



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:17 PM GMT

PDB ID : 3E5R  
Title : Crystal structure and Functional Analysis of Glyceraldehyde-3-phosphat  
eDehydrogenase from Oryza Sativa  
Authors : Tien, Y.C.; Lin, Y.H.; Chang, S.L.; Chen, C.J.  
Deposited on : 2008-08-14  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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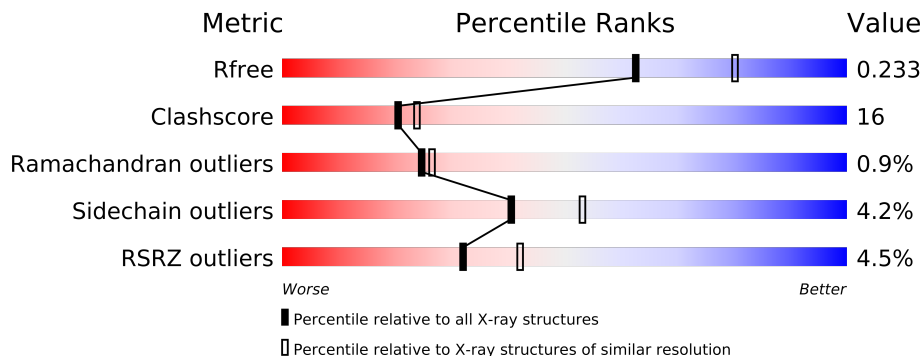
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 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	337	
1	B	337	
1	C	337	
1	O	337	

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	NAD	O	5463	-	X

## 2 Entry composition i

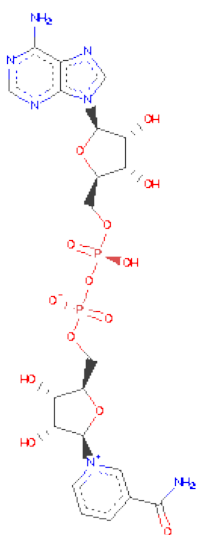
There are 3 unique types of molecules in this entry. The entry contains 11231 atoms, of which 0 are hydrogen and 0 are deuterium.

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, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	336	Total	C	N	O	S	0	0	0
			2553	1621	432	491	9			
1	A	336	Total	C	N	O	S	0	0	0
			2553	1621	432	491	9			
1	B	336	Total	C	N	O	S	0	0	0
			2553	1621	432	491	9			
1	C	336	Total	C	N	O	S	0	0	0
			2553	1621	432	491	9			

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is water.

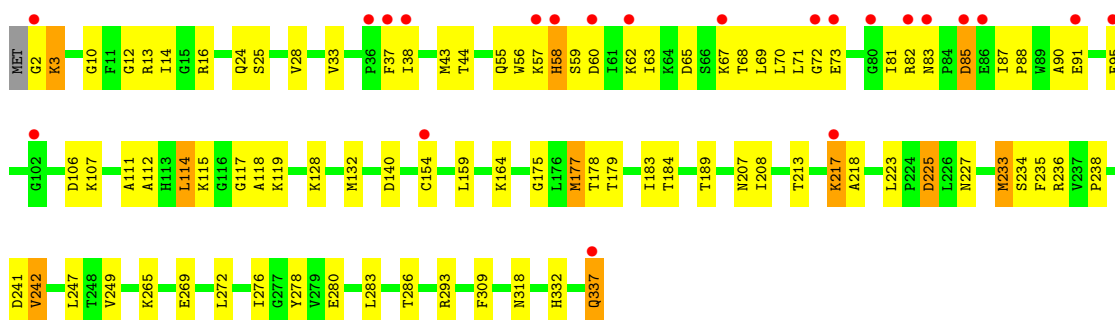
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	233	Total	O	0	0
			233	233		
3	A	194	Total	O	0	0
			194	194		
3	B	204	Total	O	0	0
			204	204		
3	C	212	Total	O	0	0
			212	212		

### 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.

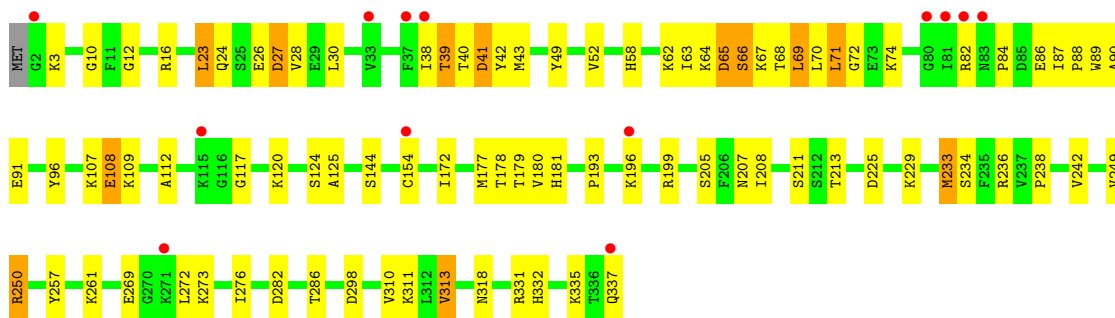
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, cytosolic

Chain O: 



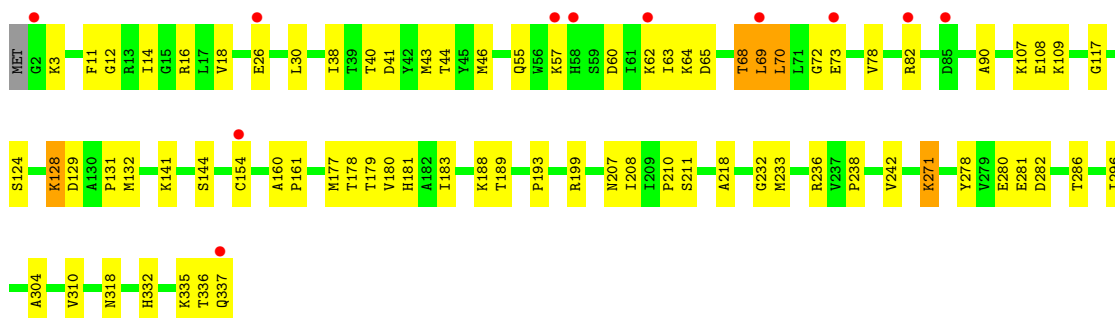
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, cytosolic

Chain A: 



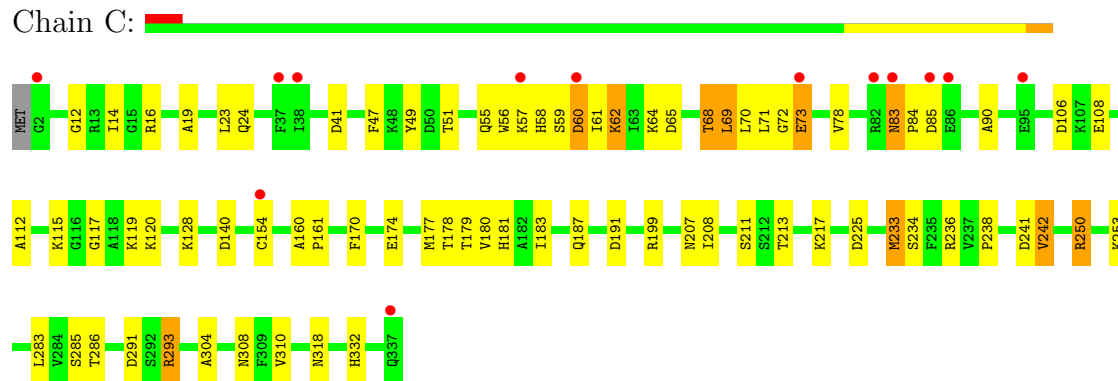
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, cytosolic

Chain B: 



- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, cytosolic

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.44Å 129.56Å 77.58Å 90.00° 117.40° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 23.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-2.30) 100.0 (23.43-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.199 , 0.239 0.237 , 0.233	Depositor DCC
$R_{free}$ test set	2965 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 10.4	EDS
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 105041 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: 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	0.38	1/2600 (0.0%)	0.70	3/3522 (0.1%)
1	B	0.36	0/2600	0.67	2/3522 (0.1%)
1	C	0.36	0/2600	0.70	3/3522 (0.1%)
1	O	0.39	0/2600	0.84	11/3522 (0.3%)
All	All	0.37	1/10400 (0.0%)	0.73	19/14088 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	LYS	CD-CE	5.39	1.64	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	67	LYS	N-CA-C	-8.92	86.92	111.00
1	O	68	THR	N-CA-C	8.18	133.09	111.00
1	O	57	LYS	C-N-CA	-7.39	103.23	121.70
1	A	3	LYS	CD-CE-NZ	7.15	128.15	111.70
1	O	85	ASP	N-CA-CB	-6.98	98.03	110.60
1	O	67	LYS	CB-CA-C	6.44	123.28	110.40
1	O	208	ILE	N-CA-C	-6.28	94.03	111.00
1	O	67	LYS	CA-CB-CG	6.21	127.06	113.40
1	O	85	ASP	CB-CG-OD2	6.14	123.82	118.30
1	B	208	ILE	N-CA-C	-5.97	94.89	111.00
1	B	180	VAL	N-CA-C	-5.83	95.25	111.00
1	A	208	ILE	N-CA-C	-5.82	95.29	111.00
1	C	208	ILE	N-CA-C	-5.82	95.30	111.00
1	O	85	ASP	CB-CG-OD1	-5.68	113.18	118.30
1	C	180	VAL	N-CA-C	-5.63	95.81	111.00
1	O	67	LYS	O-C-N	-5.12	114.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	58	HIS	O-C-N	5.09	130.85	122.70
1	C	60	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	180	VAL	N-CA-C	-5.01	97.48	111.00

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	2553	0	2576	88	1
1	B	2553	0	2576	73	0
1	C	2553	0	2576	68	0
1	O	2553	0	2576	116	0
2	A	44	0	26	9	0
2	B	44	0	24	6	0
2	C	44	0	26	10	0
2	O	44	0	26	21	0
3	A	194	0	0	11	9
3	B	204	0	0	6	2
3	C	212	0	0	17	3
3	O	233	0	0	13	9
All	All	11231	0	10406	326	12

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 16.

All (326) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:12:GLY:HA3	2:O:5463:NAD:O5B	1.32	1.29
1:O:38:ILE:HD11	1:O:43:MET:CE	1.81	1.08
1:B:107:LYS:NZ	1:B:108:GLU:OE1	1.91	1.04
1:O:12:GLY:HA3	2:O:5463:NAD:C5B	1.88	1.03
1:O:184:THR:HG23	1:O:236:ARG:HH22	1.21	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:310:VAL:HB	3:C:5782:HOH:O	1.57	1.03
1:O:83:ASN:OD1	1:O:85:ASP:HB3	1.62	0.98
1:B:69:LEU:O	1:B:70:LEU:HB2	1.63	0.97
1:O:13:ARG:N	2:O:5463:NAD:O1A	1.98	0.96
1:O:38:ILE:HD11	1:O:43:MET:HE2	1.47	0.95
1:A:64:LYS:HB2	1:A:70:LEU:HD23	1.47	0.94
1:A:107:LYS:HB3	3:A:5581:HOH:O	1.69	0.92
1:C:56:TRP:CD1	1:C:61:ILE:HD11	2.06	0.90
1:O:184:THR:CG2	1:O:236:ARG:HH22	1.85	0.89
1:A:67:LYS:HD2	3:A:5715:HOH:O	1.72	0.89
1:B:12:GLY:HA3	2:B:5465:NAD:H51A	1.55	0.88
1:A:64:LYS:HB2	1:A:70:LEU:CD2	2.06	0.86
1:O:184:THR:HG23	1:O:236:ARG:NH2	1.92	0.85
2:C:5467:NAD:H2N	2:C:5467:NAD:H51N	1.57	0.85
1:A:88:PRO:HB2	1:A:91:GLU:HG3	1.60	0.84
1:B:271:LYS:H	1:B:271:LYS:HD2	1.42	0.83
1:O:12:GLY:CA	2:O:5463:NAD:C5B	2.55	0.83
1:C:225:ASP:HB3	3:C:5599:HOH:O	1.80	0.82
1:A:82:ARG:HB2	1:A:82:ARG:NH2	1.97	0.80
1:B:40:THR:OG1	1:B:78:VAL:HG21	1.82	0.79
1:O:12:GLY:N	2:O:5463:NAD:H4B	1.97	0.79
1:A:65:ASP:O	1:A:66:SER:HB2	1.79	0.79
1:B:109:LYS:HD2	3:B:5639:HOH:O	1.81	0.79
1:O:38:ILE:HD11	1:O:43:MET:HE3	1.64	0.79
1:A:108:GLU:HG3	1:A:109:LYS:N	1.96	0.79
1:O:38:ILE:HD12	1:O:43:MET:HB2	1.65	0.78
1:O:164:LYS:HE2	3:O:5609:HOH:O	1.84	0.78
1:O:2:GLY:O	1:O:3:LYS:HB2	1.83	0.77
1:O:272:LEU:HB3	1:O:276:ILE:HG22	1.66	0.77
1:C:179:THR:HG21	3:C:5709:HOH:O	1.84	0.76
1:O:179:THR:HG21	3:O:5616:HOH:O	1.86	0.75
1:O:88:PRO:HB2	1:O:91:GLU:HG3	1.67	0.75
1:C:115:LYS:HB3	3:C:5755:HOH:O	1.85	0.75
1:O:107:LYS:HE3	3:O:5615:HOH:O	1.86	0.74
1:B:318:ASN:HD22	2:B:5465:NAD:H72N	1.36	0.73
1:O:13:ARG:H	2:O:5463:NAD:PA	2.12	0.73
1:O:13:ARG:HG2	2:O:5463:NAD:O1A	1.87	0.73
1:A:12:GLY:HA3	2:A:5466:NAD:O5B	1.89	0.73
1:O:13:ARG:HB2	2:O:5463:NAD:O1N	1.89	0.72
1:C:55:GLN:HB2	3:C:5734:HOH:O	1.87	0.72
1:O:38:ILE:HG13	1:O:38:ILE:O	1.89	0.71
1:B:131:PRO:HB2	3:B:5586:HOH:O	1.89	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:24:GLN:OE1	1:O:58:HIS:CG	2.44	0.71
1:O:24:GLN:OE1	1:O:58:HIS:CB	2.39	0.71
1:O:12:GLY:HA3	2:O:5463:NAD:PA	2.31	0.70
2:C:5467:NAD:C2N	2:C:5467:NAD:H51N	2.22	0.69
1:O:38:ILE:CD1	1:O:43:MET:HE3	2.23	0.69
1:A:58:HIS:HB2	3:A:5690:HOH:O	1.92	0.69
1:C:211:SER:HB2	3:C:5771:HOH:O	1.94	0.68
1:C:64:LYS:HE2	3:C:5752:HOH:O	1.94	0.68
1:O:159:LEU:HD22	1:O:177:MET:HE1	1.75	0.68
1:A:82:ARG:HB2	1:A:82:ARG:HH21	1.58	0.67
1:O:95:GLU:HG2	3:O:5571:HOH:O	1.94	0.67
1:O:72:GLY:O	1:O:73:GLU:HG3	1.94	0.67
1:A:144:SER:HB3	1:A:337:GLN:O	1.94	0.67
1:O:38:ILE:HD12	1:O:43:MET:CB	2.24	0.66
1:A:38:ILE:O	1:A:38:ILE:HG13	1.93	0.66
1:A:298:ASP:HB3	1:A:313:VAL:HG22	1.76	0.66
1:A:282:ASP:HB3	1:B:199:ARG:HG2	1.77	0.66
1:C:12:GLY:HA3	2:C:5467:NAD:C5B	2.27	0.65
1:A:318:ASN:HD22	2:A:5466:NAD:H72N	1.44	0.65
1:C:55:GLN:NE2	1:C:57:LYS:HE2	2.12	0.64
1:O:217:LYS:HB2	1:O:217:LYS:NZ	2.11	0.64
1:A:124:SER:O	2:A:5466:NAD:H1D	1.97	0.64
1:C:181:HIS:HB3	1:C:236:ARG:HD3	1.78	0.64
1:O:44:THR:HG21	1:O:63:ILE:HD11	1.79	0.64
1:A:63:ILE:N	1:A:63:ILE:HD12	2.13	0.64
1:A:335:LYS:HE3	3:A:5621:HOH:O	1.97	0.64
1:C:85:ASP:OD1	1:C:115:LYS:HD2	1.97	0.63
1:B:177:MET:HG2	1:B:178:THR:N	2.14	0.63
1:C:12:GLY:HA3	2:C:5467:NAD:H51A	1.81	0.62
1:O:318:ASN:HD22	2:O:5463:NAD:H72N	1.46	0.62
1:O:62:LYS:HG3	1:O:70:LEU:HB3	1.81	0.62
1:B:12:GLY:CA	2:B:5465:NAD:H51A	2.30	0.61
1:B:90:ALA:HB2	1:B:117:GLY:HA3	1.81	0.61
1:O:178:THR:HG23	1:O:233:MET:HE1	1.83	0.61
1:O:83:ASN:CG	1:O:85:ASP:HB3	2.21	0.61
1:B:62:LYS:HE3	1:B:70:LEU:HD23	1.82	0.61
1:C:24:GLN:NE2	3:C:5796:HOH:O	2.33	0.61
1:B:278:TYR:CE2	1:B:280:GLU:HG3	2.36	0.61
1:O:38:ILE:CD1	1:O:43:MET:CE	2.67	0.61
1:O:265:LYS:O	1:O:269:GLU:HG3	2.02	0.60
1:A:90:ALA:HB2	1:A:117:GLY:HA3	1.83	0.60
1:A:181:HIS:HB3	1:A:236:ARG:HD3	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:271:LYS:H	1:B:271:LYS:CD	2.05	0.60
1:O:213:THR:HG22	1:O:233:MET:HA	1.82	0.60
1:C:177:MET:HG2	1:C:178:THR:N	2.16	0.60
1:O:115:LYS:NZ	3:O:5575:HOH:O	2.34	0.60
1:O:10:GLY:HA2	2:O:5463:NAD:N3A	2.17	0.60
1:O:25:SER:OG	1:O:28:VAL:HG22	2.01	0.60
1:O:140:ASP:HB2	3:O:5610:HOH:O	2.02	0.60
1:B:107:LYS:CE	1:B:108:GLU:OE1	2.50	0.59
1:C:108:GLU:HG3	3:C:5661:HOH:O	2.02	0.59
1:C:318:ASN:O	2:C:5467:NAD:H4N	2.03	0.59
1:B:72:GLY:O	1:B:73:GLU:HB2	2.03	0.59
1:O:159:LEU:HD22	1:O:177:MET:CE	2.32	0.59
1:A:207:ASN:ND2	1:B:286:THR:HG23	2.18	0.59
1:B:69:LEU:O	1:B:70:LEU:CB	2.48	0.58
1:O:207:ASN:ND2	1:C:286:THR:HG23	2.18	0.58
1:B:64:LYS:HB3	1:B:68:THR:OG1	2.03	0.58
1:B:65:ASP:OD1	1:B:68:THR:HG23	2.02	0.58
1:A:229:LYS:HE2	3:A:5611:HOH:O	2.03	0.58
1:O:12:GLY:CA	2:O:5463:NAD:H51A	2.34	0.58
1:C:250:ARG:HD3	1:C:308:ASN:O	2.04	0.58
1:O:14:ILE:HD11	2:O:5463:NAD:C3N	2.34	0.58
1:C:83:ASN:HD22	1:C:84:PRO:HD2	1.69	0.58
1:B:271:LYS:N	1:B:271:LYS:HD2	2.17	0.57
1:A:310:VAL:HG22	1:A:311:LYS:N	2.17	0.57
1:O:217:LYS:HD3	3:O:5683:HOH:O	2.05	0.57
1:O:63:ILE:N	1:O:63:ILE:HD12	2.18	0.57
1:O:183:ILE:HD12	1:B:189:THR:HB	1.86	0.57
1:O:154:CYS:HB3	2:O:5463:NAD:H5N	1.87	0.56
1:O:12:GLY:CA	2:O:5463:NAD:H4B	2.36	0.56
1:B:12:GLY:HA3	2:B:5465:NAD:C5B	2.32	0.56
1:C:90:ALA:HB2	1:C:117:GLY:HA3	1.87	0.56
1:O:177:MET:HG2	1:O:178:THR:N	2.20	0.56
1:A:12:GLY:HA3	2:A:5466:NAD:C5B	2.36	0.56
1:A:211:SER:HB3	1:A:234:SER:OG	2.06	0.56
1:A:65:ASP:OD1	1:A:66:SER:O	2.23	0.56
1:B:60:ASP:OD1	1:B:72:GLY:HA2	2.06	0.55
1:O:55:GLN:NE2	3:O:5594:HOH:O	2.16	0.55
1:A:272:LEU:HD13	1:A:276:ILE:CD1	2.36	0.55
1:O:278:TYR:CE2	1:O:280:GLU:HG3	2.42	0.55
1:A:269:GLU:HA	1:A:273:LYS:CE	2.37	0.55
1:B:141:LYS:HG3	3:B:5480:HOH:O	2.05	0.54
1:B:124:SER:O	2:B:5465:NAD:H1D	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:112:ALA:HA	1:O:115:LYS:HD2	1.89	0.53
1:B:129:ASP:N	1:B:129:ASP:OD1	2.42	0.53
1:C:119:LYS:O	1:C:120:LYS:HD2	2.07	0.53
1:O:132:MET:HE1	1:O:218:ALA:HB1	1.90	0.53
1:A:179:THR:CG2	1:A:234:SER:HB3	2.39	0.53
1:A:207:ASN:HD22	1:B:286:THR:H	1.57	0.53
1:O:114:LEU:HD12	1:O:118:ALA:O	2.08	0.53
1:B:63:ILE:HD12	1:B:63:ILE:N	2.24	0.53
1:A:39:THR:CG2	1:A:40:THR:N	2.72	0.53
1:A:39:THR:HG22	1:A:41:ASP:N	2.24	0.53
1:A:39:THR:HG22	1:A:42:TYR:H	1.74	0.53
1:A:23:LEU:HD12	3:A:5702:HOH:O	2.08	0.53
1:C:304:ALA:CB	1:C:310:VAL:HG12	2.39	0.52
1:B:181:HIS:HB3	1:B:236:ARG:HD3	1.92	0.52
1:O:24:GLN:OE1	1:O:58:HIS:CD2	2.62	0.52
1:A:207:ASN:ND2	1:B:286:THR:H	2.07	0.52
1:C:160:ALA:HB3	1:C:161:PRO:HD3	1.92	0.52
1:B:199:ARG:HD2	1:B:210:PRO:HG2	1.90	0.52
1:O:83:ASN:OD1	1:O:85:ASP:CB	2.48	0.52
1:C:62:LYS:CB	1:C:62:LYS:NZ	2.73	0.52
1:O:88:PRO:HB2	1:O:91:GLU:CG	2.37	0.52
1:C:72:GLY:O	1:C:73:GLU:HB2	2.10	0.51
1:A:82:ARG:CB	1:A:82:ARG:HH21	2.22	0.51
1:A:125:ALA:CB	2:A:5466:NAD:O2D	2.58	0.51
1:O:111:ALA:O	1:O:114:LEU:HD22	2.09	0.51
1:O:72:GLY:O	1:O:73:GLU:CG	2.59	0.51
1:O:189:THR:HB	1:B:183:ILE:HD12	1.92	0.51
1:O:44:THR:HG21	1:O:63:ILE:CD1	2.40	0.51
1:A:177:MET:HG2	1:A:178:THR:N	2.25	0.51
1:C:291:ASP:OD1	1:C:293:ARG:HD3	2.11	0.50
1:O:38:ILE:CD1	1:O:43:MET:HG3	2.42	0.50
1:O:164:LYS:CE	3:O:5609:HOH:O	2.53	0.50
1:O:207:ASN:HD22	1:C:286:THR:H	1.58	0.50
1:O:159:LEU:HB2	1:O:177:MET:CE	2.42	0.50
1:O:12:GLY:HA2	2:O:5463:NAD:H51A	1.93	0.50
1:C:16:ARG:O	1:C:19:ALA:HB3	2.12	0.50
1:B:12:GLY:O	1:B:16:ARG:HG3	2.11	0.50
1:A:12:GLY:O	1:A:16:ARG:HG3	2.10	0.50
1:A:144:SER:CB	1:A:337:GLN:O	2.60	0.50
1:B:199:ARG:CD	1:B:210:PRO:HG2	2.42	0.50
1:A:84:PRO:HB2	1:A:112:ALA:HB3	1.94	0.50
1:B:55:GLN:O	1:B:57:LYS:HG2	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:64:LYS:O	1:C:65:ASP:CG	2.50	0.50
1:B:281:GLU:OE2	1:C:49:TYR:OH	2.28	0.50
1:O:81:ILE:HD12	1:O:87:ILE:HA	1.92	0.50
1:A:125:ALA:HB2	2:A:5466:NAD:O2D	2.12	0.50
1:A:272:LEU:HB3	1:A:276:ILE:HG13	1.94	0.50
1:B:160:ALA:HB3	1:B:161:PRO:HD3	1.94	0.49
1:C:69:LEU:HD22	1:C:78:VAL:CG2	2.42	0.49
1:B:336:THR:HG22	1:B:337:GLN:HG2	1.94	0.49
1:O:332:HIS:HE1	3:O:5604:HOH:O	1.95	0.48
1:B:14:ILE:O	1:B:18:VAL:HG23	2.13	0.48
1:C:83:ASN:HD22	1:C:84:PRO:CD	2.27	0.48
1:C:14:ILE:HG12	2:C:5467:NAD:O2N	2.13	0.48
1:B:296:ILE:N	1:B:296:ILE:HD12	2.29	0.48
1:O:12:GLY:CA	2:O:5463:NAD:C4B	2.92	0.48
1:O:13:ARG:CB	2:O:5463:NAD:O1N	2.61	0.48
1:B:107:LYS:NZ	1:B:108:GLU:CD	2.66	0.48
1:O:217:LYS:HB2	1:O:217:LYS:HZ2	1.77	0.48
1:O:247:LEU:HG	1:O:249:VAL:HG13	1.95	0.48
1:B:82:ARG:HH11	1:B:82:ARG:HG3	1.79	0.48
1:O:178:THR:HG23	1:O:233:MET:CE	2.43	0.48
1:O:309:PHE:CE2	1:C:174:GLU:HG3	2.49	0.48
1:O:2:GLY:O	1:O:3:LYS:CB	2.60	0.48
1:A:332:HIS:HE1	3:A:5666:HOH:O	1.96	0.48
1:C:56:TRP:CZ2	1:C:58:HIS:HB3	2.49	0.47
1:C:24:GLN:HG3	1:C:58:HIS:CD2	2.48	0.47
1:O:33:VAL:HG21	1:O:43:MET:SD	2.55	0.47
2:O:5463:NAD:H2N	2:O:5463:NAD:H52N	1.96	0.47
1:C:318:ASN:HD22	2:C:5467:NAD:H72N	1.62	0.47
1:O:233:MET:HE2	1:O:233:MET:C	2.34	0.47
2:A:5466:NAD:H2N	2:A:5466:NAD:H52N	1.96	0.47
1:B:304:ALA:CB	1:B:310:VAL:HG12	2.45	0.47
1:A:64:LYS:HB2	1:A:70:LEU:HD21	1.94	0.47
1:C:170:PHE:HD1	1:C:253:LYS:HE2	1.80	0.47
1:B:154:CYS:HB3	2:B:5465:NAD:H5N	1.95	0.47
1:A:335:LYS:HG3	3:A:5621:HOH:O	2.14	0.47
1:A:172:ILE:HG23	1:A:249:VAL:HG23	1.97	0.47
1:A:179:THR:HG22	1:A:234:SER:HB3	1.96	0.47
1:C:199:ARG:HG3	3:C:5634:HOH:O	2.15	0.47
1:C:293:ARG:NH1	3:C:5635:HOH:O	2.47	0.46
1:B:278:TYR:HE2	1:B:280:GLU:HG3	1.79	0.46
1:A:96:TYR:CD1	1:A:120:LYS:HB2	2.50	0.46
1:O:332:HIS:CE1	3:O:5604:HOH:O	2.67	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:ILE:HG23	1:A:249:VAL:CG2	2.46	0.46
1:A:74:LYS:HG3	1:A:74:LYS:O	2.15	0.46
1:O:337:GLN:CD	1:O:337:GLN:H	2.19	0.46
1:B:336:THR:O	1:B:337:GLN:HB2	2.16	0.46
1:A:213:THR:HG22	1:A:233:MET:HA	1.98	0.46
1:A:69:LEU:C	1:A:70:LEU:HD22	2.36	0.46
1:O:81:ILE:HD12	1:O:88:PRO:HD2	1.98	0.46
1:B:335:LYS:O	1:B:335:LYS:HG2	2.16	0.46
1:A:24:GLN:NE2	3:A:5693:HOH:O	2.49	0.46
1:A:39:THR:HG23	1:A:40:THR:N	2.31	0.45
1:O:286:THR:H	1:C:207:ASN:HD22	1.62	0.45
1:O:238:PRO:HB2	1:C:238:PRO:HB2	1.99	0.45
1:O:63:ILE:CD1	1:O:63:ILE:N	2.79	0.45
1:O:207:ASN:ND2	1:C:286:THR:H	2.15	0.45
1:C:106:ASP:CG	1:C:128:LYS:HE2	2.37	0.45
1:O:184:THR:CB	1:O:236:ARG:HH22	2.27	0.45
1:C:154:CYS:HB3	2:C:5467:NAD:H5N	1.97	0.45
1:A:27:ASP:CG	1:A:331:ARG:HE	2.20	0.45
1:C:179:THR:HG22	1:C:234:SER:HB2	1.98	0.45
1:A:65:ASP:C	1:A:66:SER:O	2.54	0.45
1:O:283:LEU:HD21	1:A:49:TYR:CZ	2.51	0.45
1:C:217:LYS:HE3	3:C:5701:HOH:O	2.16	0.45
1:O:38:ILE:CD1	1:O:43:MET:CG	2.94	0.45
1:C:304:ALA:HB1	1:C:310:VAL:HG12	1.99	0.45
1:A:310:VAL:CG2	1:A:311:LYS:N	2.79	0.45
1:O:106:ASP:OD1	1:O:128:LYS:HE2	2.17	0.45
1:O:72:GLY:C	1:O:73:GLU:HG3	2.37	0.45
1:O:119:LYS:HB2	3:O:5571:HOH:O	2.16	0.45
1:O:111:ALA:O	1:O:114:LEU:CD2	2.65	0.45
1:O:56:TRP:CD1	1:O:59:SER:O	2.70	0.45
1:A:286:THR:HG23	1:B:207:ASN:ND2	2.31	0.45
1:A:10:GLY:HA2	2:A:5466:NAD:N3A	2.32	0.44
1:O:13:ARG:N	2:O:5463:NAD:O3	2.51	0.44
1:A:38:ILE:HD11	1:A:43:MET:HG3	1.99	0.44
1:A:193:PRO:HD3	3:C:5794:HOH:O	2.16	0.44
1:B:69:LEU:HA	1:B:69:LEU:HD23	1.86	0.44
1:C:332:HIS:HD2	3:C:5792:HOH:O	2.01	0.44
1:B:278:TYR:CE2	1:B:280:GLU:CG	3.01	0.44
1:A:74:LYS:HE3	3:A:5694:HOH:O	2.17	0.44
1:C:241:ASP:O	1:C:242:VAL:HB	2.17	0.44
1:A:199:ARG:HG2	1:B:282:ASP:HB3	1.99	0.44
1:A:154:CYS:HB3	2:A:5466:NAD:H5N	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:233:MET:HE1	1:O:235:PHE:CE2	2.53	0.44
1:B:144:SER:OG	1:B:337:GLN:NE2	2.51	0.44
1:A:286:THR:H	1:B:207:ASN:ND2	2.16	0.44
1:A:74:LYS:HE3	1:A:74:LYS:HB2	1.85	0.44
1:B:38:ILE:HD13	1:B:46:MET:SD	2.57	0.44
1:A:65:ASP:O	1:A:66:SER:CB	2.54	0.43
1:O:286:THR:H	1:C:207:ASN:ND2	2.16	0.43
1:A:286:THR:H	1:B:207:ASN:HD22	1.65	0.43
1:C:23:LEU:HD13	1:C:71:LEU:HD22	1.99	0.43
1:A:282:ASP:HB3	1:B:199:ARG:CG	2.46	0.43
1:B:286:THR:HG21	1:C:51:THR:HG23	2.00	0.43
1:A:257:TYR:CE2	1:A:261:LYS:HD2	2.53	0.43
1:B:336:THR:O	1:B:337:GLN:CB	2.66	0.43
1:B:11:PHE:CE2	1:B:43:MET:HG2	2.53	0.43
1:B:177:MET:CE	1:B:179:THR:HG23	2.48	0.43
1:B:332:HIS:HE1	3:B:5554:HOH:O	2.00	0.43
1:A:272:LEU:HD13	1:A:276:ILE:HD11	2.00	0.43
1:A:249:VAL:HG22	1:A:250:ARG:N	2.34	0.43
1:C:84:PRO:HB2	1:C:112:ALA:HB3	2.01	0.43
1:C:68:THR:HG22	3:C:5746:HOH:O	2.19	0.43
1:O:175:GLY:HA3	1:O:249:VAL:HG12	2.01	0.43
1:B:44:THR:HG22	1:B:69:LEU:HD22	2.01	0.42
1:C:115:LYS:HG3	3:C:5754:HOH:O	2.19	0.42
1:B:178:THR:HA	1:B:233:MET:O	2.19	0.42
1:A:269:GLU:HA	1:A:273:LYS:HE3	2.01	0.42
1:C:62:LYS:NZ	1:C:62:LYS:HB3	2.33	0.42
1:O:90:ALA:HB2	1:O:117:GLY:HA3	2.01	0.42
1:O:24:GLN:OE1	1:O:58:HIS:HB2	2.16	0.42
1:B:177:MET:O	1:B:232:GLY:HA3	2.18	0.42
1:A:62:LYS:NZ	1:A:72:GLY:H	2.17	0.42
1:O:82:ARG:HB3	1:O:82:ARG:HE	1.50	0.42
1:C:213:THR:HG22	1:C:233:MET:HA	2.00	0.42
1:B:141:LYS:CG	3:B:5480:HOH:O	2.67	0.42
1:A:66:SER:C	1:A:68:THR:H	2.22	0.42
1:B:188:LYS:HE3	1:B:193:PRO:O	2.20	0.42
1:O:12:GLY:O	1:O:16:ARG:HG3	2.19	0.42
1:B:211:SER:HB3	3:B:5659:HOH:O	2.20	0.42
1:B:70:LEU:HD12	1:B:70:LEU:HA	1.89	0.42
1:C:115:LYS:CG	3:C:5754:HOH:O	2.68	0.41
1:O:73:GLU:OE2	1:O:73:GLU:C	2.57	0.41
1:C:12:GLY:CA	2:C:5467:NAD:H51A	2.48	0.41
1:C:70:LEU:HA	1:C:70:LEU:HD12	1.90	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:SER:O	1:A:68:THR:N	2.53	0.41
1:A:87:ILE:HG21	1:A:89:TRP:CZ2	2.55	0.41
1:A:196:LYS:HG2	1:A:196:LYS:O	2.21	0.41
1:O:179:THR:CG2	1:O:234:SER:HB2	2.51	0.41
1:O:241:ASP:O	1:O:242:VAL:HB	2.20	0.41
1:O:38:ILE:HD11	1:O:43:MET:CG	2.50	0.41
1:C:106:ASP:OD2	1:C:128:LYS:HE2	2.20	0.41
1:O:38:ILE:CD1	1:O:43:MET:CB	2.95	0.41
1:C:12:GLY:HA3	2:C:5467:NAD:O5B	2.20	0.41
1:C:47:PHE:HD1	1:C:61:ILE:HD13	1.86	0.41
1:A:87:ILE:HG21	1:A:89:TRP:CE2	2.56	0.41
1:A:63:ILE:CD1	1:A:63:ILE:N	2.83	0.41
1:C:183:ILE:HA	1:C:187:GLN:OE1	2.21	0.41
1:A:64:LYS:O	1:A:65:ASP:HB3	2.19	0.41
1:A:39:THR:CG2	1:A:41:ASP:H	2.33	0.41
1:B:128:LYS:HE3	1:B:128:LYS:HB3	1.46	0.41
1:A:205:SER:HA	1:A:238:PRO:HB3	2.03	0.41
1:O:13:ARG:CG	2:O:5463:NAD:O1N	2.69	0.41
1:A:86:GLU:CD	3:A:5661:HOH:O	2.59	0.41
1:B:132:MET:HE1	1:B:218:ALA:HB1	2.03	0.41
1:B:63:ILE:H	1:B:63:ILE:HD12	1.85	0.40
1:O:225:ASP:HB3	3:O:5678:HOH:O	2.22	0.40
1:O:38:ILE:HD11	1:O:43:MET:HG3	2.02	0.40
1:O:286:THR:HG23	1:C:207:ASN:ND2	2.36	0.40
1:A:71:LEU:CD2	1:A:71:LEU:N	2.84	0.40
1:O:37:PHE:N	1:O:37:PHE:CD2	2.89	0.40
1:O:207:ASN:HA	1:C:285:SER:OG	2.22	0.40

All (12) 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	Distance(Å)	Clash(Å)
3:O:5500:HOH:O	3:A:5665:HOH:O[1_556]	1.92	0.28
3:A:5659:HOH:O	3:C:5630:HOH:O[2_645]	1.94	0.26
3:O:5615:HOH:O	3:A:5764:HOH:O[1_556]	1.95	0.25
3:O:5601:HOH:O	3:A:5736:HOH:O[1_556]	2.02	0.18
3:O:5502:HOH:O	3:B:5586:HOH:O[1_656]	2.08	0.12
3:A:5700:HOH:O	3:C:5800:HOH:O[2_645]	2.08	0.12
1:A:225:ASP:OD1	3:O:5600:HOH:O[1_554]	2.10	0.10
3:O:5629:HOH:O	3:B:5679:HOH:O[1_656]	2.14	0.06
3:O:5603:HOH:O	3:A:5728:HOH:O[1_556]	2.15	0.05
3:A:5659:HOH:O	3:C:5606:HOH:O[2_645]	2.15	0.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:O:5602:HOH:O	3:A:5765:HOH:O[1_556]	2.17	0.03
3:O:5569:HOH:O	3:A:5715:HOH:O[1_455]	2.19	0.01

## 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	334/337 (99%)	309 (92%)	23 (7%)	2 (1%)	33	39
1	B	334/337 (99%)	311 (93%)	18 (5%)	5 (2%)	15	13
1	C	334/337 (99%)	319 (96%)	13 (4%)	2 (1%)	33	39
1	O	334/337 (99%)	313 (94%)	18 (5%)	3 (1%)	25	26
All	All	1336/1348 (99%)	1252 (94%)	72 (5%)	12 (1%)	25	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	B	3	LYS
1	B	70	LEU
1	O	3	LYS
1	C	242	VAL
1	O	242	VAL
1	A	242	VAL
1	B	242	VAL
1	B	69	LEU
1	O	65	ASP
1	C	191	ASP
1	B	238	PRO

### 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	276/277 (100%)	261 (95%)	15 (5%)	31	40
1	B	276/277 (100%)	270 (98%)	6 (2%)	64	81
1	C	276/277 (100%)	263 (95%)	13 (5%)	36	47
1	O	276/277 (100%)	264 (96%)	12 (4%)	40	52
All	All	1104/1108 (100%)	1058 (96%)	46 (4%)	40	53

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	60	ASP
1	O	69	LEU
1	O	71	LEU
1	O	114	LEU
1	O	177	MET
1	O	217	LYS
1	O	223	LEU
1	O	225	ASP
1	O	227	ASN
1	O	233	MET
1	O	293	ARG
1	O	337	GLN
1	A	23	LEU
1	A	26	GLU
1	A	27	ASP
1	A	28	VAL
1	A	30	LEU
1	A	39	THR
1	A	41	ASP
1	A	52	VAL
1	A	66	SER
1	A	69	LEU
1	A	71	LEU
1	A	108	GLU
1	A	233	MET
1	A	250	ARG
1	A	313	VAL
1	B	26	GLU
1	B	30	LEU
1	B	41	ASP
1	B	68	THR

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Mol	Chain	Res	Type
1	B	128	LYS
1	B	271	LYS
1	C	41	ASP
1	C	59	SER
1	C	60	ASP
1	C	62	LYS
1	C	68	THR
1	C	69	LEU
1	C	73	GLU
1	C	83	ASN
1	C	140	ASP
1	C	233	MET
1	C	250	ARG
1	C	283	LEU
1	C	293	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	207	ASN
1	O	227	ASN
1	O	318	ASN
1	O	332	HIS
1	A	24	GLN
1	A	83	ASN
1	A	207	ASN
1	A	318	ASN
1	A	332	HIS
1	B	24	GLN
1	B	58	HIS
1	B	207	ASN
1	B	318	ASN
1	B	332	HIS
1	C	24	GLN
1	C	55	GLN
1	C	58	HIS
1	C	83	ASN
1	C	207	ASN
1	C	332	HIS

### 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 ⓘ

4 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	5466	-	48,48,48	1.70	7 (14%)	73,73,73	3.78	32 (43%)
2	NAD	B	5465	-	48,48,48	2.50	12 (25%)	73,73,73	4.00	30 (41%)
2	NAD	C	5467	-	48,48,48	2.42	17 (35%)	73,73,73	3.82	32 (43%)
2	NAD	O	5463	-	48,48,48	1.67	6 (12%)	73,73,73	3.75	31 (42%)

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	5466	-	-	0/30/62/62	0/3/5/5
2	NAD	B	5465	-	1/1/11/11	0/30/62/62	0/3/5/5
2	NAD	C	5467	-	-	0/30/62/62	0/3/5/5
2	NAD	O	5463	-	-	0/30/62/62	0/3/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5465	NAD	PA-O3	8.41	1.75	1.59
2	B	5465	NAD	C2D-C1D	8.15	1.65	1.53
2	C	5467	NAD	O4D-C1D	6.89	1.51	1.41
2	O	5463	NAD	PA-O3	5.97	1.70	1.59
2	A	5466	NAD	PA-O3	5.77	1.70	1.59
2	C	5467	NAD	PN-O1N	5.66	1.62	1.48
2	B	5465	NAD	PN-O5D	5.25	1.76	1.60
2	C	5467	NAD	O4D-C4D	5.10	1.57	1.45
2	A	5466	NAD	O4B-C1B	4.52	1.48	1.41
2	B	5465	NAD	O4B-C1B	4.40	1.48	1.41
2	C	5467	NAD	O3D-C3D	4.11	1.52	1.43
2	C	5467	NAD	O4B-C1B	3.94	1.47	1.41
2	B	5465	NAD	O3D-C3D	-3.90	1.33	1.43
2	O	5463	NAD	O4B-C1B	3.82	1.47	1.41
2	C	5467	NAD	O5B-C5B	-3.74	1.29	1.44
2	O	5463	NAD	O4D-C1D	3.73	1.47	1.41
2	A	5466	NAD	O4D-C1D	3.69	1.47	1.41
2	O	5463	NAD	PN-O2N	3.67	1.57	1.48
2	B	5465	NAD	PN-O2N	3.56	1.57	1.48
2	A	5466	NAD	PN-O2N	3.51	1.56	1.48
2	O	5463	NAD	C2N-C3N	3.49	1.43	1.38
2	A	5466	NAD	C2N-C3N	3.45	1.43	1.38
2	C	5467	NAD	C5D-C4D	-3.35	1.40	1.51
2	C	5467	NAD	C2B-C3B	-3.32	1.44	1.53
2	B	5465	NAD	C2D-C3D	3.31	1.62	1.53
2	B	5465	NAD	C5D-C4D	-3.27	1.41	1.51
2	C	5467	NAD	PN-O5D	3.22	1.70	1.60
2	O	5463	NAD	PN-O1N	2.93	1.56	1.48
2	C	5467	NAD	C8A-N9A	2.85	1.40	1.36
2	C	5467	NAD	PA-O3	2.84	1.65	1.59
2	A	5466	NAD	PN-O1N	2.80	1.55	1.48
2	B	5465	NAD	O5D-C5D	2.73	1.56	1.44
2	C	5467	NAD	C3B-C4B	-2.64	1.45	1.53
2	B	5465	NAD	O4B-C4B	2.41	1.50	1.45
2	C	5467	NAD	C5B-C4B	-2.39	1.43	1.51
2	B	5465	NAD	PN-O3	2.35	1.65	1.60
2	B	5465	NAD	C2N-N1N	-2.34	1.32	1.35
2	C	5467	NAD	C5A-C4A	2.24	1.45	1.40
2	C	5467	NAD	C8A-N7A	-2.19	1.30	1.34
2	C	5467	NAD	C4N-C3N	2.16	1.43	1.39
2	A	5466	NAD	C2N-N1N	2.13	1.38	1.35
2	C	5467	NAD	C3D-C4D	2.11	1.58	1.53

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5466	NAD	O2N-PN-O1N	-15.65	71.51	118.72
2	O	5463	NAD	O2N-PN-O1N	-15.42	72.19	118.72
2	B	5465	NAD	C5D-C4D-C3D	14.44	173.06	115.21
2	O	5463	NAD	O3-PN-O1N	-12.29	79.48	108.83
2	A	5466	NAD	O3-PN-O1N	-11.89	80.43	108.83
2	C	5467	NAD	O4D-C1D-N1N	10.85	119.05	107.95
2	B	5465	NAD	O3-PN-O1N	10.76	134.53	108.83
2	B	5465	NAD	O4D-C4D-C5D	-10.30	72.58	109.36
2	C	5467	NAD	O4D-C4D-C5D	-10.17	73.03	109.36
2	C	5467	NAD	O4D-C4D-C3D	-10.12	84.66	105.17
2	C	5467	NAD	C4B-O4B-C1B	-9.43	99.51	109.75
2	B	5465	NAD	C4B-O4B-C1B	-9.19	99.76	109.75
2	C	5467	NAD	O3-PA-O5B	-9.14	62.52	103.41
2	O	5463	NAD	N3A-C2A-N1A	-8.79	121.36	128.71
2	A	5466	NAD	N3A-C2A-N1A	-8.74	121.41	128.71
2	B	5465	NAD	N3A-C2A-N1A	-8.60	121.52	128.71
2	C	5467	NAD	O5D-C5D-C4D	-8.44	77.96	108.94
2	C	5467	NAD	N3A-C2A-N1A	-8.35	121.73	128.71
2	A	5466	NAD	O4B-C1B-N9A	8.23	116.09	108.44
2	B	5465	NAD	C4D-O4D-C1D	8.05	118.49	109.75
2	C	5467	NAD	C2D-C3D-C4D	7.93	118.45	102.65
2	O	5463	NAD	C4B-O4B-C1B	-7.65	101.44	109.75
2	A	5466	NAD	C4B-O4B-C1B	-7.52	101.58	109.75
2	A	5466	NAD	O2N-PN-O3	7.38	128.70	108.79
2	B	5465	NAD	O5D-PN-O1N	-7.20	78.05	108.61
2	O	5463	NAD	O2N-PN-O3	7.19	128.16	108.79
2	O	5463	NAD	O4B-C1B-N9A	7.02	114.97	108.44
2	B	5465	NAD	O4B-C1B-N9A	6.83	114.79	108.44
2	B	5465	NAD	O4D-C1D-N1N	6.44	114.54	107.95
2	A	5466	NAD	O4D-C1D-N1N	6.26	114.36	107.95
2	A	5466	NAD	O5D-PN-O1N	6.19	134.88	108.61
2	O	5463	NAD	O5D-PN-O1N	6.07	134.36	108.61
2	B	5465	NAD	PN-O3-PA	-6.01	107.13	132.95
2	B	5465	NAD	O2D-C2D-C1D	5.93	129.15	111.23
2	O	5463	NAD	O4D-C1D-N1N	5.82	113.90	107.95
2	B	5465	NAD	O3D-C3D-C4D	5.72	127.94	111.08
2	C	5467	NAD	C2D-C1D-N1N	5.71	123.53	113.86
2	O	5463	NAD	PN-O3-PA	-5.50	109.34	132.95
2	A	5466	NAD	O2N-PN-O5D	-5.44	85.73	108.19
2	O	5463	NAD	O2N-PN-O5D	-5.43	85.78	108.19
2	O	5463	NAD	PN-O5D-C5D	-5.39	101.61	120.24
2	A	5466	NAD	PN-O3-PA	-5.35	109.95	132.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5467	NAD	C5D-C4D-C3D	5.31	136.50	115.21
2	A	5466	NAD	N3A-C4A-N9A	5.28	134.97	125.43
2	C	5467	NAD	N3A-C4A-N9A	5.23	134.88	125.43
2	O	5463	NAD	N3A-C4A-N9A	5.14	134.72	125.43
2	C	5467	NAD	O4B-C4B-C5B	5.06	127.42	109.36
2	A	5466	NAD	PN-O5D-C5D	-4.92	103.25	120.24
2	B	5465	NAD	O2A-PA-O3	-4.90	81.91	105.14
2	B	5465	NAD	N3A-C4A-N9A	4.76	134.04	125.43
2	C	5467	NAD	O5B-PA-O1A	4.72	127.88	109.37
2	C	5467	NAD	C4D-O4D-C1D	4.53	114.67	109.75
2	B	5465	NAD	PA-O5B-C5B	-4.46	89.97	122.03
2	A	5466	NAD	O3-PA-O1A	-4.37	79.90	111.28
2	B	5465	NAD	O3-PN-O5D	-4.37	83.85	101.36
2	B	5465	NAD	O2N-PN-O5D	-4.31	90.40	108.19
2	O	5463	NAD	O3-PN-O5D	-4.28	84.21	101.36
2	O	5463	NAD	O3-PA-O1A	-4.24	80.83	111.28
2	A	5466	NAD	O3-PN-O5D	-4.11	84.87	101.36
2	C	5467	NAD	O4B-C1B-N9A	4.03	112.19	108.44
2	B	5465	NAD	O5B-C5B-C4B	3.92	123.34	108.94
2	O	5463	NAD	O4B-C1B-C2B	-3.87	100.84	106.77
2	C	5467	NAD	PN-O5D-C5D	-3.84	106.98	120.24
2	B	5465	NAD	O2N-PN-O3	-3.84	98.45	108.79
2	A	5466	NAD	O4B-C1B-C2B	-3.83	100.91	106.77
2	C	5467	NAD	O5B-C5B-C4B	3.77	122.77	108.94
2	O	5463	NAD	O3-PA-O5B	-3.75	86.62	103.41
2	B	5465	NAD	O4D-C1D-C2D	-3.74	101.05	106.77
2	A	5466	NAD	O3-PA-O5B	-3.69	86.92	103.41
2	C	5467	NAD	C5B-C4B-C3B	-3.52	101.10	115.21
2	B	5465	NAD	O3-PA-O1A	-3.51	86.11	111.28
2	C	5467	NAD	PA-O5B-C5B	-3.45	97.23	122.03
2	C	5467	NAD	O4D-C1D-C2D	-3.37	101.61	106.77
2	A	5466	NAD	PA-O5B-C5B	-3.30	98.27	122.03
2	A	5466	NAD	O2A-PA-O3	-3.29	89.51	105.14
2	O	5463	NAD	PA-O5B-C5B	-3.25	98.68	122.03
2	O	5463	NAD	O2A-PA-O3	-3.19	89.99	105.14
2	B	5465	NAD	O5B-PA-O1A	3.14	121.66	109.37
2	A	5466	NAD	C5A-C4A-N3A	-3.05	119.07	125.70
2	B	5465	NAD	O4B-C4B-C5B	3.00	120.08	109.36
2	O	5463	NAD	C5A-C4A-N3A	-2.98	119.20	125.70
2	O	5463	NAD	O5B-PA-O1A	2.97	121.02	109.37
2	C	5467	NAD	C4A-C5A-N7A	-2.94	107.00	109.52
2	C	5467	NAD	O3-PA-O1A	-2.92	90.32	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5467	NAD	O2N-PN-O3	2.78	116.29	108.79
2	B	5465	NAD	O4B-C1B-C2B	-2.77	102.52	106.77
2	C	5467	NAD	C5A-C4A-N3A	-2.77	119.67	125.70
2	A	5466	NAD	C3D-C2D-C1D	2.74	105.19	100.91
2	O	5463	NAD	C3D-C2D-C1D	2.68	105.11	100.91
2	A	5466	NAD	C4A-C5A-N7A	-2.65	107.25	109.52
2	A	5466	NAD	C5D-C4D-C3D	-2.64	104.65	115.21
2	O	5463	NAD	C2A-N3A-C4A	2.63	121.49	114.01
2	O	5463	NAD	C5D-C4D-C3D	-2.62	104.72	115.21
2	C	5467	NAD	O7N-C7N-N7N	-2.61	118.83	122.59
2	A	5466	NAD	O4B-C4B-C5B	2.60	118.65	109.36
2	C	5467	NAD	O4B-C4B-C3B	2.60	110.44	105.17
2	A	5466	NAD	O5B-PA-O1A	2.59	119.53	109.37
2	A	5466	NAD	C2A-N3A-C4A	2.59	121.39	114.01
2	O	5463	NAD	C2D-C3D-C4D	2.59	107.81	102.65
2	B	5465	NAD	C5A-C4A-N3A	-2.57	120.09	125.70
2	O	5463	NAD	C4A-C5A-N7A	-2.57	107.32	109.52
2	A	5466	NAD	O7N-C7N-N7N	-2.55	118.91	122.59
2	C	5467	NAD	O4B-C1B-C2B	-2.53	102.90	106.77
2	O	5463	NAD	O4B-C4B-C5B	2.51	118.30	109.36
2	C	5467	NAD	C2B-C1B-N9A	-2.49	106.88	113.27
2	C	5467	NAD	O2D-C2D-C3D	2.49	119.92	111.83
2	O	5463	NAD	C5B-C4B-C3B	-2.49	105.25	115.21
2	A	5466	NAD	C2D-C3D-C4D	2.43	107.50	102.65
2	O	5463	NAD	O7N-C7N-N7N	-2.39	119.14	122.59
2	A	5466	NAD	C5B-C4B-C3B	-2.37	105.72	115.21
2	B	5465	NAD	C5B-C4B-C3B	-2.37	105.73	115.21
2	B	5465	NAD	C2A-N3A-C4A	2.34	120.68	114.01
2	C	5467	NAD	O2N-PN-O1N	-2.29	111.81	118.72
2	A	5466	NAD	O2A-PA-O1A	2.27	124.88	112.21
2	B	5465	NAD	O4B-C4B-C3B	2.27	109.76	105.17
2	B	5465	NAD	O2A-PA-O1A	2.23	124.65	112.21
2	C	5467	NAD	C2A-N3A-C4A	2.23	120.34	114.01
2	C	5467	NAD	C8A-N9A-C4A	2.15	108.54	106.90
2	B	5465	NAD	C3D-C2D-C1D	2.14	104.26	100.91
2	A	5466	NAD	O5B-C5B-C4B	2.11	116.70	108.94
2	O	5463	NAD	O5D-C5D-C4D	2.10	116.63	108.94
2	A	5466	NAD	O4D-C1D-C2D	2.09	109.97	106.77
2	A	5466	NAD	O5D-C5D-C4D	2.09	116.59	108.94
2	O	5463	NAD	O2A-PA-O1A	2.01	123.43	112.21
2	O	5463	NAD	O4D-C1D-C2D	2.01	109.85	106.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	5465	NAD	C4D

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	336/337 (99%)	0.21	13 (3%)	37 48	0, 0, 0, 1	2 (0%)
1	B	336/337 (99%)	0.20	11 (3%)	44 54	0, 0, 0, 1	2 (0%)
1	C	336/337 (99%)	0.22	13 (3%)	37 48	0, 0, 0, 0	2 (0%)
1	O	336/337 (99%)	0.30	22 (6%)	18 26	0, 0, 0, 1	2 (0%)
All	All	1344/1348 (99%)	0.23	59 (4%)	32 43	0, 0, 0, 1	8 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	154	CYS	14.1
1	C	154	CYS	13.9
1	B	154	CYS	12.7
1	A	154	CYS	12.0
1	O	2	GLY	6.7
1	A	337	GLN	5.8
1	B	2	GLY	5.7
1	C	82	ARG	4.8
1	O	337	GLN	4.8
1	O	38	ILE	4.3
1	A	2	GLY	4.3
1	A	37	PHE	4.3
1	A	271	LYS	4.2
1	C	2	GLY	4.0
1	C	37	PHE	3.8
1	B	57	LYS	3.5
1	O	37	PHE	3.4
1	O	82	ARG	3.4
1	B	73	GLU	3.1
1	O	83	ASN	3.0
1	O	60	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	337	GLN	2.9
1	O	72	GLY	2.9
1	O	73	GLU	2.9
1	O	67	LYS	2.8
1	O	80	GLY	2.8
1	B	69	LEU	2.8
1	O	57	LYS	2.7
1	A	82	ARG	2.6
1	O	85	ASP	2.5
1	C	60	ASP	2.5
1	B	82	ARG	2.5
1	O	102	GLY	2.4
1	C	38	ILE	2.4
1	B	62	LYS	2.4
1	B	26	GLU	2.4
1	O	36	PRO	2.4
1	C	57	LYS	2.4
1	A	83	ASN	2.3
1	C	86	GLU	2.3
1	O	217	LYS	2.2
1	B	58	HIS	2.2
1	C	337	GLN	2.2
1	O	91	GLU	2.2
1	B	85	ASP	2.2
1	A	196	LYS	2.2
1	C	73	GLU	2.2
1	A	33	VAL	2.2
1	A	115	LYS	2.1
1	C	95	GLU	2.1
1	O	95	GLU	2.1
1	A	81	ILE	2.1
1	O	58	HIS	2.1
1	A	80	GLY	2.0
1	C	85	ASP	2.0
1	A	38	ILE	2.0
1	C	83	ASN	2.0
1	O	62	LYS	2.0
1	O	86	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	NAD	O	5463	44/44	0.46	2.14	0,0,0,0	0
2	NAD	A	5466	44/44	0.32	1.32	0,0,0,0	0
2	NAD	C	5467	44/44	0.27	0.65	0,0,0,0	0
2	NAD	B	5465	44/44	0.17	0.16	0,0,0,0	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.