



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1GZF
Title : STRUCTURE OF THE CLOSTRIDIUM BOTULINUM C3 EXOENZYME
(WILD-TYPE) IN COMPLEX WITH NAD
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J.M.; Le Du, M.H.; Boquet, P.; Menez, A.
Deposited on : 2002-05-21
Resolution : 1.95 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

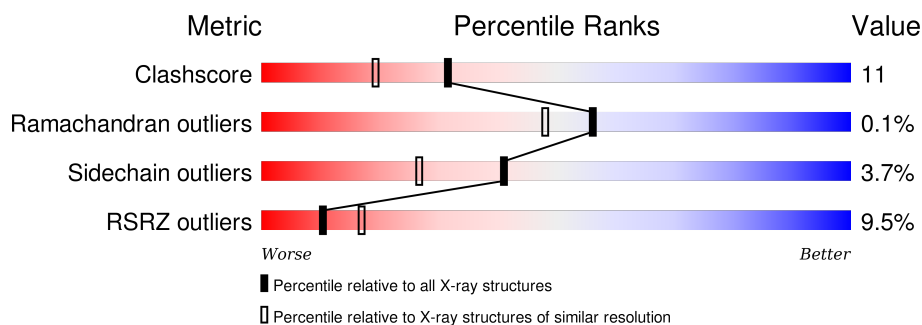
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	211	<div> <div>6%</div> <div>76%</div> <div>19%</div> <div>.</div> </div>
1	B	211	<div> <div>14%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
1	C	211	<div> <div>9%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
1	D	211	<div> <div>9%</div> <div>71%</div> <div>23%</div> <div>..</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	NAD	A	1248	X	-	-	-
2	NAD	B	1252	X	-	-	-
3	SO4	A	1249	-	X	-	-
3	SO4	B	1253	-	X	-	-
4	NIR	C	1252	X	-	-	-
5	ADP	D	1247	-	-	-	X

2 Entry composition [i](#)

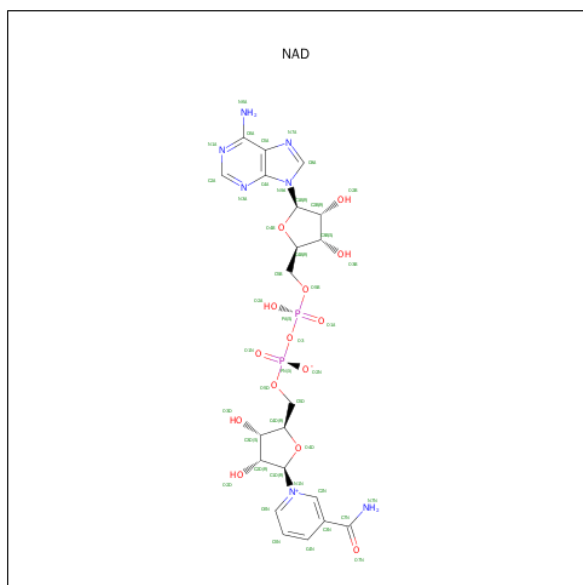
There are 6 unique types of molecules in this entry. The entry contains 7223 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MONO-ADP-RIBOSYLTRANSFERASE C3.

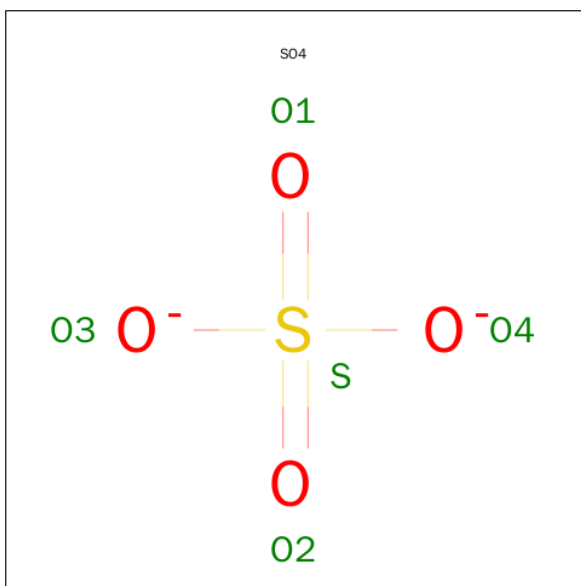
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1594	1013	271	303	7			
1	B	211	Total	C	N	O	S	0	0	0
			1658	1053	282	316	7			
1	C	208	Total	C	N	O	S	0	0	0
			1635	1038	279	311	7			
1	D	203	Total	C	N	O	S	0	0	0
			1597	1014	272	304	7			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



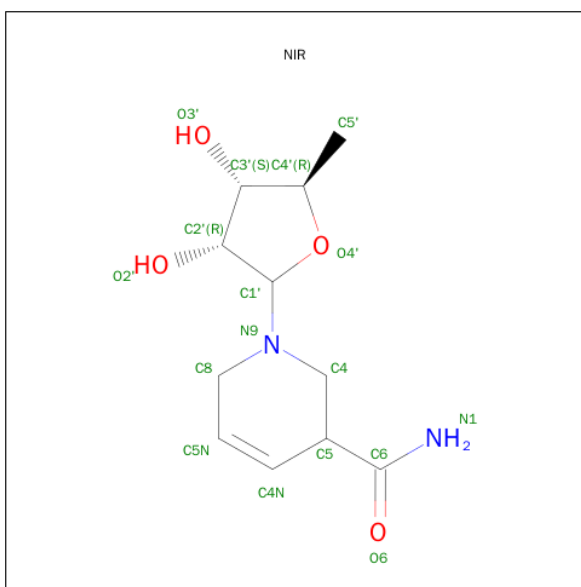
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



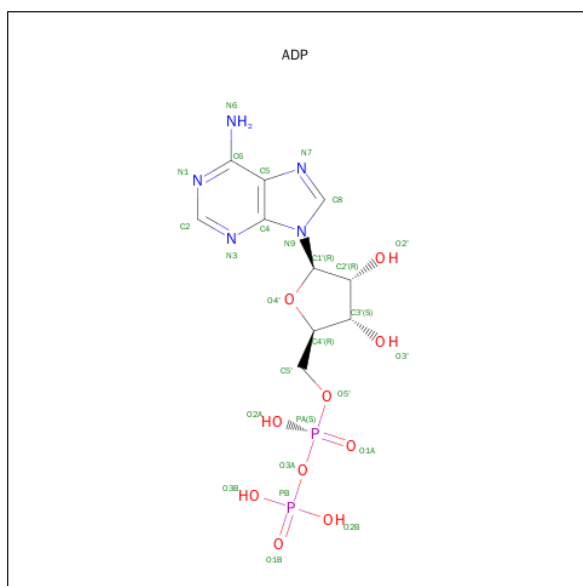
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 3-(AMINOCARBONYL)-1-[(3R,4S,5R)-3,4-DIHYDROXY-5-METHYLTETRAHYDRO-2-FURANYL]PYRIDINIUM (three-letter code: NIR) (formula: C₁₁H₁₈N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			17	11	2	4		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

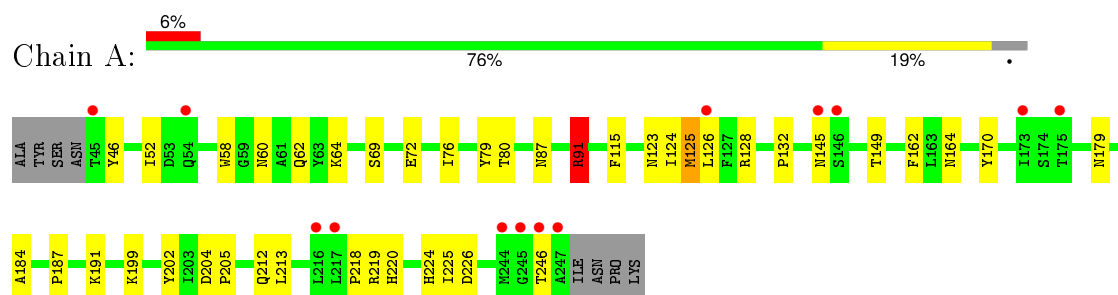
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	168	Total	O	0	0
			168	168		
6	B	125	Total	O	0	0
			125	125		
6	C	139	Total	O	0	0
			139	139		
6	D	138	Total	O	0	0
			138	138		

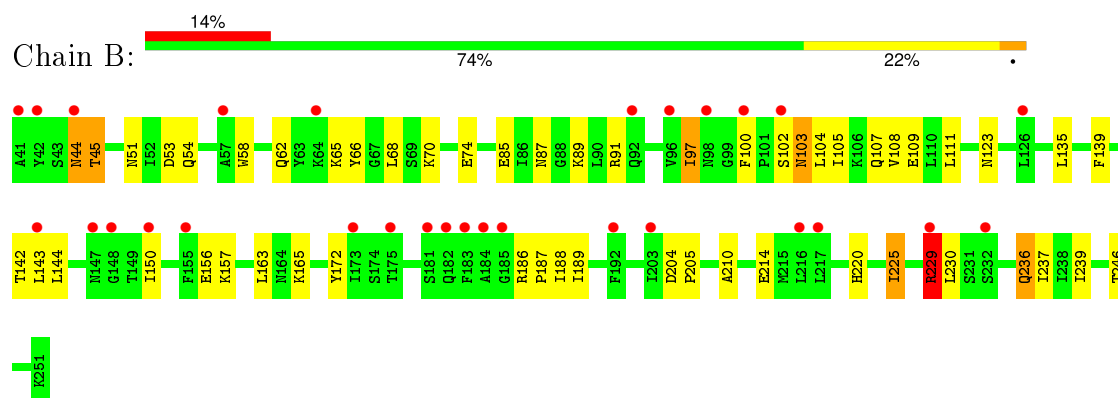
3 Residue-property plots [i](#)

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.

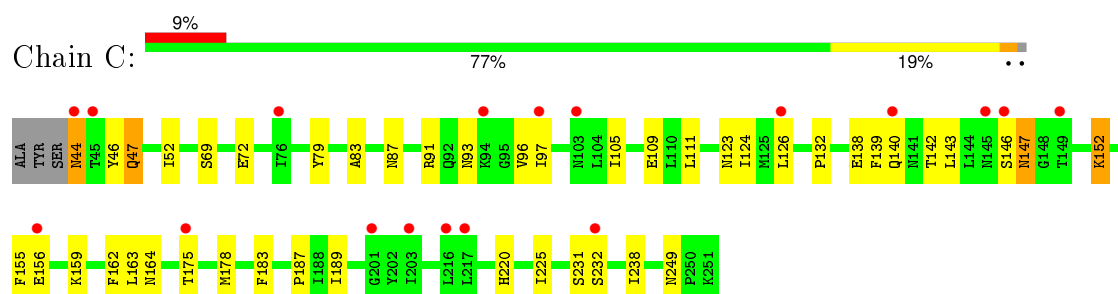
• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3



• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

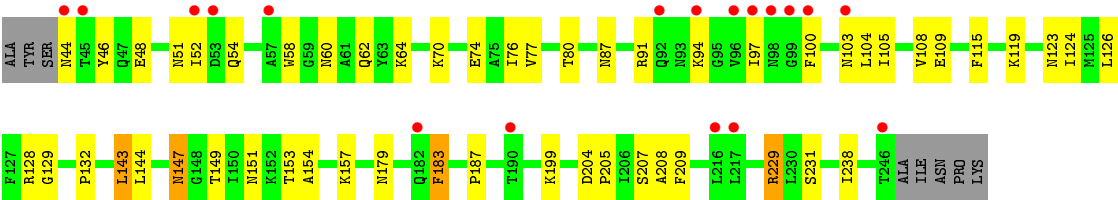


• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3



• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.95Å 74.19Å 119.68Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95 24.03 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.8 (25.00-1.95) 91.2 (24.03-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.277 0.235 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 62957 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7223	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NIR, ADP, NAD, SO4

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	0.35	0/1622	0.60	0/2178
1	B	0.44	1/1688 (0.1%)	1.04	3/2267 (0.1%)
1	C	0.40	0/1664	0.62	0/2234
1	D	0.35	0/1625	0.61	0/2182
All	All	0.39	1/6599 (0.0%)	0.74	3/8861 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	ARG	CD-NE	-9.01	1.31	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	ARG	NE-CZ-NH1	27.65	134.13	120.30
1	B	229	ARG	NE-CZ-NH2	-24.00	108.30	120.30
1	B	229	ARG	CD-NE-CZ	14.29	143.60	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Sidechain
1	A	91	ARG	Sidechain
1	B	229	ARG	Sidechain

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	1594	0	1615	30	0
1	B	1658	0	1677	46	0
1	C	1635	0	1658	30	0
1	D	1597	0	1616	38	0
2	A	44	0	25	0	0
2	B	44	0	25	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	C	17	0	16	5	0
5	C	27	0	12	1	0
5	D	27	0	12	0	0
6	A	168	0	0	1	0
6	B	125	0	0	1	0
6	C	139	0	0	4	0
6	D	138	0	0	1	0
All	All	7223	0	6656	143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (143) 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:151:ASN:HD22	1:D:154:ALA:H	1.21	0.86
1:B:229:ARG:HG2	1:B:229:ARG:O	1.75	0.85
1:B:66:TYR:HB3	1:B:68:LEU:HD13	1.59	0.85
1:B:188:ILE:HD13	1:B:237:ILE:HB	1.62	0.79
1:B:45:THR:HG23	1:B:123:ASN:HD22	1.49	0.74
1:B:44:ASN:O	1:B:45:THR:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:MET:HE3	1:A:191:LYS:HB3	1.72	0.71
1:C:162:PHE:HB3	1:C:225:ILE:HD12	1.73	0.70
1:D:129:GLY:HA3	1:D:183:PHE:HB2	1.72	0.70
1:C:105:ILE:O	1:C:109:GLU:HG3	1.91	0.69
1:D:100:PHE:HD2	1:D:104:LEU:HD22	1.58	0.68
1:B:105:ILE:O	1:B:109:GLU:HG3	1.95	0.66
1:C:152:LYS:O	1:C:156:GLU:HG2	1.95	0.66
1:D:87:ASN:HB3	1:D:91:ARG:HH22	1.63	0.64
1:B:58:TRP:O	1:B:62:GLN:HG2	1.98	0.62
1:A:46:TYR:CD2	1:A:123:ASN:HB3	2.34	0.62
1:A:125:MET:CE	1:A:191:LYS:HB3	2.30	0.62
1:B:70:LYS:O	1:B:74:GLU:HG3	2.00	0.62
1:C:147:ASN:OD1	1:C:147:ASN:N	2.30	0.62
1:C:44:ASN:HB3	6:C:2001:HOH:O	1.99	0.62
1:C:87:ASN:O	1:C:91:ARG:HG3	2.02	0.60
1:A:224:HIS:HD2	1:A:226:ASP:OD2	1.84	0.59
1:A:162:PHE:HB3	1:A:225:ILE:HD12	1.84	0.59
1:A:115:PHE:HB3	1:A:199:LYS:HD3	1.84	0.59
1:B:225:ILE:HD13	1:B:239:ILE:HG21	1.85	0.59
1:C:138:GLU:HG2	1:C:139:PHE:CD1	2.38	0.59
1:D:87:ASN:HB3	1:D:91:ARG:NH2	2.18	0.58
1:D:44:ASN:HB2	6:D:2001:HOH:O	2.03	0.58
1:C:155:PHE:CZ	1:C:159:LYS:HE3	2.38	0.58
1:D:46:TYR:CD2	1:D:123:ASN:HB3	2.38	0.58
1:B:66:TYR:HB3	1:B:68:LEU:CD1	2.32	0.57
1:C:83:ALA:HB3	4:C:1252:NIR:H5'3	1.86	0.57
1:C:93:ASN:O	1:C:96:VAL:HG22	2.05	0.57
1:B:45:THR:CG2	1:B:123:ASN:HD22	2.17	0.56
1:C:189:ILE:HB	1:C:238:ILE:HD13	1.86	0.56
1:C:132:PRO:HD3	1:C:187:PRO:HG3	1.88	0.55
1:A:87:ASN:HB3	1:A:91:ARG:HH12	1.70	0.55
1:A:162:PHE:HB3	1:A:225:ILE:CD1	2.36	0.55
1:A:164:ASN:HB2	6:A:2108:HOH:O	2.07	0.55
1:B:144:LEU:HD23	1:B:150:ILE:HD13	1.87	0.55
1:B:220:HIS:HD2	1:B:246:THR:O	1.90	0.54
1:D:124:ILE:HD12	1:D:126:LEU:HD21	1.90	0.54
1:D:51:ASN:HD21	1:D:54:GLN:HB2	1.72	0.54
1:D:151:ASN:HD21	1:D:153:THR:HB	1.73	0.54
1:C:183:PHE:CZ	4:C:1252:NIR:H4	2.43	0.54
1:C:93:ASN:HD22	1:C:96:VAL:HG23	1.71	0.53
1:B:144:LEU:CD2	1:B:150:ILE:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ILE:HA	1:D:100:PHE:CD1	2.44	0.53
1:D:229:ARG:NH1	1:D:238:ILE:HD12	2.24	0.53
1:A:124:ILE:HD13	1:A:126:LEU:HD21	1.89	0.52
1:D:119:LYS:HE2	1:D:199:LYS:HG2	1.91	0.52
1:A:60:ASN:O	1:A:64:LYS:HG3	2.09	0.52
1:B:156:GLU:HB3	6:B:2070:HOH:O	2.09	0.52
1:A:52:ILE:HD12	1:D:48:GLU:OE2	2.10	0.52
1:B:150:ILE:HG21	1:B:230:LEU:HD21	1.92	0.51
1:A:218:PRO:CG	1:A:246:THR:HG21	2.40	0.51
1:D:153:THR:O	1:D:157:LYS:HG2	2.11	0.51
1:D:76:ILE:O	1:D:80:THR:HG23	2.11	0.51
1:B:102:SER:O	1:B:105:ILE:HG22	2.10	0.51
1:D:115:PHE:HB3	1:D:199:LYS:HD3	1.93	0.51
1:B:87:ASN:O	1:B:91:ARG:HG3	2.11	0.50
1:B:102:SER:HA	1:B:105:ILE:HG22	1.94	0.50
1:C:93:ASN:ND2	1:C:96:VAL:HG23	2.27	0.49
1:B:111:LEU:HD23	1:B:172:TYR:CZ	2.46	0.49
2:B:1252:NAD:O5D	2:B:1252:NAD:C1D	2.60	0.49
1:D:179:ASN:HA	1:D:183:PHE:HE1	1.76	0.49
1:B:62:GLN:HE22	1:B:65:LYS:NZ	2.11	0.49
1:B:189:ILE:HD13	1:B:236:GLN:NE2	2.27	0.49
1:B:163:LEU:HD21	1:C:163:LEU:HD21	1.94	0.49
1:C:47:GLN:HE21	1:C:47:GLN:HA	1.76	0.49
1:B:97:ILE:HG22	1:B:100:PHE:HE2	1.77	0.49
4:C:1252:NIR:H5'1	5:C:1253:ADP:O1B	2.14	0.48
1:B:89:LYS:HE3	1:B:100:PHE:CD1	2.49	0.48
1:C:52:ILE:HD13	1:C:178:MET:SD	2.54	0.48
1:B:104:LEU:O	1:B:104:LEU:HD23	2.13	0.48
1:B:204:ASP:HB2	1:B:205:PRO:HD3	1.95	0.48
1:C:124:ILE:HD12	1:C:126:LEU:HD21	1.96	0.48
1:B:135:LEU:HD11	1:B:188:ILE:HD11	1.96	0.48
1:D:229:ARG:HH12	1:D:238:ILE:HD12	1.79	0.48
1:B:51:ASN:HD21	1:B:53:ASP:HB2	1.79	0.48
1:D:87:ASN:CB	1:D:91:ARG:HH22	2.26	0.48
1:D:132:PRO:HD3	1:D:187:PRO:HG3	1.96	0.48
1:B:89:LYS:HE3	1:B:100:PHE:CE1	2.49	0.47
1:D:64:LYS:HA	1:D:64:LYS:HZ3	1.80	0.47
1:B:97:ILE:HG22	1:B:100:PHE:CE2	2.49	0.47
1:D:105:ILE:O	1:D:109:GLU:HG3	2.15	0.47
1:B:210:ALA:HB1	1:B:214:GLU:OE2	2.14	0.46
1:B:104:LEU:O	1:B:108:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:SER:OG	1:C:72:GLU:HG3	2.14	0.46
1:B:150:ILE:HG21	1:B:230:LEU:CD2	2.44	0.46
1:C:97:ILE:HB	1:C:105:ILE:HG12	1.97	0.46
1:A:79:TYR:CD1	1:A:79:TYR:C	2.90	0.46
1:D:70:LYS:HG2	1:D:74:GLU:OE2	2.16	0.46
1:B:188:ILE:O	1:B:189:ILE:HD12	2.17	0.45
1:B:144:LEU:HD23	1:B:150:ILE:HA	1.97	0.45
1:A:69:SER:OG	1:A:72:GLU:HG3	2.16	0.45
1:C:79:TYR:HB2	1:C:111:LEU:HD11	1.99	0.45
1:A:132:PRO:HD3	1:A:187:PRO:HG3	1.98	0.45
1:D:204:ASP:HB2	1:D:205:PRO:HD3	1.99	0.45
1:D:80:THR:OG1	1:D:209:PHE:HB2	2.17	0.45
1:D:147:ASN:ND2	1:D:149:THR:H	2.15	0.45
1:C:132:PRO:HG3	1:C:143:LEU:HD23	1.98	0.45
1:B:186:ARG:HB3	1:B:187:PRO:HD2	1.98	0.45
1:A:145:ASN:HB2	1:A:149:THR:O	2.17	0.44
1:D:60:ASN:O	1:D:64:LYS:HG2	2.17	0.44
1:C:175:THR:O	4:C:1252:NIR:H5N	2.18	0.44
1:D:104:LEU:HD23	1:D:108:VAL:HG23	1.99	0.43
1:D:143:LEU:HB3	1:D:144:LEU:HD12	2.00	0.43
1:D:58:TRP:O	1:D:62:GLN:HG2	2.19	0.43
1:B:188:ILE:C	1:B:189:ILE:HD12	2.39	0.42
1:C:231:SER:O	1:C:232:SER:C	2.58	0.42
1:B:165:LYS:HE2	1:C:164:ASN:ND2	2.34	0.42
1:A:204:ASP:HB3	1:A:205:PRO:HD3	2.00	0.42
1:D:52:ILE:HG13	1:D:52:ILE:H	1.47	0.42
1:A:125:MET:HE3	1:A:191:LYS:HD2	2.01	0.42
1:A:218:PRO:HG2	1:A:246:THR:CG2	2.49	0.42
1:A:220:HIS:O	1:A:246:THR:HA	2.20	0.42
1:A:124:ILE:HG12	1:A:125:MET:N	2.35	0.42
1:B:204:ASP:N	1:B:205:PRO:CD	2.82	0.42
1:D:64:LYS:NZ	1:D:64:LYS:HA	2.34	0.42
1:C:139:PHE:HA	1:C:142:THR:OG1	2.20	0.41
1:B:103:ASN:O	1:B:107:GLN:HG3	2.20	0.41
1:B:157:LYS:HE3	1:D:208:ALA:O	2.20	0.41
1:A:212:GLN:O	1:A:213:LEU:C	2.59	0.41
1:B:139:PHE:HA	1:B:142:THR:OG1	2.20	0.41
1:A:76:ILE:O	1:A:80:THR:HG23	2.20	0.41
1:A:179:ASN:OD1	1:A:184:ALA:HB2	2.20	0.41
1:A:58:TRP:O	1:A:62:GLN:HG2	2.21	0.41
1:D:147:ASN:C	1:D:147:ASN:HD22	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ASN:ND2	1:D:153:THR:HB	2.35	0.41
1:A:170:TYR:O	1:A:219:ARG:HB2	2.21	0.41
1:B:188:ILE:HD11	1:B:237:ILE:HD12	2.02	0.41
1:B:104:LEU:HD23	1:B:104:LEU:C	2.41	0.41
1:B:225:ILE:HD13	1:B:239:ILE:CG2	2.50	0.41
1:A:202:TYR:CZ	1:A:204:ASP:HB3	2.56	0.41
1:D:204:ASP:N	1:D:205:PRO:CD	2.84	0.40
1:D:77:VAL:HG22	1:D:207:SER:HB2	2.02	0.40
4:C:1252:NIR:H3'	6:C:2033:HOH:O	2.21	0.40
1:C:220:HIS:HD2	6:C:2134:HOH:O	2.04	0.40
1:A:179:ASN:OD1	1:A:184:ALA:CB	2.69	0.40
1:A:202:TYR:CE2	1:A:204:ASP:HB3	2.57	0.40
1:C:52:ILE:HG12	6:C:2007:HOH:O	2.20	0.40
1:C:46:TYR:CD2	1:C:123:ASN:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/211 (95%)	195 (97%)	6 (3%)	0	100	100
1	B	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
1	C	206/211 (98%)	199 (97%)	6 (3%)	1 (0%)	34	21
1	D	201/211 (95%)	198 (98%)	3 (2%)	0	100	100
All	All	817/844 (97%)	794 (97%)	22 (3%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	146	SER

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	172/179 (96%)	170 (99%)	2 (1%)	78	75
1	B	179/179 (100%)	169 (94%)	10 (6%)	26	11
1	C	177/179 (99%)	171 (97%)	6 (3%)	44	30
1	D	173/179 (97%)	165 (95%)	8 (5%)	33	17
All	All	701/716 (98%)	675 (96%)	26 (4%)	41	27

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	125	MET
1	B	44	ASN
1	B	45	THR
1	B	54	GLN
1	B	85	GLU
1	B	97	ILE
1	B	103	ASN
1	B	143	LEU
1	B	225	ILE
1	B	229	ARG
1	B	236	GLN
1	C	44	ASN
1	C	47	GLN
1	C	140	GLN
1	C	147	ASN
1	C	152	LYS
1	C	249	ASN
1	D	94	LYS
1	D	103	ASN
1	D	128	ARG
1	D	143	LEU
1	D	147	ASN
1	D	183	PHE

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Mol	Chain	Res	Type
1	D	229	ARG
1	D	231	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	60	ASN
1	A	92	GLN
1	A	116	ASN
1	A	140	GLN
1	A	182	GLN
1	A	212	GLN
1	B	44	ASN
1	B	51	ASN
1	B	54	GLN
1	B	60	ASN
1	B	62	GLN
1	B	103	ASN
1	B	147	ASN
1	B	182	GLN
1	B	220	HIS
1	C	44	ASN
1	C	47	GLN
1	C	92	GLN
1	C	93	ASN
1	C	107	GLN
1	C	151	ASN
1	C	182	GLN
1	C	249	ASN
1	D	51	ASN
1	D	54	GLN
1	D	60	ASN
1	D	92	GLN
1	D	116	ASN
1	D	140	GLN
1	D	145	ASN
1	D	147	ASN
1	D	151	ASN
1	D	182	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 ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAD	A	1248	-	38,48,48	2.04	7 (18%)	47,73,73	2.82	20 (42%)
3	SO4	A	1249	-	4,4,4	4.09	4 (100%)	6,6,6	0.12	0
2	NAD	B	1252	-	38,48,48	1.06	3 (7%)	47,73,73	2.72	17 (36%)
3	SO4	B	1253	-	4,4,4	4.08	4 (100%)	6,6,6	0.17	0
4	NIR	C	1252	-	18,18,18	4.53	7 (38%)	18,26,26	3.09	6 (33%)
5	ADP	C	1253	-	22,29,29	1.06	2 (9%)	27,45,45	1.48	4 (14%)
5	ADP	D	1247	-	22,29,29	2.07	7 (31%)	27,45,45	2.62	12 (44%)

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	1248	-	1/1/11/11	0/22/62/62	0/5/5/5
3	SO4	A	1249	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	1252	-	1/1/11/11	0/22/62/62	0/5/5/5
3	SO4	B	1253	-	-	0/0/0/0	0/0/0/0
4	NIR	C	1252	-	2/2/7/9	1/8/34/34	0/2/2/2
5	ADP	C	1253	-	-	0/12/32/32	0/3/3/3
5	ADP	D	1247	-	-	0/12/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1252	NIR	C4-C5	-14.42	1.38	1.52
4	C	1252	NIR	C8-C5N	-8.02	1.34	1.49
2	A	1248	NAD	O4D-C1D	-7.68	1.31	1.41
4	C	1252	NIR	C4-N9	-5.95	1.37	1.47
4	C	1252	NIR	C5-C4N	-5.25	1.41	1.52
5	D	1247	ADP	PB-O2B	-3.43	1.42	1.54
5	D	1247	ADP	PA-O2A	-3.42	1.40	1.54
5	D	1247	ADP	O4'-C4'	-3.28	1.37	1.45
5	D	1247	ADP	C5-C4	-3.28	1.33	1.40
4	C	1252	NIR	C8-N9	-3.02	1.39	1.47
2	A	1248	NAD	PN-O1N	-2.65	1.41	1.51
5	C	1253	ADP	PB-O3B	-2.64	1.45	1.54
5	D	1247	ADP	C3'-C4'	-2.58	1.46	1.53
2	A	1248	NAD	C5A-C4A	-2.44	1.35	1.40
4	C	1252	NIR	C2'-C1'	-2.37	1.45	1.53
5	C	1253	ADP	PB-O2B	-2.03	1.47	1.54
2	A	1248	NAD	C6N-N1N	2.00	1.40	1.35
2	A	1248	NAD	C5B-C4B	2.17	1.58	1.51
2	B	1252	NAD	C2A-N1A	2.21	1.38	1.33
5	D	1247	ADP	PB-O1B	2.25	1.58	1.51
2	B	1252	NAD	C6N-N1N	2.33	1.41	1.35
2	B	1252	NAD	C3N-C7N	2.39	1.54	1.50
4	C	1252	NIR	C4N-C5N	3.12	1.41	1.32
3	A	1249	SO4	O3-S	3.61	1.60	1.47
3	B	1253	SO4	O3-S	3.80	1.61	1.47
2	A	1248	NAD	C2A-N1A	3.90	1.41	1.33
3	A	1249	SO4	O4-S	4.04	1.61	1.47
3	B	1253	SO4	O1-S	4.09	1.61	1.47
3	B	1253	SO4	O4-S	4.09	1.62	1.47
3	A	1249	SO4	O2-S	4.29	1.61	1.47
3	B	1253	SO4	O2-S	4.32	1.61	1.47
3	A	1249	SO4	O1-S	4.37	1.62	1.47
5	D	1247	ADP	C2-N1	4.66	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1248	NAD	C3N-C7N	5.61	1.59	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1247	ADP	O3B-PB-O1B	-6.75	88.87	110.58
2	B	1252	NAD	C5N-C4N-C3N	-5.79	113.05	120.33
2	B	1252	NAD	C4D-O4D-C1D	-5.62	103.55	109.72
5	D	1247	ADP	O5'-PA-O1A	-5.25	89.25	109.62
2	B	1252	NAD	O7N-C7N-N7N	-4.16	116.74	122.59
2	B	1252	NAD	C5N-C6N-N1N	-4.00	113.55	120.47
2	A	1248	NAD	C3N-C7N-N7N	-3.60	113.88	117.82
2	A	1248	NAD	O5D-PN-O1N	-3.20	97.18	109.62
2	A	1248	NAD	O2N-PN-O5D	-3.16	92.53	108.46
2	A	1248	NAD	O3-PA-O5B	-3.15	94.57	102.94
5	D	1247	ADP	O3A-PA-O5'	-3.15	94.58	102.94
2	B	1252	NAD	O3-PA-O5B	-3.01	94.96	102.94
2	A	1248	NAD	C2D-C3D-C4D	-2.95	96.55	102.61
2	A	1248	NAD	C5N-C6N-N1N	-2.78	115.66	120.47
5	D	1247	ADP	O2B-PB-O1B	-2.77	101.66	110.58
2	B	1252	NAD	C3N-C7N-N7N	-2.71	114.85	117.82
2	B	1252	NAD	PN-O3-PA	-2.70	125.14	132.73
2	A	1248	NAD	C4D-O4D-C1D	-2.66	106.80	109.72
4	C	1252	NIR	C5-C4N-C5N	-2.62	112.91	121.88
2	B	1252	NAD	N3A-C2A-N1A	-2.61	126.89	128.89
2	A	1248	NAD	C5D-C4D-C3D	-2.53	105.16	115.21
2	B	1252	NAD	O2A-PA-O1A	-2.32	99.95	112.53
2	B	1252	NAD	O3-PN-O5D	-2.31	96.80	102.94
4	C	1252	NIR	O3'-C3'-C4'	-2.31	105.01	110.36
2	A	1248	NAD	C4N-C3N-C7N	-2.23	115.21	121.09
4	C	1252	NIR	C5-C6-N1	-2.22	114.78	117.06
5	D	1247	ADP	O4'-C4'-C3'	-2.21	100.69	105.15
5	C	1253	ADP	O3A-PA-O5'	-2.21	97.08	102.94
2	A	1248	NAD	C2N-C3N-C4N	2.05	120.58	118.29
5	C	1253	ADP	O2A-PA-O3A	2.06	114.43	105.09
2	A	1248	NAD	O3B-C3B-C4B	2.10	117.35	111.05
5	D	1247	ADP	C4-C5-N7	2.22	111.52	109.48
2	B	1252	NAD	O2A-PA-O3	2.25	115.29	105.09
2	A	1248	NAD	O4B-C1B-N9A	2.25	112.81	108.10
5	D	1247	ADP	O3'-C3'-C4'	2.41	118.28	111.05
5	D	1247	ADP	C2'-C3'-C4'	2.49	107.72	102.61
5	C	1253	ADP	O3B-PB-O3A	2.51	116.50	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1252	NAD	O5D-PN-O1N	2.64	119.85	109.62
2	A	1248	NAD	O3-PN-O5D	2.64	109.93	102.94
2	B	1252	NAD	N6A-C6A-N1A	2.93	125.50	119.20
2	A	1248	NAD	C4A-C5A-N7A	2.96	112.20	109.48
2	A	1248	NAD	O2N-PN-O3	2.99	118.65	105.09
2	B	1252	NAD	C2N-C3N-C4N	3.02	121.65	118.29
5	D	1247	ADP	O2A-PA-O5'	3.11	124.14	108.46
4	C	1252	NIR	C8-C5N-C4N	3.34	129.01	123.08
5	D	1247	ADP	O2A-PA-O1A	3.47	131.36	112.53
5	C	1253	ADP	PA-O3A-PB	3.65	144.91	132.67
2	A	1248	NAD	O7N-C7N-N7N	3.86	128.02	122.59
2	A	1248	NAD	O2A-PA-O5B	4.17	129.50	108.46
5	D	1247	ADP	N6-C6-N1	4.18	128.18	119.20
2	A	1248	NAD	N6A-C6A-N1A	4.45	128.76	119.20
5	D	1247	ADP	O2B-PB-O3A	4.55	125.73	105.09
2	A	1248	NAD	N3A-C2A-N1A	4.89	132.64	128.89
2	B	1252	NAD	C6N-C5N-C4N	6.10	128.66	119.44
4	C	1252	NIR	C5'-C4'-C3'	6.27	122.34	115.80
2	B	1252	NAD	O4D-C1D-N1N	6.61	115.39	108.13
2	B	1252	NAD	O7N-C7N-C3N	8.08	128.40	119.59
4	C	1252	NIR	C2'-C1'-N9	9.30	138.74	113.39
2	A	1248	NAD	O4D-C1D-N1N	12.23	121.56	108.13

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1248	NAD	C1D
4	C	1252	NIR	C5
4	C	1252	NIR	C1'
2	B	1252	NAD	C1D

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1252	NIR	O4'-C1'-N9-C8

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1252	NAD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1252	NIR	5	0
5	C	1253	ADP	1	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, 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	203/211 (96%)	0.38	13 (6%)	23 33	24, 33, 43, 77	0
1	B	211/211 (100%)	0.82	29 (13%)	4 7	24, 38, 58, 67	0
1	C	208/211 (98%)	0.59	18 (8%)	13 20	20, 34, 57, 64	0
1	D	203/211 (96%)	0.46	18 (8%)	12 19	22, 35, 56, 71	0
All	All	825/844 (97%)	0.57	78 (9%)	10 17	20, 35, 57, 77	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	ALA	7.7
1	B	102	SER	5.6
1	A	145	ASN	4.9
1	B	183	PHE	4.9
1	C	44	ASN	4.9
1	D	44	ASN	4.9
1	B	181	SER	4.7
1	C	216	LEU	4.2
1	A	216	LEU	4.2
1	A	246	THR	4.1
1	C	146	SER	4.0
1	D	246	THR	3.9
1	D	98	ASN	3.8
1	A	244	MET	3.7
1	B	173	ILE	3.7
1	B	216	LEU	3.5
1	A	173	ILE	3.4
1	C	97	ILE	3.4
1	C	103	ASN	3.3
1	A	146	SER	3.3
1	B	100	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	100	PHE	3.2
1	B	185	GLY	3.1
1	C	140	GLN	3.1
1	A	126	LEU	3.0
1	C	126	LEU	3.0
1	B	182	GLN	3.0
1	B	217	LEU	3.0
1	B	192	PHE	3.0
1	C	149	THR	3.0
1	B	148	GLY	2.8
1	C	45	THR	2.8
1	A	217	LEU	2.8
1	B	96	VAL	2.8
1	C	232	SER	2.8
1	B	147	ASN	2.7
1	D	103	ASN	2.7
1	A	245	GLY	2.7
1	B	44	ASN	2.7
1	B	232	SER	2.7
1	B	229	ARG	2.6
1	B	184	ALA	2.5
1	C	175	THR	2.5
1	D	190	THR	2.5
1	C	217	LEU	2.5
1	D	99	GLY	2.5
1	B	64	LYS	2.5
1	D	45	THR	2.4
1	B	42	TYR	2.4
1	B	203	ILE	2.4
1	A	54	GLN	2.4
1	D	57	ALA	2.4
1	D	52	ILE	2.3
1	B	143	LEU	2.3
1	D	216	LEU	2.3
1	D	96	VAL	2.3
1	D	92	GLN	2.3
1	D	94	LYS	2.3
1	B	150	ILE	2.3
1	B	126	LEU	2.2
1	C	94	LYS	2.2
1	C	145	ASN	2.2
1	D	53	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	92	GLN	2.2
1	B	155	PHE	2.2
1	D	182	GLN	2.2
1	A	175	THR	2.2
1	D	217	LEU	2.1
1	B	98	ASN	2.1
1	C	156	GLU	2.1
1	A	45	THR	2.1
1	B	175	THR	2.0
1	C	201	GLY	2.0
1	C	76	ILE	2.0
1	C	203	ILE	2.0
1	B	41	ALA	2.0
1	B	57	ALA	2.0
1	D	97	ILE	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, 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(Å ²)	Q<0.9
5	ADP	D	1247	27/27	0.65	0.33	4.15	78,80,86,86	0
4	NIR	C	1252	17/17	0.77	0.20	1.22	45,53,70,73	0
5	ADP	C	1253	27/27	0.86	0.15	0.76	72,77,84,85	0
3	SO4	A	1249	5/5	0.95	0.12	0.58	51,52,55,55	0
2	NAD	B	1252	44/44	0.87	0.13	-0.25	37,53,71,72	0
2	NAD	A	1248	44/44	0.93	0.12	-0.36	23,33,40,43	0
3	SO4	B	1253	5/5	0.94	0.12	-0.61	51,52,54,54	0

6.5 Other polymers

There are no such residues in this entry.