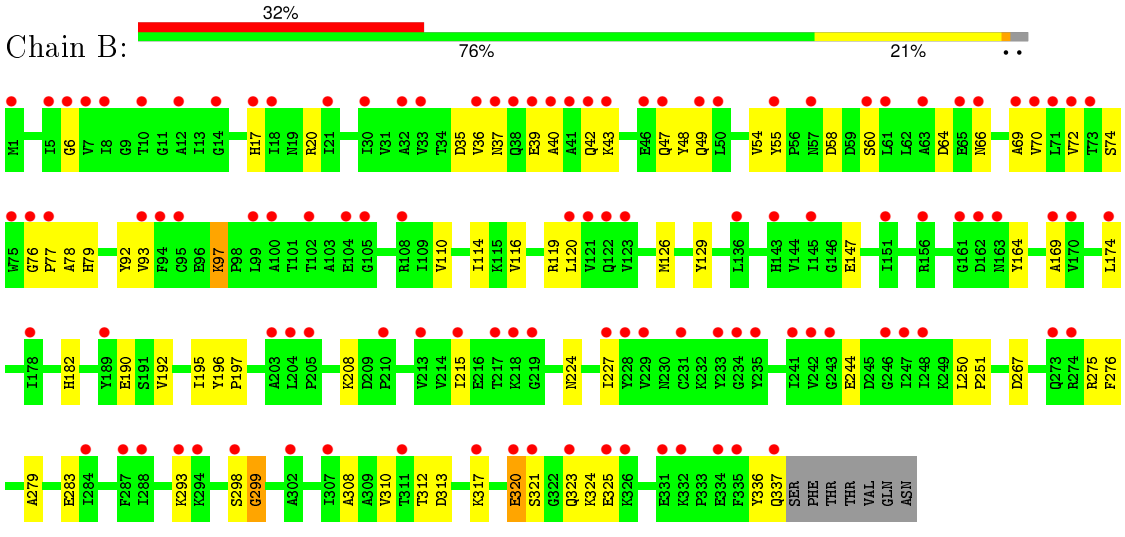
- Molecule 1: Inositol 2-dehydrogenase/D-chiro-inositol 3-dehydrogenase

Chain A:



- Molecule 1: Inositol 2-dehydrogenase/D-chiro-inositol 3-dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α, β, γ	184.37Å 184.37Å 184.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.04 – 2.30 22.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (22.04-2.30) 98.0 (22.04-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.240 , 0.286 0.240 , 0.285	Depositor DCC
R_{free} test set	2325 reflections (5.42%)	DCC
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 68.7	EDS
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Outliers	4 of 45248 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5492	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.69% 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: NAI, 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	0.29	0/2687	0.46	0/3644
1	B	0.29	0/2687	0.44	0/3644
All	All	0.29	0/5374	0.45	0/7288

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	2640	0	2635	37	0
1	B	2640	0	2635	51	0
2	A	44	0	26	3	0
3	B	44	0	27	4	0
4	A	69	0	0	0	0
4	B	55	0	0	4	0
All	All	5492	0	5323	88	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 8.

All (88) 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:165:THR:H	1:A:168:MET:HE3	1.43	0.83
1:B:182:HIS:HE1	4:B:353:HOH:O	1.66	0.79
1:B:308:ALA:O	1:B:312:THR:HG22	1.84	0.78
1:A:35:ASP:OD1	2:A:400:NAD:H1B	1.87	0.74
1:A:83:VAL:O	1:A:87:ILE:HG13	1.89	0.72
1:B:174:LEU:HD13	1:B:227:ILE:HD11	1.75	0.69
1:A:199:LYS:HE2	1:A:207:LEU:O	1.93	0.69
1:B:182:HIS:HD2	4:B:355:HOH:O	1.78	0.65
1:B:336:TYR:O	1:B:337:GLN:HB3	1.96	0.65
1:B:320:GLU:HG3	1:B:321:SER:N	2.11	0.64
1:A:192:VAL:HG12	1:A:215:ILE:HG12	1.79	0.64
1:A:116:VAL:HG11	1:A:120:LEU:HD11	1.78	0.64
1:B:97:LYS:O	1:B:97:LYS:HD3	1.98	0.64
1:A:165:THR:N	1:A:168:MET:HE3	2.14	0.61
1:B:182:HIS:CD2	4:B:355:HOH:O	2.53	0.61
1:B:69:ALA:HB2	1:B:92:TYR:HB2	1.83	0.60
1:A:68:ASP:OD2	1:A:68:ASP:N	2.35	0.59
1:B:76:GLY:N	1:B:77:PRO:HD2	2.18	0.58
1:A:199:LYS:HE2	1:A:208:LYS:HA	1.85	0.58
1:B:192:VAL:HG12	1:B:215:ILE:HG12	1.86	0.58
1:B:110:VAL:O	1:B:114:ILE:HG13	2.04	0.57
1:A:31:VAL:HG23	1:A:67:VAL:HG12	1.87	0.57
1:B:116:VAL:HG11	1:B:120:LEU:HD11	1.87	0.57
1:B:164:TYR:OH	1:B:169:ALA:HA	2.06	0.55
1:B:78:ALA:HB1	3:B:400:NAI:H61A	1.72	0.55
1:A:31:VAL:CG2	1:A:67:VAL:HG12	2.37	0.55
1:B:55:TYR:HD1	1:B:60:SER:HB2	1.73	0.54
1:B:317:LYS:HG2	1:B:325:GLU:OE2	2.08	0.53
1:B:323:GLN:HG3	1:B:324:LYS:N	2.23	0.53
1:B:35:ASP:OD1	3:B:400:NAI:H1B	2.08	0.53
1:B:70:VAL:HG23	1:B:93:VAL:HG23	1.90	0.52
1:A:64:ASP:O	1:A:67:VAL:HG22	2.09	0.52
1:B:74:SER:HB2	3:B:400:NAI:C8A	2.39	0.52
1:A:190:GLU:O	1:A:326:LYS:HD2	2.10	0.51
1:A:110:VAL:O	1:A:114:ILE:HG13	2.10	0.51
1:A:93:VAL:HG13	1:A:121:VAL:HA	1.92	0.51
1:A:331:GLU:O	1:A:333:PRO:HD3	2.11	0.51
1:B:310:VAL:O	1:B:313:ASP:HB2	2.10	0.51
1:B:17:HIS:HA	1:B:20:ARG:HH11	1.77	0.49
1:B:320:GLU:HG3	1:B:321:SER:H	1.75	0.49
1:B:37:ASN:ND2	1:B:40:ALA:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:HG11	1:A:329:LEU:HD23	1.94	0.49
1:B:323:GLN:HG3	1:B:324:LYS:H	1.76	0.49
1:A:6:GLY:O	1:A:70:VAL:HA	2.12	0.49
1:B:78:ALA:HB1	3:B:400:NAI:N6A	2.27	0.48
1:B:39:GLU:HG2	1:B:43:LYS:NZ	2.29	0.48
1:B:196:TYR:CE1	1:B:208:LYS:HD3	2.50	0.46
1:B:195:ILE:O	1:B:197:PRO:HD3	2.15	0.46
1:A:163:ASN:N	1:A:163:ASN:OD1	2.47	0.46
1:A:55:TYR:OH	1:A:64:ASP:HB2	2.16	0.46
1:B:64:ASP:OD1	1:B:66:ASN:HB2	2.17	0.45
1:A:306:TYR:O	1:A:310:VAL:HG23	2.16	0.45
1:B:227:ILE:N	1:B:227:ILE:HD12	2.32	0.45
1:A:10:THR:HB	1:A:44:VAL:HG21	1.99	0.45
1:B:119:ARG:HH21	1:B:336:TYR:HA	1.80	0.45
1:B:39:GLU:O	1:B:43:LYS:HG3	2.17	0.44
1:B:129:TYR:CE2	1:B:283:GLU:HG3	2.53	0.44
1:A:169:ALA:O	1:A:173:THR:HB	2.18	0.44
1:A:6:GLY:HA2	1:A:32:ALA:O	2.17	0.44
1:A:172:ASP:O	1:A:175:VAL:HG12	2.18	0.44
1:B:6:GLY:O	1:B:70:VAL:HA	2.18	0.43
1:A:119:ARG:HH21	1:A:336:TYR:HA	1.83	0.43
1:B:47:GLN:HG2	1:B:48:TYR:CE2	2.53	0.43
1:B:42:GLN:OE1	1:B:54:VAL:HG21	2.19	0.43
1:A:79:HIS:CE1	2:A:400:NAD:O3D	2.72	0.43
1:A:164:TYR:HA	1:A:168:MET:HE1	2.00	0.43
1:B:72:VAL:HG12	1:B:79:HIS:CD2	2.53	0.43
1:B:147:GLU:HB2	1:B:244:GLU:CD	2.38	0.43
1:B:275:ARG:HG3	1:B:276:PHE:CD2	2.54	0.43
1:B:48:TYR:O	1:B:49:GLN:C	2.57	0.43
1:B:279:ALA:O	1:B:283:GLU:HB2	2.19	0.42
1:B:298:SER:O	1:B:299:GLY:O	2.36	0.42
1:B:55:TYR:CD1	1:B:60:SER:HB2	2.52	0.42
1:A:181:LEU:O	1:A:185:VAL:HG22	2.20	0.42
1:A:250:LEU:HA	1:A:251:PRO:HD3	1.86	0.42
1:A:156:ARG:HD2	1:A:233:TYR:OH	2.20	0.41
1:A:290:SER:O	1:A:294:LYS:HB2	2.21	0.41
1:B:39:GLU:HG2	1:B:43:LYS:HZ1	1.86	0.41
1:A:128:ARG:HD2	1:A:300:PRO:HG3	2.03	0.41
1:B:250:LEU:HA	1:B:251:PRO:HD3	1.90	0.41
1:A:164:TYR:OH	1:A:169:ALA:HA	2.20	0.40
1:B:119:ARG:NH2	1:B:336:TYR:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASP:N	1:A:58:ASP:OD1	2.47	0.40
1:B:293:LYS:HE2	1:B:293:LYS:HB3	1.85	0.40
1:B:58:ASP:N	1:B:58:ASP:OD1	2.54	0.40
1:B:182:HIS:CE1	4:B:353:HOH:O	2.53	0.40
1:A:163:ASN:O	1:A:168:MET:HE1	2.20	0.40
1:A:75:TRP:HB2	2:A:400:NAD:H8A	2.03	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	335/344 (97%)	320 (96%)	15 (4%)	0	100 100
1	B	335/344 (97%)	316 (94%)	17 (5%)	2 (1%)	30 36
All	All	670/688 (97%)	636 (95%)	32 (5%)	2 (0%)	46 57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	GLY
1	B	190	GLU

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	290/297 (98%)	280 (97%)	10 (3%)	44 59
1	B	290/297 (98%)	284 (98%)	6 (2%)	61 78
All	All	580/594 (98%)	564 (97%)	16 (3%)	51 68

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	60	SER
1	A	66	ASN
1	A	68	ASP
1	A	126	MET
1	A	160	VAL
1	A	199	LYS
1	A	263	ARG
1	A	267	ASP
1	A	277	VAL
1	B	36	VAL
1	B	97	LYS
1	B	126	MET
1	B	224	ASN
1	B	267	ASP
1	B	320	GLU

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)

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	NAD	A	400	-	38,48,48	1.68	3 (7%)	47,73,73	2.00	3 (6%)
3	NAI	B	400	-	38,48,48	1.36	4 (10%)	48,73,73	1.86	9 (18%)

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	400	-	-	0/22/62/62	0/5/5/5
3	NAI	B	400	-	-	0/25/72/72	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	NAI	C4N-C5N	-4.62	1.39	1.49
3	B	400	NAI	C2N-C3N	2.48	1.40	1.34
2	A	400	NAD	C2A-N1A	2.79	1.39	1.33
3	B	400	NAI	C5A-C4A	2.95	1.47	1.40
3	B	400	NAI	C6N-C5N	3.24	1.39	1.33
2	A	400	NAD	C2A-N3A	3.79	1.38	1.32
2	A	400	NAD	O7N-C7N	8.03	1.41	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	NAD	N3A-C2A-N1A	-11.90	119.78	128.89
3	B	400	NAI	N3A-C2A-N1A	-8.34	122.51	128.89
2	A	400	NAD	PN-O3-PA	-3.64	122.50	132.73
3	B	400	NAI	C4N-C5N-C6N	-2.41	118.61	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	NAI	C4A-C5A-N7A	-2.38	107.29	109.48
3	B	400	NAI	C3N-C2N-N1N	-2.27	119.89	123.14
3	B	400	NAI	O2A-PA-O3	2.02	114.24	105.09
3	B	400	NAI	C5N-C4N-C3N	2.51	119.44	112.52
2	A	400	NAD	O4D-C1D-N1N	2.51	110.89	108.13
3	B	400	NAI	O3-PA-O5B	2.58	109.77	102.94
3	B	400	NAI	O3-PN-O5D	2.60	109.83	102.94
3	B	400	NAI	C4B-O4B-C1B	4.33	114.47	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	NAD	3	0
3	B	400	NAI	4	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	337/344 (97%)	1.51	91 (27%) 1 1	52, 76, 107, 136	0
1	B	337/344 (97%)	1.59	111 (32%) 0 0	53, 83, 112, 135	0
All	All	674/688 (97%)	1.55	202 (29%) 1 1	52, 79, 109, 136	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	LEU	12.1
1	B	7	VAL	10.5
1	B	71	LEU	10.3
1	A	7	VAL	10.1
1	A	94	PHE	7.1
1	B	70	VAL	6.7
1	B	1	MET	6.6
1	B	8	ILE	6.2
1	A	334	GLU	6.1
1	A	70	VAL	6.1
1	A	8	ILE	6.0
1	B	94	PHE	5.8
1	A	121	VAL	5.7
1	B	5	ILE	5.7
1	A	33	VAL	5.6
1	A	1	MET	5.6
1	B	334	GLU	5.5
1	B	93	VAL	5.4
1	A	18	ILE	5.3
1	A	99	LEU	5.3
1	B	77	PRO	5.3
1	B	33	VAL	5.3
1	A	66	ASN	5.3
1	A	93	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	72	VAL	5.2
1	B	6	GLY	5.2
1	B	337	GLN	5.1
1	B	204	LEU	5.1
1	B	12	ALA	5.0
1	B	75	TRP	4.9
1	B	43	LYS	4.7
1	B	30	ILE	4.7
1	B	47	GLN	4.6
1	A	123	VAL	4.6
1	B	121	VAL	4.6
1	A	95	CYS	4.6
1	A	63	ALA	4.5
1	B	63	ALA	4.5
1	B	293	LYS	4.4
1	A	213	VAL	4.4
1	A	21	ILE	4.3
1	B	18	ILE	4.3
1	B	46	GLU	4.3
1	B	248	ILE	4.3
1	A	5	ILE	4.1
1	A	227	ILE	4.1
1	A	323	GLN	4.1
1	A	6	GLY	4.1
1	A	65	GLU	4.1
1	B	227	ILE	4.0
1	B	39	GLU	4.0
1	B	36	VAL	4.0
1	B	21	ILE	4.0
1	A	30	ILE	3.9
1	A	115	LYS	3.9
1	B	228	TYR	3.9
1	A	9	GLY	3.8
1	B	65	GLU	3.8
1	A	284	ILE	3.8
1	A	61	LEU	3.7
1	B	143	HIS	3.7
1	A	287	PHE	3.7
1	A	331	GLU	3.7
1	B	242	VAL	3.7
1	A	293	LYS	3.6
1	B	66	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	229	VAL	3.5
1	A	116	VAL	3.5
1	A	242	VAL	3.5
1	A	228	TYR	3.5
1	A	104	GLU	3.5
1	B	241	ILE	3.4
1	A	17	HIS	3.4
1	B	17	HIS	3.4
1	B	287	PHE	3.4
1	A	247	ILE	3.4
1	A	317	LYS	3.4
1	B	247	ILE	3.4
1	A	337	GLN	3.4
1	B	331	GLU	3.3
1	A	59	ASP	3.3
1	A	302	ALA	3.3
1	A	162	ASP	3.3
1	A	205	PRO	3.3
1	A	215	ILE	3.3
1	B	72	VAL	3.2
1	B	231	CYS	3.2
1	A	161	GLY	3.2
1	A	163	ASN	3.2
1	A	122	GLN	3.2
1	B	325	GLU	3.2
1	B	50	LEU	3.1
1	A	156	ARG	3.1
1	B	323	GLN	3.1
1	B	162	ASP	3.1
1	B	218	LYS	3.1
1	B	307	ILE	3.1
1	B	174	LEU	3.1
1	A	321	SER	3.0
1	B	104	GLU	3.0
1	B	205	PRO	3.0
1	A	174	LEU	3.0
1	A	114	ILE	3.0
1	B	156	ARG	3.0
1	B	123	VAL	3.0
1	A	307	ILE	3.0
1	B	38	GLN	2.9
1	B	284	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	42	GLN	2.9
1	B	273	GLN	2.9
1	B	100	ALA	2.8
1	A	336	TYR	2.8
1	B	108	ARG	2.8
1	A	241	ILE	2.8
1	A	14	GLY	2.8
1	A	246	GLY	2.8
1	B	32	ALA	2.8
1	B	161	GLY	2.7
1	A	43	LYS	2.7
1	A	326	LYS	2.7
1	B	105	GLY	2.7
1	B	219	GLY	2.7
1	B	317	LYS	2.7
1	A	10	THR	2.7
1	B	163	ASN	2.6
1	B	37	ASN	2.6
1	A	83	VAL	2.6
1	A	212	ILE	2.6
1	B	102	THR	2.6
1	B	14	GLY	2.6
1	A	229	VAL	2.6
1	A	223	ILE	2.6
1	A	248	ILE	2.6
1	B	294	LYS	2.6
1	B	243	GLY	2.6
1	B	73	THR	2.5
1	B	210	PRO	2.5
1	B	95	CYS	2.5
1	A	149	LEU	2.5
1	A	237	ILE	2.5
1	A	88	LYS	2.5
1	A	243	GLY	2.5
1	A	320	GLU	2.5
1	B	178	ILE	2.5
1	B	41	ALA	2.4
1	B	169	ALA	2.4
1	A	60	SER	2.4
1	A	157	ASN	2.4
1	B	120	LEU	2.4
1	B	335	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	109	ILE	2.4
1	B	136	LEU	2.4
1	A	313	ASP	2.4
1	A	165	THR	2.4
1	A	117	GLY	2.4
1	A	271	ASP	2.4
1	B	40	ALA	2.4
1	B	122	GLN	2.3
1	A	219	GLY	2.3
1	B	69	ALA	2.3
1	B	10	THR	2.3
1	B	233	TYR	2.3
1	A	178	ILE	2.3
1	A	64	ASP	2.3
1	A	4	ARG	2.3
1	A	322	GLY	2.2
1	B	76	GLY	2.2
1	B	288	ILE	2.2
1	B	311	THR	2.2
1	B	170	VAL	2.2
1	A	214	VAL	2.2
1	B	298	SER	2.2
1	B	213	VAL	2.2
1	A	233	TYR	2.2
1	A	155	HIS	2.2
1	B	57	ASN	2.2
1	B	215	ILE	2.2
1	B	234	GLY	2.2
1	B	274	ARG	2.2
1	B	60	SER	2.2
1	B	326	LYS	2.1
1	B	151	ILE	2.1
1	B	246	GLY	2.1
1	B	99	LEU	2.1
1	A	69	ALA	2.1
1	B	320	GLU	2.1
1	A	145	ILE	2.1
1	A	291	ILE	2.1
1	B	321	SER	2.1
1	B	55	TYR	2.1
1	B	189	TYR	2.1
1	A	308	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	61	LEU	2.1
1	B	217	THR	2.1
1	B	302	ALA	2.1
1	B	49	GLN	2.1
1	A	234	GLY	2.0
1	B	332	LYS	2.0
1	B	145	ILE	2.0
1	A	273	GLN	2.0
1	B	203	ALA	2.0
1	B	235	TYR	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	NAD	A	400	44/44	0.79	0.34	2.01	77,108,121,130	0
3	NAI	B	400	44/44	0.88	0.25	0.22	74,112,127,128	0

6.5 Other polymers

There are no such residues in this entry.