



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2017 – 05:08 PM EDT

PDB ID : 3E2E  
Title : Crystal Structure of an Intermediate Complex of T7 RNAP and 7nt of RNA  
Authors : Durniak, K.J.; Bailey, S.; Steitz, T.A.  
Deposited on : unknown  
Resolution : 3.00 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.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

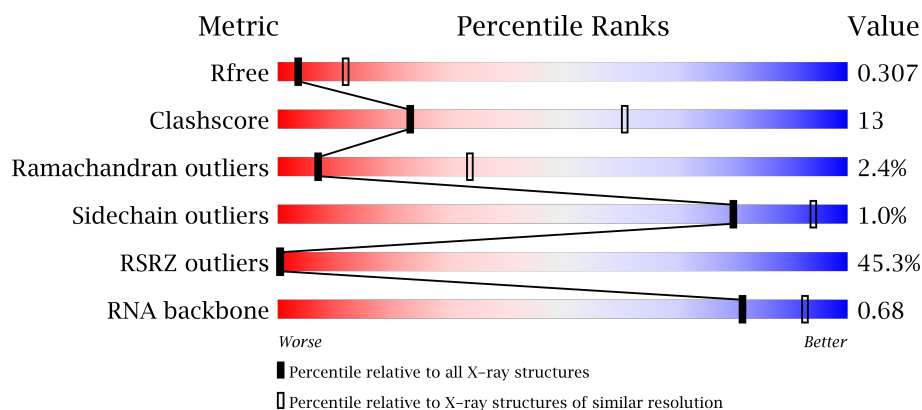
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)
RNA backbone	2435	1007 (3.34-2.66)

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	889	<div> <div>39%</div> <div> <div>72%</div> <div>19%</div> <div>• 6%</div> </div> </div>
2	R	7	<div> <div>100%</div> <div> <div>86%</div> <div>14%</div> </div> </div>
3	T	33	<div> <div>88%</div> <div> <div>52%</div> <div>39%</div> <div>• 6%</div> </div> </div>
4	N	33	<div> <div>82%</div> <div> <div>55%</div> <div>24%</div> <div>6%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8013 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 DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	832	Total	C	N	O	S	0	0	0
			6589	4206	1139	1207	37			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P00573
A	-4	HIS	-	EXPRESSION TAG	UNP P00573
A	-3	HIS	-	EXPRESSION TAG	UNP P00573
A	-2	HIS	-	EXPRESSION TAG	UNP P00573
A	-1	HIS	-	EXPRESSION TAG	UNP P00573
A	0	HIS	-	EXPRESSION TAG	UNP P00573
A	266	LEU	PRO	ENGINEERED	UNP P00573

- Molecule 2 is a RNA chain called RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*UP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	7	Total	C	N	O	P	0	0	0
			153	69	32	46	6			

- Molecule 3 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	31	Total	C	N	O	P	0	0	0
			633	301	113	188	31			

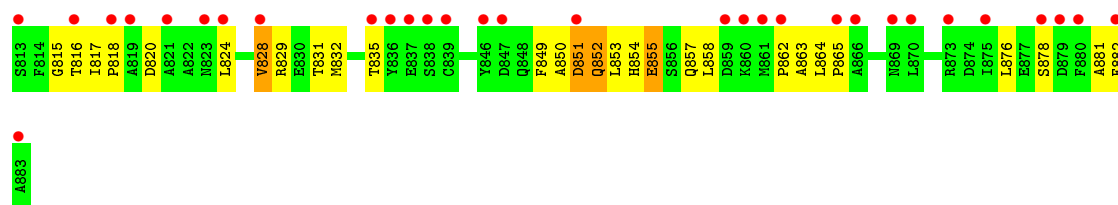
- Molecule 4 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	28	Total	C	N	O	P	0	0	0
			565	271	101	166	27			

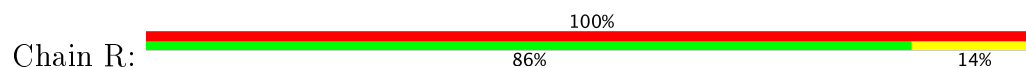
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	64	Total 64	O 64	0	0
5	R	1	Total 1	O 1	0	0
5	T	3	Total 3	O 3	0	0
5	N	5	Total 5	O 5	0	0

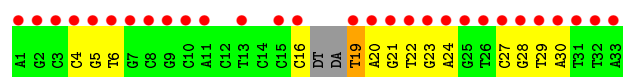
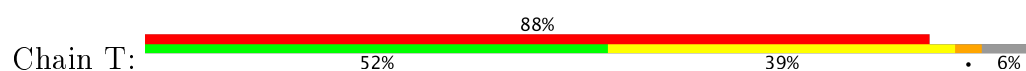




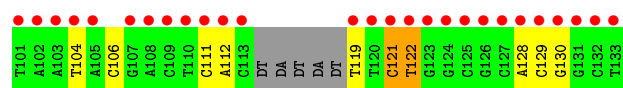
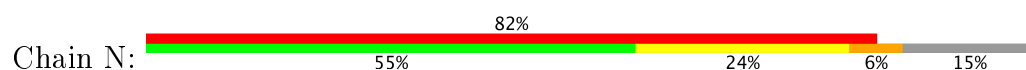
- Molecule 2: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*UP\*G)-3')



- Molecule 3: DNA (31-MER)



- Molecule 4: DNA (28-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.01Å 81.01Å 358.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.80 – 3.00 37.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (37.80-3.00) 98.5 (37.79-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.240 , 0.292 0.251 , 0.307	Depositor DCC
$R_{free}$ test set	1330 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 85.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	8013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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	0.34	0/6738	0.58	4/9109 (0.0%)
2	R	0.65	0/172	1.12	0/269
3	T	0.63	0/707	1.24	1/1086 (0.1%)
4	N	0.65	0/631	1.33	4/969 (0.4%)
All	All	0.41	0/8248	0.77	9/11433 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	19	DT	O4'-C1'-N1	8.94	114.26	108.00
4	N	122	DT	O4'-C1'-N1	7.05	112.93	108.00
1	A	43	SER	N-CA-C	6.99	129.88	111.00
4	N	121	DC	P-O3'-C3'	6.39	127.37	119.70
4	N	104	DT	C1'-O4'-C4'	-6.28	103.82	110.10
4	N	119	DT	O4'-C4'-C3'	-6.05	102.08	104.50
1	A	553	GLU	C-N-CA	5.83	136.28	121.70
1	A	43	SER	C-N-CA	5.82	136.25	121.70
1	A	44	TYR	N-CA-C	5.36	125.46	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	6589	0	6558	176	0
2	R	153	0	75	4	0
3	T	633	0	351	19	0
4	N	565	0	315	5	0
5	A	64	0	0	9	0
5	N	5	0	0	0	0
5	R	1	0	0	0	0
5	T	3	0	0	1	0
All	All	8013	0	7299	195	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 13.

All (195) 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:376:ALA:HB3	1:A:377:TRP:CB	1.72	1.19
1:A:553:GLU:CG	1:A:554:VAL:HG23	1.87	1.04
1:A:354:ALA:CA	1:A:355:ILE:HG12	1.88	1.04
1:A:131:ASN:HB3	1:A:132:THR:HA	1.06	1.03
1:A:354:ALA:HA	1:A:355:ILE:CG1	1.87	1.03
1:A:354:ALA:HB1	1:A:356:GLU:H	1.24	1.00
1:A:553:GLU:HG3	1:A:554:VAL:HG23	1.40	1.00
1:A:354:ALA:HA	1:A:355:ILE:HG12	1.01	1.00
1:A:131:ASN:CB	1:A:132:THR:HA	1.92	0.98
1:A:376:ALA:HB3	1:A:377:TRP:HB3	0.98	0.97
1:A:376:ALA:CB	1:A:377:TRP:HB3	1.94	0.96
1:A:451:PRO:HA	1:A:452:ILE:CB	1.99	0.93
1:A:451:PRO:HA	1:A:452:ILE:CG1	1.99	0.93
1:A:882:PHE:HA	5:A:907:HOH:O	1.69	0.92
1:A:556:GLY:HA3	1:A:557:ARG:HB2	1.51	0.91
3:T:19:DT:H2"	3:T:20:DA:OP1	1.69	0.89
1:A:370:ASN:HB2	1:A:371:PRO:HD2	1.55	0.89
1:A:131:ASN:HB3	1:A:132:THR:CA	2.00	0.85
1:A:349:VAL:CG2	1:A:352:ILE:HG12	2.06	0.85
1:A:850:ALA:HA	1:A:851:ASP:C	1.98	0.82
1:A:53:LYS:HB3	1:A:54:MET:HB2	1.63	0.79
1:A:556:GLY:HA3	1:A:557:ARG:CB	2.13	0.79
1:A:278:TRP:H	1:A:321:ASN:HD21	1.31	0.79
1:A:376:ALA:CB	1:A:377:TRP:CB	2.56	0.78
1:A:553:GLU:HG2	1:A:554:VAL:HG23	1.69	0.75
1:A:863:ALA:HB3	1:A:864:LEU:HA	1.68	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:PRO:HA	1:A:452:ILE:HB	1.70	0.73
1:A:354:ALA:HB3	1:A:391:ARG:HE	1.52	0.73
1:A:222:GLU:HB3	1:A:223:SER:HB3	1.68	0.73
1:A:354:ALA:HB1	1:A:356:GLU:N	2.03	0.72
1:A:451:PRO:HA	1:A:452:ILE:HG13	1.71	0.71
1:A:864:LEU:HD12	1:A:865:PRO:HD2	1.73	0.70
1:A:553:GLU:HG3	1:A:554:VAL:CG2	2.20	0.70
1:A:349:VAL:HG23	1:A:352:ILE:HG12	1.73	0.69
1:A:816:THR:HG22	1:A:817:ILE:N	2.08	0.69
1:A:710:VAL:HG21	1:A:719:LEU:HB2	1.76	0.68
1:A:550:LEU:HD11	1:A:695:ALA:HB2	1.75	0.68
1:A:784:HIS:HA	1:A:787:ASP:OD1	1.95	0.67
1:A:862:PRO:HB2	1:A:863:ALA:HB2	1.78	0.66
1:A:816:THR:HG22	1:A:817:ILE:H	1.60	0.65
1:A:375:THR:OG1	1:A:376:ALA:HA	1.97	0.65
1:A:739:TYR:H	1:A:774:GLN:NE2	1.95	0.65
2:R:1:G:C4	3:T:19:DT:H5"	2.32	0.65
1:A:452:ILE:HD11	1:A:529:ASN:HA	1.79	0.64
2:R:1:G:C5	3:T:19:DT:H5"	2.34	0.62
1:A:507:SER:HB3	1:A:510:CYS:HB2	1.80	0.62
1:A:556:GLY:CA	1:A:557:ARG:CB	2.77	0.62
1:A:224:THR:N	1:A:225:GLY:HA2	2.15	0.61
1:A:150:ARG:HH22	1:A:199:GLU:HB3	1.66	0.60
1:A:52:ARG:HA	1:A:55:PHE:HB2	1.84	0.59
1:A:180:LYS:HB3	1:A:181:ALA:HA	1.83	0.59
1:A:748:ASN:HB3	4:N:106:DC:H2"	1.84	0.59
1:A:489:ILE:HG22	1:A:490:MET:H	1.68	0.59
1:A:291:ARG:O	1:A:292:ARG:HB3	2.03	0.58
1:A:850:ALA:HA	1:A:851:ASP:O	2.02	0.58
1:A:452:ILE:CD1	1:A:529:ASN:HA	2.34	0.58
1:A:376:ALA:H	1:A:378:LYS:N	2.01	0.58
1:A:472:LYS:HG2	1:A:472:LYS:O	2.04	0.58
1:A:278:TRP:H	1:A:321:ASN:ND2	1.99	0.57
1:A:729:THR:HG22	1:A:733:PHE:HB3	1.86	0.57
1:A:710:VAL:HG11	1:A:719:LEU:N	2.19	0.57
1:A:863:ALA:HB3	1:A:864:LEU:CA	2.34	0.57
3:T:6:DT:H3	4:N:128:DA:H61	1.53	0.56
1:A:352:ILE:HD12	1:A:398:LEU:HD11	1.86	0.56
1:A:804:ILE:HG12	1:A:820:ASP:HB3	1.87	0.56
1:A:349:VAL:HG21	1:A:352:ILE:HG12	1.83	0.56
4:N:111:DC:H2"	4:N:112:DA:C8	2.40	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:VAL:HG11	1:A:719:LEU:H	1.71	0.56
1:A:829:ARG:NH2	5:A:907:HOH:O	2.38	0.56
1:A:180:LYS:HE3	1:A:183:MET:HG2	1.88	0.56
1:A:20:PRO:O	1:A:24:LEU:HB2	2.06	0.55
1:A:222:GLU:H	1:A:223:SER:C	2.09	0.55
4:N:121:DC:H4'	4:N:122:DT:OP1	2.07	0.55
3:T:22:DT:H2'	3:T:23:DG:C8	2.42	0.55
1:A:729:THR:CG2	1:A:733:PHE:HB3	2.37	0.55
1:A:224:THR:H	1:A:225:GLY:HA2	1.71	0.54
1:A:324:GLN:HA	1:A:418:TYR:HD1	1.72	0.54
1:A:760:THR:O	3:T:20:DA:H2'	2.08	0.54
1:A:681:ILE:O	1:A:685:VAL:HG12	2.08	0.54
1:A:639:TYR:HB3	1:A:780:PRO:HB3	1.89	0.54
1:A:560:ASN:O	1:A:881:ALA:HB2	2.08	0.53
1:A:383:ALA:O	1:A:387:LYS:HG3	2.09	0.53
1:A:424:GLY:HA3	5:A:897:HOH:O	2.08	0.53
1:A:408:PHE:HA	1:A:411:HIS:CD2	2.43	0.53
1:A:291:ARG:O	1:A:292:ARG:CB	2.57	0.53
1:A:375:THR:O	1:A:378:LYS:HB2	2.08	0.53
1:A:763:THR:HG22	1:A:765:LYS:H	1.73	0.53
1:A:180:LYS:HA	1:A:182:PHE:N	2.25	0.52
1:A:423:ARG:HH11	1:A:781:ASN:HD22	1.56	0.52
1:A:53:LYS:CB	1:A:54:MET:HB2	2.38	0.52
1:A:126:LEU:HD13	1:A:246:LEU:HB2	1.92	0.52
2:R:1:G:C4	3:T:19:DT:C5'	2.93	0.52
1:A:524:HIS:HB2	1:A:528:TYR:HB2	1.92	0.52
1:A:862:PRO:HB2	1:A:863:ALA:CB	2.40	0.51
3:T:20:DA:O5'	3:T:20:DA:H8	1.93	0.51
1:A:739:TYR:H	1:A:774:GLN:HE21	1.57	0.51
1:A:180:LYS:HG2	1:A:182:PHE:HD1	1.76	0.51
1:A:862:PRO:HB2	1:A:863:ALA:CA	2.41	0.51
1:A:264:ILE:N	1:A:265:SER:HB3	2.25	0.51
1:A:705:LEU:HB3	1:A:857:GLN:HE21	1.76	0.51
1:A:324:GLN:HE21	1:A:418:TYR:H	1.58	0.51
1:A:851:ASP:O	1:A:853:LEU:N	2.44	0.50
3:T:4:DC:H6	5:T:36:HOH:O	1.94	0.50
1:A:531:SER:HA	1:A:817:ILE:HG22	1.94	0.50
1:A:133:THR:HG23	1:A:136:ALA:HB2	1.93	0.50
1:A:537:ASP:O	1:A:882:PHE:HB2	2.12	0.49
1:A:362:MET:H	1:A:377:TRP:HE1	1.60	0.49
1:A:214:VAL:HG11	1:A:749:LEU:HD13	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ARG:NH1	1:A:878:SER:O	2.45	0.49
1:A:543:ILE:HD13	1:A:689:VAL:HG11	1.94	0.49
1:A:341:ILE:HD11	1:A:509:PHE:CZ	2.47	0.49
1:A:222:GLU:N	1:A:223:SER:C	2.66	0.49
1:A:376:ALA:H	1:A:378:LYS:H	1.61	0.48
1:A:747:LEU:HB2	1:A:759:PRO:HD2	1.96	0.48
1:A:816:THR:CG2	1:A:817:ILE:N	2.76	0.48
1:A:538:GLY:HA2	5:A:887:HOH:O	2.13	0.48
1:A:421:ASP:O	1:A:423:ARG:O	2.32	0.47
1:A:298:ARG:HH21	1:A:419:ASN:HB2	1.79	0.47
1:A:454:LYS:H	1:A:526:LEU:HD22	1.80	0.47
1:A:829:ARG:HB2	1:A:876:LEU:HD23	1.97	0.47
1:A:831:THR:O	1:A:835:THR:HG23	2.15	0.47
1:A:706:LEU:HD11	1:A:849:PHE:HB2	1.97	0.47
1:A:798:ALA:HB1	1:A:804:ILE:HD12	1.96	0.47
1:A:536:PHE:HB3	1:A:882:PHE:HB3	1.96	0.46
1:A:107:GLN:HB2	5:A:938:HOH:O	2.15	0.46
1:A:133:THR:HG23	1:A:136:ALA:CB	2.45	0.46
1:A:623:TYR:HB2	1:A:666:MET:SD	2.54	0.46
1:A:637:LEU:C	1:A:639:TYR:H	2.19	0.46
1:A:347:CYS:SG	1:A:349:VAL:HG22	2.56	0.46
3:T:16:DC:H2"	3:T:19:DT:O4	2.16	0.46
1:A:864:LEU:HD12	1:A:865:PRO:CD	2.44	0.46
1:A:530:CYS:SG	1:A:818:PRO:HG2	2.56	0.45
1:A:354:ALA:CB	1:A:355:ILE:HG12	2.42	0.45
1:A:794:THR:OG1	1:A:831:THR:HG21	2.15	0.45
1:A:223:SER:HA	1:A:224:THR:HA	1.70	0.45
1:A:278:TRP:CD2	1:A:284:GLY:HA3	2.52	0.45
1:A:854:HIS:O	1:A:855:GLU:HB2	2.16	0.45
1:A:816:THR:CG2	1:A:817:ILE:H	2.27	0.45
1:A:131:ASN:CB	1:A:132:THR:CA	2.76	0.45
1:A:165:ASN:HA	1:A:166:VAL:HA	1.67	0.45
1:A:376:ALA:CB	1:A:377:TRP:HB2	2.45	0.45
1:A:400:PHE:HD1	1:A:401:MET:HE2	1.82	0.45
1:A:790:HIS:NE2	1:A:832:MET:HB2	2.32	0.45
2:R:1:G:C2	3:T:19:DT:H5'	2.52	0.45
1:A:489:ILE:HG22	1:A:490:MET:N	2.32	0.45
1:A:824:LEU:O	1:A:828:VAL:HG22	2.17	0.45
4:N:129:DC:H2"	4:N:130:DG:C8	2.52	0.45
3:T:20:DA:C8	3:T:20:DA:O5'	2.70	0.45
1:A:82:ILE:HD13	1:A:112:GLU:HG3	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:LEU:HD21	1:A:809:LEU:HD13	1.99	0.44
1:A:797:TRP:CZ2	1:A:801:LYS:HD2	2.52	0.44
3:T:23:DG:H2"	3:T:24:DA:C8	2.53	0.44
1:A:376:ALA:N	1:A:378:LYS:H	2.15	0.44
1:A:534:LEU:O	1:A:815:GLY:HA2	2.18	0.44
1:A:354:ALA:CB	1:A:356:GLU:H	2.12	0.44
1:A:231:ARG:HE	1:A:234:ALA:HB2	1.83	0.43
1:A:760:THR:O	3:T:20:DA:C2'	2.65	0.43
3:T:4:DC:H2"	3:T:5:DG:C8	2.52	0.43
1:A:392:LYS:O	1:A:396:ILE:HG12	2.19	0.43
1:A:849:PHE:O	1:A:852:GLN:HB2	2.18	0.43
1:A:705:LEU:O	1:A:857:GLN:NE2	2.52	0.43
1:A:160:LYS:O	1:A:164:LYS:HG3	2.19	0.43
1:A:451:PRO:CA	1:A:452:ILE:HB	2.45	0.43
1:A:324:GLN:HA	1:A:418:TYR:CD1	2.52	0.43
1:A:53:LYS:O	1:A:57:ARG:HB3	2.19	0.43
1:A:605:ILE:HA	1:A:606:SER:HA	1.77	0.43
3:T:19:DT:H3'	3:T:20:DA:H5'	2.00	0.43
1:A:485:ASN:HB3	1:A:488:ASN:HB2	2.00	0.42
1:A:590:THR:HB	1:A:613:THR:H	1.84	0.42
1:A:616:LEU:HD13	1:A:676:TYR:HB2	2.00	0.42
1:A:374:LEU:C	1:A:376:ALA:HB2	2.40	0.42
3:T:27:DC:H2"	3:T:28:DG:C8	2.54	0.42
1:A:862:PRO:HB2	1:A:863:ALA:HA	2.02	0.42
1:A:344:TRP:O	1:A:355:ILE:HD12	2.19	0.42
1:A:354:ALA:HA	1:A:355:ILE:CB	2.46	0.42
1:A:295:ALA:O	1:A:419:ASN:ND2	2.53	0.42
1:A:556:GLY:O	1:A:561:LEU:HB2	2.19	0.42
1:A:636:THR:HA	1:A:639:TYR:HD2	1.84	0.42
1:A:355:ILE:HA	5:A:918:HOH:O	2.19	0.41
1:A:478:ARG:HH12	1:A:882:PHE:HZ	1.67	0.41
3:T:29:DT:H2"	3:T:30:DA:C8	2.55	0.41
1:A:42:GLU:HA	1:A:45:GLU:HB2	2.03	0.41
1:A:450:LYS:O	1:A:452:ILE:HG13	2.21	0.41
1:A:78:LEU:N	1:A:79:PRO:HD2	2.35	0.41
1:A:452:ILE:HG22	1:A:526:LEU:O	2.20	0.41
1:A:38:ALA:O	1:A:42:GLU:HB2	2.21	0.41
1:A:630:THR:O	1:A:634:VAL:HG23	2.21	0.41
1:A:451:PRO:HA	1:A:452:ILE:CD1	2.49	0.40
1:A:240:ASP:O	3:T:21:DG:H2"	2.21	0.40
1:A:150:ARG:NH1	5:A:940:HOH:O	2.54	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PRO:HG2	1:A:324:GLN:HG2	2.03	0.40
1:A:53:LYS:HB3	1:A:54:MET:CB	2.43	0.40
1:A:86:ASN:HD22	1:A:86:ASN:HA	1.74	0.40
1:A:452:ILE:HG23	5:A:933:HOH:O	2.21	0.40
1:A:74:ILE:HG13	5:A:903:HOH:O	2.20	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	820/889 (92%)	738 (90%)	62 (8%)	20 (2%)	7	34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	A	371	PRO
1	A	452	ILE
1	A	554	VAL
1	A	557	ARG
1	A	851	ASP
1	A	852	GLN
1	A	42	GLU
1	A	180	LYS
1	A	556	GLY
1	A	855	GLU
1	A	222	GLU
1	A	377	TRP
1	A	454	LYS
1	A	44	TYR
1	A	638	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	713	LYS
1	A	355	ILE
1	A	631	LYS
1	A	363	LYS

### 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	693/735 (94%)	686 (99%)	7 (1%)	80 94

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

Mol	Chain	Res	Type
1	A	44	TYR
1	A	133	THR
1	A	419	ASN
1	A	452	ILE
1	A	735	VAL
1	A	828	VAL
1	A	858	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	86	ASN
1	A	269	GLN
1	A	321	ASN
1	A	324	GLN
1	A	410	ASN
1	A	419	ASN
1	A	522	GLN
1	A	697	ASN
1	A	774	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	781	ASN
1	A	786	GLN
1	A	811	HIS
1	A	823	ASN
1	A	857	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	6/7 (85%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

There are no ligands in this entry.

## 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	832/889 (93%)	2.08	344 (41%) 0 0	30, 100, 101, 102	0
2	R	7/7 (100%)	5.48	7 (100%) 0 0	99, 100, 100, 101	0
3	T	31/33 (93%)	3.78	29 (93%) 0 0	97, 100, 101, 102	0
4	N	28/33 (84%)	4.27	27 (96%) 0 0	99, 100, 101, 101	0
All	All	898/962 (93%)	2.23	407 (45%) 0 0	30, 100, 101, 102	0

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	1	G	13.0
1	A	131	ASN	8.6
4	N	120	DT	8.3
1	A	716	GLY	8.0
1	A	598	THR	7.9
1	A	357	ARG	7.6
1	A	374	LEU	7.6
1	A	527	SER	7.5
1	A	646	PHE	7.5
4	N	128	DA	7.4
1	A	223	SER	7.3
1	A	385	TYR	7.1
1	A	224	THR	7.0
1	A	714	LYS	6.9
1	A	128	SER	6.9
1	A	241	SER	6.9
1	A	375	THR	6.9
1	A	369	MET	6.8
1	A	715	THR	6.7
4	N	121	DC	6.7
1	A	248	PRO	6.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	222	GLU	6.5
1	A	597	VAL	6.5
3	T	5	DG	6.5
1	A	325	ASN	6.3
1	A	671	ASN	6.3
1	A	230	HIS	6.1
1	A	54	MET	6.1
1	A	130	ASP	6.1
1	A	479	ILE	6.0
1	A	638	ALA	5.9
2	R	7	G	5.9
4	N	125	DC	5.9
1	A	10	ASP	5.8
1	A	265	SER	5.8
3	T	9	DG	5.7
4	N	130	DG	5.7
3	T	3	DC	5.7
1	A	523	HIS	5.7
1	A	596	THR	5.7
1	A	353	PRO	5.6
1	A	591	ASP	5.5
1	A	526	LEU	5.4
4	N	126	DG	5.3
3	T	33	DA	5.2
4	N	129	DC	5.2
1	A	376	ALA	5.1
1	A	358	GLU	5.1
1	A	98	LYS	5.1
4	N	127	DC	5.0
1	A	489	ILE	5.0
1	A	364	PRO	5.0
3	T	2	DG	5.0
1	A	99	ARG	5.0
1	A	605	ILE	5.0
3	T	19	DT	5.0
2	R	3	G	4.9
1	A	252	GLU	4.9
1	A	518	TYR	4.9
1	A	299	THR	4.8
3	T	1	DA	4.8
1	A	346	HIS	4.8
1	A	879	ASP	4.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	568	GLN	4.8
1	A	312	TYR	4.8
3	T	29	DT	4.8
1	A	382	ALA	4.7
3	T	20	DA	4.7
4	N	119	DT	4.7
1	A	393	SER	4.7
1	A	78	LEU	4.6
1	A	311	VAL	4.6
4	N	123	DG	4.6
1	A	354	ALA	4.5
1	A	710	VAL	4.5
4	N	101	DT	4.5
4	N	122	DT	4.5
1	A	181	ALA	4.5
1	A	381	ALA	4.4
2	R	6	U	4.4
1	A	506	ASP	4.4
4	N	104	DT	4.4
4	N	131	DG	4.4
1	A	623	TYR	4.4
4	N	111	DC	4.3
2	R	2	G	4.3
1	A	764	ASN	4.3
1	A	348	PRO	4.2
1	A	355	ILE	4.2
1	A	573	ILE	4.2
1	A	41	HIS	4.2
1	A	370	ASN	4.2
1	A	582	LEU	4.2
3	T	15	DC	4.2
1	A	127	THR	4.1
4	N	132	DC	4.1
1	A	488	ASN	4.1
3	T	6	DT	4.1
1	A	878	SER	4.1
1	A	165	ASN	4.1
1	A	239	GLN	4.1
1	A	588	ASN	4.1
1	A	449	GLY	4.0
1	A	473	VAL	4.0
1	A	371	PRO	4.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	T	11	DA	4.0
3	T	26	DT	4.0
1	A	390	ALA	4.0
1	A	253	ALA	4.0
1	A	851	ASP	3.9
1	A	797	TRP	3.9
1	A	52	ARG	3.9
1	A	344	TRP	3.9
1	A	574	VAL	3.9
1	A	482	ILE	3.9
1	A	762	ASN	3.9
4	N	124	DG	3.8
1	A	639	TYR	3.8
1	A	593	GLU	3.8
1	A	667	PHE	3.8
1	A	615	ALA	3.8
1	A	560	ASN	3.8
1	A	567	VAL	3.8
1	A	249	GLU	3.7
1	A	711	LYS	3.7
1	A	555	GLY	3.7
1	A	566	THR	3.7
1	A	373	ALA	3.7
1	A	132	THR	3.7
1	A	608	LYS	3.7
1	A	589	GLY	3.7
3	T	8	DC	3.7
1	A	345	LYS	3.7
3	T	4	DC	3.6
4	N	112	DA	3.6
1	A	499	ASN	3.6
1	A	869	ASN	3.6
1	A	721	LYS	3.6
1	A	279	THR	3.6
1	A	476	PRO	3.5
4	N	102	DA	3.5
1	A	465	ALA	3.5
1	A	360	LEU	3.5
1	A	511	PHE	3.5
1	A	76	THR	3.5
1	A	522	GLN	3.5
1	A	564	SER	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	459	TRP	3.5
1	A	388	ASP	3.5
1	A	837	GLU	3.5
1	A	343	LYS	3.5
1	A	380	ALA	3.5
1	A	389	LYS	3.4
1	A	519	ALA	3.4
1	A	865	PRO	3.4
3	T	13	DT	3.4
4	N	103	DA	3.4
4	N	105	DA	3.4
1	A	487	GLU	3.4
1	A	81	MET	3.4
1	A	835	THR	3.4
1	A	447	ALA	3.4
3	T	22	DT	3.4
1	A	554	VAL	3.3
1	A	502	TRP	3.3
1	A	644	PHE	3.3
3	T	21	DG	3.3
1	A	347	CYS	3.3
3	T	28	DG	3.3
1	A	513	ALA	3.3
1	A	575	ALA	3.3
1	A	883	ALA	3.3
3	T	24	DA	3.3
1	A	139	SER	3.3
1	A	565	GLU	3.3
3	T	23	DG	3.3
1	A	492	CYS	3.3
1	A	668	THR	3.3
1	A	90	GLU	3.3
1	A	719	LEU	3.3
1	A	803	GLY	3.2
1	A	818	PRO	3.2
1	A	468	ALA	3.2
1	A	819	ALA	3.2
1	A	517	GLU	3.2
1	A	720	ARG	3.2
1	A	859	ASP	3.2
1	A	647	ARG	3.2
1	A	361	PRO	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	578	VAL	3.2
1	A	505	GLN	3.1
1	A	813	SER	3.1
1	A	251	ALA	3.1
1	A	744	GLN	3.1
4	N	133	DT	3.1
2	R	5	G	3.1
1	A	765	LYS	3.1
1	A	654	THR	3.1
3	T	32	DT	3.1
1	A	779	ALA	3.1
1	A	607	GLU	3.1
1	A	552	ASP	3.1
1	A	28	TYR	3.1
1	A	570	ILE	3.1
1	A	480	LYS	3.0
1	A	448	LYS	3.0
1	A	616	LEU	3.0
1	A	451	PRO	3.0
1	A	406	ASN	3.0
1	A	756	ARG	3.0
1	A	79	PRO	3.0
1	A	661	SER	3.0
1	A	769	ILE	3.0
1	A	846	TYR	3.0
1	A	326	THR	3.0
3	T	7	DG	3.0
1	A	583	GLN	3.0
3	T	10	DC	3.0
1	A	362	MET	3.0
1	A	180	LYS	3.0
1	A	232	GLN	3.0
1	A	396	ILE	2.9
1	A	824	LEU	2.9
1	A	660	ASP	2.9
1	A	768	GLU	2.9
1	A	157	LEU	2.9
1	A	236	VAL	2.9
1	A	539	SER	2.9
3	T	30	DA	2.9
1	A	766	ASP	2.9
1	A	738	GLU	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	771	ALA	2.9
1	A	590	THR	2.9
3	T	16	DC	2.9
3	T	25	DG	2.9
1	A	453	GLY	2.9
1	A	717	GLU	2.8
1	A	562	LEU	2.8
1	A	640	GLY	2.8
1	A	563	PRO	2.8
1	A	543	ILE	2.8
1	A	94	ALA	2.8
1	A	197	GLY	2.8
1	A	561	LEU	2.8
1	A	466	ASN	2.8
1	A	491	ALA	2.8
1	A	770	ASP	2.8
1	A	51	PHE	2.8
1	A	352	ILE	2.8
1	A	778	ILE	2.8
1	A	551	ARG	2.8
1	A	240	ASP	2.8
1	A	752	LEU	2.8
1	A	676	TYR	2.8
1	A	57	ARG	2.8
1	A	725	VAL	2.8
1	A	379	ARG	2.7
1	A	189	ASP	2.7
1	A	472	LYS	2.7
1	A	104	GLN	2.7
1	A	718	ILE	2.7
1	A	277	PRO	2.7
2	R	4	A	2.7
1	A	498	GLU	2.7
1	A	484	GLU	2.7
1	A	190	MET	2.7
1	A	556	GLY	2.7
1	A	635	MET	2.7
1	A	613	THR	2.7
1	A	780	PRO	2.7
1	A	278	TRP	2.6
1	A	823	ASN	2.6
1	A	630	THR	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	49	ALA	2.6
1	A	202	SER	2.6
1	A	531	SER	2.6
1	A	359	GLU	2.6
1	A	627	ARG	2.6
1	A	433	ASN	2.6
1	A	342	THR	2.6
1	A	368	ASP	2.6
1	A	724	ALA	2.6
1	A	742	PRO	2.6
1	A	416	PHE	2.6
4	N	113	DC	2.6
1	A	88	TRP	2.6
1	A	755	PHE	2.5
1	A	483	GLU	2.5
1	A	77	LEU	2.5
1	A	247	ALA	2.5
1	A	141	ILE	2.5
1	A	75	THR	2.5
4	N	108	DA	2.5
1	A	486	HIS	2.5
1	A	397	SER	2.5
1	A	507	SER	2.5
1	A	275	PRO	2.5
1	A	145	ILE	2.5
1	A	525	GLY	2.5
1	A	100	PRO	2.5
1	A	739	TYR	2.5
1	A	828	VAL	2.5
1	A	184	GLN	2.5
1	A	836	TYR	2.5
1	A	93	LYS	2.4
1	A	880	PHE	2.4
1	A	30	GLU	2.4
1	A	553	GLU	2.4
1	A	327	ALA	2.4
1	A	97	GLY	2.4
1	A	166	VAL	2.4
1	A	785	SER	2.4
1	A	349	VAL	2.4
1	A	43	SER	2.4
1	A	50	ARG	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	85	ILE	2.4
1	A	378	LYS	2.4
4	N	107	DG	2.4
1	A	413	ALA	2.4
1	A	109	ILE	2.4
1	A	242	GLU	2.4
1	A	455	GLU	2.4
1	A	298	ARG	2.4
1	A	873	ARG	2.4
1	A	763	THR	2.4
3	T	27	DC	2.4
1	A	786	GLN	2.4
1	A	861	MET	2.4
1	A	620	TRP	2.4
1	A	464	GLY	2.4
1	A	633	SER	2.4
1	A	83	ALA	2.4
1	A	537	ASP	2.3
3	T	31	DT	2.3
1	A	866	ALA	2.3
1	A	383	ALA	2.3
1	A	713	LYS	2.3
1	A	882	PHE	2.3
1	A	577	LYS	2.3
4	N	109	DC	2.3
1	A	670	PRO	2.3
1	A	187	GLU	2.3
1	A	300	HIS	2.3
1	A	478	ARG	2.3
1	A	331	ASN	2.3
1	A	581	ILE	2.3
1	A	781	ASN	2.3
1	A	862	PRO	2.3
1	A	9	ASN	2.3
1	A	287	TRP	2.3
1	A	875	ILE	2.3
1	A	821	ALA	2.3
1	A	46	MET	2.3
1	A	363	LYS	2.3
1	A	23	THR	2.2
1	A	264	ILE	2.2
1	A	595	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	541	SER	2.2
1	A	533	PRO	2.2
1	A	571	TYR	2.2
1	A	73	LEU	2.2
1	A	45	GLU	2.2
4	N	110	DT	2.2
1	A	579	ASN	2.2
1	A	310	ASP	2.2
1	A	129	ALA	2.2
1	A	529	ASN	2.2
1	A	643	GLU	2.2
1	A	650	VAL	2.2
1	A	774	GLN	2.2
1	A	847	ASP	2.2
1	A	412	LYS	2.2
1	A	458	TYR	2.1
1	A	703	ALA	2.1
1	A	87	ASP	2.1
1	A	286	TYR	2.1
1	A	411	HIS	2.1
1	A	426	VAL	2.1
1	A	860	LYS	2.1
1	A	351	ASP	2.1
1	A	391	ARG	2.1
1	A	584	ALA	2.1
1	A	795	VAL	2.1
1	A	108	GLU	2.1
1	A	254	ILE	2.1
1	A	672	GLN	2.1
1	A	870	LEU	2.1
1	A	22	ASN	2.1
1	A	674	ALA	2.1
1	A	542	GLY	2.1
1	A	772	HIS	2.1
1	A	500	THR	2.1
1	A	686	SER	2.1
1	A	55	PHE	2.0
1	A	659	ILE	2.0
1	A	524	HIS	2.0
1	A	648	GLN	2.0
1	A	274	PRO	2.0
1	A	816	THR	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	838	SER	2.0
1	A	105	PHE	2.0
1	A	839	CYS	2.0
1	A	559	VAL	2.0
1	A	754	GLN	2.0
1	A	272	VAL	2.0
1	A	637	LEU	2.0
1	A	504	GLU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.