



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:32 PM BST

PDB ID : 6JDE  
Title : crystal structure of a DNA repair protein  
Authors : Yan, X.X.; Tang, Q.  
Deposited on : 2019-02-01  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

---

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 : 2.13.1  
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

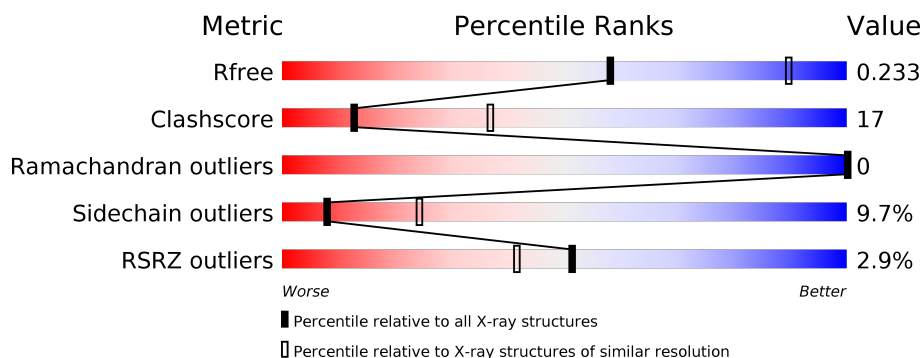
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	586	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>• •</div> </div> </div>
1	B	586	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• • •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9030 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 Putative DNA repair helicase RadD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	567	Total	C	N	O	S	1	3	0
			4386	2798	786	784	18			
1	A	560	Total	C	N	O	S	1	2	0
			4266	2722	758	769	17			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

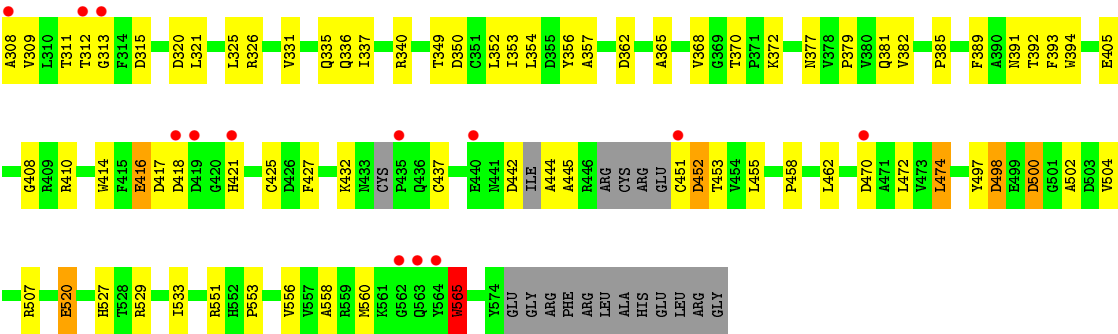
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	222	Total	O	0	0
			222	222		
3	A	154	Total	O	0	0
			154	154		

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.

- Chain B:
- 
- 29% 67% 25%
- ARG LEU ALA HIS GLU LEU ARG GLY
- Q132 I133 F3 T135 H136 K139 Y161 Y162 M169 E174 F178 R179 L185 P186 L187 R188 Y189 M190 L196 R201 M204 P205 V206 V207 Q208 R213 L214 S223 E224 A225 D226 R229 E230 Q234 Q235 R236 I237 T238 H240 P249 T241 I242 R252 G341 G342 L342 V255 V256
- Q132 I133 F3 T135 H136 K139 Y161 Y162 M169 E174 F178 R179 L185 P186 L187 R188 Y189 M190 L196 R201 M204 P205 V206 V207 Q208 R213 L214 S223 E224 A225 D226 R229 E230 Q234 Q235 R236 I237 T238 H240 P249 T241 I242 R252 G341 G342 L342 V255 V256
- I257 H264 A265 I268 V269 G270 L271 E275 D276 A277 A278 L279 I280 T284 P285 G286 A287 E288 V291 F296 K297 A298 Q299 R300 F301 R302 Y303 N306 V307 A308 T311 T312 G313 F314 D315 A316 V319 D320 L321 I322 A323 V331 Q335 G339 R340 G341 L342 V343
- I257 H264 A265 I268 V269 G270 L271 E275 D276 A277 A278 L279 I280 T284 P285 G286 A287 E288 V291 F296 K297 A298 Q299 R300 F301 R302 Y303 N306 V307 A308 T311 T312 G313 F314 D315 A316 V319 D320 L321 I322 A323 V331 Q335 G339 R340 G341 L342 V343
- I353 H354 D355 D362 L363 Y364 A365 K372 G374 K374 S375 D376 H377 V378 P379 V380 Q381 V382 F389 A390 N391 D400 G401 R410 F415 E416 D417 R428 F431 K432 R433 K434 P435 Q436 C437 N438 I443 A444 A445 R446 R447 C448 A461 G461 V456 D459 V459
- I353 H354 D355 D362 L363 Y364 A365 K372 G374 K374 S375 D376 H377 V378 P379 V380 Q381 V382 F389 A390 N391 D400 G401 R410 F415 E416 D417 R428 F431 K432 R433 K434 P435 Q436 C437 N438 I443 A444 A445 R446 R447 C448 A461 G461 V456 D459 V459
- M461 L462 K469 D470 A471 L474 R475 C476 S477 G478 D486 E489 G489 I494 D498 E499 V504 R507 F508 R509 L510 Q511 Q515 R516 F521 L522 F523 L524 R525 W527 L544 H552 P553 A558 R559 M560 K561 Y564 V565 E569 K570 Y574 Y576
- M461 L462 K469 D470 A471 L474 R475 C476 S477 G478 D486 E489 G489 I494 D498 E499 V504 R507 F508 R509 L510 Q511 Q515 R516 F521 L522 F523 L524 R525 W527 L544 H552 P553 A558 R559 M560 K561 Y564 V565 E569 K570 Y574 Y576

- Chain A:
- 
- Sequence logo for Chain A showing amino acid conservation across 300 positions. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions 1 to 300. A color scale at the top indicates conservation levels: 4% (red), 65% (green), and 27% (yellow). Amino acids are labeled at the bottom of the logo.



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.52Å 78.45Å 110.59Å 90.00° 98.50° 90.00°	Depositor
Resolution (Å)	19.95 – 2.80 19.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.95-2.80) 97.8 (19.95-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.79Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.228 , 0.240 0.232 , 0.233	Depositor DCC
$R_{free}$ test set	1580 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3604e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN

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	0.42	1/4367 (0.0%)	0.69	8/5940 (0.1%)
1	B	0.51	0/4490	0.78	17/6099 (0.3%)
All	All	0.47	1/8857 (0.0%)	0.74	25/12039 (0.2%)

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	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	SER	CB-OG	-5.42	1.35	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	561	LYS	C-N-CA	20.82	166.03	122.30
1	B	307	VAL	CB-CA-C	-11.37	89.80	111.40
1	A	294	GLU	CB-CA-C	-11.12	88.17	110.40
1	B	235	GLN	CB-CA-C	-9.96	90.48	110.40
1	B	315	ASP	N-CA-C	-9.87	84.36	111.00
1	B	474	LEU	CA-CB-CG	9.62	137.44	115.30
1	B	237	ILE	CB-CA-C	-9.10	93.40	111.60
1	B	307	VAL	N-CA-C	8.56	134.12	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	TRP	N-CA-C	8.55	134.09	111.00
1	B	308	ALA	CB-CA-C	7.91	121.96	110.10
1	A	272	LEU	CB-CA-C	7.48	124.41	110.20
1	B	315	ASP	CB-CA-C	6.99	124.37	110.40
1	A	293	ILE	CB-CA-C	-6.67	98.26	111.60
1	B	474	LEU	CB-CG-CD1	-6.47	100.01	111.00
1	B	433	ASN	CB-CA-C	-6.35	97.69	110.40
1	B	308	ALA	N-CA-C	-6.34	93.87	111.00
1	A	565	TRP	CB-CA-C	-6.03	98.35	110.40
1	A	294	GLU	N-CA-C	5.89	126.89	111.00
1	B	307	VAL	C-N-CA	5.72	136.01	121.70
1	A	187	LEU	CB-CG-CD1	-5.59	101.49	111.00
1	B	437	CYS	CB-CA-C	-5.53	99.35	110.40
1	B	204	MET	CB-CA-C	-5.41	99.57	110.40
1	A	432	LYS	CB-CA-C	5.34	121.08	110.40
1	B	433	ASN	C-N-CA	5.32	134.99	121.70
1	B	561	LYS	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	LEU	Peptide
1	A	309	VAL	Peptide
1	B	275	GLU	Peptide
1	B	307	VAL	Peptide
1	B	308	ALA	Peptide
1	B	561	LYS	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	4266	0	4072	146	0
1	B	4386	0	4228	135	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	154	0	0	7	0
3	B	222	0	0	11	0
All	All	9030	0	8300	281	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 17.

All (281) 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:234:GLN:O	1:B:237:ILE:HG12	1.23	1.27
1:B:470:ASP:OD2	1:B:559:ARG:NH1	1.70	1.25
1:A:242:ILE:HD12	1:A:271:LEU:HD22	1.16	1.13
1:A:104:LEU:HB3	1:A:136:HIS:CD2	1.90	1.05
1:A:293:ILE:HD11	3:A:701:HOH:O	1.54	1.04
1:B:428:ARG:NE	1:B:438:ASN:OD1	1.99	0.95
1:B:433:ASN:ND2	1:B:448:CYS:O	1.97	0.95
1:A:132:GLN:O	1:A:135:THR:OG1	1.85	0.94
1:B:234:GLN:O	1:B:237:ILE:CG1	2.16	0.94
1:B:400:ASP:OD1	3:B:701:HOH:O	1.86	0.93
1:A:307:VAL:HG13	1:A:308:ALA:N	1.82	0.93
1:A:307:VAL:HG13	1:A:308:ALA:H	1.38	0.87
1:A:290:ASP:HA	1:A:293:ILE:CD1	2.05	0.86
1:A:290:ASP:HA	1:A:293:ILE:HD12	1.58	0.85
1:A:349:THR:HG23	1:A:350:ASP:OD2	1.77	0.83
1:A:257:ILE:HD11	1:A:325:LEU:HD11	1.60	0.83
1:B:187:LEU:HD21	1:B:363:LEU:HG	1.59	0.83
1:A:257:ILE:HD11	1:A:325:LEU:CD1	2.10	0.81
1:A:8:TYR:OH	1:A:35:ALA:O	1.98	0.81
1:A:286:GLY:HA2	1:A:289:ARG:HB3	1.64	0.80
1:B:8:TYR:OH	1:B:35:ALA:O	1.99	0.80
1:B:187:LEU:CD2	1:B:363:LEU:HG	2.12	0.79
1:A:290:ASP:HA	1:A:293:ILE:CG1	2.13	0.78
1:B:32:PRO:HD2	1:B:185:LEU:HB3	1.65	0.78
1:A:242:ILE:CD1	1:A:271:LEU:HD22	2.07	0.78
1:A:242:ILE:HD12	1:A:271:LEU:CD2	2.08	0.77
1:B:234:GLN:C	1:B:237:ILE:HG12	2.05	0.77
1:B:433:ASN:HD22	1:B:448:CYS:C	1.89	0.76
1:B:311:THR:HG22	1:B:311:THR:O	1.85	0.75
1:A:290:ASP:CA	1:A:293:ILE:HG13	2.17	0.75
1:A:120:HIS:HA	1:A:161:ILE:HD13	1.69	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:HG12	1:B:207:VAL:H	1.54	0.73
1:B:433:ASN:O	1:B:436:GLN:HA	1.89	0.72
1:B:374:LYS:HG3	1:B:376:ASP:H	1.55	0.72
1:B:237:ILE:N	1:B:237:ILE:HD13	2.04	0.71
1:A:241:ILE:HG21	1:A:325:LEU:HD21	1.72	0.71
1:B:564:TYR:OH	3:B:702:HOH:O	2.08	0.71
1:A:290:ASP:HA	1:A:293:ILE:HG13	1.73	0.71
1:A:405:GLU:OE1	3:A:702:HOH:O	2.08	0.70
1:A:78:ILE:HA	1:A:94:PHE:O	1.92	0.69
1:A:417:ASP:OD1	1:A:418:ASP:N	2.22	0.69
1:B:475:ARG:HH11	1:B:475:ARG:HG2	1.58	0.69
1:B:437:CYS:SG	1:B:444:ALA:HA	2.33	0.69
1:A:169[A]:MET:HG2	1:A:389:PHE:HZ	1.58	0.69
1:B:314:PHE:O	1:B:316:ALA:N	2.26	0.69
1:A:372:LYS:O	1:A:377:ASN:ND2	2.26	0.68
1:A:307:VAL:CG1	1:A:308:ALA:H	2.07	0.68
1:B:255:VAL:HG22	1:B:321:LEU:HB3	1.76	0.68
1:B:315:ASP:OD2	1:B:343:ARG:NE	2.23	0.67
1:B:257:ILE:HG21	1:B:268:ILE:HG21	1.77	0.67
1:A:500:ASP:OD1	1:A:500:ASP:N	2.27	0.67
1:B:525[A]:ARG:NH1	3:B:705:HOH:O	2.27	0.67
1:B:100:VAL:HG12	1:B:133:ILE:HG12	1.77	0.67
1:A:307:VAL:CG1	1:A:308:ALA:N	2.55	0.66
1:A:311:THR:O	1:A:312:THR:HG23	1.95	0.66
1:A:451:CYS:O	1:A:453:THR:HG23	1.96	0.66
1:A:289:ARG:O	1:A:293:ILE:HD11	1.95	0.65
1:B:321:LEU:HD11	1:B:354:LEU:HG	1.78	0.65
1:B:433:ASN:ND2	1:B:448:CYS:C	2.49	0.65
1:A:474:LEU:HD11	1:A:556:VAL:HB	1.77	0.65
1:B:316:ALA:HB3	1:B:319:VAL:HG23	1.79	0.65
1:B:230:GLU:HG3	1:B:234:GLN:HE21	1.60	0.65
1:B:280:ILE:HD11	1:B:306[A]:ASN:OD1	1.98	0.64
1:A:381:GLN:HA	1:A:391:ASN:O	1.97	0.64
1:A:62:VAL:HG12	1:A:78:ILE:HD11	1.78	0.64
1:A:97:VAL:HG12	1:A:129:GLN:HB2	1.80	0.64
1:A:18:ASN:ND2	3:A:706:HOH:O	2.31	0.64
1:A:269:VAL:HG21	1:A:279:LEU:HB2	1.79	0.63
1:B:476:CYS:HB3	1:B:553:PRO:O	1.99	0.63
1:B:31:LEU:HA	1:B:185:LEU:HB3	1.80	0.63
1:B:264:HIS:O	1:B:268:ILE:HG12	1.99	0.63
1:A:311:THR:O	1:A:312:THR:CG2	2.47	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:NH2	3:B:709:HOH:O	2.33	0.61
1:B:77:ASP:N	1:B:77:ASP:OD1	2.33	0.61
1:A:104:LEU:CB	1:A:136:HIS:CD2	2.78	0.61
1:B:444:ALA:HB1	1:B:447:ARG:H	1.65	0.61
1:B:475:ARG:HH11	1:B:475:ARG:CG	2.14	0.61
1:A:3:PHE:N	3:A:707:HOH:O	2.33	0.61
1:A:349:THR:HG23	1:A:350:ASP:CG	2.21	0.60
1:A:114:LEU:HD23	1:A:146:LEU:HG	1.83	0.60
1:A:202:LEU:O	1:A:205:PRO:HD3	2.01	0.60
1:A:474:LEU:HD21	1:A:504:VAL:HG12	1.82	0.60
1:B:5:LEU:HD22	1:B:39:LEU:HB3	1.83	0.59
1:A:262:VAL:N	1:A:307:VAL:HG21	2.18	0.58
1:B:461:MET:HE3	1:B:462:LEU:HD13	1.84	0.58
1:B:469:LYS:N	1:B:469:LYS:HD3	2.19	0.58
1:B:134:LEU:HG	1:B:134:LEU:O	2.04	0.58
1:A:445:ALA:HA	1:A:451:CYS:O	2.04	0.58
1:A:202:LEU:HD22	1:A:354:LEU:CD2	2.33	0.58
1:B:169[B]:MET:HB3	1:B:389:PHE:HZ	1.69	0.58
1:B:471:ALA:HB2	1:B:559:ARG:HD3	1.84	0.57
1:B:504:VAL:HG21	1:B:558:ALA:HB2	1.86	0.57
1:A:291:VAL:HG23	1:A:292:LEU:N	2.19	0.57
1:B:339:GLY:HA2	1:B:342:LEU:HD12	1.87	0.57
1:A:246:MET:CE	1:A:272:LEU:HD23	2.35	0.57
1:B:489:GLY:HA3	1:B:511:GLN:HB2	1.87	0.56
1:A:313:GLY:C	1:A:315:ASP:OD1	2.44	0.56
1:A:520:GLU:OE2	3:A:703:HOH:O	2.17	0.56
1:B:223:SER:OG	1:B:226:ASP:HB2	2.05	0.56
1:A:202:LEU:HD22	1:A:354:LEU:HD23	1.87	0.56
1:A:290:ASP:N	1:A:293:ILE:HG13	2.22	0.54
1:B:162:TYR:HA	1:B:178:PHE:O	2.07	0.54
1:A:104:LEU:HD13	1:A:136:HIS:HB2	1.88	0.54
1:B:185:LEU:HD21	1:B:190:MET:HE3	1.89	0.54
1:B:242:ILE:HD11	1:B:268:ILE:HA	1.88	0.54
1:B:131:GLN:O	1:B:135:THR:HG23	2.08	0.54
1:B:169[B]:MET:HB3	1:B:389:PHE:CZ	2.43	0.54
1:B:206:VAL:HG12	1:B:207:VAL:N	2.21	0.54
1:B:32:PRO:HD3	1:B:185:LEU:O	2.08	0.54
1:B:331:VAL:O	1:B:335:GLN:HG2	2.07	0.54
1:B:471:ALA:CB	1:B:559:ARG:HD3	2.37	0.54
1:B:78:ILE:HA	1:B:94:PHE:O	2.08	0.54
1:B:307:VAL:O	1:B:307:VAL:HG12	1.97	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:OG1	1:A:340:ARG:NH1	2.41	0.53
1:B:188:ARG:HG3	1:B:364:TYR:CE2	2.43	0.53
1:B:17:LEU:O	1:B:21:ARG:HG3	2.09	0.53
1:A:257:ILE:HD11	1:A:325:LEU:HD12	1.87	0.53
1:A:474:LEU:CD1	1:A:556:VAL:HB	2.37	0.53
1:B:190:MET:HB3	1:B:196:LEU:HG	1.91	0.53
1:A:17:LEU:O	1:A:21:ARG:HG3	2.09	0.53
1:B:307:VAL:CG1	1:B:307:VAL:O	2.44	0.53
1:B:478:GLY:HA2	1:B:552:HIS:CD2	2.43	0.53
1:B:516:ARG:HG3	1:B:537:TRP:CZ2	2.44	0.53
1:B:206:VAL:CG1	1:B:207:VAL:H	2.19	0.53
1:A:498:ASP:HB3	1:A:500:ASP:H	1.74	0.52
1:B:169[A]:MET:HB2	1:B:389:PHE:HZ	1.74	0.52
1:B:201:ARG:HB2	1:B:353:ILE:HB	1.91	0.52
1:B:560:MET:HG2	1:B:565:TRP:CZ3	2.45	0.52
1:A:442:ASP:HA	1:A:455:LEU:HB2	1.91	0.52
1:B:381:GLN:HA	1:B:391:ASN:O	2.09	0.52
1:A:162:TYR:HA	1:A:178:PHE:O	2.10	0.52
1:B:410:ARG:NH1	3:B:712:HOH:O	2.36	0.52
1:A:437:CYS:SG	1:A:444:ALA:HB3	2.50	0.52
1:A:98:GLN:O	1:A:102:ARG:HD3	2.10	0.52
1:B:461:MET:CE	1:B:462:LEU:HD13	2.40	0.52
1:A:214:LEU:HD22	1:A:226:ASP:HB3	1.92	0.51
1:B:311:THR:CG2	1:B:311:THR:O	2.56	0.51
1:B:315:ASP:OD2	1:B:343:ARG:NH2	2.43	0.51
1:A:30:VAL:HB	1:A:184:GLU:HG3	1.93	0.51
1:A:256:MET:HG2	1:A:304:LEU:HD23	1.92	0.51
1:B:428:ARG:HH21	1:B:438:ASN:HD21	1.58	0.51
1:B:208:GLN:NE2	1:B:355:ASP:O	2.43	0.51
1:B:187:LEU:HD23	1:B:363:LEU:HG	1.91	0.51
1:B:169[A]:MET:HB2	1:B:389:PHE:CZ	2.45	0.51
1:A:442:ASP:O	1:A:455:LEU:HB2	2.10	0.51
1:A:160:TRP:CE2	1:A:171:ARG:HD2	2.46	0.51
1:A:199:PRO:HB2	1:A:353:ILE:HD11	1.92	0.50
1:B:237:ILE:HG22	1:B:237:ILE:O	2.10	0.50
1:A:372:LYS:HG2	1:A:377:ASN:HB2	1.94	0.50
1:B:475:ARG:NH1	1:B:475:ARG:CG	2.72	0.50
1:B:252:ARG:HH11	1:B:320:ASP:HB2	1.76	0.49
1:A:442:ASP:C	1:A:455:LEU:HB2	2.33	0.49
1:B:382:VAL:O	1:B:391:ASN:HB2	2.13	0.49
1:B:288:GLU:O	1:B:291:VAL:HG12	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:C	1:A:127:GLU:H	2.17	0.48
1:A:246:MET:HE2	1:A:272:LEU:HD23	1.95	0.48
1:A:265:ALA:HB1	1:A:279:LEU:HD11	1.96	0.48
1:B:207:VAL:HG12	1:B:208:GLN:N	2.28	0.48
1:A:294:GLU:OE2	1:A:300:ARG:NH1	2.46	0.48
1:A:209:TYR:HB2	1:A:357:ALA:HA	1.96	0.48
1:A:362:ASP:HB2	1:A:365:ALA:HB2	1.95	0.48
1:B:315:ASP:HB3	1:B:340:ARG:HD2	1.95	0.48
1:A:285:PRO:HB2	1:A:287:ALA:H	1.78	0.47
1:A:414:TRP:HZ3	1:A:416:GLU:HG3	1.78	0.47
1:B:300:ARG:NH2	3:B:718:HOH:O	2.46	0.47
1:A:291:VAL:HG23	1:A:292:LEU:HG	1.96	0.47
1:A:3:PHE:HB2	1:A:39:LEU:HD11	1.96	0.47
1:B:120:HIS:HA	1:B:161:ILE:HD13	1.96	0.47
1:B:185:LEU:HD11	1:B:190:MET:HE3	1.96	0.47
1:A:7:PRO:O	1:A:11:GLU:HG3	2.15	0.47
1:B:237:ILE:O	1:B:241:ILE:HD12	2.15	0.47
1:B:269:VAL:HG21	1:B:279:LEU:HB2	1.96	0.47
1:B:32:PRO:HG2	1:B:190:MET:HG3	1.96	0.47
1:B:277:ALA:HA	1:B:303:TYR:O	2.15	0.47
1:A:129:GLN:HG2	1:A:129:GLN:H	1.43	0.47
1:A:504:VAL:HG21	1:A:558:ALA:HB2	1.97	0.46
1:A:325:LEU:HD23	1:A:356:TYR:HB2	1.97	0.46
1:A:246:MET:HE3	1:A:272:LEU:HD23	1.97	0.46
1:A:527:HIS:HE1	1:A:553:PRO:HD3	1.81	0.46
1:A:169[A]:MET:HG2	1:A:389:PHE:CZ	2.44	0.46
1:A:368:VAL:HG22	1:A:392:THR:HG22	1.97	0.46
1:B:314:PHE:O	1:B:315:ASP:C	2.49	0.46
1:A:264:HIS:O	1:A:267:GLU:HB3	2.15	0.46
1:B:238:THR:HA	1:B:241:ILE:HD12	1.98	0.46
1:B:459:ASP:OD1	1:B:574:TYR:OH	2.24	0.46
1:B:486:ASP:HB2	3:B:764:HOH:O	2.16	0.46
1:A:8:TYR:CD1	1:A:185:LEU:HD22	2.51	0.45
1:A:57:HIS:CE1	1:A:97:VAL:HG21	2.52	0.45
1:A:104:LEU:HD22	1:A:136:HIS:HD2	1.81	0.45
1:A:405:GLU:HG3	1:A:529:ARG:HB3	1.98	0.45
1:B:320:ASP:OD1	1:B:320:ASP:N	2.49	0.45
1:A:154:PHE:HB2	1:A:160:TRP:CZ3	2.52	0.45
1:A:321:LEU:HD13	1:A:352:LEU:HB3	1.97	0.45
1:B:229:ARG:HE	1:B:229:ARG:HB2	1.45	0.45
1:B:313:GLY:C	1:B:315:ASP:H	2.20	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ARG:HB2	1:B:111:PHE:CE1	2.51	0.45
1:B:161:ILE:HG13	1:B:178:PHE:HD2	1.82	0.45
1:A:311:THR:C	1:A:312:THR:HG23	2.36	0.45
1:A:331:VAL:HG12	1:A:335:GLN:NE2	2.32	0.44
1:B:3:PHE:CE2	1:B:74:LEU:HD11	2.52	0.44
1:A:4:THR:HA	3:A:718:HOH:O	2.17	0.44
1:B:553:PRO:HB3	1:B:570:LYS:HB3	1.98	0.44
1:B:559:ARG:NH2	3:B:721:HOH:O	2.50	0.44
1:A:417:ASP:HB3	1:A:421:HIS:H	1.82	0.44
1:A:255:VAL:HG13	1:A:321:LEU:HG	1.98	0.44
1:A:379:PRO:HD3	1:A:394:TRP:HZ3	1.82	0.44
1:A:458:PRO:O	1:A:462:LEU:HG	2.17	0.44
1:B:296:PHE:O	1:B:298:ALA:N	2.51	0.44
1:A:257:ILE:HG23	1:A:305:VAL:HG22	2.00	0.44
1:B:132:GLN:O	1:B:135:THR:OG1	2.32	0.44
1:B:456:VAL:O	1:B:456:VAL:HG13	2.17	0.44
1:A:208:GLN:HB2	1:A:356:TYR:O	2.18	0.44
1:A:295:ASN:HB2	1:A:301:PHE:HE1	1.82	0.44
1:B:214:LEU:HD11	1:B:230:GLU:HG2	2.00	0.44
1:B:362:ASP:CG	1:B:365:ALA:HB2	2.38	0.44
1:B:428:ARG:HH21	1:B:438:ASN:ND2	2.15	0.44
1:B:521:GLN:HB3	1:B:522:LEU:HD23	1.99	0.44
1:B:471:ALA:HB2	1:B:559:ARG:CD	2.48	0.44
1:A:164:PHE:HD2	1:A:414:TRP:CD1	2.36	0.44
1:B:475:ARG:NH1	3:B:722:HOH:O	2.51	0.43
1:A:162:TYR:CE2	1:A:165:HIS:HB2	2.52	0.43
1:A:289:ARG:HE	1:A:289:ARG:HB3	1.74	0.43
1:A:295:ASN:HA	1:A:300:ARG:HH11	1.83	0.43
1:A:382:VAL:HG13	1:A:533:ILE:HD11	1.99	0.43
1:B:431:PHE:CD1	1:B:431:PHE:N	2.86	0.43
1:A:372:LYS:HE3	1:A:377:ASN:O	2.18	0.43
1:B:296:PHE:O	1:B:297:LYS:HB2	2.17	0.43
1:A:410:ARG:NH2	1:A:425:CYS:O	2.45	0.43
1:A:527:HIS:CE1	1:A:553:PRO:HD3	2.54	0.43
1:B:187:LEU:HD21	1:B:363:LEU:CG	2.39	0.43
1:A:39:LEU:HA	1:A:39:LEU:HD12	1.92	0.43
1:A:336:GLN:O	1:A:340:ARG:HG2	2.18	0.43
1:B:207:VAL:CG1	1:B:208:GLN:N	2.82	0.43
1:A:227:LEU:O	1:A:230:GLU:O	2.37	0.43
1:A:125:ASP:C	1:A:127:GLU:N	2.72	0.43
1:A:444:ALA:HA	1:A:452:ASP:OD1	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:HIS:O	1:A:139:LYS:HB2	2.19	0.42
1:A:362:ASP:HB2	1:A:365:ALA:CB	2.49	0.42
1:A:393:PHE:CG	1:A:408:GLY:HA3	2.54	0.42
1:A:560:MET:HG2	1:A:565:TRP:CE3	2.54	0.42
1:B:257:ILE:HA	1:B:323:ALA:HB3	2.01	0.42
1:B:400:ASP:OD1	1:B:401:GLY:N	2.52	0.42
1:B:494:ILE:HG12	1:B:523:PHE:CE1	2.54	0.42
1:B:39:LEU:HA	1:B:39:LEU:HD23	1.85	0.42
1:A:291:VAL:CG2	1:A:292:LEU:N	2.82	0.42
1:B:179:ARG:NE	3:B:713:HOH:O	2.39	0.42
1:A:340:ARG:HD3	1:A:340:ARG:HA	1.89	0.42
1:B:339:GLY:HA2	1:B:342:LEU:CD1	2.49	0.42
1:A:252:ARG:HB3	1:A:320:ASP:OD1	2.19	0.42
1:B:104:LEU:HB3	1:B:136:HIS:CE1	2.55	0.42
1:A:497:TYR:HA	1:A:502:ALA:O	2.20	0.42
1:A:258:PHE:CE1	1:A:337:ILE:HG12	2.55	0.41
1:B:433:ASN:O	1:B:436:GLN:CA	2.63	0.41
1:A:130:TYR:OH	1:A:146:LEU:HD11	2.20	0.41
1:A:57:HIS:ND1	1:A:97:VAL:HG21	2.35	0.41
1:B:509:ARG:O	3:B:703:HOH:O	2.22	0.41
1:B:242:ILE:HD11	1:B:268:ILE:HG23	2.01	0.41
1:B:242:ILE:CD1	1:B:271:LEU:HB2	2.50	0.41
1:A:141:ASN:HB2	1:A:144:LEU:HB2	2.03	0.41
1:A:160:TRP:CZ2	1:A:171:ARG:HD2	2.55	0.41
1:A:236:ARG:NE	3:A:714:HOH:O	2.54	0.41
1:B:315:ASP:OD2	1:B:343:ARG:CZ	2.69	0.41
1:B:443:ILE:HG22	1:B:444:ALA:O	2.21	0.41
1:A:165:HIS:CE1	1:A:167:HIS:HB2	2.56	0.41
1:A:472:LEU:HB2	1:A:565:TRP:CZ2	2.56	0.41
1:B:265:ALA:HB1	1:B:279:LEU:HD11	2.03	0.41
1:A:243:SER:O	1:A:246:MET:HB2	2.21	0.40
1:A:291:VAL:HG23	1:A:292:LEU:H	1.86	0.40
1:A:48:ALA:O	1:A:91:LYS:NZ	2.53	0.40
1:B:201:ARG:NH1	1:B:355:ASP:HB3	2.36	0.40
1:A:410:ARG:HH21	1:A:425:CYS:C	2.23	0.40
1:B:185:LEU:HD21	1:B:190:MET:CE	2.51	0.40
1:A:129:GLN:O	1:A:132:GLN:HB2	2.20	0.40
1:A:165:HIS:ND1	1:A:167:HIS:HB2	2.36	0.40
1:A:370:THR:O	1:A:394:TRP:NE1	2.37	0.40
1:B:239:PRO:HB3	1:B:271:LEU:HD22	2.03	0.40
1:A:164:PHE:HB3	1:A:414:TRP:NE1	2.36	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:MET:HA	1:A:303:TYR:OH	2.21	0.40
1:A:385:PRO:HG2	1:A:427:PHE:CZ	2.57	0.40
1:B:378:VAL:HG23	1:B:379:PRO:O	2.21	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	552/586 (94%)	492 (89%)	60 (11%)	0	100	100
1	B	558/586 (95%)	511 (92%)	47 (8%)	0	100	100
All	All	1110/1172 (95%)	1003 (90%)	107 (10%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/491 (85%)	378 (91%)	39 (9%)	8	26
1	B	436/491 (89%)	392 (90%)	44 (10%)	7	22
All	All	853/982 (87%)	770 (90%)	83 (10%)	8	24

All (83) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	B	3	PHE
1	B	6	ARG
1	B	31	LEU
1	B	33	THR
1	B	77	ASP
1	B	98	GLN
1	B	112	SER
1	B	124	ASP
1	B	128	SER
1	B	129	GLN
1	B	139	LYS
1	B	174	GLU
1	B	201	ARG
1	B	213	ARG
1	B	234	GLN
1	B	235	GLN
1	B	237	ILE
1	B	284	THR
1	B	285	PRO
1	B	291	VAL
1	B	302	ARG
1	B	306[A]	ASN
1	B	306[B]	ASN
1	B	335	GLN
1	B	372	LYS
1	B	374	LYS
1	B	400	ASP
1	B	415	PHE
1	B	416	GLU
1	B	417	ASP
1	B	433	ASN
1	B	462	LEU
1	B	469	LYS
1	B	470	ASP
1	B	474	LEU
1	B	475	ARG
1	B	498	ASP
1	B	499	GLU
1	B	507	ARG
1	B	515	GLN
1	B	521	GLN
1	B	544	LEU
1	B	564	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	569	GLU
1	A	6	ARG
1	A	38	SER
1	A	39	LEU
1	A	89	HIS
1	A	98	GLN
1	A	102	ARG
1	A	108	GLN
1	A	129	GLN
1	A	131	GLN
1	A	132	GLN
1	A	134	LEU
1	A	138	THR
1	A	139	LYS
1	A	156	LEU
1	A	187	LEU
1	A	188	ARG
1	A	201	ARG
1	A	224	GLU
1	A	226	ASP
1	A	230	GLU
1	A	236	ARG
1	A	261	THR
1	A	267	GLU
1	A	271	LEU
1	A	290	ASP
1	A	294	GLU
1	A	295	ASN
1	A	302	ARG
1	A	326	ARG
1	A	416	GLU
1	A	452	ASP
1	A	470	ASP
1	A	474	LEU
1	A	498	ASP
1	A	500	ASP
1	A	507	ARG
1	A	520	GLU
1	A	551	ARG
1	A	565	TRP

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

Mol	Chain	Res	Type
1	B	57	HIS
1	B	70	GLN
1	B	208	GLN
1	B	235	GLN
1	B	361	HIS
1	B	433	ASN
1	B	483	HIS
1	A	57	HIS
1	A	131	GLN
1	A	235	GLN
1	A	306	ASN
1	A	335	GLN
1	A	336	GLN
1	A	482	GLN
1	A	552	HIS
1	A	566	GLN

### 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 2 ligands modelled in this entry, 2 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, 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	560/586 (95%)	0.02	23 (4%) 37 27	7, 41, 76, 101	0
1	B	567/586 (96%)	-0.14	10 (1%) 68 61	11, 36, 65, 90	0
All	All	1127/1172 (96%)	-0.06	33 (2%) 51 41	7, 39, 72, 101	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	ALA	4.3
1	A	287	ALA	3.7
1	A	435	PRO	3.7
1	A	451	CYS	3.3
1	B	434	CYS	3.2
1	B	204	MET	3.1
1	A	203	ASP	3.1
1	B	433	ASN	2.7
1	A	265	ALA	2.7
1	A	421	HIS	2.7
1	B	451	CYS	2.7
1	B	287	ALA	2.7
1	A	313	GLY	2.7
1	A	564	TYR	2.6
1	A	307	VAL	2.6
1	B	445	ALA	2.5
1	A	270	GLY	2.4
1	A	562	GLY	2.4
1	A	89	HIS	2.4
1	B	313	GLY	2.4
1	B	71	ALA	2.3
1	A	282	GLY	2.3
1	A	563	GLN	2.3
1	B	564	TYR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	440	GLU	2.3
1	A	470	ASP	2.3
1	A	419	ASP	2.2
1	A	293	ILE	2.2
1	A	418	ASP	2.2
1	A	312	THR	2.1
1	A	236	ARG	2.1
1	B	225	ALA	2.0
1	A	283	ASP	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 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	ZN	A	601	1/1	0.97	0.10	38,38,38,38	0
2	ZN	B	601	1/1	0.98	0.10	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.