



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:42 PM GMT

PDB ID : 1UUR  
Title : STRUCTURE OF AN ACTIVATED DICTYOSTELIUM STAT IN ITS DNA-  
UNBOUND FORM  
Authors : Soler-Lopez, M.; Petosa, C.; Fukuzawa, M.; Ravelli, R.; Williams, J.G.; Muller,  
C.W.  
Deposited on : 2004-01-09  
Resolution : 2.70 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

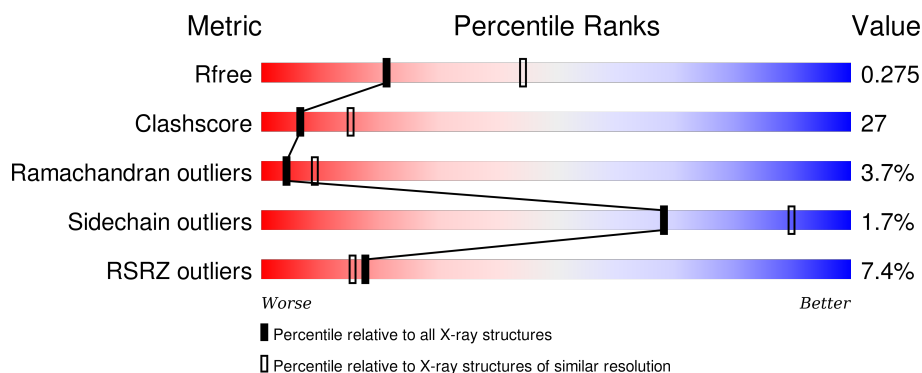
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	473	<div> <div>7%</div> <div>55%</div> <div>38%</div> <div>• •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3677 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 STATA PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	P	S	0	0	0
			3637	2322	626	676	1	12			

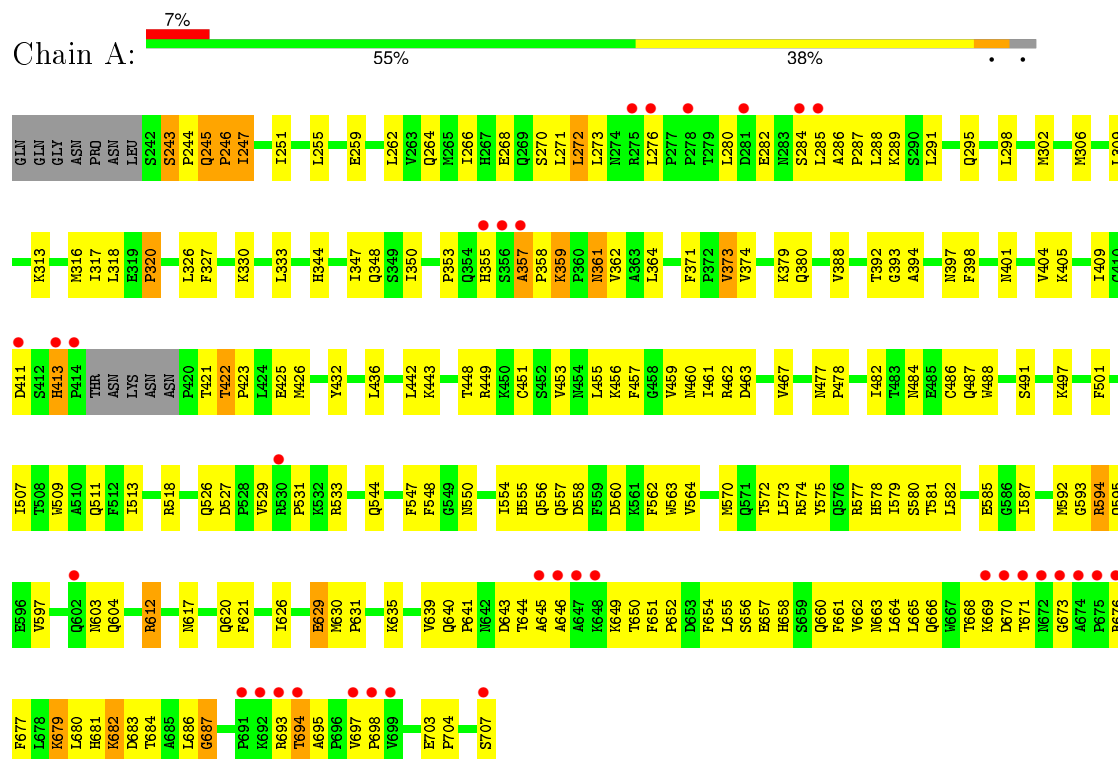
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: STATA PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.60 Å   144.00 Å   67.10 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.00-2.70) 96.0 (29.37-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 2.68 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.210   ,   0.270 0.222   ,   0.275	Depositor DCC
$R_{free}$ test set	792 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.0	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 71.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 15894 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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 [i](#)

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

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

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	0/3704	0.71	0/5022

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	413	HIS	Mainchain

### 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	3637	0	3623	198	0
2	A	40	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3677	0	3623	198	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 27.

All (198) 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:270:SER:HB2	2:A:2001:HOH:O	1.45	1.15
1:A:656:SER:HA	1:A:682:LYS:HE2	1.37	1.05
1:A:392:THR:HG22	1:A:393:GLY:H	1.23	1.01
1:A:656:SER:HA	1:A:682:LYS:CE	1.94	0.98
1:A:670:ASP:OD1	1:A:671:THR:N	2.00	0.93
1:A:270:SER:HB3	1:A:394:ALA:HB1	1.53	0.89
1:A:313:LYS:HB2	1:A:326:LEU:HD21	1.53	0.88
1:A:392:THR:HG22	1:A:393:GLY:N	1.90	0.87
1:A:526:GLN:HE22	1:A:533:ARG:H	1.23	0.86
1:A:425:GLU:HB3	1:A:443:LYS:HB3	1.58	0.86
1:A:666:GLN:OE1	1:A:680:LEU:HD11	1.74	0.86
1:A:526:GLN:NE2	1:A:533:ARG:H	1.74	0.85
1:A:459:VAL:HG23	1:A:461:ILE:HD11	1.58	0.85
1:A:276:LEU:HD11	1:A:288:LEU:HD11	1.58	0.85
1:A:693:ARG:NH1	1:A:697:VAL:HG22	1.95	0.81
1:A:604:GLN:HB2	1:A:626:ILE:HD12	1.63	0.79
1:A:404:VAL:HA	1:A:459:VAL:HG12	1.69	0.75
1:A:643:ASP:O	1:A:649:LYS:HD2	1.87	0.75
1:A:661:PHE:O	1:A:682:LYS:HD2	1.87	0.75
1:A:644:THR:HG23	1:A:649:LYS:O	1.86	0.74
1:A:704:PRO:HG2	1:A:707:SER:OXT	1.88	0.74
1:A:459:VAL:HG23	1:A:461:ILE:CD1	2.17	0.74
1:A:404:VAL:HG22	1:A:459:VAL:HG11	1.69	0.73
1:A:291:LEU:HD13	1:A:347:ILE:HD11	1.70	0.73
1:A:404:VAL:HG22	1:A:459:VAL:CG1	2.21	0.71
1:A:665:LEU:CD2	1:A:679:LYS:HG2	2.21	0.70
1:A:411:ASP:HA	1:A:413:HIS:CE1	2.25	0.70
1:A:597:VAL:HG21	1:A:612:ARG:HD2	1.74	0.70
1:A:409:ILE:HD12	1:A:456:LYS:HG3	1.71	0.69
1:A:286:ALA:N	1:A:287:PRO:HD2	2.06	0.69
1:A:693:ARG:CZ	1:A:697:VAL:HG22	2.22	0.69
1:A:655:LEU:O	1:A:682:LYS:HE3	1.93	0.69
1:A:392:THR:CG2	1:A:393:GLY:H	2.04	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD23	1:A:284:SER:OG	1.93	0.68
1:A:244:PRO:HG3	1:A:318:LEU:HD22	1.75	0.67
1:A:621:PHE:HB2	1:A:639:VAL:HG11	1.77	0.67
1:A:244:PRO:HG3	1:A:318:LEU:CD2	2.26	0.65
1:A:604:GLN:OE1	1:A:679:LYS:HE2	1.96	0.65
1:A:317:ILE:HG12	1:A:513:ILE:HD11	1.77	0.65
1:A:270:SER:CB	1:A:394:ALA:HB1	2.27	0.64
1:A:560:ASP:O	1:A:564:VAL:HG23	1.99	0.63
1:A:663:ASN:OD1	1:A:681:HIS:ND1	2.32	0.63
1:A:693:ARG:NH2	1:A:697:VAL:HA	2.14	0.63
1:A:285:LEU:HD22	1:A:288:LEU:HD12	1.81	0.62
1:A:662:VAL:O	1:A:682:LYS:HB3	1.98	0.62
1:A:262:LEU:O	1:A:266:ILE:HG13	2.00	0.62
1:A:581:THR:O	1:A:585:GLU:HG2	2.00	0.62
1:A:612:ARG:HG3	1:A:612:ARG:HH11	1.65	0.61
1:A:621:PHE:O	1:A:639:VAL:HG12	2.01	0.60
1:A:442:LEU:CD1	1:A:455:LEU:HD11	2.30	0.60
1:A:548:PHE:CD2	1:A:554:ILE:HG13	2.36	0.60
1:A:671:THR:O	1:A:671:THR:HG22	2.02	0.60
1:A:666:GLN:OE1	1:A:680:LEU:CD1	2.49	0.59
1:A:456:LYS:CG	2:A:2026:HOH:O	2.51	0.59
1:A:350:ILE:O	1:A:353:PRO:HD3	2.02	0.59
1:A:693:ARG:HH22	1:A:697:VAL:HG13	1.67	0.59
1:A:649:LYS:HD3	1:A:654:PHE:HB2	1.83	0.59
1:A:401:ASN:HD21	1:A:462:ARG:HB2	1.68	0.58
1:A:664:LEU:HD12	1:A:665:LEU:H	1.69	0.58
1:A:668:THR:HG22	1:A:669:LYS:N	2.19	0.58
1:A:432:TYR:O	1:A:436:LEU:N	2.37	0.58
1:A:573:LEU:O	1:A:580:SER:HB2	2.02	0.58
1:A:604:GLN:HB2	1:A:626:ILE:CD1	2.34	0.57
1:A:461:ILE:HD12	1:A:461:ILE:N	2.19	0.56
1:A:681:HIS:CD2	1:A:683:ASP:H	2.23	0.56
1:A:621:PHE:HB2	1:A:639:VAL:CG1	2.34	0.56
1:A:456:LYS:HD2	2:A:2026:HOH:O	2.04	0.56
1:A:509:TRP:CZ2	1:A:544:GLN:HB2	2.40	0.56
1:A:630:MET:HA	1:A:631:PRO:C	2.25	0.56
1:A:291:LEU:HD13	1:A:347:ILE:CD1	2.36	0.56
1:A:640:GLN:HB3	1:A:641:PRO:HD2	1.87	0.55
1:A:243:SER:C	1:A:245:GLN:H	2.09	0.55
1:A:656:SER:HA	1:A:682:LYS:HE3	1.85	0.55
1:A:663:ASN:OD1	1:A:681:HIS:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLN:HE22	1:A:533:ARG:N	1.99	0.54
1:A:603:ASN:O	1:A:603:ASN:OD1	2.25	0.54
1:A:665:LEU:HD21	1:A:679:LYS:HG2	1.88	0.54
1:A:501:PHE:HA	1:A:507:ILE:HG21	1.90	0.54
1:A:255:LEU:O	1:A:259:GLU:HB2	2.08	0.54
1:A:670:ASP:CG	1:A:671:THR:H	1.97	0.54
1:A:681:HIS:O	1:A:684:THR:N	2.40	0.54
1:A:693:ARG:HH21	1:A:698:PRO:CD	2.22	0.53
1:A:671:THR:C	1:A:673:GLY:H	2.12	0.53
1:A:617:ASN:HB3	1:A:620:GLN:NE2	2.24	0.53
1:A:527:ASP:O	1:A:531:PRO:HG3	2.09	0.53
1:A:693:ARG:NH2	1:A:697:VAL:HG13	2.24	0.53
1:A:286:ALA:N	1:A:287:PRO:CD	2.72	0.53
1:A:649:LYS:HE2	1:A:657:GLU:OE2	2.08	0.53
1:A:460:ASN:C	1:A:461:ILE:HD12	2.28	0.53
1:A:353:PRO:C	1:A:355:HIS:H	2.12	0.53
1:A:243:SER:N	1:A:244:PRO:CD	2.73	0.52
1:A:247:ILE:O	1:A:251:ILE:HG13	2.09	0.52
1:A:459:VAL:CG2	1:A:461:ILE:HD11	2.35	0.52
1:A:362:VAL:HG22	1:A:398:PHE:CE2	2.46	0.51
1:A:693:ARG:HH21	1:A:698:PRO:HD3	1.75	0.51
1:A:681:HIS:HD2	1:A:683:ASP:HB2	1.76	0.51
1:A:306:MET:HE1	1:A:330:LYS:HG3	1.93	0.51
1:A:641:PRO:O	1:A:644:THR:O	2.28	0.51
1:A:703:GLU:HB3	1:A:704:PRO:HD2	1.92	0.51
1:A:681:HIS:O	1:A:683:ASP:N	2.45	0.50
1:A:582:LEU:HD22	1:A:587:ILE:HG21	1.94	0.50
1:A:604:GLN:OE1	1:A:679:LYS:CE	2.59	0.50
1:A:658:HIS:C	1:A:660:GLN:H	2.14	0.50
1:A:405:LYS:O	1:A:457:PHE:HA	2.12	0.50
1:A:686:LEU:O	1:A:687:GLY:C	2.50	0.49
1:A:298:LEU:HG	1:A:302:MET:HE3	1.94	0.49
1:A:668:THR:O	1:A:676:ARG:N	2.39	0.49
1:A:482:ILE:HG22	1:A:491:SER:OG	2.12	0.49
1:A:572:THR:HG22	1:A:579:ILE:HG21	1.95	0.49
1:A:373:VAL:HG22	1:A:374:VAL:N	2.28	0.49
1:A:371:PHE:HB2	1:A:477:ASN:HB2	1.95	0.49
1:A:501:PHE:CE2	1:A:507:ILE:HG12	2.47	0.49
1:A:563:TRP:CZ3	1:A:570:MET:CE	2.95	0.49
1:A:693:ARG:NH2	1:A:698:PRO:HD2	2.28	0.48
1:A:272:LEU:HD23	1:A:288:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLU:O	1:A:426:MET:HB2	2.13	0.48
1:A:295:GLN:OE1	1:A:344:HIS:HA	2.14	0.48
1:A:612:ARG:HG3	1:A:612:ARG:NH1	2.29	0.48
1:A:582:LEU:O	1:A:587:ILE:HB	2.14	0.47
1:A:364:LEU:HD21	1:A:459:VAL:HG13	1.96	0.47
1:A:244:PRO:HB3	1:A:316:MET:CE	2.45	0.47
1:A:639:VAL:HG13	1:A:639:VAL:O	2.14	0.47
1:A:681:HIS:HD2	1:A:683:ASP:H	1.63	0.47
1:A:662:VAL:O	1:A:682:LYS:CB	2.63	0.47
1:A:592:MET:O	1:A:612:ARG:NH1	2.47	0.47
1:A:456:LYS:CD	2:A:2026:HOH:O	2.62	0.47
1:A:255:LEU:HD21	1:A:333:LEU:HD13	1.97	0.47
1:A:448:THR:HG21	1:A:451:CYS:O	2.15	0.46
1:A:442:LEU:HD11	1:A:455:LEU:HD11	1.98	0.46
1:A:544:GLN:HG2	1:A:550:ASN:HA	1.98	0.46
1:A:547:PHE:CD2	1:A:562:PHE:HA	2.51	0.46
1:A:286:ALA:H	1:A:287:PRO:HD2	1.79	0.45
1:A:597:VAL:CG2	1:A:612:ARG:HD2	2.44	0.45
1:A:401:ASN:ND2	1:A:462:ARG:HB2	2.30	0.45
1:A:456:LYS:CB	2:A:2026:HOH:O	2.64	0.45
1:A:271:LEU:C	1:A:273:LEU:H	2.20	0.45
1:A:326:LEU:O	1:A:326:LEU:HD12	2.16	0.45
1:A:421:THR:O	1:A:423:PRO:HD3	2.17	0.45
1:A:629:GLU:OE2	1:A:635:LYS:HD2	2.17	0.45
1:A:671:THR:CG2	1:A:671:THR:O	2.64	0.45
1:A:244:PRO:C	1:A:246:PRO:CD	2.85	0.45
1:A:555:HIS:CD2	1:A:557:GLN:H	2.35	0.45
1:A:270:SER:CA	1:A:394:ALA:HB1	2.46	0.45
1:A:640:GLN:CB	1:A:641:PRO:HD2	2.47	0.45
1:A:594:ARG:O	1:A:595:GLN:C	2.54	0.45
1:A:574:ARG:HG2	1:A:575:TYR:CD1	2.52	0.45
1:A:555:HIS:HD2	1:A:557:GLN:H	1.65	0.44
1:A:577:ARG:HG2	1:A:578:HIS:CD2	2.51	0.44
1:A:456:LYS:HG3	2:A:2026:HOH:O	2.17	0.44
1:A:650:THR:C	1:A:652:PRO:HD2	2.38	0.44
1:A:484:ASN:C	1:A:486:CYS:H	2.20	0.44
1:A:313:LYS:NZ	1:A:511:GLN:HE22	2.15	0.44
1:A:665:LEU:HD23	1:A:679:LYS:HG2	1.99	0.44
1:A:442:LEU:HD11	1:A:455:LEU:CD1	2.47	0.44
1:A:681:HIS:O	1:A:682:LYS:C	2.55	0.44
1:A:693:ARG:NH2	1:A:698:PRO:CD	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:CD2	1:A:288:LEU:HD23	2.48	0.43
1:A:448:THR:O	1:A:449:ARG:HB2	2.18	0.43
1:A:463:ASP:HB3	1:A:467:VAL:H	1.83	0.43
1:A:507:ILE:HB	1:A:511:GLN:HG2	2.00	0.43
1:A:487:GLN:O	1:A:488:TRP:C	2.57	0.43
1:A:285:LEU:O	1:A:289:LYS:HG3	2.18	0.43
1:A:643:ASP:O	1:A:649:LYS:CD	2.63	0.43
1:A:245:GLN:N	1:A:246:PRO:CD	2.82	0.43
1:A:694:THR:HG22	1:A:695:ALA:N	2.32	0.43
1:A:348:GLN:C	1:A:350:ILE:H	2.20	0.43
1:A:670:ASP:OD1	1:A:671:THR:CB	2.67	0.42
1:A:665:LEU:HD23	1:A:665:LEU:HA	1.83	0.42
1:A:644:THR:CG2	1:A:645:ALA:N	2.83	0.42
1:A:658:HIS:C	1:A:660:GLN:N	2.73	0.42
1:A:327:PHE:CE1	1:A:518:ARG:HD2	2.54	0.42
1:A:361:ASN:HD22	1:A:361:ASN:HA	1.56	0.42
1:A:555:HIS:HB3	1:A:558:ASP:OD2	2.20	0.42
1:A:264:GLN:O	1:A:268:GLU:HB2	2.20	0.42
1:A:357:ALA:C	1:A:359:LYS:H	2.23	0.42
1:A:697:VAL:HA	1:A:698:PRO:HD3	1.95	0.42
1:A:668:THR:CG2	1:A:669:LYS:N	2.82	0.42
1:A:662:VAL:HG12	1:A:663:ASN:N	2.35	0.41
1:A:593:GLY:O	1:A:597:VAL:HG23	2.19	0.41
1:A:422:THR:HA	1:A:423:PRO:HD2	1.87	0.41
1:A:309:LEU:HD22	1:A:326:LEU:HD13	2.02	0.41
1:A:670:ASP:O	1:A:673:GLY:N	2.54	0.41
1:A:630:MET:CE	1:A:631:PRO:HA	2.50	0.41
1:A:578:HIS:O	1:A:582:LEU:HG	2.20	0.41
1:A:651:PHE:N	1:A:652:PRO:HD2	2.35	0.41
1:A:453:VAL:O	1:A:478:PRO:HA	2.20	0.41
1:A:388:VAL:HG21	1:A:457:PHE:CD2	2.55	0.41
1:A:563:TRP:CH2	1:A:570:MET:CE	3.04	0.40
1:A:448:THR:HG22	1:A:448:THR:O	2.20	0.40
1:A:644:THR:HG22	1:A:645:ALA:N	2.35	0.40
1:A:244:PRO:O	1:A:246:PRO:N	2.54	0.40
1:A:554:ILE:N	1:A:554:ILE:CD1	2.84	0.40
1:A:630:MET:SD	1:A:631:PRO:HA	2.61	0.40
1:A:650:THR:O	1:A:651:PHE:C	2.60	0.40
1:A:497:LYS:HD3	1:A:556:GLN:HE21	1.87	0.40
1:A:557:GLN:HA	1:A:560:ASP:OD2	2.21	0.40
1:A:529:VAL:C	1:A:531:PRO:HD3	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LYS:HG2	1:A:380:GLN:N	2.36	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	456/473 (96%)	396 (87%)	43 (9%)	17 (4%)	<b>4</b> <b>9</b>

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	GLU
1	A	357	ALA
1	A	358	PRO
1	A	594	ARG
1	A	646	ALA
1	A	246	PRO
1	A	359	LYS
1	A	682	LYS
1	A	694	THR
1	A	687	GLY
1	A	272	LEU
1	A	679	LYS
1	A	247	ILE
1	A	373	VAL
1	A	245	GLN
1	A	243	SER
1	A	320	PRO

### 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	401/420 (96%)	394 (98%)	7 (2%)	68 90

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

Mol	Chain	Res	Type
1	A	320	PRO
1	A	361	ASN
1	A	397	ASN
1	A	422	THR
1	A	612	ARG
1	A	629	GLU
1	A	677	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
1	A	301	GLN
1	A	334	GLN
1	A	348	GLN
1	A	361	ASN
1	A	401	ASN
1	A	429	GLN
1	A	466	ASN
1	A	487	GLN
1	A	511	GLN
1	A	519	HIS
1	A	526	GLN
1	A	546	HIS
1	A	550	ASN
1	A	555	HIS
1	A	556	GLN
1	A	576	GLN
1	A	603	ASN

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Mol	Chain	Res	Type
1	A	620	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PTR	A	702	1	14,16,17	0.85	0	18,22,24	0.91	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	702	1	-	0/9/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	PTR	O-C-CA	-2.06	120.12	125.49
1	A	702	PTR	O3P-P-OH	2.18	113.05	105.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	460/473 (97%)	0.13	34 (7%) 17 15	21, 60, 126, 161	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	SER	7.3
1	A	673	GLY	6.7
1	A	692	LYS	6.1
1	A	672	ASN	4.8
1	A	670	ASP	4.5
1	A	674	ALA	4.4
1	A	691	PRO	4.3
1	A	285	LEU	4.3
1	A	675	PRO	4.1
1	A	356	SER	4.1
1	A	693	ARG	3.7
1	A	357	ALA	3.7
1	A	671	THR	3.5
1	A	278	PRO	3.5
1	A	413	HIS	3.4
1	A	648	LYS	3.1
1	A	355	HIS	2.8
1	A	414	PRO	2.7
1	A	411	ASP	2.7
1	A	697	VAL	2.6
1	A	694	THR	2.5
1	A	647	ALA	2.5
1	A	530	ARG	2.4
1	A	669	LYS	2.4
1	A	645	ALA	2.4
1	A	284	SER	2.3
1	A	281	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	276	LEU	2.3
1	A	698	PRO	2.3
1	A	646	ALA	2.2
1	A	676	ARG	2.2
1	A	275	ARG	2.1
1	A	699	VAL	2.0
1	A	602	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	PTR	A	702	16/17	0.97	0.14	-	45,63,72,77	0

## 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.