



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:17 am GMT

PDB ID : 2CNB  
Title : TRYPANOSOMA BRUCEI UDP-GALACTOSE-4-EPIMERASE IN  
TERNARY COMPLEX WITH NAD AND THE SUBSTRATE ANALOGUE  
UDP-4-DEOXY-4-FLUORO-ALPHA-D-GALACTOSE  
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Deposited on : 2006-05-18  
Resolution : 2.70 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

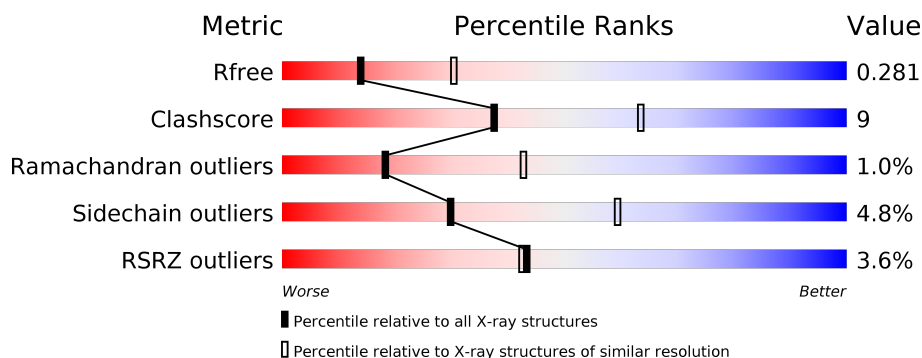
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	397	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	397	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	397	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	397	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>•</div> <div>8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UFG	A	1382	X	-	-	-
2	UFG	B	1382	X	-	-	-
2	UFG	C	1382	X	-	-	-
2	UFG	D	1382	X	-	-	-
3	NAD	A	1383	-	-	-	X
3	NAD	B	1383	-	-	-	X
3	NAD	C	1383	-	-	-	X
3	NAD	D	1383	-	-	-	X

## 2 Entry composition [i](#)

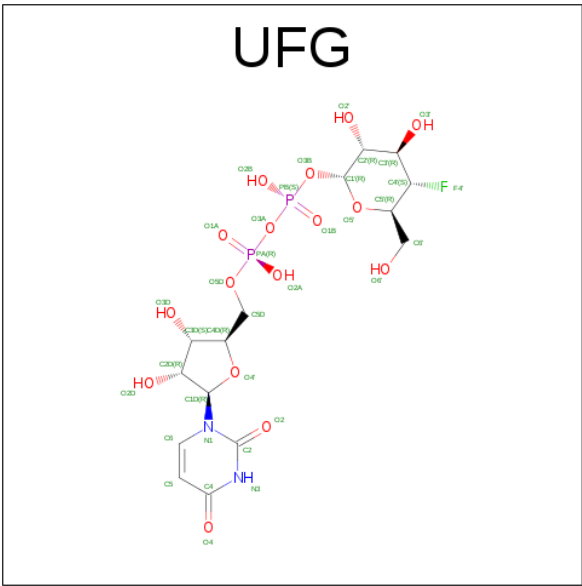
There are 4 unique types of molecules in this entry. The entry contains 12168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-GALACTOSE-4-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	3	0
			2863	1803	508	535	17			
1	B	363	Total	C	N	O	S	0	4	0
			2855	1800	512	527	16			
1	C	366	Total	C	N	O	S	0	3	0
			2863	1803	510	533	17			
1	D	364	Total	C	N	O	S	0	4	0
			2851	1796	506	533	16			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-4-DEOXY-4-FLUORO-ALPHA-D-GALACTOSE (three-letter code: UFG) (formula: C<sub>15</sub>H<sub>23</sub>FN<sub>2</sub>O<sub>16</sub>P<sub>2</sub>).



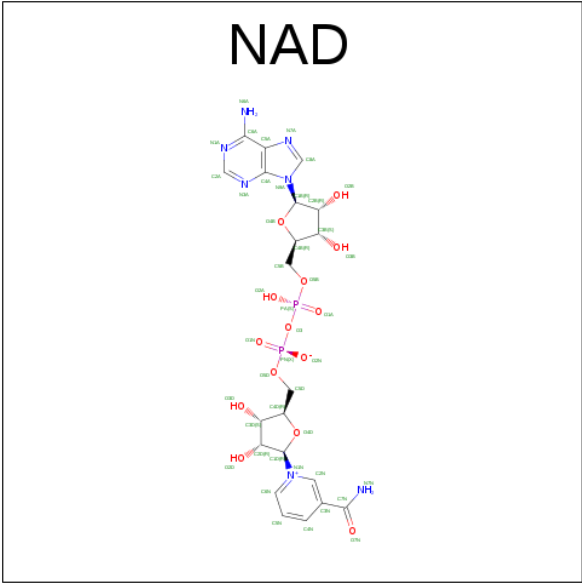
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0
			36	15	1	2	16	2	
2	B	1	Total	C	F	N	O	P	0
			36	15	1	2	16	2	

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	D	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	101	Total	O	0	0
			101	101		
4	C	118	Total	O	0	0
			118	118		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	94	Total	O	0	0
			94	94		

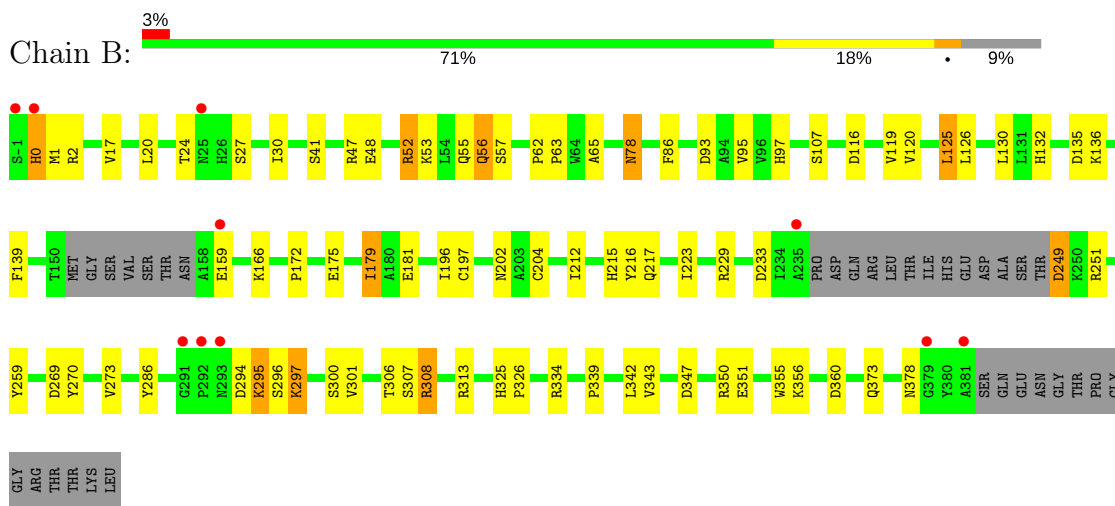
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

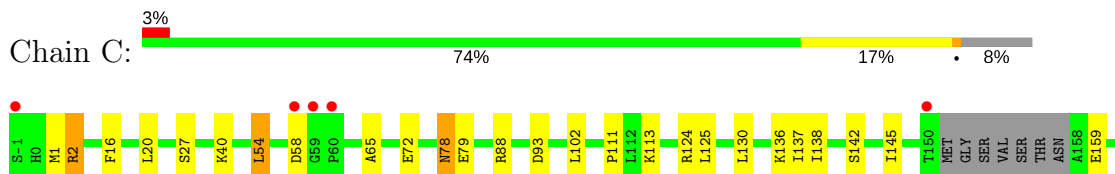
#### • Molecule 1: UDP-GALACTOSE-4-EPIMERASE

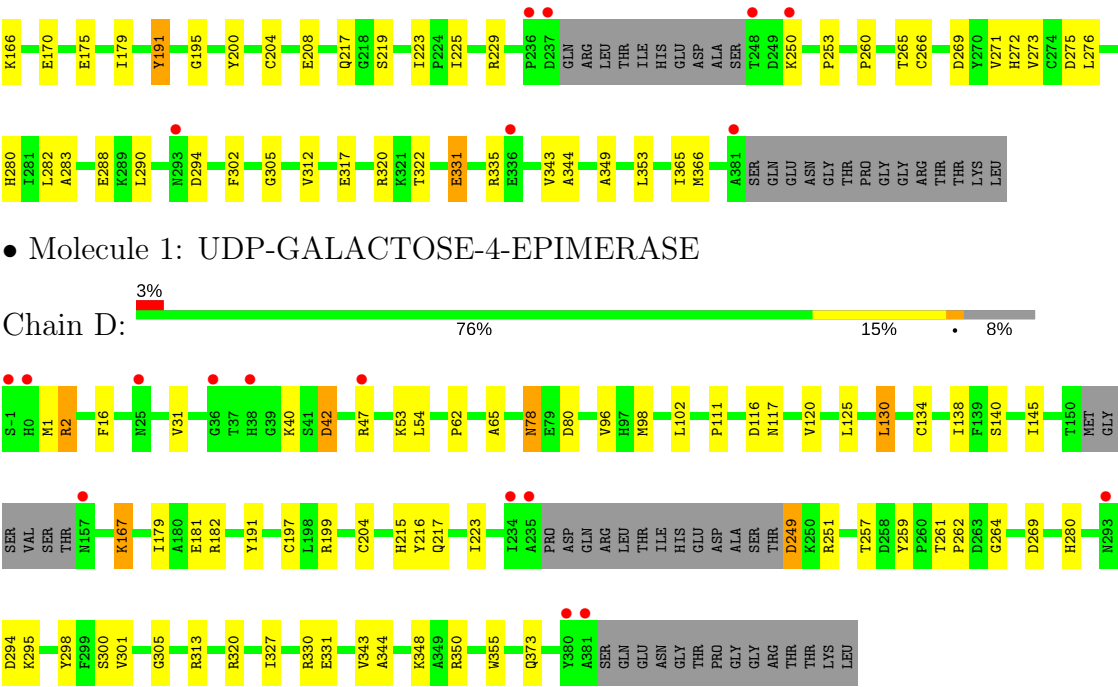


#### • Molecule 1: UDP-GALACTOSE-4-EPIMERASE



#### • Molecule 1: UDP-GALACTOSE-4-EPIMERASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.72Å 111.69Å 160.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.67 – 2.70 19.95 – 2.69	Depositor EDS
% Data completeness (in resolution range)	95.3 (91.67-2.70) 95.0 (19.95-2.69)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.199 , 0.281 0.203 , 0.281	Depositor DCC
$R_{free}$ test set	2454 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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 47.73 % 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 9.5215e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: NAD, UFG

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	0.59	0/2937	0.71	1/3978 (0.0%)
1	B	0.58	0/2929	0.69	0/3964
1	C	0.60	0/2937	0.69	0/3978
1	D	0.56	0/2926	0.66	0/3962
All	All	0.58	0/11729	0.69	1/15882 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	C-N-CA	5.14	134.56	121.70

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	2863	0	2815	54	0
1	B	2855	0	2821	56	0
1	C	2863	0	2821	48	0
1	D	2851	0	2808	45	0
2	A	36	0	21	4	0
2	B	36	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	36	0	21	5	0
2	D	36	0	21	2	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
3	C	44	0	26	1	0
3	D	44	0	26	2	0
4	A	103	0	0	6	0
4	B	101	0	0	10	0
4	C	118	0	0	8	0
4	D	94	0	0	5	0
All	All	12168	0	11453	205	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 9.

All (205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:PRO:HD2	1:B:65:ALA:HB2	1.44	0.98
1:C:159:GLU:HA	4:C:2048:HOH:O	1.67	0.94
2:D:1382:UFG:H4'	3:D:1383:NAD:C4N	2.00	0.92
1:B:308:ARG:HD2	4:B:2073:HOH:O	1.68	0.91
1:D:78:ASN:C	1:D:78:ASN:HD22	1.77	0.88
1:B:56[A]:GLN:HG3	4:B:2016:HOH:O	1.76	0.84
1:C:271:VAL:HG22	4:C:2087:HOH:O	1.77	0.84
1:B:295:LYS:O	1:B:297:LYS:N	2.14	0.80
1:A:4:LEU:HD11	1:A:31:VAL:HG12	1.64	0.79
1:C:204[B]:CYS:SG	1:C:365:ILE:HG21	2.23	0.78
1:C:204[A]:CYS:SG	1:C:223:ILE:HD12	2.24	0.78
1:A:46:THR:OG1	1:A:49:ASN:HB2	1.84	0.78
1:A:306:THR:O	1:A:307:SER:HB2	1.84	0.75
1:D:116:ASP:O	1:D:120:VAL:HB	1.88	0.73
2:A:1382:UFG:H4'	3:A:1383:NAD:C4N	2.18	0.73
1:A:47:ARG:CA	1:A:48:GLU:HB2	2.19	0.72
2:B:1382:UFG:H4'	3:B:1383:NAD:C4N	2.19	0.71
1:C:335:ARG:HH22	2:C:1382:UFG:C2D	2.03	0.71
1:A:72:GLU:OE1	1:A:88:ARG:NH2	2.23	0.71
1:A:202:ASN:OD1	1:A:268:ARG:HB3	1.91	0.70
1:B:86:PHE:HB3	1:B:132:HIS:ND1	2.07	0.70
1:A:263:ASP:OD1	1:A:265:THR:OG1	2.12	0.68
1:B:53:LYS:O	1:B:57:SER:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASN:HD22	1:B:78:ASN:C	1.97	0.67
1:B:1:MET:HG3	1:B:93:ASP:HB2	1.79	0.65
1:D:295:LYS:HA	1:D:298:TYR:CD1	2.32	0.64
1:A:47:ARG:HB3	1:A:48:GLU:HB2	1.78	0.63
1:A:172:PRO:HD3	4:A:2050:HOH:O	1.98	0.63
1:D:305:GLY:HA3	1:D:344:ALA:HB3	1.80	0.63
1:B:313:ARG:HH11	1:B:313:ARG:HG3	1.63	0.62
2:D:1382:UFG:H4'	3:D:1383:NAD:H4N	1.79	0.62
1:B:196:ILE:HD11	1:B:286:TYR:HD2	1.64	0.62
1:A:47:ARG:CB	1:A:48:GLU:HB2	2.30	0.61
1:A:78:ASN:C	1:A:78:ASN:HD22	2.04	0.61
1:A:204[B]:CYS:SG	1:A:270:TYR:HB3	2.41	0.60
1:B:197:CYS:HB2	1:B:301:VAL:HG12	1.83	0.60
1:B:249:ASP:HB3	1:B:251:ARG:HB2	1.84	0.60
1:B:48:GLU:O	1:B:52[B]:ARG:HD2	2.02	0.60
1:A:4:LEU:HD11	1:A:31:VAL:CG1	2.32	0.60
1:B:119:VAL:HG13	1:B:179:ILE:HD11	1.84	0.59
1:B:175:GLU:O	1:B:179:ILE:HG23	2.02	0.59
1:D:96:VAL:HG22	1:D:138:ILE:HB	1.84	0.58
1:B:360:ASP:HB3	4:B:2091:HOH:O	2.03	0.58
1:C:335:ARG:HH22	2:C:1382:UFG:H2D	1.66	0.58
1:B:95:VAL:HG11	1:B:125:LEU:CD1	2.33	0.58
1:B:259:TYR:CZ	1:B:334:ARG:HG2	2.38	0.58
1:B:17:VAL:HG21	1:B:30:ILE:HD11	1.85	0.58
1:D:16:PHE:CE1	1:D:280:HIS:CB	2.86	0.58
1:B:308:ARG:NH2	4:B:2074:HOH:O	2.37	0.57
1:D:313:ARG:NH2	1:D:331:GLU:OE2	2.37	0.57
1:C:2:ARG:HD3	1:C:27:SER:HB2	1.86	0.57
1:D:215:HIS:CD2	1:D:217[A]:GLN:H	2.23	0.57
1:D:215:HIS:CD2	1:D:217[B]:GLN:H	2.22	0.57
1:D:78:ASN:C	1:D:78:ASN:ND2	2.51	0.57
1:D:2:ARG:HH11	1:D:2:ARG:HB2	1.70	0.56
1:D:269:ASP:HB2	1:D:343:VAL:HA	1.87	0.56
1:B:107:SER:O	1:B:172:PRO:HG2	2.06	0.56
2:C:1382:UFG:H4'	3:C:1383:NAD:C4N	2.34	0.55
1:B:95:VAL:HG11	1:B:125:LEU:HD12	1.88	0.55
1:D:204:CYS:SG	1:D:223:ILE:HD13	2.46	0.55
1:A:297:LYS:HE2	4:A:2075:HOH:O	2.05	0.55
1:C:79:GLU:HB2	4:C:2040:HOH:O	2.07	0.55
1:D:249:ASP:HB3	1:D:251:ARG:HG3	1.88	0.55
1:A:294:ASP:HB2	1:A:295:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:SER:O	1:C:225:ILE:HD11	2.08	0.54
1:A:47:ARG:N	1:A:48:GLU:HB2	2.23	0.54
1:D:117:ASN:HB2	4:D:2025:HOH:O	2.08	0.54
1:C:111:PRO:HD2	1:D:191:TYR:CZ	2.43	0.53
1:D:320:ARG:HG3	1:D:327:ILE:HD12	1.90	0.53
1:C:113:LYS:HE3	4:C:2038:HOH:O	2.07	0.53
1:D:53:LYS:HB2	4:D:2008:HOH:O	2.06	0.53
1:B:216:TYR:H	1:B:373:GLN:HE22	1.57	0.53
1:C:272:HIS:O	4:C:2087:HOH:O	2.19	0.53
1:D:16:PHE:CE1	1:D:280:HIS:HB2	2.44	0.53
1:D:42:ASP:OD2	1:D:42:ASP:N	2.41	0.53
1:D:16:PHE:CE1	1:D:280:HIS:HB3	2.44	0.53
1:B:181:GLU:HG2	1:B:197:CYS:SG	2.49	0.52
1:B:2:ARG:HG3	1:B:27:SER:HB2	1.91	0.52
1:B:52[A]:ARG:HD2	4:B:2011:HOH:O	2.09	0.52
1:C:72:GLU:OE1	1:C:88:ARG:NH2	2.42	0.52
1:C:335:ARG:NH2	2:C:1382:UFG:O2D	2.40	0.52
1:D:261:THR:O	1:D:262:PRO:C	2.46	0.52
1:B:325:HIS:CG	1:B:326:PRO:HD2	2.44	0.52
1:C:269:ASP:HB2	1:C:343:VAL:HA	1.91	0.52
1:D:145:ILE:HD12	1:D:167:LYS:HD2	1.91	0.52
1:D:62:PRO:HD2	1:D:65:ALA:HB2	1.90	0.52
1:D:98:MET:HA	1:D:140:SER:OG	2.09	0.51
1:B:350:ARG:HG2	1:B:355:TRP:O	2.10	0.51
1:D:98:MET:HA	1:D:140:SER:HG	1.76	0.51
1:B:97:HIS:HD2	1:B:139:PHE:CE1	2.29	0.51
1:A:56:GLN:O	1:A:57:SER:HB3	2.10	0.51
1:C:276:LEU:HG	4:C:2087:HOH:O	2.10	0.51
1:A:232:SER:HB2	4:A:2065:HOH:O	2.10	0.51
1:A:119:VAL:O	1:A:122:ILE:HG22	2.10	0.50
1:D:78:ASN:HD21	1:D:80:ASP:HB2	1.76	0.50
1:B:269:ASP:HB2	1:B:343:VAL:HA	1.92	0.50
1:D:80:ASP:HA	4:D:2015:HOH:O	2.11	0.50
1:B:119:VAL:CG1	1:B:179:ILE:HD11	2.42	0.50
1:C:2:ARG:HB2	1:C:2:ARG:HH11	1.77	0.50
1:B:20:LEU:O	1:B:24:THR:OG1	2.29	0.50
1:B:229:ARG:NH1	4:B:2061:HOH:O	2.43	0.49
1:A:72:GLU:CD	1:A:88:ARG:NH2	2.65	0.49
1:B:313:ARG:NH1	1:B:313:ARG:HG3	2.26	0.49
1:C:142:SER:O	1:C:145:ILE:HG23	2.12	0.49
1:A:204[A]:CYS:SG	1:A:223:ILE:HD13	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASN:HD22	1:C:78:ASN:C	2.16	0.49
1:B:308:ARG:CD	4:B:2073:HOH:O	2.43	0.49
1:A:202:ASN:ND2	2:A:1382:UFG:H3'	2.27	0.48
1:A:150:THR:HG22	4:A:2042:HOH:O	2.13	0.48
1:B:97:HIS:HD2	1:B:139:PHE:HE1	1.61	0.48
2:A:1382:UFG:H4'	3:A:1383:NAD:H4N	1.93	0.48
1:B:116:ASP:O	1:B:120:VAL:HB	2.14	0.48
1:B:78:ASN:ND2	1:B:78:ASN:C	2.65	0.48
1:A:112:LEU:HD12	1:B:130:LEU:HD22	1.96	0.47
1:C:138:ILE:HD12	1:C:283:ALA:HB1	1.95	0.47
1:D:47:ARG:HB3	4:D:2007:HOH:O	2.13	0.47
1:A:226:ILE:O	1:A:229:ARG:N	2.47	0.47
1:B:0[B]:HIS:HE1	4:B:2005:HOH:O	1.96	0.47
1:A:130:LEU:HA	1:A:130:LEU:HD12	1.69	0.47
1:C:170:GLU:HG3	1:C:170:GLU:O	2.14	0.47
1:B:249:ASP:OD2	1:B:251:ARG:NH2	2.42	0.47
1:B:306:THR:O	1:B:307:SER:HB2	2.15	0.47
1:D:249:ASP:OD2	1:D:251:ARG:NE	2.42	0.47
1:D:216:TYR:H	1:D:373:GLN:HE22	1.63	0.47
1:D:181:GLU:HG2	1:D:197:CYS:SG	2.54	0.47
1:A:105:GLY:HA3	1:A:335:ARG:HD3	1.96	0.46
1:B:86:PHE:HB3	1:B:132:HIS:CE1	2.50	0.46
1:C:179:ILE:HG12	1:D:179:ILE:HG12	1.98	0.46
1:A:269:ASP:HB2	1:A:343:VAL:HA	1.98	0.46
1:D:350:ARG:HA	1:D:355:TRP:H	1.81	0.46
1:C:200:TYR:OH	1:C:280:HIS:NE2	2.46	0.46
1:A:145:ILE:HD12	1:A:167:LYS:HD2	1.98	0.46
1:C:282:LEU:HD13	1:C:353:LEU:O	2.16	0.46
1:A:216:TYR:H	1:A:373:GLN:HE22	1.64	0.45
1:A:202:ASN:HD22	2:A:1382:UFG:H3'	1.80	0.45
1:D:167:LYS:HE3	1:D:199:ARG:HH22	1.82	0.45
1:B:294:ASP:O	1:B:295:LYS:HB3	2.16	0.45
1:A:159:GLU:HB2	1:A:160:PRO:CD	2.47	0.45
1:C:317:GLU:OE1	1:C:320:ARG:NH1	2.49	0.45
1:B:204:CYS:SG	1:B:223:ILE:HD13	2.57	0.45
1:A:216:TYR:CD2	1:A:228:GLY:HA2	2.52	0.45
1:B:339:PRO:HG2	1:B:342:LEU:HD11	1.98	0.45
1:C:124:ARG:HD3	4:C:2041:HOH:O	2.16	0.44
1:C:191:TYR:CZ	1:D:111:PRO:HD2	2.53	0.44
1:A:163:ILE:HB	1:A:301:VAL:HG23	2.00	0.44
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LEU:HD22	1:C:294:ASP:HB3	1.98	0.44
1:A:201:PHE:HB3	4:A:2056:HOH:O	2.18	0.44
1:D:96:VAL:HG12	1:D:98:MET:HG3	1.99	0.44
1:A:32:ASP:O	1:A:73:VAL:HA	2.18	0.44
1:B:196:ILE:HD11	1:B:286:TYR:CD2	2.49	0.44
1:B:215:HIS:CD2	1:B:217:GLN:H	2.36	0.43
1:A:215:HIS:HA	1:A:373:GLN:HE22	1.84	0.43
1:C:200:TYR:OH	1:C:280:HIS:CE1	2.71	0.43
1:A:201:PHE:CE1	1:A:344:ALA:HB2	2.53	0.43
1:A:253:PRO:HA	1:A:330:ARG:O	2.18	0.43
1:A:78:ASN:HD22	1:A:80:ASP:H	1.67	0.43
1:C:16:PHE:CZ	1:C:20:LEU:HD11	2.53	0.43
1:B:378:ASN:HB3	4:B:2096:HOH:O	2.18	0.43
1:A:251:ARG:HG2	1:A:328:PRO:HB2	2.01	0.43
1:C:266:CYS:HB2	2:C:1382:UFG:O3D	2.18	0.43
1:B:347:ASP:O	1:B:351:GLU:HG3	2.19	0.42
1:C:166:LYS:HB3	1:C:166:LYS:HE2	1.79	0.42
1:A:200:TYR:OH	1:A:280:HIS:NE2	2.50	0.42
1:C:54:LEU:HD11	1:C:65:ALA:HB1	2.00	0.42
1:D:182:ARG:HG3	1:D:182:ARG:HH11	1.84	0.42
1:A:32:ASP:OD1	1:A:33:SER:N	2.51	0.42
1:A:177:LYS:HA	1:A:177:LYS:HD3	1.88	0.42
1:D:182:ARG:HG3	1:D:182:ARG:NH1	2.34	0.42
1:A:197:CYS:HB2	1:A:301:VAL:HG12	2.02	0.42
1:C:229:ARG:HH21	1:C:253:PRO:HD3	1.84	0.42
1:D:216:TYR:N	1:D:373:GLN:HE22	2.17	0.42
1:C:265:THR:HB	1:C:312:VAL:HB	2.02	0.42
1:D:130:LEU:HD12	1:D:130:LEU:HA	1.93	0.42
1:C:331:GLU:HG2	1:C:331:GLU:H	1.70	0.42
1:C:302:PHE:HB3	1:C:349:ALA:HB2	2.01	0.42
1:A:123:LEU:HB2	1:A:183:MET:HE3	2.01	0.42
1:A:56:GLN:O	1:A:57:SER:CB	2.67	0.42
1:A:294:ASP:CB	1:A:295:LYS:HA	2.49	0.41
1:A:306:THR:O	1:A:307:SER:CB	2.59	0.41
1:A:78:ASN:ND2	1:A:81:PHE:H	2.18	0.41
1:B:93:ASP:O	1:B:136:LYS:HE2	2.20	0.41
1:C:250:LYS:HA	1:C:250:LYS:HE2	2.03	0.41
1:A:83:ASN:OD1	1:A:132:HIS:NE2	2.52	0.41
1:C:322:THR:HG21	1:C:366:MET:HG3	2.01	0.41
2:B:1382:UFG:H4'	3:B:1383:NAD:H4N	2.00	0.41
1:C:130:LEU:HD12	1:C:130:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ILE:O	1:C:195:GLY:HA2	2.20	0.41
1:C:111:PRO:HD2	1:D:191:TYR:OH	2.20	0.41
1:A:141:SER:OG	1:A:142:SER:N	2.53	0.41
1:B:202:ASN:O	1:B:270:TYR:HA	2.20	0.41
1:B:95:VAL:HG11	1:B:125:LEU:HD11	2.03	0.41
1:C:208:GLU:H	1:C:208:GLU:CD	2.24	0.41
1:B:27:SER:HB3	4:B:2002:HOH:O	2.20	0.41
1:C:305:GLY:HA3	1:C:344:ALA:HB3	2.01	0.41
1:C:175:GLU:HG2	4:D:2041:HOH:O	2.21	0.40
1:D:259:TYR:O	1:D:264:GLY:HA2	2.20	0.40
1:B:1:MET:HG3	1:B:93:ASP:CB	2.49	0.40
1:D:197:CYS:HB2	1:D:301:VAL:HG12	2.03	0.40
1:D:251:ARG:HH21	1:D:330:ARG:HD3	1.86	0.40
1:A:18:ARG:HD2	1:A:207:HIS:CD2	2.57	0.40
1:A:66:ASP:HB2	4:A:2016:HOH:O	2.21	0.40
1:C:93:ASP:O	1:C:136:LYS:HE2	2.21	0.40
1:C:275:ASP:HB2	4:C:2087:HOH:O	2.21	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	363/397 (91%)	330 (91%)	25 (7%)	8 (2%)	8	20
1	B	361/397 (91%)	337 (93%)	19 (5%)	5 (1%)	13	33
1	C	363/397 (91%)	338 (93%)	23 (6%)	2 (1%)	28	56
1	D	362/397 (91%)	329 (91%)	32 (9%)	1 (0%)	44	73
All	All	1449/1588 (91%)	1334 (92%)	99 (7%)	16 (1%)	18	40

All (16) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	B	0[A]	HIS
1	B	0[B]	HIS
1	B	295	LYS
1	B	296	SER
1	D	1	MET
1	A	48	GLU
1	A	55	GLN
1	A	57	SER
1	A	334	ARG
1	A	49	ASN
1	A	56	GLN
1	A	236	PRO
1	A	294	ASP
1	C	273	VAL
1	B	63	PRO
1	C	260	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	308/331 (93%)	297 (96%)	11 (4%)	40	70
1	B	306/331 (92%)	285 (93%)	21 (7%)	18	41
1	C	308/331 (93%)	296 (96%)	12 (4%)	37	68
1	D	306/331 (92%)	290 (95%)	16 (5%)	27	55
All	All	1228/1324 (93%)	1168 (95%)	60 (5%)	30	58

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	125	LEU
1	A	130	LEU
1	A	131	LEU
1	A	135	ASP
1	A	168	SER

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Mol	Chain	Res	Type
1	A	288	GLU
1	A	293	ASN
1	A	335	ARG
1	A	358	LYS
1	A	360	ASP
1	B	41	SER
1	B	47	ARG
1	B	52[A]	ARG
1	B	52[B]	ARG
1	B	55	GLN
1	B	56[A]	GLN
1	B	56[B]	GLN
1	B	78	ASN
1	B	125	LEU
1	B	135	ASP
1	B	159	GLU
1	B	166	LYS
1	B	179	ILE
1	B	212	ILE
1	B	233	ASP
1	B	249	ASP
1	B	273	VAL
1	B	297	LYS
1	B	300	SER
1	B	308	ARG
1	B	356	LYS
1	C	1	MET
1	C	2	ARG
1	C	40	LYS
1	C	54	LEU
1	C	58	ASP
1	C	78	ASN
1	C	102	LEU
1	C	125	LEU
1	C	191	TYR
1	C	217	GLN
1	C	288	GLU
1	C	331	GLU
1	D	2	ARG
1	D	31	VAL
1	D	40	LYS
1	D	42	ASP

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Mol	Chain	Res	Type
1	D	54	LEU
1	D	78	ASN
1	D	102	LEU
1	D	125	LEU
1	D	130	LEU
1	D	134	CYS
1	D	167	LYS
1	D	249	ASP
1	D	257	THR
1	D	294	ASP
1	D	300	SER
1	D	348	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	373	GLN
1	B	49	ASN
1	B	55	GLN
1	B	78	ASN
1	B	97	HIS
1	B	373	GLN
1	C	49	ASN
1	C	78	ASN
1	C	373	GLN
1	D	49	ASN
1	D	78	ASN
1	D	97	HIS
1	D	373	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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	UFG	A	1382	-	31,38,38	1.84	3 (9%)	36,58,58	1.96	5 (13%)
3	NAD	A	1383	-	41,48,48	1.68	4 (9%)	43,73,73	1.85	3 (6%)
2	UFG	B	1382	-	31,38,38	1.21	3 (9%)	36,58,58	1.69	4 (11%)
3	NAD	B	1383	-	41,48,48	1.65	2 (4%)	43,73,73	2.08	5 (11%)
2	UFG	C	1382	-	31,38,38	1.51	5 (16%)	36,58,58	1.45	3 (8%)
3	NAD	C	1383	-	41,48,48	1.69	3 (7%)	43,73,73	2.08	8 (18%)
2	UFG	D	1382	-	31,38,38	1.29	3 (9%)	36,58,58	1.73	4 (11%)
3	NAD	D	1383	-	41,48,48	1.65	3 (7%)	43,73,73	1.84	3 (6%)

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	UFG	A	1382	-	1/1/11/11	0/19/59/59	0/3/3/3
3	NAD	A	1383	-	-	0/22/62/62	0/5/5/5
2	UFG	B	1382	-	1/1/11/11	0/19/59/59	0/3/3/3
3	NAD	B	1383	-	-	0/22/62/62	0/5/5/5
2	UFG	C	1382	-	1/1/11/11	0/19/59/59	0/3/3/3
3	NAD	C	1383	-	-	0/22/62/62	0/5/5/5
2	UFG	D	1382	-	1/1/11/11	0/19/59/59	0/3/3/3
3	NAD	D	1383	-	-	0/22/62/62	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1383	NAD	O4B-C4B	-2.14	1.40	1.45
2	C	1382	UFG	C4'-C5'	2.08	1.54	1.52
3	C	1383	NAD	C2A-N1A	2.40	1.38	1.33
2	B	1382	UFG	C4'-C3'	2.42	1.54	1.52
3	D	1383	NAD	C2A-N1A	2.59	1.38	1.33
3	A	1383	NAD	C2A-N1A	2.70	1.39	1.33
2	B	1382	UFG	C6-N1	2.87	1.39	1.35
2	D	1382	UFG	C6-N1	2.88	1.39	1.35
2	C	1382	UFG	C4'-C3'	2.90	1.54	1.52
2	C	1382	UFG	O4'-C1D	3.16	1.45	1.41
3	D	1383	NAD	C2A-N3A	3.18	1.37	1.32
2	D	1382	UFG	O4'-C1D	3.19	1.45	1.41
3	B	1383	NAD	C2A-N3A	3.35	1.37	1.32
3	C	1383	NAD	C2A-N3A	3.58	1.38	1.32
3	A	1383	NAD	C2A-N3A	3.66	1.38	1.32
2	C	1382	UFG	C6-N1	3.78	1.40	1.35
2	D	1382	UFG	C4-N3	3.88	1.40	1.33
2	B	1382	UFG	C4-N3	3.89	1.40	1.33
2	A	1382	UFG	C4-N3	4.28	1.40	1.33
2	C	1382	UFG	C4-N3	4.37	1.41	1.33
2	A	1382	UFG	O4'-C1D	4.93	1.48	1.41
2	A	1382	UFG	C6-N1	5.48	1.43	1.35
3	A	1383	NAD	O7N-C7N	8.13	1.40	1.24
3	C	1383	NAD	O7N-C7N	8.15	1.41	1.24
3	D	1383	NAD	O7N-C7N	8.34	1.41	1.24
3	B	1383	NAD	O7N-C7N	8.48	1.41	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1383	NAD	N3A-C2A-N1A	-10.47	119.74	128.86
3	C	1383	NAD	N3A-C2A-N1A	-10.46	119.75	128.86
3	D	1383	NAD	N3A-C2A-N1A	-10.12	120.05	128.86
3	A	1383	NAD	N3A-C2A-N1A	-9.85	120.28	128.86
2	A	1382	UFG	O5'-C1'-O3B	-6.02	103.50	111.36
2	D	1382	UFG	O5'-C1'-O3B	-5.53	104.13	111.36
2	B	1382	UFG	O5'-C1'-O3B	-4.97	104.87	111.36
2	D	1382	UFG	O3A-PB-O3B	-3.82	95.22	102.05
3	B	1383	NAD	O3B-C3B-C4B	-3.78	100.03	111.09
3	C	1383	NAD	O3D-C3D-C4D	-3.77	100.08	111.09
3	D	1383	NAD	O3D-C3D-C4D	-3.20	101.73	111.09
3	C	1383	NAD	O7N-C7N-C3N	-2.99	116.13	119.62
3	A	1383	NAD	O3D-C3D-C4D	-2.85	102.75	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1382	UFG	O3A-PB-O3B	-2.58	97.44	102.05
3	B	1383	NAD	C4A-C5A-N7A	-2.55	106.95	109.41
2	C	1382	UFG	O5'-C1'-O3B	-2.44	108.17	111.36
3	A	1383	NAD	C1B-N9A-C4A	-2.40	122.49	126.64
2	B	1382	UFG	C1'-O5'-C5'	-2.11	109.75	113.72
2	B	1382	UFG	O3'-C3'-C2'	-2.09	105.80	110.36
2	A	1382	UFG	C4D-O4'-C1D	-2.00	107.64	109.77
3	D	1383	NAD	C4D-O4D-C1D	2.09	111.99	109.77
3	C	1383	NAD	C2D-C3D-C4D	2.10	106.70	102.62
3	C	1383	NAD	C2N-C3N-C4N	2.16	120.72	118.26
3	C	1383	NAD	C3N-C7N-N7N	2.18	120.27	117.77
2	D	1382	UFG	O5'-C5'-C6'	2.27	111.85	106.41
3	C	1383	NAD	C2B-C3B-C4B	2.32	107.14	102.62
2	A	1382	UFG	O5'-C1'-C2'	2.40	114.93	110.30
3	C	1383	NAD	C4D-O4D-C1D	2.67	112.61	109.77
3	B	1383	NAD	C4D-O4D-C1D	2.71	112.66	109.77
3	B	1383	NAD	C3N-C7N-N7N	3.35	121.59	117.77
2	C	1382	UFG	F4'-C4'-C3'	4.41	111.72	108.49
2	D	1382	UFG	C4-N3-C2	5.61	118.95	114.13
2	C	1382	UFG	C4-N3-C2	5.69	119.02	114.13
2	B	1382	UFG	C4-N3-C2	6.95	120.10	114.13
2	A	1382	UFG	C4-N3-C2	7.93	120.94	114.13

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1382	UFG	C4'
2	B	1382	UFG	C4'
2	C	1382	UFG	C4'
2	D	1382	UFG	C4'

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1382	UFG	4	0
3	A	1383	NAD	2	0
2	B	1382	UFG	2	0
3	B	1383	NAD	2	0
2	C	1382	UFG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1383	NAD	1	0
2	D	1382	UFG	2	0
3	D	1383	NAD	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	366/397 (92%)	-0.11	18 (4%) 30 29	28, 44, 70, 91	1 (0%)
1	B	363/397 (91%)	-0.04	10 (2%) 53 54	32, 49, 68, 81	0
1	C	366/397 (92%)	-0.10	12 (3%) 47 46	29, 43, 67, 79	0
1	D	364/397 (91%)	-0.07	12 (3%) 47 46	33, 49, 66, 78	0
All	All	1459/1588 (91%)	-0.08	52 (3%) 43 42	28, 47, 68, 91	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	381	ALA	5.7
1	D	157	ASN	5.4
1	D	381	ALA	5.3
1	C	236	PRO	5.0
1	B	0[A]	HIS	5.0
1	C	237	ASP	4.9
1	B	293	ASN	4.8
1	B	381	ALA	4.7
1	A	150	THR	4.6
1	A	60	PRO	4.5
1	A	59	GLY	4.5
1	A	381	ALA	4.4
1	C	60	PRO	4.4
1	B	-1	SER	4.4
1	B	292	PRO	4.1
1	C	150	THR	3.9
1	C	248	THR	3.8
1	A	236	PRO	3.8
1	A	249	ASP	3.5
1	A	157	ASN	3.5
1	C	59	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	293	ASN	3.4
1	A	237	ASP	3.3
1	B	235	ALA	3.3
1	D	234	ILE	3.2
1	B	25	ASN	2.8
1	C	-1	SER	2.8
1	C	336	GLU	2.8
1	A	57	SER	2.7
1	C	250	LYS	2.7
1	A	55	GLN	2.7
1	D	380	TYR	2.6
1	D	-1	SER	2.6
1	A	250	LYS	2.6
1	A	52	ARG	2.6
1	D	38	HIS	2.5
1	B	291	GLY	2.5
1	B	379	GLY	2.4
1	A	-1	SER	2.3
1	D	25	ASN	2.3
1	D	0	HIS	2.2
1	A	260	PRO	2.2
1	C	293	ASN	2.1
1	C	58	ASP	2.1
1	A	47	ARG	2.1
1	D	235	ALA	2.1
1	D	36	GLY	2.1
1	A	293	ASN	2.1
1	A	330	ARG	2.1
1	A	56	GLN	2.0
1	B	159	GLU	2.0
1	D	47	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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(Å <sup>2</sup> )	Q<0.9
3	NAD	C	1383	44/44	0.88	0.25	4.66	23,33,37,38	18
3	NAD	A	1383	44/44	0.88	0.23	3.82	29,38,41,43	18
3	NAD	D	1383	44/44	0.85	0.29	3.39	38,44,49,50	18
3	NAD	B	1383	44/44	0.89	0.25	3.03	37,41,44,45	18
2	UFG	C	1382	36/36	0.96	0.16	0.16	46,52,55,56	0
2	UFG	B	1382	36/36	0.97	0.12	-0.45	31,34,37,39	0
2	UFG	A	1382	36/36	0.95	0.14	-0.59	43,47,50,50	0
2	UFG	D	1382	36/36	0.97	0.12	-0.86	33,37,41,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.