



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 AM GMT

PDB ID : 2GN8  
Title : Crystal structure of UDP-GlcNAc inverting 4,6-dehydratase in complex with NADP and UDP  
Authors : Ishiyama, N.; Creuzenet, C.; Lam, J.S.; Berghuis, A.M.  
Deposited on : 2006-04-09  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

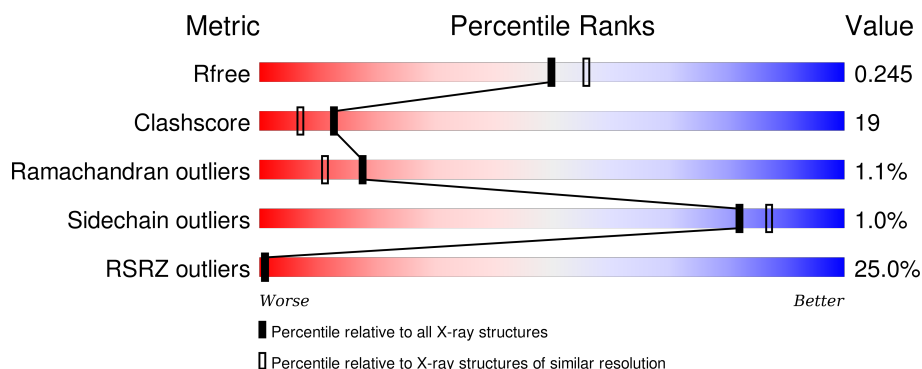
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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  $\geq 3$ , 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	
1	B	344	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5609 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	327	Total	C	N	O	S	0	0	0
			2573	1647	436	475	15			
1	B	329	Total	C	N	O	S	0	0	0
			2590	1656	440	479	15			

There are 22 discrepancies between the modelled and reference sequences:

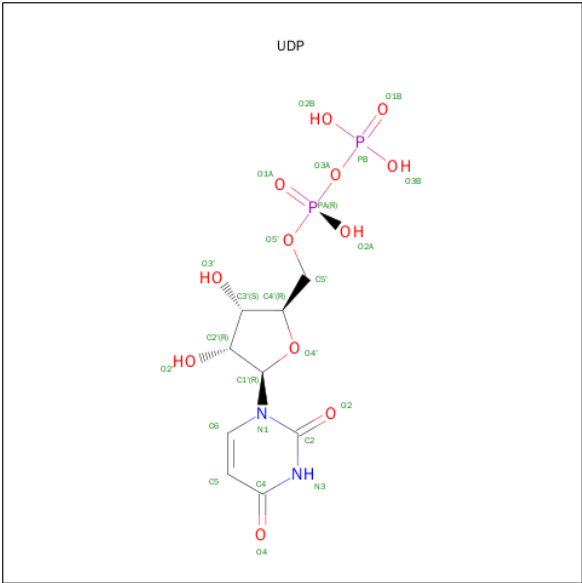
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	CLONING ARTIFACT	UNP O25511
A	-9	HIS	-	EXPRESSION TAG	UNP O25511
A	-8	HIS	-	EXPRESSION TAG	UNP O25511
A	-7	HIS	-	EXPRESSION TAG	UNP O25511
A	-6	HIS	-	EXPRESSION TAG	UNP O25511
A	-5	HIS	-	EXPRESSION TAG	UNP O25511
A	-4	HIS	-	EXPRESSION TAG	UNP 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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



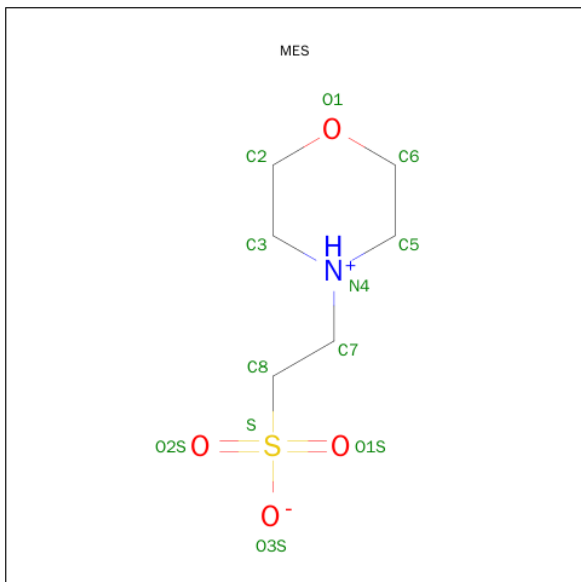
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

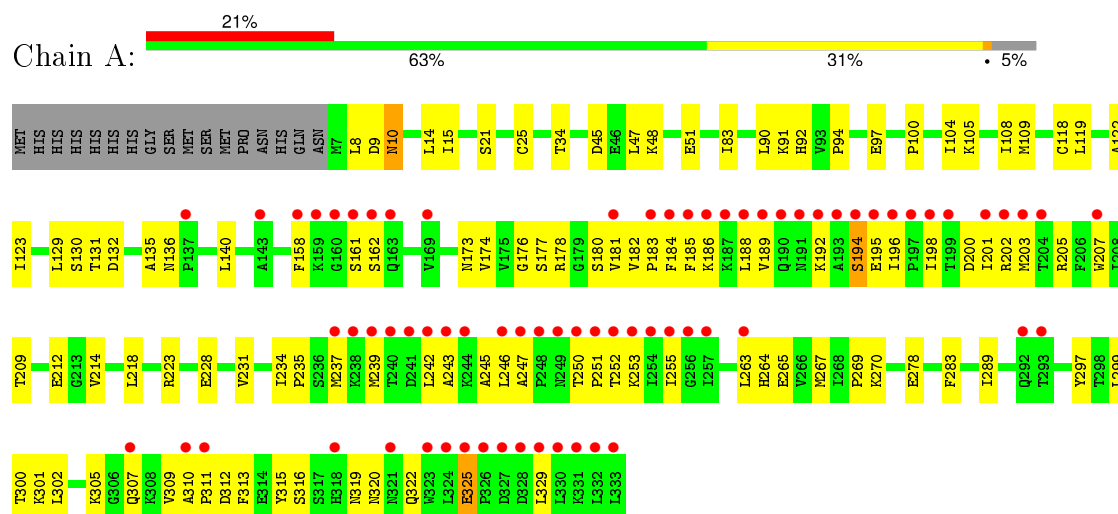
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total	O	0	0
			156	156		
5	B	132	Total	O	0	0
			132	132		

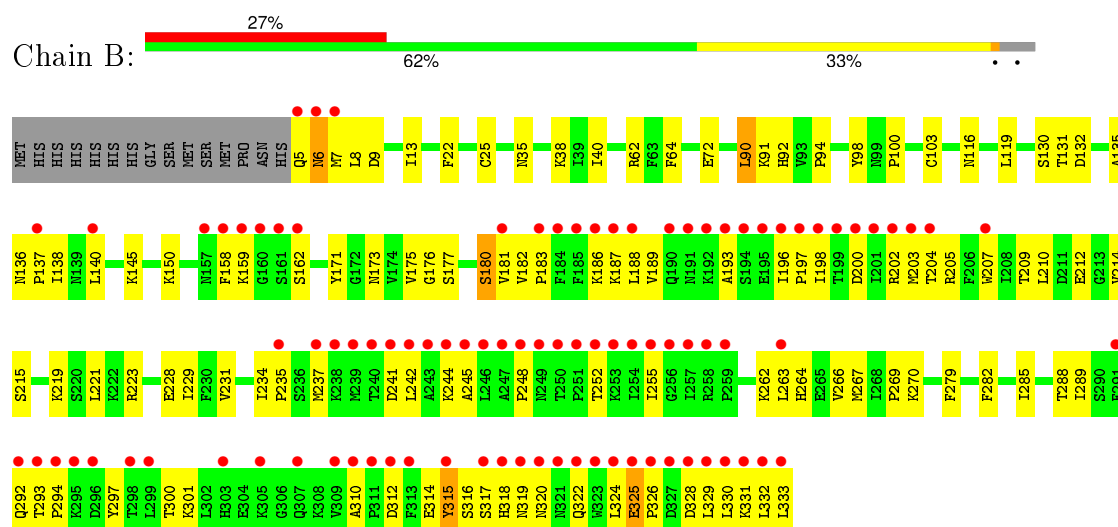
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	111.06Å 111.06Å 107.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 38.67 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.10) 97.9 (38.67-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.99 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.245 0.208 , 0.245	Depositor DCC
$R_{free}$ test set	4309 reflections (9.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.1	EDS
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 44037 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, UDP, 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	0.31	0/2624	0.58	1/3545 (0.0%)
1	B	0.31	0/2641	0.56	1/3568 (0.0%)
All	All	0.31	0/5265	0.57	2/7113 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	LEU	N-CA-C	-5.33	96.60	111.00
1	B	90	LEU	N-CA-C	-5.28	96.75	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	2573	0	2627	90	0
1	B	2590	0	2641	117	0
2	A	48	0	25	5	0
2	B	48	0	25	7	0
3	A	25	0	11	1	0
3	B	25	0	11	1	0
4	A	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	156	0	0	1	0
5	B	132	0	0	9	0
All	All	5609	0	5353	206	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 19.

All (206) 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:196:ILE:HB	1:B:252:THR:HG22	1.41	1.03
1:B:245:ALA:HB2	1:B:326:PRO:HB3	1.46	0.97
1:A:196:ILE:HB	1:A:252:THR:HG22	1.45	0.96
1:B:38:LYS:HE3	1:B:62:ARG:HG3	1.51	0.91
1:B:176:GLY:HA2	1:B:183:PRO:HD3	1.57	0.87
1:A:92:HIS:CE1	1:A:94:PRO:HG2	2.12	0.85
1:B:92:HIS:CE1	1:B:94:PRO:HG2	2.12	0.84
1:A:223:ARG:HB2	1:A:300:THR:HB	1.58	0.84
1:A:186:LYS:HE3	1:A:246:LEU:HD22	1.57	0.84
1:B:173:ASN:HD21	1:B:205:ARG:HD2	1.44	0.83
1:B:324:LEU:HD23	1:B:324:LEU:H	1.44	0.82
1:A:223:ARG:HA	1:A:301:LYS:HB2	1.60	0.80
1:B:8:LEU:HD12	1:B:13:ILE:HD11	1.64	0.79
1:B:173:ASN:ND2	1:B:205:ARG:HD2	1.97	0.78
1:A:176:GLY:HA2	1:A:183:PRO:HD3	1.65	0.76
1:B:183:PRO:HA	1:B:186:LYS:HE2	1.72	0.72
1:A:182:VAL:HB	1:A:183:PRO:HD3	1.73	0.71
1:A:8:LEU:HD23	1:A:83:ILE:HD12	1.74	0.70
1:B:242:LEU:HD12	1:B:329:LEU:HD21	1.72	0.70
1:A:8:LEU:HD12	1:A:34:THR:HG21	1.73	0.70
1:B:197:PRO:HB2	1:B:255:ILE:HD13	1.74	0.70
1:B:223:ARG:HB2	1:B:300:THR:HB	1.73	0.69
1:B:237:MET:HB2	1:B:324:LEU:HD21	1.75	0.68
1:B:223:ARG:HD2	5:B:396:HOH:O	1.94	0.67
1:B:223:ARG:HA	1:B:301:LYS:HB2	1.76	0.67
1:B:200:ASP:HB3	1:B:203:MET:HG2	1.76	0.67
1:B:328:ASP:HA	1:B:331:LYS:HD2	1.76	0.66
1:B:6:ASN:CG	1:B:7:MET:H	1.98	0.66
1:A:21:SER:OG	1:A:178:ARG:HB2	1.97	0.65
1:A:270:LYS:HE3	1:A:312:ASP:HB3	1.79	0.64
1:A:119:LEU:HD22	1:A:158:PHE:CD2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:PRO:HA	1:B:322:GLN:HB2	1.81	0.62
1:B:92:HIS:HE1	1:B:94:PRO:HG2	1.63	0.62
1:A:173:ASN:HD21	1:A:205:ARG:HD2	1.63	0.62
1:B:176:GLY:HA2	1:B:182:VAL:HB	1.81	0.62
1:A:92:HIS:HE1	1:A:94:PRO:HG2	1.61	0.61
1:A:209:THR:OG1	1:A:212:GLU:HG3	2.01	0.61
1:B:100:PRO:HA	1:B:140:LEU:CD2	2.30	0.61
1:B:231:VAL:HG11	1:B:267:MET:HG3	1.82	0.61
1:B:203:MET:SD	1:B:263:LEU:HA	2.42	0.60
1:A:194:SER:O	1:A:251:PRO:HG2	2.02	0.60
1:A:196:ILE:CB	1:A:252:THR:HG22	2.28	0.60
1:B:183:PRO:O	1:B:187:LYS:HG3	2.02	0.60
1:B:130:SER:O	2:B:334:NAP:H6N	2.02	0.60
1:B:91:LYS:HZ2	2:B:334:NAP:H72N	1.48	0.60
1:A:237:MET:HE1	1:A:329:LEU:HD22	1.83	0.59
1:A:242:LEU:HD12	1:A:329:LEU:HD21	1.84	0.59
1:A:122:ALA:HB1	1:A:162:SER:HB3	1.85	0.59
1:A:181:VAL:HG13	3:A:335:UDP:O2A	2.02	0.59
1:B:119:LEU:HD22	1:B:158:PHE:CD2	2.37	0.59
1:A:118:CYS:HA	1:A:123:ILE:HG12	1.85	0.59
1:B:181:VAL:HG13	3:B:335:UDP:O2A	2.03	0.58
1:B:6:ASN:ND2	1:B:7:MET:H	2.02	0.58
1:A:242:LEU:CD1	1:A:329:LEU:HD21	2.33	0.58
1:B:136:ASN:HD21	1:B:269:PRO:HB3	1.69	0.58
1:B:267:MET:HB3	1:B:315:TYR:HB3	1.86	0.57
1:B:325:GLU:H	1:B:325:GLU:CD	2.08	0.57
1:A:200:ASP:CG	1:A:201:ILE:H	2.06	0.57
1:B:320:ASN:HD21	1:B:322:GLN:HB2	1.70	0.57
1:B:62:ARG:HH11	1:B:62:ARG:HG3	1.70	0.56
1:A:309:VAL:HG12	1:A:310:ALA:N	2.19	0.56
1:B:241:ASP:HB3	1:B:326:PRO:HG3	1.86	0.56
1:B:159:LYS:NZ	1:B:292:GLN:HB2	2.19	0.56
1:B:159:LYS:HZ1	1:B:292:GLN:HB2	1.71	0.56
1:B:235:PRO:HG3	1:B:322:GLN:HB3	1.88	0.55
1:B:72:GLU:HG2	5:B:362:HOH:O	2.06	0.55
1:B:138:ILE:HG23	1:B:262:LYS:HE2	1.88	0.55
1:B:204:THR:HG21	1:B:317:SER:O	2.07	0.55
1:B:237:MET:HB2	1:B:324:LEU:CD2	2.36	0.55
1:A:100:PRO:HA	1:A:140:LEU:CD2	2.37	0.55
1:B:198:ILE:O	1:B:255:ILE:HG12	2.07	0.55
1:B:162:SER:HB3	5:B:456:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ILE:HG12	1:B:252:THR:HB	1.89	0.54
1:B:175:VAL:HG11	1:B:332:LEU:HD13	1.88	0.54
1:B:100:PRO:HA	1:B:140:LEU:HD22	1.89	0.54
1:A:299:LEU:HD23	1:A:299:LEU:O	2.08	0.54
1:B:209:THR:OG1	1:B:212:GLU:HG3	2.08	0.54
1:B:241:ASP:O	1:B:244:LYS:HG2	2.08	0.53
1:B:264:HIS:ND1	1:B:318:HIS:HB3	2.23	0.53
1:A:203:MET:SD	1:A:263:LEU:HA	2.49	0.53
1:B:241:ASP:HA	1:B:244:LYS:CD	2.39	0.53
1:A:173:ASN:ND2	1:A:205:ARG:HD2	2.24	0.52
1:A:10:ASN:O	1:A:10:ASN:CG	2.47	0.52
1:A:184:PHE:O	1:A:188:LEU:HG	2.09	0.52
1:A:8:LEU:CD2	1:A:83:ILE:HD12	2.39	0.52
1:A:100:PRO:HA	1:A:140:LEU:HD22	1.91	0.51
1:B:270:LYS:HB2	1:B:314:GLU:OE1	2.10	0.51
1:B:182:VAL:N	1:B:183:PRO:HD2	2.24	0.51
1:B:9:ASP:OD1	1:B:35:ASN:HB3	2.10	0.51
1:B:91:LYS:NZ	2:B:334:NAP:N7N	2.59	0.51
1:B:293:THR:HG23	1:B:293:THR:O	2.11	0.51
1:A:186:LYS:CE	1:A:246:LEU:HD22	2.36	0.51
1:A:267:MET:HB3	1:A:315:TYR:HD2	1.76	0.51
1:B:204:THR:HG22	1:B:317:SER:HB2	1.92	0.50
1:A:309:VAL:HG12	1:A:310:ALA:H	1.77	0.50
1:A:309:VAL:HG11	1:A:313:PHE:CG	2.46	0.50
1:B:328:ASP:HA	1:B:331:LYS:CD	2.40	0.50
1:A:45:ASP:OD1	1:A:48:LYS:HE2	2.12	0.50
1:A:250:THR:HG23	1:A:251:PRO:HD2	1.93	0.50
1:B:91:LYS:NZ	2:B:334:NAP:H72N	2.08	0.50
1:A:25:CYS:SG	1:A:214:VAL:HG21	2.52	0.49
1:A:97:GLU:OE1	1:B:288:THR:HG21	2.12	0.49
1:A:223:ARG:HD3	1:A:302:LEU:HD22	1.94	0.49
1:B:175:VAL:HG11	1:B:332:LEU:CD1	2.42	0.49
1:A:228:GLU:HG3	1:A:297:TYR:CE2	2.47	0.49
1:B:324:LEU:CD2	1:B:324:LEU:H	2.21	0.49
1:B:5:GLN:N	1:B:9:ASP:OD2	2.46	0.49
1:B:159:LYS:NZ	1:B:293:THR:HG22	2.28	0.49
1:A:174:VAL:HB	1:A:177:SER:HB2	1.93	0.49
1:A:231:VAL:CG1	1:A:267:MET:HG2	2.42	0.49
1:B:150:LYS:HD3	5:B:458:HOH:O	2.13	0.49
1:B:177:SER:H	1:B:180:SER:CB	2.26	0.49
1:B:229:ILE:HB	1:B:285:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PHE:O	1:A:189:VAL:HG23	2.13	0.48
1:A:176:GLY:HA2	1:A:183:PRO:CD	2.40	0.48
1:A:235:PRO:N	1:A:322:GLN:HE21	2.10	0.48
1:B:145:LYS:HE3	2:B:334:NAP:O2D	2.13	0.48
1:A:207:TRP:CD1	1:A:237:MET:HB3	2.48	0.48
1:A:181:VAL:HB	1:A:185:PHE:CE2	2.48	0.48
1:B:119:LEU:HD22	1:B:158:PHE:CE2	2.48	0.48
1:B:231:VAL:CG1	1:B:267:MET:HG3	2.44	0.48
1:B:219:LYS:O	1:B:223:ARG:HG2	2.13	0.47
1:A:237:MET:CE	1:A:329:LEU:HD22	2.43	0.47
1:A:91:LYS:HZ2	2:A:334:NAP:H72N	1.62	0.47
1:B:7:MET:CE	1:B:221:LEU:HB3	2.44	0.47
1:A:130:SER:O	2:A:334:NAP:H6N	2.15	0.47
1:B:316:SER:HB2	1:B:319:ASN:OD1	2.15	0.47
1:B:188:LEU:C	1:B:193:ALA:HB2	2.35	0.46
1:A:48:LYS:NZ	5:A:464:HOH:O	2.49	0.46
1:B:244:LYS:O	1:B:248:PRO:HB3	2.16	0.46
1:A:228:GLU:HG3	1:A:297:TYR:CD2	2.50	0.46
1:A:14:LEU:C	1:A:14:LEU:HD23	2.35	0.46
1:B:176:GLY:CA	1:B:182:VAL:HB	2.46	0.46
1:B:5:GLN:HG3	1:B:6:ASN:N	2.30	0.46
1:A:239:MET:CE	1:A:242:LEU:HD23	2.44	0.46
1:B:6:ASN:ND2	1:B:7:MET:N	2.64	0.46
1:A:181:VAL:O	1:A:184:PHE:HB3	2.16	0.46
1:B:7:MET:HE1	1:B:221:LEU:HB3	1.97	0.46
1:A:235:PRO:HG3	1:A:322:GLN:NE2	2.30	0.46
1:B:183:PRO:CA	1:B:186:LYS:HE2	2.45	0.45
1:A:181:VAL:HG23	1:A:182:VAL:N	2.32	0.45
1:B:241:ASP:HA	1:B:244:LYS:HG2	1.97	0.45
1:A:325:GLU:OE1	1:A:325:GLU:N	2.50	0.45
1:B:130:SER:OG	1:B:131:THR:N	2.50	0.45
1:A:136:ASN:HD21	1:A:269:PRO:HB3	1.82	0.45
1:B:62:ARG:NE	5:B:414:HOH:O	2.49	0.44
1:A:289:ILE:HB	1:B:98:TYR:CE1	2.53	0.44
1:B:132:ASP:HB2	1:B:266:VAL:O	2.18	0.44
1:B:62:ARG:HG3	1:B:62:ARG:NH1	2.33	0.44
1:B:40:ILE:CG2	1:B:64:PHE:HD2	2.31	0.44
1:A:195:GLU:OE1	1:A:253:LYS:HD3	2.18	0.44
1:A:122:ALA:HB1	1:A:162:SER:CB	2.47	0.43
1:A:278:GLU:HG3	1:A:283:PHE:CE1	2.53	0.43
1:B:242:LEU:CD1	1:B:329:LEU:HD21	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:SER:OG	1:B:181:VAL:N	2.51	0.43
1:A:91:LYS:NZ	2:A:334:NAP:H72N	2.16	0.43
1:A:118:CYS:CA	1:A:123:ILE:HG12	2.49	0.43
1:B:171:TYR:O	2:B:334:NAP:H5N	2.19	0.43
1:A:130:SER:OG	1:A:131:THR:N	2.52	0.43
1:B:177:SER:O	1:B:183:PRO:HG3	2.19	0.42
1:A:320:ASN:OD1	1:A:322:GLN:HG2	2.19	0.42
1:B:292:GLN:O	1:B:294:PRO:HD3	2.19	0.42
1:A:234:ILE:HA	1:A:235:PRO:HD3	1.86	0.42
1:A:305:LYS:HG3	1:A:307:GLN:NE2	2.35	0.42
1:B:135:ALA:HA	5:B:369:HOH:O	2.19	0.42
1:A:47:LEU:O	1:A:51:GLU:HG3	2.19	0.42
1:B:333:LEU:C	1:B:333:LEU:HD23	2.39	0.42
1:B:177:SER:HB3	1:B:180:SER:HB2	2.01	0.42
1:B:25:CYS:SG	1:B:214:VAL:HG21	2.59	0.42
1:A:129:LEU:HD12	2:A:334:NAP:H4D	2.01	0.42
1:A:15:ILE:HD12	1:A:15:ILE:N	2.34	0.42
1:A:189:VAL:HG22	1:A:247:ALA:HB2	2.02	0.42
1:A:105:LYS:O	1:A:109:MET:HB2	2.20	0.42
1:B:245:ALA:CB	1:B:326:PRO:HB3	2.34	0.42
1:B:245:ALA:O	1:B:330:LEU:HD21	2.19	0.42
1:B:177:SER:H	1:B:180:SER:HB2	1.84	0.42
1:B:219:LYS:HG3	5:B:464:HOH:O	2.18	0.42
1:A:198:ILE:O	1:A:255:ILE:N	2.53	0.42
1:B:207:TRP:CD1	1:B:237:MET:HB3	2.54	0.41
1:B:22:PHE:HA	1:B:210:LEU:HD11	2.02	0.41
1:B:310:ALA:C	1:B:312:ASP:H	2.24	0.41
1:A:316:SER:HB3	1:A:319:ASN:OD1	2.20	0.41
1:B:189:VAL:HA	1:B:193:ALA:CB	2.51	0.41
1:B:215:SER:O	1:B:219:LYS:HG3	2.21	0.41
1:B:264:HIS:CE1	1:B:318:HIS:HB3	2.55	0.41
1:B:288:THR:HG23	1:B:289:ILE:HG23	2.03	0.41
1:B:90:LEU:HD12	1:B:103:CYS:HA	2.01	0.41
2:B:334:NAP:H8A	5:B:339:HOH:O	2.21	0.41
1:A:91:LYS:NZ	2:A:334:NAP:N7N	2.69	0.41
1:A:132:ASP:OD2	1:A:265:GLU:HB3	2.20	0.41
1:B:328:ASP:O	1:B:331:LYS:HB2	2.20	0.41
1:B:136:ASN:N	1:B:137:PRO:CD	2.83	0.41
1:A:104:ILE:HG23	1:A:108:ILE:HD12	2.03	0.41
1:B:279:PHE:HB2	1:B:282:PHE:O	2.21	0.41
1:A:243:ALA:C	1:A:245:ALA:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:O	1:A:264:HIS:HE1	2.04	0.41
1:A:267:MET:HB3	1:A:315:TYR:CD2	2.55	0.41
1:B:116:ASN:HB2	5:B:393:HOH:O	2.21	0.41
1:A:223:ARG:HB3	1:A:302:LEU:HD22	2.03	0.40
1:B:234:ILE:HA	1:B:235:PRO:HD3	1.87	0.40
1:A:310:ALA:HA	1:A:311:PRO:HD3	1.91	0.40
1:B:177:SER:N	1:B:180:SER:HB3	2.36	0.40
1:A:242:LEU:HD13	1:A:329:LEU:HD21	2.04	0.40
1:A:237:MET:SD	1:A:329:LEU:HD22	2.61	0.40
1:A:135:ALA:O	1:A:136:ASN:C	2.59	0.40
1:B:228:GLU:HG3	1:B:297:TYR:CE1	2.56	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	325/344 (94%)	300 (92%)	20 (6%)	5 (2%)	13	7
1	B	327/344 (95%)	298 (91%)	27 (8%)	2 (1%)	30	24
All	All	652/688 (95%)	598 (92%)	47 (7%)	7 (1%)	17	11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	SER
1	A	192	LYS
1	A	194	SER
1	A	9	ASP
1	A	161	SER
1	A	180	SER
1	B	202	ARG

### 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	288/304 (95%)	285 (99%)	3 (1%)	82	87
1	B	290/304 (95%)	287 (99%)	3 (1%)	82	87
All	All	578/608 (95%)	572 (99%)	6 (1%)	82	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	218	LEU
1	A	325	GLU
1	B	6	ASN
1	B	315	TYR
1	B	325	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	11	GLN
1	A	75	ASN
1	A	125	GLN
1	A	136	ASN
1	A	173	ASN
1	A	274	HIS
1	A	286	GLN
1	A	307	GLN
1	A	322	GLN
1	B	75	ASN
1	B	136	ASN
1	B	165	GLN
1	B	173	ASN
1	B	286	GLN
1	B	320	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 ⓘ

5 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	NAP	A	334	-	42,52,52	1.53	8 (19%)	54,80,80	1.51	10 (18%)
3	UDP	A	335	-	18,26,26	1.73	4 (22%)	26,40,40	2.54	2 (7%)
4	MES	A	337	-	11,12,12	0.50	0	14,16,16	1.46	2 (14%)
2	NAP	B	334	-	42,52,52	1.56	11 (26%)	54,80,80	1.49	8 (14%)
3	UDP	B	335	-	18,26,26	1.74	4 (22%)	26,40,40	2.53	2 (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	NAP	A	334	-	-	0/27/67/67	0/5/5/5
3	UDP	A	335	-	-	0/12/32/32	0/2/2/2
4	MES	A	337	-	-	0/6/14/14	0/1/1/1
2	NAP	B	334	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	B	335	-	-	0/12/32/32	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	NAP	C3B-C2B	-2.01	1.48	1.53
3	B	335	UDP	PB-O2B	2.04	1.62	1.54
2	A	334	NAP	C7N-N7N	2.05	1.37	1.33
2	B	334	NAP	C7N-N7N	2.05	1.37	1.33
2	B	334	NAP	C5N-C4N	2.07	1.43	1.38
3	A	335	UDP	PB-O3B	2.08	1.62	1.54
2	A	334	NAP	C5N-C4N	2.11	1.43	1.38
2	B	334	NAP	P2B-O3X	2.14	1.62	1.54
2	B	334	NAP	C2N-C3N	2.22	1.42	1.39
2	A	334	NAP	C4A-N3A	2.43	1.39	1.35
2	B	334	NAP	C4A-N3A	2.50	1.39	1.35
2	A	334	NAP	PN-O1N	2.57	1.60	1.51
2	B	334	NAP	P2B-O1X	2.60	1.59	1.51
2	B	334	NAP	C4N-C3N	2.61	1.43	1.39
2	B	334	NAP	PN-O1N	2.68	1.60	1.51
2	A	334	NAP	C4N-C3N	2.72	1.43	1.39
2	A	334	NAP	PA-O1A	2.88	1.61	1.51
3	A	335	UDP	PA-O1A	2.94	1.61	1.51
3	B	335	UDP	PA-O1A	2.95	1.62	1.51
2	B	334	NAP	PA-O1A	3.03	1.62	1.51
2	A	334	NAP	C2A-N1A	3.10	1.39	1.33
2	A	334	NAP	P2B-O1X	3.17	1.61	1.51
3	A	335	UDP	PB-O1B	3.29	1.62	1.51
3	B	335	UDP	PB-O1B	3.32	1.62	1.51
2	B	334	NAP	C2A-N1A	3.52	1.40	1.33
3	B	335	UDP	C4-N3	3.69	1.40	1.33
3	A	335	UDP	C4-N3	3.71	1.40	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	334	NAP	C3N-C2N-N1N	-4.07	115.67	120.36
2	A	334	NAP	C3N-C2N-N1N	-4.00	115.75	120.36
4	A	337	MES	O2S-S-C8	-3.60	103.83	106.91
2	A	334	NAP	C3N-C7N-N7N	-3.39	114.10	117.82
2	B	334	NAP	C1B-N9A-C4A	-3.39	121.83	126.94
2	B	334	NAP	C3N-C7N-N7N	-3.36	114.14	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	335	UDP	C5-C4-N3	-3.31	114.62	123.12
3	B	335	UDP	C5-C4-N3	-3.30	114.66	123.12
2	A	334	NAP	C1B-N9A-C4A	-3.07	122.32	126.94
2	A	334	NAP	C4B-O4B-C1B	-2.50	106.97	109.72
4	A	337	MES	C7-C8-S	-2.41	105.06	112.51
2	B	334	NAP	N3A-C2A-N1A	-2.22	127.20	128.89
2	A	334	NAP	N3A-C2A-N1A	-2.14	127.26	128.89
2	A	334	NAP	C5N-C6N-N1N	-2.08	116.87	120.47
2	B	334	NAP	C4A-C5A-N7A	2.08	111.39	109.48
2	A	334	NAP	N6A-C6A-N1A	2.10	123.70	119.20
2	B	334	NAP	N6A-C6A-N1A	2.22	123.97	119.20
2	A	334	NAP	O2B-P2B-O1X	2.24	112.70	107.11
2	B	334	NAP	O2B-P2B-O1X	2.41	113.14	107.11
2	A	334	NAP	O4D-C1D-N1N	3.57	112.05	108.13
2	A	334	NAP	O7N-C7N-C3N	3.66	123.58	119.59
2	B	334	NAP	O7N-C7N-C3N	3.71	123.64	119.59
3	B	335	UDP	C4-N3-C2	11.71	125.74	114.14
3	A	335	UDP	C4-N3-C2	11.74	125.77	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	334	NAP	5	0
3	A	335	UDP	1	0
2	B	334	NAP	7	0
3	B	335	UDP	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	327/344 (95%)	1.35	71 (21%)  	10, 29, 80, 80	0
1	B	329/344 (95%)	1.70	93 (28%)  	10, 33, 80, 80	0
All	All	656/688 (95%)	1.53	164 (25%)  	10, 31, 80, 80	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ILE	15.4
1	B	333	LEU	13.7
1	B	243	ALA	13.4
1	B	161	SER	11.6
1	B	184	PHE	11.4
1	A	193	ALA	11.4
1	B	324	LEU	10.9
1	B	255	ILE	10.5
1	B	196	ILE	10.4
1	B	188	LEU	9.9
1	A	162	SER	9.8
1	A	195	GLU	9.4
1	A	330	LEU	9.3
1	B	201	ILE	9.3
1	A	246	LEU	9.1
1	A	192	LYS	8.7
1	B	186	LYS	8.3
1	B	5	GLN	8.0
1	B	247	ALA	8.0
1	B	158	PHE	7.9
1	A	190	GLN	7.9
1	B	183	PRO	7.8
1	A	247	ALA	7.4
1	A	184	PHE	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	249	ASN	7.3
1	B	187	LYS	7.3
1	B	250	THR	7.1
1	A	240	THR	7.0
1	A	255	ILE	7.0
1	A	243	ALA	6.9
1	A	189	VAL	6.9
1	B	162	SER	6.9
1	B	198	ILE	6.9
1	B	252	THR	6.8
1	B	7	MET	6.8
1	B	195	GLU	6.7
1	B	246	LEU	6.7
1	B	253	LYS	6.4
1	A	198	ILE	6.4
1	B	191	ASN	6.4
1	A	201	ILE	6.4
1	B	249	ASN	6.3
1	B	192	LYS	6.3
1	A	248	PRO	6.3
1	A	253	LYS	6.2
1	A	188	LEU	6.2
1	A	324	LEU	6.1
1	B	190	GLN	6.1
1	B	330	LEU	6.1
1	B	239	MET	6.1
1	B	193	ALA	6.0
1	B	332	LEU	6.0
1	B	323	TRP	5.9
1	B	331	LYS	5.8
1	A	327	ASP	5.5
1	B	237	MET	5.5
1	A	252	THR	5.5
1	B	299	LEU	5.5
1	A	161	SER	5.3
1	B	160	GLY	5.3
1	B	159	LYS	5.2
1	A	250	THR	5.2
1	A	194	SER	5.2
1	A	329	LEU	5.2
1	A	163	GLN	5.1
1	A	251	PRO	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	333	LEU	4.9
1	B	293	THR	5.0
1	A	256	GLY	4.9
1	B	248	PRO	4.9
1	B	292	GLN	4.8
1	A	199	THR	4.8
1	B	194	SER	4.7
1	B	313	PHE	4.7
1	A	331	LYS	4.7
1	A	187	LYS	4.6
1	A	191	ASN	4.5
1	B	203	MET	4.4
1	B	197	PRO	4.3
1	A	183	PRO	4.3
1	B	240	THR	4.3
1	A	244	LYS	4.3
1	A	242	LEU	4.2
1	A	181	VAL	4.2
1	A	326	PRO	4.2
1	B	251	PRO	4.2
1	A	328	ASP	4.2
1	B	241	ASP	4.2
1	A	160	GLY	4.1
1	A	254	ILE	4.1
1	B	326	PRO	4.0
1	B	244	LYS	4.0
1	B	254	ILE	4.0
1	A	185	PHE	3.8
1	B	202	ARG	3.8
1	A	257	ILE	3.8
1	A	332	LEU	3.7
1	B	257	ILE	3.7
1	B	245	ALA	3.7
1	A	197	PRO	3.7
1	B	327	ASP	3.7
1	B	318	HIS	3.6
1	B	328	ASP	3.6
1	A	186	LYS	3.6
1	B	312	ASP	3.6
1	B	329	LEU	3.6
1	B	321	ASN	3.5
1	B	238	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	321	ASN	3.5
1	B	319	ASN	3.4
1	B	296	ASP	3.4
1	B	204	THR	3.4
1	B	199	THR	3.3
1	A	325	GLU	3.2
1	B	310	ALA	3.2
1	A	159	LYS	3.2
1	B	207	TRP	3.1
1	A	237	MET	3.0
1	B	181	VAL	3.0
1	B	294	PRO	3.0
1	A	292	GLN	2.9
1	B	235	PRO	2.9
1	A	307	GLN	2.8
1	B	320	ASN	2.8
1	B	307	GLN	2.8
1	B	256	GLY	2.7
1	B	311	PRO	2.7
1	A	241	ASP	2.6
1	B	157	ASN	2.6
1	B	291	PHE	2.6
1	A	310	ALA	2.6
1	A	318	HIS	2.5
1	B	298	THR	2.5
1	A	311	PRO	2.5
1	A	238	LYS	2.5
1	B	263	LEU	2.4
1	A	293	THR	2.4
1	B	305	LYS	2.4
1	B	258	ARG	2.4
1	B	315	TYR	2.4
1	A	239	MET	2.3
1	A	263	LEU	2.3
1	A	203	MET	2.3
1	A	204	THR	2.3
1	B	242	LEU	2.3
1	B	185	PHE	2.2
1	B	325	GLU	2.2
1	A	207	TRP	2.2
1	A	323	TRP	2.2
1	B	259	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	309	VAL	2.2
1	B	200	ASP	2.2
1	B	137	PRO	2.2
1	A	202	ARG	2.2
1	B	6	ASN	2.2
1	B	317	SER	2.1
1	A	158	PHE	2.1
1	A	137	PRO	2.1
1	B	303	HIS	2.1
1	B	140	LEU	2.1
1	B	322	GLN	2.0
1	A	143	ALA	2.0
1	A	169	VAL	2.0
1	B	295	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	A	337	12/12	0.89	0.16	1.28	40,42,44,44	0
2	NAP	A	334	48/48	0.96	0.15	-0.01	11,29,52,54	0
2	NAP	B	334	48/48	0.96	0.14	-0.07	12,29,50,55	0
3	UDP	B	335	25/25	0.76	0.21	-0.54	65,70,72,72	0
3	UDP	A	335	25/25	0.82	0.19	-0.61	47,56,59,59	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.