Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID	:	1X87
Title	:	2.4A X-ray structure of Urocanase protein complexed with NAD
Authors	:	Tereshko, V.; Zaborske, J.; Gilbreth, R.; Dementieva, I.; Collart, F.; Joachimiak, A.; Kossiakoff, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2004-08-17
Resolution	:	2.40 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 ①) were used in the production of this report:

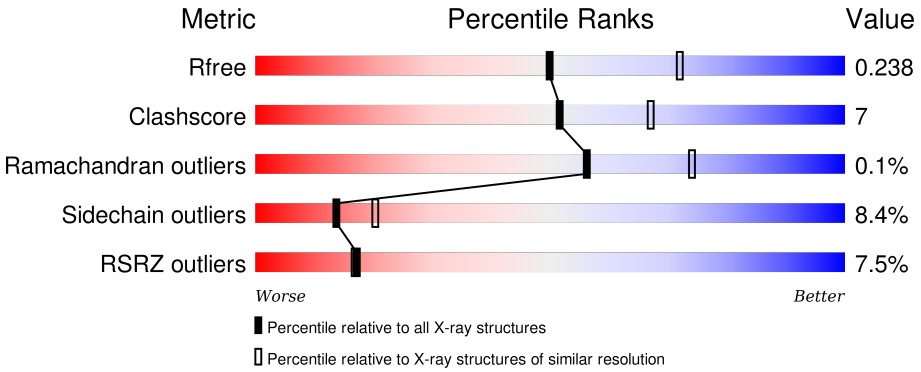
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	551	3% 71% 17% • 10%
1	B	551	10% 72% 14% • • 11%

2 Entry composition

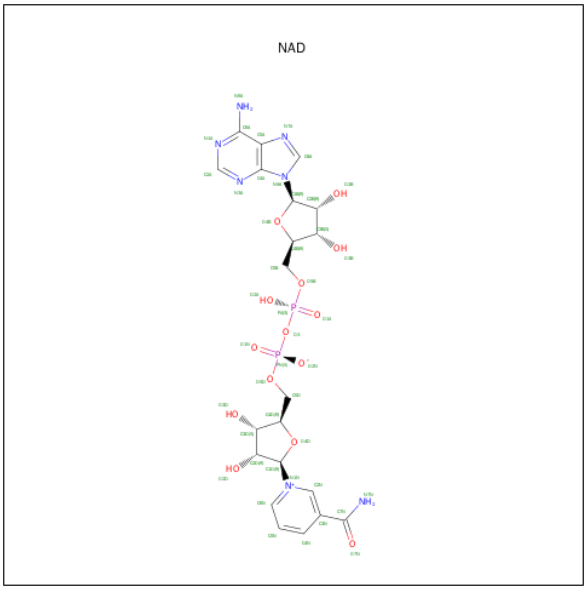
There are 3 unique types of molecules in this entry. The entry contains 7883 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Urocanase protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	Se	0	2	0
			3811	2412	681	699	5	14			
1	B	493	Total	C	N	O	S	Se	0	0	0
			3766	2371	671	705	5	14			

- 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		

- Molecule 3 is water.

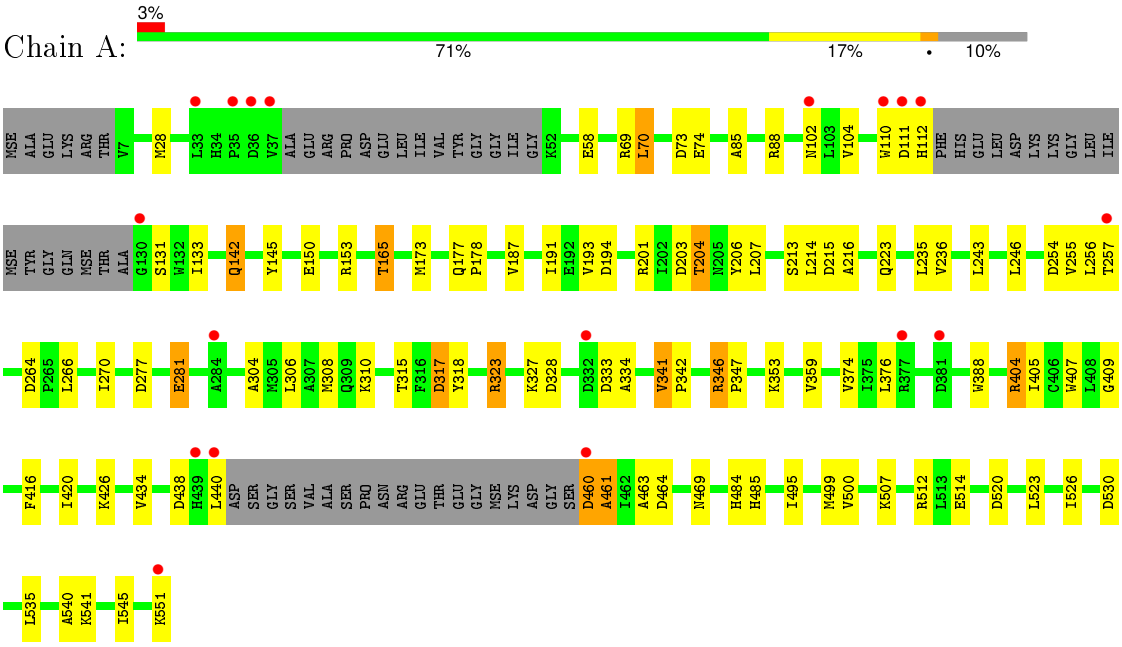
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	156	Total O 156 156	0	0
3	B	62	Total O 62 62	0	0

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.

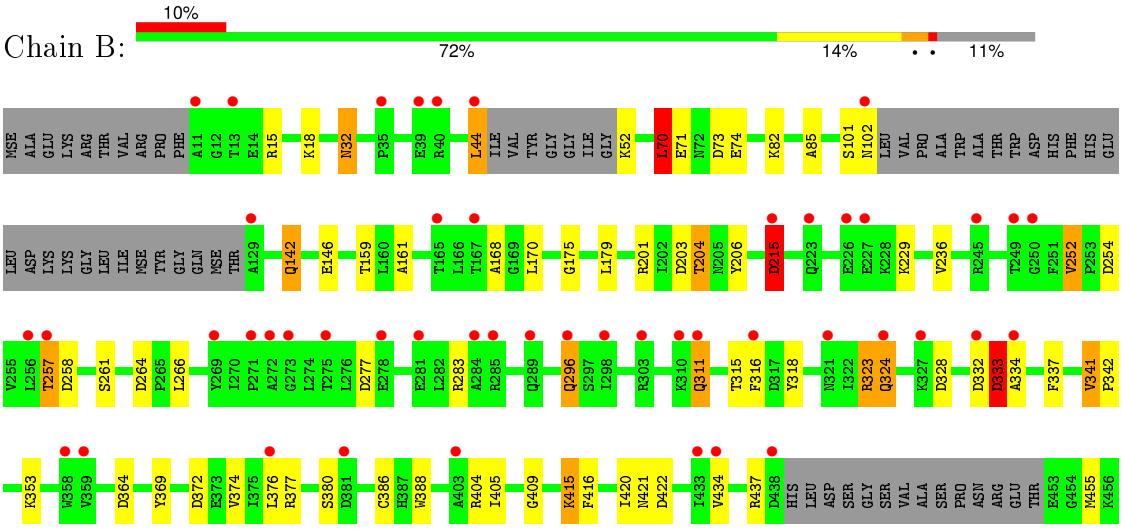
- Molecule 1: Urocanase protein

Chain A:



- Molecule 1: Urocanase protein

Chain B:




D457
G458
S459
D460
A463
N469
H485
Y489
G490
M491
G492
Y493
S494
I495
M499
V500
G505
R512
L513
E514
T519
D520
I526
R527
H528
L535
A540
K541
E542
I545
D546
M547
P548
M549
L550
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.12Å 101.61Å 113.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.40) 99.8 (19.98-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.187 , 0.232 0.192 , 0.238	Depositor DCC
R_{free} test set	2323 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.2	EDS
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 45924 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7883	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: 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	0.64	0/3887	1.04	18/5245 (0.3%)
1	B	0.54	0/3821	1.00	16/5147 (0.3%)
All	All	0.59	0/7708	1.02	34/10392 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	512	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	A	111	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	254	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	364	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	264	ASP	CB-CG-OD2	7.03	124.62	118.30
1	A	520	ASP	CB-CG-OD2	6.91	124.51	118.30
1	B	203	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	460	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	264	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	404	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	317	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	333	ASP	CB-CG-OD2	6.16	123.85	118.30
1	A	201	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	277	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	512	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	520	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	323	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	328	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	422	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	328	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	73	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	194	ASP	CB-CG-OD2	5.62	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	254	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	457	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	512	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	333	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	438	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	73	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	332	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	215	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	70	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	277	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	215	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3811	0	3806	56	0
1	B	3766	0	3758	58	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
3	A	156	0	0	0	0
3	B	62	0	0	3	0
All	All	7883	0	7616	104	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 7.

All (104) 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:324:GLN:HE21	1:B:324:GLN:HA	1.40	0.85
1:A:243:LEU:HG	1:A:308[B]:MSE:HE1	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:THR:HG23	1:A:206:TYR:HD1	1.52	0.74
1:A:150:GLU:OE1	1:A:153:ARG:NH2	2.22	0.73
1:B:463:ALA:HB1	1:B:495:ILE:HD12	1.70	0.72
1:B:415:LYS:NZ	1:B:415:LYS:HB3	2.08	0.69
1:A:526:ILE:HD13	1:B:85:ALA:HB2	1.77	0.68
1:A:461:ALA:HA	1:B:101:SER:OG	1.94	0.66
1:B:170:LEU:O	1:B:201:ARG:NH1	2.30	0.64
1:B:142:GLN:HG2	1:B:405:ILE:HG23	1.81	0.63
1:B:168:ALA:HB3	1:B:258:ASP:OD2	1.99	0.63
1:B:415:LYS:HZ2	1:B:415:LYS:HB3	1.65	0.62
1:A:317:ASP:HB2	1:A:323:ARG:HD2	1.81	0.61
1:A:374:VAL:HG22	1:A:416:PHE:HE1	1.66	0.61
1:A:526:ILE:HD13	1:B:85:ALA:CB	2.30	0.60
1:B:527:ARG:NE	3:B:856:HOH:O	2.31	0.60
1:A:142:GLN:HG2	1:A:405:ILE:HG23	1.84	0.60
1:A:464:ASP:OD2	1:B:485:HIS:NE2	2.33	0.59
1:A:28:MSE:HE2	1:A:133:ILE:HG22	1.84	0.59
1:B:416:PHE:CZ	1:B:420:ILE:HD11	2.37	0.59
1:B:266:LEU:O	1:B:283:ARG:HD3	2.02	0.59
1:A:165:THR:HB	1:A:255:VAL:HB	1.85	0.58
1:A:85:ALA:HB2	1:B:526:ILE:HD13	1.85	0.58
1:B:32:ASN:ND2	3:B:805:HOH:O	2.37	0.58
1:A:191:ILE:N	1:A:191:ILE:HD13	2.20	0.57
1:A:541:LYS:NZ	1:A:551:LYS:HG3	2.19	0.57
1:A:485[B]:HIS:CE1	1:B:495:ILE:HD11	2.40	0.56
1:A:463:ALA:HB1	1:A:495:ILE:HD12	1.88	0.56
1:A:256:LEU:HD21	1:A:308[B]:MSE:HE3	1.88	0.56
1:A:214:LEU:HD11	1:A:246:LEU:HD21	1.90	0.53
1:B:204:THR:HG23	1:B:206:TYR:HD1	1.73	0.53
1:B:257:THR:HG21	1:B:316:PHE:CE2	2.44	0.53
1:A:204:THR:HG23	1:A:206:TYR:CD1	2.38	0.53
1:A:88:ARG:NH1	1:B:514:GLU:OE2	2.42	0.52
1:B:323:ARG:HD2	1:B:337:PHE:CE1	2.44	0.52
1:A:173:MSE:HE3	2:A:600:NAD:O2N	2.10	0.52
1:B:353:LYS:HA	1:B:409:GLY:HA2	1.91	0.52
1:B:44:LEU:HA	1:B:52:LYS:HG2	1.91	0.52
1:B:159:THR:HG22	1:B:161:ALA:H	1.74	0.51
1:A:243:LEU:CG	1:A:308[B]:MSE:HE1	2.36	0.51
1:A:341:VAL:HG22	1:A:342:PRO:HD3	1.92	0.50
1:A:346:ARG:HB3	1:A:347:PRO:HD3	1.93	0.50
1:B:204:THR:HG23	1:B:206:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASP:O	1:A:461:ALA:HB2	2.12	0.50
1:B:324:GLN:HE21	1:B:324:GLN:CA	2.18	0.49
1:A:28:MSE:HE1	1:A:359:VAL:HG21	1.94	0.49
1:B:380:SER:HA	1:B:386:CYS:SG	2.52	0.49
1:A:323:ARG:HG2	1:A:334:ALA:O	2.12	0.49
1:B:215:ASP:OD2	1:B:215:ASP:N	2.45	0.49
1:A:485[B]:HIS:CE1	1:A:495:ILE:HG12	2.48	0.49
1:B:142:GLN:HE22	1:B:146:GLU:HG3	1.77	0.49
1:A:541:LYS:HZ3	1:A:551:LYS:HG3	1.78	0.48
1:B:70:LEU:HD22	1:B:74:GLU:HB2	1.95	0.48
1:A:353:LYS:HA	1:A:409:GLY:HA2	1.95	0.47
1:B:257:THR:HG22	1:B:316:PHE:O	2.14	0.47
1:A:374:VAL:HG22	1:A:416:PHE:CE1	2.49	0.47
1:B:526:ILE:HG23	1:B:547:MSE:HE3	1.97	0.47
1:B:519:THR:HG21	3:B:821:HOH:O	2.14	0.47
1:A:416:PHE:CE2	1:A:420:ILE:HD11	2.50	0.47
1:A:145:TYR:CE1	1:A:388:TRP:HB2	2.49	0.47
1:B:324:GLN:NE2	1:B:324:GLN:HA	2.19	0.47
1:B:421:ASN:ND2	1:B:505:GLY:H	2.13	0.47
1:A:177:GLN:HB2	1:A:178:PRO:HD3	1.96	0.46
1:A:193:VAL:HG21	1:A:270:ILE:HG13	1.98	0.46
1:B:526:ILE:HD11	1:B:545:ILE:CG2	2.46	0.46
1:B:296:GLN:HA	1:B:296:GLN:HE21	1.81	0.46
1:A:317:ASP:HB2	1:A:323:ARG:CD	2.45	0.46
1:A:70:LEU:HD22	1:A:74:GLU:HB2	1.97	0.46
1:A:110:TRP:O	1:A:112:HIS:N	2.49	0.46
1:B:493:TYR:HE2	1:B:495:ILE:HD11	1.81	0.45
1:A:191:ILE:HD12	1:A:235:LEU:HD23	1.98	0.45
1:B:142:GLN:HB2	1:B:388:TRP:CZ2	2.52	0.45
1:A:530:ASP:OD1	1:B:82:LYS:NZ	2.39	0.45
1:B:421:ASN:HD21	1:B:505:GLY:H	1.65	0.44
1:B:175:GLY:HA3	1:B:201:ARG:HD2	1.99	0.44
1:B:252:VAL:HG11	1:B:311:GLN:HG2	2.00	0.44
1:B:437:ARG:NE	1:B:520:ASP:OD1	2.46	0.44
1:B:437:ARG:NH2	1:B:469:ASN:HD21	2.16	0.44
1:A:102:ASN:ND2	1:A:484:HIS:NE2	2.56	0.44
1:A:434:VAL:HG13	1:A:500:VAL:HG13	1.99	0.43
1:A:142:GLN:HB3	1:A:388:TRP:CH2	2.53	0.43
1:B:341:VAL:HG22	1:B:342:PRO:HD3	2.00	0.43
1:B:333:ASP:N	1:B:333:ASP:OD1	2.41	0.43
1:B:455:MSE:HE1	1:B:528:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ILE:HD11	1:A:545:ILE:CG2	2.48	0.42
1:A:281:GLU:C	1:A:281:GLU:OE1	2.57	0.42
1:A:304:ALA:O	1:A:308[B]:MSE:HG3	2.20	0.42
1:B:333:ASP:O	1:B:334:ALA:C	2.58	0.42
1:A:460:ASP:O	1:A:461:ALA:CB	2.67	0.42
1:A:463:ALA:HB3	1:B:485:HIS:CE1	2.54	0.42
1:B:540:ALA:HA	1:B:545:ILE:HD12	2.01	0.41
1:B:434:VAL:HG13	1:B:500:VAL:HG13	2.02	0.41
1:B:369:TYR:O	1:B:372:ASP:HB2	2.20	0.41
1:A:540:ALA:HA	1:A:545:ILE:HD12	2.02	0.41
1:A:85:ALA:CB	1:B:526:ILE:HD13	2.50	0.41
1:B:257:THR:CG2	1:B:316:PHE:CE2	3.02	0.41
1:B:311:GLN:HE21	1:B:311:GLN:HA	1.86	0.41
1:A:317:ASP:OD2	1:A:323:ARG:HD3	2.21	0.41
1:A:213:SER:HB3	1:A:216:ALA:HB3	2.02	0.41
1:B:257:THR:CG2	1:B:316:PHE:CD2	3.03	0.41
1:A:142:GLN:CB	1:A:388:TRP:CH2	3.04	0.41
1:A:469:ASN:HB2	1:A:523:LEU:HD23	2.02	0.40
1:A:142:GLN:HE22	1:A:407:TRP:HE1	1.68	0.40
1:B:18:LYS:NZ	1:B:71:GLU:OE2	2.47	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	489/551 (89%)	474 (97%)	14 (3%)	1 (0%)	52 69
1	B	485/551 (88%)	463 (96%)	22 (4%)	0	100 100
All	All	974/1102 (88%)	937 (96%)	36 (4%)	1 (0%)	56 74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	ALA

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	389/414 (94%)	358 (92%)	31 (8%)	15 23
1	B	383/414 (92%)	349 (91%)	34 (9%)	12 18
All	All	772/828 (93%)	707 (92%)	65 (8%)	14 20

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	69	ARG
1	A	70	LEU
1	A	104	VAL
1	A	131	SER
1	A	142	GLN
1	A	165	THR
1	A	187	VAL
1	A	204	THR
1	A	207	LEU
1	A	223	GLN
1	A	236	VAL
1	A	257	THR
1	A	266	LEU
1	A	281	GLU
1	A	306	LEU
1	A	310	LYS
1	A	315	THR
1	A	318	TYR
1	A	327	LYS
1	A	341	VAL
1	A	346	ARG
1	A	376	LEU

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Mol	Chain	Res	Type
1	A	404	ARG
1	A	426	LYS
1	A	440	LEU
1	A	460	ASP
1	A	499	MSE
1	A	507	LYS
1	A	514	GLU
1	A	535	LEU
1	B	15	ARG
1	B	32	ASN
1	B	44	LEU
1	B	70	LEU
1	B	102	ASN
1	B	142	GLN
1	B	179	LEU
1	B	204	THR
1	B	215	ASP
1	B	229	LYS
1	B	236	VAL
1	B	252	VAL
1	B	257	THR
1	B	261	SER
1	B	296	GLN
1	B	311	GLN
1	B	315	THR
1	B	318	TYR
1	B	323	ARG
1	B	324	GLN
1	B	333	ASP
1	B	341	VAL
1	B	374	VAL
1	B	376	LEU
1	B	377	ARG
1	B	404	ARG
1	B	415	LYS
1	B	460	ASP
1	B	491	MSE
1	B	499	MSE
1	B	519	THR
1	B	527	ARG
1	B	535	LEU
1	B	549	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	223	GLN
1	A	289	GLN
1	A	324	GLN
1	A	473	ASN
1	B	102	ASN
1	B	142	GLN
1	B	296	GLN
1	B	309	GLN
1	B	311	GLN
1	B	324	GLN
1	B	421	ASN
1	B	469	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	A	600	-	38,48,48	1.66	4 (10%)	47,73,73	2.00	6 (12%)
2	NAD	B	600	-	38,48,48	1.67	3 (7%)	47,73,73	2.15	5 (10%)

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	600	-	-	0/22/62/62	0/5/5/5
2	NAD	B	600	-	-	0/22/62/62	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	NAD	O4B-C4B	-2.39	1.39	1.45
2	A	600	NAD	C2A-N1A	2.02	1.37	1.33
2	B	600	NAD	C2A-N1A	2.72	1.39	1.33
2	B	600	NAD	C2A-N3A	2.97	1.37	1.32
2	A	600	NAD	C2A-N3A	3.09	1.37	1.32
2	A	600	NAD	O7N-C7N	8.20	1.41	1.24
2	B	600	NAD	O7N-C7N	8.50	1.42	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	NAD	N3A-C2A-N1A	-12.15	119.59	128.89
2	A	600	NAD	N3A-C2A-N1A	-11.15	120.36	128.89
2	A	600	NAD	PN-O3-PA	-3.10	124.01	132.73
2	A	600	NAD	C4B-O4B-C1B	-2.85	106.59	109.72
2	B	600	NAD	C1B-N9A-C4A	-2.80	122.72	126.94
2	A	600	NAD	C1B-N9A-C4A	-2.43	123.27	126.94
2	B	600	NAD	PN-O3-PA	-2.22	126.49	132.73
2	A	600	NAD	C2N-C3N-C4N	2.34	120.89	118.29
2	B	600	NAD	C3N-C7N-N7N	2.58	120.65	117.82
2	A	600	NAD	O2A-PA-O3	2.60	116.89	105.09
2	B	600	NAD	O4D-C1D-N1N	4.65	113.24	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	NAD	1	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	482/551 (87%)	0.09	18 (3%) 45 46	34, 43, 59, 77	0
1	B	479/551 (86%)	0.48	54 (11%) 7 7	30, 51, 70, 84	0
All	All	961/1102 (87%)	0.28	72 (7%) 17 17	30, 47, 68, 84	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ASP	5.8
1	B	226	GLU	5.3
1	B	269	TYR	5.0
1	A	440	LEU	4.6
1	B	102	ASN	4.5
1	B	298	ILE	4.4
1	A	551	LYS	3.9
1	B	327	LYS	3.7
1	B	275	THR	3.7
1	B	245	ARG	3.7
1	B	332	ASP	3.7
1	A	35	PRO	3.6
1	B	257	THR	3.6
1	A	37	VAL	3.6
1	B	285	ARG	3.6
1	B	256	LEU	3.5
1	A	332	ASP	3.5
1	B	13	THR	3.5
1	B	311	GLN	3.4
1	B	458	GLY	3.3
1	B	44	LEU	3.3
1	B	542	GLU	3.2
1	B	296	GLN	3.2
1	B	381	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	284	ALA	3.0
1	B	457	ASP	3.0
1	A	33	LEU	2.9
1	A	112	HIS	2.9
1	A	110	TRP	2.8
1	B	11	ALA	2.7
1	A	102	ASN	2.7
1	B	376	LEU	2.7
1	B	273	GLY	2.7
1	A	460	ASP	2.7
1	B	334	ALA	2.6
1	B	227	GLU	2.5
1	B	303	ARG	2.5
1	B	321	ASN	2.5
1	B	289	GLN	2.4
1	B	490	GLY	2.4
1	A	439	HIS	2.4
1	A	257	THR	2.4
1	B	324	GLN	2.4
1	B	278	GLU	2.3
1	B	438	ASP	2.3
1	B	310	LYS	2.3
1	B	434	VAL	2.3
1	B	40	ARG	2.3
1	A	381	ASP	2.3
1	B	281	GLU	2.3
1	B	250	GLY	2.3
1	B	272	ALA	2.3
1	B	460	ASP	2.2
1	A	130	GLY	2.2
1	B	165	THR	2.2
1	A	377	ARG	2.2
1	B	215	ASP	2.2
1	B	129	ALA	2.2
1	B	358	TRP	2.2
1	B	359	VAL	2.1
1	B	249	THR	2.1
1	B	433	ILE	2.1
1	B	39	GLU	2.1
1	B	316	PHE	2.1
1	B	403	ALA	2.1
1	B	167	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	284	ALA	2.1
1	B	223	GLN	2.1
1	B	489	VAL	2.1
1	B	271	PRO	2.1
1	A	111	ASP	2.0
1	B	35	PRO	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	NAD	B	600	44/44	0.93	0.16	-0.13	52,55,67,68	0
2	NAD	A	600	44/44	0.95	0.12	-0.60	34,37,50,51	0

6.5 Other polymers (i)

There are no such residues in this entry.