Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:21 PM GMT

PDB ID	:	1OMO
Title	:	alanine dehydrogenase dimer w/bound NAD (archaeal)
Authors	:	Gallagher, D.T.; Smith, N.N.; Holden, M.J.; Schroeder, I.; Monbouquette, H.G.
Deposited on	:	2003-02-25
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:

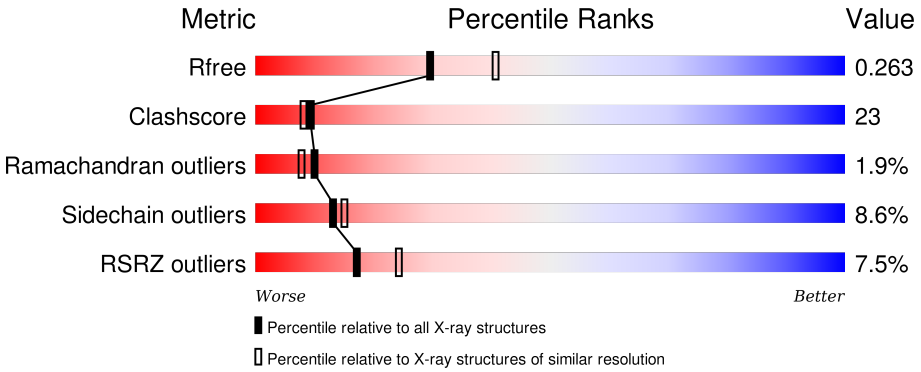
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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	322	% 69% 29%
1	B	322	14% 58% 32% 9%

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	NA	B	901	-	-	-	X
3	NAD	B	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5280 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.

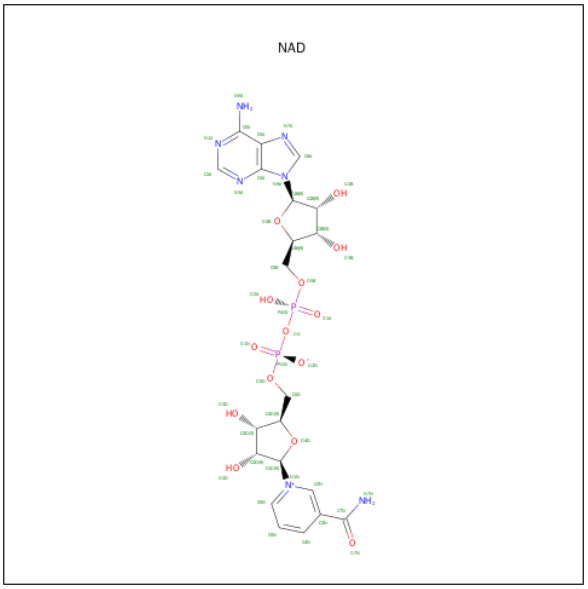
- Molecule 1 is a protein called alanine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2426	1537	406	471	12			
1	B	320	Total	C	N	O	S	0	0	0
			2426	1537	406	471	12			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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 water.

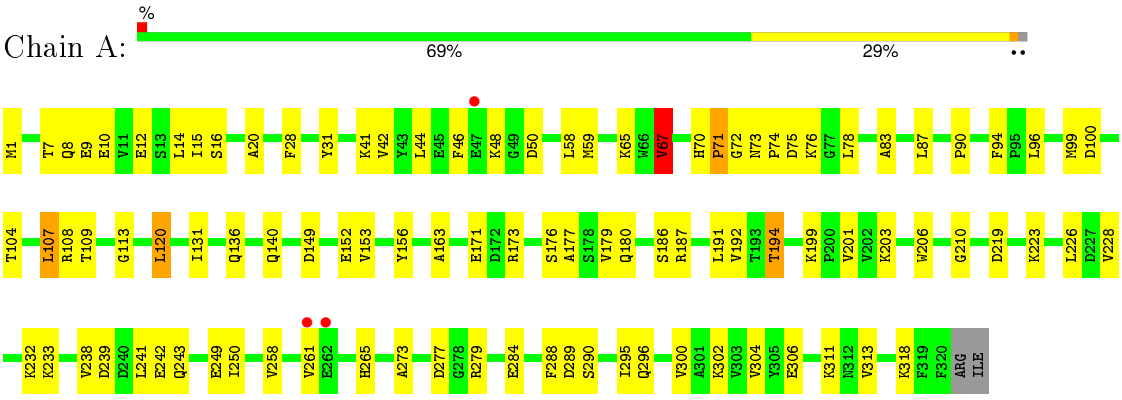
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	218	Total	O	0	0
			218	218		
4	B	120	Total	O	0	0
			120	120		

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.

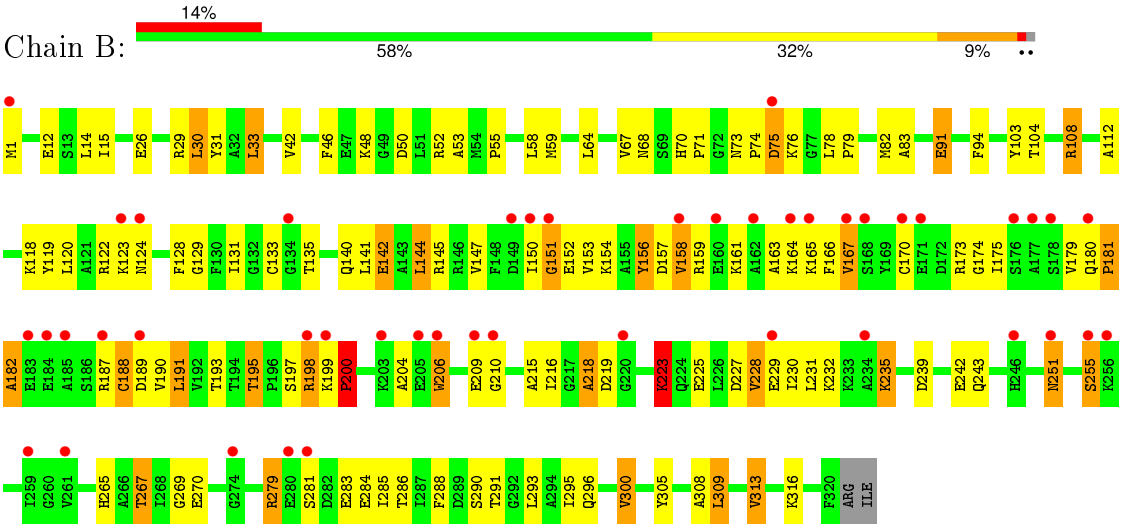
- Molecule 1: alanine dehydrogenase

Chain A:



- Molecule 1: alanine dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.70Å 55.50Å 131.30Å 90.00° 111.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.32 11.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.32) 94.5 (11.91-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	14.45 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.262 0.206 , 0.263	Depositor DCC
R_{free} test set	1190 reflections (4.02%)	DCC
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 66.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 31027 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5280	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: NA, 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	0.62	0/2466	0.86	2/3333 (0.1%)
1	B	0.55	0/2466	0.84	3/3333 (0.1%)
All	All	0.59	0/4932	0.85	5/6666 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	VAL	CB-CA-C	-6.22	99.58	111.40
1	B	174	GLY	N-CA-C	5.49	126.83	113.10
1	B	159	ARG	N-CA-C	-5.30	96.69	111.00
1	B	223	LYS	N-CA-C	5.21	125.07	111.00
1	A	99	MET	CA-CB-CG	5.13	122.02	113.30

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	2426	0	2445	88	1
1	B	2426	0	2445	140	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	26	3	0
3	B	44	0	26	5	0
4	A	218	0	0	17	0
4	B	120	0	0	20	0
All	All	5280	0	4942	224	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 23.

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ARG:HG3	1:B:279:ARG:HH21	1.06	1.10
1:B:267:THR:HG22	1:B:270:GLU:H	1.24	1.01
1:B:14:LEU:HD21	1:B:313:VAL:HG11	1.42	1.00
1:A:67:VAL:HG13	1:A:83:ALA:HB2	1.49	0.93
1:A:149:ASP:HB3	4:A:694:HOH:O	1.74	0.88
1:A:163:ALA:HB1	4:A:824:HOH:O	1.73	0.88
1:B:235:LYS:HB2	1:B:286:THR:HG22	1.58	0.85
1:B:199:LYS:HD2	1:B:200:PRO:HD2	1.58	0.85
1:B:131:ILE:HD13	1:B:191:LEU:HD21	1.62	0.81
1:B:158:VAL:HB	4:B:760:HOH:O	1.84	0.78
1:B:179:VAL:O	1:B:180:GLN:HG2	1.84	0.77
1:B:279:ARG:HG3	1:B:279:ARG:NH2	1.87	0.77
1:B:285:ILE:HG13	4:B:681:HOH:O	1.86	0.76
1:A:113:GLY:HA3	1:A:140:GLN:OE1	1.86	0.76
1:B:199:LYS:CD	1:B:200:PRO:HD2	2.16	0.75
1:A:71:PRO:O	1:A:74:PRO:HD2	1.88	0.74
1:B:235:LYS:CB	1:B:286:THR:HG22	2.17	0.74
1:A:58:LEU:HG	1:A:59:MET:HG3	1.68	0.73
1:B:150:ILE:HD13	4:B:718:HOH:O	1.87	0.73
1:B:198:ARG:HB2	4:B:787:HOH:O	1.88	0.73
1:B:122:ARG:NH2	1:B:189:ASP:HA	2.04	0.72
1:A:72:GLY:O	1:A:76:LYS:HG3	1.89	0.72
1:B:305:TYR:O	1:B:309:LEU:HD22	1.91	0.71
1:A:74:PRO:C	1:A:76:LYS:H	1.92	0.70
1:B:219:ASP:H	1:B:223:LYS:HE2	1.55	0.70
1:B:197:SER:O	1:B:223:LYS:HB3	1.90	0.70
1:A:228:VAL:HG11	1:A:258:VAL:HG11	1.75	0.69
1:A:42:VAL:HG21	1:B:42:VAL:HG21	1.74	0.69
1:B:279:ARG:HH22	1:B:286:THR:HG23	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:THR:HG22	1:B:270:GLU:N	2.02	0.69
1:B:279:ARG:HH21	1:B:279:ARG:CG	1.95	0.68
1:A:65:LYS:HE3	1:A:67:VAL:HG22	1.75	0.68
1:A:179:VAL:HA	4:A:824:HOH:O	1.93	0.68
1:B:150:ILE:HG22	1:B:151:GLY:H	1.58	0.68
1:B:279:ARG:NH2	1:B:286:THR:HG23	2.09	0.68
1:B:197:SER:O	1:B:223:LYS:CB	2.41	0.67
1:B:157:ASP:OD1	3:B:401:NAD:H1B	1.94	0.67
1:B:156:TYR:HD2	1:B:181:PRO:HA	1.59	0.67
1:A:261:VAL:HA	4:A:769:HOH:O	1.95	0.67
1:B:150:ILE:HG22	1:B:151:GLY:N	2.10	0.67
1:B:123:LYS:HG3	1:B:123:LYS:O	1.94	0.66
1:B:267:THR:HG21	4:B:557:HOH:O	1.94	0.66
1:B:305:TYR:CZ	1:B:309:LEU:HD21	2.31	0.66
1:B:156:TYR:CD2	1:B:181:PRO:HA	2.30	0.66
1:B:195:THR:N	1:B:225:GLU:OE2	2.29	0.65
1:A:65:LYS:HE3	1:A:67:VAL:CG2	2.27	0.65
1:A:70:HIS:O	1:A:73:ASN:HB2	1.97	0.65
1:A:179:VAL:HG22	4:A:824:HOH:O	1.97	0.64
1:A:318:LYS:HE3	4:B:705:HOH:O	1.98	0.64
1:B:308:ALA:HA	1:B:313:VAL:HG13	1.81	0.63
1:A:15:ILE:HG22	1:A:16:SER:N	2.12	0.63
1:A:104:THR:O	1:A:108:ARG:HG3	1.99	0.63
1:B:122:ARG:HH21	1:B:189:ASP:HA	1.64	0.62
1:B:133:CYS:HA	4:B:782:HOH:O	1.99	0.62
1:B:31:TYR:HE2	4:B:538:HOH:O	1.82	0.62
1:B:122:ARG:NH1	1:B:210:GLY:HA3	2.15	0.62
1:B:210:GLY:N	1:B:283:GLU:O	2.28	0.62
1:B:288:PHE:CE1	1:B:290:SER:HB2	2.35	0.62
1:A:250:ILE:HG23	1:A:289:ASP:OD1	2.01	0.60
1:B:128:PHE:HB2	4:B:718:HOH:O	2.01	0.60
1:A:279:ARG:NH1	1:A:284:GLU:O	2.34	0.60
1:B:293:LEU:HD12	1:B:295:ILE:HD11	1.83	0.60
1:B:74:PRO:C	1:B:76:LYS:H	2.05	0.60
1:B:135:THR:HB	3:B:401:NAD:O1N	2.02	0.59
1:B:26:GLU:HG3	1:B:30:LEU:HD22	1.82	0.59
1:B:131:ILE:HD13	1:B:191:LEU:CD2	2.33	0.59
1:A:210:GLY:HA2	1:A:279:ARG:NH1	2.17	0.59
1:A:140:GLN:HG2	1:A:192:VAL:HG11	1.84	0.59
1:B:204:ALA:HB2	1:B:227:ASP:OD2	2.03	0.59
1:A:74:PRO:C	1:A:76:LYS:N	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:HG22	4:B:718:HOH:O	2.02	0.59
1:A:15:ILE:HG13	1:A:304:VAL:CG2	2.33	0.58
1:B:73:ASN:N	1:B:74:PRO:HD2	2.18	0.58
1:A:140:GLN:HG2	1:A:192:VAL:CG1	2.33	0.58
1:B:156:TYR:CG	1:B:157:ASP:N	2.72	0.58
1:B:142:GLU:HG3	4:B:613:HOH:O	2.04	0.58
1:B:118:LYS:HB2	1:B:147:VAL:HG11	1.87	0.57
1:A:219:ASP:H	1:A:223:LYS:HD2	1.68	0.57
1:A:15:ILE:HG22	1:A:16:SER:O	2.03	0.57
1:B:161:LYS:O	1:B:165:LYS:N	2.29	0.57
1:A:76:LYS:HD2	4:A:775:HOH:O	2.03	0.57
1:A:74:PRO:O	1:A:76:LYS:N	2.37	0.57
1:A:194:THR:HG23	1:A:194:THR:O	2.04	0.57
1:A:242:GLU:HG3	4:A:785:HOH:O	2.05	0.57
1:B:150:ILE:HD12	1:B:175:ILE:HD13	1.86	0.57
1:B:129:GLY:HA2	1:B:154:LYS:O	2.04	0.57
1:A:228:VAL:CG1	1:A:258:VAL:HG11	2.35	0.56
1:B:131:ILE:O	1:B:131:ILE:HG22	2.04	0.56
1:A:9:GLU:HB2	4:A:550:HOH:O	2.05	0.55
1:A:15:ILE:HG13	1:A:304:VAL:HG22	1.88	0.55
1:B:52:ARG:NH1	1:B:219:ASP:OD2	2.40	0.55
1:A:120:LEU:O	1:A:279:ARG:HD2	2.05	0.55
1:A:265:HIS:HE1	1:A:277:ASP:O	1.88	0.55
1:B:305:TYR:CE1	1:B:309:LEU:HD21	2.42	0.55
1:B:218:ALA:HA	1:B:223:LYS:HG3	1.88	0.54
1:B:156:TYR:OH	1:B:158:VAL:HG22	2.07	0.54
1:B:122:ARG:HH21	1:B:189:ASP:CG	2.11	0.54
1:A:194:THR:HB	4:A:505:HOH:O	2.07	0.54
1:B:267:THR:CG2	1:B:270:GLU:H	2.09	0.53
1:A:109:THR:OG1	3:A:400:NAD:H4N	2.09	0.53
1:A:73:ASN:O	1:A:76:LYS:HB2	2.07	0.53
1:B:158:VAL:HG23	3:B:401:NAD:C2A	2.38	0.53
1:B:112:ALA:HB2	1:B:296:GLN:NE2	2.24	0.53
1:A:78:LEU:HD21	1:B:1:MET:SD	2.50	0.52
1:A:15:ILE:CG2	1:A:16:SER:N	2.73	0.52
1:B:33:LEU:HD23	4:B:746:HOH:O	2.08	0.52
1:A:1:MET:HB3	1:A:94:PHE:CE1	2.45	0.52
1:A:153:VAL:HB	1:A:177:ALA:HB2	1.92	0.52
1:B:122:ARG:HH11	1:B:210:GLY:HA3	1.75	0.52
1:A:41:LYS:HE3	1:A:243:GLN:NE2	2.25	0.52
1:A:199:LYS:HE3	4:A:743:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLU:OE1	1:B:145:ARG:HD3	2.10	0.51
1:B:219:ASP:HB3	1:B:223:LYS:HE2	1.92	0.51
1:B:133:CYS:HG	1:B:166:PHE:HD2	1.58	0.51
1:A:288:PHE:CE1	1:A:290:SER:HB2	2.46	0.51
1:A:194:THR:CG2	4:A:658:HOH:O	2.58	0.51
1:A:203:LYS:HD2	1:A:206:TRP:CZ2	2.45	0.51
1:B:199:LYS:CG	1:B:200:PRO:HD2	2.42	0.50
1:B:158:VAL:HG12	1:B:158:VAL:O	2.12	0.50
1:B:161:LYS:O	1:B:164:LYS:HB2	2.11	0.50
1:B:251:ASN:O	1:B:255:SER:HB2	2.10	0.50
1:B:152:GLU:HG2	1:B:153:VAL:N	2.28	0.49
1:B:197:SER:O	1:B:223:LYS:HB2	2.11	0.49
1:B:279:ARG:NH2	1:B:279:ARG:CG	2.65	0.49
1:B:108:ARG:HG3	1:B:296:GLN:HB3	1.94	0.49
1:B:150:ILE:CG2	1:B:175:ILE:HG21	2.43	0.49
1:A:226:LEU:HB2	1:A:249:GLU:OE2	2.12	0.49
1:B:68:ASN:HD22	1:B:70:HIS:CD2	2.31	0.49
1:A:1:MET:HB3	1:A:94:PHE:CZ	2.47	0.49
1:B:26:GLU:OE2	1:B:29:ARG:NH1	2.45	0.49
1:A:201:VAL:O	1:A:201:VAL:CG1	2.61	0.48
1:A:201:VAL:O	1:A:201:VAL:HG12	2.11	0.48
1:B:193:THR:OG1	1:B:215:ALA:HA	2.14	0.48
1:A:156:TYR:CE1	3:A:400:NAD:H2A	2.48	0.48
1:A:20:ALA:HB2	1:A:107:LEU:HD13	1.95	0.48
1:A:28:PHE:CZ	1:A:296:GLN:NE2	2.82	0.48
1:A:261:VAL:HG22	4:A:769:HOH:O	2.14	0.47
1:B:204:ALA:HB2	1:B:229:GLU:HB3	1.97	0.47
1:A:48:LYS:HD2	1:B:91:GLU:OE2	2.14	0.47
1:B:219:ASP:H	1:B:223:LYS:CE	2.26	0.47
1:B:228:VAL:O	1:B:231:LEU:HB2	2.14	0.47
3:B:401:NAD:H6N	4:B:684:HOH:O	2.14	0.47
1:B:128:PHE:CD2	1:B:190:VAL:HB	2.50	0.47
1:B:188:CYS:HB3	4:B:687:HOH:O	2.15	0.47
1:B:163:ALA:O	1:B:167:VAL:HB	2.15	0.47
1:A:70:HIS:HB2	1:A:73:ASN:ND2	2.30	0.47
1:A:48:LYS:HB2	4:A:673:HOH:O	2.14	0.47
1:B:1:MET:HG3	1:B:94:PHE:CZ	2.50	0.47
1:B:15:ILE:CD1	1:B:300:VAL:HG22	2.44	0.47
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.79	0.46
1:B:229:GLU:OE2	1:B:232:LYS:HD3	2.15	0.46
1:B:55:PRO:HB3	1:B:64:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ALA:HB1	1:B:179:VAL:HG22	1.97	0.46
1:B:179:VAL:O	1:B:180:GLN:CG	2.58	0.46
1:B:118:LYS:HE3	1:B:119:TYR:CE2	2.51	0.46
1:B:122:ARG:NH2	1:B:189:ASP:OD1	2.48	0.46
1:A:232:LYS:HE2	4:A:523:HOH:O	2.16	0.46
1:B:156:TYR:HE1	3:B:401:NAD:H2A	1.81	0.46
1:B:74:PRO:HG2	1:B:75:ASP:H	1.81	0.46
1:A:302:LYS:HE3	1:A:306:GLU:OE1	2.15	0.46
1:B:14:LEU:HD21	1:B:313:VAL:CG1	2.30	0.45
1:B:209:GLU:HA	4:B:681:HOH:O	2.17	0.45
1:B:156:TYR:CD1	1:B:156:TYR:C	2.87	0.45
1:B:267:THR:HG23	4:B:636:HOH:O	2.16	0.45
1:B:150:ILE:HG21	1:B:175:ILE:HG21	1.99	0.45
1:A:8:GLN:HG3	1:A:100:ASP:OD2	2.17	0.45
1:A:311:LYS:HB2	1:A:313:VAL:HG23	1.99	0.45
1:A:261:VAL:CA	4:A:769:HOH:O	2.59	0.44
1:B:243:GLN:NE2	1:B:291:THR:OG1	2.50	0.44
1:B:219:ASP:HB3	1:B:223:LYS:CE	2.46	0.44
1:B:182:ALA:HB1	1:B:206:TRP:CZ3	2.52	0.44
1:B:53:ALA:HB1	1:B:64:LEU:HD11	1.99	0.44
1:B:235:LYS:HG3	1:B:286:THR:HG22	1.98	0.44
1:A:194:THR:HG23	4:A:658:HOH:O	2.16	0.44
1:B:74:PRO:C	1:B:76:LYS:N	2.71	0.44
1:B:48:LYS:HB2	4:B:559:HOH:O	2.17	0.44
1:B:104:THR:HB	1:B:300:VAL:HG11	1.99	0.44
1:B:235:LYS:CG	1:B:286:THR:HG22	2.48	0.43
1:A:238:VAL:HG21	1:A:241:LEU:HA	1.99	0.43
1:B:161:LYS:O	1:B:165:LYS:HG2	2.18	0.43
1:B:242:GLU:HB2	4:B:668:HOH:O	2.19	0.43
1:A:104:THR:HB	1:A:300:VAL:HG11	2.01	0.43
1:B:199:LYS:O	1:B:200:PRO:C	2.56	0.43
1:B:150:ILE:CG2	1:B:151:GLY:N	2.79	0.43
1:A:90:PRO:O	1:B:70:HIS:HE1	2.02	0.43
1:B:67:VAL:HG23	1:B:83:ALA:HB2	2.00	0.43
1:B:108:ARG:CG	1:B:296:GLN:HB3	2.48	0.42
1:B:12:GLU:HG2	1:B:103:TYR:CD1	2.54	0.42
1:A:233:LYS:CG	1:A:233:LYS:O	2.67	0.42
1:A:46:PHE:CD1	1:A:50:ASP:HA	2.55	0.42
1:B:58:LEU:HG	1:B:59:MET:HG3	2.01	0.42
1:B:219:ASP:N	1:B:223:LYS:HE2	2.30	0.42
1:B:204:ALA:HA	1:B:230:ILE:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLN:O	1:A:12:GLU:HG3	2.20	0.42
1:A:187:ARG:NH1	4:A:689:HOH:O	2.52	0.42
1:A:31:TYR:HB2	1:A:295:ILE:HD13	2.00	0.42
1:B:267:THR:HB	1:B:270:GLU:OE2	2.20	0.42
1:A:50:ASP:OD1	1:A:50:ASP:C	2.58	0.42
1:B:216:ILE:HD12	4:B:778:HOH:O	2.20	0.42
1:B:46:PHE:CD1	1:B:50:ASP:HA	2.55	0.42
1:B:31:TYR:HD2	4:B:799:HOH:O	2.02	0.41
1:A:131:ILE:HG12	1:A:191:LEU:HD11	2.02	0.41
1:A:186:SER:HA	1:A:191:LEU:HD13	2.02	0.41
1:A:156:TYR:HB2	1:A:180:GLN:O	2.21	0.41
1:A:219:ASP:C	1:A:219:ASP:OD1	2.58	0.41
1:B:79:PRO:HG2	1:B:82:MET:CG	2.49	0.41
1:B:235:LYS:HE2	1:B:265:HIS:CG	2.55	0.41
1:B:140:GLN:O	1:B:144:LEU:HD22	2.21	0.41
1:A:261:VAL:O	1:A:261:VAL:HG12	2.20	0.41
1:B:70:HIS:O	1:B:73:ASN:HB2	2.21	0.41
1:B:26:GLU:OE1	1:B:29:ARG:NH1	2.51	0.41
1:A:136:GLN:NE2	1:A:136:GLN:HA	2.35	0.41
1:A:65:LYS:HE3	1:A:67:VAL:HG21	2.02	0.41
1:B:235:LYS:HA	1:B:235:LYS:HE3	2.02	0.41
1:B:122:ARG:CZ	1:B:210:GLY:O	2.69	0.41
1:A:152:GLU:HG2	1:A:153:VAL:N	2.36	0.41
1:B:267:THR:HG23	1:B:269:GLY:H	1.86	0.41
1:B:150:ILE:CG2	1:B:151:GLY:H	2.28	0.41
1:A:42:VAL:CG2	1:B:42:VAL:HG21	2.46	0.41
1:A:223:LYS:NZ	3:A:400:NAD:O2D	2.54	0.41
1:B:14:LEU:HD13	1:B:308:ALA:HB2	2.03	0.41
1:A:7:THR:HG23	1:A:10:GLU:OE2	2.21	0.41
1:B:195:THR:HG23	1:B:225:GLU:OE2	2.21	0.40
1:A:15:ILE:HG13	1:A:304:VAL:HG23	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:O	1:B:29:ARG:NH2[1_545]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	318/322 (99%)	308 (97%)	9 (3%)	1 (0%)	46 56
1	B	318/322 (99%)	279 (88%)	28 (9%)	11 (4%)	4 2
All	All	636/644 (99%)	587 (92%)	37 (6%)	12 (2%)	10 8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	B	206	TRP
1	B	151	GLY
1	B	181	PRO
1	B	182	ALA
1	B	218	ALA
1	B	158	VAL
1	B	200	PRO
1	B	228	VAL
1	B	75	ASP
1	B	71	PRO
1	B	284	GLU

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	256/258 (99%)	244 (95%)	12 (5%)	32 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	256/258 (99%)	224 (88%)	32 (12%)	6 5
All	All	512/516 (99%)	468 (91%)	44 (9%)	13 15

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	67	VAL
1	A	71	PRO
1	A	87	LEU
1	A	96	LEU
1	A	107	LEU
1	A	120	LEU
1	A	171	GLU
1	A	173	ARG
1	A	176	SER
1	A	194	THR
1	A	239	ASP
1	B	30	LEU
1	B	33	LEU
1	B	78	LEU
1	B	91	GLU
1	B	108	ARG
1	B	120	LEU
1	B	124	ASN
1	B	141	LEU
1	B	142	GLU
1	B	144	LEU
1	B	156	TYR
1	B	167	VAL
1	B	170	CYS
1	B	173	ARG
1	B	187	ARG
1	B	188	CYS
1	B	191	LEU
1	B	195	THR
1	B	198	ARG
1	B	200	PRO
1	B	223	LYS
1	B	235	LYS
1	B	239	ASP
1	B	251	ASN

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Mol	Chain	Res	Type
1	B	255	SER
1	B	267	THR
1	B	279	ARG
1	B	281	SER
1	B	300	VAL
1	B	309	LEU
1	B	313	VAL
1	B	316	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	68	ASN
1	A	243	GLN
1	A	265	HIS
1	A	312	ASN
1	B	70	HIS
1	B	243	GLN

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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	NAD	A	400	-	38,48,48	2.62	13 (34%)	47,73,73	2.65	13 (27%)
3	NAD	B	401	-	38,48,48	2.65	14 (36%)	47,73,73	2.84	16 (34%)

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
3	NAD	A	400	-	-	0/22/62/62	0/5/5/5
3	NAD	B	401	-	-	0/22/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAD	O3B-C3B	2.03	1.47	1.43
3	B	401	NAD	C3D-C4D	2.16	1.58	1.53
3	A	400	NAD	O4B-C4B	2.16	1.50	1.45
3	A	400	NAD	PN-O5D	2.19	1.69	1.59
3	A	400	NAD	C7N-N7N	2.29	1.37	1.33
3	A	400	NAD	C4A-N3A	2.30	1.39	1.35
3	B	401	NAD	C7N-N7N	2.35	1.37	1.33
3	A	400	NAD	O3B-C3B	2.41	1.48	1.43
3	B	401	NAD	C3B-C4B	2.60	1.60	1.53
3	B	401	NAD	O4B-C4B	2.70	1.51	1.45
3	A	400	NAD	C3B-C4B	2.83	1.60	1.53
3	B	401	NAD	O4D-C4D	2.92	1.51	1.45
3	A	400	NAD	O5D-C5D	3.16	1.57	1.44
3	B	401	NAD	O4B-C1B	3.24	1.45	1.41
3	B	401	NAD	C5N-C4N	3.29	1.45	1.38
3	A	400	NAD	C5N-C4N	3.39	1.45	1.38
3	B	401	NAD	O4D-C1D	3.60	1.45	1.41
3	A	400	NAD	C2N-C3N	3.73	1.44	1.39
3	B	401	NAD	C2N-C3N	3.76	1.44	1.39
3	A	400	NAD	O4D-C4D	3.87	1.54	1.45
3	B	401	NAD	O5D-C5D	4.12	1.61	1.44
3	B	401	NAD	C4A-N3A	4.97	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAD	C2A-N3A	5.36	1.41	1.32
3	A	400	NAD	C2A-N3A	5.42	1.41	1.32
3	A	400	NAD	O4D-C1D	6.09	1.48	1.41
3	B	401	NAD	C3N-C7N	9.07	1.64	1.50
3	A	400	NAD	C3N-C7N	9.10	1.64	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	NAD	N3A-C2A-N1A	-9.66	121.50	128.89
3	A	400	NAD	N3A-C2A-N1A	-7.79	122.93	128.89
3	A	400	NAD	O4D-C1D-N1N	-6.44	101.05	108.13
3	A	400	NAD	C3N-C2N-N1N	-5.73	113.76	120.36
3	B	401	NAD	C3N-C2N-N1N	-5.69	113.81	120.36
3	A	400	NAD	C5N-C4N-C3N	-5.55	113.36	120.33
3	B	401	NAD	C5N-C4N-C3N	-5.52	113.39	120.33
3	A	400	NAD	O3-PA-O5B	-5.51	88.32	102.94
3	B	401	NAD	O4D-C1D-N1N	-5.35	102.25	108.13
3	B	401	NAD	O3-PN-O5D	-3.98	92.37	102.94
3	B	401	NAD	O3-PA-O5B	-3.43	93.83	102.94
3	A	400	NAD	O4B-C1B-N9A	-2.59	102.68	108.10
3	B	401	NAD	C4D-O4D-C1D	-2.32	107.17	109.72
3	A	400	NAD	O3-PN-O5D	-2.23	97.02	102.94
3	B	401	NAD	O4B-C1B-N9A	-2.06	103.79	108.10
3	A	400	NAD	C2N-C3N-C7N	-2.05	113.35	119.31
3	B	401	NAD	C2N-C3N-C7N	-2.02	113.44	119.31
3	A	400	NAD	O5B-PA-O1A	2.16	117.98	109.62
3	B	401	NAD	O2B-C2B-C3B	2.17	118.88	111.83
3	B	401	NAD	N6A-C6A-N1A	2.26	124.05	119.20
3	A	400	NAD	O2B-C2B-C3B	2.38	119.58	111.83
3	B	401	NAD	O2N-PN-O1N	2.42	125.64	112.53
3	A	400	NAD	C6N-C5N-C4N	2.84	123.73	119.44
3	B	401	NAD	C6N-C5N-C4N	2.84	123.74	119.44
3	A	400	NAD	C2A-N1A-C6A	3.08	124.27	118.77
3	B	401	NAD	C2A-N1A-C6A	3.85	125.64	118.77
3	B	401	NAD	PN-O3-PA	5.78	148.97	132.73
3	B	401	NAD	C2N-C3N-C4N	7.58	126.72	118.29
3	A	400	NAD	C2N-C3N-C4N	7.64	126.79	118.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	NAD	3	0
3	B	401	NAD	5	0

5.7 Other polymers

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	320/322 (99%)	-0.28	3 (0%) 85 89	13, 24, 38, 52	0
1	B	320/322 (99%)	0.48	45 (14%) 4 6	14, 39, 62, 67	0
All	All	640/644 (99%)	0.10	48 (7%) 17 24	13, 27, 61, 67	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	GLU	6.2
1	B	151	GLY	6.0
1	B	187	ARG	4.5
1	B	198	ARG	4.3
1	B	149	ASP	4.1
1	B	158	VAL	4.0
1	B	255	SER	4.0
1	B	183	GLU	4.0
1	B	199	LYS	4.0
1	A	47	GLU	3.7
1	B	150	ILE	3.6
1	B	203	LYS	3.2
1	B	168	SER	3.2
1	B	205	GLU	3.1
1	B	220	GLY	3.1
1	B	209	GLU	3.0
1	B	171	GLU	3.0
1	B	280	GLU	2.9
1	B	261	VAL	2.9
1	B	178	SER	2.9
1	B	160	GLU	2.7
1	B	162	ALA	2.7
1	B	180	GLN	2.6
1	B	170	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	165	LYS	2.6
1	A	262	GLU	2.6
1	A	261	VAL	2.6
1	B	75	ASP	2.5
1	B	176	SER	2.5
1	B	206	TRP	2.5
1	B	124	ASN	2.5
1	B	210	GLY	2.5
1	B	177	ALA	2.4
1	B	167	VAL	2.3
1	B	234	ALA	2.3
1	B	189	ASP	2.3
1	B	134	GLY	2.3
1	B	274	GLY	2.3
1	B	246	HIS	2.3
1	B	256	LYS	2.2
1	B	281	SER	2.2
1	B	229	GLU	2.2
1	B	123	LYS	2.1
1	B	1	MET	2.1
1	B	185	ALA	2.1
1	B	251	ASN	2.1
1	B	259	ILE	2.1
1	B	164	LYS	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
2	NA	B	901	1/1	0.95	0.33	5.11	22,22,22,22	0
3	NAD	B	401	44/44	0.85	0.32	2.28	31,35,47,50	0
3	NAD	A	400	44/44	0.87	0.21	1.92	24,39,45,46	0
2	NA	A	900	1/1	0.96	0.12	0.38	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.