



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:42 PM GMT

PDB ID : 3RUA
Title : Specific recognition of N-acetylated substrates and domain flexibility in WbgU:
a UDP-GalNAc 4-epimerase
Authors : Bhatt, V.S.; Guan, W.; Wang, P.G.
Deposited on : 2011-05-04
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

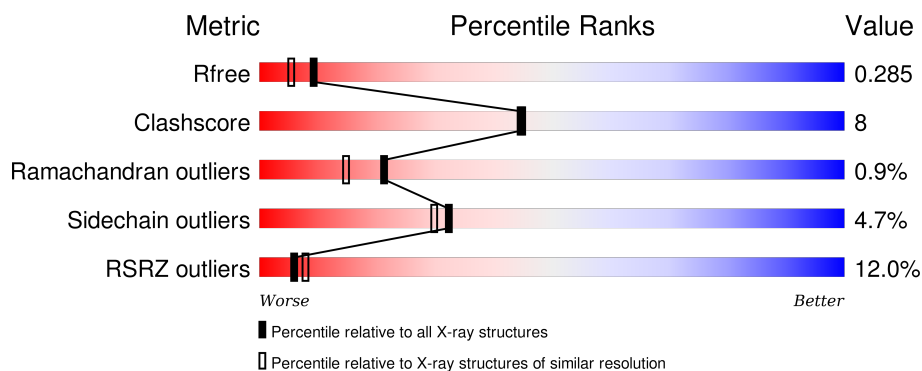
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	351	<div> <div>18%</div> <div>77%</div> <div>15%</div> <div>..</div> </div>
1	B	351	<div> <div>20%</div> <div>77%</div> <div>15%</div> <div>..</div> </div>
1	C	351	<div> <div>7%</div> <div>79%</div> <div>14%</div> <div>..</div> </div>
1	D	351	<div> <div>%</div> <div>81%</div> <div>12%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11365 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 WbgU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			
1	B	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			
1	C	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			
1	D	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			

There are 24 discrepancies between the modelled and reference sequences:

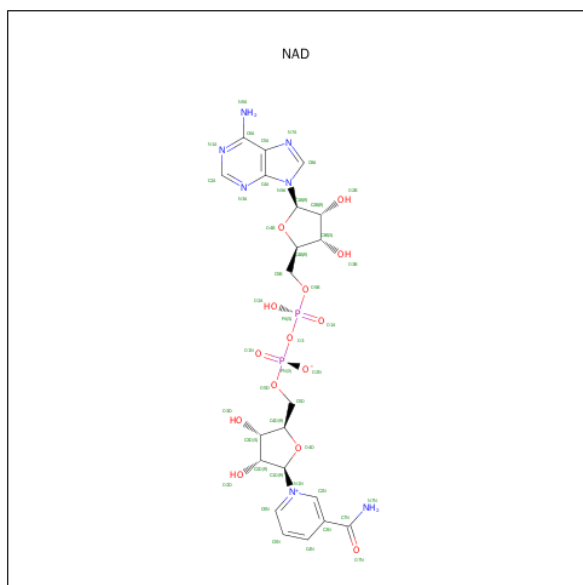
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
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 UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

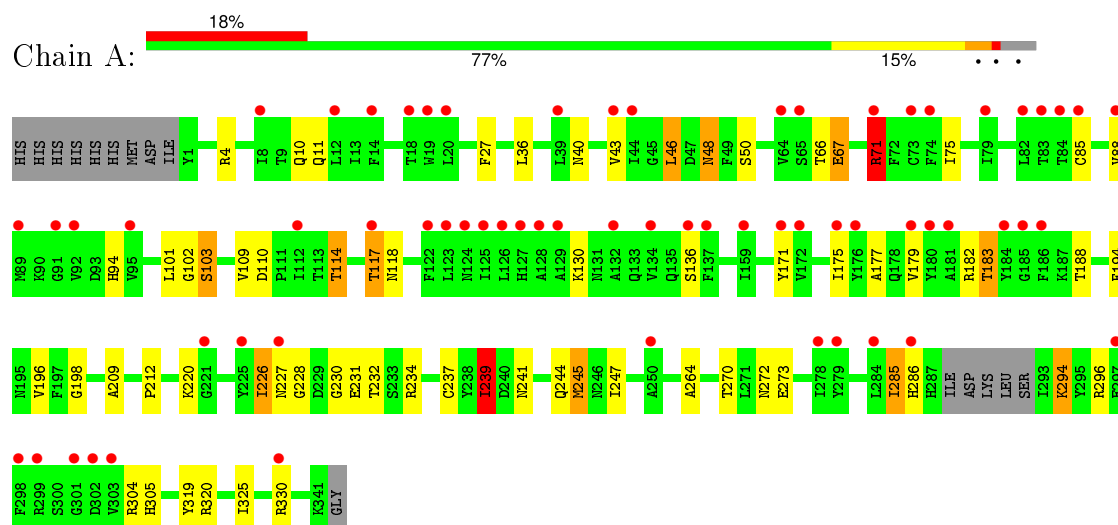
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	72	Total	O	0	0
			72	72		
5	C	106	Total	O	0	0
			106	106		
5	D	58	Total	O	0	0
			58	58		

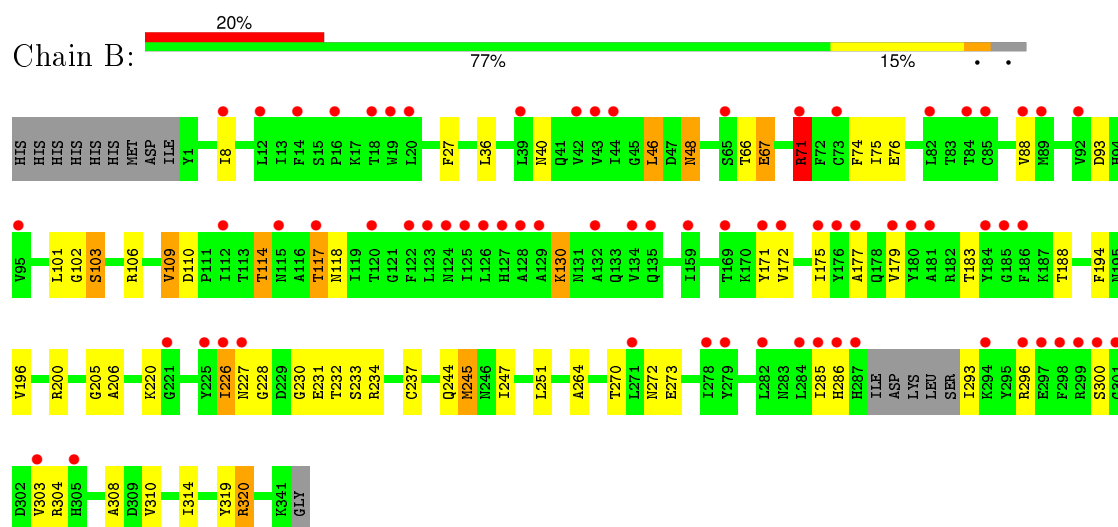
3 Residue-property plots [i](#)

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.

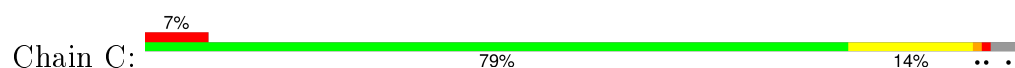
• Molecule 1: WbgU

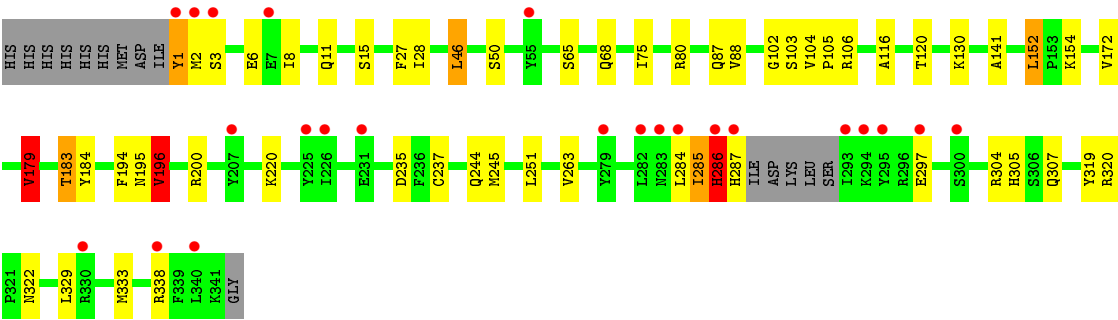


• Molecule 1: WbgU

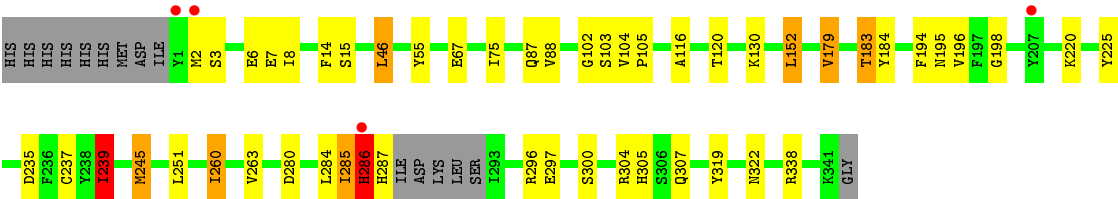
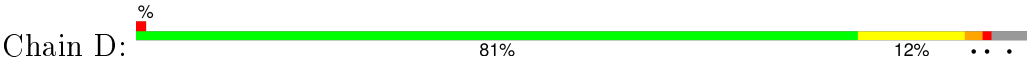


• Molecule 1: WbgU





• Molecule 1: WbgU



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	77.44Å 77.44Å 224.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 49.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.10) 99.8 (49.92-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.180 , 0.234 0.257 , 0.285	Depositor DCC
R_{free} test set	4402 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.5	EDS
Estimated twinning fraction	0.016 for -h,-k,l 0.477 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 87751 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11365	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.09	5/2739 (0.2%)	0.92	8/3717 (0.2%)
1	B	1.07	4/2739 (0.1%)	0.99	10/3717 (0.3%)
1	C	1.00	2/2739 (0.1%)	0.90	6/3717 (0.2%)
1	D	0.99	3/2739 (0.1%)	0.87	6/3717 (0.2%)
All	All	1.04	14/10956 (0.1%)	0.92	30/14868 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	THR	CB-CG2	-7.01	1.29	1.52
1	C	196	VAL	CB-CG2	-5.81	1.40	1.52
1	D	55	TYR	CD1-CE1	5.81	1.48	1.39
1	A	43	VAL	CB-CG2	5.59	1.64	1.52
1	D	55	TYR	CD2-CE2	5.58	1.47	1.39
1	B	71	ARG	CG-CD	-5.47	1.38	1.51
1	B	74	PHE	CE2-CZ	5.40	1.47	1.37
1	B	117	THR	CB-CG2	-5.38	1.34	1.52
1	C	179	VAL	CB-CG1	-5.27	1.41	1.52
1	A	27	PHE	CE2-CZ	5.23	1.47	1.37
1	A	85	CYS	CB-SG	5.16	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	VAL	CB-CG2	5.09	1.63	1.52
1	A	182	ARG	CG-CD	5.03	1.64	1.51
1	D	179	VAL	CB-CG1	-5.01	1.42	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	ARG	NE-CZ-NH2	-17.95	111.32	120.30
1	C	200	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	B	200	ARG	NE-CZ-NH1	12.67	126.63	120.30
1	A	239	ILE	CG1-CB-CG2	9.58	132.47	111.40
1	C	200	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	B	71	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	245	MET	CG-SD-CE	-7.87	87.61	100.20
1	B	245	MET	CG-SD-CE	-7.67	87.92	100.20
1	D	239	ILE	CB-CA-C	-7.53	96.54	111.60
1	D	245	MET	CG-SD-CE	-7.05	88.92	100.20
1	A	239	ILE	CB-CA-C	-6.74	98.11	111.60
1	A	71	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	71	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	71	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	D	239	ILE	CG1-CB-CG2	5.94	124.47	111.40
1	C	80	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	B	320	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	D	152	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	4	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	260	ILE	CG1-CB-CG2	-5.55	99.20	111.40
1	C	80	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	B	46	LEU	CB-CG-CD2	5.51	120.36	111.00
1	B	93	ASP	CB-CG-OD2	5.28	123.06	118.30
1	B	109	VAL	CG1-CB-CG2	5.25	119.30	110.90
1	C	46	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	46	LEU	CB-CG-CD2	5.20	119.83	111.00
1	C	152	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	46	LEU	CB-CG-CD2	5.11	119.69	111.00
1	A	4	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	200	ARG	CG-CD-NE	-5.07	101.16	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	ILE	Peptide
1	C	285	ILE	Peptide
1	D	285	ILE	Peptide

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	2681	0	2658	49	0
1	B	2681	0	2658	58	0
1	C	2681	0	2658	40	0
1	D	2681	0	2658	34	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	0	0
3	D	25	0	0	0	0
4	A	10	0	0	0	0
5	A	119	0	0	0	0
5	B	72	0	0	0	0
5	C	106	0	0	2	0
5	D	58	0	0	0	0
All	All	11365	0	10736	171	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 8.

All (171) 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:C:286:HIS:O	1:C:287:HIS:ND1	1.88	1.05
1:C:2:MET:HG3	1:C:322:ASN:HD21	1.25	1.01
1:D:2:MET:HG2	1:D:322:ASN:HD21	1.24	0.99
1:C:2:MET:CG	1:C:322:ASN:HD21	1.75	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:CE2	1:A:175:ILE:HD11	2.02	0.94
1:D:75:ILE:HD13	1:D:88:VAL:HG12	1.55	0.88
1:D:2:MET:CG	1:D:322:ASN:HD21	1.87	0.87
1:B:40:ASN:HB3	1:B:71:ARG:HH22	1.41	0.85
1:C:179:VAL:O	1:C:183:THR:HG23	1.79	0.83
1:D:179:VAL:O	1:D:183:THR:HG23	1.78	0.82
1:A:270:THR:OG1	1:A:273:GLU:HG3	1.79	0.82
1:D:286:HIS:O	1:D:287:HIS:ND1	2.14	0.79
1:C:2:MET:HG3	1:C:322:ASN:ND2	1.98	0.79
1:B:171:TYR:CE2	1:B:175:ILE:HD11	2.17	0.79
1:A:171:TYR:CZ	1:A:175:ILE:HD11	2.19	0.78
1:B:244:GLN:HE22	1:B:320:ARG:H	1.31	0.78
1:D:2:MET:HG2	1:D:322:ASN:ND2	1.99	0.77
1:B:40:ASN:HB3	1:B:71:ARG:NH2	1.98	0.77
1:A:40:ASN:HB3	1:A:71:ARG:HH22	1.50	0.77
1:B:270:THR:OG1	1:B:273:GLU:HG3	1.85	0.76
1:D:286:HIS:O	1:D:287:HIS:CG	2.39	0.76
1:B:232:THR:HG23	1:B:304:ARG:O	1.87	0.74
1:A:230:GLY:O	1:A:272:ASN:ND2	2.21	0.74
1:A:232:THR:HG23	1:A:304:ARG:O	1.88	0.73
1:C:75:ILE:HD13	1:C:88:VAL:HG12	1.70	0.73
1:A:117:THR:HG22	1:A:118:ASN:OD1	1.89	0.73
1:A:244:GLN:HE22	1:A:320:ARG:H	1.36	0.73
1:C:286:HIS:O	1:C:287:HIS:CG	2.41	0.73
1:A:67:GLU:H	1:A:67:GLU:CD	1.90	0.73
1:B:67:GLU:CD	1:B:67:GLU:H	1.93	0.71
1:B:66:THR:HB	1:B:67:GLU:OE2	1.90	0.71
1:C:27:PHE:HE2	1:C:196:VAL:HG23	1.55	0.71
1:C:244:GLN:HE22	1:C:320:ARG:H	1.39	0.69
1:B:232:THR:HG22	1:B:234:ARG:HH12	1.58	0.69
1:A:75:ILE:HD13	1:A:88:VAL:HG12	1.74	0.69
1:D:245:MET:HE2	1:D:319:TYR:CD1	2.28	0.68
1:D:280:ASP:O	1:D:284:LEU:HD13	1.94	0.68
1:A:101:LEU:HG	1:A:117:THR:HG21	1.77	0.67
1:A:66:THR:HB	1:A:67:GLU:OE2	1.94	0.67
1:C:102:GLY:O	1:C:103:SER:HB3	1.94	0.66
1:B:270:THR:OG1	1:B:273:GLU:CG	2.43	0.66
1:C:27:PHE:CE2	1:C:196:VAL:HG23	2.31	0.66
1:D:8:ILE:HG23	1:D:251:LEU:HD22	1.76	0.65
1:A:40:ASN:HB3	1:A:71:ARG:NH2	2.12	0.65
1:B:230:GLY:O	1:B:272:ASN:ND2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ILE:HD13	1:B:88:VAL:HG12	1.78	0.65
1:A:10:GLN:HE21	1:B:106:ARG:HH11	1.45	0.65
1:B:232:THR:HG22	1:B:234:ARG:NH1	2.11	0.64
1:B:244:GLN:NE2	1:B:320:ARG:H	1.96	0.64
1:A:244:GLN:NE2	1:A:320:ARG:H	1.95	0.63
1:B:245:MET:HE2	1:B:319:TYR:CE1	2.34	0.63
1:A:94:HIS:HD2	1:A:136:SER:OG	1.81	0.63
1:C:245:MET:HG2	1:C:263:VAL:HG22	1.82	0.62
1:B:228:GLY:N	1:B:296:ARG:O	2.31	0.62
1:D:245:MET:CE	1:D:319:TYR:CD1	2.84	0.61
1:A:232:THR:HG22	1:A:234:ARG:HH12	1.65	0.61
1:A:270:THR:OG1	1:A:273:GLU:CG	2.49	0.60
1:A:40:ASN:O	1:A:71:ARG:NH2	2.33	0.60
1:D:75:ILE:HD13	1:D:88:VAL:CG1	2.29	0.59
1:C:65:SER:H	1:C:68:GLN:HE21	1.50	0.59
1:B:117:THR:HG22	1:B:118:ASN:OD1	2.01	0.59
1:D:245:MET:HE2	1:D:319:TYR:CE1	2.38	0.59
1:B:102:GLY:O	1:B:103:SER:HB3	2.03	0.58
1:B:270:THR:N	1:B:273:GLU:OE1	2.31	0.57
1:C:244:GLN:NE2	1:C:320:ARG:H	2.02	0.57
1:C:285:ILE:O	1:C:285:ILE:HG22	2.04	0.57
1:B:232:THR:CG2	1:B:234:ARG:HH12	2.18	0.57
1:B:27:PHE:HE2	1:B:196:VAL:CG2	2.17	0.56
1:D:102:GLY:O	1:D:103:SER:HB3	2.04	0.56
1:A:232:THR:HG22	1:A:234:ARG:NH1	2.20	0.56
1:C:2:MET:CG	1:C:322:ASN:ND2	2.58	0.56
1:A:245:MET:HE2	1:A:319:TYR:CE1	2.41	0.55
1:B:27:PHE:HE2	1:B:196:VAL:HG22	1.70	0.55
1:B:67:GLU:CD	1:B:67:GLU:N	2.60	0.55
1:A:231:GLU:HA	1:A:231:GLU:OE2	2.07	0.55
1:A:102:GLY:O	1:A:103:SER:HB3	2.05	0.55
1:A:230:GLY:C	1:A:272:ASN:HD21	2.10	0.55
1:B:245:MET:HE2	1:B:319:TYR:CD1	2.41	0.55
1:C:245:MET:HE2	1:C:319:TYR:CD1	2.42	0.54
1:C:245:MET:HE2	1:C:319:TYR:CE1	2.42	0.54
1:C:154:LYS:HD3	5:C:423:HOH:O	2.07	0.54
1:A:10:GLN:NE2	1:B:106:ARG:HH11	2.05	0.53
1:B:226:ILE:O	1:B:226:ILE:HG22	2.08	0.53
1:A:232:THR:CG2	1:A:234:ARG:HH12	2.21	0.53
1:A:36:LEU:HD21	1:A:247:ILE:HD11	1.89	0.53
1:C:8:ILE:HG23	1:C:251:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:NZ	1:D:67:GLU:OE1	2.38	0.52
1:A:67:GLU:N	1:A:67:GLU:CD	2.60	0.52
1:B:27:PHE:CE2	1:B:196:VAL:CG2	2.93	0.52
1:B:304:ARG:HD2	1:B:304:ARG:O	2.10	0.52
1:A:179:VAL:O	1:A:183:THR:HG23	2.11	0.51
1:D:304:ARG:HG3	1:D:305:HIS:CD2	2.45	0.51
1:D:235:ASP:HB2	1:D:307:GLN:HA	1.93	0.51
1:D:245:MET:HG2	1:D:263:VAL:HG22	1.93	0.50
1:D:196:VAL:HA	1:D:237:CYS:O	2.11	0.50
1:D:179:VAL:O	1:D:183:THR:CG2	2.55	0.50
1:C:245:MET:HE1	1:C:319:TYR:CG	2.47	0.49
1:A:11:GLN:NE2	1:B:206:ALA:H	2.10	0.49
1:C:235:ASP:HB2	1:C:307:GLN:HA	1.95	0.49
1:B:40:ASN:O	1:B:71:ARG:NH2	2.36	0.49
1:B:231:GLU:OE2	1:B:231:GLU:HA	2.13	0.49
1:C:104:VAL:HB	1:C:105:PRO:HD3	1.94	0.49
1:A:110:ASP:O	1:A:114:THR:HB	2.12	0.49
1:A:245:MET:HE2	1:A:319:TYR:CD1	2.48	0.48
1:B:8:ILE:HG23	1:B:251:LEU:HD22	1.95	0.47
1:C:245:MET:CE	1:C:319:TYR:CD1	2.98	0.47
1:C:2:MET:HG2	1:C:322:ASN:HD21	1.71	0.47
1:D:198:GLY:HA3	1:D:239:ILE:CD1	2.44	0.47
1:B:314:ILE:HG23	1:B:320:ARG:NH1	2.30	0.47
1:C:65:SER:H	1:C:68:GLN:NE2	2.13	0.47
1:A:177:ALA:HB1	1:A:188:THR:OG1	2.15	0.47
1:D:245:MET:CE	1:D:319:TYR:CE1	2.99	0.46
1:A:11:GLN:HE21	1:B:206:ALA:H	1.62	0.46
1:B:233:SER:O	1:B:234:ARG:HD3	2.16	0.46
1:A:209:ALA:O	1:A:212:PRO:HD2	2.16	0.46
1:C:130:LYS:HD2	1:C:184:TYR:CG	2.51	0.46
1:B:231:GLU:O	1:B:232:THR:C	2.53	0.46
1:B:310:VAL:O	1:B:314:ILE:HG13	2.15	0.46
1:D:104:VAL:HB	1:D:105:PRO:HD3	1.98	0.46
1:B:177:ALA:HB1	1:B:188:THR:OG1	2.16	0.45
1:A:196:VAL:HA	1:A:237:CYS:O	2.17	0.45
1:C:50:SER:HB2	1:D:14:PHE:CG	2.51	0.45
1:C:1:TYR:HA	1:C:6:GLU:OE2	2.17	0.45
1:D:116:ALA:O	1:D:120:THR:HB	2.17	0.44
1:B:171:TYR:CZ	1:B:175:ILE:HD11	2.50	0.44
1:A:11:GLN:HE22	1:B:205:GLY:HA2	1.83	0.44
1:A:94:HIS:CD2	1:A:136:SER:OG	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:TYR:HB3	1:D:296:ARG:HE	1.82	0.44
1:B:101:LEU:HG	1:B:117:THR:HG21	2.00	0.44
1:B:36:LEU:HD21	1:B:247:ILE:HD11	1.99	0.43
1:C:2:MET:N	1:C:6:GLU:OE2	2.51	0.43
1:D:2:MET:N	1:D:6:GLU:OE2	2.52	0.43
1:C:194:PHE:O	1:C:195:ASN:C	2.56	0.43
1:A:228:GLY:N	1:A:296:ARG:O	2.48	0.43
1:D:245:MET:HE1	1:D:319:TYR:CG	2.54	0.43
1:B:231:GLU:O	1:B:270:THR:HG22	2.19	0.43
1:B:230:GLY:C	1:B:272:ASN:HD21	2.22	0.43
1:C:329:LEU:O	1:C:333:MET:HG2	2.19	0.43
1:A:230:GLY:C	1:A:272:ASN:ND2	2.70	0.43
1:B:245:MET:HE2	1:B:245:MET:HB2	1.87	0.43
1:A:36:LEU:HD21	1:A:247:ILE:CD1	2.49	0.43
1:B:110:ASP:O	1:B:114:THR:HB	2.19	0.43
1:C:141:ALA:HB1	5:C:383:HOH:O	2.17	0.43
1:A:294:LYS:HE2	1:A:294:LYS:HB3	1.71	0.43
1:A:194:PHE:HB2	1:A:264:ALA:HB2	2.00	0.42
1:C:196:VAL:HA	1:C:237:CYS:O	2.19	0.42
1:B:48:ASN:H	1:B:48:ASN:HD22	1.66	0.42
1:D:130:LYS:HD2	1:D:184:TYR:CG	2.54	0.42
1:B:179:VAL:O	1:B:183:THR:HG23	2.20	0.42
1:D:285:ILE:O	1:D:285:ILE:HG22	2.19	0.42
1:A:241:ASN:HB3	1:A:319:TYR:OH	2.20	0.42
1:A:48:ASN:H	1:A:48:ASN:HD22	1.68	0.42
1:B:172:VAL:HG22	1:C:172:VAL:HG22	2.01	0.42
1:D:245:MET:HB2	1:D:245:MET:HE2	1.88	0.41
1:B:36:LEU:HD21	1:B:247:ILE:CD1	2.50	0.41
1:B:264:ALA:HB3	1:B:308:ALA:HB3	2.01	0.41
1:B:196:VAL:HA	1:B:237:CYS:O	2.20	0.41
1:A:320:ARG:HH21	1:B:76:GLU:CD	2.24	0.41
1:D:194:PHE:O	1:D:195:ASN:C	2.59	0.41
1:A:171:TYR:CE2	1:A:175:ILE:CD1	2.90	0.41
1:A:226:ILE:HG22	1:A:226:ILE:O	2.19	0.41
1:D:2:MET:HG3	1:D:322:ASN:HD21	1.80	0.41
1:B:48:ASN:N	1:B:48:ASN:HD22	2.16	0.41
1:B:194:PHE:HB2	1:B:264:ALA:HB2	2.03	0.41
1:C:304:ARG:HG3	1:C:305:HIS:CD2	2.56	0.41
1:C:28:ILE:HD11	1:C:196:VAL:HG21	2.01	0.41
1:B:228:GLY:CA	1:B:296:ARG:O	2.69	0.41
1:C:116:ALA:O	1:C:120:THR:HB	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ILE:O	1:C:285:ILE:CG2	2.69	0.40
1:C:106:ARG:NH1	1:D:14:PHE:O	2.47	0.40
1:A:198:GLY:HA3	1:A:239:ILE:HG12	2.02	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	332/351 (95%)	319 (96%)	7 (2%)	6 (2%)	11	5
1	B	332/351 (95%)	313 (94%)	15 (4%)	4 (1%)	16	10
1	C	332/351 (95%)	324 (98%)	7 (2%)	1 (0%)	46	45
1	D	332/351 (95%)	322 (97%)	9 (3%)	1 (0%)	46	45
All	All	1328/1404 (95%)	1278 (96%)	38 (3%)	12 (1%)	21	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	286	HIS
1	B	227	ASN
1	C	286	HIS
1	D	286	HIS
1	B	286	HIS
1	A	50	SER
1	A	103	SER
1	A	226	ILE
1	B	103	SER
1	B	226	ILE
1	A	325	ILE

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	290/304 (95%)	276 (95%)	14 (5%)	31	29
1	B	290/304 (95%)	279 (96%)	11 (4%)	40	40
1	C	290/304 (95%)	275 (95%)	15 (5%)	29	25
1	D	290/304 (95%)	276 (95%)	14 (5%)	31	29
All	All	1160/1216 (95%)	1106 (95%)	54 (5%)	32	30

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	48	ASN
1	A	67	GLU
1	A	71	ARG
1	A	109	VAL
1	A	114	THR
1	A	130	LYS
1	A	183	THR
1	A	220	LYS
1	A	239	ILE
1	A	285	ILE
1	A	294	LYS
1	A	305	HIS
1	A	330	ARG
1	B	46	LEU
1	B	48	ASN
1	B	67	GLU
1	B	71	ARG
1	B	109	VAL
1	B	114	THR
1	B	130	LYS
1	B	220	LYS
1	B	285	ILE
1	B	293	ILE

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Mol	Chain	Res	Type
1	B	300	SER
1	C	1	TYR
1	C	3	SER
1	C	11	GLN
1	C	15	SER
1	C	46	LEU
1	C	87	GLN
1	C	152	LEU
1	C	179	VAL
1	C	183	THR
1	C	196	VAL
1	C	220	LYS
1	C	284	LEU
1	C	286	HIS
1	C	297	GLU
1	C	338	ARG
1	D	3	SER
1	D	7	GLU
1	D	15	SER
1	D	46	LEU
1	D	87	GLN
1	D	152	LEU
1	D	183	THR
1	D	220	LYS
1	D	239	ILE
1	D	260	ILE
1	D	286	HIS
1	D	297	GLU
1	D	300	SER
1	D	338	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	GLN
1	A	48	ASN
1	A	87	GLN
1	A	94	HIS
1	A	98	GLN
1	A	149	HIS
1	A	173	ASN

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Mol	Chain	Res	Type
1	A	178	GLN
1	A	244	GLN
1	A	262	ASN
1	A	272	ASN
1	B	10	GLN
1	B	11	GLN
1	B	48	ASN
1	B	87	GLN
1	B	115	ASN
1	B	173	ASN
1	B	201	GLN
1	B	244	GLN
1	B	272	ASN
1	C	68	GLN
1	C	173	ASN
1	C	244	GLN
1	C	262	ASN
1	C	322	ASN
1	D	173	ASN
1	D	322	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are unknown - leaving 6 for Mogul analysis.

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	343	-	38,48,48	1.29	4 (10%)	47,73,73	1.92	9 (19%)
4	SO4	A	345	-	4,4,4	0.34	0	6,6,6	0.34	0
4	SO4	A	346	-	4,4,4	0.39	0	6,6,6	0.41	0
2	NAD	B	343	-	38,48,48	1.25	5 (13%)	47,73,73	1.80	10 (21%)
2	NAD	C	343	-	38,48,48	1.69	8 (21%)	47,73,73	2.22	7 (14%)
2	NAD	D	343	-	38,48,48	1.36	4 (10%)	47,73,73	2.15	8 (17%)

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	343	-	-	0/22/62/62	0/5/5/5
4	SO4	A	345	-	-	0/0/0/0	0/0/0/0
4	SO4	A	346	-	-	0/0/0/0	0/0/0/0
2	NAD	B	343	-	-	0/22/62/62	0/5/5/5
2	NAD	C	343	-	-	0/22/62/62	0/5/5/5
2	NAD	D	343	-	-	0/22/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	343	NAD	PN-O2N	-2.89	1.42	1.54
2	A	343	NAD	PA-O1A	-2.57	1.41	1.51
2	A	343	NAD	PN-O1N	-2.52	1.42	1.51
2	B	343	NAD	PA-O1A	-2.46	1.42	1.51
2	C	343	NAD	PN-O2N	-2.45	1.44	1.54
2	D	343	NAD	PA-O2A	-2.29	1.45	1.54
2	C	343	NAD	PA-O2A	-2.20	1.45	1.54
2	A	343	NAD	O2D-C2D	-2.16	1.37	1.43
2	B	343	NAD	PN-O2N	-2.03	1.46	1.54
2	B	343	NAD	C8A-N7A	-2.01	1.30	1.34
2	B	343	NAD	C5D-C4D	2.02	1.58	1.51
2	B	343	NAD	C6N-N1N	2.09	1.41	1.35
2	C	343	NAD	O3D-C3D	2.28	1.48	1.43
2	C	343	NAD	C2N-C3N	2.38	1.42	1.39
2	C	343	NAD	O4D-C1D	2.42	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	343	NAD	C7N-N7N	2.48	1.38	1.33
2	C	343	NAD	C7N-N7N	2.53	1.38	1.33
2	D	343	NAD	C6N-N1N	3.36	1.44	1.35
2	C	343	NAD	C6N-N1N	3.46	1.44	1.35
2	A	343	NAD	O4B-C1B	3.57	1.45	1.41
2	C	343	NAD	O4B-C1B	5.85	1.48	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	343	NAD	N3A-C2A-N1A	-10.94	120.52	128.89
2	D	343	NAD	N3A-C2A-N1A	-10.58	120.80	128.89
2	A	343	NAD	N3A-C2A-N1A	-9.03	121.98	128.89
2	B	343	NAD	N3A-C2A-N1A	-7.29	123.31	128.89
2	C	343	NAD	C3N-C2N-N1N	-4.23	115.48	120.36
2	B	343	NAD	C4A-C5A-N7A	-4.08	105.72	109.48
2	D	343	NAD	C3N-C2N-N1N	-3.87	115.90	120.36
2	A	343	NAD	PN-O3-PA	-3.85	121.92	132.73
2	B	343	NAD	O4D-C1D-N1N	-3.57	104.20	108.13
2	B	343	NAD	PN-O3-PA	-3.25	123.60	132.73
2	B	343	NAD	C4D-O4D-C1D	-2.96	106.46	109.72
2	A	343	NAD	C4A-C5A-N7A	-2.92	106.79	109.48
2	A	343	NAD	C2B-C1B-N9A	-2.84	109.96	114.29
2	C	343	NAD	C4B-O4B-C1B	-2.72	106.73	109.72
2	B	343	NAD	C2B-C1B-N9A	-2.41	110.61	114.29
2	B	343	NAD	C3N-C2N-N1N	-2.32	117.69	120.36
2	C	343	NAD	C4A-C5A-N7A	-2.31	107.36	109.48
2	A	343	NAD	C4D-O4D-C1D	-2.24	107.26	109.72
2	C	343	NAD	C1B-N9A-C4A	-2.17	123.66	126.94
2	D	343	NAD	C4N-C3N-C7N	-2.10	115.55	121.09
2	A	343	NAD	C1B-N9A-C4A	-2.09	123.79	126.94
2	D	343	NAD	O7N-C7N-C3N	-2.07	117.33	119.59
2	A	343	NAD	O4D-C1D-N1N	-2.01	105.92	108.13
2	B	343	NAD	C2N-C3N-C4N	2.02	120.53	118.29
2	A	343	NAD	C2A-N1A-C6A	2.02	122.38	118.77
2	D	343	NAD	C4D-O4D-C1D	2.03	111.95	109.72
2	B	343	NAD	C2A-N1A-C6A	2.07	122.46	118.77
2	B	343	NAD	O2N-PN-O1N	2.09	123.86	112.53
2	A	343	NAD	C2N-C3N-C4N	2.60	121.19	118.29
2	D	343	NAD	O7N-C7N-N7N	2.79	126.52	122.59
2	D	343	NAD	O4D-C1D-N1N	3.99	112.51	108.13
2	C	343	NAD	C2N-C3N-C4N	4.20	122.96	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	343	NAD	C2N-C3N-C4N	4.93	123.78	118.29
2	C	343	NAD	O4D-C1D-N1N	5.07	113.71	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	336/351 (95%)	1.20	64 (19%) 2 2	38, 62, 100, 124	0
1	B	336/351 (95%)	1.17	70 (20%) 1 1	39, 60, 95, 117	0
1	C	336/351 (95%)	0.51	23 (6%) 20 28	33, 43, 68, 96	0
1	D	336/351 (95%)	-0.16	4 (1%) 81 85	22, 28, 42, 63	0
All	All	1344/1404 (95%)	0.68	161 (11%) 6 8	22, 47, 91, 124	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	MET	13.9
1	C	1	TYR	10.0
1	D	2	MET	7.7
1	B	279	TYR	5.8
1	C	286	HIS	5.7
1	C	295	TYR	5.7
1	A	279	TYR	5.4
1	C	225	TYR	5.4
1	B	303	VAL	4.8
1	C	293	ILE	4.7
1	A	303	VAL	4.7
1	B	221	GLY	4.6
1	D	1	TYR	4.5
1	A	286	HIS	4.4
1	C	226	ILE	4.3
1	A	225	TYR	4.1
1	A	301	GLY	4.0
1	C	207	TYR	3.9
1	A	221	GLY	3.8
1	B	301	GLY	3.7
1	B	286	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	92	VAL	3.7
1	B	92	VAL	3.6
1	B	294	LYS	3.5
1	A	129	ALA	3.5
1	A	89	MET	3.5
1	B	299	ARG	3.5
1	C	340	LEU	3.5
1	A	14	PHE	3.5
1	B	298	PHE	3.4
1	A	19	TRP	3.4
1	A	85	CYS	3.4
1	C	330	ARG	3.3
1	B	129	ALA	3.3
1	A	284	LEU	3.3
1	A	298	PHE	3.2
1	B	19	TRP	3.2
1	C	300	SER	3.2
1	B	82	LEU	3.2
1	A	184	TYR	3.1
1	A	18	THR	3.1
1	B	225	TYR	3.1
1	B	271	LEU	3.1
1	B	282	LEU	3.1
1	B	184	TYR	3.1
1	A	297	GLU	3.1
1	A	88	VAL	3.0
1	A	176	TYR	3.0
1	A	127	HIS	3.0
1	D	286	HIS	3.0
1	B	175	ILE	2.9
1	B	159	ILE	2.9
1	A	128	ALA	2.9
1	B	176	TYR	2.9
1	B	14	PHE	2.9
1	C	294	LYS	2.9
1	B	179	VAL	2.9
1	C	279	TYR	2.9
1	A	39	LEU	2.8
1	A	73	CYS	2.8
1	C	297	GLU	2.8
1	B	297	GLU	2.8
1	A	65	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	134	VAL	2.8
1	B	181	ALA	2.8
1	A	112	ILE	2.8
1	A	71	ARG	2.8
1	A	186	PHE	2.7
1	B	134	VAL	2.7
1	B	88	VAL	2.7
1	B	123	LEU	2.7
1	A	175	ILE	2.7
1	A	95	VAL	2.7
1	B	18	THR	2.7
1	A	278	ILE	2.6
1	C	283	ASN	2.6
1	A	82	LEU	2.6
1	B	278	ILE	2.6
1	A	179	VAL	2.6
1	B	8	ILE	2.6
1	B	112	ILE	2.6
1	A	8	ILE	2.6
1	A	172	VAL	2.6
1	B	171	TYR	2.5
1	B	85	CYS	2.5
1	A	299	ARG	2.5
1	B	127	HIS	2.5
1	A	91	GLY	2.5
1	C	55	TYR	2.5
1	B	39	LEU	2.5
1	B	65	SER	2.5
1	B	95	VAL	2.5
1	A	136	SER	2.5
1	B	42	VAL	2.5
1	A	137	PHE	2.5
1	B	20	LEU	2.5
1	B	305	HIS	2.5
1	B	16	PRO	2.4
1	B	185	GLY	2.4
1	B	186	PHE	2.4
1	B	284	LEU	2.4
1	B	227	ASN	2.4
1	B	120	THR	2.4
1	B	128	ALA	2.4
1	B	117	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	302	ASP	2.4
1	D	207	TYR	2.4
1	A	84	THR	2.4
1	B	132	ALA	2.4
1	C	287	HIS	2.4
1	A	185	GLY	2.3
1	A	126	LEU	2.3
1	B	89	MET	2.3
1	A	123	LEU	2.3
1	B	122	PHE	2.3
1	A	125	ILE	2.3
1	B	126	LEU	2.3
1	C	282	LEU	2.3
1	A	122	PHE	2.3
1	A	64	VAL	2.3
1	A	117	THR	2.3
1	B	84	THR	2.3
1	C	3	SER	2.2
1	A	330	ARG	2.2
1	B	287	HIS	2.2
1	A	227	ASN	2.2
1	B	172	VAL	2.2
1	C	7	GLU	2.2
1	A	12	LEU	2.2
1	A	20	LEU	2.2
1	B	124	ASN	2.2
1	B	125	ILE	2.2
1	B	177	ALA	2.2
1	B	71	ARG	2.2
1	A	181	ALA	2.2
1	A	44	ILE	2.2
1	A	159	ILE	2.2
1	B	226	ILE	2.2
1	B	180	TYR	2.1
1	C	284	LEU	2.1
1	B	73	CYS	2.1
1	A	74	PHE	2.1
1	B	12	LEU	2.1
1	C	338	ARG	2.1
1	A	83	THR	2.1
1	A	250	ALA	2.1
1	C	231	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	171	TYR	2.1
1	A	180	TYR	2.1
1	B	44	ILE	2.1
1	B	285	ILE	2.1
1	A	132	ALA	2.1
1	A	124	ASN	2.0
1	A	43	VAL	2.0
1	B	43	VAL	2.0
1	B	169	THR	2.0
1	B	296	ARG	2.0
1	B	115	ASN	2.0
1	B	300	SER	2.0
1	B	135	GLN	2.0
1	A	79	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAD	D	343	44/44	0.96	0.10	-0.01	20,28,41,45	0
2	NAD	C	343	44/44	0.96	0.10	-0.52	24,30,44,46	0
3	UNL	D	344	25/-	0.95	0.10	-0.84	26,33,37,38	0
3	UNL	C	344	25/-	0.94	0.12	-0.97	39,44,48,50	0
3	UNL	B	344	25/-	0.93	0.14	-1.01	46,65,72,76	0
3	UNL	A	344	25/-	0.94	0.14	-1.13	45,65,71,76	0
2	NAD	B	343	44/44	0.96	0.10	-1.73	24,30,42,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAD	A	343	44/44	0.96	0.10	-2.07	25,30,42,46	0
4	SO4	A	345	5/5	0.98	0.07	-2.30	28,29,31,33	0
4	SO4	A	346	5/5	0.98	0.07	-3.73	30,30,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.