

Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 07:40 PM EDT

:	1Q4K
:	The polo-box domain of Plk1 in complex with a phospho-peptide
:	Cheng, K.; Lowe, E.D.; Sinclair, J.; Nigg, E.A.; Johnson, L.N.
:	2003-08-04
:	2.30 Å(reported)
	::

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
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)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	٨	050	7%			_	
	A	259	64%	18%	•	14%	
	-		3%				
1	В	259	63%	20%	•	14%	
			8%				
1	С	259	59%	21%	•	17%	
2	D	6	50%	50%			
2	Ε	6	67%		33%		



Mol	Chain	Length	Quality of chain			
			17%			
2	\mathbf{F}	6	33%	33%	33%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5707 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	В	P 994		С	Ν	0	\mathbf{S}	0	0	0
	D	224	1822	1153	317	341	11	0	0	0
1	Λ	າາາ	Total	С	Ν	0	S	0	0	0
	A		1803	1143	312	337	11	0		
1	C	214	Total	С	Ν	0	S	0	0	0
			1744	1108	300	325	11	0	0	

• Molecule 1 is a protein called Serine/threonine-protein kinase PLK.

• Molecule 2 is a protein called Phospho-peptide sequence Met.Gln.Ser.pThr.Pro.Leu.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace				
0	р	6	Total	С	Ν	0	Р	S	0	0	0	
	D	0	49	28	7 12 1 1 0	0	0	0				
0	Б	6	Total	С	Ν	Ο	Р	S	0	0 0 0	0	0
		0	49	28	7	12	1	1		0	0	
0	Б	6	Total	С	Ν	0	Р	S	0	0	0	
		0	49	28	$\overline{7}$	12	1	1	0	0	0	

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	78	Total O 78 78	0	0
3	А	55	Total O 55 55	0	0
3	С	43	Total O 43 43	0	0
3	D	2	Total O 2 2	0	0
3	Е	8	Total O 8 8	0	0
3	F	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0





CYS GLY GLU GLU GLU PRO PRO PRO PRO PRO PRO CEU

3 Residue-property plots (i)

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.



• Molecule 1: Serine/threonine-protein kinase PLK



8450 8455 8455 8455 8455 0457 7462 7462 7463 7465	P4900 N470 S471 S471 S471 S475 M473 K474 T477 L478 L478 L478 C480 Y480	F482 R483 N484 V485 L490 L491 K492 A493 G494 G493 G493	ASN THR PRO PRO GLY GLY ESO ESO A	L508 R518 S519 1522 H523	V530 Q531 1532 N533
0536 0537 1538 1538 1541 1541 1541 1543 1543 1551	1653 1657 1658 1658 1658 1658 1658 1658 1658 1688 1888	M586 V587 D588 K589 K589 L590 L591 S593 S593 ARG SER ALA	SER ASN ARG LEU LEU LYS ALA SER		
• Molecule 2: P	'hospho-peptide se	quence Met.Gh	n.Ser.pThr.Pro	.Leu	
Chain D:	50%		50%		
M1 83 74 75 14 14					
• Molecule 2: P	'hospho-peptide se	quence Met.Gl	n.Ser.pThr.Pro	.Leu	
Chain E:	67%		<u>-</u>	33%	
M 22 25 14 14 14					
• Molecule 2: P	'hospho-peptide se	quence Met.Gh	n.Ser.pThr.Pro	.Leu	
17	%				
Chain F:	33%	33%	33	3%	
<mark>M 333 22 44 14 14 14 14 14 14 14 14 14 14 14 14 </mark>					



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	57.07Å 56.89 Å 85.05 Å	Deperitor
a, b, c, α , β , γ	91.45° 103.21° 118.50°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	29.36 - 2.30	Depositor
Resolution (A)	29.31 - 2.30	EDS
% Data completeness	96.2 (29.36-2.30)	Depositor
(in resolution range)	96.2 (29.31-2.30)	EDS
R _{merge}	0.07	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	4.04 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
D D	0.245 , 0.312	Depositor
Γ, Γ_{free}	0.237 , 0.293	DCC
R_{free} test set	1943 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	41.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.36 , 48.0	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.019 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5707	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: TPO

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).

Mal	Mal Chain		lengths	Bond angles		
WIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.58	0/1841	0.85	6/2489~(0.2%)	
1	В	0.59	0/1860	0.88	9/2514~(0.4%)	
1	С	0.47	0/1780	0.80	5/2404~(0.2%)	
2	D	0.56	0/37	0.76	0/46	
2	Е	0.75	0/37	1.13	0/46	
2	F	0.60	0/37	0.68	0/46	
All	All	0.55	0/5592	0.84	20/7545~(0.3%)	

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	А	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	В	537	ASP	CB-CG-OD2	6.85	124.46	118.30
1	С	376	ASP	CB-CG-OD2	6.68	124.31	118.30
1	В	554	ASP	CB-CG-OD2	6.46	124.12	118.30
1	А	537	ASP	CB-CG-OD2	6.37	124.03	118.30
1	С	416	ASP	CB-CG-OD2	6.29	123.96	118.30
1	С	588	ASP	CB-CG-OD2	6.00	123.70	118.30
1	В	503	ASP	CB-CG-OD2	5.84	123.56	118.30
1	А	558	ASP	CB-CG-OD2	5.81	123.53	118.30
1	В	371	ASP	CB-CG-OD2	5.71	123.44	118.30
1	В	558	ASP	CB-CG-OD2	5.66	123.40	118.30



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	457	ASP	CB-CG-OD2	5.65	123.38	118.30
1	В	376	ASP	CB-CG-OD2	5.61	123.35	118.30
1	С	503	ASP	CB-CG-OD2	5.44	123.20	118.30
1	В	588	ASP	CB-CG-OD1	5.38	123.15	118.30
1	А	573	CYS	CB-CA-C	-5.28	99.84	110.40
1	В	438	ASP	CB-CG-OD2	5.21	122.99	118.30
1	А	517	THR	N-CA-C	5.17	124.95	111.00
1	С	558	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	449	ASP	CB-CG-OD2	5.05	122.85	118.30
1	В	457	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	517	THR	Peptide
1	А	572	CYS	Peptide

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	А	1803	0	1789	35	1
1	В	1822	0	1806	27	1
1	С	1744	0	1730	29	1
2	D	49	0	48	2	0
2	Е	49	0	48	1	0
2	F	49	0	48	3	0
3	А	55	0	0	1	0
3	В	78	0	0	6	1
3	С	43	0	0	3	0
3	D	2	0	0	0	0
3	Е	8	0	0	0	0
3	F	5	0	0	0	0
All	All	5707	0	5469	90	2

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 8.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:463:LEU:HD21	1:A:469:PRO:HD2	1.54	0.89	
1:B:517:THR:C	3:B:36:HOH:O	2.16	0.82	
1:A:493:ALA:O	3:A:21:HOH:O	2.04	0.75	
1:B:432:VAL:HG12	1:B:479:LEU:HD11	1.69	0.74	
1:A:384:VAL:HA	1:A:568:GLU:HG2	1.72	0.71	
1:C:537:ASP:HB3	1:C:539:THR:HG23	1.71	0.70	
1:B:531:GLN:HE21	1:B:533:ASN:HD21	1.41	0.69	
1:B:416:ASP:OD2	1:B:516:ARG:NH1	2.27	0.67	
1:A:463:LEU:HD21	1:A:469:PRO:CD	2.25	0.66	
1:A:518:ARG:NE	1:A:518:ARG:H	1.93	0.66	
1:C:374:LEU:HD21	1:C:524:HIS:ND1	2.11	0.66	
1:A:377:MET:CE	1:A:543:LEU:HD13	2.29	0.63	
1:A:432:VAL:HG12	1:A:479:LEU:HD11	1.82	0.61	
1:B:377:MET:CE	1:B:543:LEU:HD13	2.29	0.61	
1:C:476:ILE:O	1:C:480:LYS:HG3	2.00	0.60	
1:C:377:MET:CE	1:C:543:LEU:HD13	2.31	0.60	
1:A:531:GLN:HE21	1:A:533:ASN:HD21	1.49	0.60	
1:A:377:MET:HE1	1:A:543:LEU:HB2	1.84	0.59	
1:B:407:PRO:HD3	1:B:551:THR:HG21	1.86	0.58	
1:A:522:ILE:N	1:A:522:ILE:HD12	2.19	0.57	
1:A:567:LEU:HD22	1:A:572:CYS:HB3	1.90	0.54	
1:A:435:LEU:HD13	1:A:441:ARG:HD3	1.89	0.54	
1:B:434:VAL:HG12	1:B:479:LEU:HD13	1.90	0.54	
1:B:534:PHE:CE1	1:B:579:ARG:HD2	2.43	0.54	
1:C:531:GLN:HE21	1:C:533:ASN:HD21	1.55	0.54	
1:A:573:CYS:HB3	1:A:576:LEU:H	1.74	0.53	
1:C:377:MET:HE2	1:C:587:VAL:HG21	1.91	0.53	
1:A:485:TYR:OH	2:D:2:GLN:NE2	2.43	0.52	
1:C:586:MET:HA	1:C:586:MET:CE	2.39	0.52	
1:B:468:HIS:N	1:B:468:HIS:ND1	2.57	0.52	
1:A:518:ARG:H	1:A:518:ARG:CD	2.19	0.52	
1:B:469:PRO:HD2	3:B:23:HOH:O	2.09	0.52	
1:B:377:MET:HE3	1:B:543:LEU:HD13	1.92	0.52	
1:A:463:LEU:CD2	1:A:469:PRO:HD2	2.35	0.51	
1:C:485:TYR:OH	2:F:2:GLN:NE2	2.44	0.51	
1:C:585:THR:HG21	3:C:73:HOH:O	2.10	0.51	
1:B:377:MET:SD	1:B:530:VAL:HG13	2.51	0.50	
1:C:522:ILE:HG12	1:C:586:MET:HG2	1.93	0.50	



	A h C	Interatomic	Clash		
Atom-1	Atom-2	distance (\AA)	overlap (Å)		
1:B:518:ARG:N	3:B:36:HOH:O	2.43	0.49		
1:A:377:MET:HE3	1:A:543:LEU:HD13	1.95	0.49		
1:B:575:GLU:O	1:B:579:ARG:HG2	2.12	0.49		
1:A:497:ILE:HG13	1:A:559:PHE:CD1	2.48	0.49		
1:C:374:LEU:HD21	1:C:524:HIS:CE1	2.48	0.48		
1:B:373:HIS:CD2	1:B:546:LEU:HD21	2.49	0.48		
1:A:466:SER:O	1:A:467:SER:CB	2.62	0.47		
1:A:429:ASP:O	1:A:430:ASN:HB2	2.14	0.47		
1:A:432:VAL:HG21	1:A:483:ARG:HG3	1.95	0.47		
1:B:377:MET:HE2	1:B:587:VAL:HG21	1.95	0.47		
1:B:432:VAL:HG12	1:B:479:LEU:CD1	2.42	0.47		
1:C:414:TRP:CD1	2:F:3:SER:HB3	2.49	0.47		
1:C:415:VAL:HG21	1:C:482:PHE:HD2	1.80	0.47		
1:B:485:TYR:OH	2:E:2:GLN:NE2	2.46	0.47		
1:C:575:GLU:O	1:C:579:ARG:HG2	2.16	0.46		
1:C:522:ILE:HG12	1:C:586:MET:CG	2.46	0.46		
1:C:407:PRO:CD	1:C:551:THR:HG21	2.46	0.45		
1:C:477:THR:HA	1:C:480:LYS:HE3	1.99	0.45		
1:C:463:LEU:N	1:C:463:LEU:HD12	2.31	0.45		
1:B:593:SER:HB2	3:B:55:HOH:O	2.15	0.45		
1:C:413:LYS:HD3	1:C:490:LEU:HB2	1.98	0.45		
1:A:432:VAL:HG21	1:A:483:ARG:CG	2.47	0.45		
1:B:373:HIS:NE2	1:B:546:LEU:HD21	2.32	0.44		
1:C:540:LYS:NZ	2:F:4:TPO:O1P	2.49	0.44		
1:A:384:VAL:HA	1:A:568:GLU:CG	2.46	0.44		
1:C:553:ILE:HD11	1:C:559:PHE:CE1	2.53	0.44		
1:B:468:HIS:HA	3:B:23:HOH:O	2.18	0.43		
1:A:466:SER:O	1:A:466:SER:OG	2.32	0.43		
1:B:518:ARG:NH1	1:A:568:GLU:O	2.48	0.42		
1:A:377:MET:HE1	1:A:543:LEU:CB	2.49	0.42		
1:B:567:LEU:HD22	1:B:572:CYS:HB3	2.01	0.42		
1:A:377:MET:SD	1:A:530:VAL:HG13	2.59	0.42		
1:C:382:HIS:ND1	1:C:584:ARG:NH2	2.68	0.42		
1:C:503:ASP:O	1:C:505:LEU:N	2.44	0.42		
1:C:503:ASP:C	1:C:504:GLU:HG3	2.40	0.42		
1:C:586:MET:HA	1:C:586:MET:HE2	2.01	0.42		
1:B:464:THR:O	1:B:467:SER:O	2.38	0.41		
1:A:407:PRO:CD	1:A:551:THR:HG21	2.50	0.41		
1:A:415:VAL:HG23	1:A:415:VAL:O	2.19	0.41		
1:C:377:MET:SD	1:C:530:VAL:HG13	2.60	0.41		
1:C:432:VAL:HG12	1:C:479:LEU:CD1	2.50	0.41		



Atom-1	Atom-2	Interatomic $distance (\hat{\lambda})$	Clash
		distance (A)	overlap (A)
1:B:512:ARG:HB2	1:B:524:HIS:CD2	2.55	0.41
1:A:575:GLU:OE1	1:A:579:ARG:NH2	2.54	0.41
1:A:408:ILE:HD13	1:A:500:ARG:CG	2.51	0.41
1:A:435:LEU:HD13	1:A:441:ARG:HH11	1.86	0.41
1:A:522:ILE:N	1:A:522:ILE:CD1	2.83	0.41
1:C:551:THR:HG22	3:C:46:HOH:O	2.20	0.41
1:A:414:TRP:CD1	2:D:3:SER:HB3	2.56	0.40
1:C:504:GLU:OE1	3:C:3:HOH:O	2.22	0.40
1:A:407:PRO:HD3	1:A:551:THR:HG21	2.02	0.40
1:B:524:HIS:CD2	1:B:524:HIS:C	2.95	0.40
1:B:581:ARG:NH1	3:B:58:HOH:O	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:C:589:LYS:NZ	3:B:13:HOH:O[1_554]	1.91	0.29	
1:B:419:ASP:OD2	1:A:445:TYR:OH[1_455]	2.19	0.01	

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	Perce	entiles
1	А	220/259~(85%)	206 (94%)	11 (5%)	3~(1%)	11	11
1	В	222/259~(86%)	206~(93%)	15 (7%)	1 (0%)	29	35
1	С	210/259~(81%)	198 (94%)	11 (5%)	1 (0%)	29	35
2	D	3/6~(50%)	3~(100%)	0	0	100	100
2	Ε	3/6~(50%)	3~(100%)	0	0	100	100
2	\mathbf{F}	3/6~(50%)	3~(100%)	0	0	100	100
All	All	661/795~(83%)	619 (94%)	37~(6%)	5(1%)	19	23



All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	467	SER
1	А	504	GLU
1	А	573	CYS
1	С	504	GLU
1	В	504	GLU

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Pe	erce	entiles
1	А	201/234~(86%)	182 (90%)	19 (10%)		8	10
1	В	203/234~(87%)	177~(87%)	26 (13%)		4	4
1	С	195/234~(83%)	172~(88%)	23~(12%)		5	5
2	D	5/5~(100%)	5~(100%)	0	1	00	100
2	Ε	5/5~(100%)	5~(100%)	0	1	00	100
2	F	5/5 (100%)	3(60%)	2(40%)		0	0
All	All	614/717~(86%)	544 (89%)	70 (11%)		5	6

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	371	ASP
1	В	372	CYS
1	В	379	GLN
1	В	383	SER
1	В	412	SER
1	В	423	LEU
1	В	427	LEU
1	В	434	VAL
1	В	435	LEU
1	В	441	ARG
1	В	456	ARG
1	В	467	SER



1 B 468 HIS 1 B 470 ASN 1 B 474 LYS 1 B 483 ARG 1 B 492 LYS 1 B 518 ARG 1 B 541 LEU 1 B 551 THR 1 B 554 ASP 1 B 584 ARG 1 B 591 LEU 1 B 593 SER 1 B 594 ARG 1 A 420 LYS 1 A 420 LYS 1 A 427 LEU 1 A 463 LEU 1 A 463 LEU 1 A 463 LEU 1 A 512 ARG 1 A 518 ARG 1 A 556 LYS 1	Mol	Chain	Res	Type
1 B 470 ASN 1 B 474 LYS 1 B 483 ARG 1 B 492 LYS 1 B 518 ARG 1 B 541 LEU 1 B 551 THR 1 B 554 ASP 1 B 584 ARG 1 B 591 LEU 1 B 593 SER 1 B 594 ARG 1 B 594 ARG 1 A 420 LYS 1 A 420 LYS 1 A 427 LEU 1 A 463 LEU 1 A 473 MET 1 A 503 ASP 1 A 512 ARG 1 A 518 ARG 1 A 558 ASP 1	1	В	468	HIS
1 B 474 LYS 1 B 483 ARG 1 B 518 ARG 1 B 518 ARG 1 B 541 LEU 1 B 551 THR 1 B 554 ASP 1 B 584 ARG 1 B 591 LEU 1 B 593 SER 1 B 594 ARG 1 B 594 ARG 1 A 420 LYS 1 A 427 LEU 1 A 441 ARG 1 A 443 LEU 1 A 463 LEU 1 A 473 MET 1 A 503 ASP 1 A 512 ARG 1 A 518 ARG 1 A 558 ASP 1	1	В	470	ASN
1 B 483 ARG 1 B 518 ARG 1 B 541 LEU 1 B 551 THR 1 B 554 ASP 1 B 554 ASP 1 B 584 ARG 1 B 593 SER 1 B 593 SER 1 B 594 ARG 1 B 593 SER 1 B 594 ARG 1 A 420 LYS 1 A 420 LYS 1 A 421 ARG 1 A 443 LEU 1 A 443 LEU 1 A 463 LEU 1 A 463 LEU 1 A 503 ASP 1 A 512 ARG 1 A 556 LYS 1	1	В	474	LYS
1 B 492 LYS 1 B 518 ARG 1 B 541 LEU 1 B 551 THR 1 B 554 ASP 1 B 585 THR 1 B 593 SER 1 B 594 ARG 1 B 593 SER 1 B 594 ARG 1 A 420 LYS 1 A 420 LYS 1 A 421 LEU 1 A 427 LEU 1 A 427 LEU 1 A 463 LEU 1 A 463 LEU 1 A 503 ASP 1 A 512 ARG 1 A 513 THR 1 A 556 LYS 1 A 558 ASP 1	1	В	483	ARG
1 B 518 ARG 1 B 541 LEU 1 B 551 THR 1 B 554 ASP 1 B 584 ARG 1 B 591 LEU 1 B 593 SER 1 B 594 ARG 1 B 593 SER 1 B 594 ARG 1 A 420 LYS 1 A 427 LEU 1 A 463 LEU 1 A 463 LEU 1 A 463 LEU 1 A 503 ASP 1 A 503 ASP 1 A 512 ARG 1 A 556 LYS 1 A 558 ASP 1 A 578<	1	В	492	LYS
1 B 541 LEU 1 B 551 THR 1 B 554 ASP 1 B 584 ARG 1 B 585 THR 1 B 591 LEU 1 B 593 SER 1 B 594 ARG 1 A 420 LYS 1 A 427 LEU 1 A 421 LEU 1 A 421 LEU 1 A 423 LEU 1 A 463 LEU 1 A 463 LEU 1 A 503 ASP 1 A 503 ASP 1 A 512 ARG 1 A 518 ARG 1 A 556 LYS 1 A 578<	1	В	518	ARG
1 B 551 THR 1 B 554 ASP 1 B 584 ARG 1 B 591 LEU 1 B 591 LEU 1 B 593 SER 1 B 594 ARG 1 A 420 LYS 1 A 427 LEU 1 A 427 LEU 1 A 441 ARG 1 A 427 LEU 1 A 463 LEU 1 A 463 LEU 1 A 463 LEU 1 A 503 ASP 1 A 512 ARG 1 A 518 ARG 1 A 556 LYS 1 A 556 LYS 1 A 573 CYS 1 A 584 ARG <th>1</th> <th>В</th> <th>541</th> <th>LEU</th>	1	В	541	LEU
1 B 554 ASP 1 B 584 ARG 1 B 591 LEU 1 B 593 SER 1 B 594 ARG 1 B 594 ARG 1 A 420 LYS 1 A 427 LEU 1 A 441 ARG 1 A 441 ARG 1 A 463 LEU 1 A 503 ASP 1 A 512 ARG 1 A 518 ARG 1 A 556 LYS 1 A 558 ASP 1 A 578 SER 1 A 584 ARG <th>1</th> <th>В</th> <th>551</th> <th>THR</th>	1	В	551	THR
1 B 584 ARG 1 B 591 LEU 1 B 593 SER 1 B 593 SER 1 B 594 ARG 1 A 420 LYS 1 A 427 LEU 1 A 427 LEU 1 A 441 ARG 1 A 463 LEU 1 A 463 LEU 1 A 463 LEU 1 A 463 LEU 1 A 503 ASP 1 A 503 ASP 1 A 512 ARG 1 A 518 ARG 1 A 556 LYS 1 A 558 ASP 1 A 578 SER 1 A 585 THR 1 A 585 THR 1	1	В	554	ASP
1 B 585 THR 1 B 591 LEU 1 B 593 SER 1 B 594 ARG 1 A 420 LYS 1 A 427 LEU 1 A 441 ARG 1 A 441 ARG 1 A 443 LEU 1 A 463 LEU 1 A 463 LEU 1 A 463 LEU 1 A 491 LEU 1 A 503 ASP 1 A 512 ARG 1 A 518 ARG 1 A 556 LYS 1 A 558 ASP 1 A 560 ARG 1 A 573 CYS 1 A 585 THR 1 A 585 THR 1	1	В	584	ARG
1B591LEU1B593SER1B594ARG1A420LYS1A427LEU1A441ARG1A443LEU1A463LEU1A473MET1A491LEU1A503ASP1A512ARG1A518ARG1A551THR1A556LYS1A558ASP1A560ARG1A573CYS1A578SER1A591LEU1A591LEU1C392ARG1C398GLU1C423LEU1C423LEU1C427LEU1C427LEU1C423LEU1C427LEU1C427LEU1C427LEU1C427LEU1C427LEU1C427LEU1C427LEU1C427LEU1C427LEU1C427LEU1C <th>1</th> <th>В</th> <th>585</th> <th>THR</th>	1	В	585	THR
1 B 593 SER 1 B 594 ARG 1 A 420 LYS 1 A 427 LEU 1 A 441 ARG 1 A 443 LEU 1 A 463 LEU 1 A 463 LEU 1 A 463 MET 1 A 473 MET 1 A 503 ASP 1 A 503 ASP 1 A 503 ASP 1 A 512 ARG 1 A 556 LYS 1 A 556 LYS 1 A 560 ARG 1 A 573 CYS 1 A 585 THR 1 A 585 THR 1 A 591 LEU 1 C 398 GLU 1	1	В	591	LEU
1B 594 ARG1A 420 LYS1A 427 LEU1A 441 ARG1A 463 LEU1A 463 LEU1A 473 MET1A 491 LEU1A 503 ASP1A 512 ARG1A 512 ARG1A 518 ARG1A 556 LYS1A 556 LYS1A 556 LYS1A 560 ARG1A 573 CYS1A 578 SER1A 585 THR1A 591 LEU1C 392 ARG1C 398 GLU1C 420 LYS1C 420 LYS1C 423 LEU1C 427 LEU1C 427 LEU1C 427 LEU1C 420 SER1C 420 SER1C 420 SER1C 420 SER1C 420 SER1C 420 SER1C 474 SER	1	В	593	SER
1A420LYS1A427LEU1A441ARG1A463LEU1A473MET1A491LEU1A503ASP1A512ARG1A512ARG1A518ARG1A556LYS1A556LYS1A558ASP1A560ARG1A573CYS1A578SER1A584ARG1A591LEU1C392ARG1C398GLU1C420LYS1C423LEU1C423LEU1C427LEU1C449ASP1C449ASP1C450SER1C474LYS	1	В	594	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	420	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	427	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	441	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	463	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	473	MET
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	491	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	503	ASP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	512	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	518	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	536	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	551	THR
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	А	556	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	558	ASP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	560	ARG
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	А	573	CYS
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	А	578	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	584	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	585	THR
1 C 392 ARG 1 C 398 GLU 1 C 412 SER 1 C 420 LYS 1 C 423 LEU 1 C 427 LEU 1 C 449 ASP 1 C 450 SER 1 C 474 LYS	1	A	591	LEU
1 C 398 GLU 1 C 412 SER 1 C 420 LYS 1 C 423 LEU 1 C 427 LEU 1 C 449 ASP 1 C 450 SER 1 C 474 LYS	1	С	392	ARG
1 C 412 SER 1 C 420 LYS 1 C 423 LEU 1 C 427 LEU 1 C 449 ASP 1 C 450 SER 1 C 474 LYS	1	С	398	GLU
1 C 420 LYS 1 C 423 LEU 1 C 427 LEU 1 C 449 ASP 1 C 450 SER 1 C 474 LYS	1	С	412	SER
1 C 423 LEU 1 C 427 LEU 1 C 449 ASP 1 C 450 SER 1 C 474 LYS	1	С	420	LYS
1 C 427 LEU 1 C 449 ASP 1 C 450 SER 1 C 474 LYS	1	С	423	LEU
1 C 449 ASP 1 C 450 SER 1 C 474 LYS	1	С	427	LEU
1 C 450 SER 1 C 474 LYS	1	С	449	ASP
1 C 474 LYS	1	С	450	SER
	1	С	474	LYS



Mol	Chain	Res	Type
1	С	483	ARG
1	С	492	LYS
1	С	504	GLU
1	С	508	LEU
1	С	518	ARG
1	С	519	SER
1	С	537	ASP
1	С	541	LEU
1	С	551	THR
1	С	574	LYS
1	С	584	ARG
1	C	586	MET
1	С	591	LEU
1	C	593	SER
2	F	1	MET
2	F	2	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	489	HIS
1	В	524	HIS
1	В	533	ASN
1	А	524	HIS
1	А	533	ASN
1	С	468	HIS
1	С	524	HIS
1	С	533	ASN
2	D	2	GLN
2	Е	2	GLN
2	F	2	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are 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).

Mal Trma Cl		Chain	Dec	Tink	B	Bond lengths			Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	TPO	Е	4	2	8,10,11	3.19	4 (50%)	10,14,16	2.68	4 (40%)	
2	TPO	F	4	2	8,10,11	3.57	4 (50%)	10,14,16	2.83	3 (30%)	
2	TPO	D	4	2	8,10,11	3.43	4 (50%)	10,14,16	2.80	5 (50%)	

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
2	TPO	Е	4	2	-	0/9/11/13	-
2	TPO	F	4	2	-	1/9/11/13	-
2	TPO	D	4	2	-	2/9/11/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	TPO	P-01P	6.20	1.70	1.50
2	D	4	TPO	P-01P	5.80	1.69	1.50
2	F	4	TPO	O-C	5.65	1.42	1.19
2	Е	4	TPO	O-C	5.62	1.42	1.19
2	D	4	TPO	O-C	5.54	1.42	1.19
2	Ε	4	TPO	P-O1P	5.10	1.67	1.50
2	F	4	TPO	P-O3P	3.89	1.69	1.54
2	F	4	TPO	P-O2P	3.71	1.69	1.54
2	D	4	TPO	P-O2P	3.68	1.69	1.54
2	D	4	TPO	P-O3P	3.55	1.68	1.54
2	Е	4	TPO	P-O3P	3.51	1.68	1.54
2	E	4	TPO	P-O2P	3.34	1.67	1.54

All (12) bond angle outliers are listed below:

2 F 4 TPO O2P-P-OG1 -6.26 77.96 105.9	Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
	2	F	4	TPO	O2P-P-OG1	-6.26	77.96	105.99



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	D	4	TPO	O2P-P-OG1	-5.36	81.96	105.99
2	Ε	4	TPO	O3P-P-O2P	4.83	126.10	107.64
2	F	4	TPO	O3P-P-O2P	4.45	124.63	107.64
2	D	4	TPO	O-C-CA	-4.16	113.87	124.78
2	Ε	4	TPO	O2P-P-OG1	-4.00	88.06	105.99
2	Ε	4	TPO	O-C-CA	-3.76	114.93	124.78
2	Ε	4	TPO	O3P-P-OG1	-3.42	90.68	105.99
2	F	4	TPO	O-C-CA	-3.31	116.11	124.78
2	D	4	TPO	O3P-P-O2P	2.90	118.72	107.64
2	D	4	TPO	O3P-P-O1P	2.86	121.89	110.68
2	D	4	TPO	O3P-P-OG1	-2.25	95.91	105.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4	TPO	CB-OG1-P-O2P
2	F	4	TPO	CB-OG1-P-O2P
2	D	4	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	222/259~(85%)	0.39	17 (7%) 13 17	30, 45, 59, 67	0
1	В	224/259~(86%)	0.19	9 (4%) 38 45	27, 41, 57, 65	0
1	С	214/259~(82%)	0.62	21 (9%) 7 10	35, 53, 91, 95	0
2	D	5/6~(83%)	0.62	0 100 100	51, 53, 55, 57	0
2	Е	5/6~(83%)	0.10	0 100 100	38, 40, 42, 44	0
2	F	5/6~(83%)	1.57	1 (20%) 1 1	48, 52, 56, 57	0
All	All	675/795 (84%)	0.40	48 (7%) 16 21	27, 46, 65, 95	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	372	CYS	6.6
1	В	372	CYS	6.0
1	С	469	PRO	5.3
1	С	465	VAL	5.1
1	С	463	LEU	5.0
2	F	6	LEU	4.4
1	С	464	THR	4.2
1	А	417	TYR	4.2
1	С	456	ARG	4.0
1	А	536	GLN	4.0
1	В	468	HIS	3.9
1	С	481	TYR	3.8
1	А	517	THR	3.7
1	С	471	SER	3.7
1	В	594	ARG	3.6
1	A	411	VAL	3.6
1	А	372	CYS	3.6
1	В	371	ASP	3.6
1	С	403	PRO	3.3



1	$\Omega 4K$	
-	& TT Z	

Mol	Chain	Res	Type	RSRZ	
1	С	503	ASP	3.2	
1	С	468	HIS	3.0	
1	А	503	ASP	2.7	
1	С	462	TYR	2.7	
1	А	530	VAL	2.7	
1	А	481	TYR	2.7	
1	С	557	ARG	2.6	
1	А	542	ILE	2.6	
1	А	493	ALA	2.5	
1	С	404	ALA	2.5	
1	С	457	ASP	2.5	
1	С	470	ASN	2.4	
1	С	472	LEU	2.4	
1	В	536	GLN	2.4	
1	А	456	ARG	2.4	
1	С	523	LEU	2.3	
1	С	473	MET	2.3	
1	А	504	GLU	2.3	
1	С	536	GLN	2.2	
1	А	525	LEU	2.2	
1	В	503	ASP	2.2	
1	В	522	ILE	2.2	
1	А	511	LEU	2.2	
1	А	518	ARG	2.2	
1	В	523	LEU	2.2	
1	А	593	SER	2.1	
1	А	523	LEU	2.0	
1	С	455	GLU	2.0	
1	В	404	ALA	2.0	

Continued from previous page...

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	TPO	D	4	11/12	0.95	0.12	47,49,50,51	0
2	TPO	F	4	11/12	0.96	0.10	44,47,49,49	0
2	TPO	Е	4	11/12	0.99	0.13	32,35,36,37	0



6.3 Carbohydrates (i)

There are no monosaccharides 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.

