



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:36 PM BST

PDB ID : 3VNL  
Title : Crystal structures of D-Psicose 3-epimerase with D-tagatose from *Clostridium cellulolyticum* H10  
Authors : Chan, H.C.; Zhu, Y.; Hu, Y.; Ko, T.P.; Huang, C.H.; Ren, F.; Chen, C.C.; Guo, R.T.; Sun, Y.  
Deposited on : 2012-01-16  
Resolution : 2.15 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

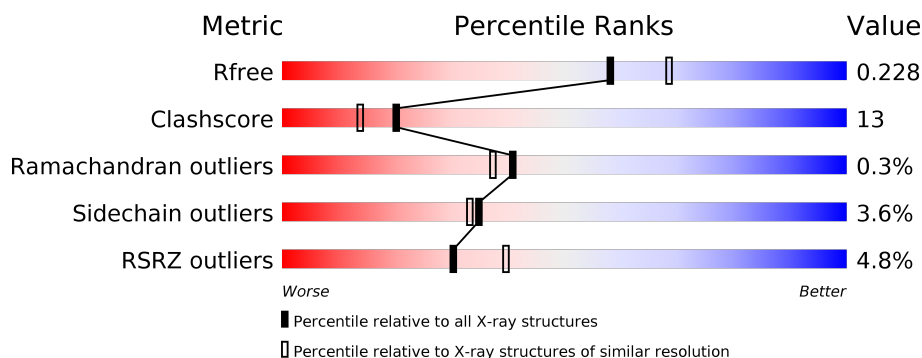
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 respectively. 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	294	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>
1	B	294	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	C	294	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	D	294	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>21%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TAG	C	301	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10140 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.

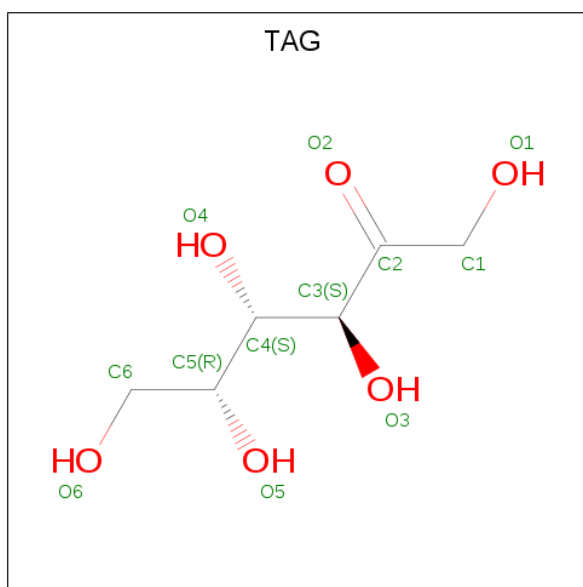
- Molecule 1 is a protein called Xylose isomerase domain protein TIM barrel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2308	1468	392	437	11			
1	B	288	Total	C	N	O	S	0	0	0
			2287	1456	387	434	10			
1	C	288	Total	C	N	O	S	0	0	0
			2287	1456	387	434	10			
1	D	289	Total	C	N	O	S	0	0	0
			2293	1459	388	435	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	EXPRESSION TAG	UNP B8I944
B	0	ALA	-	EXPRESSION TAG	UNP B8I944
C	0	ALA	-	EXPRESSION TAG	UNP B8I944
D	0	ALA	-	EXPRESSION TAG	UNP B8I944

- Molecule 2 is D-tagatose (three-letter code: TAG) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	253	Total	O	0	0
			253	253		

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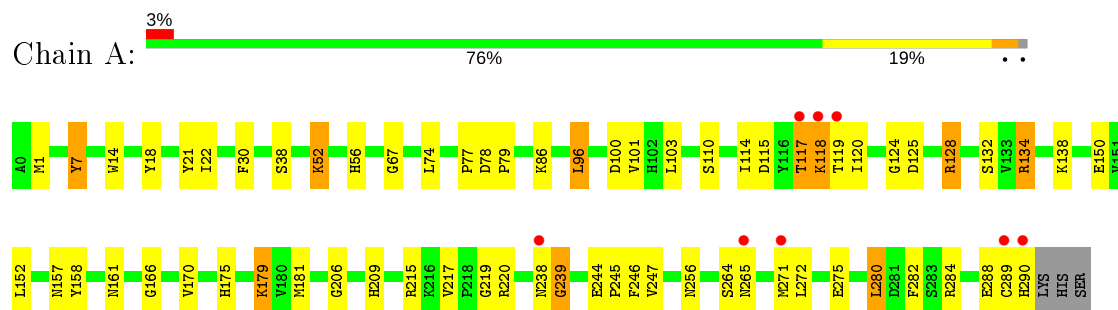
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	262	Total 262	O 262	0	0
4	C	208	Total 208	O 208	0	0
4	D	190	Total 190	O 190	0	0

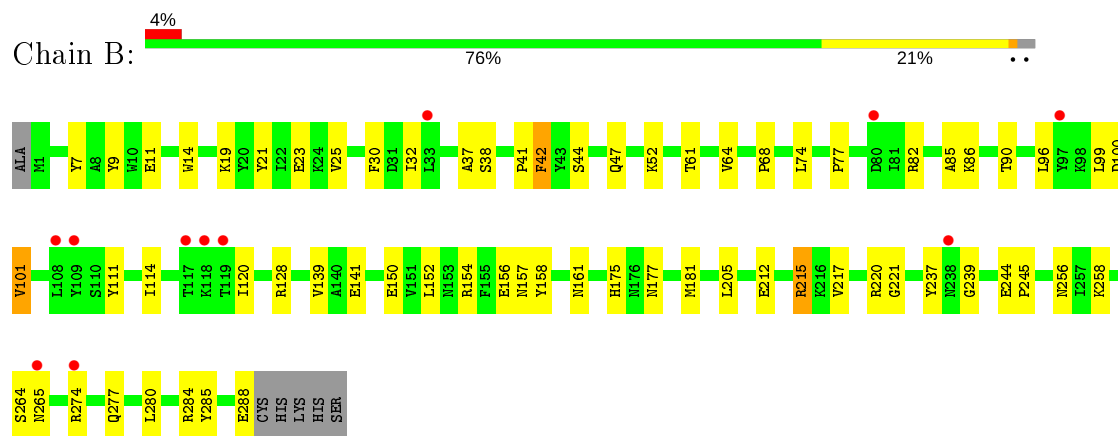
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

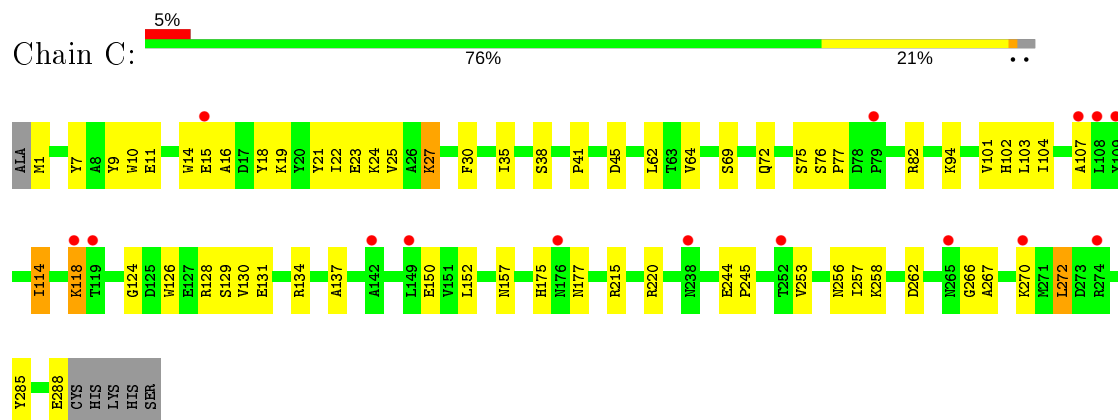
- Molecule 1: Xylose isomerase domain protein TIM barrel



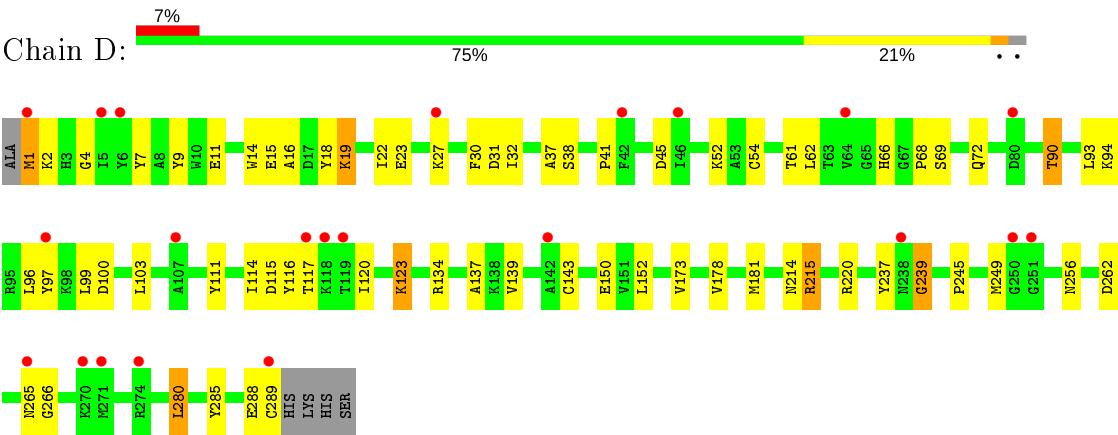
- Molecule 1: Xylose isomerase domain protein TIM barrel



- Molecule 1: Xylose isomerase domain protein TIM barrel



● Molecule 1: Xylose isomerase domain protein TIM barrel





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.07Å 115.37Å 91.53Å 90.00° 104.77° 90.00°	Depositor
Resolution (Å)	25.00 – 2.15 24.89 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.15) 95.0 (24.89-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 2.15Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.187 , 0.229 0.186 , 0.228	Depositor DCC
$R_{free}$ test set	4188 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 58.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAG, MN

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	0.74	0/2362	0.84	3/3199 (0.1%)
1	B	0.68	0/2340	0.77	1/3169 (0.0%)
1	C	0.62	0/2340	0.78	0/3169
1	D	0.64	1/2346 (0.0%)	0.78	2/3177 (0.1%)
All	All	0.67	1/9388 (0.0%)	0.79	6/12714 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	100	ASP	CB-CG	5.56	1.63	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	239	GLY	N-CA-C	6.18	128.56	113.10
1	A	215	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	67	GLY	N-CA-C	-5.64	98.99	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	215	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	TYR	Sidechain
1	A	7	TYR	Sidechain
1	B	21	TYR	Sidechain
1	B	7	TYR	Sidechain
1	C	21	TYR	Sidechain
1	D	7	TYR	Sidechain

## 5.2 Too-close contacts

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	2308	0	2240	56	0
1	B	2287	0	2223	59	0
1	C	2287	0	2223	55	0
1	D	2293	0	2228	58	0
2	A	12	0	12	5	0
2	B	12	0	12	2	0
2	C	12	0	12	6	0
2	D	12	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	253	0	0	6	1
4	B	262	0	0	3	1
4	C	208	0	0	7	0
4	D	190	0	0	3	0
All	All	10140	0	8962	228	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 13.

All (228) 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:D:90:THR:HG22	1:D:139:VAL:HG21	1.30	1.14
1:B:25:VAL:HG13	1:B:30:PHE:HB2	1.51	0.90
1:C:175:HIS:HD2	1:C:177:ASN:H	1.20	0.90
1:A:77:PRO:HA	1:A:128:ARG:HE	1.35	0.89
1:D:32:ILE:CD1	1:D:61:THR:HB	2.05	0.86
1:D:23:GLU:O	1:D:27:LYS:HG2	1.77	0.85
1:A:124:GLY:C	1:A:128:ARG:HH12	1.79	0.84
1:A:14:TRP:HE1	1:A:256:ASN:HD22	1.26	0.83
1:B:175:HIS:HD2	1:B:177:ASN:H	1.25	0.83
1:A:118:LYS:HG3	1:A:119:THR:N	1.94	0.82
1:C:215:ARG:HH22	2:C:301:TAG:H11	1.41	0.82
1:D:90:THR:CG2	1:D:139:VAL:HG21	2.11	0.79
1:A:125:ASP:N	1:A:128:ARG:HH12	1.80	0.78
1:B:274:ARG:HB3	1:B:274:ARG:NH1	1.99	0.78
1:B:244:GLU:OE2	2:B:301:TAG:H3	1.85	0.76
1:B:114:ILE:HD12	1:B:157:ASN:HA	1.68	0.75
1:A:14:TRP:HE1	1:A:256:ASN:ND2	1.85	0.75
1:A:244:GLU:OE2	2:A:7101:TAG:H3	1.89	0.73
1:B:100:ASP:OD1	4:B:557:HOH:O	2.06	0.73
1:C:244:GLU:OE2	2:C:301:TAG:H3	1.88	0.73
1:A:77:PRO:HA	1:A:128:ARG:NE	2.04	0.73
1:C:25:VAL:HG13	1:C:30:PHE:HB2	1.71	0.73
1:D:114:ILE:HD11	1:D:116:TYR:CD2	2.24	0.72
1:D:114:ILE:HD11	1:D:116:TYR:CG	2.24	0.72
2:C:301:TAG:O4	2:C:301:TAG:H12	1.91	0.69
1:C:114:ILE:HD13	1:C:157:ASN:HA	1.75	0.69
1:C:215:ARG:HH22	2:C:301:TAG:C1	2.06	0.68
1:C:175:HIS:CD2	1:C:177:ASN:H	2.08	0.67
1:A:115:ASP:OD2	1:A:117:THR:HB	1.95	0.67
1:D:111:TYR:CE2	1:D:114:ILE:HA	2.30	0.67
1:A:289:CYS:O	1:A:290:HIS:HB3	1.96	0.65
1:B:77:PRO:HD3	1:B:128:ARG:HH12	1.61	0.65
1:D:4:GLY:HA3	1:D:32:ILE:HB	1.77	0.65
1:D:19:LYS:HB2	1:D:19:LYS:NZ	2.11	0.65
1:A:244:GLU:HG2	1:A:246:PHE:CE2	2.32	0.65
1:C:75:SER:HB3	1:C:129:SER:OG	1.98	0.64
1:B:120:ILE:HD12	1:B:158:TYR:CE2	2.33	0.64
1:D:32:ILE:HD13	1:D:61:THR:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LYS:HE2	1:C:118:LYS:HA	1.80	0.63
1:B:274:ARG:CB	1:B:274:ARG:HH11	2.12	0.63
1:D:14:TRP:HE1	1:D:256:ASN:ND2	1.95	0.63
1:B:175:HIS:CD2	1:B:177:ASN:H	2.14	0.63
1:A:124:GLY:C	1:A:128:ARG:NH1	2.51	0.62
1:B:37:ALA:HB2	1:B:64:VAL:CG1	2.30	0.62
1:B:274:ARG:HB3	1:B:274:ARG:HH11	1.61	0.62
1:B:96:LEU:HG	1:B:101:VAL:HG22	1.82	0.61
1:C:23:GLU:O	1:C:27:LYS:HE2	2.01	0.61
1:B:9:TYR:CD1	1:B:245:PRO:HG2	2.36	0.61
1:B:96:LEU:HG	1:B:101:VAL:CG2	2.30	0.60
1:A:125:ASP:HA	1:A:128:ARG:NH1	2.17	0.59
1:B:90:THR:HG22	1:B:139:VAL:HG21	1.84	0.59
1:B:82:ARG:O	1:B:86:LYS:HG3	2.03	0.59
1:B:19:LYS:O	1:B:23:GLU:HG3	2.03	0.59
1:A:56:HIS:NE2	4:A:7438:HOH:O	2.27	0.59
1:D:115:ASP:OD2	1:D:117:THR:HB	2.02	0.59
1:D:38:SER:O	1:D:41:PRO:HD2	2.02	0.59
1:C:77:PRO:HB3	1:C:128:ARG:NH1	2.19	0.58
1:D:52:LYS:HB2	1:D:99:LEU:HD23	1.85	0.58
1:C:215:ARG:NH2	2:C:301:TAG:H11	2.16	0.58
1:A:74:LEU:HD22	1:A:132:SER:HB3	1.85	0.57
1:A:1:MET:HE2	1:A:288:GLU:HG2	1.85	0.57
1:D:288:GLU:O	1:D:289:CYS:HB2	2.04	0.57
1:A:77:PRO:CA	1:A:128:ARG:HE	2.13	0.57
1:B:32:ILE:HG12	1:B:61:THR:HB	1.86	0.57
1:A:117:THR:HG21	4:A:7402:HOH:O	2.03	0.56
1:C:94:LYS:NZ	4:C:475:HOH:O	2.38	0.56
1:A:181:MET:CE	1:A:209:HIS:CE1	2.89	0.56
1:A:166:GLY:O	1:A:170:VAL:HG23	2.06	0.55
1:A:114:ILE:HG13	1:A:157:ASN:HA	1.88	0.55
1:B:38:SER:O	1:B:41:PRO:HD2	2.07	0.55
1:C:10:TRP:CZ2	1:C:24:LYS:HD3	2.41	0.55
1:A:138:LYS:HD3	1:A:175:HIS:CE1	2.42	0.55
1:C:244:GLU:O	1:C:244:GLU:HG2	2.08	0.54
1:A:120:ILE:HD12	1:A:158:TYR:CE2	2.43	0.54
2:D:301:TAG:O6	2:D:301:TAG:O3	2.21	0.54
1:A:128:ARG:HH11	1:A:128:ARG:CG	2.20	0.54
1:C:77:PRO:CA	1:C:128:ARG:NH1	2.71	0.54
1:A:30:PHE:CE1	1:A:280:LEU:HG	2.43	0.54
2:A:7101:TAG:O3	2:A:7101:TAG:H62	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HG3	1:A:134:ARG:NH1	2.23	0.53
1:C:77:PRO:N	1:C:128:ARG:HH11	2.07	0.53
1:B:25:VAL:CG1	1:B:30:PHE:HB2	2.30	0.52
1:D:214:ASN:O	1:D:215:ARG:HB2	2.09	0.52
1:D:18:TYR:O	1:D:22:ILE:HG13	2.08	0.52
1:C:38:SER:O	1:C:41:PRO:HD2	2.09	0.52
1:D:1:MET:HG2	1:D:288:GLU:OE2	2.09	0.52
1:C:94:LYS:NZ	4:C:598:HOH:O	2.43	0.52
1:B:44:SER:OG	1:B:47:GLN:HG3	2.10	0.51
1:B:274:ARG:CB	1:B:274:ARG:NH1	2.72	0.51
1:C:77:PRO:CA	1:C:128:ARG:HH11	2.23	0.51
1:C:107:ALA:HB2	1:C:152:LEU:HD11	1.92	0.51
1:D:114:ILE:C	1:D:114:ILE:HD12	2.31	0.50
1:C:25:VAL:CG1	1:C:30:PHE:HB2	2.40	0.50
1:C:220:ARG:NH1	4:C:403:HOH:O	2.43	0.50
1:C:253:VAL:O	1:C:257:ILE:HG12	2.11	0.50
1:C:126:TRP:O	1:C:130:VAL:HG23	2.12	0.50
1:D:97:TYR:HB2	1:D:143:CYS:HB3	1.93	0.50
1:D:120:ILE:HG13	1:D:120:ILE:O	2.11	0.49
1:A:247:VAL:HG23	1:A:264:SER:HB3	1.94	0.49
1:A:271:MET:HB2	4:A:7278:HOH:O	2.10	0.49
1:B:244:GLU:HG2	1:B:244:GLU:O	2.12	0.49
1:B:37:ALA:HB2	1:B:64:VAL:HG11	1.93	0.49
1:A:220:ARG:NH1	1:B:285:TYR:O	2.43	0.49
1:C:18:TYR:O	1:C:22:ILE:HG13	2.13	0.49
1:B:177:ASN:HD22	1:B:177:ASN:N	2.10	0.48
1:C:7:TYR:OH	1:C:14:TRP:HA	2.13	0.48
1:D:103:LEU:C	1:D:103:LEU:HD23	2.33	0.48
1:D:9:TYR:CD1	1:D:245:PRO:HG2	2.48	0.48
1:B:280:LEU:HD21	1:B:284:ARG:HH12	1.77	0.48
1:A:77:PRO:HB3	1:A:128:ARG:HH21	1.79	0.48
1:B:150:GLU:HA	1:B:181:MET:HB3	1.95	0.48
1:B:152:LEU:O	1:B:161:ASN:HA	2.14	0.48
1:D:30:PHE:CE1	1:D:280:LEU:HG	2.48	0.48
1:A:125:ASP:CA	1:A:128:ARG:HH12	2.27	0.48
1:A:124:GLY:O	1:A:128:ARG:NH1	2.47	0.48
1:B:264:SER:O	1:B:265:ASN:HB2	2.14	0.48
1:C:103:LEU:HD23	1:C:104:ILE:N	2.28	0.48
1:C:1:MET:HE2	1:C:288:GLU:HG2	1.96	0.47
1:C:215:ARG:CD	4:C:510:HOH:O	2.62	0.47
1:B:217:VAL:HG12	1:B:245:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ILE:HD12	1:D:61:THR:HB	1.94	0.47
1:D:114:ILE:HD11	1:D:116:TYR:CD1	2.49	0.47
1:D:1:MET:HE1	1:D:237:TYR:HD2	1.80	0.47
1:D:23:GLU:O	1:D:27:LYS:HE2	2.15	0.47
1:B:77:PRO:HD3	1:B:128:ARG:NH1	2.29	0.47
1:D:90:THR:HG22	1:D:139:VAL:CG2	2.21	0.47
1:C:220:ARG:HD2	1:D:285:TYR:CE1	2.50	0.47
1:B:277:GLN:NE2	4:B:462:HOH:O	2.35	0.47
1:D:150:GLU:HA	1:D:181:MET:HB3	1.96	0.47
1:A:128:ARG:HG3	1:A:128:ARG:NH1	2.30	0.47
1:A:179:LYS:HG3	1:A:206:GLY:HA3	1.97	0.47
1:C:124:GLY:HA3	1:C:128:ARG:HH21	1.79	0.47
1:C:77:PRO:CB	1:C:128:ARG:NH1	2.78	0.47
2:A:7101:TAG:O3	2:A:7101:TAG:C6	2.63	0.47
1:A:150:GLU:OE1	2:A:7101:TAG:O3	2.22	0.46
1:D:114:ILE:HD11	1:D:116:TYR:CE2	2.50	0.46
1:A:7:TYR:OH	1:A:14:TRP:HA	2.15	0.46
1:B:74:LEU:HD23	1:B:85:ALA:CB	2.45	0.46
1:B:11:GLU:HB3	4:B:585:HOH:O	2.15	0.46
1:A:179:LYS:HE3	1:A:179:LYS:HB3	1.54	0.46
1:D:123:LYS:HE3	1:D:123:LYS:HA	1.98	0.46
1:A:128:ARG:HG3	1:A:128:ARG:HH11	1.81	0.46
1:A:96:LEU:HA	1:A:96:LEU:HD12	1.77	0.46
1:B:68:PRO:HB2	1:B:111:TYR:HA	1.98	0.46
1:A:289:CYS:O	1:A:290:HIS:CB	2.64	0.45
1:B:74:LEU:HD23	1:B:85:ALA:HB1	1.98	0.45
1:C:11:GLU:HG3	1:C:16:ALA:HB2	1.97	0.45
1:C:15:GLU:O	1:C:15:GLU:HG3	2.16	0.45
1:A:103:LEU:HD23	1:A:103:LEU:C	2.37	0.45
1:C:103:LEU:C	1:C:103:LEU:HD23	2.37	0.45
1:C:150:GLU:OE1	2:C:301:TAG:O3	2.30	0.45
1:C:69:SER:OG	1:C:72:GLN:HG3	2.17	0.45
1:D:1:MET:CE	1:D:237:TYR:HD2	2.30	0.45
1:D:66:HIS:O	1:D:68:PRO:HD3	2.15	0.45
1:A:52:LYS:HD2	1:A:100:ASP:HB2	1.97	0.45
1:A:238:ASN:HB2	4:A:7377:HOH:O	2.16	0.45
1:B:77:PRO:N	1:B:128:ARG:NH1	2.64	0.45
1:D:262:ASP:OD2	1:D:266:GLY:N	2.49	0.45
1:A:152:LEU:O	1:A:161:ASN:HA	2.16	0.45
1:C:262:ASP:OD2	1:C:266:GLY:N	2.44	0.45
1:C:64:VAL:HG23	1:C:101:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HD21	1:B:284:ARG:NH1	2.33	0.44
1:C:267:ALA:CB	1:C:272:LEU:HD13	2.47	0.44
1:D:94:LYS:HD2	1:D:143:CYS:SG	2.57	0.44
1:D:11:GLU:HG3	1:D:16:ALA:HB2	1.99	0.44
1:C:102:HIS:NE2	4:C:586:HOH:O	2.28	0.44
1:A:271:MET:HE2	1:A:275:GLU:HG2	1.99	0.44
1:B:25:VAL:HG13	1:B:30:PHE:CB	2.33	0.44
1:B:154:ARG:HD3	1:C:258:LYS:HB2	1.99	0.43
1:D:249:MET:HE2	1:D:262:ASP:HB2	2.00	0.43
1:D:256:ASN:ND2	4:D:533:HOH:O	2.43	0.43
1:D:249:MET:HE1	1:D:262:ASP:N	2.34	0.43
1:A:96:LEU:HG	1:A:101:VAL:CG1	2.48	0.43
1:B:141:GLU:HA	1:B:177:ASN:OD1	2.18	0.43
1:D:215:ARG:HB2	4:D:514:HOH:O	2.18	0.43
1:B:77:PRO:CD	1:B:128:ARG:NH1	2.82	0.43
1:A:217:VAL:HG12	1:A:245:PRO:HG3	2.01	0.43
1:D:31:ASP:O	1:D:32:ILE:HD13	2.19	0.43
1:C:175:HIS:C	1:C:175:HIS:CD2	2.92	0.42
1:C:94:LYS:HD3	1:C:94:LYS:HA	1.76	0.42
1:D:90:THR:HA	1:D:139:VAL:HG11	2.00	0.42
1:C:9:TYR:CD1	1:C:245:PRO:HG2	2.54	0.42
1:A:18:TYR:O	1:A:22:ILE:HG13	2.19	0.42
1:B:77:PRO:CA	1:B:128:ARG:NH1	2.83	0.42
1:B:96:LEU:HG	1:B:101:VAL:HG21	2.02	0.42
1:D:237:TYR:CZ	1:D:239:GLY:HA3	2.54	0.42
1:C:134:ARG:O	1:C:137:ALA:HB3	2.20	0.42
1:C:215:ARG:HD3	4:C:510:HOH:O	2.19	0.42
1:D:134:ARG:O	1:D:137:ALA:HB3	2.19	0.42
1:B:150:GLU:OE1	2:B:301:TAG:O3	2.32	0.42
1:B:52:LYS:HD2	1:B:100:ASP:CB	2.50	0.42
1:C:244:GLU:N	1:C:245:PRO:CD	2.82	0.42
1:A:125:ASP:CA	1:A:128:ARG:NH1	2.81	0.42
1:B:86:LYS:O	1:B:90:THR:HG23	2.19	0.42
1:D:69:SER:OG	1:D:72:GLN:HG3	2.19	0.42
1:B:14:TRP:HE1	1:B:256:ASN:ND2	2.17	0.42
1:C:18:TYR:CZ	1:C:35:ILE:HB	2.55	0.42
1:D:1:MET:HB3	1:D:1:MET:HE3	1.86	0.42
1:B:99:LEU:O	1:B:100:ASP:HB3	2.19	0.41
1:D:15:GLU:O	1:D:16:ALA:HB2	2.20	0.41
1:B:42:PHE:N	1:B:42:PHE:CD1	2.85	0.41
1:D:37:ALA:O	1:D:41:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLY:HA2	1:A:282:PHE:CZ	2.55	0.41
1:B:52:LYS:HD2	1:B:100:ASP:HB2	2.02	0.41
1:A:220:ARG:HH22	1:B:288:GLU:HB2	1.84	0.41
1:C:77:PRO:HB3	1:C:128:ARG:HH12	1.86	0.41
1:D:111:TYR:O	1:D:114:ILE:HG22	2.21	0.41
1:B:237:TYR:CZ	1:B:239:GLY:HA3	2.55	0.41
1:A:181:MET:HE3	1:A:209:HIS:CE1	2.55	0.41
1:A:284:ARG:HH11	1:A:284:ARG:HD2	1.72	0.41
1:D:173:VAL:HG11	1:D:178:VAL:HG21	2.02	0.41
1:B:212:GLU:CD	1:B:221:GLY:HA3	2.41	0.41
1:C:215:ARG:HD2	4:C:510:HOH:O	2.20	0.41
1:D:19:LYS:HG2	1:D:54:CYS:SG	2.61	0.41
1:D:152:LEU:HD22	2:D:301:TAG:H12	2.03	0.41
1:D:45:ASP:HB3	4:D:458:HOH:O	2.20	0.41
1:A:86:LYS:NZ	4:A:7355:HOH:O	2.54	0.41
1:D:115:ASP:OD2	1:D:117:THR:CB	2.68	0.41
1:B:77:PRO:CD	1:B:128:ARG:HH12	2.32	0.41
1:B:220:ARG:HH11	1:B:220:ARG:HG2	1.86	0.41
1:C:14:TRP:HE1	1:C:256:ASN:ND2	2.18	0.41
1:D:68:PRO:HB2	1:D:111:TYR:HA	2.02	0.40
2:A:7101:TAG:H11	2:A:7101:TAG:H4	1.75	0.40
1:A:78:ASP:HA	1:A:79:PRO:HD3	1.91	0.40
1:C:285:TYR:O	1:D:220:ARG:NH1	2.54	0.40
1:C:76:SER:O	1:C:82:ARG:HD3	2.21	0.40
1:A:56:HIS:CE1	4:A:7438:HOH:O	2.72	0.40
1:B:156:GLU:O	1:B:157:ASN:HB2	2.22	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)
4:A:7330:HOH:O	4:B:629:HOH:O[2_545]	2.01	0.19

## 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	289/294 (98%)	280 (97%)	7 (2%)	2 (1%)	22	15
1	B	286/294 (97%)	276 (96%)	10 (4%)	0	100	100
1	C	286/294 (97%)	270 (94%)	16 (6%)	0	100	100
1	D	287/294 (98%)	274 (96%)	12 (4%)	1 (0%)	41	37
All	All	1148/1176 (98%)	1100 (96%)	45 (4%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	D	239	GLY
1	A	110	SER

### 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	242/245 (99%)	231 (96%)	11 (4%)	27	24
1	B	240/245 (98%)	235 (98%)	5 (2%)	53	57
1	C	240/245 (98%)	231 (96%)	9 (4%)	33	31
1	D	241/245 (98%)	231 (96%)	10 (4%)	30	29
All	All	963/980 (98%)	928 (96%)	35 (4%)	35	33

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	52	LYS
1	A	96	LEU
1	A	117	THR
1	A	118	LYS

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Mol	Chain	Res	Type
1	A	128	ARG
1	A	134	ARG
1	A	179	LYS
1	A	265	ASN
1	A	272	LEU
1	A	280	LEU
1	B	42	PHE
1	B	101	VAL
1	B	205	LEU
1	B	215	ARG
1	B	258	LYS
1	C	19	LYS
1	C	27	LYS
1	C	45	ASP
1	C	62	LEU
1	C	114	ILE
1	C	118	LYS
1	C	131	GLU
1	C	270	LYS
1	C	272	LEU
1	D	1	MET
1	D	2	LYS
1	D	19	LYS
1	D	62	LEU
1	D	90	THR
1	D	93	LEU
1	D	96	LEU
1	D	123	LYS
1	D	265	ASN
1	D	280	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	84	ASN
1	A	175	HIS
1	A	256	ASN
1	A	277	GLN
1	B	12	GLN
1	B	47	GLN
1	B	175	HIS

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Mol	Chain	Res	Type
1	B	256	ASN
1	C	58	ASN
1	C	66	HIS
1	C	84	ASN
1	C	175	HIS
1	C	177	ASN
1	D	12	GLN
1	D	177	ASN
1	D	256	ASN
1	D	265	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - 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	TAG	D	301	3	10,11,11	0.56	0	9,14,14	0.63	0
2	TAG	C	301	3	10,11,11	0.56	0	9,14,14	0.73	0
2	TAG	B	301	3	10,11,11	0.55	0	9,14,14	1.05	1 (11%)
2	TAG	A	7101	3	10,11,11	0.56	0	9,14,14	1.07	0

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	TAG	D	301	3	-	3/16/16/16	-
2	TAG	C	301	3	-	9/16/16/16	-
2	TAG	B	301	3	-	11/16/16/16	-
2	TAG	A	7101	3	-	9/16/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	TAG	O4-C4-C3	-2.15	105.30	109.21

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	TAG	O1-C1-C2-O2
2	D	301	TAG	O1-C1-C2-C3
2	D	301	TAG	O2-C2-C3-O3
2	B	301	TAG	O1-C1-C2-O2
2	B	301	TAG	C1-C2-C3-O3
2	B	301	TAG	C1-C2-C3-C4
2	B	301	TAG	O2-C2-C3-O3
2	B	301	TAG	O2-C2-C3-C4
2	B	301	TAG	C3-C4-C5-C6
2	B	301	TAG	O4-C4-C5-O5
2	C	301	TAG	O1-C1-C2-O2
2	C	301	TAG	O1-C1-C2-C3
2	C	301	TAG	C1-C2-C3-C4
2	C	301	TAG	O2-C2-C3-O3
2	C	301	TAG	O2-C2-C3-C4
2	C	301	TAG	C3-C4-C5-O5
2	C	301	TAG	C3-C4-C5-C6
2	C	301	TAG	O4-C4-C5-O5
2	C	301	TAG	O4-C4-C5-C6
2	A	7101	TAG	O1-C1-C2-O2
2	A	7101	TAG	O1-C1-C2-C3
2	A	7101	TAG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	7101	TAG	O2-C2-C3-C4
2	A	7101	TAG	O5-C5-C6-O6
2	B	301	TAG	O4-C4-C5-C6
2	A	7101	TAG	C4-C5-C6-O6
2	B	301	TAG	C3-C4-C5-O5
2	A	7101	TAG	O3-C3-C4-O4
2	A	7101	TAG	C1-C2-C3-C4
2	B	301	TAG	O3-C3-C4-O4
2	B	301	TAG	O1-C1-C2-C3
2	A	7101	TAG	O3-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	TAG	2	0
2	C	301	TAG	6	0
2	B	301	TAG	2	0
2	A	7101	TAG	5	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	291/294 (98%)	-0.14	8 (2%) 54 63	26, 37, 56, 81	0
1	B	288/294 (97%)	0.01	11 (3%) 40 49	27, 42, 60, 76	0
1	C	288/294 (97%)	0.15	15 (5%) 27 35	31, 47, 62, 82	0
1	D	289/294 (98%)	0.23	22 (7%) 13 19	29, 48, 69, 82	0
All	All	1156/1176 (98%)	0.06	56 (4%) 30 39	26, 44, 64, 82	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	42	PHE	5.2
1	C	119	THR	5.1
1	D	238	ASN	4.8
1	D	119	THR	4.2
1	D	270	LYS	4.2
1	B	119	THR	4.1
1	A	119	THR	4.1
1	C	238	ASN	4.0
1	A	117	THR	3.9
1	C	118	LYS	3.6
1	A	289	CYS	3.4
1	B	117	THR	3.3
1	A	118	LYS	3.2
1	B	238	ASN	3.2
1	D	117	THR	3.2
1	D	274	ARG	3.2
1	D	142	ALA	3.1
1	C	149	LEU	3.1
1	C	252	THR	3.0
1	D	97	TYR	3.0
1	D	265	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	97	TYR	2.7
1	D	118	LYS	2.6
1	D	250	GLY	2.6
1	C	79	PRO	2.6
1	C	142	ALA	2.6
1	B	33	LEU	2.6
1	D	46	ILE	2.6
1	C	176	ASN	2.5
1	A	290	HIS	2.4
1	D	5	ILE	2.4
1	C	265	ASN	2.4
1	D	289	CYS	2.4
1	C	107	ALA	2.4
1	B	274	ARG	2.4
1	D	251	GLY	2.4
1	D	107	ALA	2.3
1	A	238	ASN	2.3
1	D	80	ASP	2.3
1	B	109	TYR	2.3
1	B	108	LEU	2.2
1	D	64	VAL	2.2
1	B	118	LYS	2.2
1	C	109	TYR	2.2
1	C	274	ARG	2.2
1	B	265	ASN	2.2
1	C	108	LEU	2.2
1	D	6	TYR	2.2
1	B	80	ASP	2.2
1	D	271	MET	2.1
1	C	15	GLU	2.1
1	C	270	LYS	2.1
1	A	271	MET	2.1
1	A	265	ASN	2.1
1	D	1	MET	2.0
1	D	27	LYS	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TAG	C	301	12/12	0.79	0.22	48,62,65,67	0
2	TAG	B	301	12/12	0.86	0.19	38,55,57,59	0
2	TAG	D	301	12/12	0.88	0.28	55,63,66,67	0
2	TAG	A	7101	12/12	0.88	0.20	40,47,50,53	0
3	MN	A	7102	1/1	0.99	0.09	29,29,29,29	0
3	MN	C	302	1/1	0.99	0.08	36,36,36,36	0
3	MN	B	302	1/1	1.00	0.09	33,33,33,33	0
3	MN	D	302	1/1	1.00	0.10	36,36,36,36	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.