



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:57 PM GMT

PDB ID : 1MUU
Title : 2.0 Å crystal structure of GDP-mannose dehydrogenase
Authors : Snook, C.F.; Tipton, P.A.; Beamer, L.J.
Deposited on : 2002-09-24
Resolution : 2.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

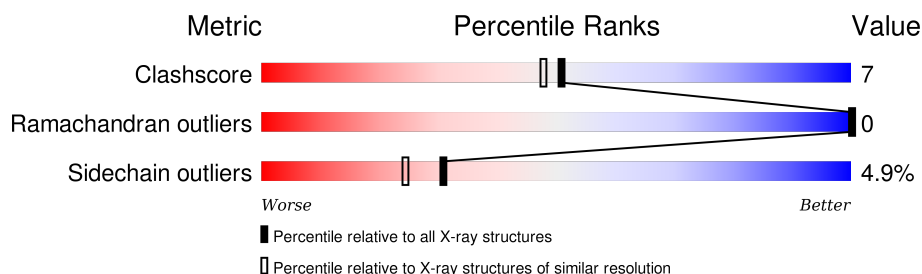
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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))
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	
1	B	436	
1	C	436	
1	D	436	

2 Entry composition [i](#)

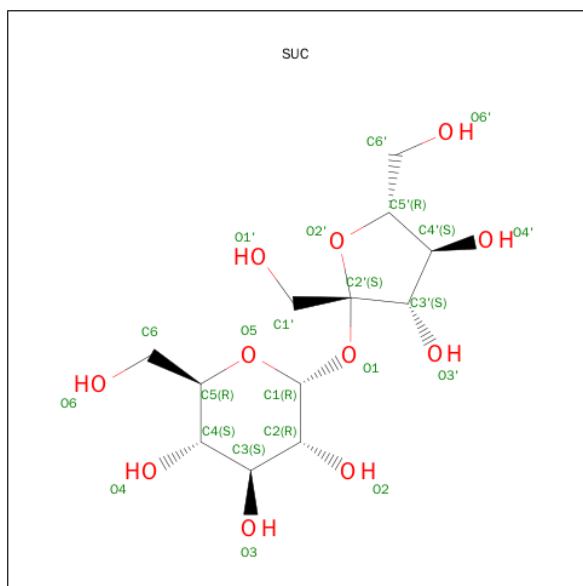
There are 5 unique types of molecules in this entry. The entry contains 14082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GDP-mannose 6-dehydrogenase.

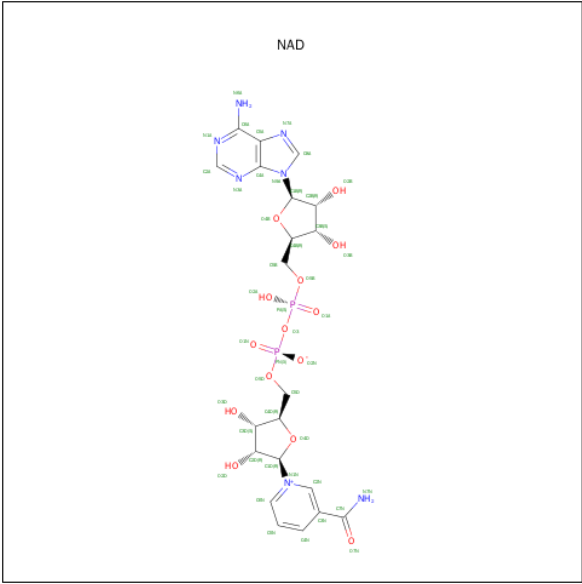
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	Se	0	0	0
			3193	2020	555	600	9	9			
1	B	436	Total	C	N	O	S	Se	0	0	0
			3210	2027	556	609	9	9			
1	C	436	Total	C	N	O	S	Se	0	0	0
			3227	2039	558	612	9	9			
1	D	436	Total	C	N	O	S	Se	0	0	0
			3226	2038	558	612	9	9			

- Molecule 2 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



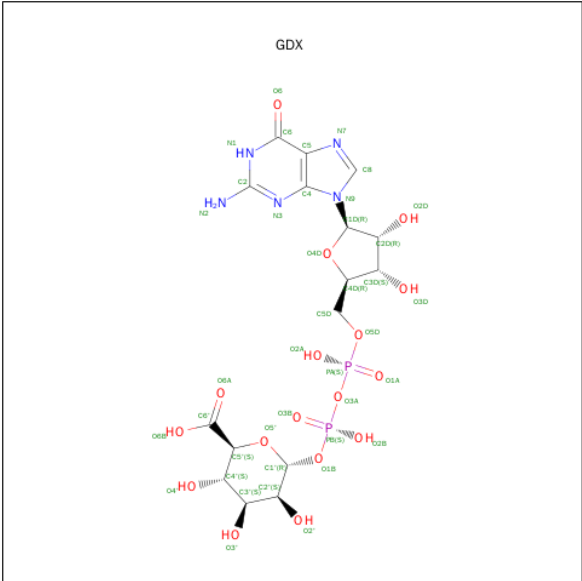
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	C	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	D	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

- Molecule 4 is GUANOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), P'-D-MANNOPYRANOSYL ESTER (three-letter code: GDX) (formula: C₁₆H₂₃N₅O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 40	C 16	N 5	O 17	P 2	0	0
4	B	1	Total 40	C 16	N 5	O 17	P 2	0	0
4	D	1	Total 40	C 16	N 5	O 17	P 2	0	0
4	D	1	Total 40	C 16	N 5	O 17	P 2	0	0

- Molecule 5 is water.

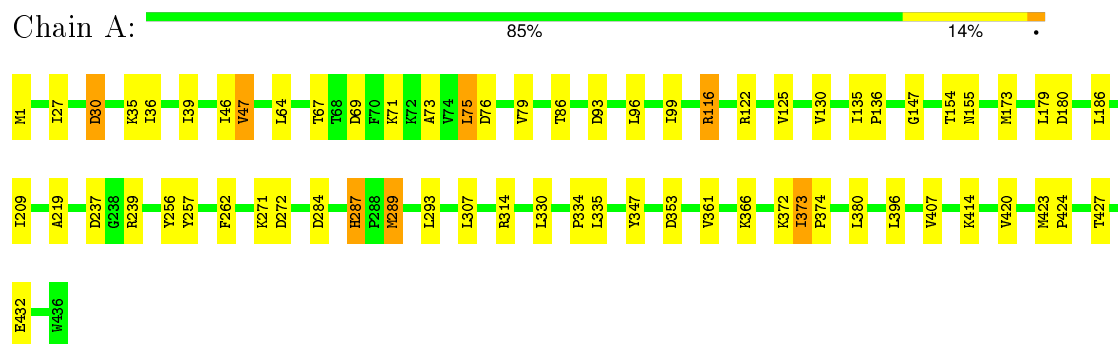
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total 183	O 183	0	0
5	B	222	Total 222	O 222	0	0
5	C	241	Total 241	O 241	0	0
5	D	257	Total 257	O 257	0	0

3 Residue-property plots

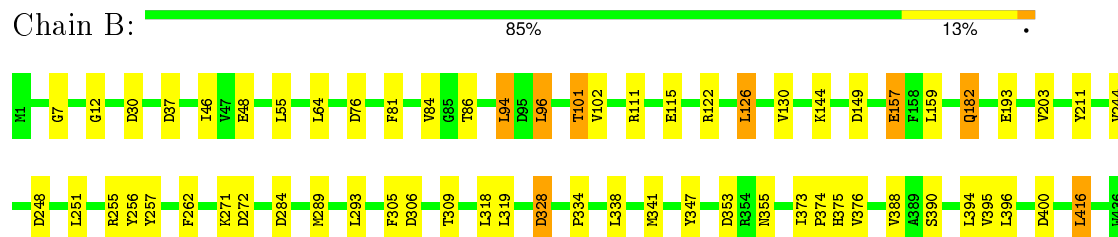
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

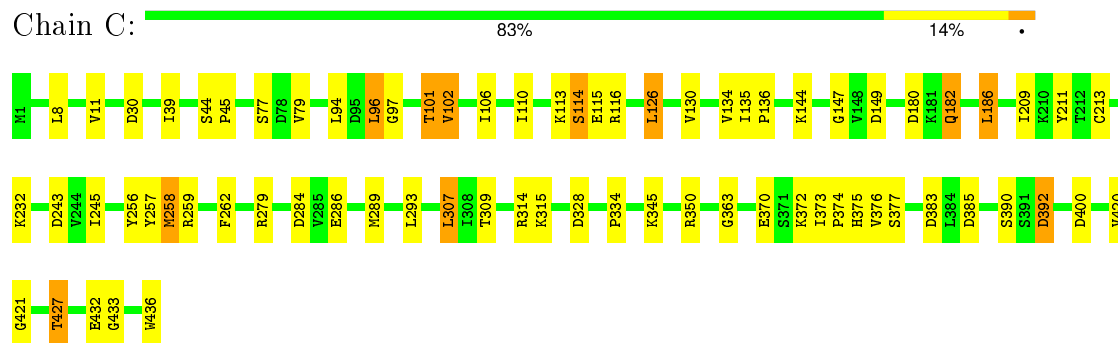
- Molecule 1: GDP-mannose 6-dehydrogenase



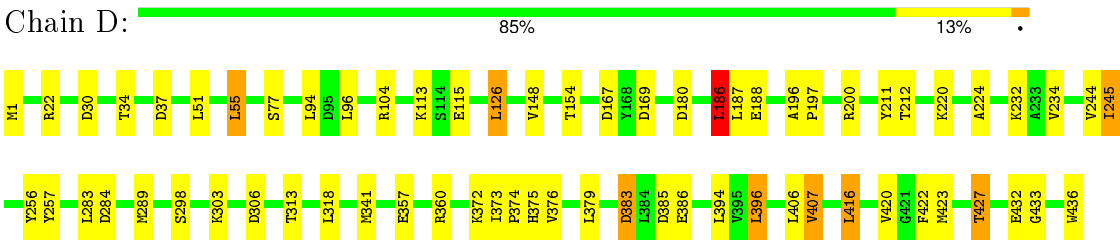
- Molecule 1: GDP-mannose 6-dehydrogenase



- Molecule 1: GDP-mannose 6-dehydrogenase



- Molecule 1: GDP-mannose 6-dehydrogenase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	82.50 Å 82.50 Å 310.17 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.02	Depositor
% Data completeness (in resolution range)	99.1 (50.00-2.02)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.209 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14082	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDX, SUC, 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	0.49	1/3238 (0.0%)	0.77	8/4391 (0.2%)
1	B	0.50	0/3254	0.77	9/4407 (0.2%)
1	C	0.51	0/3272	0.79	7/4430 (0.2%)
1	D	0.52	0/3272	0.79	9/4432 (0.2%)
All	All	0.50	1/13036 (0.0%)	0.78	33/17660 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	MSE	SE-CE	-5.14	1.65	1.95

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	284	ASP	CB-CG-OD2	6.46	124.11	118.30
1	D	306	ASP	CB-CG-OD2	6.17	123.85	118.30
1	C	284	ASP	CB-CG-OD2	6.08	123.78	118.30
1	D	385	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	272	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	400	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	306	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	30	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	383	ASP	CB-CG-OD2	5.83	123.55	118.30
1	D	284	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	284	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	180	ASP	CB-CG-OD2	5.68	123.41	118.30
1	D	37	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	392	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	30	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	180	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	328	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	167	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	353	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	272	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	69	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	400	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	149	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	186	LEU	CA-CB-CG	5.15	127.14	115.30
1	B	37	ASP	CB-CG-OD2	5.15	122.93	118.30
1	C	328	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	353	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	76	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	93	ASP	CB-CG-OD2	5.05	122.84	118.30
1	C	180	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	30	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3193	0	3111	53	0
1	B	3210	0	3155	44	0
1	C	3227	0	3182	67	1
1	D	3226	0	3173	47	1
2	C	23	0	22	2	0
3	A	35	0	19	1	0
3	B	35	0	19	0	0
3	C	35	0	19	1	0
3	D	35	0	19	0	0
4	B	80	0	32	0	0
4	D	80	0	32	0	0
5	A	183	0	0	2	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	222	0	0	3	6
5	C	241	0	0	9	3
5	D	257	0	0	1	5
All	All	14082	0	12783	180	9

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 (180) 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:315:LYS:NZ	5:C:1232:HOH:O	1.81	1.11
1:C:392:ASP:OD1	2:C:1009:SUC:H62	1.52	1.07
1:A:289:MSE:HE3	1:B:293:LEU:CD2	1.91	1.01
1:A:116:ARG:NH2	1:A:147:GLY:O	1.99	0.94
1:A:1:MSE:HE1	1:A:186:LEU:HD21	1.52	0.90
1:A:361:VAL:O	1:A:366:LYS:NZ	2.09	0.85
1:C:293:LEU:CD2	1:D:289:MSE:HE3	2.10	0.82
1:A:289:MSE:HE3	1:B:293:LEU:HD21	1.59	0.82
1:C:286:GLU:OE2	5:C:1044:HOH:O	1.98	0.82
1:A:293:LEU:HD21	1:B:289:MSE:HE3	1.64	0.79
1:A:289:MSE:CE	1:B:293:LEU:HD21	2.11	0.79
1:B:86:THR:HB	1:B:94:LEU:HD12	1.65	0.77
1:C:392:ASP:OD1	2:C:1009:SUC:C6	2.32	0.76
1:B:94:LEU:HD21	1:B:96:LEU:HD11	1.65	0.76
1:B:94:LEU:HD21	1:B:96:LEU:CD1	2.16	0.76
1:C:427:THR:HB	1:C:432:GLU:HA	1.67	0.76
1:C:314:ARG:NH1	5:C:1179:HOH:O	2.18	0.75
1:C:293:LEU:HD21	1:D:289:MSE:HE3	1.68	0.75
1:A:237:ASP:OD1	1:A:239:ARG:HD3	1.89	0.73
1:A:373:ILE:O	1:A:373:ILE:HG23	1.90	0.71
1:C:383:ASP:OD2	1:C:385:ASP:HB2	1.91	0.71
1:B:94:LEU:HB2	5:B:1205:HOH:O	1.90	0.71
1:D:427:THR:CG2	1:D:436:TRP:OXT	2.40	0.70
1:A:373:ILE:N	1:A:374:PRO:HD3	2.08	0.69
1:A:1:MSE:HE2	1:A:79:VAL:HG12	1.73	0.69
1:D:427:THR:HB	1:D:432:GLU:HA	1.74	0.69
1:C:114:SER:O	5:C:1141:HOH:O	2.11	0.68
1:B:81:PHE:HD2	1:B:122:ARG:HG3	1.59	0.67
1:D:427:THR:HG22	1:D:433:GLY:H	1.60	0.67
1:A:71:LYS:O	1:A:75:LEU:HD22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ILE:N	1:C:374:PRO:HD3	2.11	0.66
1:A:122:ARG:HD2	1:A:155:ASN:O	1.96	0.65
1:A:173:MSE:HE3	1:B:248:ASP:HB2	1.79	0.65
1:A:256:TYR:HD2	1:A:257:TYR:CE2	2.15	0.65
1:D:188:GLU:OE1	1:D:200:ARG:NH1	2.29	0.65
1:C:182:GLN:HE21	1:C:182:GLN:H	1.43	0.64
1:D:126:LEU:HD13	1:D:211:TYR:CZ	2.32	0.64
1:A:289:MSE:HE3	1:B:293:LEU:HD23	1.75	0.63
1:C:375:HIS:CD2	1:C:376:VAL:HG23	2.33	0.63
1:A:27:ILE:HD13	1:A:73:ALA:HA	1.80	0.63
1:C:245:ILE:CD1	1:D:212:THR:CG2	2.77	0.63
1:C:245:ILE:HD11	1:D:212:THR:CG2	2.29	0.63
1:A:289:MSE:CE	1:B:293:LEU:CD2	2.69	0.63
1:A:271:LYS:HD2	1:B:86:THR:O	1.98	0.62
1:B:262:PHE:CE2	1:B:334:PRO:HB2	2.34	0.62
1:C:256:TYR:HD2	1:C:257:TYR:CE2	2.18	0.62
1:C:97:GLY:O	1:C:101:THR:HG23	2.00	0.61
1:C:94:LEU:CD2	1:C:96:LEU:HD11	2.31	0.60
1:A:47:VAL:CG1	1:B:328:ASP:HB3	2.31	0.60
1:A:293:LEU:CD2	1:B:289:MSE:HE3	2.29	0.60
1:C:427:THR:CG2	1:C:436:TRP:OXT	2.50	0.60
1:C:116:ARG:NH2	1:C:147:GLY:O	2.35	0.59
1:C:126:LEU:HD13	1:C:211:TYR:CZ	2.38	0.59
1:C:259:ARG:HH11	1:C:259:ARG:HG2	1.68	0.59
1:A:373:ILE:CG2	1:A:373:ILE:O	2.51	0.58
1:C:245:ILE:HD11	1:D:212:THR:HB	1.86	0.58
1:C:77:SER:O	1:C:113:LYS:NZ	2.37	0.58
1:C:293:LEU:HD21	1:D:289:MSE:CE	2.33	0.58
1:A:27:ILE:HD11	1:A:67:THR:HG21	1.85	0.57
1:A:287:HIS:N	1:A:287:HIS:ND1	2.52	0.57
1:C:427:THR:HG22	1:C:436:TRP:OXT	2.04	0.57
1:B:305:PHE:CD1	1:B:341:MSE:HE2	2.41	0.56
1:A:396:LEU:HD12	1:A:396:LEU:N	2.20	0.56
1:D:77:SER:O	1:D:113:LYS:NZ	2.39	0.56
1:A:361:VAL:C	1:A:366:LYS:NZ	2.60	0.55
1:C:245:ILE:CD1	1:D:212:THR:HG22	2.37	0.55
1:C:370:GLU:O	1:C:374:PRO:HG3	2.07	0.55
1:D:256:TYR:HD2	1:D:257:TYR:CE2	2.24	0.54
1:A:373:ILE:N	1:A:374:PRO:CD	2.70	0.54
1:C:258:MSE:HA	1:C:258:MSE:HE3	1.89	0.54
1:D:115:GLU:CD	1:D:115:GLU:H	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:CD2	1:B:96:LEU:HD13	2.38	0.54
1:C:372:LYS:C	1:C:374:PRO:HD3	2.28	0.54
1:D:375:HIS:CD2	1:D:376:VAL:HG23	2.42	0.53
1:D:22:ARG:NH2	1:D:169:ASP:OD1	2.30	0.53
1:C:427:THR:HG21	1:D:232:LYS:NZ	2.25	0.52
1:D:427:THR:HG22	1:D:436:TRP:OXT	2.10	0.52
1:D:1:MSE:HE1	1:D:186:LEU:HD11	1.92	0.52
1:B:373:ILE:N	1:B:374:PRO:HD3	2.23	0.52
1:B:46:ILE:CD1	1:B:48:GLU:HB2	2.40	0.52
1:C:245:ILE:HD11	1:D:212:THR:CB	2.40	0.52
1:A:47:VAL:HG12	1:B:328:ASP:HB3	1.91	0.52
1:C:258:MSE:CE	1:C:258:MSE:HA	2.39	0.52
1:C:374:PRO:HA	1:C:377:SER:OG	2.10	0.51
1:B:182:GLN:H	1:B:182:GLN:HE21	1.56	0.51
1:B:309:THR:HG22	1:B:347:TYR:CZ	2.45	0.51
1:A:27:ILE:HD11	1:A:67:THR:CG2	2.41	0.51
1:C:363:GLY:HA3	5:C:1194:HOH:O	2.09	0.51
1:B:388:VAL:HA	1:B:394:LEU:HD21	1.92	0.51
1:B:94:LEU:CD2	1:B:96:LEU:CD1	2.89	0.50
1:D:423:MSE:HE1	1:D:427:THR:HA	1.92	0.50
1:B:126:LEU:HD13	1:B:211:TYR:CZ	2.46	0.50
1:C:309:THR:HG22	1:C:309:THR:O	2.11	0.50
1:A:396:LEU:HD21	1:A:407:VAL:HG22	1.94	0.50
1:C:309:THR:O	1:C:309:THR:CG2	2.59	0.50
1:C:94:LEU:HG	1:C:96:LEU:CD1	2.42	0.49
1:B:115:GLU:OE1	1:B:115:GLU:N	2.42	0.49
1:C:258:MSE:CE	1:D:224:ALA:HB2	2.42	0.49
1:A:427:THR:CG2	1:A:432:GLU:HG3	2.41	0.49
1:D:407:VAL:HG11	1:D:422:PHE:HB3	1.95	0.49
1:A:237:ASP:OD1	1:A:239:ARG:CD	2.57	0.49
1:A:372:LYS:C	1:A:374:PRO:HD3	2.33	0.49
1:D:51:LEU:HG	1:D:55:LEU:HD22	1.94	0.49
1:A:256:TYR:CD2	1:A:257:TYR:CE2	2.99	0.49
1:C:94:LEU:HD23	1:C:96:LEU:HD11	1.93	0.49
1:C:334:PRO:HG2	5:C:1074:HOH:O	2.13	0.48
1:A:209:ILE:HD13	1:B:244:VAL:HG21	1.94	0.48
1:A:135:ILE:HB	1:A:136:PRO:HD3	1.95	0.48
1:A:71:LYS:O	1:A:75:LEU:CD2	2.60	0.48
1:D:234:VAL:HG12	1:D:234:VAL:O	2.13	0.48
1:C:245:ILE:HD13	1:D:212:THR:HG22	1.95	0.48
1:B:94:LEU:HD21	1:B:96:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:THR:HG21	5:B:1077:HOH:O	2.14	0.48
1:B:86:THR:HB	1:B:94:LEU:CD1	2.38	0.47
1:A:396:LEU:CD1	1:A:396:LEU:N	2.77	0.47
1:C:106:ILE:HG22	1:C:110:ILE:HD12	1.97	0.47
1:B:256:TYR:HD2	1:B:257:TYR:CE2	2.32	0.47
1:B:375:HIS:CD2	1:B:376:VAL:HG23	2.50	0.47
1:C:262:PHE:CE2	1:C:334:PRO:HB2	2.49	0.47
1:C:130:VAL:HA	1:C:134:VAL:HG22	1.95	0.47
1:B:394:LEU:HB2	1:B:416:LEU:HD12	1.97	0.47
1:A:256:TYR:HD2	1:A:257:TYR:CD2	2.33	0.47
1:B:305:PHE:CG	1:B:341:MSE:HE2	2.50	0.46
1:D:427:THR:HG23	1:D:436:TRP:OXT	2.16	0.46
1:A:219:ALA:HA	1:A:289:MSE:HE1	1.96	0.46
1:C:232:LYS:NZ	1:D:427:THR:HG21	2.30	0.46
1:C:258:MSE:HE2	1:D:224:ALA:HB2	1.97	0.46
1:A:262:PHE:CE2	1:A:334:PRO:HB2	2.51	0.46
1:C:350:ARG:CD	1:C:390:SER:OG	2.64	0.46
1:D:303:LYS:HE2	5:D:1095:HOH:O	2.16	0.45
1:A:1:MSE:HE1	1:A:186:LEU:CD2	2.35	0.45
1:D:373:ILE:N	1:D:374:PRO:HD3	2.32	0.45
1:D:394:LEU:HB2	1:D:416:LEU:HD12	1.99	0.44
1:C:256:TYR:CD2	1:C:257:TYR:CE2	3.02	0.44
1:D:94:LEU:CD2	1:D:96:LEU:CD2	2.95	0.44
1:C:8:LEU:HD13	1:C:39:ILE:CD1	2.48	0.44
1:C:256:TYR:HD2	1:C:257:TYR:CD2	2.36	0.44
1:A:47:VAL:HG11	1:B:355:ASN:HB3	1.99	0.44
1:C:102:VAL:HG23	3:C:1003:NAD:C6A	2.48	0.44
1:D:357:GLU:O	1:D:360:ARG:HG2	2.18	0.44
1:D:396:LEU:N	1:D:396:LEU:HD22	2.32	0.44
1:A:314:ARG:HD3	5:A:1172:HOH:O	2.17	0.43
1:D:256:TYR:CD2	1:D:257:TYR:CE2	3.06	0.43
1:D:372:LYS:C	1:D:374:PRO:HD3	2.38	0.43
1:C:289:MSE:HE3	1:D:289:MSE:HE2	2.00	0.43
1:C:213:CYS:SG	1:D:245:ILE:HD12	2.58	0.43
1:C:307:LEU:HD13	5:C:1092:HOH:O	2.18	0.43
1:C:427:THR:HG22	1:C:433:GLY:H	1.84	0.42
1:C:373:ILE:N	1:C:374:PRO:CD	2.82	0.42
1:A:135:ILE:HD11	1:A:179:LEU:HD21	2.01	0.42
1:A:99:ILE:HD12	1:A:125:VAL:HG11	2.01	0.42
1:B:157:GLU:HG2	1:B:159:LEU:H	1.85	0.42
1:B:193:GLU:HB2	5:B:1206:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:MSE:CE	1:D:289:MSE:HE2	2.50	0.42
1:B:84:VAL:HG11	1:B:102:VAL:HG21	2.01	0.42
1:C:135:ILE:HB	1:C:136:PRO:HD3	2.00	0.42
1:A:86:THR:O	1:B:271:LYS:HD2	2.20	0.42
1:A:30:ASP:O	1:A:36:ILE:HD11	2.20	0.42
1:C:363:GLY:CA	5:C:1194:HOH:O	2.68	0.42
1:B:182:GLN:NE2	1:B:182:GLN:H	2.17	0.42
1:D:234:VAL:CG1	1:D:234:VAL:O	2.68	0.41
1:B:130:VAL:HB	1:B:203:VAL:HG11	2.01	0.41
1:B:144:LYS:HB3	1:B:149:ASP:CB	2.50	0.41
1:D:341:MSE:HB2	1:D:341:MSE:HE3	2.01	0.41
1:A:423:MSE:HA	1:A:424:PRO:HD3	1.91	0.41
1:C:44:SER:HA	1:C:45:PRO:HD3	1.93	0.41
1:C:421:GLY:HA2	1:C:436:TRP:CZ2	2.55	0.41
1:C:209:ILE:HD13	1:D:244:VAL:HG11	2.03	0.41
1:B:7:GLY:O	1:B:12:GLY:HA3	2.20	0.41
1:A:179:LEU:HA	1:A:179:LEU:HD12	1.88	0.41
1:D:196:ALA:HB1	1:D:197:PRO:HD2	2.02	0.41
1:C:94:LEU:HD12	5:C:1160:HOH:O	2.20	0.41
1:C:113:LYS:O	1:C:144:LYS:NZ	2.54	0.41
1:A:130:VAL:HG21	1:A:154:THR:CG2	2.51	0.41
3:A:1001:NAD:H8A	5:A:1051:HOH:O	2.21	0.41
1:A:314:ARG:HA	1:A:347:TYR:CD2	2.57	0.40
1:C:258:MSE:HE3	1:D:220:LYS:O	2.22	0.40
1:D:383:ASP:OD2	1:D:386:GLU:N	2.53	0.40
1:C:79:VAL:CG2	1:C:186:LEU:HD23	2.51	0.40
1:A:35:LYS:O	1:A:39:ILE:HG12	2.22	0.40

All (9) 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)
5:A:1163:HOH:O	5:C:1045:HOH:O[3_464]	1.88	0.32
5:B:1090:HOH:O	5:D:1157:HOH:O[1_565]	1.92	0.28
1:D:104:ARG:NE	5:B:1100:HOH:O[3_554]	2.03	0.17
5:B:1090:HOH:O	5:D:1184:HOH:O[1_565]	2.03	0.17
5:B:1091:HOH:O	5:D:1044:HOH:O[1_565]	2.06	0.14
5:C:1213:HOH:O	5:D:1135:HOH:O[4_545]	2.11	0.09
5:A:1038:HOH:O	5:B:1208:HOH:O[1_655]	2.12	0.08
5:B:1194:HOH:O	5:C:1164:HOH:O[1_565]	2.16	0.04
1:C:115:GLU:OE1	5:D:1241:HOH:O[4_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	434/436 (100%)	416 (96%)	18 (4%)	0	100	100
1	B	434/436 (100%)	422 (97%)	12 (3%)	0	100	100
1	C	434/436 (100%)	422 (97%)	12 (3%)	0	100	100
1	D	434/436 (100%)	422 (97%)	12 (3%)	0	100	100
All	All	1736/1744 (100%)	1682 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/361 (91%)	313 (96%)	14 (4%)	35	30
1	B	336/361 (93%)	318 (95%)	18 (5%)	27	21
1	C	340/361 (94%)	325 (96%)	15 (4%)	35	29
1	D	340/361 (94%)	321 (94%)	19 (6%)	26	19
All	All	1343/1444 (93%)	1277 (95%)	66 (5%)	31	24

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	47	VAL

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Mol	Chain	Res	Type
1	A	64	LEU
1	A	75	LEU
1	A	96	LEU
1	A	116	ARG
1	A	287	HIS
1	A	307	LEU
1	A	330	LEU
1	A	335	LEU
1	A	373	ILE
1	A	380	LEU
1	A	414	LYS
1	A	420	VAL
1	B	55	LEU
1	B	64	LEU
1	B	94	LEU
1	B	96	LEU
1	B	101	THR
1	B	111	ARG
1	B	126	LEU
1	B	157	GLU
1	B	182	GLN
1	B	251	LEU
1	B	255	ARG
1	B	318	LEU
1	B	319	LEU
1	B	338	LEU
1	B	390	SER
1	B	395	VAL
1	B	396	LEU
1	B	416	LEU
1	C	11	VAL
1	C	96	LEU
1	C	101	THR
1	C	102	VAL
1	C	114	SER
1	C	126	LEU
1	C	182	GLN
1	C	186	LEU
1	C	243	ASP
1	C	258	MSE
1	C	279	ARG
1	C	307	LEU

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Mol	Chain	Res	Type
1	C	345	LYS
1	C	420	VAL
1	C	427	THR
1	D	34	THR
1	D	55	LEU
1	D	126	LEU
1	D	148	VAL
1	D	154	THR
1	D	186	LEU
1	D	187	LEU
1	D	245	ILE
1	D	283	LEU
1	D	298	SER
1	D	313	THR
1	D	318	LEU
1	D	379	LEU
1	D	396	LEU
1	D	406	LEU
1	D	407	VAL
1	D	416	LEU
1	D	420	VAL
1	D	427	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	B	182	GLN
1	C	182	GLN
1	D	247	GLN
1	D	362	HIS
1	D	365	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 ⓘ

9 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$
3	NAD	A	1001	-	31,38,48	1.04	2 (6%)	39,58,73	2.26	5 (12%)
3	NAD	B	1002	-	31,38,48	1.08	2 (6%)	39,58,73	2.28	5 (12%)
4	GDX	B	1005	-	32,43,43	4.05	13 (40%)	45,67,67	1.88	10 (22%)
4	GDX	B	1006	-	32,43,43	3.92	13 (40%)	45,67,67	1.79	10 (22%)
3	NAD	C	1003	-	31,38,48	1.07	2 (6%)	39,58,73	2.27	6 (15%)
2	SUC	C	1009	-	24,24,24	0.42	0	36,36,36	0.79	2 (5%)
3	NAD	D	1004	-	31,38,48	1.05	2 (6%)	39,58,73	2.30	4 (10%)
4	GDX	D	1007	-	32,43,43	4.00	13 (40%)	45,67,67	2.02	10 (22%)
4	GDX	D	1008	-	32,43,43	3.86	14 (43%)	45,67,67	1.94	11 (24%)

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	1001	-	-	0/18/51/62	0/4/4/5
3	NAD	B	1002	-	-	0/18/51/62	0/4/4/5
4	GDX	B	1005	-	-	0/17/61/61	0/4/4/4
4	GDX	B	1006	-	-	0/17/61/61	0/4/4/4
3	NAD	C	1003	-	-	0/18/51/62	0/4/4/5
2	SUC	C	1009	-	-	0/12/51/51	0/2/2/2
3	NAD	D	1004	-	-	0/18/51/62	0/4/4/5
4	GDX	D	1007	-	-	0/17/61/61	0/4/4/4
4	GDX	D	1008	-	-	0/17/61/61	0/4/4/4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1007	GDX	C4'-C5'	-8.48	1.35	1.53
4	B	1005	GDX	C4'-C5'	-8.46	1.35	1.53
4	B	1006	GDX	C4'-C5'	-8.39	1.35	1.53
4	D	1008	GDX	C4'-C5'	-8.20	1.35	1.53
4	B	1005	GDX	O3'-C3'	-7.76	1.24	1.43
4	B	1005	GDX	O2D-C2D	-7.68	1.24	1.43
4	D	1007	GDX	O3'-C3'	-7.65	1.24	1.43
4	B	1006	GDX	O4'-C4'	-7.36	1.25	1.43
4	B	1005	GDX	O2'-C2'	-7.35	1.25	1.43
4	B	1006	GDX	O3'-C3'	-7.34	1.25	1.43
4	D	1008	GDX	O2'-C2'	-7.24	1.25	1.43
4	D	1007	GDX	O4'-C4'	-7.21	1.25	1.43
4	D	1008	GDX	O4'-C4'	-7.14	1.25	1.43
4	B	1006	GDX	O2'-C2'	-7.13	1.25	1.43
4	B	1006	GDX	O2D-C2D	-7.11	1.25	1.43
4	D	1007	GDX	O2D-C2D	-7.10	1.26	1.43
4	D	1008	GDX	O2D-C2D	-7.04	1.26	1.43
4	B	1005	GDX	O4'-C4'	-6.83	1.26	1.43
4	D	1007	GDX	O2'-C2'	-6.83	1.26	1.43
4	D	1008	GDX	O3'-C3'	-6.75	1.26	1.43
4	B	1005	GDX	C3D-C4D	-6.72	1.34	1.53
4	B	1005	GDX	C3D-C2D	-6.60	1.35	1.53
4	B	1006	GDX	C3D-C2D	-6.50	1.35	1.53
4	D	1007	GDX	C3D-C4D	-6.49	1.35	1.53
4	D	1007	GDX	C3D-C2D	-6.44	1.35	1.53
4	B	1005	GDX	C4'-C3'	-6.37	1.35	1.52
4	D	1008	GDX	C3D-C4D	-6.30	1.36	1.53
4	B	1006	GDX	C3D-C4D	-6.24	1.36	1.53
4	D	1007	GDX	C3'-C2'	-6.20	1.36	1.52
4	D	1008	GDX	C3D-C2D	-6.06	1.36	1.53
4	B	1006	GDX	C3'-C2'	-5.98	1.36	1.52
4	D	1007	GDX	C4'-C3'	-5.97	1.36	1.52
4	B	1006	GDX	C4'-C3'	-5.94	1.36	1.52
4	D	1008	GDX	C4'-C3'	-5.88	1.37	1.52
4	D	1008	GDX	C3'-C2'	-5.69	1.37	1.52
4	B	1005	GDX	C3'-C2'	-5.66	1.37	1.52
4	D	1007	GDX	C1'-C2'	-5.47	1.36	1.52
4	B	1005	GDX	C1'-C2'	-5.36	1.36	1.52
4	B	1006	GDX	C1'-C2'	-5.34	1.36	1.52
4	D	1008	GDX	C1'-C2'	-4.95	1.37	1.52
4	B	1006	GDX	O4D-C1D	2.03	1.43	1.41
4	D	1008	GDX	O5'-C1'	2.14	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	NAD	C2A-N1A	2.14	1.38	1.33
3	D	1004	NAD	C2A-N1A	2.25	1.38	1.33
3	B	1002	NAD	C2A-N1A	2.27	1.38	1.33
3	A	1001	NAD	C2A-N1A	2.41	1.38	1.33
4	B	1006	GDX	C5-C4	2.50	1.46	1.40
4	B	1005	GDX	O4D-C1D	2.51	1.44	1.41
4	D	1008	GDX	C5-C4	2.88	1.47	1.40
4	B	1006	GDX	C6-C5	2.88	1.47	1.41
4	D	1007	GDX	C5-C4	2.99	1.47	1.40
4	D	1008	GDX	C6-C5	3.14	1.47	1.41
4	D	1008	GDX	O4D-C1D	3.20	1.45	1.41
4	B	1005	GDX	C5-C4	3.26	1.47	1.40
3	A	1001	NAD	C2A-N3A	3.38	1.38	1.32
3	B	1002	NAD	C2A-N3A	3.47	1.38	1.32
4	D	1007	GDX	O4D-C1D	3.49	1.45	1.41
4	B	1005	GDX	C6-C5	3.50	1.48	1.41
4	D	1007	GDX	C6-C5	3.63	1.48	1.41
3	D	1004	NAD	C2A-N3A	3.72	1.38	1.32
3	C	1003	NAD	C2A-N3A	3.74	1.38	1.32

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1004	NAD	N3A-C2A-N1A	-12.36	119.43	128.89
3	C	1003	NAD	N3A-C2A-N1A	-11.92	119.77	128.89
3	B	1002	NAD	N3A-C2A-N1A	-11.67	119.96	128.89
3	A	1001	NAD	N3A-C2A-N1A	-11.62	120.00	128.89
4	D	1007	GDX	O5'-C1'-O1B	-4.95	104.83	111.36
4	D	1007	GDX	C4D-O4D-C1D	-4.85	104.39	109.72
4	D	1008	GDX	C5-C6-N1	-4.71	117.15	123.59
4	D	1008	GDX	C4D-O4D-C1D	-4.68	104.57	109.72
3	A	1001	NAD	PN-O3-PA	-4.51	120.06	132.73
4	D	1007	GDX	C5-C6-N1	-4.31	117.70	123.59
4	B	1006	GDX	C4D-O4D-C1D	-4.21	105.09	109.72
3	D	1004	NAD	PN-O3-PA	-4.03	121.40	132.73
4	B	1006	GDX	C5-C6-N1	-4.02	118.09	123.59
4	B	1005	GDX	C5-C6-N1	-3.98	118.14	123.59
4	B	1005	GDX	C6-C5-C4	-3.69	116.49	120.90
4	B	1005	GDX	O5'-C1'-O1B	-3.49	106.76	111.36
4	D	1007	GDX	C6-C5-C4	-3.38	116.86	120.90
3	C	1003	NAD	PN-O3-PA	-3.24	123.63	132.73
4	D	1008	GDX	C6-C5-C4	-3.21	117.06	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	NAD	C1B-N9A-C4A	-3.17	122.16	126.94
4	B	1006	GDX	O5'-C1'-O1B	-3.15	107.21	111.36
4	B	1005	GDX	N3-C2-N1	-2.99	122.88	127.44
3	C	1003	NAD	C4B-O4B-C1B	-2.87	106.56	109.72
3	B	1002	NAD	PN-O3-PA	-2.83	124.78	132.73
4	D	1008	GDX	N3-C2-N1	-2.83	123.14	127.44
4	B	1006	GDX	N3-C2-N1	-2.75	123.25	127.44
4	B	1006	GDX	C6-C5-C4	-2.69	117.69	120.90
3	B	1002	NAD	C4B-O4B-C1B	-2.64	106.81	109.72
4	D	1007	GDX	N3-C2-N1	-2.60	123.49	127.44
3	D	1004	NAD	C1B-N9A-C4A	-2.57	123.07	126.94
3	C	1003	NAD	C4A-C5A-N7A	-2.45	107.22	109.48
4	B	1005	GDX	C4D-O4D-C1D	-2.43	107.05	109.72
3	A	1001	NAD	C4A-C5A-N7A	-2.41	107.26	109.48
3	C	1003	NAD	O3-PN-O5D	-2.41	96.55	102.94
4	D	1008	GDX	O5'-C1'-O1B	-2.38	108.22	111.36
4	D	1008	GDX	O3D-C3D-C4D	-2.37	103.95	111.05
3	D	1004	NAD	C4B-O4B-C1B	-2.33	107.16	109.72
4	D	1007	GDX	C4-C5-N7	-2.27	107.39	109.48
3	A	1001	NAD	C4B-O4B-C1B	-2.24	107.26	109.72
3	A	1001	NAD	C1B-N9A-C4A	-2.18	123.65	126.94
4	D	1008	GDX	PB-O3A-PA	-2.14	126.71	132.73
4	B	1005	GDX	O3A-PB-O1B	2.08	109.62	103.63
2	C	1009	SUC	C1-O5-C5	2.08	117.79	113.75
3	C	1003	NAD	C2B-C1B-N9A	2.12	117.53	114.29
2	C	1009	SUC	O5-C5-C4	2.32	114.03	109.68
3	B	1002	NAD	O4B-C1B-N9A	2.63	113.60	108.10
4	B	1006	GDX	C2D-C3D-C4D	2.76	108.28	102.61
4	B	1006	GDX	O4D-C1D-N9	2.79	113.94	108.10
4	D	1007	GDX	O4D-C1D-N9	2.92	114.22	108.10
4	B	1006	GDX	O3A-PB-O1B	2.97	112.17	103.63
4	D	1007	GDX	C2D-C3D-C4D	3.15	109.08	102.61
4	D	1008	GDX	C2D-C3D-C4D	3.28	109.34	102.61
4	B	1005	GDX	C2D-C3D-C4D	3.35	109.50	102.61
4	B	1006	GDX	C6-N1-C2	3.67	121.04	115.94
4	D	1008	GDX	C2D-C1D-N9	3.88	120.22	114.29
4	D	1008	GDX	O4D-C1D-N9	4.00	116.48	108.10
4	B	1005	GDX	C6-N1-C2	4.30	121.91	115.94
4	B	1006	GDX	C2D-C1D-N9	4.32	120.89	114.29
4	B	1005	GDX	O4D-C1D-N9	4.43	117.36	108.10
4	B	1005	GDX	C2D-C1D-N9	4.43	121.06	114.29
4	D	1007	GDX	C6-N1-C2	4.59	122.31	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1008	GDX	C6-N1-C2	4.76	122.55	115.94
4	D	1007	GDX	C2D-C1D-N9	4.93	121.83	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	NAD	1	0
3	C	1003	NAD	1	0
2	C	1009	SUC	2	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.