



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:24 PM GMT

PDB ID : 2X0N
Title : STRUCTURE OF GLYCOSOMAL GLYCERALDEHYDE-3-PHOSPHAT
EDEHYDROGENASE FROM TRYPANOSOMA BRUCEI DETERMINED
FROM LAUE DATA
Authors : Vellieux, F.M.D.; Hajdu, J.; Hol, W.G.J.
Deposited on : 2009-12-16
Resolution : 3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

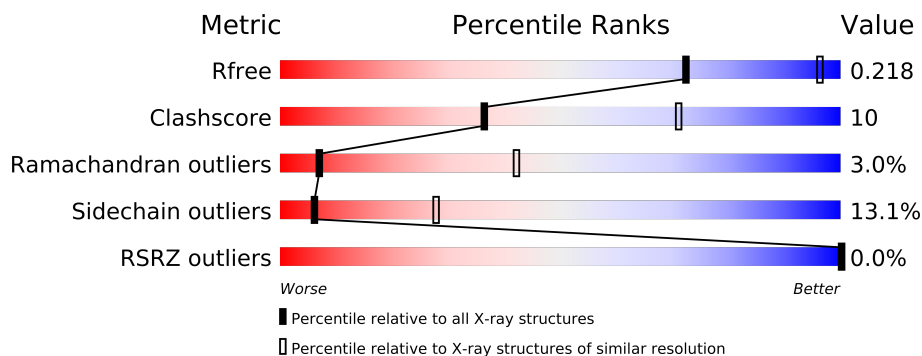
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	359	
1	B	359	
1	O	359	
1	P	359	
1	Q	359	
1	R	359	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	360	-	X
2	SO4	B	360	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	O	360	-	X
2	SO4	P	360	-	X
2	SO4	Q	360	-	X
2	SO4	R	360	-	X

2 Entry composition

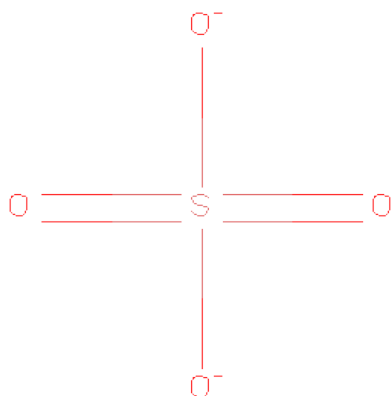
There are 3 unique types of molecules in this entry. The entry contains 16734 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE, GLYCOSOMAL.

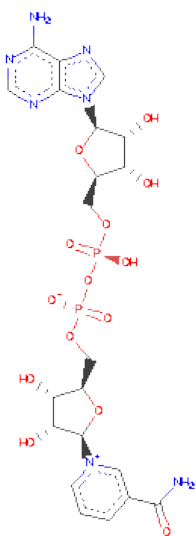
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	B	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	O	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	P	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	Q	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			
1	R	358	Total	C	N	O	S	0	0	0
			2735	1718	490	514	13			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0

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

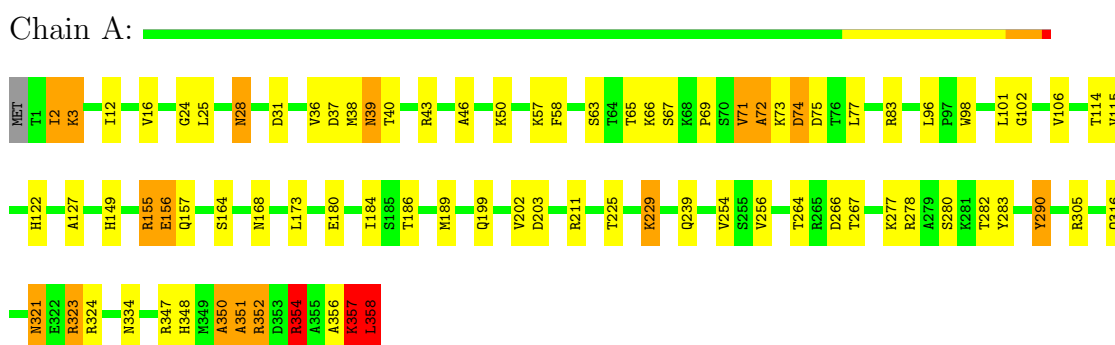


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	O	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	P	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	Q	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	R	1	Total 44	C 21	N 7	O 14	P 2	0	0

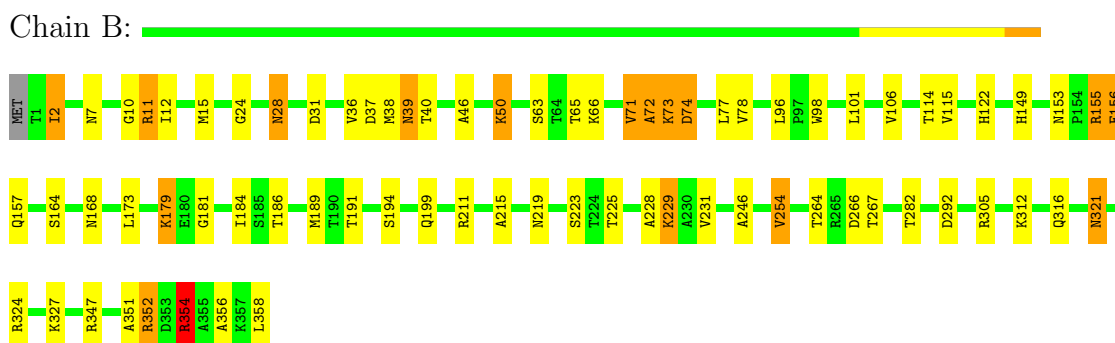
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

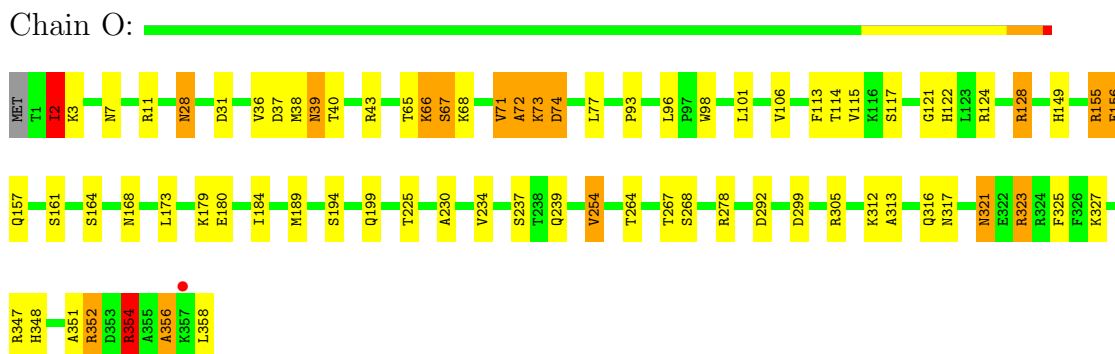
- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE, GLYCOSOMAL



- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE, GLYCOSOMAL

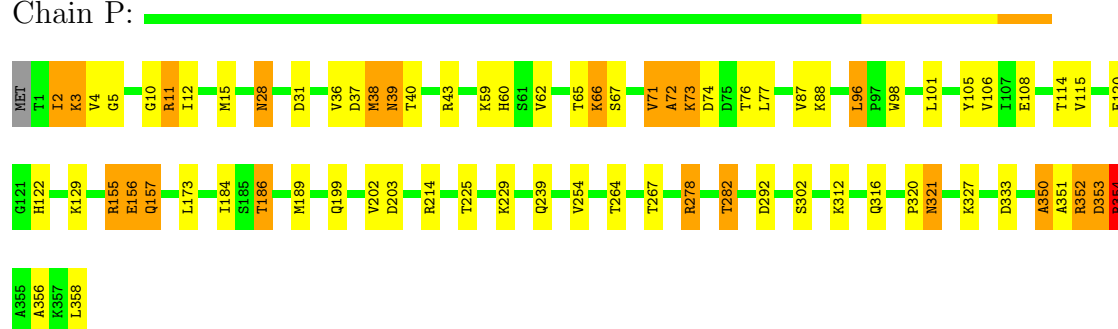


- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE, GLYCOSOMAL



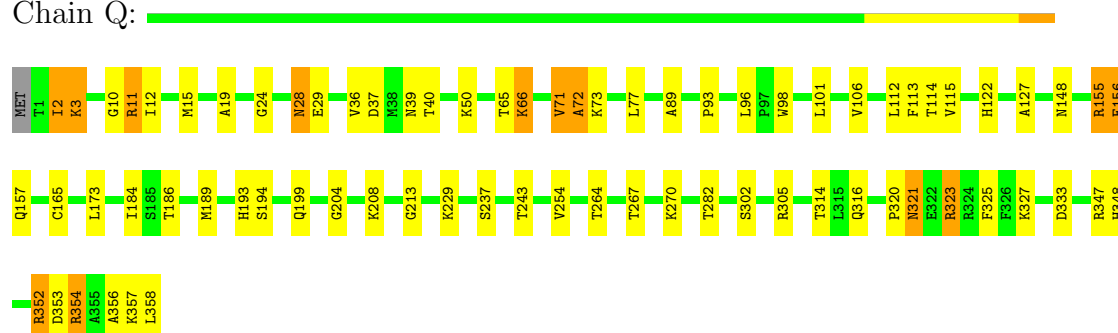
- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE, GLYCOSOMAL

Chain P:



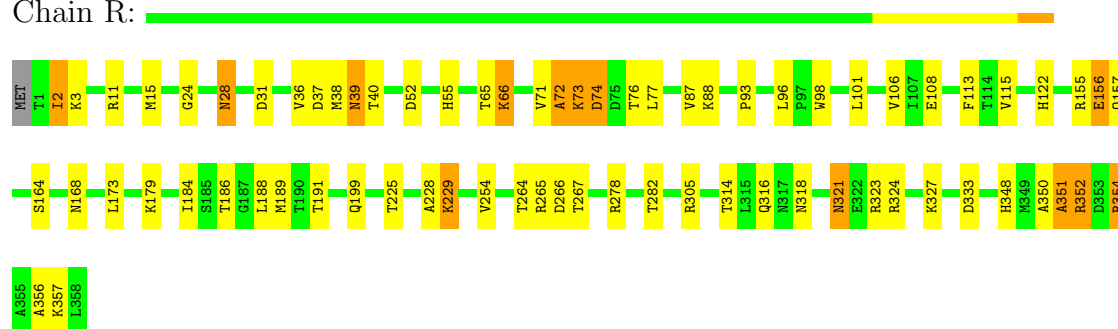
- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE, GLYCOSOMAL

Chain Q:



- Molecule 1: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE, GLYCOSOMAL

Chain R:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.52Å 256.27Å 114.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.40 – 3.20 7.40 – 3.20	Depositor EDS
% Data completeness (in resolution range)	57.3 (7.40-3.20) 57.3 (7.40-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 3.22Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.150 , 0.218 0.149 , 0.218	Depositor DCC
R_{free} test set	1798 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 34998 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16734	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.26 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.9661e-03.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.44	0/2785	0.65	2/3770 (0.1%)
1	B	0.42	0/2785	0.64	0/3770
1	O	0.45	0/2785	0.66	0/3770
1	P	0.45	0/2785	0.66	0/3770
1	Q	0.43	0/2785	0.63	0/3770
1	R	0.44	0/2785	0.67	2/3770 (0.1%)
All	All	0.44	0/16710	0.65	4/22620 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	155	ARG	NE-CZ-NH2	9.21	124.91	120.30
1	R	155	ARG	CD-NE-CZ	-5.67	115.67	123.60
1	A	25	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	358	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2735	0	12	32	0
1	B	2735	0	0	29	0
1	O	2735	0	0	30	0
1	P	2735	0	0	33	0
1	Q	2735	0	0	24	0
1	R	2735	0	0	27	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	O	10	0	0	1	0
2	P	10	0	0	1	0
2	Q	10	0	0	0	0
2	R	10	0	0	1	0
3	A	44	0	26	1	0
3	B	44	0	26	2	0
3	O	44	0	26	1	0
3	P	44	0	26	2	0
3	Q	44	0	26	2	0
3	R	44	0	26	1	0
All	All	16734	0	168	174	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (174) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:128:ARG:CG	1:O:128:ARG:NH1	2.49	0.74
1:A:156:GLU:OE1	1:A:156:GLU:CA	2.43	0.66
1:O:155:ARG:NH1	1:O:155:ARG:CG	2.59	0.64
1:O:323:ARG:NH1	1:O:323:ARG:CG	2.60	0.64
1:R:156:GLU:OE1	1:R:156:GLU:CA	2.46	0.64
1:A:323:ARG:CG	1:A:323:ARG:NH1	2.60	0.63
1:Q:155:ARG:NH1	1:Q:155:ARG:CG	2.61	0.63
1:B:156:GLU:CA	1:B:156:GLU:OE1	2.47	0.63
1:R:2:ILE:O	1:R:31:ASP:N	2.32	0.63
1:A:357:LYS:CG	1:A:358:LEU:N	2.62	0.62
1:O:347:ARG:NH2	1:O:358:LEU:CD2	2.62	0.62
1:P:28:ASN:OD1	1:P:28:ASN:N	2.33	0.62
1:B:225:THR:OG1	2:B:360:SO4:O4	2.17	0.61
1:Q:10:GLY:O	1:Q:12:ILE:N	2.33	0.61
1:O:37:ASP:OD1	3:O:361:NAD:H1B	2.01	0.60
1:O:28:ASN:OD1	1:O:28:ASN:N	2.35	0.60
1:P:225:THR:OG1	2:P:360:SO4:O4	2.20	0.60
1:Q:37:ASP:OD1	3:Q:361:NAD:H1B	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:155:ARG:CG	1:B:155:ARG:NH1	2.63	0.60
1:P:350:ALA:O	1:P:352:ARG:N	2.34	0.60
1:P:155:ARG:NH1	1:P:155:ARG:CG	2.65	0.59
1:B:37:ASP:OD1	3:B:361:NAD:H1B	2.02	0.59
1:B:292:ASP:O	1:B:312:LYS:NZ	2.35	0.59
1:P:302:SER:N	1:P:333:ASP:OD2	2.36	0.59
1:R:65:THR:CG2	1:R:66:LYS:N	2.66	0.58
1:P:37:ASP:OD1	3:P:361:NAD:H1B	2.03	0.58
1:A:155:ARG:NH1	1:A:155:ARG:CG	2.67	0.58
1:Q:352:ARG:C	1:Q:354:ARG:N	2.57	0.58
1:Q:71:VAL:O	1:Q:72:ALA:CB	2.51	0.58
1:P:352:ARG:C	1:P:354:ARG:N	2.57	0.58
1:B:98:TRP:NE1	1:B:122:HIS:ND1	2.52	0.58
1:Q:323:ARG:NH1	1:Q:323:ARG:CG	2.66	0.58
1:B:65:THR:CG2	1:B:66:LYS:N	2.67	0.57
1:A:347:ARG:NH2	1:A:358:LEU:CD2	2.67	0.57
1:R:37:ASP:OD1	3:R:361:NAD:H1B	2.03	0.57
1:B:194:SER:OG	1:B:254:VAL:O	2.23	0.56
1:A:28:ASN:N	1:A:28:ASN:OD1	2.38	0.56
1:A:352:ARG:C	1:A:354:ARG:N	2.59	0.56
1:P:292:ASP:O	1:P:312:LYS:NZ	2.39	0.56
1:P:156:GLU:OE1	1:P:156:GLU:CA	2.53	0.56
1:A:350:ALA:O	1:A:352:ARG:N	2.37	0.56
1:A:321:ASN:ND2	1:A:321:ASN:N	2.54	0.56
1:O:156:GLU:CA	1:O:156:GLU:OE1	2.54	0.55
1:P:71:VAL:O	1:P:72:ALA:CB	2.53	0.55
1:A:71:VAL:O	1:A:72:ALA:CB	2.54	0.55
1:P:65:THR:CG2	1:P:66:LYS:N	2.70	0.55
1:Q:2:ILE:CG2	1:Q:3:LYS:N	2.69	0.55
1:Q:156:GLU:CA	1:Q:156:GLU:OE1	2.53	0.55
1:O:71:VAL:O	1:O:72:ALA:CB	2.53	0.55
1:B:28:ASN:OD1	1:B:28:ASN:N	2.39	0.55
1:B:266:ASP:OD1	1:B:324:ARG:NE	2.40	0.55
1:O:180:GLU:OE1	1:O:278:ARG:NH2	2.41	0.53
1:A:65:THR:CG2	1:A:66:LYS:N	2.72	0.53
1:A:164:SER:O	1:A:168:ASN:ND2	2.42	0.53
1:A:38:MET:O	1:A:39:ASN:CB	2.56	0.53
1:R:350:ALA:O	1:R:352:ARG:N	2.42	0.52
3:P:361:NAD:O2A	3:P:361:NAD:O1N	2.25	0.52
1:R:28:ASN:N	1:R:28:ASN:OD1	2.42	0.52
1:Q:347:ARG:NH2	1:Q:358:LEU:CD2	2.73	0.52
1:B:10:GLY:O	1:B:12:ILE:N	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:71:VAL:O	1:R:72:ALA:CB	2.57	0.52
1:B:71:VAL:O	1:B:72:ALA:CB	2.58	0.51
1:A:37:ASP:OD1	3:A:361:NAD:H1B	2.10	0.51
1:B:11:ARG:O	1:B:15:MET:CG	2.58	0.51
1:P:2:ILE:CG2	1:P:3:LYS:N	2.73	0.51
1:R:352:ARG:C	1:R:354:ARG:N	2.63	0.51
1:B:46:ALA:O	1:B:50:LYS:CG	2.58	0.50
1:P:59:LYS:O	1:P:60:HIS:CD2	2.63	0.50
1:P:2:ILE:O	1:P:31:ASP:N	2.44	0.50
1:R:225:THR:OG1	2:R:360:SO4:O1	2.30	0.50
1:B:63:SER:O	1:B:78:VAL:N	2.45	0.50
1:A:46:ALA:O	1:A:50:LYS:CG	2.60	0.50
1:Q:28:ASN:OD1	1:Q:28:ASN:N	2.45	0.49
1:R:38:MET:O	1:R:39:ASN:CB	2.60	0.49
1:R:87:VAL:CG1	1:R:88:LYS:N	2.75	0.49
1:R:11:ARG:O	1:R:15:MET:CG	2.60	0.49
1:A:73:LYS:O	1:A:74:ASP:C	2.50	0.49
1:Q:65:THR:CG2	1:Q:66:LYS:N	2.76	0.49
1:A:3:LYS:CG	1:A:102:GLY:O	2.60	0.49
1:B:164:SER:O	1:B:168:ASN:ND2	2.46	0.48
1:O:164:SER:O	1:O:168:ASN:ND2	2.46	0.48
1:R:350:ALA:C	1:R:352:ARG:N	2.65	0.48
1:B:321:ASN:N	1:B:321:ASN:ND2	2.62	0.48
1:P:87:VAL:CG1	1:P:88:LYS:N	2.76	0.48
1:O:67:SER:OG	1:O:68:LYS:N	2.46	0.48
1:R:108:GLU:OE2	1:R:122:HIS:NE2	2.47	0.48
1:P:10:GLY:O	1:P:12:ILE:N	2.47	0.48
1:B:38:MET:O	1:B:39:ASN:CB	2.61	0.48
1:R:321:ASN:N	1:R:321:ASN:ND2	2.62	0.48
1:A:266:ASP:OD1	1:A:324:ARG:NE	2.46	0.48
1:O:352:ARG:C	1:O:354:ARG:N	2.67	0.48
1:P:352:ARG:CG	1:P:352:ARG:NH1	2.77	0.47
1:R:348:HIS:CE1	1:R:352:ARG:NH2	2.82	0.47
1:Q:165:CYS:CB	3:Q:361:NAD:H4N	2.44	0.47
1:A:348:HIS:CE1	1:A:352:ARG:NH2	2.83	0.47
1:R:352:ARG:NH1	1:R:352:ARG:CG	2.78	0.47
1:O:348:HIS:CE1	1:O:352:ARG:NH2	2.83	0.47
1:A:202:VAL:O	1:A:203:ASP:C	2.52	0.47
1:Q:112:LEU:C	1:Q:113:PHE:CD2	2.89	0.46
1:B:223:SER:O	1:B:246:ALA:N	2.48	0.46
1:A:98:TRP:NE1	1:A:122:HIS:ND1	2.64	0.46
1:O:313:ALA:O	1:O:317:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:347:ARG:NH2	1:B:358:LEU:CD2	2.79	0.46
1:O:65:THR:CG2	1:O:66:LYS:N	2.80	0.45
1:B:352:ARG:C	1:B:354:ARG:N	2.69	0.45
1:R:350:ALA:O	1:R:351:ALA:C	2.55	0.45
1:O:98:TRP:NE1	1:O:122:HIS:ND1	2.64	0.45
1:B:73:LYS:O	1:B:74:ASP:C	2.55	0.45
1:A:352:ARG:CG	1:A:352:ARG:NH1	2.80	0.44
1:O:292:ASP:O	1:O:312:LYS:NZ	2.50	0.44
1:A:350:ALA:C	1:A:352:ARG:N	2.70	0.44
1:R:314:THR:O	1:R:318:ASN:ND2	2.49	0.44
1:P:108:GLU:OE2	1:P:122:HIS:NE2	2.50	0.44
1:A:180:GLU:OE2	1:A:283:TYR:OH	2.35	0.44
1:P:350:ALA:C	1:P:352:ARG:N	2.71	0.44
1:O:352:ARG:NH1	1:O:352:ARG:CG	2.79	0.44
1:R:164:SER:O	1:R:168:ASN:ND2	2.51	0.44
1:O:194:SER:OG	1:O:254:VAL:O	2.36	0.44
1:P:105:TYR:OH	1:P:353:ASP:OD2	2.35	0.44
1:Q:302:SER:N	1:Q:333:ASP:OD2	2.51	0.44
1:A:12:ILE:O	1:A:16:VAL:N	2.50	0.44
1:Q:352:ARG:CG	1:Q:352:ARG:NH1	2.78	0.43
1:P:4:VAL:CG1	1:P:5:GLY:N	2.81	0.43
1:A:350:ALA:O	1:A:351:ALA:C	2.56	0.43
1:Q:193:HIS:ND1	1:Q:194:SER:O	2.52	0.43
1:Q:320:PRO:O	1:Q:321:ASN:CB	2.66	0.43
1:P:11:ARG:O	1:P:15:MET:CG	2.66	0.43
1:A:2:ILE:O	1:A:31:ASP:N	2.51	0.43
1:P:278:ARG:O	1:P:282:THR:OG1	2.36	0.43
1:R:266:ASP:OD1	1:R:324:ARG:NE	2.51	0.43
1:O:321:ASN:ND2	1:O:321:ASN:N	2.67	0.43
1:Q:93:PRO:CG	1:Q:113:PHE:CE1	3.01	0.43
1:O:2:ILE:O	1:O:31:ASP:N	2.52	0.43
1:P:352:ARG:O	1:P:354:ARG:N	2.52	0.43
1:O:354:ARG:O	1:O:356:ALA:N	2.51	0.43
1:O:38:MET:O	1:O:39:ASN:CB	2.66	0.43
1:Q:204:GLY:N	1:Q:213:GLY:O	2.52	0.43
1:Q:321:ASN:ND2	1:Q:321:ASN:N	2.67	0.43
1:P:11:ARG:O	1:P:15:MET:N	2.51	0.42
1:R:52:ASP:OD1	1:R:55:HIS:N	2.52	0.42
1:O:225:THR:OG1	2:O:360:SO4:O4	2.38	0.42
1:A:2:ILE:CG2	1:A:3:LYS:N	2.83	0.42
1:B:7:ASN:ND2	1:B:122:HIS:CE1	2.88	0.42
1:P:202:VAL:O	1:P:203:ASP:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:129:LYS:NZ	1:P:157:GLN:O	2.53	0.42
1:P:73:LYS:O	1:P:74:ASP:C	2.58	0.41
1:B:179:LYS:C	1:B:181:GLY:N	2.73	0.41
1:O:7:ASN:ND2	1:O:122:HIS:CE1	2.88	0.41
1:R:228:ALA:O	1:R:229:LYS:C	2.58	0.41
1:B:2:ILE:O	1:B:31:ASP:N	2.53	0.41
1:B:215:ALA:O	1:B:219:ASN:ND2	2.53	0.41
1:O:73:LYS:O	1:O:74:ASP:C	2.58	0.41
1:P:320:PRO:O	1:P:321:ASN:CB	2.68	0.41
1:A:290:TYR:CD2	1:A:290:TYR:C	2.94	0.41
1:O:121:GLY:O	1:O:124:ARG:N	2.54	0.41
1:Q:11:ARG:O	1:Q:15:MET:CG	2.69	0.41
1:Q:348:HIS:CE1	1:Q:352:ARG:NH2	2.88	0.41
3:B:361:NAD:O1N	3:B:361:NAD:O2A	2.38	0.41
1:P:38:MET:O	1:P:39:ASN:CB	2.68	0.41
1:P:96:LEU:CD1	1:P:98:TRP:CZ2	3.04	0.41
1:R:73:LYS:O	1:R:74:ASP:C	2.59	0.41
1:Q:325:PHE:CE2	1:R:188:LEU:CD1	3.04	0.41
1:O:325:PHE:CD2	1:P:186:THR:CG2	3.04	0.40
1:A:277:LYS:O	1:A:280:SER:CB	2.69	0.40
1:O:299:ASP:OD1	1:P:214:ARG:NH2	2.54	0.40
1:B:153:ASN:C	1:B:153:ASN:OD1	2.60	0.40
1:A:67:SER:N	1:A:75:ASP:OD1	2.54	0.40
1:Q:122:HIS:O	1:Q:127:ALA:CB	2.69	0.40
1:R:333:ASP:OD1	1:R:333:ASP:C	2.60	0.40
1:B:228:ALA:O	1:B:231:VAL:N	2.54	0.40
1:A:122:HIS:O	1:A:127:ALA:CB	2.69	0.40
1:B:228:ALA:O	1:B:229:LYS:C	2.60	0.40
1:R:93:PRO:CG	1:R:113:PHE:CE1	3.04	0.40
1:O:93:PRO:CG	1:O:113:PHE:CE1	3.04	0.40

There are no symmetry-related clashes.

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	356/359 (99%)	309 (87%)	35 (10%)	12 (3%)	6	38
1	B	356/359 (99%)	308 (86%)	38 (11%)	10 (3%)	8	44
1	O	356/359 (99%)	305 (86%)	39 (11%)	12 (3%)	6	38
1	P	356/359 (99%)	306 (86%)	39 (11%)	11 (3%)	7	41
1	Q	356/359 (99%)	308 (86%)	36 (10%)	12 (3%)	6	38
1	R	356/359 (99%)	303 (85%)	45 (13%)	8 (2%)	10	53
All	All	2136/2154 (99%)	1839 (86%)	232 (11%)	65 (3%)	7	42

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	72	ALA
1	A	351	ALA
1	A	356	ALA
1	B	11	ARG
1	B	39	ASN
1	B	72	ALA
1	O	11	ARG
1	O	72	ALA
1	O	356	ALA
1	P	72	ALA
1	P	351	ALA
1	P	354	ARG
1	Q	11	ARG
1	Q	72	ALA
1	R	72	ALA
1	A	2	ILE
1	A	254	VAL
1	B	2	ILE
1	B	254	VAL
1	B	354	ARG
1	B	356	ALA
1	O	2	ILE
1	O	74	ASP
1	O	230	ALA
1	O	254	VAL
1	O	351	ALA
1	P	2	ILE
1	P	11	ARG
1	P	254	VAL

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Mol	Chain	Res	Type
1	P	356	ALA
1	Q	2	ILE
1	Q	24	GLY
1	Q	254	VAL
1	Q	356	ALA
1	R	2	ILE
1	R	24	GLY
1	R	39	ASN
1	R	254	VAL
1	R	351	ALA
1	R	356	ALA
1	A	354	ARG
1	B	74	ASP
1	O	39	ASN
1	O	354	ARG
1	P	39	ASN
1	P	67	SER
1	Q	19	ALA
1	Q	39	ASN
1	A	24	GLY
1	A	229	LYS
1	A	357	LYS
1	O	67	SER
1	P	353	ASP
1	Q	89	ALA
1	Q	314	THR
1	Q	353	ASP
1	R	74	ASP
1	A	74	ASP
1	A	350	ALA
1	B	24	GLY
1	B	351	ALA
1	P	350	ALA
1	Q	148	ASN
1	O	237	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	295/296 (100%)	250 (85%)	45 (15%)	4	18
1	B	295/296 (100%)	261 (88%)	34 (12%)	8	35
1	O	295/296 (100%)	256 (87%)	39 (13%)	6	27
1	P	295/296 (100%)	257 (87%)	38 (13%)	6	28
1	Q	295/296 (100%)	255 (86%)	40 (14%)	5	25
1	R	295/296 (100%)	259 (88%)	36 (12%)	7	31
All	All	1770/1776 (100%)	1538 (87%)	232 (13%)	6	28

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	28	ASN
1	A	36	VAL
1	A	40	THR
1	A	43	ARG
1	A	57	LYS
1	A	58	PHE
1	A	63	SER
1	A	69	PRO
1	A	71	VAL
1	A	77	LEU
1	A	83	ARG
1	A	96	LEU
1	A	101	LEU
1	A	106	VAL
1	A	114	THR
1	A	115	VAL
1	A	149	HIS
1	A	155	ARG
1	A	156	GLU
1	A	157	GLN
1	A	173	LEU
1	A	184	ILE
1	A	186	THR
1	A	189	MET
1	A	199	GLN
1	A	211	ARG
1	A	225	THR
1	A	229	LYS
1	A	239	GLN

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Mol	Chain	Res	Type
1	A	256	VAL
1	A	264	THR
1	A	267	THR
1	A	278	ARG
1	A	282	THR
1	A	290	TYR
1	A	305	ARG
1	A	316	GLN
1	A	321	ASN
1	A	323	ARG
1	A	334	ASN
1	A	352	ARG
1	A	354	ARG
1	A	357	LYS
1	A	358	LEU
1	B	28	ASN
1	B	36	VAL
1	B	40	THR
1	B	50	LYS
1	B	71	VAL
1	B	73	LYS
1	B	77	LEU
1	B	96	LEU
1	B	101	LEU
1	B	106	VAL
1	B	114	THR
1	B	115	VAL
1	B	149	HIS
1	B	155	ARG
1	B	156	GLU
1	B	157	GLN
1	B	173	LEU
1	B	179	LYS
1	B	184	ILE
1	B	186	THR
1	B	189	MET
1	B	191	THR
1	B	199	GLN
1	B	211	ARG
1	B	229	LYS
1	B	264	THR
1	B	267	THR

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Mol	Chain	Res	Type
1	B	282	THR
1	B	305	ARG
1	B	316	GLN
1	B	321	ASN
1	B	327	LYS
1	B	352	ARG
1	B	354	ARG
1	O	2	ILE
1	O	3	LYS
1	O	28	ASN
1	O	36	VAL
1	O	40	THR
1	O	43	ARG
1	O	66	LYS
1	O	71	VAL
1	O	73	LYS
1	O	77	LEU
1	O	96	LEU
1	O	101	LEU
1	O	106	VAL
1	O	114	THR
1	O	115	VAL
1	O	117	SER
1	O	128	ARG
1	O	149	HIS
1	O	155	ARG
1	O	156	GLU
1	O	157	GLN
1	O	161	SER
1	O	173	LEU
1	O	179	LYS
1	O	184	ILE
1	O	189	MET
1	O	199	GLN
1	O	234	VAL
1	O	239	GLN
1	O	264	THR
1	O	267	THR
1	O	268	SER
1	O	305	ARG
1	O	316	GLN
1	O	321	ASN

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Mol	Chain	Res	Type
1	O	323	ARG
1	O	327	LYS
1	O	352	ARG
1	O	354	ARG
1	P	3	LYS
1	P	28	ASN
1	P	36	VAL
1	P	38	MET
1	P	40	THR
1	P	43	ARG
1	P	62	VAL
1	P	66	LYS
1	P	71	VAL
1	P	73	LYS
1	P	76	THR
1	P	77	LEU
1	P	96	LEU
1	P	101	LEU
1	P	106	VAL
1	P	114	THR
1	P	115	VAL
1	P	120	GLU
1	P	155	ARG
1	P	156	GLU
1	P	157	GLN
1	P	173	LEU
1	P	184	ILE
1	P	186	THR
1	P	189	MET
1	P	199	GLN
1	P	229	LYS
1	P	239	GLN
1	P	264	THR
1	P	267	THR
1	P	278	ARG
1	P	282	THR
1	P	316	GLN
1	P	321	ASN
1	P	327	LYS
1	P	352	ARG
1	P	354	ARG
1	P	358	LEU

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Mol	Chain	Res	Type
1	Q	3	LYS
1	Q	28	ASN
1	Q	29	GLU
1	Q	36	VAL
1	Q	40	THR
1	Q	50	LYS
1	Q	66	LYS
1	Q	71	VAL
1	Q	73	LYS
1	Q	77	LEU
1	Q	96	LEU
1	Q	98	TRP
1	Q	101	LEU
1	Q	106	VAL
1	Q	114	THR
1	Q	115	VAL
1	Q	155	ARG
1	Q	156	GLU
1	Q	157	GLN
1	Q	173	LEU
1	Q	184	ILE
1	Q	186	THR
1	Q	189	MET
1	Q	199	GLN
1	Q	208	LYS
1	Q	229	LYS
1	Q	237	SER
1	Q	243	THR
1	Q	264	THR
1	Q	267	THR
1	Q	270	LYS
1	Q	282	THR
1	Q	305	ARG
1	Q	316	GLN
1	Q	321	ASN
1	Q	323	ARG
1	Q	327	LYS
1	Q	352	ARG
1	Q	354	ARG
1	Q	357	LYS
1	R	3	LYS
1	R	28	ASN

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Mol	Chain	Res	Type
1	R	36	VAL
1	R	40	THR
1	R	66	LYS
1	R	73	LYS
1	R	76	THR
1	R	77	LEU
1	R	96	LEU
1	R	98	TRP
1	R	101	LEU
1	R	106	VAL
1	R	115	VAL
1	R	156	GLU
1	R	157	GLN
1	R	173	LEU
1	R	179	LYS
1	R	184	ILE
1	R	186	THR
1	R	189	MET
1	R	191	THR
1	R	199	GLN
1	R	229	LYS
1	R	264	THR
1	R	265	ARG
1	R	267	THR
1	R	278	ARG
1	R	282	THR
1	R	305	ARG
1	R	316	GLN
1	R	321	ASN
1	R	323	ARG
1	R	327	LYS
1	R	352	ARG
1	R	354	ARG
1	R	357	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

18 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	SO4	A	359	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	A	360	-	4,4,4	0.50	0	6,6,6	0.37	0
3	NAD	A	361	-	48,48,48	1.67	8 (16%)	73,73,73	2.10	20 (27%)
2	SO4	B	359	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	B	360	-	4,4,4	0.45	0	6,6,6	0.24	0
3	NAD	B	361	-	48,48,48	1.71	10 (20%)	73,73,73	2.24	21 (28%)
2	SO4	O	359	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	O	360	-	4,4,4	0.48	0	6,6,6	0.36	0
3	NAD	O	361	-	48,48,48	1.79	13 (27%)	73,73,73	2.15	15 (20%)
2	SO4	P	359	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	P	360	-	4,4,4	0.43	0	6,6,6	0.19	0
3	NAD	P	361	-	48,48,48	1.75	12 (25%)	73,73,73	2.19	21 (28%)
2	SO4	Q	359	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	Q	360	-	4,4,4	0.59	0	6,6,6	0.12	0
3	NAD	Q	361	-	48,48,48	1.71	9 (18%)	73,73,73	2.18	20 (27%)
2	SO4	R	359	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	R	360	-	4,4,4	0.60	0	6,6,6	0.34	0
3	NAD	R	361	-	48,48,48	1.80	13 (27%)	73,73,73	2.24	21 (28%)

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	SO4	A	359	-	-	0/0/0/0	0/0/0/0
2	SO4	A	360	-	-	0/0/0/0	0/0/0/0
3	NAD	A	361	-	-	0/30/62/62	0/3/5/5
2	SO4	B	359	-	-	0/0/0/0	0/0/0/0
2	SO4	B	360	-	-	0/0/0/0	0/0/0/0
3	NAD	B	361	-	-	0/30/62/62	0/3/5/5
2	SO4	O	359	-	-	0/0/0/0	0/0/0/0
2	SO4	O	360	-	-	0/0/0/0	0/0/0/0
3	NAD	O	361	-	-	0/30/62/62	0/3/5/5
2	SO4	P	359	-	-	0/0/0/0	0/0/0/0
2	SO4	P	360	-	-	0/0/0/0	0/0/0/0
3	NAD	P	361	-	-	0/30/62/62	0/3/5/5
2	SO4	Q	359	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	360	-	-	0/0/0/0	0/0/0/0
3	NAD	Q	361	-	-	0/30/62/62	0/3/5/5
2	SO4	R	359	-	-	0/0/0/0	0/0/0/0
2	SO4	R	360	-	-	0/0/0/0	0/0/0/0
3	NAD	R	361	-	-	0/30/62/62	0/3/5/5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	361	NAD	O4D-C1D	5.23	1.49	1.41
3	Q	361	NAD	C7N-N7N	5.18	1.44	1.33
3	A	361	NAD	C7N-N7N	5.15	1.44	1.33
3	R	361	NAD	C7N-N7N	5.13	1.44	1.33
3	Q	361	NAD	O4D-C1D	5.11	1.49	1.41
3	P	361	NAD	C7N-N7N	5.11	1.44	1.33
3	O	361	NAD	C7N-N7N	5.10	1.44	1.33
3	R	361	NAD	O4D-C1D	5.01	1.49	1.41
3	O	361	NAD	O4D-C1D	5.01	1.49	1.41
3	B	361	NAD	C7N-N7N	5.00	1.44	1.33
3	A	361	NAD	O4D-C1D	4.98	1.49	1.41
3	P	361	NAD	O4D-C1D	4.87	1.48	1.41
3	P	361	NAD	O4D-C4D	-3.10	1.37	1.45
3	O	361	NAD	C2B-C3B	-3.02	1.45	1.53
3	R	361	NAD	C2B-C3B	-3.00	1.45	1.53
3	A	361	NAD	O4D-C4D	-2.98	1.38	1.45
3	O	361	NAD	O4D-C4D	-2.97	1.38	1.45
3	R	361	NAD	C4A-N9A	-2.97	1.33	1.37
3	R	361	NAD	O4D-C4D	-2.96	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	361	NAD	O4D-C4D	-2.87	1.38	1.45
3	P	361	NAD	C4A-N9A	-2.87	1.33	1.37
3	Q	361	NAD	C2D-C1D	-2.81	1.49	1.53
3	B	361	NAD	C2B-C3B	-2.76	1.45	1.53
3	Q	361	NAD	O4D-C4D	-2.75	1.38	1.45
3	O	361	NAD	C6A-N6A	2.74	1.43	1.35
3	Q	361	NAD	C6A-N6A	2.71	1.43	1.35
3	R	361	NAD	C6A-N6A	2.68	1.43	1.35
3	B	361	NAD	C6A-N6A	2.62	1.43	1.35
3	O	361	NAD	C2B-C1B	-2.59	1.49	1.53
3	O	361	NAD	C2D-C1D	-2.58	1.49	1.53
3	P	361	NAD	C2B-C1B	-2.55	1.49	1.53
3	P	361	NAD	C6A-N6A	2.51	1.43	1.35
3	A	361	NAD	C6A-N6A	2.50	1.43	1.35
3	R	361	NAD	C1D-N1N	2.48	1.56	1.48
3	A	361	NAD	C1D-N1N	2.47	1.56	1.48
3	Q	361	NAD	C2B-C3B	-2.45	1.46	1.53
3	O	361	NAD	O3D-C3D	-2.42	1.37	1.43
3	R	361	NAD	O3D-C3D	-2.38	1.37	1.43
3	Q	361	NAD	O3D-C3D	-2.37	1.37	1.43
3	P	361	NAD	O3D-C3D	-2.36	1.37	1.43
3	P	361	NAD	C1D-N1N	2.34	1.56	1.48
3	B	361	NAD	C1D-N1N	2.29	1.55	1.48
3	R	361	NAD	C2D-C1D	-2.29	1.50	1.53
3	P	361	NAD	O4B-C1B	-2.27	1.37	1.41
3	B	361	NAD	C2D-C1D	-2.24	1.50	1.53
3	B	361	NAD	O3D-C3D	-2.20	1.37	1.43
3	R	361	NAD	O4B-C1B	-2.18	1.38	1.41
3	O	361	NAD	C4A-N9A	-2.18	1.34	1.37
3	O	361	NAD	O3B-C3B	-2.17	1.37	1.43
3	Q	361	NAD	C1D-N1N	2.17	1.55	1.48
3	P	361	NAD	C2B-C3B	-2.16	1.47	1.53
3	O	361	NAD	O2D-C2D	-2.14	1.37	1.43
3	R	361	NAD	C2B-C1B	-2.13	1.50	1.53
3	O	361	NAD	O2B-C2B	-2.12	1.37	1.43
3	B	361	NAD	O2D-C2D	-2.10	1.37	1.43
3	A	361	NAD	O2D-C2D	-2.07	1.38	1.43
3	P	361	NAD	O4B-C4B	-2.06	1.40	1.45
3	P	361	NAD	C2D-C1D	-2.06	1.50	1.53
3	A	361	NAD	C2B-C3B	-2.05	1.47	1.53
3	R	361	NAD	C2D-C3D	-2.05	1.47	1.53
3	A	361	NAD	O3D-C3D	-2.04	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	361	NAD	C1D-N1N	2.03	1.55	1.48
3	B	361	NAD	C2D-C3D	-2.03	1.47	1.53
3	R	361	NAD	O2D-C2D	-2.02	1.38	1.43
3	Q	361	NAD	O2D-C2D	-2.01	1.38	1.43

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	361	NAD	O4D-C1D-N1N	8.85	117.00	107.95
3	R	361	NAD	O4D-C1D-N1N	8.78	116.94	107.95
3	B	361	NAD	N3A-C2A-N1A	-8.12	121.92	128.71
3	R	361	NAD	N3A-C2A-N1A	-8.09	121.94	128.71
3	Q	361	NAD	O4D-C1D-N1N	8.09	116.22	107.95
3	Q	361	NAD	N3A-C2A-N1A	-7.71	122.26	128.71
3	P	361	NAD	N3A-C2A-N1A	-7.63	122.33	128.71
3	O	361	NAD	O4D-C1D-N1N	7.51	115.64	107.95
3	O	361	NAD	N3A-C2A-N1A	-7.45	122.48	128.71
3	A	361	NAD	N3A-C2A-N1A	-7.42	122.51	128.71
3	P	361	NAD	O4D-C1D-N1N	7.26	115.38	107.95
3	A	361	NAD	O4D-C1D-N1N	6.83	114.94	107.95
3	Q	361	NAD	O3-PA-O5B	-6.05	76.36	103.41
3	O	361	NAD	O4B-C1B-N9A	5.53	113.59	108.44
3	P	361	NAD	C4B-O4B-C1B	-5.49	103.78	109.75
3	A	361	NAD	O3-PA-O5B	-5.16	80.31	103.41
3	O	361	NAD	N3A-C4A-N9A	5.03	134.52	125.43
3	B	361	NAD	O3-PA-O5B	-5.01	80.98	103.41
3	B	361	NAD	N3A-C4A-N9A	4.86	134.20	125.43
3	R	361	NAD	O3-PA-O1A	-4.74	77.25	111.28
3	R	361	NAD	O4B-C1B-N9A	4.65	112.76	108.44
3	Q	361	NAD	N3A-C4A-N9A	4.59	133.72	125.43
3	A	361	NAD	N3A-C4A-N9A	4.47	133.51	125.43
3	P	361	NAD	O3-PA-O5B	-4.40	83.71	103.41
3	A	361	NAD	C2D-C1D-N1N	4.32	121.17	113.86
3	O	361	NAD	O3-PA-O1A	-4.28	80.59	111.28
3	B	361	NAD	O2A-PA-O3	-4.19	85.28	105.14
3	P	361	NAD	O2A-PA-O3	-4.10	85.69	105.14
3	Q	361	NAD	C8A-N9A-C4A	4.05	109.99	106.90
3	O	361	NAD	C8A-N9A-C4A	4.00	109.96	106.90
3	R	361	NAD	O3-PA-O5B	-3.96	85.71	103.41
3	Q	361	NAD	C4B-O4B-C1B	-3.94	105.47	109.75
3	P	361	NAD	O3-PA-O1A	-3.93	83.10	111.28
3	A	361	NAD	O3-PA-O1A	-3.93	83.10	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	361	NAD	O3-PA-O5B	-3.90	85.98	103.41
3	P	361	NAD	C8A-N9A-C4A	3.88	109.86	106.90
3	R	361	NAD	N3A-C4A-N9A	3.86	132.41	125.43
3	Q	361	NAD	O5B-PA-O1A	3.86	124.50	109.37
3	P	361	NAD	N3A-C4A-N9A	3.81	132.31	125.43
3	R	361	NAD	C2D-C1D-N1N	3.75	120.20	113.86
3	B	361	NAD	O4B-C1B-N9A	3.70	111.89	108.44
3	Q	361	NAD	O3-PA-O1A	-3.67	84.91	111.28
3	B	361	NAD	O3-PA-O1A	-3.60	85.43	111.28
3	O	361	NAD	O2A-PA-O3	-3.58	88.16	105.14
3	R	361	NAD	C3N-C7N-N7N	3.37	121.60	117.77
3	P	361	NAD	C1B-N9A-C4A	-3.34	120.86	126.64
3	P	361	NAD	C2D-C1D-N1N	3.33	119.50	113.86
3	A	361	NAD	O2A-PA-O3	-3.26	89.66	105.14
3	R	361	NAD	O2A-PA-O3	-3.26	89.69	105.14
3	R	361	NAD	O5B-PA-O1A	3.22	121.98	109.37
3	Q	361	NAD	O5D-C5D-C4D	3.21	120.70	108.94
3	B	361	NAD	O5B-C5B-C4B	3.17	120.56	108.94
3	A	361	NAD	C4B-O4B-C1B	-3.10	106.38	109.75
3	B	361	NAD	C8A-N9A-C4A	3.07	109.24	106.90
3	A	361	NAD	C8A-N9A-C4A	3.02	109.20	106.90
3	O	361	NAD	O2N-PN-O1N	-3.00	109.68	118.72
3	A	361	NAD	C3D-C2D-C1D	3.00	105.59	100.91
3	B	361	NAD	C3N-C7N-N7N	2.96	121.14	117.77
3	B	361	NAD	O5B-PA-O1A	2.95	120.92	109.37
3	A	361	NAD	O5B-PA-O1A	2.91	120.78	109.37
3	B	361	NAD	C2D-C1D-N1N	2.90	118.76	113.86
3	R	361	NAD	C4B-O4B-C1B	-2.87	106.63	109.75
3	R	361	NAD	O5B-C5B-C4B	2.85	119.40	108.94
3	Q	361	NAD	O2N-PN-O1N	-2.83	110.19	118.72
3	O	361	NAD	O5B-C5B-C4B	2.81	119.26	108.94
3	P	361	NAD	C3N-C7N-N7N	2.81	120.96	117.77
3	B	361	NAD	O2N-PN-O1N	-2.80	110.27	118.72
3	R	361	NAD	C8A-N9A-C4A	2.76	109.00	106.90
3	O	361	NAD	O5B-PA-O1A	2.75	120.16	109.37
3	A	361	NAD	O4B-C1B-N9A	2.75	111.00	108.44
3	R	361	NAD	O5D-C5D-C4D	2.75	119.02	108.94
3	Q	361	NAD	C4A-C5A-N7A	-2.75	107.17	109.52
3	P	361	NAD	O2N-PN-O1N	-2.75	110.44	118.72
3	P	361	NAD	C3D-C2D-C1D	2.73	105.19	100.91
3	P	361	NAD	O5D-C5D-C4D	2.64	118.64	108.94
3	A	361	NAD	O2N-PN-O1N	-2.61	110.86	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	361	NAD	C2D-C1D-N1N	2.59	118.24	113.86
3	Q	361	NAD	O3-PN-O5D	2.55	111.57	101.36
3	P	361	NAD	O5B-PA-O1A	2.54	119.31	109.37
3	R	361	NAD	O2N-PN-O1N	-2.54	111.07	118.72
3	B	361	NAD	C5A-C4A-N3A	-2.53	120.20	125.70
3	Q	361	NAD	O2A-PA-O3	-2.51	93.22	105.14
3	R	361	NAD	O4B-C1B-C2B	-2.50	102.94	106.77
3	P	361	NAD	O5B-C5B-C4B	2.49	118.06	108.94
3	Q	361	NAD	C5A-C4A-N3A	-2.45	120.36	125.70
3	O	361	NAD	C5A-C4A-N3A	-2.41	120.45	125.70
3	B	361	NAD	PN-O3-PA	-2.41	122.61	132.95
3	P	361	NAD	O4B-C1B-N9A	2.40	110.68	108.44
3	B	361	NAD	O2A-PA-O5B	2.38	120.52	108.51
3	Q	361	NAD	N7A-C8A-N9A	-2.37	107.66	114.36
3	P	361	NAD	C2D-C3D-C4D	2.36	107.35	102.65
3	A	361	NAD	C5A-C4A-N3A	-2.33	120.63	125.70
3	P	361	NAD	N7A-C8A-N9A	-2.32	107.80	114.36
3	R	361	NAD	C4A-C5A-N7A	-2.30	107.56	109.52
3	Q	361	NAD	O4B-C1B-N9A	2.27	110.55	108.44
3	R	361	NAD	C5A-C4A-N3A	-2.27	120.76	125.70
3	A	361	NAD	C1B-N9A-C4A	-2.27	122.72	126.64
3	B	361	NAD	O5D-C5D-C4D	2.23	117.13	108.94
3	A	361	NAD	O4B-C1B-C2B	-2.21	103.39	106.77
3	A	361	NAD	O7N-C7N-N7N	-2.21	119.41	122.59
3	A	361	NAD	C2D-C3D-C4D	2.19	107.02	102.65
3	Q	361	NAD	C3B-C2B-C1B	2.17	104.30	100.91
3	O	361	NAD	N7A-C8A-N9A	-2.17	108.23	114.36
3	A	361	NAD	O5B-C5B-C4B	2.16	116.86	108.94
3	O	361	NAD	C2D-C3D-C4D	2.16	106.95	102.65
3	B	361	NAD	C2A-N3A-C4A	2.13	120.06	114.01
3	R	361	NAD	C1B-N9A-C4A	-2.12	122.97	126.64
3	Q	361	NAD	C1B-N9A-C4A	-2.11	123.00	126.64
3	P	361	NAD	C4A-C5A-N7A	-2.09	107.73	109.52
3	B	361	NAD	C4B-O4B-C1B	-2.08	107.48	109.75
3	R	361	NAD	C2A-N3A-C4A	2.08	119.94	114.01
3	P	361	NAD	O7N-C7N-N7N	-2.07	119.61	122.59
3	R	361	NAD	N7A-C8A-N9A	-2.05	108.57	114.36
3	Q	361	NAD	C2A-N3A-C4A	2.04	119.81	114.01
3	A	361	NAD	N7A-C8A-N9A	-2.03	108.60	114.36
3	B	361	NAD	O4B-C1B-C2B	-2.03	103.67	106.77
3	O	361	NAD	C2D-C1D-N1N	2.02	117.27	113.86
3	B	361	NAD	C2D-C3D-C4D	2.00	106.64	102.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	358/359 (99%)	-0.76	0 100 100	3, 26, 78, 196	0
1	B	358/359 (99%)	-0.73	0 100 100	4, 28, 74, 188	0
1	O	358/359 (99%)	-0.75	1 (0%) 91 58	6, 27, 72, 187	0
1	P	358/359 (99%)	-0.75	0 100 100	4, 26, 76, 188	0
1	Q	358/359 (99%)	-0.73	0 100 100	9, 29, 77, 189	0
1	R	358/359 (99%)	-0.76	0 100 100	5, 27, 76, 190	0
All	All	2148/2154 (99%)	-0.75	1 (0%) 100 100	3, 27, 76, 196	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	357	LYS	2.2

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	360	5/5	0.14	3.98	86,92,92,93	0
2	SO4	B	360	5/5	0.16	2.99	106,108,110,111	0
2	SO4	P	360	5/5	0.17	2.59	116,118,121,121	0
2	SO4	O	360	5/5	0.15	2.53	96,97,98,100	0
2	SO4	Q	360	5/5	0.15	2.51	95,95,97,99	0
2	SO4	R	360	5/5	0.15	2.06	83,86,89,90	0
2	SO4	O	359	5/5	0.15	1.86	95,99,101,102	0
2	SO4	Q	359	5/5	0.14	1.52	102,104,105,106	0
2	SO4	B	359	5/5	0.14	1.35	99,103,105,108	0
2	SO4	P	359	5/5	0.13	1.22	79,84,85,87	0
2	SO4	A	359	5/5	0.12	0.71	81,84,88,92	0
2	SO4	R	359	5/5	0.11	0.21	79,86,86,88	0
3	NAD	P	361	44/44	0.11	0.20	5,42,54,194	0
3	NAD	A	361	44/44	0.09	-0.06	4,43,57,155	0
3	NAD	O	361	44/44	0.09	-0.19	0,47,63,155	0
3	NAD	R	361	44/44	0.09	-0.29	0,37,49,124	0
3	NAD	B	361	44/44	0.09	-0.31	16,48,74,138	0
3	NAD	Q	361	44/44	0.09	-0.35	0,44,63,202	0

6.5 Other polymers ⓘ

There are no such residues in this entry.