



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:07 AM GMT

PDB ID : 2PI5  
Title : T7 RNA polymerase complexed with a phi10 promoter  
Authors : Kennedy, W.P.; Momand, J.R.; Yin, Y.W.  
Deposited on : 2007-04-12  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

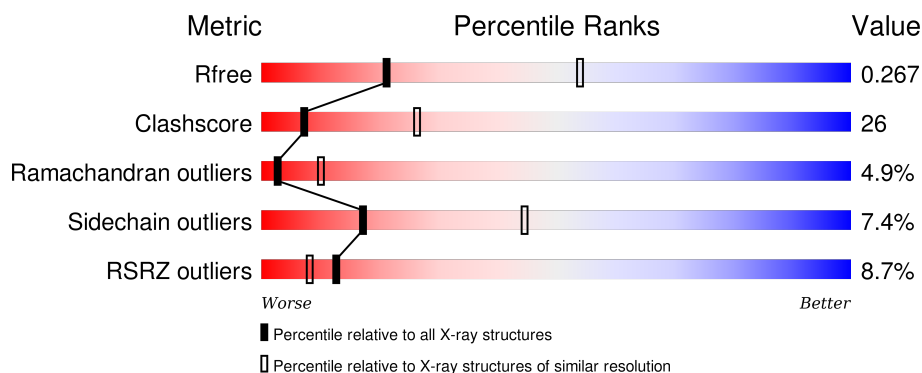
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	T	22	<div> <div>9%</div> <div>18% 64% 18%</div> </div>
2	P	14	<div> <div>7%</div> <div>29% 64% 7%</div> </div>
3	A	878	<div> <div>9%</div> <div>54% 37% 7%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7451 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 DNA chain called 5'-D(\*CP\*TP\*TP\*C\*CP\*TP\*AP\*TP\*AP\*GP\*TP\*GP\*AP\*GP\*TP\*CP\*GP\*TP\*AP\*TP\*TP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	18	Total	C	N	O	P	0	0	0
			368	178	65	108	17			

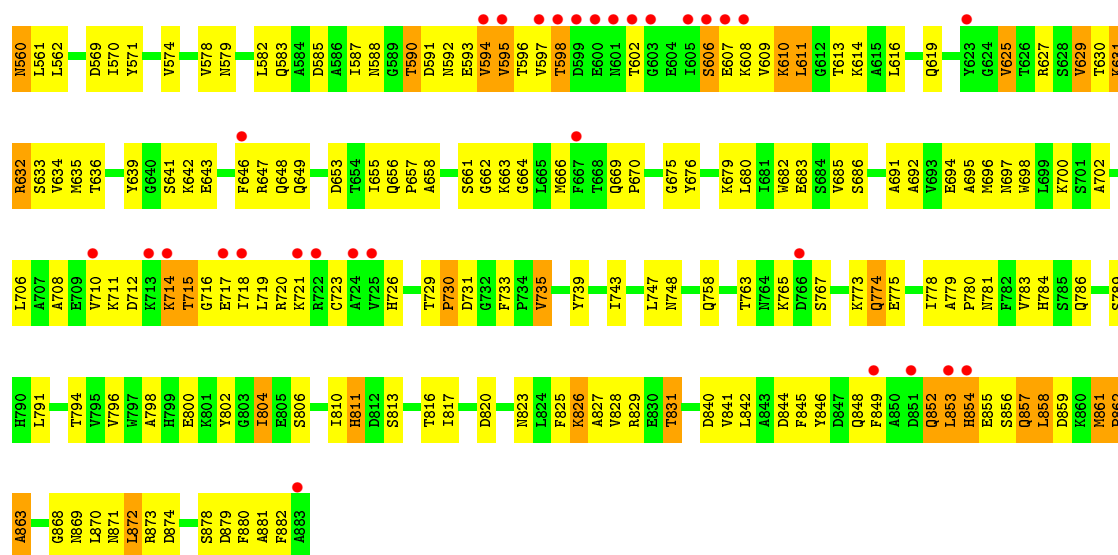
- Molecule 2 is a DNA chain called 5'-D(\*TP\*AP\*AP\*TP\*AP\*CP\*GP\*AP\*CP\*TP\*CP\*AP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	14	Total	C	N	O	P	0	0	0
			280	136	50	81	13			

- Molecule 3 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	862	Total	C	N	O	S	0	0	0
			6803	4334	1178	1254	37			





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.45 Å   73.79 Å   80.31 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	39.04 – 2.90 39.18 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.4 (39.04-2.90) 89.5 (39.18-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.90 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.249   ,   0.268 0.249   ,   0.267	Depositor DCC
$R_{free}$ test set	1233 reflections (4.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 29685 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	T	0.69	0/412	0.82	0/635
2	P	0.59	0/313	0.93	1/480 (0.2%)
3	A	0.49	0/6959	0.64	0/9416
All	All	0.50	0/7684	0.67	1/10531 (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	T	0	3
2	P	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	106	DC	O4'-C1'-N1	5.39	111.77	108.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	106	DC	Sidechain
1	T	10	DG	Sidechain
1	T	11	DT	Sidechain
1	T	9	DA	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	T	368	0	207	12	0
2	P	280	0	160	9	0
3	A	6803	0	6764	362	0
All	All	7451	0	7131	379	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 26.

All (379) 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)
3:A:473:VAL:HG22	3:A:474:PRO:HD2	1.20	1.18
3:A:804:ILE:HG12	3:A:820:ASP:HB3	1.48	0.94
3:A:278:TRP:H	3:A:321:ASN:HD21	0.92	0.91
3:A:595:VAL:HG12	3:A:608:LYS:HA	1.51	0.90
3:A:774:GLN:HA	3:A:774:GLN:HE21	1.36	0.90
3:A:816:THR:HG22	3:A:817:ILE:H	1.39	0.87
3:A:425:ARG:HH21	3:A:811:HIS:HB3	1.39	0.87
3:A:473:VAL:CG2	3:A:474:PRO:HD2	2.06	0.85
2:P:103:DA:H2''	2:P:104:DT:H5'	1.57	0.85
3:A:305:LEU:HD22	3:A:305:LEU:O	1.76	0.85
3:A:663:LYS:HG2	3:A:664:GLY:H	1.40	0.85
3:A:595:VAL:HG23	3:A:597:VAL:H	1.40	0.85
3:A:278:TRP:H	3:A:321:ASN:ND2	1.74	0.84
3:A:367:ILE:HD12	3:A:374:LEU:HD21	1.60	0.81
3:A:594:VAL:HG13	3:A:595:VAL:H	1.46	0.81
3:A:278:TRP:N	3:A:321:ASN:HD21	1.76	0.80
3:A:324:GLN:HE21	3:A:418:TYR:H	1.31	0.79
1:T:5:DC:H4'	3:A:422:TRP:HZ3	1.49	0.78
3:A:170:LEU:O	3:A:174:VAL:HG23	1.84	0.78
2:P:108:DA:H2''	2:P:109:DC:H5'	1.65	0.77
3:A:729:THR:HG22	3:A:733:PHE:O	1.85	0.77
3:A:427:TYR:HA	3:A:435:GLN:HE22	1.50	0.76
3:A:636:THR:HA	3:A:639:TYR:HD2	1.50	0.76
3:A:590:THR:HB	3:A:613:THR:H	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:846:TYR:HA	3:A:849:PHE:CE1	2.22	0.75
3:A:829:ARG:NH1	3:A:878:SER:O	2.19	0.75
3:A:706:LEU:HD21	3:A:849:PHE:HB2	1.68	0.74
3:A:585:ASP:O	3:A:614:LYS:HA	1.88	0.74
3:A:841:VAL:HG23	3:A:842:LEU:HD22	1.70	0.74
3:A:454:LYS:N	3:A:526:LEU:HD13	2.04	0.73
1:T:5:DC:H4'	3:A:422:TRP:CZ3	2.24	0.72
3:A:544:GLN:HG2	3:A:559:VAL:HG11	1.69	0.72
3:A:729:THR:CG2	3:A:733:PHE:HB3	2.19	0.72
3:A:861:MET:H	3:A:862:PRO:HD2	1.53	0.71
3:A:281:ILE:HD11	3:A:305:LEU:HD13	1.72	0.71
3:A:669:GLN:HE21	3:A:669:GLN:HA	1.54	0.71
3:A:632:ARG:HA	3:A:635:MET:HG2	1.71	0.71
3:A:594:VAL:HG22	3:A:595:VAL:HG22	1.73	0.70
3:A:106:LEU:HA	3:A:109:ILE:HD12	1.72	0.70
3:A:386:ARG:NH1	3:A:386:ARG:HB2	2.06	0.70
3:A:854:HIS:CG	3:A:855:GLU:N	2.60	0.69
3:A:616:LEU:HD23	3:A:676:TYR:HB2	1.75	0.69
3:A:397:SER:O	3:A:401:MET:HG2	1.93	0.68
3:A:778:ILE:HG23	3:A:779:ALA:H	1.59	0.68
3:A:425:ARG:NH2	3:A:811:HIS:HB3	2.09	0.67
3:A:596:THR:HG23	3:A:607:GLU:HB3	1.76	0.67
3:A:871:ASN:HB3	3:A:874:ASP:OD2	1.95	0.67
3:A:50:ARG:NH1	3:A:50:ARG:HB2	2.08	0.67
3:A:6:ILE:HD12	3:A:8:LYS:HD2	1.76	0.67
3:A:550:LEU:HD11	3:A:695:ALA:HB2	1.78	0.66
3:A:853:LEU:HD13	3:A:854:HIS:HB3	1.77	0.66
3:A:540:CYS:SG	3:A:543:ILE:HD12	2.35	0.66
3:A:6:ILE:HG21	3:A:8:LYS:HZ3	1.59	0.66
3:A:416:PHE:CE2	3:A:434:PRO:HD3	2.30	0.66
3:A:311:VAL:O	3:A:312:TYR:HB3	1.94	0.66
3:A:849:PHE:O	3:A:853:LEU:HB3	1.96	0.65
3:A:692:ALA:O	3:A:696:MET:HG3	1.97	0.65
3:A:854:HIS:NE2	3:A:856:SER:C	2.50	0.65
3:A:730:PRO:CD	3:A:786:GLN:HE22	2.08	0.65
3:A:731:ASP:OD1	3:A:789:SER:HB2	1.97	0.65
3:A:50:ARG:HH11	3:A:50:ARG:HB2	1.61	0.64
3:A:669:GLN:NE2	3:A:669:GLN:HA	2.11	0.64
3:A:794:THR:OG1	3:A:831:THR:HG21	1.97	0.64
3:A:428:ALA:H	3:A:435:GLN:HE21	1.44	0.64
3:A:729:THR:HG21	3:A:733:PHE:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:630:THR:O	3:A:634:VAL:HG12	1.98	0.64
3:A:185:VAL:HG22	3:A:186:VAL:N	2.13	0.64
3:A:366:ASP:HB3	3:A:369:MET:HG2	1.80	0.64
3:A:452:ILE:HG23	3:A:453:GLY:N	2.13	0.63
3:A:169:GLN:HE21	3:A:171:ASN:HB2	1.64	0.63
2:P:108:DA:H2''	2:P:109:DC:C5'	2.28	0.62
3:A:425:ARG:HH21	3:A:811:HIS:CB	2.13	0.62
3:A:8:LYS:O	3:A:9:ASN:HB3	1.98	0.62
3:A:798:ALA:O	3:A:804:ILE:HB	1.99	0.61
3:A:438:ASP:OD2	3:A:509:PHE:HB2	2.00	0.61
3:A:647:ARG:HE	3:A:675:GLY:HA2	1.66	0.61
3:A:594:VAL:HG22	3:A:595:VAL:N	2.14	0.61
3:A:594:VAL:HG13	3:A:595:VAL:N	2.14	0.61
3:A:778:ILE:HG23	3:A:779:ALA:N	2.15	0.61
3:A:150:ARG:O	3:A:152:GLY:N	2.34	0.60
3:A:706:LEU:HG	3:A:853:LEU:HG	1.83	0.60
2:P:103:DA:H2''	2:P:104:DT:C5'	2.31	0.60
3:A:164:LYS:C	3:A:164:LYS:HD2	2.21	0.60
1:T:19:DA:H1'	1:T:20:DT:H5'	1.84	0.60
3:A:551:ARG:O	3:A:868:GLY:HA3	2.00	0.60
3:A:853:LEU:HD22	3:A:854:HIS:N	2.16	0.60
1:T:7:DA:H2'	1:T:8:DT:H72	1.84	0.60
3:A:625:VAL:HA	3:A:629:VAL:HG21	1.84	0.60
1:T:5:DC:H2''	1:T:6:DT:H5'	1.83	0.59
3:A:702:ALA:O	3:A:706:LEU:HD12	2.02	0.59
3:A:609:VAL:HG11	3:A:669:GLN:OE1	2.02	0.59
3:A:739:TYR:CD1	3:A:773:LYS:HE3	2.38	0.59
3:A:473:VAL:HG22	3:A:474:PRO:CD	2.12	0.59
3:A:395:ARG:O	3:A:399:GLU:HG2	2.02	0.59
3:A:425:ARG:HH11	3:A:784:HIS:CG	2.21	0.58
3:A:452:ILE:HG12	3:A:457:TYR:N	2.18	0.58
3:A:594:VAL:HG11	3:A:598:THR:HG21	1.86	0.58
3:A:386:ARG:HH11	3:A:386:ARG:HB2	1.67	0.58
3:A:633:SER:HA	3:A:649:GLN:OE1	2.02	0.58
3:A:743:ILE:HD11	3:A:767:SER:HB3	1.84	0.58
3:A:862:PRO:O	3:A:863:ALA:CB	2.52	0.58
3:A:335:LEU:HD22	3:A:335:LEU:O	2.03	0.58
3:A:590:THR:HG22	3:A:591:ASP:N	2.19	0.58
3:A:335:LEU:HD22	3:A:339:ASN:ND2	2.20	0.57
2:P:102:DA:H1'	2:P:103:DA:C8	2.39	0.57
3:A:747:LEU:O	3:A:758:GLN:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:853:LEU:HD22	3:A:854:HIS:H	1.68	0.57
3:A:73:LEU:HG	3:A:260:ALA:HB1	1.86	0.57
3:A:643:GLU:CD	3:A:679:LYS:HD2	2.24	0.57
3:A:147:ASP:OD1	3:A:292:ARG:HD2	2.04	0.56
3:A:861:MET:HB3	3:A:862:PRO:CD	2.35	0.56
3:A:862:PRO:O	3:A:863:ALA:HB3	2.05	0.56
3:A:806:SER:O	3:A:816:THR:HG23	2.04	0.56
3:A:452:ILE:HG23	3:A:453:GLY:H	1.70	0.56
3:A:106:LEU:HD21	3:A:212:VAL:HG13	1.88	0.56
3:A:159:ALA:HA	3:A:162:PHE:CE2	2.41	0.56
3:A:560:ASN:O	3:A:881:ALA:HB2	2.05	0.56
3:A:796:VAL:O	3:A:800:GLU:HG3	2.06	0.56
3:A:139:SER:OG	3:A:206:LYS:HE2	2.05	0.56
3:A:569:ASP:OD2	3:A:627:ARG:HD2	2.06	0.56
3:A:427:TYR:HA	3:A:435:GLN:NE2	2.19	0.55
3:A:366:ASP:CB	3:A:369:MET:HG2	2.37	0.55
3:A:12:SER:OG	3:A:15:GLU:HG3	2.07	0.55
3:A:639:TYR:HA	3:A:780:PRO:HB3	1.89	0.55
3:A:592:ASN:OD1	3:A:611:LEU:HA	2.07	0.55
3:A:845:PHE:O	3:A:848:GLN:HB2	2.07	0.55
1:T:6:DT:OP2	1:T:7:DA:H4'	2.07	0.55
3:A:763:THR:HG22	3:A:765:LYS:H	1.72	0.55
3:A:311:VAL:O	3:A:312:TYR:CB	2.54	0.54
3:A:551:ARG:HH11	3:A:551:ARG:HG3	1.72	0.54
3:A:281:ILE:HD11	3:A:305:LEU:O	2.07	0.54
3:A:324:GLN:HE21	3:A:418:TYR:N	2.04	0.54
3:A:804:ILE:HG23	3:A:816:THR:HG21	1.89	0.54
3:A:176:HIS:CD2	3:A:177:VAL:H	2.25	0.54
3:A:424:GLY:O	3:A:425:ARG:C	2.46	0.54
3:A:386:ARG:HH11	3:A:386:ARG:CB	2.20	0.54
3:A:647:ARG:HH11	3:A:647:ARG:HG2	1.73	0.54
3:A:473:VAL:HG21	3:A:477:GLU:CD	2.28	0.54
1:T:17:DG:H1'	1:T:18:DT:H5'	1.89	0.54
3:A:643:GLU:OE1	3:A:679:LYS:HD2	2.08	0.54
3:A:679:LYS:HG3	3:A:683:GLU:OE2	2.08	0.54
3:A:364:PRO:C	3:A:366:ASP:H	2.09	0.53
3:A:632:ARG:O	3:A:636:THR:HG23	2.09	0.53
3:A:720:ARG:HD2	3:A:721:LYS:O	2.10	0.52
3:A:619:GLN:NE2	3:A:666:MET:O	2.42	0.52
3:A:324:GLN:NE2	3:A:418:TYR:H	2.05	0.52
3:A:6:ILE:HG21	3:A:8:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:TRP:CE3	3:A:512:LEU:HB2	2.45	0.52
3:A:459:TRP:HA	3:A:462:ILE:HB	1.91	0.52
3:A:367:ILE:HG23	3:A:368:ASP:OD1	2.10	0.51
3:A:861:MET:HB3	3:A:862:PRO:HD3	1.92	0.51
3:A:186:VAL:HG12	3:A:187:GLU:N	2.25	0.51
3:A:254:ILE:HG22	3:A:399:GLU:HG3	1.91	0.51
3:A:570:ILE:HG23	3:A:571:TYR:CD1	2.45	0.51
3:A:486:HIS:CE1	3:A:490:MET:HG3	2.45	0.51
3:A:272:VAL:O	3:A:415:TRP:HZ3	1.93	0.51
3:A:871:ASN:C	3:A:873:ARG:H	2.14	0.51
3:A:729:THR:HG23	3:A:733:PHE:H	1.75	0.51
3:A:711:LYS:HG2	3:A:712:ASP:N	2.25	0.51
3:A:802:TYR:OH	3:A:826:LYS:HE3	2.09	0.51
3:A:579:ASN:HA	3:A:582:LEU:HD12	1.91	0.51
1:T:14:DG:H1'	1:T:15:DT:H5''	1.93	0.51
3:A:816:THR:HG22	3:A:817:ILE:N	2.17	0.51
3:A:153:ARG:HH11	3:A:153:ARG:HG2	1.76	0.51
3:A:685:VAL:HG23	3:A:686:SER:N	2.26	0.51
3:A:370:ASN:ND2	3:A:375:THR:OG1	2.44	0.51
3:A:570:ILE:HG23	3:A:571:TYR:N	2.26	0.51
3:A:861:MET:O	3:A:862:PRO:O	2.29	0.50
1:T:14:DG:H2''	1:T:15:DT:H5'	1.92	0.50
3:A:593:GLU:HG3	3:A:594:VAL:H	1.77	0.50
3:A:636:THR:HA	3:A:639:TYR:CD2	2.40	0.50
3:A:593:GLU:HB3	3:A:610:LYS:CB	2.41	0.50
3:A:710:VAL:HG13	3:A:719:LEU:HB2	1.92	0.50
3:A:507:SER:HB3	3:A:510:CYS:HB2	1.94	0.50
3:A:199:GLU:OE2	3:A:199:GLU:HA	2.11	0.49
3:A:574:VAL:O	3:A:578:VAL:HG23	2.12	0.49
3:A:99:ARG:HG2	3:A:99:ARG:HH11	1.77	0.49
3:A:19:ILE:HB	3:A:20:PRO:HD3	1.93	0.49
3:A:537:ASP:OD1	3:A:813:SER:OG	2.11	0.49
3:A:163:LYS:HA	3:A:163:LYS:NZ	2.28	0.49
3:A:176:HIS:O	3:A:179:LYS:HE2	2.12	0.49
3:A:169:GLN:HG2	3:A:172:LYS:NZ	2.27	0.49
3:A:370:ASN:N	3:A:371:PRO:CD	2.76	0.49
3:A:857:GLN:O	3:A:858:LEU:HB3	2.13	0.49
3:A:607:GLU:C	3:A:609:VAL:H	2.15	0.49
2:P:107:DG:H2''	2:P:108:DA:H5'	1.94	0.49
3:A:72:PRO:HB3	3:A:262:ALA:HB3	1.93	0.49
3:A:641:SER:HB3	3:A:646:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:421:ASP:OD2	3:A:423:ARG:HD3	2.13	0.48
3:A:6:ILE:HD12	3:A:8:LYS:CD	2.42	0.48
3:A:224:THR:O	3:A:226:MET:N	2.41	0.48
3:A:523:HIS:O	3:A:524:HIS:ND1	2.46	0.48
3:A:337:VAL:HG21	3:A:512:LEU:HD21	1.96	0.48
3:A:6:ILE:HB	3:A:8:LYS:HZ2	1.78	0.48
3:A:147:ASP:CG	3:A:292:ARG:HD2	2.34	0.48
2:P:106:DC:H2"	3:A:748:ASN:HB3	1.96	0.48
3:A:511:PHE:O	3:A:514:PHE:N	2.46	0.48
3:A:240:ASP:OD1	3:A:241:SER:N	2.46	0.48
3:A:595:VAL:CG1	3:A:608:LYS:HA	2.34	0.48
3:A:367:ILE:HD12	3:A:374:LEU:CD2	2.37	0.48
3:A:853:LEU:HD13	3:A:853:LEU:C	2.34	0.48
3:A:823:ASN:O	3:A:826:LYS:HG2	2.14	0.48
3:A:729:THR:CG2	3:A:733:PHE:H	2.27	0.48
3:A:337:VAL:O	3:A:341:ILE:HG12	2.14	0.48
3:A:475:PHE:O	3:A:476:PRO:C	2.52	0.48
3:A:544:GLN:CG	3:A:559:VAL:HG11	2.40	0.47
3:A:229:LEU:HG	3:A:242:GLU:HG3	1.96	0.47
3:A:561:LEU:O	3:A:878:SER:HB2	2.13	0.47
3:A:698:TRP:HZ3	3:A:863:ALA:N	2.12	0.47
3:A:308:TYR:HA	3:A:311:VAL:HG23	1.95	0.47
3:A:24:LEU:HD11	3:A:273:VAL:HG21	1.96	0.47
3:A:422:TRP:CD2	3:A:423:ARG:HD2	2.49	0.47
3:A:201:TRP:HB2	3:A:302:LYS:HD3	1.95	0.47
3:A:590:THR:HB	3:A:613:THR:N	2.25	0.47
3:A:559:VAL:O	3:A:560:ASN:CB	2.63	0.47
3:A:363:LYS:HG2	3:A:364:PRO:HD2	1.96	0.47
3:A:201:TRP:HZ2	3:A:299:THR:O	1.98	0.47
3:A:36:GLN:NE2	3:A:273:VAL:HG22	2.30	0.47
3:A:783:VAL:HG23	3:A:784:HIS:H	1.79	0.47
3:A:308:TYR:HA	3:A:311:VAL:CG2	2.44	0.47
3:A:827:ALA:O	3:A:831:THR:HG22	2.14	0.47
3:A:710:VAL:HG12	3:A:720:ARG:O	2.14	0.47
3:A:517:GLU:HG3	3:A:532:LEU:HB2	1.97	0.47
3:A:46:MET:HG3	3:A:47:GLY:N	2.29	0.47
3:A:663:LYS:HG2	3:A:664:GLY:N	2.20	0.47
3:A:679:LYS:HE2	3:A:683:GLU:OE1	2.15	0.47
3:A:719:LEU:HD22	3:A:719:LEU:N	2.30	0.46
3:A:451:PRO:HA	3:A:528:TYR:O	2.15	0.46
3:A:361:PRO:HD3	3:A:384:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:453:GLY:HA2	3:A:526:LEU:HB3	1.96	0.46
3:A:502:TRP:O	3:A:505:GLN:HG2	2.15	0.46
3:A:371:PRO:O	3:A:372:GLU:HG2	2.15	0.46
3:A:726:HIS:HD2	3:A:735:VAL:O	1.98	0.46
3:A:852:GLN:O	3:A:853:LEU:HB2	2.15	0.46
3:A:452:ILE:CG2	3:A:453:GLY:N	2.78	0.46
3:A:159:ALA:O	3:A:163:LYS:HG2	2.15	0.46
3:A:185:VAL:HG22	3:A:186:VAL:H	1.78	0.46
3:A:562:LEU:HD21	3:A:870:LEU:CD1	2.46	0.46
3:A:632:ARG:HA	3:A:635:MET:CG	2.44	0.46
3:A:22:ASN:C	3:A:24:LEU:N	2.69	0.46
3:A:593:GLU:HB3	3:A:610:LYS:HB2	1.98	0.46
3:A:425:ARG:NH1	3:A:784:HIS:CG	2.83	0.46
3:A:775:GLU:O	3:A:778:ILE:HG22	2.16	0.46
3:A:272:VAL:HG12	3:A:272:VAL:O	2.15	0.46
3:A:224:THR:O	3:A:224:THR:OG1	2.34	0.46
3:A:648:GLN:CD	3:A:648:GLN:H	2.19	0.46
3:A:631:LYS:O	3:A:634:VAL:HG12	2.15	0.45
3:A:199:GLU:HA	3:A:302:LYS:HZ3	1.80	0.45
3:A:455:GLU:OE1	3:A:455:GLU:HA	2.16	0.45
1:T:6:DT:OP2	1:T:7:DA:C4'	2.63	0.45
3:A:857:GLN:NE2	3:A:857:GLN:HA	2.30	0.45
3:A:347:CYS:SG	3:A:348:PRO:HD2	2.56	0.45
3:A:474:PRO:HA	3:A:880:PHE:CZ	2.52	0.45
3:A:664:GLY:HA2	3:A:666:MET:SD	2.56	0.45
3:A:841:VAL:HG23	3:A:842:LEU:N	2.32	0.45
3:A:169:GLN:HG2	3:A:172:LYS:HZ3	1.80	0.45
3:A:783:VAL:HG23	3:A:784:HIS:N	2.32	0.45
3:A:12:SER:HG	3:A:15:GLU:HG3	1.82	0.45
3:A:23:THR:O	3:A:27:HIS:HD2	1.98	0.45
3:A:656:GLN:HA	3:A:656:GLN:OE1	2.17	0.45
3:A:606:SER:O	3:A:607:GLU:C	2.53	0.45
3:A:457:TYR:CD1	3:A:521:VAL:HG11	2.52	0.45
3:A:663:LYS:CG	3:A:664:GLY:H	2.19	0.45
3:A:846:TYR:C	3:A:848:GLN:H	2.20	0.44
3:A:186:VAL:HG12	3:A:187:GLU:H	1.82	0.44
3:A:404:GLN:CA	3:A:404:GLN:HE21	2.31	0.44
2:P:111:DC:H2''	2:P:112:DA:C8	2.52	0.44
3:A:246:LEU:HD21	3:A:254:ILE:HD12	1.98	0.44
1:T:16:DC:H2''	1:T:17:DG:C8	2.53	0.44
3:A:22:ASN:C	3:A:24:LEU:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:454:LYS:C	3:A:454:LYS:HD3	2.37	0.44
3:A:871:ASN:O	3:A:873:ARG:N	2.50	0.44
3:A:696:MET:O	3:A:700:LYS:HG3	2.17	0.44
3:A:102:ALA:CB	3:A:215:ARG:HG3	2.48	0.44
3:A:729:THR:OG1	3:A:789:SER:HB3	2.18	0.44
3:A:829:ARG:NH2	3:A:882:PHE:HD1	2.15	0.44
3:A:557:ARG:NH1	3:A:557:ARG:HG2	2.31	0.44
3:A:594:VAL:HG11	3:A:598:THR:CG2	2.47	0.44
1:T:20:DT:O2	3:A:97:GLY:HA2	2.18	0.44
3:A:237:VAL:HG12	3:A:237:VAL:O	2.18	0.44
3:A:316:VAL:O	3:A:320:ILE:HG12	2.18	0.44
3:A:344:TRP:CE3	3:A:348:PRO:HD3	2.52	0.44
3:A:561:LEU:HD22	3:A:561:LEU:N	2.33	0.43
3:A:559:VAL:O	3:A:560:ASN:CG	2.57	0.43
3:A:574:VAL:HG12	3:A:574:VAL:O	2.17	0.43
2:P:110:DT:H1'	2:P:111:DC:H5''	2.00	0.43
3:A:871:ASN:C	3:A:873:ARG:N	2.71	0.43
3:A:330:ILE:HB	3:A:409:ALA:HA	1.99	0.43
3:A:333:LYS:O	3:A:336:ALA:HB3	2.19	0.43
3:A:656:GLN:HB3	3:A:657:PRO:CD	2.49	0.43
3:A:855:GLU:OE2	3:A:856:SER:HB3	2.18	0.43
3:A:169:GLN:NE2	3:A:171:ASN:HB2	2.31	0.43
3:A:739:TYR:H	3:A:774:GLN:HE22	1.66	0.43
3:A:404:GLN:HA	3:A:404:GLN:NE2	2.33	0.43
3:A:853:LEU:HD13	3:A:854:HIS:CB	2.48	0.43
3:A:698:TRP:CZ3	3:A:862:PRO:HA	2.54	0.43
3:A:842:LEU:O	3:A:845:PHE:HB3	2.19	0.43
3:A:781:ASN:HA	3:A:781:ASN:HD22	1.65	0.43
3:A:281:ILE:HD11	3:A:305:LEU:CD1	2.44	0.43
3:A:854:HIS:CD2	3:A:858:LEU:N	2.87	0.43
3:A:452:ILE:CG2	3:A:453:GLY:H	2.31	0.43
3:A:523:HIS:C	3:A:524:HIS:ND1	2.72	0.43
3:A:553:GLU:OE2	3:A:869:ASN:N	2.52	0.43
3:A:774:GLN:HA	3:A:774:GLN:NE2	2.17	0.43
3:A:594:VAL:HG22	3:A:595:VAL:H	1.80	0.43
3:A:344:TRP:C	3:A:346:HIS:H	2.23	0.43
3:A:730:PRO:HD2	3:A:786:GLN:HE22	1.84	0.42
3:A:342:THR:O	3:A:395:ARG:NH2	2.48	0.42
3:A:791:LEU:HD23	3:A:791:LEU:C	2.40	0.42
3:A:706:LEU:HA	3:A:853:LEU:CD2	2.49	0.42
3:A:783:VAL:O	3:A:784:HIS:C	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:779:ALA:N	3:A:780:PRO:HD2	2.34	0.42
3:A:570:ILE:HG23	3:A:571:TYR:H	1.84	0.42
3:A:697:ASN:HD22	3:A:697:ASN:HA	1.63	0.42
3:A:669:GLN:HA	3:A:670:PRO:HD2	1.85	0.42
3:A:416:PHE:CD2	3:A:434:PRO:HD3	2.54	0.42
3:A:185:VAL:CG2	3:A:186:VAL:N	2.80	0.42
3:A:19:ILE:HG22	3:A:195:LEU:HD21	2.00	0.42
3:A:324:GLN:HE21	3:A:417:PRO:HA	1.83	0.42
3:A:164:LYS:O	3:A:164:LYS:HD2	2.19	0.42
3:A:828:VAL:O	3:A:831:THR:HG23	2.19	0.42
3:A:109:ILE:HG22	3:A:110:LYS:N	2.35	0.42
3:A:428:ALA:H	3:A:435:GLN:NE2	2.13	0.42
3:A:854:HIS:NE2	3:A:856:SER:O	2.52	0.42
3:A:691:ALA:O	3:A:692:ALA:C	2.58	0.42
3:A:159:ALA:O	3:A:163:LYS:CG	2.68	0.42
3:A:72:PRO:O	3:A:75:THR:OG1	2.37	0.42
3:A:492:CYS:HA	3:A:499:ASN:HB2	2.02	0.42
3:A:676:TYR:O	3:A:680:LEU:HD13	2.20	0.42
3:A:176:HIS:CG	3:A:177:VAL:H	2.38	0.42
3:A:298:ARG:HH12	3:A:427:TYR:HB2	1.85	0.41
3:A:551:ARG:NH1	3:A:551:ARG:HG3	2.35	0.41
3:A:717:GLU:O	3:A:719:LEU:HD22	2.20	0.41
3:A:870:LEU:C	3:A:870:LEU:HD23	2.40	0.41
3:A:379:ARG:O	3:A:382:ALA:HB3	2.20	0.41
3:A:856:SER:O	3:A:857:GLN:C	2.59	0.41
3:A:583:GLN:O	3:A:587:ILE:HG12	2.20	0.41
3:A:590:THR:CG2	3:A:591:ASP:N	2.82	0.41
3:A:448:LYS:H	3:A:448:LYS:HD2	1.85	0.41
3:A:274:PRO:HA	3:A:275:PRO:HD3	1.76	0.41
3:A:32:LEU:O	3:A:33:ALA:C	2.56	0.41
3:A:739:TYR:HD1	3:A:773:LYS:HE3	1.84	0.41
3:A:177:VAL:O	3:A:179:LYS:HG2	2.20	0.41
3:A:609:VAL:CG2	3:A:611:LEU:HG	2.50	0.41
3:A:857:GLN:HE21	3:A:857:GLN:HA	1.84	0.41
3:A:710:VAL:O	3:A:710:VAL:HG13	2.20	0.41
3:A:714:LYS:O	3:A:715:THR:OG1	2.35	0.41
3:A:78:LEU:O	3:A:82:ILE:HG13	2.20	0.41
3:A:551:ARG:HE	3:A:872:LEU:HD11	1.86	0.41
3:A:712:ASP:OD2	3:A:715:THR:HB	2.20	0.41
3:A:715:THR:O	3:A:717:GLU:N	2.53	0.41
3:A:394:ARG:HG2	3:A:394:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:6:ILE:HD12	3:A:8:LYS:CE	2.50	0.41
3:A:691:ALA:O	3:A:694:GLU:N	2.54	0.41
3:A:366:ASP:N	3:A:366:ASP:OD2	2.52	0.41
3:A:551:ARG:HB2	3:A:868:GLY:H	1.86	0.41
3:A:718:ILE:HG21	3:A:721:LYS:HG3	2.03	0.41
3:A:557:ARG:HH11	3:A:557:ARG:HG2	1.85	0.41
3:A:655:ILE:O	3:A:658:ALA:HB3	2.20	0.41
3:A:6:ILE:CG2	3:A:8:LYS:NZ	2.84	0.41
3:A:840:ASP:O	3:A:844:ASP:OD2	2.39	0.41
3:A:552:ASP:HB2	3:A:691:ALA:HB2	2.03	0.40
3:A:579:ASN:O	3:A:583:GLN:HG2	2.21	0.40
3:A:373:ALA:C	3:A:375:THR:H	2.24	0.40
3:A:545:HIS:O	3:A:549:MET:HG2	2.21	0.40
3:A:719:LEU:CD2	3:A:719:LEU:H	2.34	0.40
3:A:419:ASN:HA	3:A:419:ASN:HD22	1.49	0.40
3:A:555:GLY:O	3:A:559:VAL:HG23	2.21	0.40
3:A:485:ASN:O	3:A:489:ILE:HG13	2.20	0.40
3:A:421:ASP:HB3	3:A:427:TYR:CE1	2.57	0.40
3:A:332:LYS:HE2	3:A:409:ALA:O	2.22	0.40
3:A:661:SER:OG	3:A:662:GLY:N	2.53	0.40
3:A:642:LYS:HA	3:A:642:LYS:HD3	1.96	0.40
3:A:313:MET:N	3:A:314:PRO:HD3	2.37	0.40
3:A:739:TYR:HD2	3:A:774:GLN:NE2	2.18	0.40
3:A:842:LEU:HA	3:A:842:LEU:HD13	1.93	0.40
3:A:825:PHE:CE1	3:A:829:ARG:NH2	2.90	0.40
3:A:682:TRP:HA	3:A:685:VAL:HG22	2.03	0.40
3:A:204:TRP:O	3:A:205:HIS:C	2.58	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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
3	A	858/878 (98%)	693 (81%)	123 (14%)	42 (5%)	<b>3</b> <b>10</b>

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	168	GLU
3	A	176	HIS
3	A	373	ALA
3	A	560	ASN
3	A	594	VAL
3	A	606	SER
3	A	611	LEU
3	A	857	GLN
3	A	859	ASP
3	A	862	PRO
3	A	863	ALA
3	A	151	PHE
3	A	372	GLU
3	A	602	THR
3	A	715	THR
3	A	104	GLN
3	A	169	GLN
3	A	174	VAL
3	A	177	VAL
3	A	178	TYR
3	A	270	PRO
3	A	312	TYR
3	A	350	GLU
3	A	508	PRO
3	A	631	LYS
3	A	861	MET
3	A	872	LEU
3	A	248	PRO
3	A	425	ARG
3	A	595	VAL
3	A	708	ALA
3	A	716	GLY
3	A	811	HIS
3	A	858	LEU
3	A	590	THR
3	A	588	ASN
3	A	625	VAL
3	A	629	VAL

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Mol	Chain	Res	Type
3	A	810	ILE
3	A	213	GLY
3	A	364	PRO
3	A	804	ILE

### 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	
3	A	714/724 (99%)	661 (93%)	53 (7%)	17	44

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	31	ARG
3	A	35	GLU
3	A	46	MET
3	A	99	ARG
3	A	131	ASN
3	A	163	LYS
3	A	164	LYS
3	A	183	MET
3	A	223	SER
3	A	245	GLU
3	A	249	GLU
3	A	265	SER
3	A	274	PRO
3	A	276	LYS
3	A	291	ARG
3	A	292	ARG
3	A	305	LEU
3	A	313	MET
3	A	335	LEU
3	A	351	ASP
3	A	370	ASN
3	A	375	THR

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Mol	Chain	Res	Type
3	A	394	ARG
3	A	400	PHE
3	A	404	GLN
3	A	410	ASN
3	A	419	ASN
3	A	422	TRP
3	A	423	ARG
3	A	426	VAL
3	A	448	LYS
3	A	459	TRP
3	A	471	ASP
3	A	473	VAL
3	A	487	GLU
3	A	514	PHE
3	A	523	HIS
3	A	537	ASP
3	A	598	THR
3	A	610	LYS
3	A	632	ARG
3	A	653	ASP
3	A	714	LYS
3	A	723	CYS
3	A	730	PRO
3	A	735	VAL
3	A	774	GLN
3	A	826	LYS
3	A	831	THR
3	A	852	GLN
3	A	853	LEU
3	A	854	HIS
3	A	879	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	22	ASN
3	A	27	HIS
3	A	86	ASN
3	A	131	ASN
3	A	165	ASN
3	A	169	GLN
3	A	171	ASN

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Mol	Chain	Res	Type
3	A	176	HIS
3	A	269	GLN
3	A	289	ASN
3	A	321	ASN
3	A	324	GLN
3	A	370	ASN
3	A	404	GLN
3	A	410	ASN
3	A	411	HIS
3	A	419	ASN
3	A	435	GLN
3	A	463	HIS
3	A	485	ASN
3	A	486	HIS
3	A	544	GLN
3	A	619	GLN
3	A	669	GLN
3	A	672	GLN
3	A	697	ASN
3	A	726	HIS
3	A	737	GLN
3	A	744	GLN
3	A	764	ASN
3	A	774	GLN
3	A	781	ASN
3	A	786	GLN
3	A	823	ASN
3	A	848	GLN
3	A	852	GLN
3	A	857	GLN
3	A	869	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](#)

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	T	18/22 (81%)	-0.00	2 (11%) <b>7</b> <b>4</b>	64, 72, 123, 136	0
2	P	14/14 (100%)	0.02	1 (7%) <b>19</b> <b>13</b>	53, 70, 106, 147	0
3	A	862/878 (98%)	0.55	75 (8%) <b>13</b> <b>8</b>	48, 81, 129, 149	0
All	All	894/914 (97%)	0.53	78 (8%) <b>13</b> <b>8</b>	48, 81, 129, 149	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	602	THR	10.7
3	A	180	LYS	9.1
3	A	598	THR	8.1
3	A	601	ASN	7.8
3	A	599	ASP	7.0
3	A	608	LYS	6.8
3	A	600	GLU	6.6
3	A	361	PRO	6.4
3	A	175	GLY	6.3
3	A	362	MET	6.2
3	A	607	GLU	5.8
3	A	368	ASP	5.6
3	A	603	GLY	5.6
3	A	374	LEU	5.5
3	A	606	SER	5.2
3	A	883	ALA	5.0
3	A	597	VAL	5.0
3	A	360	LEU	4.6
3	A	714	LYS	4.6
3	A	367	ILE	4.4
3	A	370	ASN	4.4
3	A	385	TYR	4.2
3	A	181	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
3	A	378	LYS	4.1
3	A	377	TRP	4.0
3	A	178	TYR	3.9
2	P	114	DT	3.8
3	A	166	VAL	3.8
3	A	169	GLN	3.8
3	A	177	VAL	3.6
3	A	168	GLU	3.6
3	A	853	LEU	3.4
3	A	849	PHE	3.4
3	A	235	GLY	3.4
3	A	363	LYS	3.4
3	A	766	ASP	3.3
3	A	171	ASN	3.3
3	A	174	VAL	3.3
3	A	375	THR	3.2
3	A	725	VAL	3.2
3	A	372	GLU	3.1
3	A	176	HIS	3.1
1	T	6	DT	3.0
3	A	369	MET	3.0
3	A	364	PRO	2.9
3	A	300	HIS	2.8
3	A	28	TYR	2.8
3	A	376	ALA	2.8
3	A	851	ASP	2.7
3	A	98	LYS	2.7
3	A	605	ILE	2.7
3	A	667	PHE	2.7
3	A	55	PHE	2.6
3	A	381	ALA	2.6
3	A	371	PRO	2.6
3	A	721	LYS	2.6
3	A	380	ALA	2.5
3	A	713	LYS	2.5
3	A	646	PHE	2.4
3	A	623	TYR	2.4
3	A	234	ALA	2.3
3	A	717	GLU	2.3
3	A	172	LYS	2.3
3	A	447	ALA	2.3
3	A	52	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	594	VAL	2.3
3	A	724	ALA	2.3
3	A	718	ILE	2.2
1	T	5	DC	2.2
3	A	267	MET	2.2
3	A	365	GLU	2.2
3	A	722	ARG	2.1
3	A	710	VAL	2.1
3	A	854	HIS	2.1
3	A	379	ARG	2.0
3	A	373	ALA	2.0
3	A	167	GLU	2.0
3	A	595	VAL	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.