



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 08:57 AM EDT

PDB ID : 2GN4  
Title : Crystal structure of UDP-GlcNAc inverting 4,6-dehydratase in complex with NADPH and UDP-GlcNAc  
Authors : Ishiyama, N.; Creuzenet, C.; Lam, J.S.; Berghuis, A.M.  
Deposited on : unknown  
Resolution : 1.90 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 : rb-20030345  
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) : rb-20030345

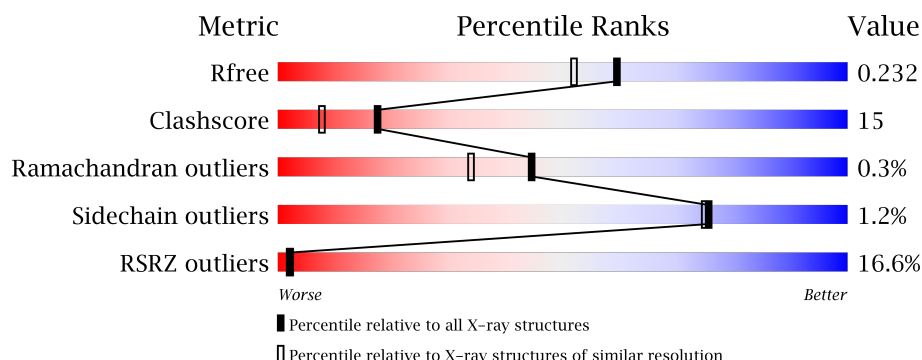
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	344	<div> <div>17%</div> <div>69%</div> <div>26%</div> <div>• •</div> </div>
1	B	344	<div> <div>15%</div> <div>71%</div> <div>24%</div> <div>5%</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
4	MES	B	337	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5719 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-GlcNAc C6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	3	0
			2615	1670	445	484	16			
1	B	327	Total	C	N	O	S	0	3	0
			2598	1661	441	480	16			

There are 22 discrepancies between the modelled and reference sequences:

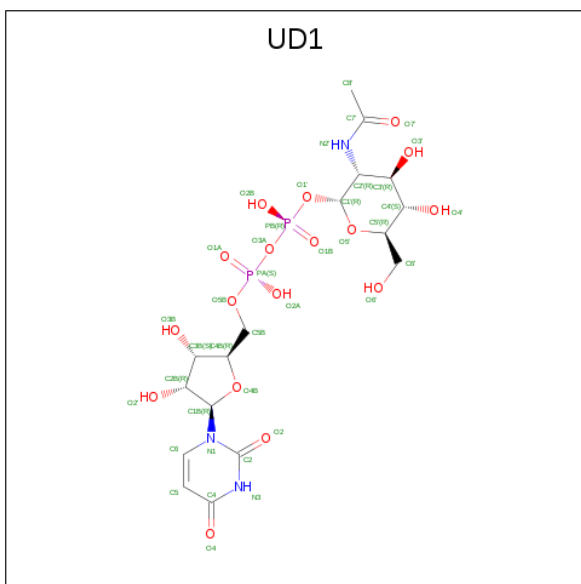
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	cloning artifact	UNP O25511
A	-9	HIS	-	EXPRESSION TAG	UNP O25511
A	-8	HIS	-	EXPRESSION TAG	UNP O25511
A	-7	HIS	-	EXPRESSION TAG	UNP O25511
A	-6	HIS	-	EXPRESSION TAG	UNP O25511
A	-5	HIS	-	EXPRESSION TAG	UNP O25511
A	-4	HIS	-	EXPRESSION TAG	UNP O25511
A	-3	GLY	-	cloning artifact	UNP O25511
A	-2	SER	-	cloning artifact	UNP O25511
A	-1	MET	-	cloning artifact	UNP O25511
A	0	SER	-	cloning artifact	UNP O25511
B	-10	MET	-	cloning artifact	UNP O25511
B	-9	HIS	-	EXPRESSION TAG	UNP O25511
B	-8	HIS	-	EXPRESSION TAG	UNP O25511
B	-7	HIS	-	EXPRESSION TAG	UNP O25511
B	-6	HIS	-	EXPRESSION TAG	UNP O25511
B	-5	HIS	-	EXPRESSION TAG	UNP O25511
B	-4	HIS	-	EXPRESSION TAG	UNP O25511
B	-3	GLY	-	cloning artifact	UNP O25511
B	-2	SER	-	cloning artifact	UNP O25511
B	-1	MET	-	cloning artifact	UNP O25511
B	0	SER	-	cloning artifact	UNP O25511

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula:  $C_{17}H_{27}N_3O_{17}P_2$ ).



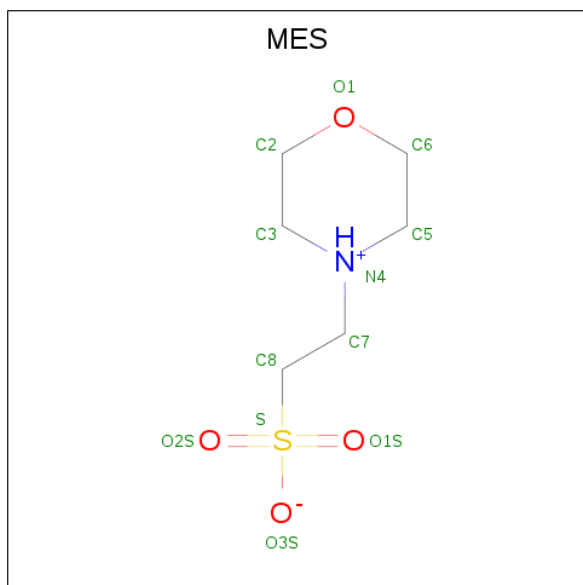
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

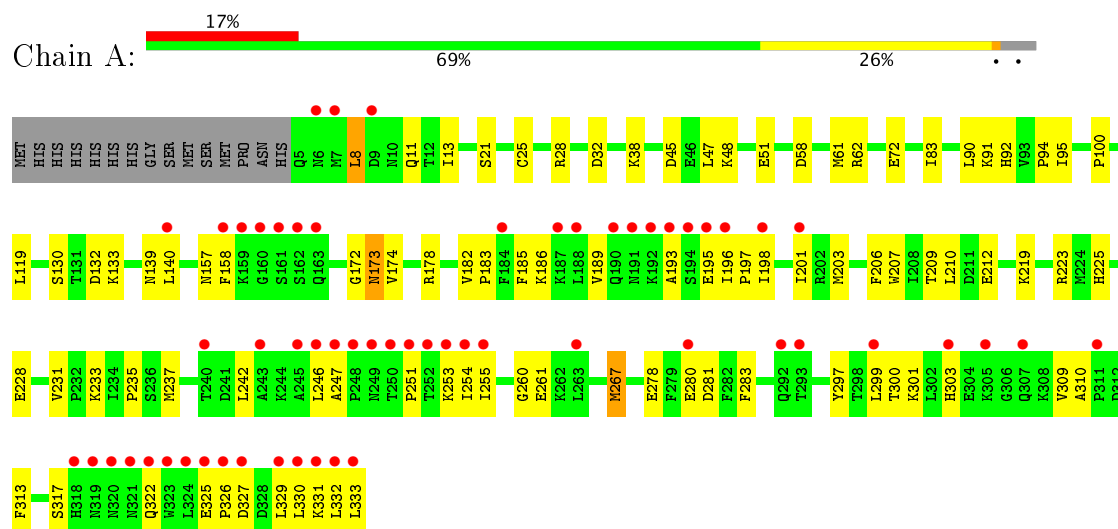
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total	O	0	0
			145	145		
5	B	163	Total	O	0	0
			163	163		

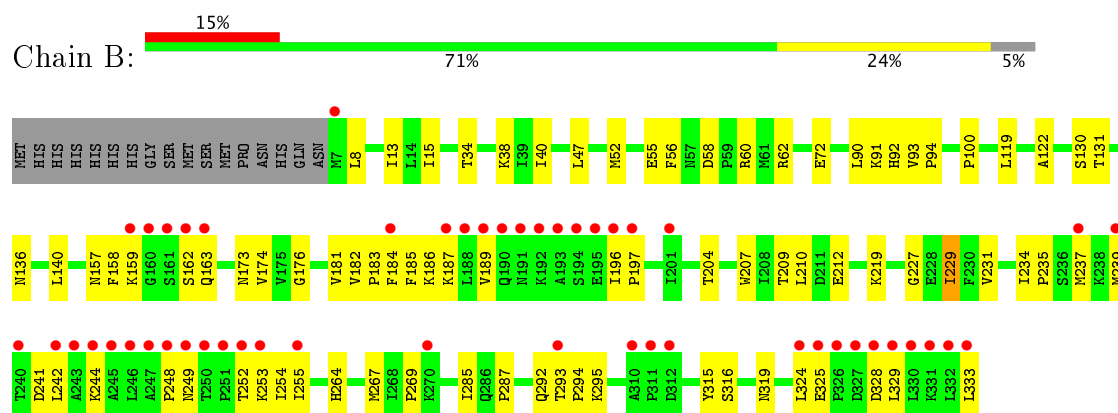
### 3 Residue-property plots [i](#)

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-GlcNAc C6 dehydratase



#### • Molecule 1: UDP-GlcNAc C6 dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.36Å 111.36Å 107.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 49.49 – 1.89	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-1.90) 94.9 (49.49-1.89)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.197 , 0.229 0.200 , 0.232	Depositor DCC
$R_{free}$ test set	5824 reflections (10.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: NDP, UD1, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/2667	0.57	1/3603 (0.0%)
1	B	0.31	0/2650	0.59	2/3580 (0.1%)
All	All	0.31	0/5317	0.58	3/7183 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	LEU	N-CA-C	-5.74	95.50	111.00
1	A	90	LEU	N-CA-C	-5.59	95.89	111.00
1	B	229	ILE	N-CA-C	-5.00	97.49	111.00

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	2615	0	2656	89	0
1	B	2598	0	2642	78	0
2	A	48	0	26	2	0
2	B	48	0	26	1	0
3	A	39	0	25	2	0
3	B	39	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	26	0	0
5	A	145	0	0	6	0
5	B	163	0	0	7	0
All	All	5719	0	5426	167	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 15.

All (167) 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:242:LEU:HD13	1:B:329:LEU:HD21	1.42	1.02
1:A:189:VAL:HA	1:A:193:ALA:HB2	1.45	0.99
1:A:223:ARG:HB2	1:A:300:THR:HB	1.54	0.88
1:B:8:LEU:HD12	1:B:34:THR:HG21	1.61	0.80
1:A:92[A]:HIS:CE1	1:A:94:PRO:HG2	2.17	0.79
1:A:223:ARG:HA	1:A:301:LYS:HB2	1.68	0.74
1:B:231:VAL:HG13	1:B:267:MET:HG2	1.71	0.71
1:B:184:PHE:HA	1:B:187:LYS:HE2	1.72	0.70
1:B:174:VAL:HG11	1:B:210:LEU:HD13	1.73	0.70
1:B:237:MET:SD	1:B:329:LEU:HD22	2.32	0.70
1:B:196:ILE:HB	1:B:252:THR:HG22	1.73	0.70
1:A:203:MET:HE3	1:A:261:GLU:OE2	1.91	0.70
1:B:100:PRO:HA	1:B:140:LEU:HD22	1.73	0.70
1:B:231:VAL:CG1	1:B:267:MET:HG2	2.21	0.69
1:A:38:LYS:HD2	1:A:62:ARG:HG3	1.73	0.69
1:A:197:PRO:HB3	1:A:255:ILE:HD12	1.74	0.69
1:B:186:LYS:HZ3	1:B:333:LEU:HG	1.59	0.68
1:B:176:GLY:HA2	1:B:183:PRO:HD3	1.75	0.68
1:A:309:VAL:HG12	1:A:310:ALA:H	1.60	0.67
1:A:182:VAL:HB	1:A:183:PRO:HD3	1.77	0.67
1:A:242:LEU:HD12	1:A:329:LEU:HD22	1.76	0.66
1:A:173:ASN:H	1:A:173:ASN:HD22	1.43	0.66
1:B:159:LYS:HE3	1:B:292:GLN:HB2	1.77	0.66
1:B:38:LYS:NZ	1:B:62:ARG:HH11	1.94	0.66
1:B:55:GLU:HG3	1:B:56:PHE:CD1	2.31	0.66
1:A:100:PRO:HA	1:A:140:LEU:HD22	1.79	0.65
1:A:196:ILE:HD11	1:A:247:ALA:HB3	1.78	0.65
1:A:173:ASN:N	1:A:173:ASN:HD22	1.95	0.65
1:A:8:LEU:HD11	1:A:13:ILE:HD11	1.77	0.65
1:B:119:LEU:HD22	1:B:158:PHE:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:GLU:HB3	1:A:326:PRO:HD2	1.78	0.65
1:B:136:ASN:HD21	1:B:269:PRO:HB3	1.61	0.64
1:B:316:SER:HB2	1:B:319:ASN:OD1	1.97	0.64
1:A:225:HIS:ND1	1:A:301:LYS:HE3	2.13	0.63
1:B:55:GLU:HG3	1:B:56:PHE:HD1	1.62	0.63
1:B:186:LYS:NZ	1:B:333:LEU:HG	2.13	0.63
1:A:130:SER:O	2:A:334:NDP:H6N	1.98	0.62
1:A:174:VAL:HG11	1:A:210:LEU:HD13	1.81	0.62
1:B:237:MET:HE3	1:B:324:LEU:HG	1.82	0.62
1:B:184:PHE:HA	1:B:187:LYS:CE	2.32	0.60
1:B:100:PRO:HA	1:B:140:LEU:CD2	2.31	0.59
1:B:93:VAL:HB	1:B:94:PRO:HD3	1.85	0.58
1:A:235:PRO:HA	1:A:322:GLN:HG3	1.84	0.58
1:B:52:MET:HA	1:B:55:GLU:HG2	1.85	0.57
1:B:242:LEU:HD13	1:B:329:LEU:CD2	2.27	0.57
1:A:195:GLU:HG2	1:A:253:LYS:HB2	1.86	0.57
1:A:242:LEU:HD12	1:A:329:LEU:CD2	2.35	0.57
1:A:309:VAL:HG11	1:A:313:PHE:CG	2.40	0.56
1:B:219:LYS:HD2	5:B:486:HOH:O	2.06	0.56
1:A:91:LYS:HB2	3:A:335:UD1:O3'	2.06	0.56
1:B:92[B]:HIS:ND1	1:B:94:PRO:HD2	2.21	0.56
1:A:231:VAL:CG1	1:A:267:MET:HG2	2.36	0.55
1:B:209:THR:OG1	1:B:212:GLU:HG3	2.07	0.55
1:B:244:LYS:O	1:B:248:PRO:HG3	2.07	0.55
1:A:309:VAL:HG12	1:A:310:ALA:N	2.22	0.55
1:B:136:ASN:ND2	1:B:269:PRO:HB3	2.22	0.55
1:B:122:ALA:HB1	1:B:162:SER:HB2	1.88	0.55
1:A:92[A]:HIS:HE1	1:A:94:PRO:HG2	1.69	0.55
1:B:72[A]:GLU:HG3	5:B:370:HOH:O	2.06	0.54
1:B:159:LYS:HG2	5:B:485:HOH:O	2.07	0.54
1:A:48:LYS:NZ	5:A:471:HOH:O	2.40	0.54
1:A:132:ASP:OD2	1:A:172:GLY:HA2	2.08	0.54
1:A:72[A]:GLU:HG3	5:A:362:HOH:O	2.07	0.53
1:A:45:ASP:HB3	1:A:48:LYS:HE3	1.90	0.53
1:A:8:LEU:HD12	1:A:11:GLN:HB2	1.90	0.53
1:B:91:LYS:HB2	3:B:335:UD1:O3'	2.09	0.53
1:B:197:PRO:HB2	1:B:255:ILE:HD13	1.91	0.53
1:A:209:THR:OG1	1:A:212:GLU:HG3	2.08	0.52
1:B:173:ASN:HD22	1:B:173:ASN:H	1.56	0.52
1:A:231:VAL:HG13	1:A:267:MET:HG2	1.91	0.52
1:B:92[A]:HIS:HE1	5:B:382:HOH:O	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD12	1:B:242:LEU:O	2.10	0.51
1:A:235:PRO:N	1:A:322:GLN:HE21	2.08	0.51
1:B:38:LYS:HZ1	1:B:62:ARG:HH11	1.59	0.51
1:A:119:LEU:HD22	1:A:158:PHE:CD2	2.45	0.51
1:A:92[A]:HIS:HB3	1:A:95:ILE:HB	1.92	0.51
1:B:185:PHE:O	1:B:189:VAL:HG23	2.11	0.51
1:A:189:VAL:HG21	1:A:246:LEU:O	2.11	0.50
1:A:299:LEU:HD23	1:A:300:THR:O	2.11	0.50
1:B:181:VAL:HG13	1:B:182:VAL:N	2.26	0.50
1:A:196:ILE:HD11	1:A:247:ALA:CB	2.41	0.50
1:A:100:PRO:HA	1:A:140:LEU:CD2	2.41	0.50
1:A:233:LYS:HD2	1:A:281:ASP:HA	1.94	0.50
1:A:140:LEU:HG	1:A:140:LEU:O	2.09	0.49
1:A:38:LYS:HD2	1:A:62:ARG:CG	2.42	0.49
1:A:139:ASN:HB3	1:A:260:GLY:O	2.12	0.48
1:A:195:GLU:CG	1:A:253:LYS:HB2	2.43	0.48
1:A:235:PRO:HG3	1:A:322:GLN:HE21	1.79	0.47
1:B:325:GLU:HB2	1:B:328:ASP:HB2	1.94	0.47
1:B:253:LYS:HG2	1:B:254:ILE:N	2.29	0.47
1:A:58:ASP:HB3	1:A:61:MET:HG2	1.96	0.47
1:A:8:LEU:HD13	1:A:83:ILE:HD12	1.97	0.47
1:B:38:LYS:HZ2	1:B:62:ARG:HH11	1.62	0.47
1:B:100:PRO:CA	1:B:140:LEU:HD22	2.44	0.47
1:A:299:LEU:CD2	1:A:303:HIS:HA	2.45	0.47
1:A:333:LEU:C	1:A:333:LEU:HD23	2.35	0.47
1:B:237:MET:HE3	1:B:324:LEU:CG	2.44	0.47
1:B:173:ASN:HD22	1:B:173:ASN:N	2.13	0.46
1:B:204:THR:HB	1:B:264:HIS:ND1	2.30	0.46
1:A:198:ILE:O	1:A:254:ILE:HA	2.15	0.46
1:A:299:LEU:HD21	1:A:303:HIS:HA	1.96	0.46
1:B:207:TRP:CD1	1:B:237:MET:HB3	2.51	0.46
1:B:231:VAL:HG11	1:B:267:MET:HG2	1.96	0.46
1:A:278:GLU:HG3	1:A:283:PHE:CE1	2.51	0.45
1:B:92[B]:HIS:CE1	1:B:94:PRO:HD2	2.52	0.45
1:A:206:PHE:CE1	1:A:317:SER:HB3	2.51	0.45
1:B:163:GLN:NE2	5:B:429:HOH:O	2.49	0.45
1:B:8:LEU:HD22	1:B:13:ILE:HD11	1.98	0.45
1:A:195:GLU:CD	1:A:253:LYS:HB2	2.37	0.45
1:A:195:GLU:HA	1:A:251:PRO:O	2.17	0.45
1:B:15:ILE:O	1:B:15:ILE:HG23	2.17	0.45
1:A:133:LYS:HE2	3:A:335:UD1:O1'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLU:OE1	1:A:253:LYS:HD3	2.16	0.44
1:B:186:LYS:HE2	1:B:333:LEU:CD1	2.47	0.44
1:B:58:ASP:OD1	1:B:60:ARG:HG2	2.18	0.44
1:A:228:GLU:HG3	1:A:297:TYR:CE2	2.53	0.44
1:A:100:PRO:CA	1:A:140:LEU:HD22	2.48	0.44
1:B:52:MET:HA	1:B:55:GLU:CG	2.47	0.43
1:A:185:PHE:O	1:A:189:VAL:HG23	2.18	0.43
1:B:140:LEU:O	1:B:140:LEU:HG	2.15	0.43
1:B:181:VAL:HG21	1:B:239:MET:HE2	2.00	0.43
1:B:229:ILE:HB	1:B:285:ILE:HB	2.00	0.43
1:A:235:PRO:CG	1:A:322:GLN:HE21	2.32	0.43
5:A:389:HOH:O	1:B:47:LEU:HD23	2.17	0.43
1:B:130:SER:O	2:B:334:NDP:H6N	2.19	0.43
1:B:294:PRO:O	1:B:295:LYS:HD3	2.19	0.43
1:A:207:TRP:CD1	1:A:237:MET:HB3	2.54	0.43
1:A:25[B]:CYS:SG	1:A:210:LEU:HD23	2.58	0.43
1:A:330:LEU:C	1:A:332:LEU:H	2.22	0.43
1:A:197:PRO:HB3	1:A:255:ILE:CD1	2.45	0.43
1:A:173:ASN:ND2	1:A:173:ASN:N	2.64	0.43
1:A:280:GLU:HB3	5:A:473:HOH:O	2.18	0.42
1:A:327:ASP:O	1:A:331:LYS:HG3	2.18	0.42
1:A:47:LEU:O	1:A:51:GLU:HG3	2.18	0.42
1:B:159:LYS:CE	1:B:292:GLN:HB2	2.47	0.42
1:B:58:ASP:OD1	1:B:60:ARG:CG	2.67	0.42
1:B:187:LYS:HG3	5:B:473:HOH:O	2.19	0.42
1:A:28:ARG:HD2	1:A:32:ASP:OD1	2.19	0.42
1:A:92[A]:HIS:ND1	1:A:94:PRO:HG2	2.32	0.42
1:B:239:MET:CE	1:B:242:LEU:HD23	2.49	0.42
1:A:255:ILE:HG23	5:A:447:HOH:O	2.20	0.42
1:A:235:PRO:CD	1:A:322:GLN:HE21	2.33	0.42
1:B:159:LYS:HE2	5:B:485:HOH:O	2.20	0.42
1:A:21:SER:OG	1:A:178:ARG:HB2	2.20	0.42
1:A:235:PRO:HG3	1:A:322:GLN:NE2	2.34	0.42
1:A:326:PRO:O	1:A:330:LEU:HG	2.19	0.42
1:B:159:LYS:NZ	1:B:293:THR:HB	2.35	0.42
1:B:234:ILE:HA	1:B:235:PRO:HD3	1.89	0.42
1:A:173:ASN:ND2	5:A:419:HOH:O	2.53	0.41
1:A:45:ASP:OD1	1:A:48:LYS:HE2	2.19	0.41
1:A:201:ILE:HD11	1:A:254:ILE:HD11	2.01	0.41
1:A:45:ASP:HB3	2:A:334:NDP:O1X	2.20	0.41
1:B:181:VAL:O	1:B:184:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:PRO:O	1:B:187:LYS:HG3	2.20	0.41
1:A:219:LYS:O	1:A:223:ARG:HG2	2.19	0.41
1:A:255:ILE:HG22	1:A:255:ILE:O	2.21	0.41
1:B:122:ALA:HB1	1:B:162:SER:CB	2.50	0.41
1:B:38:LYS:HE2	1:B:40:ILE:HG12	2.03	0.41
1:A:186:LYS:NZ	1:A:333:LEU:HD23	2.35	0.41
1:A:196:ILE:CD1	1:A:247:ALA:HB3	2.49	0.41
1:A:8:LEU:HD12	1:A:11:GLN:CB	2.51	0.41
1:B:325:GLU:HB2	1:B:328:ASP:CB	2.51	0.41
1:B:227:GLY:O	1:B:287:PRO:HG3	2.21	0.41
1:A:25[B]:CYS:SG	1:A:210:LEU:CD2	3.09	0.40
1:B:293:THR:HG23	1:B:293:THR:O	2.21	0.40
1:A:206:PHE:CD1	1:A:317:SER:HB3	2.56	0.40
1:B:181:VAL:HG11	1:B:239:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/344 (96%)	315 (96%)	14 (4%)	1 (0%)	44	34
1	B	328/344 (95%)	320 (98%)	7 (2%)	1 (0%)	44	34
All	All	658/688 (96%)	635 (96%)	21 (3%)	2 (0%)	44	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	B	249	ASN

### 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	293/304 (96%)	290 (99%)	3 (1%)	80	80
1	B	291/304 (96%)	287 (99%)	4 (1%)	71	69
All	All	584/608 (96%)	577 (99%)	7 (1%)	75	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	173	ASN
1	A	267	MET
1	B	131	THR
1	B	157	ASN
1	B	241	ASP
1	B	315	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	173	ASN
1	A	191	ASN
1	A	286	GLN
1	A	307	GLN
1	A	322	GLN
1	B	35	ASN
1	B	75	ASN
1	B	136	ASN
1	B	165	GLN
1	B	173	ASN
1	B	274	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 ⓘ

6 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	NDP	A	334	-	43,52,52	1.31	6 (13%)	49,80,80	1.23	6 (12%)
3	UD1	A	335	-	34,41,41	1.29	3 (8%)	43,62,62	2.54	3 (6%)
2	NDP	B	334	-	43,52,52	1.28	5 (11%)	49,80,80	1.21	6 (12%)
3	UD1	B	335	-	34,41,41	1.25	3 (8%)	43,62,62	2.53	3 (6%)
4	MES	B	336	-	12,12,12	0.72	0	14,16,16	1.59	1 (7%)
4	MES	B	337	-	12,12,12	0.69	0	14,16,16	1.35	1 (7%)

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	NDP	A	334	-	-	0/30/77/77	0/5/5/5
3	UD1	A	335	-	-	0/22/63/63	0/3/3/3
2	NDP	B	334	-	-	0/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UD1	B	335	-	-	0/22/63/63	0/3/3/3
4	MES	B	336	-	-	0/6/14/14	0/1/1/1
4	MES	B	337	-	-	0/6/14/14	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	NDP	C2A-N3A	2.02	1.35	1.32
2	A	334	NDP	C2A-N3A	2.06	1.35	1.32
2	A	334	NDP	C4A-N3A	2.29	1.38	1.35
2	B	334	NDP	P2B-O1X	2.55	1.59	1.50
2	B	334	NDP	PN-O1N	2.61	1.60	1.50
2	A	334	NDP	P2B-O1X	2.69	1.59	1.50
2	A	334	NDP	PN-O1N	2.75	1.61	1.50
3	B	335	UD1	PB-O1B	2.92	1.61	1.50
3	B	335	UD1	PA-O1A	2.93	1.61	1.50
3	A	335	UD1	PA-O1A	2.95	1.62	1.50
2	B	334	NDP	PA-O1A	2.96	1.62	1.50
2	A	334	NDP	PA-O1A	3.00	1.62	1.50
3	A	335	UD1	PB-O1B	3.01	1.62	1.50
2	B	334	NDP	C2A-N1A	3.05	1.39	1.33
2	A	334	NDP	C2A-N1A	3.21	1.39	1.33
3	B	335	UD1	C4-N3	3.71	1.39	1.33
3	A	335	UD1	C4-N3	3.88	1.40	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	335	UD1	O5'-C1'-O1'	-6.68	102.63	111.36
3	B	335	UD1	O5'-C1'-O1'	-6.43	102.95	111.36
4	B	336	MES	O2S-S-C8	-4.80	102.67	106.79
3	A	335	UD1	C5-C4-N3	-3.53	114.68	123.12
3	B	335	UD1	C5-C4-N3	-3.49	114.78	123.12
4	B	337	MES	O1S-S-C8	-3.23	104.02	106.79
2	B	334	NDP	C1B-N9A-C4A	-2.84	121.73	126.64
2	A	334	NDP	C1B-N9A-C4A	-2.77	121.85	126.64
2	A	334	NDP	C3N-C2N-N1N	-2.46	119.50	123.08
2	B	334	NDP	O3B-C3B-C4B	-2.26	104.48	111.09
2	B	334	NDP	C3N-C2N-N1N	-2.13	119.99	123.08
2	B	334	NDP	N3A-C2A-N1A	-2.12	127.01	128.86
2	A	334	NDP	C1D-N1N-C6N	-2.06	116.30	120.77
2	B	334	NDP	C1D-N1N-C6N	-2.05	116.31	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	334	NDP	O4D-C1D-N1N	2.00	112.10	108.07
2	A	334	NDP	C4A-C5A-N7A	2.08	111.42	109.41
2	B	334	NDP	N6A-C6A-N1A	2.51	123.74	118.77
2	A	334	NDP	N6A-C6A-N1A	2.65	124.02	118.77
3	A	335	UD1	C4-N3-C2	13.51	125.74	114.13
3	B	335	UD1	C4-N3-C2	13.60	125.81	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	334	NDP	2	0
3	A	335	UD1	2	0
2	B	334	NDP	1	0
3	B	335	UD1	1	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	329/344 (95%)	1.02	59 (17%) <b>2</b> <b>2</b>	16, 36, 80, 80	0
1	B	327/344 (95%)	0.87	50 (15%) <b>2</b> <b>2</b>	15, 32, 74, 80	0
All	All	656/688 (95%)	0.94	109 (16%) <b>2</b> <b>2</b>	15, 33, 78, 80	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ALA	9.3
1	B	161	SER	9.1
1	B	250	THR	8.8
1	A	162	SER	8.8
1	A	161	SER	7.9
1	A	324	LEU	7.8
1	B	162	SER	7.8
1	B	246	LEU	7.8
1	B	193	ALA	7.8
1	A	243	ALA	7.6
1	B	330	LEU	7.3
1	A	326	PRO	7.1
1	A	159	LYS	6.8
1	A	7	MET	6.8
1	A	160	GLY	6.8
1	B	328	ASP	6.8
1	B	247	ALA	6.8
1	B	249	ASN	6.7
1	B	333	LEU	6.6
1	B	201	ILE	6.1
1	A	319	ASN	6.1
1	B	248	PRO	6.0
1	A	333	LEU	5.9
1	B	191	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	194	SER	5.6
1	B	324	LEU	5.5
1	A	247	ALA	5.5
1	B	331	LYS	5.5
1	A	192	LYS	5.3
1	B	327	ASP	5.2
1	B	190	GLN	5.2
1	B	196	ILE	5.1
1	A	191	ASN	5.1
1	B	240	THR	5.0
1	A	329	LEU	5.0
1	A	158	PHE	4.9
1	A	6	ASN	4.8
1	A	201	ILE	4.7
1	A	293	THR	4.7
1	B	237	MET	4.6
1	A	249	ASN	4.5
1	B	244	LYS	4.4
1	B	332	LEU	4.3
1	A	331	LYS	4.3
1	B	325	GLU	4.3
1	A	163	GLN	4.3
1	A	250	THR	4.2
1	A	323	TRP	4.2
1	B	329	LEU	4.1
1	A	195	GLU	4.1
1	B	195	GLU	4.0
1	B	159	LYS	4.0
1	A	193	ALA	4.0
1	A	196	ILE	3.9
1	B	310	ALA	3.8
1	B	163	GLN	3.8
1	A	325	GLU	3.8
1	B	311	PRO	3.7
1	B	160	GLY	3.7
1	B	251	PRO	3.7
1	B	189	VAL	3.7
1	A	311	PRO	3.6
1	B	192	LYS	3.6
1	A	330	LEU	3.6
1	B	187	LYS	3.5
1	A	299	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	307	GLN	3.5
1	A	246	LEU	3.4
1	A	190	GLN	3.4
1	B	242	LEU	3.4
1	B	184	PHE	3.3
1	B	188	LEU	3.3
1	B	253	LYS	3.2
1	A	252	THR	3.2
1	A	327	ASP	3.2
1	A	198	ILE	3.2
1	A	332	LEU	3.1
1	A	263	LEU	3.1
1	A	303	HIS	3.0
1	B	7	MET	3.0
1	A	248	PRO	2.9
1	A	318	HIS	2.9
1	B	326	PRO	2.9
1	A	194	SER	2.9
1	B	270	LYS	2.8
1	A	292	GLN	2.8
1	B	239	MET	2.8
1	A	240	THR	2.8
1	A	320	ASN	2.7
1	B	312	ASP	2.6
1	A	254	ILE	2.5
1	A	9	ASP	2.5
1	A	188	LEU	2.4
1	A	321	ASN	2.4
1	A	253	LYS	2.4
1	A	255	ILE	2.4
1	B	255	ILE	2.3
1	A	245	ALA	2.3
1	A	184	PHE	2.3
1	A	251	PRO	2.2
1	A	280	GLU	2.2
1	A	187	LYS	2.2
1	B	252	THR	2.2
1	A	140	LEU	2.1
1	B	245	ALA	2.1
1	B	197	PRO	2.1
1	B	293	THR	2.1
1	A	322	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	305	LYS	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
4	MES	B	337	12/12	0.72	0.24	2.98	47,50,55,58	0
3	UD1	A	335	39/39	0.90	0.15	0.19	35,47,51,55	0
3	UD1	B	335	39/39	0.91	0.14	0.02	33,43,49,53	0
2	NDP	B	334	48/48	0.97	0.12	-0.28	14,27,35,38	0
4	MES	B	336	12/12	0.94	0.11	-0.48	32,37,39,41	0
2	NDP	A	334	48/48	0.97	0.12	-0.57	13,28,39,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.