



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:20 am BST

PDB ID : 3NPY
Title : Crystal Structure of Tyrosinase from *Bacillus megaterium* soaked in CuSO₄
Authors : Sendovski, M.; Kanteev, M.; Adir, N.; Fishman, A.
Deposited on : 2010-06-29
Resolution : 2.19 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

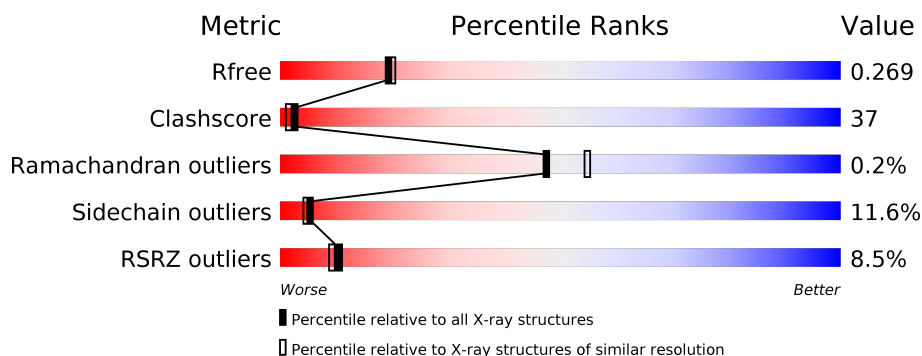
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	303	
1	B	303	

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	CL	A	513	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4831 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2300	1466	412	414	8			
1	B	285	Total	C	N	O	S	0	0	0
			2337	1487	422	420	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	299	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	300	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	301	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	302	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	303	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	298	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	299	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	300	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	301	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	302	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	303	HIS	-	EXPRESSION TAG	UNP B2ZB02

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cu	0	2
			4	4		
2	A	2	Total	Cu	0	2
			4	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Zn 3	0	0
3	A	5	Total 5	Zn 5	0	0

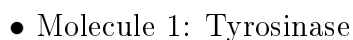
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	Cl 3	0	0
4	A	3	Total 3	Cl 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total 87	O 87	0	0
5	B	85	Total 85	O 85	0	0

- Molecule 1: Tyrosinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.55Å 82.13Å 146.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.19 54.71 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.19) 98.1 (54.71-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.20Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0072	Depositor
R, R_{free}	0.249 , 0.275 0.259 , 0.269	Depositor DCC
R_{free} test set	1563 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4831	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: ZN, CU, CL

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	1/2377 (0.0%)	0.69	0/3240
1	B	0.76	1/2415 (0.0%)	0.70	1/3291 (0.0%)
All	All	0.75	2/4792 (0.0%)	0.69	1/6531 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	250	TYR	CD1-CE1	-5.30	1.31	1.39
1	A	226	VAL	CB-CG2	-5.27	1.41	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ALA	CB-CA-C	-5.07	102.49	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	GLY	Peptide

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	2300	0	2180	165	0
1	B	2337	0	2221	168	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	5	0	0	1	0
3	B	3	0	0	0	0
4	A	3	0	0	3	0
4	B	3	0	0	1	0
5	A	87	0	0	9	0
5	B	85	0	0	10	0
All	All	4831	0	4401	332	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 37.

All (332) 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:244:ILE:HG22	1:A:245:HIS:ND1	1.39	1.32
1:B:4:LYS:CG	1:B:280:ARG:HG2	1.63	1.28
1:B:4:LYS:HG3	1:B:280:ARG:CG	1.61	1.28
1:B:254:LYS:HD2	1:B:255:ASN:H	1.03	1.17
1:B:200:GLY:HA2	1:B:202:GLN:HG2	1.28	1.13
1:B:254:LYS:HD2	1:B:255:ASN:N	1.61	1.13
1:A:244:ILE:CG2	1:A:245:HIS:CE1	2.32	1.12
1:A:193:GLN:HG2	1:A:198:ILE:HD12	1.28	1.11
1:A:20:ARG:HG2	1:A:24:ARG:NH2	1.69	1.07
1:B:123:ASP:O	1:B:124:PHE:CD1	2.08	1.07
1:A:244:ILE:CG2	1:A:245:HIS:ND1	2.19	1.06
1:B:4:LYS:HG3	1:B:280:ARG:HG2	1.11	1.05
1:B:99:GLN:NE2	1:B:165:ARG:HH21	1.56	1.03
1:B:64:ALA:HB1	1:B:266:MET:HE3	1.35	1.02
1:B:4:LYS:CG	1:B:280:ARG:CG	2.30	1.02
1:B:254:LYS:CD	1:B:255:ASN:H	1.73	1.01
1:B:96:THR:HG22	1:B:165:ARG:HH22	1.24	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HG21	1:A:245:HIS:CE1	1.96	0.99
1:A:175:THR:HG23	5:A:390:HOH:O	1.63	0.98
1:B:99:GLN:HE22	1:B:165:ARG:HH21	1.04	0.98
1:A:94:TRP:CE3	1:A:163:PRO:HG2	1.98	0.97
1:A:215:MET:HE3	1:A:227:PHE:HB2	1.46	0.96
1:A:67:PRO:HG2	1:A:266:MET:CE	1.94	0.96
1:A:254:LYS:O	1:A:255:ASN:HB2	1.63	0.96
1:A:224:ASP:OD1	1:A:226:VAL:HG23	1.64	0.95
1:A:67:PRO:HG2	1:A:266:MET:HE1	1.48	0.95
1:A:254:LYS:HE2	1:A:255:ASN:OD1	1.67	0.94
1:B:215:MET:HE3	1:B:227:PHE:HB2	1.49	0.94
1:B:49:HIS:CE1	5:B:388:HOH:O	2.20	0.94
1:B:119:ASN:HD22	1:B:120:PRO:HD2	1.33	0.94
1:A:113:PHE:O	1:A:130:PRO:HD2	1.69	0.93
1:A:267:TYR:CD1	1:A:268:PRO:HA	2.04	0.92
1:B:4:LYS:HG3	1:B:280:ARG:HG3	1.49	0.91
1:A:261:ASN:HB2	1:A:264:ASP:OD2	1.70	0.91
1:A:20:ARG:HG2	1:A:24:ARG:HH22	1.34	0.90
1:B:200:GLY:CA	1:B:202:GLN:HG2	2.03	0.89
1:B:215:MET:CE	1:B:221:ALA:O	2.20	0.88
1:B:4:LYS:HG2	1:B:280:ARG:HG2	1.55	0.88
1:A:244:ILE:HG22	1:A:245:HIS:HD1	1.30	0.87
1:B:149:LEU:HD22	1:B:150:LYS:N	1.90	0.87
1:A:127:ASP:HA	1:A:132:ALA:HB1	1.57	0.86
1:B:62:SER:HB3	5:B:348:HOH:O	1.76	0.85
1:A:244:ILE:HG22	1:A:245:HIS:CE1	2.01	0.85
1:A:57:ASN:HD21	1:A:60:HIS:HD1	1.24	0.85
1:A:101:GLN:NE2	1:A:101:GLN:HA	1.91	0.85
1:B:215:MET:HE3	1:B:221:ALA:O	1.79	0.83
1:A:94:TRP:HE3	1:A:163:PRO:HG2	1.44	0.82
1:B:267:TYR:CD1	1:B:268:PRO:HA	2.16	0.81
1:B:123:ASP:O	1:B:124:PHE:HD1	1.60	0.81
1:B:144:ASN:OD1	4:B:512:CL:CL	2.35	0.81
1:B:8:ARG:HG2	1:B:89:LEU:O	1.81	0.81
1:A:8:ARG:HG2	1:A:89:LEU:O	1.81	0.81
1:B:57:ASN:HD21	1:B:60:HIS:HD1	1.27	0.81
1:A:254:LYS:CE	1:A:255:ASN:OD1	2.29	0.80
1:A:254:LYS:CD	1:A:255:ASN:OD1	2.30	0.79
1:B:119:ASN:HD22	1:B:120:PRO:CD	1.95	0.79
1:A:6:ARG:HD3	1:A:81:GLN:OE1	1.82	0.79
1:A:254:LYS:HD3	1:A:255:ASN:OD1	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:HG3	1:B:85:PRO:HA	1.63	0.78
1:A:267:TYR:CG	1:A:268:PRO:HA	2.18	0.78
1:B:119:ASN:ND2	1:B:120:PRO:HD2	2.00	0.77
1:A:64:ALA:H	1:A:260:GLN:HE22	1.32	0.75
1:A:95:GLU:OE2	1:A:236:ARG:NH2	2.20	0.75
1:A:101:GLN:HE21	1:A:101:GLN:HA	1.52	0.74
1:B:49:HIS:HE1	5:B:388:HOH:O	1.64	0.73
1:A:94:TRP:CE3	1:A:163:PRO:CG	2.72	0.73
1:A:20:ARG:HG2	1:A:24:ARG:CZ	2.19	0.72
1:A:254:LYS:CD	1:A:255:ASN:CG	2.59	0.71
1:B:215:MET:HE2	1:B:221:ALA:O	1.89	0.71
1:B:64:ALA:H	1:B:260:GLN:HE22	1.37	0.70
1:B:99:GLN:NE2	1:B:165:ARG:NH2	2.35	0.70
1:A:215:MET:HE1	1:A:221:ALA:HB1	1.74	0.70
1:A:67:PRO:HG2	1:A:266:MET:HE3	1.73	0.70
1:B:149:LEU:CD2	1:B:150:LYS:H	2.04	0.70
1:A:278:ASN:HA	5:A:361:HOH:O	1.92	0.69
1:A:244:ILE:HG22	1:A:245:HIS:CG	2.27	0.69
1:B:279:HIS:HD2	5:B:379:HOH:O	1.76	0.69
1:B:152:ASN:ND2	1:B:155:ALA:CB	2.56	0.69
1:B:149:LEU:CD2	1:B:150:LYS:N	2.56	0.69
1:A:101:GLN:HE21	1:A:101:GLN:CA	2.05	0.68
1:A:236:ARG:HA	1:A:286:TYR:CE2	2.28	0.68
1:B:149:LEU:HD22	1:B:150:LYS:H	1.59	0.68
1:B:94:TRP:CE3	1:B:163:PRO:HG2	2.29	0.68
1:A:57:ASN:ND2	1:A:60:HIS:H	1.93	0.67
1:B:254:LYS:CG	1:B:255:ASN:H	2.08	0.67
3:A:505:ZN:ZN	4:A:511:CL:CL	1.81	0.67
1:A:263:ARG:O	1:A:264:ASP:OD1	2.13	0.66
1:A:221:ALA:HB3	1:A:222:PRO:HD3	1.78	0.66
1:B:64:ALA:HB1	1:B:266:MET:CE	2.19	0.66
1:A:236:ARG:HB2	1:A:286:TYR:CE1	2.30	0.66
1:B:96:THR:HG22	1:B:165:ARG:NH2	2.05	0.66
1:B:152:ASN:ND2	1:B:155:ALA:HB3	2.10	0.66
1:B:123:ASP:O	1:B:124:PHE:CG	2.49	0.66
1:B:221:ALA:HB3	1:B:222:PRO:HD3	1.78	0.66
1:B:215:MET:HE1	1:B:221:ALA:HB1	1.78	0.65
1:A:14:LEU:HD11	1:A:90:PRO:HB3	1.76	0.65
1:A:64:ALA:HB1	1:A:266:MET:HE2	1.79	0.65
1:B:57:ASN:ND2	1:B:60:HIS:H	1.94	0.65
1:B:38:TYR:OH	1:B:76:PHE:HA	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ASN:HD22	1:A:119:ASN:C	1.98	0.64
1:B:267:TYR:CG	1:B:268:PRO:HA	2.33	0.64
1:B:28:ILE:CG2	1:B:32:LYS:HE2	2.26	0.64
1:A:141:GLU:HG2	1:A:219:PRO:HB2	1.79	0.64
1:B:215:MET:HE2	1:B:215:MET:HA	1.80	0.63
1:A:235:ASP:HB3	1:A:286:TYR:OH	1.98	0.63
1:B:141:GLU:O	1:B:141:GLU:HG2	1.99	0.62
1:A:20:ARG:HD2	1:A:24:ARG:HH12	1.64	0.62
1:A:101:GLN:NE2	1:A:101:GLN:CA	2.54	0.62
1:A:254:LYS:HD3	1:A:255:ASN:CG	2.20	0.62
1:A:64:ALA:H	1:A:260:GLN:NE2	1.98	0.61
1:A:119:ASN:HD22	1:A:120:PRO:N	1.98	0.61
1:B:121:ILE:O	1:B:121:ILE:CG2	2.48	0.61
1:A:113:PHE:O	1:A:130:PRO:CD	2.46	0.61
1:B:68:TRP:N	1:B:266:MET:HE1	2.15	0.61
1:B:198:ILE:O	1:B:198:ILE:HG22	2.01	0.61
1:B:233:ASN:O	1:B:237:ILE:HG12	2.00	0.60
1:A:115:GLY:HA3	1:A:128:THR:O	2.02	0.60
1:A:68:TRP:N	1:A:266:MET:HE1	2.16	0.60
1:A:142:GLN:HE21	1:A:144:ASN:ND2	2.00	0.60
1:B:59:ALA:HB3	1:B:60:HIS:CE1	2.37	0.60
1:A:119:ASN:ND2	1:A:121:ILE:H	2.00	0.59
1:B:158:GLU:OE2	1:B:201:PRO:HD3	2.01	0.59
1:A:126:VAL:HG13	5:A:367:HOH:O	2.03	0.59
1:B:64:ALA:CB	1:B:266:MET:HE3	2.22	0.59
1:B:254:LYS:CD	1:B:255:ASN:N	2.43	0.59
1:B:142:GLN:HE21	1:B:144:ASN:ND2	2.00	0.59
1:A:236:ARG:HB2	1:A:286:TYR:CZ	2.38	0.58
1:B:133:ALA:HB2	1:B:148:GLY:HA3	1.86	0.58
1:A:254:LYS:HD3	1:A:255:ASN:CB	2.33	0.58
1:A:241:TRP:O	1:A:245:HIS:ND1	2.29	0.58
1:A:62:SER:OG	1:A:260:GLN:CD	2.43	0.57
1:B:9:LYS:HG2	1:B:287:ASP:OD1	2.03	0.57
1:A:109:TRP:O	1:A:115:GLY:O	2.21	0.57
1:B:123:ASP:O	1:B:124:PHE:CB	2.52	0.57
1:B:256:GLY:N	1:B:261:ASN:HD21	2.01	0.57
1:B:193:GLN:HG2	1:B:198:ILE:HD12	1.86	0.57
1:A:20:ARG:CD	1:A:24:ARG:HH12	2.18	0.57
1:B:29:LEU:HD22	1:B:80:LEU:HD23	1.86	0.56
1:A:165:ARG:HB2	5:A:325:HOH:O	2.04	0.56
1:A:114:MET:O	1:A:151:ARG:NH1	2.26	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLU:HG2	1:B:201:PRO:CD	2.36	0.56
1:A:195:GLU:O	1:A:204:HIS:HB3	2.06	0.56
1:B:215:MET:HE1	1:B:227:PHE:HD2	1.70	0.56
1:B:261:ASN:HB2	1:B:264:ASP:OD2	2.05	0.56
1:B:243:ILE:O	1:B:246:ARG:HG2	2.05	0.56
1:A:117:ASN:ND2	1:A:118:GLY:H	2.05	0.55
1:B:68:TRP:NE1	1:B:267:TYR:O	2.32	0.55
1:A:254:LYS:HD3	1:A:254:LYS:C	2.26	0.55
1:A:101:GLN:HB3	5:A:316:HOH:O	2.07	0.55
1:A:57:ASN:HD22	1:A:59:ALA:H	1.54	0.55
1:A:188:ASN:O	1:A:188:ASN:ND2	2.39	0.55
1:B:117:ASN:ND2	1:B:118:GLY:H	2.05	0.55
1:B:9:LYS:HA	1:B:287:ASP:CG	2.27	0.55
1:B:4:LYS:CB	1:B:280:ARG:CG	2.84	0.55
1:B:68:TRP:HB2	1:B:266:MET:CE	2.37	0.55
1:B:150:LYS:O	1:B:213:GLY:HA3	2.07	0.55
1:A:215:MET:HA	1:A:215:MET:HE2	1.88	0.55
1:B:5:TYR:HB3	5:B:334:HOH:O	2.07	0.54
1:B:64:ALA:O	1:B:68:TRP:HB2	2.07	0.54
1:B:94:TRP:HE1	1:B:230:HIS:HD2	1.53	0.54
1:A:174:ILE:HD11	1:A:193:GLN:HG3	1.88	0.54
1:B:64:ALA:H	1:B:260:GLN:NE2	2.06	0.54
1:B:4:LYS:CG	1:B:280:ARG:HG3	2.19	0.54
1:B:57:ASN:HD22	1:B:59:ALA:H	1.54	0.54
1:A:20:ARG:CG	1:A:24:ARG:NH1	2.71	0.53
1:B:84:ASN:HD22	1:B:86:GLU:H	1.57	0.53
1:A:84:ASN:HD22	1:A:86:GLU:H	1.56	0.53
1:B:118:GLY:HA3	1:B:124:PHE:O	2.09	0.53
1:B:4:LYS:CB	1:B:280:ARG:HG3	2.39	0.53
1:A:20:ARG:CG	1:A:24:ARG:CZ	2.87	0.53
1:B:215:MET:CE	1:B:221:ALA:HB1	2.39	0.52
1:B:235:ASP:HB3	1:B:286:TYR:OH	2.10	0.52
1:B:142:GLN:HE21	1:B:144:ASN:HD22	1.57	0.52
1:A:256:GLY:H	1:A:261:ASN:HD21	1.57	0.52
1:B:181:PRO:HG2	1:B:183:ASP:OD2	2.09	0.52
1:A:254:LYS:CD	1:A:255:ASN:CB	2.88	0.52
1:A:87:VAL:HG22	5:A:387:HOH:O	2.08	0.52
1:B:193:GLN:HG2	1:B:198:ILE:CD1	2.40	0.52
1:B:20:ARG:O	1:B:20:ARG:HG2	2.09	0.52
1:B:245:HIS:HB3	1:B:248:GLN:HB2	1.91	0.52
1:A:181:PRO:HG2	1:A:183:ASP:CG	2.29	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:CE	1:A:221:ALA:HB1	2.40	0.52
1:A:119:ASN:HD22	1:A:120:PRO:CD	2.23	0.52
1:A:127:ASP:CA	1:A:132:ALA:HB1	2.37	0.51
1:A:194:LEU:HA	1:A:203:LEU:HD13	1.91	0.51
1:A:62:SER:HB3	1:A:260:GLN:OE1	2.11	0.51
1:A:64:ALA:HB1	1:A:266:MET:CE	2.39	0.51
1:B:163:PRO:HB3	5:B:352:HOH:O	2.09	0.51
1:B:68:TRP:HB2	1:B:266:MET:HE2	1.93	0.51
1:A:254:LYS:CD	1:A:255:ASN:HB2	2.41	0.51
1:A:262:PHE:CD2	1:A:263:ARG:HG3	2.45	0.51
1:A:53:GLY:N	5:A:351:HOH:O	2.31	0.51
1:A:95:GLU:HB2	1:A:165:ARG:HA	1.92	0.51
1:A:57:ASN:ND2	1:A:60:HIS:HD1	2.00	0.51
1:A:142:GLN:HE21	1:A:144:ASN:HD22	1.57	0.50
1:B:149:LEU:HD11	1:B:224:ASP:CG	2.31	0.50
1:B:38:TYR:CZ	1:B:76:PHE:HA	2.46	0.50
1:B:279:HIS:CD2	5:B:379:HOH:O	2.56	0.50
1:A:14:LEU:HD11	1:A:90:PRO:CB	2.42	0.50
1:A:254:LYS:CD	1:A:254:LYS:C	2.80	0.50
1:B:17:THR:HG23	1:B:18:GLU:N	2.26	0.50
1:B:57:ASN:ND2	1:B:60:HIS:HD1	2.02	0.50
1:B:29:LEU:CD2	1:B:80:LEU:HD23	2.42	0.49
1:A:267:TYR:CG	1:A:268:PRO:CA	2.92	0.49
1:A:29:LEU:HD22	1:A:80:LEU:HD23	1.93	0.49
1:B:254:LYS:CG	1:B:255:ASN:N	2.72	0.49
1:A:254:LYS:HD2	1:A:255:ASN:HB2	1.95	0.49
1:A:49:HIS:HA	1:A:56:ARG:O	2.12	0.49
1:A:8:ARG:CG	1:A:89:LEU:O	2.57	0.49
1:A:68:TRP:NE1	1:A:267:TYR:O	2.40	0.49
1:B:28:ILE:HG23	1:B:32:LYS:HE2	1.95	0.49
1:A:152:ASN:ND2	1:A:155:ALA:HB2	2.28	0.49
1:A:174:ILE:HD13	1:A:190:PHE:HA	1.95	0.49
1:A:62:SER:CB	1:A:260:GLN:OE1	2.61	0.48
1:B:250:TYR:HB2	1:B:277:MET:CE	2.43	0.48
1:B:126:VAL:HG13	1:B:149:LEU:O	2.12	0.48
1:B:200:GLY:CA	1:B:201:PRO:C	2.82	0.48
1:A:174:ILE:CD1	1:A:193:GLN:HG3	2.43	0.48
1:A:49:HIS:CE1	4:A:513:CL:CL	3.03	0.48
1:A:49:HIS:HA	1:A:57:ASN:HA	1.94	0.48
1:B:236:ARG:HA	1:B:286:TYR:CE1	2.48	0.48
1:B:256:GLY:H	1:B:261:ASN:HD21	1.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:C	1:A:282:LEU:N	2.66	0.48
1:B:4:LYS:HD2	1:B:4:LYS:N	2.29	0.47
1:B:84:ASN:C	1:B:84:ASN:HD22	2.17	0.47
1:B:127:ASP:N	1:B:127:ASP:OD1	2.47	0.47
1:A:119:ASN:ND2	1:A:119:ASN:C	2.66	0.47
1:A:53:GLY:CA	5:A:351:HOH:O	2.63	0.47
1:B:224:ASP:OD1	1:B:226:VAL:HG23	2.15	0.47
1:B:117:ASN:HD21	1:B:153:PHE:H	1.63	0.47
1:A:145:PRO:CD	1:B:53:GLY:HA2	2.44	0.47
1:A:57:ASN:ND2	1:A:60:HIS:N	2.62	0.47
1:B:243:ILE:HG22	1:B:244:ILE:N	2.29	0.47
1:B:6:ARG:HD3	1:B:81:GLN:OE1	2.15	0.47
1:B:119:ASN:HA	1:B:120:PRO:HD3	1.66	0.46
1:B:123:ASP:O	1:B:124:PHE:HB2	2.15	0.46
1:B:149:LEU:HD23	1:B:150:LYS:H	1.77	0.46
1:B:254:LYS:HA	1:B:261:ASN:ND2	2.31	0.46
1:B:11:VAL:CG1	1:B:11:VAL:O	2.62	0.46
1:A:261:ASN:HB2	1:A:264:ASP:CG	2.33	0.46
1:B:4:LYS:CA	1:B:280:ARG:HG3	2.45	0.46
1:B:6:ARG:NH2	1:B:282:LEU:O	2.49	0.46
1:B:57:ASN:ND2	1:B:60:HIS:N	2.62	0.46
1:B:8:ARG:CG	1:B:89:LEU:O	2.58	0.46
1:A:182:TRP:CE3	1:A:252:PRO:HD3	2.50	0.46
1:A:254:LYS:HD3	1:A:255:ASN:N	2.30	0.46
1:B:280:ARG:HE	1:B:280:ARG:HB2	1.49	0.46
1:A:84:ASN:HD22	1:A:84:ASN:C	2.17	0.46
1:A:215:MET:HE1	1:A:227:PHE:HD2	1.81	0.46
1:A:215:MET:HE2	1:A:221:ALA:O	2.16	0.46
1:A:174:ILE:CD1	1:A:190:PHE:HA	2.46	0.45
1:A:215:MET:CE	1:A:227:PHE:HD2	2.30	0.45
1:B:11:VAL:HG12	1:B:11:VAL:O	2.16	0.45
1:A:254:LYS:O	1:A:255:ASN:CB	2.39	0.45
1:A:280:ARG:HB2	1:A:280:ARG:HE	1.56	0.45
1:B:215:MET:CE	1:B:227:PHE:HD2	2.29	0.45
1:B:69:HIS:O	1:B:73:LEU:HG	2.17	0.45
1:A:207:VAL:HB	1:A:230:HIS:CE1	2.52	0.45
1:A:244:ILE:HG22	1:A:245:HIS:N	2.31	0.45
1:B:133:ALA:CB	1:B:148:GLY:HA3	2.47	0.45
1:A:145:PRO:HG2	1:B:53:GLY:HA3	1.99	0.44
1:A:69:HIS:O	1:A:73:LEU:HG	2.17	0.44
1:B:121:ILE:HG23	1:B:121:ILE:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLY:HA3	1:B:202:GLN:O	2.17	0.44
1:B:51:PRO:O	1:B:54:SER:HB3	2.17	0.44
1:B:112:ASP:OD1	1:B:112:ASP:C	2.54	0.44
1:A:236:ARG:CA	1:A:286:TYR:CE2	3.00	0.44
1:A:13:HIS:CD2	1:A:13:HIS:N	2.85	0.44
1:B:165:ARG:HG3	5:B:384:HOH:O	2.18	0.44
1:A:111:ALA:O	1:A:129:GLY:HA2	2.17	0.44
1:A:56:ARG:HA	1:A:61:MET:HB2	1.99	0.44
1:B:108:ILE:HD11	1:B:229:LEU:HD23	2.00	0.44
1:B:204:HIS:HD1	1:B:205:ASN:ND2	2.15	0.44
1:B:207:VAL:HB	1:B:230:HIS:CE1	2.52	0.44
1:B:4:LYS:HE3	5:B:368:HOH:O	2.17	0.44
1:A:180:PRO:HA	1:A:182:TRP:N	2.33	0.44
1:B:62:SER:OG	1:B:63:SER:N	2.50	0.44
1:A:67:PRO:CG	1:A:266:MET:HE1	2.35	0.43
1:B:50:THR:HA	1:B:51:PRO:HA	1.87	0.43
1:B:93:GLU:OE1	1:B:96:THR:HG21	2.18	0.43
1:A:111:ALA:O	1:A:130:PRO:HD3	2.17	0.43
1:A:62:SER:CB	1:A:260:GLN:CD	2.87	0.43
1:A:59:ALA:HB3	1:A:60:HIS:CE1	2.53	0.43
1:A:113:PHE:HB3	1:A:114:MET:H	1.61	0.43
1:A:244:ILE:CG2	1:A:245:HIS:N	2.80	0.43
1:A:267:TYR:CZ	1:A:268:PRO:HB3	2.53	0.43
1:B:169:LEU:HA	1:B:169:LEU:HD12	1.86	0.43
1:B:243:ILE:O	1:B:246:ARG:CG	2.66	0.43
1:A:126:VAL:O	1:A:132:ALA:HA	2.18	0.43
1:B:61:MET:HB3	5:B:310:HOH:O	2.18	0.43
1:B:24:ARG:HH11	1:B:24:ARG:HG2	1.82	0.43
1:A:162:LEU:HB3	1:A:163:PRO:HD2	1.99	0.43
1:A:254:LYS:HD2	1:A:255:ASN:CG	2.37	0.43
1:A:51:PRO:O	1:A:54:SER:HB3	2.19	0.43
1:A:233:ASN:O	1:A:237:ILE:HG13	2.19	0.42
1:B:191:ARG:C	1:B:191:ARG:HD2	2.39	0.42
1:B:149:LEU:HD11	1:B:224:ASP:OD2	2.19	0.42
1:B:182:TRP:CZ2	1:B:252:PRO:HB3	2.54	0.42
1:B:24:ARG:HA	1:B:24:ARG:HD3	1.84	0.42
1:A:279:HIS:O	1:A:282:LEU:HB2	2.19	0.42
1:A:108:ILE:HD11	1:A:229:LEU:HD23	2.00	0.42
1:B:254:LYS:HD3	1:B:254:LYS:HA	1.73	0.42
1:A:175:THR:HA	5:A:390:HOH:O	2.19	0.42
1:A:49:HIS:HE1	4:A:513:CL:CL	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:OD2	1:A:61:MET:SD	2.77	0.42
1:B:125:ILE:O	1:B:125:ILE:HG22	2.19	0.42
1:A:117:ASN:HD21	1:A:153:PHE:H	1.68	0.42
1:B:114:MET:HG3	1:B:226:VAL:HG22	2.02	0.42
1:A:262:PHE:O	1:A:273:PRO:HD2	2.20	0.41
1:A:284:TYR:C	1:A:285:VAL:HG13	2.40	0.41
1:B:280:ARG:C	1:B:282:LEU:N	2.72	0.41
1:B:57:ASN:HD21	1:B:60:HIS:N	2.18	0.41
1:A:125:ILE:HD12	1:A:150:LYS:HE2	2.01	0.41
1:A:191:ARG:C	1:A:191:ARG:HD2	2.40	0.41
1:A:152:ASN:N	1:A:211:VAL:O	2.53	0.41
1:B:4:LYS:HA	1:B:280:ARG:HG3	2.01	0.41
1:B:117:ASN:HD22	1:B:118:GLY:H	1.66	0.41
1:B:279:HIS:O	1:B:282:LEU:HB2	2.20	0.41
1:A:178:ASP:HA	1:A:189:SER:OG	2.21	0.41
1:A:150:LYS:O	1:A:213:GLY:HA3	2.21	0.41
1:B:180:PRO:HA	1:B:182:TRP:N	2.35	0.41
1:B:14:LEU:HD13	1:B:19:LYS:HG2	2.03	0.41
1:A:57:ASN:HD21	1:A:60:HIS:N	2.18	0.41
1:A:198:ILE:O	1:A:199:ASN:HB2	2.21	0.41
1:B:42:HIS:CE1	1:B:218:VAL:O	2.74	0.41
1:B:6:ARG:HB2	1:B:283:GLY:O	2.21	0.40
1:A:62:SER:HB3	1:A:260:GLN:CD	2.41	0.40
1:B:158:GLU:HG2	1:B:201:PRO:HD2	2.02	0.40
1:A:127:ASP:O	1:A:132:ALA:CB	2.70	0.40
1:A:244:ILE:CG2	1:A:245:HIS:CG	2.97	0.40
1:B:100:MET:O	1:B:101:GLN:C	2.56	0.40
1:B:170:ASN:HA	1:B:173:LYS:HD3	2.03	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	277/303 (91%)	265 (96%)	12 (4%)	0	100	100
1	B	283/303 (93%)	270 (95%)	12 (4%)	1 (0%)	34	37
All	All	560/606 (92%)	535 (96%)	24 (4%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	PHE

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	244/266 (92%)	217 (89%)	27 (11%)	6	5
1	B	248/266 (93%)	218 (88%)	30 (12%)	5	4
All	All	492/532 (92%)	435 (88%)	57 (12%)	5	5

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	THR
1	A	20	ARG
1	A	29	LEU
1	A	57	ASN
1	A	62	SER
1	A	84	ASN
1	A	89	LEU
1	A	94	TRP
1	A	112	ASP
1	A	113	PHE
1	A	114	MET
1	A	117	ASN
1	A	119	ASN
1	A	141	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	LEU
1	A	152	ASN
1	A	157	LYS
1	A	165	ARG
1	A	169	LEU
1	A	184	MET
1	A	194	LEU
1	A	217	VAL
1	A	254	LYS
1	A	280	ARG
1	A	281	LYS
1	A	288	ILE
1	B	20	ARG
1	B	24	ARG
1	B	29	LEU
1	B	47	LYS
1	B	55	ASP
1	B	57	ASN
1	B	60	HIS
1	B	63	SER
1	B	81	GLN
1	B	84	ASN
1	B	89	LEU
1	B	94	TRP
1	B	117	ASN
1	B	119	ASN
1	B	123	ASP
1	B	125	ILE
1	B	126	VAL
1	B	127	ASP
1	B	137	THR
1	B	146	SER
1	B	149	LEU
1	B	169	LEU
1	B	173	LYS
1	B	193	GLN
1	B	194	LEU
1	B	254	LYS
1	B	255	ASN
1	B	271	THR
1	B	280	ARG
1	B	281	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	84	ASN
1	A	101	GLN
1	A	117	ASN
1	A	119	ASN
1	A	142	GLN
1	A	144	ASN
1	A	152	ASN
1	A	188	ASN
1	A	199	ASN
1	A	202	GLN
1	A	205	ASN
1	A	260	GLN
1	A	261	ASN
1	A	270	ASN
1	A	278	ASN
1	B	57	ASN
1	B	84	ASN
1	B	99	GLN
1	B	117	ASN
1	B	119	ASN
1	B	142	GLN
1	B	144	ASN
1	B	202	GLN
1	B	205	ASN
1	B	230	HIS
1	B	247	ASN
1	B	251	GLN
1	B	260	GLN
1	B	261	ASN
1	B	278	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	281/303 (92%)	0.61	22 (7%) 13 11	19, 36, 72, 101	0
1	B	285/303 (94%)	0.55	26 (9%) 9 8	20, 37, 72, 116	0
All	All	566/606 (93%)	0.58	48 (8%) 10 9	19, 36, 72, 116	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	ASN	5.2
1	B	148	GLY	4.8
1	A	121	ILE	4.6
1	B	169	LEU	4.3
1	B	287	ASP	4.0
1	B	53	GLY	3.8
1	A	53	GLY	3.6
1	B	147	GLY	3.4
1	B	198	ILE	3.4
1	B	187	GLN	3.3
1	A	174	ILE	3.3
1	A	62	SER	3.2
1	B	194	LEU	3.2
1	A	165	ARG	2.9
1	B	244	ILE	2.9
1	B	152	ASN	2.9
1	B	288	ILE	2.8
1	A	5	TYR	2.8
1	A	249	ASN	2.8
1	B	123	ASP	2.7
1	B	247	ASN	2.7
1	A	285	VAL	2.7
1	B	137	THR	2.7
1	B	199	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	146	SER	2.6
1	B	200	GLY	2.6
1	A	55	ASP	2.6
1	B	101	GLN	2.6
1	B	142	GLN	2.6
1	A	176	GLN	2.5
1	B	155	ALA	2.5
1	A	125	ILE	2.4
1	A	14	LEU	2.4
1	A	7	VAL	2.4
1	A	142	GLN	2.3
1	B	174	ILE	2.3
1	A	199	ASN	2.3
1	B	267	TYR	2.2
1	A	183	ASP	2.2
1	A	184	MET	2.2
1	B	82	SER	2.1
1	B	141	GLU	2.1
1	A	120	PRO	2.1
1	A	61	MET	2.1
1	A	163	PRO	2.0
1	A	155	ALA	2.0
1	B	135	ARG	2.0
1	B	165	ARG	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. 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	B-factors(\AA^2)	Q<0.9
3	ZN	A	506	1/1	0.65	0.21	34,34,34,34	1
4	CL	A	513	1/1	0.69	0.17	31,31,31,31	1
4	CL	B	512	1/1	0.72	0.17	31,31,31,31	1
3	ZN	A	507	1/1	0.81	0.13	30,30,30,30	1
3	ZN	A	508	1/1	0.85	0.09	34,34,34,34	1
3	ZN	B	507	1/1	0.93	0.17	34,34,34,34	1
3	ZN	A	505	1/1	0.96	0.10	34,34,34,34	0
2	CU	B	501[A]	1/1	0.97	0.14	34,34,34,34	1
2	CU	B	501[B]	1/1	0.97	0.14	30,30,30,30	1
4	CL	A	510	1/1	0.98	0.05	34,34,34,34	0
2	CU	B	502[B]	1/1	0.98	0.16	31,31,31,31	1
4	CL	B	509	1/1	0.98	0.07	34,34,34,34	0
2	CU	B	502[A]	1/1	0.98	0.16	34,34,34,34	1
3	ZN	A	509	1/1	0.98	0.10	34,34,34,34	1
3	ZN	B	505	1/1	0.99	0.07	34,34,34,34	0
2	CU	A	501[A]	1/1	0.99	0.18	34,34,34,34	1
4	CL	A	511	1/1	0.99	0.08	31,31,31,31	1
2	CU	A	502[A]	1/1	0.99	0.15	34,34,34,34	1
4	CL	B	508	1/1	0.99	0.07	34,34,34,34	0
2	CU	A	502[B]	1/1	0.99	0.15	31,31,31,31	1
3	ZN	B	506	1/1	0.99	0.12	34,34,34,34	1
2	CU	A	501[B]	1/1	0.99	0.18	31,31,31,31	1

6.5 Other polymers ⓘ

There are no such residues in this entry.