



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:58 PM GMT

PDB ID : 1MV8
Title : 1.55 Å crystal structure of a ternary complex of GDP-mannose dehydrogenase from *Pseudomonas aeruginosa*
Authors : Snook, C.F.; Tipton, P.A.; Beamer, L.J.
Deposited on : 2002-09-24
Resolution : 1.55 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) : 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

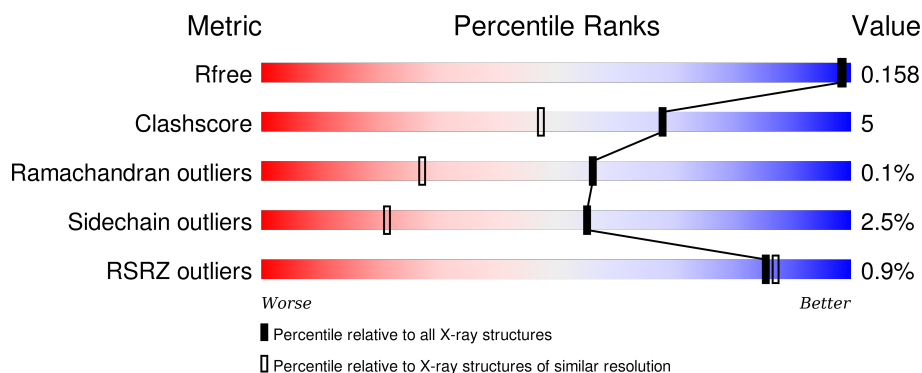
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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.

Mol	Chain	Length	Quality of chain
1	A	436	<div> <div></div> <div>86%12%•</div> </div>
1	B	436	<div> <div></div> <div>91%8%•</div> </div>
1	C	436	<div> <div></div> <div>91%8%</div> </div>
1	D	436	<div> <div></div> <div>89%10%•</div> </div>

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	SUC	B	2012	-	-	-	X
2	SUC	D	2013	-	-	-	X
4	GDX	A	2006	-	-	-	X
5	ACY	C	2010	-	-	X	X

2 Entry composition [i](#)

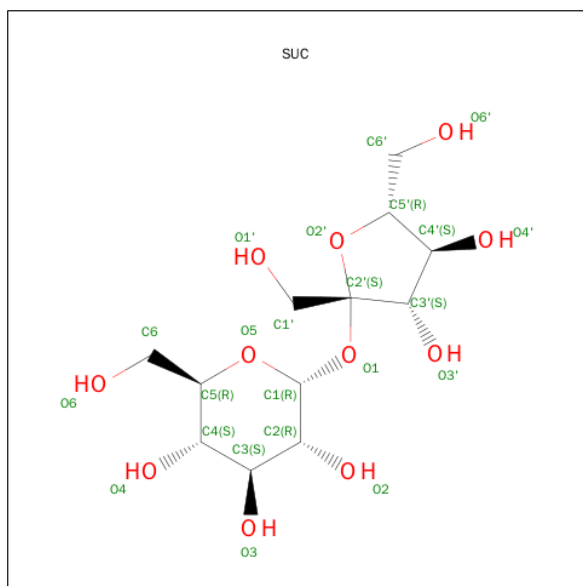
There are 7 unique types of molecules in this entry. The entry contains 14879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

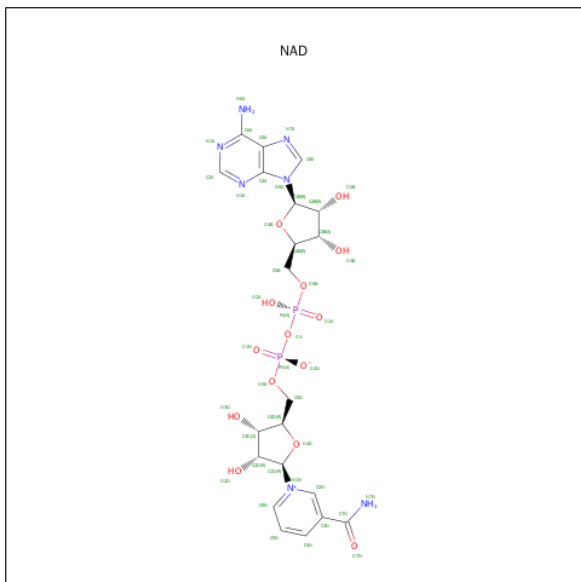
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3280	2065	562	635	18			
1	B	436	Total	C	N	O	S	0	0	0
			3273	2066	562	627	18			
1	C	436	Total	C	N	O	S	0	0	0
			3297	2077	566	636	18			
1	D	436	Total	C	N	O	S	0	0	0
			3291	2075	565	633	18			

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



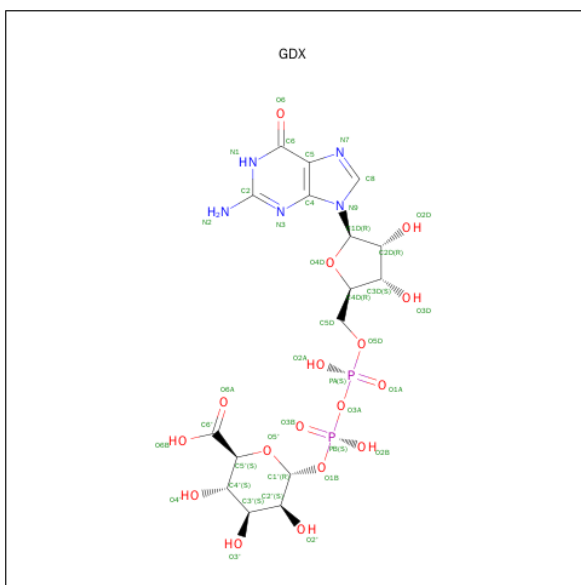
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

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



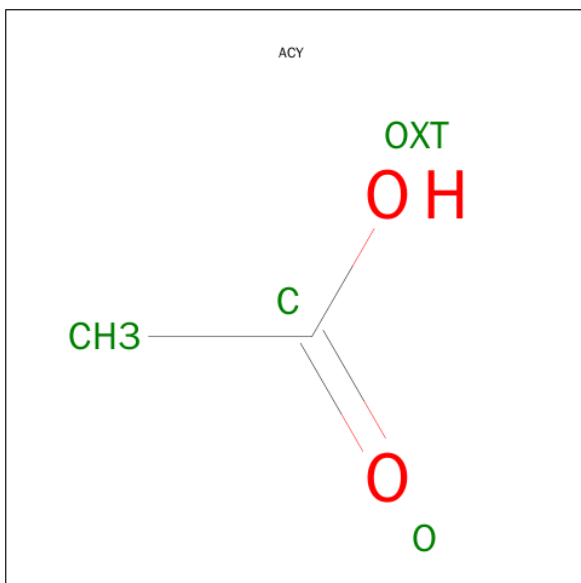
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	C	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	D	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

- Molecule 4 is GUANOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), P'-D-MANNOPYRANOSYL ESTER (three-letter code: GDX) (formula: $C_{16}H_{23}N_5O_{17}P_2$).



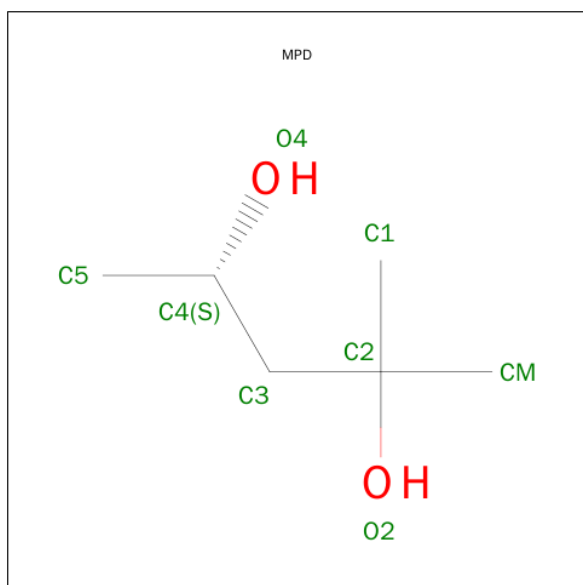
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 40	C 16	N 5	O 17	P 2	0	0
4	A	1	Total 40	C 16	N 5	O 17	P 2	0	0
4	D	1	Total 40	C 16	N 5	O 17	P 2	0	0
4	D	1	Total 40	C 16	N 5	O 17	P 2	0	0

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: $\text{C}_2\text{H}_4\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			8	6	2		

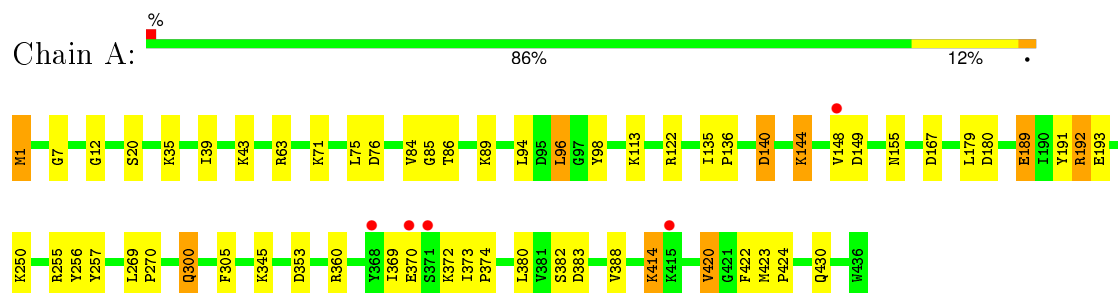
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	289	Total	O	0	0
			289	289		
7	B	301	Total	O	0	0
			301	301		
7	C	386	Total	O	0	0
			386	386		
7	D	400	Total	O	0	0
			400	400		

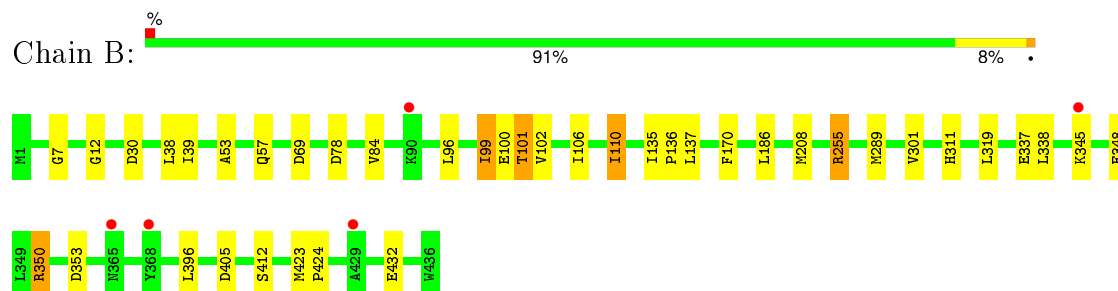
3 Residue-property plots [i](#)

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.

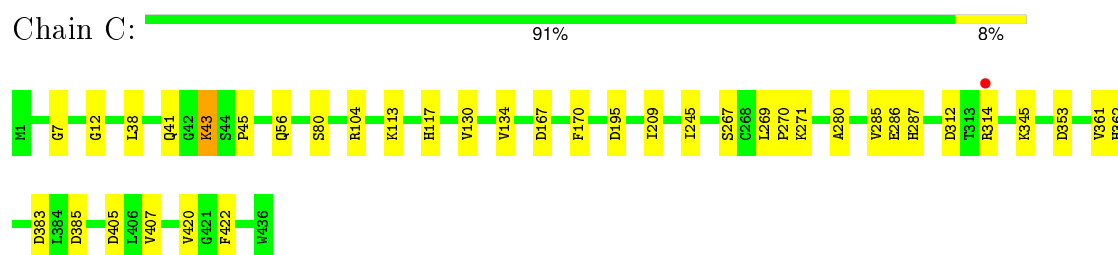
- Molecule 1: GDP-mannose 6-dehydrogenase



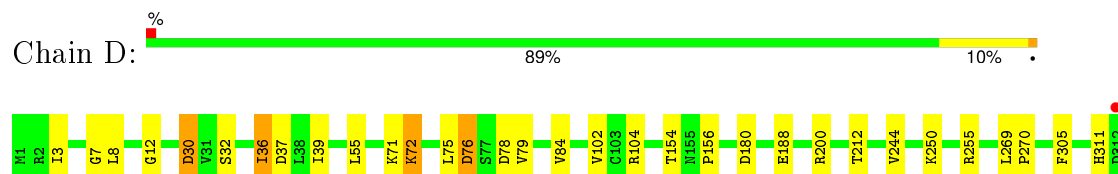
- Molecule 1: GDP-mannose 6-dehydrogenase

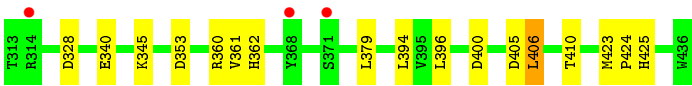


- Molecule 1: GDP-mannose 6-dehydrogenase



- Molecule 1: GDP-mannose 6-dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	82.47Å 82.47Å 309.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.55 49.55 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.55) 99.0 (49.55-1.55)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.174 , 0.194 0.151 , 0.158	Depositor DCC
R_{free} test set	14843 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.8	EDS
Estimated twinning fraction	0.176 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 294148 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14879	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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, MPD, SUC, ACY, 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	0.40	0/3333	0.73	6/4520 (0.1%)
1	B	0.41	1/3327 (0.0%)	0.75	5/4511 (0.1%)
1	C	0.40	0/3351	0.74	5/4543 (0.1%)
1	D	0.41	0/3345	0.75	9/4533 (0.2%)
All	All	0.41	1/13356 (0.0%)	0.74	25/18107 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	MET	SD-CE	-7.28	1.37	1.77

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ASP	CB-CG-OD2	6.00	123.70	118.30
1	C	405	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	405	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	405	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	195	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	312	ASP	CB-CG-OD2	5.47	123.23	118.30
1	D	76	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	353	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	180	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	37	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	30	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	180	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	140	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	167	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	328	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	353	ASP	CB-CG-OD2	5.12	122.91	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	69	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	383	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	76	ASP	CB-CG-OD2	5.07	122.87	118.30
1	C	353	ASP	CB-CG-OD2	5.07	122.87	118.30
1	D	353	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	78	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	400	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	78	ASP	CB-CG-OD2	5.02	122.82	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	3280	0	3256	40	0
1	B	3273	0	3255	25	0
1	C	3297	0	3281	26	0
1	D	3291	0	3281	42	0
2	B	23	0	22	0	0
2	D	23	0	22	0	0
3	A	35	0	19	2	0
3	B	35	0	19	0	0
3	C	35	0	19	0	0
3	D	35	0	19	0	0
4	A	80	0	32	0	0
4	D	80	0	32	0	0
5	C	8	0	6	3	0
6	C	8	0	14	0	0
7	A	289	0	0	2	0
7	B	301	0	0	3	0
7	C	386	0	0	7	1
7	D	400	0	0	8	1
All	All	14879	0	13277	127	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 5.

All (127) 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:D:305:PHE:HZ	1:D:345:LYS:CD	1.47	1.26
1:B:348:GLU:OE2	1:B:350:ARG:NH2	1.82	1.11
1:D:305:PHE:CZ	1:D:345:LYS:CD	2.35	1.08
1:D:305:PHE:HZ	1:D:345:LYS:HD3	1.15	1.05
1:D:305:PHE:CZ	1:D:345:LYS:HD3	1.94	1.02
1:A:382:SER:OG	7:A:2295:HOH:O	1.78	1.00
1:B:350:ARG:HG3	1:B:350:ARG:HH11	1.33	0.94
1:D:188:GLU:OE2	1:D:200:ARG:HD2	1.69	0.93
1:A:360:ARG:HD2	1:A:370:GLU:OE2	1.69	0.92
1:D:305:PHE:CZ	1:D:345:LYS:HD2	2.05	0.89
1:C:383:ASP:OD2	1:C:385:ASP:HB2	1.75	0.86
1:A:122:ARG:NH1	1:A:191:TYR:OH	2.10	0.85
1:B:106:ILE:O	1:B:110:ILE:HG23	1.74	0.85
1:D:360:ARG:HD2	7:D:2401:HOH:O	1.76	0.84
1:A:122:ARG:NH1	1:A:155:ASN:OD1	2.12	0.83
1:D:30:ASP:HB3	1:D:36:ILE:HD11	1.63	0.80
1:A:122:ARG:NH1	1:A:191:TYR:HH	1.82	0.77
1:D:188:GLU:OE2	1:D:200:ARG:CD	2.32	0.77
1:B:255:ARG:NH1	7:B:2126:HOH:O	2.19	0.76
5:C:2009:ACY:C	5:C:2010:ACY:O	2.34	0.75
1:B:345:LYS:HE3	1:D:340:GLU:OE1	1.86	0.74
1:C:286:GLU:OE2	7:C:2063:HOH:O	2.07	0.71
1:A:84:VAL:HG11	1:A:98:TYR:HB3	1.72	0.70
1:A:71:LYS:O	1:A:75:LEU:HD23	1.93	0.68
1:B:350:ARG:HG3	1:B:350:ARG:NH1	2.06	0.67
1:D:255:ARG:NH1	7:D:2413:HOH:O	2.28	0.66
1:B:84:VAL:HG11	1:B:102:VAL:HG21	1.77	0.65
1:C:267:SER:O	1:C:271:LYS:NZ	2.26	0.64
1:D:361:VAL:HG22	1:D:362:HIS:CD2	2.32	0.64
1:C:280:ALA:HB2	7:C:2376:HOH:O	1.97	0.64
1:B:345:LYS:CE	1:D:340:GLU:OE1	2.46	0.63
1:A:84:VAL:HG12	1:A:85:GLY:N	2.14	0.63
1:C:285:VAL:O	1:C:287:HIS:HD2	1.83	0.61
1:B:345:LYS:HE3	1:D:340:GLU:CD	2.20	0.61
1:C:45:PRO:HG2	7:C:2330:HOH:O	2.00	0.60
1:D:30:ASP:CB	1:D:36:ILE:HD11	2.30	0.59
1:D:30:ASP:HB3	1:D:36:ILE:CD1	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:SER:OG	1:C:117:HIS:HE1	1.85	0.59
1:A:122:ARG:HD2	1:A:155:ASN:O	2.02	0.59
1:D:32:SER:O	1:D:36:ILE:HD13	2.04	0.57
1:D:8:LEU:HD13	1:D:39:ILE:HD13	1.87	0.57
1:B:101:THR:HG21	7:B:2072:HOH:O	2.05	0.56
1:B:311:HIS:HE1	1:B:432:GLU:OE2	1.88	0.56
1:B:99:ILE:HG13	1:B:100:GLU:N	2.21	0.56
1:A:420:VAL:HG11	1:A:422:PHE:CE2	2.40	0.56
1:D:84:VAL:HG11	1:D:102:VAL:HG21	1.88	0.55
1:D:305:PHE:HZ	1:D:345:LYS:CE	2.18	0.55
1:C:314:ARG:CZ	7:C:2076:HOH:O	2.53	0.55
1:A:84:VAL:HG13	3:A:2001:NAD:C8A	2.37	0.55
1:A:372:LYS:C	1:A:374:PRO:HD2	2.27	0.55
1:C:113:LYS:HZ3	1:C:117:HIS:HD2	1.55	0.54
1:A:84:VAL:CG1	1:A:98:TYR:HB3	2.38	0.54
1:C:113:LYS:NZ	1:C:117:HIS:HD2	2.05	0.54
1:A:373:ILE:N	1:A:374:PRO:CD	2.71	0.53
1:C:287:HIS:HE1	7:C:2081:HOH:O	1.91	0.53
1:B:350:ARG:CG	1:B:350:ARG:NH1	2.71	0.53
1:D:71:LYS:O	1:D:75:LEU:HD13	2.09	0.53
1:B:53:ALA:O	1:B:57:GLN:HG3	2.09	0.52
1:D:305:PHE:CZ	1:D:345:LYS:NZ	2.73	0.52
1:D:311:HIS:HE1	7:D:2240:HOH:O	1.92	0.51
1:D:424:PRO:HB2	1:D:425:HIS:CD2	2.45	0.51
1:C:420:VAL:O	5:C:2010:ACY:H1	2.11	0.51
1:A:84:VAL:CG1	3:A:2001:NAD:C8A	2.89	0.50
1:A:84:VAL:HG12	1:A:85:GLY:H	1.77	0.50
1:C:41:GLN:HB2	1:C:43:LYS:HG3	1.93	0.50
1:D:104:ARG:CZ	7:D:2360:HOH:O	2.59	0.50
1:A:20:SER:O	1:A:63:ARG:NH1	2.45	0.49
1:A:86:THR:HB	1:A:94:LEU:HD11	1.96	0.48
1:A:250:LYS:NZ	1:B:170:PHE:O	2.43	0.48
1:A:135:ILE:HB	1:A:136:PRO:HD3	1.96	0.47
1:A:189:GLU:OE1	1:A:192:ARG:NE	2.36	0.47
1:C:383:ASP:OD2	1:C:385:ASP:CB	2.56	0.47
1:D:72:LYS:HD3	1:D:76:ASP:OD2	2.15	0.46
1:B:7:GLY:O	1:B:12:GLY:HA3	2.16	0.46
1:D:410:THR:HG21	7:D:2337:HOH:O	2.15	0.46
1:A:420:VAL:HG11	1:A:422:PHE:HE2	1.80	0.46
1:D:3:ILE:HG12	1:D:79:VAL:CG1	2.45	0.46
1:D:7:GLY:O	1:D:12:GLY:HA3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ARG:NH2	7:D:2413:HOH:O	2.48	0.46
1:C:170:PHE:O	1:D:250:LYS:NZ	2.40	0.45
1:B:311:HIS:CE1	1:B:432:GLU:OE2	2.67	0.45
1:D:36:ILE:CD1	1:D:36:ILE:N	2.79	0.45
1:C:209:ILE:HD13	1:D:244:VAL:HG11	1.98	0.45
1:A:7:GLY:O	1:A:12:GLY:HA3	2.17	0.45
1:C:420:VAL:HG13	5:C:2010:ACY:H2	1.99	0.45
1:D:305:PHE:CE2	1:D:345:LYS:NZ	2.78	0.45
1:B:135:ILE:HB	1:B:136:PRO:HD3	1.99	0.44
1:B:423:MET:HA	1:B:424:PRO:HD2	1.90	0.44
1:D:396:LEU:N	1:D:396:LEU:HD22	2.32	0.44
1:B:301:VAL:HG11	1:B:337:GLU:OE1	2.18	0.44
1:A:360:ARG:HG2	1:A:369:ILE:HG21	2.00	0.43
1:A:75:LEU:HD13	1:A:113:LYS:HG3	2.00	0.43
1:A:89:LYS:HE3	7:A:2237:HOH:O	2.16	0.43
1:A:373:ILE:N	1:A:374:PRO:HD2	2.32	0.43
1:A:269:LEU:HB2	1:A:270:PRO:HD3	2.01	0.43
1:C:7:GLY:O	1:C:12:GLY:HA3	2.18	0.43
1:A:84:VAL:CG1	1:A:85:GLY:N	2.79	0.43
1:D:394:LEU:HD13	1:D:406:LEU:HD11	1.99	0.43
1:A:144:LYS:HG2	1:A:149:ASP:HB3	2.01	0.43
1:A:360:ARG:CD	1:A:370:GLU:OE2	2.55	0.42
1:B:186:LEU:C	1:B:186:LEU:HD23	2.40	0.42
1:D:423:MET:HA	1:D:424:PRO:HD3	1.94	0.42
1:A:256:TYR:HD2	1:A:257:TYR:CE2	2.37	0.42
1:B:319:LEU:HD12	1:B:396:LEU:HD23	2.01	0.42
1:C:104:ARG:NH2	7:C:2308:HOH:O	2.51	0.42
1:A:388:VAL:O	1:A:414:LYS:HE3	2.19	0.42
1:A:300:GLN:HA	1:A:300:GLN:HE21	1.84	0.42
1:C:245:ILE:HD11	1:D:212:THR:HB	2.02	0.42
1:C:269:LEU:HB2	1:C:270:PRO:HD3	2.01	0.42
1:B:255:ARG:HG2	7:B:2027:HOH:O	2.20	0.41
1:D:269:LEU:HB2	1:D:270:PRO:HD3	2.02	0.41
1:C:407:VAL:HG21	1:C:422:PHE:HB3	2.03	0.41
1:D:255:ARG:CZ	7:D:2413:HOH:O	2.64	0.41
1:C:104:ARG:NE	7:C:2308:HOH:O	2.53	0.41
1:A:35:LYS:O	1:A:39:ILE:HG12	2.20	0.41
1:A:94:LEU:HG	1:A:96:LEU:HD13	2.03	0.41
1:A:305:PHE:HZ	1:A:345:LYS:HG3	1.86	0.41
1:D:311:HIS:CE1	7:D:2240:HOH:O	2.70	0.41
1:C:130:VAL:HA	1:C:134:VAL:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB2	1:A:1:MET:HE2	1.84	0.41
1:B:348:GLU:CD	1:B:350:ARG:HH22	2.08	0.41
1:C:361:VAL:HG23	1:C:362:HIS:CD2	2.55	0.41
1:A:423:MET:HA	1:A:424:PRO:HD3	1.97	0.40
1:C:113:LYS:NZ	1:C:117:HIS:CD2	2.88	0.40
1:A:84:VAL:CG1	1:A:85:GLY:H	2.34	0.40
1:B:100:GLU:HG2	1:B:137:LEU:HD11	2.03	0.40
1:D:154:THR:HG22	1:D:156:PRO:HD3	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)
7:C:2358:HOH:O	7:D:2112:HOH:O[4_545]	1.98	0.22

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%)	421 (97%)	12 (3%)	1 (0%)	52	25
1	B	434/436 (100%)	420 (97%)	14 (3%)	0	100	100
1	C	434/436 (100%)	421 (97%)	13 (3%)	0	100	100
1	D	434/436 (100%)	422 (97%)	12 (3%)	0	100	100
All	All	1736/1744 (100%)	1684 (97%)	51 (3%)	1 (0%)	56	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ARG

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	356/370 (96%)	341 (96%)	15 (4%)	36	7
1	B	353/370 (95%)	342 (97%)	11 (3%)	47	14
1	C	359/370 (97%)	355 (99%)	4 (1%)	80	58
1	D	358/370 (97%)	353 (99%)	5 (1%)	74	48
All	All	1426/1480 (96%)	1391 (98%)	35 (2%)	55	21

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	43	LYS
1	A	96	LEU
1	A	140	ASP
1	A	144	LYS
1	A	148	VAL
1	A	179	LEU
1	A	189	GLU
1	A	193	GLU
1	A	255	ARG
1	A	300	GLN
1	A	380	LEU
1	A	414	LYS
1	A	420	VAL
1	A	430	GLN
1	B	38	LEU
1	B	39	ILE
1	B	96	LEU
1	B	99	ILE
1	B	101	THR
1	B	110	ILE
1	B	208	MET
1	B	255	ARG
1	B	338	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	350	ARG
1	B	412	SER
1	C	38	LEU
1	C	43	LYS
1	C	56	GLN
1	C	345	LYS
1	D	36	ILE
1	D	55	LEU
1	D	72	LYS
1	D	379	LEU
1	D	406	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	300	GLN
1	B	229	ASN
1	B	311	HIS
1	B	362	HIS
1	B	425	HIS
1	C	117	HIS
1	C	229	ASN
1	C	287	HIS
1	D	300	GLN
1	D	311	HIS
1	D	425	HIS

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

13 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	2001	-	31,38,48	0.97	1 (3%)	39,58,73	2.14	6 (15%)
4	GDX	A	2005	-	32,43,43	3.69	14 (43%)	45,67,67	2.00	12 (26%)
4	GDX	A	2006	-	32,43,43	3.70	13 (40%)	45,67,67	2.08	14 (31%)
3	NAD	B	2002	-	31,38,48	1.12	3 (9%)	39,58,73	2.42	6 (15%)
2	SUC	B	2012	-	24,24,24	0.43	0	36,36,36	0.71	0
3	NAD	C	2003	-	31,38,48	1.08	1 (3%)	39,58,73	2.07	5 (12%)
5	ACY	C	2009	-	1,3,3	0.44	0	0,3,3	0.00	-
5	ACY	C	2010	-	1,3,3	0.93	0	0,3,3	0.00	-
6	MPD	C	2011	-	6,7,7	0.27	0	7,10,10	0.48	0
3	NAD	D	2004	-	31,38,48	1.10	2 (6%)	39,58,73	2.08	5 (12%)
4	GDX	D	2007	-	32,43,43	3.66	14 (43%)	45,67,67	2.04	14 (31%)
4	GDX	D	2008	-	32,43,43	3.72	15 (46%)	45,67,67	2.09	14 (31%)
2	SUC	D	2013	-	24,24,24	0.41	0	36,36,36	0.59	0

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	2001	-	-	0/18/51/62	0/4/4/5
4	GDX	A	2005	-	-	0/17/61/61	0/4/4/4
4	GDX	A	2006	-	-	0/17/61/61	0/4/4/4
3	NAD	B	2002	-	-	0/18/51/62	0/4/4/5
2	SUC	B	2012	-	-	0/12/51/51	0/2/2/2
3	NAD	C	2003	-	-	0/18/51/62	0/4/4/5
5	ACY	C	2009	-	-	0/0/0/0	0/0/0/0
5	ACY	C	2010	-	-	0/0/0/0	0/0/0/0
6	MPD	C	2011	-	-	0/5/5/5	0/0/0/0
3	NAD	D	2004	-	-	0/18/51/62	0/4/4/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDX	D	2007	-	-	0/17/61/61	0/4/4/4
4	GDX	D	2008	-	-	0/17/61/61	0/4/4/4
2	SUC	D	2013	-	-	0/12/51/51	0/2/2/2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2007	GDX	C4'-C5'	-7.86	1.36	1.53
4	D	2008	GDX	C4'-C5'	-7.84	1.36	1.53
4	A	2005	GDX	C4'-C5'	-7.75	1.36	1.53
4	A	2006	GDX	C4'-C5'	-7.73	1.36	1.53
4	A	2006	GDX	O2'-C2'	-7.06	1.26	1.43
4	A	2006	GDX	O3'-C3'	-6.87	1.26	1.43
4	D	2008	GDX	O4'-C4'	-6.75	1.26	1.43
4	A	2005	GDX	O3'-C3'	-6.71	1.26	1.43
4	A	2005	GDX	O2'-C2'	-6.69	1.26	1.43
4	D	2008	GDX	O2'-C2'	-6.67	1.27	1.43
4	D	2008	GDX	O3'-C3'	-6.60	1.27	1.43
4	D	2007	GDX	O4'-C4'	-6.55	1.27	1.43
4	D	2007	GDX	O3'-C3'	-6.55	1.27	1.43
4	A	2006	GDX	O4'-C4'	-6.53	1.27	1.43
4	D	2007	GDX	O2'-C2'	-6.43	1.27	1.43
4	A	2005	GDX	O2D-C2D	-6.42	1.27	1.43
4	A	2005	GDX	O4'-C4'	-6.31	1.27	1.43
4	A	2006	GDX	C3D-C2D	-6.23	1.36	1.53
4	D	2008	GDX	C3D-C4D	-6.18	1.36	1.53
4	A	2005	GDX	C3D-C4D	-6.16	1.36	1.53
4	D	2007	GDX	O2D-C2D	-6.14	1.28	1.43
4	D	2008	GDX	O2D-C2D	-6.10	1.28	1.43
4	D	2008	GDX	C3D-C2D	-6.09	1.36	1.53
4	D	2007	GDX	C3D-C2D	-6.08	1.36	1.53
4	A	2005	GDX	C3D-C2D	-6.02	1.37	1.53
4	D	2007	GDX	C3D-C4D	-5.96	1.36	1.53
4	A	2006	GDX	C3D-C4D	-5.91	1.37	1.53
4	A	2006	GDX	O2D-C2D	-5.80	1.29	1.43
4	A	2006	GDX	C3'-C2'	-5.71	1.37	1.52
4	A	2005	GDX	C4'-C3'	-5.60	1.37	1.52
4	A	2006	GDX	C4'-C3'	-5.60	1.37	1.52
4	A	2005	GDX	C3'-C2'	-5.53	1.37	1.52
4	D	2008	GDX	C4'-C3'	-5.33	1.38	1.52
4	D	2007	GDX	C3'-C2'	-5.30	1.38	1.52
4	D	2008	GDX	C3'-C2'	-5.20	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2007	GDX	C4'-C3'	-5.17	1.38	1.52
4	D	2007	GDX	C1'-C2'	-5.13	1.37	1.52
4	D	2008	GDX	C1'-C2'	-5.03	1.37	1.52
4	A	2006	GDX	C1'-C2'	-5.02	1.37	1.52
4	A	2005	GDX	C1'-C2'	-4.85	1.38	1.52
3	B	2002	NAD	PN-O2N	-2.16	1.45	1.54
4	D	2008	GDX	O5'-C1'	2.11	1.47	1.41
4	A	2005	GDX	O4D-C1D	2.13	1.43	1.41
4	A	2006	GDX	O5'-C5'	2.18	1.46	1.43
3	B	2002	NAD	C2A-N1A	2.22	1.38	1.33
4	D	2007	GDX	O5'-C5'	2.25	1.47	1.43
3	D	2004	NAD	C2A-N1A	2.26	1.38	1.33
4	A	2005	GDX	O5'-C5'	2.36	1.47	1.43
4	D	2008	GDX	O5'-C5'	2.57	1.47	1.43
4	D	2007	GDX	O4D-C1D	2.84	1.44	1.41
4	D	2008	GDX	O4D-C1D	2.89	1.44	1.41
4	D	2007	GDX	C5-C4	3.03	1.47	1.40
4	A	2006	GDX	C5-C4	3.15	1.47	1.40
4	D	2008	GDX	C5-C4	3.17	1.47	1.40
3	A	2001	NAD	C2A-N3A	3.25	1.37	1.32
4	A	2005	GDX	C5-C4	3.29	1.47	1.40
4	A	2006	GDX	C6-C5	3.38	1.48	1.41
4	A	2005	GDX	C6-C5	3.48	1.48	1.41
4	D	2007	GDX	C6-C5	3.60	1.48	1.41
3	B	2002	NAD	C2A-N3A	3.68	1.38	1.32
3	D	2004	NAD	C2A-N3A	3.79	1.38	1.32
3	C	2003	NAD	C2A-N3A	3.89	1.39	1.32
4	D	2008	GDX	C6-C5	3.93	1.49	1.41

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	NAD	N3A-C2A-N1A	-12.24	119.53	128.89
3	A	2001	NAD	N3A-C2A-N1A	-10.92	120.53	128.89
3	C	2003	NAD	N3A-C2A-N1A	-10.52	120.84	128.89
3	D	2004	NAD	N3A-C2A-N1A	-10.37	120.96	128.89
4	D	2007	GDX	C5-C6-N1	-5.18	116.50	123.59
4	D	2008	GDX	C5-C6-N1	-4.87	116.93	123.59
4	A	2005	GDX	C5-C6-N1	-4.85	116.96	123.59
4	A	2006	GDX	C5-C6-N1	-4.63	117.26	123.59
3	B	2002	NAD	PN-O3-PA	-4.09	121.23	132.73
4	D	2008	GDX	C4D-O4D-C1D	-3.94	105.39	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2006	GDX	O5'-C1'-O1B	-3.92	106.19	111.36
3	B	2002	NAD	C1B-N9A-C4A	-3.79	121.22	126.94
4	A	2006	GDX	C4D-O4D-C1D	-3.79	105.55	109.72
4	A	2005	GDX	C4D-O4D-C1D	-3.69	105.67	109.72
3	D	2004	NAD	C4B-O4B-C1B	-3.60	105.76	109.72
3	B	2002	NAD	C4B-O4B-C1B	-3.57	105.80	109.72
4	D	2007	GDX	C4D-O4D-C1D	-3.53	105.84	109.72
3	C	2003	NAD	PN-O3-PA	-3.51	122.87	132.73
4	A	2006	GDX	C6-C5-C4	-3.50	116.71	120.90
4	D	2008	GDX	C6-C5-C4	-3.47	116.75	120.90
4	A	2005	GDX	C6-C5-C4	-3.23	117.04	120.90
3	A	2001	NAD	PN-O3-PA	-3.16	123.86	132.73
3	C	2003	NAD	C4B-O4B-C1B	-3.07	106.35	109.72
4	D	2007	GDX	C6-C5-C4	-3.02	117.29	120.90
4	D	2008	GDX	N3-C2-N1	-2.98	122.91	127.44
3	C	2003	NAD	C1B-N9A-C4A	-2.85	122.64	126.94
4	A	2006	GDX	N3-C2-N1	-2.81	123.16	127.44
3	A	2001	NAD	C4B-O4B-C1B	-2.69	106.76	109.72
3	A	2001	NAD	C1B-N9A-C4A	-2.58	123.04	126.94
4	D	2007	GDX	PB-O3A-PA	-2.56	125.55	132.73
4	D	2007	GDX	N3-C2-N1	-2.55	123.56	127.44
4	D	2008	GDX	O5'-C1'-O1B	-2.50	108.07	111.36
4	A	2005	GDX	N3-C2-N1	-2.41	123.77	127.44
3	D	2004	NAD	PN-O3-PA	-2.31	126.24	132.73
4	A	2005	GDX	O3D-C3D-C4D	-2.27	104.23	111.05
4	D	2008	GDX	O3D-C3D-C4D	-2.25	104.30	111.05
3	D	2004	NAD	C1B-N9A-C4A	-2.24	123.56	126.94
4	A	2006	GDX	PB-O3A-PA	-2.21	126.51	132.73
4	D	2007	GDX	C1D-N9-C4	-2.20	123.62	126.94
4	D	2008	GDX	PB-O3A-PA	-2.17	126.64	132.73
3	A	2001	NAD	C4A-C5A-N7A	-2.16	107.50	109.48
4	A	2006	GDX	C1D-N9-C4	-2.10	123.78	126.94
4	D	2008	GDX	C4-C5-N7	-2.03	107.61	109.48
4	D	2007	GDX	O5'-C1'-O1B	-2.03	108.69	111.36
4	A	2006	GDX	C4'-C3'-C2'	2.02	114.56	110.79
3	B	2002	NAD	O2N-PN-O3	2.06	114.45	105.09
4	D	2007	GDX	C1'-C2'-C3'	2.08	114.08	109.97
4	A	2005	GDX	O4'-C4'-C3'	2.12	115.10	110.34
4	A	2006	GDX	O4'-C4'-C3'	2.12	115.12	110.34
4	D	2008	GDX	C4'-C3'-C2'	2.14	114.79	110.79
3	C	2003	NAD	O4B-C1B-N9A	2.19	112.69	108.10
4	D	2008	GDX	C1'-C2'-C3'	2.21	114.34	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2007	GDX	C4'-C3'-C2'	2.25	114.99	110.79
3	B	2002	NAD	O2A-PA-O3	2.26	115.36	105.09
4	D	2007	GDX	O4'-C4'-C3'	2.30	115.52	110.34
4	A	2005	GDX	C1'-C2'-C3'	2.31	114.52	109.97
4	A	2005	GDX	C4'-C3'-C2'	2.43	115.32	110.79
4	A	2006	GDX	C1'-C2'-C3'	2.46	114.82	109.97
3	A	2001	NAD	O4B-C1B-N9A	2.53	113.39	108.10
4	D	2008	GDX	C2D-C3D-C4D	2.58	107.92	102.61
4	D	2008	GDX	O4D-C1D-N9	2.69	113.73	108.10
4	D	2007	GDX	C2D-C3D-C4D	2.81	108.38	102.61
3	D	2004	NAD	O4B-C1B-N9A	2.89	114.15	108.10
4	A	2006	GDX	O4D-C1D-N9	2.94	114.26	108.10
4	A	2005	GDX	C2D-C3D-C4D	3.05	108.89	102.61
4	A	2006	GDX	C2D-C3D-C4D	3.33	109.46	102.61
4	D	2007	GDX	O4D-C1D-N9	3.62	115.67	108.10
4	A	2005	GDX	O4D-C1D-N9	3.71	115.87	108.10
4	A	2006	GDX	C6-N1-C2	4.81	122.62	115.94
4	A	2005	GDX	C6-N1-C2	4.88	122.72	115.94
4	D	2007	GDX	C6-N1-C2	4.93	122.78	115.94
4	D	2008	GDX	C6-N1-C2	5.10	123.01	115.94
4	A	2005	GDX	C2D-C1D-N9	5.40	122.54	114.29
4	D	2007	GDX	C2D-C1D-N9	5.76	123.09	114.29
4	A	2006	GDX	C2D-C1D-N9	5.88	123.28	114.29
4	D	2008	GDX	C2D-C1D-N9	6.45	124.15	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NAD	2	0
5	C	2009	ACY	1	0
5	C	2010	ACY	3	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, 95th 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	436/436 (100%)	-0.32	5 (1%)	82	84	4, 9, 18, 25	1 (0%)
1	B	436/436 (100%)	-0.37	5 (1%)	82	84	4, 9, 17, 23	2 (0%)
1	C	436/436 (100%)	-0.44	1 (0%)	95	95	3, 8, 16, 21	0
1	D	436/436 (100%)	-0.42	4 (0%)	85	87	3, 7, 16, 25	0
All	All	1744/1744 (100%)	-0.39	15 (0%)	85	87	3, 8, 17, 25	3 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	TYR	4.6
1	D	368	TYR	3.6
1	B	345	LYS	3.5
1	A	371	SER	2.9
1	A	148	VAL	2.7
1	B	368	TYR	2.6
1	B	90	LYS	2.6
1	D	371	SER	2.5
1	D	312	ASP	2.5
1	B	365	ASN	2.5
1	A	415	LYS	2.3
1	A	370	GLU	2.1
1	B	429	ALA	2.1
1	D	314	ARG	2.1
1	C	314	ARG	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 [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, 95th 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(\AA^2)	Q<0.9
2	SUC	B	2012	23/23	0.77	0.22	3.93	31,34,40,41	0
5	ACY	C	2010	4/4	0.93	0.10	3.19	26,26,26,27	0
2	SUC	D	2013	23/23	0.88	0.13	2.30	25,27,30,32	0
4	GDX	A	2006	40/40	0.97	0.08	2.20	12,14,16,18	0
4	GDX	A	2005	40/40	0.97	0.08	1.46	13,15,16,17	0
4	GDX	D	2007	40/40	0.98	0.07	1.11	11,13,14,16	0
3	NAD	C	2003	35/44	0.98	0.07	0.50	12,16,18,19	0
4	GDX	D	2008	40/40	0.98	0.07	0.37	11,13,15,16	0
3	NAD	D	2004	35/44	0.98	0.06	0.13	12,15,16,18	0
3	NAD	B	2002	35/44	0.98	0.06	-0.35	15,17,19,19	0
3	NAD	A	2001	35/44	0.98	0.06	-0.45	14,17,21,23	0
5	ACY	C	2009	4/4	0.94	0.06	-	26,26,27,27	0
6	MPD	C	2011	8/8	0.53	0.38	-	38,39,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.