



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:17 AM GMT

PDB ID : 3OM9  
Title : T. Gondii bradyzoite-specific LDH (LDH1) in complex with NAD and OXQ  
Authors : Susko, M.S.; Wilson, D.K.  
Deposited on : 2010-08-26  
Resolution : 1.98 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](mailto: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.

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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 : 1.7 (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

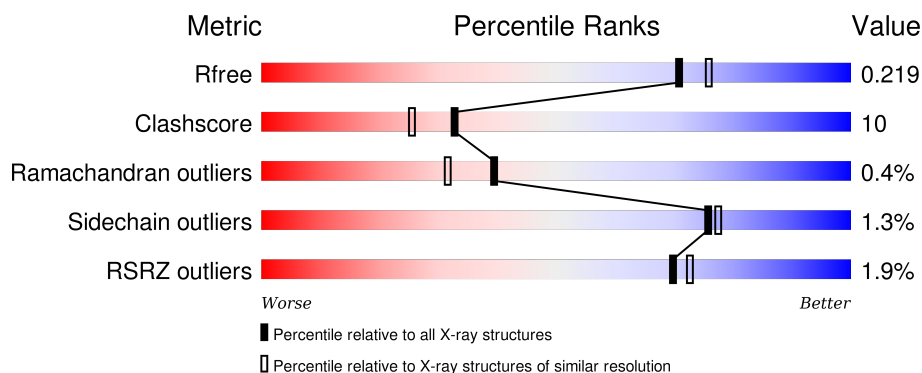
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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  $\geq 3$ , 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	329	<div> <div>2%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	B	329	<div> <div>2%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	C	329	<div> <div>2%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>
1	D	329	<div> <div>2%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10521 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 Lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2479	1568	419	469	23			
1	B	329	Total	C	N	O	S	0	0	0
			2479	1568	419	469	23			
1	C	326	Total	C	N	O	S	0	0	0
			2462	1558	416	465	23			
1	D	326	Total	C	N	O	S	0	0	0
			2462	1558	416	465	23			

There are 8 discrepancies between the modelled and reference sequences:

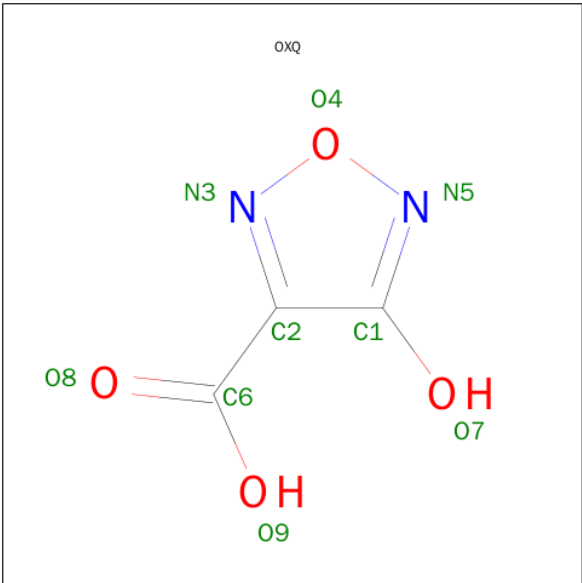
Chain	Residue	Modelled	Actual	Comment	Reference
A	334	PRO	-	EXPRESSION TAG	UNP P90613
A	335	GLY	-	EXPRESSION TAG	UNP P90613
B	334	PRO	-	EXPRESSION TAG	UNP P90613
B	335	GLY	-	EXPRESSION TAG	UNP P90613
C	334	PRO	-	EXPRESSION TAG	UNP P90613
C	335	GLY	-	EXPRESSION TAG	UNP P90613
D	334	PRO	-	EXPRESSION TAG	UNP P90613
D	335	GLY	-	EXPRESSION TAG	UNP P90613

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 3 is 4-HYDROXY-1,2,5-OXADIAZOLE-3-CARBOXYLIC ACID (three-letter code: OXQ) (formula: C<sub>3</sub>H<sub>2</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 3 2 4	0	0
3	B	1	Total C N O 9 3 2 4	0	0
3	C	1	Total C N O 9 3 2 4	0	0
3	D	1	Total C N O 9 3 2 4	0	0

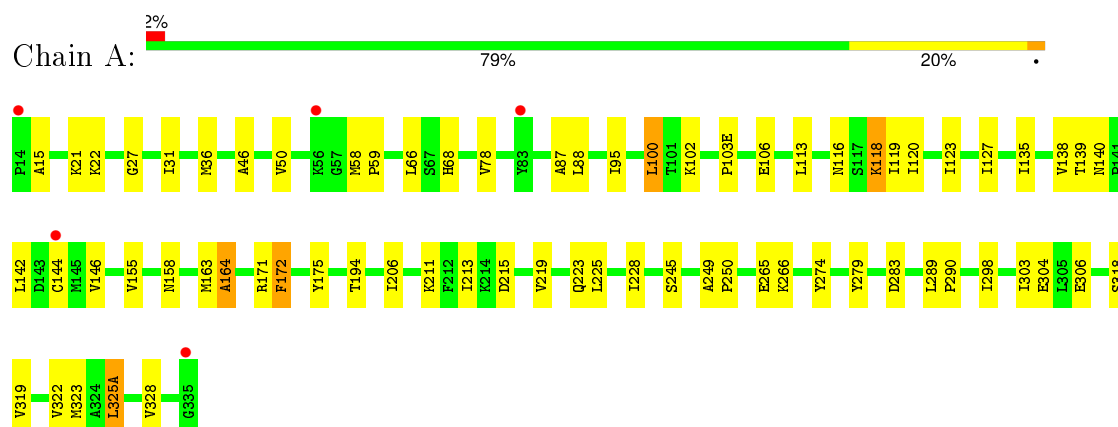
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	131	Total O 131 131	0	0
4	B	104	Total O 104 104	0	0
4	C	98	Total O 98 98	0	0
4	D	94	Total O 94 94	0	0

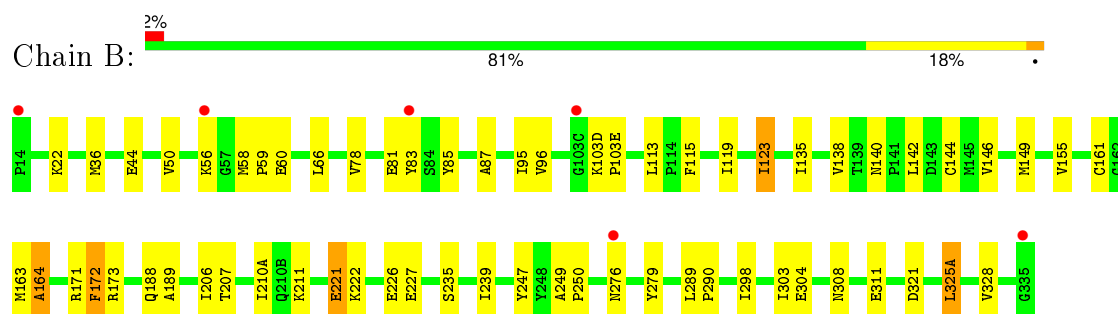
### 3 Residue-property plots [i](#)

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

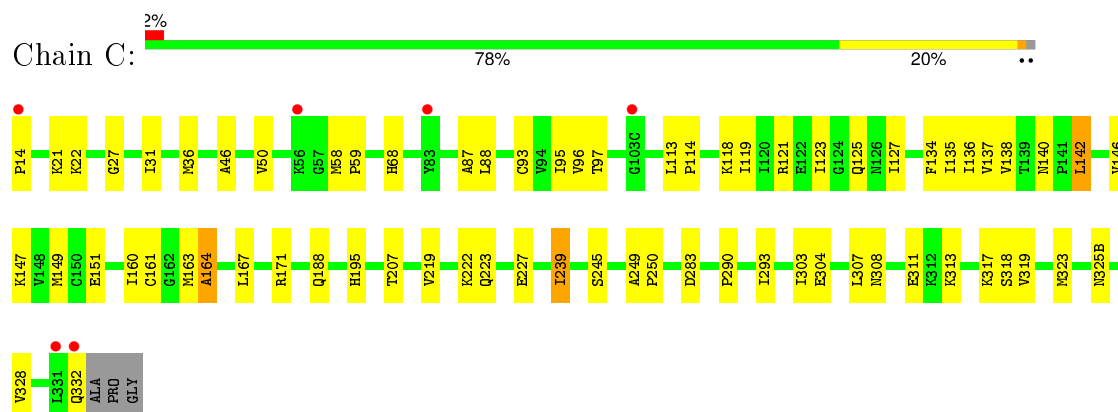
#### • Molecule 1: Lactate dehydrogenase



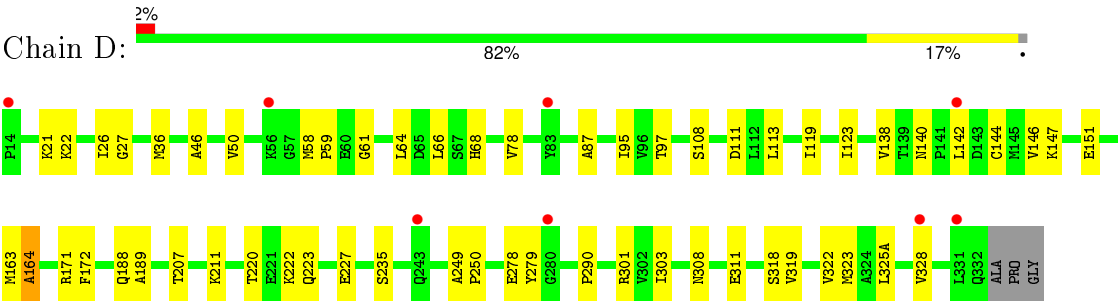
#### • Molecule 1: Lactate dehydrogenase



#### • Molecule 1: Lactate dehydrogenase



● Molecule 1: Lactate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.31 Å 124.46 Å 86.72 Å 90.00° 105.61° 90.00°	Depositor
Resolution (Å)	30.00 – 1.98 38.43 – 1.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.98) 98.4 (38.43-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	26.73 (at 1.98 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.196 , 0.223 0.196 , 0.219	Depositor DCC
$R_{free}$ test set	2822 reflections (3.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.7	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 92721 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10521	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OXQ, 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	0.30	0/2518	0.59	1/3405 (0.0%)
1	B	0.30	0/2518	0.59	0/3405
1	C	0.30	0/2500	0.58	1/3381 (0.0%)
1	D	0.29	0/2500	0.58	1/3381 (0.0%)
All	All	0.30	0/10036	0.58	3/13572 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	GLY	N-CA-C	-5.31	99.82	113.10
1	A	27	GLY	N-CA-C	-5.06	100.44	113.10
1	D	27	GLY	N-CA-C	-5.04	100.50	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2479	0	2533	61	0
1	B	2479	0	2533	57	0
1	C	2462	0	2518	62	0
1	D	2462	0	2518	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	4	0
2	D	44	0	26	1	0
3	A	9	0	0	1	0
3	B	9	0	0	0	0
3	C	9	0	0	2	0
3	D	9	0	0	1	0
4	A	131	0	0	1	0
4	B	104	0	0	1	0
4	C	98	0	0	4	0
4	D	94	0	0	2	0
All	All	10521	0	10206	212	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 10.

All (212) 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:142:LEU:HD22	1:D:164:ALA:HB2	1.42	0.99
1:A:213:ILE:HD13	1:A:219:VAL:HG23	1.46	0.93
1:B:325(A):LEU:HG	4:B:422:HOH:O	1.77	0.85
1:B:119:ILE:O	1:B:123:ILE:HD13	1.75	0.84
1:C:123:ILE:O	1:C:127:ILE:HD13	1.77	0.83
1:C:113:LEU:HD11	1:C:328:VAL:CG1	2.06	0.83
1:A:175:TYR:HB3	1:A:228:ILE:HD12	1.57	0.83
1:A:325(A):LEU:O	1:A:328:VAL:HG23	1.83	0.79
1:C:119:ILE:HD12	2:C:705:NAD:H61A	1.48	0.78
1:A:120:ILE:HD11	1:A:139:THR:HG21	1.66	0.78
1:D:220:THR:OG1	1:D:223:GLN:HG3	1.85	0.75
1:C:135:ILE:HB	1:C:160:ILE:HD13	1.69	0.75
1:C:134:PHE:CD2	1:C:136:ILE:HD11	2.21	0.75
1:D:26:ILE:HG21	1:D:123:ILE:HD12	1.71	0.73
1:D:142:LEU:HD22	1:D:164:ALA:CB	2.18	0.72
1:C:93:CYS:SG	1:C:136:ILE:HD13	2.30	0.72
1:A:103(E):PRO:HG2	1:A:106:GLU:HG3	1.71	0.72
1:C:119:ILE:HD12	2:C:705:NAD:N6A	2.05	0.71
1:D:113:LEU:HD21	1:D:328:VAL:CG2	2.21	0.70
1:C:14:PRO:HB3	4:D:371:HOH:O	1.92	0.69
1:D:222:LYS:O	1:D:227:GLU:HG3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ILE:HD11	1:D:64:LEU:HB2	1.75	0.69
1:B:325(A):LEU:O	1:B:328:VAL:HG23	1.94	0.68
1:B:113:LEU:HD22	1:B:325(A):LEU:HD13	1.76	0.68
1:A:123:ILE:O	1:A:127:ILE:HD13	1.93	0.68
1:A:116:ASN:O	1:A:120:ILE:HD13	1.94	0.68
1:A:135:ILE:HD13	1:A:155:VAL:HG21	1.74	0.68
1:B:161:CYS:HB3	1:B:298:ILE:HD11	1.77	0.67
1:A:15:ALA:HB1	4:A:5:HOH:O	1.95	0.66
1:C:303:ILE:N	1:C:303:ILE:HD12	2.11	0.65
1:B:135:ILE:HD12	1:B:135:ILE:N	2.10	0.65
1:C:113:LEU:HD11	1:C:328:VAL:HG13	1.77	0.65
1:A:158:ASN:O	1:A:298:ILE:HD12	1.97	0.64
1:B:113:LEU:HD11	1:B:328:VAL:HG22	1.79	0.64
1:A:144:CYS:SG	1:A:325(A):LEU:HB2	2.38	0.64
1:A:50:VAL:HG11	1:A:87:ALA:HA	1.80	0.63
1:B:115:PHE:O	1:B:119:ILE:HD13	1.99	0.63
1:D:50:VAL:HG11	1:D:87:ALA:HA	1.81	0.62
1:A:135:ILE:N	1:A:135:ILE:HD12	2.15	0.62
1:A:113:LEU:HD21	1:A:328:VAL:HG22	1.81	0.61
1:C:121:ARG:NH1	1:C:332:GLN:HG3	2.15	0.61
1:D:113:LEU:HD21	1:D:328:VAL:HG23	1.83	0.61
1:A:113:LEU:HD11	1:A:328:VAL:HG22	1.82	0.61
1:D:144:CYS:SG	1:D:328:VAL:HG21	2.42	0.60
1:A:135:ILE:HD11	1:A:155:VAL:HG11	1.84	0.60
1:C:293:ILE:HD12	1:C:293:ILE:N	2.16	0.60
1:D:142:LEU:O	1:D:146:VAL:HG23	2.03	0.59
1:D:290:PRO:HB2	1:D:303:ILE:HB	1.84	0.59
1:B:113:LEU:HD22	1:B:325(A):LEU:CD1	2.33	0.59
1:B:144:CYS:SG	1:B:328:VAL:HG21	2.43	0.58
1:C:121:ARG:O	1:C:125:GLN:HG3	2.03	0.58
1:B:221:GLU:OE2	1:B:226:GLU:HG3	2.02	0.58
1:A:306:GLU:HG3	1:D:211:LYS:HD3	1.86	0.58
1:B:142:LEU:HG	1:B:164:ALA:HB2	1.85	0.58
1:D:22:LYS:HE3	1:D:50:VAL:HG21	1.84	0.58
1:C:142:LEU:O	1:C:146:VAL:HG23	2.04	0.57
1:D:322:VAL:HA	1:D:325(A):LEU:HD12	1.86	0.57
1:C:136:ILE:N	1:C:136:ILE:HD12	2.19	0.57
1:A:144:CYS:SG	1:A:325(A):LEU:CB	2.92	0.57
1:A:68:HIS:CE1	1:C:171:ARG:HG2	2.39	0.57
1:B:239:ILE:HD12	1:D:61:GLY:O	2.04	0.57
1:B:140:ASN:HA	1:B:142:LEU:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:LYS:HG2	1:C:317:LYS:HE3	1.87	0.57
1:B:239:ILE:HD11	1:D:64:LEU:CB	2.34	0.57
1:A:319:VAL:O	1:A:323:MET:HG3	2.05	0.57
1:B:119:ILE:H	1:B:119:ILE:HD12	1.69	0.57
1:B:135:ILE:HD13	1:B:155:VAL:HG21	1.87	0.56
1:C:140:ASN:HA	1:C:142:LEU:N	2.21	0.56
1:B:119:ILE:HD12	1:B:119:ILE:N	2.20	0.56
1:C:142:LEU:HG	1:C:164:ALA:HB2	1.88	0.56
1:A:194:THR:H	1:A:318:SER:HB2	1.69	0.56
1:C:50:VAL:HG11	1:C:87:ALA:HA	1.87	0.56
1:C:308:ASN:OD1	1:C:311:GLU:HG3	2.06	0.56
1:D:140:ASN:HA	1:D:142:LEU:N	2.20	0.56
1:B:142:LEU:O	1:B:146:VAL:HG23	2.06	0.55
1:C:222:LYS:O	1:C:227:GLU:HG3	2.06	0.55
1:A:172:PHE:CZ	1:A:206:ILE:HD11	2.41	0.55
1:D:301:ARG:HD3	1:D:303:ILE:HD11	1.89	0.55
1:B:290:PRO:HG2	1:B:303:ILE:HB	1.88	0.55
1:A:36:MET:SD	1:A:95:ILE:HG21	2.47	0.55
1:B:172:PHE:CZ	1:B:206:ILE:HD11	2.41	0.55
1:B:222:LYS:O	1:B:227:GLU:HG3	2.06	0.54
1:B:113:LEU:HD11	1:B:328:VAL:CG2	2.37	0.54
1:D:119:ILE:O	1:D:123:ILE:HG12	2.07	0.54
1:C:22:LYS:HE3	1:C:50:VAL:HG21	1.88	0.54
1:D:138:VAL:O	2:D:707:NAD:H2N	2.06	0.54
1:B:138:VAL:O	2:B:703:NAD:H2N	2.07	0.53
1:C:135:ILE:C	1:C:136:ILE:HD12	2.28	0.53
1:A:171:ARG:HG2	1:C:68:HIS:CE1	2.44	0.53
1:A:113:LEU:HD11	1:A:328:VAL:CG2	2.38	0.52
1:A:213:ILE:CD1	1:A:219:VAL:HG23	2.30	0.52
1:A:223:GLN:O	1:A:228:ILE:HG12	2.10	0.52
1:A:135:ILE:H	1:A:135:ILE:HD12	1.75	0.52
1:A:142:LEU:HG	1:A:164:ALA:HB2	1.92	0.52
1:A:140:ASN:HA	1:A:142:LEU:N	2.24	0.52
1:D:66:LEU:HB2	1:D:78:VAL:HG11	1.92	0.52
1:B:22:LYS:HE2	1:B:50:VAL:HG21	1.91	0.52
1:B:36:MET:SD	1:B:95:ILE:HG21	2.50	0.52
1:B:60:GLU:HG3	1:B:83:TYR:OH	2.10	0.52
1:C:147:LYS:O	1:C:151:GLU:HG3	2.10	0.52
1:C:21:LYS:O	1:C:46:ALA:HB1	2.10	0.52
1:C:313:LYS:HE2	1:C:317:LYS:NZ	2.25	0.51
1:C:249:ALA:HB3	1:C:250:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HD11	1:A:225:LEU:CD1	2.41	0.51
1:D:22:LYS:HE3	1:D:50:VAL:CG2	2.40	0.51
1:D:308:ASN:OD1	1:D:311:GLU:HG3	2.10	0.51
1:B:279:TYR:CE2	1:B:289:LEU:HD22	2.45	0.51
1:A:194:THR:HG21	1:A:322:VAL:HB	1.92	0.50
1:B:172:PHE:CE2	1:B:206:ILE:HD11	2.46	0.50
1:B:50:VAL:HG11	1:B:87:ALA:HA	1.93	0.50
1:C:138:VAL:O	2:C:705:NAD:H2N	2.11	0.50
1:D:188:GLN:HB2	1:D:207:THR:OG1	2.10	0.49
1:B:96:VAL:HG21	1:B:149:MET:HE3	1.93	0.49
1:A:290:PRO:HG2	1:A:303:ILE:HB	1.94	0.49
1:B:85:TYR:OH	1:B:123:ILE:HD12	2.12	0.49
1:A:279:TYR:CE2	1:A:289:LEU:HD22	2.46	0.49
1:A:303:ILE:HD12	1:A:303:ILE:N	2.28	0.48
1:A:211:LYS:HE2	4:D:349:HOH:O	2.13	0.48
1:A:172:PHE:CE2	1:A:206:ILE:HD11	2.48	0.48
1:C:222:LYS:HG3	4:C:345:HOH:O	2.14	0.48
1:A:138:VAL:O	2:A:701:NAD:H2N	2.13	0.48
1:A:118:LYS:HE3	1:A:119:ILE:HG13	1.95	0.48
1:C:58:MET:HB3	1:C:59:PRO:HD3	1.95	0.48
1:B:135:ILE:HD11	1:B:155:VAL:HG11	1.95	0.47
1:A:21:LYS:O	1:A:46:ALA:HB1	2.14	0.47
1:A:213:ILE:HD11	1:A:225:LEU:HD11	1.97	0.47
1:C:219:VAL:HG23	1:C:223:GLN:CD	2.35	0.47
1:C:97:THR:HB	2:C:705:NAD:H51N	1.96	0.47
1:A:22:LYS:HE3	1:A:50:VAL:HG21	1.96	0.47
1:C:195:HIS:NE2	3:C:706:OXQ:O7	2.44	0.47
1:B:119:ILE:H	1:B:119:ILE:CD1	2.28	0.46
1:C:239:ILE:HD13	4:C:394:HOH:O	2.14	0.46
1:C:160:ILE:HD12	1:C:161:CYS:H	1.80	0.46
1:D:26:ILE:CG2	1:D:123:ILE:HD12	2.43	0.46
1:C:245:SER:HB2	3:C:706:OXQ:N3	2.31	0.46
1:A:66:LEU:HB2	1:A:78:VAL:HG11	1.96	0.46
1:A:249:ALA:N	1:A:250:PRO:CD	2.79	0.46
1:A:58:MET:HB3	1:A:59:PRO:HD3	1.96	0.46
1:A:142:LEU:O	1:A:146:VAL:HG23	2.16	0.45
1:D:249:ALA:HB3	1:D:250:PRO:HD3	1.99	0.45
1:D:319:VAL:O	1:D:323:MET:HG3	2.17	0.45
1:B:247:TYR:C	1:B:250:PRO:HD2	2.38	0.45
1:D:97:THR:HG22	1:D:138:VAL:HB	1.97	0.45
1:A:245:SER:HB2	3:A:702:OXQ:N3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:HD13	1:A:127:ILE:HD12	1.99	0.44
1:C:303:ILE:N	1:C:303:ILE:CD1	2.80	0.44
1:A:211:LYS:HE3	1:A:215:ASP:OD2	2.16	0.44
1:C:134:PHE:CE2	1:C:136:ILE:HD11	2.52	0.44
1:D:58:MET:HB3	1:D:59:PRO:HD3	1.99	0.44
1:D:163:MET:SD	1:D:163:MET:C	2.96	0.44
1:C:167:LEU:HD22	1:C:250:PRO:HG3	1.99	0.44
1:C:188:GLN:HB2	1:C:207:THR:OG1	2.18	0.44
1:C:88:LEU:CD1	1:C:127:ILE:HD12	2.48	0.44
1:A:171:ARG:HG2	1:C:68:HIS:CG	2.53	0.44
1:C:163:MET:C	1:C:163:MET:SD	2.96	0.44
1:D:36:MET:SD	1:D:95:ILE:HG21	2.58	0.44
1:B:171:ARG:HG2	1:D:68:HIS:CE1	2.53	0.44
1:C:22:LYS:HE3	1:C:50:VAL:CG2	2.47	0.43
1:C:319:VAL:O	1:C:323:MET:HG3	2.17	0.43
1:C:160:ILE:HD12	1:C:161:CYS:N	2.32	0.43
1:C:290:PRO:HB2	1:C:303:ILE:HB	2.00	0.43
1:C:239:ILE:CD1	4:C:394:HOH:O	2.66	0.43
1:D:21:LYS:O	1:D:46:ALA:HB1	2.18	0.43
1:C:31:ILE:O	1:C:36:MET:HG3	2.17	0.43
1:B:66:LEU:HB2	1:B:78:VAL:HG11	2.00	0.43
1:C:325(B):ASN:HA	1:C:328:VAL:HG22	2.01	0.43
1:A:194:THR:CG2	1:A:322:VAL:HB	2.49	0.43
1:B:211:LYS:HE2	1:C:304:GLU:O	2.19	0.43
1:D:108:SER:HB3	1:D:111:ASP:OD2	2.19	0.43
1:D:171:ARG:HD3	1:D:235:SER:HB2	2.01	0.43
1:A:100:LEU:HD13	1:A:102:LYS:O	2.19	0.43
1:B:249:ALA:N	1:B:250:PRO:CD	2.82	0.42
1:B:173:ARG:HG3	1:B:189:ALA:HB3	2.01	0.42
1:B:321:ASP:O	1:B:325(A):LEU:HD23	2.19	0.42
1:C:135:ILE:CB	1:C:160:ILE:HD13	2.45	0.42
1:A:22:LYS:HE3	1:A:50:VAL:CG2	2.50	0.42
1:B:279:TYR:CZ	1:B:304:GLU:HA	2.55	0.42
1:D:249:ALA:N	1:D:250:PRO:CD	2.83	0.42
1:B:188:GLN:HB2	1:B:207:THR:OG1	2.19	0.42
1:A:279:TYR:CZ	1:A:304:GLU:HA	2.54	0.42
1:A:265:GLU:OE2	1:B:44:GLU:OE2	2.37	0.42
1:A:274:TYR:CE1	1:A:283:ASP:HA	2.54	0.42
1:B:172:PHE:CD2	1:B:189:ALA:HB1	2.55	0.42
1:B:58:MET:HB3	1:B:59:PRO:HD3	2.02	0.42
1:B:163:MET:C	1:B:163:MET:SD	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:PHE:CD2	1:D:189:ALA:HB1	2.55	0.41
1:B:308:ASN:OD1	1:B:311:GLU:HG3	2.20	0.41
1:D:278:GLU:O	1:D:279:TYR:HB2	2.21	0.41
1:B:103(D):LYS:HA	1:B:103(E):PRO:HD3	1.94	0.41
1:A:163:MET:SD	1:A:163:MET:C	2.98	0.41
1:D:140:ASN:ND2	3:D:708:OXQ:N5	2.68	0.41
1:C:113:LEU:HB3	1:C:114:PRO:CD	2.51	0.41
1:C:164:ALA:HB3	4:C:419:HOH:O	2.21	0.41
1:A:265:GLU:O	1:A:266:LYS:HB2	2.21	0.41
1:B:142:LEU:C	1:B:142:LEU:HD13	2.41	0.41
1:B:56:LYS:HG2	1:B:83:TYR:CE2	2.55	0.41
1:C:307:LEU:HB3	1:C:311:GLU:HB2	2.02	0.41
1:B:206:ILE:HB	1:B:210(A):ILE:HB	2.02	0.41
1:B:22:LYS:HE2	1:B:50:VAL:CG2	2.50	0.41
1:B:171:ARG:HD3	1:B:235:SER:HB2	2.03	0.41
1:C:36:MET:SD	1:C:95:ILE:HG21	2.61	0.41
1:C:137:VAL:HG23	1:C:160:ILE:HD11	2.03	0.41
1:D:301:ARG:HD3	1:D:303:ILE:CD1	2.50	0.40
1:B:211:LYS:HD2	1:B:211:LYS:HA	1.88	0.40
1:D:147:LYS:O	1:D:151:GLU:HG3	2.20	0.40
1:A:144:CYS:SG	1:A:325(A):LEU:HB3	2.61	0.40
1:C:134:PHE:HD2	1:C:136:ILE:HD11	1.82	0.40
1:C:96:VAL:HG21	1:C:149:MET:HE3	2.02	0.40
1:A:120:ILE:HD12	1:A:120:ILE:N	2.37	0.40
1:A:31:ILE:O	1:A:36:MET:HG3	2.21	0.40
1:C:88:LEU:HD13	1:C:127:ILE:HD12	2.03	0.40
1:B:50:VAL:HG13	1:B:81:GLU:HG2	2.03	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	327/329 (99%)	318 (97%)	8 (2%)	1 (0%)	46	39
1	B	327/329 (99%)	319 (98%)	7 (2%)	1 (0%)	46	39
1	C	324/329 (98%)	316 (98%)	6 (2%)	2 (1%)	30	21
1	D	324/329 (98%)	316 (98%)	7 (2%)	1 (0%)	46	39
All	All	1302/1316 (99%)	1269 (98%)	28 (2%)	5 (0%)	39	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	ALA
1	D	164	ALA
1	B	164	ALA
1	C	164	ALA
1	C	142	LEU

### 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	270/270 (100%)	266 (98%)	4 (2%)	72	73
1	B	270/270 (100%)	265 (98%)	5 (2%)	65	65
1	C	269/270 (100%)	265 (98%)	4 (2%)	72	73
1	D	269/270 (100%)	268 (100%)	1 (0%)	93	95
All	All	1078/1080 (100%)	1064 (99%)	14 (1%)	76	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	118	LYS
1	A	172	PHE
1	A	325(A)	LEU
1	B	123	ILE
1	B	172	PHE

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Mol	Chain	Res	Type
1	B	221	GLU
1	B	276	ASN
1	B	325(A)	LEU
1	C	118	LYS
1	C	239	ILE
1	C	283	ASP
1	C	318	SER
1	D	318	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	B	276	ASN
1	C	332	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	701	-	38,48,48	1.76	8 (21%)	47,73,73	1.92	10 (21%)
3	OXQ	A	702	-	3,9,9	1.00	0	0,12,12	0.00	-
2	NAD	B	703	-	38,48,48	1.80	9 (23%)	47,73,73	1.89	10 (21%)
3	OXQ	B	704	-	3,9,9	0.99	0	0,12,12	0.00	-
2	NAD	C	705	-	38,48,48	1.73	9 (23%)	47,73,73	1.90	11 (23%)
3	OXQ	C	706	-	3,9,9	0.97	0	0,12,12	0.00	-
2	NAD	D	707	-	38,48,48	1.77	9 (23%)	47,73,73	1.87	8 (17%)
3	OXQ	D	708	-	3,9,9	0.97	0	0,12,12	0.00	-

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	701	-	-	0/22/62/62	0/5/5/5
3	OXQ	A	702	-	-	0/0/4/4	0/0/1/1
2	NAD	B	703	-	-	0/22/62/62	0/5/5/5
3	OXQ	B	704	-	-	0/0/4/4	0/0/1/1
2	NAD	C	705	-	-	0/22/62/62	0/5/5/5
3	OXQ	C	706	-	-	0/0/4/4	0/0/1/1
2	NAD	D	707	-	-	0/22/62/62	0/5/5/5
3	OXQ	D	708	-	-	0/0/4/4	0/0/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	705	NAD	PA-O1A	-2.75	1.41	1.51
2	A	701	NAD	PA-O1A	-2.73	1.41	1.51
2	D	707	NAD	PA-O1A	-2.72	1.41	1.51
2	B	703	NAD	PA-O1A	-2.57	1.41	1.51
2	C	705	NAD	C5N-C4N	2.01	1.43	1.38
2	D	707	NAD	C6N-C5N	2.02	1.43	1.38
2	A	701	NAD	C5N-C4N	2.02	1.43	1.38
2	D	707	NAD	C5N-C4N	2.06	1.43	1.38
2	B	703	NAD	C5N-C4N	2.18	1.43	1.38
2	C	705	NAD	C4A-N3A	2.19	1.38	1.35
2	B	703	NAD	C6N-C5N	2.20	1.43	1.38
2	C	705	NAD	C6N-C5N	2.22	1.43	1.38
2	A	701	NAD	C4A-N3A	2.54	1.39	1.35
2	D	707	NAD	C4A-N3A	2.56	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	703	NAD	C4A-N3A	2.76	1.39	1.35
2	B	703	NAD	C6N-N1N	3.09	1.43	1.35
2	C	705	NAD	C6N-N1N	3.18	1.44	1.35
2	A	701	NAD	C6N-N1N	3.21	1.44	1.35
2	D	707	NAD	C6N-N1N	3.22	1.44	1.35
2	A	701	NAD	O4D-C1D	3.33	1.45	1.41
2	D	707	NAD	O4D-C1D	3.46	1.45	1.41
2	C	705	NAD	O4D-C1D	3.46	1.45	1.41
2	C	705	NAD	C2A-N1A	3.64	1.40	1.33
2	B	703	NAD	O4D-C1D	3.71	1.45	1.41
2	B	703	NAD	C2A-N1A	3.77	1.41	1.33
2	D	707	NAD	C2A-N1A	3.93	1.41	1.33
2	A	701	NAD	C2A-N1A	3.94	1.41	1.33
2	A	701	NAD	C2A-N3A	4.00	1.39	1.32
2	C	705	NAD	C2A-N3A	4.02	1.39	1.32
2	D	707	NAD	C2A-N3A	4.12	1.39	1.32
2	B	703	NAD	C2A-N3A	4.19	1.39	1.32
2	C	705	NAD	C4N-C3N	4.51	1.47	1.39
2	B	703	NAD	C4N-C3N	4.57	1.47	1.39
2	A	701	NAD	C4N-C3N	4.60	1.47	1.39
2	D	707	NAD	C4N-C3N	4.60	1.47	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAD	N3A-C2A-N1A	-8.06	122.73	128.89
2	B	703	NAD	N3A-C2A-N1A	-7.88	122.86	128.89
2	D	707	NAD	N3A-C2A-N1A	-7.88	122.86	128.89
2	C	705	NAD	N3A-C2A-N1A	-7.61	123.06	128.89
2	D	707	NAD	O4D-C1D-N1N	-4.90	102.74	108.13
2	B	703	NAD	O4D-C1D-N1N	-4.89	102.76	108.13
2	C	705	NAD	O4D-C1D-N1N	-4.70	102.96	108.13
2	A	701	NAD	O4D-C1D-N1N	-4.46	103.23	108.13
2	A	701	NAD	C1B-N9A-C4A	-3.29	121.98	126.94
2	D	707	NAD	C1B-N9A-C4A	-3.24	122.05	126.94
2	C	705	NAD	C1B-N9A-C4A	-3.21	122.10	126.94
2	B	703	NAD	C1B-N9A-C4A	-3.10	122.27	126.94
2	B	703	NAD	C2B-C1B-N9A	-3.05	109.63	114.29
2	C	705	NAD	C2B-C1B-N9A	-2.82	109.99	114.29
2	A	701	NAD	O7N-C7N-C3N	-2.76	116.58	119.59
2	A	701	NAD	C2B-C1B-N9A	-2.71	110.16	114.29
2	D	707	NAD	C2B-C1B-N9A	-2.61	110.31	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	705	NAD	O7N-C7N-C3N	-2.60	116.74	119.59
2	C	705	NAD	O5B-C5B-C4B	-2.50	99.91	109.12
2	D	707	NAD	O7N-C7N-C3N	-2.49	116.86	119.59
2	D	707	NAD	O5B-C5B-C4B	-2.40	100.28	109.12
2	B	703	NAD	O5B-C5B-C4B	-2.39	100.32	109.12
2	B	703	NAD	O7N-C7N-C3N	-2.38	116.99	119.59
2	A	701	NAD	O5B-C5B-C4B	-2.37	100.38	109.12
2	C	705	NAD	C5N-C4N-C3N	-2.14	117.64	120.33
2	B	703	NAD	C5N-C4N-C3N	-2.07	117.73	120.33
2	C	705	NAD	O3B-C3B-C4B	-2.06	104.86	111.05
2	A	701	NAD	C4B-O4B-C1B	-2.06	107.46	109.72
2	A	701	NAD	O4B-C1B-N9A	2.12	112.54	108.10
2	B	703	NAD	O4B-C1B-N9A	2.22	112.73	108.10
2	C	705	NAD	O4B-C1B-N9A	2.29	112.89	108.10
2	D	707	NAD	C3N-C7N-N7N	2.29	120.32	117.82
2	B	703	NAD	C3N-C7N-N7N	2.32	120.35	117.82
2	C	705	NAD	C3N-C7N-N7N	2.44	120.49	117.82
2	A	701	NAD	C3N-C7N-N7N	2.66	120.73	117.82
2	D	707	NAD	C2N-C3N-C4N	2.93	121.55	118.29
2	B	703	NAD	C2N-C3N-C4N	3.04	121.67	118.29
2	A	701	NAD	C2N-C3N-C4N	3.08	121.72	118.29
2	C	705	NAD	C2N-C3N-C4N	3.10	121.75	118.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NAD	1	0
3	A	702	OXQ	1	0
2	B	703	NAD	1	0
2	C	705	NAD	4	0
3	C	706	OXQ	2	0
2	D	707	NAD	1	0
3	D	708	OXQ	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	329/329 (100%)	-0.15	5 (1%) 76 79	9, 14, 29, 48	0
1	B	329/329 (100%)	-0.11	6 (1%) 71 74	8, 14, 29, 44	0
1	C	326/329 (99%)	-0.07	6 (1%) 71 74	9, 15, 26, 43	0
1	D	326/329 (99%)	-0.01	8 (2%) 61 64	9, 15, 29, 45	0
All	All	1310/1316 (99%)	-0.08	25 (1%) 70 73	8, 15, 29, 48	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	GLY	9.0
1	C	14	PRO	8.2
1	B	83	TYR	7.8
1	B	335	GLY	7.7
1	D	83	TYR	4.9
1	D	14	PRO	4.8
1	A	83	TYR	4.7
1	B	103(C)	GLY	4.4
1	D	56	LYS	4.2
1	A	14	PRO	3.9
1	B	56	LYS	3.6
1	D	331	LEU	3.5
1	A	56	LYS	3.2
1	B	14	PRO	3.2
1	C	56	LYS	3.2
1	A	144	CYS	3.1
1	C	83	TYR	2.9
1	B	276	ASN	2.8
1	C	103(C)	GLY	2.6
1	C	332	GLN	2.6
1	D	280	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	331	LEU	2.2
1	D	142	LEU	2.1
1	D	243	GLN	2.1
1	D	328	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OXQ	B	704	9/9	0.95	0.11	1.78	13,14,15,15	0
3	OXQ	D	708	9/9	0.93	0.11	1.48	14,16,17,19	0
3	OXQ	A	702	9/9	0.96	0.10	0.67	12,14,15,16	0
2	NAD	C	705	44/44	0.95	0.12	0.25	11,15,22,26	0
2	NAD	B	703	44/44	0.96	0.10	0.20	11,13,24,26	0
3	OXQ	C	706	9/9	0.96	0.09	0.10	12,13,15,16	0
2	NAD	A	701	44/44	0.96	0.09	-0.29	9,13,25,31	0
2	NAD	D	707	44/44	0.96	0.10	-0.31	9,15,23,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.