Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:16 AM GMT

PDB ID	:	3OA0
Title	:	Crystal structure of the WlbA (WbpB) Dehydrogenase from Thermus thermophilus in complex with NAD and UDP-GlcNAcA
Authors	:	Holden, H.M.; Thoden, J.B.
Deposited on	:	2010-08-04
Resolution	:	2.00 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:

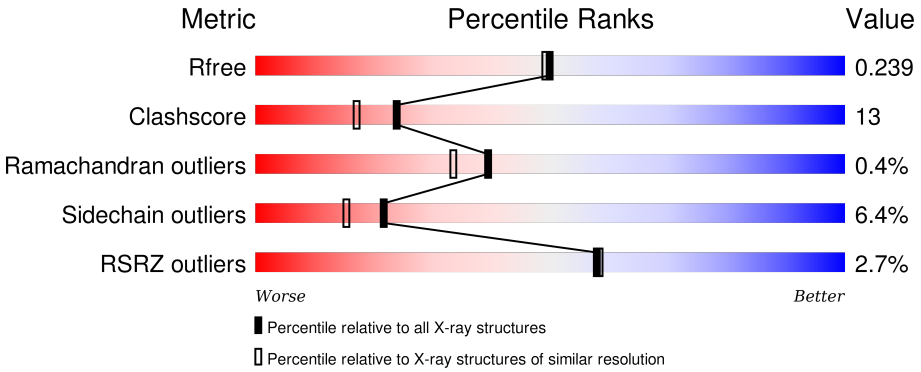
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	312	4% 75% 21%
1	B	312	2% 77% 20%
1	C	312	2% 82% 13%
1	D	312	3% 77% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10599 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.

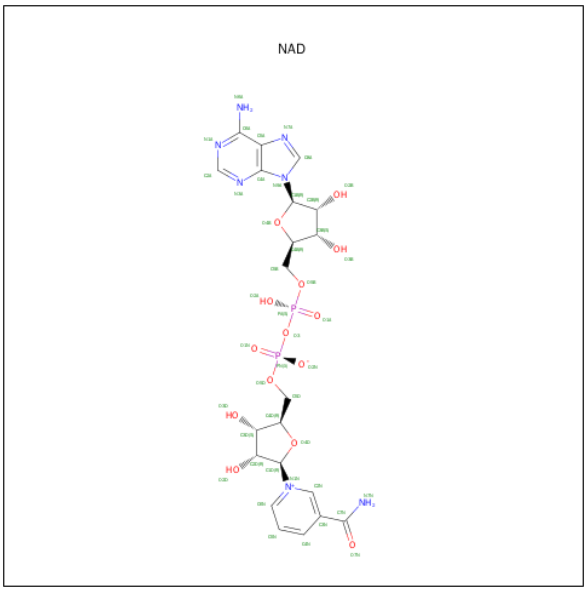
- Molecule 1 is a protein called Lipopolysaccharide biosynthesis protein wbpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	3	0
			2473	1588	437	445	3			
1	B	310	Total	C	N	O	S	0	2	0
			2465	1582	436	445	2			
1	C	310	Total	C	N	O	S	0	0	0
			2451	1573	432	444	2			
1	D	307	Total	C	N	O	S	0	0	0
			2428	1558	429	439	2			

There are 8 discrepancies between the modelled and reference sequences:

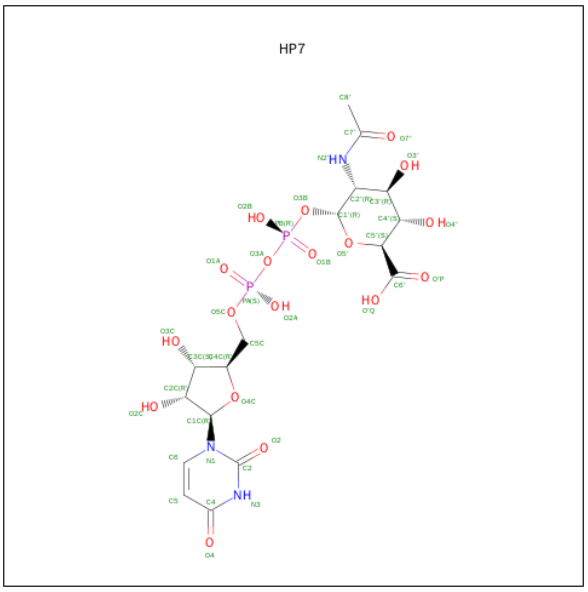
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q72KX8
A	0	HIS	-	EXPRESSION TAG	UNP Q72KX8
B	-1	GLY	-	EXPRESSION TAG	UNP Q72KX8
B	0	HIS	-	EXPRESSION TAG	UNP Q72KX8
C	-1	GLY	-	EXPRESSION TAG	UNP Q72KX8
C	0	HIS	-	EXPRESSION TAG	UNP Q72KX8
D	-1	GLY	-	EXPRESSION TAG	UNP Q72KX8
D	0	HIS	-	EXPRESSION TAG	UNP Q72KX8

- 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		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (2S,3S,4R,5R,6R)-5-ACETAMIDO-6-[[[(2R,3S,4R,5R)-5-(2,4-DIOXOPYRIMIDIN-1-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHOXY-HYDROXY-PHOSPHORYL]OXY-HYDROXY-PHOSPHORYL]OXY-3,4-DIHYDROXY-OXANE-2-CARBOXYLIC ACID (three-letter code: HP7) (formula: $C_{17}H_{25}N_3O_{18}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 40 17 3 18 2	0	0
3	B	1	Total C N O P 40 17 3 18 2	0	0
3	C	1	Total C N O P 40 17 3 18 2	0	0
3	D	1	Total C N O P 40 17 3 18 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	109	Total O 109 109	0	0

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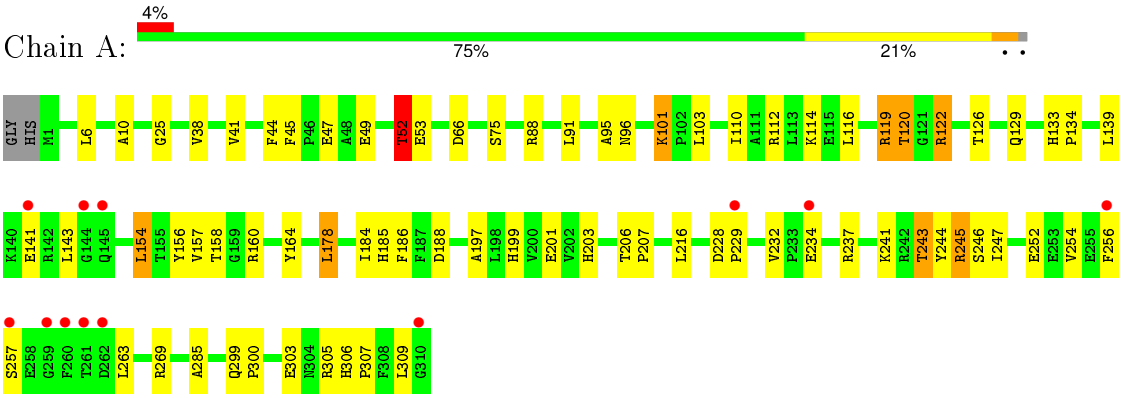
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	98	Total O 98 98	0	0
5	C	125	Total O 125 125	0	0
5	D	110	Total O 110 110	0	0

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.

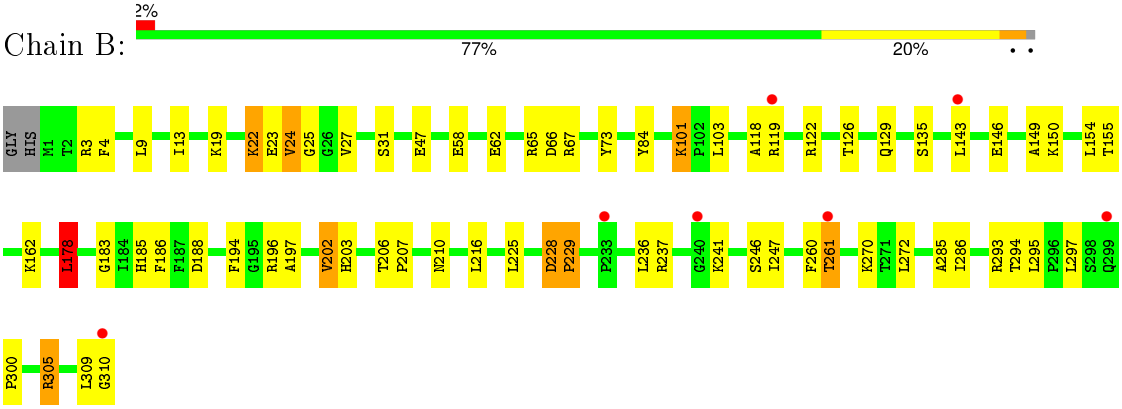
- Molecule 1: Lipopolysaccharide biosynthesis protein wbpB

Chain A:



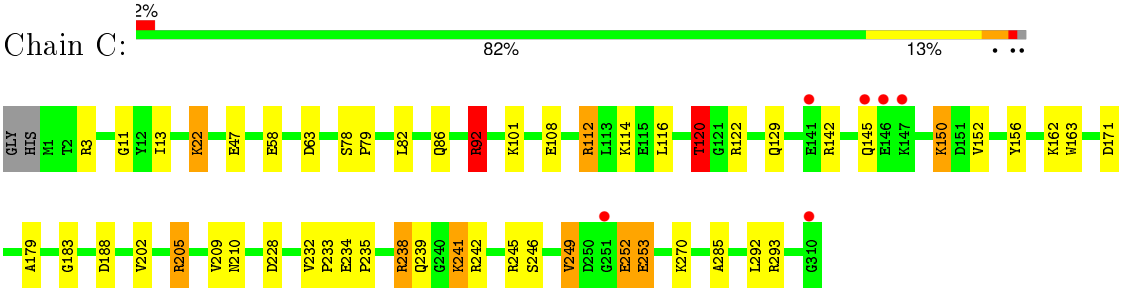
- Molecule 1: Lipopolysaccharide biosynthesis protein wbpB

Chain B:



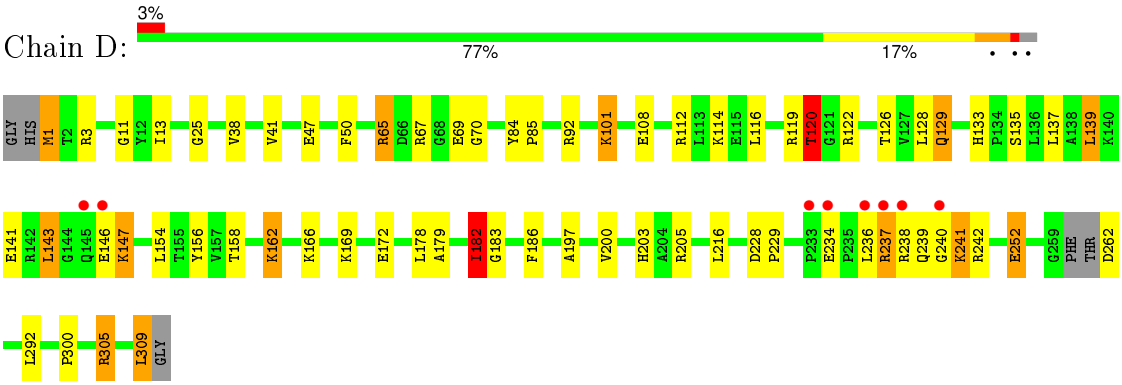
- Molecule 1: Lipopolysaccharide biosynthesis protein wbpB

Chain C:



- Molecule 1: Lipopolysaccharide biosynthesis protein wbpB

Chain D:


3%
77%
17%
GLY HIS M1 T2 R3 G11 Y12 I13 G25 V38 V41 E47 F50 R65 D66 R67 G68 E69 G70 Y84 P85 R92 K101 E108 R112 L113 K114 E115 L116 R119 T120 G121 R122 T126 V127 L128 Q129 H133 P134 S135 L136 L137 A138 L139 K140
E141 R142 L143 G144 Q145 E146 K147 L154 T155 Y156 V157 T158 K162 K166 K169 E172 L178 A179 I182 G183 F186 A197 V200 H203 A204 R205 L216 D228 P229 P233 E234 P235 L236 R237 R238 Q239 G240 K241 R242 E252 G259 PHE THR D262
L292 P300 R305 I309 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.10Å 68.32Å 164.12Å 90.00° 94.51° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 36.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.00-2.00) 91.8 (36.82-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	17.71 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.189 , 0.248 0.186 , 0.239	Depositor DCC
R_{free} test set	4966 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	1.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.3	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 98909 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10599	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: HP7, NAD, CL

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	0.60	0/2539	1.00	3/3440 (0.1%)
1	B	0.58	0/2531	1.01	4/3431 (0.1%)
1	C	0.59	1/2511 (0.0%)	1.07	9/3405 (0.3%)
1	D	0.56	0/2486	1.01	8/3371 (0.2%)
All	All	0.58	1/10067 (0.0%)	1.02	24/13647 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	241	LYS	CD-CE	6.52	1.67	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	92	ARG	NE-CZ-NH2	-13.74	113.43	120.30
1	C	92	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	C	205	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	C	205	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	C	92	ARG	CG-CD-NE	-6.56	98.02	111.80
1	C	293	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	120	THR	N-CA-CB	-6.23	98.46	110.30
1	D	119	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	B	122	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	D	65	ARG	CG-CD-NE	-5.78	99.65	111.80
1	D	242	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	178	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	B	293	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	92	ARG	CD-NE-CZ	5.47	131.26	123.60
1	A	52	THR	N-CA-CB	-5.42	100.01	110.30
1	B	178	LEU	CA-CB-CG	5.37	127.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	156	TYR	CA-CB-CG	5.37	123.61	113.40
1	D	205	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	88	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	C	63	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	182	ILE	CG1-CB-CG2	5.23	122.91	111.40
1	C	120	THR	N-CA-CB	-5.10	100.60	110.30
1	B	228	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	D	205	ARG	NE-CZ-NH1	-5.03	117.78	120.30

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	2473	0	2489	73	1
1	B	2465	0	2476	82	0
1	C	2451	0	2455	48	1
1	D	2428	0	2435	56	0
2	A	44	0	26	4	0
2	B	44	0	26	5	0
2	C	44	0	26	8	0
2	D	44	0	26	6	0
3	A	40	0	22	6	0
3	B	40	0	22	3	0
3	C	40	0	22	2	0
3	D	40	0	22	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	109	0	0	2	0
5	B	98	0	0	2	0
5	C	125	0	0	3	0
5	D	110	0	0	4	0
All	All	10599	0	10047	264	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 13.

All (264) 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:300:PRO:CG	1:B:305:ARG:HH12	1.47	1.28
1:C:120:THR:HG22	1:C:122:ARG:H	1.11	1.14
1:B:300:PRO:HG2	1:B:305:ARG:NH1	1.66	1.09
1:B:305:ARG:HB2	1:B:305:ARG:HH11	1.15	1.08
2:D:311:NAD:N7N	5:D:402:HOH:O	1.88	1.06
1:B:300:PRO:HG2	1:B:305:ARG:HH12	0.90	1.05
1:D:300:PRO:HG2	1:D:305:ARG:NH2	1.72	1.04
1:D:241:LYS:HD2	1:D:241:LYS:N	1.73	1.01
1:C:129:GLN:HE22	2:C:311:NAD:H72N	1.08	1.01
1:B:305:ARG:NH1	1:B:305:ARG:HB2	1.78	0.98
1:A:154:LEU:HD12	1:A:247:ILE:HG12	1.46	0.98
1:B:118:ALA:HB3	1:B:119[A]:ARG:NH1	1.80	0.96
1:C:120:THR:CG2	1:C:122:ARG:H	1.79	0.95
1:B:129:GLN:HE22	2:B:311:NAD:H72N	1.14	0.95
1:B:305:ARG:HD3	1:B:310:GLY:O	1.66	0.95
1:A:158:THR:HA	1:A:243:THR:HG23	1.48	0.93
1:B:236:LEU:HB3	1:B:241:LYS:HD3	1.49	0.93
1:A:160:ARG:NH2	3:A:312:HP7:O'P	2.04	0.91
1:D:300:PRO:HG2	1:D:305:ARG:HH21	1.32	0.89
2:B:311:NAD:C4N	3:B:312:HP7:H3'	2.02	0.88
1:A:116:LEU:O	1:A:120:THR:HB	1.74	0.87
1:C:242:ARG:NH2	5:C:416:HOH:O	1.81	0.86
1:D:120:THR:HG22	1:D:122:ARG:H	1.38	0.86
1:A:120:THR:HG22	1:A:122:ARG:H	1.41	0.85
1:B:305:ARG:CB	1:B:305:ARG:HH11	1.89	0.85
1:A:103:LEU:HD13	1:A:126:THR:HB	1.58	0.85
1:A:129:GLN:HE22	2:A:311:NAD:H72N	1.22	0.85
1:B:300:PRO:CG	1:B:305:ARG:NH1	2.28	0.84
1:C:116:LEU:O	1:C:120:THR:HB	1.77	0.84
1:A:120:THR:HG23	1:A:122:ARG:HB2	1.59	0.84
1:D:120:THR:CG2	1:D:122:ARG:H	1.90	0.83
2:D:311:NAD:O5D	2:D:311:NAD:H6N	1.80	0.81
1:D:300:PRO:CG	1:D:305:ARG:NH2	2.44	0.80
1:A:245:ARG:HH11	1:A:245:ARG:CG	1.94	0.80
1:A:245:ARG:HH11	1:A:245:ARG:CB	1.95	0.79
1:C:129:GLN:NE2	2:C:311:NAD:H72N	1.80	0.79
1:B:62:GLU:OE2	1:C:92:ARG:HD3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:O	1:B:24:VAL:CG1	2.31	0.78
1:A:120:THR:CG2	1:A:122:ARG:HB2	2.14	0.78
1:A:101:LYS:HE3	1:A:101:LYS:O	1.82	0.78
1:B:237:ARG:HH21	1:B:237:ARG:CB	1.97	0.78
1:C:3:ARG:HH21	1:C:3:ARG:HG2	1.47	0.78
2:C:311:NAD:C4N	3:C:312:HP7:H3'	2.14	0.77
1:D:116:LEU:O	1:D:120:THR:HB	1.85	0.77
2:A:311:NAD:C4N	3:A:312:HP7:H3'	2.15	0.76
1:B:118:ALA:HB3	1:B:119[A]:ARG:HH11	1.49	0.76
1:B:237:ARG:HH21	1:B:237:ARG:HB3	1.52	0.75
1:C:234:GLU:OE2	1:C:238:ARG:NH1	2.20	0.74
1:B:300:PRO:HG3	1:B:305:ARG:HH12	1.48	0.74
1:B:237:ARG:NH2	1:B:237:ARG:HB2	2.02	0.74
1:B:24:VAL:HG11	1:B:272:LEU:CD1	2.18	0.72
1:B:260:PHE:O	1:B:261:THR:C	2.26	0.72
1:A:49:GLU:OE2	1:B:162:LYS:HE2	1.90	0.71
1:B:237:ARG:NH2	1:B:237:ARG:CB	2.54	0.71
1:B:65:ARG:NH2	1:B:66:ASP:OD1	2.24	0.71
1:D:137:LEU:O	5:D:391:HOH:O	2.08	0.71
1:A:160:ARG:HH21	3:A:312:HP7:C6'	2.04	0.71
1:B:67:ARG:O	1:B:67:ARG:HG3	1.89	0.70
1:B:101:LYS:HD2	1:B:185:HIS:CE1	2.27	0.70
1:D:234:GLU:HG2	1:D:234:GLU:O	1.92	0.70
2:D:311:NAD:C4N	3:D:312:HP7:H3'	2.22	0.69
1:A:101:LYS:HE3	1:A:101:LYS:C	2.11	0.69
1:C:108:GLU:HB3	1:C:112:ARG:HH12	1.57	0.69
1:D:139:LEU:HD22	1:D:143:LEU:HD22	1.75	0.68
2:B:311:NAD:C3N	3:B:312:HP7:H3'	2.24	0.68
1:B:228:ASP:OD2	5:B:396:HOH:O	2.10	0.68
1:C:3:ARG:NH2	1:C:3:ARG:HG2	2.06	0.67
1:B:118:ALA:CB	1:B:119[A]:ARG:NH1	2.56	0.67
2:C:311:NAD:H6N	2:C:311:NAD:O5D	1.94	0.66
1:A:25:GLY:HA2	5:A:365:HOH:O	1.93	0.66
1:D:179:ALA:O	1:D:183:GLY:HA3	1.95	0.66
1:C:120:THR:CG2	1:C:122:ARG:N	2.58	0.65
1:B:236:LEU:HB3	1:B:241:LYS:CD	2.27	0.65
1:A:120:THR:CG2	1:A:122:ARG:H	2.10	0.64
1:B:24:VAL:O	1:B:24:VAL:HG12	1.96	0.64
1:A:52:THR:HG22	1:A:53:GLU:HG2	1.78	0.64
1:B:305:ARG:O	1:B:305:ARG:HG2	1.96	0.64
1:A:129:GLN:NE2	2:A:311:NAD:H72N	1.92	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLN:NE2	2:B:311:NAD:H72N	1.91	0.63
1:A:185:HIS:CD2	1:A:185:HIS:H	2.15	0.63
1:D:237:ARG:O	1:D:240:GLY:N	2.29	0.63
1:D:237:ARG:O	1:D:239:GLN:N	2.32	0.62
1:C:246:SER:HB2	1:C:253:GLU:OE1	2.00	0.61
1:C:142:ARG:NH2	1:C:252:GLU:OE2	2.32	0.61
1:B:196:ARG:HG2	1:B:197:ALA:N	2.16	0.61
1:B:146:GLU:OE2	1:B:150:LYS:NZ	2.35	0.60
1:A:245:ARG:HH11	1:A:245:ARG:HG3	1.65	0.60
1:B:24:VAL:HG11	1:B:272:LEU:HD12	1.83	0.59
1:A:234:GLU:HB2	1:A:237:ARG:HH21	1.67	0.59
1:D:3:ARG:NH1	1:D:69:GLU:HG3	2.17	0.59
1:B:236:LEU:O	1:B:241:LYS:HG3	2.02	0.59
1:B:202:VAL:HG22	1:B:297:LEU:HD23	1.84	0.59
1:D:1:MET:HG2	1:D:25:GLY:O	2.03	0.58
1:A:203:HIS:CE1	1:A:300:PRO:HB3	2.38	0.58
1:B:101:LYS:C	1:B:101:LYS:HE2	2.24	0.58
1:D:101:LYS:O	1:D:101:LYS:HD3	2.03	0.58
1:B:305:ARG:CD	1:B:310:GLY:O	2.47	0.58
1:B:202:VAL:HG12	1:B:295:LEU:HD23	1.84	0.58
1:C:202:VAL:CG2	1:C:292:LEU:HD22	2.35	0.57
5:C:341:HOH:O	1:D:162:LYS:HG2	2.04	0.57
1:B:62:GLU:OE2	1:C:92:ARG:CD	2.53	0.57
1:D:240:GLY:C	1:D:241:LYS:HD2	2.23	0.57
2:A:311:NAD:C5N	3:A:312:HP7:H3'	2.33	0.57
1:D:241:LYS:N	1:D:241:LYS:CD	2.58	0.56
1:B:178:LEU:HD23	1:B:225:LEU:HD23	1.86	0.56
1:A:139:LEU:HD22	1:A:254:VAL:HG11	1.88	0.56
1:A:66:ASP:OD2	1:D:112:ARG:NH1	2.39	0.55
1:C:13:ILE:HD13	2:C:311:NAD:C4N	2.35	0.55
1:A:245:ARG:HG3	1:A:256:PHE:CZ	2.41	0.55
1:C:120:THR:HG22	1:C:122:ARG:N	1.97	0.55
1:A:158:THR:HG23	1:A:158:THR:O	2.07	0.55
1:A:157:VAL:O	1:A:243:THR:HG22	2.07	0.54
1:A:245:ARG:NH1	1:A:245:ARG:HG3	2.19	0.54
1:C:142:ARG:HH21	1:C:252:GLU:CD	2.11	0.54
1:B:154:LEU:HD13	1:B:154:LEU:C	2.28	0.54
1:D:158:THR:HG21	1:D:182:ILE:HD12	1.90	0.54
1:A:234:GLU:HG2	1:A:234:GLU:O	2.06	0.54
1:D:172:GLU:HB2	5:D:442:HOH:O	2.07	0.54
1:B:143:LEU:HD13	1:B:194:PHE:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ALA:CB	1:B:119[A]:ARG:HH11	2.19	0.53
1:B:150:LYS:N	1:B:150:LYS:HD3	2.23	0.53
1:C:179:ALA:O	1:C:183:GLY:HA3	2.08	0.53
1:B:178:LEU:CD2	1:B:225:LEU:HD23	2.39	0.53
1:A:229:PRO:O	1:A:232:VAL:HG23	2.08	0.53
1:D:234:GLU:O	1:D:234:GLU:CG	2.57	0.53
1:B:118:ALA:HB3	1:B:119[A]:ARG:HH12	1.69	0.52
1:B:101:LYS:CD	1:B:185:HIS:CE1	2.92	0.52
1:A:300:PRO:HG2	1:A:305:ARG:HH11	1.75	0.52
1:B:206:THR:HB	1:B:207:PRO:HD2	1.91	0.52
1:D:228:ASP:C	1:D:228:ASP:OD1	2.48	0.52
1:B:27:VAL:HG13	1:B:27:VAL:O	2.09	0.52
1:C:209:VAL:C	1:C:210:ASN:HD22	2.14	0.51
1:D:300:PRO:HG2	1:D:305:ARG:HH22	1.70	0.51
1:B:24:VAL:O	1:B:24:VAL:HG13	2.08	0.51
1:B:19:LYS:O	1:B:23:GLU:HG3	2.10	0.51
1:B:178:LEU:HD23	1:B:225:LEU:CD2	2.41	0.51
1:A:129:GLN:HB2	1:A:263:LEU:HB3	1.91	0.50
1:B:24:VAL:HG11	1:B:272:LEU:HD11	1.92	0.50
1:A:101:LYS:HD2	1:A:184:ILE:CG2	2.41	0.50
1:C:114:LYS:HE3	5:C:314:HOH:O	2.12	0.50
1:A:156:TYR:CD2	1:A:186:PHE:HE1	2.30	0.50
1:C:232:VAL:HG13	1:C:233:PRO:HD2	1.93	0.50
1:A:160:ARG:CZ	3:A:312:HP7:O'P	2.59	0.50
1:D:120:THR:HG23	1:D:122:ARG:HB2	1.94	0.50
1:A:245:ARG:HG2	1:A:246:SER:N	2.27	0.50
1:C:3:ARG:CG	1:C:3:ARG:HH21	2.18	0.50
1:D:120:THR:CG2	1:D:122:ARG:HB2	2.42	0.49
1:B:149:ALA:C	1:B:150:LYS:HD3	2.33	0.49
1:A:234:GLU:CG	1:A:234:GLU:O	2.61	0.49
1:C:239:GLN:OE1	1:C:241:LYS:HE2	2.12	0.49
1:D:183:GLY:HA2	1:D:186:PHE:CE1	2.47	0.49
1:A:6:LEU:HD12	1:A:75:SER:O	2.11	0.49
1:A:38:VAL:O	1:A:41:VAL:HG12	2.12	0.49
1:B:84:TYR:OH	5:B:393:HOH:O	2.12	0.49
1:B:197:ALA:HA	1:B:216:LEU:HD23	1.94	0.49
1:D:133:HIS:CE1	1:D:135:SER:HB2	2.47	0.49
1:B:188:ASP:HA	1:B:285:ALA:HB2	1.95	0.48
1:D:101:LYS:C	1:D:101:LYS:HD3	2.34	0.48
1:B:22:LYS:O	1:B:25:GLY:N	2.45	0.48
1:C:112:ARG:O	1:C:116:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ALA:O	1:A:122:ARG:HG2	2.14	0.48
1:A:120:THR:CG2	1:A:122:ARG:N	2.77	0.48
1:B:305:ARG:CG	1:B:305:ARG:O	2.60	0.48
1:D:237:ARG:C	1:D:239:GLN:N	2.67	0.48
1:C:228:ASP:C	1:C:228:ASP:OD1	2.52	0.48
1:C:188:ASP:HA	1:C:285:ALA:HB2	1.96	0.47
1:D:120:THR:CG2	1:D:122:ARG:N	2.69	0.47
1:D:158:THR:HG23	1:D:158:THR:O	2.14	0.47
1:B:154:LEU:HD13	1:B:155:THR:N	2.29	0.47
1:D:197:ALA:HA	1:D:216:LEU:HD22	1.97	0.47
1:D:84:TYR:HB3	1:D:85:PRO:CD	2.45	0.47
1:C:202:VAL:HG22	1:C:292:LEU:HD22	1.97	0.47
1:D:179:ALA:O	1:D:183:GLY:CA	2.63	0.46
1:D:108:GLU:HG2	5:D:344:HOH:O	2.14	0.46
1:B:9:LEU:HD22	1:B:31:SER:CB	2.46	0.46
1:A:228:ASP:OD1	1:A:228:ASP:C	2.53	0.46
1:A:185:HIS:HD2	1:A:185:HIS:H	1.61	0.46
1:D:200:VAL:CG1	1:D:292:LEU:HD21	2.45	0.46
1:A:110:ILE:HG22	1:A:114:LYS:HE3	1.96	0.46
1:A:241:LYS:HA	1:A:241:LYS:HD3	1.66	0.46
1:A:197:ALA:HA	1:A:216:LEU:HD23	1.97	0.46
1:B:24:VAL:CG1	1:B:272:LEU:HD12	2.46	0.46
1:D:169:LYS:NZ	3:D:312:HP7:O4	2.49	0.46
1:D:300:PRO:CG	1:D:305:ARG:HH22	2.24	0.46
1:C:22:LYS:HE2	1:C:22:LYS:HB2	1.76	0.46
1:A:101:LYS:HD2	1:A:184:ILE:HG23	1.98	0.46
1:A:245:ARG:HB3	1:A:245:ARG:HH11	1.74	0.46
1:A:303:GLU:H	1:A:303:GLU:CD	2.19	0.45
1:A:299:GLN:HA	1:A:299:GLN:NE2	2.31	0.45
1:C:82:LEU:O	1:C:86:GLN:HG3	2.15	0.45
1:A:157:VAL:O	1:A:243:THR:CG2	2.65	0.45
1:B:196:ARG:O	1:B:216:LEU:HA	2.16	0.45
1:B:103:LEU:HB3	1:B:286:ILE:HD11	1.99	0.45
1:D:129:GLN:CD	1:D:129:GLN:H	2.18	0.45
1:C:171:ASP:C	1:C:171:ASP:OD2	2.55	0.45
1:D:67:ARG:O	1:D:67:ARG:HG3	2.16	0.45
1:B:300:PRO:HG3	1:B:305:ARG:NH1	2.18	0.45
1:B:196:ARG:CG	1:B:197:ALA:N	2.80	0.45
1:D:252:GLU:HG3	1:D:252:GLU:O	2.16	0.45
1:A:188:ASP:HA	1:A:285:ALA:HB2	1.99	0.45
1:B:203:HIS:CE1	1:B:300:PRO:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD13	1:B:126:THR:HB	1.98	0.44
1:C:78:SER:HB2	1:C:79:PRO:HD2	1.99	0.44
1:D:13:ILE:HD13	2:D:311:NAD:C4N	2.48	0.44
1:A:133:HIS:CE1	1:A:256:PHE:HB2	2.52	0.44
1:D:237:ARG:C	1:D:239:GLN:H	2.21	0.44
1:D:228:ASP:HA	1:D:229:PRO:HD3	1.82	0.44
1:B:101:LYS:HG2	1:B:185:HIS:CE1	2.52	0.44
2:D:311:NAD:C3N	3:D:312:HP7:H3'	2.47	0.44
1:A:245:ARG:CZ	1:A:256:PHE:CE1	3.01	0.44
1:A:25:GLY:CA	5:A:365:HOH:O	2.61	0.43
2:C:311:NAD:C3N	3:C:312:HP7:H3'	2.48	0.43
1:C:152:VAL:HG22	1:C:249:VAL:HB	1.99	0.43
1:B:13:ILE:HD13	2:B:311:NAD:C4N	2.49	0.43
1:A:160:ARG:HD3	1:A:160:ARG:HA	1.78	0.43
1:A:160:ARG:HG3	1:A:164:TYR:CD1	2.54	0.43
1:B:58:GLU:OE2	1:C:58:GLU:OE2	2.36	0.43
1:B:183:GLY:HA2	1:B:186:PHE:CE1	2.53	0.43
1:D:120:THR:HG23	1:D:122:ARG:N	2.33	0.43
1:D:203:HIS:CE1	1:D:300:PRO:HB3	2.54	0.43
1:A:91:LEU:HD22	1:A:122:ARG:HB3	2.01	0.43
1:C:246:SER:CB	1:C:253:GLU:OE1	2.65	0.43
1:B:178:LEU:C	1:B:178:LEU:HD23	2.39	0.43
1:B:154:LEU:CD1	1:B:154:LEU:C	2.87	0.43
1:C:163:TRP:HA	1:D:50:PHE:HB3	2.00	0.43
1:C:129:GLN:HE22	2:C:311:NAD:C7N	2.29	0.43
1:C:78:SER:HB2	1:C:79:PRO:CD	2.49	0.43
1:B:19:LYS:HB2	1:B:19:LYS:HE3	1.69	0.42
1:D:147:LYS:H	1:D:147:LYS:HD3	1.82	0.42
1:C:270:LYS:HB3	1:C:270:LYS:HE3	1.85	0.42
1:A:95:ALA:C	1:A:122:ARG:HG2	2.39	0.42
1:A:156:TYR:CZ	1:A:158:THR:HB	2.54	0.42
1:A:299:GLN:HE21	1:A:299:GLN:HA	1.85	0.42
1:A:44:PHE:HB3	1:A:45:PHE:CD2	2.54	0.42
1:A:199:HIS:NE2	1:A:201:GLU:OE2	2.49	0.42
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.79	0.42
1:C:232:VAL:CG1	1:C:233:PRO:HD2	2.49	0.42
1:D:38:VAL:O	1:D:41:VAL:HG12	2.19	0.42
1:D:309:LEU:HA	1:D:309:LEU:HD12	1.83	0.42
1:A:96:ASN:OD1	1:A:122:ARG:HG3	2.20	0.42
1:A:119:ARG:HG3	1:A:119:ARG:O	2.19	0.42
1:A:306:HIS:ND1	1:A:307:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HB	1:A:207:PRO:HD2	2.02	0.41
1:D:126:THR:HG23	1:D:128:LEU:HG	2.02	0.41
1:C:234:GLU:O	1:C:235:PRO:C	2.59	0.41
1:D:147:LYS:N	1:D:147:LYS:HD3	2.35	0.41
1:B:185:HIS:NE2	3:B:312:HP7:O3'	2.36	0.41
1:A:160:ARG:NE	3:A:312:HP7:O'P	2.53	0.41
1:A:133:HIS:HA	1:A:134:PRO:HD3	1.89	0.41
1:B:4:PHE:CD2	1:B:73:TYR:HB2	2.56	0.41
1:B:228:ASP:HA	1:B:229:PRO:HD3	1.84	0.41
1:D:11:GLY:HA3	2:D:311:NAD:O5B	2.21	0.41
1:D:141:GLU:OE2	1:D:141:GLU:HA	2.21	0.41
1:B:247:ILE:O	1:B:247:ILE:HG23	2.21	0.41
1:B:270:LYS:HE3	1:B:270:LYS:HB3	1.68	0.41
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.76	0.41
1:A:300:PRO:HG2	1:A:305:ARG:NH1	2.35	0.41
1:C:205:ARG:NH2	1:C:292:LEU:O	2.54	0.41
1:C:150:LYS:HG3	1:C:249:VAL:CG2	2.51	0.41
1:C:156:TYR:CZ	1:C:245:ARG:HD3	2.56	0.40
1:C:120:THR:CG2	1:C:122:ARG:HB2	2.52	0.40
1:A:10:ALA:HB2	1:A:38:VAL:CG1	2.51	0.40
1:B:3:ARG:NH2	1:B:3:ARG:HG2	2.36	0.40
1:C:11:GLY:HA3	2:C:311:NAD:O5B	2.22	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:257:SER:OG	1:C:239:GLN:NE2[1_455]	2.13	0.07

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	311/312 (100%)	298 (96%)	12 (4%)	1 (0%)	46 41
1	B	310/312 (99%)	300 (97%)	9 (3%)	1 (0%)	46 41
1	C	308/312 (99%)	300 (97%)	7 (2%)	1 (0%)	46 41
1	D	303/312 (97%)	288 (95%)	13 (4%)	2 (1%)	26 19
All	All	1232/1248 (99%)	1186 (96%)	41 (3%)	5 (0%)	39 33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	THR
1	D	238	ARG
1	A	244	TYR
1	D	70	GLY
1	C	238	ARG

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	255/253 (101%)	240 (94%)	15 (6%)	24 18
1	B	254/253 (100%)	241 (95%)	13 (5%)	29 23
1	C	252/253 (100%)	240 (95%)	12 (5%)	31 26
1	D	250/253 (99%)	226 (90%)	24 (10%)	10 6
All	All	1011/1012 (100%)	947 (94%)	64 (6%)	22 16

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	52	THR
1	A	101	LYS
1	A	112	ARG
1	A	119	ARG
1	A	120	THR

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Mol	Chain	Res	Type
1	A	122	ARG
1	A	141	GLU
1	A	143	LEU
1	A	154	LEU
1	A	243	THR
1	A	245	ARG
1	A	252	GLU
1	A	269	ARG
1	A	309	LEU
1	B	22	LYS
1	B	24	VAL
1	B	47	GLU
1	B	101	LYS
1	B	135	SER
1	B	178	LEU
1	B	202	VAL
1	B	210	ASN
1	B	229	PRO
1	B	246	SER
1	B	294	THR
1	B	305	ARG
1	B	309	LEU
1	C	22	LYS
1	C	47	GLU
1	C	92	ARG
1	C	101	LYS
1	C	112	ARG
1	C	120	THR
1	C	145	GLN
1	C	150	LYS
1	C	162	LYS
1	C	249	VAL
1	C	252	GLU
1	C	253	GLU
1	D	1	MET
1	D	47	GLU
1	D	65	ARG
1	D	92	ARG
1	D	101	LYS
1	D	114	LYS
1	D	120	THR
1	D	129	GLN

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Mol	Chain	Res	Type
1	D	139	LEU
1	D	143	LEU
1	D	146	GLU
1	D	147	LYS
1	D	154	LEU
1	D	162	LYS
1	D	166	LYS
1	D	178	LEU
1	D	182	ILE
1	D	236	LEU
1	D	237	ARG
1	D	241	LYS
1	D	252	GLU
1	D	262	ASP
1	D	305	ARG
1	D	309	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	185	HIS
1	A	299	GLN
1	B	81	HIS
1	B	129	GLN
1	B	239	GLN
1	C	81	HIS
1	C	129	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 (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	NAD	A	311	-	38,48,48	1.06	3 (7%)	47,73,73	3.07	20 (42%)
3	HP7	A	312	-	30,42,42	0.72	1 (3%)	44,64,64	2.26	9 (20%)
2	NAD	B	311	-	38,48,48	0.97	2 (5%)	47,73,73	2.52	19 (40%)
3	HP7	B	312	-	30,42,42	0.77	1 (3%)	44,64,64	1.91	9 (20%)
2	NAD	C	311	-	38,48,48	1.01	2 (5%)	47,73,73	2.50	15 (31%)
3	HP7	C	312	-	30,42,42	0.77	1 (3%)	44,64,64	2.25	8 (18%)
2	NAD	D	311	-	38,48,48	0.90	1 (2%)	47,73,73	2.82	20 (42%)
3	HP7	D	312	-	30,42,42	0.67	1 (3%)	44,64,64	1.59	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	311	-	-	0/22/62/62	0/5/5/5
3	HP7	A	312	-	-	0/20/65/65	0/3/3/3
2	NAD	B	311	-	-	0/22/62/62	0/5/5/5
3	HP7	B	312	-	-	0/20/65/65	0/3/3/3
2	NAD	C	311	-	-	0/22/62/62	0/5/5/5
3	HP7	C	312	-	-	0/20/65/65	0/3/3/3
2	NAD	D	311	-	-	0/22/62/62	0/5/5/5
3	HP7	D	312	-	-	0/20/65/65	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	311	NAD	C8A-N7A	-2.20	1.30	1.34
2	C	311	NAD	C4A-N3A	-2.01	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	311	NAD	O4D-C1D	2.06	1.43	1.41
2	D	311	NAD	O4B-C1B	2.18	1.44	1.41
2	B	311	NAD	O4B-C1B	2.21	1.44	1.41
3	D	312	HP7	O4C-C1C	2.22	1.44	1.41
2	C	311	NAD	O4B-C1B	2.24	1.44	1.41
3	A	312	HP7	O4C-C1C	2.31	1.44	1.41
2	B	311	NAD	O4D-C1D	2.57	1.44	1.41
3	B	312	HP7	O4C-C1C	3.12	1.45	1.41
3	C	312	HP7	O4C-C1C	3.14	1.45	1.41
2	A	311	NAD	O4B-C1B	3.31	1.45	1.41

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	311	NAD	N3A-C2A-N1A	-13.48	118.58	128.89
2	D	311	NAD	N3A-C2A-N1A	-10.95	120.51	128.89
2	C	311	NAD	N3A-C2A-N1A	-8.36	122.50	128.89
2	B	311	NAD	N3A-C2A-N1A	-7.91	122.84	128.89
2	A	311	NAD	C4B-O4B-C1B	-5.11	104.11	109.72
2	C	311	NAD	PN-O3-PA	-4.45	120.24	132.73
2	A	311	NAD	PN-O3-PA	-4.42	120.32	132.73
2	D	311	NAD	PN-O3-PA	-4.40	120.36	132.73
2	B	311	NAD	C5B-C4B-C3B	-4.39	97.78	115.21
2	D	311	NAD	C1B-N9A-C4A	-4.33	120.41	126.94
2	B	311	NAD	PN-O3-PA	-4.25	120.80	132.73
2	A	311	NAD	O5D-PN-O1N	-4.20	93.30	109.62
2	D	311	NAD	C5B-C4B-C3B	-4.12	98.88	115.21
2	C	311	NAD	O2N-PN-O1N	-4.07	90.46	112.53
3	B	312	HP7	PB-O3A-PA	-4.00	121.50	132.73
2	D	311	NAD	O2N-PN-O1N	-4.00	90.84	112.53
2	C	311	NAD	C5B-C4B-C3B	-3.86	99.88	115.21
2	B	311	NAD	C1B-N9A-C4A	-3.71	121.34	126.94
2	A	311	NAD	C1B-N9A-C4A	-3.66	121.43	126.94
3	C	312	HP7	O5'-C1'-O3B	-3.50	106.75	111.36
2	A	311	NAD	C5B-C4B-C3B	-3.42	101.66	115.21
2	B	311	NAD	O5D-PN-O1N	-3.41	96.37	109.62
2	D	311	NAD	O7N-C7N-N7N	-3.37	117.85	122.59
2	D	311	NAD	C4A-C5A-N7A	-3.37	106.38	109.48
2	A	311	NAD	O3B-C3B-C4B	-3.29	101.18	111.05
2	C	311	NAD	C4B-O4B-C1B	-3.23	106.17	109.72
3	B	312	HP7	C2'-N2'-C7'	-3.14	115.06	123.10
3	A	312	HP7	PB-O3A-PA	-3.10	124.03	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	311	NAD	O5B-PA-O1A	-3.04	97.81	109.62
2	C	311	NAD	O5D-PN-O1N	-3.00	97.99	109.62
3	D	312	HP7	O7'-C7'-N2'	-2.88	115.98	121.86
2	D	311	NAD	C4B-O4B-C1B	-2.84	106.59	109.72
3	C	312	HP7	O3C-C3C-C4C	-2.79	102.67	111.05
2	D	311	NAD	O3D-C3D-C4D	-2.63	103.17	111.05
2	D	311	NAD	O5D-PN-O1N	-2.62	99.43	109.62
3	C	312	HP7	C5-C4-N3	-2.61	116.41	123.12
2	A	311	NAD	C5N-C4N-C3N	-2.61	117.05	120.33
2	C	311	NAD	O3D-C3D-C4D	-2.57	103.35	111.05
2	C	311	NAD	C1B-N9A-C4A	-2.53	123.12	126.94
3	A	312	HP7	C5-C4-N3	-2.52	116.66	123.12
2	A	311	NAD	C2B-C1B-N9A	-2.52	110.45	114.29
3	A	312	HP7	O7'-C7'-C8'	-2.51	117.45	122.06
2	D	311	NAD	O5B-PA-O1A	-2.51	99.86	109.62
2	B	311	NAD	C4A-C5A-N7A	-2.51	107.17	109.48
2	D	311	NAD	O3B-C3B-C4B	-2.51	103.54	111.05
3	A	312	HP7	C5C-C4C-C3C	-2.44	105.54	115.21
2	B	311	NAD	O7N-C7N-C3N	-2.35	117.02	119.59
3	B	312	HP7	C5-C4-N3	-2.34	117.12	123.12
2	A	311	NAD	O5B-PA-O1A	-2.33	100.56	109.62
2	B	311	NAD	O5B-PA-O1A	-2.28	100.77	109.62
2	D	311	NAD	O3D-C3D-C2D	-2.22	104.60	111.83
2	B	311	NAD	C4B-O4B-C1B	-2.21	107.29	109.72
3	D	312	HP7	O5'-C1'-O3B	-2.20	108.46	111.36
2	A	311	NAD	O7N-C7N-N7N	-2.17	119.54	122.59
3	C	312	HP7	O3A-PB-O3B	-2.11	97.55	103.63
2	B	311	NAD	O2N-PN-O1N	-2.09	101.17	112.53
2	A	311	NAD	O3D-C3D-C4D	-2.09	104.78	111.05
3	B	312	HP7	C3'-C2'-N2'	2.06	114.94	110.66
3	D	312	HP7	O4C-C1C-N1	2.11	112.54	108.08
3	B	312	HP7	C3'-C4'-C5'	2.13	112.79	108.66
2	C	311	NAD	C2N-C3N-C7N	2.15	125.57	119.31
2	C	311	NAD	C2A-N1A-C6A	2.23	122.75	118.77
2	A	311	NAD	N6A-C6A-N1A	2.25	124.03	119.20
3	D	312	HP7	C4C-O4C-C1C	2.25	112.19	109.72
3	A	312	HP7	O3A-PA-O5C	2.27	108.96	102.94
3	D	312	HP7	O3B-C1'-C2'	2.28	112.61	108.42
3	B	312	HP7	O2B-PB-O3B	2.36	115.97	106.49
3	D	312	HP7	C1'-O5'-C5'	2.36	115.84	112.17
2	B	311	NAD	N6A-C6A-N1A	2.42	124.40	119.20
3	B	312	HP7	C4C-O4C-C1C	2.43	112.39	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	311	NAD	C2A-N1A-C6A	2.46	123.17	118.77
2	A	311	NAD	C4D-O4D-C1D	2.48	112.44	109.72
3	B	312	HP7	O4C-C1C-N1	2.54	113.43	108.08
2	A	311	NAD	O4B-C4B-C3B	2.59	110.36	105.15
2	D	311	NAD	C4D-O4D-C1D	2.59	112.56	109.72
3	C	312	HP7	O3B-C1'-C2'	2.74	113.46	108.42
2	D	311	NAD	O4B-C1B-N9A	2.77	113.91	108.10
2	A	311	NAD	C3N-C7N-N7N	2.87	120.96	117.82
2	D	311	NAD	C2A-N1A-C6A	2.87	123.90	118.77
2	C	311	NAD	O4B-C1B-N9A	3.05	114.48	108.10
2	B	311	NAD	O4D-C1D-N1N	3.16	111.60	108.13
2	B	311	NAD	O3-PA-O5B	3.24	111.54	102.94
3	C	312	HP7	C8'-C7'-N2'	3.26	122.35	116.11
3	D	312	HP7	C8'-C7'-N2'	3.30	122.43	116.11
2	B	311	NAD	O3-PN-O5D	3.37	111.87	102.94
3	A	312	HP7	C8'-C7'-N2'	3.39	122.59	116.11
3	A	312	HP7	O3B-C1'-C2'	3.41	114.70	108.42
2	D	311	NAD	O3-PN-O5D	3.54	112.33	102.94
3	A	312	HP7	C3'-C2'-N2'	3.72	118.36	110.66
2	B	311	NAD	C3N-C7N-N7N	3.76	121.93	117.82
2	C	311	NAD	O2N-PN-O3	3.93	122.92	105.09
2	D	311	NAD	O7N-C7N-C3N	3.97	123.92	119.59
2	B	311	NAD	C4D-O4D-C1D	3.98	114.10	109.72
3	C	312	HP7	C1'-O5'-C5'	3.99	118.36	112.17
2	A	311	NAD	O4B-C1B-N9A	4.11	116.69	108.10
2	A	311	NAD	O3-PA-O5B	4.11	113.84	102.94
2	B	311	NAD	O4B-C1B-N9A	4.42	117.34	108.10
2	B	311	NAD	O2N-PN-O3	4.48	125.43	105.09
2	A	311	NAD	C2A-N1A-C6A	4.53	126.85	118.77
2	D	311	NAD	O3-PA-O5B	4.65	115.26	102.94
2	D	311	NAD	O2N-PN-O3	4.82	126.94	105.09
2	A	311	NAD	O2N-PN-O3	4.99	127.73	105.09
3	D	312	HP7	C4-N3-C2	5.37	119.46	114.14
2	C	311	NAD	O3-PN-O5D	5.62	117.84	102.94
2	C	311	NAD	O3-PA-O5B	5.90	118.58	102.94
3	B	312	HP7	C4-N3-C2	7.96	122.03	114.14
3	C	312	HP7	C4-N3-C2	10.58	124.62	114.14
3	A	312	HP7	C4-N3-C2	10.93	124.97	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	311	NAD	4	0
3	A	312	HP7	6	0
2	B	311	NAD	5	0
3	B	312	HP7	3	0
2	C	311	NAD	8	0
3	C	312	HP7	2	0
2	D	311	NAD	6	0
3	D	312	HP7	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	310/312 (99%)	-0.05	12 (3%) 43 45	16, 28, 51, 64	0
1	B	310/312 (99%)	-0.19	7 (2%) 64 64	13, 31, 81, 168	0
1	C	310/312 (99%)	-0.29	6 (1%) 70 70	15, 26, 68, 169	0
1	D	307/312 (98%)	-0.16	8 (2%) 59 60	16, 29, 92, 205	0
All	All	1237/1248 (99%)	-0.17	33 (2%) 58 58	13, 29, 77, 205	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	310	GLY	7.1
1	A	310	GLY	5.9
1	A	259	GLY	5.0
1	D	145	GLN	4.8
1	B	310	GLY	4.5
1	C	251	GLY	4.3
1	A	260	PHE	4.1
1	D	146	GLU	3.9
1	A	261	THR	3.8
1	C	145	GLN	3.6
1	D	237	ARG	3.4
1	A	257	SER	2.8
1	A	144	GLY	2.7
1	A	141	GLU	2.7
1	B	240	GLY	2.6
1	C	146	GLU	2.6
1	D	238	ARG	2.5
1	A	145	GLN	2.5
1	A	229	PRO	2.5
1	D	233	PRO	2.5
1	A	262	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	143	LEU	2.4
1	A	234	GLU	2.3
1	B	233	PRO	2.3
1	D	240	GLY	2.3
1	C	147	LYS	2.3
1	D	236	LEU	2.3
1	B	299	GLN	2.2
1	D	234	GLU	2.2
1	A	256	PHE	2.2
1	C	141	GLU	2.2
1	B	261	THR	2.1
1	B	119[A]	ARG	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
3	HP7	A	312	40/40	0.84	0.17	1.63	30,59,491,500	0
3	HP7	B	312	40/40	0.89	0.15	1.48	24,47,396,500	0
2	NAD	B	311	44/44	0.97	0.11	0.19	12,17,41,66	0
2	NAD	C	311	44/44	0.98	0.10	0.14	10,18,62,500	0
3	HP7	D	312	40/40	0.94	0.11	0.07	24,40,55,58	0
2	NAD	A	311	44/44	0.97	0.10	-0.23	12,19,32,42	0
2	NAD	D	311	44/44	0.98	0.10	-0.28	11,20,84,500	0
3	HP7	C	312	40/40	0.96	0.08	-0.83	20,31,44,49	0
4	CL	B	313	1/1	0.98	0.08	-0.88	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CL	D	313	1/1	1.00	0.08	-1.78	24,24,24,24	0
4	CL	C	313	1/1	0.99	0.08	-2.63	23,23,23,23	0
4	CL	A	313	1/1	0.99	0.09	-	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.