



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:42 PM GMT

PDB ID : 3RUE
Title : Alternative analogs as viable substrates of UDP-hexose 4-epimerases
Authors : Bhatt, V.S.; Guan, W.; Wang, P.G.
Deposited on : 2011-05-05
Resolution : 2.80 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

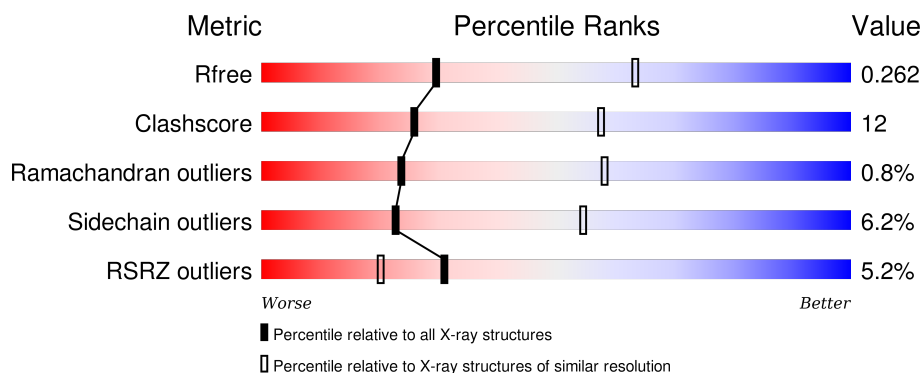
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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>3%</div> <div>68%</div> <div>24%</div> <div>• •</div> </div>
1	B	351	<div> <div>3%</div> <div>64%</div> <div>29%</div> <div>• •</div> </div>
1	S	351	<div> <div>7%</div> <div>70%</div> <div>23%</div> <div>• •</div> </div>
1	b	351	<div> <div>6%</div> <div>90%</div> <div>5%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNL	B	344	-	-	X	-
3	UNL	S	344	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11018 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	S	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			

There are 24 discrepancies between the modelled and reference sequences:

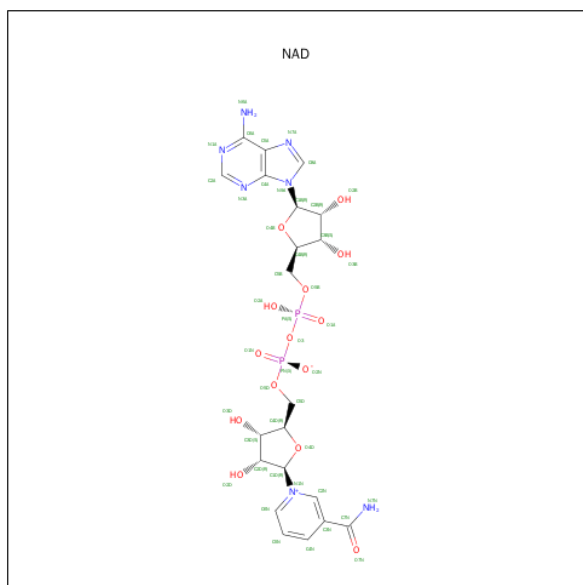
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9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

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Chain	Residue	Modelled	Actual	Comment	Reference
b	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
b	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
b	-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	S	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		

- 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	S	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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

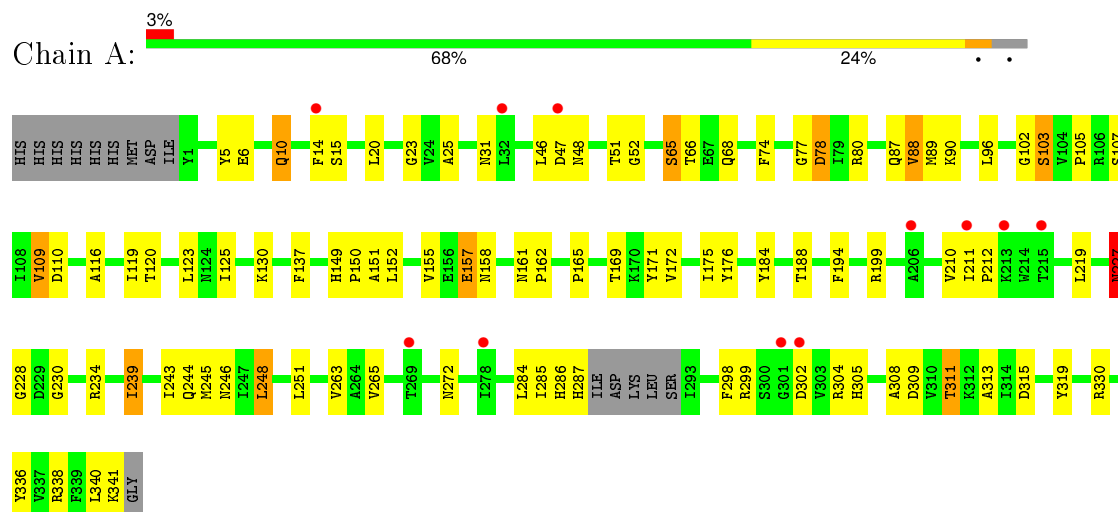
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	6	Total	O	0	0
			6	6		
4	S	4	Total	O	0	0
			4	4		
4	b	2	Total	O	0	0
			2	2		

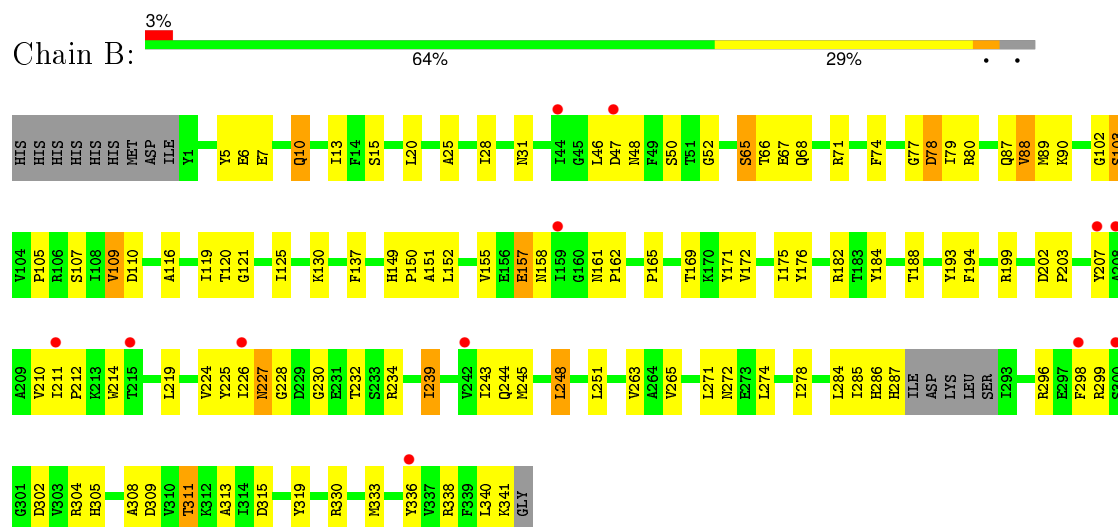
3 Residue-property plots

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

• Molecule 1: WbgU

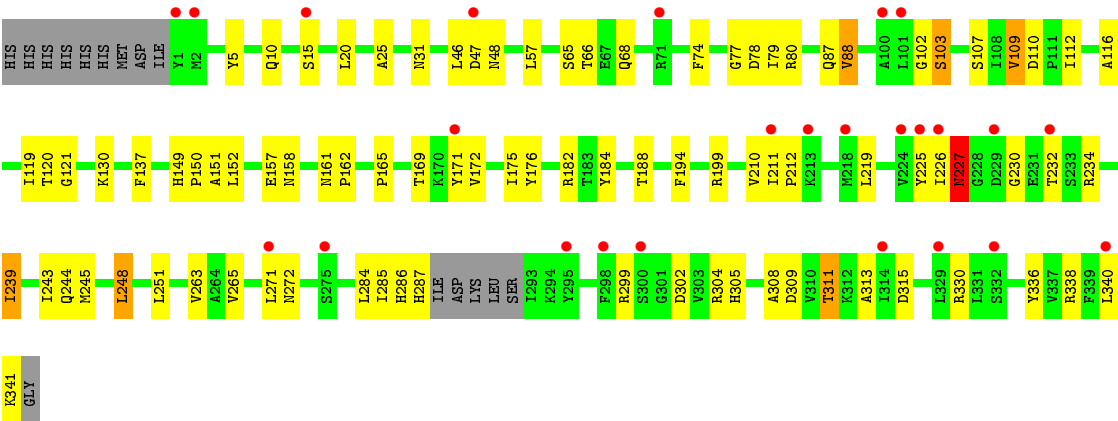


• Molecule 1: WbgU

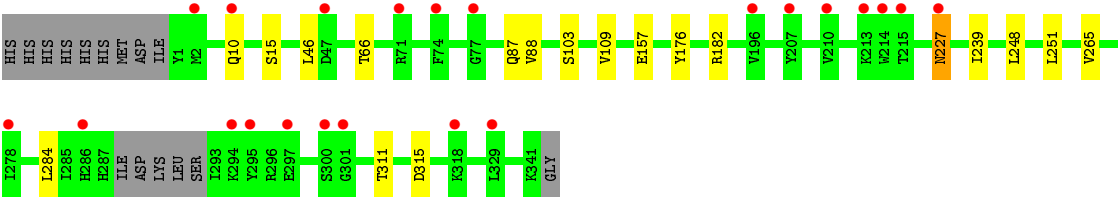
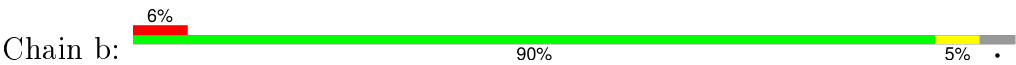


• Molecule 1: WbgU





● Molecule 1: WbgU



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	78.45Å 78.45Å 226.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.50 – 2.80 43.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (75.50-2.80) 99.4 (43.50-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.264 0.229 , 0.262	Depositor DCC
R_{free} test set	1900 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.3	EDS
Estimated twinning fraction	0.014 for -h,-k,l 0.429 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 38003 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11018	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: UNL, 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	0.46	0/2739	0.58	0/3717
1	B	0.46	0/2739	0.58	0/3717
1	S	0.46	0/2739	0.57	0/3717
1	b	0.46	0/2739	0.57	0/3717
All	All	0.46	0/10956	0.58	0/14868

There are no bond length outliers.

There are no bond angle outliers.

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	2681	0	2658	85	1
1	B	2681	0	2658	112	1
1	S	2681	0	2658	82	0
1	b	2681	0	2658	0	0
2	A	44	0	26	4	0
2	B	44	0	26	7	0
2	S	44	0	26	2	0
2	b	44	0	26	0	0
3	A	25	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	17	0
3	S	25	0	0	12	0
3	b	25	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	S	4	0	0	0	0
4	b	2	0	0	0	0
All	All	11018	0	10736	269	1

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 12.

All (269) 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:A:298:PHE:HB3	1:A:302:ASP:OD2	1.56	1.05
1:B:271:LEU:CD1	3:B:344:UNL:C1B	3.65	0.91
1:B:71:ARG:HH22	1:S:109:VAL:HG11	45.24	0.90
1:A:47:ASP:HB2	2:A:344:NAD:O2B	1.72	0.88
1:A:110:ASP:HB3	1:B:10:GLN:HE22	1.39	0.87
1:B:67:GLU:HB3	1:S:109:VAL:CG2	47.24	0.85
1:A:309:ASP:OD1	1:A:311:THR:HG23	1.77	0.84
1:B:309:ASP:OD1	1:B:311:THR:HG23	1.77	0.84
1:S:25:ALA:HB2	1:S:47:ASP:OD2	1.78	0.84
1:B:271:LEU:HD11	3:B:344:UNL:O2'	4.50	0.83
1:S:309:ASP:OD1	1:S:311:THR:HG23	1.77	0.83
1:B:271:LEU:HD13	3:B:344:UNL:C1B	3.41	0.83
1:B:71:ARG:HH22	1:S:109:VAL:CG1	44.62	0.82
1:B:271:LEU:HD11	3:B:344:UNL:C1B	2.99	0.81
1:S:245:MET:HG2	1:S:263:VAL:HG22	1.63	0.80
1:B:25:ALA:HB2	1:B:47:ASP:OD2	1.84	0.79
1:B:47:ASP:OD1	1:B:74:PHE:CZ	2.36	0.79
1:B:67:GLU:HB3	1:S:109:VAL:HG23	47.68	0.78
1:B:245:MET:HG2	1:B:263:VAL:HG22	1.66	0.78
1:A:110:ASP:HB3	1:B:10:GLN:NE2	2.00	0.77
1:B:47:ASP:OD1	1:B:74:PHE:HZ	1.69	0.76
1:A:245:MET:HG2	1:A:263:VAL:HG22	1.69	0.75
1:A:47:ASP:OD1	1:A:74:PHE:CZ	2.41	0.73
1:B:71:ARG:NH2	1:S:109:VAL:HG11	45.90	0.73
1:A:25:ALA:HB2	1:A:47:ASP:OD2	1.87	0.73
1:S:47:ASP:OD1	1:S:74:PHE:CZ	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:SER:HB2	1:B:165:PRO:HB2	1.71	0.71
1:S:285:ILE:HG22	1:S:285:ILE:O	1.90	0.71
1:B:71:ARG:NH1	1:S:109:VAL:HG21	47.36	0.71
1:A:107:SER:HB2	1:A:165:PRO:HB2	1.72	0.71
1:B:285:ILE:HG22	1:B:285:ILE:O	1.90	0.71
1:B:271:LEU:CD1	3:B:344:UNL:O2'	5.26	0.70
1:S:271:LEU:CD1	3:S:344:UNL:C1B	2.69	0.70
1:B:271:LEU:HD21	3:B:344:UNL:O4B	2.67	0.69
1:A:47:ASP:OD1	1:A:74:PHE:HZ	1.75	0.69
1:A:285:ILE:HG22	1:A:285:ILE:O	1.91	0.69
1:B:67:GLU:HB3	1:S:109:VAL:HG22	47.20	0.69
1:S:271:LEU:HD11	3:S:344:UNL:O2'	1.92	0.68
1:A:304:ARG:HG3	1:A:305:HIS:CD2	2.28	0.68
1:B:102:GLY:O	1:B:103:SER:HB3	1.93	0.68
1:S:102:GLY:O	1:S:103:SER:HB3	1.94	0.68
1:B:20:LEU:HD13	1:B:88:VAL:HG13	1.76	0.68
1:S:47:ASP:OD1	1:S:74:PHE:HZ	1.77	0.67
1:B:171:TYR:CZ	1:B:175:ILE:HD11	2.37	0.67
1:B:304:ARG:HG3	1:B:305:HIS:CD2	2.29	0.67
1:A:20:LEU:HD13	1:A:88:VAL:HG13	1.77	0.67
1:B:226:ILE:HA	3:B:344:UNL:O2	2.93	0.66
1:S:227:ASN:OD1	3:S:344:UNL:N3	2.28	0.66
1:B:71:ARG:HH22	1:S:109:VAL:CB	45.22	0.65
1:S:65:SER:HB3	1:S:68:GLN:OE1	1.97	0.65
1:A:227:ASN:OD1	3:A:343:UNL:N3	2.29	0.65
1:B:271:LEU:HD11	3:B:344:UNL:C2B	4.10	0.65
1:B:65:SER:HB3	1:B:68:GLN:OE1	2.10	0.65
1:S:171:TYR:CZ	1:S:175:ILE:HD11	2.32	0.64
1:S:25:ALA:CB	1:S:47:ASP:OD2	2.44	0.64
1:A:171:TYR:CZ	1:A:175:ILE:HD11	2.32	0.64
1:B:25:ALA:CB	1:B:47:ASP:OD2	2.51	0.64
1:S:271:LEU:HD13	3:S:344:UNL:C1B	2.27	0.64
2:B:343:NAD:O2N	2:B:343:NAD:N7N	3.70	0.64
3:B:344:UNL:C5B	3:B:344:UNL:C6	4.10	0.64
1:S:304:ARG:HG3	1:S:305:HIS:CD2	2.32	0.64
1:A:102:GLY:O	1:A:103:SER:HB3	1.97	0.63
1:S:20:LEU:HD13	1:S:88:VAL:HG13	1.80	0.63
1:A:234:ARG:HH11	1:A:234:ARG:HG2	1.63	0.63
1:S:119:ILE:HG13	1:S:169:THR:HG22	1.81	0.63
2:S:343:NAD:N7N	2:S:343:NAD:O2N	2.30	0.62
1:B:227:ASN:OD1	3:B:344:UNL:N3	4.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:CZ	1:S:109:VAL:HG21	48.08	0.62
1:S:245:MET:HE1	1:S:313:ALA:HB1	1.82	0.62
1:S:271:LEU:HD11	3:S:344:UNL:C1B	2.30	0.61
1:S:130:LYS:HE3	1:S:184:TYR:CD1	2.35	0.61
1:B:119:ILE:HG13	1:B:169:THR:HG22	1.82	0.61
1:S:149:HIS:HD2	1:S:151:ALA:H	1.49	0.60
1:B:244:GLN:HG2	1:B:248:LEU:HD22	1.82	0.60
1:B:244:GLN:HE21	1:B:248:LEU:HD21	1.66	0.60
1:S:107:SER:HB2	1:S:165:PRO:HB2	1.83	0.60
1:A:244:GLN:HE21	1:A:248:LEU:HD21	1.67	0.60
1:B:149:HIS:HD2	1:B:151:ALA:H	1.54	0.60
1:S:225:TYR:O	3:S:344:UNL:N3	2.34	0.60
1:B:245:MET:HE1	1:B:313:ALA:HB1	1.87	0.59
1:B:130:LYS:HE3	1:B:184:TYR:CD1	2.38	0.59
1:S:244:GLN:HG2	1:S:248:LEU:HD22	1.85	0.59
1:B:225:TYR:O	3:B:344:UNL:N3	2.69	0.59
1:B:234:ARG:HG2	1:B:234:ARG:HH11	1.68	0.58
1:B:116:ALA:O	1:B:120:THR:HB	2.10	0.58
1:A:25:ALA:CB	1:A:47:ASP:OD2	2.51	0.58
1:A:245:MET:HE1	1:A:313:ALA:HB1	1.86	0.58
1:B:244:GLN:HG2	1:B:248:LEU:CD2	2.34	0.58
1:A:244:GLN:HG2	1:A:248:LEU:HD22	1.85	0.58
1:A:244:GLN:HG2	1:A:248:LEU:CD2	2.34	0.58
1:B:31:ASN:HB3	1:B:243:ILE:HD11	1.85	0.57
1:S:244:GLN:HE21	1:S:248:LEU:HD21	1.70	0.57
1:A:227:ASN:OD1	3:A:343:UNL:C2	2.52	0.57
1:S:78:ASP:OD1	1:S:80:ARG:HB2	2.05	0.57
1:S:234:ARG:HH11	1:S:234:ARG:HG2	1.70	0.57
1:A:130:LYS:HE3	1:A:184:TYR:CD1	2.40	0.57
1:A:31:ASN:HB3	1:A:243:ILE:HD11	1.85	0.57
1:B:152:LEU:HD11	1:B:305:HIS:HB3	1.87	0.56
1:S:244:GLN:HG2	1:S:248:LEU:CD2	2.35	0.56
1:B:227:ASN:OD1	1:B:296:ARG:NE	2.38	0.56
1:S:271:LEU:CD1	3:S:344:UNL:O2'	2.54	0.56
1:A:152:LEU:HD11	1:A:305:HIS:HB3	1.88	0.56
1:S:152:LEU:HD11	1:S:305:HIS:HB3	1.86	0.56
1:A:119:ILE:HG13	1:A:169:THR:HG22	1.88	0.56
1:B:271:LEU:CD2	3:B:344:UNL:O4B	3.39	0.55
1:S:226:ILE:HA	3:S:344:UNL:O2	2.06	0.55
1:S:227:ASN:N	3:S:344:UNL:O2	2.36	0.55
1:B:52:GLY:HA3	2:B:343:NAD:O3B	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ILE:O	1:B:287:HIS:CD2	2.61	0.55
1:A:285:ILE:O	1:A:287:HIS:CD2	2.60	0.55
1:B:137:PHE:HB3	1:B:188:THR:HG22	1.88	0.55
1:S:31:ASN:HB3	1:S:243:ILE:HD11	1.89	0.55
1:A:149:HIS:HD2	1:A:151:ALA:H	1.54	0.55
1:S:116:ALA:O	1:S:120:THR:HB	2.06	0.55
1:S:285:ILE:O	1:S:287:HIS:CD2	2.60	0.54
1:B:78:ASP:OD1	1:B:80:ARG:HB2	2.09	0.54
1:A:109:VAL:HG21	1:B:13:ILE:HG22	1.89	0.54
1:A:149:HIS:CE1	1:A:158:ASN:HB3	2.42	0.54
1:S:161:ASN:HD22	1:S:161:ASN:N	2.06	0.54
1:A:137:PHE:HB3	1:A:188:THR:HG22	1.89	0.54
1:B:193:TYR:HB2	2:B:343:NAD:C5N	2.38	0.54
1:S:119:ILE:HD13	1:S:172:VAL:HG11	1.91	0.53
1:A:116:ALA:O	1:A:120:THR:HB	2.09	0.53
1:A:51:THR:OG1	2:A:344:NAD:O2A	2.22	0.52
1:A:51:THR:HG22	1:B:7:GLU:OE1	2.09	0.52
1:B:28:ILE:HD12	2:B:343:NAD:H51N	3.06	0.52
1:A:299:ARG:HB2	1:A:302:ASP:HB3	1.91	0.52
1:B:330:ARG:HH11	1:B:330:ARG:HG2	1.75	0.52
1:S:137:PHE:HB3	1:S:188:THR:HG22	1.90	0.52
1:B:161:ASN:N	1:B:161:ASN:HD22	2.17	0.52
1:S:299:ARG:HB2	1:S:302:ASP:HB2	1.92	0.52
1:S:271:LEU:HD21	3:S:344:UNL:O4B	2.09	0.52
1:A:78:ASP:OD1	1:A:80:ARG:HB2	2.09	0.52
1:A:230:GLY:O	1:A:272:ASN:ND2	2.43	0.52
1:S:330:ARG:HG2	1:S:330:ARG:HH11	1.73	0.52
1:A:330:ARG:HH11	1:A:330:ARG:HG2	1.75	0.51
1:S:227:ASN:OD1	3:S:344:UNL:C2	2.59	0.51
1:A:65:SER:HB3	1:A:68:GLN:OE1	2.10	0.51
1:B:299:ARG:HB2	1:B:302:ASP:HB2	1.94	0.51
1:B:302:ASP:OD1	3:B:344:UNL:O3B	2.29	0.51
1:A:149:HIS:CD2	1:A:150:PRO:HD2	2.45	0.51
1:B:230:GLY:O	1:B:272:ASN:ND2	2.44	0.51
1:S:109:VAL:HG12	1:S:110:ASP:N	2.26	0.51
1:S:194:PHE:CE2	1:S:308:ALA:HB2	2.46	0.51
1:B:212:PRO:HB3	1:B:336:TYR:OH	2.10	0.51
1:B:149:HIS:CE1	1:B:158:ASN:HB3	2.46	0.50
1:B:194:PHE:CE2	1:B:308:ALA:HB2	2.50	0.50
1:A:212:PRO:HB3	1:A:336:TYR:OH	2.11	0.50
3:A:343:UNL:O5B	3:A:343:UNL:O1B	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:H	1:B:239:ILE:HD11	1.81	0.50
1:S:149:HIS:CE1	1:S:158:ASN:HB3	2.47	0.50
1:S:230:GLY:O	1:S:272:ASN:ND2	2.45	0.49
1:S:219:LEU:HD12	1:S:340:LEU:HD12	1.94	0.49
1:B:338:ARG:O	1:B:341:LYS:HG2	2.15	0.49
1:B:149:HIS:CD2	1:B:150:PRO:HD2	2.48	0.48
2:B:343:NAD:O5D	2:B:343:NAD:H2N	2.76	0.48
1:S:338:ARG:O	1:S:341:LYS:HG2	2.14	0.48
1:A:285:ILE:O	1:A:287:HIS:HD2	1.97	0.48
1:B:285:ILE:O	1:B:285:ILE:CG2	2.61	0.48
1:B:285:ILE:O	1:B:287:HIS:HD2	1.97	0.47
1:B:219:LEU:HD12	1:B:340:LEU:HD12	1.96	0.47
1:A:219:LEU:HD12	1:A:340:LEU:HD12	1.96	0.47
1:A:299:ARG:NH2	3:A:343:UNL:C2B	2.77	0.47
1:B:227:ASN:N	3:B:344:UNL:O2	2.64	0.47
1:B:109:VAL:HG12	1:B:110:ASP:N	2.31	0.47
1:A:245:MET:HE1	1:A:319:TYR:CG	2.49	0.47
1:S:245:MET:HG2	1:S:263:VAL:CG2	2.41	0.47
1:A:285:ILE:O	1:A:285:ILE:CG2	2.62	0.47
1:A:103:SER:OG	1:A:105:PRO:HD2	2.14	0.46
1:B:119:ILE:HD11	1:B:169:THR:HA	1.98	0.46
1:A:109:VAL:HG12	1:A:110:ASP:N	2.30	0.46
1:B:210:VAL:HB	3:B:344:UNL:C5B	2.99	0.46
3:B:344:UNL:O5B	3:B:344:UNL:O1B	2.33	0.46
1:A:23:GLY:HA2	2:A:344:NAD:H1B	1.97	0.46
1:A:5:TYR:CG	1:A:244:GLN:HG3	2.51	0.46
1:S:285:ILE:O	1:S:287:HIS:HD2	1.97	0.46
1:A:194:PHE:CE2	1:A:308:ALA:HB2	2.49	0.46
1:S:79:ILE:HG13	1:S:121:GLY:HA3	1.98	0.46
1:A:338:ARG:O	1:A:341:LYS:HG2	2.14	0.46
1:S:109:VAL:CG1	1:S:110:ASP:N	2.77	0.46
1:S:285:ILE:O	1:S:285:ILE:CG2	2.61	0.46
1:B:65:SER:HB3	1:B:68:GLN:CD	2.39	0.46
1:B:5:TYR:CG	1:B:244:GLN:HG3	2.51	0.46
1:S:271:LEU:HD11	3:S:344:UNL:C2B	2.46	0.45
1:B:47:ASP:OD1	1:B:74:PHE:CE1	2.70	0.45
1:B:20:LEU:CD1	1:B:88:VAL:HG13	2.46	0.45
1:A:52:GLY:HA3	2:A:344:NAD:O3B	2.16	0.45
1:A:171:TYR:CE2	1:A:175:ILE:HD11	2.51	0.45
1:S:149:HIS:CD2	1:S:150:PRO:HD2	2.52	0.45
1:A:299:ARG:O	1:A:302:ASP:CG	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:48:ASN:HB3	1:S:77:GLY:O	2.17	0.45
1:S:152:LEU:HD11	1:S:305:HIS:CB	2.47	0.45
2:S:343:NAD:H2N	2:S:343:NAD:O5D	2.16	0.45
1:B:119:ILE:HD13	1:B:172:VAL:HG11	2.06	0.45
1:S:199:ARG:H	1:S:239:ILE:HD11	1.82	0.45
1:S:171:TYR:CE2	1:S:175:ILE:HD11	2.52	0.44
1:S:210:VAL:HG13	1:S:211:ILE:N	2.32	0.44
1:S:227:ASN:N	1:S:227:ASN:OD1	2.50	0.44
1:A:234:ARG:HG2	1:A:234:ARG:NH1	2.31	0.44
1:B:210:VAL:HG13	1:B:211:ILE:N	2.35	0.44
1:A:20:LEU:CD1	1:A:88:VAL:HG13	2.47	0.44
1:S:65:SER:HB3	1:S:68:GLN:CD	2.36	0.44
1:S:286:HIS:O	1:S:287:HIS:CD2	2.71	0.44
1:B:48:ASN:HB3	1:B:77:GLY:O	2.18	0.44
1:B:286:HIS:O	1:B:287:HIS:CD2	2.73	0.44
1:A:119:ILE:HD11	1:A:169:THR:HA	2.00	0.44
1:A:109:VAL:CG1	1:A:110:ASP:N	2.78	0.44
1:B:152:LEU:HD11	1:B:305:HIS:CB	2.48	0.44
1:A:6:GLU:O	1:A:10:GLN:HG2	2.18	0.43
1:A:65:SER:HB3	1:A:68:GLN:CG	2.48	0.43
1:B:245:MET:HE1	1:B:319:TYR:CG	2.53	0.43
1:A:161:ASN:N	1:A:161:ASN:HD22	2.16	0.43
1:B:227:ASN:N	1:B:227:ASN:OD1	3.26	0.43
1:B:65:SER:HB3	1:B:68:GLN:CG	2.48	0.43
1:A:5:TYR:CD2	1:A:244:GLN:HG3	2.53	0.43
1:A:48:ASN:HB3	1:A:77:GLY:O	2.19	0.43
1:A:89:MET:O	1:A:90:LYS:C	2.57	0.43
1:B:245:MET:HG2	1:B:263:VAL:CG2	2.43	0.43
1:A:155:VAL:HG12	1:A:157:GLU:OE2	2.18	0.43
1:A:199:ARG:H	1:A:239:ILE:HD11	1.84	0.43
1:B:6:GLU:O	1:B:10:GLN:HG2	2.19	0.43
1:B:109:VAL:CG1	1:B:110:ASP:N	2.79	0.43
1:A:152:LEU:HD11	1:A:305:HIS:CB	2.49	0.42
1:B:125:ILE:HD13	1:B:125:ILE:HA	1.88	0.42
1:A:109:VAL:CG2	1:B:13:ILE:HG22	2.50	0.42
1:S:232:THR:CG2	1:S:234:ARG:HH12	2.32	0.42
1:B:161:ASN:HA	1:B:162:PRO:HD3	1.76	0.42
1:B:171:TYR:CE2	1:B:175:ILE:HD11	2.55	0.42
1:A:96:LEU:HD22	1:A:246:ASN:OD1	2.19	0.42
1:S:161:ASN:HA	1:S:162:PRO:HD3	1.75	0.42
1:B:232:THR:CG2	1:B:234:ARG:HH12	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:SER:HB3	1:A:68:GLN:CD	2.40	0.42
1:A:286:HIS:O	1:A:287:HIS:CD2	2.73	0.42
1:B:89:MET:O	1:B:90:LYS:C	2.58	0.42
1:B:67:GLU:CB	1:S:109:VAL:HG22	47.06	0.41
1:B:214:TRP:CD1	1:B:224:VAL:HG13	2.55	0.41
1:A:125:ILE:HA	1:A:125:ILE:HD13	1.90	0.41
1:B:50:SER:OG	2:B:343:NAD:H2B	2.40	0.41
1:A:123:LEU:HG	1:S:112:ILE:HD13	2.02	0.41
1:A:228:GLY:HA3	1:A:298:PHE:CD1	2.56	0.41
1:B:155:VAL:HG12	1:B:157:GLU:OE2	2.20	0.41
1:B:274:LEU:O	1:B:278:ILE:HG13	2.23	0.41
1:B:47:ASP:CG	1:B:74:PHE:CE1	2.94	0.41
1:B:52:GLY:CA	2:B:343:NAD:O3B	2.68	0.41
1:S:212:PRO:HB3	1:S:336:TYR:OH	2.19	0.41
1:A:227:ASN:N	3:A:343:UNL:O2	2.50	0.41
1:B:234:ARG:NH1	1:B:234:ARG:HG2	2.34	0.41
1:A:119:ILE:HD13	1:A:172:VAL:HG11	2.02	0.41
1:A:31:ASN:OD1	1:A:239:ILE:HD12	2.21	0.41
1:A:161:ASN:HA	1:A:162:PRO:HD3	1.76	0.41
1:B:71:ARG:HH22	1:S:109:VAL:HB	45.37	0.41
1:A:47:ASP:OD1	1:A:74:PHE:CE1	2.74	0.41
1:B:10:GLN:HE21	1:B:10:GLN:HB3	1.70	0.41
1:B:103:SER:OG	1:B:105:PRO:HD2	2.20	0.41
1:B:5:TYR:CD2	1:B:244:GLN:HG3	2.56	0.41
1:B:333:MET:CE	1:B:333:MET:HA	2.51	0.41
1:A:227:ASN:OD1	1:A:227:ASN:N	2.54	0.41
1:B:227:ASN:H	3:B:344:UNL:C2	2.45	0.41
1:B:79:ILE:HG13	1:B:121:GLY:HA3	2.05	0.41
1:S:57:LEU:HD11	1:S:74:PHE:CE1	2.56	0.40
1:S:5:TYR:CG	1:S:244:GLN:HG3	2.56	0.40
1:A:245:MET:HE1	1:A:319:TYR:CD2	2.57	0.40
1:A:210:VAL:HG13	1:A:211:ILE:N	2.36	0.40
1:S:47:ASP:OD1	1:S:74:PHE:CE1	2.75	0.40
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.96	0.40
1:B:228:GLY:HA3	1:B:298:PHE:CD1	2.57	0.40
1:A:47:ASP:C	1:A:47:ASP:OD1	2.60	0.40
1:S:130:LYS:HE3	1:S:184:TYR:CG	2.56	0.40
1:B:202:ASP:HA	1:B:203:PRO:HD3	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PHE:CD2	1:B:207:TYR:OH[1_455]	2.14	0.06

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%)	312 (94%)	17 (5%)	3 (1%)	21	55
1	B	332/351 (95%)	312 (94%)	17 (5%)	3 (1%)	21	55
1	S	332/351 (95%)	309 (93%)	21 (6%)	2 (1%)	30	65
1	b	332/351 (95%)	310 (93%)	20 (6%)	2 (1%)	30	65
All	All	1328/1404 (95%)	1243 (94%)	75 (6%)	10 (1%)	24	58

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	B	227	ASN
1	S	227	ASN
1	b	227	ASN
1	A	227	ASN
1	B	103	SER
1	A	103	SER
1	S	103	SER
1	b	103	SER
1	B	65	SER

5.3.2 Protein sidechains [i](#)

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%)	272 (94%)	18 (6%)	23	54
1	B	290/304 (95%)	272 (94%)	18 (6%)	23	54
1	S	290/304 (95%)	272 (94%)	18 (6%)	23	54
1	b	290/304 (95%)	272 (94%)	18 (6%)	23	54
All	All	1160/1216 (95%)	1088 (94%)	72 (6%)	23	54

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	15	SER
1	A	46	LEU
1	A	66	THR
1	A	78	ASP
1	A	87	GLN
1	A	88	VAL
1	A	109	VAL
1	A	157	GLU
1	A	176	TYR
1	A	227	ASN
1	A	239	ILE
1	A	248	LEU
1	A	251	LEU
1	A	265	VAL
1	A	284	LEU
1	A	311	THR
1	A	315	ASP
1	B	10	GLN
1	B	15	SER
1	B	46	LEU
1	B	66	THR
1	B	78	ASP
1	B	87	GLN
1	B	88	VAL
1	B	109	VAL
1	B	157	GLU
1	B	176	TYR
1	B	182	ARG
1	B	239	ILE
1	B	248	LEU

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Mol	Chain	Res	Type
1	B	251	LEU
1	B	265	VAL
1	B	284	LEU
1	B	311	THR
1	B	315	ASP
1	S	10	GLN
1	S	15	SER
1	S	46	LEU
1	S	66	THR
1	S	87	GLN
1	S	88	VAL
1	S	109	VAL
1	S	157	GLU
1	S	176	TYR
1	S	182	ARG
1	S	227	ASN
1	S	239	ILE
1	S	248	LEU
1	S	251	LEU
1	S	265	VAL
1	S	284	LEU
1	S	311	THR
1	S	315	ASP
1	b	10	GLN
1	b	15	SER
1	b	46	LEU
1	b	66	THR
1	b	87	GLN
1	b	88	VAL
1	b	109	VAL
1	b	157	GLU
1	b	176	TYR
1	b	182	ARG
1	b	227	ASN
1	b	239	ILE
1	b	248	LEU
1	b	251	LEU
1	b	265	VAL
1	b	284	LEU
1	b	311	THR
1	b	315	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	GLN
1	A	149	HIS
1	A	161	ASN
1	A	244	GLN
1	A	287	HIS
1	B	10	GLN
1	B	11	GLN
1	B	149	HIS
1	B	161	ASN
1	B	244	GLN
1	B	287	HIS
1	S	10	GLN
1	S	11	GLN
1	S	149	HIS
1	S	161	ASN
1	S	244	GLN
1	S	287	HIS
1	b	10	GLN
1	b	11	GLN
1	b	149	HIS
1	b	161	ASN
1	b	244	GLN
1	b	287	HIS

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 8 ligands modelled in this entry, 4 are unknown - leaving 4 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	344	-	38,48,48	1.75	13 (34%)	47,73,73	2.43	13 (27%)
2	NAD	B	343	-	38,48,48	0.69	0	47,73,73	1.89	5 (10%)
2	NAD	S	343	-	38,48,48	0.71	0	47,73,73	1.82	4 (8%)
2	NAD	b	343	-	38,48,48	0.71	0	47,73,73	1.78	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	NAD	A	344	-	-	0/22/62/62	0/5/5/5
2	NAD	B	343	-	-	0/22/62/62	0/5/5/5
2	NAD	S	343	-	-	0/22/62/62	0/5/5/5
2	NAD	b	343	-	-	0/22/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	344	NAD	PA-O2A	-3.07	1.41	1.54
2	A	344	NAD	PN-O2N	-2.99	1.42	1.54
2	A	344	NAD	O4B-C4B	-2.88	1.38	1.45
2	A	344	NAD	PN-O1N	-2.79	1.41	1.51
2	A	344	NAD	O4D-C1D	-2.72	1.37	1.41
2	A	344	NAD	PN-O5D	-2.69	1.46	1.59
2	A	344	NAD	C5A-N7A	-2.47	1.31	1.39
2	A	344	NAD	PA-O1A	-2.44	1.42	1.51
2	A	344	NAD	C2D-C3D	-2.42	1.46	1.53
2	A	344	NAD	C5A-C4A	-2.21	1.35	1.40
2	A	344	NAD	C4A-N3A	-2.19	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	344	NAD	PA-O5B	-2.07	1.49	1.59
2	A	344	NAD	O5D-C5D	-2.05	1.36	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	344	NAD	N3A-C2A-N1A	-10.48	120.87	128.89
2	B	343	NAD	N3A-C2A-N1A	-9.86	121.35	128.89
2	b	343	NAD	N3A-C2A-N1A	-9.72	121.45	128.89
2	S	343	NAD	N3A-C2A-N1A	-9.52	121.61	128.89
2	A	344	NAD	C4D-O4D-C1D	-5.22	103.98	109.72
2	S	343	NAD	PN-O3-PA	-4.27	120.75	132.73
2	b	343	NAD	PN-O3-PA	-4.17	121.03	132.73
2	B	343	NAD	PN-O3-PA	-4.06	121.32	132.73
2	A	344	NAD	O4D-C1D-N1N	-3.90	103.84	108.13
2	A	344	NAD	O3D-C3D-C2D	-3.13	101.65	111.83
2	A	344	NAD	O4B-C1B-N9A	-3.10	101.62	108.10
2	A	344	NAD	C4A-C5A-N7A	-2.76	106.94	109.48
2	S	343	NAD	C4A-C5A-N7A	-2.37	107.30	109.48
2	A	344	NAD	C3N-C7N-N7N	-2.35	115.24	117.82
2	b	343	NAD	C4A-C5A-N7A	-2.35	107.32	109.48
2	B	343	NAD	C4A-C5A-N7A	-2.26	107.40	109.48
2	A	344	NAD	C4B-O4B-C1B	-2.23	107.27	109.72
2	A	344	NAD	O4B-C4B-C3B	-2.21	100.69	105.15
2	A	344	NAD	O7N-C7N-N7N	2.02	125.44	122.59
2	A	344	NAD	O5B-C5B-C4B	2.13	116.96	109.12
2	B	343	NAD	C2N-C3N-C4N	2.24	120.79	118.29
2	B	343	NAD	O4D-C1D-N1N	3.21	111.65	108.13
2	S	343	NAD	O4D-C1D-N1N	3.29	111.75	108.13
2	A	344	NAD	C2N-C3N-C4N	3.65	122.35	118.29
2	A	344	NAD	C2B-C1B-N9A	5.24	122.30	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	344	NAD	4	0
2	B	343	NAD	7	0
2	S	343	NAD	2	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, 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%)	0.25	11 (3%) 50 38	51, 69, 117, 148	0
1	B	336/351 (95%)	0.26	12 (3%) 46 34	51, 69, 117, 148	0
1	S	336/351 (95%)	0.33	25 (7%) 17 9	51, 70, 118, 148	0
1	b	336/351 (95%)	0.41	22 (6%) 22 13	51, 69, 117, 149	0
All	All	1344/1404 (95%)	0.31	70 (5%) 31 20	51, 69, 118, 149	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	b	2	MET	8.1
1	b	300	SER	7.5
1	b	47	ASP	5.9
1	S	2	MET	5.7
1	S	226	ILE	4.6
1	S	47	ASP	4.2
1	A	47	ASP	4.2
1	b	295	TYR	4.0
1	A	32	LEU	3.9
1	A	14	PHE	3.8
1	S	1	TYR	3.7
1	S	224	VAL	3.6
1	b	301	GLY	3.5
1	S	232	THR	3.3
1	A	302	ASP	3.2
1	S	15	SER	3.2
1	S	275	SER	3.2
1	b	318	LYS	3.1
1	b	196	VAL	3.0
1	B	215	THR	2.9
1	B	207	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	298	PHE	2.8
1	S	340	LEU	2.8
1	S	314	ILE	2.7
1	b	215	THR	2.7
1	B	336	TYR	2.7
1	A	301	GLY	2.7
1	A	211	ILE	2.6
1	S	211	ILE	2.6
1	A	269	THR	2.5
1	S	71	ARG	2.5
1	B	208	ALA	2.5
1	A	215	THR	2.5
1	B	44	ILE	2.5
1	b	71	ARG	2.4
1	B	47	ASP	2.4
1	b	213	LYS	2.4
1	b	286	HIS	2.4
1	A	206	ALA	2.3
1	S	225	TYR	2.3
1	S	218	MET	2.3
1	S	101	LEU	2.3
1	b	210	VAL	2.3
1	b	74	PHE	2.3
1	b	207	TYR	2.3
1	b	227	ASN	2.3
1	B	300	SER	2.2
1	S	329	LEU	2.2
1	B	159	ILE	2.2
1	B	211	ILE	2.2
1	B	242	VAL	2.2
1	S	271	LEU	2.2
1	S	229	ASP	2.2
1	S	213	LYS	2.2
1	b	294	LYS	2.2
1	S	295	TYR	2.2
1	b	77	GLY	2.2
1	b	214	TRP	2.1
1	S	300	SER	2.1
1	A	213	LYS	2.1
1	b	329	LEU	2.1
1	S	171	TYR	2.1
1	S	100	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	298	PHE	2.1
1	A	278	ILE	2.1
1	B	226	ILE	2.1
1	S	332	SER	2.0
1	b	10	GLN	2.0
1	b	278	ILE	2.0
1	b	297	GLU	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	b	343	44/44	0.92	0.20	-0.33	61,63,70,70	0
2	NAD	B	343	44/44	0.92	0.18	-0.49	59,60,65,66	0
2	NAD	A	344	44/44	0.91	0.17	-0.61	54,58,64,66	0
2	NAD	S	343	44/44	0.94	0.16	-0.77	59,62,68,68	0
3	UNL	b	344	25/-	0.86	0.21	-0.83	75,78,79,79	0
3	UNL	S	344	25/-	0.85	0.18	-0.98	77,79,80,80	0
3	UNL	B	344	25/-	0.93	0.18	-1.09	78,83,84,85	0
3	UNL	A	343	25/-	0.91	0.14	-1.23	80,85,86,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.